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Towards first principles prediction of pK_a :

COSMO-RS and the cluster-continuum approach

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Abstract:

The COSMO-RS method, a post quantum chemistry extension of the quantum chemical dielectric continuum solvation model COSMO with a statistical thermodynamics treatment for realistic solvation simulation, has been applied to the prediction of aqueous pK_a of acids and bases. The combination of the COSMO-RS approach to pK_a prediction with the cluster-continuum approach (explicit solvation of the solute compound with one or more solvent molecules) was used on three data sets consisting of 94 acids and 75 bases. Correlation of the calculated free energies of dissociation in water with the experimental aqueous pK_a of the solute acids and bases in their bare state and explicitly solvated by one or two solvent molecules showed an increase of the regression slope with the number of explicit solvent molecules thus showing a regression slope that is closer to the theoretical value than the slope found for bare solutes. It was found that the cluster-continuum approach is limited to a pK_a range of strong to moderately weak acids and bases, because the optimizations of the solvent-solute complexes of the ionic species of very weak acids (such as the anion of *tert*-butanol) did not lead to the desired complexes but yielded dissociation products.

Keywords: pK_a ; acidity; basicity; COSMO; COSMO-RS; explicit solvation; cluster-continuum model;

Introduction

The transfer of protons is one of the central processes in biology, organic, and inorganic chemistry. Consequently, the detailed analysis of the thermodynamics of the proton transfer reaction and the prediction of dissociation constants of acids and bases in different solvents have found substantial interest in many areas of chemistry and biochemistry. Experimental measurement of aqueous phase pK_a values nowadays has become an inexpensive standard application¹. However, there are broad classes of chemicals that are not readily amenable to experimental characterization (e.g. reaction intermediates, very strong and very weak acids or bases with a pK_a outside the pK_a range that can be conveniently measured). Therefore, considerable and ongoing effort has been devoted to the development of first principle prediction methods for pK_a values. The computational prediction of high quality gas phase dissociation constants has become feasible with high level (post-Hartree-Fock) *ab initio* quantum chemistry methods, which nowadays can be as good or even more accurate than the experimentally challenging measurements of this property²⁻⁶. In the liquid phase, which is of much larger practical importance, the situation seems reversed: at least for solvent water there is a large number of reliable experimental dissociation constant data available, but the theoretical prediction from first principles is extremely challenging because of the strong solvation effects of the neutral and ionic species involved in the proton transfer reaction. Thus the prediction of dissociation constants can be seen as the ultimate challenge for quantum chemistry (QC) based solvation models, where the general goal is to improve the reliability of the computational approach so as to have a realistic comparison with the available experimental data. A large number of attempts in this direction have been reported, but a consistent and generally applicable method is still lacking. Nevertheless, the rapid development of efficient QC methods in recent years has opened new perspectives for the modeling of acid-base equilibria in solution

and the rigorous prediction of the associated pK_a values in the liquid. The effect of the solvent on the proton transfer reaction can be included in quantum chemical computations in two ways: either the solvent molecules are accounted for explicitly, as in the molecular dynamics (MD) simulation framework⁷, or implicitly, using a continuum solvation model. Due to its considerable computational cost, the MD based explicit solvation approach yet remained restricted to a limited number of small systems. Of the different implicit QC methodologies available for the computation of pK_a values the Dielectric Continuum Solvation Methods (DCSMs) have become most popular⁹, because they are able to describe long range electrostatic interactions of solutes with a solvent at moderate computational cost in the context of quantum chemical programs¹⁰⁻¹⁷. Thus QC based DCSM methods may help to shed some light on the particulars of the relationship between molecular structure and pK_a value. In DCSMs the interactions of a solute molecule with the solvent are treated by means of putting the solute in a cavity that is surrounded by a dielectric continuum, which represents the solvent. Solvent-related properties like the size and shape of the cavity are treated as adjustable parameters and obtained from physically motivated modeling procedures. DCSMs are distinguished by the construction of the cavity and how the solute-solvent interactions are treated. Despite the well known deficiencies of DCSM methods, (i.e. the neglect of hydrogen bonding and the inadequate treatment of the short range electrostatics^{10,18-21}, which can be much stronger in ions than in neutrals and thus can introduce a large asymmetry to the solvation energy of an acid compared to its conjugate base) it is possible to correlate the quantum chemical dissociation free energy of a solvated molecule ΔG_{diss} with its pK_a via a linear free energy relationship (LFER)¹⁰:

$$pK_a = c_1 \Delta G_{\text{diss}} + c_2 \quad (1)$$

From the basic thermodynamics c_1 is expected to be unity if ΔG_{diss} would be calculated without a systematic error and the LFER axis intercept c_2 is expected to be equal to $-\log[\text{Solvent}]$ ²². Looking in detail into the DCSM studies,¹⁰⁻¹⁷ in the regression of pK_a values versus the calculated dissociation free energy ΔG_{diss} the studies report slopes that are significantly lower than the theoretically expected value

of $1/RT\ln(10)$, which was first noted and discussed by Klamt *et al.*¹⁰. Such a behavior has been reported for aqueous¹⁰⁻¹² and non-aqueous acids^{10,13-15,23} as well as for bases.^{16,17,24} This drawback is common to all simple DCSMs unless considerable effort is taken in the (often physically hardly justifiable) adjustment of numerous additional and often physically doubtful parameters of the DCSM. Atom type or hybridization specific cavity radii and cavity definitions that depend on the charge of the molecule are examples of such parameters²⁵. Although such models became quite popular and successful applications for water and nonaqueous solvents have been reported^{10-17, 22-27}, it remains doubtful if the predictive power of such empirical adjustments persists for more complex chemically multifunctional solutes or for solutes such as free radicals, zwitterions or excited states²³. In particular empirical models are very likely to fail if electron delocalization is important in the anions or cations involved in the proton exchange reaction^{8,28}. Pliego and Riveros²⁹ showed that the error of such DCSM methods in pK_a predictions can become as large as 7 pK_a units when solutes with different functional groups are considered. They proposed that the neglect of specific solute-solvent interactions may cause this significant error²⁹.

A promising approach to the pK_a problem, which does not artificially modify the cavity to try to reproduce hydrogen bonding and short-range solute-solvent interaction behavior that is not accounted for by the DCSM, is the addition of explicit solvent molecules to the solute ions²⁹⁻³⁴, which in the context of pK_a prediction by DCSM's has been reported in the literature as "Cluster-Continuum"^{29,30,33}, "Supermolecule"^{32,34}, or "Implicit-Explicit Solvation"³¹ approach. The solute and its according ionic form are represented by a cluster of the neutral and ionic solute molecule with one or more surrounding solvent molecules that form a partial or full solvation shell around the compound, accounting for local solute-solvent interactions such as Hydrogen Bonding (HB) and electrostatic charge-dipole interactions in a physical way. Compared to simple DCSMs, this approach appears to increase the slope of the aqueous pK_a LFER with each added explicit water²⁹⁻³⁴, but its practical application leads to some ambiguities and problems: there is no natural choice of the number of solvent molecules that represent the solvent shell, retaining some level of arbitrariness involved, where a choice has to be taken.

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However, what in practice might turn out to be the much harder problem, is the optimization of the solute-solvent cluster. For complex, multifunctional solutes, as most chemically or biologically interesting drug-like compounds are, it is very difficult and computationally demanding to find the global minimum of the weakly bonded solute-solvent complex³⁴. If the solvent itself is a complex multifunctional compound, or if a mixture of several solvent compounds is used, it easily may become impossible to find and optimize the global minimum of the cluster at all. To avoid the problematic optimization of weakly bound complexes Adam³⁴ suggested to use only one or two explicit solvent molecules only if there are strong hydrogen bonds between the solute and solvent, so that the resulting complex is stable in the gas phase and thus can be observed experimentally³⁴. Unfortunately this criterion does not resolve the problem of getting the right number of explicit solvent molecules, nor does it seem to be applicable to complex multifunctional compounds or compounds with electron delocalization, where it might not be easy to decide if there is strong or weak bonding in the complex.

To be able to overcome the arbitrariness involved in the choice of the number of explicit solvent molecules added to the solute, Ding *et al.*³² proposed for each solute to pick from the set of bare, mono- or di-solvated solutes that species, which minimizes the calculated total free energy of dissociation, thus introducing an additional local descriptor of the chemical nature of the solute-solvent interactions. They argue that the minimum dissociation energy species should be the compound with the highest thermodynamic stability in the framework of the quantum chemical dielectric continuum solvation model used. This approach reflects some known defects of DCSM's for protic and polar solvents, in particular the neglect of Hydrogen Bonding interactions between solute and solute, which are introduced when explicit solvent molecules are added. Thus for protic and polar solvents such as water or dimethylsulfoxide the addition of a solvent sphere may lead to improved correlation of ΔG_{diss} with experimental pK_a , while solvents of low polarity are well represented by the DCSM on the bare solute compound. It must be noted, that while being physically plausible, this criterion is hardly applicable in

1 practical predictions, because for any solute it involves the conformational search and optimization of
2 bare solutes, *mono-*, *di-* and probably even higher solvated solute-solvent clusters.
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4 A different criterion for the choice of the number of explicit solvent molecules was introduced by Pliego
5 and Riveros²⁹. In their reasoning the cluster with the number of explicit solvent molecules that
6 minimizes the free energy of solvation of the anionic or cationic form of the solute acid or base,
7 respectively, should lead to the best predictions of the property based on the cluster-continuum model,
8 based on the assumption that for a rigid cluster, the complex with minimum free energy of solvation will
9 be closest the *real* free energy of solvation of the ion in solution. They found that for aqueous pK_a
10 typically three explicit water molecules minimize the free energy of solvation of the anions or cations.
11 Apart from the significant theoretical and practical problems that are raised by finding the global
12 minimum of a cluster consisting of four weakly bonded compounds, the free energy of solvation of the
13 ionic form only partly reflects the physics of the dissociation reaction, totally neglecting the solvation of
14 the neutral solute and the influence of the quantum chemical method, both of which are accounted for by
15 the criterion of Ding *et al.*³².
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28 Another set of rather heuristic criteria for explicit solvation of acids was proposed by Kelly *et al.*³¹. In
29 combination with their post-DSCM method SM6³⁵, they proposed to add a single explicit water
30 molecule to the anionic form of a solute acid only (*semi-solvation*), either if the anion consists of less
31 than three atoms, or if the charge of the anionic form of the acid is localized on one or more oxygen
32 atoms in a way that the oxygen(s) bear a more negative partial charge than the oxygen of the solvent
33 water. Obviously, for both criteria a certain amount of arbitrariness remains. In particular, the quite
34 arbitrary partition of the solute anions into species that form a strong hydrogen bond with water (the
35 ones whose oxygens have a more negative partial charge than the water oxygen) and those who do not,
36 is doubtful. If explicit solvation is trying to compensate the shortcomings of the DCSM, which does not
37 account for Hydrogen Bonding interactions at all, the division into strong and weak hydrogen bonds
38 does not seem useful. Neither does this separation make sense if one tries to account for shortcomings of
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the underlying quantum chemistry or DFT methods, which have or don't have the same problems for strong and weak Hydrogen Bonds.

The DCSM-based implicit/explicit pK_a models already mentioned use the combination of a gas phase dissociation energy of the cluster compounds (the explicit solvation part) computed by a high-level QC method, with the cluster free energy of solvation³⁶⁻³⁸ computed by a DCSM model (the implicit solvation part), which connects the gas phase to the liquid state. These approaches all rely on explicit solvation to correct the shortcomings of the DCSM method. In this work we chose a different approach: the Conductor-like Screening Model for Real Solvents (COSMO-RS)¹⁸⁻²¹. COSMO-RS goes beyond the DCSM concept in that it combines the electrostatic advantages and the computational efficiency of the DCSM COSMO³⁹ with a statistical thermodynamics method for local interaction of surfaces, which takes into account local deviations from dielectric behavior as well as hydrogen bonding. In this approach all information about solutes and solvents is extracted from initial QC-COSMO calculations, and only very few parameters have been adjusted to experimental values of partition coefficients and vapor pressures of a wide range of neutral organic compounds. COSMO-RS is capable of predicting partition coefficients, vapor pressures, and solvation free energies of neutral compounds with a root mean square error (rmse) of 0.3 log-units and better and a lot of experience has been gathered during the past years about its surprising ability to predict mixture thermodynamics¹⁸⁻²⁰. Although COSMO-RS could successfully be applied to the first principles prediction of aqueous acidity¹⁰ and basicity²⁴ as well as acid and base pK_a in non-aqueous solvents^{10,28}, there remained some problematic aspects: most prominently, the correlation of COSMO-RS predicted free energy of dissociation with experimental pK_a showed a slope that is lower than the one expected from thermodynamic theory^{10,24}. I.e. COSMO-RS was not able to solve the slope problem of the underlying DCSM COSMO. In addition it was found that the systematic deviations known from DCSMs for aliphatic amine compounds were also present in COSMO-RS predictions of aqueous base pK_a ²⁴. This study tries to assess if the combination of the COSMO-RS method for predicting pK_a with the explicit solvation approach is able to resolve these issues. In addition, the performance and stability of different criteria for the choice of the number of

explicit solvent molecules is tested. We decided to perform this study on the data sets for aqueous acids and base pK_a already published^{10,24}. The standard COSMO-RS method implemented in the COSMOtherm program⁴⁰ based on Turbomole DFT/COSMO calculations⁴¹⁻⁴⁶ was used for this purpose.

Theoretical calculations

Our theoretical calculations of ΔG_{diss} of aqueous acids are based on the reaction model



The theoretical calculations of ΔG_{diss} of aqueous bases are based on the reaction model



Unlike the DCSM methods mentioned, COSMO-RS is able to directly calculate the free energy of each species in aqueous solution. Thus no gas phase energies were computed. We applied our standard procedure for COSMO-RS calculations to all four species appearing in eqs. 2 and 3, which consists of two steps:

1) Full DFT geometry optimization with the Turbomole program package⁴³ using B-P density functional^{44,45} with TZVP quality basis set using the RI approximation.⁴⁶ During these calculations the COSMO continuum solvation model was applied in the conductor limit ($\epsilon = \infty$). Optimized element-specific radii from the COSMO-RS parameterizations^{19,20} have been used for the COSMO cavity construction. Such calculations end up with the self-consistent state of the solute in the presence of a virtual conductor that surrounds the solute outside the cavity.

2) COSMO-RS calculations have been done using the COSMOtherm program³⁶. In these calculations the deviations of the real solvent, in this case water, compared to an ideal conductor are taken into account in a model of pair-wise interacting molecular surfaces. For this purpose, electrostatic energy differences and hydrogen bonding energies are quantified as functions of the local COSMO polarization

charge densities σ and σ' of the two interacting surface pieces. The chemical potential differences arising from these interactions are evaluated using an exact statistical thermodynamics algorithm for independently pair-wise interacting surfaces, which is implemented in *COSMOtherm*. More detailed descriptions of the COSMO-RS method are given elsewhere¹⁸⁻²¹.

If more than one cluster conformation or different deprotonation or protonation sites were considered to be potentially relevant for the neutral, anionic, or cationic form of the acids AH and bases B, several conformations were calculated in step 1 and a thermodynamic Boltzmann average over the total Gibbs free energies of the conformers was consistently calculated by the *COSMOtherm* program in step 2. For this study the geometries of all molecules taken from refs. 10 and 24 have been re-optimized on BP/TZVP/COSMO level. In addition all compounds have been carefully rechecked for possible conformations, and if necessary, additional conformations have been added to the *COSMOtherm* calculations in step 2.

To avoid the human bias and ambiguity involved in the construction of the clusters of the solute with one or two explicit water molecules, their geometries were created with a novel COSMO-RS based procedure: starting from the optimized BP/TZVP/COSMO geometries of the bare solute molecule and the water molecule, the pair-interaction energies of all possible contacts of the cavities of the two molecules are scanned and the minimum energy contact, which for both molecules is the site where the contact probability between the molecule is largest and thus the site where a cluster is most likely to be formed, will be identified. Along the bond defined by this contact site, the solvent molecule is arranged at different torsional angles between 0° and 360° , in steps of 45° and the resulting cluster geometries were optimized independently at BP/TZVP/COSMO level of theory. Of the cluster conformer thus found, the minimum energy cluster is used in the COSMO-RS computation of step 2. The clusters with two explicit water molecules are created the same way, using the *mono*-solvated solute cluster as starting structure instead of the bare solute. This procedure is applicable in the same manner to neutral and ionic species, and to any solvent or solute (which itself can be a cluster). Thus it can be automated quite

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easily. Although the cluster generation procedure via COSMO-RS created cluster geometries is not a global optimization procedure and thus can not guarantee that the optimized clusters are the absolute minimum energy structures of the phase space spanned by the atomic coordinates of the complexes, it provides a reliable, consistent - and what is even more important for practical application: simple, automatic, and unbiased - procedure for finding cluster geometries that are very likely to be the best (and minimum energy) structures in the framework of the QC/COSMO-RS approach used. For a small subset of the clusters, a global approach to finding the minimum energy conformations of the clusters was tested: *ab initio* MD simulated annealing of the geometries on BP/TZVP/COSMO level of theory, as provided by Turbomole⁴³. For the compounds tested (*tert*-butanol, oxalic acid, indole, melamine) the MD procedure was not able to find lower energy cluster conformations than the COSMO-RS contact probability based method, which is strong indicator for the soundness of the COSMO-RS provided geometries. The optimized geometries of all the acids, bases, ions and explicitly solvated cluster-compounds are given in the Supplementary Material section of this journal.

For all acids AH, the Gibbs free energy of dissociation (ΔG_{diss}) has been calculated as the difference of the total free energy of the anion A^- and the neutral acid AH. The free energy difference of H_3O^+ and H_2O is a constant additional contribution:

$$\Delta G_{\text{diss}} = G_{\text{tot}}(A^-) - G_{\text{tot}}(AH) + [G_{\text{tot}}(H_3O^+) - G_{\text{tot}}(H_2O)] \quad (4)$$

For all bases B, the Gibbs free energy of dissociation (ΔG_{diss}) has been calculated as the difference of the total free energy of the protonated cation BH^+ and the base B. To this free energy difference the free energy difference of H_3O^+ and H_2O is a constant additional contribution:

$$\Delta G_{\text{diss}} = G_{\text{tot}}(B) - G_{\text{tot}}(BH^+) + [G_{\text{tot}}(H_3O^+) - G_{\text{tot}}(H_2O)] \quad (5)$$

From the calculation procedure described above, we get $G_{\text{tot}}(H_3O^+) - G_{\text{tot}}(H_2O) = 1124.47$ kJ/mol. This value is in good agreement with literature estimates²³. Zero point vibrational energies are not taken into account. Consequently, the geometries optimized in step 1 were not analyzed for the nature of the stationary point of the optimized geometry. We make the common assumption that the difference in zero

point energy between the neutral and the deprotonated acid or protonated base is small and systematic¹⁰.

All regressions of the dissociation free energy vs. experimental pK_a have been cross-validated by a “leave-one-out” cross-validation procedure. The cross-validated regression coefficients q^2 are given together with the regression coefficients r^2 .

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Aqueous Acids

For the purpose of finding the LFER coefficients of eq. 1, a data set of 94 acids in solvent water was used. The data set consists of the reference data set of 5 alcohols, 23 carboxylic acids, 8 inorganic acids, 16 phenols, and 12 heterocyclic compounds as reported in ref. 10. A set of 30 multifunctional substituted benzoic acids⁵¹ has been added to the initial data set, to be able to assess the performance of the explicit solvation on more challenging solutes. The acids experimental pK_a values range from 0 to 19. No compound has been removed from the data set for any reason during the study.

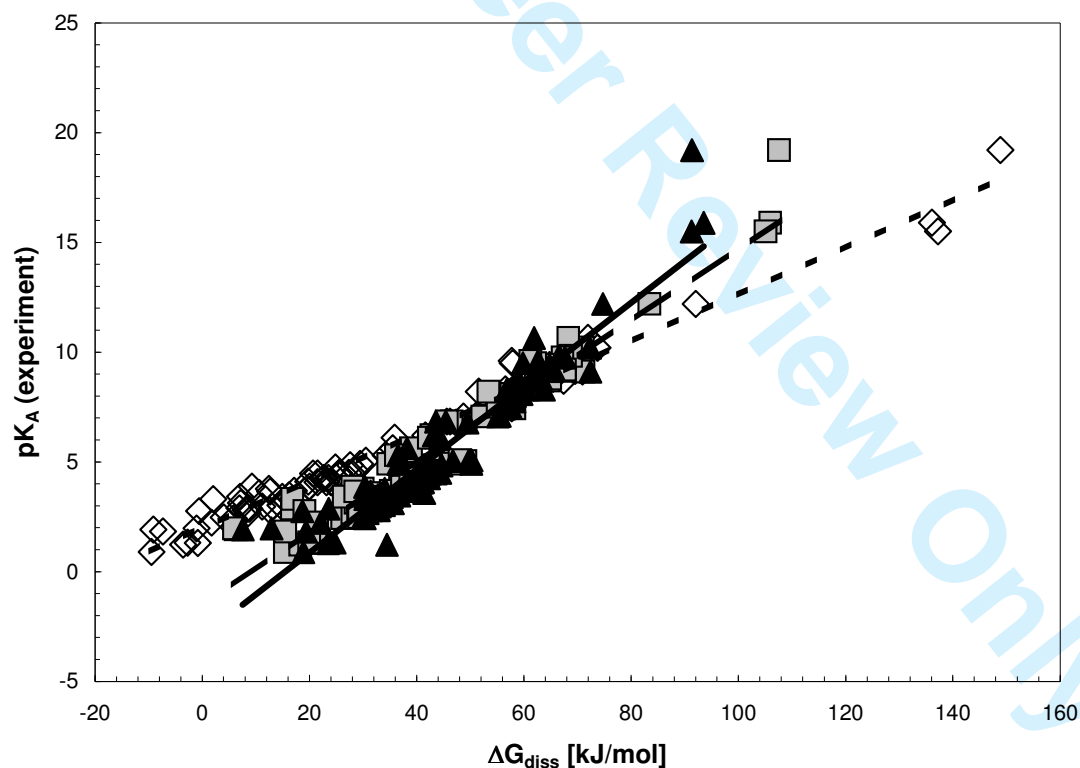


FIGURE 1: Calculated Gibbs free energy of dissociation vs. experimental acids pK_a in solvent water. Open rhombus: bare acids and anions. Dotted line: regression line (eq. 4) for bare acids ($r^2 = 0.978$, $q^2 = 0.976$, $c_1 = 0.107$, $c_2 = 1.94$). Filled squares: acids and anions with one explicit water molecule. Striped line: regression line (eq. 5) for *mono*-solvated compounds ($r^2 = 0.935$, $q^2 = 0.932$, $c_1 = 0.164$, $c_2 = -1.56$). Filled triangles: acids and anions with two explicit water molecules, respectively. Solid line: regression line (eq. 6) for *di*-solvated compounds ($r^2 = 0.899$, $q^2 = 0.893$, $c_1 = 0.190$, $c_2 = -2.94$).

The results for all 94 acids are shown in Table 1 and Figure 1. The free energies of all individual species are given in the Supplementary Material section of this journal. The regression of the calculated aqueous Gibbs free energy of dissociation (ΔG_{diss}) vs. experimental pK_a for the bare neutral and ionic compounds results in a correlation coefficient of $r^2 = 0.978$ ($q^2 = 0.976$). The regression equation for the bare acids pK_a in aqueous solution reads

$$pK_a = 0.107(\pm 0.01)\Delta G_{\text{diss}} + 1.94(\pm 0.1) \quad (4)$$

If we would have omitted the free energy difference of H_3O^+ and H_2O , which we calculate as

-1124.47 kJ/mol, in the definition of ΔG_{diss} we would have got a regression constant of $\hat{c}_2 = -118.75$.

Including this energy difference, the calculated axis intercept of 1.9 is reasonably close to the theoretical value of $c_2 = -\log[H_2O] = -1.74$. In accordance with previous work¹⁰ on aqueous acidity of bare compounds we found that the slope of the regression is lower than the theoretical value of $1/RT\ln(10) = 0.1759$.

The regression equation for the *mono*-solvated neutral and ionic compounds ($r^2 = 0.935$, $q^2 = 0.932$) reads

$$pK_a = 0.164(\pm 0.01)\Delta G_{\text{diss}} - 1.56(\pm 0.1) \quad (5)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -185.42$.

Thus, in comparison with the bare compound regression, the slope of the *mono*-solvated solutes is closer to the theoretical value. Yet the slope remains to be somewhat smaller than the theoretical value.

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Moreover, the correlation of ΔG_{diss} with the experimental $\text{p}K_{\text{a}}$ data is worse than for the bare compounds. If the explicit solvation is applied to the ionic form of the compound set only (*semi*-solvation, as proposed by Kelly *et al.*³¹) the slope of the regression (with $r^2 = 0.929$, $q^2 = 0.926$) decreases to $c_1 = 0.139$ and the regression constant is $c_2 = 27875.09$, which omitting the free energy difference of H_3O^+ and H_2O , yields $\hat{c}_2 = -317.98$. Thus the *semi*-solvation expectably yields to a regression that is somewhat in between the regression of the bare and the *mono*-solvated solutes.

The regression equation for the *di*-solvated neutral and ionic compounds ($r^2 = 0.899$, $q^2 = 0.893$) reads

$$\text{p}K_{\text{a}} = 0.190(\pm 0.01) \frac{\Delta G_{\text{diss}}}{RT \ln(10)} - 2.94(\pm 0.1) \quad (6)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -216.54$.

Both slope and regression constant are closer to the theoretical values for the *di*-solvated compounds compared to the bare compounds or the *mono*-solvated compounds, the slope is even higher than the theoretical value. Again, the correlation of ΔG_{diss} with the experimental $\text{p}K_{\text{a}}$ data for *di*-solvated compounds is worse than for the *mono*-solvated and bare compounds.

These results corroborate the claims given in the literature²⁹⁻³⁴ that the explicit solvation approach is able to solve the *slope problem*¹⁰ of the quantum chemical DCSCM's. However, they lead to new problems: First, even when quite careful choice of the minimum energy structure of the solvent-solute cluster is applied, the overall correlation deteriorates with increasing number of explicit solvent molecules. Second, even though the slope of the ΔG_{diss} vs. $\text{p}K_{\text{a}}$ correlations is closer to the theoretical slope for the *mono*- or *di*-solvated solutes, it is still somewhat different, and for the *di*-solvated solutes even overshoots the theoretical value. A convergence of the slope appears to be reached at *di*-solvation, because the change in slope from *mono*- to *di*-solvation is much smaller than from bare solutes to *mono*-solvation.

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If, following Ding *et al.*³², we introduce the additional solute specific category of minimal ΔG_{diss} in the choice of the cluster or bare solute for the correlation with $\text{p}K_{\text{a}}$, a look at the ΔG_{diss} values in Table 1 reveals an important trend: while for strong and medium acids with $\text{p}K_{\text{a}} < 10$ the bare solute is preferred, weak acids show minimum dissociation free energy if they are solvated with one or, for very weak acids with $\text{p}K_{\text{a}} > 12$, two explicit water molecules. When looking at dissociation energy as computed on the DCSCM level only (i.e. BP/TZVP/COSMO without COSMO-RS), the doubly solvated solute is preferred throughout the entire $\text{p}K_{\text{a}}$ range. This implies that a major portion of the interaction effects that are missing in the DCSCM already is taken into account by COSMO-RS, which however has problems with very weak acids. This flaw can be explained quite well in the framework of COSMO-RS theory: as yet, non-local long range electrostatic effects and strong hydrogen bonding are not explicitly taken into account by COSMO-RS⁴⁷. Now, the dissociation of very weak acids leads to anions where the charge is very concentrated and often localized on only one atom. It is exactly this type of ions where the COSMO-RS neglect of non-local electrostatic effects and strong hydrogen bonding may lead to increased errors – and, in turn, explicit solvation captures some of these neglected interactions. Thus the combination of COSMO-RS computed free energies of dissociation with the approach of Ding *et al.*³², does not seem to be very promising: the overall correlation of the minimum ΔG_{diss} with $\text{p}K_{\text{a}}$ is worse than the one for the bare solutes ($r^2 = 0.915$, $q^2 = 0.912$) and it leads to a slope that is significantly lower than the theoretical: $c_1 = 0.127$ and the regression constant is $c_2 = 1.54$, which omitting the free energy difference of H_3O^+ and H_2O , yields $\hat{c}_2 = -141.58$.

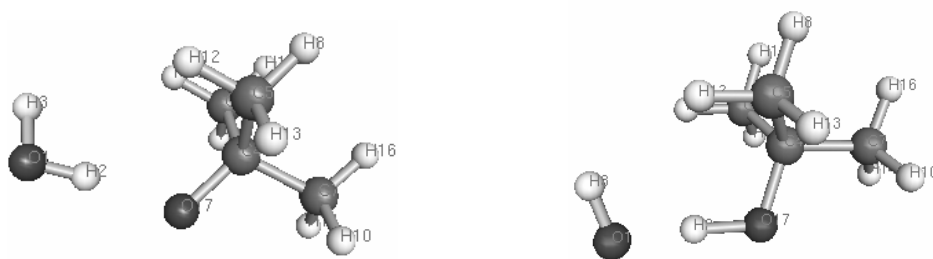


FIGURE 2: Optimized geometries for $(\text{CH}_3)_3\text{C-O}^{(-)}\cdots\text{H-O-H}$ and $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}$.

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5 Critical inspection of Table 1 and Figure 1 shows that there is one significant outlier in the regression of
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7 the mono- and di-solvated compounds, but not in the regression of the bare ions. It is *tert*-butanol, the
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9 weakest acid in the data set. A closer look at the optimized geometries of the explicitly solvated *tert*-
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11 butanol and *tert*-butoxy-anion revealed that the quantum chemical optimization of the *tert*-butoxy-anion
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13 - water and di-water clusters yielded an unexpected structure: Instead of the anion - water cluster
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15 $(\text{CH}_3)_3\text{C-O}^{(-)}\cdots\text{H-O-H}$, a complex of *tert*-butanol with an hydroxy-anion $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}$, or in the
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17 case of two explicit water molecules the anion $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}\cdots\text{H-O-H}$, was optimized (see Figure
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19 2). The exact same artifact can also be observed in the data published by Kelly *et al.*³¹. A deeper
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21 investigation of the configurational space of the *tert*-butoxy-anion cluster showed that any free
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23 optimization of the *tert*-butoxy-anion – water cluster always yielded in a *tert*-butanol - hydroxy-anion
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25 cluster. A constrained optimization of the *tert*-butoxy-anion – water complex with the contacting
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27 hydrogen atom of the water molecule fixed at the equilibrium bond distance of the isolated water
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29 molecule with a subsequent potential energy surface scan along the $\text{O}^{(-)}\cdots\text{H-O-H}$ bond resulted in a
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31 minimum energy structure with the expected $(\text{CH}_3)_3\text{C-O}^{(-)}\cdots\text{H-O-H}$ geometry, which however was 73
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33 kJ/mol higher in energy than the $(\text{CH}_3)_3\text{C-OH}\cdots\text{O}^{(-)}\text{-H}$ structure and thus lead to an even worse
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35 regression with the experimental pK_a . Obviously, for the anions of very weak acids like *tert*-butanol,
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37 which have their negative charge sharply localized on one atom, the hydrogen-transfer of a hydrogen
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39 atom from the water to the anionic site leads to an energetically much favoured structure, compared to
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41 the hydrogen bonded anion – water cluster expected from the explicit solvation model – at least on the
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43 quantum chemical level of theory employed in this study. This implies that the cluster-continuum model
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45 can not be applied to very weak acids like *tert*-butanol. Thus the applicability range of the cluster-
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47 continuum model seems to be restricted to acids of medium strength, (again that is, for the quantum
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49 chemical BP//TZVP//COSMO level of theory used in this study). As a consequence, *tert*-butanol was

removed from the regression. The new correlation for 93 acids leads to the following regression

equations: The regression equation for the bare solutes ($r^2 = 0.975$, $q^2 = 0.973$) reads

$$\text{p}K_{\text{a}} = 0.105(\pm 0.01)\Delta G_{\text{diss}} + 1.99(\pm 0.1) \quad (7)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -116.40$.

The regression equation for the *mono*-solvated neutral and ionic compounds ($r^2 = 0.934$, $q^2 = 0.929$) reads

$$\text{p}K_{\text{a}} = 0.157(\pm 0.01)\Delta G_{\text{diss}} - 1.32(\pm 0.1) \quad (8)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -177.83$.

The regression equation for the *di*-solvated neutral and ionic compounds ($r^2 = 0.907$, $q^2 = 0.901$) reads

$$\text{p}K_{\text{a}} = 0.180(\pm 0.01)\Delta G_{\text{diss}} - 2.56(\pm 0.1) \quad (9)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -205.20$.

Thus even if the problematic compound is removed from the data set, the general trends of decreasing correlation quality and non-theoretical slope with increasing number of explicit solvent molecules remained.

Aqueous Bases

For the purpose of finding the eq. 1 LFER correlations of the base protonation reaction, a data set of 43 bases was taken from ref. 24. Experimental base $\text{p}K_{\text{a}}$ values range between -5 and 14. This set consists of 35 bases that are protonated at a nitrogen atom, namely five anilines, four amidines, six benzodiazepines, four guanidines, and 16 five- or six-ring heterocyclic compounds, and eight bases that

are protonated at a carbon atom, namely four pyrroles and four indoles. For the pyrroles and indoles we considered all possible protonation sites in the conformer equilibrium calculations of the cations.

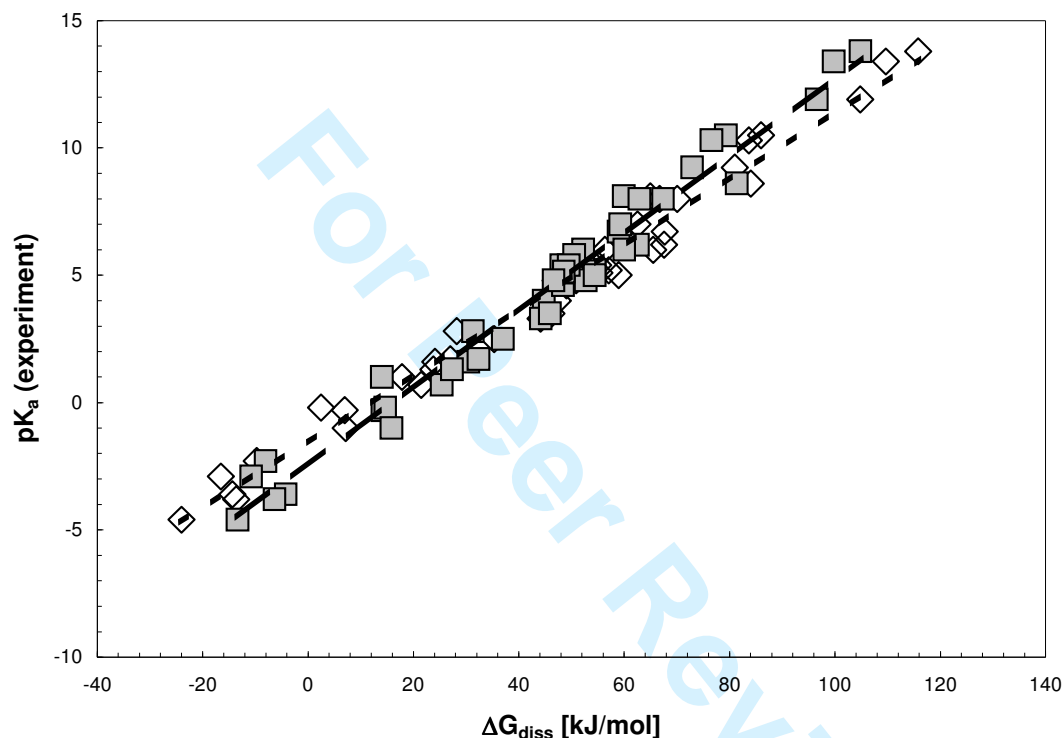


FIGURE 3: Calculated Gibbs free energy of dissociation vs. experimental bases pK_a in solvent water. Open rhombus: bare bases and cations. Dotted line: regression line (eq. 10) for bare bases ($r^2 = 0.981$, $q^2 = 0.979$, $c_1 = 0.130$, $c_2 = -1.57$). Filled squares: bases and cations with one explicit water molecule. Striped line: regression line (eq. 11) for mono-solvated compounds ($r^2 = 0.973$, $q^2 = 0.970$, $c_1 = 0.153$, $c_2 = -2.48$).

The results for all 43 bases are shown in Table 2 and Figure 3. The free energies of all the individual species are given in the Supplementary Material section of this journal. The regression of the calculated

aqueous Gibbs free energy of dissociation (ΔG_{diss}) vs. experimental base $\text{p}K_{\text{a}}$ for the bare neutral and cationic compounds results in a correlation coefficient of $r^2 = 0.981$ ($q^2 = 0.979$). The regression equation for the bare bases $\text{p}K_{\text{a}}$ in aqueous solution reads

$$\text{p}K_{\text{a}} = 0.130(\pm 0.01) \frac{\Delta G_{\text{diss}}}{RT \ln(10)} - 1.57(\pm 0.1) \quad (10)$$

If we would have omitted the free energy difference of H_3O^+ and H_2O in the definition of ΔG_{diss} we would have got a regression constant of $\hat{c}_2 = -147.96$. Including this energy difference, the calculated axis intercept of 1.9 is very close to the theoretical value of $c_2 = -\log[\text{H}_2\text{O}] = -1.74$. In accordance with previous work²⁴ on aqueous basicity of bare compounds we found that the slope of the regression is lower than the theoretical value of $1/RT \ln(10) = 0.1759$.

The regression equation for the *mono*-solvated base compounds ($r^2 = 0.973$, $q^2 = 0.970$) reads

$$\text{p}K_{\text{a}} = 0.153(\pm 0.01) \frac{\Delta G_{\text{diss}}}{RT \ln(10)} - 2.47(\pm 0.1) \quad (11)$$

which omitting the free energy difference of H_3O^+ and H_2O , yields a regression constant of $\hat{c}_2 = -174.24$. Thus, in comparison with the bare compound regression, the slope of the *mono*-solvated solutes is closer to the theoretical value. Yet the slope remains to be significantly smaller than the theoretical value. Moreover, the correlation of ΔG_{diss} with the experimental $\text{p}K_{\text{a}}$ data is worse than for the bare compounds.

If, again following Ding *et al.*³², we introduce the additional solute specific category of minimal ΔG_{diss} in the choice of the cluster or bare solute for the correlation with $\text{p}K_{\text{a}}$, the ΔG_{diss} values in Table 2 follow the same trend that was spotted for the acidic solutes: for strong bases with base $\text{p}K_{\text{a}} < 5$ the bare solute is preferred, while weak bases show minimum dissociation free energy for the solvated molecules, which is essentially the same behavior as recognized for acids. The overall correlation of the minimum

ΔG_{diss} with base $\text{p}K_{\text{a}}$ is worse than the one for the bare solutes ($r^2 = 0.974$, $q^2 = 0.972$) and it leads to a

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slope that is significantly lower than the theoretical: $c_1 = 0.140$ and the regression constant is $c_2 = -1.61$,

which omitting the free energy difference of H_3O^+ and H_2O , yields $\hat{c}_2 = -159.17$.

Another important aspect of the base $\text{p}K_a$ prediction using DCSM's is the systematic deviation that is found for aliphatic amines²⁴. This group of compounds is known to cause considerable problems in most quantum chemical continuum solvation models^{21,48-50}, which also has consequences in the COSMO-RS prediction of $\text{p}K_a$, namely a systematic deviation for *secondary* and *tertiary* aliphatic amines. COSMO-RS computations of ΔG_{diss} of bare and mono-solvated bases is given in Table 3 for 32 *primary*, *secondary* and *tertiary* aliphatic amines. The $\text{p}K_a$ values for these compounds have been calculated using eq. 10 for bare solutes and eq. 11 for mono-solvated solutes, respectively. The root mean square error (RMSE) is 1.38 for bare amine solutes and 1.76 for mono-solvated amines. The systematic deviation of the *secondary* and *tertiary* aliphatic amines is more pronounced for the mono-solvated amines than for the bare amines. Thus it must be concluded that the explicit solvation approach is not capable of curing the flaws that DCSM's and COSMO-RS show for aliphatic amines.

Conclusions

Linear relations between $\text{p}K_a$ and the free energy of dissociation in aqueous solution ΔG_{diss} , as computed by the post-DCSM method COSMO-RS on the basis of quantum chemical DFT/COSMO calculations, have been obtained for the deprotonation and protonation reactions of acids and bases, respectively. Without any special adjustments of radii or other parameters this led to a prediction model for acid and base $\text{p}K_a$ values in water. This allows for prediction of absolute aqueous acid and base $\text{p}K_a$ values with an average error of typically less than 0.6 $\text{p}K_a$ units. From the observation that the slope of the experimental $\text{p}K_a$ versus theoretical ΔG_{diss} was found to be significantly lower than the theoretical value $1/RT\ln(10)$ if bare solutes and their respective ionic species were used in the COSMO-RS computation, the explicit solvation approach, as first proposed by Pliego and Riveros^{29,38}, was used to comprise local

interaction effects that play an important role in the protonation reaction, but are not, or not sufficiently accounted for by the COSMO-RS method. The application of the COSMO-RS method to the calculation of acids pK_a in acetonitrile²⁸ showed a better performance of the COSMO-RS model on acids that produced anions with delocalized charges, as they are less affected by solvation, while acids that formed localized anions showed a systematic deviation. This observation is corroborated by a recent study, which used multipole derived charge analysis to assess the degree of charge delocalization in anion species formed from aqueous dissociation reactions⁸. Both findings are, at least in part, related to the capability of the solvent to solvate and thus stabilize the anions or cations. Apparently this effect is not captured sufficiently by COSMO-RS and its underlying QC/DCSM method DFT/COSMO if there are short-range interactions in the solvation of ions with localized charges. In this study it was found that the explicit solvation approach in combination with COSMO-RS was able to remove these deficits in parts: while the slope of the pK_a versus ΔG_{diss} correlation was closer to the theoretical slope when the number of explicit solvent atoms in the calculations was increased, the correlation decreased, which may have been expected due to the increasing number of ambiguities with increasing number of explicit solvent molecules. Moreover, it was found that for weak acids, such as *tert*-butanol, the quantum chemical geometry optimization of the solvent-solute complex of the according *tert*-butoxy anion was not possible, which makes the explicit solvation approach inapplicable for such compounds. In addition, the systematic deviation found for aliphatic amines was not resolved by the cluster method. Application of only *mono*- or only *di*-solvated clusters of neutral and ionic solute species lead to an improved, yet not fully theoretical slope of the pK_a versus ΔG_{diss} correlation. Other criteria proposed for the choice of the number of explicit solvent molecules used, such as *semi*-solvation of only ions³¹, or from a list of bare, *mono*- or *di*-solvated solutes, choice of the species that minimizes the free energy of dissociation³² performed worse than the simple decision to use one or two explicit solvent molecule for all solutes involved. Thus the choice of the explicit solvent molecules remains ambiguous and must be considered an unsolved issue. From a practical standpoint it remains difficult or even impossible to find the global minimum energy cluster geometries for weakly bonded clusters with more than one explicit solvent

1 molecules. Even for the medium number of compounds used in this study it was impossible to apply
2 global conformational search procedures for finding the cluster geometries of each solute and ion. To
3 avoid this general problem, an automatic procedure, based on COSMO-RS contact interaction energies
4 was proposed, creating “good” or at least sufficiently low energy cluster geometries, without a guarantee
5 of obtaining the actual global minimum, however. Thus it can be concluded that the combination of
6 COSMO-RS with the explicit solvation methodology leads to a *theoretical* improvement in the slope of
7 the correlation of the free energy of dissociation with pK_a and thus a better understanding of the physics
8 of the protonation reaction in solution, but suffers from serious disadvantages that – at least for now -
9 prevent it from being a *practical* prediction method for everyday production work: the simple linear
10 relation between pK_a and the dissociation free energies of the bare solutes and ions proved to be the
11 more robust approach for pK_a prediction.
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24 **Supplementary Material**

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26 Free energies of all species involved in the computation of the dissociation energies (Tables S1, S2, and
27 S3). List of optimized geometries used in the free energy calculations (Table S4).
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TABLE 1: Experimental pK_a and Gibbs free energies of dissociation of bare, mono-solvated and di-solvated aqueous acids.

| Compound | $pK_a(\text{exp})^a$ | $G_{\text{diss}}(\text{bare})^b$ | $\Delta G_{\text{diss}}(\text{H}_2\text{O})^b$ | $\Delta G_{\text{diss}}(2\text{H}_2\text{O})^b$ |
|----------------------------|----------------------|----------------------------------|--|---|
| Ethanol | 15.9 | 136.08 | 105.94 | 93.53 |
| 2,2,2-trichloroethanol | 12.2 | 92.04 | 83.43 | 74.74 |
| formic acid | 3.77 | 12.43 | 29.97 | 34.06 |
| acetic acid | 4.75 | 24.83 | 39.69 | 42.86 |
| Nitromethane | 10.2 | 73.69 | 71.03 | 72.31 |
| dichloroacetic acid | 1.3 | -0.81 | 21.69 | 23.47 |
| trichloroacetic acid | 0.89 | -9.46 | 15.42 | 18.86 |
| n-pentanoic acid | 4.84 | 27.56 | 42.44 | 44.66 |
| 2,2-dimethylpropanoic acid | 5.05 | 30.50 | 44.45 | 46.77 |
| benzoic acid | 4.27 | 23.53 | 39.46 | 40.93 |
| oxalic acid | 1.23 | -3.61 | 18.30 | 34.47 |
| maleic acid | 1.83 | -7.35 | 15.52 | 19.36 |
| fumaric acid | 3.03 | 14.59 | 33.21 | 33.91 |
| acrylic acid | 4.26 | 22.85 | 38.68 | 42.33 |
| bromoacetic acid | 2.87 | 8.51 | 28.40 | 30.93 |
| chloroacetic acid | 2.81 | 8.07 | 28.65 | 31.53 |
| cyanoacetic acid | 2.44 | 5.88 | 26.08 | 30.29 |
| fluoroacetic acid | 2.66 | 8.52 | 28.07 | 30.84 |
| iodoacetic acid | 3.13 | 7.22 | 28.64 | 32.52 |
| 2-hydroxypropanoic acid | 3.87 | 9.23 | 28.01 | 30.36 |
| 2-chloropropanoic acid | 2.8 | 12.58 | 29.71 | 32.95 |
| 3-chloropropanoic acid | 4.1 | 19.76 | 36.88 | 38.34 |
| nitroacetic acid | 1.32 | -2.75 | 19.99 | 24.66 |
| 2-acetylbutanedioic acid | 2.86 | 8.81 | 16.73 | 23.54 |
| carbonic acid | 3.58 | 10.60 | 31.62 | 41.37 |
| hypochlorous acid | 7.43 | 57.75 | 58.25 | 56.35 |
| hypobromous acid | 8.7 | 67.41 | 64.64 | 59.08 |
| hypoiodous acid | 10.64 | 71.94 | 68.28 | 61.87 |
| nitrous acid | 3.3 | 2.04 | 16.80 | 30.42 |
| sulfurous acid | 1.92 | -9.09 | 6.22 | 7.57 |
| phosphoric acid | 1.97 | -1.03 | 5.92 | 12.89 |
| boric acid | 9.12 | 70.92 | 71.10 | 72.38 |
| pentachlorophenol | 4.9 | 29.41 | 34.67 | 36.55 |
| 2,3,4,6-tetrachlorophenol | 5.62 | 35.52 | 38.96 | 38.19 |
| 2,3,4-trichlorophenol | 7.1 | 51.03 | 53.73 | 55.52 |
| 2,3-dichlorophenol | 7.76 | 55.05 | 56.73 | 58.24 |
| 2,4,5-trichlorophenol | 7.07 | 48.73 | 52.22 | 55.17 |
| 2,4,6-trichlorophenol | 6.21 | 41.62 | 42.76 | 43.19 |
| 2,4-dichlorophenol | 8.09 | 56.88 | 57.71 | 59.56 |
| 2,5-dichlorophenol | 7.51 | 53.01 | 55.10 | 57.45 |
| 2,6-dichlorophenol | 6.79 | 47.36 | 47.81 | 49.47 |
| 2-chlorophenol | 8.29 | 60.88 | 60.80 | 63.71 |
| 3,4-dichlorophenol | 8.68 | 62.51 | 62.24 | 61.19 |
| 3,5-dichlorophenol | 8.27 | 57.87 | 58.91 | 58.01 |
| 3-chlorophenol | 8.78 | 65.41 | 64.91 | 63.21 |

| | | | | | |
|----|------------------------------------|------|--------|--------|-------|
| 1 | 4-chlorophenol | 9.14 | 69.57 | 67.63 | 65.17 |
| 2 | phenol | 9.82 | 70.87 | 68.82 | 66.57 |
| 3 | 5-nitouracil | 5.3 | 34.18 | 36.17 | 36.53 |
| 4 | cis-5-formyluracil | 6.84 | 46.20 | 46.58 | 43.60 |
| 5 | thymine | 9.75 | 68.64 | 67.21 | 67.64 |
| 6 | trans-5-formyluracil | 6.84 | 45.61 | 45.64 | 45.44 |
| 7 | uracil | 9.42 | 64.78 | 64.13 | 64.79 |
| 8 | fluorouracil | 8 | 54.99 | 58.34 | 57.85 |
| 9 | methylthiouracil | 8.2 | 51.60 | 53.38 | 57.35 |
| 10 | phenytoin | 8.3 | 56.53 | 59.71 | 56.83 |
| 11 | 3,3-methylphenylglutarimide | 9.2 | 64.17 | 67.65 | 65.55 |
| 12 | 3,3-dimethylsuccinimide | 9.5 | 57.89 | 62.08 | 59.80 |
| 13 | dimethadione | 6.1 | 35.86 | 42.26 | 44.33 |
| 14 | phthalimide | 8.3 | 58.09 | 61.04 | 60.47 |
| 15 | succinimide | 9.6 | 57.76 | 61.20 | 62.62 |
| 16 | phthalic acid | 2.76 | -0.61 | 19.06 | 18.70 |
| 17 | methanol | 15.5 | 137.22 | 105.05 | 91.27 |
| 18 | hypophosphorous acid | 2.23 | 1.72 | 21.44 | 22.11 |
| 19 | 4-methylbenzoic acid | 4.47 | 25.56 | 40.87 | 42.31 |
| 20 | 4-ethylbenzoic acid | 4.47 | 25.40 | 41.26 | 42.49 |
| 21 | 4-propylbenzoic acid | 4.47 | 25.51 | 41.08 | 42.11 |
| 22 | 4-(1-methylethyl)-benzoic acid | 4.47 | 25.44 | 40.40 | 43.60 |
| 23 | 4-butylbenzoic acid | 4.47 | 25.52 | 41.27 | 41.64 |
| 24 | 4-(1,1-dimethylethyl)-benzoic acid | 4.4 | 25.51 | 41.39 | 42.06 |
| 25 | 4-phenylbenzoic acid | 4.07 | 23.99 | 40.19 | 41.02 |
| 26 | 4-fluorobenzoic acid | 4.07 | 23.17 | 39.27 | 40.84 |
| 27 | 4-chlorobenzoic acid | 4.07 | 21.50 | 38.01 | 39.74 |
| 28 | 4-bromobenzoic acid | 4.47 | 21.52 | 38.14 | 40.56 |
| 29 | 4-iodobenzoic acid | 4.47 | 20.68 | 37.66 | 39.99 |
| 30 | 4-methoxybenzoic acid | 4.5 | 27.33 | 42.67 | 44.36 |
| 31 | 4-hydroxybenzoic acid | 4.58 | 28.58 | 42.70 | 43.75 |
| 32 | 4-nitrobenzoic acid | 3.4 | 14.92 | 34.05 | 35.39 |
| 33 | 4-hydroxymethylbenzoic acid | 4.27 | 22.68 | 38.95 | 40.09 |
| 34 | 4-cyanobenzoic acid | 3.47 | 16.19 | 34.72 | 36.76 |
| 35 | 4-aminobenzoic acid | 4.92 | 36.24 | 46.32 | 50.17 |
| 36 | 4-methylaminobenzoic acid | 5.04 | 36.15 | 49.09 | 49.67 |
| 37 | 4-dimethylaminobenzoic acid | 5.07 | 35.04 | 48.01 | 50.23 |
| 38 | 4-trifluoromethylbenzoic acid | 3.67 | 19.09 | 36.47 | 38.60 |
| 39 | 4-sulfamoylbenzoic acid | 3.67 | 17.14 | 35.17 | 36.75 |
| 40 | 4-carbamoylbenzoic acid | 3.87 | 20.01 | 37.27 | 39.77 |
| 41 | salicylic acid | 2.97 | 13.13 | 31.28 | 32.75 |
| 42 | 2,4-dihydroxybenzoic acid | 3.11 | 18.08 | 34.85 | 35.57 |
| 43 | 5-iodo-2-hydroxybenzoic acid | 2.89 | 6.91 | 29.06 | 31.52 |
| 44 | 3-hydroxybenzoic acid | 4.08 | 24.19 | 38.86 | 41.19 |
| 45 | mandelic acid | 3.41 | 7.04 | 26.43 | 30.56 |
| 46 | 3-hydroxy-2-naphtoic acid | 2.97 | 11.16 | 30.58 | 33.13 |
| 47 | anthracene-9-carboxylic acid | 3.65 | 12.65 | 28.61 | 31.41 |
| 48 | pamoic acid | 2.47 | 4.01 | 29.28 | 30.03 |
| 49 | tert-butanol | 19.2 | 148.88 | 107.60 | 91.32 |

^a pK_a^{Exp} : Experimental aqueous pKa value of acids, taken from refs. 10, 51.

^b ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. 4 in [kJ·mol⁻¹].

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TABLE 2: Experimental base pK_a and Gibbs free energies of dissociation of bare and mono-solvated aqueous bases.

| Compound | $pK_a(\text{Exp})^a$ | $\Delta G_{\text{diss}}(\text{bare})^b$ | $\Delta G_{\text{diss}}(\text{H}_2\text{O})^b$ |
|---|----------------------|---|--|
| hydroxyimidazo(2,3-a)isoindole | 8.6 | 84.03 | 81.42 |
| imidazo[2,3-b]thioxazole | 8 | 70.10 | 67.38 |
| tetrahydrozoline | 10.5 | 85.97 | 79.31 |
| tolazoline | 10.3 | 83.64 | 76.58 |
| 4-chloroaniline | 4 | 47.44 | 44.78 |
| 4-methoxyaniline | 5.2 | 57.04 | 54.43 |
| 4-nitroaniline | 1 | 17.79 | 14.03 |
| aniline | 4.6 | 49.04 | 48.42 |
| p-toluidine | 5.1 | 55.31 | 49.08 |
| 1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one | 3.3 | 44.14 | 44.16 |
| 1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one | 1.6 | 24.12 | 30.42 |
| 1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one | 1.7 | 27.01 | 32.37 |
| 1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one | 3.5 | 46.25 | 45.91 |
| 2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine | 6.2 | 67.59 | 62.62 |
| 3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine | 4.8 | 50.84 | 52.73 |
| clonidine | 8.1 | 64.95 | 59.94 |
| debrisoquin | 11.9 | 104.81 | 96.56 |
| guanidine | 13.8 | 115.78 | 104.87 |
| methylguanidine | 13.4 | 109.68 | 99.79 |
| 2-aminopyridine | 6.71 | 67.69 | 58.98 |
| 2-aminothiazole | 5.4 | 55.09 | 48.11 |
| 2-methylimidazole | 8 | 66.68 | 62.94 |
| 3-aminopyridine | 6 | 65.51 | 60.04 |
| 4-aminopyridine | 9.23 | 81.02 | 72.89 |
| 4-methylpyridine | 6 | 56.34 | 52.25 |
| benzimidazole | 5.8 | 52.15 | 50.55 |
| imidazole | 7 | 62.51 | 59.27 |
| isoquinoline | 5.4 | 52.84 | 49.51 |
| melamine | 5 | 58.94 | 54.44 |
| pyrazine | 0.7 | 21.47 | 25.39 |
| pyrazole | 2.5 | 35.36 | 36.96 |
| pyridine | 5.14 | 51.55 | 48.55 |
| pyrimidine | 1.3 | 23.74 | 27.33 |
| quinoline | 4.8 | 46.99 | 46.62 |
| thiazole | 2.8 | 28.25 | 31.32 |
| 1-methylindole | -2.3 | -9.71 | -8.02 |
| 1-methylpyrrole | -2.9 | -16.56 | -10.76 |
| 2-methylindole | -0.3 | 6.96 | 14.10 |
| 2-methylpyrrole | -0.2 | 2.42 | 14.66 |
| 3-methylindole | -4.6 | -24.06 | -13.34 |
| 3-methylpyrrole | -1 | 7.11 | 15.84 |
| indole | -3.6 | -14.37 | -4.23 |
| pyrrole | -3.8 | -13.64 | -6.38 |

^a pK_a^{Exp} : Experimental aqueous base pKa value taken from ref. 24.

^b ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. 5 in [kJ·mol⁻¹].

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TABLE 3: Experimental aqueous base pK_a and Gibbs free energies of dissociation of bare and mono-solvated aliphatic amine bases.

| Compound | Base-Type | $pK_a(\text{Exp})^a$ | $\Delta G_{\text{diss}}(\text{bare})^b$ | $\Delta G_{\text{diss}}(\text{H}_2\text{O})^b$ | $pK_a^{\text{calc}}(\text{bare})^c$ | $pK_a^{\text{calc}}(\text{H}_2\text{O})^d$ | $\Delta pK_a(\text{bare})$ | $\Delta pK_a(\text{H}_2\text{O})$ |
|------------------------------|-----------|----------------------|---|--|-------------------------------------|--|----------------------------|-----------------------------------|
| 1 methylamine | primary | 10.6 | 104.07 | 88.78 | 11.97 | 11.09 | -1.37 | -0.49 |
| 2 ethylamine | primary | 10.9 | 100.39 | 86.62 | 11.50 | 10.76 | -0.60 | 0.14 |
| 3 n-propylamine | primary | 10.7 | 99.45 | 85.81 | 11.37 | 10.64 | -0.67 | 0.06 |
| 4 n-butylamine | primary | 10.8 | 99.17 | 85.81 | 11.34 | 10.64 | -0.54 | 0.16 |
| 5 n-pentylamine | primary | 10.6 | 98.93 | 85.84 | 11.31 | 10.64 | -0.71 | -0.04 |
| 6 n-hexylamine | primary | 10.6 | 98.92 | 85.18 | 11.30 | 10.54 | -0.70 | 0.06 |
| 7 n-heptylamine | primary | 10.7 | 98.84 | 85.08 | 11.29 | 10.53 | -0.59 | 0.17 |
| 8 n-octylamine | primary | 10.7 | 98.76 | 85.15 | 11.28 | 10.54 | -0.58 | 0.16 |
| 9 iso-propylamine | primary | 10.6 | 95.54 | 83.76 | 10.86 | 10.32 | -0.26 | 0.28 |
| 10 sec-butylamine | primary | 10.56 | 91.95 | 81.99 | 10.40 | 10.05 | 0.16 | 0.51 |
| 11 tert-butylamine | primary | 10.7 | 93.11 | 81.53 | 10.55 | 9.98 | 0.15 | 0.72 |
| 12 neo-pentylamine | primary | 10.21 | 94.59 | 80.82 | 10.74 | 9.87 | -0.53 | 0.34 |
| 13 cyclohexylamine | primary | 10.6 | 95.11 | 82.76 | 10.81 | 10.17 | -0.21 | 0.43 |
| 14 dimethylamine | secondary | 10.7 | 96.12 | 79.30 | 10.94 | 9.64 | -0.24 | 1.06 |
| 15 diethylamine | secondary | 11.1 | 88.89 | 78.44 | 10.00 | 9.51 | 1.10 | 1.59 |
| 16 di-n-propylamine | secondary | 11 | 87.51 | 76.91 | 9.82 | 9.28 | 1.18 | 1.72 |
| 17 di-iso-propylamine | secondary | 11.1 | 85.10 | 76.66 | 9.50 | 9.24 | 1.60 | 1.86 |
| 18 di-n-butylamine | secondary | 11.4 | 87.21 | 76.31 | 9.78 | 9.19 | 1.62 | 2.21 |
| 19 di-iso-butylamine | secondary | 10.5 | 77.93 | 64.94 | 8.57 | 7.45 | 1.93 | 3.05 |
| 20 di-sec-butylamine | secondary | 11.01 | 80.87 | 75.10 | 8.95 | 9.00 | 2.06 | 2.01 |
| 21 tert-butylcyclohexylamine | secondary | 11.23 | 81.90 | 73.15 | 9.09 | 8.70 | 2.14 | 2.53 |
| 22 trimethylamine | tertiary | 9.8 | 80.69 | 66.81 | 8.93 | 7.73 | 0.87 | 2.07 |
| 23 dimethylethylamine | tertiary | 10.2 | 78.60 | 67.65 | 8.66 | 7.86 | 1.54 | 2.34 |
| 24 dimethyl-n-propylamine | tertiary | 9.99 | 77.48 | 66.97 | 8.51 | 7.76 | 1.48 | 2.23 |
| 25 dimethyl-iso-propylamine | tertiary | 10.3 | 77.00 | 68.84 | 8.45 | 8.04 | 1.85 | 2.26 |
| 26 dimethyl-n-butylamine | tertiary | 10.02 | 77.22 | 66.78 | 8.48 | 7.73 | 1.54 | 2.29 |
| 27 dimethyl-iso-butylamine | tertiary | 9.91 | 74.43 | 65.50 | 8.11 | 7.53 | 1.80 | 2.38 |
| 28 dimethyl-sec-butylamine | tertiary | 10.4 | 77.84 | 68.69 | 8.56 | 8.02 | 1.84 | 2.38 |
| 29 dimethyl-tert-butylamine | tertiary | 10.52 | 80.82 | 71.46 | 8.95 | 8.45 | 1.57 | 2.07 |
| 30 triethylamine | tertiary | 10.8 | 78.65 | 71.56 | 8.66 | 8.46 | 2.14 | 2.34 |
| 31 tri-n-propylamine | tertiary | 10.7 | 78.96 | 69.69 | 8.71 | 8.17 | 1.99 | 2.53 |
| 32 tri-n-butylamine | tertiary | 10.89 | 78.47 | 69.36 | 8.64 | 8.12 | 2.25 | 2.77 |

^a pK_a^{Exp} : Experimental aqueous base pK_a value taken from ref. 24.

^b ΔG_{diss} : Gibbs free energies of dissociation calculated from eq. 5 in [kJ·mol⁻¹].

^c $pK_a^{\text{calc}}(\text{bare})$: pK_a of bare amine bases calculated from eq. 10.

^d $pK_a^{\text{calc}}(\text{H}_2\text{O})$: pK_a of mono-solvated amine bases calculated from eq. 11.

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Supplementary Material to:

First principles prediction of pK_a: COSMO-RS and the cluster-continuum approach

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KEYWORDS: pK_a; acidity; basicity; COSMO; COSMO-RS; density functional theory;

TABLE S1: Experimental pK_a and Gibbs free energies of bare, mono-solvated and di-solvated aqueous acids.

| Compound | $pK_a(\text{Exp})^a$ | $G(\text{AH})^b$ | $G(\text{A}^-)^b$ | $G(\text{AH}\cdot\text{H}_2\text{O})^b$ | $G(\text{A}^-\cdot\text{H}_2\text{O})^b$ | $G(\text{AH}\cdot 2\text{H}_2\text{O})^b$ | $G(\text{A}^-\cdot 2\text{H}_2\text{O})^b$ |
|----------------------------|----------------------|------------------|-------------------|---|--|---|--|
| ethanol | 15.9 | -407192.75 | -405932.1933 | -607976.05 | -606745.64 | -808761.49 | -807543.49 |
| 2,2,2-trichloroethanol | 12.2 | -4027063.85 | -4025847.339 | -4227856.50 | -4226648.60 | -4428641.71 | -4427442.50 |
| formic acid | 3.77 | -498419.13 | -497282.2218 | -699210.35 | -698055.91 | -899997.73 | -898839.19 |
| acetic acid | 4.75 | -601684.32 | -600535.0143 | -802473.84 | -801309.68 | -1003259.56 | -1002092.23 |
| nitromethane | 10.2 | -643528.89 | -642330.7273 | -844302.27 | -843106.77 | -1045086.79 | -1043890.01 |
| dichloroacetic acid | 1.3 | -3014912.86 | -3013789.195 | -3215708.21 | -3214562.05 | -3416493.77 | -3415345.82 |
| trichloroacetic acid | 0.89 | -4221505.27 | -4220390.258 | -4422303.25 | -4421163.36 | -4623090.73 | -4621947.40 |
| n-pentanoic acid | 4.84 | -911383.95 | -910231.9169 | -1112173.20 | -1111006.29 | -1312958.43 | -1311789.29 |
| 2,2-dimethylpropanoic acid | 5.05 | -911379.72 | -910224.755 | -1112168.43 | -1110999.50 | -1312954.03 | -1311782.78 |
| benzoic acid | 4.27 | -1105183.13 | -1104035.132 | -1305972.59 | -1304808.66 | -1506757.71 | -1505592.30 |
| oxalic acid | 1.23 | -993682.13 | -992561.2674 | -1194476.68 | -1193333.90 | -1395275.89 | -1394116.95 |
| maleic acid | 1.83 | -1196956.99 | -1195839.864 | -1397753.04 | -1396613.05 | -1598539.50 | -1597395.67 |
| fumaric acid | 3.03 | -1196967.63 | -1195828.574 | -1397758.39 | -1396600.71 | -1598553.49 | -1597395.11 |
| acrylic acid | 4.26 | -701679.58 | -700532.255 | -902469.38 | -901306.23 | -1103254.40 | -1102087.59 |
| bromoacetic acid | 2.87 | -7358183.68 | -7357050.701 | -7558976.50 | -7557823.62 | -7759760.56 | -7758605.15 |
| chloroacetic acid | 2.81 | -1808304.94 | -1807172.396 | -2009097.83 | -2007944.70 | -2209882.06 | -2208726.05 |
| cyanoacetic acid | 2.44 | -843914.94 | -842784.5871 | -1044708.49 | -1043557.94 | -1245493.73 | -1244338.97 |
| fluoroacetic acid | 2.66 | -862284.69 | -861151.695 | -1063077.34 | -1061924.80 | -1263861.99 | -1262706.68 |
| iodoacetic acid | 3.13 | -630170.59 | -629038.8935 | -830964.67 | -829811.56 | -1031750.65 | -1030593.65 |
| 2-hydroxypropanoic acid | 3.87 | -902477.35 | -901343.6465 | -1103269.20 | -1102116.71 | -1304053.44 | -1302898.61 |
| 2-chloropropanoic acid | 2.8 | -1911547.21 | -1910410.158 | -2112338.93 | -2111184.75 | -2313123.36 | -2311965.94 |
| 3-chloropropanoic acid | 4.1 | -1911557.21 | -1910412.972 | -2112347.78 | -2111186.43 | -2313131.32 | -2311968.50 |
| nitroacetic acid | 1.32 | -1138790.10 | -1137668.378 | -1339585.59 | -1338441.12 | -1540370.81 | -1539221.67 |
| 2-acetylbutanedioic acid | 2.86 | -1601062.73 | -1599929.447 | -1801854.80 | -1800713.60 | -2002637.00 | -2001488.99 |
| carbonic acid | 3.58 | -696063.66 | -694928.5828 | -896855.56 | -895699.46 | -1097648.86 | -1096483.02 |
| hypochlorous acid | 7.43 | -1407217.85 | -1406035.623 | -1608010.03 | -1606827.30 | -1808796.91 | -1807616.09 |
| hypobromous acid | 8.7 | -6957132.58 | -6955940.694 | -7157923.29 | -7156734.17 | -7358708.79 | -7357525.24 |
| hypoiodous acid | 10.64 | -229155.38 | -227958.9666 | -429946.84 | -428754.09 | -630733.26 | -629546.92 |
| nitrous acid | 3.3 | -540300.54 | -539174.0233 | -741089.51 | -739948.23 | -941886.43 | -940731.54 |
| sulfurous acid | 1.92 | -1641240.08 | -1640124.693 | -1842029.71 | -1840899.02 | -2042817.45 | -2041685.41 |
| phosphoric acid | 1.97 | -1691557.18 | -1690433.734 | -1892350.57 | -1891220.18 | -2093144.26 | -2092006.90 |
| boric acid | 9.12 | -663171.83 | -661976.44 | -863958.05 | -862762.47 | -1064744.19 | -1063547.34 |
| pentachlorophenol | 4.9 | -6840598.39 | -6839444.506 | -7041383.83 | -7040224.69 | -7242169.77 | -7241008.74 |
| 2,3,4,6-tetrachlorophenol | 5.62 | -5633988.50 | -5632828.508 | -5834773.01 | -5833609.58 | -6035558.82 | -6034396.15 |
| 2,3,4-trichlorophenol | 7.1 | -4427367.41 | -4426191.903 | -4628156.05 | -4626977.85 | -4828942.19 | -4827762.20 |
| 2,3-dichlorophenol | 7.76 | -3220743.41 | -3219563.891 | -3421531.41 | -3420350.20 | -3622317.22 | -3621134.50 |
| 2,4,5-trichlorophenol | 7.07 | -4427376.94 | -4426203.737 | -4628166.28 | -4626989.59 | -4828952.12 | -4827772.48 |
| 2,4,6-trichlorophenol | 6.21 | -4427374.18 | -4426208.085 | -4628158.50 | -4626991.26 | -4828944.52 | -4827776.86 |
| 2,4-dichlorophenol | 8.09 | -3220750.81 | -3219569.449 | -3421538.79 | -3420356.61 | -3622324.86 | -3621140.83 |
| 2,5-dichlorophenol | 7.51 | -3220753.12 | -3219575.638 | -3421541.64 | -3420362.07 | -3622327.12 | -3621145.20 |
| 2,6-dichlorophenol | 6.79 | -3220742.78 | -3219570.947 | -3421526.15 | -3420353.87 | -3622311.80 | -3621137.85 |
| 2-chlorophenol | 8.29 | -2014114.41 | -2012929.057 | -2214901.51 | -2213716.24 | -2415687.32 | -2414499.14 |
| 3,4-dichlorophenol | 8.68 | -3220747.30 | -3219560.318 | -3421535.27 | -3420348.56 | -3622321.71 | -3621136.04 |
| 3,5-dichlorophenol | 8.27 | -3220756.86 | -3219574.512 | -3421545.42 | -3420362.03 | -3622331.64 | -3621149.16 |
| 3-chlorophenol | 8.78 | -2014119.59 | -2012929.705 | -2214907.33 | -2213717.95 | -2415693.09 | -2414505.40 |
| 4-chlorophenol | 9.14 | -2014118.05 | -2012924.008 | -2214905.55 | -2213713.45 | -2415690.81 | -2414501.17 |
| phenol | 9.82 | -807476.99 | -806281.6423 | -1008263.81 | -1007070.52 | -1209049.16 | -1207858.12 |
| 5-nitouracil | 5.3 | -1626604.26 | -1625445.605 | -1827385.29 | -1826224.65 | -2028170.63 | -2027009.62 |
| cis-5-formyluracil | 6.84 | -1387126.03 | -1385955.365 | -1587905.80 | -1586734.75 | -1788690.61 | -1787522.54 |
| thymine | 9.75 | -1192743.49 | -1191550.382 | -1393523.03 | -1392331.35 | -1594308.61 | -1593116.50 |
| trans-5-formyluracil | 6.84 | -1387126.80 | -1385956.72 | -1587906.25 | -1586736.14 | -1788690.49 | -1787520.58 |

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|----|------------------------------------|------|-------------|--------------|-------------|-------------|-------------|-------------|
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| 4 | uracil | 9.42 | -1089497.97 | -1088308.718 | -1290277.91 | -1289089.31 | -1491063.39 | -1489874.12 |
| 5 | fluorouracil | 8 | -1350092.82 | -1348913.347 | -1550873.31 | -1549690.50 | -1751657.53 | -1750475.21 |
| 6 | methylthiouracil | 8.2 | -2040569.26 | -2039393.19 | -2241345.72 | -2240167.86 | -2442134.11 | -2440952.29 |
| 7 | phenytoin | 8.3 | -2202875.30 | -2201694.294 | -2403655.06 | -2402470.88 | -2604440.43 | -2603259.12 |
| 8 | 3,3-methylphenylglutarimide | 9.2 | -1760440.91 | -1759252.26 | -1961218.09 | -1960025.97 | -2162001.52 | -2160811.49 |
| 9 | 3,3-dimethylsuccinimide | 9.5 | -1153722.82 | -1152540.452 | -1354502.51 | -1353315.96 | -1555287.70 | -1554103.43 |
| 10 | dimethadione | 6.1 | -1248067.53 | -1246907.195 | -1448849.90 | -1447683.17 | -1649635.83 | -1648467.03 |
| 11 | phthalimide | 8.3 | -1347506.31 | -1346323.738 | -1548286.07 | -1547100.56 | -1749071.94 | -1747887.00 |
| 12 | succinimide | 9.6 | -947253.37 | -946071.131 | -1148032.98 | -1146847.30 | -1348818.45 | -1347631.36 |
| 13 | phthalic acid | 2.76 | -1600451.16 | -1599327.289 | -1801244.53 | -1800101.00 | -2002026.77 | -2000883.60 |
| 14 | methanol | 15.5 | -303944.85 | -302683.1629 | -504728.69 | -503499.17 | -705514.01 | -704298.27 |
| 15 | hypophosphorous acid | 2.23 | -1296181.52 | -1295055.33 | -1496980.74 | -1495834.83 | -1697768.92 | -1696622.33 |
| 16 | 4-methylbenzoic acid | 4.47 | -1208429.73 | -1207279.699 | -1409219.11 | -1408053.76 | -1610003.58 | -1608836.79 |
| 17 | 4-ethylbenzoic acid | 4.47 | -1311661.86 | -1310511.979 | -1512451.32 | -1511285.58 | -1713236.34 | -1712069.38 |
| 18 | 4-propylbenzoic acid | 4.47 | -1414896.30 | -1413746.319 | -1615685.65 | -1614520.09 | -1816470.40 | -1815303.82 |
| 19 | 4-(1-methylethyl)-benzoic acid | 4.47 | -1414894.16 | -1413744.25 | -1615682.93 | -1614518.05 | -1816469.17 | -1815301.09 |
| 20 | 4-butylbenzoic acid | 4.47 | -1518129.79 | -1516979.803 | -1718919.20 | -1717753.46 | -1919703.85 | -1918537.73 |
| 21 | 4-(1,1-dimethylethyl)-benzoic acid | 4.4 | -1518120.53 | -1516970.554 | -1718910.22 | -1717744.36 | -1919694.43 | -1918527.90 |
| 22 | 4-phenylbenzoic acid | 4.07 | -1711933.61 | -1710785.145 | -1912723.38 | -1911558.71 | -2113508.03 | -2112342.53 |
| 23 | 4-fluorobenzoic acid | 4.07 | -1365814.05 | -1364666.409 | -1566603.79 | -1565440.04 | -1767388.73 | -1766223.42 |
| 24 | 4-chlorobenzoic acid | 4.07 | -2311823.82 | -2310677.843 | -2512613.70 | -2511451.22 | -2713399.04 | -2712234.83 |
| 25 | 4-bromobenzoic acid | 4.47 | -7861698.99 | -7860552.997 | -8062488.85 | -8061326.24 | -8263274.78 | -8262109.75 |
| 26 | 4-iodobenzoic acid | 4.47 | -1133680.18 | -1132535.028 | -1334470.31 | -1333308.18 | -1535256.61 | -1534092.14 |
| 27 | 4-methoxybenzoic acid | 4.5 | -1405956.62 | -1404804.816 | -1606745.65 | -1605578.51 | -1807530.40 | -1806361.57 |
| 28 | 4-hydroxybenzoic acid | 4.58 | -1302780.78 | -1301627.725 | -1503568.82 | -1502401.65 | -1704361.16 | -1703192.94 |
| 29 | 4-nitrobenzoic acid | 3.4 | -1642310.23 | -1641170.834 | -1843101.90 | -1841943.38 | -2043886.92 | -2042727.05 |
| 30 | 4-hydroxymethylbenzoic acid | 4.27 | -1405982.04 | -1404834.881 | -1606771.60 | -1605608.18 | -1807556.39 | -1806391.84 |
| 31 | 4-cyanobenzoic acid | 3.47 | -1347430.97 | -1346290.307 | -1548222.28 | -1547063.09 | -1749007.41 | -1747846.18 |
| 32 | 4-aminobenzoic acid | 4.92 | -1250609.21 | -1249448.504 | -1451396.14 | -1450225.35 | -1652183.29 | -1651008.64 |
| 33 | 4-methylaminobenzoic acid | 5.04 | -1353813.87 | -1352653.242 | -1554600.86 | -1553427.29 | -1755385.15 | -1754211.00 |
| 34 | 4-dimethylaminobenzoic acid | 5.07 | -1457011.07 | -1455851.555 | -1657798.34 | -1656625.86 | -1858582.64 | -1857407.94 |
| 35 | 4-trifluoromethylbenzoic acid | 3.67 | -1990349.42 | -1989205.856 | -2191139.87 | -2189978.93 | -2391925.76 | -2390762.68 |
| 36 | 4-sulfamoylbenzoic acid | 3.67 | -2691002.97 | -2689861.36 | -2891793.37 | -2890633.73 | -3092578.83 | -3091417.61 |
| 37 | 4-carbamoylbenzoic acid | 3.87 | -1548296.73 | -1547152.255 | -1749086.91 | -1747925.16 | -1949872.98 | -1948708.74 |
| 38 | salicylic acid | 2.97 | -1302781.05 | -1301643.449 | -1503572.26 | -1502416.50 | -1704357.38 | -1703200.15 |
| 39 | 2,4-dihydroxybenzoic acid | 3.11 | -1500379.49 | -1499236.936 | -1701169.59 | -1700010.27 | -1901962.21 | -1900802.17 |
| 40 | 5-iodo-2-hydroxybenzoic acid | 2.89 | -1331275.18 | -1330143.798 | -1532067.89 | -1530914.36 | -1732854.39 | -1731698.40 |
| 41 | 3-hydroxybenzoic acid | 4.08 | -1302772.24 | -1301623.573 | -1503560.22 | -1502396.89 | -1704353.11 | -1703187.44 |
| 42 | mandelic acid | 3.41 | -1405965.98 | -1404834.467 | -1606758.61 | -1605607.71 | -1807544.47 | -1806389.44 |
| 43 | 3-hydroxy-2-naphthoic acid | 2.97 | -1706239.82 | -1705104.186 | -1907031.97 | -1905876.92 | -2107818.67 | -2106661.06 |
| 44 | anthracene-9-carboxylic acid | 3.65 | -1912066.61 | -1910929.486 | -2112858.36 | -2111705.28 | -2313643.82 | -2312487.94 |
| 45 | pamoic acid | 2.47 | -3512537.22 | -3511408.744 | -3713327.51 | -3712173.75 | -3914119.46 | -3912964.95 |
| 46 | tert-butanol | 19.2 | -613681.06 | -612407.7033 | -814465.54 | -813233.47 | -1015246.84 | -1014031.04 |

^a pK_a^{Exp} : Experimental pK_a value of acids in water..

^b G : Gibbs free energies in [kJ·mol⁻¹].

TABLE S2: Experimental base pK_a and Gibbs free energies of bare and mono-solvated aqueous bases.

| Compound | $pK_a(\text{Exp})^a$ | $G(\text{B})^b$ | $G(\text{BH}^+)^b$ | $G(\text{B-H}_2\text{O})^b$ | $G(\text{BH}^+\text{-H}_2\text{O})^b$ |
|---|----------------------|-----------------|--------------------|-----------------------------|---------------------------------------|
| hydroxyimidazo(2,3-a)isoindole | 8.6 | -1747137.48 | -1748345.98 | -1947921.18 | -1949127.07 |
| imidazo[2,3-b]thioxazole | 8 | -2088269.45 | -2089464.03 | -2289054.14 | -2290245.99 |
| tetrahydrozoline | 10.5 | -1613792.59 | -1615003.04 | -1814578.71 | -1815782.50 |
| tolazoline | 10.3 | -1307246.76 | -1308454.87 | -1508033.01 | -1509234.06 |
| 4-chloroaniline | 4 | -1961939.83 | -1963111.75 | -2162726.60 | -2163895.85 |
| 4-methoxyaniline | 5.2 | -1056058.83 | -1057240.34 | -1256843.90 | -1258022.80 |
| 4-nitroaniline | 1 | -1292458.99 | -1293601.26 | -1493249.66 | -1494388.17 |
| aniline | 4.6 | -755300.38 | -756473.89 | -956084.38 | -957257.27 |
| p-toluidine | 5.1 | -858541.01 | -859720.79 | -1059327.74 | -1060501.29 |
| 1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one | 3.3 | -2108407.13 | -2109575.74 | -2309189.75 | -2310358.39 |
| 1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one | 1.6 | -2305987.13 | -2307135.73 | -2506764.53 | -2507919.42 |
| 1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one | 1.7 | -2202786.39 | -2203937.88 | -2403564.50 | -2404721.34 |
| 1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one | 3.5 | -2005206.89 | -2006377.61 | -2205989.94 | -2207160.32 |
| 2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine | 6.2 | -1913920.45 | -1915112.51 | -2114706.02 | -2115893.12 |
| 3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine | 4.8 | -2253639.16 | -2254814.48 | -2454417.22 | -2455594.42 |
| clonidine | 8.1 | -3762692.20 | -3763881.63 | -3963474.07 | -3964658.48 |
| debrisoquin | 11.9 | -1452665.25 | -1453894.53 | -1653451.72 | -1654672.75 |
| guanidine | 13.8 | -539448.31 | -540688.56 | -740232.78 | -741462.12 |
| methylguanidine | 13.4 | -642651.50 | -643885.65 | -843437.72 | -844661.98 |
| 2-aminopyridine | 6.71 | -797461.96 | -798654.13 | -998245.68 | -999429.14 |
| 2-aminothiazole | 5.4 | -1639571.03 | -1640750.59 | -1840353.64 | -1841526.22 |
| 2-methylimidazole | 8 | -697390.05 | -698581.20 | -898175.66 | -899363.08 |
| 3-aminopyridine | 6 | -797438.34 | -798628.33 | -998225.57 | -999410.08 |
| 4-aminopyridine | 9.23 | -797457.41 | -798662.91 | -998245.21 | -999442.57 |
| 4-methylpyridine | 6 | -755276.85 | -756457.67 | -956063.31 | -957240.03 |
| benzimidazole | 5.8 | -997614.32 | -998790.94 | -1198398.63 | -1199573.66 |
| imidazole | 7 | -594137.28 | -595324.27 | -794922.61 | -796106.36 |
| isoquinoline | 5.4 | -1055491.82 | -1056669.13 | -1256277.98 | -1257451.97 |
| melamine | 5 | -1172700.67 | -1173884.09 | -1373479.11 | -1374658.03 |
| pyrazine | 0.7 | -694144.42 | -695290.37 | -894927.94 | -896077.80 |
| pyrazole | 2.5 | -594086.49 | -595246.32 | -794869.01 | -796030.45 |
| pyridine | 5.14 | -652027.79 | -653203.81 | -852813.94 | -853986.95 |
| pyrimidine | 1.3 | -694163.24 | -695311.45 | -894946.47 | -896098.28 |
| quinoline | 4.8 | -1055495.90 | -1056667.36 | -1256280.84 | -1257451.93 |
| thiazole | 2.8 | -1494148.96 | -1495301.69 | -1694932.21 | -1696088.00 |
| 1-methylindole | -2.3 | -1058643.42 | -1059758.17 | -1259414.79 | -1260531.24 |
| 1-methylpyrrole | -2.9 | -655168.18 | -656276.09 | -855937.98 | -857051.70 |
| 2-methylindole | -0.3 | -1058683.99 | -1059815.42 | -1259462.09 | -1260600.66 |
| 2-methylpyrrole | -0.2 | -655207.87 | -656334.76 | -855980.94 | -857120.07 |
| 3-methylindole | -4.6 | -1058679.73 | -1059780.14 | -1259454.52 | -1260565.65 |
| 3-methylpyrrole | -1 | -655199.67 | -656331.26 | -855973.02 | -857113.34 |
| indole | -3.6 | -955437.39 | -956547.49 | -1156212.31 | -1157332.55 |
| pyrrole | -3.8 | -551960.55 | -553071.38 | -752735.34 | -753853.44 |

^a pK_a^{Exp} : Experimental pK_a value of bases in water..

^b G : Gibbs free energies in [$\text{kJ}\cdot\text{mol}^{-1}$].

TABLE S3: Experimental aqueous base pK_a and Gibbs free energies of bare and mono-solvated aliphatic amines.

| Compound | Base-Type | $pK_a(\text{Exp})$ | $G(\text{B})$ | $G(\text{BH}^+)$ | $G(\text{B-H}_2\text{O})$ | $G(\text{BH}^+-\text{H}_2\text{O})$ |
|---------------------------|-----------|--------------------|---------------|------------------|---------------------------|-------------------------------------|
| methylamine | primary | 10.6 | -251766.85 | -252993.48 | -452559.44 | -453772.6972 |
| ethylamine | primary | 10.9 | -355007.93 | -356230.91 | -555799.60 | -557010.6987 |
| n-propylamine | primary | 10.7 | -458241.12 | -459463.14 | -659032.76 | -660243.044 |
| n-butylamine | primary | 10.8 | -561474.48 | -562696.40 | -762266.01 | -763476.2888 |
| n-pentylamine | primary | 10.6 | -664708.10 | -665929.85 | -865499.55 | -866709.865 |
| n-hexylamine | primary | 10.6 | -767941.75 | -769163.33 | -968733.09 | -969942.734 |
| n-heptylamine | primary | 10.7 | -871175.29 | -872396.82 | -1071966.63 | -1073176.187 |
| n-octylamine | primary | 10.7 | -974408.94 | -975630.37 | -1175200.31 | -1176409.932 |
| iso-propylamine | primary | 10.6 | -458250.20 | -459468.87 | -659040.90 | -660249.1431 |
| sec-butylamine | primary | 10.56 | -561481.27 | -562696.14 | -762271.30 | -763477.7667 |
| tert-butylamine | primary | 10.7 | -561489.55 | -562705.66 | -762279.98 | -763485.9896 |
| neo-pentylamine | primary | 10.21 | -664705.68 | -665923.02 | -865496.88 | -866702.1767 |
| cyclohexylamine | primary | 10.6 | -764791.27 | -766009.29 | -965581.98 | -966789.2147 |
| dimethylamine | secondary | 10.7 | -354980.45 | -356191.32 | -555765.71 | -556969.4821 |
| diethylamine | secondary | 11.1 | -561460.56 | -562665.28 | -762244.69 | -763447.601 |
| di-n-propylamine | secondary | 11 | -767926.45 | -769129.86 | -968710.65 | -969912.0297 |
| di-iso-propylamine | secondary | 11.1 | -767930.46 | -769133.70 | -968715.06 | -969916.1912 |
| di-n-butylamine | secondary | 11.4 | -974393.18 | -975596.37 | -1175177.28 | -1176378.07 |
| di-iso-butylamine | secondary | 10.5 | -974392.56 | -975588.00 | -1175175.99 | -1176365.403 |
| di-sec-butylamine | secondary | 11.01 | -974390.37 | -975589.42 | -1175174.33 | -1176373.912 |
| tert-butylcyclohexylamine | secondary | 11.23 | -1177699.78 | -1178900.20 | -1378483.85 | -1379681.473 |
| trimethylamine | tertiary | 9.8 | -458196.12 | -459387.58 | -658976.61 | -660167.8995 |
| dimethylethylamine | tertiary | 10.2 | -561431.11 | -562621.17 | -762211.64 | -763403.7712 |
| dimethyl-n-propylamine | tertiary | 9.99 | -664663.97 | -665853.12 | -865444.01 | -866635.4592 |
| dimethyl-iso-propylamine | tertiary | 10.3 | -664661.48 | -665849.88 | -865440.42 | -866633.729 |
| dimethyl-n-butylamine | tertiary | 10.02 | -767897.33 | -769086.03 | -968677.40 | -969868.6602 |
| dimethyl-iso-butylamine | tertiary | 9.91 | -767890.97 | -769081.87 | -968674.39 | -969864.3698 |
| dimethyl-sec-butylamine | tertiary | 10.4 | -767887.91 | -769077.14 | -968667.41 | -969860.5798 |
| dimethyl-tert-butylamine | tertiary | 10.52 | -767884.44 | -769080.15 | -968668.05 | -969863.9856 |
| triethylamine | tertiary | 10.8 | -767892.51 | -769088.86 | -968675.78 | -969871.8192 |
| tri-n-propylamine | tertiary | 10.7 | -1077590.04 | -1078783.91 | -1278373.11 | -1279567.279 |
| tri-n-butylamine | tertiary | 10.89 | -1387289.99 | -1388483.44 | -1588073.28 | -1589267.115 |

^a pK_a^{Exp} : Experimental pK_a value of bases in water..

^b G : Gibbs free energies in $[\text{kJ}\cdot\text{mol}^{-1}]$.


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0.3245 0.3500 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
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-1.2936 2.2882 -0.0002 Cl 0 0 0 0 0 0 0 0 0 0 0 0 12
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6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
1.2155 -0.9108 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
1.1918 0.4802 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0000 1.2988 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.1918 0.4802 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2155 -0.9108 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0000 -1.5987 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0000 2.5726 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.7450 1.3470 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
2.7450 1.3470 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 9
0.0000 -3.3792 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 10
2.1639 -1.4476 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.1639 -1.4476 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
1.2068 0.4404 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
1.1983 -0.9531 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.0301 -1.6143 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2381 -0.9175 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.1914 0.4743 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0186 1.1943 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0559 -3.3814 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 7
0.0860 2.5466 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 8
2.7452 1.2941 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 9
2.1362 -1.5056 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1938 -1.4385 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.6908 1.4051 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12
-0.8263 2.9098 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
8 6 0 0 0 0
8 13 0 0 0 0
M END
$$$$
2,4-dichlorophenol0-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000

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1
2
3 1.9556 0.0851 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
4 1.4643 -1.2190 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
5 0.0827 -1.4332 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
6 -0.8072 -0.3557 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
7 -0.2903 0.9372 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
8 1.1181 1.2583 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
9 -0.5628 -3.0984 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 7
10 1.5806 2.4556 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 8
11 3.0360 0.2519 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
12 2.1532 -2.0657 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
13 -1.8850 -0.5198 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
14 -1.4380 2.3030 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12
15
16 2 1 0 0 0 0
17 6 1 0 0 0 0
18 9 1 0 0 0 0
19 3 2 0 0 0 0
20 10 2 0 0 0 0
21 4 3 0 0 0 0
22 7 3 0 0 0 0
23 5 4 0 0 0 0
24 11 4 0 0 0 0
25 6 5 0 0 0 0
26 8 6 0 0 0 0
27 5 12 0 0 0 0
28 M END
29 \$\$\$\$
30 2,4-dichlorophenol0.sdf
31 COSMOTHERM 3D 0
32
33 13 13 0 0 0 0 0 0 0 0 0 0 V2000
34 -1.4557 -1.2285 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
35 -1.9390 0.0795 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
36 -1.0605 1.1725 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
37 0.3222 0.9132 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
38 0.8291 -0.3856 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
39 -0.0761 -1.4469 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
40 -1.5848 2.4296 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
41 1.4300 2.2920 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
42 0.5472 -3.1057 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 9
43 -2.1509 -2.0674 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
44 -3.0129 0.2701 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
45 1.9042 -0.5580 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
46 -0.8529 3.0827 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
47
48 2 1 0 0 0 0
49 6 1 0 0 0 0
50 10 1 0 0 0 0
51 3 2 0 0 0 0
52 11 2 0 0 0 0
53 4 3 0 0 0 0
54 7 3 0 0 0 0
55 5 4 0 0 0 0
56 8 4 0 0 0 0
57 6 5 0 0 0 0
58 12 5 0 0 0 0
59 9 6 0 0 0 0
60 7 13 0 0 0 0
M END
\$\$\$\$
2,4-dichlorophenol1-anion.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
1.9555 0.0851 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 1
1.4643 -1.2191 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0827 -1.4332 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.8073 -0.3557 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2903 0.9372 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1181 1.2582 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.5629 -3.0983 0.0003 Cl 0 0 0 0 0 0 0 0 0 0 0 7
1.5807 2.4555 0.0009 O 0 0 0 0 0 0 0 0 0 0 0 8
3.0359 0.2519 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1531 -2.0658 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.8850 -0.5198 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.4380 2.3030 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0
M END
\$\$\$\$
2,4-dichlorophenol1.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-1.4604 -1.2291 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.9420 0.0809 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.0650 1.1759 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.3189 0.9217 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
0.8202 -0.3796 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0819 -1.4442 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.4913 2.4704 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 7
1.4451 2.2790 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
0.5467 -3.1014 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 9
-2.1563 -2.0673 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.0191 0.2619 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
1.8955 -0.5513 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.4678 2.4888 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 13

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2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
9 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid-anion0.sdf
COSMOtherm 3D 0
16 17 0 0 0 0 0 0 0 0 0 V2000
1.5941 -1.3908 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.2041 -1.4553 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.5977 -0.3016 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0492 0.9685 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4535 1.0466 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.2138 -0.1263 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.0980 -0.3895 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.6725 -1.5067 0.0033 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.7328 0.7507 -0.0030 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.6803 2.1049 0.0006 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5875 -0.1022 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.6808 1.7205 -0.0016 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
3.8955 0.8242 0.0020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.2073 -2.2927 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.2976 -2.4250 -0.0024 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.9366 2.0268 0.0026 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 9 0 0 0 0
12 10 0 0 0 0
13 11 0 0 0 0
5 16 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid-anion1.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 0 V2000
1.5302 -1.4156 -0.0202 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.1374 -1.4040 -0.0164 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6334 -0.2259 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0842 0.9983 0.0122 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4889 1.0087 0.0118 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.2099 -0.1879 -0.0047 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.1577 -0.3607 -0.0039 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.6195 -1.5465 0.0645 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.8609 0.6924 -0.0757 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.5844 2.1967 0.0325 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5805 -0.0989 -0.0040 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.0828 2.9108 0.0505 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
3.9595 -0.9985 -0.0143 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.0857 -2.3562 -0.0300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.4149 -2.3449 -0.0242 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
2.0280 1.9595 0.0263 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 10 0 0 0 0
13 11 0 0 0 0
5 16 0 0 0 0
M END
$$$$
2,4-dihydroxybenzoicacid0.sdf
COSMOtherm 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
1.5723 -1.4046 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.1901 -1.4473 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.5868 -0.2655 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0868 0.9926 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4864 1.0397 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.2204 -0.1495 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.0428 -0.2854 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.6034 -1.5138 0.0018 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.7494 0.7444 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9

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M END
$$$$
2,5-dichlorophenol0-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
0.7628 1.0465 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
1.5078 -0.1231 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
0.9400 -1.3999 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.4629 -1.4675 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2303 -0.3100 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.6821 1.0268 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.5478 -2.3028 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.3881 2.0947 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 8
1.2515 2.0221 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
3.2997 0.0049 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-0.9534 -2.4425 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
-3.0088 -0.4571 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0

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M END
$$$$
2,5-dichlorophenol1.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 V2000
-1.5278 -0.1262 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7607 1.0357 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
0.6382 0.9316 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2203 -0.3498 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4380 -1.5018 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9561 -1.4001 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
1.3649 2.0814 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 7
2.9859 -0.4608 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
-3.2931 0.0250 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 9
-1.2200 2.0238 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
0.9136 -2.4825 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.5743 -2.2964 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
2.3199 1.8553 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 6 0 0 0 0
7 13 0 0 0 0

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M END
$$$$
2,5-dichlorophenol1-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
0.7628 1.0465 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
1.5078 -0.1231 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
0.9400 -1.3999 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.4629 -1.4675 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2303 -0.3100 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.6821 1.0268 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.5478 -2.3028 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.3881 2.0947 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 8
1.2515 2.0222 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
3.2997 0.0049 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-0.9534 -2.4425 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
-3.0088 -0.4571 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
5 12 0 0 0 0

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M END
$$$$
2,5-dichlorophenol1.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 V2000
-1.5289 -0.1298 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7646 1.0355 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 2
0.6358 0.9404 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2281 -0.3365 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4456 -1.4890 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9498 -1.3986 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.4439 2.0355 -0.0004 O 0 0 0 0 0 0 0 0 0 0 0 7

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2.9875 -0.4694 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 8
-3.2949 0.0150 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 9
-1.2392 2.0179 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 10
0.9267 -2.4671 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.5614 -2.2994 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 12
0.8976 2.8452 0.0010 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2,6-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
1.2079 -1.6352 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
1.1906 -0.2449 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0000 0.5750 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.1906 -0.2449 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2079 -1.6352 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0000 -2.3471 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0001 1.8509 -0.0009 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.7476 0.6299 0.0004 Cl 0 0 0 0 0 0 0 0 0 0 0 8
2.7476 0.6299 0.0004 Cl 0 0 0 0 0 0 0 0 0 0 0 9
2.1627 -2.1639 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1627 -2.1639 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 11
0.0000 -3.4371 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
2,6-dichlorophenol.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
1.2175 -1.6473 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
1.2016 -0.2539 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.0037 0.4723 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.1977 -0.2745 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2066 -1.6667 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0108 -2.3534 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0308 1.8282 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.7189 0.6323 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
2.7218 0.6426 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 9
2.1717 -2.1736 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1544 -2.2040 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 11
0.0193 -3.4432 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.8914 2.1655 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid0-anion.sdf
COSMOTHERM 3D 0
18 17 0 0 0 0 0 0 0 0 0 V2000
2.2232 0.3007 0.1407 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8777 0.7708 -0.4678 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.3557 0.1722 0.2088 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.6165 1.0646 0.0963 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.5113 2.2501 -0.1966 O 0 0 0 0 0 0 0 0 0 0 0 5
-2.9498 0.4386 0.4105 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6266 -1.2443 -0.2720 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.9322 -2.0884 0.7436 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.5854 -1.6051 -1.4402 O 0 0 0 0 0 0 0 0 0 0 0 9
3.2463 0.4332 -0.5992 O 0 0 0 0 0 0 0 0 0 0 0 10
2.2135 -0.1409 1.3304 O 0 0 0 0 0 0 0 0 0 0 0 11
0.8693 0.5646 -1.5468 H 0 0 0 0 0 0 0 0 0 0 0 12
0.8323 1.8656 -0.3542 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.1498 0.1091 1.2935 H 0 0 0 0 0 0 0 0 0 0 0 14
-3.7234 1.2106 0.4889 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.2240 -0.2612 -0.3961 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.9002 -0.1491 1.3383 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.1216 -2.9726 0.3583 H 0 0 0 0 0 0 0 0 0 0 0 18

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2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
8 18 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid0.sdf
COSMOTHERM 3D 0
19 18 0 0 0 0 0 0 0 0 0 V2000
2.1182 0.2652 0.2160 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8190 0.8846 -0.2428 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.4119 0.1673 0.3022 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.6943 1.0309 0.1293 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.5952 2.2153 -0.1614 O 0 0 0 0 0 0 0 0 0 0 0 5
-3.0218 0.3685 0.3709 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.5729 -1.2158 -0.3164 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.0632 -2.1156 0.5642 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.3037 -1.4879 -1.4767 O 0 0 0 0 0 0 0 0 0 0 0 9
3.1783 0.8193 -0.4200 O 0 0 0 0 0 0 0 0 0 0 0 10
2.2332 -0.6124 1.0597 O 0 0 0 0 0 0 0 0 0 0 0 11
0.8055 0.9116 -1.3414 H 0 0 0 0 0 0 0 0 0 0 0 12
0.8083 1.9337 0.0887 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.3183 0.0267 1.3922 H 0 0 0 0 0 0 0 0 0 0 0 14
-3.8153 1.1228 0.4116 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.2368 -0.3319 -0.4527 H 0 0 0 0 0 0 0 0 0 0 0 16
-3.0061 -0.2246 1.2961 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.1795 -2.9730 0.0980 H 0 0 0 0 0 0 0 0 0 0 0 18
3.9963 0.4024 -0.0712 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 8 0 0 0 0
10 19 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid0a-anion.sdf
COSMOTHERM 3D 0
18 17 0 0 0 0 0 0 0 0 0 V2000
2.1110 0.2524 -0.2723 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7944 0.9168 0.0530 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.4231 0.1126 -0.3838 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.5558 -1.1962 0.3766 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.0692 -1.3381 1.5023 O 0 0 0 0 0 0 0 0 0 0 0 5
-1.3304 -2.2988 -0.2997 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.7793 0.9239 -0.1608 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.7525 0.5756 -0.8853 O 0 0 0 0 0 0 0 0 0 0 0 8
-1.7555 1.8239 0.7215 O 0 0 0 0 0 0 0 0 0 0 0 9
3.1595 0.9487 0.2445 O 0 0 0 0 0 0 0 0 0 0 0 10
2.2660 -0.7701 -0.9259 O 0 0 0 0 0 0 0 0 0 0 0 11
0.7942 1.9048 -0.4328 H 0 0 0 0 0 0 0 0 0 0 0 12
0.7596 1.1140 1.1329 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.3842 -0.1153 -1.4577 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.6086 -3.0795 0.4186 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.2176 -1.8857 -0.8007 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.6959 -2.7425 -1.0847 H 0 0 0 0 0 0 0 0 0 0 0 17
3.9862 0.4877 -0.0172 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 18 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid1.sdf
COSMOTHERM 3D 0
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19 18 0 0 0 0 0 0 0 0 0 V2000
  1.7993  0.2424  0.1129 C  0 0 0 0 0 0 0 0 0 0 0 1
  1.0119 -1.0494  0.0978 C  0 0 0 0 0 0 0 0 0 0 0 2
 -0.4962 -0.8069 -0.0072 C  0 0 0 0 0 0 0 0 0 0 0 3
 -1.1433 -0.1380  1.2128 C  0 0 0 0 0 0 0 0 0 0 0 4
 -2.1830  0.5245  1.0840 O  0 0 0 0 0 0 0 0 0 0 0 5
 -0.5585 -0.3837  2.5677 C  0 0 0 0 0 0 0 0 0 0 0 6
 -0.8612 -0.1841 -1.3738 C  0 0 0 0 0 0 0 0 0 0 0 7
 -2.0155  0.4863 -1.4435 O  0 0 0 0 0 0 0 0 0 0 0 8
 -0.1540 -0.3378 -2.3591 O  0 0 0 0 0 0 0 0 0 0 0 9
  3.1252  0.0248 -0.0217 O  0 0 0 0 0 0 0 0 0 0 0 10
  1.3087  1.3552  0.2460 O  0 0 0 0 0 0 0 0 0 0 0 11
  1.2616 -1.6191  1.0047 H  0 0 0 0 0 0 0 0 0 0 0 12
  1.3526 -1.6624 -0.7460 H  0 0 0 0 0 0 0 0 0 0 0 13
 -0.9808 -1.8040 -0.0244 H  0 0 0 0 0 0 0 0 0 0 0 14
 -1.2276  0.0117  3.3392 H  0 0 0 0 0 0 0 0 0 0 0 15
 -0.3922 -1.4600  2.7266 H  0 0 0 0 0 0 0 0 0 0 0 16
  0.4228  0.1076  2.6531 H  0 0 0 0 0 0 0 0 0 0 0 17
 -2.3569  0.5898 -0.4849 H  0 0 0 0 0 0 0 0 0 0 0 18
  3.5873  0.8908  0.0207 H  0 0 0 0 0 0 0 0 0 0 0 19

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2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 8 0 0 0 0
10 19 0 0 0 0

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M END

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2-acetylbutanedioicacid1a-anion.sdf

COSMOTHERM 3D 0

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18 18 0 0 0 0 0 0 0 0 0 V2000
  1.8988  0.3241 -0.1301 C  0 0 0 0 0 0 0 0 0 0 0 1
  0.8545  0.0358 -1.2124 C  0 0 0 0 0 0 0 0 0 0 0 2
 -0.6155 -0.2323 -0.7696 C  0 0 0 0 0 0 0 0 0 0 0 3
 -0.6746 -1.4581  0.1653 C  0 0 0 0 0 0 0 0 0 0 0 4
 -0.6148 -2.5834 -0.3246 O  0 0 0 0 0 0 0 0 0 0 0 5
 -0.7863 -1.2440  1.6514 C  0 0 0 0 0 0 0 0 0 0 0 6
 -1.3957  0.9889 -0.2248 C  0 0 0 0 0 0 0 0 0 0 0 7
 -0.7354  1.9067  0.4119 O  0 0 0 0 0 0 0 0 0 0 0 8
 -2.6266  1.0284 -0.4206 O  0 0 0 0 0 0 0 0 0 0 0 9
  1.5867  1.2370  0.7723 O  0 0 0 0 0 0 0 0 0 0 0 10
  2.9958 -0.2465 -0.1313 O  0 0 0 0 0 0 0 0 0 0 0 11
  1.2057 -0.8277 -1.7901 H  0 0 0 0 0 0 0 0 0 0 0 12
  0.8465  0.9020 -1.8941 H  0 0 0 0 0 0 0 0 0 0 0 13
 -1.1478 -0.5491 -1.6775 H  0 0 0 0 0 0 0 0 0 0 0 14
 -0.7085 -2.1991  2.1824 H  0 0 0 0 0 0 0 0 0 0 0 15
 -0.0130 -0.5464  2.0068 H  0 0 0 0 0 0 0 0 0 0 0 16
 -1.7572 -0.7753  1.8804 H  0 0 0 0 0 0 0 0 0 0 0 17
  0.5248  1.5858  0.6053 H  0 0 0 0 0 0 0 0 0 0 0 18

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2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
8 18 0 0 0 0
10 18 0 0 0 0

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M END

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2-acetylbutanedioicacid2.sdf

COSMOTHERM 3D 0

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19 18 0 0 0 0 0 0 0 0 0 V2000
 -0.0479 -1.7929  0.2574 C  0 0 0 0 0 0 0 0 0 0 0 1
 -0.0204 -1.0201 -1.0430 C  0 0 0 0 0 0 0 0 0 0 0 2
  0.0038  0.4953 -0.8130 C  0 0 0 0 0 0 0 0 0 0 0 3
 -1.2558  1.0691 -0.1522 C  0 0 0 0 0 0 0 0 0 0 0 4
 -1.1890  2.0778  0.5650 O  0 0 0 0 0 0 0 0 0 0 0 5
 -2.5788  0.4457 -0.4692 C  0 0 0 0 0 0 0 0 0 0 0 6
  1.3489  0.9351 -0.1914 C  0 0 0 0 0 0 0 0 0 0 0 7
  1.3405  2.0376  0.5626 O  0 0 0 0 0 0 0 0 0 0 0 8
  2.3857  0.3266 -0.4158 O  0 0 0 0 0 0 0 0 0 0 0 9
  0.0965 -3.1200  0.0580 O  0 0 0 0 0 0 0 0 0 0 0 10
 -0.1939 -1.2884  1.3626 O  0 0 0 0 0 0 0 0 0 0 0 11
 -0.8883 -1.3197 -1.6476 H  0 0 0 0 0 0 0 0 0 0 0 12
  0.8655 -1.3234 -1.6157 H  0 0 0 0 0 0 0 0 0 0 0 13
 -0.0019  0.9686 -1.8153 H  0 0 0 0 0 0 0 0 0 0 0 14
 -3.3887  1.0788 -0.0915 H  0 0 0 0 0 0 0 0 0 0 0 15
 -2.6870  0.2975 -1.5542 H  0 0 0 0 0 0 0 0 0 0 0 16
 -2.6515 -0.5482 -0.0012 H  0 0 0 0 0 0 0 0 0 0 0 17
  0.3613  2.3104  0.6823 H  0 0 0 0 0 0 0 0 0 0 0 18

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1
2
3      0.0520  -3.5717  0.9294 H  0  0  0  0  0  0  0  0  0  0  0  19
4      2  1  0  0  0  0
5     10  1  0  0  0  0
6     11  1  0  0  0  0
7     3  2  0  0  0  0
8     12  2  0  0  0  0
9     13  2  0  0  0  0
10    4  3  0  0  0  0
11    7  3  0  0  0  0
12   14  3  0  0  0  0
13    5  4  0  0  0  0
14    6  4  0  0  0  0
15   15  6  0  0  0  0
16   16  6  0  0  0  0
17   17  6  0  0  0  0
18    8  7  0  0  0  0
19    9  7  0  0  0  0
20   18  8  0  0  0  0
21   10  19  0  0  0  0
22 M  END
23 $$$$
24 2-acetylbutanedioicacid2a-anion.sdf
25 COSMOTHERM      3D      0
26
27 18 18 0 0 0 0 0 0 0 0 0 V2000
28 0.3217 -0.1268 1.9017 C 0 0 0 0 0 0 0 0 0 0 0 0 1
29 0.0297 -1.2086 0.8580 C 0 0 0 0 0 0 0 0 0 0 0 0 2
30 -0.2316 -0.7694 -0.6141 C 0 0 0 0 0 0 0 0 0 0 0 0 3
31 -1.4577 0.1650 -0.6804 C 0 0 0 0 0 0 0 0 0 0 0 0 4
32 -2.5826 -0.3246 -0.6119 O 0 0 0 0 0 0 0 0 0 0 0 0 5
33 -1.2441 1.6497 -0.8079 C 0 0 0 0 0 0 0 0 0 0 0 0 6
34 0.9919 -0.2280 -1.3925 C 0 0 0 0 0 0 0 0 0 0 0 0 7
35 1.0370 -0.4309 -2.6221 O 0 0 0 0 0 0 0 0 0 0 0 0 8
36 1.9062 0.4142 -0.7323 O 0 0 0 0 0 0 0 0 0 0 0 0 9
37 1.2282 0.7802 1.5856 O 0 0 0 0 0 0 0 0 0 0 0 0 10
38 -0.2417 -0.1330 3.0027 O 0 0 0 0 0 0 0 0 0 0 0 0 11
39 -0.8377 -1.7812 1.2082 H 0 0 0 0 0 0 0 0 0 0 0 0 12
40 0.8920 -1.8954 0.8549 H 0 0 0 0 0 0 0 0 0 0 0 0 13
41 -0.5471 -1.6788 -1.1447 H 0 0 0 0 0 0 0 0 0 0 0 0 14
42 -2.2003 2.1807 -0.7445 H 0 0 0 0 0 0 0 0 0 0 0 0 15
43 -0.5547 2.0135 -0.0309 H 0 0 0 0 0 0 0 0 0 0 0 0 16
44 -0.7655 1.8692 -1.7760 H 0 0 0 0 0 0 0 0 0 0 0 0 17
45 1.5795 0.6114 0.5228 H 0 0 0 0 0 0 0 0 0 0 0 0 18
46
47 2 1 0 0 0 0
48 10 1 0 0 0 0
49 11 1 0 0 0 0
50 3 2 0 0 0 0
51 12 2 0 0 0 0
52 13 2 0 0 0 0
53 4 3 0 0 0 0
54 7 3 0 0 0 0
55 14 3 0 0 0 0
56 5 4 0 0 0 0
57 6 4 0 0 0 0
58 15 6 0 0 0 0
59 16 6 0 0 0 0
60 17 6 0 0 0 0
61 8 7 0 0 0 0
62 9 7 0 0 0 0
63 9 18 0 0 0 0
64 10 18 0 0 0 0
65 M  END
66 $$$$
67 2-acetylbutanedioicacid4.sdf
68 COSMOTHERM      3D      0
69
70 19 18 0 0 0 0 0 0 0 0 0 V2000
71 0.0350 1.9702 0.0466 C 0 0 0 0 0 0 0 0 0 0 0 0 1
72 0.1428 0.9714 -1.1028 C 0 0 0 0 0 0 0 0 0 0 0 0 2
73 0.0832 -0.5287 -0.7368 C 0 0 0 0 0 0 0 0 0 0 0 0 3
74 1.2980 -1.1205 0.0023 C 0 0 0 0 0 0 0 0 0 0 0 0 4
75 1.1892 -2.2279 0.5455 O 0 0 0 0 0 0 0 0 0 0 0 0 5
76 2.5997 -0.3924 -0.0267 C 0 0 0 0 0 0 0 0 0 0 0 0 6
77 -1.2695 -0.9704 -0.1519 C 0 0 0 0 0 0 0 0 0 0 0 0 7
78 -1.3372 -2.2013 0.3341 O 0 0 0 0 0 0 0 0 0 0 0 0 8
79 -2.2619 -0.2391 -0.1695 O 0 0 0 0 0 0 0 0 0 0 0 0 9
80 -1.1598 2.0471 0.6665 O 0 0 0 0 0 0 0 0 0 0 0 0 10
81 0.9497 2.7061 0.3894 O 0 0 0 0 0 0 0 0 0 0 0 0 11
82 1.0789 1.1757 -1.6325 H 0 0 0 0 0 0 0 0 0 0 0 0 12
83 -0.6773 1.1751 -1.8060 H 0 0 0 0 0 0 0 0 0 0 0 0 13
84 0.1258 -1.0683 -1.7045 H 0 0 0 0 0 0 0 0 0 0 0 0 14
85 3.3622 -0.9676 0.5086 H 0 0 0 0 0 0 0 0 0 0 0 0 15
86 2.9138 -0.2384 -1.0714 H 0 0 0 0 0 0 0 0 0 0 0 0 16
87 2.4961 0.6095 0.4176 H 0 0 0 0 0 0 0 0 0 0 0 0 17
88 -0.3730 -2.5345 0.4277 H 0 0 0 0 0 0 0 0 0 0 0 0 18
89 -1.7662 1.3371 0.2991 H 0 0 0 0 0 0 0 0 0 0 0 0 19
90
91 2 1 0 0 0 0
92 10 1 0 0 0 0
93 11 1 0 0 0 0
94 3 2 0 0 0 0
95 12 2 0 0 0 0
96 13 2 0 0 0 0
97 4 3 0 0 0 0
98 7 3 0 0 0 0
99 14 3 0 0 0 0
100 5 4 0 0 0 0
101 6 4 0 0 0 0
102 15 6 0 0 0 0
103 16 6 0 0 0 0
104 17 6 0 0 0 0
105 8 7 0 0 0 0
106 9 7 0 0 0 0
107 9 18 0 0 0 0
108 10 18 0 0 0 0
109 M  END

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2-chlorophenol0-anion.sdf
COSMOTHERM      3D              0

12 12 0 0 0 0 0 0 0 0 0 V2000
  1.6501  1.0496 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
  2.4322 -0.1044  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
  1.8425 -1.3791  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.4417 -1.4679  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
 -0.3288 -0.3092 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
  0.2084  1.0303  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
  2.4494 -2.2854  0.0002 H 0 0 0 0 0 0 0 0 0 0 0 7
 -0.5123  2.0953  0.0001 O 0 0 0 0 0 0 0 0 0 0 0 8
  2.1236  2.0360 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
  3.5220 -0.0112  0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
 -0.0507 -2.4427  0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
 -2.1137 -0.4687  0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12

  2 1 0 0 0 0
  6 1 0 0 0 0
  9 1 0 0 0 0
  3 2 0 0 0 0
 10 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
 11 4 0 0 0 0
  6 5 0 0 0 0
  8 6 0 0 0 0
  5 12 0 0 0 0

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M  END
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2-chlorophenol0.sdf
COSMOTHERM      3D              0

13 13 0 0 0 0 0 0 0 0 0 V2000
  0.0588 -2.4380  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
 -1.0749 -1.6238  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
 -0.9446 -0.2269  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.3503  0.3219  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
  1.4877 -0.4839  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
  1.3413 -1.8748  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
 -2.0774  0.5341  0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
  0.5037  2.0904  0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 8
 -1.8234  1.4817 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 9
 -0.0629 -3.5222  0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
 -2.0784 -2.0525 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
  2.4764 -0.0243  0.0001 H 0 0 0 0 0 0 0 0 0 0 0 12
  2.2275 -2.5098  0.0000 H 0 0 0 0 0 0 0 0 0 0 0 13

  2 1 0 0 0 0
  6 1 0 0 0 0
 10 1 0 0 0 0
  3 2 0 0 0 0
 11 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
  8 4 0 0 0 0
  6 5 0 0 0 0
 12 5 0 0 0 0
  9 7 0 0 0 0
  6 13 0 0 0 0

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M  END
$$$$
2-chlorophenol1-anion.sdf
COSMOTHERM      3D              0

12 12 0 0 0 0 0 0 0 0 0 V2000
  1.6499  1.0498 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
  2.4320 -0.1042  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
  1.8426 -1.3790  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.4419 -1.4679  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
 -0.3287 -0.3092 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
  0.2082  1.0304  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
  2.4497 -2.2852  0.0004 H 0 0 0 0 0 0 0 0 0 0 0 7
 -0.5126  2.0953  0.0003 O 0 0 0 0 0 0 0 0 0 0 0 8
  2.1233  2.0362 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
  3.5218 -0.0109  0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
 -0.0505 -2.4427  0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
 -2.1134 -0.4690  0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 12

  2 1 0 0 0 0
  6 1 0 0 0 0
  9 1 0 0 0 0
  3 2 0 0 0 0
 10 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
 11 4 0 0 0 0
  6 5 0 0 0 0
  8 6 0 0 0 0
  5 12 0 0 0 0

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M  END
$$$$
2-chlorophenol1.sdf
COSMOTHERM      3D              0

13 13 0 0 0 0 0 0 0 0 0 V2000
  0.0877 -2.4388  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
 -1.0563 -1.6375 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
 -0.9479 -0.2378  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.3372  0.3334 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
  1.4823 -0.4624  0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
  1.3599 -1.8561  0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
 -2.0342  0.5900  0.0002 O 0 0 0 0 0 0 0 0 0 0 0 7
  0.4957  2.0962 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 8

```

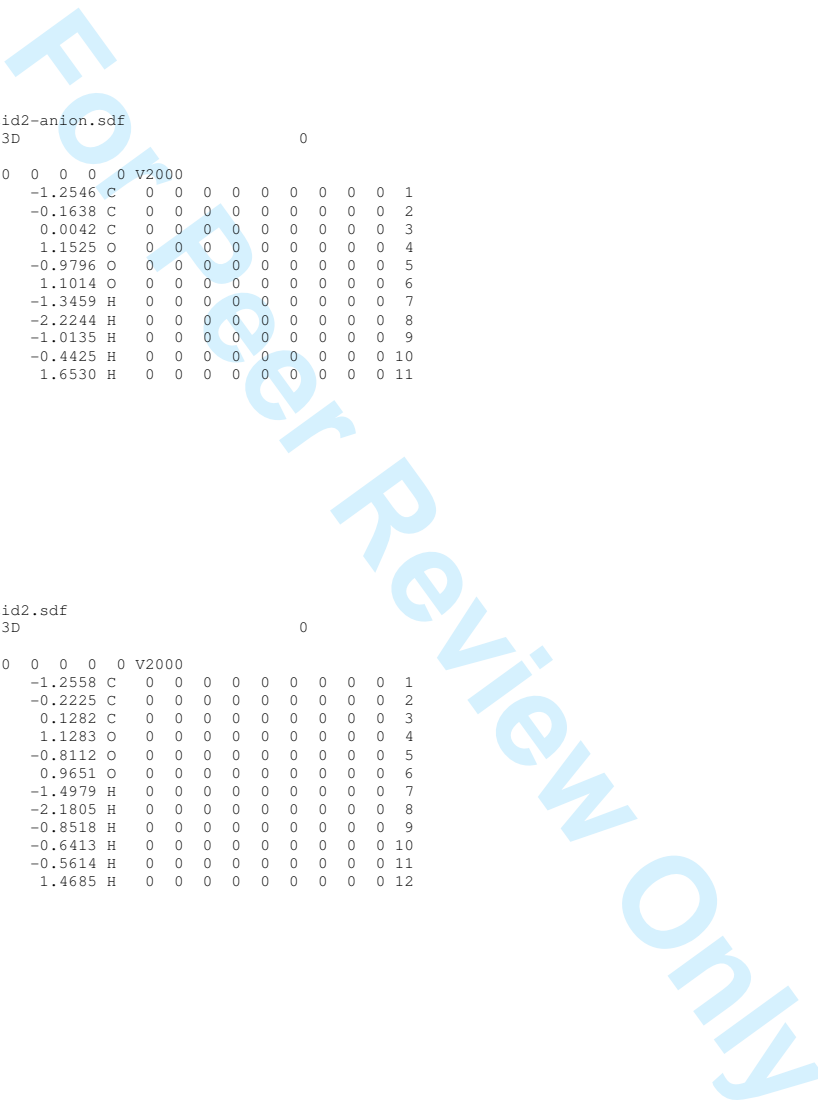


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1
2
3      1.8527   0.8029   0.7562 O   0 0 0 0 0 0 0 0 0 0 5
4     -1.5569  -0.1409   0.6733 Cl  0 0 0 0 0 0 0 0 0 0 6
5     -1.4781   0.6359  -2.1965 H   0 0 0 0 0 0 0 0 0 0 7
6      0.2753   0.6627  -2.5040 H   0 0 0 0 0 0 0 0 0 0 8
7     -0.5164  -0.8657  -2.0316 H   0 0 0 0 0 0 0 0 0 0 9
8     -0.3039   1.6536  -0.2492 H   0 0 0 0 0 0 0 0 0 0 10
9      2.2055  -1.4462   0.2093 H   0 0 0 0 0 0 0 0 0 0 11
10
11     2 1 0 0 0 0
12     7 1 0 0 0 0
13     8 1 0 0 0 0
14     9 1 0 0 0 0
15     3 2 0 0 0 0
16     6 2 0 0 0 0
17    10 2 0 0 0 0
18     4 3 0 0 0 0
19     5 3 0 0 0 0
20     4 11 0 0 0 0
21 M END
22 $$$$
23 2-hydroxypropanoicacid0-anion.sdf
24 COSMOTHERM      3D          0
25
26    11 10 0 0 0 0 0 0 0 0 0 0 V2000
27     1.3699   0.4374  -1.2545 C   0 0 0 0 0 0 0 0 0 0 1
28     0.7044  -0.3973  -0.1596 C   0 0 0 0 0 0 0 0 0 0 2
29    -0.8025  -0.0481   0.0023 C   0 0 0 0 0 0 0 0 0 0 3
30    -1.1337   0.3953   1.1526 O   0 0 0 0 0 0 0 0 0 0 4
31    -1.5639  -0.2270  -0.9867 O   0 0 0 0 0 0 0 0 0 0 5
32     1.3654  -0.2009   1.1057 O   0 0 0 0 0 0 0 0 0 0 6
33     2.4352   0.1777  -1.3398 H   0 0 0 0 0 0 0 0 0 0 7
34     0.8878   0.2518  -2.2243 H   0 0 0 0 0 0 0 0 0 0 8
35     1.2911   1.5106  -1.0223 H   0 0 0 0 0 0 0 0 0 0 9
36     0.7665  -1.4674  -0.4310 H   0 0 0 0 0 0 0 0 0 0 10
37     0.6104   0.1402   1.6567 H   0 0 0 0 0 0 0 0 0 0 11
38
39     2 1 0 0 0 0
40     7 1 0 0 0 0
41     8 1 0 0 0 0
42     9 1 0 0 0 0
43     3 2 0 0 0 0
44     6 2 0 0 0 0
45    10 2 0 0 0 0
46     4 3 0 0 0 0
47     5 3 0 0 0 0
48     6 11 0 0 0 0
49 M END
50 $$$$
51 2-hydroxypropanoicacid0.sdf
52 COSMOTHERM      3D          0
53
54    12 11 0 0 0 0 0 0 0 0 0 0 V2000
55     1.2591  -1.2440  -0.6320 C   0 0 0 0 0 0 0 0 0 0 1
56     0.7077  -0.2273   0.3784 C   0 0 0 0 0 0 0 0 0 0 2
57    -0.7342   0.1267   0.0141 C   0 0 0 0 0 0 0 0 0 0 3
58    -1.0505   1.1150  -0.6314 O   0 0 0 0 0 0 0 0 0 0 4
59    -1.6147  -0.7971   0.4549 O   0 0 0 0 0 0 0 0 0 0 5
60     1.5012   0.9589   0.4507 O   0 0 0 0 0 0 0 0 0 0 6
61     2.2947  -1.4913  -0.3641 H   0 0 0 0 0 0 0 0 0 0 7
62     0.6655  -2.1687  -0.6270 H   0 0 0 0 0 0 0 0 0 0 8
63     1.2459  -0.8228  -1.6481 H   0 0 0 0 0 0 0 0 0 0 9
64     0.7176  -0.6608   1.3876 H   0 0 0 0 0 0 0 0 0 0 10
65    -2.5120  -0.5488   0.1403 H   0 0 0 0 0 0 0 0 0 0 11
66     1.3752   1.4474  -0.3865 H   0 0 0 0 0 0 0 0 0 0 12
67
68     2 1 0 0 0 0
69     7 1 0 0 0 0
70     8 1 0 0 0 0
71     9 1 0 0 0 0
72     3 2 0 0 0 0
73     6 2 0 0 0 0
74    10 2 0 0 0 0
75     4 3 0 0 0 0
76     5 3 0 0 0 0
77    11 5 0 0 0 0
78     6 12 0 0 0 0
79 M END
80 $$$$
81 2-hydroxypropanoicacid1-anion.sdf
82 COSMOTHERM      3D          0
83
84    11 10 0 0 0 0 0 0 0 0 0 0 V2000
85     1.3803   0.4201  -1.2530 C   0 0 0 0 0 0 0 0 0 0 1
86     0.7068  -0.3977  -0.1509 C   0 0 0 0 0 0 0 0 0 0 2
87    -0.8031  -0.0489  -0.0033 C   0 0 0 0 0 0 0 0 0 0 3
88    -1.5537  -0.2086  -1.0024 O   0 0 0 0 0 0 0 0 0 0 4
89    -1.1470   0.3733   1.1527 O   0 0 0 0 0 0 0 0 0 0 5
90     1.3581  -0.1788   1.1160 O   0 0 0 0 0 0 0 0 0 0 6
91     2.4508   0.1746  -1.3106 H   0 0 0 0 0 0 0 0 0 0 7
92     0.9202   0.2026  -2.2269 H   0 0 0 0 0 0 0 0 0 0 8
93     1.2815   1.4976  -1.0508 H   0 0 0 0 0 0 0 0 0 0 9
94     0.7715  -1.4720  -0.4060 H   0 0 0 0 0 0 0 0 0 0 10
95     0.5887   0.1376   1.6631 H   0 0 0 0 0 0 0 0 0 0 11
96
97     2 1 0 0 0 0
98     7 1 0 0 0 0
99     8 1 0 0 0 0
100    9 1 0 0 0 0
101    3 2 0 0 0 0
102    6 2 0 0 0 0
103   10 2 0 0 0 0
104    4 3 0 0 0 0
105    5 3 0 0 0 0
106    6 11 0 0 0 0
107 M END
108 $$$$
109 2-hydroxypropanoicacid1.sdf
110 COSMOTHERM      3D          0
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12 11 0 0 0 0 0 0 0 0 0 0 V2000
-1.3160 1.1794 -0.6690 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7142 0.2399 0.3842 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7766 0.0394 0.0960 C 0 0 0 0 0 0 0 0 0 0 0 3
1.6518 0.8102 0.4612 O 0 0 0 0 0 0 0 0 0 0 0 4
1.0149 -1.0634 -0.6485 O 0 0 0 0 0 0 0 0 0 0 0 5
-1.4327 -0.9936 0.4943 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.3684 1.3710 -0.4213 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.7804 2.1385 -0.6915 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.2636 0.7252 -1.6697 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.7748 0.7071 1.3761 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9785 -1.1119 -0.8334 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.4399 -1.4194 -0.3840 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid2-anion.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 V2000
1.3659 0.4451 -1.2546 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7036 -0.3980 -0.1638 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.8024 -0.0481 0.0042 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.1275 0.4050 1.1525 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.5688 -0.2346 -0.9796 O 0 0 0 0 0 0 0 0 0 0 0 5
1.3681 -0.2104 1.1014 O 0 0 0 0 0 0 0 0 0 0 0 6
2.4306 0.1851 -1.3459 H 0 0 0 0 0 0 0 0 0 0 0 7
0.8803 0.2680 -2.2244 H 0 0 0 0 0 0 0 0 0 0 0 8
1.2890 1.5164 -1.0135 H 0 0 0 0 0 0 0 0 0 0 0 9
0.7652 -1.4659 -0.4425 H 0 0 0 0 0 0 0 0 0 0 0 10
0.6187 0.1418 1.6530 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
6 11 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid2.sdf
COSMOTHERM 3D 0
12 11 0 0 0 0 0 0 0 0 V2000
1.2563 0.6166 -1.2558 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7093 -0.3794 -0.2225 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7338 -0.0184 0.1282 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.0542 0.6067 1.1283 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.6085 -0.4351 -0.8112 O 0 0 0 0 0 0 0 0 0 0 0 5
1.5027 -0.4273 0.9651 O 0 0 0 0 0 0 0 0 0 0 0 6
2.2932 0.3492 -1.4979 H 0 0 0 0 0 0 0 0 0 0 0 7
0.6632 0.5931 -2.1805 H 0 0 0 0 0 0 0 0 0 0 0 8
1.2386 1.6395 -0.8518 H 0 0 0 0 0 0 0 0 0 0 0 9
0.7236 -1.3951 -0.6413 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.5076 -0.1267 -0.5614 H 0 0 0 0 0 0 0 0 0 0 0 11
1.3237 0.3915 1.4685 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
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9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide0-anion.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 V2000
-0.8095 -0.5649 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
0.5722 -1.2426 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.4141 0.9411 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
0.9388 1.1404 0.0004 N 0 0 0 0 0 0 0 0 0 0 0 4
1.5653 -0.0734 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6317 -0.8790 1.2624 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.6321 -0.8795 -1.2621 C 0 0 0 0 0 0 0 0 0 0 0 7
2.8062 -0.2310 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 8
-1.2619 1.8575 -0.0004 O 0 0 0 0 0 0 0 0 0 0 0 9
0.7483 -1.8731 -0.8849 H 0 0 0 0 0 0 0 0 0 0 0 10
0.7483 -1.8732 0.8846 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.0532 -0.6780 2.1773 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.5432 -0.2645 1.2905 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.9291 -1.9389 1.2731 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.0540 -0.6781 -2.1771 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.5439 -0.2656 -1.2898 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.9288 -1.9396 -1.2726 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
    
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6 1 0 0 0 0
7 1 0 0 0 0
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10 2 0 0 0 0
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5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
7 17 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimide0.sdf
COSMOTHERM 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-0.8230 -0.5670 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.5684 -1.2495 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.4835 0.9348 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.8988 1.0718 -0.0007 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.5945 -0.1316 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.6377 -0.8941 1.2663 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.6365 -0.8939 -1.2671 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
2.8166 -0.2259 0.0004 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2703 1.8741 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.3649 1.9807 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.7355 -1.8818 -0.8830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.7353 -1.8808 0.8848 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.0681 -0.6693 2.1800 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.5703 -0.3141 1.2850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.8927 -1.9634 1.2738 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.0663 -0.6687 -2.1803 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.5693 -0.3141 -1.2865 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.8914 -1.9633 -1.2752 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
11 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
7 18 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimidel-anion.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
-0.8095 -0.5649 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.5722 -1.2426 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.4141 0.9411 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.9388 1.1404 0.0004 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.5653 -0.0734 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.6317 -0.8790 1.2624 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.6321 -0.8795 -1.2621 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
2.8062 -0.2310 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2619 1.8575 -0.0004 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.7483 -1.8731 -0.8849 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.7483 -1.8732 0.8846 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.0532 -0.6780 2.1773 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.5432 -0.2645 1.2905 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.9291 -1.9389 1.2731 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.0540 -0.6781 -2.1771 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.5439 -0.2656 -1.2898 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-1.9288 -1.9396 -1.2726 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
7 17 0 0 0 0
M END
$$$$
3,3-dimethylsuccinimidel.sdf
COSMOTHERM 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-0.8436 -0.5574 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.5415 -1.2443 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
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-0.4528  0.9440  -0.0002  C  0  0  0  0  0  0  0  0  0  0  0  3
 0.9469  1.1222  0.0000  N  0  0  0  0  0  0  0  0  0  0  0  4
 1.4738  -0.0726  -0.0004  C  0  0  0  0  0  0  0  0  0  0  0  5
-1.6592  -0.8731  1.2669  C  0  0  0  0  0  0  0  0  0  0  0  6
-1.6619  -0.8731  -1.2652  C  0  0  0  0  0  0  0  0  0  0  0  7
 2.7813  -0.2912  0.0000  O  0  0  0  0  0  0  0  0  0  0  0  8
-1.2462  1.8795  0.0000  O  0  0  0  0  0  0  0  0  0  0  0  9
 0.7211  -1.8719  -0.8867  H  0  0  0  0  0  0  0  0  0  0  0  10
 0.7218  -1.8738  0.8826  H  0  0  0  0  0  0  0  0  0  0  0  11
-1.0844  -0.6589  2.1801  H  0  0  0  0  0  0  0  0  0  0  0  12
-2.5790  -0.2725  1.2872  H  0  0  0  0  0  0  0  0  0  0  0  13
-1.9386  -1.9367  1.2775  H  0  0  0  0  0  0  0  0  0  0  0  14
-1.0888  -0.6597  -2.1797  H  0  0  0  0  0  0  0  0  0  0  0  15
-2.5814  -0.2720  -1.2839  H  0  0  0  0  0  0  0  0  0  0  0  16
-1.9421  -1.9365  -1.2749  H  0  0  0  0  0  0  0  0  0  0  0  17
 3.2550  0.5702  0.0015  H  0  0  0  0  0  0  0  0  0  0  0  18

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2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
8 18 0 0 0 0

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M END

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3,3-dimethylsuccinimide2-anion.sdf

COSMOTHERM 3D 0

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17 17 0 0 0 0 0 0 0 0 0 V2000
-0.8095  -0.5649  0.0000  C  0  0  0  0  0  0  0  0  0  0  0  1
 0.5722  -1.2426  -0.0001  C  0  0  0  0  0  0  0  0  0  0  0  2
-0.4141  0.9411  -0.0001  C  0  0  0  0  0  0  0  0  0  0  0  3
 0.9388  1.1404  0.0004  N  0  0  0  0  0  0  0  0  0  0  0  4
 1.5653  -0.0734  0.0000  C  0  0  0  0  0  0  0  0  0  0  0  5
-1.6317  -0.8790  1.2624  C  0  0  0  0  0  0  0  0  0  0  0  6
-1.6321  -0.8795  -1.2621  C  0  0  0  0  0  0  0  0  0  0  0  7
 2.8062  -0.2310  -0.0002  O  0  0  0  0  0  0  0  0  0  0  0  8
-1.2619  1.8575  -0.0004  O  0  0  0  0  0  0  0  0  0  0  0  9
 0.7483  -1.8731  -0.8849  H  0  0  0  0  0  0  0  0  0  0  0  10
 0.7483  -1.8732  0.8846  H  0  0  0  0  0  0  0  0  0  0  0  11
-1.0532  -0.6780  2.1773  H  0  0  0  0  0  0  0  0  0  0  0  12
-2.5432  -0.2645  1.2905  H  0  0  0  0  0  0  0  0  0  0  0  13
-1.9291  -1.9389  1.2731  H  0  0  0  0  0  0  0  0  0  0  0  14
-1.0540  -0.6781  -2.1771  H  0  0  0  0  0  0  0  0  0  0  0  15
-2.5439  -0.2656  -1.2898  H  0  0  0  0  0  0  0  0  0  0  0  16
-1.9288  -1.9396  -1.2726  H  0  0  0  0  0  0  0  0  0  0  0  17

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2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
7 17 0 0 0 0

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M END

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3,3-dimethylsuccinimide2.sdf

COSMOTHERM 3D 0

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18 18 0 0 0 0 0 0 0 0 0 V2000
-0.7936  -0.5908  0.0001  C  0  0  0  0  0  0  0  0  0  0  0  1
 0.6013  -1.2587  0.0012  C  0  0  0  0  0  0  0  0  0  0  0  2
-0.3698  0.8684  0.0001  C  0  0  0  0  0  0  0  0  0  0  0  3
 0.9064  1.1448  -0.0002  N  0  0  0  0  0  0  0  0  0  0  0  4
 1.5876  -0.0917  0.0003  C  0  0  0  0  0  0  0  0  0  0  0  5
-1.6123  -0.9116  1.2679  C  0  0  0  0  0  0  0  0  0  0  0  6
-1.6096  -0.9115  -1.2695  C  0  0  0  0  0  0  0  0  0  0  0  7
 2.8119  -0.1821  0.0001  O  0  0  0  0  0  0  0  0  0  0  0  8
-1.3116  1.8004  0.0003  O  0  0  0  0  0  0  0  0  0  0  0  9
 0.7773  -1.8874  -0.8830  H  0  0  0  0  0  0  0  0  0  0  0  10
 0.7767  -1.8853  0.8871  H  0  0  0  0  0  0  0  0  0  0  0  11
-1.0425  -0.6842  2.1805  H  0  0  0  0  0  0  0  0  0  0  0  12
-2.5477  -0.3364  1.2870  H  0  0  0  0  0  0  0  0  0  0  0  13
-1.8643  -1.9813  1.2762  H  0  0  0  0  0  0  0  0  0  0  0  14
-1.0388  -0.6820  -2.1809  H  0  0  0  0  0  0  0  0  0  0  0  15
-2.5461  -0.3379  -1.2896  H  0  0  0  0  0  0  0  0  0  0  0  16
-1.8598  -1.9816  -1.2796  H  0  0  0  0  0  0  0  0  0  0  0  17
-0.8915  2.6887  -0.0010  H  0  0  0  0  0  0  0  0  0  0  0  18

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2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0

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4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 18 0 0 0 0

```

M END

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3,3-methylphenylglutarimide0-anion.sdf

COSMOTHERM 3D 0

```

27 28 0 0 0 0 0 0 0 0 0 V2000
2.2998 -0.2222 1.1824 C 0 0 0 0 0 0 0 0 0 0 0 0 1
2.9743 -0.2331 0.0011 N 0 0 0 0 0 0 0 0 0 0 0 0 2
2.3027 -0.2092 -1.1818 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.7730 -0.1887 -1.2395 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1033 0.4480 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.7699 -0.2019 1.2358 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.9287 -0.2351 -2.2718 O 0 0 0 0 0 0 0 0 0 0 0 0 7
2.9225 -0.2599 2.2736 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.4053 0.1477 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.3945 1.9607 0.0089 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.4499 -1.2377 -1.3471 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.4719 0.3297 -2.1614 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.4464 -1.2521 1.3308 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.4663 0.3063 2.1625 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-4.1792 -0.4676 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 15
-3.2250 -1.4932 -0.0162 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-1.8620 -1.1863 -0.0163 C 0 0 0 0 0 0 0 0 0 0 0 0 17
-2.3778 1.1625 0.0125 C 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.7472 0.8609 0.0125 C 0 0 0 0 0 0 0 0 0 0 0 0 19
1.4788 2.1389 0.0099 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.0221 2.4462 0.9035 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.0226 2.4558 -0.8801 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-5.2449 -0.7040 -0.0015 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-3.5430 -2.5377 -0.0274 H 0 0 0 0 0 0 0 0 0 0 0 0 24
-1.1437 -2.0094 -0.0273 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-2.0768 2.2096 0.0238 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-4.4759 1.6742 0.0239 H 0 0 0 0 0 0 0 0 0 0 0 0 27

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2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
19 27 0 0 0 0

```

M END

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3,3-methylphenylglutarimide0.sdf

COSMOTHERM 3D 0

```

28 29 0 0 0 0 0 0 0 0 0 V2000
2.2522 0.2135 -1.2480 C 0 0 0 0 0 0 0 0 0 0 0 0 1
2.8693 0.2514 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 0 2
2.2516 0.2192 1.2475 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.7401 0.2137 1.2521 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.0954 -0.4377 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.7407 0.2080 -1.2533 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.9356 0.2250 2.2705 O 0 0 0 0 0 0 0 0 0 0 0 0 7
2.9367 0.2144 -2.2707 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.4162 -0.1437 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.3978 -1.9483 0.0042 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.8930 0.2645 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.4335 1.2696 1.3357 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.4124 -0.2854 2.1738 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.4341 1.2634 -1.3422 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.4135 -0.2954 -2.1728 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-4.1878 0.4534 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.2414 1.4858 -0.0067 C 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.8766 1.1878 -0.0059 C 0 0 0 0 0 0 0 0 0 0 0 0 18
-2.3783 -1.1667 0.0056 C 0 0 0 0 0 0 0 0 0 0 0 0 19
-3.7489 -0.8727 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 0 20
1.4818 -2.1310 0.0048 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.0173 -2.4399 -0.8867 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-0.0174 -2.4358 0.8972 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-5.2549 0.6832 -0.0023 H 0 0 0 0 0 0 0 0 0 0 0 0 24
-3.5660 2.5280 -0.0116 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.1644 2.0164 -0.0102 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-2.0707 -2.2117 0.0108 H 0 0 0 0 0 0 0 0 0 0 0 0 27

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1
2
3 -4.4727 -1.6901 0.0097 H 0 0 0 0 0 0 0 0 0 0 0 28
4 2 1 0 0 0 0
5 6 1 0 0 0 0
6 8 1 0 0 0 0
7 3 2 0 0 0 0
8 11 2 0 0 0 0
9 4 3 0 0 0 0
10 7 3 0 0 0 0
11 5 4 0 0 0 0
12 12 4 0 0 0 0
13 13 4 0 0 0 0
14 6 5 0 0 0 0
15 9 5 0 0 0 0
16 10 5 0 0 0 0
17 14 6 0 0 0 0
18 15 6 0 0 0 0
19 18 9 0 0 0 0
20 19 9 0 0 0 0
21 21 10 0 0 0 0
22 22 10 0 0 0 0
23 23 10 0 0 0 0
24 17 16 0 0 0 0
25 20 16 0 0 0 0
26 24 16 0 0 0 0
27 18 17 0 0 0 0
28 25 17 0 0 0 0
29 26 18 0 0 0 0
30 20 19 0 0 0 0
31 27 19 0 0 0 0
32 20 28 0 0 0 0

M END

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3,3-methylphenylglutarimide1-anion.sdf
COSMOtherm 3D 0

27 28 0 0 0 0 0 0 0 0 0 V2000
0.9051 -1.6836 1.0375 C 0 0 0 0 0 0 0 0 0 0 0 1
1.0659 -2.0718 -0.2578 N 0 0 0 0 0 0 0 0 0 0 0 2
0.0554 -1.9165 -1.1567 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2703 -1.2643 -0.7573 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.1651 -0.2885 0.4252 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4069 -1.0658 1.5235 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1793 -2.3316 -2.3372 O 0 0 0 0 0 0 0 0 0 0 0 7
1.8277 -1.8523 1.8746 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.5821 0.0770 0.9182 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.4125 1.0057 0.0673 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.9501 -2.0824 -0.4602 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.7186 -0.8043 -1.6486 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.0505 -1.8931 1.8734 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.1888 -0.4431 2.4010 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9041 3.4502 -0.5252 C 0 0 0 0 0 0 0 0 0 0 0 15
0.6326 2.5273 -1.5386 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.0182 1.3212 -1.2439 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.1283 1.9484 1.0757 C 0 0 0 0 0 0 0 0 0 0 0 18
0.5190 3.1531 0.7881 C 0 0 0 0 0 0 0 0 0 0 0 19
-3.1383 -0.8330 1.1911 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.5435 0.7295 1.8026 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.1454 0.6030 0.1323 H 0 0 0 0 0 0 0 0 0 0 0 22
1.4096 4.3904 -0.7537 H 0 0 0 0 0 0 0 0 0 0 0 23
0.9268 2.7415 -2.5683 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.2125 0.6243 -2.0597 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.4211 1.7450 2.1081 H 0 0 0 0 0 0 0 0 0 0 0 26
0.7225 3.8628 1.5929 H 0 0 0 0 0 0 0 0 0 0 0 27

2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
17 10 0 0 0 0
18 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
19 27 0 0 0 0

M END

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3,3-methylphenylglutarimide1.sdf
COSMOtherm 3D 0

28 29 0 0 0 0 0 0 0 0 0 V2000
-1.1369 0.8472 1.6490 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2009 1.0040 2.0059 N 0 0 0 0 0 0 0 0 0 0 0 2
1.2244 0.0701 1.8598 C 0 0 0 0 0 0 0 0 0 0 0 3
0.8266 -1.2615 1.2650 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3751 -1.1955 0.3003 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.5179 -0.5004 1.0819 C 0 0 0 0 0 0 0 0 0 0 0 6
2.3654 0.3447 2.2305 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.9328 1.7689 1.8259 O 0 0 0 0 0 0 0 0 0 0 0 8

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-0.8056 -2.6341 -0.0581 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0571 -0.4252 -0.9960 C 0 0 0 0 0 0 0 0 0 0 0 10
0.4628 1.9082 2.4082 H 0 0 0 0 0 0 0 0 0 0 0 11
0.5522 -1.9127 2.1131 H 0 0 0 0 0 0 0 0 0 0 0 12
1.7171 -1.7111 0.8084 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.8025 -1.1377 1.9378 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.4225 -0.3638 0.4777 H 0 0 0 0 0 0 0 0 0 0 0 15
0.4579 0.9241 -3.4356 C 0 0 0 0 0 0 0 0 0 0 0 16
1.5030 0.6236 -2.5590 C 0 0 0 0 0 0 0 0 0 0 0 17
1.2471 -0.0450 -1.3543 C 0 0 0 0 0 0 0 0 0 0 0 18
-1.0980 -0.1181 -1.8941 C 0 0 0 0 0 0 0 0 0 0 0 19
-0.8474 0.5470 -3.0970 C 0 0 0 0 0 0 0 0 0 0 0 20
-1.0494 -3.2023 0.8521 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.6918 -2.6285 -0.7078 H 0 0 0 0 0 0 0 0 0 0 0 22
0.0034 -3.1568 -0.5886 H 0 0 0 0 0 0 0 0 0 0 0 23
0.6559 1.4458 -4.3736 H 0 0 0 0 0 0 0 0 0 0 0 24
2.5272 0.9086 -2.8074 H 0 0 0 0 0 0 0 0 0 0 0 25
2.0909 -0.2680 -0.7007 H 0 0 0 0 0 0 0 0 0 0 0 26
-2.1252 -0.4051 -1.6601 H 0 0 0 0 0 0 0 0 0 0 0 27
-1.6756 0.7714 -3.7721 H 0 0 0 0 0 0 0 0 0 0 0 28
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 9 0 0 0 0
18 10 0 0 0 0
19 10 0 0 0 0
17 16 0 0 0 0
20 16 0 0 0 0
24 16 0 0 0 0
18 17 0 0 0 0
25 17 0 0 0 0
26 18 0 0 0 0
20 19 0 0 0 0
27 19 0 0 0 0
20 28 0 0 0 0
M END
$$$$
3,3-methylphenylglutarimide2-anion.sdf
COSMOTHERM 3D 0
27 28 0 0 0 0 0 0 0 0 0 V2000
2.2986 1.1836 0.2183 C 0 0 0 0 0 0 0 0 0 0 0 1
2.9742 0.0031 0.2337 N 0 0 0 0 0 0 0 0 0 0 0 2
2.3037 -1.1805 0.2132 C 0 0 0 0 0 0 0 0 0 0 0 3
0.7740 -1.2394 0.1929 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1033 -0.0022 -0.4487 C 0 0 0 0 0 0 0 0 0 0 0 5
0.7687 1.2360 0.1966 C 0 0 0 0 0 0 0 0 0 0 0 6
2.9305 -2.2697 0.2424 O 0 0 0 0 0 0 0 0 0 0 0 7
2.9203 2.2757 0.2532 O 0 0 0 0 0 0 0 0 0 0 0 8
-1.4052 -0.0031 -0.1479 C 0 0 0 0 0 0 0 0 0 0 0 9
0.3943 0.0005 -1.9615 C 0 0 0 0 0 0 0 0 0 0 0 10
0.4511 -1.3431 1.2423 H 0 0 0 0 0 0 0 0 0 0 0 11
0.4737 -2.1636 -0.3218 H 0 0 0 0 0 0 0 0 0 0 0 12
0.4445 1.3352 1.2461 H 0 0 0 0 0 0 0 0 0 0 0 13
0.4648 2.1604 -0.3155 H 0 0 0 0 0 0 0 0 0 0 0 14
-4.1789 0.0004 0.4683 C 0 0 0 0 0 0 0 0 0 0 0 15
-3.2244 -0.0085 1.4936 C 0 0 0 0 0 0 0 0 0 0 0 16
-1.8615 -0.0102 1.1862 C 0 0 0 0 0 0 0 0 0 0 0 17
-2.3780 0.0055 -1.1625 C 0 0 0 0 0 0 0 0 0 0 0 18
-3.7474 0.0072 -0.8605 C 0 0 0 0 0 0 0 0 0 0 0 19
1.4786 0.0009 -2.1398 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.0224 0.8933 -2.4502 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.0226 -0.8905 -2.4532 H 0 0 0 0 0 0 0 0 0 0 0 22
-5.2445 0.0019 0.7051 H 0 0 0 0 0 0 0 0 0 0 0 23
-3.5420 -0.0140 2.5383 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.1430 -0.0168 2.0091 H 0 0 0 0 0 0 0 0 0 0 0 25
-2.0773 0.0112 -2.2098 H 0 0 0 0 0 0 0 0 0 0 0 26
-4.4764 0.0140 -1.6736 H 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0

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3 24 16 0 0 0 0
4 25 17 0 0 0 0
5 19 18 0 0 0 0
6 26 18 0 0 0 0
7 19 27 0 0 0 0
8 M END
9 \$\$\$\$
10 3,3-methylphenylglutarimide2.sdf
11 COSMOTHERM 3D 0
12
13 28 29 0 0 0 0 0 0 0 0 0 V2000
14 2.2410 1.1280 0.0428 C 0 0 0 0 0 0 0 0 0 0 0 1
15 2.9404 0.0524 0.2585 N 0 0 0 0 0 0 0 0 0 0 0 2
16 2.2688 -1.1678 0.3989 C 0 0 0 0 0 0 0 0 0 0 0 3
17 0.7502 -1.1809 0.4671 C 0 0 0 0 0 0 0 0 0 0 0 4
18 0.0892 -0.1121 -0.4438 C 0 0 0 0 0 0 0 0 0 0 0 5
19 0.7534 1.2456 -0.1032 C 0 0 0 0 0 0 0 0 0 0 0 6
20 2.9262 -2.2068 0.5040 O 0 0 0 0 0 0 0 0 0 0 0 7
21 2.8766 2.3007 -0.0551 O 0 0 0 0 0 0 0 0 0 0 0 8
22 -1.4182 -0.0357 -0.1447 C 0 0 0 0 0 0 0 0 0 0 0 9
23 0.3800 -0.4582 -1.9165 C 0 0 0 0 0 0 0 0 0 0 0 10
24 0.4818 -0.9993 1.5212 H 0 0 0 0 0 0 0 0 0 0 0 11
25 0.3992 -2.1893 0.2111 H 0 0 0 0 0 0 0 0 0 0 0 12
26 0.3777 1.6384 0.8556 H 0 0 0 0 0 0 0 0 0 0 0 13
27 0.5237 2.0078 -0.8615 H 0 0 0 0 0 0 0 0 0 0 0 14
28 -4.1836 0.1181 0.4617 C 0 0 0 0 0 0 0 0 0 0 0 15
29 -3.2267 0.3495 1.4577 C 0 0 0 0 0 0 0 0 0 0 0 16
30 -1.8649 0.2733 1.1554 C 0 0 0 0 0 0 0 0 0 0 0 17
31 -2.3910 -0.2654 -1.1311 C 0 0 0 0 0 0 0 0 0 0 0 18
32 -3.7585 -0.1903 -0.8327 C 0 0 0 0 0 0 0 0 0 0 0 19
33 1.4631 -0.4907 -2.1015 H 0 0 0 0 0 0 0 0 0 0 0 20
34 -0.0468 0.2929 -2.5958 H 0 0 0 0 0 0 0 0 0 0 0 21
35 -0.0292 -1.4427 -2.1832 H 0 0 0 0 0 0 0 0 0 0 0 22
36 -5.2482 0.1780 0.6949 H 0 0 0 0 0 0 0 0 0 0 0 23
37 -3.5410 0.5914 2.4748 H 0 0 0 0 0 0 0 0 0 0 0 24
38 -1.1441 0.4583 1.9551 H 0 0 0 0 0 0 0 0 0 0 0 25
39 -2.0936 -0.5074 -2.1509 H 0 0 0 0 0 0 0 0 0 0 0 26
40 -4.4907 -0.3735 -1.6217 H 0 0 0 0 0 0 0 0 0 0 0 27
41 3.8366 2.1430 0.0933 H 0 0 0 0 0 0 0 0 0 0 0 28
42
43 2 1 0 0 0 0
44 6 1 0 0 0 0
45 8 1 0 0 0 0
46 3 2 0 0 0 0
47 4 3 0 0 0 0
48 7 3 0 0 0 0
49 5 4 0 0 0 0
50 11 4 0 0 0 0
51 12 4 0 0 0 0
52 6 5 0 0 0 0
53 9 5 0 0 0 0
54 10 5 0 0 0 0
55 13 6 0 0 0 0
56 14 6 0 0 0 0
57 17 9 0 0 0 0
58 18 9 0 0 0 0
59 20 10 0 0 0 0
60 21 10 0 0 0 0
22 10 0 0 0 0
16 15 0 0 0 0
19 15 0 0 0 0
23 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
19 18 0 0 0 0
26 18 0 0 0 0
27 19 0 0 0 0
8 28 0 0 0 0
M END
\$\$\$\$
3,3-methylphenylglutarimide3-anion.sdf
COSMOTHERM 3D 0
27 28 0 0 0 0 0 0 0 0 0 V2000
0.9051 -1.6836 1.0375 C 0 0 0 0 0 0 0 0 0 0 0 1
1.0659 -2.0718 -0.2578 N 0 0 0 0 0 0 0 0 0 0 0 2
0.0554 -1.9165 -1.1567 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2703 -1.2643 -0.7573 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.1651 -0.2885 0.4252 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4069 -1.0658 1.5235 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1793 -2.3316 -2.3372 O 0 0 0 0 0 0 0 0 0 0 0 7
1.8277 -1.8523 1.8746 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.5821 0.0770 0.9182 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.4125 1.0057 0.0673 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.9501 -2.0824 -0.4602 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.7186 -0.8043 -1.6486 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.0505 -1.8931 1.8734 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.1888 -0.4431 2.4010 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9041 3.4502 -0.5252 C 0 0 0 0 0 0 0 0 0 0 0 15
0.6326 2.5273 -1.5386 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.0182 1.3212 -1.2439 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.1283 1.9484 1.0757 C 0 0 0 0 0 0 0 0 0 0 0 18
0.5190 3.1531 0.7881 C 0 0 0 0 0 0 0 0 0 0 0 19
-3.1383 -0.8330 1.1911 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.5435 0.7295 1.8026 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.1454 0.6030 0.1323 H 0 0 0 0 0 0 0 0 0 0 0 22
1.4096 4.3904 -0.7537 H 0 0 0 0 0 0 0 0 0 0 0 23
0.9268 2.7415 -2.5683 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.2125 0.6243 -2.0597 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.4211 1.7450 2.1081 H 0 0 0 0 0 0 0 0 0 0 0 26
0.7225 3.8628 1.5929 H 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0


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2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
9 6 0 0 0 0
4 12 0 0 0 0
M END
$$$$
3,4-dichlorophenol.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.1348 0.6171 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.5079 -0.7337 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.4871 -1.7173 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.8344 -1.3656 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
2.2006 -0.0111 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2131 0.9835 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.2007 -1.2241 0.0001 C1 0 0 0 0 0 0 0 0 0 0 0 7
0.1995 -2.7686 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 8
2.6059 -2.1358 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
3.5361 0.2849 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 10
1.4875 2.0392 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.3466 1.8959 -0.0001 C1 0 0 0 0 0 0 0 0 0 0 0 12
3.6624 1.2530 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
10 13 0 0 0 0
M END
$$$$
3,5-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
0.2651 -1.1813 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1191 -1.2230 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.8893 -0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.1192 1.2229 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2650 1.1814 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.0176 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-3.1750 -0.0001 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 7
1.1705 2.7296 0.0000 C1 0 0 0 0 0 0 0 0 0 0 0 8
1.1705 -2.7296 0.0000 C1 0 0 0 0 0 0 0 0 0 0 0 9
-1.6517 -2.1748 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.6518 2.1747 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
2.1046 0.0000 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
3,5-dichlorophenol.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-3.1543 0.0674 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7903 0.0017 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.0947 1.2213 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.2961 1.1876 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1828 2.7203 0.0000 C1 0 0 0 0 0 0 0 0 0 0 0 5
1.0278 -0.0028 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2943 -1.1902 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
1.1757 -2.7259 0.0000 C1 0 0 0 0 0 0 0 0 0 0 0 8
-1.0989 -1.2201 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 9
-3.5298 -0.8341 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.6429 2.1623 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
2.1156 -0.0040 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.6403 -2.1666 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
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12 6 0 0 0 0
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9 13 0 0 0 0
M END
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3-chlorophenol-anion.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
-0.9068 0.0000 -1.8240 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.9260 0.0000 -0.8751 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.6532 -0.0001 0.5399 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2522 -0.0001 0.8965 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7257 0.0000 -0.0875 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4525 0.0000 -1.4586 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.5837 0.0001 1.4353 O 0 0 0 0 0 0 0 0 0 0 0 7
2.4537 0.0000 0.4269 Cl 0 0 0 0 0 0 0 0 0 0 0 8
-1.1626 -0.0001 -2.8872 H 0 0 0 0 0 0 0 0 0 0 0 9
-2.9726 0.0002 -1.1917 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0165 -0.0001 1.9543 H 0 0 0 0 0 0 0 0 0 0 0 11
1.2488 0.0002 -2.2012 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$
3-chlorophenol.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2407 0.8828 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7584 -0.0877 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.4796 -1.4560 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.8642 -1.8488 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.8954 -0.9061 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.5800 0.4614 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.2825 -2.1918 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.5372 1.4423 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.0029 1.9460 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
2.4534 0.4453 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-1.1093 -2.9119 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.9395 -1.2257 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
-3.4228 1.0313 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
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9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
8 6 0 0 0 0
8 13 0 0 0 0
M END
$$$$
3-chloropropanoicacid0-anion.sdf
COSMOtherm 3D 0

10 9 0 0 0 0 0 0 0 0 0 V2000
-0.7343 -0.5148 -0.2079 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2837 0.5534 0.1273 C 0 0 0 0 0 0 0 0 0 0 0 2
1.7454 0.0307 0.0239 C 0 0 0 0 0 0 0 0 0 0 0 3
2.6470 0.9137 -0.0889 O 0 0 0 0 0 0 0 0 0 0 0 4
1.9260 -1.2239 0.0852 O 0 0 0 0 0 0 0 0 0 0 0 5
0.1364 0.9052 1.1615 H 0 0 0 0 0 0 0 0 0 0 0 6
-2.4728 0.1131 0.0260 Cl 0 0 0 0 0 0 0 0 0 0 0 7
-0.6935 -0.8257 -1.2564 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.6542 -1.3883 0.4436 H 0 0 0 0 0 0 0 0 0 0 0 9
0.1711 1.4271 -0.5297 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 10 0 0 0 0
M END
$$$$
3-chloropropanoicacid0.sdf
COSMOtherm 3D 0

11 10 0 0 0 0 0 0 0 0 0 V2000
-0.7923 -0.5857 -0.0217 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2456 0.5226 0.0172 C 0 0 0 0 0 0 0 0 0 0 0 2
1.6531 -0.0326 0.0040 C 0 0 0 0 0 0 0 0 0 0 0 3
2.5754 0.9591 -0.0115 O 0 0 0 0 0 0 0 0 0 0 0 4
1.9487 -1.2190 0.0089 O 0 0 0 0 0 0 0 0 0 0 0 5
0.1318 1.1389 0.9219 H 0 0 0 0 0 0 0 0 0 0 0 6
-2.4809 0.1364 0.0019 Cl 0 0 0 0 0 0 0 0 0 0 0 7
-0.7342 -1.1790 -0.9385 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.7353 -1.2411 0.8518 H 0 0 0 0 0 0 0 0 0 0 0 9
0.1343 1.2009 -0.8417 H 0 0 0 0 0 0 0 0 0 0 0 10
3.4673 0.5474 -0.0132 H 0 0 0 0 0 0 0 0 0 0 0 11

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2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 11 0 0 0 0
M END
$$$$
3-chloropropanoicacid1-anion.sdf
COSMOtherm 3D 0
10 9 0 0 0 0 0 0 0 0 0 V2000
-0.7349 -0.5338 -0.1532 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2838 0.5566 0.0966 C 0 0 0 0 0 0 0 0 0 0 0 2
1.7457 0.0321 0.0174 C 0 0 0 0 0 0 0 0 0 0 0 3
1.9232 -1.2237 0.0646 O 0 0 0 0 0 0 0 0 0 0 0 4
2.6501 0.9153 -0.0684 O 0 0 0 0 0 0 0 0 0 0 0 5
0.1428 0.9866 1.1014 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.6893 -0.9325 -1.1710 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.6641 -1.3500 0.5701 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.4727 0.1182 0.0185 Cl 0 0 0 0 0 0 0 0 0 0 0 9
0.1653 1.3793 -0.6230 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 10 0 0 0 0
M END
$$$$
3-chloropropanoicacid1.sdf
COSMOtherm 3D 0
11 10 0 0 0 0 0 0 0 0 0 V2000
-0.9512 1.0698 0.0607 C 0 0 0 0 0 0 0 0 0 0 0 1
0.3671 0.8780 0.7875 C 0 0 0 0 0 0 0 0 0 0 0 2
1.3722 -0.0169 0.0920 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4481 0.2246 -1.2376 O 0 0 0 0 0 0 0 0 0 0 0 4
2.0693 -0.8466 0.6579 O 0 0 0 0 0 0 0 0 0 0 0 5
0.2126 0.4914 1.8019 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.6099 1.7445 0.6141 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.8209 1.4242 -0.9652 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.8755 -0.5202 -0.0773 Cl 0 0 0 0 0 0 0 0 0 0 0 9
0.8332 1.8748 0.8841 H 0 0 0 0 0 0 0 0 0 0 0 10
2.1272 -0.3734 -1.6196 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 11 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid-anion0.sdf
COSMOtherm 3D 0
21 23 0 0 0 0 0 0 0 0 0 V2000
3.8273 0.2954 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
3.5764 -1.1026 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 2
2.2758 -1.5704 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1745 -0.6679 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4276 0.7531 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 5
2.7822 1.1999 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1714 -1.1142 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2401 -0.2332 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9780 1.1859 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 9
0.3323 1.6516 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.6662 -0.7481 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 11
-2.8864 -1.9828 0.0006 O 0 0 0 0 0 0 0 0 0 0 0 12
-3.5939 0.1607 -0.0008 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.0135 2.0576 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.8543 1.4117 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 15
4.8577 0.6565 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 16
4.4135 -1.8030 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 17
2.0737 -2.6445 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 18
2.9827 2.2740 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.3838 -2.1860 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 20
0.5136 2.7290 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
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14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 13 0 0 0 0
15 14 0 0 0 0
10 21 0 0 0 0
M  END
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3-hydroxy-2-naphtoicacid-anion1.sdf
COSMOTHERM 3D 0

21 22 0 0 0 0 0 0 0 0 0 V2000
3.8241 0.2396 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 1
3.5381 -1.1515 -0.0037 C 0 0 0 0 0 0 0 0 0 0 0 0 2
2.2266 -1.5890 -0.0048 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1491 -0.6584 -0.0023 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4396 0.7504 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.8014 1.1699 0.0026 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.2090 -1.0632 -0.0021 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2771 -0.1760 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9661 1.2277 0.0021 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.3551 1.6607 0.0034 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.7009 -0.7650 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.7797 -2.0344 0.0179 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.6838 0.0323 -0.0194 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.9847 2.1470 0.0045 O 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.5800 3.0371 0.0086 H 0 0 0 0 0 0 0 0 0 0 0 0 15
4.8633 0.5744 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 0 16
4.3581 -1.8718 -0.0057 H 0 0 0 0 0 0 0 0 0 0 0 0 17
1.9988 -2.6578 -0.0077 H 0 0 0 0 0 0 0 0 0 0 0 0 18
3.0268 2.2390 0.0057 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.4519 -2.1277 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 0 20
0.5635 2.7353 0.0064 H 0 0 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
19 6 0 0 0 0
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11 8 0 0 0 0
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14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 14 0 0 0 0
10 21 0 0 0 0
M  END
$$$$
3-hydroxy-2-naphtoicacid0.sdf
COSMOTHERM 3D 0

22 23 0 0 0 0 0 0 0 0 0 V2000
3.8316 0.2671 -0.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 1
3.5657 -1.1293 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 2
2.2634 -1.5845 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1735 -0.6654 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4420 0.7529 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.8000 1.1855 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.1693 -1.0991 0.0018 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2292 -0.1949 0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9536 1.2204 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.3597 1.6651 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.6276 -0.6489 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.7910 -1.9852 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.6004 0.1250 -0.0025 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.9577 2.1354 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 14
-3.7543 -2.1743 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.8145 1.6135 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 0 16
4.8663 0.6148 -0.0034 H 0 0 0 0 0 0 0 0 0 0 0 0 17
4.3960 -1.8371 -0.0024 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2.0477 -2.6554 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 19
3.0131 2.2565 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.3804 -2.1691 0.0017 H 0 0 0 0 0 0 0 0 0 0 0 0 21
0.5527 2.7395 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
18 2 0 0 0 0
4 3 0 0 0 0
19 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
20 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
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11 8 0 0 0 0
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12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0

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16 14 0 0 0 0
10 22 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid1.sdf
COSMOtherm 3D 0
22 23 0 0 0 0 0 0 0 0 V2000
3.8356 0.2787 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
3.5773 -1.1192 -0.0062 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
2.2776 -1.5827 -0.0070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1830 -0.6693 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4442 0.7488 0.0024 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.7989 1.1912 0.0032 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.1585 -1.1036 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2304 -0.2128 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9596 1.2035 0.0045 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.3542 1.6496 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.5892 -0.8050 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-3.5823 0.1383 -0.0346 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.8459 -2.0007 0.0283 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.9358 2.1548 0.0097 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-4.4569 -0.3067 -0.0216 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.8155 1.7071 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
4.8685 0.6321 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
4.4119 -1.8219 -0.0096 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
2.0687 -2.6549 -0.0109 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
3.0052 -2.2636 0.0070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.3762 -2.1732 -0.0057 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
0.5392 2.7255 0.0115 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
18 2 0 0 0 0
4 3 0 0 0 0
19 3 0 0 0 0
5 4 0 0 0 0
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6 5 0 0 0 0
10 5 0 0 0 0
20 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0
16 14 0 0 0 0
10 22 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid2.sdf
COSMOtherm 3D 0
22 23 0 0 0 0 0 0 0 0 V2000
3.8371 0.2528 -0.0041 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
3.5617 -1.1412 -0.0070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
2.2558 -1.5887 -0.0058 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1735 -0.6620 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4526 0.7504 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.8109 1.1781 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.1748 -1.0788 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2421 -0.1836 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9507 1.2252 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.3675 1.6589 0.0062 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.6008 -0.7955 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-3.6285 0.0846 -0.0445 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.7966 -2.0095 0.0329 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.9818 2.1197 0.0152 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-4.4538 -0.4486 -0.0412 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.6071 3.0224 0.0192 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
4.8741 0.5936 -0.0052 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
4.3874 -1.8544 -0.0102 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
2.0336 -2.6583 -0.0082 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
3.0302 2.2479 0.0027 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.4035 -2.1457 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
0.5718 2.7333 0.0106 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
18 2 0 0 0 0
4 3 0 0 0 0
19 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
20 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0
16 14 0 0 0 0
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M END

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3-hydroxybenzoicacid-anion.sdf
COSMOTHERM      3D      0

15 15 0 0 0 0 0 0 0 0 0 V2000
  1.1373 -1.8685 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 0 1
 -0.2128 -1.4995 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 2
 -0.5718 -0.1417 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.4364 0.8343 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 4
  1.7858 0.4590 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 5
  2.1433 -0.8978 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 6
 -2.0464 0.2811 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 7
  2.8078 1.3840 -0.0015 O 0 0 0 0 0 0 0 0 0 0 0 0 8
 -2.2906 1.5276 0.0029 O 0 0 0 0 0 0 0 0 0 0 0 0 9
 -2.9127 -0.6472 -0.0034 O 0 0 0 0 0 0 0 0 0 0 0 0 10
  1.4154 -2.9246 0.0021 H 0 0 0 0 0 0 0 0 0 0 0 0 11
 -1.0019 -2.2520 0.0016 H 0 0 0 0 0 0 0 0 0 0 0 0 12
  0.1502 1.8890 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 13
  3.1984 -1.1768 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 14
  2.4256 2.2821 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 15

  2 1 0 0 0 0
  6 1 0 0 0 0
 11 1 0 0 0 0
  3 2 0 0 0 0
 12 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
 13 4 0 0 0 0
  6 5 0 0 0 0
  8 5 0 0 0 0
 14 6 0 0 0 0
  9 7 0 0 0 0
 10 7 0 0 0 0
  8 15 0 0 0 0
M END

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3-hydroxybenzoicacid.sdf
COSMOTHERM      3D      0

16 16 0 0 0 0 0 0 0 0 0 V2000
  1.1774 -1.8678 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 1
 -0.1768 -1.5251 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 2
 -0.5459 -0.1696 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.4386 0.8340 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 4
  1.7917 0.4753 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 5
  2.1635 -0.8788 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 6
 -1.9959 0.1697 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 7
  2.7992 1.4055 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 0 8
 -2.2324 1.5068 0.0032 O 0 0 0 0 0 0 0 0 0 0 0 0 9
 -2.9043 -0.6553 -0.0035 O 0 0 0 0 0 0 0 0 0 0 0 0 10
  1.4729 -2.9179 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 0 11
 -0.9497 -2.2932 0.0016 H 0 0 0 0 0 0 0 0 0 0 0 0 12
  0.1535 1.8869 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 0 13
  3.2225 -1.1414 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 0 14
  2.4160 2.3035 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 0 15
 -3.2051 1.6365 0.0030 H 0 0 0 0 0 0 0 0 0 0 0 0 16

  2 1 0 0 0 0
  6 1 0 0 0 0
 11 1 0 0 0 0
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 12 2 0 0 0 0
  4 3 0 0 0 0
  7 3 0 0 0 0
  5 4 0 0 0 0
 13 4 0 0 0 0
  6 5 0 0 0 0
  8 5 0 0 0 0
 14 6 0 0 0 0
  9 7 0 0 0 0
 10 7 0 0 0 0
 15 8 0 0 0 0
  9 16 0 0 0 0
M END

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4-(1,1-dimethylethyl)-benzoicacid-anion.sdf
COSMOTHERM      3D      0

26 26 0 0 0 0 0 0 0 0 0 V2000
 -0.4275 0.0017 -1.2251 C 0 0 0 0 0 0 0 0 0 0 0 0 1
  0.9727 0.0015 -1.2132 C 0 0 0 0 0 0 0 0 0 0 0 0 2
  1.6878 0.0003 -0.0077 C 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.9530 -0.0007 1.1901 C 0 0 0 0 0 0 0 0 0 0 0 0 4
 -0.4426 -0.0010 1.1774 C 0 0 0 0 0 0 0 0 0 0 0 0 5
 -1.1698 0.0004 -0.0311 C 0 0 0 0 0 0 0 0 0 0 0 0 6
  3.2171 -0.0001 0.0047 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 -2.7081 -0.0001 -0.0038 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 -3.2062 -1.2638 0.7384 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 -3.3201 0.0039 -1.4169 C 0 0 0 0 0 0 0 0 0 0 0 0 10
 -3.2070 1.2588 0.7459 C 0 0 0 0 0 0 0 0 0 0 0 0 11
  3.8074 -0.0027 -1.1209 O 0 0 0 0 0 0 0 0 0 0 0 0 12
  3.7879 0.0021 1.1407 O 0 0 0 0 0 0 0 0 0 0 0 0 13
 -0.9408 0.0029 -2.1873 H 0 0 0 0 0 0 0 0 0 0 0 0 14
  1.5307 0.0022 -2.1516 H 0 0 0 0 0 0 0 0 0 0 0 0 15
  1.4972 -0.0015 2.1366 H 0 0 0 0 0 0 0 0 0 0 0 0 16
 -0.9754 -0.0020 2.1312 H 0 0 0 0 0 0 0 0 0 0 0 0 17
 -4.3066 -1.2735 0.7706 H 0 0 0 0 0 0 0 0 0 0 0 0 18
 -2.8379 -1.2981 1.7736 H 0 0 0 0 0 0 0 0 0 0 0 0 19
 -2.8704 -2.1783 0.2263 H 0 0 0 0 0 0 0 0 0 0 0 0 20
 -4.4172 0.0033 -1.3390 H 0 0 0 0 0 0 0 0 0 0 0 0 21
 -3.0268 0.8976 -1.9880 H 0 0 0 0 0 0 0 0 0 0 0 0 22
 -3.0262 -0.8861 -1.9935 H 0 0 0 0 0 0 0 0 0 0 0 0 23
 -4.3076 1.2703 0.7734 H 0 0 0 0 0 0 0 0 0 0 0 0 24
 -2.8674 2.1766 0.2423 H 0 0 0 0 0 0 0 0 0 0 0 0 25
 -2.8433 1.2846 1.7829 H 0 0 0 0 0 0 0 0 0 0 0 0 26

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2 1 0 0 0 0
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14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
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16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
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11 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
24 11 0 0 0 0
25 11 0 0 0 0
11 26 0 0 0 0
M END
$$$$
4-(1,1-dimethylethyl)-benzoicacid.sdf
COSMOTHERM 3D 0
27 27 0 0 0 0 0 0 0 0 0 V2000
-0.4569 0.0007 -1.2386 C 0 0 0 0 0 0 0 0 0 0 1
0.9388 0.0003 -1.2411 C 0 0 0 0 0 0 0 0 0 0 2
1.6538 -0.0007 -0.0334 C 0 0 0 0 0 0 0 0 0 0 3
0.9380 -0.0018 1.1787 C 0 0 0 0 0 0 0 0 0 0 4
-0.4542 -0.0020 1.1693 C 0 0 0 0 0 0 0 0 0 0 5
-1.1872 -0.0003 -0.0361 C 0 0 0 0 0 0 0 0 0 0 6
3.1369 -0.0001 -0.0787 C 0 0 0 0 0 0 0 0 0 0 7
-2.7230 0.0003 0.0039 C 0 0 0 0 0 0 0 0 0 0 8
-3.2116 -1.2637 0.7529 C 0 0 0 0 0 0 0 0 0 0 9
-3.3465 0.0036 -1.4041 C 0 0 0 0 0 0 0 0 0 0 10
-3.2104 1.2615 0.7583 C 0 0 0 0 0 0 0 0 0 0 11
3.8072 -0.0016 -1.1080 O 0 0 0 0 0 0 0 0 0 0 12
3.7106 0.0028 1.1542 O 0 0 0 0 0 0 0 0 0 0 13
-0.9775 0.0019 -2.1957 H 0 0 0 0 0 0 0 0 0 0 14
1.4854 0.0009 -2.1853 H 0 0 0 0 0 0 0 0 0 0 15
1.4734 -0.0027 2.1282 H 0 0 0 0 0 0 0 0 0 0 16
-0.9800 -0.0030 2.1256 H 0 0 0 0 0 0 0 0 0 0 17
-4.3114 -1.2718 0.7924 H 0 0 0 0 0 0 0 0 0 0 18
-2.8365 -1.2958 1.7854 H 0 0 0 0 0 0 0 0 0 0 19
-2.8801 -2.1786 0.2393 H 0 0 0 0 0 0 0 0 0 0 20
-4.4425 0.0034 -1.3151 H 0 0 0 0 0 0 0 0 0 0 21
-3.0591 0.8973 -1.9780 H 0 0 0 0 0 0 0 0 0 0 22
-3.0590 -0.8872 -1.9824 H 0 0 0 0 0 0 0 0 0 0 23
-4.3103 1.2736 0.7927 H 0 0 0 0 0 0 0 0 0 0 24
-2.8729 2.1783 0.2520 H 0 0 0 0 0 0 0 0 0 0 25
-2.8401 1.2860 1.7928 H 0 0 0 0 0 0 0 0 0 0 26
4.6835 0.0038 1.0262 H 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
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10 8 0 0 0 0
11 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
24 11 0 0 0 0
25 11 0 0 0 0
26 11 0 0 0 0
13 27 0 0 0 0
M END
$$$$
4-(1-methylethyl)-benzoicacid-anion.sdf
COSMOTHERM 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
-0.6182 0.0021 1.3698 C 0 0 0 0 0 0 0 0 0 0 1
0.7769 0.0016 1.2700 C 0 0 0 0 0 0 0 0 0 0 2
1.4086 0.0000 0.0170 C 0 0 0 0 0 0 0 0 0 0 3
0.5995 -0.0009 -1.1322 C 0 0 0 0 0 0 0 0 0 0 4
-0.7936 -0.0007 -1.0316 C 0 0 0 0 0 0 0 0 0 0 5
-1.4309 0.0011 0.2233 C 0 0 0 0 0 0 0 0 0 0 6
2.9342 -0.0003 -0.0963 C 0 0 0 0 0 0 0 0 0 0 7
-2.9479 0.0012 0.3453 C 0 0 0 0 0 0 0 0 0 0 8
-3.5713 1.2676 -0.2730 C 0 0 0 0 0 0 0 0 0 0 9
-3.5698 -1.2703 -0.2642 C 0 0 0 0 0 0 0 0 0 0 10
3.5974 0.0011 0.9879 O 0 0 0 0 0 0 0 0 0 0 11
3.4288 -0.0018 -1.2674 O 0 0 0 0 0 0 0 0 0 0 12
-1.0897 0.0035 2.3566 H 0 0 0 0 0 0 0 0 0 0 13

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1.3974 0.0023 2.1683 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.0849 -0.0023 -2.1100 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.3932 -0.0013 -1.9456 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.1820 0.0048 1.4229 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-4.6618 1.2705 -0.1248 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.1609 2.1796 0.1849 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-3.3796 1.3159 -1.3562 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-4.6606 -1.2728 -0.1176 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.1596 -2.1785 0.2014 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-3.3763 -1.3267 -1.3467 H 0 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
10 23 0 0 0 0
M END
$$$$
4-(1-methylethyl)-benzoicacid.sdf
COSMOtherm 3D 0
24 24 0 0 0 0 0 0 0 0 0 V2000
-0.6472 0.0023 1.3838 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7444 0.0022 1.2982 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.3760 0.0008 0.0430 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.5848 -0.0003 -1.1216 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.8052 0.0001 -1.0243 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.4485 0.0013 0.2280 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.8590 -0.0002 -0.0086 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.9644 0.0009 0.3367 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-3.5780 1.2683 -0.2901 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-3.5759 -1.2721 -0.2808 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5947 0.0006 0.9749 O 0 0 0 0 0 0 0 0 0 0 0 0 11
3.3511 -0.0024 -1.2762 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.1256 0.0031 2.3659 H 0 0 0 0 0 0 0 0 0 0 0 0 13
1.3538 0.0033 2.2031 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.0604 -0.0013 -2.1022 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.3979 -0.0009 -1.9414 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.2090 0.0046 1.4113 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-4.6692 1.2708 -0.1499 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.1709 2.1802 0.1706 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-3.3780 1.3142 -1.3716 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-4.6674 -1.2743 -0.1427 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.1691 -2.1797 0.1882 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-3.3735 -1.3267 -1.3615 H 0 0 0 0 0 0 0 0 0 0 0 0 23
4.3302 -0.0039 -1.2121 H 0 0 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
12 24 0 0 0 0
M END
$$$$
4-aminobenzoicacid-anion.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 0 V2000
1.4503 1.2142 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0577 1.2023 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6743 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0577 -1.2023 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4503 -1.2142 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.1809 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.1928 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7
3.5533 0.0000 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.7812 1.1305 0.0009 O 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.7812 -1.1305 -0.0007 O 0 0 0 0 0 0 0 0 0 0 0 0 10
4.0773 -0.8667 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 0 11
4.0773 0.8666 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 12
```

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1
2
3      1.9926    2.1634   -0.0008 H    0  0  0  0  0  0  0  0  0  0  13
4     -0.4933    2.1451   -0.0008 H    0  0  0  0  0  0  0  0  0  0  14
5     -0.4933   -2.1451    0.0004 H    0  0  0  0  0  0  0  0  0  0  15
6      1.9926   -2.1634    0.0008 H    0  0  0  0  0  0  0  0  0  0  16
7
8      2  1  0  0  0  0
9      6  1  0  0  0  0
10     13  1  0  0  0  0
11      3  2  0  0  0  0
12     14  2  0  0  0  0
13      4  3  0  0  0  0
14      7  3  0  0  0  0
15      5  4  0  0  0  0
16     15  4  0  0  0  0
17      6  5  0  0  0  0
18      8  6  0  0  0  0
19      9  7  0  0  0  0
20     10  7  0  0  0  0
21     11  8  0  0  0  0
22     12  8  0  0  0  0
23      5 16  0  0  0  0
```

M END

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4-aminobenzoicacid.sdf
COSMOtherm 3D

0

```
17 17 0 0 0 0 0 0 0 0 0 0 V2000
1.4808    1.2198    0.0001 C    0  0  0  0  0  0  0  0  0  0  1
0.0961    1.2282    0.0001 C    0  0  0  0  0  0  0  0  0  0  2
-0.6450    0.0255    0.0003 C    0  0  0  0  0  0  0  0  0  0  3
0.0655   -1.1962    0.0003 C    0  0  0  0  0  0  0  0  0  0  4
1.4511   -1.2189    0.0004 C    0  0  0  0  0  0  0  0  0  0  5
2.1950   -0.0088   -0.0001 C    0  0  0  0  0  0  0  0  0  0  6
-2.1104    0.0888    0.0000 C    0  0  0  0  0  0  0  0  0  0  7
3.5561   -0.0257   -0.0005 N    0  0  0  0  0  0  0  0  0  0  8
-2.7816    1.1242    0.0000 O    0  0  0  0  0  0  0  0  0  0  9
-2.7110   -1.1410   -0.0004 O    0  0  0  0  0  0  0  0  0  0 10
4.0705   -0.8991   -0.0003 H    0  0  0  0  0  0  0  0  0  0 11
4.0923    0.8344    0.0001 H    0  0  0  0  0  0  0  0  0  0 12
2.0358    2.1603   -0.0002 H    0  0  0  0  0  0  0  0  0  0 13
-0.4392    2.1791    0.0002 H    0  0  0  0  0  0  0  0  0  0 14
-0.4817   -2.1392    0.0005 H    0  0  0  0  0  0  0  0  0  0 15
1.9831   -2.1726    0.0004 H    0  0  0  0  0  0  0  0  0  0 16
-3.6792   -0.9860   -0.0013 H    0  0  0  0  0  0  0  0  0  0 17
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2  1  0  0  0  0
6  1  0  0  0  0
13  1  0  0  0  0
3  2  0  0  0  0
14  2  0  0  0  0
4  3  0  0  0  0
7  3  0  0  0  0
5  4  0  0  0  0
15  4  0  0  0  0
6  5  0  0  0  0
16  5  0  0  0  0
8  6  0  0  0  0
9  7  0  0  0  0
10  7  0  0  0  0
11  8  0  0  0  0
12  8  0  0  0  0
10 17  0  0  0  0
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M END

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4-bromobenzoicacid-anion.sdf
COSMOtherm 3D

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```
14 14 0 0 0 0 0 0 0 0 0 0 V2000
0.1197    1.2204   -0.0011 C    0  0  0  0  0  0  0  0  0  0  1
-1.2787    1.2070   -0.0009 C    0  0  0  0  0  0  0  0  0  0  2
-1.9955    0.0000   -0.0002 C    0  0  0  0  0  0  0  0  0  0  3
-1.2788   -1.2070    0.0008 C    0  0  0  0  0  0  0  0  0  0  4
0.1197   -1.2204    0.0008 C    0  0  0  0  0  0  0  0  0  0  5
0.7987    0.0000    0.0000 C    0  0  0  0  0  0  0  0  0  0  6
-3.5282    0.0000    0.0000 C    0  0  0  0  0  0  0  0  0  0  7
2.7311    0.0000    0.0000 Br   0  0  0  0  0  0  0  0  0  0  8
-4.1032    1.1318    0.0020 O    0  0  0  0  0  0  0  0  0  0  9
-4.1031   -1.1318   -0.0018 O    0  0  0  0  0  0  0  0  0  0 10
0.6667    2.1635   -0.0018 H    0  0  0  0  0  0  0  0  0  0 11
-1.8326    2.1471   -0.0015 H    0  0  0  0  0  0  0  0  0  0 12
-1.8327   -2.1470    0.0014 H    0  0  0  0  0  0  0  0  0  0 13
0.6667   -2.1635    0.0018 H    0  0  0  0  0  0  0  0  0  0 14
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2  1  0  0  0  0
6  1  0  0  0  0
11  1  0  0  0  0
3  2  0  0  0  0
12  2  0  0  0  0
4  3  0  0  0  0
7  3  0  0  0  0
5  4  0  0  0  0
13  4  0  0  0  0
6  5  0  0  0  0
8  6  0  0  0  0
9  7  0  0  0  0
10  7  0  0  0  0
5 14  0  0  0  0
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M END

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4-bromobenzoicacid.sdf
COSMOtherm 3D

0

```
15 15 0 0 0 0 0 0 0 0 0 0 V2000
0.1496    1.2325   -0.0005 C    0  0  0  0  0  0  0  0  0  0  1
-1.2448    1.2334   -0.0004 C    0  0  0  0  0  0  0  0  0  0  2
-1.9610    0.0243    0.0004 C    0  0  0  0  0  0  0  0  0  0  3
-1.2622   -1.1956    0.0012 C    0  0  0  0  0  0  0  0  0  0  4
0.1332   -1.2111    0.0011 C    0  0  0  0  0  0  0  0  0  0  5
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0.8200   0.0057   0.0002 C  0  0  0  0  0  0  0  0  0  0  6
-3.4476   0.0812   0.0001 C  0  0  0  0  0  0  0  0  0  0  7
 2.7427  -0.0077  -0.0002 Br  0  0  0  0  0  0  0  0  0  0  8
-4.1036   1.1178   0.0012 O  0  0  0  0  0  0  0  0  0  0  9
-4.0257  -1.1463  -0.0019 O  0  0  0  0  0  0  0  0  0  0 10
 0.7021   2.1715  -0.0014 H  0  0  0  0  0  0  0  0  0  0 11
-1.7868   2.1796  -0.0009 H  0  0  0  0  0  0  0  0  0  0 12
-1.8059  -2.1397   0.0017 H  0  0  0  0  0  0  0  0  0  0 13
 0.6728  -2.1576   0.0018 H  0  0  0  0  0  0  0  0  0  0 14
-4.9986  -1.0175  -0.0027 H  0  0  0  0  0  0  0  0  0  0 15
 2  1  0  0  0  0
 6  1  0  0  0  0
11  1  0  0  0  0
 3  2  0  0  0  0
12  2  0  0  0  0
 4  3  0  0  0  0
 7  3  0  0  0  0
 5  4  0  0  0  0
13  4  0  0  0  0
 6  5  0  0  0  0
14  5  0  0  0  0
 8  6  0  0  0  0
 9  7  0  0  0  0
10  7  0  0  0  0
10 15  0  0  0  0
M END
$$$$
4-butylbenzoicacid-anion.sdf
COSMOtherm 3D 0
26 26 0 0 0 0 0 0 0 0 v2000
-0.0196  -0.4742   1.2350 C  0  0  0  0  0  0  0  0  0  0  1
 1.3393  -0.1465   1.2146 C  0  0  0  0  0  0  0  0  0  0  2
 2.0317  -0.0154  -0.0004 C  0  0  0  0  0  0  0  0  0  0  3
 1.3217  -0.2246  -1.1944 C  0  0  0  0  0  0  0  0  0  0  4
-0.0368  -0.5531  -1.1738 C  0  0  0  0  0  0  0  0  0  0  5
-0.7343  -0.6813   0.0413 C  0  0  0  0  0  0  0  0  0  0  6
 3.5194   0.3414  -0.0226 C  0  0  0  0  0  0  0  0  0  0  7
-2.2134  -0.9936   0.0614 C  0  0  0  0  0  0  0  0  0  0  8
-3.0969   0.2704  -0.0137 C  0  0  0  0  0  0  0  0  0  0  9
-4.5981  -0.0437   0.0067 C  0  0  0  0  0  0  0  0  0  0 10
-5.4752   1.2116  -0.0710 C  0  0  0  0  0  0  0  0  0  0 11
 4.0948   0.5010   1.0995 O  0  0  0  0  0  0  0  0  0  0 12
 4.0726   0.4538  -1.1615 O  0  0  0  0  0  0  0  0  0  0 13
-0.5371  -0.5759   2.1930 H  0  0  0  0  0  0  0  0  0  0 14
 1.8869   0.0079   2.1462 H  0  0  0  0  0  0  0  0  0  0 15
 1.8558  -0.1308  -2.1418 H  0  0  0  0  0  0  0  0  0  0 16
-0.5674  -0.7176  -2.1158 H  0  0  0  0  0  0  0  0  0  0 17
-2.4605  -1.5469   0.9822 H  0  0  0  0  0  0  0  0  0  0 18
-2.4628  -1.6523  -0.7863 H  0  0  0  0  0  0  0  0  0  0 19
-2.8500   0.8293  -0.9328 H  0  0  0  0  0  0  0  0  0  0 20
-2.8479   0.9353   0.8309 H  0  0  0  0  0  0  0  0  0  0 21
-4.8374  -0.6054   0.9260 H  0  0  0  0  0  0  0  0  0  0 22
-4.8383  -0.7147  -0.8355 H  0  0  0  0  0  0  0  0  0  0 23
-6.5451   0.9555  -0.0546 H  0  0  0  0  0  0  0  0  0  0 24
-5.2798   1.7755  -0.9965 H  0  0  0  0  0  0  0  0  0  0 25
-5.2787   1.8853   0.7773 H  0  0  0  0  0  0  0  0  0  0 26
 2  1  0  0  0  0
 6  1  0  0  0  0
14  1  0  0  0  0
 3  2  0  0  0  0
15  2  0  0  0  0
 4  3  0  0  0  0
 7  3  0  0  0  0
 5  4  0  0  0  0
16  4  0  0  0  0
 6  5  0  0  0  0
17  5  0  0  0  0
 8  6  0  0  0  0
12  7  0  0  0  0
13  7  0  0  0  0
 9  8  0  0  0  0
18  8  0  0  0  0
19  8  0  0  0  0
10  9  0  0  0  0
20  9  0  0  0  0
21  9  0  0  0  0
11 10  0  0  0  0
22 10  0  0  0  0
23 10  0  0  0  0
24 11  0  0  0  0
25 11  0  0  0  0
11 26  0  0  0  0
M END
$$$$
4-butylbenzoicacid.sdf
COSMOtherm 3D 0
27 27 0 0 0 0 0 0 0 0 v2000
-0.0485  -0.4639   1.2590 C  0  0  0  0  0  0  0  0  0  0  1
 1.3059  -0.1365   1.2447 C  0  0  0  0  0  0  0  0  0  0  2
 1.9951  -0.0219   0.0239 C  0  0  0  0  0  0  0  0  0  0  3
 1.2999  -0.2445  -1.1795 C  0  0  0  0  0  0  0  0  0  0  4
-0.0551  -0.5723  -1.1542 C  0  0  0  0  0  0  0  0  0  0  5
-0.7547  -0.6856   0.0616 C  0  0  0  0  0  0  0  0  0  0  6
 3.4375   0.3267   0.0509 C  0  0  0  0  0  0  0  0  0  0  7
-2.2313  -0.9971   0.0774 C  0  0  0  0  0  0  0  0  0  0  8
-3.1070   0.2723  -0.0178 C  0  0  0  0  0  0  0  0  0  0  9
-4.6091  -0.0382  -0.0103 C  0  0  0  0  0  0  0  0  0  0 10
-5.4799   1.2200  -0.1060 C  0  0  0  0  0  0  0  0  0  0 11
 4.0920   0.5252   1.0712 O  0  0  0  0  0  0  0  0  0  0 12
 3.9916   0.4120  -1.1882 O  0  0  0  0  0  0  0  0  0  0 13
-0.5699  -0.5547   2.2146 H  0  0  0  0  0  0  0  0  0  0 14
 1.8447   0.0291   2.1787 H  0  0  0  0  0  0  0  0  0  0 15
 1.8223  -0.1660  -2.1328 H  0  0  0  0  0  0  0  0  0  0 16

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1
2
3 -0.5814 -0.7484 -2.0951 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
4 -2.4839 -1.5379 1.0035 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
5 -2.4759 -1.6630 -0.7653 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
6 -2.8484 0.8217 -0.9393 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
7 -2.8640 0.9428 0.8238 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
8 -4.8592 -0.5922 0.9106 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
9 -4.8425 -0.7141 -0.8503 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
10 -6.5506 0.9674 -0.0991 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
11 -5.2729 1.7765 -1.0334 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
12 -5.2898 1.8988 0.7396 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
13 4.9381 0.6432 -1.0725 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
14 2 1 0 0 0 0
15 6 1 0 0 0 0
16 14 1 0 0 0 0
17 3 2 0 0 0 0
18 15 2 0 0 0 0
19 4 3 0 0 0 0
20 7 3 0 0 0 0
21 5 4 0 0 0 0
22 16 4 0 0 0 0
23 6 5 0 0 0 0
24 17 5 0 0 0 0
25 8 6 0 0 0 0
26 12 7 0 0 0 0
27 13 7 0 0 0 0
28 9 8 0 0 0 0
29 18 8 0 0 0 0
30 19 8 0 0 0 0
31 10 9 0 0 0 0
32 20 9 0 0 0 0
33 21 9 0 0 0 0
34 11 10 0 0 0 0
35 22 10 0 0 0 0
36 23 10 0 0 0 0
37 24 11 0 0 0 0
38 25 11 0 0 0 0
39 26 11 0 0 0 0
40 13 27 0 0 0 0
41 M END
42 $$$$
43 4-carbamoylbenzoicacid-anion.sdf
44 COSMOtherm 3D 0
45
46 18 18 0 0 0 0 0 0 0 0 0 0 V2000
47 -0.6927 1.2026 0.1178 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
48 0.7020 1.1987 0.1309 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
49 1.4198 -0.0020 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
50 0.7034 -1.2015 -0.1364 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
51 -0.6929 -1.2070 -0.1334 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
52 -1.4066 -0.0020 -0.0026 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
53 2.9540 -0.0031 0.0042 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
54 -2.9088 0.0575 -0.0210 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
55 -3.5141 1.0805 -0.3970 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
56 -3.5656 -1.0531 0.3950 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
57 3.5285 1.1199 0.1456 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
58 3.5283 -1.1261 -0.1350 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
59 -4.5822 -1.0608 0.3918 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
60 -3.0864 -1.8552 0.7904 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
61 -1.2464 2.1387 0.2082 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
62 1.2589 2.1308 0.2380 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
63 1.2604 -2.1326 -0.2508 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
64 -1.2204 -2.1543 -0.2642 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
65 2 1 0 0 0 0
66 6 1 0 0 0 0
67 15 1 0 0 0 0
68 3 2 0 0 0 0
69 16 2 0 0 0 0
70 4 3 0 0 0 0
71 7 3 0 0 0 0
72 5 4 0 0 0 0
73 17 4 0 0 0 0
74 6 5 0 0 0 0
75 8 6 0 0 0 0
76 11 7 0 0 0 0
77 12 7 0 0 0 0
78 9 8 0 0 0 0
79 10 8 0 0 0 0
80 13 10 0 0 0 0
81 14 10 0 0 0 0
82 5 18 0 0 0 0
83 M END
84 $$$$
85 4-carbamoylbenzoicacid.sdf
86 COSMOtherm 3D 0
87
88 19 19 0 0 0 0 0 0 0 0 0 0 V2000
89 -0.7225 0.1296 -1.2110 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
90 0.6693 0.1420 -1.2223 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
91 1.3870 0.0040 -0.0214 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
92 0.6909 -0.1419 1.1907 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
93 -0.7039 -0.1373 1.2004 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
94 -1.4221 0.0021 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
95 2.8762 0.0133 -0.0792 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
96 -2.9289 -0.0228 -0.0476 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
97 -3.5313 -0.4307 -1.0575 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
98 -3.5744 0.4188 1.0571 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
99 3.5295 0.1470 -1.1084 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
100 3.4549 -0.1426 1.1371 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
101 -4.5910 0.4195 1.0731 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
102 -3.0887 0.8380 1.8434 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
103 -1.2829 0.2251 -2.1416 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
104 1.2135 0.2548 -2.1604 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
105 1.2380 -0.2628 2.1249 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
106 -1.2250 -0.2720 2.1496 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
107 4.4279 -0.1245 1.0100 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
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2 1 0 0 0 0
6 1 0 0 0 0
15 1 0 0 0 0
3 2 0 0 0 0
16 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 19 0 0 0 0
M END
$$$$
4-chlorobenzoicacid-anion.sdf
COSMOTHERM 3D 0

14 14 0 0 0 0 0 0 0 0 V2000
0.9353 1.2201 -0.0010 C 0 0 0 0 0 0 0 0 0 0 1
-0.4626 1.2070 -0.0007 C 0 0 0 0 0 0 0 0 0 0 2
-1.1796 0.0000 -0.0002 C 0 0 0 0 0 0 0 0 0 0 3
-0.4626 -1.2070 0.0007 C 0 0 0 0 0 0 0 0 0 0 4
0.9353 -1.2201 0.0005 C 0 0 0 0 0 0 0 0 0 0 5
1.6147 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-2.7120 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
3.3914 0.0000 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 8
-3.2874 1.1317 0.0016 O 0 0 0 0 0 0 0 0 0 0 9
-3.2873 -1.1317 -0.0013 O 0 0 0 0 0 0 0 0 0 0 10
1.4865 2.1609 -0.0017 H 0 0 0 0 0 0 0 0 0 0 11
-1.0167 2.1468 -0.0010 H 0 0 0 0 0 0 0 0 0 0 12
-1.0167 -2.1468 0.0011 H 0 0 0 0 0 0 0 0 0 0 13
1.4865 -2.1609 0.0013 H 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
5 14 0 0 0 0
M END
$$$$
4-chlorobenzoicacid.sdf
COSMOTHERM 3D 0

15 15 0 0 0 0 0 0 0 0 V2000
0.9654 1.2282 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-0.4283 1.2316 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-1.1470 0.0238 0.0004 C 0 0 0 0 0 0 0 0 0 0 3
-0.4500 -1.1974 0.0008 C 0 0 0 0 0 0 0 0 0 0 4
0.9448 -1.2152 0.0007 C 0 0 0 0 0 0 0 0 0 0 5
1.6337 0.0004 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
-2.6331 0.0835 0.0001 C 0 0 0 0 0 0 0 0 0 0 7
3.4008 -0.0150 -0.0003 Cl 0 0 0 0 0 0 0 0 0 0 8
-3.2875 1.1211 0.0005 O 0 0 0 0 0 0 0 0 0 0 9
-3.2139 -1.1430 -0.0012 O 0 0 0 0 0 0 0 0 0 0 10
1.5237 2.1639 -0.0008 H 0 0 0 0 0 0 0 0 0 0 11
-0.9689 2.1786 -0.0002 H 0 0 0 0 0 0 0 0 0 0 12
-0.9955 -2.1404 0.0011 H 0 0 0 0 0 0 0 0 0 0 13
1.4869 -2.1604 0.0012 H 0 0 0 0 0 0 0 0 0 0 14
-4.1864 -1.0119 -0.0022 H 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
10 15 0 0 0 0
M END
$$$$
4-chlorophenol-anion.sdf
COSMOTHERM 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
0.1684 1.2153 0.0002 C 0 0 0 0 0 0 0 0 0 0 1
-1.2270 1.2140 0.0007 C 0 0 0 0 0 0 0 0 0 0 2
-2.0031 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
-1.2270 -1.2140 0.0006 C 0 0 0 0 0 0 0 0 0 0 4
0.1684 -1.2153 0.0003 C 0 0 0 0 0 0 0 0 0 0 5
0.8606 0.0000 0.0005 C 0 0 0 0 0 0 0 0 0 0 6
-3.2979 0.0000 -0.0009 O 0 0 0 0 0 0 0 0 0 0 7
2.6522 0.0000 -0.0004 Cl 0 0 0 0 0 0 0 0 0 0 8
0.7173 2.1598 0.0005 H 0 0 0 0 0 0 0 0 0 0 9
-1.7646 2.1666 0.0004 H 0 0 0 0 0 0 0 0 0 0 10

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1
2
3 -1.7646 -2.1666 0.0002 H 0 0 0 0 0 0 0 0 0 0 11
4 0.7173 -2.1598 0.0006 H 0 0 0 0 0 0 0 0 0 0 12
5
6 2 1 0 0 0 0
7 6 1 0 0 0 0
8 9 1 0 0 0 0
9 3 2 0 0 0 0
10 10 2 0 0 0 0
11 4 3 0 0 0 0
12 7 3 0 0 0 0
13 5 4 0 0 0 0
14 11 4 0 0 0 0
15 6 5 0 0 0 0
16 8 6 0 0 0 0
17 5 12 0 0 0 0
18 M END
19 \$\$\$\$
20 4-chlorophenol.sdf
21 COSMOTHERM 3D 0
22
23 13 13 0 0 0 0 0 0 0 0 0 V2000
24 1.2136 1.1990 -0.0003 C 0 0 0 0 0 0 0 0 0 0 1
25 1.2156 -0.1970 0.0001 C 0 0 0 0 0 0 0 0 0 0 2
26 -0.0015 -0.8823 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
27 -1.2180 -0.1991 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4
28 -1.2163 1.1989 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
29 -0.0014 1.9006 0.0001 C 0 0 0 0 0 0 0 0 0 0 6
30 0.0001 -2.6600 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 7
31 0.0597 3.2715 0.0001 O 0 0 0 0 0 0 0 0 0 0 8
32 2.1550 1.7501 -0.0001 H 0 0 0 0 0 0 0 0 0 0 9
33 2.1597 -0.7418 0.0004 H 0 0 0 0 0 0 0 0 0 0 10
34 -2.1622 -0.7437 -0.0003 H 0 0 0 0 0 0 0 0 0 0 11
35 -2.1644 1.7416 0.0000 H 0 0 0 0 0 0 0 0 0 0 12
36 -0.8451 3.6379 0.0012 H 0 0 0 0 0 0 0 0 0 0 13
37 2 1 0 0 0 0
38 6 1 0 0 0 0
39 9 1 0 0 0 0
40 3 2 0 0 0 0
41 10 2 0 0 0 0
42 4 3 0 0 0 0
43 7 3 0 0 0 0
44 5 4 0 0 0 0
45 11 4 0 0 0 0
46 6 5 0 0 0 0
47 12 5 0 0 0 0
48 8 6 0 0 0 0
49 8 13 0 0 0 0
50 M END
51 \$\$\$\$
52 4-cyanobenzoicacid-anion.sdf
53 COSMOTHERM 3D 0
54
55 15 15 0 0 0 0 0 0 0 0 0 V2000
56 1.0942 1.2228 -0.0008 C 0 0 0 0 0 0 0 0 0 0 1
57 -0.2988 1.2104 -0.0009 C 0 0 0 0 0 0 0 0 0 0 2
58 -1.0116 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
59 -0.2989 -1.2105 0.0007 C 0 0 0 0 0 0 0 0 0 0 4
60 1.0941 -1.2230 0.0007 C 0 0 0 0 0 0 0 0 0 0 5
1.7976 -0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-2.5482 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 7
3.2248 0.0000 0.0001 C 0 0 0 0 0 0 0 0 0 0 8
4.3931 0.0002 0.0001 N 0 0 0 0 0 0 0 0 0 0 9
-3.1184 1.1326 0.0017 O 0 0 0 0 0 0 0 0 0 0 10
-3.1185 -1.1324 -0.0015 O 0 0 0 0 0 0 0 0 0 0 11
1.6426 2.1655 -0.0015 H 0 0 0 0 0 0 0 0 0 0 12
-0.8581 2.1467 -0.0015 H 0 0 0 0 0 0 0 0 0 0 13
-0.8583 -2.1468 0.0011 H 0 0 0 0 0 0 0 0 0 0 14
1.6425 -2.1657 0.0014 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
5 15 0 0 0 0
M END
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4-cyanobenzoicacid.sdf
COSMOTHERM 3D 0
16 16 0 0 0 0 0 0 0 0 0 V2000
1.1235 1.2298 -0.0012 C 0 0 0 0 0 0 0 0 0 0 1
-0.2673 1.2329 -0.0008 C 0 0 0 0 0 0 0 0 0 0 2
-0.9802 0.0222 0.0003 C 0 0 0 0 0 0 0 0 0 0 3
-0.2881 -1.2013 0.0016 C 0 0 0 0 0 0 0 0 0 0 4
1.1038 -1.2180 0.0016 C 0 0 0 0 0 0 0 0 0 0 5
1.8126 -0.0002 0.0000 C 0 0 0 0 0 0 0 0 0 0 6
-2.4728 0.0823 0.0002 C 0 0 0 0 0 0 0 0 0 0 7
3.2415 -0.0126 -0.0003 C 0 0 0 0 0 0 0 0 0 0 8
4.4086 -0.0224 -0.0004 N 0 0 0 0 0 0 0 0 0 0 9
-3.1199 1.1225 0.0023 O 0 0 0 0 0 0 0 0 0 0 10
-3.0487 -1.1426 -0.0029 O 0 0 0 0 0 0 0 0 0 0 11
1.6784 2.1677 -0.0024 H 0 0 0 0 0 0 0 0 0 0 12
-0.8127 2.1767 -0.0016 H 0 0 0 0 0 0 0 0 0 0 13
-0.8374 -2.1416 0.0026 H 0 0 0 0 0 0 0 0 0 0 14
1.6434 -2.1648 0.0028 H 0 0 0 0 0 0 0 0 0 0 15
-4.0224 -1.0180 -0.0035 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0

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6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
11 16 0 0 0 0
M END
$$$$
4-dimethylaminobenzoicacid-anion.sdf
COSMOtherm 3D 0

22 22 0 0 0 0 0 0 0 0 0 V2000
-0.7029 0.0066 1.2146 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.6897 0.0056 1.1998 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.4242 0.0002 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.6898 -0.0050 -1.1999 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.7028 -0.0049 -1.2148 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.4459 0.0010 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.9418 -0.0004 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.8221 0.0019 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 8
-3.5580 0.0040 -1.2595 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-3.5582 -0.0070 1.2596 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5306 -0.0057 1.1305 O 0 0 0 0 0 0 0 0 0 0 0 0 11
3.5308 0.0046 -1.1304 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.2221 0.0117 2.1727 H 0 0 0 0 0 0 0 0 0 0 0 0 13
1.2385 0.0096 2.1441 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.2385 -0.0097 -2.1442 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.2220 -0.0104 -2.1728 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-4.6309 0.0208 -1.0424 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-3.3185 0.8903 -1.8709 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.3440 -0.8954 -1.8618 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-4.6312 -0.0178 1.0424 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-3.3221 -0.8985 1.8650 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.3407 0.8873 1.8680 H 0 0 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
10 22 0 0 0 0
M END
$$$$
4-dimethylaminobenzoicacid.sdf
COSMOtherm 3D 0

23 23 0 0 0 0 0 0 0 0 0 V2000
-0.7321 0.0039 1.2288 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.6526 0.0039 1.2300 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.3926 0.0006 0.0275 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.6751 -0.0024 -1.1892 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.7105 -0.0026 -1.2099 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.4636 0.0006 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.8571 -0.0004 0.0853 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.8295 0.0002 -0.0103 N 0 0 0 0 0 0 0 0 0 0 0 0 8
-3.5584 0.0041 -1.2786 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-3.5832 -0.0058 1.2432 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5331 -0.0018 1.1181 O 0 0 0 0 0 0 0 0 0 0 0 0 11
3.4536 0.0006 -1.1472 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.2601 0.0075 2.1810 H 0 0 0 0 0 0 0 0 0 0 0 0 13
1.1887 0.0068 2.1807 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.2167 -0.0054 -2.1356 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.2215 -0.0061 -2.1712 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-4.6319 0.0172 -1.0677 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-3.3143 0.8936 -1.8812 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.3348 -0.8941 -1.8766 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-4.6523 -0.0203 1.0109 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-3.3501 -0.8955 1.8499 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.3730 0.8922 1.8462 H 0 0 0 0 0 0 0 0 0 0 0 0 22
4.4222 -0.0022 -0.9950 H 0 0 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0

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8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 23 0 0 0 0
M  END
$$$$
4-ethylbenzoicacid-anion.sdf
COSMOtherm 3D 0

20 20 0 0 0 0 0 0 0 0 0 V2000
1.0330 -1.2117 0.2584 C 0 0 0 0 0 0 0 0 0 0 1
-0.3574 -1.2078 0.1141 C 0 0 0 0 0 0 0 0 0 0 2
-1.0720 -0.0007 0.0430 C 0 0 0 0 0 0 0 0 0 0 3
-0.3513 1.2023 0.1238 C 0 0 0 0 0 0 0 0 0 0 4
1.0389 1.1982 0.2683 C 0 0 0 0 0 0 0 0 0 0 5
1.7580 -0.0089 0.3349 C 0 0 0 0 0 0 0 0 0 0 6
-2.5938 0.0037 -0.1151 C 0 0 0 0 0 0 0 0 0 0 7
3.2666 -0.0126 0.4483 C 0 0 0 0 0 0 0 0 0 0 8
3.9678 0.0214 -0.9239 C 0 0 0 0 0 0 0 0 0 0 9
-3.1739 -1.1254 -0.1806 O 0 0 0 0 0 0 0 0 0 0 10
-3.1683 1.1362 -0.1710 O 0 0 0 0 0 0 0 0 0 0 11
1.5679 -2.1639 0.3163 H 0 0 0 0 0 0 0 0 0 0 12
-0.9124 -2.1463 0.0595 H 0 0 0 0 0 0 0 0 0 0 13
-0.9018 2.1439 0.0770 H 0 0 0 0 0 0 0 0 0 0 14
1.5782 2.1475 0.3343 H 0 0 0 0 0 0 0 0 0 0 15
3.5896 -0.9114 0.9967 H 0 0 0 0 0 0 0 0 0 0 16
3.5907 0.8578 1.0402 H 0 0 0 0 0 0 0 0 0 0 17
5.0611 0.0194 -0.8025 H 0 0 0 0 0 0 0 0 0 0 18
3.6892 0.9245 -1.4872 H 0 0 0 0 0 0 0 0 0 0 19
3.6906 -0.8537 -1.5303 H 0 0 0 0 0 0 0 0 0 0 20

2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
9 20 0 0 0 0
M  END
$$$$
4-ethylbenzoicacid.sdf
COSMOtherm 3D 0

21 21 0 0 0 0 0 0 0 0 0 V2000
1.0620 -1.2238 0.2495 C 0 0 0 0 0 0 0 0 0 0 1
-0.3239 -1.2345 0.1056 C 0 0 0 0 0 0 0 0 0 0 2
-1.0398 -0.0255 0.0433 C 0 0 0 0 0 0 0 0 0 0 3
-0.3388 1.1918 0.1297 C 0 0 0 0 0 0 0 0 0 0 4
1.0480 1.1914 0.2743 C 0 0 0 0 0 0 0 0 0 0 5
1.7737 -0.0124 0.3346 C 0 0 0 0 0 0 0 0 0 0 6
-2.5153 -0.0788 -0.1066 C 0 0 0 0 0 0 0 0 0 0 7
3.2797 -0.0033 0.4499 C 0 0 0 0 0 0 0 0 0 0 8
3.9758 0.0511 -0.9252 C 0 0 0 0 0 0 0 0 0 0 9
-3.1758 -1.1120 -0.1790 O 0 0 0 0 0 0 0 0 0 0 10
-3.0939 1.1507 -0.1585 O 0 0 0 0 0 0 0 0 0 0 11
1.6045 -2.1706 0.3018 H 0 0 0 0 0 0 0 0 0 0 12
-0.8663 -2.1792 0.0451 H 0 0 0 0 0 0 0 0 0 0 13
-0.8809 2.1365 0.0895 H 0 0 0 0 0 0 0 0 0 0 14
1.5793 2.1433 0.3464 H 0 0 0 0 0 0 0 0 0 0 15
3.6099 -0.9049 0.9882 H 0 0 0 0 0 0 0 0 0 0 16
3.5939 0.8654 1.0487 H 0 0 0 0 0 0 0 0 0 0 17
5.0684 0.0593 -0.8025 H 0 0 0 0 0 0 0 0 0 0 18
3.6874 0.9570 -1.4786 H 0 0 0 0 0 0 0 0 0 0 19
3.7072 -0.8214 -1.5388 H 0 0 0 0 0 0 0 0 0 0 20
-4.0610 1.0172 -0.2561 H 0 0 0 0 0 0 0 0 0 0 21

2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0

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1
2
3 11 21 0 0 0 0
4 M END
5 $$$$
6 4-fluorobenzoicacid-anion.sdf
7 COSMOtherm 3D 0
8
9 14 14 0 0 0 0 0 0 0 0 0 V2000
10 1.3944 1.2219 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 1
11 -0.0039 1.2085 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 2
12 -0.7202 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
13 -0.0039 -1.2085 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 4
14 1.3944 -1.2219 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 5
15 2.0613 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
16 -2.2516 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
17 3.4334 0.0000 0.0002 F 0 0 0 0 0 0 0 0 0 0 0 8
18 -2.8287 1.1314 0.0012 O 0 0 0 0 0 0 0 0 0 0 0 9
19 -2.8287 -1.1314 -0.0009 O 0 0 0 0 0 0 0 0 0 0 0 10
20 1.9590 2.1553 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 11
21 -0.5603 2.1468 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 12
22 -0.5602 -2.1468 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
23 1.9590 -2.1553 0.0010 H 0 0 0 0 0 0 0 0 0 0 0 14
24 2 1 0 0 0 0
25 6 1 0 0 0 0
26 11 1 0 0 0 0
27 3 2 0 0 0 0
28 12 2 0 0 0 0
29 4 3 0 0 0 0
30 7 3 0 0 0 0
31 5 4 0 0 0 0
32 13 4 0 0 0 0
33 6 5 0 0 0 0
34 8 6 0 0 0 0
35 9 7 0 0 0 0
36 10 7 0 0 0 0
37 5 14 0 0 0 0
38 M END
39 $$$$
40 4-fluorobenzoicacid.sdf
41 COSMOtherm 3D 0
42
43 15 15 0 0 0 0 0 0 0 0 V2000
44 1.4251 1.2249 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
45 0.0317 1.2312 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 2
46 -0.6896 0.0234 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 3
47 0.0036 -1.2014 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
48 1.3980 -1.2235 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
49 2.0767 -0.0070 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
50 -2.1738 0.0868 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
51 3.4398 -0.0223 -0.0003 F 0 0 0 0 0 0 0 0 0 0 0 8
52 -2.8276 1.1256 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 9
53 -2.7597 -1.1383 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 10
54 2.0000 2.1509 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
55 -0.5089 2.1779 0.0007 H 0 0 0 0 0 0 0 0 0 0 0 12
56 -0.5467 -2.1414 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 13
57 1.9521 -2.1622 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 14
58 -3.7314 -1.0021 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 15
59 2 1 0 0 0 0
60 6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
10 15 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0
15 15 0 0 0 0 0 0 0 0 V2000
1.4351 1.2150 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0402 1.2041 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6844 -0.0011 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0384 -1.2058 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4350 -1.2161 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 5
2.1372 -0.0006 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.2104 -0.0005 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.7931 -1.1310 -0.0010 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.7918 1.1308 0.0009 O 0 0 0 0 0 0 0 0 0 0 0 9
3.5103 0.0580 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 10
3.8721 -0.8488 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 11
1.9918 2.1542 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5134 2.1447 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5147 -2.1466 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 14
1.9841 -2.1617 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
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11 10 0 0 0 0
5 15 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 V2000
1.4658 1.2181 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0771 1.2279 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6544 0.0232 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0455 -1.1992 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4369 -1.2199 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.1523 -0.0096 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.1307 0.0873 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.7239 -1.1389 -0.0015 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.7908 1.1251 0.0015 O 0 0 0 0 0 0 0 0 0 0 0 0 9
3.5152 0.0346 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-3.6940 -0.9936 -0.0020 H 0 0 0 0 0 0 0 0 0 0 0 0 11
3.8753 -0.8736 0.0015 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2.0342 2.1491 -0.0016 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.4604 2.1769 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.5028 -2.1409 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.9749 -2.1706 0.0012 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
11 8 0 0 0 0
12 10 0 0 0 0
5 16 0 0 0 0
M END
$$$$
4-hydroxymethylbenzoicacid-anion.sdf
COSMOtherm 3D 0
18 18 0 0 0 0 0 0 0 0 V2000
-0.9914 -0.2400 1.2259 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.3991 -0.0988 1.2146 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.1054 -0.0419 0.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.3830 -0.1319 -1.1995 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.0067 -0.2753 -1.1891 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.7128 -0.3308 0.0243 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.6304 0.1095 -0.0100 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-3.2142 -0.4489 0.0344 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-3.7822 0.8851 -0.0563 O 0 0 0 0 0 0 0 0 0 0 0 0 9
3.2141 0.1711 1.1164 O 0 0 0 0 0 0 0 0 0 0 0 0 10
3.1967 0.1631 -1.1458 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-4.7517 0.7800 -0.0592 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.5263 -0.2863 2.1783 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.9600 -0.0346 2.1486 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.9320 -0.0938 -2.1421 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.5533 -0.3507 -2.1329 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.5495 -0.9370 0.9651 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-3.5527 -1.0577 -0.8211 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
12 9 0 0 0 0
8 18 0 0 0 0
M END
$$$$
4-hydroxymethylbenzoicacid.sdf
COSMOtherm 3D 0
19 19 0 0 0 0 0 0 0 0 V2000
-1.0217 -0.2358 1.2347 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.3653 -0.0947 1.2394 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.0731 -0.0429 0.0261 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.3718 -0.1339 -1.1901 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.0156 -0.2771 -1.1847 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.7283 -0.3292 0.0243 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.5531 0.1014 0.0741 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-3.2308 -0.4494 0.0201 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-3.7893 0.8852 -0.0743 O 0 0 0 0 0 0 0 0 0 0 0 0 9
3.2139 0.1710 1.1058 O 0 0 0 0 0 0 0 0 0 0 0 0 10
3.1247 0.1500 -1.1567 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-4.7592 0.7853 -0.0874 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.5648 -0.2785 2.1812 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.9125 -0.0275 2.1805 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.9126 -0.0997 -2.1355 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.5536 -0.3537 -2.1320 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.5727 -0.9394 0.9468 H 0 0 0 0 0 0 0 0 0 0 0 0 17
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3 3.0964 -1.2966 -0.0057 O 0 0 0 0 0 0 0 0 0 0 11
4 -1.3871 2.3872 -0.0052 H 0 0 0 0 0 0 0 0 0 0 12
5 1.1065 2.1676 -0.0032 H 0 0 0 0 0 0 0 0 0 0 13
6 0.7394 -2.1067 0.0028 H 0 0 0 0 0 0 0 0 0 0 14
7 -1.7333 -1.9227 0.0024 H 0 0 0 0 0 0 0 0 0 0 15
8 -4.9633 -0.2733 0.0048 H 0 0 0 0 0 0 0 0 0 0 16
9 -3.7917 -1.2932 -0.8930 H 0 0 0 0 0 0 0 0 0 0 17
10 -3.7875 -1.2846 0.9071 H 0 0 0 0 0 0 0 0 0 0 18
11 2 1 0 0 0 0
12 6 1 0 0 0 0
13 12 1 0 0 0 0
14 3 2 0 0 0 0
15 13 2 0 0 0 0
16 4 3 0 0 0 0
17 7 3 0 0 0 0
18 5 4 0 0 0 0
19 14 4 0 0 0 0
20 6 5 0 0 0 0
21 15 5 0 0 0 0
22 8 6 0 0 0 0
23 10 7 0 0 0 0
24 11 7 0 0 0 0
25 9 8 0 0 0 0
26 16 9 0 0 0 0
27 17 9 0 0 0 0
28 9 18 0 0 0 0
29 M END
30 \$\$\$\$
31 4-methoxybenzoicacid.sdf
32 COSMOTHERM 3D 0
33 19 19 0 0 0 0 0 0 0 0 0 0 V2000
34 -0.9403 1.4156 -0.0022 C 0 0 0 0 0 0 0 0 0 0 1
35 0.4414 1.3055 -0.0020 C 0 0 0 0 0 0 0 0 0 0 2
36 1.0641 0.0394 -0.0006 C 0 0 0 0 0 0 0 0 0 0 3
37 0.2579 -1.1126 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
38 -1.1331 -1.0159 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
39 -1.7404 0.2534 -0.0013 C 0 0 0 0 0 0 0 0 0 0 6
40 2.5398 -0.0285 0.0008 C 0 0 0 0 0 0 0 0 0 0 7
41 -3.0855 0.4603 -0.0018 O 0 0 0 0 0 0 0 0 0 0 8
42 -3.9526 -0.6957 0.0042 C 0 0 0 0 0 0 0 0 0 0 9
43 3.2895 0.9467 0.0052 O 0 0 0 0 0 0 0 0 0 0 10
44 3.0216 -1.3026 -0.0033 O 0 0 0 0 0 0 0 0 0 0 11
45 -1.4261 2.3923 -0.0032 H 0 0 0 0 0 0 0 0 0 0 12
46 1.0598 2.2040 -0.0025 H 0 0 0 0 0 0 0 0 0 0 13
47 0.7204 -2.0993 0.0011 H 0 0 0 0 0 0 0 0 0 0 14
48 -1.7319 -1.9252 0.0004 H 0 0 0 0 0 0 0 0 0 0 15
49 -4.9706 -0.2943 0.0060 H 0 0 0 0 0 0 0 0 0 0 16
50 -3.7959 -1.3082 -0.8956 H 0 0 0 0 0 0 0 0 0 0 17
51 -3.7904 -1.3028 0.9066 H 0 0 0 0 0 0 0 0 0 0 18
52 4.0008 -1.2446 -0.0002 H 0 0 0 0 0 0 0 0 0 0 19
53 2 1 0 0 0 0
54 6 1 0 0 0 0
55 12 1 0 0 0 0
56 3 2 0 0 0 0
57 13 2 0 0 0 0
58 4 3 0 0 0 0
59 7 3 0 0 0 0
60 5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
16 9 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
11 19 0 0 0 0
M END
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4-methylaminobenzoicacid-anion.sdf
COSMOTHERM 3D 0
19 19 0 0 0 0 0 0 0 0 0 0 V2000
-0.9039 1.4182 -0.0037 C 0 0 0 0 0 0 0 0 0 0 1
0.4788 1.2800 -0.0025 C 0 0 0 0 0 0 0 0 0 0 2
1.0977 0.0129 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
0.2586 -1.1142 0.0024 C 0 0 0 0 0 0 0 0 0 0 4
-1.1323 -1.0020 0.0021 C 0 0 0 0 0 0 0 0 0 0 5
-1.7482 0.2752 -0.0011 C 0 0 0 0 0 0 0 0 0 0 6
2.6090 -0.1275 0.0004 C 0 0 0 0 0 0 0 0 0 0 7
-3.1113 0.4253 -0.0020 N 0 0 0 0 0 0 0 0 0 0 8
-4.0576 -0.6750 0.0030 C 0 0 0 0 0 0 0 0 0 0 9
3.2996 0.9439 0.0075 O 0 0 0 0 0 0 0 0 0 0 10
3.0913 -1.3073 -0.0068 O 0 0 0 0 0 0 0 0 0 0 11
-3.4821 1.3690 -0.0031 H 0 0 0 0 0 0 0 0 0 0 12
-1.3579 2.4129 -0.0061 H 0 0 0 0 0 0 0 0 0 0 13
1.1140 2.1682 -0.0041 H 0 0 0 0 0 0 0 0 0 0 14
0.7212 -2.1034 0.0043 H 0 0 0 0 0 0 0 0 0 0 15
-1.7461 -1.9037 0.0046 H 0 0 0 0 0 0 0 0 0 0 16
-5.0718 -0.2604 0.0023 H 0 0 0 0 0 0 0 0 0 0 17
-3.9476 -1.3174 -0.8874 H 0 0 0 0 0 0 0 0 0 0 18
-3.9460 -1.3107 0.8981 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0

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16 5 0 0 0 0
8 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
9 19 0 0 0 0
M END
$$$$
4-methylaminobenzoicacid.sdf
COSMOtherm 3D 0

20 20 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-0.9334 1.4307 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.4431 1.3104 -0.0015 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.0685 0.0409 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.2459 -1.1058 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.1383 -1.0018 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.7654 0.2739 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
2.5323 -0.0343 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-3.1193 0.4097 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-4.0629 -0.6965 0.0019 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
3.2983 0.9335 0.0035 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.0151 -1.3154 -0.0023 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-3.4979 1.3514 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.3984 2.4191 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
1.0655 2.2068 -0.0022 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
0.7021 -2.0961 0.0010 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.7439 -1.9078 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-5.0772 -0.2837 0.0043 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-3.9482 -1.3307 -0.8921 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.9439 -1.3308 0.8951 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
3.9935 -1.2516 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0 0
6 1 0 0 0 0 0
13 1 0 0 0 0 0
3 2 0 0 0 0 0
14 2 0 0 0 0 0
4 3 0 0 0 0 0
7 3 0 0 0 0 0
5 4 0 0 0 0 0
15 4 0 0 0 0 0
6 5 0 0 0 0 0
16 5 0 0 0 0 0
8 6 0 0 0 0 0
10 7 0 0 0 0 0
11 7 0 0 0 0 0
9 8 0 0 0 0 0
12 8 0 0 0 0 0
17 9 0 0 0 0 0
18 9 0 0 0 0 0
19 9 0 0 0 0 0
11 20 0 0 0 0 0
M END
$$$$
4-methylbenzoicacid-anion.sdf
COSMOtherm 3D 0

17 17 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
1.4618 1.2047 -0.0101 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0640 1.2046 -0.0045 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6582 0.0001 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0643 -1.2044 -0.0050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4619 -1.2045 -0.0105 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.1880 0.0003 -0.0095 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
3.6968 -0.0001 0.0185 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.1878 -0.0001 0.0033 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.7686 1.1306 0.0046 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.7683 -1.1310 0.0056 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
2.0019 2.1555 -0.0176 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.4903 2.1450 -0.0067 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.4899 -2.1449 -0.0076 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.0019 -2.1553 -0.0185 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
4.0700 -0.0358 1.0553 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
4.1075 0.9080 -0.4443 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
4.1082 -0.8750 -0.5043 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0 0
6 1 0 0 0 0 0
11 1 0 0 0 0 0
3 2 0 0 0 0 0
12 2 0 0 0 0 0
4 3 0 0 0 0 0
8 3 0 0 0 0 0
5 4 0 0 0 0 0
13 4 0 0 0 0 0
6 5 0 0 0 0 0
14 5 0 0 0 0 0
7 6 0 0 0 0 0
15 7 0 0 0 0 0
16 7 0 0 0 0 0
9 8 0 0 0 0 0
10 8 0 0 0 0 0
7 17 0 0 0 0 0
M END
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4-methylbenzoicacid.sdf
COSMOtherm 3D 0

18 18 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
1.4921 1.2082 -0.0093 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0990 1.2280 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6281 0.0242 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0707 -1.1972 -0.0047 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
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1.4648 -1.2064 -0.0103 C 0 0 0 0 0 0 0 0 0 0 0 5
2.2014 -0.0076 -0.0092 C 0 0 0 0 0 0 0 0 0 0 0 6
3.7072 -0.0262 0.0169 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.1104 0.0868 0.0029 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.7686 1.1239 0.0040 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.6992 -1.1391 0.0051 O 0 0 0 0 0 0 0 0 0 0 0 10
2.0430 2.1513 -0.0164 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4397 2.1767 -0.0056 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.4783 -2.1388 -0.0072 H 0 0 0 0 0 0 0 0 0 0 0 13
1.9940 -2.1619 -0.0182 H 0 0 0 0 0 0 0 0 0 0 0 14
4.0735 -0.0657 1.0559 H 0 0 0 0 0 0 0 0 0 0 0 15
4.1283 0.8773 -0.4442 H 0 0 0 0 0 0 0 0 0 0 0 16
4.1065 -0.9081 -0.5023 H 0 0 0 0 0 0 0 0 0 0 0 17
-3.6703 -0.9992 0.0065 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 18 0 0 0 0
M END
$$$$
4-nitrobenzoicacid-anion.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 v2000
0.6867 1.2239 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7066 1.2115 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.4190 -0.0001 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.7065 -1.2117 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 4
0.6867 -1.2241 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 5
1.3651 -0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.9566 0.0000 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
2.8380 -0.0001 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 8
3.4291 -1.0930 -0.0155 O 0 0 0 0 0 0 0 0 0 0 0 9
3.4287 1.0933 0.0153 O 0 0 0 0 0 0 0 0 0 0 0 10
-3.5248 1.1329 -0.0168 O 0 0 0 0 0 0 0 0 0 0 0 11
-3.5251 -1.1327 0.0165 O 0 0 0 0 0 0 0 0 0 0 0 12
1.2446 2.1591 0.0023 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2654 2.1477 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.2654 -2.1479 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 15
1.2447 -2.1594 -0.0022 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
5 16 0 0 0 0
M END
$$$$
4-nitrobenzoicacid.sdf
COSMOtherm 3D 0
17 17 0 0 0 0 0 0 0 0 v2000
0.7162 1.2326 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6758 1.2353 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.3872 0.0235 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.6954 -1.2005 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 4
0.6975 -1.2165 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 5
1.3790 0.0025 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.8815 0.0823 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 7
2.8610 -0.0097 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 8
3.4357 -1.1077 -0.0200 O 0 0 0 0 0 0 0 0 0 0 0 9
3.4539 1.0786 0.0193 O 0 0 0 0 0 0 0 0 0 0 0 10
-3.5276 1.1223 -0.0170 O 0 0 0 0 0 0 0 0 0 0 0 11
-3.4543 -1.1427 0.0165 O 0 0 0 0 0 0 0 0 0 0 0 12
1.2808 2.1632 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2211 2.1788 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.2439 -2.1410 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 15
1.2479 -2.1556 0.0012 H 0 0 0 0 0 0 0 0 0 0 0 16
-4.4286 -1.0222 0.0114 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
8 6 0 0 0 0

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1
2
3 11 7 0 0 0 0
4 12 7 0 0 0 0
5 9 8 0 0 0 0
6 10 8 0 0 0 0
7 12 17 0 0 0 0
8 M END
9 $$$$
10 4-phenylbenzoicacid-anion.sdf
11 COSMOTHERM 3D 0
12
13 24 25 0 0 0 0 0 0 0 0 0 V2000
14 -0.2565 1.1704 -0.2985 C 0 0 0 0 0 0 0 0 0 0 0 1
15 -1.6523 1.1671 -0.2990 C 0 0 0 0 0 0 0 0 0 0 0 2
16 -2.3740 -0.0001 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 3
17 -1.6522 -1.1675 0.2976 C 0 0 0 0 0 0 0 0 0 0 0 4
18 -0.2563 -1.1707 0.2964 C 0 0 0 0 0 0 0 0 0 0 0 5
19 0.4715 -0.0001 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 6
20 1.9563 0.0001 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 7
21 -3.9047 0.0001 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 8
22 4.0796 -1.1204 -0.4532 C 0 0 0 0 0 0 0 0 0 0 0 9
23 2.6818 -1.1210 -0.4535 C 0 0 0 0 0 0 0 0 0 0 0 10
24 2.6810 1.1214 0.4522 C 0 0 0 0 0 0 0 0 0 0 0 11
25 4.0788 1.1206 0.4551 C 0 0 0 0 0 0 0 0 0 0 0 12
26 4.7854 0.0000 0.0018 C 0 0 0 0 0 0 0 0 0 0 0 13
27 -4.4831 1.0967 -0.2762 O 0 0 0 0 0 0 0 0 0 0 0 14
28 -4.4831 -1.0967 0.2785 O 0 0 0 0 0 0 0 0 0 0 0 15
29 0.2781 2.0875 -0.5549 H 0 0 0 0 0 0 0 0 0 0 0 16
30 -2.2066 2.0760 -0.5397 H 0 0 0 0 0 0 0 0 0 0 0 17
31 -2.2062 -2.0764 0.5385 H 0 0 0 0 0 0 0 0 0 0 0 18
32 0.2784 -2.0878 0.5525 H 0 0 0 0 0 0 0 0 0 0 0 19
33 4.6198 -1.9968 -0.8166 H 0 0 0 0 0 0 0 0 0 0 0 20
34 2.1459 -1.9944 -0.8300 H 0 0 0 0 0 0 0 0 0 0 0 21
35 2.1444 1.9946 0.8281 H 0 0 0 0 0 0 0 0 0 0 0 22
36 4.6183 1.9969 0.8199 H 0 0 0 0 0 0 0 0 0 0 0 23
37 5.8768 -0.0001 0.0032 H 0 0 0 0 0 0 0 0 0 0 0 24
38
39 2 1 0 0 0 0 0
40 6 1 0 0 0 0 0
41 16 1 0 0 0 0 0
42 3 2 0 0 0 0 0
43 17 2 0 0 0 0 0
44 4 3 0 0 0 0 0
45 8 3 0 0 0 0 0
46 5 4 0 0 0 0 0
47 18 4 0 0 0 0 0
48 6 5 0 0 0 0 0
49 19 5 0 0 0 0 0
50 7 6 0 0 0 0 0
51 10 7 0 0 0 0 0
52 11 7 0 0 0 0 0
53 14 8 0 0 0 0 0
54 15 8 0 0 0 0 0
55 10 9 0 0 0 0 0
56 13 9 0 0 0 0 0
57 20 9 0 0 0 0 0
58 21 10 0 0 0 0 0
59 12 11 0 0 0 0 0
60 22 11 0 0 0 0 0
13 12 0 0 0 0 0
23 12 0 0 0 0 0
13 24 0 0 0 0 0
M END
$$$$
4-phenylbenzoicacid.sdf
COSMOTHERM 3D 0
25 26 0 0 0 0 0 0 0 0 0 V2000
-0.2278 1.1884 -0.2988 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.6195 1.1954 -0.3017 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.3382 0.0242 -0.0035 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.6318 -1.1546 0.2980 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2390 -1.1573 0.2976 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4915 0.0117 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 6
1.9745 0.0026 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 7
-3.8223 0.0750 -0.0204 C 0 0 0 0 0 0 0 0 0 0 0 8
4.0860 -1.1273 -0.4702 C 0 0 0 0 0 0 0 0 0 0 0 9
2.6887 -1.1190 -0.4685 C 0 0 0 0 0 0 0 0 0 0 0 10
2.7041 1.1139 0.4677 C 0 0 0 0 0 0 0 0 0 0 0 11
4.1015 1.1016 0.4715 C 0 0 0 0 0 0 0 0 0 0 0 12
4.7985 -0.0180 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 13
-4.4844 1.0730 -0.2895 O 0 0 0 0 0 0 0 0 0 0 0 14
-4.4013 -1.1140 0.2944 O 0 0 0 0 0 0 0 0 0 0 0 15
0.3112 2.1022 -0.5537 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.1643 2.1086 -0.5444 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.1739 -2.0681 0.5411 H 0 0 0 0 0 0 0 0 0 0 0 18
0.2913 -2.0756 0.5541 H 0 0 0 0 0 0 0 0 0 0 0 19
4.6202 -2.0011 -0.8478 H 0 0 0 0 0 0 0 0 0 0 0 20
2.1459 -1.9827 -0.8567 H 0 0 0 0 0 0 0 0 0 0 0 21
2.1736 1.9855 0.8554 H 0 0 0 0 0 0 0 0 0 0 0 22
4.6480 1.9674 0.8500 H 0 0 0 0 0 0 0 0 0 0 0 23
5.8899 -0.0261 0.0024 H 0 0 0 0 0 0 0 0 0 0 0 24
-5.3738 -0.9881 0.2578 H 0 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0 0
6 1 0 0 0 0 0
16 1 0 0 0 0 0
3 2 0 0 0 0 0
17 2 0 0 0 0 0
4 3 0 0 0 0 0
8 3 0 0 0 0 0
5 4 0 0 0 0 0
18 4 0 0 0 0 0
6 5 0 0 0 0 0
19 5 0 0 0 0 0
7 6 0 0 0 0 0
10 7 0 0 0 0 0
11 7 0 0 0 0 0

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1
2
3 14 8 0 0 0 0
4 15 8 0 0 0 0
5 10 9 0 0 0 0
6 13 9 0 0 0 0
7 20 9 0 0 0 0
8 21 10 0 0 0 0
9 12 11 0 0 0 0
10 22 11 0 0 0 0
11 13 12 0 0 0 0
12 23 12 0 0 0 0
13 24 13 0 0 0 0
14 15 25 0 0 0 0
15 M END
16 $$$$
17 4-propylbenzoicacid-anion.sdf
18 COSMOTHERM 3D 0
19
20 23 23 0 0 0 0 0 0 0 0 0 V2000
21 -0.5333 -0.3469 1.2153 C 0 0 0 0 0 0 0 0 0 0 0 1
22 0.8491 -0.1397 1.2089 C 0 0 0 0 0 0 0 0 0 0 0 2
23 1.5582 -0.0403 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 3
24 0.8403 -0.1572 -1.2013 C 0 0 0 0 0 0 0 0 0 0 0 4
25 -0.5419 -0.3649 -1.1947 C 0 0 0 0 0 0 0 0 0 0 0 5
26 -1.2558 -0.4606 0.0138 C 0 0 0 0 0 0 0 0 0 0 0 6
27 3.0713 0.1862 -0.0064 C 0 0 0 0 0 0 0 0 0 0 0 7
28 -2.7565 -0.6415 0.0202 C 0 0 0 0 0 0 0 0 0 0 0 8
29 -3.5264 0.6968 -0.0205 C 0 0 0 0 0 0 0 0 0 0 0 9
30 -5.0463 0.5036 -0.0115 C 0 0 0 0 0 0 0 0 0 0 0 10
31 3.6499 0.2768 1.1217 O 0 0 0 0 0 0 0 0 0 0 0 11
32 3.6406 0.2690 -1.1399 O 0 0 0 0 0 0 0 0 0 0 0 12
33 -1.0639 -0.4263 2.1684 H 0 0 0 0 0 0 0 0 0 0 0 13
34 1.4022 -0.0569 2.1464 H 0 0 0 0 0 0 0 0 0 0 0 14
35 1.3867 -0.0879 -2.1438 H 0 0 0 0 0 0 0 0 0 0 0 15
36 -1.0789 -0.4589 -2.1428 H 0 0 0 0 0 0 0 0 0 0 0 16
37 -3.0574 -1.1972 0.9236 H 0 0 0 0 0 0 0 0 0 0 0 17
38 -3.0590 -1.2510 -0.8472 H 0 0 0 0 0 0 0 0 0 0 0 18
39 -3.2257 1.2562 -0.9219 H 0 0 0 0 0 0 0 0 0 0 0 19
40 -3.2222 1.3114 0.8428 H 0 0 0 0 0 0 0 0 0 0 0 20
41 -5.5715 1.4696 -0.0411 H 0 0 0 0 0 0 0 0 0 0 0 21
42 -5.3732 -0.0287 0.8953 H 0 0 0 0 0 0 0 0 0 0 0 22
43 -5.3763 -0.0852 -0.8816 H 0 0 0 0 0 0 0 0 0 0 0 23
44
45 2 1 0 0 0 0
46 6 1 0 0 0 0
47 13 1 0 0 0 0
48 3 2 0 0 0 0
49 14 2 0 0 0 0
50 4 3 0 0 0 0
51 7 3 0 0 0 0
52 5 4 0 0 0 0
53 15 4 0 0 0 0
54 6 5 0 0 0 0
55 16 5 0 0 0 0
56 8 6 0 0 0 0
57 11 7 0 0 0 0
58 12 7 0 0 0 0
59 9 8 0 0 0 0
60 17 8 0 0 0 0
18 8 0 0 0 0
19 10 9 0 0 0 0
20 19 9 0 0 0 0
21 20 9 0 0 0 0
22 21 10 0 0 0 0
23 22 10 0 0 0 0
24 10 23 0 0 0 0
25 M END
26 $$$$
27 4-propylbenzoicacid.sdf
28 COSMOTHERM 3D 0
29
30 24 24 0 0 0 0 0 0 0 0 0 V2000
31 -0.5616 -0.3352 1.2343 C 0 0 0 0 0 0 0 0 0 0 0 1
32 0.8165 -0.1288 1.2377 C 0 0 0 0 0 0 0 0 0 0 0 2
33 1.5237 -0.0422 0.0250 C 0 0 0 0 0 0 0 0 0 0 0 3
34 0.8222 -0.1684 -1.1885 C 0 0 0 0 0 0 0 0 0 0 0 4
35 -0.5566 -0.3759 -1.1810 C 0 0 0 0 0 0 0 0 0 0 0 5
36 -1.2739 -0.4613 0.0267 C 0 0 0 0 0 0 0 0 0 0 0 6
37 2.9912 0.1743 0.0709 C 0 0 0 0 0 0 0 0 0 0 0 7
38 -2.7719 -0.6435 0.0250 C 0 0 0 0 0 0 0 0 0 0 0 8
39 -3.5364 0.6985 -0.0369 C 0 0 0 0 0 0 0 0 0 0 0 9
40 -5.0561 0.5066 -0.0412 C 0 0 0 0 0 0 0 0 0 0 0 10
41 3.6528 0.2779 1.1008 O 0 0 0 0 0 0 0 0 0 0 0 11
42 3.5608 0.2512 -1.1615 O 0 0 0 0 0 0 0 0 0 0 0 12
43 -1.0972 -0.4056 2.1838 H 0 0 0 0 0 0 0 0 0 0 0 13
44 1.3595 -0.0370 2.1794 H 0 0 0 0 0 0 0 0 0 0 0 14
45 1.3578 -0.1099 -2.1360 H 0 0 0 0 0 0 0 0 0 0 0 15
46 -1.0882 -0.4790 -2.1298 H 0 0 0 0 0 0 0 0 0 0 0 16
47 -3.0781 -1.1872 0.9331 H 0 0 0 0 0 0 0 0 0 0 0 17
48 -3.0668 -1.2609 -0.8387 H 0 0 0 0 0 0 0 0 0 0 0 18
49 -3.2255 1.2472 -0.9411 H 0 0 0 0 0 0 0 0 0 0 0 19
50 -3.2393 1.3204 0.8233 H 0 0 0 0 0 0 0 0 0 0 0 20
51 -5.5778 1.4738 -0.0853 H 0 0 0 0 0 0 0 0 0 0 0 21
52 -5.3929 -0.0159 0.8676 H 0 0 0 0 0 0 0 0 0 0 0 22
53 -5.3781 -0.0897 -0.9090 H 0 0 0 0 0 0 0 0 0 0 0 23
54 4.5233 0.3919 -1.0331 H 0 0 0 0 0 0 0 0 0 0 0 24
55
56 2 1 0 0 0 0
57 6 1 0 0 0 0
58 13 1 0 0 0 0
59 3 2 0 0 0 0
60 14 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0

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8 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
23 10 0 0 0 0
12 24 0 0 0 0

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M END
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4-sulfamoylbenzoicacid-anion.sdf
COSMOtherm 3D 0

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19 19 0 0 0 0 0 0 0 0 0 V2000
-0.0481 -0.0551 1.2165 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
1.3476 -0.0233 1.2076 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
2.0623 0.0002 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.3532 -0.0029 -1.2129 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0433 -0.0307 -1.2289 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.7253 -0.0552 -0.0080 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
3.5989 0.0249 0.0035 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.5391 -0.0849 -0.0073 S 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.9886 -0.7789 1.2362 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.9977 -0.5703 -1.3423 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-3.1272 1.5023 0.1238 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
4.1654 0.0557 1.1374 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
4.1733 0.0117 -1.1270 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.8241 1.9378 1.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.8282 2.0721 -0.6747 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.5986 -0.0876 2.1575 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.9036 -0.0251 2.1459 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
1.9135 0.0087 -2.1486 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.5916 -0.0411 -2.1714 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19

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2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
5 19 0 0 0 0

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M END
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4-sulfamoylbenzoicacid.sdf
COSMOtherm 3D 0

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20 20 0 0 0 0 0 0 0 0 0 V2000
-0.0765 -0.0461 1.2276 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
1.3166 -0.0166 1.2336 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
2.0303 0.0073 0.0234 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.3407 0.0074 -1.2007 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0546 -0.0163 -1.2189 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.7415 -0.0423 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
3.5225 0.0229 0.0850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.5619 -0.0865 -0.0186 S 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-3.0022 -0.8491 1.1851 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.9957 -0.5079 -1.3814 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-3.1552 1.4840 0.1899 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
4.1691 0.0531 1.1250 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
4.0998 -0.0035 -1.1393 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.8745 1.8760 1.0945 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.8638 2.1000 -0.5761 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.6319 -0.0809 2.1651 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.8601 -0.0215 2.1785 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
1.8903 0.0210 -2.1408 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.5966 -0.0235 -2.1643 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
5.0733 0.0090 -1.0139 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20

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2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
13 20 0 0 0 0

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M END
$$$$

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1
2
3 4-trifluoromethylbenzoic acid-anion.sdf
4 COSMOtherm 3D 0
5 17 17 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
6 0.2651 1.2178 -0.0294 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
7 -1.1306 1.2087 -0.0163 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
8 -1.8443 0.0002 -0.0123 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
9 -1.1288 -1.2076 -0.0292 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
10 0.2667 -1.2144 -0.0443 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
11 0.9647 0.0024 -0.0470 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
12 -3.3801 -0.0007 0.0105 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
13 2.4672 0.0010 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
14 2.9450 -0.0595 1.2888 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
15 3.0147 1.1232 -0.5539 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
16 3.0157 -1.0668 -0.6547 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
17 -3.9530 1.1310 0.0062 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
18 -3.9513 -1.1331 0.0336 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
19 0.8061 2.1649 -0.0321 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
20 -1.6881 2.1462 -0.0074 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
21 -1.6851 -2.1458 -0.0292 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
22 0.8089 -2.1609 -0.0588 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0 0
3 1 0 0 0 0 0
4 1 0 0 0 0 0
5 2 0 0 0 0 0
6 3 0 0 0 0 0
7 3 0 0 0 0 0
8 4 0 0 0 0 0
9 4 0 0 0 0 0
10 5 0 0 0 0 0
11 6 0 0 0 0 0
12 6 0 0 0 0 0
13 7 0 0 0 0 0
14 7 0 0 0 0 0
15 8 0 0 0 0 0
16 8 0 0 0 0 0
17 8 0 0 0 0 0
18 5 17 0 0 0 0

M END
26 \$\$\$\$
27 4-trifluoromethylbenzoic acid.sdf
28 COSMOtherm 3D 0
29 18 18 0 0 0 0 0 0 0 0 0 V2000
30 0.2943 1.2296 -0.0284 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
31 -1.0989 1.2345 -0.0147 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
32 -1.8109 0.0244 -0.0116 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
33 -1.1147 -1.1960 -0.0271 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
34 0.2793 -1.2053 -0.0420 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
35 0.9810 0.0077 -0.0434 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
36 -3.3026 0.0808 0.0076 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
37 2.4885 -0.0054 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
38 2.9576 -0.0682 1.2879 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
39 3.0375 1.1115 -0.5564 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
40 3.0206 -1.0775 -0.6551 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
41 -3.9541 1.1187 0.0063 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
42 -3.8768 -1.1453 0.0288 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
43 0.8411 2.1724 -0.0315 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
44 -1.6441 2.1784 -0.0052 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
45 -1.6604 -2.1385 -0.0288 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
46 0.8144 -2.1548 -0.0561 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
47 -4.8504 -1.0215 0.0396 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
4 1 0 0 0 0 0
5 2 0 0 0 0 0
6 3 2 0 0 0 0
7 3 0 0 0 0 0
8 4 0 0 0 0 0
9 4 0 0 0 0 0
10 5 0 0 0 0 0
11 6 5 0 0 0 0
12 7 5 0 0 0 0
13 8 6 0 0 0 0
14 12 7 0 0 0 0
15 13 7 0 0 0 0
16 9 8 0 0 0 0
17 10 8 0 0 0 0
18 11 8 0 0 0 0
19 13 18 0 0 0 0

M END
51 \$\$\$\$
52 5-fluorouracil0-anion.sdf
53 COSMOtherm 3D 0
54 11 11 0 0 0 0 0 0 0 0 0 V2000
55 -1.4982 0.0296 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
56 -0.6920 1.0886 0.0007 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
57 0.6744 0.8749 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
58 1.0716 -0.5146 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
59 0.1502 -1.5256 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
60 -1.1916 -1.2750 0.0004 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.4969 1.8325 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.8349 0.3365 -0.0009 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4153 -0.8074 -0.0005 F 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.4649 -2.5726 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-3.3179 -0.5147 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0 0
3 1 0 0 0 0 0
4 1 0 0 0 0 0
5 2 0 0 0 0 0
6 3 2 0 0 0 0
7 3 0 0 0 0 0
8 4 3 0 0 0 0
9 7 3 0 0 0 0
10 5 4 0 0 0 0
11 9 4 0 0 0 0

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6 5 0 0 0 0
10 5 0 0 0 0
8 11 0 0 0 0
M END
$$$$
5-fluorouracil0.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 V2000
-1.6641 0.0462 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.6838 1.0337 -0.0002 N 0 0 0 0 0 0 0 0 0 0 2
0.7109 0.8728 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.1050 -0.5246 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.1938 -1.5277 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-1.1483 -1.2402 -0.0001 N 0 0 0 0 0 0 0 0 0 0 6
1.4769 1.8416 0.0001 O 0 0 0 0 0 0 0 0 0 0 7
-2.8710 0.2920 0.0001 O 0 0 0 0 0 0 0 0 0 0 8
2.4325 -0.7908 0.0000 F 0 0 0 0 0 0 0 0 0 0 9
-1.0263 1.9962 -0.0002 H 0 0 0 0 0 0 0 0 0 0 10
-1.8239 -2.0023 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
0.4707 -2.5802 0.0002 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 6 0 0 0 0
5 12 0 0 0 0
M END
$$$$
5-fluorouracil1-anion.sdf
COSMOTHERM 3D 0
11 11 0 0 0 0 0 0 0 0 V2000
-0.1043 -1.6198 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1096 -0.7060 0.0001 N 0 0 0 0 0 0 0 0 0 0 2
-0.8816 0.6455 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.5132 1.0782 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
1.5313 0.1853 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.2246 -1.1505 -0.0004 N 0 0 0 0 0 0 0 0 0 0 6
-1.8244 1.4831 -0.0002 O 0 0 0 0 0 0 0 0 0 0 7
-0.2884 -2.8635 0.0003 O 0 0 0 0 0 0 0 0 0 0 8
0.7835 2.4215 0.0002 F 0 0 0 0 0 0 0 0 0 0 9
1.9714 -1.8421 -0.0004 H 0 0 0 0 0 0 0 0 0 0 10
2.5842 0.4632 0.0000 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 6 0 0 0 0
5 11 0 0 0 0
M END
$$$$
5-fluorouracil1.sdf
COSMOTHERM 3D 0
12 12 0 0 0 0 0 0 0 0 V2000
-0.1142 -1.6391 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-1.1024 -0.6803 0.0003 N 0 0 0 0 0 0 0 0 0 0 2
-0.7927 0.5992 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
0.5550 1.0585 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
1.5576 0.1364 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.2186 -1.1785 0.0004 N 0 0 0 0 0 0 0 0 0 0 6
-1.8191 1.4678 0.0000 O 0 0 0 0 0 0 0 0 0 0 7
-0.3420 -2.8580 -0.0005 O 0 0 0 0 0 0 0 0 0 0 8
0.8082 2.3956 -0.0002 F 0 0 0 0 0 0 0 0 0 0 9
1.9543 -1.8850 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10
2.6152 0.3938 -0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-1.4829 2.3885 -0.0011 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
10 6 0 0 0 0
7 12 0 0 0 0
M END
$$$$
5-fluorouracil2-anion.sdf
COSMOTHERM 3D 0
11 11 0 0 0 0 0 0 0 0 V2000
-1.6487 -0.0175 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.6826 1.0118 -0.0004 N 0 0 0 0 0 0 0 0 0 0 2
0.7089 0.8650 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.0793 -0.5178 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
0.1329 -1.5144 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-1.2065 -1.3076 0.0001 N 0 0 0 0 0 0 0 0 0 0 6
1.4743 1.8547 0.0002 O 0 0 0 0 0 0 0 0 0 0 7
-2.8626 0.3027 0.0001 O 0 0 0 0 0 0 0 0 0 0 8

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2
3      2.4199  -0.8186  0.0000 F  0  0  0  0  0  0  0  0  0  0  9
4     -1.0351  1.9705  0.0001 H  0  0  0  0  0  0  0  0  0  0 10
5      0.4662  -2.5577  0.0001 H  0  0  0  0  0  0  0  0  0  0 11
6
7      2  1  0  0  0  0
8      6  1  0  0  0  0
9      8  1  0  0  0  0
10     3  2  0  0  0  0
11     10  2  0  0  0  0
12     4  3  0  0  0  0
13     7  3  0  0  0  0
14     5  4  0  0  0  0
15     9  4  0  0  0  0
16     6  5  0  0  0  0
17     5  11 0  0  0  0
18 M  END
19 $$$$
20 5-fluorouracil2.sdf
21 COSMOTHERM 3D 0
22
23 12 12 0 0 0 0 0 0 0 0 0 V2000
24 -0.0324  1.5451 -0.0001 C  0  0  0  0  0  0  0  0  0  0  0  1
25  1.0154  0.6759 -0.0001 N  0  0  0  0  0  0  0  0  0  0  0  2
26  0.8684 -0.7261  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  3
27 -0.5271 -1.1002 -0.0001 C  0  0  0  0  0  0  0  0  0  0  0  4
28 -1.5286 -0.1716  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  5
29 -1.2920  1.1788  0.0001 N  0  0  0  0  0  0  0  0  0  0  0  6
30  1.8481 -1.4808  0.0002 O  0  0  0  0  0  0  0  0  0  0  0  7
31  0.3292  2.8338 -0.0001 O  0  0  0  0  0  0  0  0  0  0  0  8
32 -0.8008 -2.4293 -0.0001 F  0  0  0  0  0  0  0  0  0  0  0  9
33  1.9704  1.0426 -0.0003 H  0  0  0  0  0  0  0  0  0  0  0 10
34 -2.5740 -0.4864  0.0002 H  0  0  0  0  0  0  0  0  0  0  0 11
35 -0.4860  3.3784  0.0015 H  0  0  0  0  0  0  0  0  0  0  0 12
36
37  2  1  0  0  0  0
38  6  1  0  0  0  0
39  8  1  0  0  0  0
40  3  2  0  0  0  0
41  10  2  0  0  0  0
42  4  3  0  0  0  0
43  7  3  0  0  0  0
44  5  4  0  0  0  0
45  9  4  0  0  0  0
46  6  5  0  0  0  0
47  11  5  0  0  0  0
48  8  12 0  0  0  0
49 M  END
50 $$$$
51 5-fluorouracil3-anion.sdf
52 COSMOTHERM 3D 0
53
54 11 11 0 0 0 0 0 0 0 0 0 V2000
55 -1.6263  0.0552  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  1
56 -0.6875  1.0861  0.0000 N  0  0  0  0  0  0  0  0  0  0  0  2
57  0.5976  0.7819  0.0001 C  0  0  0  0  0  0  0  0  0  0  0  3
58  1.0358 -0.5504 -0.0004 C  0  0  0  0  0  0  0  0  0  0  0  4
59  0.0759 -1.5455  0.0004 C  0  0  0  0  0  0  0  0  0  0  0  5
60 -1.2385 -1.2813  0.0005 N  0  0  0  0  0  0  0  0  0  0  0  6
61  1.4715  1.8299  0.0004 O  0  0  0  0  0  0  0  0  0  0  0  7
62 -2.8569  0.3468 -0.0005 O  0  0  0  0  0  0  0  0  0  0  0  8
63  2.3871 -0.8343 -0.0004 F  0  0  0  0  0  0  0  0  0  0  0  9
64  0.3842 -2.5967  0.0005 H  0  0  0  0  0  0  0  0  0  0  0 10
65  2.3872  1.4846  0.0002 H  0  0  0  0  0  0  0  0  0  0  0 11
66
67  2  1  0  0  0  0
68  6  1  0  0  0  0
69  8  1  0  0  0  0
70  3  2  0  0  0  0
71  4  3  0  0  0  0
72  7  3  0  0  0  0
73  5  4  0  0  0  0
74  9  4  0  0  0  0
75  6  5  0  0  0  0
76  10  5  0  0  0  0
77  7  11 0  0  0  0
78 M  END
79 $$$$
80 5-fluorouracil3.sdf
81 COSMOTHERM 3D 0
82
83 12 12 0 0 0 0 0 0 0 0 0 V2000
84 -1.5186  0.0377 -0.0002 C  0  0  0  0  0  0  0  0  0  0  0  1
85 -0.6733  1.0780  0.0003 N  0  0  0  0  0  0  0  0  0  0  0  2
86  0.6248  0.7852  0.0001 C  0  0  0  0  0  0  0  0  0  0  0  3
87  1.0560 -0.5544 -0.0005 C  0  0  0  0  0  0  0  0  0  0  0  4
88  0.1054 -1.5537  0.0007 C  0  0  0  0  0  0  0  0  0  0  0  5
89 -1.2136 -1.2670  0.0010 N  0  0  0  0  0  0  0  0  0  0  0  6
90  1.4718  1.8298  0.0007 O  0  0  0  0  0  0  0  0  0  0  0  7
91 -2.8251  0.3802 -0.0010 O  0  0  0  0  0  0  0  0  0  0  0  8
92  2.3910 -0.8275 -0.0009 F  0  0  0  0  0  0  0  0  0  0  0  9
93  0.3991 -2.6055  0.0015 H  0  0  0  0  0  0  0  0  0  0  0 10
94 -3.3491 -0.4472  0.0005 H  0  0  0  0  0  0  0  0  0  0  0 11
95  2.3979  1.5109 -0.0002 H  0  0  0  0  0  0  0  0  0  0  0 12
96
97  2  1  0  0  0  0
98  6  1  0  0  0  0
99  8  1  0  0  0  0
100  3  2  0  0  0  0
101  4  3  0  0  0  0
102  7  3  0  0  0  0
103  5  4  0  0  0  0
104  9  4  0  0  0  0
105  6  5  0  0  0  0
106  10  5  0  0  0  0
107  11  8  0  0  0  0
108  7  12 0  0  0  0
109 M  END
110 $$$$
111 5-iodo-2-hydroxybenzoicacid-anion0.sdf

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1
2
3 COSMOTHERM 3D 0
4
5 15 15 0 0 0 0 0 0 0 0 0 V2000
6 0.4178 -0.2671 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
7 -0.5551 0.7270 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
8 -0.1783 2.0796 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
9 1.2039 2.4188 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 4
10 2.1699 1.3934 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 5
11 1.7822 0.0544 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 6
12 -1.2325 3.1659 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
13 -0.7777 4.3836 -0.0024 O 0 0 0 0 0 0 0 0 0 0 0 8
14 -2.4487 2.8627 0.0021 O 0 0 0 0 0 0 0 0 0 0 0 9
15 1.5952 3.7097 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 10
16 -0.1741 -2.3321 -0.0001 I 0 0 0 0 0 0 0 0 0 0 0 11
17 0.6631 4.2231 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 12
18 -1.6199 0.4927 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 13
19 3.2288 1.6585 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 14
20 2.5428 -0.7267 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 15
21
22 2 1 0 0 0 0
23 6 1 0 0 0 0
24 3 2 0 0 0 0
25 13 2 0 0 0 0
26 4 3 0 0 0 0
27 7 3 0 0 0 0
28 5 4 0 0 0 0
29 10 4 0 0 0 0
30 6 5 0 0 0 0
31 14 5 0 0 0 0
32 8 7 0 0 0 0
33 9 7 0 0 0 0
34 12 8 0 0 0 0
35 12 10 0 0 0 0
36 6 15 0 0 0 0
37 M END
38 $$$$
39 5-iodo-2-hydroxybenzoicacid-anion1.sdf
40 COSMOTHERM 3D 0
41
42 15 14 0 0 0 0 0 0 0 0 V2000
43 0.4311 -0.2631 0.0224 C 0 0 0 0 0 0 0 0 0 0 0 1
44 -0.5317 0.7469 0.0161 C 0 0 0 0 0 0 0 0 0 0 0 2
45 -0.1466 2.0967 0.0225 C 0 0 0 0 0 0 0 0 0 0 0 3
46 1.2295 2.4040 0.0722 C 0 0 0 0 0 0 0 0 0 0 0 4
47 2.1849 1.3777 0.1086 C 0 0 0 0 0 0 0 0 0 0 0 5
48 1.7937 0.0357 0.0737 C 0 0 0 0 0 0 0 0 0 0 0 6
49 -1.2286 3.1793 -0.0332 C 0 0 0 0 0 0 0 0 0 0 0 7
50 -1.1748 3.9842 -1.0077 O 0 0 0 0 0 0 0 0 0 0 0 8
51 -2.1000 3.1536 0.8863 O 0 0 0 0 0 0 0 0 0 0 0 9
52 1.5980 3.7257 0.1121 O 0 0 0 0 0 0 0 0 0 0 0 10
53 -0.1956 -2.3171 -0.0292 I 0 0 0 0 0 0 0 0 0 0 0 11
54 2.5686 3.7800 0.2028 H 0 0 0 0 0 0 0 0 0 0 0 12
55 -1.5952 0.5066 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 13
56 3.2479 1.6276 0.1610 H 0 0 0 0 0 0 0 0 0 0 0 14
57 2.5495 -0.7490 0.0903 H 0 0 0 0 0 0 0 0 0 0 0 15
58
59 2 1 0 0 0 0
60 6 1 0 0 0 0
61 3 2 0 0 0 0
62 13 2 0 0 0 0
63 4 3 0 0 0 0
64 7 3 0 0 0 0
65 5 4 0 0 0 0
66 10 4 0 0 0 0
67 6 5 0 0 0 0
68 14 5 0 0 0 0
69 8 7 0 0 0 0
70 9 7 0 0 0 0
71 12 10 0 0 0 0
72 6 15 0 0 0 0
73 M END
74 $$$$
75 5-iodo-2-hydroxybenzoicacid0.sdf
76 COSMOTHERM 3D 0
77
78 16 15 0 0 0 0 0 0 0 0 V2000
79 0.4212 -0.2788 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
80 -0.5442 0.7160 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
81 -0.1521 2.0725 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
82 1.2314 2.4058 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
83 2.1869 1.3743 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 5
84 1.7891 0.0422 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 6
85 -1.1416 3.1581 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
86 -2.4248 2.7577 0.0012 O 0 0 0 0 0 0 0 0 0 0 0 8
87 -0.8303 4.3623 -0.0011 O 0 0 0 0 0 0 0 0 0 0 0 9
88 1.6670 3.6837 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 10
89 -0.1747 -2.3332 -0.0001 I 0 0 0 0 0 0 0 0 0 0 0 11
90 -2.9960 3.5562 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
91 0.8426 4.2602 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 13
92 -1.6055 0.4740 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 14
93 3.2461 1.6343 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 15
94 2.5456 -0.7424 0.0007 H 0 0 0 0 0 0 0 0 0 0 0 16
95
96 2 1 0 0 0 0
97 6 1 0 0 0 0
98 3 2 0 0 0 0
99 14 2 0 0 0 0
100 4 3 0 0 0 0
101 7 3 0 0 0 0
102 5 4 0 0 0 0
103 10 4 0 0 0 0
104 6 5 0 0 0 0
105 15 5 0 0 0 0
106 8 7 0 0 0 0
107 9 7 0 0 0 0
108 12 8 0 0 0 0
109 13 10 0 0 0 0
110 6 16 0 0 0 0
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9 13 0 0 0 0
M END
\$\$\$\$
5-nitrouracil-anion1.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
0.1753 -1.3717 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6070 -0.2001 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0531 1.0972 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4492 0.9519 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 4
2.1942 -0.2315 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.4982 -1.4298 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.4409 2.2327 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 7
3.4349 -0.1800 0.0003 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.0237 -0.3279 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 9
-0.3546 -2.3277 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9797 1.8252 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.5277 -1.4842 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.7404 0.6988 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 9 0 0 0 0
9 13 0 0 0 0
M END
\$\$\$\$
5-nitrouracil.sdf
COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
0.1145 -1.3626 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6205 -0.2010 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0513 1.1042 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4579 0.9722 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 4
2.2273 -0.1744 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
1.4577 -1.3500 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.4501 2.2234 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 7
3.4511 -0.1917 0.0003 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.0634 -0.3258 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 9
-0.3668 -2.3389 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9768 1.8529 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
1.9740 -2.2304 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.5520 -1.4745 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.7516 0.7058 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
\$\$\$\$
5-nitrouracil2-anion.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2417 -1.4325 -0.0038 C 0 0 0 0 0 0 0 0 0 0 0 1
0.5633 -0.2680 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.1321 0.9893 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.4459 1.0454 -0.0018 N 0 0 0 0 0 0 0 0 0 0 0 4
-2.1793 -0.1361 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.5544 -1.4042 -0.0042 N 0 0 0 0 0 0 0 0 0 0 0 6
0.5358 2.1501 -0.0035 O 0 0 0 0 0 0 0 0 0 0 0 7
-3.4264 -0.0886 0.0063 O 0 0 0 0 0 0 0 0 0 0 0 8
1.9630 -0.3653 0.0016 N 0 0 0 0 0 0 0 0 0 0 0 9
0.2498 -2.4097 -0.0067 H 0 0 0 0 0 0 0 0 0 0 0 10
2.5286 -1.4778 0.0008 O 0 0 0 0 0 0 0 0 0 0 0 11
2.6527 0.7193 0.0041 O 0 0 0 0 0 0 0 0 0 0 0 12
1.5153 1.8869 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
7 13 0 0 0 0
M END
\$\$\$\$
aceticacid-anion.sdf
COSMOtherm 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000

1
2
3 1.4421 -0.0806 -0.0002 C 0 0 0 0 0 0 0 0 0 0 1
4 -0.0963 -0.0003 -0.0011 C 0 0 0 0 0 0 0 0 0 0 2
5 -0.7505 -1.0903 0.0003 O 0 0 0 0 0 0 0 0 0 0 3
6 -0.6054 1.1662 0.0003 O 0 0 0 0 0 0 0 0 0 0 4
7 1.8011 -1.1172 -0.0340 H 0 0 0 0 0 0 0 0 0 0 5
8 1.8457 0.4703 -0.8631 H 0 0 0 0 0 0 0 0 0 0 6
9 1.8376 0.4064 0.9044 H 0 0 0 0 0 0 0 0 0 0 7

2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
1 7 0 0 0 0

M END

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aceticacid.sdf

COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
1.4608 0.0493 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.0345 -0.0960 -0.0011 C 0 0 0 0 0 0 0 0 0 0 2
-0.6519 -1.1529 0.0002 O 0 0 0 0 0 0 0 0 0 0 3
-0.6624 1.1098 -0.0001 O 0 0 0 0 0 0 0 0 0 0 4
1.9331 -0.9368 -0.0341 H 0 0 0 0 0 0 0 0 0 0 5
1.7812 0.6484 -0.8639 H 0 0 0 0 0 0 0 0 0 0 6
1.7813 0.5833 0.9059 H 0 0 0 0 0 0 0 0 0 0 7
-1.6307 0.9458 0.0044 H 0 0 0 0 0 0 0 0 0 0 8

2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
4 8 0 0 0 0

M END

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acrylicacid0-anion.sdf

COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
2.0014 -0.0221 -0.0049 C 0 0 0 0 0 0 0 0 0 0 1
0.8399 0.6448 0.0067 C 0 0 0 0 0 0 0 0 0 0 2
-0.5250 -0.0220 0.0014 C 0 0 0 0 0 0 0 0 0 0 3
-1.5247 0.7691 -0.0044 O 0 0 0 0 0 0 0 0 0 0 4
-0.5800 -1.2906 0.0022 O 0 0 0 0 0 0 0 0 0 0 5
2.9643 0.4941 -0.0031 H 0 0 0 0 0 0 0 0 0 0 6
2.0101 -1.1152 -0.0167 H 0 0 0 0 0 0 0 0 0 0 7
0.8306 1.7397 0.0177 H 0 0 0 0 0 0 0 0 0 0 8

2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 8 0 0 0 0

M END

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acrylicacid0.sdf

COSMOTHERM 3D 0

9 8 0 0 0 0 0 0 0 0 0 V2000
2.0284 -0.0188 -0.0018 C 0 0 0 0 0 0 0 0 0 0 1
0.8624 0.6403 0.0023 C 0 0 0 0 0 0 0 0 0 0 2
-0.4343 -0.0766 0.0006 C 0 0 0 0 0 0 0 0 0 0 3
-1.4784 0.7954 -0.0014 O 0 0 0 0 0 0 0 0 0 0 4
-0.5894 -1.2932 0.0007 O 0 0 0 0 0 0 0 0 0 0 5
2.9779 0.5175 -0.0011 H 0 0 0 0 0 0 0 0 0 0 6
2.0605 -1.1104 -0.0059 H 0 0 0 0 0 0 0 0 0 0 7
0.8207 1.7308 0.0059 H 0 0 0 0 0 0 0 0 0 0 8
-2.3096 0.2726 -0.0022 H 0 0 0 0 0 0 0 0 0 0 9

2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 9 0 0 0 0

M END

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acrylicacid1-anion.sdf

COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
2.0015 -0.0221 -0.0042 C 0 0 0 0 0 0 0 0 0 0 1
0.8400 0.6447 0.0057 C 0 0 0 0 0 0 0 0 0 0 2
-0.5250 -0.0220 0.0012 C 0 0 0 0 0 0 0 0 0 0 3
-0.5802 -1.2906 0.0019 O 0 0 0 0 0 0 0 0 0 0 4
-1.5246 0.7692 -0.0038 O 0 0 0 0 0 0 0 0 0 0 5
2.9643 0.4943 -0.0029 H 0 0 0 0 0 0 0 0 0 0 6
2.0103 -1.1152 -0.0139 H 0 0 0 0 0 0 0 0 0 0 7
0.8307 1.7396 0.0147 H 0 0 0 0 0 0 0 0 0 0 8

2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 8 0 0 0 0

M END

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acrylicacid1.sdf

COSMOTHERM 3D 0

9 8 0 0 0 0 0 0 0 0 0 V2000

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1.9957 -0.0510 -0.0032 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8631 0.6661 0.0042 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.4979 0.0887 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.5273 -1.2683 0.0018 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.5203 0.7705 -0.0028 O 0 0 0 0 0 0 0 0 0 0 0 5
2.9682 0.4438 -0.0022 H 0 0 0 0 0 0 0 0 0 0 0 6
1.9872 -1.1419 -0.0107 H 0 0 0 0 0 0 0 0 0 0 0 7
0.8811 1.7573 0.0105 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.4683 -1.5460 -0.0032 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 9 0 0 0 0
M END
$$$$
anthracene-9-carboxylicacid-anion.sdf
COSMOtherm 3D 0
26 28 0 0 0 0 0 0 0 0 0 0 V2000
3.6682 -1.3855 -0.0205 C 0 0 0 0 0 0 0 0 0 0 0 1
3.6753 0.0403 -0.0130 C 0 0 0 0 0 0 0 0 0 0 0 2
2.4922 0.7444 -0.0024 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2272 0.0730 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 4
1.2232 -1.3777 -0.0064 C 0 0 0 0 0 0 0 0 0 0 0 5
2.4758 -2.0717 -0.0165 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0000 0.7784 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2272 0.0730 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.2232 -1.3777 0.0064 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0000 -2.0662 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.4922 0.7444 0.0035 C 0 0 0 0 0 0 0 0 0 0 0 11
-3.6753 0.0404 0.0131 C 0 0 0 0 0 0 0 0 0 0 0 12
-3.6682 -1.3854 0.0207 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.4758 -2.0716 0.0158 C 0 0 0 0 0 0 0 0 0 0 0 14
0.0000 2.3055 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 15
0.1316 2.8724 1.1246 O 0 0 0 0 0 0 0 0 0 0 0 16
-0.1315 2.8722 -1.1251 O 0 0 0 0 0 0 0 0 0 0 0 17
4.6147 -1.9293 -0.0286 H 0 0 0 0 0 0 0 0 0 0 0 18
4.6279 0.5735 -0.0149 H 0 0 0 0 0 0 0 0 0 0 0 19
2.5085 1.8358 0.0100 H 0 0 0 0 0 0 0 0 0 0 0 20
2.4645 -3.1643 -0.0216 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.0001 -3.1594 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 22
-2.5085 1.8359 -0.0082 H 0 0 0 0 0 0 0 0 0 0 0 23
-4.6279 0.5736 0.0166 H 0 0 0 0 0 0 0 0 0 0 0 24
-4.6148 -1.9293 0.0288 H 0 0 0 0 0 0 0 0 0 0 0 25
-2.4646 -3.1643 0.0214 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
6 1 0 0 0 0
18 1 0 0 0 0
3 2 0 0 0 0
19 2 0 0 0 0
4 3 0 0 0 0
20 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
21 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
13 12 0 0 0 0
24 12 0 0 0 0
14 13 0 0 0 0
25 13 0 0 0 0
16 15 0 0 0 0
17 15 0 0 0 0
14 26 0 0 0 0
M END
$$$$
anthracene-9-carboxylicacid.sdf
COSMOtherm 3D 0
27 29 0 0 0 0 0 0 0 0 0 0 V2000
3.6791 -1.3995 -0.0593 C 0 0 0 0 0 0 0 0 0 0 0 1
3.6874 0.0247 -0.0481 C 0 0 0 0 0 0 0 0 0 0 0 2
2.5112 0.7397 -0.0188 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2424 0.0757 0.0083 C 0 0 0 0 0 0 0 0 0 0 0 4
1.2384 -1.3738 -0.0187 C 0 0 0 0 0 0 0 0 0 0 0 5
2.4839 -2.0777 -0.0466 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0009 0.7631 0.0151 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2326 0.0622 0.0164 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.2115 -1.3881 0.0038 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0172 -2.0616 -0.0185 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.5098 0.7083 0.0767 C 0 0 0 0 0 0 0 0 0 0 0 11
-3.6768 -0.0216 0.0936 C 0 0 0 0 0 0 0 0 0 0 0 12
-3.6516 -1.4452 0.0581 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.4483 -2.1077 0.0163 C 0 0 0 0 0 0 0 0 0 0 0 14
0.0136 2.2602 0.0615 C 0 0 0 0 0 0 0 0 0 0 0 15
0.5507 2.9260 0.9380 O 0 0 0 0 0 0 0 0 0 0 0 16
-0.6269 2.8249 -0.9915 O 0 0 0 0 0 0 0 0 0 0 0 17
4.6234 -1.9458 -0.0812 H 0 0 0 0 0 0 0 0 0 0 0 18
4.6407 0.5558 -0.0673 H 0 0 0 0 0 0 0 0 0 0 0 19
2.5472 1.8286 -0.0069 H 0 0 0 0 0 0 0 0 0 0 0 20
2.4613 -3.1695 -0.0629 H 0 0 0 0 0 0 0 0 0 0 0 21
0.0232 -3.1545 -0.0345 H 0 0 0 0 0 0 0 0 0 0 0 22

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1
2
3      3 2 0 0 0 0
4      6 2 0 0 0 0
5      7 2 0 0 0 0
6      4 3 0 0 0 0
7      5 3 0 0 0 0
8      4 8 0 0 0 0
9 M  END
10 $$$$
11 carbonicacid0-anion.sdf
12 COSMOTHERM      3D      0
13
14      5 4 0 0 0 0 0 0 0 0 0 V2000
15      -0.1133 -0.0487 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
16      -0.0620 -1.3081 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 2
17      1.1382 0.6301 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3
18      -1.1060 0.7187 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 4
19      1.8234 -0.0665 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 5
20      2 1 0 0 0 0
21      3 1 0 0 0 0
22      4 1 0 0 0 0
23      3 5 0 0 0 0
24 M  END
25 $$$$
26 carbonicacid0.sdf
27 COSMOTHERM      3D      0
28
29      6 5 0 0 0 0 0 0 0 0 0 V2000
30      -0.0002 -0.0991 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
31      -0.0019 -1.3196 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 2
32      1.0909 0.6885 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 3
33      -1.0888 0.6915 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 4
34      1.8797 0.1090 -0.0012 H 0 0 0 0 0 0 0 0 0 0 0 0 5
35      -1.8794 0.1144 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 0 6
36      2 1 0 0 0 0
37      3 1 0 0 0 0
38      4 1 0 0 0 0
39      5 3 0 0 0 0
40      4 6 0 0 0 0
41 M  END
42 $$$$
43 carbonicacid1.sdf
44 COSMOTHERM      3D      0
45
46      6 5 0 0 0 0 0 0 0 0 0 V2000
47      0.0683 -0.0825 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
48      0.8932 -0.9774 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 2
49      0.3372 1.2425 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 3
50      -1.2538 -0.3218 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 4
51      1.3096 1.3606 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 0 5
52      -1.7525 0.5215 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 6
53      2 1 0 0 0 0
54      3 1 0 0 0 0
55      4 1 0 0 0 0
56      5 3 0 0 0 0
57      4 6 0 0 0 0
58 M  END
59 $$$$
60 chloroaceticacid0-anion.sdf
    COSMOTHERM      3D      0
    7 6 0 0 0 0 0 0 0 0 0 V2000
    -0.0332 -1.7617 -0.0041 C1 0 0 0 0 0 0 0 0 0 0 0 0 1
    0.8419 -0.1342 0.0132 C 0 0 0 0 0 0 0 0 0 0 0 0 2
    -0.0664 1.1152 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 3
    -1.3180 1.0040 0.0044 O 0 0 0 0 0 0 0 0 0 0 0 0 4
    0.6236 2.1807 -0.0089 O 0 0 0 0 0 0 0 0 0 0 0 0 5
    1.4907 -0.1378 -0.8689 H 0 0 0 0 0 0 0 0 0 0 0 0 6
    1.4592 -0.1408 0.9179 H 0 0 0 0 0 0 0 0 0 0 0 0 7
    2 1 0 0 0 0
    3 2 0 0 0 0
    6 2 0 0 0 0
    4 3 0 0 0 0
    5 3 0 0 0 0
    2 7 0 0 0 0
M  END
$$$$
chloroaceticacid0.sdf
COSMOTHERM      3D      0
8 7 0 0 0 0 0 0 0 0 0 V2000
-0.0428 -1.7452 -0.0080 C1 0 0 0 0 0 0 0 0 0 0 0 0 1
0.8763 -0.1782 0.0242 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.0480 1.0899 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.2808 0.9110 0.0097 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.5988 2.1806 -0.0167 O 0 0 0 0 0 0 0 0 0 0 0 0 5
1.5418 -0.1724 -0.8458 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.4841 -0.1768 0.9359 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.7089 1.7958 -0.0027 H 0 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M  END
$$$$
chloroaceticacid1-anion.sdf
COSMOTHERM      3D      0
7 6 0 0 0 0 0 0 0 0 0 V2000
1.7617 0.0332 0.0049 C1 0 0 0 0 0 0 0 0 0 0 0 0 1
0.1342 -0.8419 -0.0156 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.1152 0.0664 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-2.1807 -0.6236 0.0105 O 0 0 0 0 0 0 0 0 0 0 0 0 4

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2
3 -1.0040 1.3180 -0.0052 O 0 0 0 0 0 0 0 0 0 5
4 0.1375 -1.4935 0.8645 H 0 0 0 0 0 0 0 0 0 6
5 0.1412 -1.4564 -0.9222 H 0 0 0 0 0 0 0 0 0 7
6 2 1 0 0 0 0
7 3 2 0 0 0 0
8 6 2 0 0 0 0
9 4 3 0 0 0 0
10 5 3 0 0 0 0
11 2 7 0 0 0 0

M END

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chloroaceticacid1.sdf

COSMOtherm 3D 0

8 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
1.7597 0.0337 0.0067 C1 0 0 0 0 0 0 0 0 0 0 0 0 1
0.1842 -0.8458 -0.0204 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.0068 0.0967 -0.0033 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-2.1422 -0.6366 0.0134 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.9756 1.3124 -0.0069 O 0 0 0 0 0 0 0 0 0 0 0 0 5
0.1501 -1.5049 0.8541 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1563 -1.4583 -0.9287 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.9087 -0.0222 0.0157 H 0 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0 0
3 2 0 0 0 0 0
6 2 0 0 0 0 0
7 2 0 0 0 0 0
4 3 0 0 0 0 0
5 3 0 0 0 0 0
4 8 0 0 0 0 0

M END

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cis-5-formyluracil-anion0.sdf

COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
0.0850 -1.5082 0.0083 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.8309 -0.4735 0.0046 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.3039 0.9149 0.0044 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.0621 1.0961 -0.0021 N 0 0 0 0 0 0 0 0 0 0 0 0 4
1.9319 0.0679 -0.0034 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.4029 -1.2639 0.0055 N 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.0681 1.9089 0.0111 O 0 0 0 0 0 0 0 0 0 0 0 0 7
3.1778 0.1769 -0.0109 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.2285 -0.8618 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.2205 -2.5569 0.0118 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.0742 -2.0311 0.0060 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-3.2245 -0.1286 -0.0164 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.3697 -1.9728 0.0136 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0 0
6 1 0 0 0 0 0
10 1 0 0 0 0 0
3 2 0 0 0 0 0
9 2 0 0 0 0 0
4 3 0 0 0 0 0
7 3 0 0 0 0 0
5 4 0 0 0 0 0
6 5 0 0 0 0 0
8 5 0 0 0 0 0
11 6 0 0 0 0 0
12 9 0 0 0 0 0
9 13 0 0 0 0 0

M END

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cis-5-formyluracil-anion1.sdf

COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.4955 -0.1407 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.4785 0.8347 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.8989 0.3699 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.9941 -1.0296 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0595 -1.9541 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3500 -1.4625 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 6
1.9353 1.0557 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 0 7
0.1974 -3.1726 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.8761 2.2206 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.5330 0.2186 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.9396 -1.4170 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.1491 3.2272 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.9875 2.3523 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0 0
6 1 0 0 0 0 0
10 1 0 0 0 0 0
3 2 0 0 0 0 0
9 2 0 0 0 0 0
4 3 0 0 0 0 0
7 3 0 0 0 0 0
5 4 0 0 0 0 0
11 4 0 0 0 0 0
6 5 0 0 0 0 0
8 5 0 0 0 0 0
12 9 0 0 0 0 0
9 13 0 0 0 0 0

M END

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cis-5-formyluracil.sdf

COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.5038 -0.0801 0.0065 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.4879 0.8503 0.0054 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.9005 0.3779 0.0042 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.0164 -1.0302 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 4
0.0071 -1.9739 -0.0028 C 0 0 0 0 0 0 0 0 0 0 0 0 5

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-1.2761 -1.4096 0.0020 N 0 0 0 0 0 0 0 0 0 0 0 6
1.9182 1.0687 0.0078 O 0 0 0 0 0 0 0 0 0 0 0 7
0.1927 -3.1862 -0.0082 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.8756 2.2589 0.0034 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.5527 0.2200 0.0091 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9688 -1.4009 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.0573 -2.0655 0.0007 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.1210 3.2302 -0.0153 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.9821 2.4079 0.0186 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
cis-5-formyluracil2-anion.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 V2000
-1.5697 -0.2689 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6003 0.7615 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7620 0.3063 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 3
1.0980 -0.9662 0.0007 N 0 0 0 0 0 0 0 0 0 0 0 4
0.0784 -1.9169 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2847 -1.5566 0.0011 N 0 0 0 0 0 0 0 0 0 0 0 6
1.7540 1.2161 0.0010 O 0 0 0 0 0 0 0 0 0 0 0 7
0.3755 -3.1331 -0.0021 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.9264 2.1462 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.6326 0.0048 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.0615 3.0674 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.0016 2.4161 -0.0015 H 0 0 0 0 0 0 0 0 0 0 0 12
1.2870 2.1234 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
7 13 0 0 0 0
M END
$$$$
cyanoaceticacid0-anion.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 V2000
1.5333 -0.2852 -0.0038 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2303 -0.9179 -0.0502 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.9912 0.0851 -0.0028 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.7398 1.3183 -0.0254 O 0 0 0 0 0 0 0 0 0 0 0 4
-2.1144 -0.4860 0.0450 O 0 0 0 0 0 0 0 0 0 0 0 5
2.5768 0.2336 0.0397 N 0 0 0 0 0 0 0 0 0 0 0 6
0.1413 -1.6236 0.7893 H 0 0 0 0 0 0 0 0 0 0 0 7
0.1517 -1.5105 -0.9747 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 8 0 0 0 0
M END
$$$$
cyanoaceticacid0.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 V2000
1.5649 -0.2644 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 1
0.2567 -0.8959 -0.0431 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.8906 0.1119 -0.0066 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.7710 1.3226 -0.0197 O 0 0 0 0 0 0 0 0 0 0 0 4
-2.0666 -0.5426 0.0362 O 0 0 0 0 0 0 0 0 0 0 0 5
2.6204 0.2221 0.0332 N 0 0 0 0 0 0 0 0 0 0 0 6
0.1569 -1.5940 0.8023 H 0 0 0 0 0 0 0 0 0 0 0 7
0.1698 -1.5003 -0.9600 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.7918 0.1203 0.0472 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 9 0 0 0 0
M END
$$$$
cyanoaceticacid1-anion.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 V2000
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1.5200 -0.1306 -0.0167 C 0 0 0 0 0 0 0 0 0 0 1
0.3263 -0.9477 -0.0627 C 0 0 0 0 0 0 0 0 0 0 2
-0.9792 -0.0384 0.0034 C 0 0 0 0 0 0 0 0 0 0 3
-1.4561 0.3117 -1.1080 O 0 0 0 0 0 0 0 0 0 0 4
-1.3919 0.2372 1.1606 O 0 0 0 0 0 0 0 0 0 0 5
2.4613 0.5588 0.0199 N 0 0 0 0 0 0 0 0 0 0 6
0.3393 -1.6409 0.7904 H 0 0 0 0 0 0 0 0 0 0 7
0.3312 -1.5296 -0.9950 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 8 0 0 0 0
M END
$$$$
cyanoaceticacid1.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 0 0 V2000
1.5357 -0.2679 0.0081 C 0 0 0 0 0 0 0 0 0 0 1
0.2500 -0.9214 0.1954 C 0 0 0 0 0 0 0 0 0 0 2
-0.9787 -0.0310 0.0078 C 0 0 0 0 0 0 0 0 0 0 3
-2.0920 -0.4873 -0.1735 O 0 0 0 0 0 0 0 0 0 0 4
-0.6923 1.2792 0.1021 O 0 0 0 0 0 0 0 0 0 0 5
2.5717 0.2366 -0.1521 N 0 0 0 0 0 0 0 0 0 0 6
0.2014 -1.3323 1.2176 H 0 0 0 0 0 0 0 0 0 0 7
0.1664 -1.7739 -0.4932 H 0 0 0 0 0 0 0 0 0 0 8
-1.5262 1.7900 0.0034 H 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 9 0 0 0 0
M END
$$$$
dichloroaceticacid0-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 0 V2000
-1.0342 0.0138 1.4985 Cl 0 0 0 0 0 0 0 0 0 0 1
-0.1317 -0.5202 -0.0003 C 0 0 0 0 0 0 0 0 0 0 2
1.3310 0.0351 0.0013 C 0 0 0 0 0 0 0 0 0 0 3
1.4849 1.2800 0.0043 O 0 0 0 0 0 0 0 0 0 0 4
2.2015 -0.8797 -0.0006 O 0 0 0 0 0 0 0 0 0 0 5
-1.0310 0.0157 -1.5005 Cl 0 0 0 0 0 0 0 0 0 0 6
-0.1681 -1.6104 -0.0010 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
dichloroaceticacid0.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 0 V2000
1.4996 1.0305 -0.0156 Cl 0 0 0 0 0 0 0 0 0 0 1
0.0008 0.1748 0.5137 C 0 0 0 0 0 0 0 0 0 0 2
-0.0066 -1.2357 -0.0945 C 0 0 0 0 0 0 0 0 0 0 3
-0.0155 -1.4781 -1.2841 O 0 0 0 0 0 0 0 0 0 0 4
-0.0008 -2.1457 0.8929 O 0 0 0 0 0 0 0 0 0 0 5
-1.4903 1.0465 -0.0096 Cl 0 0 0 0 0 0 0 0 0 0 6
0.0032 0.1556 1.6039 H 0 0 0 0 0 0 0 0 0 0 7
-0.0039 -3.0456 0.4959 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 8 0 0 0 0
M END
$$$$
dimethadione0-anion.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 0 0 0 V2000
0.7500 -0.5547 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
0.4961 0.9706 0.0000 C 0 0 0 0 0 0 0 0 0 0 2
-0.6162 -1.0791 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
-1.4856 0.0182 0.0000 C 0 0 0 0 0 0 0 0 0 0 4
-0.8385 1.2206 0.0002 N 0 0 0 0 0 0 0 0 0 0 5
1.4632 -1.0082 -1.2721 C 0 0 0 0 0 0 0 0 0 0 6
1.4633 -1.0081 1.2721 C 0 0 0 0 0 0 0 0 0 0 7
1.4126 1.8145 -0.0001 O 0 0 0 0 0 0 0 0 0 0 8
-2.7021 -0.1934 -0.0001 O 0 0 0 0 0 0 0 0 0 0 9
0.8953 -0.7152 -2.1664 H 0 0 0 0 0 0 0 0 0 0 10
2.4565 -0.5411 -1.3225 H 0 0 0 0 0 0 0 0 0 0 11
1.5892 -2.1002 -1.2731 H 0 0 0 0 0 0 0 0 0 0 12
0.8952 -0.7155 2.1664 H 0 0 0 0 0 0 0 0 0 0 13
2.4564 -0.5407 1.3227 H 0 0 0 0 0 0 0 0 0 0 14
1.5898 -2.1001 1.2730 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
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2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
  9 16 0 0 0 0

```

M END
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dimethadione2-anion.sdf
COSMOtherm      3D      0

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15 15 0 0 0 0 0 0 0 0 0 0 0 0 V2000
  0.7500 -0.5547  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
  0.4961  0.9706  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
 -0.6162 -1.0791  0.0000 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
 -1.4856  0.0182  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
 -0.8385  1.2206  0.0002 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
  1.4632 -1.0082 -1.2721 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
  1.4633 -1.0081  1.2721 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
  1.4126  1.8145 -0.0001 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
 -2.7021 -0.1934 -0.0001 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
  0.8953 -0.7152 -2.1664 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 10
  2.4565 -0.5411 -1.3225 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 11
  1.5892 -2.1002 -1.2731 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 12
  0.8952 -0.7155  2.1664 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 13
  2.4564 -0.5407  1.3227 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 14
  1.5898 -2.1001  1.2730 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 15

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2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
  7 15 0 0 0 0

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M END
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dimethadione2.sdf
COSMOtherm      3D      0

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16 16 0 0 0 0 0 0 0 0 0 0 0 0 V2000
  0.7304 -0.5871  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
  0.4584  0.9028 -0.0001 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
 -0.6541 -1.0790  0.0000 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
 -1.5041  0.0088  0.0000 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
 -0.7982  1.2284 -0.0001 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
  1.4300 -1.0515 -1.2771 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
  1.4299 -1.0511  1.2774 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
  1.4755  1.7414 -0.0002 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
 -2.7132 -0.1291  0.0000 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
  0.8760 -0.7320 -2.1696 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 10
  2.4427 -0.6294 -1.3188 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 11
  1.5066 -2.1464 -1.2733 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 12
  0.8756 -0.7314  2.1697 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 13
  2.4425 -0.6288  1.3191 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 14
  1.5066 -2.1460  1.2739 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 15
  1.1478  2.6679  0.0009 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0 16

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2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
  8 16 0 0 0 0

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M END
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ethanol-anion.sdf
COSMOtherm      3D      0

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8 7 0 0 0 0 0 0 0 0 0 0 0 0 V2000
  1.2659  0.0000  0.2319 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
 -0.0831  0.0000 -0.5238 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
 -1.1861  0.0000  0.2918 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
  2.1301  0.0011 -0.4578 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
  1.3407  0.8908  0.8781 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
  1.3417 -0.8918  0.8767 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
 -0.0400 -0.8873 -1.2254 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
 -0.0400  0.8874 -1.2252 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
  2 1 0 0 0 0

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4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
2 8 0 0 0 0
M END
$$$$
ethanol.sdf
COSMOtherm 3D 0
9 8 0 0 0 0 0 0 0 0 0 V2000
1.2720 0.0000 0.2530 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0012 0.0000 -0.5761 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.1321 0.0000 0.3241 O 0 0 0 0 0 0 0 0 0 0 0 3
2.1521 0.0008 -0.4063 H 0 0 0 0 0 0 0 0 0 0 0 4
1.3239 0.8929 0.8933 H 0 0 0 0 0 0 0 0 0 0 0 5
1.3246 -0.8937 0.8922 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0318 -0.8924 -1.2259 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.0318 0.8925 -1.2258 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.9393 -0.0004 -0.2211 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 2 0 0 0 0
3 9 0 0 0 0
M END
$$$$
fluoroaceticacid0-anion.sdf
COSMOtherm 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
-0.0701 -1.8291 -0.0065 F 0 0 0 0 0 0 0 0 0 0 0 1
0.7532 -0.6667 0.0096 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.0496 0.6469 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.3090 0.5981 0.0030 O 0 0 0 0 0 0 0 0 0 0 0 4
0.6892 1.6789 -0.0055 O 0 0 0 0 0 0 0 0 0 0 0 5
1.4027 -0.7141 -0.8765 H 0 0 0 0 0 0 0 0 0 0 0 6
1.3718 -0.7184 0.9175 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
fluoroaceticacid0.sdf
COSMOtherm 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
-0.0925 -1.8060 -0.0073 F 0 0 0 0 0 0 0 0 0 0 0 1
0.7798 -0.7071 0.0102 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0619 0.6286 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2773 0.5276 0.0039 O 0 0 0 0 0 0 0 0 0 0 0 4
0.6813 1.6813 -0.0060 O 0 0 0 0 0 0 0 0 0 0 0 5
1.4296 -0.7595 -0.8750 H 0 0 0 0 0 0 0 0 0 0 0 6
1.3968 -0.7632 0.9186 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.6534 1.4359 -0.0018 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
fluoroaceticacid1-anion.sdf
COSMOtherm 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
1.8290 0.0701 0.0005 F 0 0 0 0 0 0 0 0 0 0 0 1
0.6666 -0.7533 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6469 0.0496 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.6789 -0.6890 0.0004 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.5980 1.3090 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 5
0.7160 -1.3887 0.8956 H 0 0 0 0 0 0 0 0 0 0 0 6
0.7162 -1.3862 -0.8988 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
fluoroaceticacid1.sdf
COSMOtherm 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
1.8340 0.0683 0.0074 F 0 0 0 0 0 0 0 0 0 0 0 1
0.7052 -0.7562 -0.0105 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.5548 0.0914 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.6436 -0.7060 0.0061 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.5847 1.3082 -0.0032 O 0 0 0 0 0 0 0 0 0 0 0 5
0.7247 -1.4072 0.8754 H 0 0 0 0 0 0 0 0 0 0 0 6
0.7308 -1.3750 -0.9193 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.4473 -0.1412 0.0045 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0

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7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
formicacid-anion.sdf
COSMOTHERM 3D 0

4 3 0 0 0 0 0 0 0 0 0 V2000
-0.3690 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
0.1857 1.1375 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 2
0.1857 -1.1375 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 3
-1.4974 0.0000 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 4
2 1 0 0 0 0
3 1 0 0 0 0
1 4 0 0 0 0
M END
$$$$
formicacid.sdf
COSMOTHERM 3D 0

5 4 0 0 0 0 0 0 0 0 0 V2000
-0.4154 -0.0935 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
0.1224 1.1398 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 2
0.2155 -1.1348 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 3
-1.5169 -0.0240 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 4
1.1032 1.0584 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
2 5 0 0 0 0
M END
$$$$
fumaricacid-anion.sdf
COSMOTHERM 3D 0

11 10 0 0 0 0 0 0 0 0 0 V2000
0.4898 0.3983 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.5575 -0.4432 -0.0051 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.0068 0.0182 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 3
1.8859 -0.0842 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 4
2.2540 -1.2553 -0.0160 O 0 0 0 0 0 0 0 0 0 0 0 5
2.7666 0.9554 0.0178 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.8702 -0.9152 0.0204 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.2364 1.2646 -0.0175 O 0 0 0 0 0 0 0 0 0 0 0 8
0.3271 1.4779 0.0057 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.3870 -1.5238 -0.0101 H 0 0 0 0 0 0 0 0 0 0 0 10
3.6743 0.5809 0.0156 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
4 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
6 11 0 0 0 0
M END
$$$$
fumaricacid.sdf
COSMOTHERM 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
0.5222 0.4207 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.5222 -0.4208 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.9185 0.0858 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 3
1.9185 -0.0858 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 4
2.2500 -1.2642 -0.0096 O 0 0 0 0 0 0 0 0 0 0 0 5
2.8032 0.9402 0.0110 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.8033 -0.9402 0.0109 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.2499 1.2642 -0.0096 O 0 0 0 0 0 0 0 0 0 0 0 8
0.3752 1.5021 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.3752 -1.5022 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 10
3.7109 0.5642 0.0105 H 0 0 0 0 0 0 0 0 0 0 0 11
-3.7109 -0.5641 0.0105 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
4 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 6 0 0 0 0
7 12 0 0 0 0
M END
$$$$
hypobromousacid-anion.sdf
COSMOTHERM 3D 0

2 0 0 0 0 0 0 0 0 0 0 V2000
-1.5538 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 1
0.3111 0.0000 0.0000 Br 0 0 0 0 0 0 0 0 0 0 0 2
M END
$$$$
hypobromousacid.sdf
COSMOTHERM 3D 0

3 1 0 0 0 0 0 0 0 0 0 V2000
-1.5419 0.0632 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 1
0.3313 -0.0015 0.0000 Br 0 0 0 0 0 0 0 0 0 0 0 2
-1.7912 -0.8853 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 3

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1 3 0 0 0 0
M END
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hypochlorousacid-anion.sdf
COSMOtherm 3D 0

2 1 0 0 0 0 0 0 0 0 0 V2000
-1.2070 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.5447 0.0000 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 2
1 2 0 0 0 0
M END
$$$$
hypochlorousacid.sdf
COSMOtherm 3D 0

3 2 0 0 0 0 0 0 0 0 0 V2000
-1.1727 0.0638 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.5697 -0.0036 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 2
-1.4219 -0.8856 0.0000 H 0 0 0 0 0 0 0 0 0 0 3
2 1 0 0 0 0
1 3 0 0 0 0
M END
$$$$
hypiodousacid-anion.sdf
COSMOtherm 3D 0

2 0 0 0 0 0 0 0 0 0 V2000
-1.8041 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.2274 0.0000 0.0000 I 0 0 0 0 0 0 0 0 0 0 2
M END
$$$$
hypiodousacid.sdf
COSMOtherm 3D 0

3 1 0 0 0 0 0 0 0 0 0 V2000
-1.8114 0.0626 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.2448 -0.0009 0.0000 I 0 0 0 0 0 0 0 0 0 0 2
-2.0735 -0.8813 0.0000 H 0 0 0 0 0 0 0 0 0 0 3
1 3 0 0 0 0
M END
$$$$
hypophosphorousacid-anion.sdf
COSMOtherm 3D 0

5 4 0 0 0 0 0 0 0 0 0 V2000
1.3430 -0.4208 0.0000 O 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.3520 0.0000 P 0 0 0 0 0 0 0 0 0 0 2
-1.3430 -0.4208 0.0000 O 0 0 0 0 0 0 0 0 0 0 3
0.0000 1.2710 1.1157 H 0 0 0 0 0 0 0 0 0 0 4
0.0001 1.2711 -1.1157 H 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
2 5 0 0 0 0
M END
$$$$
hypophosphorousacid.sdf
COSMOtherm 3D 0

6 5 0 0 0 0 0 0 0 0 0 V2000
-0.0222 1.1316 1.2714 H 0 0 0 0 0 0 0 0 0 0 1
0.0815 -0.0004 0.4132 P 0 0 0 0 0 0 0 0 0 0 2
-0.0175 -1.1343 1.2692 H 0 0 0 0 0 0 0 0 0 0 3
1.2913 0.0010 -0.5059 O 0 0 0 0 0 0 0 0 0 0 4
-1.3133 -0.0016 -0.4605 O 0 0 0 0 0 0 0 0 0 0 5
-2.1151 0.0223 0.1008 H 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
5 6 0 0 0 0
M END
$$$$
iodoaceticacid0-anion.sdf
COSMOtherm 3D 0

7 5 0 0 0 0 0 0 0 0 0 V2000
-0.0077 -1.0024 -0.0018 I 0 0 0 0 0 0 0 0 0 0 1
0.8993 1.0299 0.0231 C 0 0 0 0 0 0 0 0 0 0 2
-0.0767 2.2226 0.0013 C 0 0 0 0 0 0 0 0 0 0 3
-1.3214 2.0633 0.0082 O 0 0 0 0 0 0 0 0 0 0 4
0.5725 3.3153 -0.0171 O 0 0 0 0 0 0 0 0 0 0 5
1.5525 1.0389 -0.8544 H 0 0 0 0 0 0 0 0 0 0 6
1.5048 1.0362 0.9346 H 0 0 0 0 0 0 0 0 0 0 7
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
iodoaceticacid0.sdf
COSMOtherm 3D 0

8 6 0 0 0 0 0 0 0 0 0 V2000
-0.0101 -1.0009 -0.0031 I 0 0 0 0 0 0 0 0 0 0 1
0.9342 0.9722 0.0364 C 0 0 0 0 0 0 0 0 0 0 2
0.0422 2.1901 0.0025 C 0 0 0 0 0 0 0 0 0 0 3
-1.2783 1.9541 0.0153 O 0 0 0 0 0 0 0 0 0 0 4
0.5379 3.3079 -0.0279 O 0 0 0 0 0 0 0 0 0 0 5
1.6045 0.9980 -0.8279 H 0 0 0 0 0 0 0 0 0 0 6
1.5313 0.9952 0.9536 H 0 0 0 0 0 0 0 0 0 0 7
-1.7452 2.8190 -0.0032 H 0 0 0 0 0 0 0 0 0 0 8
3 2 0 0 0 0
6 2 0 0 0 0

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7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
iodoaceticacid1-anion.sdf
COSMOTHERM 3D 0

7 5 0 0 0 0 0 0 0 0 0 V2000
1.0024 0.0077 0.0018 I 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.0299 -0.8993 -0.0224 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.2227 0.0768 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-3.3153 -0.5725 0.0165 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.0634 1.3214 -0.0080 O 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.0388 -1.5517 0.8558 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.0363 -1.5057 -0.9333 H 0 0 0 0 0 0 0 0 0 0 0 0 7
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
$$$$
iodoaceticacid1.sdf
COSMOTHERM 3D 0

8 6 0 0 0 0 0 0 0 0 0 V2000
1.0043 0.0083 0.0030 I 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.9625 -0.9064 -0.0359 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.0981 0.0956 -0.0056 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-3.2728 -0.5780 0.0258 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.0150 1.3097 -0.0132 O 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.0172 -1.5732 0.8302 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.0109 -1.5042 -0.9518 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-4.0036 0.0787 0.0338 H 0 0 0 0 0 0 0 0 0 0 0 0 8
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
maleicacid3-anion.sdf
COSMOTHERM 3D 0

11 11 0 0 0 0 0 0 0 0 0 V2000
0.6754 -1.1413 -0.0155 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.6754 -1.1413 -0.0156 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.6558 -0.0014 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.6558 -0.0011 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.2076 1.2286 -0.0084 O 0 0 0 0 0 0 0 0 0 0 0 0 5
2.8710 -0.2770 0.0211 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.8711 -0.2770 0.0212 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2075 1.2285 -0.0083 O 0 0 0 0 0 0 0 0 0 0 0 0 8
1.1731 -2.1144 -0.0247 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.1732 -2.1144 -0.0250 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0010 1.2511 -0.0129 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
9 1 0 0 0 0
4 2 0 0 0 0
10 2 0 0 0 0
5 3 0 0 0 0
6 3 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
5 11 0 0 0 0
8 11 0 0 0 0
M END
$$$$
maleicacid3.sdf
COSMOTHERM 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
0.6669 -1.1230 -0.0048 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.6827 -1.1277 -0.0089 C 0 0 0 0 0 0 0 0 0 0 0 0 2
1.5784 0.0394 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.6979 -0.0244 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.2471 1.2338 -0.0077 O 0 0 0 0 0 0 0 0 0 0 0 0 5
2.8603 -0.3417 0.0104 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.8929 -0.3162 0.0079 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.3114 1.2538 0.0012 O 0 0 0 0 0 0 0 0 0 0 0 0 8
1.1744 -2.0888 -0.0074 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.1660 -2.1063 -0.0131 H 0 0 0 0 0 0 0 0 0 0 0 0 10
3.4323 0.4579 0.0127 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.2913 1.3341 -0.0068 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
9 1 0 0 0 0
4 2 0 0 0 0
10 2 0 0 0 0
5 3 0 0 0 0
6 3 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
11 6 0 0 0 0
8 12 0 0 0 0
M END
$$$$
mandelicacid-anion0.sdf
COSMOTHERM 3D 0

18 18 0 0 0 0 0 0 0 0 0 V2000

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2
3 -3.1021 -0.0161 -0.4438 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
4 -2.6068 -0.9577 0.4658 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
5 -1.2691 -0.9026 0.8755 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
6 -0.4077 0.0894 0.3821 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
7 -0.9151 1.0345 -0.5251 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
8 -2.2509 0.9826 -0.9357 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
9 1.0489 0.1251 0.8015 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
10 1.5025 1.4599 1.0622 O 0 0 0 0 0 0 0 0 0 0 0 0 0 8
11 1.9744 -0.5071 -0.3011 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
12 1.7957 -1.7133 -0.6039 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
13 2.8437 0.2936 -0.7770 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
14 2.2373 1.5412 0.3942 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
15 -4.1458 -0.0545 -0.7616 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
16 -3.2649 -1.7330 0.8636 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
17 -0.8896 -1.6351 1.5923 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
18 -0.2575 1.8213 -0.9005 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
19 -2.6304 1.7240 -1.6422 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
20 1.1701 -0.4912 1.7097 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
21 2 1 0 0 0 0
22 6 1 0 0 0 0
23 13 1 0 0 0 0
24 3 2 0 0 0 0
25 14 2 0 0 0 0
26 4 3 0 0 0 0
27 15 3 0 0 0 0
28 5 4 0 0 0 0
29 7 4 0 0 0 0
30 6 5 0 0 0 0
31 16 5 0 0 0 0
32 17 6 0 0 0 0
33 8 7 0 0 0 0
34 9 7 0 0 0 0
35 12 8 0 0 0 0
36 10 9 0 0 0 0
37 11 9 0 0 0 0
38 7 18 0 0 0 0
39 M END
40 $$$$
41 mandelicacid-anion1.sdf
42 COSMOtherm 3D 0
43
44 18 18 0 0 0 0 0 0 0 0 0 V2000
45 0.0608 -0.4269 -3.1006 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
46 -1.0239 -0.8298 -2.3116 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
47 -1.1116 -0.4262 -0.9744 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
48 -0.1166 0.3845 -0.4051 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
49 0.9624 0.7928 -1.2062 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
50 1.0537 0.3881 -2.5425 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
51 -0.1839 0.7888 1.0552 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
52 -1.5296 0.9607 1.5119 O 0 0 0 0 0 0 0 0 0 0 0 0 0 8
53 0.5178 -0.2840 1.9694 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
54 -0.2592 -0.8381 2.8137 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
55 1.7457 -0.4903 1.8058 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
56 -1.5752 0.2687 2.2269 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
57 0.1279 -0.7390 -4.1447 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
58 -1.8063 -1.4604 -2.7395 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
59 -1.9638 -0.7295 -0.3634 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
60 1.7359 1.4349 -0.7784 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
61 1.8979 0.7168 -3.1525 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
62 0.3753 1.7318 1.1878 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
63 2 1 0 0 0 0
64 6 1 0 0 0 0
65 13 1 0 0 0 0
66 3 2 0 0 0 0
67 14 2 0 0 0 0
68 4 3 0 0 0 0
69 15 3 0 0 0 0
70 5 4 0 0 0 0
71 7 4 0 0 0 0
72 6 5 0 0 0 0
73 16 5 0 0 0 0
74 17 6 0 0 0 0
75 8 7 0 0 0 0
76 9 7 0 0 0 0
77 12 8 0 0 0 0
78 10 9 0 0 0 0
79 11 9 0 0 0 0
80 7 18 0 0 0 0
81 M END
82 $$$$
83 mandelicacid0.sdf
84 COSMOtherm 3D 0
85
86 19 19 0 0 0 0 0 0 0 0 0 V2000
87 0.4695 -0.0128 -3.0938 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
88 -0.5099 -0.9012 -2.6371 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
89 -0.9291 -0.8572 -1.3021 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
90 -0.3719 0.0745 -0.4160 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
91 0.6076 0.9668 -0.8790 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
92 1.0251 0.9238 -2.2122 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
93 -0.8301 0.1233 1.0384 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
94 -1.2043 1.4376 1.4489 O 0 0 0 0 0 0 0 0 0 0 0 0 0 8
95 0.2804 -0.3854 1.9636 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
96 0.5243 -1.6952 1.8157 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
97 0.8728 0.3499 2.7423 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
98 -0.5081 1.7381 2.0732 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
99 1.2574 -1.9530 2.4172 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
100 0.7956 -0.0449 -4.1349 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
101 -0.9532 -1.6274 -3.3210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
102 -1.6993 -1.5471 -0.9493 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
103 1.0368 1.7063 -0.1994 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
104 1.7873 1.6214 -2.5645 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
105 -1.6962 -0.5470 1.1583 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
106 2 1 0 0 0 0
107 6 1 0 0 0 0
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14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
7 19 0 0 0 0
M END
$$$$
mandelicacid1.sdf
COSMOTHERM 3D 0
19 19 0 0 0 0 0 0 0 0 0 V2000
0.1979 0.4805 -3.0994 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.4300 -0.8489 -2.7293 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.2618 -1.2454 -1.3977 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1413 -0.3175 -0.4264 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3696 1.0173 -0.8035 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.2046 1.4125 -2.1344 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.3661 -0.7714 1.0123 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.7475 -0.7717 1.3922 O 0 0 0 0 0 0 0 0 0 0 0 0 8
0.5261 0.0462 1.9577 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.1464 1.0468 2.5666 O 0 0 0 0 0 0 0 0 0 0 0 0 10
1.7173 -0.1690 2.1168 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.0823 0.1439 1.3418 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.4844 1.5543 3.1235 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.3304 0.7910 -4.1372 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.7417 -1.5799 -3.4775 H 0 0 0 0 0 0 0 0 0 0 0 0 15
0.4393 -2.2844 -1.1112 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.6767 1.7566 -0.0594 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.3835 2.4512 -2.4174 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.0339 -1.8133 1.1094 H 0 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
7 19 0 0 0 0
M END
$$$$
methanol-anion.sdf
COSMOTHERM 3D 0
5 4 0 0 0 0 0 0 0 0 0 V2000
-0.6612 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7119 0.0000 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.1400 0.3315 0.9691 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.1400 0.6732 -0.7717 H 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.1402 -1.0049 -0.1973 H 0 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
1 5 0 0 0 0
M END
$$$$
methanol.sdf
COSMOTHERM 3D 0
6 5 0 0 0 0 0 0 0 0 0 V2000
-0.7382 0.0127 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7000 -0.0651 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.1138 -1.0183 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.1211 0.5268 -0.8972 H 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.1211 0.5269 0.8971 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.0413 0.8466 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
2 6 0 0 0 0
M END
$$$$
methylthiouracil0-anion.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.8379 -0.0328 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.3249 1.1936 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 2
1.0644 1.2997 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8112 0.0645 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1467 -1.1460 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.2236 -1.2205 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 6

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1
2
3     1.6084    2.4440    0.0001 O    0 0 0 0 0 0 0 0 0 0 0 0 7
4    -2.6542   -0.0480    0.0000 S    0 0 0 0 0 0 0 0 0 0 0 0 8
5     2.9018    0.1062    0.0000 H    0 0 0 0 0 0 0 0 0 0 0 0 9
6     1.8724   -2.4645   -0.0002 C    0 0 0 0 0 0 0 0 0 0 0 0 10
7    -2.7814   -1.4020   -0.0005 H    0 0 0 0 0 0 0 0 0 0 0 0 11
8     1.5908   -3.0572   -0.8842 H    0 0 0 0 0 0 0 0 0 0 0 0 12
9     2.9609   -2.3248   -0.0018 H    0 0 0 0 0 0 0 0 0 0 0 0 13
10    1.5934   -3.0561    0.8854 H    0 0 0 0 0 0 0 0 0 0 0 0 14
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M END
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methylthiouracil0.sdf
COSMOtherm 3D 0

15 15 0 0 0 0 0 0 0 0 0 V2000
-0.9915 -0.0143 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.2822 1.1540 0.0010 N 0 0 0 0 0 0 0 0 0 0 0 0 2
1.1275 1.2923 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8404 0.0384 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1669 -1.1506 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.2154 -1.1440 0.0002 N 0 0 0 0 0 0 0 0 0 0 0 0 6
1.6263 2.4258 -0.0010 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.6818 -0.0750 -0.0003 S 0 0 0 0 0 0 0 0 0 0 0 0 8
2.9274 0.0619 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.8244 2.0196 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.7177 -2.0315 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.8159 -2.4963 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 12
1.5167 -3.0671 -0.8927 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.9060 -2.3960 0.0063 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.5058 -3.0743 0.8831 H 0 0 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
11 6 0 0 0 0
13 12 0 0 0 0
14 12 0 0 0 0
12 15 0 0 0 0

M END
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methylthiouracil1-anion.sdf
COSMOtherm 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
-0.9476 0.0740 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.3047 1.2402 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 2
1.0855 1.2826 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8201 0.0283 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1448 -1.1595 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.2297 -1.1173 0.0009 N 0 0 0 0 0 0 0 0 0 0 0 0 6
1.6738 2.3982 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.6809 -0.0609 -0.0002 S 0 0 0 0 0 0 0 0 0 0 0 0 8
2.9092 0.0449 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.7668 -1.9832 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.7796 -2.5159 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 11
1.4764 -3.0886 0.8893 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2.8717 -2.4272 -0.0053 H 0 0 0 0 0 0 0 0 0 0 0 0 13
1.4688 -3.0916 -0.8858 H 0 0 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0
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3 2 0 0 0 0
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12 11 0 0 0 0
13 11 0 0 0 0
11 14 0 0 0 0

M END
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methylthiouracil1.sdf
COSMOtherm 3D 0

15 15 0 0 0 0 0 0 0 0 0 V2000
-0.9747 0.0419 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.2969 1.2150 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 0 2
1.0337 1.1901 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8151 0.0103 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1311 -1.1842 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.2344 -1.1349 0.0004 N 0 0 0 0 0 0 0 0 0 0 0 0 6
1.6839 2.3652 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 0 7

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-2.6789 -0.0519 0.0000 S 0 0 0 0 0 0 0 0 0 0 8
2.9014 0.0457 -0.0012 H 0 0 0 0 0 0 0 0 0 0 9
-0.7658 -2.0068 0.0003 H 0 0 0 0 0 0 0 0 0 0 10
1.7724 -2.5321 0.0003 C 0 0 0 0 0 0 0 0 0 0 11
1.0133 3.0827 0.0022 H 0 0 0 0 0 0 0 0 0 0 12
1.4656 -3.1038 -0.8882 H 0 0 0 0 0 0 0 0 0 0 13
2.8632 -2.4372 0.0019 H 0 0 0 0 0 0 0 0 0 0 14
1.4631 -3.1045 0.8875 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
10 6 0 0 0 0
12 7 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
11 15 0 0 0 0
M END
$$$$
methylthiouracil2-anion.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
-0.9463 -0.1026 0.0005 C 0 0 0 0 0 0 0 0 0 0 1
-0.2906 1.1179 0.0016 N 0 0 0 0 0 0 0 0 0 0 2
1.1026 1.2938 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.8230 0.0566 0.0002 C 0 0 0 0 0 0 0 0 0 0 4
1.1329 -1.1440 0.0003 C 0 0 0 0 0 0 0 0 0 0 5
-0.2326 -1.2363 0.0005 N 0 0 0 0 0 0 0 0 0 0 6
1.5829 2.4511 -0.0010 O 0 0 0 0 0 0 0 0 0 0 7
-2.6808 -0.0880 -0.0006 S 0 0 0 0 0 0 0 0 0 0 8
2.9117 0.0899 -0.0004 H 0 0 0 0 0 0 0 0 0 0 9
-0.8641 1.9626 0.0013 H 0 0 0 0 0 0 0 0 0 0 10
1.8617 -2.4609 -0.0005 C 0 0 0 0 0 0 0 0 0 0 11
1.5825 -3.0481 -0.8888 H 0 0 0 0 0 0 0 0 0 0 12
2.9500 -2.3239 0.0056 H 0 0 0 0 0 0 0 0 0 0 13
1.5729 -3.0549 0.8801 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
11 14 0 0 0 0
M END
$$$$
methylthiouracil2.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 V2000
-0.8832 -0.0735 -0.0003 C 0 0 0 0 0 0 0 0 0 0 1
-0.2627 1.1394 -0.0010 N 0 0 0 0 0 0 0 0 0 0 2
1.1461 1.2858 0.0001 C 0 0 0 0 0 0 0 0 0 0 3
1.8367 0.0264 0.0006 C 0 0 0 0 0 0 0 0 0 0 4
1.1397 -1.1618 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
-0.2408 -1.2162 -0.0001 N 0 0 0 0 0 0 0 0 0 0 6
1.6436 2.4245 0.0003 O 0 0 0 0 0 0 0 0 0 0 7
-2.6649 -0.0237 0.0003 S 0 0 0 0 0 0 0 0 0 0 8
2.9255 0.0442 0.0012 H 0 0 0 0 0 0 0 0 0 0 9
-0.8077 2.0043 -0.0015 H 0 0 0 0 0 0 0 0 0 0 10
1.8279 -2.4938 -0.0002 C 0 0 0 0 0 0 0 0 0 0 11
-2.7868 -1.3778 0.0021 H 0 0 0 0 0 0 0 0 0 0 12
1.5270 -3.0738 0.8856 H 0 0 0 0 0 0 0 0 0 0 13
2.9186 -2.3846 -0.0025 H 0 0 0 0 0 0 0 0 0 0 14
1.5233 -3.0753 -0.8837 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 8 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
11 15 0 0 0 0
M END
$$$$
methylthiouracil3-anion.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
-0.9337 -0.0229 0.0006 C 0 0 0 0 0 0 0 0 0 0 1
-0.2970 1.1876 -0.0038 N 0 0 0 0 0 0 0 0 0 0 2
1.0323 1.1763 0.0003 C 0 0 0 0 0 0 0 0 0 0 3
1.7986 0.0016 0.0106 C 0 0 0 0 0 0 0 0 0 0 4
1.0751 -1.1949 0.0103 C 0 0 0 0 0 0 0 0 0 0 5
-0.2739 -1.2181 0.0083 N 0 0 0 0 0 0 0 0 0 0 6

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1
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3 1.6019 2.4178 -0.0049 O 0 0 0 0 0 0 0 0 0 0 7
4 -2.6840 -0.0342 -0.0014 S 0 0 0 0 0 0 0 0 0 0 8
5 2.8888 0.0182 0.0172 H 0 0 0 0 0 0 0 0 0 0 9
6 1.7758 -2.5269 -0.0107 C 0 0 0 0 0 0 0 0 0 0 10
7 2.5746 2.3251 -0.0033 H 0 0 0 0 0 0 0 0 0 0 11
8 1.7933 -2.9264 -1.0375 H 0 0 0 0 0 0 0 0 0 0 12
9 2.8138 -2.4442 0.3363 H 0 0 0 0 0 0 0 0 0 0 13
10 1.2378 -3.2528 0.6138 H 0 0 0 0 0 0 0 0 0 0 14
11 2 1 0 0 0 0
12 6 1 0 0 0 0
13 8 1 0 0 0 0
14 3 2 0 0 0 0
15 4 3 0 0 0 0
16 7 3 0 0 0 0
17 5 4 0 0 0 0
18 9 4 0 0 0 0
19 6 5 0 0 0 0
20 10 5 0 0 0 0
21 11 7 0 0 0 0
22 12 10 0 0 0 0
23 13 10 0 0 0 0
24 10 14 0 0 0 0

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M END

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methylthiouracil3.sdf

COSMOTHERM 3D

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15 15 0 0 0 0 0 0 0 0 0 V2000
1 -0.8636 -0.0436 0.0005 C 0 0 0 0 0 0 0 0 0 0 1
2 -0.3057 1.1771 -0.0026 N 0 0 0 0 0 0 0 0 0 0 2
3 1.0314 1.1961 -0.0001 C 0 0 0 0 0 0 0 0 0 0 3
4 1.8044 0.0236 0.0062 C 0 0 0 0 0 0 0 0 0 0 4
5 1.1140 -1.1875 0.0057 C 0 0 0 0 0 0 0 0 0 0 5
6 -0.2445 -1.2274 0.0044 N 0 0 0 0 0 0 0 0 0 0 6
7 1.5698 2.4358 -0.0025 O 0 0 0 0 0 0 0 0 0 0 7
8 -2.6540 -0.0140 -0.0008 S 0 0 0 0 0 0 0 0 0 0 8
9 2.8939 0.0587 0.0107 H 0 0 0 0 0 0 0 0 0 0 9
10 1.8253 -2.5078 -0.0059 C 0 0 0 0 0 0 0 0 0 0 10
11 -2.8002 -1.3659 0.0039 H 0 0 0 0 0 0 0 0 0 0 11
12 2.5455 2.3727 -0.0015 H 0 0 0 0 0 0 0 0 0 0 12
13 1.6687 -3.0081 -0.9744 H 0 0 0 0 0 0 0 0 0 0 13
14 2.9032 -2.3871 0.1542 H 0 0 0 0 0 0 0 0 0 0 14
15 1.4135 -3.1685 0.7702 H 0 0 0 0 0 0 0 0 0 0 15

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2 1 0 0 0 0

6 1 0 0 0 0

8 1 0 0 0 0

3 2 0 0 0 0

4 3 0 0 0 0

7 3 0 0 0 0

5 4 0 0 0 0

9 4 0 0 0 0

6 5 0 0 0 0

10 5 0 0 0 0

12 7 0 0 0 0

11 8 0 0 0 0

13 10 0 0 0 0

14 10 0 0 0 0

10 15 0 0 0 0

M END

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n-pentanoicacid-anion.sdf

COSMOTHERM 3D

0

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16 15 0 0 0 0 0 0 0 0 0 V2000
1 3.4621 0.3252 0.0088 C 0 0 0 0 0 0 0 0 0 0 1
2 2.2171 -0.5690 -0.0087 C 0 0 0 0 0 0 0 0 0 0 2
3 0.9015 0.2218 0.0055 C 0 0 0 0 0 0 0 0 0 0 3
4 -0.3385 -0.6732 -0.0111 C 0 0 0 0 0 0 0 0 0 0 4
5 -1.7095 0.0430 -0.0004 C 0 0 0 0 0 0 0 0 0 0 5
6 -1.7358 1.3116 -0.0065 O 0 0 0 0 0 0 0 0 0 0 6
7 -2.7340 -0.7150 0.0118 O 0 0 0 0 0 0 0 0 0 0 7
8 4.3881 -0.2692 -0.0039 H 0 0 0 0 0 0 0 0 0 0 8
9 3.4825 0.9937 -0.8666 H 0 0 0 0 0 0 0 0 0 0 9
10 3.4833 0.9575 0.9105 H 0 0 0 0 0 0 0 0 0 0 10
11 2.2415 -1.2493 0.8608 H 0 0 0 0 0 0 0 0 0 0 11
12 2.2421 -1.2158 -0.9032 H 0 0 0 0 0 0 0 0 0 0 12
13 0.8724 0.9023 -0.8623 H 0 0 0 0 0 0 0 0 0 0 13
14 0.8725 0.8696 0.8982 H 0 0 0 0 0 0 0 0 0 0 14
15 -0.3237 -1.3597 0.8537 H 0 0 0 0 0 0 0 0 0 0 15
16 -0.3223 -1.3268 -0.9012 H 0 0 0 0 0 0 0 0 0 0 16

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2 1 0 0 0 0

8 1 0 0 0 0

9 1 0 0 0 0

10 1 0 0 0 0

3 2 0 0 0 0

11 2 0 0 0 0

12 2 0 0 0 0

4 3 0 0 0 0

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14 3 0 0 0 0

5 4 0 0 0 0

15 4 0 0 0 0

6 5 0 0 0 0

7 5 0 0 0 0

4 16 0 0 0 0

M END

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n-pentanoicacid.sdf

COSMOTHERM 3D

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17 16 0 0 0 0 0 0 0 0 0 V2000
1 3.4908 0.3137 0.0067 C 0 0 0 0 0 0 0 0 0 0 1
2 2.2388 -0.5694 -0.0064 C 0 0 0 0 0 0 0 0 0 0 2
3 0.9359 0.2407 0.0041 C 0 0 0 0 0 0 0 0 0 0 3
4 -0.3026 -0.6552 -0.0086 C 0 0 0 0 0 0 0 0 0 0 4

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-1.6132 0.0935 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.7512 1.3089 -0.0046 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.6757 -0.7567 0.0087 O 0 0 0 0 0 0 0 0 0 0 0 0 7
4.4085 -0.2927 -0.0020 H 0 0 0 0 0 0 0 0 0 0 0 0 8
3.5190 0.9759 -0.8728 H 0 0 0 0 0 0 0 0 0 0 0 0 9
3.5184 0.9498 0.9053 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.2542 -1.2441 0.8668 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2.2551 -1.2192 -0.8983 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.9116 0.9125 -0.8696 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.9109 0.8881 0.8959 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.3075 -1.3363 0.8591 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.3061 -1.3112 -0.8957 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.4954 -0.2160 0.0093 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
11 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
7 17 0 0 0 0
M END
$$$$
nitroaceticacid0-anion.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 0 0 V2000
-0.0836 -1.3018 0.0018 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.9223 -0.0761 -0.0275 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.3130 -1.0607 0.0315 O 0 0 0 0 0 0 0 0 0 0 0 0 3
0.5215 -2.4048 -0.0101 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.2090 1.2254 -0.0054 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.1410 1.7207 -1.0900 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0739 1.7207 1.0984 O 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5644 -0.1145 0.8578 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.5104 -0.1133 -0.9496 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
2 9 0 0 0 0
M END
$$$$
nitroaceticacid0.sdf
COSMOTHERM 3D 0
10 9 0 0 0 0 0 0 0 0 0 0 V2000
1.2892 -0.0350 -0.0202 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0663 -0.9418 -0.0924 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.9834 1.2698 -0.0459 O 0 0 0 0 0 0 0 0 0 0 0 0 3
2.4130 -0.4967 0.0329 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.2385 -0.1875 0.0126 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.6403 0.0951 1.1454 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.8141 0.1132 -1.0382 O 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0667 -1.4686 -1.0531 H 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0973 -1.6563 0.7368 H 0 0 0 0 0 0 0 0 0 0 0 0 9
1.8144 1.7936 -0.0107 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
9 2 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
3 10 0 0 0 0
M END
$$$$
nitroaceticacid1-anion.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 0 0 V2000
-0.0836 -1.3019 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.9222 -0.0759 0.0277 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.5218 -2.4047 0.0041 O 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.3133 -1.0610 -0.0175 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.2090 1.2254 0.0027 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.1313 1.7294 1.0864 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0834 1.7122 -1.1025 O 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5101 -0.1119 0.9500 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.5645 -0.1158 -0.8575 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
2 9 0 0 0 0
M END
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nitroaceticacid1.sdf
COSMOTHERM 3D 0
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10 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
  1.2067 0.0699 -0.0774 C 0 0 0 0 0 0 0 0 0 0 0 0 1
  0.0526 -0.8445 0.3197 C 0 0 0 0 0 0 0 0 0 0 0 0 2
  2.3685 -0.5317 0.2317 O 0 0 0 0 0 0 0 0 0 0 0 0 3
  1.0959 1.1587 -0.6053 O 0 0 0 0 0 0 0 0 0 0 0 0 4
  -1.2618 -0.1421 0.1013 N 0 0 0 0 0 0 0 0 0 0 0 0 5
  -1.9578 -0.5063 -0.8509 O 0 0 0 0 0 0 0 0 0 0 0 0 6
  -1.5538 0.7621 0.8884 O 0 0 0 0 0 0 0 0 0 0 0 0 7
  0.0564 -1.7534 -0.2908 H 0 0 0 0 0 0 0 0 0 0 0 0 8
  0.1125 -1.1005 1.3838 H 0 0 0 0 0 0 0 0 0 0 0 0 9
  3.1095 0.0482 -0.0529 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
9 2 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
3 10 0 0 0 0
```

M END

```
$$$$
nitroaceticacid2-anion.sdf
COSMOtherm 3D 0
```

```
9 8 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-0.0832 -1.3016 -0.0071 C 0 0 0 0 0 0 0 0 0 0 0 0 1
  0.9218 -0.0763 0.0380 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.3115 -1.0604 -0.0680 O 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.5209 -2.4048 0.0243 O 0 0 0 0 0 0 0 0 0 0 0 0 4
  0.2087 1.2254 0.0121 N 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.1711 1.7055 1.0938 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0442 1.7358 -1.0920 O 0 0 0 0 0 0 0 0 0 0 0 0 7
  1.4986 -0.1165 0.9671 H 0 0 0 0 0 0 0 0 0 0 0 0 8
  1.5748 -0.1112 -0.8395 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
2 9 0 0 0 0
```

M END

```
$$$$
nitroaceticacid2.sdf
COSMOtherm 3D 0
```

```
10 9 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
  1.3161 -0.1167 -0.0066 C 0 0 0 0 0 0 0 0 0 0 0 0 1
  0.0008 -0.8006 -0.3947 C 0 0 0 0 0 0 0 0 0 0 0 0 2
  1.3341 1.2138 0.0994 O 0 0 0 0 0 0 0 0 0 0 0 0 3
  2.3165 -0.7940 0.1434 O 0 0 0 0 0 0 0 0 0 0 0 0 4
  -1.2794 -0.0784 -0.0311 N 0 0 0 0 0 0 0 0 0 0 0 0 5
  -1.2901 1.1675 -0.0953 O 0 0 0 0 0 0 0 0 0 0 0 0 6
  -2.2492 -0.7588 0.2744 O 0 0 0 0 0 0 0 0 0 0 0 0 7
  -0.0288 -0.8920 -1.4912 H 0 0 0 0 0 0 0 0 0 0 0 0 8
  -0.0566 -1.7940 0.0559 H 0 0 0 0 0 0 0 0 0 0 0 0 9
  0.4049 1.5557 -0.0481 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
9 2 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
3 10 0 0 0 0
```

M END

```
$$$$
nitromethane-anion.sdf
COSMOtherm 3D 0
```

```
6 5 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.3632 -0.0032 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.0301 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 2
  0.6403 1.1208 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.6456 -1.1179 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 4
  -1.8719 -0.9617 0.0007 H 0 0 0 0 0 0 0 0 0 0 0 0 5
  -1.8765 0.9530 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
5 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
1 6 0 0 0 0
```

M END

```
$$$$
nitromethane.sdf
COSMOtherm 3D 0
```

```
7 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.4172 -0.0663 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
  0.0823 -0.0004 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 2
  0.6013 1.1225 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.7207 -1.0602 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 4
  -1.7180 -1.1151 -0.0012 H 0 0 0 0 0 0 0 0 0 0 0 0 5
  -1.7609 0.4593 -0.8975 H 0 0 0 0 0 0 0 0 0 0 0 0 6
  -1.7610 0.4614 -0.8961 H 0 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
1 7 0 0 0 0
```

M END


```
1
2
3
4 nitrousacid-anion.sdf
5 COSMOtherm 3D 0
6 3 2 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
7 0.0000 -0.4717 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
8 -1.0785 0.2065 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
9 1.0785 0.2065 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
10 2 1 0 0 0 0
11 1 3 0 0 0 0
```

M END

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```
12 nitrousacid.sdf
13 COSMOtherm 3D 0
14 4 3 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
15 0.1449 -0.5058 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
16 -1.1286 0.1212 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
17 1.0626 0.2522 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
18 -0.9674 1.1007 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
19 2 1 0 0 0 0
20 3 1 0 0 0 0
21 2 4 0 0 0 0
```

M END

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```
22 oxalicacid0.sdf
23 COSMOtherm 3D 0
24 8 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
25 0.7669 0.1136 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
26 -0.7668 -0.1136 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
27 1.2892 1.2109 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
28 -1.4058 1.0623 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
29 -1.2892 -1.2109 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
30 1.4058 -1.0623 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
31 -2.3737 0.8904 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
32 2.3737 -0.8904 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
33 2 1 0 0 0 0
34 3 1 0 0 0 0
35 6 1 0 0 0 0
36 4 2 0 0 0 0
37 5 2 0 0 0 0
38 7 4 0 0 0 0
39 6 8 0 0 0 0
```

M END

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```
41 oxalicacid2--anion.sdf
42 COSMOtherm 3D 0
43 7 6 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
44 0.7547 -0.1253 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
45 -0.8215 -0.0393 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
46 1.4226 -1.1457 -0.0008 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
47 -1.4691 -1.1065 0.0009 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
48 -1.2374 1.1645 -0.0009 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
49 1.3037 1.1049 0.0010 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
50 0.4819 1.6887 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
51 2 1 0 0 0 0
52 3 1 0 0 0 0
53 6 1 0 0 0 0
54 4 2 0 0 0 0
55 5 2 0 0 0 0
56 6 7 0 0 0 0
```

M END

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```
58 pamoicacid-anion0.sdf
59 COSMOtherm 3D 0
60 44 48 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
61 4.6749 -2.6323 -0.4341 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
62 3.5586 -3.0106 -1.2204 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
63 2.4672 -2.1726 -1.3604 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
64 2.4154 -0.8927 -0.7262 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
65 3.5749 -0.5060 0.0422 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
66 4.6783 -1.3958 0.1780 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
67 1.2980 0.0024 -0.8287 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
68 1.4098 1.3004 -0.3011 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
69 2.5759 1.6820 0.4523 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
70 3.6077 0.7746 0.6346 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
71 0.0154 -0.4033 -1.5507 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
72 -1.2595 -0.4812 -0.7149 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
73 -1.6059 -1.6301 0.0584 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
74 -2.8867 -1.6866 0.7305 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
75 -3.7755 -0.5931 0.6126 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
76 -3.4381 0.5319 -0.1184 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
77 -2.1594 0.5983 -0.7887 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
78 -1.1131 -3.8581 0.9598 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
79 -2.3728 -3.9075 1.6092 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
80 -3.2371 -2.8370 1.4931 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
81 -0.7419 -2.7569 0.2102 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
82 -1.8336 1.7072 -1.4623 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
83 0.4525 2.2421 -0.4266 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
84 -4.3972 1.6784 -0.2007 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
85 2.7313 3.0573 0.9995 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
86 -2.9698 2.4649 -1.2400 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
87 -0.3937 1.9597 -0.9364 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
88 -3.9659 2.7369 -0.8933 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 28
89 -5.5142 1.6678 0.3306 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29
90 2.3147 4.0937 0.4974 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 30
91 3.4498 3.0627 2.1609 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 31
92 5.5254 -3.3074 -0.3286 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 32
93 3.5592 -3.9768 -1.7287 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 33
94 1.6460 -2.5029 -1.9955 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 34
95 5.5352 -1.0714 0.7730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 35
96 4.4817 1.0647 1.2184 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 36
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3.4463 4.1253 2.4071 H 0 0 0 0 0 0 0 0 0 0 0 44
2 1 0 0 0 0
6 1 0 0 0 0
32 1 0 0 0 0
3 2 0 0 0 0
33 2 0 0 0 0
4 3 0 0 0 0
34 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
35 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
25 9 0 0 0 0
36 10 0 0 0 0
12 11 0 0 0 0
37 11 0 0 0 0
38 11 0 0 0 0
13 12 0 0 0 0
17 12 0 0 0 0
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22 17 0 0 0 0
19 18 0 0 0 0
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40 18 0 0 0 0
20 19 0 0 0 0
41 19 0 0 0 0
42 20 0 0 0 0
43 21 0 0 0 0
26 22 0 0 0 0
27 23 0 0 0 0
28 24 0 0 0 0
29 24 0 0 0 0
30 25 0 0 0 0
31 25 0 0 0 0
28 26 0 0 0 0
31 44 0 0 0 0

```

```

M END
$$$$
pamoicacid-anion2.sdf
COSMOTHERM 3D 0

```

```

44 48 0 0 0 0 0 0 0 0 0 V2000
3.8317 -1.7658 -1.2969 C 0 0 0 0 0 0 0 0 0 0 1
3.5234 -1.0012 -0.1423 C 0 0 0 0 0 0 0 0 0 0 2
2.4170 -0.1729 -0.1066 C 0 0 0 0 0 0 0 0 0 0 3
1.5482 -0.0531 -1.2311 C 0 0 0 0 0 0 0 0 0 0 4
1.8858 -0.8106 -2.4142 C 0 0 0 0 0 0 0 0 0 0 5
3.0288 -1.6630 -2.4125 C 0 0 0 0 0 0 0 0 0 0 6
0.3921 0.7891 -1.2212 C 0 0 0 0 0 0 0 0 0 0 7
-0.3429 0.9297 -2.4022 C 0 0 0 0 0 0 0 0 0 0 8
-0.0026 0.1836 -3.5870 C 0 0 0 0 0 0 0 0 0 0 9
1.0909 -0.6740 -3.5690 C 0 0 0 0 0 0 0 0 0 0 10
-0.0160 1.5827 0.0152 C 0 0 0 0 0 0 0 0 0 0 11
-0.4137 0.7784 1.2488 C 0 0 0 0 0 0 0 0 0 0 12
-1.5756 -0.0543 1.2710 C 0 0 0 0 0 0 0 0 0 0 13
-1.9027 -0.8036 2.4622 C 0 0 0 0 0 0 0 0 0 0 14
-1.0828 -0.6664 3.6079 C 0 0 0 0 0 0 0 0 0 0 15
0.0185 0.1677 3.6126 C 0 0 0 0 0 0 0 0 0 0 16
0.3403 0.9154 2.4229 C 0 0 0 0 0 0 0 0 0 0 17
-3.5737 -0.9944 0.2073 C 0 0 0 0 0 0 0 0 0 0 18
-3.8740 -1.7465 1.3705 C 0 0 0 0 0 0 0 0 0 0 19
-3.0533 -1.6417 2.4765 C 0 0 0 0 0 0 0 0 0 0 20
-2.4593 -0.1764 0.1572 C 0 0 0 0 0 0 0 0 0 0 21
1.4160 1.7382 2.4488 O 0 0 0 0 0 0 0 0 0 0 22
-1.4102 1.7752 -2.4180 O 0 0 0 0 0 0 0 0 0 0 23
0.8625 0.3105 4.8646 C 0 0 0 0 0 0 0 0 0 0 24
-0.8206 0.3465 -4.7980 C 0 0 0 0 0 0 0 0 0 0 25
1.7846 1.6092 3.4454 H 0 0 0 0 0 0 0 0 0 0 26
-1.8020 1.7189 -3.3430 H 0 0 0 0 0 0 0 0 0 0 27
1.8701 1.1277 4.7803 O 0 0 0 0 0 0 0 0 0 0 28
0.5707 -0.3409 5.8945 O 0 0 0 0 0 0 0 0 0 0 29
-1.8058 1.1035 -4.8697 O 0 0 0 0 0 0 0 0 0 0 30
-0.4297 -0.3931 -5.8519 O 0 0 0 0 0 0 0 0 0 0 31
4.7063 -2.4183 -1.3019 H 0 0 0 0 0 0 0 0 0 0 32
4.1741 -1.0659 0.7322 H 0 0 0 0 0 0 0 0 0 0 33
2.2214 0.4177 0.7878 H 0 0 0 0 0 0 0 0 0 0 34
3.2575 -2.2288 -3.3186 H 0 0 0 0 0 0 0 0 0 0 35
1.3455 -1.2447 -4.4625 H 0 0 0 0 0 0 0 0 0 0 36
-0.8459 2.2448 -0.2672 H 0 0 0 0 0 0 0 0 0 0 37
0.8170 2.2397 0.3036 H 0 0 0 0 0 0 0 0 0 0 38
-1.3188 -1.2288 4.5141 H 0 0 0 0 0 0 0 0 0 0 39
-4.2335 -1.0589 -0.6607 H 0 0 0 0 0 0 0 0 0 0 40
-4.7543 -2.3913 1.3927 H 0 0 0 0 0 0 0 0 0 0 41
-3.2771 -2.2014 3.3882 H 0 0 0 0 0 0 0 0 0 0 42
-2.2676 0.4056 -0.7432 H 0 0 0 0 0 0 0 0 0 0 43
-1.0402 -0.2064 -6.5977 H 0 0 0 0 0 0 0 0 0 0 44
2 1 0 0 0 0
6 1 0 0 0 0
32 1 0 0 0 0
3 2 0 0 0 0
33 2 0 0 0 0
4 3 0 0 0 0

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For Peer Review Only

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34 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
35 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
25 9 0 0 0 0
36 10 0 0 0 0
12 11 0 0 0 0
37 11 0 0 0 0
38 11 0 0 0 0
13 12 0 0 0 0
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14 13 0 0 0 0
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16 15 0 0 0 0
39 15 0 0 0 0
17 16 0 0 0 0
24 16 0 0 0 0
22 17 0 0 0 0
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40 18 0 0 0 0
20 19 0 0 0 0
41 19 0 0 0 0
42 20 0 0 0 0
43 21 0 0 0 0
26 22 0 0 0 0
27 23 0 0 0 0
28 24 0 0 0 0
29 24 0 0 0 0
30 25 0 0 0 0
31 25 0 0 0 0
28 26 0 0 0 0
31 44 0 0 0 0
M END
$$$$
pamoicacid-anion3.sdf
COSMOtherm 3D 0
44 48 0 0 0 0 0 0 0 0 0 V2000
4.9618 1.1051 -2.1600 C 0 0 0 0 0 0 0 0 0 0 1
3.8007 1.7790 -2.6176 C 0 0 0 0 0 0 0 0 0 0 2
2.6109 1.7081 -1.9181 C 0 0 0 0 0 0 0 0 0 0 3
2.4981 0.9599 -0.7059 C 0 0 0 0 0 0 0 0 0 0 4
3.6899 0.2773 -0.2483 C 0 0 0 0 0 0 0 0 0 0 5
4.9005 0.3702 -0.9959 C 0 0 0 0 0 0 0 0 0 0 6
1.2832 0.8562 0.0445 C 0 0 0 0 0 0 0 0 0 0 7
1.2957 0.1437 1.2490 C 0 0 0 0 0 0 0 0 0 0 8
2.4778 -0.5458 1.6973 C 0 0 0 0 0 0 0 0 0 0 9
3.6444 -0.4676 0.9458 C 0 0 0 0 0 0 0 0 0 0 10
0.0006 1.5595 -0.3772 C 0 0 0 0 0 0 0 0 0 0 11
-1.2531 0.7051 -0.5046 C 0 0 0 0 0 0 0 0 0 0 12
-1.3446 -0.3854 -1.4209 C 0 0 0 0 0 0 0 0 0 0 13
-2.5650 -1.1556 -1.5059 C 0 0 0 0 0 0 0 0 0 0 14
-3.6614 -0.7954 -0.6869 C 0 0 0 0 0 0 0 0 0 0 15
-3.5950 0.2794 0.1800 C 0 0 0 0 0 0 0 0 0 0 16
-2.3798 1.0504 0.2548 C 0 0 0 0 0 0 0 0 0 0 17
-0.3948 -1.8195 -3.1709 C 0 0 0 0 0 0 0 0 0 0 18
-1.5921 -2.5764 -3.2398 C 0 0 0 0 0 0 0 0 0 0 19
-2.6534 -2.2424 -2.4215 C 0 0 0 0 0 0 0 0 0 0 20
-0.2736 -0.7617 -2.2881 C 0 0 0 0 0 0 0 0 0 0 21
-2.3396 2.1171 1.0856 O 0 0 0 0 0 0 0 0 0 0 22
0.1652 0.1190 1.9955 O 0 0 0 0 0 0 0 0 0 0 23
-4.7974 0.6462 1.0296 C 0 0 0 0 0 0 0 0 0 0 24
2.4321 -1.3070 2.9548 C 0 0 0 0 0 0 0 0 0 0 25
-3.3071 2.1107 1.5217 H 0 0 0 0 0 0 0 0 0 0 26
0.3706 -0.4458 2.7997 H 0 0 0 0 0 0 0 0 0 0 27
-4.6567 1.6848 1.7977 O 0 0 0 0 0 0 0 0 0 0 28
-5.8440 -0.0417 0.9621 O 0 0 0 0 0 0 0 0 0 0 29
1.4256 -1.3819 3.6817 O 0 0 0 0 0 0 0 0 0 0 30
3.5775 -1.9371 3.2783 O 0 0 0 0 0 0 0 0 0 0 31
5.8921 1.1729 -2.7258 H 0 0 0 0 0 0 0 0 0 0 32
3.8462 2.3647 -3.5377 H 0 0 0 0 0 0 0 0 0 0 33
1.7488 2.2484 -2.3078 H 0 0 0 0 0 0 0 0 0 0 34
5.7817 -0.1561 -0.6221 H 0 0 0 0 0 0 0 0 0 0 35
4.5417 -0.9860 1.2846 H 0 0 0 0 0 0 0 0 0 0 36
0.1664 2.0827 -1.3287 H 0 0 0 0 0 0 0 0 0 0 37
-0.2195 2.3430 0.3625 H 0 0 0 0 0 0 0 0 0 0 38
-4.5886 -1.3705 -0.7371 H 0 0 0 0 0 0 0 0 0 0 39
0.4428 -2.0756 -3.8233 H 0 0 0 0 0 0 0 0 0 0 40
-1.6728 -3.4098 -3.9399 H 0 0 0 0 0 0 0 0 0 0 41
-3.5875 -2.8082 -2.4662 H 0 0 0 0 0 0 0 0 0 0 42
0.6596 -0.2012 -2.2602 H 0 0 0 0 0 0 0 0 0 0 43
3.4346 -2.4091 4.1271 H 0 0 0 0 0 0 0 0 0 0 44
2 1 0 0 0 0
6 1 0 0 0 0
32 1 0 0 0 0
3 2 0 0 0 0
33 2 0 0 0 0
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11 7 0 0 0 0
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30 25 0 0 0 0
31 25 0 0 0 0
28 26 0 0 0 0
31 44 0 0 0 0
M END
$$$$
pamoicacid0.sdf
COSMOTHERM 3D 0
45 48 0 0 0 0 0 0 0 0 0 V2000
4.9793 -2.1643 1.0661 C 0 0 0 0 0 0 0 0 0 0 0 1
3.8258 -2.6199 1.7539 C 0 0 0 0 0 0 0 0 0 0 0 2
2.6350 -1.9208 1.6940 C 0 0 0 0 0 0 0 0 0 0 0 3
2.5168 -0.7071 0.9500 C 0 0 0 0 0 0 0 0 0 0 0 4
3.7019 -0.2486 0.2571 C 0 0 0 0 0 0 0 0 0 0 0 5
4.9132 -0.9961 0.3378 C 0 0 0 0 0 0 0 0 0 0 0 6
1.3010 0.0428 0.8528 C 0 0 0 0 0 0 0 0 0 0 0 7
1.3076 1.2508 0.1477 C 0 0 0 0 0 0 0 0 0 0 0 8
2.4848 1.7029 -0.5472 C 0 0 0 0 0 0 0 0 0 0 0 9
3.6509 0.9501 -0.4810 C 0 0 0 0 0 0 0 0 0 0 0 10
0.0251 -0.3805 1.5683 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.2329 -0.5024 0.7199 C 0 0 0 0 0 0 0 0 0 0 0 12
-1.3295 -1.4270 -0.3635 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.5461 -1.5111 -1.1396 C 0 0 0 0 0 0 0 0 0 0 0 14
-3.6404 -0.6959 -0.7908 C 0 0 0 0 0 0 0 0 0 0 0 15
-3.5678 0.1783 0.2879 C 0 0 0 0 0 0 0 0 0 0 0 16
-2.3516 0.2656 1.0558 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.3832 -3.1831 -1.7852 C 0 0 0 0 0 0 0 0 0 0 0 18
-1.5769 -3.2501 -2.5499 C 0 0 0 0 0 0 0 0 0 0 0 19
-2.6356 -2.4281 -2.2279 C 0 0 0 0 0 0 0 0 0 0 0 20
-0.2617 -2.3006 -0.7288 C 0 0 0 0 0 0 0 0 0 0 0 21
-2.2806 1.1039 2.1213 O 0 0 0 0 0 0 0 0 0 0 0 22
0.1738 1.9923 0.1290 O 0 0 0 0 0 0 0 0 0 0 0 23
-4.7171 1.0140 0.6657 C 0 0 0 0 0 0 0 0 0 0 0 24
2.4355 2.9685 -1.2949 C 0 0 0 0 0 0 0 0 0 0 0 25
-3.1679 1.5727 2.1711 H 0 0 0 0 0 0 0 0 0 0 0 26
0.3728 2.7986 -0.4358 H 0 0 0 0 0 0 0 0 0 0 0 27
-4.7017 1.8266 1.6078 O 0 0 0 0 0 0 0 0 0 0 0 28
-5.8196 0.8363 -0.0864 O 0 0 0 0 0 0 0 0 0 0 0 29
1.4260 3.6920 -1.3615 O 0 0 0 0 0 0 0 0 0 0 0 30
3.5800 3.3031 -1.9196 O 0 0 0 0 0 0 0 0 0 0 0 31
5.9102 -2.7300 1.1251 H 0 0 0 0 0 0 0 0 0 0 0 32
3.8759 -3.5422 2.3357 H 0 0 0 0 0 0 0 0 0 0 0 33
1.7796 -2.3090 2.2461 H 0 0 0 0 0 0 0 0 0 0 0 34
5.7891 -0.6225 -0.1974 H 0 0 0 0 0 0 0 0 0 0 0 35
4.5434 1.2889 -1.0075 H 0 0 0 0 0 0 0 0 0 0 0 36
-0.1819 0.3490 2.3636 H 0 0 0 0 0 0 0 0 0 0 0 37
0.1895 -1.3397 2.0768 H 0 0 0 0 0 0 0 0 0 0 0 38
-4.5595 -0.7588 -1.3738 H 0 0 0 0 0 0 0 0 0 0 0 39
0.4514 -3.8414 -2.0348 H 0 0 0 0 0 0 0 0 0 0 0 40
-1.6531 -3.9518 -3.3818 H 0 0 0 0 0 0 0 0 0 0 0 41
-3.5669 -2.4694 -2.7973 H 0 0 0 0 0 0 0 0 0 0 0 42
0.6684 -2.2764 -0.1638 H 0 0 0 0 0 0 0 0 0 0 0 43
-6.5154 1.4436 0.2464 H 0 0 0 0 0 0 0 0 0 0 0 44
3.4360 4.1572 -2.3817 H 0 0 0 0 0 0 0 0 0 0 0 45
2 1 0 0 0 0
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3 2 0 0 0 0
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4 3 0 0 0 0
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6 5 0 0 0 0
10 5 0 0 0 0
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10 9 0 0 0 0
25 9 0 0 0 0
36 10 0 0 0 0

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3 21 13 0 0 0 0
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9 24 16 0 0 0 0
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14 20 19 0 0 0 0
15 41 19 0 0 0 0
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18 26 22 0 0 0 0
19 27 23 0 0 0 0
20 28 24 0 0 0 0
21 29 24 0 0 0 0
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23 31 25 0 0 0 0
24 44 29 0 0 0 0
25 31 45 0 0 0 0
26 M END
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30
31 45 48 0 0 0 0 0 0 0 0 0 v2000
32 5.0157 -2.1027 1.0764 C 0 0 0 0 0 0 0 0 0 0 0 1
33 3.8679 -2.5811 1.7581 C 0 0 0 0 0 0 0 0 0 0 0 2
34 2.6655 -1.9021 1.6968 C 0 0 0 0 0 0 0 0 0 0 0 3
35 2.5285 -0.6916 0.9507 C 0 0 0 0 0 0 0 0 0 0 0 4
36 3.7056 -0.2126 0.2616 C 0 0 0 0 0 0 0 0 0 0 0 5
37 4.9296 -0.9387 0.3434 C 0 0 0 0 0 0 0 0 0 0 0 6
38 1.3044 0.0434 0.8519 C 0 0 0 0 0 0 0 0 0 0 0 7
39 1.2881 1.2532 0.1466 C 0 0 0 0 0 0 0 0 0 0 0 8
40 2.4558 1.7226 -0.5532 C 0 0 0 0 0 0 0 0 0 0 0 9
41 3.6289 0.9815 -0.4794 C 0 0 0 0 0 0 0 0 0 0 0 10
42 0.0348 -0.4042 1.5659 C 0 0 0 0 0 0 0 0 0 0 0 11
43 -1.2259 -0.5286 0.7204 C 0 0 0 0 0 0 0 0 0 0 0 12
44 -1.3072 -1.4415 -0.3732 C 0 0 0 0 0 0 0 0 0 0 0 13
45 -2.5207 -1.5292 -1.1501 C 0 0 0 0 0 0 0 0 0 0 0 14
46 -3.6169 -0.7226 -0.7932 C 0 0 0 0 0 0 0 0 0 0 0 15
47 -3.5638 0.1446 0.2926 C 0 0 0 0 0 0 0 0 0 0 0 16
48 -2.3519 0.2274 1.0673 C 0 0 0 0 0 0 0 0 0 0 0 17
49 -0.3430 -3.1755 -1.8089 C 0 0 0 0 0 0 0 0 0 0 0 18
50 -1.5354 -3.2459 -2.5753 C 0 0 0 0 0 0 0 0 0 0 0 19
51 -2.6021 -2.4368 -2.2467 C 0 0 0 0 0 0 0 0 0 0 0 20
52 -0.2300 -2.3011 -0.7447 C 0 0 0 0 0 0 0 0 0 0 0 21
53 -2.2501 1.0398 2.1559 O 0 0 0 0 0 0 0 0 0 0 0 22
54 0.1234 1.9535 0.1637 O 0 0 0 0 0 0 0 0 0 0 0 23
55 -4.7939 0.9283 0.5626 C 0 0 0 0 0 0 0 0 0 0 0 24
56 2.5131 2.9669 -1.3593 C 0 0 0 0 0 0 0 0 0 0 0 25
57 -3.1034 1.5225 2.2731 H 0 0 0 0 0 0 0 0 0 0 0 26
58 0.2342 2.7697 -0.3808 H 0 0 0 0 0 0 0 0 0 0 0 27
59 -5.8324 0.8652 -0.0811 O 0 0 0 0 0 0 0 0 0 0 0 28
60 -4.6759 1.7713 1.6369 O 0 0 0 0 0 0 0 0 0 0 0 29
61 3.4871 3.3633 -1.9845 O 0 0 0 0 0 0 0 0 0 0 0 30
62 1.3381 3.6711 -1.3521 O 0 0 0 0 0 0 0 0 0 0 0 31
63 5.9561 -2.6523 1.1372 H 0 0 0 0 0 0 0 0 0 0 0 32
64 3.9334 -3.5011 2.3419 H 0 0 0 0 0 0 0 0 0 0 0 33
65 1.8153 -2.3070 2.2447 H 0 0 0 0 0 0 0 0 0 0 0 34
66 5.8003 -0.5493 -0.1890 H 0 0 0 0 0 0 0 0 0 0 0 35
67 4.5108 1.3441 -1.0098 H 0 0 0 0 0 0 0 0 0 0 0 36
68 -0.1740 0.3082 2.3753 H 0 0 0 0 0 0 0 0 0 0 0 37
69 0.2124 -1.3704 2.0562 H 0 0 0 0 0 0 0 0 0 0 0 38
70 -4.5392 -0.7766 -1.3736 H 0 0 0 0 0 0 0 0 0 0 0 39
71 0.4982 -3.8230 -2.0644 H 0 0 0 0 0 0 0 0 0 0 0 40
72 -1.6047 -3.9412 -3.4131 H 0 0 0 0 0 0 0 0 0 0 0 41
73 -3.5321 -2.4806 -2.8180 H 0 0 0 0 0 0 0 0 0 0 0 42
74 0.6999 -2.2732 -0.1794 H 0 0 0 0 0 0 0 0 0 0 0 43
75 -5.5193 2.2559 1.7674 H 0 0 0 0 0 0 0 0 0 0 0 44
76 1.4339 4.4751 -1.9068 H 0 0 0 0 0 0 0 0 0 0 0 45
77 2 1 0 0 0 0 0
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85 7 4 0 0 0 0 0
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100 17 12 0 0 0 0 0
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102 21 13 0 0 0 0 0
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104 20 14 0 0 0 0 0
105 16 15 0 0 0 0 0
106 39 15 0 0 0 0 0
107 17 16 0 0 0 0 0

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5 19 18 0 0 0 0
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8 20 19 0 0 0 0
9 41 19 0 0 0 0
10 42 20 0 0 0 0
11 43 21 0 0 0 0
12 26 22 0 0 0 0
13 27 23 0 0 0 0
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15 29 24 0 0 0 0
16 30 25 0 0 0 0
17 31 25 0 0 0 0
18 44 29 0 0 0 0
19 31 45 0 0 0 0
20 M END
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23 COSMOTHERM 3D 0
24
25 45 48 0 0 0 0 0 0 0 0 0 V2000
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27 3.6428 -1.3041 -2.9453 C 0 0 0 0 0 0 0 0 0 0 0 2
28 2.5259 -1.3882 -2.1349 C 0 0 0 0 0 0 0 0 0 0 0 3
29 2.4801 -0.7485 -0.8597 C 0 0 0 0 0 0 0 0 0 0 0 4
30 3.6631 -0.0292 -0.4456 C 0 0 0 0 0 0 0 0 0 0 0 5
31 4.7938 0.0474 -1.3101 C 0 0 0 0 0 0 0 0 0 0 0 6
32 1.3447 -0.7984 0.0134 C 0 0 0 0 0 0 0 0 0 0 0 7
33 1.4573 -0.2551 1.2942 C 0 0 0 0 0 0 0 0 0 0 0 8
34 2.6286 0.4632 1.7120 C 0 0 0 0 0 0 0 0 0 0 0 9
35 3.6953 0.5685 0.8290 C 0 0 0 0 0 0 0 0 0 0 0 10
36 0.0459 -1.5009 -0.3706 C 0 0 0 0 0 0 0 0 0 0 0 11
37 -1.2319 -0.6638 -0.4358 C 0 0 0 0 0 0 0 0 0 0 0 12
38 -1.5100 0.1661 -1.5715 C 0 0 0 0 0 0 0 0 0 0 0 13
39 -2.8118 0.7674 -1.7167 C 0 0 0 0 0 0 0 0 0 0 0 14
40 -3.7875 0.5406 -0.7208 C 0 0 0 0 0 0 0 0 0 0 0 15
41 -3.5028 -0.2016 0.4136 C 0 0 0 0 0 0 0 0 0 0 0 16
42 -2.2102 -0.8054 0.5554 C 0 0 0 0 0 0 0 0 0 0 0 17
43 -0.8704 1.1962 -3.6994 C 0 0 0 0 0 0 0 0 0 0 0 18
44 -2.1525 1.7833 -3.8335 C 0 0 0 0 0 0 0 0 0 0 0 19
45 -3.1026 1.5708 -2.8553 C 0 0 0 0 0 0 0 0 0 0 0 20
46 -0.5587 0.4110 -2.6038 C 0 0 0 0 0 0 0 0 0 0 0 21
47 -2.0006 -1.5836 1.6590 O 0 0 0 0 0 0 0 0 0 0 0 22
48 0.3957 -0.4414 2.1371 O 0 0 0 0 0 0 0 0 0 0 0 23
49 -4.5966 -0.3024 1.4248 C 0 0 0 0 0 0 0 0 0 0 0 24
50 2.7968 1.1045 3.0399 C 0 0 0 0 0 0 0 0 0 0 0 25
51 -1.0557 -1.4581 1.9249 H 0 0 0 0 0 0 0 0 0 0 0 26
52 0.5820 -0.0068 3.0078 H 0 0 0 0 0 0 0 0 0 0 0 27
53 -5.7886 -0.3124 1.1279 O 0 0 0 0 0 0 0 0 0 0 0 28
54 -4.1780 -0.3186 2.7109 O 0 0 0 0 0 0 0 0 0 0 0 29
55 3.7717 1.7474 3.3988 O 0 0 0 0 0 0 0 0 0 0 0 30
56 1.7225 0.9101 3.8685 O 0 0 0 0 0 0 0 0 0 0 0 31
57 5.6570 -0.5124 -3.1970 H 0 0 0 0 0 0 0 0 0 0 0 32
58 3.6424 -1.8139 -3.9104 H 0 0 0 0 0 0 0 0 0 0 0 33
59 1.6788 -1.9780 -2.4837 H 0 0 0 0 0 0 0 0 0 0 0 34
60 5.6704 0.6027 -0.9696 H 0 0 0 0 0 0 0 0 0 0 0 35
61 4.5824 1.1200 1.1438 H 0 0 0 0 0 0 0 0 0 0 0 36
62 -0.1207 -2.3334 0.3308 H 0 0 0 0 0 0 0 0 0 0 0 37
63 0.1712 -1.9785 -1.3496 H 0 0 0 0 0 0 0 0 0 0 0 38
64 -4.7779 0.9855 -0.8298 H 0 0 0 0 0 0 0 0 0 0 0 39
65 -0.1166 1.3685 -4.4700 H 0 0 0 0 0 0 0 0 0 0 0 40
66 -2.3824 2.3999 -4.7037 H 0 0 0 0 0 0 0 0 0 0 0 41
67 -4.0970 2.0148 -2.9392 H 0 0 0 0 0 0 0 0 0 0 0 42
68 0.4407 -0.0134 -2.5283 H 0 0 0 0 0 0 0 0 0 0 0 43
69 -4.9820 -0.3580 3.2743 H 0 0 0 0 0 0 0 0 0 0 0 44
70 1.8790 1.3566 4.7284 H 0 0 0 0 0 0 0 0 0 0 0 45
71 2 1 0 0 0 0
72 6 1 0 0 0 0
73 32 1 0 0 0 0
74 3 2 0 0 0 0
75 33 2 0 0 0 0
76 4 3 0 0 0 0
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79 7 4 0 0 0 0
80 6 5 0 0 0 0
81 10 5 0 0 0 0
82 35 6 0 0 0 0
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84 11 7 0 0 0 0
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103 22 17 0 0 0 0
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105 21 18 0 0 0 0
106 40 18 0 0 0 0
107 20 19 0 0 0 0

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3 29 24 0 0 0 0
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5 31 25 0 0 0 0
6 44 29 0 0 0 0
7 31 45 0 0 0 0
8 M END
9 $$$$
10 pentachlorophenol-anion.sdf
11 COSMOTHERM 3D 0
12 12 12 0 0 0 0 0 0 0 0 V2000
13 0.4489 1.2096 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
14 -0.9459 1.2075 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
15 -1.7440 0.0000 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 3
16 -0.9459 -1.2075 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
17 0.4489 -1.2096 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
18 1.1690 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
19 -3.0121 0.0000 -0.0005 O 0 0 0 0 0 0 0 0 0 0 0 7
20 -1.8479 2.7192 0.0002 Cl 0 0 0 0 0 0 0 0 0 0 0 8
21 1.3301 2.7349 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 9
22 2.9266 0.0000 -0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 10
23 1.3301 -2.7349 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 11
24 -1.8480 -2.7192 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 12
25 2 1 0 0 0 0
26 6 1 0 0 0 0
27 9 1 0 0 0 0
28 3 2 0 0 0 0
29 8 2 0 0 0 0
30 4 3 0 0 0 0
31 7 3 0 0 0 0
32 5 4 0 0 0 0
33 6 5 0 0 0 0
34 11 5 0 0 0 0
35 10 6 0 0 0 0
36 4 12 0 0 0 0
37 M END
38 $$$$
39 pentachlorophenol.sdf
40 COSMOTHERM 3D 0
41 13 13 0 0 0 0 0 0 0 0 V2000
42 0.4687 1.2149 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
43 -0.9327 1.2089 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
44 -1.6437 -0.0048 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
45 -0.9185 -1.2102 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
46 0.4815 -1.2146 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
47 1.1828 0.0030 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
48 -2.9929 0.0373 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 7
49 -1.8495 2.6950 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 8
50 1.3262 2.7343 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 9
51 2.9293 0.0096 -0.0002 Cl 0 0 0 0 0 0 0 0 0 0 0 10
52 1.3435 -2.7310 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 11
53 -1.8424 -2.6987 0.0001 Cl 0 0 0 0 0 0 0 0 0 0 0 12
54 -3.3420 -0.8815 0.0018 H 0 0 0 0 0 0 0 0 0 0 0 13
55 2 1 0 0 0 0
56 6 1 0 0 0 0
57 9 1 0 0 0 0
58 3 2 0 0 0 0
59 8 2 0 0 0 0
60 4 3 0 0 0 0
61 7 3 0 0 0 0
62 5 4 0 0 0 0
63 12 4 0 0 0 0
64 6 5 0 0 0 0
65 11 5 0 0 0 0
66 10 6 0 0 0 0
67 7 13 0 0 0 0
68 M END
69 $$$$
70 phenol-anion.sdf
71 COSMOTHERM 3D 0
72 12 12 0 0 0 0 0 0 0 0 V2000
73 1.2060 -1.1540 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
74 1.2142 0.2421 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
75 0.0000 1.0174 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
76 -1.2142 0.2421 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 4
77 -1.2060 -1.1540 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
78 0.0000 -1.8763 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
79 0.0000 2.3153 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 7
80 2.1585 -1.6937 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 8
81 2.1640 0.7866 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
82 -2.1640 0.7866 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
83 -2.1585 -1.6937 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 11
84 0.0000 -2.9678 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 12
85 2 1 0 0 0 0
86 6 1 0 0 0 0
87 8 1 0 0 0 0
88 3 2 0 0 0 0
89 9 2 0 0 0 0
90 4 3 0 0 0 0
91 7 3 0 0 0 0
92 5 4 0 0 0 0
93 10 4 0 0 0 0
94 6 5 0 0 0 0
95 11 5 0 0 0 0
96 6 12 0 0 0 0
97 M END
98 $$$$
99 phenol.sdf
100 COSMOTHERM 3D 0
101 13 13 0 0 0 0 0 0 0 0 V2000
102 -1.8845 -0.0020 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
103 -1.1762 1.2074 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2

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11 7 0 0 0 0
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14 10 0 0 0 0
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22 11 0 0 0 0
13 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
24 13 0 0 0 0
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16 15 0 0 0 0
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17 16 0 0 0 0
27 16 0 0 0 0
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28 17 0 0 0 0
19 18 0 0 0 0
29 18 0 0 0 0
19 30 0 0 0 0
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M END
$$$$
phenytoin1.sdf
COSMOTHERM
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3D

0

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31 33 0 0 0 0 0 0 0 0 0 V2000
-0.9493 2.5609 0.2123 N 0 0 0 0 0 0 0 0 0 0 0 1
0.4403 2.6153 0.1747 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.3416 1.2418 0.1526 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0063 0.4464 0.0267 C 0 0 0 0 0 0 0 0 0 0 0 4
1.0556 1.4897 0.0839 N 0 0 0 0 0 0 0 0 0 0 0 5
0.1106 -0.3056 -1.3141 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1018 -0.5253 1.2155 C 0 0 0 0 0 0 0 0 0 0 0 7
0.9824 3.8356 0.2346 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.4903 0.8227 0.2096 O 0 0 0 0 0 0 0 0 0 0 0 9
1.0265 -1.1504 3.3759 C 0 0 0 0 0 0 0 0 0 0 0 10
0.9715 -0.2730 2.2857 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.7147 -1.6682 1.2535 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.6652 -2.5380 2.3467 C 0 0 0 0 0 0 0 0 0 0 0 13
0.2081 -2.2838 3.4119 C 0 0 0 0 0 0 0 0 0 0 0 14
-1.0068 -0.6452 -2.0894 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.8490 -1.3572 -3.2866 C 0 0 0 0 0 0 0 0 0 0 0 16
0.4234 -1.7363 -3.7217 C 0 0 0 0 0 0 0 0 0 0 0 17
1.5435 -1.3993 -2.9503 C 0 0 0 0 0 0 0 0 0 0 0 18
1.3888 -0.6891 -1.7577 C 0 0 0 0 0 0 0 0 0 0 0 19
-1.5742 3.3585 0.3193 H 0 0 0 0 0 0 0 0 0 0 0 20
1.7134 -0.9439 4.1990 H 0 0 0 0 0 0 0 0 0 0 0 21
1.6117 0.6087 2.2571 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.3920 -1.8818 0.4257 H 0 0 0 0 0 0 0 0 0 0 0 23
-1.3069 -3.4211 2.3630 H 0 0 0 0 0 0 0 0 0 0 0 24
0.2510 -2.9670 4.2621 H 0 0 0 0 0 0 0 0 0 0 0 25
-2.0079 -0.3626 -1.7638 H 0 0 0 0 0 0 0 0 0 0 0 26
-1.7297 -1.6107 -3.8799 H 0 0 0 0 0 0 0 0 0 0 0 27
0.5442 -2.2893 -4.6550 H 0 0 0 0 0 0 0 0 0 0 0 28
2.5432 -1.6878 -3.2807 H 0 0 0 0 0 0 0 0 0 0 0 29
2.2641 -0.4202 -1.1657 H 0 0 0 0 0 0 0 0 0 0 0 30
1.9576 3.7430 0.2000 H 0 0 0 0 0 0 0 0 0 0 0 31
```

```
2 1 0 0 0 0
3 1 0 0 0 0
20 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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15 6 0 0 0 0
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11 7 0 0 0 0
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11 10 0 0 0 0
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22 11 0 0 0 0
13 12 0 0 0 0
23 12 0 0 0 0
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25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
17 16 0 0 0 0
27 16 0 0 0 0
18 17 0 0 0 0
28 17 0 0 0 0
19 18 0 0 0 0
29 18 0 0 0 0
30 19 0 0 0 0
8 31 0 0 0 0
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M END
$$$$
phenytoin2-anion.sdf
COSMOTHERM
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30 32 0 0 0 0 0 0 0 0 V2000
-0.8564 2.6146 -0.0241 N 0 0 0 0 0 0 0 0 0 0 0 1
0.6245 2.6262 -0.0658 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.1518 1.3646 0.0493 C 0 0 0 0 0 0 0 0 0 0 0 3
0.0697 0.4371 -0.0072 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1676 1.4067 -0.0679 N 0 0 0 0 0 0 0 0 0 0 0 5
0.0851 -0.4164 1.2776 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1040 -0.4283 -1.2780 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2209 3.7363 -0.1256 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.3929 0.8569 0.1348 O 0 0 0 0 0 0 0 0 0 0 0 9
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1.2144 -2.1791 -2.5622 C 0 0 0 0 0 0 0 0 0 0 10
1.0841 -1.4308 -1.3898 C 0 0 0 0 0 0 0 0 0 0 11
-0.7474 -0.2013 -2.3697 C 0 0 0 0 0 0 0 0 0 0 12
-0.6207 -0.9524 -3.5459 C 0 0 0 0 0 0 0 0 0 0 13
0.3594 -1.9440 -3.6474 C 0 0 0 0 0 0 0 0 0 0 14
0.8828 -0.0452 2.3684 C 0 0 0 0 0 0 0 0 0 0 15
0.8605 -0.7889 3.5554 C 0 0 0 0 0 0 0 0 0 0 16
0.0400 -1.9171 3.6655 C 0 0 0 0 0 0 0 0 0 0 17
-0.7575 -2.2970 2.5780 C 0 0 0 0 0 0 0 0 0 0 18
-0.7333 -1.5533 1.3942 C 0 0 0 0 0 0 0 0 0 0 19
1.9848 -2.9502 -2.6296 H 0 0 0 0 0 0 0 0 0 0 20
1.7535 -1.6235 -0.5491 H 0 0 0 0 0 0 0 0 0 0 21
-1.5227 0.5646 -2.3133 H 0 0 0 0 0 0 0 0 0 0 22
-1.2968 -0.7618 -4.3819 H 0 0 0 0 0 0 0 0 0 0 23
0.4561 -2.5320 -4.5621 H 0 0 0 0 0 0 0 0 0 0 24
1.5247 0.8311 2.2695 H 0 0 0 0 0 0 0 0 0 0 25
1.4880 -0.4849 4.3961 H 0 0 0 0 0 0 0 0 0 0 26
0.0222 -2.4980 4.5896 H 0 0 0 0 0 0 0 0 0 0 27
-1.4001 -3.1769 2.6513 H 0 0 0 0 0 0 0 0 0 0 28
-1.3583 -1.8600 0.5537 H 0 0 0 0 0 0 0 0 0 0 29
-3.0292 1.6024 0.1732 H 0 0 0 0 0 0 0 0 0 0 30
2 1 0 0 0 0
3 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
15 6 0 0 0 0
19 6 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
20 10 0 0 0 0
21 11 0 0 0 0
13 12 0 0 0 0
22 12 0 0 0 0
14 13 0 0 0 0
23 13 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
29 19 0 0 0 0
9 30 0 0 0 0
M END
$$$$
phenytoin2.sdf
COSMOTHERM 3D 0
31 33 0 0 0 0 0 0 0 0 0 V2000
-0.8514 2.6179 -0.1383 N 0 0 0 0 0 0 0 0 0 0 1
0.5741 2.6842 -0.2704 C 0 0 0 0 0 0 0 0 0 0 2
-1.1420 1.3630 -0.0181 C 0 0 0 0 0 0 0 0 0 0 3
0.0554 0.4007 -0.0152 C 0 0 0 0 0 0 0 0 0 0 4
1.0997 1.4247 -0.1174 N 0 0 0 0 0 0 0 0 0 0 5
0.0866 -0.3624 1.3232 C 0 0 0 0 0 0 0 0 0 0 6
0.0933 -0.5249 -1.2432 C 0 0 0 0 0 0 0 0 0 0 7
1.2042 3.7209 -0.4768 O 0 0 0 0 0 0 0 0 0 0 8
-2.3602 0.8637 0.1207 O 0 0 0 0 0 0 0 0 0 0 9
1.1169 -2.4073 -2.3940 C 0 0 0 0 0 0 0 0 0 0 10
0.9932 -1.6030 -1.2577 C 0 0 0 0 0 0 0 0 0 0 11
-0.6797 -0.2666 -2.3849 C 0 0 0 0 0 0 0 0 0 0 12
-0.5615 -1.0781 -3.5188 C 0 0 0 0 0 0 0 0 0 0 13
0.3363 -2.1500 -3.5269 C 0 0 0 0 0 0 0 0 0 0 14
0.8912 0.0748 2.3840 C 0 0 0 0 0 0 0 0 0 0 15
0.8788 -0.6061 3.6078 C 0 0 0 0 0 0 0 0 0 0 16
0.0539 -1.7210 3.7861 C 0 0 0 0 0 0 0 0 0 0 17
-0.7583 -2.1557 2.7311 C 0 0 0 0 0 0 0 0 0 0 18
-0.7427 -1.4813 1.5074 C 0 0 0 0 0 0 0 0 0 0 19
1.8222 -3.2404 -2.3916 H 0 0 0 0 0 0 0 0 0 0 20
1.6008 -1.8180 -0.3769 H 0 0 0 0 0 0 0 0 0 0 21
-1.3846 0.5665 -2.4025 H 0 0 0 0 0 0 0 0 0 0 22
-1.1760 -0.8698 -4.3964 H 0 0 0 0 0 0 0 0 0 0 23
0.4271 -2.7829 -4.4114 H 0 0 0 0 0 0 0 0 0 0 24
1.5360 0.9440 2.2522 H 0 0 0 0 0 0 0 0 0 0 25
1.5170 -0.2603 4.4229 H 0 0 0 0 0 0 0 0 0 0 26
0.0444 -2.2510 4.7401 H 0 0 0 0 0 0 0 0 0 0 27
-1.4057 -3.0249 2.8595 H 0 0 0 0 0 0 0 0 0 0 28
-1.3746 -1.8329 0.6908 H 0 0 0 0 0 0 0 0 0 0 29
2.0609 1.2066 -0.3677 H 0 0 0 0 0 0 0 0 0 0 30
-3.0145 1.5964 0.1225 H 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
3 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
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30 5 0 0 0 0
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11 7 0 0 0 0
12 7 0 0 0 0
11 10 0 0 0 0

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14 10 0 0 0 0
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26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
29 19 0 0 0 0
9 31 0 0 0 0
M END
$$$$
phenytoin3-anion.sdf
COSMOtherm 3D 0
30 32 0 0 0 0 0 0 0 0 0 V2000
-2.6042 -1.0045 0.2574 N 0 0 0 0 0 0 0 0 0 0 0 1
-2.6092 0.3681 0.1980 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.2892 -1.3272 0.1711 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.4557 0.0196 0.0280 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.5046 1.0549 0.0858 N 0 0 0 0 0 0 0 0 0 0 0 5
0.2905 0.1169 -1.3129 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5216 0.1120 1.2049 C 0 0 0 0 0 0 0 0 0 0 0 7
-3.8296 0.9653 0.2651 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.7974 -2.4726 0.2182 O 0 0 0 0 0 0 0 0 0 0 0 9
1.1330 0.9969 3.3922 C 0 0 0 0 0 0 0 0 0 0 0 10
0.2596 0.9519 2.2983 C 0 0 0 0 0 0 0 0 0 0 0 11
1.6810 -0.6841 1.2312 C 0 0 0 0 0 0 0 0 0 0 0 12
2.5518 -0.6427 2.3248 C 0 0 0 0 0 0 0 0 0 0 0 13
2.2824 0.1992 3.4118 C 0 0 0 0 0 0 0 0 0 0 0 14
0.6872 1.3879 -1.7686 C 0 0 0 0 0 0 0 0 0 0 0 15
1.3784 1.5343 -2.9740 C 0 0 0 0 0 0 0 0 0 0 0 16
1.6882 0.4095 -3.7509 C 0 0 0 0 0 0 0 0 0 0 0 17
1.2985 -0.8572 -3.3067 C 0 0 0 0 0 0 0 0 0 0 0 18
0.6061 -1.0032 -2.0960 C 0 0 0 0 0 0 0 0 0 0 0 19
0.9133 1.6608 4.2313 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.6349 1.5752 2.2772 H 0 0 0 0 0 0 0 0 0 0 0 21
1.9033 -1.3408 0.3893 H 0 0 0 0 0 0 0 0 0 0 0 22
3.4470 -1.2685 2.3269 H 0 0 0 0 0 0 0 0 0 0 0 23
2.9645 0.2347 4.2635 H 0 0 0 0 0 0 0 0 0 0 0 24
0.4368 2.2670 -1.1731 H 0 0 0 0 0 0 0 0 0 0 0 25
1.6755 2.5300 -3.3103 H 0 0 0 0 0 0 0 0 0 0 0 26
2.2262 0.5223 -4.6942 H 0 0 0 0 0 0 0 0 0 0 0 27
1.5302 -1.7417 -3.9041 H 0 0 0 0 0 0 0 0 0 0 0 28
0.3119 -1.9962 -1.7538 H 0 0 0 0 0 0 0 0 0 0 0 29
-3.6803 1.9317 0.2116 H 0 0 0 0 0 0 0 0 0 0 0 30
2 1 0 0 0 0
3 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
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17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
29 19 0 0 0 0
8 30 0 0 0 0
M END
$$$$
phenytoin3.sdf
COSMOtherm 3D 0
31 33 0 0 0 0 0 0 0 0 0 V2000
-2.6104 -0.8648 0.0648 N 0 0 0 0 0 0 0 0 0 0 0 1
-2.5659 0.5437 -0.0128 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.3489 -1.1784 0.0667 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.4241 0.0474 -0.0024 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4178 1.1457 -0.0369 N 0 0 0 0 0 0 0 0 0 0 0 5
0.4153 0.1064 -1.2881 C 0 0 0 0 0 0 0 0 0 0 0 6
0.4468 0.0817 1.2672 C 0 0 0 0 0 0 0 0 0 0 0 7
-3.7615 1.1500 -0.0558 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.8643 -2.4081 0.1482 O 0 0 0 0 0 0 0 0 0 0 0 9
0.8835 0.8813 3.5204 C 0 0 0 0 0 0 0 0 0 0 0 10
0.1040 0.8936 2.3568 C 0 0 0 0 0 0 0 0 0 0 0 11
1.5788 -0.7456 1.3584 C 0 0 0 0 0 0 0 0 0 0 0 12
2.3533 -0.7595 2.5216 C 0 0 0 0 0 0 0 0 0 0 0 13

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2.0081 0.0546 3.6078 C 0 0 0 0 0 0 0 0 0 0 0 14
1.3182 1.1728 -1.4417 C 0 0 0 0 0 0 0 0 0 0 0 15
2.0664 1.3069 -2.6126 C 0 0 0 0 0 0 0 0 0 0 0 16
1.9243 0.3758 -3.6502 C 0 0 0 0 0 0 0 0 0 0 0 17
1.0271 -0.6849 -3.5053 C 0 0 0 0 0 0 0 0 0 0 0 18
0.2729 -0.8181 -2.3314 C 0 0 0 0 0 0 0 0 0 0 0 19
0.6088 1.5232 4.3596 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.7676 1.5444 2.2863 H 0 0 0 0 0 0 0 0 0 0 0 21
1.8611 -1.3778 0.5151 H 0 0 0 0 0 0 0 0 0 0 0 22
3.2307 -1.4065 2.5783 H 0 0 0 0 0 0 0 0 0 0 0 23
2.6153 0.0459 4.5147 H 0 0 0 0 0 0 0 0 0 0 0 24
1.4353 1.9014 -0.6375 H 0 0 0 0 0 0 0 0 0 0 0 25
2.7633 2.1408 -2.7164 H 0 0 0 0 0 0 0 0 0 0 0 26
2.5121 0.4777 -4.5643 H 0 0 0 0 0 0 0 0 0 0 0 27
0.9078 -1.4168 -4.3063 H 0 0 0 0 0 0 0 0 0 0 0 28
-0.4177 -1.6573 -2.2417 H 0 0 0 0 0 0 0 0 0 0 0 29
-1.6053 -3.0506 0.2043 H 0 0 0 0 0 0 0 0 0 0 0 30
-3.6153 2.1173 -0.1094 H 0 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
3 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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15 6 0 0 0 0
19 6 0 0 0 0
11 7 0 0 0 0
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11 10 0 0 0 0
14 10 0 0 0 0
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21 11 0 0 0 0
13 12 0 0 0 0
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16 15 0 0 0 0
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17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
29 19 0 0 0 0
8 31 0 0 0 0
M END
$$$$
phosphoricacid0-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
0.1316 -0.0075 -0.0009 P 0 0 0 0 0 0 0 0 0 0 0 1
0.9365 1.2956 0.0703 O 0 0 0 0 0 0 0 0 0 0 0 2
-0.9075 -0.0801 1.3150 O 0 0 0 0 0 0 0 0 0 0 0 3
-0.9184 0.0701 -1.3073 O 0 0 0 0 0 0 0 0 0 0 0 4
0.7830 -1.3856 -0.0837 O 0 0 0 0 0 0 0 0 0 0 0 5
-1.1711 0.8216 1.5805 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.1832 0.9963 -1.4656 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 3 0 0 0 0
4 7 0 0 0 0
M END
$$$$
phosphoricacid0.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
0.0322 -0.0463 -0.0996 P 0 0 0 0 0 0 0 0 0 0 0 1
1.1937 0.8369 0.6317 O 0 0 0 0 0 0 0 0 0 0 0 2
-0.3935 -1.0569 1.0988 O 0 0 0 0 0 0 0 0 0 0 0 3
-1.2940 0.8822 -0.2237 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3985 -0.6358 -1.4344 O 0 0 0 0 0 0 0 0 0 0 0 5
1.7224 1.3447 -0.0169 H 0 0 0 0 0 0 0 0 0 0 0 6
0.3162 -1.6923 1.3229 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.5166 1.3528 0.6048 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
7 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
phosphoricacid1-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
-0.0066 -0.1317 0.0009 P 0 0 0 0 0 0 0 0 0 0 0 1
0.1223 0.9169 1.3045 O 0 0 0 0 0 0 0 0 0 0 0 2
-1.3775 -0.7887 0.1428 O 0 0 0 0 0 0 0 0 0 0 0 3
-0.1413 0.9088 -1.3088 O 0 0 0 0 0 0 0 0 0 0 0 4
1.2958 -0.9303 -0.1284 O 0 0 0 0 0 0 0 0 0 0 0 5
1.0543 1.1812 1.4258 H 0 0 0 0 0 0 0 0 0 0 0 6
0.7472 1.1732 -1.6149 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0

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3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
7 4 7 0 0 0 0
M END
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phosphoricacid1.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
0.0495 -0.0253 0.0995 P 0 0 0 0 0 0 0 0 0 0 1
1.0212 0.3502 -1.1462 O 0 0 0 0 0 0 0 0 0 0 2
-0.9031 1.2865 0.1683 O 0 0 0 0 0 0 0 0 0 0 3
-0.8234 -1.2493 -0.5369 O 0 0 0 0 0 0 0 0 0 0 4
0.6715 -0.2989 1.4417 O 0 0 0 0 0 0 0 0 0 0 5
1.6434 -0.3715 -1.3691 H 0 0 0 0 0 0 0 0 0 0 6
-1.3335 1.4975 -0.6848 H 0 0 0 0 0 0 0 0 0 0 7
-1.2959 -1.7516 0.1575 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
7 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
phosphoricacid2-anion.sdf
COSMOTHERM 3D 0
7 6 0 0 0 0 0 0 0 0 0 V2000
-0.0017 0.0077 -0.1316 P 0 0 0 0 0 0 0 0 0 0 1
1.3034 0.2022 0.9059 O 0 0 0 0 0 0 0 0 0 0 2
-1.2937 -0.1923 0.9203 O 0 0 0 0 0 0 0 0 0 0 3
-0.2150 1.3721 -0.7821 O 0 0 0 0 0 0 0 0 0 0 4
0.1907 -1.2832 -0.9367 O 0 0 0 0 0 0 0 0 0 0 5
1.6539 -0.6720 1.1634 H 0 0 0 0 0 0 0 0 0 0 6
-1.3681 -1.1313 1.1763 H 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
3 7 0 0 0 0
M END
$$$$
phosphoricacid2.sdf
COSMOTHERM 3D 0
8 7 0 0 0 0 0 0 0 0 0 V2000
-0.0004 -0.1182 0.0013 P 0 0 0 0 0 0 0 0 0 0 1
1.2113 0.5964 -0.8134 O 0 0 0 0 0 0 0 0 0 0 2
0.0963 0.6231 1.4447 O 0 0 0 0 0 0 0 0 0 0 3
-1.3022 0.6060 -0.6496 O 0 0 0 0 0 0 0 0 0 0 4
-0.0049 -1.6257 0.0160 O 0 0 0 0 0 0 0 0 0 0 5
1.4109 0.1311 -1.6507 H 0 0 0 0 0 0 0 0 0 0 6
0.7265 0.1747 2.0441 H 0 0 0 0 0 0 0 0 0 0 7
-2.1338 0.1563 -0.3973 H 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 2 0 0 0 0
7 3 0 0 0 0
4 8 0 0 0 0
M END
$$$$
phthalicacid0-anion.sdf
COSMOTHERM 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
-1.5099 -2.3763 0.0036 C 0 0 0 0 0 0 0 0 0 0 1
-0.1860 -2.8314 -0.0130 C 0 0 0 0 0 0 0 0 0 0 2
0.8644 -1.9098 -0.0122 C 0 0 0 0 0 0 0 0 0 0 3
0.6169 -0.5293 0.0084 C 0 0 0 0 0 0 0 0 0 0 4
-0.7172 -0.0802 0.0127 C 0 0 0 0 0 0 0 0 0 0 5
-1.7749 -1.0034 0.0173 C 0 0 0 0 0 0 0 0 0 0 6
1.7695 0.4714 0.0662 C 0 0 0 0 0 0 0 0 0 0 7
-1.0747 1.3812 0.0306 C 0 0 0 0 0 0 0 0 0 0 8
2.9452 0.0296 -0.0938 O 0 0 0 0 0 0 0 0 0 0 9
1.4378 1.6782 0.2877 O 0 0 0 0 0 0 0 0 0 0 10
-1.5274 1.9691 1.0061 O 0 0 0 0 0 0 0 0 0 0 11
-1.0574 1.9287 -1.2132 O 0 0 0 0 0 0 0 0 0 0 12
-2.3377 -3.0875 0.0052 H 0 0 0 0 0 0 0 0 0 0 13
0.0249 -3.9025 -0.0232 H 0 0 0 0 0 0 0 0 0 0 14
1.9033 -2.2436 -0.0169 H 0 0 0 0 0 0 0 0 0 0 15
-2.8073 -0.6481 0.0239 H 0 0 0 0 0 0 0 0 0 0 16
-1.3522 2.8621 -1.1321 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
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8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0

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12 17 0 0 0 0
M END
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phthalicacid0.sdf
COSMOTHERM          3D          0

18 18 0 0 0 0 0 0 0 0 0 V2000
-2.8234 -0.0134 -0.0085 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.4705 -1.3660 -0.0093 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.1227 -1.7387 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1174 -0.7639 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.4706 0.6041 0.0186 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.8280 0.9656 0.0083 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.3031 -1.2488 -0.0528 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.5841 1.6467 0.1662 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.8004 -1.9909 0.7817 O 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.9377 -0.8588 -1.1804 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
1.6910 1.4423 0.6505 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.1822 2.8661 -0.2639 O 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.8736 0.2810 -0.0122 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-3.2433 -2.1358 -0.0176 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.8470 -2.7939 -0.0151 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.0992 2.0203 0.0390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2.8521 -1.2184 -1.1584 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
0.9064 3.5035 -0.0814 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 10 0 0 0 0
12 18 0 0 0 0
M END
$$$$
phthalicacid1-anion.sdf
COSMOTHERM          3D          0

17 17 0 0 0 0 0 0 0 0 0 V2000
0.1883 -2.8314 -0.0124 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
1.5117 -2.3750 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.7755 -1.0018 0.0167 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.7169 -0.0797 0.0124 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.6167 -0.5300 0.0081 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.8630 -1.9109 -0.0097 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.0729 1.3821 0.0317 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.7698 0.4703 0.0645 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.5206 1.9703 1.0095 O 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.0618 1.9296 -1.2121 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.9456 0.0270 -0.0941 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.4387 1.6774 0.2831 O 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.0215 -3.9027 -0.0231 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.3402 -3.0854 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2.8075 -0.6456 0.0230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.9017 -2.2455 -0.0142 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.3565 2.8629 -1.1291 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
10 17 0 0 0 0
M END
$$$$
phthalicacid1.sdf
COSMOTHERM          3D          0

18 18 0 0 0 0 0 0 0 0 0 V2000
-0.5046 -2.7893 -0.0106 C 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.8897 -2.6876 0.0108 C 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.4978 -1.4299 0.0173 C 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.7216 -0.2623 -0.0042 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.6885 -0.3641 0.0112 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.2870 -1.6328 -0.0113 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.4591 1.0375 -0.1053 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.6011 0.8149 0.1176 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4264 1.3339 0.5817 O 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.9840 1.8201 -1.1015 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.6991 0.8870 -0.4188 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.1079 1.7786 0.9299 O 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.9847 -3.7687 -0.0198 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
1.5070 -3.5868 0.0182 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2.5851 -1.3455 0.0069 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.3752 -1.7037 0.0028 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16

```

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1
2
3      1.5041    2.6537   -1.1113 H   0 0 0 0 0 0 0 0 0 0 0 17
4     -1.7424    2.5284    0.9376 H   0 0 0 0 0 0 0 0 0 0 0 18
5
6      2 1 0 0 0 0
7      6 1 0 0 0 0
8     13 1 0 0 0 0
9      3 2 0 0 0 0
10     14 2 0 0 0 0
11     4 3 0 0 0 0
12     15 3 0 0 0 0
13     5 4 0 0 0 0
14     7 4 0 0 0 0
15     6 5 0 0 0 0
16     8 5 0 0 0 0
17     16 6 0 0 0 0
18     9 7 0 0 0 0
19     10 7 0 0 0 0
20     11 8 0 0 0 0
21     12 8 0 0 0 0
22     17 10 0 0 0 0
23     12 18 0 0 0 0

```

M END

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phthalicacid2-anion.sdf
COSMOtherm 3D

0

```

17 17 0 0 0 0 0 0 0 0 0 0 V2000
2.3757 -1.5106 0.0054 C 0 0 0 0 0 0 0 0 0 0 0 1
2.8311 -0.1869 -0.0151 C 0 0 0 0 0 0 0 0 0 0 0 2
1.9099 0.8637 -0.0156 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5293 0.6166 0.0070 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0799 -0.7174 0.0136 C 0 0 0 0 0 0 0 0 0 0 0 5
1.0028 -1.7754 0.0210 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4709 1.7695 0.0670 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.3816 -1.0746 0.0297 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.6776 1.4384 0.2881 O 0 0 0 0 0 0 0 0 0 0 0 9
-0.0280 2.9454 -0.0904 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.9705 -1.5286 1.0040 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.9281 -1.0545 -1.2144 O 0 0 0 0 0 0 0 0 0 0 0 12
3.0867 -2.3386 0.0085 H 0 0 0 0 0 0 0 0 0 0 0 13
3.9022 0.0236 -0.0268 H 0 0 0 0 0 0 0 0 0 0 0 14
2.2437 1.9026 -0.0221 H 0 0 0 0 0 0 0 0 0 0 0 15
0.6471 -2.8076 0.0302 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.8617 -1.3491 -1.1347 H 0 0 0 0 0 0 0 0 0 0 0 17

```

```

2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
12 17 0 0 0 0

```

M END

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phthalicacid2.sdf
COSMOtherm 3D

0

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18 18 0 0 0 0 0 0 0 0 0 0 V2000
-0.5672 -2.7529 0.0162 C 0 0 0 0 0 0 0 0 0 0 0 1
0.8274 -2.6855 -0.0166 C 0 0 0 0 0 0 0 0 0 0 0 2
1.4661 -1.4417 -0.0349 C 0 0 0 0 0 0 0 0 0 0 0 3
0.7179 -0.2561 -0.0243 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6930 -0.3240 0.0218 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.3229 -1.5766 0.0339 C 0 0 0 0 0 0 0 0 0 0 0 6
1.4304 1.0474 -0.2073 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.5226 0.9074 -0.2042 C 0 0 0 0 0 0 0 0 0 0 0 8
1.0757 1.9281 -0.9781 O 0 0 0 0 0 0 0 0 0 0 0 9
2.5604 1.1199 0.5352 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.2223 1.8424 0.9333 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.6851 0.8500 -0.4884 O 0 0 0 0 0 0 0 0 0 0 0 12
-1.0714 -3.7200 0.0326 H 0 0 0 0 0 0 0 0 0 0 0 13
1.4228 -3.5992 -0.0315 H 0 0 0 0 0 0 0 0 0 0 0 14
2.5536 -1.3878 -0.0849 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.4104 -1.6280 0.0858 H 0 0 0 0 0 0 0 0 0 0 0 16
3.0179 1.9602 0.3112 H 0 0 0 0 0 0 0 0 0 0 0 17
-3.2113 1.6487 -0.2643 H 0 0 0 0 0 0 0 0 0 0 0 18

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2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 10 0 0 0 0
12 18 0 0 0 0

```

M END

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phthalicacid3-anion.sdf

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```
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 10 0 0 0 0
12 18 0 0 0 0
```

```
M END
$$$$
phthalimide0-anion.sdf
COSMOtherm 3D 0
15 16 0 0 0 0 0 0 0 0 0 0 0 V2000
-2.6044 0.7013 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.6044 -0.7013 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.3970 -1.4253 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.2118 -0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2118 0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3970 1.4252 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.2447 1.1146 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.2447 -1.1146 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.0502 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 9
1.6432 -2.2963 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 10
1.6431 2.2963 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-3.5555 1.2371 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.5555 -1.2371 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.3971 -2.5172 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.3971 2.5171 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
12 1 0 0 0 0
3 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
9 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
6 15 0 0 0 0
```

```
M END
$$$$
phthalimide0.sdf
COSMOtherm 3D 0
16 17 0 0 0 0 0 0 0 0 0 0 V2000
-2.6101 0.7013 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.6101 -0.7013 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.4073 -1.4274 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.2219 -0.7018 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2219 0.7018 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.4073 1.4274 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1975 1.1682 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.1975 -1.1682 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.9708 0.0000 0.0005 N 0 0 0 0 0 0 0 0 0 0 0 0 9
1.6396 -2.3108 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 10
1.6396 2.3108 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 0 11
2.9900 0.0000 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.5605 1.2369 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-3.5604 -1.2369 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.4068 -2.5181 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.4068 2.5181 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
9 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 9 0 0 0 0
6 16 0 0 0 0
```

```
M END
$$$$
phthalimide1-anion.sdf
COSMOtherm 3D 0
15 16 0 0 0 0 0 0 0 0 0 0 V2000
-2.6044 0.7013 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.6044 -0.7013 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.3970 -1.4253 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.2118 -0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2118 0.6990 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3970 1.4252 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 6
```

```

1
2
3      1.2447    1.1146    0.0000 C    0 0 0 0 0 0 0 0 0 0 7
4      1.2447   -1.1146    0.0000 C    0 0 0 0 0 0 0 0 0 0 8
5      2.0502    0.0000    0.0000 N    0 0 0 0 0 0 0 0 0 0 9
6      1.6432   -2.2963   -0.0001 O    0 0 0 0 0 0 0 0 0 0 10
7      1.6431    2.2963    0.0001 O    0 0 0 0 0 0 0 0 0 0 11
8     -3.5555    1.2371   -0.0002 H    0 0 0 0 0 0 0 0 0 0 12
9     -3.5555   -1.2371    0.0002 H    0 0 0 0 0 0 0 0 0 0 13
10    -1.3971   -2.5172    0.0004 H    0 0 0 0 0 0 0 0 0 0 14
11    -1.3971    2.5171   -0.0003 H    0 0 0 0 0 0 0 0 0 0 15

```

```

12      2 1 0 0 0 0
13      6 1 0 0 0 0
14      12 1 0 0 0 0
15      3 2 0 0 0 0
16      13 2 0 0 0 0
17      4 3 0 0 0 0
18      14 3 0 0 0 0
19      5 4 0 0 0 0
20      8 4 0 0 0 0
21      6 5 0 0 0 0
22      7 5 0 0 0 0
23      9 7 0 0 0 0
24      11 7 0 0 0 0
25      9 8 0 0 0 0
26      10 8 0 0 0 0
27      6 15 0 0 0 0

```

M END

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phthalimide1.sdf

COSMOtherm 3D 0

```

21      16 17 0 0 0 0 0 0 0 0 0 0 V2000
22     -2.5883    0.7685    0.0004 C    0 0 0 0 0 0 0 0 0 0 1
23     -2.6384   -0.6312   -0.0005 C    0 0 0 0 0 0 0 0 0 0 2
24     -1.4596   -1.4030   -0.0008 C    0 0 0 0 0 0 0 0 0 0 3
25     -0.2518   -0.7218   -0.0002 C    0 0 0 0 0 0 0 0 0 0 4
26     -0.2048    0.6804    0.0005 C    0 0 0 0 0 0 0 0 0 0 5
27     -1.3585    1.4540    0.0009 C    0 0 0 0 0 0 0 0 0 0 6
28      1.2404    0.9976    0.0000 C    0 0 0 0 0 0 0 0 0 0 7
29      1.1832   -1.1859    0.0001 C    0 0 0 0 0 0 0 0 0 0 8
30      2.0364   -0.0463    0.0002 N    0 0 0 0 0 0 0 0 0 0 9
31      1.5891   -2.3419    0.0004 O    0 0 0 0 0 0 0 0 0 0 10
32      1.6518    2.2538   -0.0007 O    0 0 0 0 0 0 0 0 0 0 11
33     -3.5183    1.3385    0.0006 H    0 0 0 0 0 0 0 0 0 0 12
34     -3.6077   -1.1319   -0.0009 H    0 0 0 0 0 0 0 0 0 0 13
35     -1.5013   -2.4931   -0.0013 H    0 0 0 0 0 0 0 0 0 0 14
36     -1.3239    2.5438    0.0013 H    0 0 0 0 0 0 0 0 0 0 15
37      2.6346    2.2780   -0.0021 H    0 0 0 0 0 0 0 0 0 0 16

```

```

38      2 1 0 0 0 0
39      6 1 0 0 0 0
40      12 1 0 0 0 0
41      3 2 0 0 0 0
42      13 2 0 0 0 0
43      4 3 0 0 0 0
44      14 3 0 0 0 0
45      5 4 0 0 0 0
46      8 4 0 0 0 0
47      6 5 0 0 0 0
48      7 5 0 0 0 0
49      15 6 0 0 0 0
50      9 7 0 0 0 0
51      11 7 0 0 0 0
52      9 8 0 0 0 0
53      10 8 0 0 0 0
54      11 16 0 0 0 0

```

M END

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salicylicacid-anion0.sdf

COSMOtherm 3D 0

```

55      15 16 0 0 0 0 0 0 0 0 0 0 V2000
56      1.9959   -1.4216   -0.0003 C    0 0 0 0 0 0 0 0 0 0 1
57      2.6365   -0.1708    0.0001 C    0 0 0 0 0 0 0 0 0 0 2
58      1.8937    1.0093    0.0001 C    0 0 0 0 0 0 0 0 0 0 3
59      0.4858    0.9587    0.0002 C    0 0 0 0 0 0 0 0 0 0 4
60     -0.1751   -0.3024   -0.0002 C    0 0 0 0 0 0 0 0 0 0 5
61      0.6014   -1.4728   -0.0002 C    0 0 0 0 0 0 0 0 0 0 6
62     -0.2268    2.1088    0.0003 O    0 0 0 0 0 0 0 0 0 0 7
63     -1.6841   -0.3704    0.0000 C    0 0 0 0 0 0 0 0 0 0 8
64     -2.2666   -1.4824    0.0006 O    0 0 0 0 0 0 0 0 0 0 9
65     -2.3019    0.7751   -0.0006 O    0 0 0 0 0 0 0 0 0 0 10
66      2.5832   -2.3412   -0.0002 H    0 0 0 0 0 0 0 0 0 0 11
67      3.7274   -0.1162    0.0001 H    0 0 0 0 0 0 0 0 0 0 12
68      2.3862    1.9840    0.0003 H    0 0 0 0 0 0 0 0 0 0 13
69      0.0777   -2.4311   -0.0004 H    0 0 0 0 0 0 0 0 0 0 14
70     -1.2267    1.7479   -0.0001 H    0 0 0 0 0 0 0 0 0 0 15

```

```

71      2 1 0 0 0 0
72      6 1 0 0 0 0
73      11 1 0 0 0 0
74      3 2 0 0 0 0
75      12 2 0 0 0 0
76      4 3 0 0 0 0
77      13 3 0 0 0 0
78      5 4 0 0 0 0
79      7 4 0 0 0 0
80      6 5 0 0 0 0
81      8 5 0 0 0 0
82      14 6 0 0 0 0
83      9 8 0 0 0 0
84      10 8 0 0 0 0
85      7 15 0 0 0 0
86      10 15 0 0 0 0

```

M END

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salicylicacid-anion1.sdf

COSMOtherm 3D 0

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```

15 15 0 0 0 0 0 0 0 0 0 V2000
  1.8791 -0.0117 1.5268 C 0 0 0 0 0 0 0 0 0 0 1
  2.6213 -0.0034 0.3387 C 0 0 0 0 0 0 0 0 0 0 2
  1.9603 0.0060 -0.8882 C 0 0 0 0 0 0 0 0 0 0 3
  0.5533 0.0059 -0.9557 C 0 0 0 0 0 0 0 0 0 0 4
 -0.2183 -0.0018 0.2336 C 0 0 0 0 0 0 0 0 0 0 5
  0.4861 -0.0100 1.4534 C 0 0 0 0 0 0 0 0 0 0 6
 -0.0555 0.0164 -2.1866 O 0 0 0 0 0 0 0 0 0 0 7
 -1.7536 -0.0017 0.2902 C 0 0 0 0 0 0 0 0 0 0 8
 -2.2730 0.0347 1.4519 O 0 0 0 0 0 0 0 0 0 0 9
 -2.3987 -0.0388 -0.7997 O 0 0 0 0 0 0 0 0 0 0 10
  2.3821 -0.0191 2.4953 H 0 0 0 0 0 0 0 0 0 0 11
  3.7128 -0.0034 0.3633 H 0 0 0 0 0 0 0 0 0 0 12
  2.5332 0.0137 -1.8202 H 0 0 0 0 0 0 0 0 0 0 13
 -0.1188 -0.0140 2.3616 H 0 0 0 0 0 0 0 0 0 0 14
  0.6488 0.0261 -2.8644 H 0 0 0 0 0 0 0 0 0 0 15
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
  11 1 0 0 0 0 0
  3 2 0 0 0 0 0
  12 2 0 0 0 0 0
  4 3 0 0 0 0 0
  13 3 0 0 0 0 0
  5 4 0 0 0 0 0
  7 4 0 0 0 0 0
  6 5 0 0 0 0 0
  8 5 0 0 0 0 0
  14 6 0 0 0 0 0
  9 8 0 0 0 0 0
  10 8 0 0 0 0 0
  7 15 0 0 0 0 0
M END
$$$$
salicylicacid-anion2.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
  1.9626 -1.4503 -0.0138 C 0 0 0 0 0 0 0 0 0 0 1
  2.6334 -0.2225 -0.0041 C 0 0 0 0 0 0 0 0 0 0 2
  1.9050 0.9727 0.0087 C 0 0 0 0 0 0 0 0 0 0 3
  0.5036 0.9394 0.0087 C 0 0 0 0 0 0 0 0 0 0 4
 -0.1889 -0.2866 -0.0016 C 0 0 0 0 0 0 0 0 0 0 5
  0.5617 -1.4715 -0.0113 C 0 0 0 0 0 0 0 0 0 0 6
 -0.2521 2.0934 0.0224 O 0 0 0 0 0 0 0 0 0 0 7
 -1.7161 -0.3256 -0.0035 C 0 0 0 0 0 0 0 0 0 0 8
 -2.2847 -0.3944 1.1267 O 0 0 0 0 0 0 0 0 0 0 9
 -2.2835 -0.3015 -1.1362 O 0 0 0 0 0 0 0 0 0 0 10
  2.5241 -2.3861 -0.0237 H 0 0 0 0 0 0 0 0 0 0 11
  3.7243 -0.1873 -0.0051 H 0 0 0 0 0 0 0 0 0 0 12
  2.4221 1.9362 -0.0180 H 0 0 0 0 0 0 0 0 0 0 13
  0.0359 -2.4297 -0.0180 H 0 0 0 0 0 0 0 0 0 0 14
  0.3463 2.8644 0.0254 H 0 0 0 0 0 0 0 0 0 0 15
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
  11 1 0 0 0 0 0
  3 2 0 0 0 0 0
  12 2 0 0 0 0 0
  4 3 0 0 0 0 0
  13 3 0 0 0 0 0
  5 4 0 0 0 0 0
  7 4 0 0 0 0 0
  6 5 0 0 0 0 0
  8 5 0 0 0 0 0
  14 6 0 0 0 0 0
  9 8 0 0 0 0 0
  10 8 0 0 0 0 0
  7 15 0 0 0 0 0
M END
$$$$
salicylicacid0.sdf
COSMOTHERM 3D 0
16 16 0 0 0 0 0 0 0 0 0 V2000
  1.9437 -1.4792 -0.0009 C 0 0 0 0 0 0 0 0 0 0 1
  2.6327 -0.2522 0.0005 C 0 0 0 0 0 0 0 0 0 0 2
  1.9427 0.9560 0.0010 C 0 0 0 0 0 0 0 0 0 0 3
  0.5371 0.9648 0.0003 C 0 0 0 0 0 0 0 0 0 0 4
 -0.1718 -0.2708 -0.0006 C 0 0 0 0 0 0 0 0 0 0 5
  0.5549 -1.4820 -0.0012 C 0 0 0 0 0 0 0 0 0 0 6
 -0.0979 2.1606 0.0003 O 0 0 0 0 0 0 0 0 0 0 7
 -1.6370 -0.2430 -0.0003 C 0 0 0 0 0 0 0 0 0 0 8
 -2.3052 0.8076 -0.0017 O 0 0 0 0 0 0 0 0 0 0 9
 -2.2310 -1.4522 0.0023 O 0 0 0 0 0 0 0 0 0 0 10
  2.4950 -2.4198 -0.0015 H 0 0 0 0 0 0 0 0 0 0 11
  3.7241 -0.2427 0.0010 H 0 0 0 0 0 0 0 0 0 0 12
  2.4727 1.9094 0.0020 H 0 0 0 0 0 0 0 0 0 0 13
  0.0072 -2.4245 -0.0022 H 0 0 0 0 0 0 0 0 0 0 14
 -1.0821 1.9529 -0.0002 H 0 0 0 0 0 0 0 0 0 0 15
 -3.2027 -1.3130 0.0010 H 0 0 0 0 0 0 0 0 0 0 16
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
  11 1 0 0 0 0 0
  3 2 0 0 0 0 0
  12 2 0 0 0 0 0
  4 3 0 0 0 0 0
  13 3 0 0 0 0 0
  5 4 0 0 0 0 0
  7 4 0 0 0 0 0
  6 5 0 0 0 0 0
  8 5 0 0 0 0 0
  14 6 0 0 0 0 0
  15 7 0 0 0 0 0
  9 8 0 0 0 0 0
  10 8 0 0 0 0 0

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For Peer Review Only

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1
2
3 10 16 0 0 0 0
4 M END
5 $$$
6 salicylicacid1.sdf
7 COSMOtherm 3D 0
8
9 16 16 0 0 0 0 0 0 0 0 0 V2000
10 1.9715 -1.4610 -0.0320 C 0 0 0 0 0 0 0 0 0 0 0 1
11 2.6400 -0.2246 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 2
12 1.9244 0.9673 0.0219 C 0 0 0 0 0 0 0 0 0 0 0 3
13 0.5178 0.9589 0.0163 C 0 0 0 0 0 0 0 0 0 0 0 4
14 -0.1720 -0.2862 -0.0092 C 0 0 0 0 0 0 0 0 0 0 0 5
15 0.5836 -1.4800 -0.0308 C 0 0 0 0 0 0 0 0 0 0 0 6
16 -0.0920 2.1735 0.0418 O 0 0 0 0 0 0 0 0 0 0 0 7
17 -1.6436 -0.4208 0.0039 C 0 0 0 0 0 0 0 0 0 0 0 8
18 -2.2655 -1.4717 0.0889 O 0 0 0 0 0 0 0 0 0 0 0 9
19 -2.2911 0.7850 -0.0999 O 0 0 0 0 0 0 0 0 0 0 0 10
20 2.5351 -2.3940 -0.0536 H 0 0 0 0 0 0 0 0 0 0 0 11
21 3.7310 -0.1927 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 12
22 2.4359 1.9307 0.0437 H 0 0 0 0 0 0 0 0 0 0 0 13
23 0.0408 -2.4259 -0.0498 H 0 0 0 0 0 0 0 0 0 0 0 14
24 -1.0702 2.0368 0.0097 H 0 0 0 0 0 0 0 0 0 0 0 15
25 -3.2603 0.6394 -0.0506 H 0 0 0 0 0 0 0 0 0 0 0 16
26
27 2 1 0 0 0 0
28 6 1 0 0 0 0
29 11 1 0 0 0 0
30 3 2 0 0 0 0
31 12 2 0 0 0 0
32 4 3 0 0 0 0
33 13 3 0 0 0 0
34 5 4 0 0 0 0
35 7 4 0 0 0 0
36 6 5 0 0 0 0
37 8 5 0 0 0 0
38 14 6 0 0 0 0
39 15 7 0 0 0 0
40 9 8 0 0 0 0
41 10 8 0 0 0 0
42 10 16 0 0 0 0
43 M END
44 $$$
45 salicylicacid2.sdf
46 COSMOtherm 3D 0
47
48 16 16 0 0 0 0 0 0 0 0 0 V2000
49 1.9317 -1.4943 -0.0426 C 0 0 0 0 0 0 0 0 0 0 0 1
50 2.6385 -0.2825 -0.0182 C 0 0 0 0 0 0 0 0 0 0 0 2
51 1.9533 0.9281 0.0169 C 0 0 0 0 0 0 0 0 0 0 0 3
52 0.5467 0.9625 0.0248 C 0 0 0 0 0 0 0 0 0 0 0 4
53 -0.1830 -0.2553 -0.0031 C 0 0 0 0 0 0 0 0 0 0 0 5
54 0.5426 -1.4666 -0.0311 C 0 0 0 0 0 0 0 0 0 0 0 6
55 -0.1079 2.1566 0.0694 O 0 0 0 0 0 0 0 0 0 0 0 7
56 -1.6636 -0.3820 0.0043 C 0 0 0 0 0 0 0 0 0 0 0 8
57 -2.2529 -1.4555 0.1264 O 0 0 0 0 0 0 0 0 0 0 0 9
58 -2.3413 0.7817 -0.1506 O 0 0 0 0 0 0 0 0 0 0 0 10
59 2.4632 -2.4459 -0.0703 H 0 0 0 0 0 0 0 0 0 0 0 11
60 3.7298 -0.2802 -0.0257 H 0 0 0 0 0 0 0 0 0 0 0 12
61 2.5024 1.8728 0.0404 H 0 0 0 0 0 0 0 0 0 0 0 13
62 -0.0288 -2.3952 -0.0481 H 0 0 0 0 0 0 0 0 0 0 0 14
63 0.5561 2.8732 0.1006 H 0 0 0 0 0 0 0 0 0 0 0 15
64 -3.2967 0.5540 -0.1305 H 0 0 0 0 0 0 0 0 0 0 0 16
65
66 2 1 0 0 0 0
67 6 1 0 0 0 0
68 11 1 0 0 0 0
69 3 2 0 0 0 0
70 12 2 0 0 0 0
71 4 3 0 0 0 0
72 13 3 0 0 0 0
73 5 4 0 0 0 0
74 7 4 0 0 0 0
75 6 5 0 0 0 0
76 8 5 0 0 0 0
77 14 6 0 0 0 0
78 15 7 0 0 0 0
79 9 8 0 0 0 0
80 10 8 0 0 0 0
81 10 16 0 0 0 0
82 M END
83 $$$
84 succinimide0-anion.sdf
85 COSMOtherm 3D 0
86
87 11 11 0 0 0 0 0 0 0 0 0 V2000
88 -0.7642 -1.3025 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
89 -1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
90 0.7642 -1.3025 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
91 1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
92 0.0000 0.9894 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 5
93 2.2894 0.6213 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 6
94 -2.2894 0.6213 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
95 -1.2087 -1.7807 -0.8848 H 0 0 0 0 0 0 0 0 0 0 0 8
96 -1.2079 -1.7800 0.8861 H 0 0 0 0 0 0 0 0 0 0 0 9
97 1.2079 -1.7800 -0.8861 H 0 0 0 0 0 0 0 0 0 0 0 10
98 1.2087 -1.7806 0.8848 H 0 0 0 0 0 0 0 0 0 0 0 11
99
100 2 1 0 0 0 0
101 3 1 0 0 0 0
102 8 1 0 0 0 0
103 9 1 0 0 0 0
104 5 2 0 0 0 0
105 7 2 0 0 0 0
106 4 3 0 0 0 0
107 10 3 0 0 0 0
108 5 4 0 0 0 0
109 6 4 0 0 0 0
110 3 11 0 0 0 0
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M END
$$$$
succinimide0.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 0 V2000
-0.7686 -1.3091 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1700 0.1577 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7686 -1.3091 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1700 0.1577 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0000 0.9110 -0.0005 N 0 0 0 0 0 0 0 0 0 0 0 5
2.3005 0.6308 0.0003 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.3005 0.6307 0.0003 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.2031 -1.7935 -0.8850 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.2029 -1.7935 0.8851 H 0 0 0 0 0 0 0 0 0 0 0 9
1.2029 -1.7935 -0.8852 H 0 0 0 0 0 0 0 0 0 0 0 10
1.2030 -1.7936 0.8849 H 0 0 0 0 0 0 0 0 0 0 0 11
0.0000 1.9318 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
5 12 0 0 0 0

M END
$$$$
succinimidel-anion.sdf
COSMOtherm 3D 0

11 11 0 0 0 0 0 0 0 0 V2000
-0.7642 -1.3025 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7642 -1.3025 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1140 0.1968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0000 0.9894 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 5
2.2894 0.6213 0.0001 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.2894 0.6213 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.2087 -1.7807 -0.8848 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.2079 -1.7800 0.8861 H 0 0 0 0 0 0 0 0 0 0 0 9
1.2079 -1.7800 -0.8861 H 0 0 0 0 0 0 0 0 0 0 0 10
1.2087 -1.7806 0.8848 H 0 0 0 0 0 0 0 0 0 0 0 11

2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
3 11 0 0 0 0

M END
$$$$
succinimidel.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
-0.8108 -1.3030 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1547 0.1908 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7226 -1.3195 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 3
1.0279 0.1510 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0185 0.9790 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 5
2.2943 0.5414 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 6
-2.2849 0.6685 -0.0003 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.2528 -1.7802 -0.8842 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.2506 -1.7784 0.8879 H 0 0 0 0 0 0 0 0 0 0 0 9
1.1627 -1.7975 -0.8874 H 0 0 0 0 0 0 0 0 0 0 0 10
1.1647 -1.7988 0.8843 H 0 0 0 0 0 0 0 0 0 0 0 11
2.3328 1.5235 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 12

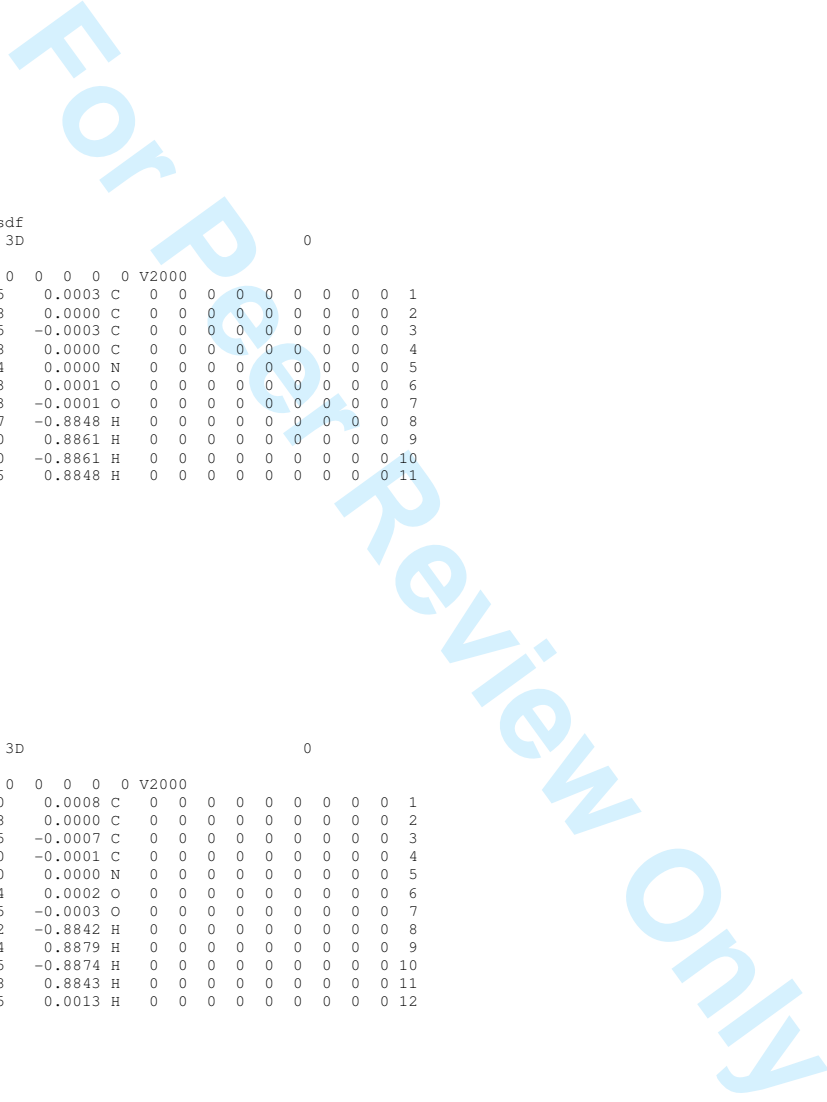
2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
6 12 0 0 0 0

M END
$$$$
sulfurousacid-anion.sdf
COSMOtherm 3D 0

5 4 0 0 0 0 0 0 0 0 V2000
-0.3954 0.0003 0.1433 S 0 0 0 0 0 0 0 0 0 0 0 1
0.1242 -0.0091 -1.5871 O 0 0 0 0 0 0 0 0 0 0 0 2
0.2999 -1.2545 0.7067 O 0 0 0 0 0 0 0 0 0 0 0 3
0.2988 1.2627 0.6908 O 0 0 0 0 0 0 0 0 0 0 0 4
1.1052 0.0044 -1.5476 H 0 0 0 0 0 0 0 0 0 0 0 5

2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
2 5 0 0 0 0

M END
$$$$
```



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1
2
3 sulfurousacid.sdf
4 COSMOTHERM 3D 0
5
6 6 5 0 0 0 0 0 0 0 0 0 0 V2000
7 0.4172 0.1054 -0.0001 S 0 0 0 0 0 0 0 0 0 0 0 1
8 -0.1871 -0.7785 1.3068 O 0 0 0 0 0 0 0 0 0 0 0 2
9 -0.1870 -0.7838 -1.3034 O 0 0 0 0 0 0 0 0 0 0 0 3
10 -0.3205 1.4166 -0.0032 O 0 0 0 0 0 0 0 0 0 0 0 4
11 -1.1245 -0.5183 1.4602 H 0 0 0 0 0 0 0 0 0 0 0 5
12 -1.1235 -0.5222 -1.4601 H 0 0 0 0 0 0 0 0 0 0 0 6
13
14 2 1 0 0 0 0
15 3 1 0 0 0 0
16 4 1 0 0 0 0
17 5 2 0 0 0 0
18 3 6 0 0 0 0
19 M END
20 $$$
21 tert-butanol-anion.sdf
22 COSMOTHERM 3D 0
23
24 14 13 0 0 0 0 0 0 0 0 V2000
25 -0.0001 0.0001 -0.0570 C 0 0 0 0 0 0 0 0 0 0 0 1
26 0.3766 -1.4050 0.4983 C 0 0 0 0 0 0 0 0 0 0 0 2
27 -1.4036 0.3761 0.5019 C 0 0 0 0 0 0 0 0 0 0 0 3
28 1.0288 1.0274 0.4996 C 0 0 0 0 0 0 0 0 0 0 0 4
29 0.3925 -1.4571 1.6017 H 0 0 0 0 0 0 0 0 0 0 0 5
30 -1.6873 1.3747 0.1304 H 0 0 0 0 0 0 0 0 0 0 0 6
31 2.0347 0.7740 0.1265 H 0 0 0 0 0 0 0 0 0 0 0 7
32 -1.4533 0.3896 1.6055 H 0 0 0 0 0 0 0 0 0 0 0 8
33 -0.3472 -2.1494 0.1276 H 0 0 0 0 0 0 0 0 0 0 0 9
34 1.3742 -1.6889 0.1247 H 0 0 0 0 0 0 0 0 0 0 0 10
35 0.7753 2.0343 0.1291 H 0 0 0 0 0 0 0 0 0 0 0 11
36 -2.1485 -0.3469 0.1305 H 0 0 0 0 0 0 0 0 0 0 0 12
37 1.0683 1.0641 1.6031 H 0 0 0 0 0 0 0 0 0 0 0 13
38 -0.0018 0.0013 -1.4347 O 0 0 0 0 0 0 0 0 0 0 0 14
39
40 2 1 0 0 0 0
41 3 1 0 0 0 0
42 4 1 0 0 0 0
43 5 2 0 0 0 0
44 9 2 0 0 0 0
45 10 2 0 0 0 0
46 6 3 0 0 0 0
47 8 3 0 0 0 0
48 12 3 0 0 0 0
49 7 4 0 0 0 0
50 11 4 0 0 0 0
51 13 4 0 0 0 0
52 1 14 0 0 0 0
53 M END
54 $$$
55 tert-butanol.sdf
56 COSMOTHERM 3D 0
57
58 15 14 0 0 0 0 0 0 0 0 V2000
59 -0.0041 0.0395 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
60 -0.7622 0.4654 1.2644 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7622 0.4661 -1.2642 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4217 0.5918 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8723 1.5591 1.3080 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.2242 0.1351 -2.1645 H 0 0 0 0 0 0 0 0 0 0 0 6
1.9667 0.2520 0.8931 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.8722 1.5599 -1.3073 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.7705 0.0233 1.2790 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.2242 0.1341 2.1646 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9666 0.2525 -0.8929 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.7705 0.0241 -1.2790 H 0 0 0 0 0 0 0 0 0 0 0 12
1.4077 1.6905 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 13
0.1518 -1.4146 -0.0004 O 0 0 0 0 0 0 0 0 0 0 0 14
-0.7445 -1.7999 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 15
61
62 2 1 0 0 0 0
63 3 1 0 0 0 0
64 4 1 0 0 0 0
65 14 1 0 0 0 0
66 5 2 0 0 0 0
67 9 2 0 0 0 0
68 10 2 0 0 0 0
69 6 3 0 0 0 0
70 8 3 0 0 0 0
71 12 3 0 0 0 0
72 7 4 0 0 0 0
73 11 4 0 0 0 0
74 13 4 0 0 0 0
75 14 15 0 0 0 0
76 M END
77 $$$
78 thymine-anion1.sdf
79 COSMOTHERM 3D 0
80
81 14 14 0 0 0 0 0 0 0 0 V2000
82 -0.1734 1.5170 0.0055 C 0 0 0 0 0 0 0 0 0 0 0 1
83 -1.1718 0.5559 0.0048 C 0 0 0 0 0 0 0 0 0 0 0 2
84 -0.7553 -0.8208 0.0019 C 0 0 0 0 0 0 0 0 0 0 0 3
85 0.6345 -0.9920 -0.0067 N 0 0 0 0 0 0 0 0 0 0 0 4
86 1.6060 0.0243 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 5
87 1.1684 1.3130 0.0025 N 0 0 0 0 0 0 0 0 0 0 0 6
88 -1.5073 -1.8275 0.0058 O 0 0 0 0 0 0 0 0 0 0 0 7
89 2.8210 -0.3042 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 8
90 -2.6372 0.8905 -0.0085 C 0 0 0 0 0 0 0 0 0 0 0 9
91 -0.4738 2.5726 0.0070 H 0 0 0 0 0 0 0 0 0 0 0 10
92 0.9758 -1.9544 -0.0070 H 0 0 0 0 0 0 0 0 0 0 0 11
93 -3.1477 0.5373 0.9026 H 0 0 0 0 0 0 0 0 0 0 0 12
94 -3.1544 0.4199 -0.8599 H 0 0 0 0 0 0 0 0 0 0 0 13
95 -2.7864 1.9773 -0.0783 H 0 0 0 0 0 0 0 0 0 0 0 14
96
97 2 1 0 0 0 0
98 6 1 0 0 0 0
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10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 9 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
thymine.sdf
COSMOTHERM 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
-0.2358 -1.5308 0.0005 C 0 0 0 0 0 0 0 0 0 0 1
-1.1931 -0.5610 0.0012 C 0 0 0 0 0 0 0 0 0 0 2
-0.7573 0.8299 0.0002 C 0 0 0 0 0 0 0 0 0 0 3
0.6382 1.0148 0.0015 N 0 0 0 0 0 0 0 0 0 0 4
1.6228 0.0390 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.1098 -1.2457 -0.0010 N 0 0 0 0 0 0 0 0 0 0 6
-1.5071 1.8174 -0.0011 O 0 0 0 0 0 0 0 0 0 0 7
2.8316 0.2902 -0.0004 O 0 0 0 0 0 0 0 0 0 0 8
-2.6630 -0.8607 -0.0002 C 0 0 0 0 0 0 0 0 0 0 9
-0.4772 -2.5931 0.0004 H 0 0 0 0 0 0 0 0 0 0 10
0.9694 1.9810 0.0019 H 0 0 0 0 0 0 0 0 0 0 11
1.7880 -2.0053 -0.0018 H 0 0 0 0 0 0 0 0 0 0 12
-3.1480 -0.4549 -0.9011 H 0 0 0 0 0 0 0 0 0 0 13
-3.1600 -0.4000 0.8667 H 0 0 0 0 0 0 0 0 0 0 14
-2.8404 -1.9432 0.0313 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
9 15 0 0 0 0
M END
$$$$
trans-5-formyluracil-anion0.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2798 -1.3087 -0.0001 C 0 0 0 0 0 0 0 0 0 0 1
-0.9153 -0.0847 0.0001 C 0 0 0 0 0 0 0 0 0 0 2
-0.0774 1.1359 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.2907 0.9994 0.0000 N 0 0 0 0 0 0 0 0 0 0 4
1.8897 -0.2079 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.0596 -1.3779 -0.0001 N 0 0 0 0 0 0 0 0 0 0 6
-0.6008 2.2805 0.0000 O 0 0 0 0 0 0 0 0 0 0 7
3.1253 -0.3988 0.0001 O 0 0 0 0 0 0 0 0 0 0 8
-2.3637 -0.0062 -0.0003 C 0 0 0 0 0 0 0 0 0 0 9
-0.8290 -2.2518 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10
1.5337 -2.2806 -0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-3.1410 -0.9756 0.0003 O 0 0 0 0 0 0 0 0 0 0 12
-2.7665 1.0298 -0.0012 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 6 0 0 0 0
12 9 0 0 0 0
9 13 0 0 0 0
M END
$$$$
trans-5-formyluracil-anion1.sdf
COSMOTHERM 3D 0
13 13 0 0 0 0 0 0 0 0 0 V2000
-0.2325 -1.3051 0.0000 C 0 0 0 0 0 0 0 0 0 0 1
-0.9240 -0.0791 -0.0003 C 0 0 0 0 0 0 0 0 0 0 2
-0.1404 1.1418 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
1.2390 0.9038 0.0006 N 0 0 0 0 0 0 0 0 0 0 4
1.8773 -0.3441 0.0000 C 0 0 0 0 0 0 0 0 0 0 5
1.0863 -1.4787 0.0000 N 0 0 0 0 0 0 0 0 0 0 6
-0.5688 2.3129 -0.0001 O 0 0 0 0 0 0 0 0 0 0 7
3.1211 -0.3936 -0.0002 O 0 0 0 0 0 0 0 0 0 0 8
-2.3648 -0.0173 -0.0003 C 0 0 0 0 0 0 0 0 0 0 9
-0.8348 -2.2210 0.0001 H 0 0 0 0 0 0 0 0 0 0 10
1.8441 1.7270 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-3.1365 -0.9955 0.0003 O 0 0 0 0 0 0 0 0 0 0 12
-2.7856 1.0133 -0.0008 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0

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7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 9 0 0 0 0
9 13 0 0 0 0
M END
\$\$\$\$
trans-5-formyluracil.sdf
COSMOTHERM 3D 0

14 14 0 0 0 0 0 0 0 0 0 V2000
-0.2914 -1.2943 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.9385 -0.0802 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.1445 1.1475 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.2468 0.9277 0.0006 N 0 0 0 0 0 0 0 0 0 0 0 0 4
1.9141 -0.2832 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.0539 -1.3916 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5863 2.2999 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 7
3.1347 -0.3996 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.3993 -0.0103 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.8435 -2.2347 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.8389 1.7607 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.5034 -2.3076 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.1466 -0.9923 0.0004 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.8163 1.0190 -0.0012 H 0 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
12 6 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
\$\$\$\$
trans-5-formyluracil2-anion.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
-1.5697 -0.2689 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.6003 0.7615 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 2
0.7620 0.3063 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.0980 -0.9662 0.0007 N 0 0 0 0 0 0 0 0 0 0 0 0 4
0.0784 -1.9169 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.2847 -1.5566 0.0011 N 0 0 0 0 0 0 0 0 0 0 0 0 6
1.7540 1.2161 0.0010 O 0 0 0 0 0 0 0 0 0 0 0 0 7
0.3755 -3.1331 -0.0021 O 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9264 2.1462 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.6326 0.0048 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.0615 3.0674 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.0016 2.4161 -0.0015 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.2870 2.1234 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
7 13 0 0 0 0
M END
\$\$\$\$
trichloroaceticacid-anion.sdf
COSMOTHERM 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
0.5429 -0.9834 1.4795 Cl 0 0 0 0 0 0 0 0 0 0 0 0 1
0.1183 0.0008 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.4656 0.3101 0.0022 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.7804 1.5177 0.0029 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.1651 -0.7259 0.0022 O 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5400 -0.9721 -1.4876 Cl 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1542 1.4928 0.0050 Cl 0 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 7 0 0 0 0
M END
\$\$\$\$
trichloroaceticacid.sdf
COSMOTHERM 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
0.4436 -1.0530 1.4593 Cl 0 0 0 0 0 0 0 0 0 0 0 0 1
0.1685 -0.0162 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.3106 0.4953 0.0139 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.6056 1.6688 0.0200 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.1550 -0.5380 0.0139 O 0 0 0 0 0 0 0 0 0 0 0 0 5
0.4295 -0.9851 -1.5075 Cl 0 0 0 0 0 0 0 0 0 0 0 0 6
1.2984 1.3710 0.0274 Cl 0 0 0 0 0 0 0 0 0 0 0 0 7

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-3.0760 -0.1950 0.0170 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
5 8 0 0 0 0
M END
$$$$
uracil-anion1.sdf
COSMOtherm 3D 0
11 11 0 0 0 0 0 0 0 0 0 V2000
-1.7175 -0.0934 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1520 1.1701 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
0.2744 1.2861 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.9235 0.0429 0.0002 N 0 0 0 0 0 0 0 0 0 0 0 4
0.3106 -1.2236 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.0540 -1.2735 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 6
0.9526 2.3436 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 7
1.0423 -2.2442 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 8
-1.7627 2.0714 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
-2.8100 -0.1813 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9446 0.0575 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
4 11 0 0 0 0
M END
$$$$
uracil.sdf
COSMOtherm 3D 0
12 12 0 0 0 0 0 0 0 0 0 V2000
-1.7458 -0.0178 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1435 1.2015 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 2
0.3006 1.2898 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.9514 0.0380 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
0.3676 -1.2192 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.0204 -1.1808 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 6
0.9722 2.3320 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 7
1.0127 -2.2697 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 8
-1.7286 2.1172 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
-2.8272 -0.1450 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
1.9727 0.0527 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.4980 -2.0805 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
6 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
6 12 0 0 0 0
M END
$$$$

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S4 b) Mono-solvated Acids & Anions

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2,2,2-trichloroethanol-anion.sdf
COSMOtherm 3D 0
11 9 0 0 0 0 0 0 0 0 0 V2000
-3.6769 0.3261 -0.1977 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8189 -0.2320 -0.4323 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.3556 1.0180 0.4044 H 0 0 0 0 0 0 0 0 0 0 0 3
0.4442 0.0021 -0.1189 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.5978 -0.3217 -1.2362 C 0 0 0 0 0 0 0 0 0 0 0 5
1.8215 1.0060 -0.8113 Cl 0 0 0 0 0 0 0 0 0 0 0 6
-0.3203 0.9475 1.2462 Cl 0 0 0 0 0 0 0 0 0 0 0 7
1.1489 -1.5258 0.5881 Cl 0 0 0 0 0 0 0 0 0 0 0 8
-1.6380 -1.0768 -0.8202 O 0 0 0 0 0 0 0 0 0 0 0 9
0.0305 -0.7975 -2.0288 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.8733 0.6927 -1.6205 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
5 11 0 0 0 0
M END
$$$$
2,2,2-trichloroethanol.sdf
COSMOtherm 3D 0

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12 10 0 0 0 0 0 0 0 0 0 V2000
-3.7463 -0.1444 -0.2754 O 0 0 0 0 0 0 0 0 0 0 1
-4.1383 -0.8906 -0.7645 H 0 0 0 0 0 0 0 0 0 0 2
-3.6522 0.5606 -0.9411 H 0 0 0 0 0 0 0 0 0 0 3
0.4943 -0.1048 -0.0131 C 0 0 0 0 0 0 0 0 0 0 4
-0.4905 -1.2470 0.3210 C 0 0 0 0 0 0 0 0 0 0 5
1.8410 -0.7910 -1.0234 Cl 0 0 0 0 0 0 0 0 0 0 6
-0.3344 1.2146 -0.9466 Cl 0 0 0 0 0 0 0 0 0 0 7
1.1920 0.6075 1.5014 Cl 0 0 0 0 0 0 0 0 0 0 8
-1.5531 -0.8387 1.1413 O 0 0 0 0 0 0 0 0 0 0 9
0.0952 -2.0150 0.8479 H 0 0 0 0 0 0 0 0 0 0 10
-0.8304 -1.6628 -0.6415 H 0 0 0 0 0 0 0 0 0 0 11
-2.3191 -0.5464 0.5673 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
9 12 0 0 0 0
M END
$$$$
2,2-dimethylpropanoicacid-anion.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-3.5942 -0.1554 0.0014 O 0 0 0 0 0 0 0 0 0 0 1
-2.6125 -0.4207 -0.0002 H 0 0 0 0 0 0 0 0 0 0 2
-3.5437 0.8166 -0.0025 H 0 0 0 0 0 0 0 0 0 0 3
2.0250 1.2678 -0.0139 C 0 0 0 0 0 0 0 0 0 0 4
1.2526 -0.0598 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
1.6186 -0.8592 1.2686 C 0 0 0 0 0 0 0 0 0 0 6
1.6210 -0.8871 -1.2495 C 0 0 0 0 0 0 0 0 0 0 7
-0.2917 0.1845 -0.0023 C 0 0 0 0 0 0 0 0 0 0 8
-0.7329 1.3673 -0.0019 O 0 0 0 0 0 0 0 0 0 0 9
-1.0278 -0.8674 -0.0029 O 0 0 0 0 0 0 0 0 0 0 10
3.1096 1.0743 -0.0116 H 0 0 0 0 0 0 0 0 0 0 11
1.7828 1.8602 -0.9079 H 0 0 0 0 0 0 0 0 0 0 12
1.7820 1.8793 0.8668 H 0 0 0 0 0 0 0 0 0 0 13
2.6995 -1.0724 1.2881 H 0 0 0 0 0 0 0 0 0 0 14
1.0747 -1.8133 1.2968 H 0 0 0 0 0 0 0 0 0 0 15
1.3701 -0.2936 2.1806 H 0 0 0 0 0 0 0 0 0 0 16
2.7019 -1.1007 -1.2621 H 0 0 0 0 0 0 0 0 0 0 17
1.0767 -1.8413 -1.2577 H 0 0 0 0 0 0 0 0 0 0 18
1.3744 -0.3418 -2.1743 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0
M END
$$$$
2,2-dimethylpropanoicacid.sdf
COSMOTHERM 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-3.6236 -0.0263 0.1980 O 0 0 0 0 0 0 0 0 0 0 1
-3.8516 -0.5483 -0.5932 H 0 0 0 0 0 0 0 0 0 0 2
-3.9862 0.8606 0.0180 H 0 0 0 0 0 0 0 0 0 0 3
2.1551 0.0265 -1.1735 C 0 0 0 0 0 0 0 0 0 0 4
1.2852 -0.0005 0.0924 C 0 0 0 0 0 0 0 0 0 0 5
1.5802 1.2441 0.9616 C 0 0 0 0 0 0 0 0 0 0 6
1.5755 -1.2846 0.9045 C 0 0 0 0 0 0 0 0 0 0 7
-0.1994 0.0071 -0.3029 C 0 0 0 0 0 0 0 0 0 0 8
-0.6120 0.0134 -1.4605 O 0 0 0 0 0 0 0 0 0 0 9
-1.0254 0.0018 0.7585 O 0 0 0 0 0 0 0 0 0 0 10
3.2170 0.0139 -0.8876 H 0 0 0 0 0 0 0 0 0 0 11
1.9592 -0.8459 -1.8121 H 0 0 0 0 0 0 0 0 0 0 12
1.9690 0.9321 -1.7678 H 0 0 0 0 0 0 0 0 0 0 13
2.6458 1.2522 1.2353 H 0 0 0 0 0 0 0 0 0 0 14
0.9859 1.2371 1.8847 H 0 0 0 0 0 0 0 0 0 0 15
1.3631 2.1732 0.4134 H 0 0 0 0 0 0 0 0 0 0 16
2.6409 -1.3089 1.1783 H 0 0 0 0 0 0 0 0 0 0 17
0.9802 -1.3171 1.8264 H 0 0 0 0 0 0 0 0 0 0 18
1.3556 -2.1871 0.3145 H 0 0 0 0 0 0 0 0 0 0 19
-1.9947 0.0035 0.4452 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
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3 19 7 0 0 0 0
4 9 8 0 0 0 0
5 10 8 0 0 0 0
6 10 20 0 0 0 0
7 M END
8 $$$
9 2,3,4,6-tetrachlorophenol-anion.sdf
10 COSMOTHERM 3D 0
11
12 15 14 0 0 0 0 0 0 0 0 0 V2000
13 -4.8073 -0.8001 -0.5123 O 0 0 0 0 0 0 0 0 0 0 0 1
14 -3.8395 -0.7857 -0.2498 H 0 0 0 0 0 0 0 0 0 0 0 2
15 -5.0111 0.1257 -0.7273 H 0 0 0 0 0 0 0 0 0 0 0 3
16 0.0775 1.7612 0.0246 C 0 0 0 0 0 0 0 0 0 0 0 4
17 -1.0981 1.0271 0.0961 C 0 0 0 0 0 0 0 0 0 0 0 5
18 -1.1580 -0.4079 0.1235 C 0 0 0 0 0 0 0 0 0 0 0 6
19 0.1500 -1.0213 0.0657 C 0 0 0 0 0 0 0 0 0 0 0 7
20 1.3470 -0.2995 -0.0054 C 0 0 0 0 0 0 0 0 0 0 0 8
21 1.3082 1.1038 -0.0274 C 0 0 0 0 0 0 0 0 0 0 0 9
22 -2.2361 -1.0951 0.1965 O 0 0 0 0 0 0 0 0 0 0 0 10
23 0.1729 -2.7818 0.0919 Cl 0 0 0 0 0 0 0 0 0 0 0 11
24 2.8951 -1.1370 -0.0702 Cl 0 0 0 0 0 0 0 0 0 0 0 12
25 2.7840 2.0707 -0.1141 Cl 0 0 0 0 0 0 0 0 0 0 0 13
26 -2.6354 1.9082 0.1686 Cl 0 0 0 0 0 0 0 0 0 0 0 14
27 0.0450 2.8500 0.0099 H 0 0 0 0 0 0 0 0 0 0 0 15
28
29 2 1 0 0 0 0
30 3 1 0 0 0 0
31 5 4 0 0 0 0
32 9 4 0 0 0 0
33 6 5 0 0 0 0
34 14 5 0 0 0 0
35 7 6 0 0 0 0
36 10 6 0 0 0 0
37 8 7 0 0 0 0
38 11 7 0 0 0 0
39 9 8 0 0 0 0
40 12 8 0 0 0 0
41 13 9 0 0 0 0
42 4 15 0 0 0 0
43 M END
44 $$$
45 2,3,4,6-tetrachlorophenol.sdf
46 COSMOTHERM 3D 0
47
48 16 15 0 0 0 0 0 0 0 0 V2000
49 -4.3041 0.0409 -1.5728 O 0 0 0 0 0 0 0 0 0 0 0 1
50 -4.3084 -0.6487 -2.2610 H 0 0 0 0 0 0 0 0 0 0 0 2
51 -4.4164 0.8761 -2.0621 H 0 0 0 0 0 0 0 0 0 0 0 3
52 -0.3255 -0.0089 -0.7504 C 0 0 0 0 0 0 0 0 0 0 0 4
53 1.0752 -0.0010 -0.6249 C 0 0 0 0 0 0 0 0 0 0 0 5
54 1.6486 0.0046 0.6537 C 0 0 0 0 0 0 0 0 0 0 0 6
55 0.8363 0.0029 1.7873 C 0 0 0 0 0 0 0 0 0 0 0 7
56 -0.5448 -0.0042 1.6447 C 0 0 0 0 0 0 0 0 0 0 0 8
57 -1.1743 -0.0094 0.3800 C 0 0 0 0 0 0 0 0 0 0 0 9
58 3.3929 0.0144 0.8707 Cl 0 0 0 0 0 0 0 0 0 0 0 10
59 -2.5139 -0.0207 0.3449 O 0 0 0 0 0 0 0 0 0 0 0 11
60 -1.0668 -0.0193 -2.3383 Cl 0 0 0 0 0 0 0 0 0 0 0 12
61 2.0851 0.0001 -2.0520 Cl 0 0 0 0 0 0 0 0 0 0 0 13
62 1.2841 0.0075 2.7795 H 0 0 0 0 0 0 0 0 0 0 0 14
63 -1.5521 -0.0057 3.0867 Cl 0 0 0 0 0 0 0 0 0 0 0 15
64 -2.9541 0.0083 -0.5662 H 0 0 0 0 0 0 0 0 0 0 0 16
65
66 2 1 0 0 0 0
67 3 1 0 0 0 0
68 5 4 0 0 0 0
69 9 4 0 0 0 0
70 12 4 0 0 0 0
71 6 5 0 0 0 0
72 13 5 0 0 0 0
73 7 6 0 0 0 0
74 10 6 0 0 0 0
75 8 7 0 0 0 0
76 14 7 0 0 0 0
77 9 8 0 0 0 0
78 15 8 0 0 0 0
79 11 9 0 0 0 0
80 11 16 0 0 0 0
81 M END
82 $$$
83 2,3,4-trichlorophenol-anion.sdf
84 COSMOTHERM 3D 0
85
86 15 14 0 0 0 0 0 0 0 0 V2000
87 -4.8410 -0.0444 1.4948 O 0 0 0 0 0 0 0 0 0 0 0 1
88 -4.0333 -0.0101 0.8812 H 0 0 0 0 0 0 0 0 0 0 0 2
89 -4.8468 0.8208 1.9384 H 0 0 0 0 0 0 0 0 0 0 0 3
90 -1.2265 -0.0064 1.5919 C 0 0 0 0 0 0 0 0 0 0 0 4
91 0.0934 -0.0051 2.0259 C 0 0 0 0 0 0 0 0 0 0 0 5
92 1.1482 -0.0018 1.1080 C 0 0 0 0 0 0 0 0 0 0 0 6
93 0.8642 0.0002 -0.2677 C 0 0 0 0 0 0 0 0 0 0 0 7
94 -0.4674 -0.0007 -0.7025 C 0 0 0 0 0 0 0 0 0 0 0 8
95 -1.5872 -0.0027 0.2069 C 0 0 0 0 0 0 0 0 0 0 0 9
96 2.8142 0.0005 1.7076 Cl 0 0 0 0 0 0 0 0 0 0 0 10
97 -2.8103 -0.0029 -0.2105 O 0 0 0 0 0 0 0 0 0 0 0 11
98 -2.0358 -0.0132 2.3247 H 0 0 0 0 0 0 0 0 0 0 0 12
99 0.3179 -0.0072 3.0934 H 0 0 0 0 0 0 0 0 0 0 0 13
100 2.1847 0.0031 -1.4378 Cl 0 0 0 0 0 0 0 0 0 0 0 14
101 -0.8465 0.0010 -2.4261 Cl 0 0 0 0 0 0 0 0 0 0 0 15
102
103 2 1 0 0 0 0
104 3 1 0 0 0 0
105 5 4 0 0 0 0
106 9 4 0 0 0 0
107 12 4 0 0 0 0
108 6 5 0 0 0 0
109 13 5 0 0 0 0
110 7 6 0 0 0 0

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10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
\$\$\$\$
2,3,4-trichlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-4.6384 0.0030 1.5542 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.1834 -0.8050 1.5313 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.2725 0.7341 1.4365 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0609 0.0011 2.0153 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.2513 0.0012 1.5516 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.5308 0.0008 0.1736 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.4445 0.0002 -0.7301 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.8812 0.0002 -0.2660 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.1281 0.0003 1.1163 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.7831 0.0004 -0.3272 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.7968 -0.0004 -2.4490 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
2.2110 -0.0004 -1.4062 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
2.7745 -0.0001 1.7451 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
0.2606 0.0014 3.0864 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.0787 0.0022 2.2620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-3.4737 -0.0003 0.4166 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 9 0 0 0 0
10 16 0 0 0 0
M END
\$\$\$\$
2,3-dichlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
-4.6680 -0.0414 -0.1072 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.6763 -0.0126 -0.3310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.8342 0.7907 0.3677 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.4122 -0.0080 1.4709 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3781 -0.0058 2.4015 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.9666 -0.0016 2.0031 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.2403 0.0003 0.6316 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.2182 -0.0018 -0.3207 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.1753 -0.0029 0.0579 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.7802 0.0010 2.7268 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.1232 -0.0011 -0.8236 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.4530 -0.0158 1.8022 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.6131 -0.0087 3.4684 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.9467 0.0043 0.1273 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
0.5797 0.0001 -2.0511 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
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2,3-dichlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-4.5363 -0.0092 0.0042 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.0499 -0.7579 -0.3510 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.0335 0.7842 -0.2674 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.4281 0.0016 2.3772 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.4377 0.0035 1.4156 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.1194 0.0029 0.0450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2436 0.0013 -0.3342 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.2428 -0.0004 0.6482 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.9196 -0.0001 2.0071 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.0542 0.0045 -0.9311 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.6373 0.0010 -2.0468 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
2.9465 -0.0028 0.1869 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.9885 0.0017 -0.5396 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.6923 0.0020 3.4355 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.4877 0.0043 1.7114 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.7119 -0.0014 2.7543 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0

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6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 10 0 0 0 0
9 16 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol-anion.sdf
COSMOTHERM      3D      0
15 14 0 0 0 0 0 0 0 0 0 V2000
-3.3026 3.2156 0.0065 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.3210 2.9607 -0.0019 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.6270 2.9590 -0.8734 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.1848 0.3035 0.0213 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.7324 -1.0105 0.0109 C 0 0 0 0 0 0 0 0 0 0 0 5
0.6382 -1.3052 -0.0039 C 0 0 0 0 0 0 0 0 0 0 0 6
1.5515 -0.2443 -0.0072 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0962 1.0679 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.2950 1.4294 0.0161 C 0 0 0 0 0 0 0 0 0 0 0 9
1.2486 -2.9643 -0.0205 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-0.7084 2.6525 0.0225 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.2566 0.5052 0.0360 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.9335 -2.3176 0.0162 Cl 0 0 0 0 0 0 0 0 0 0 0 13
2.6210 -0.4536 -0.0178 H 0 0 0 0 0 0 0 0 0 0 0 14
2.2900 2.3823 0.0012 Cl 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2,4,5-trichlorophenol.sdf
COSMOTHERM      3D      0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.3246 -0.0105 -2.8674 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6428 -0.7450 -3.4235 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.6762 0.7942 -3.2906 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.7075 0.0009 1.0244 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.1784 0.0023 -0.2881 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.2869 0.0031 -1.3759 C 0 0 0 0 0 0 0 0 0 0 0 6
1.0952 0.0008 -1.0902 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5690 0.0002 0.2179 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6689 -0.0006 1.2868 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.6945 0.0079 -2.6602 O 0 0 0 0 0 0 0 0 0 0 0 10
2.2476 -0.0015 -2.4242 Cl 0 0 0 0 0 0 0 0 0 0 0 11
1.3010 -0.0014 2.9295 Cl 0 0 0 0 0 0 0 0 0 0 0 12
-1.8823 0.0003 2.3359 Cl 0 0 0 0 0 0 0 0 0 0 0 13
-2.2517 0.0037 -0.4784 H 0 0 0 0 0 0 0 0 0 0 0 14
2.6410 -0.0017 0.4098 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.7084 0.0034 -2.7257 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
12 9 0 0 0 0
10 16 0 0 0 0
M END
$$$$
2,4,6-trichlorophenol-anion.sdf
COSMOTHERM      3D      0
15 14 0 0 0 0 0 0 0 0 0 V2000
-4.1763 0.2917 -1.0099 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.3671 0.0083 -0.4825 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.0925 1.2588 -1.0677 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5516 -0.9830 -0.0559 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2050 -1.3038 0.0865 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8635 -0.3487 0.2208 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.3774 1.0059 0.1844 C 0 0 0 0 0 0 0 0 0 0 0 7
0.9581 1.3718 0.0392 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9158 0.3643 -0.0825 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.0975 -0.6792 0.3633 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.5829 2.3001 0.3567 Cl 0 0 0 0 0 0 0 0 0 0 0 11
-0.2520 -3.0196 0.1181 Cl 0 0 0 0 0 0 0 0 0 0 0 12
3.6292 0.8036 -0.2684 Cl 0 0 0 0 0 0 0 0 0 0 0 13
2.2997 -1.7692 -0.1494 H 0 0 0 0 0 0 0 0 0 0 0 14
1.2434 2.4231 0.0234 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0

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5 4 0 0 0 0
 9 4 0 0 0 0
 14 4 0 0 0 0
 6 5 0 0 0 0
 12 5 0 0 0 0
 7 6 0 0 0 0
 10 6 0 0 0 0
 8 7 0 0 0 0
 11 7 0 0 0 0
 9 8 0 0 0 0
 13 9 0 0 0 0
 8 15 0 0 0 0

M END

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2,4,6-trichlorophenol.sdf
 COSMOTHERM 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
 -4.3902 0.0737 -0.3079 O 0 0 0 0 0 0 0 0 0 0 1
 -4.6586 -0.6530 -0.8987 H 0 0 0 0 0 0 0 0 0 0 2
 -4.6285 0.8842 -0.7935 H 0 0 0 0 0 0 0 0 0 0 3
 0.2953 -0.0061 1.3121 C 0 0 0 0 0 0 0 0 0 0 4
 1.6356 0.0051 0.9359 C 0 0 0 0 0 0 0 0 0 0 5
 1.9443 0.0076 -0.4242 C 0 0 0 0 0 0 0 0 0 0 6
 0.9460 -0.0018 -1.3950 C 0 0 0 0 0 0 0 0 0 0 7
 -0.3870 -0.0142 -0.9828 C 0 0 0 0 0 0 0 0 0 0 8
 -0.7665 -0.0147 0.3775 C 0 0 0 0 0 0 0 0 0 0 9
 3.6404 0.0226 -0.9263 Cl 0 0 0 0 0 0 0 0 0 0 10
 -2.0248 -0.0301 0.8453 O 0 0 0 0 0 0 0 0 0 0 11
 -0.1036 -0.0091 3.0287 Cl 0 0 0 0 0 0 0 0 0 0 12
 2.4177 0.0121 1.6930 H 0 0 0 0 0 0 0 0 0 0 13
 1.1893 -0.0013 -2.4560 H 0 0 0 0 0 0 0 0 0 0 14
 -1.6443 -0.0321 -2.2198 Cl 0 0 0 0 0 0 0 0 0 0 15
 -2.7638 0.0080 0.1571 H 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 9 4 0 0 0 0
 12 4 0 0 0 0
 6 5 0 0 0 0
 13 5 0 0 0 0
 7 6 0 0 0 0
 10 6 0 0 0 0
 8 7 0 0 0 0
 14 7 0 0 0 0
 9 8 0 0 0 0
 15 8 0 0 0 0
 11 9 0 0 0 0
 11 16 0 0 0 0

M END

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2,4-dichlorophenol-anion.sdf
 COSMOTHERM 3D 0

15 14 0 0 0 0 0 0 0 0 0 V2000
 -2.2785 -3.9859 0.0307 O 0 0 0 0 0 0 0 0 0 0 1
 -1.4803 -3.3532 0.0077 H 0 0 0 0 0 0 0 0 0 0 2
 -2.6902 -3.8923 -0.8452 H 0 0 0 0 0 0 0 0 0 0 3
 -1.4855 -0.4651 0.0203 C 0 0 0 0 0 0 0 0 0 0 4
 -1.5916 0.9246 0.0139 C 0 0 0 0 0 0 0 0 0 0 5
 -0.4303 1.7013 0.0015 C 0 0 0 0 0 0 0 0 0 0 6
 0.8314 1.1021 -0.0046 C 0 0 0 0 0 0 0 0 0 0 7
 0.9100 -0.2884 0.0025 C 0 0 0 0 0 0 0 0 0 0 8
 -0.2313 -1.1609 0.0107 C 0 0 0 0 0 0 0 0 0 0 9
 -0.5486 3.4811 -0.0069 Cl 0 0 0 0 0 0 0 0 0 0 10
 -0.1316 -2.4531 0.0124 O 0 0 0 0 0 0 0 0 0 0 11
 -2.3934 -1.0725 0.0321 H 0 0 0 0 0 0 0 0 0 0 12
 -2.5738 1.4000 0.0196 H 0 0 0 0 0 0 0 0 0 0 13
 1.7391 1.7056 -0.0122 H 0 0 0 0 0 0 0 0 0 0 14
 2.5233 -1.0415 -0.0049 Cl 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 9 4 0 0 0 0
 12 4 0 0 0 0
 6 5 0 0 0 0
 13 5 0 0 0 0
 7 6 0 0 0 0
 10 6 0 0 0 0
 8 7 0 0 0 0
 14 7 0 0 0 0
 9 8 0 0 0 0
 11 9 0 0 0 0
 8 15 0 0 0 0

M END

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2,4-dichlorophenol.sdf
 COSMOTHERM 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
 -2.3387 -0.0153 -3.7655 O 0 0 0 0 0 0 0 0 0 0 1
 -2.5232 -0.8833 -4.1690 H 0 0 0 0 0 0 0 0 0 0 2
 -2.3443 0.6116 -4.5121 H 0 0 0 0 0 0 0 0 0 0 3
 -1.5842 0.0164 0.9106 C 0 0 0 0 0 0 0 0 0 0 4
 -1.4621 0.0238 -0.4796 C 0 0 0 0 0 0 0 0 0 0 5
 -0.2014 0.0159 -1.1060 C 0 0 0 0 0 0 0 0 0 0 6
 0.9384 0.0025 -0.2747 C 0 0 0 0 0 0 0 0 0 0 7
 0.8387 -0.0043 1.1161 C 0 0 0 0 0 0 0 0 0 0 8
 -0.4307 0.0020 1.6947 C 0 0 0 0 0 0 0 0 0 0 9
 -0.0369 0.0198 -2.4478 O 0 0 0 0 0 0 0 0 0 0 10
 2.5412 -0.0063 -1.0174 Cl 0 0 0 0 0 0 0 0 0 0 11
 -0.5694 -0.0085 3.4639 Cl 0 0 0 0 0 0 0 0 0 0 12
 -2.5714 0.0216 1.3720 H 0 0 0 0 0 0 0 0 0 0 13
 -2.3595 0.0357 -1.1003 H 0 0 0 0 0 0 0 0 0 0 14
 1.7384 -0.0150 1.7295 H 0 0 0 0 0 0 0 0 0 0 15

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3 M END
4 \$\$\$
5 2,5-dichlorophenol-anion.sdf
6 COSMOTHERM 3D 0
7
8 15 14 0 1
9 4.0237 0.5231 0.0377 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
10 3.0594 0.8424 0.0129 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
11 4.1609 0.0972 -0.8256 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
12 0.6507 -0.7522 0.0099 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
13 -0.4691 -1.5722 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
14 -1.7775 -1.0840 -0.0078 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
15 -1.9360 0.3103 -0.0090 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
16 -0.8294 1.1505 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
17 0.5287 0.6801 0.0070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
18 -2.6400 -1.7479 -0.0155 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
19 1.5524 1.4698 0.0126 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
20 1.6552 -1.1774 0.0203 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
21 -0.2253 -3.3476 0.0028 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
22 -2.9400 0.7374 -0.0166 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
23 -1.0863 2.9132 -0.0020 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
24
25 2 1 0 0 0 0
26 3 1 0 0 0 0
27 5 4 0 0 0 0
28 9 4 0 0 0 0
29 12 4 0 0 0 0
30 6 5 0 0 0 0
31 13 5 0 0 0 0
32 7 6 0 0 0 0
33 10 6 0 0 0 0
34 8 7 0 0 0 0
35 14 7 0 0 0 0
36 9 8 0 0 0 0
37 11 9 0 0 0 0
38 8 15 0 0 0 0
39
40 M END
41 \$\$\$
42 2,5-dichlorophenol.sdf
43 COSMOTHERM 3D 0
44
45 16 15 0 1
46 -3.8682 0.0009 -0.1412 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
47 -4.4151 -0.7764 -0.3584 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
48 -4.4232 0.7682 -0.3730 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
49 0.5334 0.0001 1.5466 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
50 -0.6168 -0.0001 0.7613 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
51 -0.5018 -0.0001 -0.6427 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
52 0.7949 0.0001 -1.2002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
53 1.9321 0.0002 -0.3965 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
54 1.8152 0.0003 0.9976 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
55 -1.5732 -0.0005 -1.4634 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
56 0.9692 0.0000 -2.9589 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
57 0.3523 -0.0001 3.3128 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
58 -1.6072 -0.0003 1.2167 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
59 2.9195 0.0004 -0.8584 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
60 2.7029 0.0003 1.6278 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.4390 0.0006 -0.9353 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
10 16 0 0 0 0
M END
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2,6-dichlorophenol-anion.sdf
COSMOTHERM 3D 0
15 14 0 1
-2.6990 -2.6474 -0.3543 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.9003 -2.0738 -0.1364 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-3.4099 -2.0086 -0.5310 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
2.0530 1.2950 -0.1452 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
1.4868 0.0325 -0.0062 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.0746 -0.2303 0.0950 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.6977 0.9822 0.0309 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.1614 2.2583 -0.1096 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.2261 2.4249 -0.1995 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.4148 -1.4124 0.2324 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.4701 0.8169 0.1510 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
2.5646 -1.3855 0.0554 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
3.1372 1.3968 -0.2129 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.8270 3.1218 -0.1482 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.6571 3.4203 -0.3085 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
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10 6 0 0 0 0
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11 7 0 0 0 0
9 8 0 0 0 0

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14 8 0 0 0 0
9 15 0 0 0 0

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M END

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2,6-dichlorophenol.sdf
COSMOtherm 3D 0

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16 15 0 0 0 0 0 0 0 0 V2000
-2.8135 0.0210 2.4644 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4113 -0.7262 2.2804 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.3596 0.8127 2.3081 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1047 0.0096 -1.2582 C 0 0 0 0 0 0 0 0 0 0 0 4
1.5099 0.0007 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1072 -0.0049 0.1807 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6660 -0.0017 -1.0011 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0905 0.0075 -2.2716 C 0 0 0 0 0 0 0 0 0 0 0 8
1.2994 0.0132 -2.4012 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.3736 -0.0141 1.4377 O 0 0 0 0 0 0 0 0 0 0 0 10
-2.4298 -0.0109 -0.8638 Cl 0 0 0 0 0 0 0 0 0 0 0 11
2.5351 -0.0040 1.4403 Cl 0 0 0 0 0 0 0 0 0 0 0 12
3.1914 0.0136 -1.3403 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.7340 0.0100 -3.1512 H 0 0 0 0 0 0 0 0 0 0 0 14
1.7557 0.0206 -3.3911 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.3774 -0.0066 1.5311 H 0 0 0 0 0 0 0 0 0 0 0 16

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
10 16 0 0 0 0

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M END

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2-acetylbutanedioicacid-anion.sdf
COSMOtherm 3D 0

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21 20 0 0 0 0 0 0 0 0 V2000
-4.5938 0.2740 -0.7253 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.7744 0.1322 -0.1689 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.4030 1.0864 -1.2249 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.3266 0.2400 0.5208 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.1093 -0.0003 1.4254 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2478 -0.2499 0.7122 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1882 -1.3849 -0.3249 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6879 -1.2554 -1.4387 O 0 0 0 0 0 0 0 0 0 0 0 8
0.5237 -2.6679 0.1074 C 0 0 0 0 0 0 0 0 0 0 0 9
1.9136 0.9943 0.1011 C 0 0 0 0 0 0 0 0 0 0 0 10
1.1442 1.7968 -0.6114 O 0 0 0 0 0 0 0 0 0 0 0 11
3.1147 1.2192 0.2721 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.4401 -0.2130 0.8882 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.1506 0.9165 -0.5632 O 0 0 0 0 0 0 0 0 0 0 0 14
-0.3355 -0.8433 2.0893 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.0049 0.8837 2.0751 H 0 0 0 0 0 0 0 0 0 0 0 16
1.9453 -0.6131 1.4855 H 0 0 0 0 0 0 0 0 0 0 0 17
0.7474 -3.4645 -0.6112 H 0 0 0 0 0 0 0 0 0 0 0 18
0.8466 -2.9610 1.1168 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.5685 -2.5266 0.1510 H 0 0 0 0 0 0 0 0 0 0 0 20
0.1044 1.4115 -0.6295 H 0 0 0 0 0 0 0 0 0 0 0 21

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
11 21 0 0 0 0
14 21 0 0 0 0

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M END

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2-acetylbutanedioicacid.sdf
COSMOtherm 3D 0

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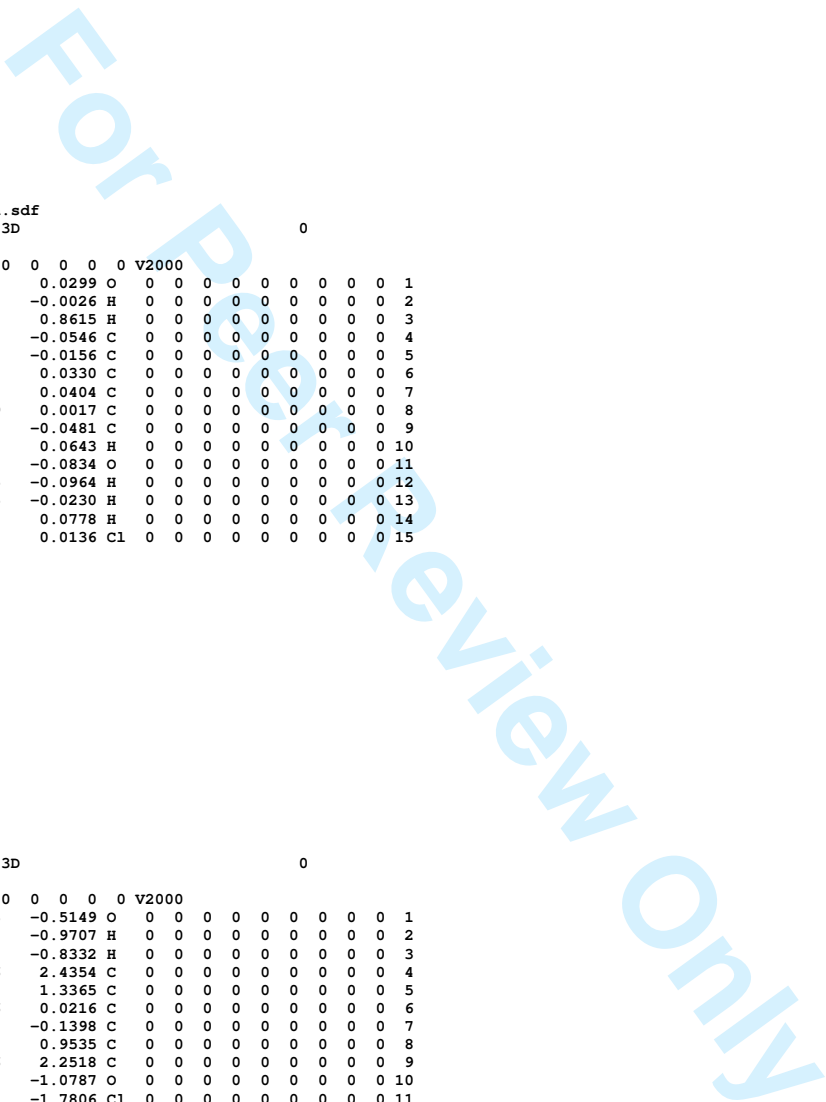
```

22 20 0 0 0 0 0 0 0 0 V2000
-4.5000 0.0121 -0.8767 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.5065 -0.7781 -1.4476 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5297 0.7646 -1.4959 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.2909 -0.0461 0.3251 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2071 -0.0110 1.3868 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1959 0.0058 0.7688 C 0 0 0 0 0 0 0 0 0 0 0 6
1.5626 -1.2564 -0.0192 C 0 0 0 0 0 0 0 0 0 0 0 7
2.3389 -1.1983 -0.9847 O 0 0 0 0 0 0 0 0 0 0 0 8
1.0438 -2.5763 0.4602 C 0 0 0 0 0 0 0 0 0 0 0 9
1.4617 1.3463 0.0483 C 0 0 0 0 0 0 0 0 0 0 0 10
2.3223 1.3295 -0.9736 O 0 0 0 0 0 0 0 0 0 0 0 11
0.9458 2.3895 0.4255 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.5153 0.1062 0.8347 O 0 0 0 0 0 0 0 0 0 0 0 13

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-1.0543 -0.2096 -0.8704 O 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.3391 -0.8750 -0.8750 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.3487 0.8794 2.0125 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.9177 -0.0020 1.6103 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
1.5484 -3.3902 -0.0716 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
1.1943 -2.6807 1.5452 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.0397 -2.6457 0.2790 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
2.5411 0.3469 -1.1614 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.2249 0.0585 0.0945 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
21 11 0 0 0 0
13 22 0 0 0 0
M END
$$$$
2-chlorophenol-anion.sdf
COSMOtherm 3D 0
15 14 0 0 0 0 0 0 0 0 0 V2000
-3.9304 -0.5244 0.0299 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.9164 -0.6410 -0.0026 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.0944 -0.0481 0.8615 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.8842 1.4030 -0.0546 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.0349 2.4511 -0.0156 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
1.4148 2.2001 0.0330 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.8558 0.8688 0.0404 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.9298 -0.1699 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.4918 0.0228 -0.0481 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.1378 3.0162 0.0643 H 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.3393 -0.9617 -0.0834 O 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.9563 1.6125 -0.0964 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.3300 3.4815 -0.0230 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.9224 0.6387 0.0778 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
1.5299 -1.8541 0.0136 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
8 15 0 0 0 0
M END
$$$$
2-chlorophenol.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.8343 -0.0003 -0.5149 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.2977 -0.7268 -0.9707 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.2730 0.8100 -0.8332 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0820 -0.0016 2.4354 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.9441 -0.0037 1.3365 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4387 -0.0026 0.0216 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.9622 0.0002 -0.1398 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.8272 0.0024 0.9535 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.3054 0.0016 2.2518 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.2294 -0.0044 -1.0787 O 0 0 0 0 0 0 0 0 0 0 0 0 0 10
1.6335 0.0011 -1.7806 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.2070 -0.0006 -0.8227 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.5020 -0.0024 3.4427 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.0263 -0.0069 1.4811 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2.9047 0.0047 0.7851 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.9819 0.0034 3.1070 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
12 10 0 0 0 0
9 16 0 0 0 0
M END
$$$$
2-chloropropanoicacid-anion.sdf
COSMOtherm 3D 0
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13 11 0 0 0 0 0 0 0 0 0 V2000
-3.6800 0.7084 -0.2821 O 0 0 0 0 0 0 0 0 0 0 1
-2.6740 0.6378 -0.2909 H 0 0 0 0 0 0 0 0 0 0 2
-3.9651 -0.1442 0.0890 H 0 0 0 0 0 0 0 0 0 0 3
1.4551 -1.4915 -0.9427 C 0 0 0 0 0 0 0 0 0 0 4
1.0243 -0.6153 0.2247 C 0 0 0 0 0 0 0 0 0 0 5
-0.5079 -0.3844 0.2359 C 0 0 0 0 0 0 0 0 0 0 6
-1.1502 -1.2937 0.8288 O 0 0 0 0 0 0 0 0 0 0 7
-0.9867 0.6208 -0.3730 O 0 0 0 0 0 0 0 0 0 0 8
1.9757 0.9906 0.1621 Cl 0 0 0 0 0 0 0 0 0 0 9
2.5354 -1.6853 -0.9169 H 0 0 0 0 0 0 0 0 0 0 10
0.9294 -2.4557 -0.8736 H 0 0 0 0 0 0 0 0 0 0 11
1.1983 -1.0225 -1.9025 H 0 0 0 0 0 0 0 0 0 0 12
1.3256 -1.0505 1.1827 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 13 0 0 0 0
M END
$$$$
2-chloropropanoicacid.sdf
COSMOtherm 3D 0
14 12 0 0 0 0 0 0 0 0 V2000
-3.7186 0.4046 -0.0182 O 0 0 0 0 0 0 0 0 0 0 1
-4.0492 -0.4400 -0.3758 H 0 0 0 0 0 0 0 0 0 0 2
-3.8832 1.0546 -0.7260 H 0 0 0 0 0 0 0 0 0 0 3
1.8130 -1.6321 0.2712 C 0 0 0 0 0 0 0 0 0 0 4
1.0307 -0.3737 0.5662 C 0 0 0 0 0 0 0 0 0 0 5
-0.4060 -0.4026 0.0361 C 0 0 0 0 0 0 0 0 0 0 6
-1.2277 0.3390 0.7812 O 0 0 0 0 0 0 0 0 0 0 7
-0.7430 -1.0394 -0.9546 O 0 0 0 0 0 0 0 0 0 0 8
1.8293 1.0929 -0.2536 Cl 0 0 0 0 0 0 0 0 0 0 9
2.8435 -1.5389 0.6350 H 0 0 0 0 0 0 0 0 0 0 10
1.3371 -2.4749 0.7961 H 0 0 0 0 0 0 0 0 0 0 11
1.8195 -1.8530 -0.8034 H 0 0 0 0 0 0 0 0 0 0 12
1.0314 -0.1165 1.6297 H 0 0 0 0 0 0 0 0 0 0 13
-2.1812 0.3215 0.3961 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 14 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid-anion.sdf
COSMOtherm 3D 0
14 12 0 0 0 0 0 0 0 0 V2000
-3.5184 -0.1169 -0.0702 O 0 0 0 0 0 0 0 0 0 0 1
-2.5399 -0.3212 0.0635 H 0 0 0 0 0 0 0 0 0 0 2
-3.5201 0.7802 -0.4452 H 0 0 0 0 0 0 0 0 0 0 3
1.8879 -1.3884 -0.4831 C 0 0 0 0 0 0 0 0 0 0 4
1.4007 -0.2219 0.3765 C 0 0 0 0 0 0 0 0 0 0 5
-0.0880 0.1199 0.1052 C 0 0 0 0 0 0 0 0 0 0 6
-0.3200 1.2894 -0.3249 O 0 0 0 0 0 0 0 0 0 0 7
-0.9463 -0.7888 0.3346 O 0 0 0 0 0 0 0 0 0 0 8
2.1952 0.9544 0.1371 O 0 0 0 0 0 0 0 0 0 0 9
2.9461 -1.5990 -0.2723 H 0 0 0 0 0 0 0 0 0 0 10
1.3036 -2.2939 -0.2700 H 0 0 0 0 0 0 0 0 0 0 11
1.7867 -1.1473 -1.5521 H 0 0 0 0 0 0 0 0 0 0 12
1.4839 -0.4976 1.4438 H 0 0 0 0 0 0 0 0 0 0 13
1.5029 1.5985 -0.1660 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
9 14 0 0 0 0
M END
$$$$
2-hydroxypropanoicacid.sdf
COSMOtherm 3D 0
15 13 0 0 0 0 0 0 0 0 V2000
-3.4289 -0.0743 0.1351 O 0 0 0 0 0 0 0 0 0 0 1
-3.6127 -0.9739 -0.1922 H 0 0 0 0 0 0 0 0 0 0 2
-3.8090 0.5189 -0.5388 H 0 0 0 0 0 0 0 0 0 0 3
1.8198 -0.5247 1.4109 C 0 0 0 0 0 0 0 0 0 0 4
1.4079 0.3722 0.2378 C 0 0 0 0 0 0 0 0 0 0 5
-0.0319 0.0936 -0.1954 C 0 0 0 0 0 0 0 0 0 0 6
-0.2855 -0.3875 -1.3002 O 0 0 0 0 0 0 0 0 0 0 7
-0.9371 0.4060 0.7249 O 0 0 0 0 0 0 0 0 0 0 8
2.2745 0.1814 -0.8864 O 0 0 0 0 0 0 0 0 0 0 9
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2.8660 -0.3178 1.6729 H 0 0 0 0 0 0 0 0 0 10
1.1943 -0.3293 2.2923 H 0 0 0 0 0 0 0 0 0 11
1.7288 -1.5855 1.1361 H 0 0 0 0 0 0 0 0 0 12
1.4639 1.4292 0.5493 H 0 0 0 0 0 0 0 0 0 13
-1.8903 0.1855 0.4019 H 0 0 0 0 0 0 0 0 0 14
1.7064 -0.2204 -1.5815 H 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
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13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
14 8 0 0 0 0
9 15 0 0 0 0
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M END
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3,3-dimethylsuccinimide-anion.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 V2000
-3.4991 1.0516 -0.0097 O 0 0 0 0 0 0 0 0 0 1
-2.5708 0.6385 -0.0005 H 0 0 0 0 0 0 0 0 0 2
-3.3296 2.0096 -0.0090 H 0 0 0 0 0 0 0 0 0 3
1.4611 0.0243 -0.0038 C 0 0 0 0 0 0 0 0 0 4
0.9693 -1.4348 -0.0052 C 0 0 0 0 0 0 0 0 0 5
0.1186 0.8084 0.0078 C 0 0 0 0 0 0 0 0 0 6
-0.9725 -0.0207 0.0111 N 0 0 0 0 0 0 0 0 0 7
-0.5591 -1.3252 0.0035 C 0 0 0 0 0 0 0 0 0 8
2.2541 0.3897 -1.2712 C 0 0 0 0 0 0 0 0 0 9
2.2717 0.3815 1.2549 C 0 0 0 0 0 0 0 0 0 10
-1.3222 -2.3116 0.0029 O 0 0 0 0 0 0 0 0 0 11
0.0568 2.0514 0.0128 O 0 0 0 0 0 0 0 0 0 12
1.2985 -2.0060 0.8761 H 0 0 0 0 0 0 0 0 0 13
1.2885 -2.0009 -0.8936 H 0 0 0 0 0 0 0 0 0 14
1.6933 0.1321 -2.1826 H 0 0 0 0 0 0 0 0 0 15
2.4691 1.4680 -1.2936 H 0 0 0 0 0 0 0 0 0 16
3.2104 -0.1543 -1.2928 H 0 0 0 0 0 0 0 0 0 17
1.7235 0.1180 2.1723 H 0 0 0 0 0 0 0 0 0 18
2.4870 1.4597 1.2812 H 0 0 0 0 0 0 0 0 0 19
3.2281 -0.1626 1.2598 H 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
13 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
11 8 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
17 9 0 0 0 0
18 10 0 0 0 0
19 10 0 0 0 0
10 20 0 0 0 0

M END
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3,3-dimethylsuccinimide.sdf
COSMOtherm 3D 0
21 20 0 0 0 0 0 0 0 0 V2000
-3.5316 -0.0012 1.0718 O 0 0 0 0 0 0 0 0 0 1
-4.0472 -0.7741 0.7785 H 0 0 0 0 0 0 0 0 0 2
-4.0571 0.7640 0.7759 H 0 0 0 0 0 0 0 0 0 3
1.5002 -0.0006 -0.0190 C 0 0 0 0 0 0 0 0 0 4
0.9240 0.0000 -1.4561 C 0 0 0 0 0 0 0 0 0 5
0.2383 0.0012 0.8659 C 0 0 0 0 0 0 0 0 0 6
-0.8833 0.0010 0.0494 N 0 0 0 0 0 0 0 0 0 7
-0.5874 0.0007 -1.3062 C 0 0 0 0 0 0 0 0 0 8
2.3257 1.2644 0.2852 C 0 0 0 0 0 0 0 0 0 9
2.3218 -1.2681 0.2854 C 0 0 0 0 0 0 0 0 0 10
-1.4281 0.0010 -2.2012 O 0 0 0 0 0 0 0 0 0 11
0.2016 0.0025 2.0924 O 0 0 0 0 0 0 0 0 0 12
-1.8617 0.0022 0.4195 H 0 0 0 0 0 0 0 0 0 13
1.2216 -0.8840 -2.0382 H 0 0 0 0 0 0 0 0 0 14
1.2222 0.8842 -2.0376 H 0 0 0 0 0 0 0 0 0 15
1.7513 2.1788 0.0760 H 0 0 0 0 0 0 0 0 0 16
2.6326 1.2802 1.3403 H 0 0 0 0 0 0 0 0 0 17
3.2299 1.2747 -0.3398 H 0 0 0 0 0 0 0 0 0 18
1.7445 -2.1808 0.0762 H 0 0 0 0 0 0 0 0 0 19
2.6286 -1.2848 1.3404 H 0 0 0 0 0 0 0 0 0 20
3.2260 -1.2813 -0.3396 H 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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8 5 0 0 0 0
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17 9 0 0 0 0
18 9 0 0 0 0
19 10 0 0 0 0
20 10 0 0 0 0
10 21 0 0 0 0

M END
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3,3-methylphenylglutarimide-anion.sdf
COSMOtherm 3D 0

30 30 0 0 0 0 0 0 0 0 0 V2000
-3.8285 -2.0707 0.6172 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.1343 -1.3309 0.5215 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.0012 -2.3250 -0.3062 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.3713 0.6418 1.2145 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.9606 -0.1046 0.2361 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.6459 0.0725 -1.0800 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5932 1.0985 -1.4980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.4641 1.3972 -0.4216 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.3406 1.7135 0.8598 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.2354 -0.5853 -1.9694 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.6856 0.4807 2.4167 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
1.2913 2.6308 -0.8443 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
1.4182 0.2129 -0.1762 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.1337 2.0373 -1.7119 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.1498 0.7766 -2.4500 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.8920 2.6580 0.7032 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
0.3062 1.8672 1.7334 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
3.2587 -1.8943 0.2999 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
2.3277 -1.9873 -0.7379 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
1.4201 -0.9450 -0.9723 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
2.3640 0.2884 0.8651 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
3.2726 -0.7467 1.1025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
0.6296 3.4931 -1.0181 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
2.0187 2.9090 -0.0686 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
1.8449 2.4282 -1.7738 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
3.9667 -2.7048 0.4828 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
2.3025 -2.8750 -1.3734 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
0.7084 -1.0528 -1.7912 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 28
2.3991 1.1735 1.5037 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29
3.9941 -0.6559 1.9171 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 30

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
16 9 0 0 0 0
17 9 0 0 0 0
23 12 0 0 0 0
24 12 0 0 0 0
25 12 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
19 18 0 0 0 0
22 18 0 0 0 0
26 18 0 0 0 0
20 19 0 0 0 0
27 19 0 0 0 0
28 20 0 0 0 0
22 21 0 0 0 0
29 21 0 0 0 0
22 30 0 0 0 0

M END
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3,3-methylphenylglutarimide.sdf
COSMOtherm 3D 0

31 31 0 0 0 0 0 0 0 0 0 V2000
-3.8756 0.4543 2.1072 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.3923 -0.3620 2.2338 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.5445 1.1265 1.8830 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.3621 1.2514 -0.5332 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.8959 0.1070 0.0480 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.5485 -1.2053 -0.2497 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.4996 -1.4025 -1.3226 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.5102 -0.2439 -1.4475 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.3372 1.0406 -1.6260 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.1063 -2.1385 0.3314 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.7478 2.3649 -0.1716 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
1.3730 -0.4663 -2.7089 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
1.4324 -0.1182 -0.2200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.6239 0.2444 0.7855 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.0435 -1.4893 -2.2794 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.0171 -2.3738 -1.1546 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.8934 0.9691 -2.5773 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
0.2764 1.9474 -1.6873 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
3.2126 0.1488 1.9704 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
2.3793 -0.9674 1.8677 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
1.5012 -1.0989 0.7836 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
2.2831 0.9982 -0.1022 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
3.1614 1.1328 0.9759 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
0.7359 -0.5515 -3.6020 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
2.0695 0.3700 -2.8620 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
1.9633 -1.3892 -2.6137 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
3.8963 0.2526 2.8149 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27

1
2
3 2.4074 -1.7455 2.6332 H 0 0 0 0 0 0 0 0 0 0 0 28
4 0.8719 -1.9881 0.7362 H 0 0 0 0 0 0 0 0 0 0 0 29
5 2.2695 1.7786 -0.8658 H 0 0 0 0 0 0 0 0 0 0 0 30
6 3.8082 2.0102 1.0383 H 0 0 0 0 0 0 0 0 0 0 0 31
7 2 1 0 0 0 0
8 3 1 0 0 0 0
9 5 4 0 0 0 0
10 9 4 0 0 0 0
11 11 4 0 0 0 0
12 6 5 0 0 0 0
13 14 5 0 0 0 0
14 7 6 0 0 0 0
15 10 6 0 0 0 0
16 8 7 0 0 0 0
17 15 7 0 0 0 0
18 16 7 0 0 0 0
19 9 8 0 0 0 0
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21 13 8 0 0 0 0
22 17 9 0 0 0 0
23 18 9 0 0 0 0
24 24 12 0 0 0 0
25 25 12 0 0 0 0
26 26 12 0 0 0 0
27 21 13 0 0 0 0
28 22 13 0 0 0 0
29 20 19 0 0 0 0
30 23 19 0 0 0 0
31 27 19 0 0 0 0
32 21 20 0 0 0 0
33 28 20 0 0 0 0
34 29 21 0 0 0 0
35 23 22 0 0 0 0
36 30 22 0 0 0 0
37 23 31 0 0 0 0
38 M END
39 \$\$\$
40 3,4-dichlorophenol-anion.sdf
41 COSMOtherm 3D 0
42
43 15 14 0 0 0 0 0 0 0 0 0 V2000
44 -5.0613 0.4722 0.0263 O 0 0 0 0 0 0 0 0 0 0 0 1
45 -4.1866 -0.0533 0.0050 H 0 0 0 0 0 0 0 0 0 0 0 2
46 -5.0789 0.9512 -0.8196 H 0 0 0 0 0 0 0 0 0 0 0 3
47 -0.2335 1.5531 0.0114 C 0 0 0 0 0 0 0 0 0 0 0 4
48 -1.5038 0.9859 0.0160 C 0 0 0 0 0 0 0 0 0 0 0 5
49 -1.6977 -0.4342 0.0103 C 0 0 0 0 0 0 0 0 0 0 0 6
50 -0.5013 -1.2262 0.0043 C 0 0 0 0 0 0 0 0 0 0 0 7
51 0.7598 -0.6401 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 8
52 0.9168 0.7534 0.0034 C 0 0 0 0 0 0 0 0 0 0 0 9
53 -2.8744 -0.9921 0.0126 O 0 0 0 0 0 0 0 0 0 0 0 10
54 2.1849 -1.7055 -0.0086 Cl 0 0 0 0 0 0 0 0 0 0 0 11
55 2.5135 1.5228 -0.0024 Cl 0 0 0 0 0 0 0 0 0 0 0 12
56 -0.1209 2.6389 0.0149 H 0 0 0 0 0 0 0 0 0 0 0 13
57 -2.3824 1.6342 0.0262 H 0 0 0 0 0 0 0 0 0 0 0 14
58 -0.5939 -2.3132 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 15
59 2 1 0 0 0 0
60 3 1 0 0 0 0
61 5 4 0 0 0 0
62 9 4 0 0 0 0
63 13 4 0 0 0 0
64 6 5 0 0 0 0
65 14 5 0 0 0 0
66 7 6 0 0 0 0
67 10 6 0 0 0 0
68 8 7 0 0 0 0
69 9 8 0 0 0 0
70 11 8 0 0 0 0
71 12 9 0 0 0 0
72 7 15 0 0 0 0
73 M END
74 \$\$\$
75 3,4-dichlorophenol.sdf
76 COSMOtherm 3D 0
77
78 16 15 0 0 0 0 0 0 0 0 0 V2000
79 -1.1488 0.0438 -4.2917 O 0 0 0 0 0 0 0 0 0 0 0 1
80 -1.2907 -0.7591 -4.8256 H 0 0 0 0 0 0 0 0 0 0 0 2
81 -1.1674 0.7757 -4.9351 H 0 0 0 0 0 0 0 0 0 0 0 3
82 -0.4937 -0.0078 0.3841 C 0 0 0 0 0 0 0 0 0 0 0 4
83 0.6296 0.0035 1.2208 C 0 0 0 0 0 0 0 0 0 0 0 5
84 1.9054 0.0059 0.6465 C 0 0 0 0 0 0 0 0 0 0 0 6
85 2.0622 -0.0029 -0.7367 C 0 0 0 0 0 0 0 0 0 0 0 7
86 0.9334 -0.0150 -1.5761 C 0 0 0 0 0 0 0 0 0 0 0 8
87 -0.3515 -0.0183 -1.0046 C 0 0 0 0 0 0 0 0 0 0 0 9
88 0.4764 0.0155 2.9784 Cl 0 0 0 0 0 0 0 0 0 0 0 10
89 2.7822 0.0153 1.2941 H 0 0 0 0 0 0 0 0 0 0 0 11
90 3.0598 -0.0003 -1.1769 H 0 0 0 0 0 0 0 0 0 0 0 12
91 1.1347 -0.0274 -2.9188 O 0 0 0 0 0 0 0 0 0 0 0 13
92 -1.2371 -0.0268 -1.6402 H 0 0 0 0 0 0 0 0 0 0 0 14
93 -2.1258 -0.0112 1.0549 Cl 0 0 0 0 0 0 0 0 0 0 0 15
94 0.2593 -0.0053 -3.4226 H 0 0 0 0 0 0 0 0 0 0 0 16
95 2 1 0 0 0 0
96 3 1 0 0 0 0
97 5 4 0 0 0 0
98 9 4 0 0 0 0
99 15 4 0 0 0 0
100 6 5 0 0 0 0
101 10 5 0 0 0 0
102 7 6 0 0 0 0
103 11 6 0 0 0 0
104 8 7 0 0 0 0
105 12 7 0 0 0 0
106 9 8 0 0 0 0
107 13 8 0 0 0 0

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14 9 0 0 0 0
13 16 0 0 0 0
M END
$$$$
3,5-dichlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 V2000
-4.3366 -0.0302 1.4849 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.3357 -0.0071 1.6682 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5354 0.8434 1.1072 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4997 0.0013 0.4850 C 0 0 0 0 0 0 0 0 0 0 0 4
0.5447 -0.0046 1.4896 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8530 -0.0102 1.1575 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.1785 -0.0096 -0.2425 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.1677 -0.0031 -1.1915 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1973 0.0033 -0.8820 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.7645 -0.0159 2.0830 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.6203 -0.0025 -2.9225 Cl 0 0 0 0 0 0 0 0 0 0 0 11
3.2279 0.0078 0.9470 Cl 0 0 0 0 0 0 0 0 0 0 0 12
0.8341 -0.0058 2.5407 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.2271 -0.0179 -0.5405 H 0 0 0 0 0 0 0 0 0 0 0 14
1.9681 0.0086 -1.6487 H 0 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
9 15 0 0 0 0
M END
$$$$
3,5-dichlorophenol.sdf
COSMOtherm 3D 0

16 15 0 0 0 0 0 0 0 0 V2000
-4.1729 -0.0063 -1.3906 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6544 -0.7825 -1.7316 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.6653 0.7612 -1.7358 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.6378 0.0056 -2.1905 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.7605 0.0033 -1.1578 C 0 0 0 0 0 0 0 0 0 0 0 5
0.6118 0.0020 -1.4741 C 0 0 0 0 0 0 0 0 0 0 0 6
1.5366 -0.0003 -0.4360 C 0 0 0 0 0 0 0 0 0 0 0 7
3.2642 -0.0023 -0.8361 Cl 0 0 0 0 0 0 0 0 0 0 0 8
1.1694 -0.0009 0.9127 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.2002 0.0008 1.1838 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.7209 0.0004 2.8793 Cl 0 0 0 0 0 0 0 0 0 0 0 11
-1.1748 0.0029 0.1887 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.5948 0.0015 -1.8622 H 0 0 0 0 0 0 0 0 0 0 0 13
0.9270 0.0022 -2.5166 H 0 0 0 0 0 0 0 0 0 0 0 14
1.9110 -0.0026 1.7083 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.2347 0.0044 0.4402 H 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 9 0 0 0 0
15 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
12 16 0 0 0 0
M END
$$$$
3-chlorophenol-anion.sdf
COSMOtherm 3D 0

15 14 0 0 0 0 0 0 0 0 V2000
-4.5282 0.0705 0.2863 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5501 0.0160 0.5805 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5941 0.9195 -0.1828 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.1073 -0.0238 -1.9379 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.2073 -0.0566 -1.0833 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.0518 -0.0617 0.3420 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2993 -0.0292 0.8291 C 0 0 0 0 0 0 0 0 0 0 0 7
1.3635 0.0017 -0.0620 C 0 0 0 0 0 0 0 0 0 0 0 8
1.2110 0.0072 -1.4510 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.0611 -0.0928 1.1684 O 0 0 0 0 0 0 0 0 0 0 0 10
3.0318 0.0415 0.6059 Cl 0 0 0 0 0 0 0 0 0 0 0 11
-0.2681 -0.0214 -3.0192 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.2201 -0.0841 -1.4924 H 0 0 0 0 0 0 0 0 0 0 0 13
0.4688 -0.0314 1.9069 H 0 0 0 0 0 0 0 0 0 0 0 14
2.0699 0.0326 -2.1197 H 0 0 0 0 0 0 0 0 0 0 0 15

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0

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14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
9 15 0 0 0 0
M END
$$$$
3-chlorophenol.sdf
COSMOTHERM 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
-4.4971 0.2757 0.0146 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.7624 -0.3314 0.7292 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.8122 -0.1492 -0.8039 H 0 0 0 0 0 0 0 0 0 0 0 3
0.3313 0.8307 -0.0023 C 0 0 0 0 0 0 0 0 0 0 0 4
1.3969 -0.0651 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2198 -1.4501 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0936 -1.9357 -0.0024 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.1899 -1.0702 -0.0055 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9815 0.3219 -0.0043 C 0 0 0 0 0 0 0 0 0 0 0 9
2.0732 -2.1266 0.0026 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.9983 1.2257 -0.0053 O 0 0 0 0 0 0 0 0 0 0 0 11
0.4945 1.9082 -0.0022 H 0 0 0 0 0 0 0 0 0 0 0 12
3.0516 0.5891 0.0031 Cl 0 0 0 0 0 0 0 0 0 0 0 13
-0.2628 -3.0139 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.2058 -1.4686 -0.0089 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.8954 0.7691 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
11 9 0 0 0 0
11 16 0 0 0 0
M END
$$$$
3-chloropropanoicacid-anion.sdf
COSMOTHERM 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-4.3547 -0.0171 0.0841 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4274 -0.0009 -0.3196 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.1707 -0.0275 1.0396 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4415 0.0227 0.5583 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4515 -0.0111 -0.5875 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.0149 0.0064 -0.0937 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.2368 0.0030 1.1479 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.9029 0.0204 -1.0140 O 0 0 0 0 0 0 0 0 0 0 0 8
0.5952 -0.9158 -1.1976 H 0 0 0 0 0 0 0 0 0 0 0 9
1.3719 0.9392 1.1504 H 0 0 0 0 0 0 0 0 0 0 0 10
1.3607 -0.8498 1.2120 H 0 0 0 0 0 0 0 0 0 0 0 11
3.1890 -0.0087 -0.0746 Cl 0 0 0 0 0 0 0 0 0 0 0 12
0.6004 0.8496 -1.2565 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 13 0 0 0 0
M END
$$$$
3-chloropropanoicacid.sdf
COSMOTHERM 3D 0

14 12 0 0 0 0 0 0 0 0 0 V2000
-4.3705 0.0076 0.1087 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6486 -0.8101 -0.3434 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5989 0.7232 -0.5128 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5247 -0.0213 -0.5790 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4766 0.0017 0.5191 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9306 0.0010 -0.0516 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.8624 -0.0028 0.9110 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.1869 0.0059 -1.2526 O 0 0 0 0 0 0 0 0 0 0 0 8
0.5883 0.8955 1.1514 H 0 0 0 0 0 0 0 0 0 0 0 9
3.2112 0.0053 0.1550 Cl 0 0 0 0 0 0 0 0 0 0 0 10
1.4786 -0.9327 -1.1815 H 0 0 0 0 0 0 0 0 0 0 0 11
1.4693 0.8575 -1.2273 H 0 0 0 0 0 0 0 0 0 0 0 12
0.5804 -0.8690 1.1836 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.8008 0.0000 0.5021 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 14 0 0 0 0
M END
$$$$

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1  
2  
3 3-hydroxy-2-naphtoicacid-anion.sdf  
4 COSMOtherm 3D 0  
5  
6 24 25 0 0 0 0 0 0 0 0 0 V2000  
7 -5.3919 -1.4569 0.0296 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1  
8 -4.3943 -1.3496 0.0075 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2  
9 -5.7210 -0.5419 0.0062 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3  
10 4.3276 -0.2922 0.0081 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4  
11 3.8190 -1.6185 0.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5  
12 2.4541 -1.8341 -0.0032 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6  
13 1.5421 -0.7406 -0.0025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7  
14 2.0570 0.6071 0.0037 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8  
15 3.4710 0.7922 0.0089 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9  
16 0.1372 -0.9272 -0.0076 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10  
17 -0.7470 0.1399 -0.0067 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11  
18 -0.2234 1.4840 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12  
19 1.1501 1.6951 0.0044 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13  
20 -2.2398 -0.0934 -0.0118 C 0 0 0 0 0 0 0 0 0 0 0 0 0 14  
21 -2.6805 -1.2785 -0.0201 O 0 0 0 0 0 0 0 0 0 0 0 0 0 15  
22 -2.9892 0.9564 -0.0078 O 0 0 0 0 0 0 0 0 0 0 0 0 0 16  
23 -1.0738 2.5384 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 0 0 17  
24 -2.0157 2.0781 -0.0021 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18  
25 5.4076 -0.1306 0.0121 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19  
26 4.5097 -2.4634 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20  
27 2.0536 -2.8507 -0.0080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21  
28 3.8694 1.8097 0.0137 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22  
29 -0.2717 -1.9401 -0.0123 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23  
30 1.5300 2.7192 0.0092 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24  
31 2 1 0 0 0 0 0  
32 3 1 0 0 0 0 0  
33 5 4 0 0 0 0 0  
34 9 4 0 0 0 0 0  
35 19 4 0 0 0 0 0  
36 6 5 0 0 0 0 0  
37 20 5 0 0 0 0 0  
38 7 6 0 0 0 0 0  
39 21 6 0 0 0 0 0  
40 8 7 0 0 0 0 0  
41 10 7 0 0 0 0 0  
42 9 8 0 0 0 0 0  
43 13 8 0 0 0 0 0  
44 22 9 0 0 0 0 0  
45 11 10 0 0 0 0 0  
46 23 10 0 0 0 0 0  
47 12 11 0 0 0 0 0  
48 14 11 0 0 0 0 0  
49 13 12 0 0 0 0 0  
50 17 12 0 0 0 0 0  
51 15 14 0 0 0 0 0  
52 16 14 0 0 0 0 0  
53 18 16 0 0 0 0 0  
54 18 17 0 0 0 0 0  
55 13 24 0 0 0 0 0  
56 M END  
57 $$$  
58 3-hydroxy-2-naphtoicacid.sdf  
59 COSMOtherm 3D 0  
60  
61 25 25 0 0 0 0 0 0 0 0 0 V2000  
62 -5.2205 -0.0279 1.5676 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1  
63 -5.6891 -0.7255 1.0733 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2  
64 -5.6789 0.7985 1.3279 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3  
65 4.3136 -0.0075 0.3705 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4  
66 3.7701 -0.0029 1.6837 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5  
67 2.4021 0.0024 1.8647 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6  
68 1.5210 0.0029 0.7444 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7  
69 2.0712 -0.0017 -0.5892 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8  
70 3.4888 -0.0070 -0.7374 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9  
71 0.1168 0.0074 0.8964 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10  
72 -0.7379 0.0068 -0.2018 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11  
73 -0.1805 0.0018 -1.5308 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12  
74 1.1959 -0.0021 -1.7015 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13  
75 -2.2070 0.0082 -0.0358 C 0 0 0 0 0 0 0 0 0 0 0 0 0 14  
76 -2.6424 0.0146 1.2188 O 0 0 0 0 0 0 0 0 0 0 0 0 0 15  
77 -2.9847 0.0024 -1.0146 O 0 0 0 0 0 0 0 0 0 0 0 0 0 16  
78 -0.9825 0.0005 -2.6269 O 0 0 0 0 0 0 0 0 0 0 0 0 0 17  
79 -3.6723 0.0058 1.2517 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18  
80 -1.9269 0.0019 -2.2709 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19  
81 5.3974 -0.0118 0.2390 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20  
82 4.4392 -0.0035 2.5455 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21  
83 1.9737 0.0058 2.8694 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22  
84 3.9146 -0.0106 -1.7433 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23  
85 -0.3098 0.0106 1.9004 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24  
86 1.6026 -0.0056 -2.7146 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25  
87 2 1 0 0 0 0 0  
88 3 1 0 0 0 0 0  
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91 20 4 0 0 0 0 0  
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96 8 7 0 0 0 0 0  
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106 17 12 0 0 0 0 0  
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13 -4.6337 -0.8075 0.0085 O 0 0 0 0 0 0 0 0 0 0 0 0 1
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20 2.2508 -0.7255 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 8
21 2.8847 0.5260 0.0042 C 0 0 0 0 0 0 0 0 0 0 0 0 9
22 -1.4506 0.2643 -0.0052 C 0 0 0 0 0 0 0 0 0 0 0 0 10
23 3.0560 -1.8432 0.0004 O 0 0 0 0 0 0 0 0 0 0 0 0 11
24 -1.9531 -0.9144 -0.0053 O 0 0 0 0 0 0 0 0 0 0 0 0 12
25 -2.1113 1.3403 -0.0071 O 0 0 0 0 0 0 0 0 0 0 0 0 13
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28 0.3540 -1.7815 -0.0054 H 0 0 0 0 0 0 0 0 0 0 0 0 16
29 3.9750 0.5774 0.0068 H 0 0 0 0 0 0 0 0 0 0 0 0 17
30 2.4950 -2.6420 -0.0032 H 0 0 0 0 0 0 0 0 0 0 0 0 18
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56 2.6421 -3.1605 -0.7971 H 0 0 0 0 0 0 0 0 0 0 0 0 3
57 -2.4915 0.3502 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 4
58 -1.5191 1.3533 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 5
59 -0.1611 0.9926 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 6
60 0.2165 -0.3615 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.7672 -1.3631 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.1267 -0.9979 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.8580 2.0773 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.4665 -2.6909 -0.0008 O 0 0 0 0 0 0 0 0 0 0 0 0 11
2.1349 1.6139 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 12
0.5999 3.2774 0.0000 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-3.5492 0.6183 0.0030 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.7975 2.4067 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.2713 -0.6352 -0.0058 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.8852 -1.7827 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 0 17
0.5281 -2.8420 0.0020 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2.7319 2.3926 0.0016 H 0 0 0 0 0 0 0 0 0 0 0 0 19
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-1.0915 0.1311 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 0 6
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0.9780 -1.1540 0.0022 C 0 0 0 0 0 0 0 0 0 0 0 0 8
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-2.6127 0.2028 0.0022 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.2967 -0.0808 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 11

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3.7601 -0.8461 1.2623 C 0 0 0 0 0 0 0 0 0 0 12
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-3.1553 1.3446 0.0039 O 0 0 0 0 0 0 0 0 0 0 15
-3.2421 -0.9145 0.0006 O 0 0 0 0 0 0 0 0 0 0 16
1.6350 2.1842 -0.0041 H 0 0 0 0 0 0 0 0 0 0 17
-0.8336 2.2658 -0.0021 H 0 0 0 0 0 0 0 0 0 0 18
-1.0022 -2.0224 0.0047 H 0 0 0 0 0 0 0 0 0 0 19
1.4653 -2.1316 0.0034 H 0 0 0 0 0 0 0 0 0 0 20
4.8578 -0.9294 1.2710 H 0 0 0 0 0 0 0 0 0 0 21
3.3440 -1.8630 1.2963 H 0 0 0 0 0 0 0 0 0 0 22
3.4495 -0.3191 2.1772 H 0 0 0 0 0 0 0 0 0 0 23
5.0660 1.1733 -0.0044 H 0 0 0 0 0 0 0 0 0 0 24
3.7067 1.8876 -0.8970 H 0 0 0 0 0 0 0 0 0 0 25
3.7076 1.8914 0.8866 H 0 0 0 0 0 0 0 0 0 0 26
4.8566 -0.9342 -1.2709 H 0 0 0 0 0 0 0 0 0 0 27
3.4466 -0.3289 -2.1778 H 0 0 0 0 0 0 0 0 0 0 28
3.3434 -1.8689 -1.2898 H 0 0 0 0 0 0 0 0 0 0 29
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-1.0552 -0.0067 -0.2066 C 0 0 0 0 0 0 0 0 0 0 6
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0.9680 0.0041 1.1366 C 0 0 0 0 0 0 0 0 0 0 8
1.7817 -0.0023 -0.0154 C 0 0 0 0 0 0 0 0 0 0 9
-2.5392 -0.0020 -0.3519 C 0 0 0 0 0 0 0 0 0 0 10
3.3122 0.0031 0.1273 C 0 0 0 0 0 0 0 0 0 0 11
3.7460 1.2764 0.8939 C 0 0 0 0 0 0 0 0 0 0 12
4.0282 -0.0115 -1.2362 C 0 0 0 0 0 0 0 0 0 0 13
3.7535 -1.2484 0.9245 C 0 0 0 0 0 0 0 0 0 0 14
-3.1148 0.0234 -1.4419 O 0 0 0 0 0 0 0 0 0 0 15
-3.1961 -0.0288 0.8207 O 0 0 0 0 0 0 0 0 0 0 16
1.7187 -0.0181 -2.1843 H 0 0 0 0 0 0 0 0 0 0 17
-0.7403 -0.0180 -2.3399 H 0 0 0 0 0 0 0 0 0 0 18
-1.0232 0.0062 1.9597 H 0 0 0 0 0 0 0 0 0 0 19
1.4279 0.0121 2.1263 H 0 0 0 0 0 0 0 0 0 0 20
4.8407 1.2898 1.0073 H 0 0 0 0 0 0 0 0 0 0 21
3.3018 1.3178 1.8983 H 0 0 0 0 0 0 0 0 0 0 22
3.4470 2.1846 0.3491 H 0 0 0 0 0 0 0 0 0 0 23
5.1157 -0.0052 -1.0743 H 0 0 0 0 0 0 0 0 0 0 24
3.7827 -0.9122 -1.8185 H 0 0 0 0 0 0 0 0 0 0 25
3.7757 0.8716 -1.8416 H 0 0 0 0 0 0 0 0 0 0 26
4.8485 -1.2533 1.0366 H 0 0 0 0 0 0 0 0 0 0 27
3.4586 -2.1714 0.4029 H 0 0 0 0 0 0 0 0 0 0 28
3.3112 -1.2674 1.9304 H 0 0 0 0 0 0 0 0 0 0 29
-4.2033 -0.0154 0.6577 H 0 0 0 0 0 0 0 0 0 0 30
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For Peer Review Only

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9 M END
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11 4-(1-methylethyl)-benzoicacid-anion.sdf
12 COSMOtherm 3D 0
13
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16 -4.6272 -0.0014 0.4867 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
17 -5.6586 0.0589 -0.6723 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
18 1.1906 0.0204 1.3603 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
19 -0.2009 0.0147 1.2200 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
20 -0.7930 -0.0033 -0.0523 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
21 0.0489 -0.0170 -1.1775 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
22 1.4377 -0.0132 -1.0351 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
23 2.0367 0.0063 0.2384 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
24 -2.3071 -0.0076 -0.2212 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
25 3.5494 0.0105 0.4047 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
26 4.1885 -1.2721 -0.1624 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12
27 4.1898 1.2654 -0.2197 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13
28 -3.0058 -0.0174 0.8545 O 0 0 0 0 0 0 0 0 0 0 0 0 0 14
29 -2.7756 -0.0010 -1.3947 O 0 0 0 0 0 0 0 0 0 0 0 0 0 15
30 1.6324 0.0357 2.3604 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
31 -0.8455 0.0249 2.1006 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
32 -0.4066 -0.0305 -2.1694 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
33 2.0641 -0.0252 -1.9306 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
34 3.7518 0.0348 1.4883 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
35 5.2736 -1.2738 0.0215 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
36 3.7608 -2.1719 0.3038 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
37 4.0320 -1.3457 -1.2498 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
38 5.2742 1.2763 -0.0323 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24
39 3.7602 2.1860 0.2021 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25
40 4.0375 1.2878 -1.3099 H 0 0 0 0 0 0 0 0 0 0 0 0 0 26
41
42 2 1 0 0 0 0
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45 9 4 0 0 0 0
46 16 4 0 0 0 0
47 6 5 0 0 0 0
48 17 5 0 0 0 0
49 7 6 0 0 0 0
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52 18 7 0 0 0 0
53 9 8 0 0 0 0
54 19 8 0 0 0 0
55 11 9 0 0 0 0
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57 15 10 0 0 0 0
58 12 11 0 0 0 0
59 13 11 0 0 0 0
60 20 11 0 0 0 0
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13 26 0 0 0 0
M END
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4-(1-methylethyl)-benzoicacid.sdf
COSMOtherm 3D 0
27 26 0 0 0 0 0 0 0 0 0 V2000
-5.4969 -0.0215 0.8029 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.8656 -0.3928 -0.0199 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.8766 0.8750 0.8584 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.3747 0.0012 -1.4007 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0197 0.0007 -1.4371 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.7609 -0.0021 -0.2437 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0739 -0.0045 0.9845 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.3202 -0.0039 1.0109 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.0720 -0.0009 -0.1797 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.2503 -0.0025 -0.3201 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5921 0.0009 -0.1563 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
4.1474 1.2746 0.5107 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12
4.1524 -1.2654 0.5201 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.8764 0.0026 -1.3824 O 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.8530 -0.0113 0.8816 O 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.9372 0.0038 -2.3376 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
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-0.6361 -0.0064 1.9186 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
1.8301 -0.0053 1.9768 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
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3.7759 2.1821 0.0126 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
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6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0

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15 27 0 0 0 0
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4-aminobenzoicacid-anion.sdf
COSMOtherm      3D          0
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 1.9931 0.0069 -1.2635 C 0 0 0 0 0 0 0 0 0 0 4
 0.6041 0.0072 -1.1574 C 0 0 0 0 0 0 0 0 0 0 5
-0.0381 0.0049  0.0947 C 0 0 0 0 0 0 0 0 0 0 6
 0.7732 0.0052  1.2443 C 0 0 0 0 0 0 0 0 0 0 7
 2.1631 0.0052  1.1565 C 0 0 0 0 0 0 0 0 0 0 8
 2.8028 0.0043 -0.1044 C 0 0 0 0 0 0 0 0 0 0 9
-1.5475 0.0033  0.2119 C 0 0 0 0 0 0 0 0 0 0 10
 4.1868 -0.0629 -0.2010 N 0 0 0 0 0 0 0 0 0 0 11
-2.2156 0.0048 -0.8868 O 0 0 0 0 0 0 0 0 0 0 12
-2.0623 -0.0002  1.3687 O 0 0 0 0 0 0 0 0 0 0 13
 4.7106 0.2555  0.6113 H 0 0 0 0 0 0 0 0 0 0 14
 4.5934 0.2580 -1.0767 H 0 0 0 0 0 0 0 0 0 0 15
 2.4685 0.0088 -2.2478 H 0 0 0 0 0 0 0 0 0 0 16
-0.0092 0.0115 -2.0603 H 0 0 0 0 0 0 0 0 0 0 17
 0.2890 0.0081  2.2227 H 0 0 0 0 0 0 0 0 0 0 18
 2.7706 0.0062  2.0650 H 0 0 0 0 0 0 0 0 0 0 19

 2 1 0 0 0 0
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M  END
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4-aminobenzoicacid.sdf
COSMOtherm      3D          0
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-5.1878  0.8876  0.4030 H 0 0 0 0 0 0 0 0 0 0 3
 2.2290 0.0060 -1.1351 C 0 0 0 0 0 0 0 0 0 0 4
 0.8500 0.0024 -1.2730 C 0 0 0 0 0 0 0 0 0 0 5
-0.0014 -0.0038 -0.1474 C 0 0 0 0 0 0 0 0 0 0 6
 0.5916 -0.0070  1.1340 C 0 0 0 0 0 0 0 0 0 0 7
 1.9702 -0.0034  1.2878 C 0 0 0 0 0 0 0 0 0 0 8
 2.8248 0.0032  0.1540 C 0 0 0 0 0 0 0 0 0 0 9
-1.4626 -0.0057 -0.3472 C 0 0 0 0 0 0 0 0 0 0 10
 4.1802 0.0067  0.2986 N 0 0 0 0 0 0 0 0 0 0 11
-2.0107 -0.0018 -1.4567 O 0 0 0 0 0 0 0 0 0 0 12
-2.1739 -0.0137  0.8036 O 0 0 0 0 0 0 0 0 0 0 13
 4.6107 0.0074  1.2162 H 0 0 0 0 0 0 0 0 0 0 14
 4.7944 0.0117 -0.5076 H 0 0 0 0 0 0 0 0 0 0 15
 2.8694 0.0109 -2.0197 H 0 0 0 0 0 0 0 0 0 0 16
 0.4053 0.0047 -2.2695 H 0 0 0 0 0 0 0 0 0 0 17
-0.0434 -0.0120  2.0204 H 0 0 0 0 0 0 0 0 0 0 18
 2.4103 -0.0057  2.2873 H 0 0 0 0 0 0 0 0 0 0 19
-3.1666 -0.0083  0.5908 H 0 0 0 0 0 0 0 0 0 0 20

 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 9 4 0 0 0 0
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 6 5 0 0 0 0
17 5 0 0 0 0
 7 6 0 0 0 0
10 6 0 0 0 0
 8 7 0 0 0 0
18 7 0 0 0 0
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12 10 0 0 0 0
13 10 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
13 20 0 0 0 0
```

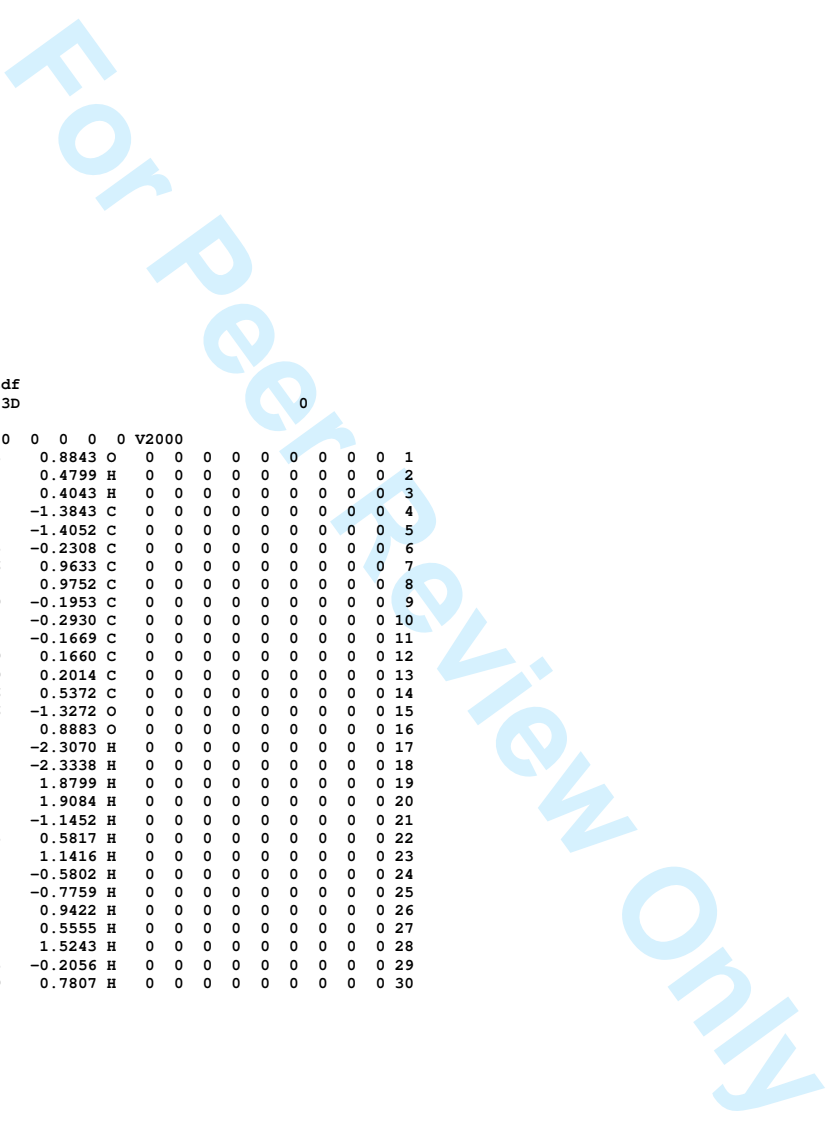
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3 M END
4 $$$$
5 4-bromobenzoicacid-anion.sdf
6 COSMOtherm 3D 0
7
8 17 16 0 0 0 0 0 0 0 0 V2000
9 -6.2493 -0.0142 -0.5404 O 0 0 0 0 0 0 0 0 0 0 0 1
10 -5.2433 -0.0061 -0.6393 H 0 0 0 0 0 0 0 0 0 0 0 2
11 -6.3782 -0.0721 0.4220 H 0 0 0 0 0 0 0 0 0 0 0 3
12 0.6193 0.0067 -1.1810 C 0 0 0 0 0 0 0 0 0 0 0 4
13 -0.7769 0.0084 -1.1026 C 0 0 0 0 0 0 0 0 0 0 0 5
14 -1.4339 0.0048 0.1379 C 0 0 0 0 0 0 0 0 0 0 0 6
15 -0.6619 -0.0008 1.3102 C 0 0 0 0 0 0 0 0 0 0 0 7
16 0.7349 -0.0035 1.2572 C 0 0 0 0 0 0 0 0 0 0 0 8
17 1.3553 0.0005 0.0060 C 0 0 0 0 0 0 0 0 0 0 0 9
18 -2.9577 0.0071 0.2210 C 0 0 0 0 0 0 0 0 0 0 0 10
19 3.2848 -0.0027 -0.0851 Br 0 0 0 0 0 0 0 0 0 0 0 11
20 -3.5893 0.0032 -0.8930 O 0 0 0 0 0 0 0 0 0 0 0 12
21 -3.4863 0.0113 1.3673 O 0 0 0 0 0 0 0 0 0 0 0 13
22 1.1213 0.0096 -2.1487 H 0 0 0 0 0 0 0 0 0 0 0 14
23 -1.3719 0.0125 -2.0169 H 0 0 0 0 0 0 0 0 0 0 0 15
24 -1.1705 -0.0036 2.2754 H 0 0 0 0 0 0 0 0 0 0 0 16
25 1.3255 -0.0080 2.1735 H 0 0 0 0 0 0 0 0 0 0 0 17
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27 2 1 0 0 0 0
28 3 1 0 0 0 0
29 5 4 0 0 0 0
30 9 4 0 0 0 0
31 14 4 0 0 0 0
32 6 5 0 0 0 0
33 15 5 0 0 0 0
34 7 6 0 0 0 0
35 10 6 0 0 0 0
36 8 7 0 0 0 0
37 16 7 0 0 0 0
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39 11 9 0 0 0 0
40 12 10 0 0 0 0
41 13 10 0 0 0 0
42 8 17 0 0 0 0
43 M END
44 $$$$
45 4-bromobenzoicacid.sdf
46 COSMOtherm 3D 0
47
48 18 17 0 0 0 0 0 0 0 0 V2000
49 -6.1691 -0.0241 0.6974 O 0 0 0 0 0 0 0 0 0 0 0 1
50 -6.5382 -0.6800 0.0775 H 0 0 0 0 0 0 0 0 0 0 0 2
51 -6.5623 0.8244 0.4215 H 0 0 0 0 0 0 0 0 0 0 0 3
52 0.7814 -0.0072 -1.2761 C 0 0 0 0 0 0 0 0 0 0 0 4
53 -0.6110 -0.0053 -1.3611 C 0 0 0 0 0 0 0 0 0 0 0 5
54 -1.4012 0.0028 -0.1998 C 0 0 0 0 0 0 0 0 0 0 0 6
55 -0.7771 0.0093 1.0593 C 0 0 0 0 0 0 0 0 0 0 0 7
56 0.6154 0.0086 1.1609 C 0 0 0 0 0 0 0 0 0 0 0 8
57 1.3754 0.0000 -0.0112 C 0 0 0 0 0 0 0 0 0 0 0 9
58 -2.8892 0.0061 -0.3455 C 0 0 0 0 0 0 0 0 0 0 0 10
59 3.2959 -0.0016 0.1195 Br 0 0 0 0 0 0 0 0 0 0 0 11
60 -3.4582 0.0191 -1.4376 O 0 0 0 0 0 0 0 0 0 0 0 12
61 -3.5410 -0.0070 0.8266 O 0 0 0 0 0 0 0 0 0 0 0 13
62 1.3899 -0.0145 -2.1797 H 0 0 0 0 0 0 0 0 0 0 0 14
63 -1.0957 -0.0100 -2.3380 H 0 0 0 0 0 0 0 0 0 0 0 15
64 -1.3795 0.0159 1.9672 H 0 0 0 0 0 0 0 0 0 0 0 16
65 1.0966 0.0148 2.1386 H 0 0 0 0 0 0 0 0 0 0 0 17
66 -4.5520 -0.0034 0.6700 H 0 0 0 0 0 0 0 0 0 0 0 18
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68 2 1 0 0 0 0
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85 M END
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87 4-butylbenzoicacid-anion.sdf
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90 29 28 0 0 0 0 0 0 0 0 V2000
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92 -5.1342 -0.7448 -0.3962 H 0 0 0 0 0 0 0 0 0 0 0 2
93 -6.2235 0.3100 -0.7258 H 0 0 0 0 0 0 0 0 0 0 0 3
94 0.6272 -1.0442 0.7500 C 0 0 0 0 0 0 0 0 0 0 0 4
95 -0.7450 -1.0409 0.4852 C 0 0 0 0 0 0 0 0 0 0 0 5
96 -1.4108 0.1511 0.1538 C 0 0 0 0 0 0 0 0 0 0 0 6
97 -0.6618 1.3379 0.0953 C 0 0 0 0 0 0 0 0 0 0 0 7
98 0.7103 1.3327 0.3587 C 0 0 0 0 0 0 0 0 0 0 0 8
99 1.3813 0.1420 0.6915 C 0 0 0 0 0 0 0 0 0 0 0 9
100 -2.9078 0.1681 -0.1292 C 0 0 0 0 0 0 0 0 0 0 0 10
101 2.8721 0.1314 0.9417 C 0 0 0 0 0 0 0 0 0 0 0 11
102 3.6984 -0.1219 -0.3366 C 0 0 0 0 0 0 0 0 0 0 0 12
103 5.2111 -0.1291 -0.0807 C 0 0 0 0 0 0 0 0 0 0 0 13
104 6.0339 -0.3842 -1.3480 C 0 0 0 0 0 0 0 0 0 0 0 14
105 -3.5165 -0.9596 -0.0749 O 0 0 0 0 0 0 0 0 0 0 0 15
106 -3.4516 1.2770 -0.3967 O 0 0 0 0 0 0 0 0 0 0 0 16
107 1.1236 -1.9821 1.0139 H 0 0 0 0 0 0 0 0 0 0 0 17
108 -1.3207 -1.9665 0.5384 H 0 0 0 0 0 0 0 0 0 0 0 18
109 -1.1747 2.2681 -0.1557 H 0 0 0 0 0 0 0 0 0 0 0 19

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1.2726 2.2694 0.3132 H 0 0 0 0 0 0 0 0 0 0 0 20
3.1152 -0.6477 1.6824 H 0 0 0 0 0 0 0 0 0 0 0 21
3.1782 1.0964 1.3779 H 0 0 0 0 0 0 0 0 0 0 0 22
3.4547 0.6525 -1.0840 H 0 0 0 0 0 0 0 0 0 0 0 23
3.3948 -1.0869 -0.7781 H 0 0 0 0 0 0 0 0 0 0 0 24
5.4460 -0.8995 0.6737 H 0 0 0 0 0 0 0 0 0 0 0 25
5.5069 0.8370 0.3636 H 0 0 0 0 0 0 0 0 0 0 0 26
7.1129 -0.3845 -1.1330 H 0 0 0 0 0 0 0 0 0 0 0 27
5.8436 0.3903 -2.1072 H 0 0 0 0 0 0 0 0 0 0 0 28
5.7820 -1.3584 -1.7958 H 0 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
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15 10 0 0 0 0
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24 12 0 0 0 0
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26 13 0 0 0 0
27 14 0 0 0 0
28 14 0 0 0 0
14 29 0 0 0 0
M END
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4-butylbenzoicacid.sdf
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-6.3339 1.2994 0.4043 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7586 -0.2980 -1.3843 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6088 -0.0271 -1.4052 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.3737 -0.1365 -0.2308 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.7383 -0.5236 0.9633 C 0 0 0 0 0 0 0 0 0 0 0 7
0.6305 -0.7932 0.9752 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4041 -0.6859 -0.1953 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.8351 0.1544 -0.2930 C 0 0 0 0 0 0 0 0 0 0 0 10
2.8921 -0.9401 -0.1669 C 0 0 0 0 0 0 0 0 0 0 0 11
3.7091 0.3269 0.1660 C 0 0 0 0 0 0 0 0 0 0 0 12
5.2209 0.0679 0.2014 C 0 0 0 0 0 0 0 0 0 0 0 13
6.0357 1.3216 0.5372 C 0 0 0 0 0 0 0 0 0 0 0 14
-3.4180 0.4876 -1.3272 O 0 0 0 0 0 0 0 0 0 0 0 15
-3.4629 0.0211 0.8883 O 0 0 0 0 0 0 0 0 0 0 0 16
1.3377 -0.2148 -2.3070 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.1002 0.2674 -2.3338 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.3206 -0.6180 1.8799 H 0 0 0 0 0 0 0 0 0 0 0 19
1.1089 -1.0998 1.9084 H 0 0 0 0 0 0 0 0 0 0 0 20
3.2179 -1.3284 -1.1452 H 0 0 0 0 0 0 0 0 0 0 0 21
3.1177 -1.7165 0.5817 H 0 0 0 0 0 0 0 0 0 0 0 22
3.3797 0.7232 1.1416 H 0 0 0 0 0 0 0 0 0 0 0 23
3.4854 1.1084 -0.5802 H 0 0 0 0 0 0 0 0 0 0 0 24
5.5423 -0.3310 -0.7759 H 0 0 0 0 0 0 0 0 0 0 0 25
5.4347 -0.7214 0.9422 H 0 0 0 0 0 0 0 0 0 0 0 26
7.1144 1.1061 0.5555 H 0 0 0 0 0 0 0 0 0 0 0 27
5.7580 1.7231 1.5243 H 0 0 0 0 0 0 0 0 0 0 0 28
5.8655 2.1165 -0.2056 H 0 0 0 0 0 0 0 0 0 0 0 29
-4.4564 0.2279 0.7807 H 0 0 0 0 0 0 0 0 0 0 0 30
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24 12 0 0 0 0
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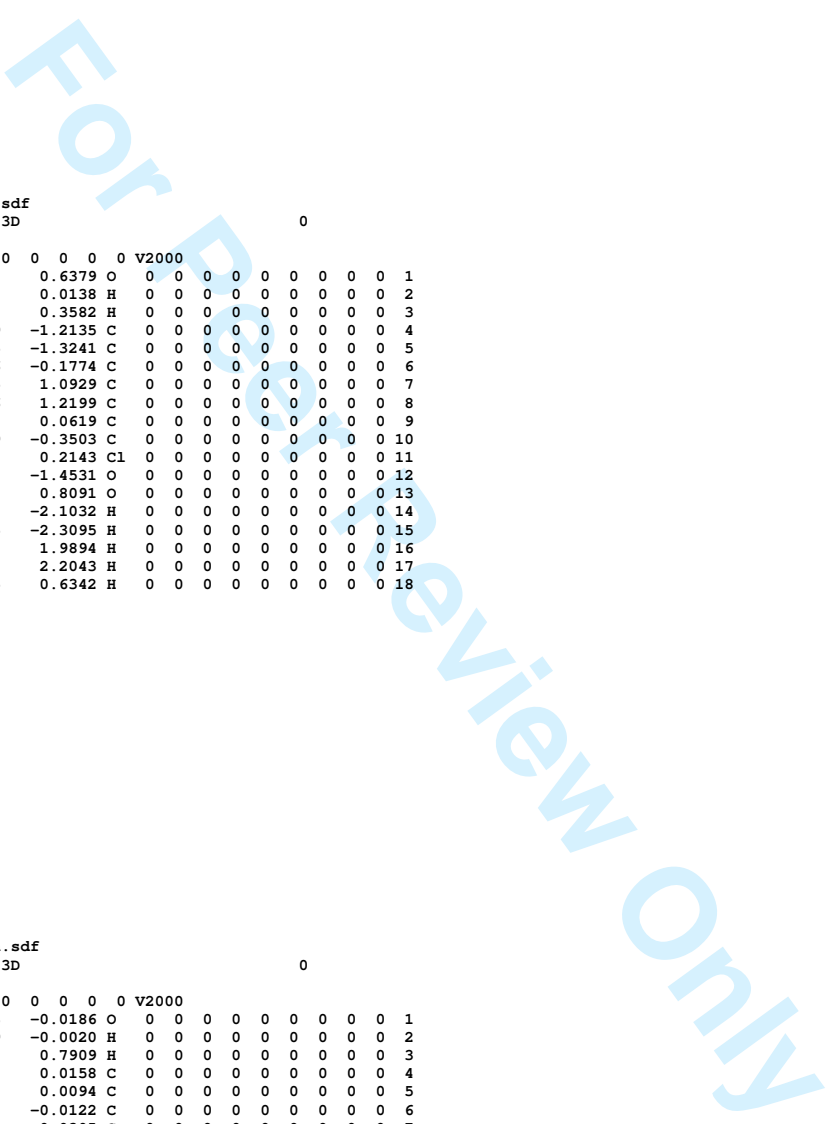


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-0.5600   0.1183  -0.0026 C  0  0  0  0  0  0  0  0  0  0  6
 0.2250   1.2822  -0.0014 C  0  0  0  0  0  0  0  0  0  0  7
 1.6207   1.2134   0.0002 C  0  0  0  0  0  0  0  0  0  0  8
 2.2273  -0.0443   0.0008 C  0  0  0  0  0  0  0  0  0  0  9
-2.0831   0.2183  -0.0047 C  0  0  0  0  0  0  0  0  0  0 10
 4.0003  -0.1477   0.0030 Cl 0  0  0  0  0  0  0  0  0  0 11
-2.7267  -0.8888  -0.0098 O  0  0  0  0  0  0  0  0  0  0 12
-2.5993   1.3701  -0.0014 O  0  0  0  0  0  0  0  0  0  0 13
 1.9733  -2.1940   0.0004 H  0  0  0  0  0  0  0  0  0  0 14
-0.5218  -2.0368  -0.0032 H  0  0  0  0  0  0  0  0  0  0 15
-0.2732   2.2526  -0.0016 H  0  0  0  0  0  0  0  0  0  0 16
 2.2251   2.1208   0.0010 H  0  0  0  0  0  0  0  0  0  0 17
 2  1  0  0  0  0  0
 3  1  0  0  0  0  0
 5  4  0  0  0  0  0
 9  4  0  0  0  0  0
14  4  0  0  0  0  0
 6  5  0  0  0  0  0
15  5  0  0  0  0  0
 7  6  0  0  0  0  0
10  6  0  0  0  0  0
 8  7  0  0  0  0  0
16  7  0  0  0  0  0
 9  8  0  0  0  0  0
11  9  0  0  0  0  0
12 10  0  0  0  0  0
13 10  0  0  0  0  0
 8 17  0  0  0  0  0
M END
$$$$
4-chlorobenzoicacid.sdf
COSMOtherm      3D      0
18 17  0  0  0  0  0  0  0  0  0  0 v2000
-5.3123  -0.0004   0.6379 O  0  0  0  0  0  0  0  0  0  0  1
-5.6866  -0.6490   0.0138 H  0  0  0  0  0  0  0  0  0  0  2
-5.6862   0.8554   0.3582 H  0  0  0  0  0  0  0  0  0  0  3
 1.6745   0.0059  -1.2135 C  0  0  0  0  0  0  0  0  0  0  4
 0.2845   0.0035  -1.3241 C  0  0  0  0  0  0  0  0  0  0  5
-0.5271  -0.0036  -0.1774 C  0  0  0  0  0  0  0  0  0  0  6
 0.0741  -0.0085   1.0929 C  0  0  0  0  0  0  0  0  0  0  7
 1.4640  -0.0066   1.2199 C  0  0  0  0  0  0  0  0  0  0  8
 2.2453   0.0007   0.0619 C  0  0  0  0  0  0  0  0  0  0  9
-2.0118  -0.0049  -0.3503 C  0  0  0  0  0  0  0  0  0  0 10
 4.0081   0.0037   0.2143 Cl 0  0  0  0  0  0  0  0  0  0 11
-2.5607  -0.0062  -1.4531 O  0  0  0  0  0  0  0  0  0  0 12
-2.6855  -0.0040   0.8091 O  0  0  0  0  0  0  0  0  0  0 13
 2.3035   0.0118  -2.1032 H  0  0  0  0  0  0  0  0  0  0 14
-0.1823   0.0075  -2.3095 H  0  0  0  0  0  0  0  0  0  0 15
-0.5450  -0.0142   1.9894 H  0  0  0  0  0  0  0  0  0  0 16
 1.9315  -0.0104   2.2043 H  0  0  0  0  0  0  0  0  0  0 17
-3.6933  -0.0025   0.6342 H  0  0  0  0  0  0  0  0  0  0 18
 2  1  0  0  0  0  0
 3  1  0  0  0  0  0
 5  4  0  0  0  0  0
 9  4  0  0  0  0  0
14  4  0  0  0  0  0
 6  5  0  0  0  0  0
15  5  0  0  0  0  0
 7  6  0  0  0  0  0
10  6  0  0  0  0  0
 8  7  0  0  0  0  0
16  7  0  0  0  0  0
 9  8  0  0  0  0  0
17  8  0  0  0  0  0
11  9  0  0  0  0  0
12 10  0  0  0  0  0
13 10  0  0  0  0  0
13 18  0  0  0  0  0
M END
$$$$
4-chlorophenol-anion.sdf
COSMOtherm      3D      0
15 14  0  0  0  0  0  0  0  0  0  0 v2000
 1.0209   4.4203  -0.0186 O  0  0  0  0  0  0  0  0  0  0  1
 0.3252   3.6669  -0.0020 H  0  0  0  0  0  0  0  0  0  0  2
 1.5432   4.2904   0.7909 H  0  0  0  0  0  0  0  0  0  0  3
-1.2919  -1.0410   0.0158 C  0  0  0  0  0  0  0  0  0  0  4
-1.5882   0.3228   0.0094 C  0  0  0  0  0  0  0  0  0  0  5
-0.5667   1.3267  -0.0122 C  0  0  0  0  0  0  0  0  0  0  6
 0.7816   0.8417  -0.0305 C  0  0  0  0  0  0  0  0  0  0  7
 1.0815  -0.5219  -0.0244 C  0  0  0  0  0  0  0  0  0  0  8
 0.0428  -1.4564  -0.0018 C  0  0  0  0  0  0  0  0  0  0  9
-0.8606   2.6021  -0.0143 O  0  0  0  0  0  0  0  0  0  0 10
 0.4254  -3.2046   0.0081 Cl 0  0  0  0  0  0  0  0  0  0 11
-2.0976  -1.7775   0.0333 H  0  0  0  0  0  0  0  0  0  0 12
-2.6316   0.6478   0.0238 H  0  0  0  0  0  0  0  0  0  0 13
 1.5963   1.5695  -0.0525 H  0  0  0  0  0  0  0  0  0  0 14
 2.1211  -0.8545  -0.0375 H  0  0  0  0  0  0  0  0  0  0 15
 2  1  0  0  0  0  0
 3  1  0  0  0  0  0
 5  4  0  0  0  0  0
 9  4  0  0  0  0  0
12  4  0  0  0  0  0
 6  5  0  0  0  0  0
13  5  0  0  0  0  0
 7  6  0  0  0  0  0
10  6  0  0  0  0  0
 8  7  0  0  0  0  0
14  7  0  0  0  0  0
 9  8  0  0  0  0  0
11  9  0  0  0  0  0
 8 15  0  0  0  0  0
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4-chlorophenol.sdf
COSMOtherm          3D          0

16 15 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
1.0105 4.3857 -0.0118 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
1.6704 4.3586 -0.7281 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.5332 4.4803 0.8052 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.6023 0.2789 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.2902 -1.0816 -0.0020 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.0498 -1.4757 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.0792 -0.5344 0.0056 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.7626 0.8275 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.5808 1.2457 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.4505 -3.2096 -0.0021 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.9482 2.5577 0.0016 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.6445 0.6015 -0.0036 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.0873 -1.8254 -0.0052 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.1223 -0.8512 0.0082 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
1.5661 1.5660 0.0119 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.1456 3.1633 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
12 4 0 0 0 0 0
6 5 0 0 0 0 0
13 5 0 0 0 0 0
7 6 0 0 0 0 0
10 6 0 0 0 0 0
8 7 0 0 0 0 0
14 7 0 0 0 0 0
9 8 0 0 0 0 0
15 8 0 0 0 0 0
11 9 0 0 0 0 0
11 16 0 0 0 0 0
M END
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$$$$
4-cyanobenzoicacid-anion.sdf
COSMOtherm          3D          0

18 17 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-5.2051 -0.4934 -0.0142 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.2020 -0.6096 -0.0011 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.3163 0.4712 -0.0751 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.6501 -1.2344 0.0021 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.2605 -1.1364 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.3737 0.1167 0.0044 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.4118 1.2811 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.8024 1.2067 -0.0026 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4277 -0.0576 -0.0017 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9009 0.2229 0.0076 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.8525 -0.1460 -0.0047 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
5.0184 -0.2175 -0.0067 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.5439 -0.8824 0.0092 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.4070 1.3776 0.0073 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2.1387 -2.2092 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.3530 -2.0378 0.0079 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.0880 2.2503 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2.4076 2.1137 -0.0054 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
15 4 0 0 0 0 0
6 5 0 0 0 0 0
16 5 0 0 0 0 0
7 6 0 0 0 0 0
10 6 0 0 0 0 0
8 7 0 0 0 0 0
17 7 0 0 0 0 0
9 8 0 0 0 0 0
11 9 0 0 0 0 0
13 10 0 0 0 0 0
14 10 0 0 0 0 0
12 11 0 0 0 0 0
8 18 0 0 0 0 0
M END
$$$$

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$$$$
4-cyanobenzoicacid.sdf
COSMOtherm          3D          0

19 18 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0
-5.1214 0.0027 0.6330 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.4905 -0.6689 0.0302 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.4953 0.8474 0.3211 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.8509 -0.0038 -1.2035 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.4644 -0.0069 -1.3164 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.3443 -0.0072 -0.1680 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2494 -0.0045 1.1055 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.6359 -0.0007 1.2343 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4403 0.0000 0.0772 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.8346 -0.0045 -0.3449 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.8637 0.0053 0.2023 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
5.0266 0.0105 0.3036 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.3737 0.0116 -1.4508 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.5065 -0.0170 0.8113 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2.4785 -0.0034 -2.0944 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.0056 -0.0079 -2.2999 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.3753 -0.0040 1.9977 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2.0986 0.0027 2.2210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.5177 -0.0015 0.6378 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0

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9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
14 19 0 0 0 0
```

M END
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4-dimethylaminobenzoicacid-anion.sdf
COSMOtherm 3D

0

```
25 24 0 0 0 0 0 0 0 0 0 V2000
-5.5995 0.0024 -0.4610 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.5940 -0.0107 -0.6059 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.6763 -0.0419 0.5080 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2472 0.0260 -1.2032 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.1426 0.0096 -1.1199 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8138 0.0086 0.1162 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0206 0.0191 1.2777 C 0 0 0 0 0 0 0 0 0 0 0 7
1.3700 0.0368 1.2210 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0508 0.0558 -0.0288 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.3223 -0.0150 0.2046 C 0 0 0 0 0 0 0 0 0 0 0 10
3.4287 0.1125 -0.0980 N 0 0 0 0 0 0 0 0 0 0 0 11
4.2235 -0.0702 1.1140 C 0 0 0 0 0 0 0 0 0 0 0 12
4.0990 -0.0816 -1.3810 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.9719 -0.0084 -0.9060 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.8602 -0.0397 1.3515 O 0 0 0 0 0 0 0 0 0 0 0 15
1.7151 0.0153 -2.1867 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.7347 -0.0099 -2.0370 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.5200 0.0063 2.2486 H 0 0 0 0 0 0 0 0 0 0 0 18
1.9341 0.0354 2.1529 H 0 0 0 0 0 0 0 0 0 0 0 19
5.2805 0.0766 0.8668 H 0 0 0 0 0 0 0 0 0 0 0 20
3.9516 0.6713 1.8792 H 0 0 0 0 0 0 0 0 0 0 0 21
4.1037 -1.0788 1.5509 H 0 0 0 0 0 0 0 0 0 0 0 22
5.1749 0.0699 -1.2421 H 0 0 0 0 0 0 0 0 0 0 0 23
3.9392 -1.0950 -1.7932 H 0 0 0 0 0 0 0 0 0 0 0 24
3.7503 0.6514 -2.1231 H 0 0 0 0 0 0 0 0 0 0 0 25
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 13 0 0 0 0
24 13 0 0 0 0
13 25 0 0 0 0
```

M END
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4-dimethylaminobenzoicacid.sdf
COSMOtherm 3D

0

```
26 25 0 0 0 0 0 0 0 0 0 V2000
-5.5824 -0.0258 0.6270 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.9239 -0.5663 -0.1089 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.9621 0.8590 0.4760 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4302 -0.0023 -1.2330 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0477 -0.0008 -1.3306 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7753 0.0020 -0.1847 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1442 0.0037 1.0776 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2379 0.0026 1.1962 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0741 0.0002 0.0405 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.2401 0.0038 -0.3440 C 0 0 0 0 0 0 0 0 0 0 0 10
3.4376 -0.0005 0.1481 N 0 0 0 0 0 0 0 0 0 0 0 11
4.0754 0.0013 1.4634 C 0 0 0 0 0 0 0 0 0 0 0 12
4.2754 -0.0045 -1.0499 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.8193 0.0144 -1.4384 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.9204 -0.0102 0.8258 O 0 0 0 0 0 0 0 0 0 0 0 15
2.0232 -0.0053 -2.1463 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4214 -0.0022 -2.3161 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.7523 0.0056 1.9829 H 0 0 0 0 0 0 0 0 0 0 0 18
1.6804 0.0042 2.1909 H 0 0 0 0 0 0 0 0 0 0 0 19
5.1612 0.0033 1.3286 H 0 0 0 0 0 0 0 0 0 0 0 20
3.7990 0.8950 2.0464 H 0 0 0 0 0 0 0 0 0 0 0 21
3.8023 -0.8927 2.0476 H 0 0 0 0 0 0 0 0 0 0 0 22
5.3262 -0.0029 -0.7446 H 0 0 0 0 0 0 0 0 0 0 0 23
4.0966 -0.9003 -1.6664 H 0 0 0 0 0 0 0 0 0 0 0 24
4.0960 0.8869 -1.6726 H 0 0 0 0 0 0 0 0 0 0 0 25
-3.9179 -0.0058 0.6382 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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9 4 0 0 0 0
 16 4 0 0 0 0
 6 5 0 0 0 0
 17 5 0 0 0 0
 7 6 0 0 0 0
 10 6 0 0 0 0
 8 7 0 0 0 0
 18 7 0 0 0 0
 9 8 0 0 0 0
 19 8 0 0 0 0
 11 9 0 0 0 0
 14 10 0 0 0 0
 15 10 0 0 0 0
 12 11 0 0 0 0
 13 11 0 0 0 0
 20 12 0 0 0 0
 21 12 0 0 0 0
 22 12 0 0 0 0
 23 13 0 0 0 0
 24 13 0 0 0 0
 25 13 0 0 0 0
 15 26 0 0 0 0

M END

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4-ethylbenzoicacid-anion.sdf

COSMOtherm

3D

0

23 22 0 0 0 0 0 0 0 0 0 V2000
 -5.2314 -0.4470 0.2623 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -4.2366 -0.6051 0.1597 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -5.2850 0.5203 0.3499 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 1.7332 1.1979 -0.2249 C 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.3418 1.2723 -0.1242 C 0 0 0 0 0 0 0 0 0 0 0 0 5
 -0.4424 0.1071 -0.1069 C 0 0 0 0 0 0 0 0 0 0 0 0 6
 0.2078 -1.1350 -0.1939 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 1.6000 -1.2078 -0.2928 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 2.3889 -0.0434 -0.3110 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 -1.9595 0.1995 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 10
 3.8979 -0.1233 -0.3785 C 0 0 0 0 0 0 0 0 0 0 0 0 11
 4.5536 -0.1883 1.0149 C 0 0 0 0 0 0 0 0 0 0 0 0 12
 -2.4818 1.3476 0.0811 O 0 0 0 0 0 0 0 0 0 0 0 0 13
 -2.6062 -0.9077 0.0016 O 0 0 0 0 0 0 0 0 0 0 0 0 14
 2.3233 2.1184 -0.2450 H 0 0 0 0 0 0 0 0 0 0 0 0 15
 -0.1592 2.2402 -0.0630 H 0 0 0 0 0 0 0 0 0 0 0 0 16
 -0.3946 -2.0450 -0.1869 H 0 0 0 0 0 0 0 0 0 0 0 0 17
 2.0857 -2.1849 -0.3658 H 0 0 0 0 0 0 0 0 0 0 0 0 18
 4.2860 0.7539 -0.9195 H 0 0 0 0 0 0 0 0 0 0 0 0 19
 4.1916 -1.0130 -0.9575 H 0 0 0 0 0 0 0 0 0 0 0 0 20
 5.6487 -0.2431 0.9272 H 0 0 0 0 0 0 0 0 0 0 0 0 21
 4.2112 -1.0737 1.5711 H 0 0 0 0 0 0 0 0 0 0 0 0 22
 4.3037 0.7024 1.6104 H 0 0 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0

3 1 0 0 0 0

5 4 0 0 0 0

9 4 0 0 0 0

15 4 0 0 0 0

6 5 0 0 0 0

16 5 0 0 0 0

7 6 0 0 0 0

10 6 0 0 0 0

8 7 0 0 0 0

17 7 0 0 0 0

9 8 0 0 0 0

18 8 0 0 0 0

11 9 0 0 0 0

13 10 0 0 0 0

14 10 0 0 0 0

12 11 0 0 0 0

19 11 0 0 0 0

20 11 0 0 0 0

21 12 0 0 0 0

22 12 0 0 0 0

12 23 0 0 0 0

M END

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4-ethylbenzoicacid.sdf

COSMOtherm

3D

0

24 23 0 0 0 0 0 0 0 0 0 V2000
 -5.1912 0.2092 0.6380 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -5.6117 -0.5207 0.1474 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -5.5033 1.0172 0.1909 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 1.7920 -0.2099 -1.2045 C 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.4073 -0.1021 -1.3228 C 0 0 0 0 0 0 0 0 0 0 0 0 5
 -0.4064 -0.0974 -0.1764 C 0 0 0 0 0 0 0 0 0 0 0 0 6
 0.1975 -0.2061 1.0892 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 1.5844 -0.3125 1.1984 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 2.4065 -0.3156 0.0568 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 -1.8837 0.0202 -0.3437 C 0 0 0 0 0 0 0 0 0 0 0 0 10
 3.9105 -0.3891 0.1830 C 0 0 0 0 0 0 0 0 0 0 0 0 11
 4.5599 1.0023 0.3201 C 0 0 0 0 0 0 0 0 0 0 0 0 12
 -2.4359 0.1239 -1.4410 O 0 0 0 0 0 0 0 0 0 0 0 0 13
 -2.5621 0.0052 0.8168 O 0 0 0 0 0 0 0 0 0 0 0 0 14
 2.4099 -0.2183 -2.1056 H 0 0 0 0 0 0 0 0 0 0 0 0 15
 -0.0600 -0.0245 -2.3055 H 0 0 0 0 0 0 0 0 0 0 0 0 16
 -0.4218 -0.2101 1.9863 H 0 0 0 0 0 0 0 0 0 0 0 0 17
 2.0395 -0.4014 2.1877 H 0 0 0 0 0 0 0 0 0 0 0 0 18
 4.3260 -0.8976 -0.7006 H 0 0 0 0 0 0 0 0 0 0 0 0 19
 4.1739 -0.9992 1.0608 H 0 0 0 0 0 0 0 0 0 0 0 0 20
 5.6521 0.9109 0.4096 H 0 0 0 0 0 0 0 0 0 0 0 0 21
 4.1866 1.5260 1.2125 H 0 0 0 0 0 0 0 0 0 0 0 0 22
 4.3408 1.6286 -0.5572 H 0 0 0 0 0 0 0 0 0 0 0 0 23
 -3.5632 0.0916 0.6380 H 0 0 0 0 0 0 0 0 0 0 0 0 24

2 1 0 0 0 0

3 1 0 0 0 0

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5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
20 11 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
14 24 0 0 0 0

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M END

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4-fluorobenzoicacid-anion.sdf

COSMOtherm 3D

0

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17 16 0 0 0 0 0 0 0 0 0 V2000
-4.9128 -0.4385 0.0394 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.9098 -0.5722 0.0151 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.0069 0.5297 0.0258 H 0 0 0 0 0 0 0 0 0 0 0 3
1.9284 -1.2710 -0.0047 C 0 0 0 0 0 0 0 0 0 0 0 4
0.5353 -1.1560 -0.0127 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0886 0.1028 -0.0093 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7137 1.2560 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1083 1.1665 0.0104 C 0 0 0 0 0 0 0 0 0 0 0 8
2.6834 -0.1013 0.0067 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.6079 0.2259 -0.0173 C 0 0 0 0 0 0 0 0 0 0 0 10
4.0507 -0.2020 0.0152 F 0 0 0 0 0 0 0 0 0 0 0 11
-2.2702 -0.8711 -0.0214 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.1086 1.3851 -0.0193 O 0 0 0 0 0 0 0 0 0 0 0 13
2.4230 -2.2432 -0.0072 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.0856 -2.0525 -0.0212 H 0 0 0 0 0 0 0 0 0 0 0 15
0.2279 2.2326 0.0037 H 0 0 0 0 0 0 0 0 0 0 0 16
2.7394 2.0560 0.0194 H 0 0 0 0 0 0 0 0 0 0 0 17

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
8 17 0 0 0 0

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M END

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4-fluorobenzoicacid.sdf

COSMOtherm 3D

0

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18 17 0 0 0 0 0 0 0 0 0 V2000
-4.8584 -0.0236 0.5657 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.2027 -0.6683 -0.0794 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.2480 0.8281 0.2951 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1663 0.0004 -1.1453 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7790 0.0029 -1.2837 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0555 0.0030 -0.1522 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5187 0.0009 1.1319 C 0 0 0 0 0 0 0 0 0 0 0 7
1.9054 -0.0018 1.2880 C 0 0 0 0 0 0 0 0 0 0 0 8
2.6977 -0.0019 0.1425 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.5348 0.0053 -0.3554 C 0 0 0 0 0 0 0 0 0 0 0 10
4.0549 -0.0046 0.2877 F 0 0 0 0 0 0 0 0 0 0 0 11
-2.0633 0.0027 -1.4682 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.2336 0.0090 0.7908 O 0 0 0 0 0 0 0 0 0 0 0 13
2.8265 0.0005 -2.0127 H 0 0 0 0 0 0 0 0 0 0 0 14
0.3300 0.0052 -2.2771 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.1208 0.0012 2.0138 H 0 0 0 0 0 0 0 0 0 0 0 16
2.3674 -0.0037 2.2755 H 0 0 0 0 0 0 0 0 0 0 0 17
-3.2365 0.0080 0.5940 H 0 0 0 0 0 0 0 0 0 0 0 18

```

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
13 18 0 0 0 0

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M END

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4-hydroxybenzoicacid-anion.sdf

COSMOtherm 3D

0

```
18 17 0 0 0 0 0 0 0 0 0 V2000
-4.8622 0.0133 -0.4164 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8599 0.0061 -0.5684 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.9343 -0.0378 0.5526 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1479 0.0041 1.1586 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7567 0.0021 1.2468 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0505 -0.0012 0.0950 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5833 -0.0033 -1.1588 C 0 0 0 0 0 0 0 0 0 0 0 7
1.9754 -0.0023 -1.2669 C 0 0 0 0 0 0 0 0 0 0 0 8
2.7619 0.0018 -0.1039 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.5652 -0.0035 0.2147 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.2305 -0.0059 -0.8830 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.0731 -0.0074 1.3726 O 0 0 0 0 0 0 0 0 0 0 0 12
4.1344 0.0034 -0.1421 O 0 0 0 0 0 0 0 0 0 0 0 13
4.4322 0.0021 -1.0718 H 0 0 0 0 0 0 0 0 0 0 0 14
2.7691 0.0072 2.0561 H 0 0 0 0 0 0 0 0 0 0 0 15
0.2711 0.0037 2.2240 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.0321 -0.0063 -2.0598 H 0 0 0 0 0 0 0 0 0 0 0 17
2.4563 -0.0044 -2.2487 H 0 0 0 0 0 0 0 0 0 0 0 18
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
14 13 0 0 0 0
8 18 0 0 0 0
M END
$$$$
4-hydroxybenzoicacid.sdf
COSMOTHERM 3D 0
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19 18 0 0 0 0 0 0 0 0 0 V2000
-1.1619 0.0031 -4.4682 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.1716 -0.7809 -5.0475 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.1441 0.7620 -5.0798 H 0 0 0 0 0 0 0 0 0 0 0 3
1.6542 0.0004 -0.5782 C 0 0 0 0 0 0 0 0 0 0 0 4
1.3675 0.0008 0.7797 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0340 0.0001 1.2384 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.0085 -0.0008 0.2897 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7323 -0.0009 -1.0736 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6055 -0.0005 -1.5222 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.2197 0.0002 2.6917 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.5458 0.0002 3.0098 O 0 0 0 0 0 0 0 0 0 0 0 11
0.6514 0.0003 3.5616 O 0 0 0 0 0 0 0 0 0 0 0 12
0.9391 -0.0019 -2.8332 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.6102 0.0009 3.9886 H 0 0 0 0 0 0 0 0 0 0 0 14
0.1194 0.0007 -3.4263 H 0 0 0 0 0 0 0 0 0 0 0 15
2.6861 0.0007 -0.9322 H 0 0 0 0 0 0 0 0 0 0 0 16
2.1795 0.0014 1.5080 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.0460 -0.0014 0.6234 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.5461 -0.0019 -1.8005 H 0 0 0 0 0 0 0 0 0 0 0 19
```

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
14 11 0 0 0 0
15 13 0 0 0 0
8 19 0 0 0 0
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M END
$$$$
4-hydroxymethylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
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```
21 20 0 0 0 0 0 0 0 0 0 V2000
-5.2857 -0.4589 -0.2023 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.2846 -0.5943 -0.1372 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.3712 0.5075 -0.2755 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5515 -1.2231 0.2693 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1606 -1.1397 0.1614 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4779 0.1092 0.0914 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3096 1.2717 0.1343 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6993 1.1878 0.2446 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3388 -0.0610 0.3130 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9965 0.2130 -0.0211 C 0 0 0 0 0 0 0 0 0 0 0 10
3.8401 -0.1501 0.3964 C 0 0 0 0 0 0 0 0 0 0 0 11
4.3773 -0.1370 -0.9529 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.6470 -0.8910 -0.0312 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.5082 1.3650 -0.0963 O 0 0 0 0 0 0 0 0 0 0 0 14
5.3481 -0.1785 -0.8709 H 0 0 0 0 0 0 0 0 0 0 0 15
2.0348 -2.2019 0.3261 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4489 -2.0442 0.1340 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.1877 2.2417 0.0856 H 0 0 0 0 0 0 0 0 0 0 0 18
2.2978 2.1015 0.2835 H 0 0 0 0 0 0 0 0 0 0 0 19
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4.1368 -1.0803 0.9099 H 0 0 0 0 0 0 0 0 0 0 0 20
4.2392 0.7060 0.9662 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
15 12 0 0 0 0
11 21 0 0 0 0
M END
$$$$
4-hydroxymethylbenzoicacid.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
-5.2315 0.2116 0.6140 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.6667 -0.5638 0.2128 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.5481 0.9703 0.0891 H 0 0 0 0 0 0 0 0 0 0 0 3
1.7589 -0.2420 -1.1766 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3755 -0.1350 -1.3082 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4436 -0.0960 -0.1664 C 0 0 0 0 0 0 0 0 0 0 0 6
0.1458 -0.1669 1.1075 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5324 -0.2722 1.2312 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3546 -0.3115 0.0941 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.9229 0.0161 -0.3494 C 0 0 0 0 0 0 0 0 0 0 0 10
3.8532 -0.3921 0.2315 C 0 0 0 0 0 0 0 0 0 0 0 11
4.3848 0.9563 0.1870 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.4611 0.1094 -1.4537 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.6100 0.0070 0.8036 O 0 0 0 0 0 0 0 0 0 0 0 14
5.3553 0.8795 0.2432 H 0 0 0 0 0 0 0 0 0 0 0 15
2.3868 -0.2778 -2.0695 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.0861 -0.0848 -2.2952 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.4821 -0.1411 1.9978 H 0 0 0 0 0 0 0 0 0 0 0 18
1.9835 -0.3285 2.2242 H 0 0 0 0 0 0 0 0 0 0 0 19
4.2757 -0.9913 -0.5926 H 0 0 0 0 0 0 0 0 0 0 0 20
4.1198 -0.8742 1.1869 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.6112 0.0892 0.6175 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
15 12 0 0 0 0
14 22 0 0 0 0
M END
$$$$
4-iodobenzoicacid-anion.sdf
COSMOtherm 3D 0
17 15 0 0 0 0 0 0 0 0 0 V2000
-6.9293 -0.5578 -0.0118 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.9231 -0.6601 0.0040 H 0 0 0 0 0 0 0 0 0 0 0 2
-7.0525 0.4056 -0.0668 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.0581 -1.1612 0.0026 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4554 -1.0928 0.0041 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.1211 0.1427 0.0035 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.3572 1.3200 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0407 1.2764 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6728 0.0300 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 9
-3.6461 0.2150 0.0055 C 0 0 0 0 0 0 0 0 0 0 0 10
2.8149 -0.0567 -0.0014 I 0 0 0 0 0 0 0 0 0 0 0 11
-4.2691 -0.9036 0.0081 O 0 0 0 0 0 0 0 0 0 0 0 12
-4.1827 1.3575 0.0043 O 0 0 0 0 0 0 0 0 0 0 0 13
0.4441 -2.1288 0.0031 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.0435 -2.0116 0.0057 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.8718 2.2821 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 16
0.6187 2.2006 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
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10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0

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9 8 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
8 17 0 0 0 0
M END
$$$$
4-iodobenzoicacid.sdf
COSMOTHERM 3D 0

18 16 0 0 0 0 0 0 0 0 0 V2000
-6.8490 -0.0028 0.7379 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-7.2459 -0.6559 0.1328 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-7.2347 0.8507 0.4674 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0854 -0.0066 -1.3053 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.3083 -0.0077 -1.3791 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.0887 -0.0051 -0.2115 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.4538 -0.0017 1.0419 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0599 0.0003 1.1316 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.6936 -0.0022 -0.0460 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-3.5783 -0.0018 -0.3442 C 0 0 0 0 0 0 0 0 0 0 0 0 10
2.8277 0.0016 0.0815 I 0 0 0 0 0 0 0 0 0 0 0 0 11
-4.1566 0.0153 -1.4315 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-4.2197 -0.0175 0.8332 O 0 0 0 0 0 0 0 0 0 0 0 0 13
0.6804 -0.0092 -2.2181 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.8007 -0.0101 -2.3523 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.0482 0.0009 1.9553 H 0 0 0 0 0 0 0 0 0 0 0 0 16
0.4231 0.0044 2.1083 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-5.2322 -0.0065 0.6862 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
13 18 0 0 0 0
M END
$$$$
4-methoxybenzoicacid-anion.sdf
COSMOTHERM 3D 0

21 20 0 0 0 0 0 0 0 0 0 V2000
-5.2950 0.0169 0.2474 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.3024 -0.0005 0.4529 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.3121 0.0449 -0.7250 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4933 0.0002 1.4062 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1116 -0.0032 1.2402 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4688 -0.0045 -0.0427 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.3868 -0.0034 -1.1536 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.7782 -0.0002 -1.0097 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.3377 0.0014 0.2791 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9769 -0.0075 -0.2282 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.6835 0.0043 0.5390 O 0 0 0 0 0 0 0 0 0 0 0 0 11
4.5853 0.0067 -0.5855 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.6885 -0.0120 0.8401 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.4351 -0.0052 -1.4068 O 0 0 0 0 0 0 0 0 0 0 0 0 14
1.9410 0.0019 2.4019 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.5425 -0.0040 2.1134 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.0540 -0.0041 -2.1519 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.4108 0.0008 -1.8966 H 0 0 0 0 0 0 0 0 0 0 0 0 18
5.5915 0.0093 -0.1542 H 0 0 0 0 0 0 0 0 0 0 0 0 19
4.4505 -0.8939 -1.2035 H 0 0 0 0 0 0 0 0 0 0 0 0 20
4.4458 0.9064 -1.2037 H 0 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
19 12 0 0 0 0
20 12 0 0 0 0
12 21 0 0 0 0
M END
$$$$
4-methoxybenzoicacid.sdf
COSMOTHERM 3D 0

22 21 0 0 0 0 0 0 0 0 0 V2000
-5.1836 -0.0015 0.8186 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.5860 -0.6814 0.2478 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.5631 0.8393 0.5036 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7072 -0.0077 -1.3933 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3207 -0.0069 -1.4318 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4358 -0.0021 -0.2416 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2425 0.0032 0.9888 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.6371 0.0033 1.0436 C 0 0 0 0 0 0 0 0 0 0 0 0 8

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2.3775 -0.0024 -0.1525 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9181 -0.0003 -0.3306 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.7391 -0.0042 -0.2143 O 0 0 0 0 0 0 0 0 0 0 0 0 11
4.4760 0.0124 1.0279 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.5370 0.0218 -1.3985 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.5346 -0.0273 0.8662 O 0 0 0 0 0 0 0 0 0 0 0 0 14
2.2951 -0.0125 -2.3123 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.1985 -0.0102 -2.3911 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.3252 0.0074 1.9193 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.1347 0.0080 2.0122 H 0 0 0 0 0 0 0 0 0 0 0 0 18
5.5317 0.0148 0.7392 H 0 0 0 0 0 0 0 0 0 0 0 0 19
4.2476 0.9185 1.6081 H 0 0 0 0 0 0 0 0 0 0 0 0 20
4.2569 -0.8834 1.6272 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.5448 -0.0171 0.7358 H 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
19 12 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
14 22 0 0 0 0
M END
$$$$
4-methylaminobenzoicacid-anion.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 V2000
-5.2730 -0.2012 0.0272 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.2862 -0.4420 0.0178 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.2481 0.7716 0.0300 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4991 -1.4168 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1197 -1.2515 0.0078 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4699 0.0295 -0.0098 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.3912 1.1395 -0.0336 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.7787 0.9967 -0.0420 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.3659 -0.2926 -0.0317 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9707 0.2124 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.7299 -0.4766 -0.0816 N 0 0 0 0 0 0 0 0 0 0 0 0 11
4.6838 0.6053 0.1117 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.6878 -0.8558 0.0069 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.4363 1.3908 -0.0012 O 0 0 0 0 0 0 0 0 0 0 0 0 14
4.0606 -1.4096 0.1466 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.9322 -2.4205 0.0129 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.5317 -2.1271 0.0319 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.0498 2.1382 -0.0414 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2.4105 1.8853 -0.0569 H 0 0 0 0 0 0 0 0 0 0 0 0 19
5.6956 0.1862 0.0730 H 0 0 0 0 0 0 0 0 0 0 0 0 20
4.5967 1.3560 -0.6887 H 0 0 0 0 0 0 0 0 0 0 0 0 21
4.5538 1.1202 1.0810 H 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
12 22 0 0 0 0
M END
$$$$
4-methylaminobenzoicacid.sdf
COSMOtherm 3D 0
23 22 0 0 0 0 0 0 0 0 0 V2000
-5.1921 -0.0057 0.8235 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.5839 -0.5868 0.1459 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.5661 0.8747 0.6353 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7063 -0.0047 -1.4106 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3236 -0.0049 -1.4378 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4352 -0.0038 -0.2444 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2602 -0.0010 0.9820 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.6491 0.0011 1.0280 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4098 -0.0010 -0.1723 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.9067 -0.0022 -0.3247 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.7724 -0.0009 -0.1627 N 0 0 0 0 0 0 0 0 0 0 0 0 11
4.5916 0.0110 1.0382 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.5430 0.0185 -1.3864 O 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.5240 -0.0278 0.8795 O 0 0 0 0 0 0 0 0 0 0 0 0 14
4.2493 0.0047 -1.0585 H 0 0 0 0 0 0 0 0 0 0 0 0 15

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3 2.2741 -0.0067 -2.3441 H 0 0 0 0 0 0 0 0 0 0 0 16
4 -0.2001 -0.0066 -2.3954 H 0 0 0 0 0 0 0 0 0 0 0 17
5 -0.3012 0.0010 1.9170 H 0 0 0 0 0 0 0 0 0 0 0 18
6 2.1541 0.0056 1.9939 H 0 0 0 0 0 0 0 0 0 0 0 19
7 5.6445 -0.0012 0.7368 H 0 0 0 0 0 0 0 0 0 0 0 20
8 4.4147 0.9145 1.6446 H 0 0 0 0 0 0 0 0 0 0 0 21
9 4.4016 -0.8724 1.6691 H 0 0 0 0 0 0 0 0 0 0 0 22
10 -3.5298 -0.0129 0.7445 H 0 0 0 0 0 0 0 0 0 0 0 23
11 2 1 0 0 0 0 0
12 3 1 0 0 0 0 0
13 5 4 0 0 0 0 0
14 9 4 0 0 0 0 0
15 16 4 0 0 0 0 0
16 6 5 0 0 0 0 0
17 17 5 0 0 0 0 0
18 7 6 0 0 0 0 0
19 10 6 0 0 0 0 0
20 8 7 0 0 0 0 0
21 18 7 0 0 0 0 0
22 9 8 0 0 0 0 0
23 19 8 0 0 0 0 0
24 11 9 0 0 0 0 0
25 13 10 0 0 0 0 0
26 14 10 0 0 0 0 0
27 12 11 0 0 0 0 0
28 15 11 0 0 0 0 0
29 20 12 0 0 0 0 0
30 21 12 0 0 0 0 0
31 22 12 0 0 0 0 0
32 14 23 0 0 0 0 0

M END

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4-methylbenzoicacid-anion.sdf

COSMOtherm

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20 19 0 0 0 0 0 0 0 0 0 0 V2000
24 -4.8384 -0.0034 -0.4293 O 0 0 0 0 0 0 0 0 0 0 0 1
25 -3.8348 0.0002 -0.5695 H 0 0 0 0 0 0 0 0 0 0 0 2
26 -4.9240 -0.0094 0.5398 H 0 0 0 0 0 0 0 0 0 0 0 3
27 2.0063 -0.0082 -1.2579 C 0 0 0 0 0 0 0 0 0 0 0 4
28 0.6124 -0.0019 -1.1570 C 0 0 0 0 0 0 0 0 0 0 0 5
29 -0.0181 0.0003 0.0979 C 0 0 0 0 0 0 0 0 0 0 0 6
30 0.7892 -0.0064 1.2474 C 0 0 0 0 0 0 0 0 0 0 0 7
31 2.1822 -0.0131 1.1453 C 0 0 0 0 0 0 0 0 0 0 0 8
32 2.8181 -0.0102 -0.1094 C 0 0 0 0 0 0 0 0 0 0 0 9
33 4.3228 0.0167 -0.2178 C 0 0 0 0 0 0 0 0 0 0 0 10
34 -1.5366 0.0050 0.2201 C 0 0 0 0 0 0 0 0 0 0 0 11
35 -2.2018 0.0035 -0.8763 O 0 0 0 0 0 0 0 0 0 0 0 12
36 -2.0409 0.0105 1.3789 O 0 0 0 0 0 0 0 0 0 0 0 13
37 2.4759 -0.0140 -2.2452 H 0 0 0 0 0 0 0 0 0 0 0 14
38 -0.0063 -0.0023 -2.0561 H 0 0 0 0 0 0 0 0 0 0 0 15
39 0.3049 -0.0102 2.2256 H 0 0 0 0 0 0 0 0 0 0 0 16
40 2.7898 -0.0229 2.0541 H 0 0 0 0 0 0 0 0 0 0 0 17
41 4.6974 1.0536 -0.2087 H 0 0 0 0 0 0 0 0 0 0 0 18
42 4.6670 -0.4457 -1.1533 H 0 0 0 0 0 0 0 0 0 0 0 19
43 4.7956 -0.5065 0.6251 H 0 0 0 0 0 0 0 0 0 0 0 20

2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
14 4 0 0 0 0 0
6 5 0 0 0 0 0
15 5 0 0 0 0 0
7 6 0 0 0 0 0
11 6 0 0 0 0 0
8 7 0 0 0 0 0
16 7 0 0 0 0 0
9 8 0 0 0 0 0
17 8 0 0 0 0 0
10 9 0 0 0 0 0
18 10 0 0 0 0 0
19 10 0 0 0 0 0
12 11 0 0 0 0 0
13 11 0 0 0 0 0
10 20 0 0 0 0 0

M END

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4-methylbenzoicacid.sdf

COSMOtherm

3D

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21 20 0 0 0 0 0 0 0 0 0 0 V2000
51 -4.7971 -0.0001 0.5584 O 0 0 0 0 0 0 0 0 0 0 0 1
52 -5.1508 -0.5968 -0.1265 H 0 0 0 0 0 0 0 0 0 0 0 2
53 -5.1632 0.8752 0.3345 H 0 0 0 0 0 0 0 0 0 0 0 3
54 2.2418 -0.0039 -1.1225 C 0 0 0 0 0 0 0 0 0 0 0 4
55 0.8563 -0.0021 -1.2745 C 0 0 0 0 0 0 0 0 0 0 0 5
56 0.0160 -0.0045 -0.1475 C 0 0 0 0 0 0 0 0 0 0 0 6
57 0.5959 -0.0117 1.1337 C 0 0 0 0 0 0 0 0 0 0 0 7
58 1.9835 -0.0135 1.2771 C 0 0 0 0 0 0 0 0 0 0 0 8
59 2.8320 -0.0059 0.1550 C 0 0 0 0 0 0 0 0 0 0 0 9
60 4.3299 0.0253 0.3160 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.4611 -0.0036 -0.3509 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.9938 0.0018 -1.4629 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.1638 -0.0096 0.7953 O 0 0 0 0 0 0 0 0 0 0 0 13
2.8801 -0.0064 -2.0089 H 0 0 0 0 0 0 0 0 0 0 0 14
0.4095 -0.0019 -2.2697 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.0425 -0.0190 2.0172 H 0 0 0 0 0 0 0 0 0 0 0 16
2.4192 -0.0234 2.2788 H 0 0 0 0 0 0 0 0 0 0 0 17
4.6910 1.0655 0.3694 H 0 0 0 0 0 0 0 0 0 0 0 18
4.8352 -0.4524 -0.5344 H 0 0 0 0 0 0 0 0 0 0 0 19
4.6452 -0.4767 1.2411 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.1638 -0.0022 0.5934 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0

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9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
18 10 0 0 0 0
19 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
13 21 0 0 0 0
M END
$$$$
4-nitrobenzoicacid-anion.sdf
COSMOtherm 3D 0
19 18 0 0 0 0 0 0 0 0 0 V2000
-5.6415 -0.5179 0.0209 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6376 -0.6212 0.0045 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.7662 0.4459 0.0639 H 0 0 0 0 0 0 0 0 0 0 0 3
1.3619 1.2328 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.0295 1.3012 -0.0031 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8095 0.1322 -0.0052 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1703 -1.1193 -0.0037 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2201 -1.2111 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9675 -0.0283 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.3382 0.2317 -0.0098 C 0 0 0 0 0 0 0 0 0 0 0 10
3.4386 -0.1138 0.0040 N 0 0 0 0 0 0 0 0 0 0 0 11
3.9644 -1.2394 -0.0060 O 0 0 0 0 0 0 0 0 0 0 0 12
4.0914 0.9432 0.0158 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.8476 1.3843 -0.0143 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.9741 -0.8772 -0.0085 O 0 0 0 0 0 0 0 0 0 0 0 15
1.9724 2.1344 0.0024 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.5329 2.2682 -0.0045 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.7794 -2.0232 -0.0049 H 0 0 0 0 0 0 0 0 0 0 0 18
1.7232 -2.1767 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
8 19 0 0 0 0
M END
$$$$
4-nitrobenzoicacid.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-5.5407 -0.0020 0.6619 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.9135 -0.7433 0.1502 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.9294 0.7980 0.2629 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4079 0.0006 -1.2406 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0196 -0.0005 -1.3452 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7809 -0.0009 -0.1902 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1792 -0.0011 1.0800 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2088 -0.0015 1.1995 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9787 -0.0001 0.0349 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.2749 -0.0010 -0.3541 C 0 0 0 0 0 0 0 0 0 0 0 10
3.4541 0.0006 0.1569 N 0 0 0 0 0 0 0 0 0 0 0 11
3.9459 -0.0139 1.2956 O 0 0 0 0 0 0 0 0 0 0 0 12
4.1284 0.0154 -0.8831 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.8217 -0.0128 -1.4563 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.9330 0.0123 0.8087 O 0 0 0 0 0 0 0 0 0 0 0 15
2.0395 0.0013 -2.1268 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4560 -0.0013 -2.3257 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.7974 -0.0016 1.9763 H 0 0 0 0 0 0 0 0 0 0 0 18
1.6891 -0.0021 2.1762 H 0 0 0 0 0 0 0 0 0 0 0 19
-3.9486 0.0102 0.6539 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 20 0 0 0 0

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3 M END
4 $$$$
5 4-phenylbenzoicacid-anion.sdf
6 COSMOtherm 3D 0
7
8 27 27 0 0 0 0 0 0 0 0 V2000
9 -6.5743 -0.5328 0.1106 O 0 0 0 0 0 0 0 0 0 0 0 1
10 -5.5690 -0.6498 0.1330 H 0 0 0 0 0 0 0 0 0 0 0 2
11 -6.6786 0.4219 -0.0456 H 0 0 0 0 0 0 0 0 0 0 0 3
12 0.2947 -1.1218 0.2705 C 0 0 0 0 0 0 0 0 0 0 0 4
13 -1.1000 -1.0705 0.2601 C 0 0 0 0 0 0 0 0 0 0 0 5
14 -1.7763 0.1270 -0.0248 C 0 0 0 0 0 0 0 0 0 0 0 6
15 -1.0126 1.2724 -0.3025 C 0 0 0 0 0 0 0 0 0 0 0 7
16 0.3817 1.2247 -0.2965 C 0 0 0 0 0 0 0 0 0 0 0 8
17 1.0659 0.0256 -0.0083 C 0 0 0 0 0 0 0 0 0 0 0 9
18 2.5498 -0.0258 0.0026 C 0 0 0 0 0 0 0 0 0 0 0 10
19 -3.2989 0.1926 -0.0367 C 0 0 0 0 0 0 0 0 0 0 0 11
20 4.7068 1.0302 0.4516 C 0 0 0 0 0 0 0 0 0 0 0 12
21 3.3101 1.0782 0.4404 C 0 0 0 0 0 0 0 0 0 0 0 13
22 3.2396 -1.1794 -0.4235 C 0 0 0 0 0 0 0 0 0 0 0 14
23 4.6364 -1.2270 -0.4124 C 0 0 0 0 0 0 0 0 0 0 0 15
24 5.3774 -0.1225 0.0250 C 0 0 0 0 0 0 0 0 0 0 0 16
25 -3.9215 -0.9059 0.1851 O 0 0 0 0 0 0 0 0 0 0 0 17
26 -3.8434 1.3098 -0.2616 O 0 0 0 0 0 0 0 0 0 0 0 18
27 0.7935 -2.0604 0.5197 H 0 0 0 0 0 0 0 0 0 0 0 19
28 -1.6848 -1.9640 0.4840 H 0 0 0 0 0 0 0 0 0 0 0 20
29 -1.5319 2.2042 -0.5326 H 0 0 0 0 0 0 0 0 0 0 0 21
30 0.9488 2.1253 -0.5402 H 0 0 0 0 0 0 0 0 0 0 0 22
31 5.2737 1.8947 0.8027 H 0 0 0 0 0 0 0 0 0 0 0 23
32 2.8024 1.9764 0.7968 H 0 0 0 0 0 0 0 0 0 0 0 24
33 2.6774 -2.0410 -0.7885 H 0 0 0 0 0 0 0 0 0 0 0 25
34 5.1484 -2.1284 -0.7551 H 0 0 0 0 0 0 0 0 0 0 0 26
35 6.4681 -0.1598 0.0338 H 0 0 0 0 0 0 0 0 0 0 0 27
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37 2 1 0 0 0 0
38 3 1 0 0 0 0
39 5 4 0 0 0 0
40 9 4 0 0 0 0
41 19 4 0 0 0 0
42 6 5 0 0 0 0
43 20 5 0 0 0 0
44 7 6 0 0 0 0
45 11 6 0 0 0 0
46 8 7 0 0 0 0
47 21 7 0 0 0 0
48 9 8 0 0 0 0
49 22 8 0 0 0 0
50 10 9 0 0 0 0
51 13 10 0 0 0 0
52 14 10 0 0 0 0
53 17 11 0 0 0 0
54 18 11 0 0 0 0
55 13 12 0 0 0 0
56 16 12 0 0 0 0
57 23 12 0 0 0 0
58 24 13 0 0 0 0
59 15 14 0 0 0 0
60 25 14 0 0 0 0
61 16 15 0 0 0 0
62 26 15 0 0 0 0
63 16 27 0 0 0 0
64 M END
65 $$$$
66 4-phenylbenzoicacid.sdf
67 COSMOtherm 3D 0
68
69 28 28 0 0 0 0 0 0 0 0 V2000
70 -6.5044 0.1720 0.7282 O 0 0 0 0 0 0 0 0 0 0 0 1
71 -6.8950 -0.5998 0.2785 H 0 0 0 0 0 0 0 0 0 0 0 2
72 -6.8750 0.9425 0.2595 H 0 0 0 0 0 0 0 0 0 0 0 3
73 0.4280 -0.2856 -1.2613 C 0 0 0 0 0 0 0 0 0 0 0 4
74 -0.9619 -0.3002 -1.3367 C 0 0 0 0 0 0 0 0 0 0 0 5
75 -1.7418 -0.0461 -0.1956 C 0 0 0 0 0 0 0 0 0 0 0 6
76 -1.0959 0.2227 1.0242 C 0 0 0 0 0 0 0 0 0 0 0 7
77 0.2956 0.2381 1.0963 C 0 0 0 0 0 0 0 0 0 0 0 8
78 1.0870 -0.0157 -0.0431 C 0 0 0 0 0 0 0 0 0 0 0 9
79 2.5686 0.0034 0.0356 C 0 0 0 0 0 0 0 0 0 0 0 10
80 -3.2284 -0.0708 -0.3186 C 0 0 0 0 0 0 0 0 0 0 0 11
81 4.6331 -0.4140 1.2702 C 0 0 0 0 0 0 0 0 0 0 0 12
82 3.2379 -0.4333 1.1970 C 0 0 0 0 0 0 0 0 0 0 0 13
83 3.3441 0.4617 -1.0490 C 0 0 0 0 0 0 0 0 0 0 0 14
84 4.7391 0.4835 -0.9735 C 0 0 0 0 0 0 0 0 0 0 0 15
85 5.3903 0.0451 0.1858 C 0 0 0 0 0 0 0 0 0 0 0 16
86 -3.8156 -0.2927 -1.3794 O 0 0 0 0 0 0 0 0 0 0 0 17
87 -3.8687 0.1710 0.8372 O 0 0 0 0 0 0 0 0 0 0 0 18
88 1.0121 -0.5087 -2.1554 H 0 0 0 0 0 0 0 0 0 0 0 19
89 -1.4595 -0.5176 -2.2827 H 0 0 0 0 0 0 0 0 0 0 0 20
90 -1.6870 0.4300 1.9161 H 0 0 0 0 0 0 0 0 0 0 0 21
91 0.7757 0.4721 2.0475 H 0 0 0 0 0 0 0 0 0 0 0 22
92 5.1314 -0.7657 2.1755 H 0 0 0 0 0 0 0 0 0 0 0 23
93 2.6627 -0.8143 2.0427 H 0 0 0 0 0 0 0 0 0 0 0 24
94 2.8509 0.8270 -1.9515 H 0 0 0 0 0 0 0 0 0 0 0 25
95 5.3197 0.8513 -1.8216 H 0 0 0 0 0 0 0 0 0 0 0 26
96 6.4800 0.0614 0.2437 H 0 0 0 0 0 0 0 0 0 0 0 27
97 -4.8789 0.1482 0.6895 H 0 0 0 0 0 0 0 0 0 0 0 28
98
99 2 1 0 0 0 0
100 3 1 0 0 0 0
101 5 4 0 0 0 0
102 9 4 0 0 0 0
103 19 4 0 0 0 0
104 6 5 0 0 0 0
105 20 5 0 0 0 0
106 7 6 0 0 0 0
107 11 6 0 0 0 0
108 8 7 0 0 0 0
109 21 7 0 0 0 0
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9 8 0 0 0 0
22 8 0 0 0 0
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14 10 0 0 0 0
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13 12 0 0 0 0
16 12 0 0 0 0
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24 13 0 0 0 0
15 14 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
27 16 0 0 0 0
18 28 0 0 0 0
M END
$$$$
4-propylbenzoicacid-anion.sdf
COSMOtherm 3D 0
26 25 0 0 0 0 0 0 0 0 0 V2000
-5.7020 -0.5127 -0.3680 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.7038 -0.6446 -0.2546 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.7914 0.4562 -0.3789 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1159 -1.1666 0.4314 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2712 -1.1110 0.2686 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9299 0.1220 0.1300 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1592 1.2961 0.1605 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2270 1.2389 0.3232 C 0 0 0 0 0 0 0 0 0 0 0 8
1.8915 0.0066 0.4601 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.4411 0.1957 -0.0461 C 0 0 0 0 0 0 0 0 0 0 0 10
3.3957 -0.0548 0.5926 C 0 0 0 0 0 0 0 0 0 0 0 11
4.1186 -0.1361 -0.7698 C 0 0 0 0 0 0 0 0 0 0 0 12
5.6431 -0.1853 -0.6268 C 0 0 0 0 0 0 0 0 0 0 0 13
-3.0744 -0.9198 -0.0568 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.9718 1.3357 -0.1705 O 0 0 0 0 0 0 0 0 0 0 0 15
1.6079 -2.1368 0.5434 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.8633 -2.0277 0.2522 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.6670 2.2570 0.0594 H 0 0 0 0 0 0 0 0 0 0 0 18
1.8065 2.1659 0.3499 H 0 0 0 0 0 0 0 0 0 0 0 19
3.6785 -0.9315 1.1980 H 0 0 0 0 0 0 0 0 0 0 0 20
3.7545 0.8375 1.1318 H 0 0 0 0 0 0 0 0 0 0 0 21
3.8284 0.7339 -1.3818 H 0 0 0 0 0 0 0 0 0 0 0 22
3.7641 -1.0290 -1.3110 H 0 0 0 0 0 0 0 0 0 0 0 23
6.1340 -0.2457 -1.6093 H 0 0 0 0 0 0 0 0 0 0 0 24
5.9584 -1.0614 -0.0389 H 0 0 0 0 0 0 0 0 0 0 0 25
6.0228 0.7136 -0.1166 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
13 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
24 13 0 0 0 0
25 13 0 0 0 0
13 26 0 0 0 0
M END
$$$$
4-propylbenzoicacid.sdf
COSMOtherm 3D 0
27 26 0 0 0 0 0 0 0 0 0 V2000
-5.6453 0.3270 0.7304 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.0872 -0.1804 0.0252 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.9236 1.2491 0.5807 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2758 -0.2745 -1.2812 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.1064 -0.1119 -1.3632 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8948 -0.1287 -0.1989 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2679 -0.3134 1.0468 C 0 0 0 0 0 0 0 0 0 0 0 7
1.1159 -0.4760 1.1194 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9129 -0.4583 -0.0401 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.3706 0.0480 -0.3268 C 0 0 0 0 0 0 0 0 0 0 0 10
3.4143 -0.5915 0.0487 C 0 0 0 0 0 0 0 0 0 0 0 11
4.1272 0.7661 0.2392 C 0 0 0 0 0 0 0 0 0 0 0 12
5.6502 0.6228 0.3234 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.9425 0.2113 -1.4071 O 0 0 0 0 0 0 0 0 0 0 0 14
-3.0231 0.0160 0.8479 O 0 0 0 0 0 0 0 0 0 0 0 15
1.8742 -0.2637 -2.1954 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.5911 0.0269 -2.3307 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.8678 -0.3352 1.9568 H 0 0 0 0 0 0 0 0 0 0 0 18
1.5884 -0.6252 2.0932 H 0 0 0 0 0 0 0 0 0 0 0 19
3.7960 -1.0688 -0.8684 H 0 0 0 0 0 0 0 0 0 0 0 20
3.6764 -1.2520 0.8910 H 0 0 0 0 0 0 0 0 0 0 0 21
3.7449 1.2467 1.1546 H 0 0 0 0 0 0 0 0 0 0 0 22
3.8596 1.4322 -0.5976 H 0 0 0 0 0 0 0 0 0 0 0 23
6.1340 1.6013 0.4595 H 0 0 0 0 0 0 0 0 0 0 0 24
6.0579 0.1713 -0.5944 H 0 0 0 0 0 0 0 0 0 0 0 25
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-4.6243 -0.0037 0.6635 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
19 4 0 0 0 0
6 5 0 0 0 0
20 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
11 9 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
17 14 0 0 0 0
18 14 0 0 0 0
16 23 0 0 0 0
M END
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4-trifluoromethylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
20 19 0 0 0 0 0 0 0 0 V2000
-6.0797 0.1181 -0.5241 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.0772 0.0488 -0.6318 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.1950 0.1881 0.4394 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7776 -0.0617 -1.1867 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6162 -0.0650 -1.1082 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2661 -0.0501 0.1353 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4918 -0.0410 1.3063 C 0 0 0 0 0 0 0 0 0 0 0 7
0.9017 -0.0385 1.2425 C 0 0 0 0 0 0 0 0 0 0 0 8
1.5367 -0.0507 -0.0082 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.7936 -0.0374 0.2241 C 0 0 0 0 0 0 0 0 0 0 0 10
3.0371 0.0168 -0.0790 C 0 0 0 0 0 0 0 0 0 0 0 11
3.4994 1.3112 -0.0054 F 0 0 0 0 0 0 0 0 0 0 0 12
3.5364 -0.4979 -1.2398 F 0 0 0 0 0 0 0 0 0 0 0 13
3.6437 -0.6567 0.9438 F 0 0 0 0 0 0 0 0 0 0 0 14
-3.4255 -0.0532 -0.8883 O 0 0 0 0 0 0 0 0 0 0 0 15
-3.3152 -0.0062 1.3715 O 0 0 0 0 0 0 0 0 0 0 0 16
1.2703 -0.0725 -2.1594 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.2173 -0.0769 -2.0180 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.0000 -0.0334 2.2712 H 0 0 0 0 0 0 0 0 0 0 0 19
1.4908 -0.0321 2.1605 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
8 20 0 0 0 0
M END
$$$$

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4-trifluoromethylbenzoicacid.sdf
COSMOTHERM 3D 0
21 20 0 0 0 0 0 0 0 0 V2000
-5.9974 -0.0471 0.6916 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.3554 -0.6547 0.0185 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.4122 0.8128 0.4942 H 0 0 0 0 0 0 0 0 0 0 0 3
0.9466 -0.0139 -1.2686 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.4439 0.0034 -1.3630 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2347 0.0122 -0.2033 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6179 0.0078 1.0585 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7727 -0.0098 1.1594 C 0 0 0 0 0 0 0 0 0 0 0 8
1.5526 -0.0276 -0.0050 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.7271 0.0163 -0.3528 C 0 0 0 0 0 0 0 0 0 0 0 10
3.0555 -0.0101 0.1095 C 0 0 0 0 0 0 0 0 0 0 0 11
3.5457 1.2688 0.2102 F 0 0 0 0 0 0 0 0 0 0 0 12
3.6705 -0.5734 -0.9690 F 0 0 0 0 0 0 0 0 0 0 0 13
3.5009 -0.6780 1.2135 F 0 0 0 0 0 0 0 0 0 0 0 14
-3.2895 0.0095 -1.4472 O 0 0 0 0 0 0 0 0 0 0 0 15
-3.3776 0.0238 0.8171 O 0 0 0 0 0 0 0 0 0 0 0 16
1.5531 -0.0258 -2.1741 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.9280 0.0067 -2.3397 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.2257 0.0140 1.9622 H 0 0 0 0 0 0 0 0 0 0 0 19
1.2454 -0.0189 2.1416 H 0 0 0 0 0 0 0 0 0 0 0 20
-4.3908 0.0115 0.6638 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0

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19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
11 9 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 11 0 0 0 0
16 21 0 0 0 0

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M END

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5-fluorouracil-anion.sdf
COSMOtherm 3D 0

```

14 13 0 0 0 0 0 0 0 0 0 V2000
-3.7914 -0.0069 1.1967 O 0 0 0 0 0 0 0 0 0 0 1
-2.8562 -0.0079 0.8114 H 0 0 0 0 0 0 0 0 0 0 2
-3.8603 0.8454 1.6602 H 0 0 0 0 0 0 0 0 0 0 3
-0.8644 -0.0147 -1.0683 C 0 0 0 0 0 0 0 0 0 0 4
0.5086 0.0094 -1.3888 N 0 0 0 0 0 0 0 0 0 0 5
1.5883 0.0140 -0.4990 C 0 0 0 0 0 0 0 0 0 0 6
1.1375 -0.0099 0.8625 C 0 0 0 0 0 0 0 0 0 0 7
-0.1977 -0.0327 1.1750 C 0 0 0 0 0 0 0 0 0 0 8
-1.1971 -0.0363 0.2569 N 0 0 0 0 0 0 0 0 0 0 9
2.7708 0.0376 -0.9005 O 0 0 0 0 0 0 0 0 0 0 10
-1.7027 -0.0159 -1.9974 O 0 0 0 0 0 0 0 0 0 0 11
2.0927 -0.0084 1.8472 F 0 0 0 0 0 0 0 0 0 0 12
0.7423 0.0263 -2.3830 H 0 0 0 0 0 0 0 0 0 0 13
-0.5009 -0.0510 2.2264 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
8 14 0 0 0 0

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M END

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5-fluorouracil.sdf
COSMOtherm 3D 0

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15 14 0 0 0 0 0 0 0 0 0 V2000
-1.2340 0.0219 3.7206 O 0 0 0 0 0 0 0 0 0 0 1
-0.8340 0.6890 4.3072 H 0 0 0 0 0 0 0 0 0 0 2
-1.1409 -0.8176 4.2069 H 0 0 0 0 0 0 0 0 0 0 3
1.1142 -0.0050 0.8419 C 0 0 0 0 0 0 0 0 0 0 4
1.4045 -0.0013 -0.5219 N 0 0 0 0 0 0 0 0 0 0 5
0.5056 0.0030 -1.5989 C 0 0 0 0 0 0 0 0 0 0 6
-0.8758 -0.0010 -1.1588 C 0 0 0 0 0 0 0 0 0 0 7
-1.2090 -0.0079 0.1562 C 0 0 0 0 0 0 0 0 0 0 8
-0.2397 -0.0075 1.1251 N 0 0 0 0 0 0 0 0 0 0 9
0.8947 0.0095 -2.7726 O 0 0 0 0 0 0 0 0 0 0 10
1.9914 -0.0058 1.7094 O 0 0 0 0 0 0 0 0 0 0 11
-1.8316 -0.0002 -2.1210 F 0 0 0 0 0 0 0 0 0 0 12
2.3973 0.0022 -0.7627 H 0 0 0 0 0 0 0 0 0 0 13
-0.5272 -0.0134 2.1334 H 0 0 0 0 0 0 0 0 0 0 14
-2.2433 -0.0115 0.4971 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
14 9 0 0 0 0
8 15 0 0 0 0

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M END

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5-iodo-2-hydroxybenzoicacid-anion.sdf
COSMOtherm 3D 0

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18 17 0 0 0 0 0 0 0 0 0 V2000
-5.3732 -2.8086 -0.0218 O 0 0 0 0 0 0 0 0 0 0 1
-4.4985 -2.3172 -0.0058 H 0 0 0 0 0 0 0 0 0 0 2
-6.0372 -2.0980 -0.0292 H 0 0 0 0 0 0 0 0 0 0 3
0.7179 0.5374 -0.0010 C 0 0 0 0 0 0 0 0 0 0 4
-0.4627 -0.1969 0.0064 C 0 0 0 0 0 0 0 0 0 0 5
-1.7019 0.4646 0.0059 C 0 0 0 0 0 0 0 0 0 0 6
-1.7333 1.8869 -0.0014 C 0 0 0 0 0 0 0 0 0 0 7
-0.5233 2.6072 -0.0092 C 0 0 0 0 0 0 0 0 0 0 8
0.6996 1.9392 -0.0089 C 0 0 0 0 0 0 0 0 0 0 9
-2.9892 -0.3207 0.0117 C 0 0 0 0 0 0 0 0 0 0 10
-4.0798 0.3698 0.0094 O 0 0 0 0 0 0 0 0 0 0 11
-2.9465 -1.5835 0.0167 O 0 0 0 0 0 0 0 0 0 0 12
-2.9075 2.5520 -0.0010 O 0 0 0 0 0 0 0 0 0 0 13
2.6046 -0.4874 -0.0003 I 0 0 0 0 0 0 0 0 0 0 14
-3.6118 1.7662 0.0031 H 0 0 0 0 0 0 0 0 0 0 15
-0.4624 -1.2870 0.0122 H 0 0 0 0 0 0 0 0 0 0 16
-0.5538 3.6982 -0.0151 H 0 0 0 0 0 0 0 0 0 0 17
1.6265 2.5128 -0.0150 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0

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9 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
15 11 0 0 0 0
15 13 0 0 0 0
9 18 0 0 0 0
M END
$$$$
5-iodo-2-hydroxybenzoicacid.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-5.1021 -0.0135 2.8996 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.6507 -0.8081 2.7647 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.7034 0.7365 2.7364 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7187 -0.0011 -0.5470 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.4667 0.0039 0.1734 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.7013 0.0036 -0.5080 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.7171 -0.0018 -1.9302 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.4997 -0.0073 -2.6339 C 0 0 0 0 0 0 0 0 0 0 0 8
0.7118 -0.0070 -1.9508 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.9839 0.0084 0.2238 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.8886 0.0108 1.5470 O 0 0 0 0 0 0 0 0 0 0 0 11
-4.0818 0.0099 -0.3746 O 0 0 0 0 0 0 0 0 0 0 0 12
-2.8701 -0.0021 -2.6345 O 0 0 0 0 0 0 0 0 0 0 0 13
2.5899 0.0001 0.4931 I 0 0 0 0 0 0 0 0 0 0 0 14
-3.8208 0.0078 1.9903 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.6073 0.0033 -1.9405 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4686 0.0083 1.2621 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.5186 -0.0117 -3.7244 H 0 0 0 0 0 0 0 0 0 0 0 18
1.6448 -0.0113 -2.5141 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
15 11 0 0 0 0
16 13 0 0 0 0
9 19 0 0 0 0
M END
$$$$
5-nitrouracil-anion.sdf
COSMOTHERM 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.7511 -0.1078 -2.0922 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.9974 -0.0414 -1.4342 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.9499 0.8161 -2.3221 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3357 0.0270 -0.9117 C 0 0 0 0 0 0 0 0 0 0 0 4
0.8822 0.0047 -0.2132 C 0 0 0 0 0 0 0 0 0 0 0 5
0.8708 -0.0123 1.2434 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4431 -0.0018 1.7386 N 0 0 0 0 0 0 0 0 0 0 0 7
-1.6402 0.0194 1.0183 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.5436 0.0315 -0.3659 N 0 0 0 0 0 0 0 0 0 0 0 9
1.8200 -0.0332 2.0364 O 0 0 0 0 0 0 0 0 0 0 0 10
-2.7273 0.0260 1.6124 O 0 0 0 0 0 0 0 0 0 0 0 11
2.0948 0.0037 -0.9617 N 0 0 0 0 0 0 0 0 0 0 0 12
-0.2947 0.0368 -2.0035 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5268 -0.0119 2.7569 H 0 0 0 0 0 0 0 0 0 0 0 14
2.0286 0.0234 -2.2196 O 0 0 0 0 0 0 0 0 0 0 0 15
3.1919 -0.0171 -0.3610 O 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 12 0 0 0 0
12 16 0 0 0 0
M END
$$$$
5-nitrouracil.sdf
COSMOTHERM 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-2.1028 -3.5784 0.0025 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.9729 -4.2456 0.7011 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.1392 -4.0909 -0.8260 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.9333 -0.2794 0.0012 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2068 0.8915 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2588 0.8513 0.0034 C 0 0 0 0 0 0 0 0 0 0 0 6

```

1
2
3 1.7454 -0.4734 0.0026 N 0 0 0 0 0 0 0 0 0 0 0 7
4 1.0389 -1.6627 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 8
5 -0.3519 -1.4871 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 9
6 2.0529 1.7877 0.0077 O 0 0 0 0 0 0 0 0 0 0 0 10
7 1.5625 -2.7712 -0.0031 O 0 0 0 0 0 0 0 0 0 0 0 11
8 -0.9426 2.1350 -0.0010 N 0 0 0 0 0 0 0 0 0 0 0 12
9 -2.0222 -0.2597 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 13
10 2.7635 -0.5629 0.0041 H 0 0 0 0 0 0 0 0 0 0 0 14
11 -0.9569 -2.3559 -0.0023 H 0 0 0 0 0 0 0 0 0 0 0 15
12 -2.1912 2.0799 0.0207 O 0 0 0 0 0 0 0 0 0 0 0 16
13 -0.3125 3.2043 -0.0258 O 0 0 0 0 0 0 0 0 0 0 0 17
14 2 1 0 0 0 0
15 3 1 0 0 0 0
16 5 4 0 0 0 0
17 9 4 0 0 0 0
18 13 4 0 0 0 0
19 6 5 0 0 0 0
20 12 5 0 0 0 0
21 7 6 0 0 0 0
22 10 6 0 0 0 0
23 8 7 0 0 0 0
24 14 7 0 0 0 0
25 9 8 0 0 0 0
26 11 8 0 0 0 0
27 15 9 0 0 0 0
28 16 12 0 0 0 0
29 12 17 0 0 0 0
30 M END
31 \$\$\$
32 aceticacid-anion.sdf
33 COSMOTHERM 3D 0
34 10 8 0 0 0 0 0 0 0 0 0 V2000
35 -2.6444 -0.0635 -0.0058 O 0 0 0 0 0 0 0 0 0 0 0 1
36 -1.6798 -0.3817 0.0017 H 0 0 0 0 0 0 0 0 0 0 0 2
37 -2.5492 0.9048 -0.0039 H 0 0 0 0 0 0 0 0 0 0 0 3
38 2.1955 -0.3112 -0.0073 C 0 0 0 0 0 0 0 0 0 0 0 4
39 0.7003 0.0343 0.0054 C 0 0 0 0 0 0 0 0 0 0 0 5
40 -0.1274 -0.9468 0.0074 O 0 0 0 0 0 0 0 0 0 0 0 6
41 0.3779 1.2565 0.0033 O 0 0 0 0 0 0 0 0 0 0 0 7
42 2.3728 -1.3892 0.0936 H 0 0 0 0 0 0 0 0 0 0 0 8
43 2.6397 0.0363 -0.9527 H 0 0 0 0 0 0 0 0 0 0 0 9
44 2.7089 0.2225 0.8058 H 0 0 0 0 0 0 0 0 0 0 0 10
45 2 1 0 0 0 0
46 3 1 0 0 0 0
47 5 4 0 0 0 0
48 8 4 0 0 0 0
49 9 4 0 0 0 0
50 6 5 0 0 0 0
51 7 5 0 0 0 0
52 4 10 0 0 0 0
53 M END
54 \$\$\$
55 aceticacid.sdf
56 COSMOTHERM 3D 0
57 11 9 0 0 0 0 0 0 0 0 0 V2000
58 -2.6632 -0.0231 0.0932 O 0 0 0 0 0 0 0 0 0 0 0 1
59 -2.8339 -0.5955 -0.6771 H 0 0 0 0 0 0 0 0 0 0 0 2
60 -2.9948 0.8534 -0.1753 H 0 0 0 0 0 0 0 0 0 0 0 3
1 2.2026 -0.0055 0.4247 C 0 0 0 0 0 0 0 0 0 0 0 4
2 0.7914 0.0037 -0.1040 C 0 0 0 0 0 0 0 0 0 0 0 5
3 0.4952 0.0091 -1.2971 O 0 0 0 0 0 0 0 0 0 0 0 6
4 -0.1272 0.0009 0.8789 O 0 0 0 0 0 0 0 0 0 0 0 7
5 2.9163 0.0324 -0.4042 H 0 0 0 0 0 0 0 0 0 0 0 8
6 2.3613 0.8523 1.0931 H 0 0 0 0 0 0 0 0 0 0 0 9
7 2.3721 -0.9165 1.0166 H 0 0 0 0 0 0 0 0 0 0 0 10
8 -1.0668 0.0031 0.4835 H 0 0 0 0 0 0 0 0 0 0 0 11
9 2 1 0 0 0 0
10 3 1 0 0 0 0
11 5 4 0 0 0 0
12 8 4 0 0 0 0
13 9 4 0 0 0 0
14 10 4 0 0 0 0
15 6 5 0 0 0 0
16 7 5 0 0 0 0
17 7 11 0 0 0 0
18 M END
19 \$\$\$
20 acrylicacid-anion.sdf
21 COSMOTHERM 3D 0
22 11 9 0 0 0 0 0 0 0 0 0 V2000
23 -3.0979 0.0891 -0.0036 O 0 0 0 0 0 0 0 0 0 0 0 1
24 -2.1603 -0.2967 -0.0023 H 0 0 0 0 0 0 0 0 0 0 0 2
25 -2.9385 1.0483 0.0325 H 0 0 0 0 0 0 0 0 0 0 0 3
26 2.7509 0.2383 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 4
27 1.6817 -0.5680 -0.0029 C 0 0 0 0 0 0 0 0 0 0 0 5
28 0.2534 -0.0659 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 6
29 -0.6462 -0.9855 0.0038 O 0 0 0 0 0 0 0 0 0 0 0 7
30 0.0309 1.1766 -0.0002 O 0 0 0 0 0 0 0 0 0 0 0 8
31 3.7696 -0.1553 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
32 2.6250 1.3241 0.0036 H 0 0 0 0 0 0 0 0 0 0 0 10
33 1.8040 -1.6556 -0.0048 H 0 0 0 0 0 0 0 0 0 0 0 11
34 2 1 0 0 0 0
35 3 1 0 0 0 0
36 5 4 0 0 0 0
37 9 4 0 0 0 0
38 10 4 0 0 0 0
39 6 5 0 0 0 0
40 7 6 0 0 0 0
41 8 6 0 0 0 0
42 5 11 0 0 0 0
43 M END
44 \$\$\$


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1
2
3     -3.4957   0.5498   0.1903 C   0 0 0 0 0 0 0 0 0 0 0 9
4     0.2475   0.2296  -0.1203 C   0 0 0 0 0 0 0 0 0 0 0 10
5     0.4198  -1.1739  -0.0612 C   0 0 0 0 0 0 0 0 0 0 0 11
6    -0.7518  -2.0202   0.0659 C   0 0 0 0 0 0 0 0 0 0 0 12
7    -2.0222  -1.4329   0.1473 C   0 0 0 0 0 0 0 0 0 0 0 13
8     1.6997  -1.8098  -0.1587 C   0 0 0 0 0 0 0 0 0 0 0 14
9     1.8169  -3.1805  -0.1199 C   0 0 0 0 0 0 0 0 0 0 0 15
10    0.6649  -4.0084   0.0156 C   0 0 0 0 0 0 0 0 0 0 0 16
11   -0.5839  -3.4409   0.1059 C   0 0 0 0 0 0 0 0 0 0 0 17
12    1.4459   1.1228  -0.3038 C   0 0 0 0 0 0 0 0 0 0 0 18
13    1.6481   1.7697  -1.3289 O   0 0 0 0 0 0 0 0 0 0 0 19
14    2.2564   1.1426   0.7607 O   0 0 0 0 0 0 0 0 0 0 0 20
15   -4.6518   2.3548   0.2201 H   0 0 0 0 0 0 0 0 0 0 0 21
16   -2.6579   3.8450  -0.0208 H   0 0 0 0 0 0 0 0 0 0 0 22
17   -0.3971   2.9015  -0.1962 H   0 0 0 0 0 0 0 0 0 0 0 23
18   -4.3596  -0.1095   0.3003 H   0 0 0 0 0 0 0 0 0 0 0 24
19   -2.9001  -2.0758   0.2510 H   0 0 0 0 0 0 0 0 0 0 0 25
20    2.5964  -1.1976  -0.2607 H   0 0 0 0 0 0 0 0 0 0 0 26
21    2.8032  -3.6418  -0.1961 H   0 0 0 0 0 0 0 0 0 0 0 27
22    0.7809  -5.0931   0.0456 H   0 0 0 0 0 0 0 0 0 0 0 28
23   -1.4742  -4.0657   0.2046 H   0 0 0 0 0 0 0 0 0 0 0 29
24    3.0615   1.7588   0.5926 H   0 0 0 0 0 0 0 0 0 0 0 30

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25  2 1 0 0 0 0
26  3 1 0 0 0 0
27  5 4 0 0 0 0
28  9 4 0 0 0 0
29 21 4 0 0 0 0
30  6 5 0 0 0 0
31 22 5 0 0 0 0
32  7 6 0 0 0 0
33 23 6 0 0 0 0
34  8 7 0 0 0 0
35 10 7 0 0 0 0
36  9 8 0 0 0 0
37 13 8 0 0 0 0
38 24 9 0 0 0 0
39 11 10 0 0 0 0
40 18 10 0 0 0 0
41 12 11 0 0 0 0
42 14 11 0 0 0 0
43 13 12 0 0 0 0
44 17 12 0 0 0 0
45 25 13 0 0 0 0
46 15 14 0 0 0 0
47 26 14 0 0 0 0
48 16 15 0 0 0 0
49 27 15 0 0 0 0
50 17 16 0 0 0 0
51 28 16 0 0 0 0
52 29 17 0 0 0 0
53 19 18 0 0 0 0
54 20 18 0 0 0 0
55 20 30 0 0 0 0

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M END

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benzoicacid-anion.sdf
COSMOtherm 3D

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56 17 16 0 0 0 0 0 0 0 0 0 0 V2000
57 -4.3945 -0.3391 0.0040 O 0 0 0 0 0 0 0 0 0 0 0 1
58 -3.3979 -0.5181 0.0029 H 0 0 0 0 0 0 0 0 0 0 0 2
59 -4.4394 0.6325 0.0276 H 0 0 0 0 0 0 0 0 0 0 0 3
60  2.4269 -1.3406 0.0020 C 0 0 0 0 0 0 0 0 0 0 0 4
61  1.0343 -1.2087 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
62  0.4357 0.0624 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 6
63  1.2605 1.1998 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 7
64  2.6531 1.0720 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 8
65  3.2403 -0.1999 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 9
66 -1.0830 0.2161 -0.0028 C 0 0 0 0 0 0 0 0 0 0 0 10
67 -1.7684 -0.8670 -0.0060 O 0 0 0 0 0 0 0 0 0 0 0 11
68 -1.5618 1.3847 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 12
69  2.8806 -2.3341 0.0032 H 0 0 0 0 0 0 0 0 0 0 0 13
70  0.3922 -2.0909 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 14
71  0.7902  2.1845 -0.0022 H 0 0 0 0 0 0 0 0 0 0 0 15
72  3.2827  1.9642 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 16
73  4.3274 -0.3020 0.0040 H 0 0 0 0 0 0 0 0 0 0 0 17

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74  2 1 0 0 0 0
75  3 1 0 0 0 0
76  5 4 0 0 0 0
77  9 4 0 0 0 0
78 13 4 0 0 0 0
79  6 5 0 0 0 0
80 14 5 0 0 0 0
81  7 6 0 0 0 0
82 10 6 0 0 0 0
83  8 7 0 0 0 0
84 15 7 0 0 0 0
85  9 8 0 0 0 0
86 16 8 0 0 0 0
87 11 10 0 0 0 0
88 12 10 0 0 0 0
89  9 17 0 0 0 0

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M END

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benzoicacid.sdf
COSMOtherm 3D

0

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90 18 17 0 0 0 0 0 0 0 0 0 0 V2000
91 -4.3632 0.0074 0.4523 O 0 0 0 0 0 0 0 0 0 0 0 1
92 -4.7151 -0.6120 -0.2134 H 0 0 0 0 0 0 0 0 0 0 0 2
93 -4.7170 0.8776 0.1908 H 0 0 0 0 0 0 0 0 0 0 0 3
94  2.3790 0.0004 1.4007 C 0 0 0 0 0 0 0 0 0 0 0 4
95  0.9959 -0.0067 1.2045 C 0 0 0 0 0 0 0 0 0 0 0 5
96  0.4698 -0.0047 -0.0996 C 0 0 0 0 0 0 0 0 0 0 0 6
97  1.3438 0.0046 -1.2005 C 0 0 0 0 0 0 0 0 0 0 0 7

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2.7252 0.0115 -1.0009 C 0 0 0 0 0 0 0 0 0 0 0 8
3.2452 0.0097 0.3002 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.0027 -0.0103 -0.3564 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.7440 -0.0203 0.7627 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.4912 -0.0079 -1.4875 O 0 0 0 0 0 0 0 0 0 0 0 12
2.7831 -0.0019 2.4147 H 0 0 0 0 0 0 0 0 0 0 0 13
0.3209 -0.0140 2.0603 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9271 0.0070 -2.2085 H 0 0 0 0 0 0 0 0 0 0 0 15
3.3987 0.0184 -1.8597 H 0 0 0 0 0 0 0 0 0 0 0 16
4.3258 0.0160 0.4564 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.7390 -0.0141 0.5287 H 0 0 0 0 0 0 0 0 0 0 0 18

```

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
17 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
11 18 0 0 0 0

```

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M END
$$$$
boricacid-anion.sdf
COSMOTHERM 3D 0
9 7 0 0 0 0 0 0 0 0 0 0 V2000
-2.4159 -0.0065 0.0547 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.5369 0.5655 0.0124 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.7885 0.0284 -0.8435 H 0 0 0 0 0 0 0 0 0 0 0 3
0.6613 0.0582 -0.0009 B 0 0 0 0 0 0 0 0 0 0 0 4
2.0833 0.0900 -0.0062 O 0 0 0 0 0 0 0 0 0 0 0 5
-0.1275 1.1357 0.0036 O 0 0 0 0 0 0 0 0 0 0 0 6
0.1863 -1.2824 0.0008 O 0 0 0 0 0 0 0 0 0 0 0 7
2.3755 1.0177 -0.0063 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.7971 -1.2330 0.0077 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
7 9 0 0 0 0

```

```

M END
$$$$
boricacid.sdf
COSMOTHERM 3D 0
10 8 0 0 0 0 0 0 0 0 0 0 V2000
-2.4306 -0.0050 0.0090 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.0005 -0.7952 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0410 0.7542 -0.0043 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7305 0.0020 -0.0050 B 0 0 0 0 0 0 0 0 0 0 0 4
2.1146 -0.0081 -0.0608 O 0 0 0 0 0 0 0 0 0 0 0 5
0.0702 0.0067 -1.2204 O 0 0 0 0 0 0 0 0 0 0 0 6
0.0878 0.0070 1.2223 O 0 0 0 0 0 0 0 0 0 0 0 7
2.5119 -0.0115 0.8275 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.9061 0.0098 -1.0733 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8916 0.0106 1.0956 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
9 6 0 0 0 0
7 10 0 0 0 0

```

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M END
$$$$
bromoaceticacid-anion.sdf
COSMOTHERM 3D 0
10 7 0 0 0 0 0 0 0 0 0 0 V2000
-4.0676 -1.1434 0.0017 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.0911 -0.8958 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5225 -0.2836 0.0048 H 0 0 0 0 0 0 0 0 0 0 0 3
1.7111 -0.2743 0.0014 Br 0 0 0 0 0 0 0 0 0 0 0 4
0.2933 1.1430 -0.0080 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.1640 0.6498 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.9817 1.6113 0.0062 O 0 0 0 0 0 0 0 0 0 0 0 7
-1.4257 -0.5887 -0.0064 O 0 0 0 0 0 0 0 0 0 0 0 8
0.4911 1.7332 -0.9081 H 0 0 0 0 0 0 0 0 0 0 0 9
0.4947 1.7493 0.8803 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0

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M END
$$$$
bromoaceticacid.sdf
COSMOTHERM 3D 0
11 8 0 0 0 0 0 0 0 0 0 0 V2000
-4.4823 0.0128 -0.2467 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6753 -0.7812 -0.7785 H 0 0 0 0 0 0 0 0 0 0 0 2

```

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1
2
3   -4.6437   0.7622  -0.8494 H   0 0 0 0 0 0 0 0 0 0 3
4     1.8363   0.0052  -0.0963 Br  0 0 0 0 0 0 0 0 0 0 4
5     0.1822  -0.0221   0.9630 C   0 0 0 0 0 0 0 0 0 0 5
6    -1.0784  -0.0094   0.1094 C   0 0 0 0 0 0 0 0 0 0 6
7    -2.1470   0.0093   0.9126 O   0 0 0 0 0 0 0 0 0 0 7
8    -1.1183  -0.0191  -1.1115 O   0 0 0 0 0 0 0 0 0 0 8
9     0.2079   0.8556   1.6167 H   0 0 0 0 0 0 0 0 0 0 9
10    0.2128  -0.9291   1.5757 H   0 0 0 0 0 0 0 0 0 0 10
11   -3.0196   0.0091   0.3662 H   0 0 0 0 0 0 0 0 0 0 11
12
13   2 1 0 0 0 0
14   3 1 0 0 0 0
15   6 5 0 0 0 0
16   9 5 0 0 0 0
17  10 5 0 0 0 0
18   7 6 0 0 0 0
19   8 6 0 0 0 0
20   7 11 0 0 0 0
21 M  END
22 $$$
23 carbonicacid-anion.sdf
24 COSMOTHERM          3D          0
25
26   8 6 0 0 0 0 0 0 0 0 0 V2000
27   -2.7019  -0.0378  -0.0070 O   0 0 0 0 0 0 0 0 0 0 1
28   -1.7426  -0.3446  -0.0030 H   0 0 0 0 0 0 0 0 0 0 2
29   -2.6325   0.9275   0.0888 H   0 0 0 0 0 0 0 0 0 0 3
30   0.6704   0.0340   0.0005 C   0 0 0 0 0 0 0 0 0 0 4
31   0.4603   1.2701  -0.0015 O   0 0 0 0 0 0 0 0 0 0 5
32   2.0126  -0.3983  -0.0014 O   0 0 0 0 0 0 0 0 0 0 6
33  -0.1600  -0.9222   0.0044 O   0 0 0 0 0 0 0 0 0 0 7
34   2.5600   0.4114  -0.0037 H   0 0 0 0 0 0 0 0 0 0 8
35
36   2 1 0 0 0 0
37   3 1 0 0 0 0
38   5 4 0 0 0 0
39   6 4 0 0 0 0
40   7 4 0 0 0 0
41   6 8 0 0 0 0
42 M  END
43 $$$
44 carbonicacid.sdf
45 COSMOTHERM          3D          0
46
47   9 7 0 0 0 0 0 0 0 0 0 V2000
48   -2.6404   0.0053   0.0548 O   0 0 0 0 0 0 0 0 0 0 1
49   -2.9165  -0.7935  -0.4317 H   0 0 0 0 0 0 0 0 0 0 2
50   -2.8856   0.7493  -0.5258 H   0 0 0 0 0 0 0 0 0 0 3
51   0.7465  -0.0005  -0.0871 C   0 0 0 0 0 0 0 0 0 0 4
52   0.5495  -0.0026  -1.2964 O   0 0 0 0 0 0 0 0 0 0 5
53   1.9764   0.0032   0.4837 O   0 0 0 0 0 0 0 0 0 0 6
54  -0.1760  -0.0023   0.8699 O   0 0 0 0 0 0 0 0 0 0 7
55   2.6347  -0.0041  -0.2401 H   0 0 0 0 0 0 0 0 0 0 8
56  -1.1165  -0.0014   0.4566 H   0 0 0 0 0 0 0 0 0 0 9
57
58   2 1 0 0 0 0
59   3 1 0 0 0 0
60   5 4 0 0 0 0
61   6 4 0 0 0 0
62   7 4 0 0 0 0
63   8 6 0 0 0 0
64   7 9 0 0 0 0
65 M  END
66 $$$
67 chloroaceticacid-anion.sdf
68 COSMOTHERM          3D          0
69
70  10 8 0 0 0 0 0 0 0 0 0 V2000
71  -3.4582  -0.8948   0.0042 O   0 0 0 0 0 0 0 0 0 0 1
72  -2.4577  -0.7761  -0.0009 H   0 0 0 0 0 0 0 0 0 0 2
73  -3.7929   0.0185   0.0173 H   0 0 0 0 0 0 0 0 0 0 3
74   2.2625  -0.5579   0.0009 Cl  0 0 0 0 0 0 0 0 0 0 4
75   1.1148   0.8849   0.0045 C   0 0 0 0 0 0 0 0 0 0 5
76  -0.3882   0.5466  -0.0025 C   0 0 0 0 0 0 0 0 0 0 6
77  -0.7688  -0.6618  -0.0077 O   0 0 0 0 0 0 0 0 0 0 7
78  -1.1100   1.5812  -0.0021 O   0 0 0 0 0 0 0 0 0 0 8
79   1.3678   1.4704  -0.8854 H   0 0 0 0 0 0 0 0 0 0 9
80   1.3614   1.4607   0.9026 H   0 0 0 0 0 0 0 0 0 0 10
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82   2 1 0 0 0 0
83   3 1 0 0 0 0
84   5 4 0 0 0 0
85   6 5 0 0 0 0
86   9 5 0 0 0 0
87   7 6 0 0 0 0
88   8 6 0 0 0 0
89   5 10 0 0 0 0
90 M  END
91 $$$
92 chloroaceticacid_270.sdf
93 COSMOTHERM          3D          0
94
95  11 9 0 0 0 0 0 0 0 0 0 V2000
96  -3.7212  -0.0019  -0.1683 O   0 0 0 0 0 0 0 0 0 0 1
97  -3.9278  -0.7977  -0.6924 H   0 0 0 0 0 0 0 0 0 0 2
98  -3.9107   0.7459  -0.7646 H   0 0 0 0 0 0 0 0 0 0 3
99   2.4612  -0.0025  -0.1807 Cl  0 0 0 0 0 0 0 0 0 0 4
100  0.9862   0.0007   0.8665 C   0 0 0 0 0 0 0 0 0 0 5
101  -0.3086   0.0027   0.0629 C   0 0 0 0 0 0 0 0 0 0 6
102  -1.3462   0.0038   0.9048 O   0 0 0 0 0 0 0 0 0 0 7
103  -0.3898   0.0039  -1.1559 O   0 0 0 0 0 0 0 0 0 0 8
104   1.0317   0.8929   1.5007 H   0 0 0 0 0 0 0 0 0 0 9
105   1.0285  -0.8909   1.5017 H   0 0 0 0 0 0 0 0 0 0 10
106  -2.2388   0.0037   0.3914 H   0 0 0 0 0 0 0 0 0 0 11
107
108   2 1 0 0 0 0
109   3 1 0 0 0 0
110   5 4 0 0 0 0
111   6 5 0 0 0 0
112   9 5 0 0 0 0

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10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 11 0 0 0 0

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M END

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cis-5-formyluracil-anion.sdf
COSMOtherm 3D 0

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16 15 0 0 0 0 0 0 0 0 0 V2000
-3.8198 -0.0183 1.7575 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.9687 -0.0185 1.2203 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.9854 0.9224 1.9407 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.2625 -0.0273 1.0768 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.0450 -0.0074 0.5631 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.2015 0.0108 -0.8837 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0281 0.0077 -1.5602 N 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.3106 -0.0125 -0.9992 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.3976 -0.0307 0.3811 N 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2590 0.0280 -1.5338 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.3091 -0.0144 -1.7382 O 0 0 0 0 0 0 0 0 0 0 0 0 11
2.1385 -0.0105 1.5057 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.3801 -0.0425 2.1676 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.0194 0.0196 -2.5807 H 0 0 0 0 0 0 0 0 0 0 0 0 14
3.3548 0.0064 1.2638 O 0 0 0 0 0 0 0 0 0 0 0 0 15
1.7937 -0.0298 2.5700 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 12 0 0 0 0
12 16 0 0 0 0

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M END

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cis-5-formyluracil.sdf
COSMOtherm 3D 0

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17 16 0 0 0 0 0 0 0 0 0 V2000
-1.7705 0.0238 -3.6982 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.7186 -0.7922 -4.2288 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.5137 0.7339 -4.3144 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.1032 -0.0121 -0.2167 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.5690 -0.0035 1.0563 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.8888 0.0038 1.2025 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.5754 0.0011 -0.0302 N 0 0 0 0 0 0 0 0 0 0 0 0 7
1.0438 -0.0062 -1.3077 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.3542 -0.0135 -1.3353 N 0 0 0 0 0 0 0 0 0 0 0 0 9
1.5304 0.0116 2.2539 O 0 0 0 0 0 0 0 0 0 0 0 0 10
1.7254 -0.0065 -2.3297 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.5063 -0.0033 2.1739 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.1841 -0.0185 -0.3724 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.5959 0.0067 0.0253 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.8204 -0.0197 -2.2805 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.2274 0.0043 3.3733 O 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.5747 -0.0112 1.8481 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
15 9 0 0 0 0
16 12 0 0 0 0
12 17 0 0 0 0

```

M END

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cyanoaceticacid-anion.sdf
COSMOtherm 3D 0

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```

11 9 0 0 0 0 0 0 0 0 0 V2000
-3.2330 -1.0223 -0.0108 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.2427 -0.8419 0.0086 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.6260 -0.1329 -0.0346 H 0 0 0 0 0 0 0 0 0 0 0 0 3
2.1766 -0.2380 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.3058 0.9211 0.0276 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.2313 0.5919 0.0079 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5611 -0.6338 0.0391 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.9841 1.5934 -0.0301 O 0 0 0 0 0 0 0 0 0 0 0 0 8
2.8725 -1.1729 -0.0314 N 0 0 0 0 0 0 0 0 0 0 0 0 9
1.5356 1.5688 -0.8315 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.5195 1.5079 0.9342 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0

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1
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5 11 0 0 0 0
M END
$$$$
cyanoaceticacid.sdf
COSMOTHERM 3D 0
12 10 0 0 0 0 0 0 0 0 0 V2000
-3.5386 -0.0110 -0.2633 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.7068 -0.7890 -0.8264 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.7173 0.7557 -0.8385 H 0 0 0 0 0 0 0 0 0 0 0 0 3
2.3388 -0.0045 0.1020 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1412 0.0122 0.9245 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.1527 0.0087 0.0985 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.1860 0.0185 -1.1233 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2126 -0.0042 0.9024 O 0 0 0 0 0 0 0 0 0 0 0 0 8
3.3055 -0.0184 -0.5452 N 0 0 0 0 0 0 0 0 0 0 0 0 9
1.1517 0.9044 1.5704 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.1448 -0.8609 1.5955 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.0870 -0.0027 0.3572 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
8 12 0 0 0 0
M END
$$$$
dichloroaceticacid-anion.sdf
COSMOTHERM 3D 0
10 8 0 0 0 0 0 0 0 0 0 V2000
-3.9580 -0.6585 0.0135 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.9549 -0.6254 -0.0082 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.2200 0.2776 0.0449 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4953 -0.2293 1.5204 Cl 0 0 0 0 0 0 0 0 0 0 0 0 4
0.8396 0.5387 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.7177 0.4697 -0.0317 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.2446 -0.6792 -0.0291 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2746 1.5949 -0.0554 O 0 0 0 0 0 0 0 0 0 0 0 0 8
1.5561 -0.2630 -1.4780 Cl 0 0 0 0 0 0 0 0 0 0 0 0 9
1.2061 1.5659 -0.0056 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0
M END
$$$$
dichloroaceticacid.sdf
COSMOTHERM 3D 0
11 9 0 0 0 0 0 0 0 0 0 V2000
-4.0484 0.0000 0.0828 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.3079 -0.7642 -0.4646 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.3146 0.7830 -0.4340 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.6062 -1.4969 -0.0065 Cl 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7350 -0.0003 0.5151 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.6766 0.0033 -0.1024 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.8819 0.0099 -1.3054 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.5908 -0.0031 0.8577 O 0 0 0 0 0 0 0 0 0 0 0 0 8
1.6144 1.4924 -0.0019 Cl 0 0 0 0 0 0 0 0 0 0 0 0 9
0.7133 -0.0025 1.6052 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.5532 -0.0009 0.4621 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
8 11 0 0 0 0
M END
$$$$
dimethadione-anion.sdf
COSMOTHERM 3D 0
18 17 0 0 0 0 0 0 0 0 0 V2000
-3.6149 -0.0411 0.8752 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.6496 -0.0235 0.5847 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.8216 0.8876 1.0767 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4169 0.0067 0.0588 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1237 -0.0128 0.9049 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.8799 0.0107 -1.3046 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5119 -0.0048 -1.2133 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.9583 -0.0184 0.0805 N 0 0 0 0 0 0 0 0 0 0 0 0 8
2.2188 1.2865 0.2859 C 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2452 -1.2593 0.2678 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.1164 -0.0212 2.1470 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.1797 -0.0048 -2.2483 O 0 0 0 0 0 0 0 0 0 0 0 0 12
1.6069 2.1755 0.0778 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.5523 1.3301 1.3319 H 0 0 0 0 0 0 0 0 0 0 0 0 14
3.1044 1.3031 -0.3648 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.6519 -2.1577 0.0467 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.5796 -1.3109 1.3131 H 0 0 0 0 0 0 0 0 0 0 0 0 17
3.1309 -1.2483 -0.3829 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0

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5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
17 10 0 0 0 0
10 18 0 0 0 0
M END
$$$$
dimethadione.sdf
COSMOtherm          3D          0
19 18 0 0 0 0 0 0 0 0 0 0 V2000
-3.5434 -0.0016 0.9055 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.0496 -0.7842 0.6219 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.0675 0.7562 0.5888 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4375 -0.0013 0.0582 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1800 0.0025 0.9440 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.8664 -0.0007 -1.3106 O 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.4937 0.0012 -1.2479 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.8927 0.0042 0.0833 N 0 0 0 0 0 0 0 0 0 0 0 0 8
2.2479 -1.2792 0.2469 C 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2543 1.2730 0.2453 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.1462 0.0035 2.1676 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.2091 0.0009 -2.2327 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.9041 0.0038 0.3707 H 0 0 0 0 0 0 0 0 0 0 0 0 13
1.6337 -2.1698 0.0576 H 0 0 0 0 0 0 0 0 0 0 0 0 14
2.6227 -1.3226 1.2782 H 0 0 0 0 0 0 0 0 0 0 0 0 15
3.1053 -1.2806 -0.4390 H 0 0 0 0 0 0 0 0 0 0 0 0 16
1.6446 2.1664 0.0551 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.6292 1.3157 1.2766 H 0 0 0 0 0 0 0 0 0 0 0 0 18
3.1118 1.2692 -0.4405 H 0 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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9 4 0 0 0 0
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11 5 0 0 0 0
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8 7 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
17 10 0 0 0 0
18 10 0 0 0 0
10 19 0 0 0 0
M END
$$$$
ethanol-anion.sdf
COSMOtherm          3D          0
11 10 0 0 0 0 0 0 0 0 0 V2000
-2.1626 -0.0818 -0.4034 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.1989 0.1183 0.1648 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.9491 0.0950 -1.3348 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.6899 0.1740 -0.7831 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.9362 -0.4516 0.4030 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.1076 0.3459 0.8870 O 0 0 0 0 0 0 0 0 0 0 0 0 6
2.5249 -0.4645 -1.1207 H 0 0 0 0 0 0 0 0 0 0 0 0 7
1.0093 0.3245 -1.6364 H 0 0 0 0 0 0 0 0 0 0 0 0 8
2.1017 1.1564 -0.5007 H 0 0 0 0 0 0 0 0 0 0 0 0 9
1.6830 -0.6579 1.2051 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.5714 -1.4571 0.0763 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
6 2 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
5 11 0 0 0 0
M END
$$$$
ethanol.sdf
COSMOtherm          3D          0
12 10 0 0 0 0 0 0 0 0 0 V2000
-2.6448 0.0041 -0.0905 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.9169 -0.7967 -0.5739 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.8884 0.7371 -0.6843 H 0 0 0 0 0 0 0 0 0 0 0 0 3
2.3421 0.0006 -0.0340 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.8934 -0.0036 -0.4914 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.0379 0.0024 0.6676 O 0 0 0 0 0 0 0 0 0 0 0 0 6
3.0160 -0.0027 -0.9034 H 0 0 0 0 0 0 0 0 0 0 0 0 7
2.5609 0.8964 0.5660 H 0 0 0 0 0 0 0 0 0 0 0 0 8
2.5634 -0.8887 0.5748 H 0 0 0 0 0 0 0 0 0 0 0 0 9
0.6966 -0.8985 -1.1105 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.6949 0.8838 -1.1208 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.9025 0.0010 0.3529 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0

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5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
6 12 0 0 0 0
M END
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fluoroaceticacid-anion.sdf
COSMOtherm 3D 0
10 8 0 0 0 0 0 0 0 0 0 V2000
-3.1347 0.0075 0.5646 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.1261 0.0009 0.5713 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.3585 -0.0334 -0.3810 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2604 0.0002 0.8647 F 0 0 0 0 0 0 0 0 0 0 0 4
1.6800 0.0069 -0.4326 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1439 -0.0024 -0.4135 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4463 -0.0087 0.7113 O 0 0 0 0 0 0 0 0 0 0 0 7
-0.3841 -0.0021 -1.5590 O 0 0 0 0 0 0 0 0 0 0 0 8
2.0475 -0.8835 -0.9633 H 0 0 0 0 0 0 0 0 0 0 0 9
2.0359 0.9105 -0.9488 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 10 0 0 0 0
M END
$$$$
fluoroaceticacid.sdf
COSMOtherm 3D 0
11 9 0 0 0 0 0 0 0 0 0 V2000
-3.2375 0.0056 -0.0564 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4816 -0.7893 -0.5652 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4394 0.7530 -0.6491 H 0 0 0 0 0 0 0 0 0 0 0 3
2.5721 -0.0097 -0.2316 F 0 0 0 0 0 0 0 0 0 0 0 4
1.5311 0.0178 0.7069 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1826 0.0007 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.8084 -0.0113 0.8952 O 0 0 0 0 0 0 0 0 0 0 0 7
0.0453 0.0016 -1.2141 O 0 0 0 0 0 0 0 0 0 0 0 8
1.6243 0.9333 1.3090 H 0 0 0 0 0 0 0 0 0 0 0 9
1.6238 -0.8605 1.3618 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.7275 -0.0073 0.4314 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
7 11 0 0 0 0
M END
$$$$
formicacid-anion.sdf
COSMOtherm 3D 0
7 5 0 0 0 0 0 0 0 0 0 V2000
-2.1773 0.2336 0.0005 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.2740 -0.2195 0.0038 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.9545 1.1801 -0.0311 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1851 -0.2583 -0.0046 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1672 0.9993 0.0032 O 0 0 0 0 0 0 0 0 0 0 0 5
0.1857 -1.0517 0.0027 O 0 0 0 0 0 0 0 0 0 0 0 6
2.1905 -0.7601 -0.0192 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
4 7 0 0 0 0
M END
$$$$
formicacid.sdf
COSMOtherm 3D 0
8 6 0 0 0 0 0 0 0 0 0 V2000
-2.1614 0.0015 -0.2298 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.3313 -0.7855 -0.7790 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.3101 0.7578 -0.8264 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2470 -0.0012 0.2592 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1513 0.0014 1.0169 O 0 0 0 0 0 0 0 0 0 0 0 5
1.2745 -0.0002 -0.9643 O 0 0 0 0 0 0 0 0 0 0 0 6
2.1568 -0.0040 0.8882 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.6996 0.0022 0.4417 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
5 8 0 0 0 0
M END
$$$$
fumaricacid-anion.sdf
COSMOtherm 3D 0
14 12 0 0 0 0 0 0 0 0 0 V2000
-4.6310 0.0519 0.0034 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6951 -0.3253 0.0029 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.4754 1.0125 0.0103 H 0 0 0 0 0 0 0 0 0 0 0 3

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1.1952 0.3899 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1660 -0.4728 -0.0042 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2829 -0.0263 -0.0027 C 0 0 0 0 0 0 0 0 0 0 0 6
2.6022 -0.0622 0.0012 C 0 0 0 0 0 0 0 0 0 0 0 7
2.9944 -1.2250 -0.0019 O 0 0 0 0 0 0 0 0 0 0 0 8
3.4573 0.9976 0.0044 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.1378 -0.9819 0.0030 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.5419 1.2074 -0.0064 O 0 0 0 0 0 0 0 0 0 0 0 11
1.0098 1.4659 0.0053 H 0 0 0 0 0 0 0 0 0 0 0 12
0.3524 -1.5503 -0.0084 H 0 0 0 0 0 0 0 0 0 0 0 13
4.3743 0.6462 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
9 14 0 0 0 0
M END
$$$$
fumaricacid.sdf
COSMOtherm 3D 0
15 13 0 0 0 0 0 0 0 0 0 V2000
-4.6194 0.0106 0.1322 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.9049 -0.8119 -0.3067 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.8611 0.7205 -0.4910 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2480 0.0004 -0.4144 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1906 -0.0038 0.4109 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2042 -0.0035 -0.1175 C 0 0 0 0 0 0 0 0 0 0 0 6
2.6378 0.0007 0.1049 C 0 0 0 0 0 0 0 0 0 0 0 7
2.9621 -0.0066 1.2859 O 0 0 0 0 0 0 0 0 0 0 0 8
3.5336 0.0095 -0.9135 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.1054 0.0087 0.8736 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.4890 -0.0125 -1.3135 O 0 0 0 0 0 0 0 0 0 0 0 11
1.1126 0.0032 -1.4974 H 0 0 0 0 0 0 0 0 0 0 0 12
0.3222 -0.0058 1.4946 H 0 0 0 0 0 0 0 0 0 0 0 13
4.4370 0.0059 -0.5277 H 0 0 0 0 0 0 0 0 0 0 0 14
-3.0592 0.0084 0.4927 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
13 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
14 9 0 0 0 0
10 15 0 0 0 0
M END
$$$$
hypobromousacid-anion.sdf
COSMOtherm 3D 0
5 2 0 0 0 0 0 0 0 0 0 V2000
-2.8958 -0.0595 0.3746 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.9839 -0.0209 -0.1272 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1596 0.8710 0.4733 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.7130 0.0041 -0.9832 O 0 0 0 0 0 0 0 0 0 0 0 4
0.7874 0.0004 0.1175 Br 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
M END
$$$$
hypobromousacid.sdf
COSMOtherm 3D 0
6 3 0 0 0 0 0 0 0 0 0 V2000
-2.7993 -0.0165 0.4151 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4604 -0.6421 0.0660 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.2525 0.8467 0.4140 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.6180 0.0104 -1.0964 O 0 0 0 0 0 0 0 0 0 0 0 4
0.7871 -0.0014 0.1367 Br 0 0 0 0 0 0 0 0 0 0 0 5
-1.4453 0.0050 -0.5059 H 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 1 0 0 0 0
4 6 0 0 0 0
M END
$$$$
hypochlorousacid-anion.sdf
COSMOtherm 3D 0
5 3 0 0 0 0 0 0 0 0 0 V2000
-2.3659 0.2896 0.0592 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.4202 -0.1415 0.0162 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.4965 0.6832 -0.8200 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.0842 -0.9022 -0.0176 O 0 0 0 0 0 0 0 0 0 0 0 4
1.2171 0.2611 0.0041 Cl 0 0 0 0 0 0 0 0 0 0 0 5
2 1 0 0 0 0
3 1 0 0 0 0
4 5 0 0 0 0
M END
$$$$
hypochlorousacid.sdf
COSMOtherm 3D 0
6 4 0 0 0 0 0 0 0 0 0 V2000

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-2.2723 -0.0113 0.3352 O 0 0 0 0 0 0 0 0 0 0 0 0 1  
-2.8788 -0.6891 -0.0155 H 0 0 0 0 0 0 0 0 0 0 0 0 2  
-2.7569 0.8289 0.2402 H 0 0 0 0 0 0 0 0 0 0 0 0 3  
0.0126 0.0079 -0.9742 O 0 0 0 0 0 0 0 0 0 0 0 0 4  
1.2047 -0.0025 0.2950 Cl 0 0 0 0 0 0 0 0 0 0 0 0 5  
-0.8701 0.0027 -0.4595 H 0 0 0 0 0 0 0 0 0 0 0 0 6  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
4 6 0 0 0 0
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M END
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hypoiodousacid-anion.sdf
COSMOtherm 3D 0

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5 2 0 0 0 0 0 0 0 0 0 0 V2000  
-3.2394 -0.0573 -0.4281 O 0 0 0 0 0 0 0 0 0 0 0 0 1  
-2.3436 -0.0217 0.1086 H 0 0 0 0 0 0 0 0 0 0 0 0 2  
-3.5621 0.8599 -0.4295 H 0 0 0 0 0 0 0 0 0 0 0 0 3  
-1.1204 -0.0008 1.0103 O 0 0 0 0 0 0 0 0 0 0 0 0 4  
0.5966 0.0007 -0.0709 I 0 0 0 0 0 0 0 0 0 0 0 0 5  
2 1 0 0 0 0  
3 1 0 0 0 0
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M END
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hypoiodousacid.sdf
COSMOtherm 3D 0

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6 3 0 0 0 0 0 0 0 0 0 0 V2000  
-3.1660 0.0074 0.4760 O 0 0 0 0 0 0 0 0 0 0 0 0 1  
-3.6826 -0.8135 0.3740 H 0 0 0 0 0 0 0 0 0 0 0 0 2  
-3.7857 0.7190 0.2298 H 0 0 0 0 0 0 0 0 0 0 0 0 3  
-1.0344 -0.0044 -1.1480 O 0 0 0 0 0 0 0 0 0 0 0 0 4  
0.6034 0.0004 0.0840 I 0 0 0 0 0 0 0 0 0 0 0 0 5  
-1.8226 0.0014 -0.5153 H 0 0 0 0 0 0 0 0 0 0 0 0 6  
2 1 0 0 0 0  
3 1 0 0 0 0  
4 6 0 0 0 0
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M END
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hypophosphorousacid-anion.sdf
COSMOtherm 3D 0

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8 6 0 0 0 0 0 0 0 0 0 0 V2000  
-2.8099 -0.1697 0.3622 O 0 0 0 0 0 0 0 0 0 0 0 0 1  
-1.9056 0.0768 -0.0066 H 0 0 0 0 0 0 0 0 0 0 0 0 2  
-3.0263 0.5547 0.9736 H 0 0 0 0 0 0 0 0 0 0 0 0 3  
-0.4335 0.4850 -0.6914 O 0 0 0 0 0 0 0 0 0 0 0 0 4  
0.9001 -0.2271 -0.3075 P 0 0 0 0 0 0 0 0 0 0 0 0 5  
1.6589 0.1955 0.9711 O 0 0 0 0 0 0 0 0 0 0 0 0 6  
0.6487 -1.6457 -0.2622 H 0 0 0 0 0 0 0 0 0 0 0 0 7  
1.7764 -0.1164 -1.4447 H 0 0 0 0 0 0 0 0 0 0 0 0 8  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 5 0 0 0 0  
7 5 0 0 0 0  
5 8 0 0 0 0
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M END
\$\$\$\$
hypophosphorousacid.sdf
COSMOtherm 3D 0

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9 7 0 0 0 0 0 0 0 0 0 0 V2000  
-0.4413 2.5662 -0.1387 O 0 0 0 0 0 0 0 0 0 0 0 0 1  
0.1073 3.2172 -0.6141 H 0 0 0 0 0 0 0 0 0 0 0 0 2  
-0.7671 3.0413 0.6479 H 0 0 0 0 0 0 0 0 0 0 0 0 3  
0.2747 -0.6548 -1.6453 H 0 0 0 0 0 0 0 0 0 0 0 0 4  
0.2783 -0.9412 -0.2484 P 0 0 0 0 0 0 0 0 0 0 0 0 5  
1.3654 -1.8317 -0.0404 H 0 0 0 0 0 0 0 0 0 0 0 0 6  
-1.0692 -1.4545 0.2526 O 0 0 0 0 0 0 0 0 0 0 0 0 7  
0.8868 0.3942 0.4562 O 0 0 0 0 0 0 0 0 0 0 0 0 8  
0.3675 1.2478 0.2356 H 0 0 0 0 0 0 0 0 0 0 0 0 9  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 5 0 0 0 0  
7 5 0 0 0 0  
8 5 0 0 0 0  
8 9 0 0 0 0
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M END
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iodoaceticacid-anion.sdf
COSMOtherm 3D 0

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10 7 0 0 0 0 0 0 0 0 0 0 V2000  
-4.5085 -1.2652 0.0007 O 0 0 0 0 0 0 0 0 0 0 0 0 1  
-3.5440 -0.9744 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 2  
-4.9996 -0.4258 0.0231 H 0 0 0 0 0 0 0 0 0 0 0 0 3  
1.3945 -0.1694 0.0000 I 0 0 0 0 0 0 0 0 0 0 0 0 4  
-0.2970 1.2682 0.0029 C 0 0 0 0 0 0 0 0 0 0 0 0 5  
-1.7130 0.6738 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 0 6  
-1.8960 -0.5784 -0.0025 O 0 0 0 0 0 0 0 0 0 0 0 0 7  
-2.5925 1.5809 -0.0019 O 0 0 0 0 0 0 0 0 0 0 0 0 8  
-0.1307 1.8801 -0.8888 H 0 0 0 0 0 0 0 0 0 0 0 0 9  
-0.1332 1.8735 0.8994 H 0 0 0 0 0 0 0 0 0 0 0 0 10  
2 1 0 0 0 0  
3 1 0 0 0 0  
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7 6 0 0 0 0  
8 6 0 0 0 0  
5 10 0 0 0 0
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M END
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iodoaceticacid.sdf
COSMOtherm 3D 0
11 8 0 0 0 0 0 0 0 0 0 V2000
-4.3805 1.0434 0.2759 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.8817 0.3082 0.6746 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.9844 1.4226 -0.3895 H 0 0 0 0 0 0 0 0 0 0 0 3
1.3507 0.1848 0.0749 I 0 0 0 0 0 0 0 0 0 0 0 4
-0.2133 -1.1297 -0.7433 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.5568 -0.7441 -0.1717 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.1011 0.3084 -0.7881 O 0 0 0 0 0 0 0 0 0 0 0 7
-2.0866 -1.3572 0.7517 O 0 0 0 0 0 0 0 0 0 0 0 8
0.0702 -2.1368 -0.4359 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.1589 -0.9954 -1.8261 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.0039 0.5430 -0.3566 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0 0
3 1 0 0 0 0 0
6 5 0 0 0 0 0
9 5 0 0 0 0 0
10 5 0 0 0 0 0
7 6 0 0 0 0 0
8 6 0 0 0 0 0
7 11 0 0 0 0 0

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M END
$$$$
maleicacid-anion.sdf
COSMOtherm 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-4.3194 0.6438 -0.0344 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4738 0.1124 -0.0060 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.1528 1.3887 0.5681 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5510 -1.0866 -0.0045 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2268 -1.3521 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 5
2.2931 0.2170 -0.0012 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.9532 -0.4194 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6161 1.3496 -0.0159 O 0 0 0 0 0 0 0 0 0 0 0 8
3.5336 0.1952 0.0142 O 0 0 0 0 0 0 0 0 0 0 0 9
-2.0925 -0.9571 0.0093 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.7663 0.8580 -0.0038 O 0 0 0 0 0 0 0 0 0 0 0 11
2.2311 -1.9418 -0.0049 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0675 -2.4045 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 13
0.5114 1.1512 -0.0137 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
12 4 0 0 0 0 0
7 5 0 0 0 0 0
13 5 0 0 0 0 0
8 6 0 0 0 0 0
9 6 0 0 0 0 0
10 7 0 0 0 0 0
11 7 0 0 0 0 0
8 14 0 0 0 0 0
11 14 0 0 0 0 0

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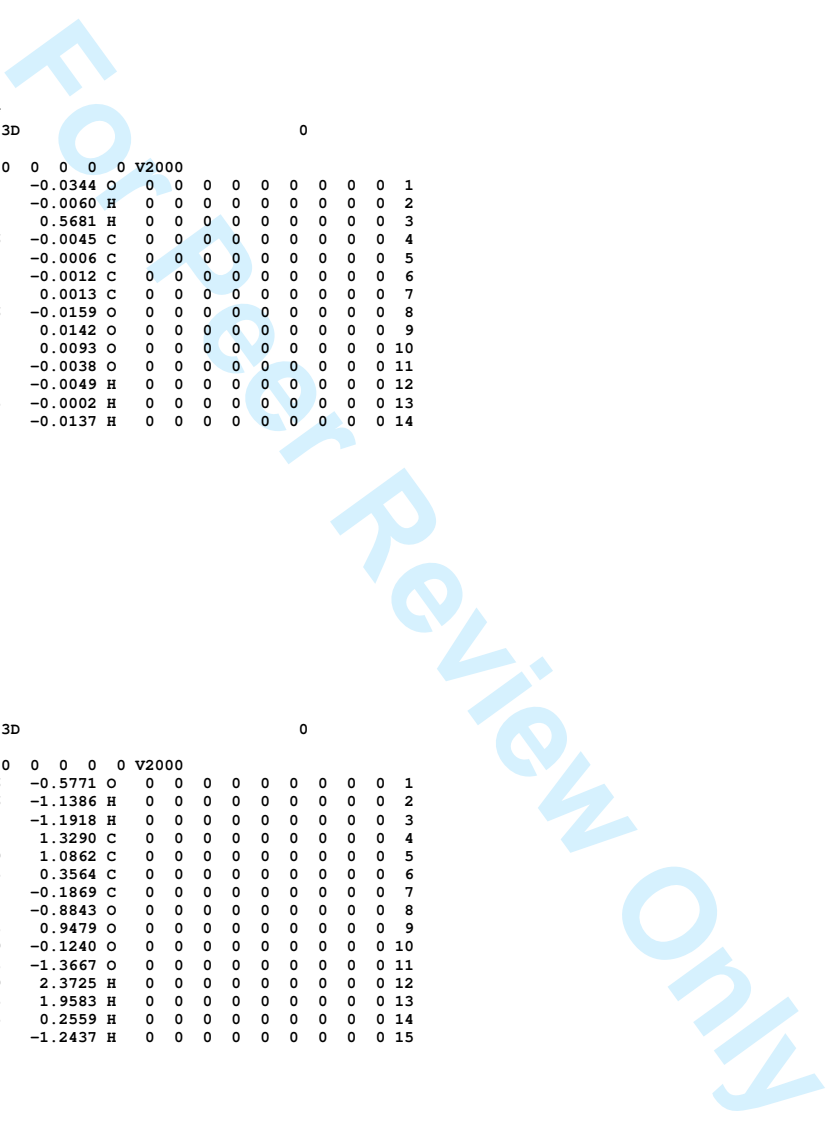
M END
$$$$
maleicacid.sdf
COSMOtherm 3D 0
15 13 0 0 0 0 0 0 0 0 0 V2000
-4.1677 -0.0146 -0.5771 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.2492 -0.8076 -1.1386 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.2403 0.7388 -1.1918 H 0 0 0 0 0 0 0 0 0 0 0 3
0.2005 0.0028 1.3290 C 0 0 0 0 0 0 0 0 0 0 0 4
1.5282 0.0009 1.0862 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9195 0.0085 0.3564 C 0 0 0 0 0 0 0 0 0 0 0 6
2.3195 -0.0031 -0.1869 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7867 0.0157 -0.8843 O 0 0 0 0 0 0 0 0 0 0 0 8
-2.0990 0.0053 0.9479 O 0 0 0 0 0 0 0 0 0 0 0 9
3.5497 -0.0159 -0.1240 O 0 0 0 0 0 0 0 0 0 0 0 10
1.6985 0.0063 -1.3667 O 0 0 0 0 0 0 0 0 0 0 0 11
-0.1190 0.0009 2.3725 H 0 0 0 0 0 0 0 0 0 0 0 12
2.1847 -0.0045 1.9583 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.8779 0.0025 0.2559 H 0 0 0 0 0 0 0 0 0 0 0 14
0.6720 0.0134 -1.2437 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
12 4 0 0 0 0 0
7 5 0 0 0 0 0
13 5 0 0 0 0 0
8 6 0 0 0 0 0
9 6 0 0 0 0 0
10 7 0 0 0 0 0
11 7 0 0 0 0 0
14 9 0 0 0 0 0
11 15 0 0 0 0 0

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M END
$$$$
mandelicacid-anion.sdf
COSMOtherm 3D 0
21 20 0 0 0 0 0 0 0 0 0 V2000
-4.0212 0.4854 1.9522 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.1980 0.1164 1.5055 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.4540 1.0007 1.2500 H 0 0 0 0 0 0 0 0 0 0 0 3
3.2838 0.4961 1.0465 C 0 0 0 0 0 0 0 0 0 0 0 4
2.7428 -0.7771 1.2609 C 0 0 0 0 0 0 0 0 0 0 0 5
1.5935 -1.1773 0.5697 C 0 0 0 0 0 0 0 0 0 0 0 6
0.9677 -0.3125 -0.3412 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5194 0.9611 -0.5546 C 0 0 0 0 0 0 0 0 0 0 0 8
2.6693 1.3625 0.1329 C 0 0 0 0 0 0 0 0 0 0 0 9

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-4.2400 0.3361 0.0190 O 0 0 0 0 0 0 0 0 0 0 1
-3.3554 -0.1644 0.0081 H 0 0 0 0 0 0 0 0 0 0 2
-3.9511 1.2655 0.0086 H 0 0 0 0 0 0 0 0 0 0 3
4.1650 0.5314 0.0097 C 0 0 0 0 0 0 0 0 0 0 4
2.9965 -0.4606 0.0082 C 0 0 0 0 0 0 0 0 0 0 5
1.6228 0.2240 -0.0057 C 0 0 0 0 0 0 0 0 0 0 6
0.4572 -0.7658 -0.0043 C 0 0 0 0 0 0 0 0 0 0 7
-0.9543 -0.1465 -0.0091 C 0 0 0 0 0 0 0 0 0 0 8
-1.0867 1.1078 -0.0152 O 0 0 0 0 0 0 0 0 0 0 9
-1.9262 -0.9891 -0.0059 O 0 0 0 0 0 0 0 0 0 0 10
5.1360 0.0138 0.0210 H 0 0 0 0 0 0 0 0 0 0 11
4.1398 1.1750 -0.8839 H 0 0 0 0 0 0 0 0 0 0 12
4.1260 1.1880 0.8933 H 0 0 0 0 0 0 0 0 0 0 13
3.0682 -1.1139 0.8952 H 0 0 0 0 0 0 0 0 0 0 14
3.0807 -1.1260 -0.8688 H 0 0 0 0 0 0 0 0 0 0 15
1.5468 0.8766 -0.8917 H 0 0 0 0 0 0 0 0 0 0 16
1.5362 0.8903 0.8689 H 0 0 0 0 0 0 0 0 0 0 17
0.5197 -1.4288 0.8761 H 0 0 0 0 0 0 0 0 0 0 18
0.5231 -1.4361 -0.8789 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0
M END
$$$$
n-pentanoicacid.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-4.3288 -0.0036 -0.1320 O 0 0 0 0 0 0 0 0 0 0 1
-4.5339 -0.8131 -0.6347 H 0 0 0 0 0 0 0 0 0 0 2
-4.5220 0.7243 -0.7510 H 0 0 0 0 0 0 0 0 0 0 3
4.2394 0.0052 -0.4316 C 0 0 0 0 0 0 0 0 0 0 4
3.0299 -0.0118 0.5088 C 0 0 0 0 0 0 0 0 0 0 5
1.6903 0.0058 -0.2391 C 0 0 0 0 0 0 0 0 0 0 6
0.4912 -0.0097 0.7082 C 0 0 0 0 0 0 0 0 0 0 7
-0.8560 0.0025 0.0159 C 0 0 0 0 0 0 0 0 0 0 8
-1.0208 -0.0017 -1.2012 O 0 0 0 0 0 0 0 0 0 0 9
-1.8775 0.0177 0.8938 O 0 0 0 0 0 0 0 0 0 0 10
5.1851 -0.0099 0.1302 H 0 0 0 0 0 0 0 0 0 0 11
4.2340 -0.8693 -1.1011 H 0 0 0 0 0 0 0 0 0 0 12
4.2389 0.9082 -1.0621 H 0 0 0 0 0 0 0 0 0 0 13
3.0788 0.8569 1.1880 H 0 0 0 0 0 0 0 0 0 0 14
3.0755 -0.9078 1.1516 H 0 0 0 0 0 0 0 0 0 0 15
1.6344 -0.8631 -0.9153 H 0 0 0 0 0 0 0 0 0 0 16
1.6388 0.9009 -0.8808 H 0 0 0 0 0 0 0 0 0 0 17
0.5182 0.8549 1.3928 H 0 0 0 0 0 0 0 0 0 0 18
0.5164 -0.8997 1.3599 H 0 0 0 0 0 0 0 0 0 0 19
-2.7682 0.0155 0.3998 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 20 0 0 0 0
M END
$$$$
nitroaceticacid-anion.sdf
COSMOtherm 3D 0
12 10 0 0 0 0 0 0 0 0 0 V2000
-3.5623 -0.0125 1.1098 O 0 0 0 0 0 0 0 0 0 0 1
-2.5939 -0.0119 0.8466 H 0 0 0 0 0 0 0 0 0 0 2
-4.0192 0.3617 0.3372 H 0 0 0 0 0 0 0 0 0 0 3
-0.5900 -0.0071 -0.6877 C 0 0 0 0 0 0 0 0 0 0 4
0.9429 -0.0012 -1.0471 C 0 0 0 0 0 0 0 0 0 0 5
-0.9015 -0.0136 0.5364 O 0 0 0 0 0 0 0 0 0 0 6
-1.3319 -0.0042 -1.6956 O 0 0 0 0 0 0 0 0 0 0 7
1.8018 0.0040 0.1695 N 0 0 0 0 0 0 0 0 0 0 8
2.1087 1.1003 0.6636 O 0 0 0 0 0 0 0 0 0 0 9
2.1124 -1.0892 0.6689 O 0 0 0 0 0 0 0 0 0 0 10
1.1869 -0.9036 -1.6163 H 0 0 0 0 0 0 0 0 0 0 11
1.1786 0.9021 -1.6180 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
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9 8 0 0 0 0
10 8 0 0 0 0
5 12 0 0 0 0
M END
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nitroaceticacid.sdf
COSMOtherm 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-3.9122 0.0075 -0.2555 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.1002 -0.7614 -0.8251 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.0823 0.7858 -0.8180 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.5400 0.0132 0.1148 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7319 -0.0331 0.9693 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6069 -0.0517 0.9007 O 0 0 0 0 0 0 0 0 0 0 0 6
-0.5406 0.1019 -1.1033 O 0 0 0 0 0 0 0 0 0 0 0 7
1.9430 -0.0168 0.0788 N 0 0 0 0 0 0 0 0 0 0 0 8
2.4459 1.0793 -0.1856 O 0 0 0 0 0 0 0 0 0 0 0 9
2.3431 -1.1009 -0.3581 O 0 0 0 0 0 0 0 0 0 0 0 10
0.7853 0.8444 1.6225 H 0 0 0 0 0 0 0 0 0 0 0 11
0.7650 -0.9559 1.5581 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.4860 -0.0174 0.3500 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
6 13 0 0 0 0
M END
\$\$\$\$
nitromethane-anion.sdf
COSMOtherm 3D 0

9 7 0 0 0 0 0 0 0 0 0 V2000
-2.5945 0.0071 -0.0427 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6366 -0.0137 -0.3581 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.4955 0.0465 0.9244 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1000 0.0136 -0.2417 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7960 -0.0021 0.0082 N 0 0 0 0 0 0 0 0 0 0 0 5
-0.0694 -0.0112 -0.9931 O 0 0 0 0 0 0 0 0 0 0 0 6
0.3232 -0.0088 1.2167 O 0 0 0 0 0 0 0 0 0 0 0 7
2.7781 0.0204 0.6053 H 0 0 0 0 0 0 0 0 0 0 0 8
2.4233 0.0177 -1.2771 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
4 9 0 0 0 0
M END
\$\$\$\$
nitromethane.sdf
COSMOtherm 3D 0

10 8 0 0 0 0 0 0 0 0 0 V2000
-2.9359 0.0843 -0.0271 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.2711 -0.8260 0.0452 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.9759 -0.0253 -0.2029 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2019 0.0384 -0.4329 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7796 -0.0116 0.0367 N 0 0 0 0 0 0 0 0 0 0 0 5
0.5725 -0.0133 1.2512 O 0 0 0 0 0 0 0 0 0 0 0 6
-0.1175 -0.0458 -0.8230 O 0 0 0 0 0 0 0 0 0 0 0 7
2.2081 0.0087 -1.5236 H 0 0 0 0 0 0 0 0 0 0 0 8
2.6322 0.9679 -0.0444 H 0 0 0 0 0 0 0 0 0 0 0 9
2.7149 -0.8230 0.0078 H 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
4 10 0 0 0 0
M END
\$\$\$\$
nitrousacid-anion.sdf
COSMOtherm 3D 0

6 4 0 0 0 0 0 0 0 0 0 V2000
-1.0327 0.0013 -0.2995 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.2103 -0.0023 -1.2866 N 0 0 0 0 0 0 0 0 0 0 0 2
1.0139 0.0012 -0.9815 O 0 0 0 0 0 0 0 0 0 0 0 3
1.1094 -0.0023 2.0527 H 0 0 0 0 0 0 0 0 0 0 0 4
0.1471 -0.0005 2.1983 O 0 0 0 0 0 0 0 0 0 0 0 5
-0.2245 0.0030 1.2667 H 0 0 0 0 0 0 0 0 0 0 0 6
2 1 0 0 0 0
3 2 0 0 0 0
5 4 0 0 0 0
5 6 0 0 0 0
M END
\$\$\$\$
nitrousacid.sdf
COSMOtherm 3D 0

7 5 0 0 0 0 0 0 0 0 0 V2000
-2.4332 -0.0005 -0.1442 O 0 0 0 0 0 0 0 0 0 0 0 1
0.0440 -0.0006 0.7156 O 0 0 0 0 0 0 0 0 0 0 0 2
0.8652 0.0001 -0.4228 N 0 0 0 0 0 0 0 0 0 0 0 3
2.0263 0.0004 -0.1356 O 0 0 0 0 0 0 0 0 0 0 0 4

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3      -2.6739   -0.7678   -0.6952 H   0 0 0 0 0 0 0 0 0 0 0 5
4      -2.6802   0.7776   -0.6771 H   0 0 0 0 0 0 0 0 0 0 0 6
5      -0.9092  -0.0004   0.3304 H   0 0 0 0 0 0 0 0 0 0 0 7
6      5 1 0 0 0 0
7      6 1 0 0 0 0
8      3 2 0 0 0 0
9      4 3 0 0 0 0
10     2 7 0 0 0 0
11 M END
12 $$$
13 oh.sdf
14 COSMOtherm      3D      0
15
16 5 4 0 0 0 0 0 0 0 0 0 V2000
17 -1.2254 -0.0372 -0.0452 O 0 0 0 0 0 0 0 0 0 0 0 1
18 -0.0275 -0.0006 -0.0162 H 0 0 0 0 0 0 0 0 0 0 0 2
19 -1.5188 0.4761 0.7263 H 0 0 0 0 0 0 0 0 0 0 0 3
20 1.5209 -0.4761 0.7262 H 0 0 0 0 0 0 0 0 0 0 0 4
21 1.2270 0.0372 -0.0453 O 0 0 0 0 0 0 0 0 0 0 0 5
22 2 1 0 0 0 0
23 3 1 0 0 0 0
24 2 5 0 0 0 0
25 4 5 0 0 0 0
26 M END
27 $$$
28 oxalicacid-anion.sdf
29 COSMOtherm      3D      0
30
31 10 8 0 0 0 0 0 0 0 0 0 V2000
32 -3.0490 -0.0228 0.0774 O 0 0 0 0 0 0 0 0 0 0 0 1
33 -2.1819 -0.0079 -0.4123 H 0 0 0 0 0 0 0 0 0 0 0 2
34 -2.7545 -0.0010 1.0049 H 0 0 0 0 0 0 0 0 0 0 0 3
35 0.5831 0.0050 0.7458 C 0 0 0 0 0 0 0 0 0 0 0 4
36 0.4611 0.0049 -0.8267 C 0 0 0 0 0 0 0 0 0 0 0 5
37 -0.3408 0.0302 1.5413 O 0 0 0 0 0 0 0 0 0 0 0 6
38 -0.6887 0.0148 -1.3330 O 0 0 0 0 0 0 0 0 0 0 0 7
39 1.5851 -0.0026 -1.4089 O 0 0 0 0 0 0 0 0 0 0 0 8
40 1.8719 -0.0248 1.1307 O 0 0 0 0 0 0 0 0 0 0 0 9
41 2.3590 -0.0257 0.2524 H 0 0 0 0 0 0 0 0 0 0 0 10
42 2 1 0 0 0 0
43 3 1 0 0 0 0
44 5 4 0 0 0 0
45 6 4 0 0 0 0
46 9 4 0 0 0 0
47 7 5 0 0 0 0
48 8 5 0 0 0 0
49 9 10 0 0 0 0
50 M END
51 $$$
52 oxalicacid.sdf
53 COSMOtherm      3D      0
54
55 11 9 0 0 0 0 0 0 0 0 0 V2000
56 -3.3974 -0.0174 0.1857 O 0 0 0 0 0 0 0 0 0 0 0 1
57 -3.6508 -0.6408 -0.5205 H 0 0 0 0 0 0 0 0 0 0 0 2
58 -3.7411 0.8471 -0.1074 H 0 0 0 0 0 0 0 0 0 0 0 3
59 -0.0604 0.0025 -0.2552 C 0 0 0 0 0 0 0 0 0 0 0 4
60 1.4202 0.0001 0.2163 C 0 0 0 0 0 0 0 0 0 0 0 5
61 -0.3697 0.0125 -1.4370 O 0 0 0 0 0 0 0 0 0 0 0 6
62 2.2482 -0.0067 -0.8385 O 0 0 0 0 0 0 0 0 0 0 0 7
63 1.7654 0.0044 1.3826 O 0 0 0 0 0 0 0 0 0 0 0 8
64 -0.8836 -0.0069 0.7788 O 0 0 0 0 0 0 0 0 0 0 0 9
65 3.1727 -0.0084 -0.5050 H 0 0 0 0 0 0 0 0 0 0 0 10
66 -1.8718 -0.0038 0.4608 H 0 0 0 0 0 0 0 0 0 0 0 11
67 2 1 0 0 0 0
68 3 1 0 0 0 0
69 5 4 0 0 0 0
70 6 4 0 0 0 0
71 9 4 0 0 0 0
72 7 5 0 0 0 0
73 8 5 0 0 0 0
74 10 7 0 0 0 0
75 9 11 0 0 0 0
76 M END
77 $$$
78 pamoicacid-anion.sdf
79 COSMOtherm      3D      0
80
81 47 50 0 0 0 0 0 0 0 0 0 V2000
82 -7.7945 1.1666 0.0813 O 0 0 0 0 0 0 0 0 0 0 0 1
83 -8.1328 1.1968 -0.8326 H 0 0 0 0 0 0 0 0 0 0 0 2
84 -7.8014 2.0947 0.3802 H 0 0 0 0 0 0 0 0 0 0 0 3
85 -0.6540 -3.9777 1.7692 C 0 0 0 0 0 0 0 0 0 0 0 4
86 0.4793 -3.5816 1.0134 C 0 0 0 0 0 0 0 0 0 0 0 5
87 0.4358 -2.4748 0.1856 C 0 0 0 0 0 0 0 0 0 0 0 6
88 -0.7514 -1.6939 0.0581 C 0 0 0 0 0 0 0 0 0 0 0 7
89 -1.9106 -2.1207 0.8072 C 0 0 0 0 0 0 0 0 0 0 0 8
90 -1.8269 -3.2609 1.6590 C 0 0 0 0 0 0 0 0 0 0 0 9
91 -0.8249 -0.5397 -0.7838 C 0 0 0 0 0 0 0 0 0 0 0 10
92 -2.0580 0.1041 -0.9301 C 0 0 0 0 0 0 0 0 0 0 0 11
93 -3.2193 -0.3252 -0.1926 C 0 0 0 0 0 0 0 0 0 0 0 12
94 -3.1225 -1.4144 0.6625 C 0 0 0 0 0 0 0 0 0 0 0 13
95 0.3782 -0.0399 -1.5763 C 0 0 0 0 0 0 0 0 0 0 0 14
96 1.5802 0.4484 -0.7743 C 0 0 0 0 0 0 0 0 0 0 0 15
97 1.5178 1.6109 0.0562 C 0 0 0 0 0 0 0 0 0 0 0 16
98 2.6842 2.0291 0.7997 C 0 0 0 0 0 0 0 0 0 0 0 17
99 3.8878 1.2970 0.6602 C 0 0 0 0 0 0 0 0 0 0 0 18
100 3.9726 0.1974 -0.1721 C 0 0 0 0 0 0 0 0 0 0 0 19
101 2.8073 -0.2153 -0.9140 C 0 0 0 0 0 0 0 0 0 0 0 20
102 0.3093 3.5241 0.9982 C 0 0 0 0 0 0 0 0 0 0 0 21
103 1.4502 3.9144 1.7435 C 0 0 0 0 0 0 0 0 0 0 0 22
104 2.6148 3.1793 1.6360 C 0 0 0 0 0 0 0 0 0 0 0 23
105 0.3401 2.4072 0.1821 C 0 0 0 0 0 0 0 0 0 0 0 24
106 2.9111 -1.2883 -1.7346 O 0 0 0 0 0 0 0 0 0 0 0 25
107 -2.1531 1.1693 -1.7727 O 0 0 0 0 0 0 0 0 0 0 0 26

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| 2.7023 | 1.0108 | -1.7037 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 29 |
| -2.4888 | -0.2125 | 1.3315 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 30 |
| 2.8392 | 2.2110 | -2.8504 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 31 |
| 1.4317 | 2.8253 | -4.5069 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 32 |
| -2.9776 | 0.5812 | 2.6669 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 33 |
| -1.8111 | 1.2698 | 4.4741 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 34 |
| 5.0384 | -0.7561 | 3.8914 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 35 |
| 5.0764 | -1.8719 | 1.6516 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 36 |
| 3.0680 | -1.9969 | 0.2726 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 37 |
| 2.9107 | 0.2271 | 4.7356 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 38 |
| 0.5471 | 0.6972 | 4.4613 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 39 |
| -0.2666 | -2.5383 | -0.3549 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 40 |
| 1.4290 | -2.2151 | -0.6508 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 41 |
| -0.5855 | 1.5114 | -4.6995 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 42 |
| -3.8980 | -2.9456 | -2.6670 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 43 |
| -4.3095 | -1.4378 | -4.6218 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 44 |
| -2.6609 | 0.3513 | -5.1586 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 45 |
| -1.9151 | -2.6841 | -1.2697 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 46 |
| 2.1594 | 3.4681 | -4.6523 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 47 |
| -2.7327 | 1.6157 | 4.7766 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 48 |
| 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 8 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 13 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 38 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 26 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 28 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 16 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 18 | 17 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | 17 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 18 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 27 | 19 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 25 | 20 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 22 | 21 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 24 | 21 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 43 | 21 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | 22 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 44 | 22 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 46 | 24 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 29 | 25 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 30 | 26 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 31 | 27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 32 | 27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 33 | 28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| \$\$\$\$ | | | | | | | | | | | | | | | | |
| pentachlorophenol-anion.sdf | | | | | | | | | | | | | | | | |
| COSMOTHERM | 3D | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | | |
| 15 | 14 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| -4.8565 | -1.1301 | 0.5175 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 |
| -3.8898 | -1.1144 | 0.2587 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 |
| -5.0477 | -0.2182 | 0.7945 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 |
| 0.1156 | 1.3459 | -0.0242 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 |
| -1.0940 | 0.6512 | -0.0971 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 |
| -1.1774 | -0.7869 | -0.1214 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 |
| 0.1053 | -1.4435 | -0.0678 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 |
| 1.3164 | -0.7538 | 0.0035 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 |
| 1.3384 | 0.6530 | 0.0281 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 |
| -2.2752 | -1.4377 | -0.1891 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 |
| -2.6206 | 1.5227 | -0.1760 | Cl | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 |
| 0.1205 | 3.1046 | 0.0011 | Cl | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 |
| 2.8603 | 1.5245 | 0.1204 | Cl | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 14 |
| 2.8342 | -1.6408 | 0.0665 | Cl | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 |
| 0.0734 | -3.2011 | -0.0957 | Cl | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 16 |
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| 12 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
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| 14 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

For Peer Review Only

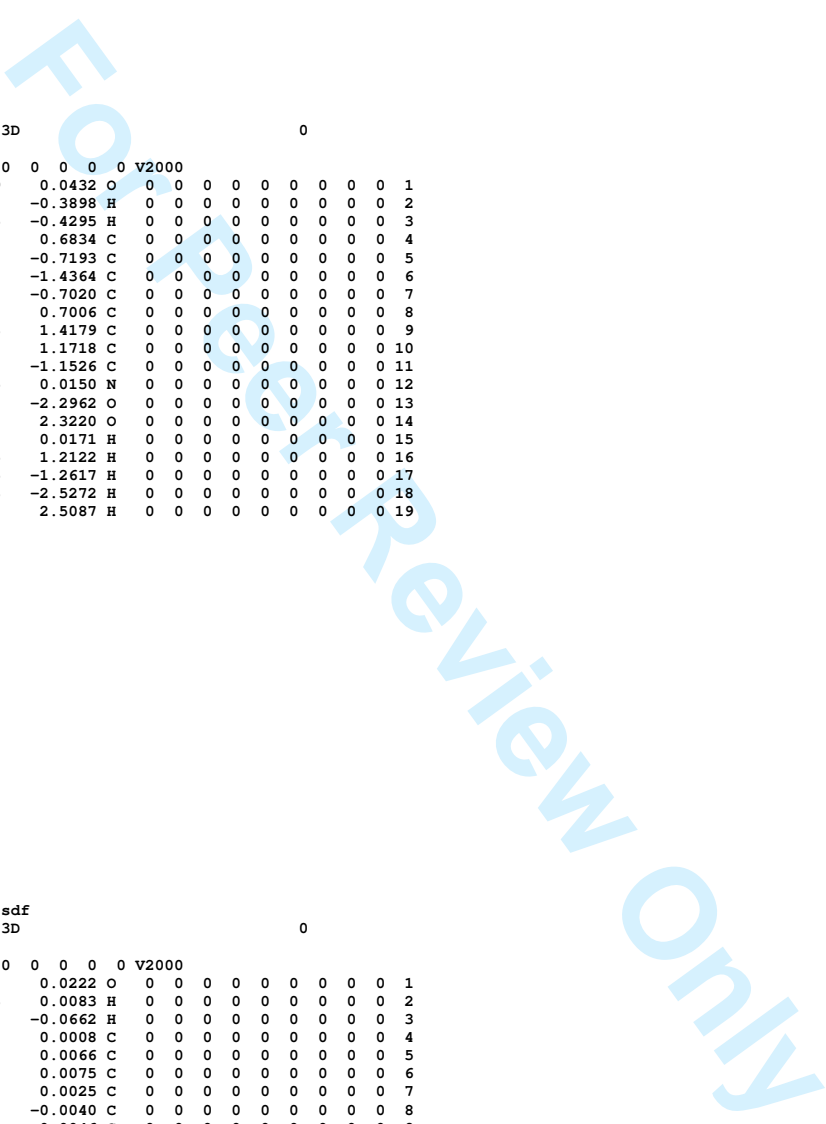
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 -5.1347 -0.8783 1.7408 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 -2.3916 -0.1564 0.3786 N 0 0 0 0 0 0 0 0 0 0 0 0 4
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 -1.2079 -0.8091 0.3120 C 0 0 0 0 0 0 0 0 0 0 0 0 6
 -0.0363 0.2205 0.0373 C 0 0 0 0 0 0 0 0 0 0 0 0 7
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 -1.0159 -2.0286 0.4425 O 0 0 0 0 0 0 0 0 0 0 0 0 12
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 1.0295 0.9693 2.2379 C 0 0 0 0 0 0 0 0 0 0 0 0 14
 1.9403 -0.9620 1.1065 C 0 0 0 0 0 0 0 0 0 0 0 0 15
 2.8697 -1.1297 2.1370 C 0 0 0 0 0 0 0 0 0 0 0 0 16
 2.8868 -0.2449 3.2228 C 0 0 0 0 0 0 0 0 0 0 0 0 17
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 0.5187 -0.8276 -3.6355 C 0 0 0 0 0 0 0 0 0 0 0 0 19
 1.6379 -0.0609 -3.9736 C 0 0 0 0 0 0 0 0 0 0 0 0 20
 2.2252 0.7649 -3.0068 C 0 0 0 0 0 0 0 0 0 0 0 0 21
 1.6962 0.8169 -1.7143 C 0 0 0 0 0 0 0 0 0 0 0 0 22
 -0.4867 2.3107 -0.3543 H 0 0 0 0 0 0 0 0 0 0 0 0 23
 1.9693 1.5028 4.1083 H 0 0 0 0 0 0 0 0 0 0 0 0 24
 0.3093 1.7879 2.2766 H 0 0 0 0 0 0 0 0 0 0 0 0 25
 1.9370 -1.6531 0.2626 H 0 0 0 0 0 0 0 0 0 0 0 0 26
 3.5860 -1.9526 2.0902 H 0 0 0 0 0 0 0 0 0 0 0 0 27
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 3.1009 1.3666 -3.2579 H 0 0 0 0 0 0 0 0 0 0 0 0 32
 2.1688 1.4567 -0.9656 H 0 0 0 0 0 0 0 0 0 0 0 0 33
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 -5.1697 0.2938 -1.7777 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 -2.3532 -0.1929 -0.1021 N 0 0 0 0 0 0 0 0 0 0 0 0 4
 -2.1391 -0.0434 1.2838 C 0 0 0 0 0 0 0 0 0 0 0 0 5
 -1.1890 -0.1637 -0.8212 C 0 0 0 0 0 0 0 0 0 0 0 0 6
 -0.0217 -0.0078 0.2136 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 -0.7860 -0.0135 1.4686 N 0 0 0 0 0 0 0 0 0 0 0 0 8
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 0.9014 -1.2253 0.0734 C 0 0 0 0 0 0 0 0 0 0 0 0 10
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 -1.0721 -0.2559 -2.0366 O 0 0 0 0 0 0 0 0 0 0 0 0 12
 1.6667 -3.4134 0.8039 C 0 0 0 0 0 0 0 0 0 0 0 0 13
 0.8400 -2.2962 0.9748 C 0 0 0 0 0 0 0 0 0 0 0 0 14
 1.7930 -1.2932 -1.0104 C 0 0 0 0 0 0 0 0 0 0 0 0 15
 2.6114 -2.4119 -1.1839 C 0 0 0 0 0 0 0 0 0 0 0 0 16
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1.2664 -0.0121 -0.1606 C 0 0 0 0 0 0 0 0 0 0 0 7
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1.9083 0.0132 1.4325 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7276 -0.0038 0.6990 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7357 -0.0067 -0.6989 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9251 0.0108 -1.4184 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.7137 -0.0273 -1.1295 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.7266 -0.0288 1.1127 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.5225 -0.0415 -0.0130 N 0 0 0 0 0 0 0 0 0 0 0 12
-1.1335 -0.0373 2.2879 O 0 0 0 0 0 0 0 0 0 0 0 13
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-1.1071 -0.0316 -2.3094 O 0 0 0 0 0 0 0 0 0 0 0 14
4.0814 0.0459 -1.2174 H 0 0 0 0 0 0 0 0 0 0 0 15
4.0668 0.0472 1.2569 H 0 0 0 0 0 0 0 0 0 0 0 16
1.9016 0.0136 2.5243 H 0 0 0 0 0 0 0 0 0 0 0 17
1.9314 0.0094 -2.5102 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
9 18 0 0 0 0
M END
$$$$
phthalimide.sdf
COSMOTHERM 3D 0
19 19 0 0 0 0 0 0 0 0 0 V2000
-4.2758 -0.0009 0.0432 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.6637 -0.7828 -0.3898 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.6682 0.7555 -0.4295 H 0 0 0 0 0 0 0 0 0 0 0 3
3.1453 -0.0010 0.6834 C 0 0 0 0 0 0 0 0 0 0 0 4
3.1353 -0.0010 -0.7193 C 0 0 0 0 0 0 0 0 0 0 0 5
1.9270 -0.0004 -1.4364 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7469 0.0002 -0.7020 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7568 0.0001 0.7006 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9474 -0.0003 1.4179 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.6632 0.0010 1.1718 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.6794 0.0008 -1.1526 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.4487 0.0015 0.0150 N 0 0 0 0 0 0 0 0 0 0 0 12
-1.1242 0.0008 -2.2962 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.0907 0.0012 2.3220 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.4936 0.0012 0.0171 H 0 0 0 0 0 0 0 0 0 0 0 15
4.0996 -0.0015 1.2122 H 0 0 0 0 0 0 0 0 0 0 0 16
4.0818 -0.0015 -1.2617 H 0 0 0 0 0 0 0 0 0 0 0 17
1.9184 -0.0003 -2.5272 H 0 0 0 0 0 0 0 0 0 0 0 18
1.9548 -0.0004 2.5087 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 12 0 0 0 0
9 19 0 0 0 0
M END
$$$$
salicylicacid-anion.sdf
COSMOTHERM 3D 0
18 18 0 0 0 0 0 0 0 0 0 V2000
-4.5414 -0.4262 0.0222 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5514 -0.5993 0.0083 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.6069 0.5402 -0.0662 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2980 -1.7028 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 4
3.1516 -0.5862 0.0066 C 0 0 0 0 0 0 0 0 0 0 0 5
2.6317 0.7072 0.0075 C 0 0 0 0 0 0 0 0 0 0 0 6
1.2378 0.9084 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3625 -0.2147 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 8
0.9173 -1.5059 -0.0046 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7456 2.1693 0.0032 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.1282 -0.0074 -0.0091 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.8968 -1.0132 -0.0102 O 0 0 0 0 0 0 0 0 0 0 0 12
-1.5444 1.2159 -0.0120 O 0 0 0 0 0 0 0 0 0 0 0 13
2.7119 -2.7123 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 14
4.2346 -0.7276 0.0106 H 0 0 0 0 0 0 0 0 0 0 0 15
3.2894 1.5787 0.0122 H 0 0 0 0 0 0 0 0 0 0 0 16
0.2330 -2.3563 -0.0093 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.2935 2.0056 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
17 9 0 0 0 0
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3 12 11 0 0 0 0
4 13 11 0 0 0 0
5 10 18 0 0 0 0
6 13 18 0 0 0 0
7 M END
8 $$$
9 salicylicacid.sdf
10 COSMOtherm 3D 0
11
12 19 18 0 0 0 0 0 0 0 0 0 V2000
13 -4.4471 -0.0150 0.4652 O 0 0 0 0 0 0 0 0 0 0 0 1
14 -4.7314 -0.5387 -0.3066 H 0 0 0 0 0 0 0 0 0 0 0 2
15 -4.8093 0.8765 0.3073 H 0 0 0 0 0 0 0 0 0 0 0 3
16 2.2205 0.0040 1.7646 C 0 0 0 0 0 0 0 0 0 0 0 4
17 3.1266 0.0043 0.6887 C 0 0 0 0 0 0 0 0 0 0 0 5
18 2.6732 0.0010 -0.6274 C 0 0 0 0 0 0 0 0 0 0 0 6
19 1.2932 -0.0015 -0.8973 C 0 0 0 0 0 0 0 0 0 0 0 7
20 0.3658 -0.0030 0.1836 C 0 0 0 0 0 0 0 0 0 0 0 8
21 0.8545 -0.0003 1.5070 C 0 0 0 0 0 0 0 0 0 0 0 9
22 0.8866 -0.0025 -2.1892 O 0 0 0 0 0 0 0 0 0 0 0 10
23 -1.0772 -0.0017 -0.1154 C 0 0 0 0 0 0 0 0 0 0 0 11
24 -1.5136 0.0122 -1.2887 O 0 0 0 0 0 0 0 0 0 0 0 12
25 -1.8841 -0.0192 0.9416 O 0 0 0 0 0 0 0 0 0 0 0 13
26 2.5858 0.0076 2.7919 H 0 0 0 0 0 0 0 0 0 0 0 14
27 4.2009 0.0081 0.8829 H 0 0 0 0 0 0 0 0 0 0 0 15
28 3.3715 0.0020 -1.4656 H 0 0 0 0 0 0 0 0 0 0 0 16
29 0.1384 -0.0001 2.3290 H 0 0 0 0 0 0 0 0 0 0 0 17
30 -0.1246 0.0071 -2.1500 H 0 0 0 0 0 0 0 0 0 0 0 18
31 -2.8706 -0.0081 0.6513 H 0 0 0 0 0 0 0 0 0 0 0 19
32 2 1 0 0 0 0
33 3 1 0 0 0 0
34 5 4 0 0 0 0
35 9 4 0 0 0 0
36 14 4 0 0 0 0
37 6 5 0 0 0 0
38 15 5 0 0 0 0
39 7 6 0 0 0 0
40 16 6 0 0 0 0
41 8 7 0 0 0 0
42 10 7 0 0 0 0
43 9 8 0 0 0 0
44 11 8 0 0 0 0
45 17 9 0 0 0 0
46 18 10 0 0 0 0
47 12 11 0 0 0 0
48 13 11 0 0 0 0
49 13 19 0 0 0 0
50 M END
51 $$$
52 succinimide-anion.sdf
53 COSMOtherm 3D 0
54
55 14 13 0 0 0 0 0 0 0 0 0 V2000
56 -3.1345 -0.3613 -0.0460 O 0 0 0 0 0 0 0 0 0 0 0 1
57 -2.1233 -0.2684 -0.0163 H 0 0 0 0 0 0 0 0 0 0 0 2
58 -3.4574 0.3853 0.4872 H 0 0 0 0 0 0 0 0 0 0 0 3
59 1.7388 1.0098 -0.0105 C 0 0 0 0 0 0 0 0 0 0 0 4
60 0.2069 1.1367 0.0024 C 0 0 0 0 0 0 0 0 0 0 0 5
1 1.9693 -0.5017 -0.0128 C 0 0 0 0 0 0 0 0 0 0 0 6
2 0.5450 -1.0799 0.0067 C 0 0 0 0 0 0 0 0 0 0 0 7
3 -0.4031 -0.0906 0.0139 N 0 0 0 0 0 0 0 0 0 0 0 8
4 0.2983 -2.3012 0.0140 O 0 0 0 0 0 0 0 0 0 0 0 9
5 -0.3939 2.2281 0.0052 O 0 0 0 0 0 0 0 0 0 0 0 10
6 2.1519 1.5190 0.8723 H 0 0 0 0 0 0 0 0 0 0 0 11
7 2.1383 1.5208 -0.8984 H 0 0 0 0 0 0 0 0 0 0 0 12
8 2.5222 -0.8677 0.8644 H 0 0 0 0 0 0 0 0 0 0 0 13
9 2.4960 -0.8676 -0.9061 H 0 0 0 0 0 0 0 0 0 0 0 14
10 2 1 0 0 0 0
11 3 1 0 0 0 0
12 5 4 0 0 0 0
13 6 4 0 0 0 0
14 11 4 0 0 0 0
15 12 4 0 0 0 0
16 8 5 0 0 0 0
17 10 5 0 0 0 0
18 7 6 0 0 0 0
19 13 6 0 0 0 0
20 8 7 0 0 0 0
21 9 7 0 0 0 0
22 6 14 0 0 0 0
23 M END
24 $$$
25 succinimide.sdf
26 COSMOtherm 3D 0
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28 15 14 0 0 0 0 0 0 0 0 0 V2000
29 -3.1705 -0.0001 0.1081 O 0 0 0 0 0 0 0 0 0 0 0 1
30 -3.5705 -0.7714 -0.3329 H 0 0 0 0 0 0 0 0 0 0 0 2
31 -3.5728 0.7670 -0.3381 H 0 0 0 0 0 0 0 0 0 0 0 3
32 1.9147 -0.0003 0.7222 C 0 0 0 0 0 0 0 0 0 0 0 4
33 0.4556 0.0001 1.1569 C 0 0 0 0 0 0 0 0 0 0 0 5
34 1.8742 -0.0003 -0.8131 C 0 0 0 0 0 0 0 0 0 0 0 6
35 0.3941 0.0001 -1.1697 C 0 0 0 0 0 0 0 0 0 0 0 7
36 -0.3332 0.0000 0.0137 N 0 0 0 0 0 0 0 0 0 0 0 8
37 -0.1023 0.0004 -2.2923 O 0 0 0 0 0 0 0 0 0 0 0 9
38 0.0199 0.0004 2.3046 O 0 0 0 0 0 0 0 0 0 0 0 10
39 2.4094 -0.8855 1.1449 H 0 0 0 0 0 0 0 0 0 0 0 11
40 2.4099 0.8846 1.1449 H 0 0 0 0 0 0 0 0 0 0 0 12
41 2.3459 -0.8855 -1.2613 H 0 0 0 0 0 0 0 0 0 0 0 13
42 2.3463 0.8846 -1.2612 H 0 0 0 0 0 0 0 0 0 0 0 14
43 -1.3784 0.0005 0.0375 H 0 0 0 0 0 0 0 0 0 0 0 15
44 2 1 0 0 0 0
45 3 1 0 0 0 0
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47 6 4 0 0 0 0

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11 4 0 0 0 0
12 4 0 0 0 0
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10 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
8 15 0 0 0 0
M END
$$$$
sulfurousacid-anion.sdf
COSMOtherm 3D 0
8 6 0 0 0 0 0 0 0 0 0 V2000
-2.4129 -0.0777 0.4723 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.1362 1.4151 -0.3776 O 0 0 0 0 0 0 0 0 0 0 0 2
0.8751 -0.0444 -0.3264 S 0 0 0 0 0 0 0 0 0 0 0 3
1.3459 -0.1055 1.1345 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.1831 -1.1680 -0.5690 O 0 0 0 0 0 0 0 0 0 0 0 5
-1.0105 1.1348 0.0115 H 0 0 0 0 0 0 0 0 0 0 0 6
-3.1084 -0.0451 -0.2086 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.7150 -0.6921 0.0993 H 0 0 0 0 0 0 0 0 0 0 0 8
7 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
1 8 0 0 0 0
M END
$$$$
sulfurousacid.sdf
COSMOtherm 3D 0
9 7 0 0 0 0 0 0 0 0 0 V2000
-2.2515 -0.0001 0.3788 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.5222 0.0116 1.3157 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0823 -0.0061 -0.1323 H 0 0 0 0 0 0 0 0 0 0 0 3
0.9256 0.0012 -0.2169 S 0 0 0 0 0 0 0 0 0 0 0 4
-0.0693 -1.2979 -0.6307 O 0 0 0 0 0 0 0 0 0 0 0 5
-0.0817 1.2839 -0.6496 O 0 0 0 0 0 0 0 0 0 0 0 6
1.0223 0.0125 1.2879 O 0 0 0 0 0 0 0 0 0 0 0 7
-0.9597 -1.1324 -0.1988 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.9720 1.1131 -0.2171 H 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
6 9 0 0 0 0
M END
$$$$
tert-butanol-anion.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-2.6693 -0.0044 0.0878 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.4218 -0.0208 0.5344 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.5795 0.0638 -0.8775 H 0 0 0 0 0 0 0 0 0 0 0 3
0.6201 0.0000 -0.0066 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4773 1.2893 -0.8457 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4914 -1.2346 -0.9264 C 0 0 0 0 0 0 0 0 0 0 0 6
1.9936 -0.0132 0.6840 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2402 1.3548 -1.6384 H 0 0 0 0 0 0 0 0 0 0 0 8
0.6123 -2.1563 -0.3362 H 0 0 0 0 0 0 0 0 0 0 0 9
2.0925 0.8587 1.3490 H 0 0 0 0 0 0 0 0 0 0 0 10
1.2468 -1.2354 -1.7290 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5155 1.3254 -1.3198 H 0 0 0 0 0 0 0 0 0 0 0 12
0.5769 2.1727 -0.1960 H 0 0 0 0 0 0 0 0 0 0 0 13
2.1033 -0.9240 1.2927 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.5061 -1.2560 -1.3911 H 0 0 0 0 0 0 0 0 0 0 0 15
2.8168 0.0154 -0.0477 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.3770 -0.0393 1.0087 O 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
13 5 0 0 0 0
9 6 0 0 0 0
11 6 0 0 0 0
15 6 0 0 0 0
10 7 0 0 0 0
14 7 0 0 0 0
16 7 0 0 0 0
2 17 0 0 0 0
4 17 0 0 0 0
M END
$$$$
tert-butanol.sdf
COSMOtherm 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-2.9378 0.0008 0.0920 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.2268 -0.7770 -0.4184 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.2135 0.7599 -0.4527 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7440 0.0005 -0.0308 C 0 0 0 0 0 0 0 0 0 0 0 4
0.5994 1.2815 -0.8674 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5960 -1.2458 -0.9177 C 0 0 0 0 0 0 0 0 0 0 0 6
2.0843 -0.0160 0.7078 C 0 0 0 0 0 0 0 0 0 0 0 7
1.3747 1.3361 -1.6468 H 0 0 0 0 0 0 0 0 0 0 0 8

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1
2
3      0.6815  -2.1592  -0.3109 H  0  0  0  0  0  0  0  0  0  0  9
4      2.1727  0.8631  1.3633 H  0  0  0  0  0  0  0  0  0  0  10
5      1.3726  -1.2730  -1.6973 H  0  0  0  0  0  0  0  0  0  0  11
6     -0.3820  1.3111  -1.3652 H  0  0  0  0  0  0  0  0  0  0  12
7      0.6903  2.1700  -0.2254 H  0  0  0  0  0  0  0  0  0  0  13
8      2.1712  -0.9218  1.3260 H  0  0  0  0  0  0  0  0  0  0  14
9     -0.3846  -1.2518  -1.4180 H  0  0  0  0  0  0  0  0  0  0  15
10     2.9214  -0.0015  -0.0049 H  0  0  0  0  0  0  0  0  0  0  16
11    -0.2728  -0.0188  1.0092 O  0  0  0  0  0  0  0  0  0  0  17
12    -1.1638  -0.0107  0.5760 H  0  0  0  0  0  0  0  0  0  0  18
13     2  1  0  0  0  0
14     3  1  0  0  0  0
15     5  4  0  0  0  0
16     6  4  0  0  0  0
17     7  4  0  0  0  0
18    17  4  0  0  0  0
19     8  5  0  0  0  0
20    12  5  0  0  0  0
21    13  5  0  0  0  0
22     9  6  0  0  0  0
23    11  6  0  0  0  0
24    15  6  0  0  0  0
25    10  7  0  0  0  0
26    14  7  0  0  0  0
27    16  7  0  0  0  0
28    17  18  0  0  0  0
29 M END
30 $$$
31 thymine-anion.sdf
32 COSMOTHERM 3D 0
33
34 17 16 0 0 0 0 0 0 0 0 0 0 V2000
35   -3.7378  -0.0331  -1.2111 O  0  0  0  0  0  0  0  0  0  0  1
36   -2.7966  -0.0211  -0.8297 H  0  0  0  0  0  0  0  0  0  0  2
37   -3.9778  0.9064  -1.2859 H  0  0  0  0  0  0  0  0  0  0  3
38   -0.1453  -0.0164  -1.2008 C  0  0  0  0  0  0  0  0  0  0  4
39    1.2114  -0.0046  -0.9356 C  0  0  0  0  0  0  0  0  0  0  5
40    1.6108  0.0075  0.4488 C  0  0  0  0  0  0  0  0  0  0  6
41    0.5393  0.0056  1.3502 N  0  0  0  0  0  0  0  0  0  0  7
42   -0.8289  -0.0083  1.0333 C  0  0  0  0  0  0  0  0  0  0  8
43   -1.1548  -0.0192  -0.2910 N  0  0  0  0  0  0  0  0  0  0  9
44    2.7886  0.0188  0.8810 O  0  0  0  0  0  0  0  0  0  0  10
45   -1.6703  -0.0102  1.9637 O  0  0  0  0  0  0  0  0  0  0  11
46    2.2619  -0.0025  -2.0100 C  0  0  0  0  0  0  0  0  0  0  12
47   -0.4755  -0.0249  -2.2461 H  0  0  0  0  0  0  0  0  0  0  13
48    0.7771  0.0134  2.3432 H  0  0  0  0  0  0  0  0  0  0  14
49    2.9337  -0.8714  -1.9219 H  0  0  0  0  0  0  0  0  0  0  15
50    2.8988  0.8952  -1.9547 H  0  0  0  0  0  0  0  0  0  0  16
51    1.7983  -0.0295  -3.0059 H  0  0  0  0  0  0  0  0  0  0  17
52     2  1  0  0  0  0
53     3  1  0  0  0  0
54     5  4  0  0  0  0
55     9  4  0  0  0  0
56    13  4  0  0  0  0
57     6  5  0  0  0  0
58    12  5  0  0  0  0
59     7  6  0  0  0  0
60    10  6  0  0  0  0
61     8  7  0  0  0  0
62    14  7  0  0  0  0
63     9  8  0  0  0  0
64    11  8  0  0  0  0
65    15  12  0  0  0  0
66    16  12  0  0  0  0
67    12  17  0  0  0  0
68 M END
69 $$$
70 thymine.sdf
71 COSMOTHERM 3D 0
72
73 18 17 0 0 0 0 0 0 0 0 0 0 V2000
74   -3.7154  -0.0052  1.2303 O  0  0  0  0  0  0  0  0  0  0  1
75   -4.2437  -0.7725  0.9453 H  0  0  0  0  0  0  0  0  0  0  2
76   -4.2467  0.7668  0.9637 H  0  0  0  0  0  0  0  0  0  0  3
77   -0.1090  0.0032  1.2297 C  0  0  0  0  0  0  0  0  0  0  4
78    1.2269  0.0013  0.9517 C  0  0  0  0  0  0  0  0  0  0  5
79    1.6299  -0.0013  -0.4472 C  0  0  0  0  0  0  0  0  0  0  6
80    0.5667  -0.0016  -1.3677 N  0  0  0  0  0  0  0  0  0  0  7
81   -0.7943  0.0018  -1.0914 C  0  0  0  0  0  0  0  0  0  0  8
82   -1.0804  0.0035  0.2592 N  0  0  0  0  0  0  0  0  0  0  9
83    2.8011  -0.0039  -0.8593 O  0  0  0  0  0  0  0  0  0  0  10
84   -1.6594  0.0029  -1.9749 O  0  0  0  0  0  0  0  0  0  0  11
85    2.2866  0.0008  2.0136 C  0  0  0  0  0  0  0  0  0  0  12
86   -0.4865  0.0045  2.2526 H  0  0  0  0  0  0  0  0  0  0  13
87    0.8202  -0.0028  -2.3569 H  0  0  0  0  0  0  0  0  0  0  14
88   -2.0869  0.0033  0.5385 H  0  0  0  0  0  0  0  0  0  0  15
89    2.9358  0.8853  1.9255 H  0  0  0  0  0  0  0  0  0  0  16
90    2.9362  -0.8832  1.9240 H  0  0  0  0  0  0  0  0  0  0  17
91    1.8360  -0.0001  3.0144 H  0  0  0  0  0  0  0  0  0  0  18
92     2  1  0  0  0  0
93     3  1  0  0  0  0
94     5  4  0  0  0  0
95     9  4  0  0  0  0
96    13  4  0  0  0  0
97     6  5  0  0  0  0
98    12  5  0  0  0  0
99     7  6  0  0  0  0
100    10  6  0  0  0  0
101     8  7  0  0  0  0
102    14  7  0  0  0  0
103     9  8  0  0  0  0
104    11  8  0  0  0  0
105    15  9  0  0  0  0
106    16  12  0  0  0  0
107    17  12  0  0  0  0
```



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2
3 12 18 0 0 0 0
4 M END
5 $$$
6 trans-5-formyluracil-anion.sdf
7 COSMOtherm 3D 0
8
9 16 15 0 0 0 0 0 0 0 0 0 V2000
10 -3.5639 -0.0749 -1.9373 O 0 0 0 0 0 0 0 0 0 0 0 1
11 -2.7607 -0.0286 -1.3330 H 0 0 0 0 0 0 0 0 0 0 0 2
12 -3.7862 0.8555 -2.1130 H 0 0 0 0 0 0 0 0 0 0 0 3
13 -0.0736 0.0085 -0.9682 C 0 0 0 0 0 0 0 0 0 0 0 4
14 1.1791 0.0012 -0.3353 C 0 0 0 0 0 0 0 0 0 0 0 5
15 1.2089 -0.0051 1.1162 C 0 0 0 0 0 0 0 0 0 0 0 6
16 -0.0683 0.0000 1.6896 N 0 0 0 0 0 0 0 0 0 0 0 7
17 -1.2956 0.0078 1.0157 C 0 0 0 0 0 0 0 0 0 0 0 8
18 -1.2627 0.0123 -0.3690 N 0 0 0 0 0 0 0 0 0 0 0 9
19 2.2176 -0.0140 1.8467 O 0 0 0 0 0 0 0 0 0 0 0 10
20 -2.3557 0.0106 1.6624 O 0 0 0 0 0 0 0 0 0 0 0 11
21 2.4122 -0.0005 -1.0870 C 0 0 0 0 0 0 0 0 0 0 0 12
22 -0.0906 0.0125 -2.0636 H 0 0 0 0 0 0 0 0 0 0 0 13
23 -0.1107 -0.0041 2.7104 H 0 0 0 0 0 0 0 0 0 0 0 14
24 2.5065 0.0065 -2.3280 O 0 0 0 0 0 0 0 0 0 0 0 15
25 3.3349 -0.0087 -0.4649 H 0 0 0 0 0 0 0 0 0 0 0 16
26
27 2 1 0 0 0 0
28 3 1 0 0 0 0
29 5 4 0 0 0 0
30 9 4 0 0 0 0
31 13 4 0 0 0 0
32 6 5 0 0 0 0
33 12 5 0 0 0 0
34 7 6 0 0 0 0
35 10 6 0 0 0 0
36 8 7 0 0 0 0
37 14 7 0 0 0 0
38 9 8 0 0 0 0
39 11 8 0 0 0 0
40 15 12 0 0 0 0
41 12 16 0 0 0 0
42 M END
43 $$$
44 trans-5-formyluracil.sdf
45 COSMOtherm 3D 0
46
47 17 16 0 0 0 0 0 0 0 0 V2000
48 -1.9653 3.4283 0.0117 O 0 0 0 0 0 0 0 0 0 0 0 1
49 -2.0287 3.8719 -0.8538 H 0 0 0 0 0 0 0 0 0 0 0 2
50 -1.7122 4.1363 0.6318 H 0 0 0 0 0 0 0 0 0 0 0 3
51 -0.9856 0.0203 0.0056 C 0 0 0 0 0 0 0 0 0 0 0 4
52 -0.3280 -1.1912 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
53 1.1326 -1.2003 -0.0014 C 0 0 0 0 0 0 0 0 0 0 0 6
54 1.7080 0.0836 -0.0045 N 0 0 0 0 0 0 0 0 0 0 0 7
55 1.0560 1.3056 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 8
56 -0.3402 1.2019 0.0046 N 0 0 0 0 0 0 0 0 0 0 0 9
57 1.8569 -2.2014 -0.0006 O 0 0 0 0 0 0 0 0 0 0 0 10
58 1.6372 2.3874 -0.0011 O 0 0 0 0 0 0 0 0 0 0 0 11
59 -1.0698 -2.4489 0.0020 C 0 0 0 0 0 0 0 0 0 0 0 12
60 -2.0759 0.0662 0.0105 H 0 0 0 0 0 0 0 0 0 0 0 13
61 2.7292 0.1248 -0.0065 H 0 0 0 0 0 0 0 0 0 0 0 14
62 -0.8890 2.1010 0.0089 H 0 0 0 0 0 0 0 0 0 0 0 15
63 -2.3020 -2.5384 -0.0016 O 0 0 0 0 0 0 0 0 0 0 0 16
64 -0.4376 -3.3624 0.0072 H 0 0 0 0 0 0 0 0 0 0 0 17
65
66 2 1 0 0 0 0
67 3 1 0 0 0 0
68 5 4 0 0 0 0
69 9 4 0 0 0 0
70 13 4 0 0 0 0
71 6 5 0 0 0 0
72 12 5 0 0 0 0
73 7 6 0 0 0 0
74 10 6 0 0 0 0
75 8 7 0 0 0 0
76 14 7 0 0 0 0
77 9 8 0 0 0 0
78 11 8 0 0 0 0
79 15 9 0 0 0 0
80 16 12 0 0 0 0
81 12 17 0 0 0 0
82 M END
83 $$$
84 trichloroaceticacid-anion.sdf
85 COSMOtherm 3D 0
86
87 10 8 0 0 0 0 0 0 0 0 V2000
88 -4.3883 -0.0641 0.0317 O 0 0 0 0 0 0 0 0 0 0 0 1
89 -3.4013 -0.2175 -0.0096 H 0 0 0 0 0 0 0 0 0 0 0 2
90 -4.4923 0.8734 -0.2056 H 0 0 0 0 0 0 0 0 0 0 0 3
91 0.9349 -1.0183 1.4816 Cl 0 0 0 0 0 0 0 0 0 0 0 4
92 0.6035 -0.0050 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 5
93 -0.9517 0.3955 -0.0296 C 0 0 0 0 0 0 0 0 0 0 0 6
94 -1.2130 1.6101 -0.0268 O 0 0 0 0 0 0 0 0 0 0 0 7
95 -1.7100 -0.6097 -0.0540 O 0 0 0 0 0 0 0 0 0 0 0 8
96 1.0007 -0.9865 -1.4847 Cl 0 0 0 0 0 0 0 0 0 0 0 9
97 1.7063 1.4313 0.0410 Cl 0 0 0 0 0 0 0 0 0 0 0 10
98
99 2 1 0 0 0 0
100 3 1 0 0 0 0
101 5 4 0 0 0 0
102 6 5 0 0 0 0
103 9 5 0 0 0 0
104 7 6 0 0 0 0
105 8 6 0 0 0 0
106 5 10 0 0 0 0
107 M END
108 $$$
109 trichloroaceticacid.sdf
110 COSMOtherm 3D 0

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11 9 0 0 0 0 0 0 0 0 0 V2000
-4.1733 -0.0159 0.0556 O 0 0 0 0 0 0 0 0 0 0 1
-4.4380 -0.6336 -0.6510 H 0 0 0 0 0 0 0 0 0 0 2
-4.5322 0.8495 -0.2143 H 0 0 0 0 0 0 0 0 0 0 3
0.9388 1.4765 1.0174 Cl 0 0 0 0 0 0 0 0 0 0 4
0.6269 -0.0001 0.0110 C 0 0 0 0 0 0 0 0 0 0 5
-0.8774 0.0046 -0.4470 C 0 0 0 0 0 0 0 0 0 0 6
-1.1849 0.0122 -1.6246 O 0 0 0 0 0 0 0 0 0 0 7
-1.6818 -0.0018 0.5933 O 0 0 0 0 0 0 0 0 0 0 8
0.9358 -1.4903 0.9972 Cl 0 0 0 0 0 0 0 0 0 0 9
1.7188 0.0086 -1.4104 Cl 0 0 0 0 0 0 0 0 0 0 10
-2.6879 0.0011 0.2964 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 5 0 0 0 0 0
9 5 0 0 0 0 0
10 5 0 0 0 0 0
7 6 0 0 0 0 0
8 6 0 0 0 0 0
8 11 0 0 0 0 0
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M END

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uracil--anion.sdf

COSMOTHERM

3D

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14 13 0 0 0 0 0 0 0 0 0 V2000
-3.7266 0.6094 0.0010 O 0 0 0 0 0 0 0 0 0 0 1
-2.7252 0.4471 0.0089 H 0 0 0 0 0 0 0 0 0 0 2
-3.8940 1.0380 -0.8558 H 0 0 0 0 0 0 0 0 0 0 3
-0.2351 1.4086 0.0426 C 0 0 0 0 0 0 0 0 0 0 4
1.1447 1.4486 0.0162 C 0 0 0 0 0 0 0 0 0 0 5
1.8718 0.2139 -0.0134 C 0 0 0 0 0 0 0 0 0 0 6
1.0378 -0.9145 -0.0114 N 0 0 0 0 0 0 0 0 0 0 7
-0.3672 -0.9230 0.0155 C 0 0 0 0 0 0 0 0 0 0 8
-1.0002 0.2899 0.0438 N 0 0 0 0 0 0 0 0 0 0 9
3.1171 0.0682 -0.0389 O 0 0 0 0 0 0 0 0 0 0 10
-0.9695 -2.0203 0.0139 O 0 0 0 0 0 0 0 0 0 0 11
1.6909 2.3902 0.0171 H 0 0 0 0 0 0 0 0 0 0 12
-0.7979 2.3477 0.0653 H 0 0 0 0 0 0 0 0 0 0 13
1.4974 -1.8263 -0.0312 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
13 4 0 0 0 0 0
6 5 0 0 0 0 0
12 5 0 0 0 0 0
7 6 0 0 0 0 0
10 6 0 0 0 0 0
8 7 0 0 0 0 0
9 8 0 0 0 0 0
11 8 0 0 0 0 0
7 14 0 0 0 0 0
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M END

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uracil.sdf

COSMOTHERM

3D

0

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15 14 0 0 0 0 0 0 0 0 0 V2000
-3.6919 0.0025 0.6561 O 0 0 0 0 0 0 0 0 0 0 1
-4.1805 -0.6598 0.1345 H 0 0 0 0 0 0 0 0 0 0 2
-4.1114 0.8510 0.4241 H 0 0 0 0 0 0 0 0 0 0 3
-0.1782 -0.0119 1.4571 C 0 0 0 0 0 0 0 0 0 0 4
1.1837 -0.0032 1.4533 C 0 0 0 0 0 0 0 0 0 0 5
1.8946 0.0037 0.1947 C 0 0 0 0 0 0 0 0 0 0 6
1.0522 0.0039 -0.9355 N 0 0 0 0 0 0 0 0 0 0 7
-0.3362 -0.0038 -0.9562 C 0 0 0 0 0 0 0 0 0 0 8
-0.9140 -0.0137 0.3032 N 0 0 0 0 0 0 0 0 0 0 9
3.1270 0.0097 0.0451 O 0 0 0 0 0 0 0 0 0 0 10
-0.9926 -0.0027 -2.0018 O 0 0 0 0 0 0 0 0 0 0 11
1.7506 -0.0030 2.3807 H 0 0 0 0 0 0 0 0 0 0 12
-0.7604 -0.0182 2.3782 H 0 0 0 0 0 0 0 0 0 0 13
1.5100 0.0092 -1.8485 H 0 0 0 0 0 0 0 0 0 0 14
-1.9588 -0.0144 0.3523 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
13 4 0 0 0 0 0
6 5 0 0 0 0 0
12 5 0 0 0 0 0
7 6 0 0 0 0 0
10 6 0 0 0 0 0
8 7 0 0 0 0 0
14 7 0 0 0 0 0
9 8 0 0 0 0 0
11 8 0 0 0 0 0
9 15 0 0 0 0 0
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M END

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S4 c) Di-solvated Acids & Anions

2,2,2-trichloroethanol--anion.sdf

COSMOTHERM

3D

0

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14 11 0 0 0 0 0 0 0 0 0 V2000
-2.3352 0.2149 2.8476 O 0 0 0 0 0 0 0 0 0 0 1
-1.4184 0.2833 2.3839 H 0 0 0 0 0 0 0 0 0 0 2
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-2.8748 -0.3169 2.2388 H 0 0 0 0 0 0 0 0 0 0 0 3
2.3407 0.2110 2.8389 O 0 0 0 0 0 0 0 0 0 0 0 4
1.4219 0.2831 2.3795 H 0 0 0 0 0 0 0 0 0 0 0 5
2.8888 -0.2823 2.2058 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0009 0.0994 -0.6836 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0018 1.0625 0.5386 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0048 1.0717 -2.2372 Cl 0 0 0 0 0 0 0 0 0 0 0 9
1.4761 -0.9691 -0.6763 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-1.4736 -0.9753 -0.6726 Cl 0 0 0 0 0 0 0 0 0 0 0 11
0.0009 0.4229 1.7418 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.8979 1.7026 0.3713 H 0 0 0 0 0 0 0 0 0 0 0 13
0.8910 1.7067 0.3692 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
2,2,2-trichloroethanol.sdf
COSMOtherm 3D 0
15 12 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
1.2372 -4.1821 -0.0446 O 0 0 0 0 0 0 0 0 0 0 0 0 1
1.9033 -3.8530 0.5855 H 0 0 0 0 0 0 0 0 0 0 0 0 2
1.6490 -4.0684 -0.9201 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.2727 -3.1606 0.2053 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.6546 -3.6927 0.9258 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.3330 -3.4876 0.1130 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.0521 0.9057 0.1037 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.6703 0.0999 1.2061 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.4362 1.8056 0.8668 Cl 0 0 0 0 0 0 0 0 0 0 0 0 9
0.6983 -0.1951 -1.1861 Cl 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.0786 2.0994 -0.6640 Cl 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.7863 -0.6014 0.7308 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.9919 0.8333 1.9615 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.0866 -0.5611 1.6603 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.5155 -1.5444 0.5009 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
12 15 0 0 0 0
M END
$$$$
2,2-dimethylpropanoicacid-anion.sdf
COSMOtherm 3D 0
22 19 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-4.6509 0.4669 0.7999 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.9291 0.1017 0.2070 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.3280 1.3454 1.0640 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-2.7486 -0.6201 -0.7992 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.8205 -0.6194 -0.3402 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.5958 -0.0802 -1.5955 H 0 0 0 0 0 0 0 0 0 0 0 0 6
2.8253 0.8076 -0.7289 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.8862 0.0497 0.2209 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.8408 0.7671 1.5877 C 0 0 0 0 0 0 0 0 0 0 0 0 9
2.3990 -1.3925 0.4169 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.4345 -0.0095 -0.3515 C 0 0 0 0 0 0 0 0 0 0 0 0 11
0.1704 0.5557 -1.4475 O 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.4235 -0.6532 0.3588 O 0 0 0 0 0 0 0 0 0 0 0 0 13
3.8429 0.8408 -0.3078 H 0 0 0 0 0 0 0 0 0 0 0 0 14
2.8759 0.3192 -1.7128 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2.4839 1.8408 -0.8868 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.8478 0.8025 2.0336 H 0 0 0 0 0 0 0 0 0 0 0 0 17
1.1713 0.2406 2.2821 H 0 0 0 0 0 0 0 0 0 0 0 0 18
1.4814 1.8028 1.4814 H 0 0 0 0 0 0 0 0 0 0 0 0 19
3.4127 -1.3813 0.8484 H 0 0 0 0 0 0 0 0 0 0 0 0 20
1.7385 -1.9520 1.0936 H 0 0 0 0 0 0 0 0 0 0 0 0 21
2.4455 -1.9316 -0.5423 H 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
17 9 0 0 0 0
18 9 0 0 0 0
19 9 0 0 0 0
20 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
10 22 0 0 0 0
M END
$$$$

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1
2
3 2,2-dimethylpropanoicacid.sdf
4 COSMOTHERM      3D      0
5
6 23 20 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
7 -1.2902 3.2387 0.0671 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
8 -1.3329 2.2469 -0.0082 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
9 -1.7079 3.5781 -0.7446 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
10 1.3522 2.9043 0.0398 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
11 0.4000 3.2285 -0.0085 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
12 1.7902 3.2433 -0.7618 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
13 -1.5118 -2.2240 0.0610 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
14 -0.0593 -1.7286 0.0012 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
15 0.6145 -2.2276 -1.2994 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
16 0.7261 -2.2477 1.2275 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
17 -0.0297 -0.1941 0.0008 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
18 -1.0556 0.5003 -0.0176 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
19 1.2004 0.3130 0.0157 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
20 -1.5220 -3.3238 0.0576 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
21 -2.0158 -1.8787 0.9748 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
22 -2.0925 -1.8716 -0.8027 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
23 0.5868 -3.3269 -1.3222 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
24 1.6629 -1.9058 -1.3549 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
25 0.0869 -1.8550 -2.1902 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
26 0.6996 -3.3473 1.2356 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
27 1.7752 -1.9264 1.1959 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
28 0.2798 -1.8896 2.1673 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
29 1.2066 1.3519 0.0016 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
30
31 2 1 0 0 0 0 0
32 3 1 0 0 0 0 0
33 5 4 0 0 0 0 0
34 6 4 0 0 0 0 0
35 8 7 0 0 0 0 0
36 14 7 0 0 0 0 0
37 15 7 0 0 0 0 0
38 16 7 0 0 0 0 0
39 9 8 0 0 0 0 0
40 10 8 0 0 0 0 0
41 11 8 0 0 0 0 0
42 17 9 0 0 0 0 0
43 18 9 0 0 0 0 0
44 19 9 0 0 0 0 0
45 20 10 0 0 0 0 0
46 21 10 0 0 0 0 0
47 22 10 0 0 0 0 0
48 12 11 0 0 0 0 0
49 13 11 0 0 0 0 0
50 13 23 0 0 0 0 0
51 M END
52 $$$$

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53 2,3,4,6-tetrachlorophenol-anion.sdf
54 COSMOTHERM      3D      0
55
56 18 16 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
57 -1.1870 2.6366 4.3085 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
58 -0.8420 1.6995 4.2754 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
59 -1.8494 2.6234 5.0204 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
60 -0.2269 0.0697 4.2771 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3004 -0.3688 3.3644 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.7283 0.0921 4.4622 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.8215 0.0147 -0.5909 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.2912 -0.4193 0.6163 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.1015 -0.6839 0.8395 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.9136 -0.4439 -0.3292 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.3994 -0.0085 -1.5566 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.9793 0.2248 -1.6845 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.5933 -1.0984 1.9506 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.6386 -0.7374 -0.1409 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.4671 0.2541 -2.9316 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.6873 0.7744 -3.2064 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2.3993 -0.6913 1.9735 Cl 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2.8920 0.1901 -0.6904 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
61
62 2 1 0 0 0 0 0
63 3 1 0 0 0 0 0
64 5 4 0 0 0 0 0
65 6 4 0 0 0 0 0
66 8 7 0 0 0 0 0
67 12 7 0 0 0 0 0
68 9 8 0 0 0 0 0
69 17 8 0 0 0 0 0
70 10 9 0 0 0 0 0
71 13 9 0 0 0 0 0
72 11 10 0 0 0 0 0
73 14 10 0 0 0 0 0
74 12 11 0 0 0 0 0
75 15 11 0 0 0 0 0
76 16 12 0 0 0 0 0
77 7 18 0 0 0 0 0
78 M END
79 $$$$

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80 2,3,4,6-tetrachlorophenol.sdf
81 COSMOTHERM      3D      0
82
83 19 17 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
84 -1.2725 -5.3102 -1.1426 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
85 -0.8371 -6.1063 -1.4985 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
86 -1.4682 -4.7706 -1.9299 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
87 0.2782 -4.0988 0.7202 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
88 -0.3062 -4.5280 0.0286 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
89 -0.2093 -4.1816 1.5587 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
90 -0.4825 -0.2025 0.1592 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
91 -0.8924 1.1385 0.0448 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
92 0.0742 2.1422 -0.1027 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
93 1.4288 1.8112 -0.1352 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
94 1.8152 0.4828 -0.0199 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
95 0.8837 -0.5709 0.1315 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12

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-0.3809    3.8343   -0.2490 Cl  0 0 0 0 0 0 0 0 0 0 13
 1.3569   -1.8172    0.2251 O  0 0 0 0 0 0 0 0 0 0 14
-1.6787   -1.4707    0.3367 Cl  0 0 0 0 0 0 0 0 0 0 15
-2.5933    1.5445    0.0838 Cl  0 0 0 0 0 0 0 0 0 0 16
  2.1790    2.5918   -0.2484 H  0 0 0 0 0 0 0 0 0 0 17
  3.5298    0.0882   -0.0611 Cl  0 0 0 0 0 0 0 0 0 0 18
  0.7005   -2.5838    0.4112 H  0 0 0 0 0 0 0 0 0 0 19
 2  1  0  0  0  0
 3  1  0  0  0  0
 5  4  0  0  0  0
 6  4  0  0  0  0
 8  7  0  0  0  0
12  7  0  0  0  0
15  7  0  0  0  0
 9  8  0  0  0  0
16  8  0  0  0  0
10  9  0  0  0  0
13  9  0  0  0  0
11 10  0  0  0  0
17 10  0  0  0  0
12 11  0  0  0  0
18 11  0  0  0  0
14 12  0  0  0  0
14 19  0  0  0  0
M  END
$$$$
2,3,4-trichlorophenol-anion.sdf
COSMOtherm      3D              0
18 16  0  0  0  0  0  0  0  0  0  0 v2000
 -1.8845    0.7401    5.1930 O  0 0 0 0 0 0 0 0 0 0 1
 -1.0308    0.2814    4.9391 H  0 0 0 0 0 0 0 0 0 0 2
 -1.9076    1.5375    4.6370 H  0 0 0 0 0 0 0 0 0 0 3
  0.4359   -0.5458    4.5701 O  0 0 0 0 0 0 0 0 0 0 4
  0.7165   -0.3986    3.5883 H  0 0 0 0 0 0 0 0 0 0 5
  0.2923   -1.5048    4.6537 H  0 0 0 0 0 0 0 0 0 0 6
 -0.9538   -0.2263    1.2465 C  0 0 0 0 0 0 0 0 0 0 7
 -1.7958   -0.2106    0.1411 C  0 0 0 0 0 0 0 0 0 0 8
 -1.2770   -0.0940   -1.1517 C  0 0 0 0 0 0 0 0 0 0 9
  0.1121    0.0128   -1.3299 C  0 0 0 0 0 0 0 0 0 0 10
  0.9586   -0.0034   -0.2137 C  0 0 0 0 0 0 0 0 0 0 11
  0.4678   -0.1241    1.1354 C  0 0 0 0 0 0 0 0 0 0 12
 -2.3880   -0.0810   -2.5296 Cl  0 0 0 0 0 0 0 0 0 0 13
  1.2682   -0.1360    2.1534 O  0 0 0 0 0 0 0 0 0 0 14
 -1.3817   -0.3106    2.2474 H  0 0 0 0 0 0 0 0 0 0 15
 -2.8754   -0.2905    0.2755 H  0 0 0 0 0 0 0 0 0 0 16
  0.7819    0.1647   -2.9541 Cl  0 0 0 0 0 0 0 0 0 0 17
  2.7064    0.1282   -0.4140 Cl  0 0 0 0 0 0 0 0 0 0 18
 2  1  0  0  0  0
 3  1  0  0  0  0
 5  4  0  0  0  0
 6  4  0  0  0  0
 8  7  0  0  0  0
12  7  0  0  0  0
15  7  0  0  0  0
 9  8  0  0  0  0
16  8  0  0  0  0
10  9  0  0  0  0
13  9  0  0  0  0
11 10  0  0  0  0
17 10  0  0  0  0
12 11  0  0  0  0
14 12  0  0  0  0
11 18  0  0  0  0
M  END
$$$$
2,3,4-trichlorophenol.sdf
COSMOtherm      3D              0
19 17  0  0  0  0  0  0  0  0  0 v2000
 -1.0125    0.4387   -6.2050 O  0 0 0 0 0 0 0 0 0 0 1
 -0.8013   -0.4095   -6.6356 H  0 0 0 0 0 0 0 0 0 0 2
 -0.9936    1.0902   -6.9294 H  0 0 0 0 0 0 0 0 0 0 3
  0.6519    1.0613   -4.1780 O  0 0 0 0 0 0 0 0 0 0 4
  0.0698    0.8257   -4.9620 H  0 0 0 0 0 0 0 0 0 0 5
  1.5636    1.0699   -4.5201 H  0 0 0 0 0 0 0 0 0 0 6
  0.1490    1.9783    0.4071 C  0 0 0 0 0 0 0 0 0 0 7
  0.2807    1.3986   -0.8511 C  0 0 0 0 0 0 0 0 0 0 8
  0.2627    0.0007   -1.0099 C  0 0 0 0 0 0 0 0 0 0 9
  0.1076   -0.7997    0.1456 C  0 0 0 0 0 0 0 0 0 0 10
 -0.0257   -0.2181    1.4169 C  0 0 0 0 0 0 0 0 0 0 11
 -0.0034    1.1801    1.5415 C  0 0 0 0 0 0 0 0 0 0 12
  0.3873   -0.6087   -2.2035 O  0 0 0 0 0 0 0 0 0 0 13
  0.0850   -2.5435   -0.0532 Cl  0 0 0 0 0 0 0 0 0 0 14
 -0.2167   -1.2336    2.8321 Cl  0 0 0 0 0 0 0 0 0 0 15
 -0.1671    1.9555    3.1163 Cl  0 0 0 0 0 0 0 0 0 0 16
  0.1655    3.0628    0.5120 H  0 0 0 0 0 0 0 0 0 0 17
  0.3972    2.0302   -1.7321 H  0 0 0 0 0 0 0 0 0 0 18
  0.4971    0.0733   -2.9629 H  0 0 0 0 0 0 0 0 0 0 19
 2  1  0  0  0  0
 3  1  0  0  0  0
 5  4  0  0  0  0
 6  4  0  0  0  0
 8  7  0  0  0  0
12  7  0  0  0  0
17  7  0  0  0  0
 9  8  0  0  0  0
18  8  0  0  0  0
10  9  0  0  0  0
13  9  0  0  0  0
11 10  0  0  0  0
14 10  0  0  0  0
12 11  0  0  0  0
15 11  0  0  0  0
16 12  0  0  0  0
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1
2
3 13 19 0 0 0 0
4 M END
5 $$$
6 2,3-dichlorophenol-anion.sdf
7 COSMOTHERM 3D 0
8
9 18 16 0 0 0 0 0 0 0 0 V2000
10 -1.0148 0.6403 5.1994 O 0 0 0 0 0 0 0 0 0 0 0 1
11 -0.2368 0.2272 4.7212 H 0 0 0 0 0 0 0 0 0 0 0 2
12 -1.2014 1.4549 4.7020 H 0 0 0 0 0 0 0 0 0 0 0 3
13 1.1119 -0.5278 3.9650 O 0 0 0 0 0 0 0 0 0 0 0 4
14 1.1246 -0.3490 2.9457 H 0 0 0 0 0 0 0 0 0 0 0 5
15 1.0303 -1.4935 4.0554 H 0 0 0 0 0 0 0 0 0 0 0 6
16 -1.1023 -0.2051 1.1423 C 0 0 0 0 0 0 0 0 0 0 0 7
17 -2.2006 -0.2379 0.2884 C 0 0 0 0 0 0 0 0 0 0 0 8
18 -2.0498 -0.1546 -1.1027 C 0 0 0 0 0 0 0 0 0 0 0 9
19 -0.7538 -0.0321 -1.6125 C 0 0 0 0 0 0 0 0 0 0 0 10
20 0.3634 0.0034 -0.7743 C 0 0 0 0 0 0 0 0 0 0 0 11
21 0.2390 -0.0827 0.6595 C 0 0 0 0 0 0 0 0 0 0 0 12
22 -2.9058 -0.1791 -1.7751 H 0 0 0 0 0 0 0 0 0 0 0 13
23 1.2787 -0.0463 1.4350 O 0 0 0 0 0 0 0 0 0 0 0 14
24 -1.2442 -0.2642 2.2236 H 0 0 0 0 0 0 0 0 0 0 0 15
25 -3.2053 -0.3314 0.7065 H 0 0 0 0 0 0 0 0 0 0 0 16
26 -0.5636 0.0779 -3.3772 Cl 0 0 0 0 0 0 0 0 0 0 0 17
27 1.9962 0.1589 -1.4318 Cl 0 0 0 0 0 0 0 0 0 0 0 18
28
29 2 1 0 0 0 0
30 3 1 0 0 0 0
31 5 4 0 0 0 0
32 6 4 0 0 0 0
33 8 7 0 0 0 0
34 12 7 0 0 0 0
35 15 7 0 0 0 0
36 9 8 0 0 0 0
37 16 8 0 0 0 0
38 10 9 0 0 0 0
39 13 9 0 0 0 0
40 11 10 0 0 0 0
41 17 10 0 0 0 0
42 12 11 0 0 0 0
43 14 12 0 0 0 0
44 11 18 0 0 0 0
45 M END
46 $$$
47 2,3-dichlorophenol.sdf
48 COSMOTHERM 3D 0
49
50 19 17 0 0 0 0 0 0 0 0 V2000
51 -5.6465 -0.4216 1.0804 O 0 0 0 0 0 0 0 0 0 0 0 1
52 -5.7636 -1.3895 1.0754 H 0 0 0 0 0 0 0 0 0 0 0 2
53 -6.5449 -0.0689 0.9449 H 0 0 0 0 0 0 0 0 0 0 0 3
54 -3.8703 0.4728 -0.7449 O 0 0 0 0 0 0 0 0 0 0 0 4
55 -4.5572 0.1198 -0.1036 H 0 0 0 0 0 0 0 0 0 0 0 5
56 -4.2300 0.3049 -1.6342 H 0 0 0 0 0 0 0 0 0 0 0 6
57 0.3573 2.4523 -0.0119 C 0 0 0 0 0 0 0 0 0 0 0 7
58 -0.7238 1.5965 -0.2173 C 0 0 0 0 0 0 0 0 0 0 0 8
59 -0.5360 0.2017 -0.2613 C 0 0 0 0 0 0 0 0 0 0 0 9
60 0.7740 -0.3076 -0.0933 C 0 0 0 0 0 0 0 0 0 0 0 10
61 1.8469 0.5698 0.1114 C 0 0 0 0 0 0 0 0 0 0 0 11
62 1.6519 1.9519 0.1542 C 0 0 0 0 0 0 0 0 0 0 0 12
63 -1.5432 -0.6733 -0.4572 O 0 0 0 0 0 0 0 0 0 0 0 13
64 1.0078 -2.0491 -0.1493 Cl 0 0 0 0 0 0 0 0 0 0 0 14
65 3.4833 -0.0569 0.3205 Cl 0 0 0 0 0 0 0 0 0 0 0 15
66 -2.4398 -0.1916 -0.5676 H 0 0 0 0 0 0 0 0 0 0 0 16
67 0.1925 3.5303 0.0196 H 0 0 0 0 0 0 0 0 0 0 0 17
68 -1.7316 1.9934 -0.3468 H 0 0 0 0 0 0 0 0 0 0 0 18
69 2.4998 2.6165 0.3141 H 0 0 0 0 0 0 0 0 0 0 0 19
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71 2 1 0 0 0 0
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73 5 4 0 0 0 0
74 6 4 0 0 0 0
75 8 7 0 0 0 0
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77 17 7 0 0 0 0
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82 11 10 0 0 0 0
83 14 10 0 0 0 0
84 12 11 0 0 0 0
85 15 11 0 0 0 0
86 16 13 0 0 0 0
87 12 19 0 0 0 0
88 M END
89 $$$
90 2,4,5-trichlorophenol-anion.sdf
91 COSMOTHERM 3D 0
92
93 18 16 0 0 0 0 0 0 0 0 V2000
94 2.4166 -4.5640 1.0951 O 0 0 0 0 0 0 0 0 0 0 0 1
95 1.6990 -4.3802 0.4229 H 0 0 0 0 0 0 0 0 0 0 0 2
96 2.1216 -5.3726 1.5479 H 0 0 0 0 0 0 0 0 0 0 0 3
97 0.4649 -4.1138 -0.7541 O 0 0 0 0 0 0 0 0 0 0 0 4
98 -0.1446 -3.3026 -0.5815 H 0 0 0 0 0 0 0 0 0 0 0 5
99 0.8346 -3.9791 -1.6438 H 0 0 0 0 0 0 0 0 0 0 0 6
100 0.5846 -0.5454 -0.2584 C 0 0 0 0 0 0 0 0 0 0 0 7
101 0.9947 0.7782 -0.1430 C 0 0 0 0 0 0 0 0 0 0 0 8
102 0.0662 1.8081 0.0613 C 0 0 0 0 0 0 0 0 0 0 0 9
103 -1.2918 1.4794 0.1477 C 0 0 0 0 0 0 0 0 0 0 0 10
104 -1.6980 0.1560 0.0323 C 0 0 0 0 0 0 0 0 0 0 0 11
105 -0.7916 -0.9374 -0.1784 C 0 0 0 0 0 0 0 0 0 0 0 12
106 0.5509 3.5012 0.2107 Cl 0 0 0 0 0 0 0 0 0 0 0 13
107 -1.1838 -2.1662 -0.2843 O 0 0 0 0 0 0 0 0 0 0 0 14
108 1.3291 -1.3263 -0.4160 H 0 0 0 0 0 0 0 0 0 0 0 15
109 2.7278 1.1378 -0.2592 Cl 0 0 0 0 0 0 0 0 0 0 0 16
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-2.0284    2.2669    0.3060 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  17
-3.4295   -0.2156    0.1480 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  18
 2   1   0   0   0   0   0
 3   1   0   0   0   0   0
 5   4   0   0   0   0   0
 6   4   0   0   0   0   0
 8   7   0   0   0   0   0
12   7   0   0   0   0   0
15   7   0   0   0   0   0
 9   8   0   0   0   0   0
16   8   0   0   0   0   0
10   9   0   0   0   0   0
13   9   0   0   0   0   0
11  10   0   0   0   0   0
17  10   0   0   0   0   0
12  11   0   0   0   0   0
14  12   0   0   0   0   0
11  18   0   0   0   0   0

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M  END
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2,4,5-trichlorophenol.sdf
COSMOtherm      3D                        0

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19 17   0   0   0   0   0   0   0   0   0 V2000
-5.5912    1.5439    1.0458 O   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  1
-6.3673    0.9933    0.8354 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  2
-5.9467    2.4484    1.1204 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  3
-3.5750    1.3576   -0.7269 O   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  4
-4.3614    1.4274   -0.1055 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  5
-3.9411    1.4173   -1.6274 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  6
 1.0313    0.9829   -0.0952 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  7
-0.3344    0.7612   -0.2666 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  8
-0.8664   -0.5417   -0.2397 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  9
 0.0356   -1.6097   -0.0383 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 10
 1.3988   -1.3923    0.1328 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 11
 1.9081   -0.0915    0.1042 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 12
-2.1759   -0.8027   -0.3989 O   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 13
-0.5839   -3.2598    0.0003 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 14
 3.6384    0.1492    0.3238 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 15
 1.6223    2.6416   -0.1390 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 16
-1.0067    1.6053   -0.4206 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 17
 2.0708   -2.2354    0.2873 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 18
-2.7188    0.0600   -0.5303 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 19

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 2   1   0   0   0   0   0
 3   1   0   0   0   0   0
 5   4   0   0   0   0   0
 6   4   0   0   0   0   0
 8   7   0   0   0   0   0
12   7   0   0   0   0   0
16   7   0   0   0   0   0
 9   8   0   0   0   0   0
17   8   0   0   0   0   0
10   9   0   0   0   0   0
13   9   0   0   0   0   0
11  10   0   0   0   0   0
14  10   0   0   0   0   0
12  11   0   0   0   0   0
18  11   0   0   0   0   0
15  12   0   0   0   0   0
13  19   0   0   0   0   0

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M  END
$$$$
2,4,6-trichlorophenol-anion.sdf
COSMOtherm      3D                        0

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18 16   0   0   0   0   0   0   0   0   0 V2000
-2.5580    4.2129    0.2005 O   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  1
-1.5946    4.0610   -0.0204 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  2
-2.5373    4.7624    1.0025 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  3
 0.0776    3.8686   -0.4506 O   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  4
 0.4405    2.9703   -0.1339 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  5
 0.1425    3.8297   -1.4209 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  6
-0.1322   -1.8143    1.0344 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  7
 0.3008   -0.5162    1.2873 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  8
 0.6168    0.4588    0.2786 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0  9
 0.4291   -0.0603   -1.0493 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 10
-0.0050   -1.3492   -1.3476 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 11
-0.2847   -2.2187   -0.2928 C   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 12
 1.0287    1.6480    0.5488 O   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 13
 0.8065    1.0254   -2.4045 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 14
 0.4897   -0.0081    2.9768 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 15
-0.8402   -3.8706   -0.6455 Cl  0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 16
-0.3505   -2.4940    1.8573 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 17
-0.1187   -1.6674   -2.3833 H   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0   0 18

```

```

 2   1   0   0   0   0   0
 3   1   0   0   0   0   0
 5   4   0   0   0   0   0
 6   4   0   0   0   0   0
 8   7   0   0   0   0   0
12   7   0   0   0   0   0
17   7   0   0   0   0   0
 9   8   0   0   0   0   0
15   8   0   0   0   0   0
10   9   0   0   0   0   0
13   9   0   0   0   0   0
11  10   0   0   0   0   0
14  10   0   0   0   0   0
12  11   0   0   0   0   0
16  12   0   0   0   0   0
11  18   0   0   0   0   0

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M  END
$$$$
2,4,6-trichlorophenol.sdf
COSMOtherm      3D                        0

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1
2
3 19 17 0 0 0 0 0 0 0 0 0 V2000
4 -1.3309 -5.2770 0.6266 O 0 0 0 0 0 0 0 0 0 0 1
5 -1.5192 -6.0354 0.0442 H 0 0 0 0 0 0 0 0 0 0 2
6 -2.1666 -4.7763 0.6480 H 0 0 0 0 0 0 0 0 0 0 3
7 0.7835 -3.8511 -0.2970 O 0 0 0 0 0 0 0 0 0 0 4
8 0.0038 -4.3669 0.0636 H 0 0 0 0 0 0 0 0 0 0 5
9 1.5018 -3.9836 0.3463 H 0 0 0 0 0 0 0 0 0 0 6
10 0.0005 0.8802 -1.3133 C 0 0 0 0 0 0 0 0 0 0 7
11 -0.1431 2.1562 -0.7764 C 0 0 0 0 0 0 0 0 0 0 8
12 -0.1067 2.3012 0.6101 C 0 0 0 0 0 0 0 0 0 0 9
13 0.0674 1.2037 1.4490 C 0 0 0 0 0 0 0 0 0 0 10
14 0.2079 -0.0616 0.8773 C 0 0 0 0 0 0 0 0 0 0 11
15 0.1816 -0.2784 -0.5191 C 0 0 0 0 0 0 0 0 0 0 12
16 -0.2866 3.9131 1.3171 Cl 0 0 0 0 0 0 0 0 0 0 13
17 0.3058 -1.4582 -1.1409 O 0 0 0 0 0 0 0 0 0 0 14
18 -0.0425 0.6901 -3.0653 Cl 0 0 0 0 0 0 0 0 0 0 15
19 -0.2790 3.0150 -1.4312 H 0 0 0 0 0 0 0 0 0 0 16
20 0.0944 1.3192 2.5312 H 0 0 0 0 0 0 0 0 0 0 17
21 0.4213 -1.4401 1.9571 Cl 0 0 0 0 0 0 0 0 0 0 18
22 0.4823 -2.2897 -0.5705 H 0 0 0 0 0 0 0 0 0 0 19
23
24 2 1 0 0 0 0
25 3 1 0 0 0 0
26 5 4 0 0 0 0
27 6 4 0 0 0 0
28 8 7 0 0 0 0
29 12 7 0 0 0 0
30 15 7 0 0 0 0
31 9 8 0 0 0 0
32 16 8 0 0 0 0
33 10 9 0 0 0 0
34 13 9 0 0 0 0
35 11 10 0 0 0 0
36 17 10 0 0 0 0
37 12 11 0 0 0 0
38 18 11 0 0 0 0
39 14 12 0 0 0 0
40 14 19 0 0 0 0

M END

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2,4-dichlorophenol-anion.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 V2000
29 2.5039 0.5807 -4.2998 O 0 0 0 0 0 0 0 0 0 0 1
30 1.5882 0.1834 -4.2052 H 0 0 0 0 0 0 0 0 0 0 2
31 2.4741 1.3906 -3.7624 H 0 0 0 0 0 0 0 0 0 0 3
32 0.0267 -0.5273 -4.0960 O 0 0 0 0 0 0 0 0 0 0 4
33 -0.4047 -0.3602 -3.1678 H 0 0 0 0 0 0 0 0 0 0 5
34 0.1104 -1.4943 -4.1683 H 0 0 0 0 0 0 0 0 0 0 6
35 0.9096 -0.1768 -0.6261 C 0 0 0 0 0 0 0 0 0 0 7
36 1.5945 -0.1644 0.5880 C 0 0 0 0 0 0 0 0 0 0 8
37 0.8769 -0.0488 1.7805 C 0 0 0 0 0 0 0 0 0 0 9
38 -0.5155 0.0594 1.7701 C 0 0 0 0 0 0 0 0 0 0 10
39 -1.1767 0.0439 0.5440 C 0 0 0 0 0 0 0 0 0 0 11
40 -0.5155 -0.0707 -0.7244 C 0 0 0 0 0 0 0 0 0 0 12
41 1.7399 -0.0311 3.3408 Cl 0 0 0 0 0 0 0 0 0 0 13
42 -1.1603 -0.0767 -1.8529 O 0 0 0 0 0 0 0 0 0 0 14
43 1.4747 -0.2614 -1.5573 H 0 0 0 0 0 0 0 0 0 0 15
44 2.6824 -0.2475 0.6040 H 0 0 0 0 0 0 0 0 0 0 16
45 -1.0782 0.1509 2.6989 H 0 0 0 0 0 0 0 0 0 0 17
46 -2.9505 0.1808 0.5409 Cl 0 0 0 0 0 0 0 0 0 0 18
47
48 2 1 0 0 0 0
49 3 1 0 0 0 0
50 5 4 0 0 0 0
51 6 4 0 0 0 0
52 8 7 0 0 0 0
53 12 7 0 0 0 0
54 15 7 0 0 0 0
55 9 8 0 0 0 0
56 16 8 0 0 0 0
57 10 9 0 0 0 0
58 13 9 0 0 0 0
59 11 10 0 0 0 0
60 17 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
11 18 0 0 0 0

M END

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2,4-dichlorophenol.sdf
COSMOtherm 3D 0

19 17 0 0 0 0 0 0 0 0 V2000
51 -0.8438 0.9055 -5.7649 O 0 0 0 0 0 0 0 0 0 0 1
52 -0.5787 0.0906 -6.2289 H 0 0 0 0 0 0 0 0 0 0 2
53 -0.7518 1.6074 -6.4346 H 0 0 0 0 0 0 0 0 0 0 3
54 0.6109 1.3765 -3.5392 O 0 0 0 0 0 0 0 0 0 0 4
55 0.0903 1.2016 -4.3795 H 0 0 0 0 0 0 0 0 0 0 5
56 1.5352 1.4904 -3.8238 H 0 0 0 0 0 0 0 0 0 0 6
57 0.1243 1.6504 1.1472 C 0 0 0 0 0 0 0 0 0 0 7
58 0.2579 1.2414 -0.1808 C 0 0 0 0 0 0 0 0 0 0 8
59 0.2173 -0.1206 -0.5400 C 0 0 0 0 0 0 0 0 0 0 9
60 0.0356 -1.0589 0.4990 C 0 0 0 0 0 0 0 0 0 0 10
-0.0993 -0.6721 1.8318 C 0 0 0 0 0 0 0 0 0 0 11
-0.0519 0.6878 2.1411 C 0 0 0 0 0 0 0 0 0 0 12
0.3435 -0.5585 -1.8098 O 0 0 0 0 0 0 0 0 0 0 13
-0.0244 -2.7790 0.0979 Cl 0 0 0 0 0 0 0 0 0 0 14
-0.2199 1.1915 3.8349 Cl 0 0 0 0 0 0 0 0 0 0 15
0.1596 2.7100 1.3980 H 0 0 0 0 0 0 0 0 0 0 16
0.3934 1.9879 -0.9651 H 0 0 0 0 0 0 0 0 0 0 17
-0.2377 -1.4225 2.6088 H 0 0 0 0 0 0 0 0 0 0 18
0.4637 0.2211 -2.4629 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0


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12 11 0 0 0 0
17 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
19 16 0 0 0 0
20 17 0 0 0 0
11 23 0 0 0 0
M END
$$$$
2,5-dichlorophenol-anion.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 V2000
-4.3079 1.7869 -1.0748 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6450 2.0233 -0.3631 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.7360 2.6317 -1.2957 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.5226 2.4667 0.8660 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.5509 2.1674 0.6879 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.7609 2.0866 1.7293 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.5210 -0.4742 0.2466 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0457 -1.7628 0.0441 C 0 0 0 0 0 0 0 0 0 0 0 8
1.2935 -2.0519 -0.2251 C 0 0 0 0 0 0 0 0 0 0 0 9
2.1798 -0.9661 -0.2873 C 0 0 0 0 0 0 0 0 0 0 0 10
1.7260 0.3321 -0.0877 C 0 0 0 0 0 0 0 0 0 0 0 11
0.3566 0.6603 0.1926 C 0 0 0 0 0 0 0 0 0 0 0 12
1.6425 -3.0712 -0.3805 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.0522 1.8760 0.3793 O 0 0 0 0 0 0 0 0 0 0 0 14
-1.5768 -0.2958 0.4529 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.2076 -3.1224 0.1314 Cl 0 0 0 0 0 0 0 0 0 0 0 16
3.2358 -1.1444 -0.4956 H 0 0 0 0 0 0 0 0 0 0 0 17
2.8903 1.6753 -0.1783 Cl 0 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2,5-dichlorophenol.sdf
COSMOtherm 3D 0

19 17 0 0 0 0 0 0 0 0 V2000
-5.0823 1.1694 0.9141 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.8208 0.5750 0.6890 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.4934 2.0486 1.0013 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.0461 1.1240 -0.8480 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.8375 1.1402 -0.2307 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.4126 1.1165 -1.7503 H 0 0 0 0 0 0 0 0 0 0 0 6
1.5659 1.1285 0.0426 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2321 0.8179 -0.2079 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1837 -0.5294 -0.2080 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7909 -1.5191 0.0476 C 0 0 0 0 0 0 0 0 0 0 0 10
2.1201 -1.1864 0.2954 C 0 0 0 0 0 0 0 0 0 0 0 11
2.5283 0.1517 0.2959 C 0 0 0 0 0 0 0 0 0 0 0 12
-1.4582 -0.8994 -0.4398 O 0 0 0 0 0 0 0 0 0 0 0 13
0.3018 -3.2178 0.0521 Cl 0 0 0 0 0 0 0 0 0 0 0 14
2.0531 2.8364 0.0356 Cl 0 0 0 0 0 0 0 0 0 0 0 15
-0.5005 1.6008 -0.4040 H 0 0 0 0 0 0 0 0 0 0 0 16
2.8471 -1.9752 0.4896 H 0 0 0 0 0 0 0 0 0 0 0 17
3.5669 0.4145 0.4889 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.0611 -0.0864 -0.6021 H 0 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
18 12 0 0 0 0
13 19 0 0 0 0
M END
$$$$
2,6-dichlorophenol-anion.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 V2000
-4.1808 -1.4341 1.7405 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8355 -0.6528 1.2193 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.0620 -1.1527 2.0402 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.2348 0.7098 0.3319 O 0 0 0 0 0 0 0 0 0 0 0 4
-2.2154 0.7117 0.3436 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.4712 0.6069 -0.6059 H 0 0 0 0 0 0 0 0 0 0 0 6
2.7324 -0.5524 0.0655 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6121 -0.0206 0.6950 C 0 0 0 0 0 0 0 0 0 0 0 8
0.3673 0.2830 0.0402 C 0 0 0 0 0 0 0 0 0 0 0 9

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3 0.4138 -0.0247 -1.3635 C 0 0 0 0 0 0 0 0 0 0 10
4 1.5185 -0.5578 -2.0215 C 0 0 0 0 0 0 0 0 0 0 11
5 2.6915 -0.8293 -1.3071 C 0 0 0 0 0 0 0 0 0 0 12
6 -0.6482 0.7776 0.6603 O 0 0 0 0 0 0 0 0 0 0 13
7 -1.0494 0.3270 -2.3211 C1 0 0 0 0 0 0 0 0 0 0 14
8 1.6941 0.3178 2.4422 C1 0 0 0 0 0 0 0 0 0 0 15
9 3.6343 -0.7524 0.6461 H 0 0 0 0 0 0 0 0 0 0 16
10 1.4628 -0.7582 -3.0925 H 0 0 0 0 0 0 0 0 0 0 17
11 3.5622 -1.2467 -1.8130 H 0 0 0 0 0 0 0 0 0 0 18
12 2 1 0 0 0 0
13 3 1 0 0 0 0
14 5 4 0 0 0 0
15 6 4 0 0 0 0
16 8 7 0 0 0 0
17 12 7 0 0 0 0
18 16 7 0 0 0 0
19 9 8 0 0 0 0
20 15 8 0 0 0 0
21 10 9 0 0 0 0
22 13 9 0 0 0 0
23 11 10 0 0 0 0
24 14 10 0 0 0 0
25 12 11 0 0 0 0
26 17 11 0 0 0 0
27 12 18 0 0 0 0
28 M END
29 \$\$\$\$
30 2,6-dichlorophenol.sdf
31 COSMOtherm 3D 0
32
33 19 17 0 0 0 0 0 0 0 0 0 0 V2000
34 -4.6682 -1.1539 -1.1131 O 0 0 0 0 0 0 0 0 0 0 1
35 -4.8261 -2.0801 -1.3719 H 0 0 0 0 0 0 0 0 0 0 2
36 -4.3614 -0.7237 -1.9317 H 0 0 0 0 0 0 0 0 0 0 3
37 -2.9315 -1.0402 0.9702 O 0 0 0 0 0 0 0 0 0 0 4
38 -3.5640 -1.0498 0.1941 H 0 0 0 0 0 0 0 0 0 0 5
39 -3.2695 -0.3522 1.5700 H 0 0 0 0 0 0 0 0 0 0 6
40 2.8428 0.4641 -0.3286 C 0 0 0 0 0 0 0 0 0 0 7
41 1.8370 -0.4642 -0.0778 C 0 0 0 0 0 0 0 0 0 0 8
42 0.4834 -0.0961 0.1162 C 0 0 0 0 0 0 0 0 0 0 9
43 0.2102 1.2884 0.0381 C 0 0 0 0 0 0 0 0 0 0 10
44 1.2033 2.2362 -0.2113 C 0 0 0 0 0 0 0 0 0 0 11
45 2.5243 1.8240 -0.3953 C 0 0 0 0 0 0 0 0 0 0 12
46 -0.4122 -1.0688 0.3482 O 0 0 0 0 0 0 0 0 0 0 13
47 -1.4551 1.8465 0.2563 C1 0 0 0 0 0 0 0 0 0 0 14
48 2.2514 -2.1813 0.0076 C1 0 0 0 0 0 0 0 0 0 0 15
49 3.8682 0.1228 -0.4688 H 0 0 0 0 0 0 0 0 0 0 16
50 0.9351 3.2920 -0.2613 H 0 0 0 0 0 0 0 0 0 0 17
51 3.3045 2.5596 -0.5906 H 0 0 0 0 0 0 0 0 0 0 18
52 -1.3725 -0.7909 0.5522 H 0 0 0 0 0 0 0 0 0 0 19
53 2 1 0 0 0 0
54 3 1 0 0 0 0
55 5 4 0 0 0 0
56 6 4 0 0 0 0
57 8 7 0 0 0 0
58 12 7 0 0 0 0
59 16 7 0 0 0 0
60 9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
18 12 0 0 0 0
13 19 0 0 0 0
M END
\$\$\$\$
2-acetylbutanedioicacid-anion.sdf
COSMOtherm 3D 0
24 22 0 0 0 0 0 0 0 0 0 0 V2000
-0.9899 0.6208 5.5458 O 0 0 0 0 0 0 0 0 0 0 1
-0.2207 0.5123 4.9184 H 0 0 0 0 0 0 0 0 0 0 2
-1.5183 1.3389 5.1576 H 0 0 0 0 0 0 0 0 0 0 3
1.1702 0.2478 3.8993 O 0 0 0 0 0 0 0 0 0 0 4
0.9359 -0.2671 3.0618 H 0 0 0 0 0 0 0 0 0 0 5
1.5272 1.0937 3.5761 H 0 0 0 0 0 0 0 0 0 0 6
0.6737 -0.6589 0.6346 C 0 0 0 0 0 0 0 0 0 0 7
0.3551 -1.4718 -0.6277 C 0 0 0 0 0 0 0 0 0 0 8
-0.2706 -0.6914 -1.8148 C 0 0 0 0 0 0 0 0 0 0 9
-1.5244 0.1109 -1.4242 C 0 0 0 0 0 0 0 0 0 0 10
-1.6856 1.2652 -1.8095 O 0 0 0 0 0 0 0 0 0 0 11
-2.5550 -0.6027 -0.5859 C 0 0 0 0 0 0 0 0 0 0 12
0.7022 0.1974 -2.6067 C 0 0 0 0 0 0 0 0 0 0 13
1.5057 0.9794 -1.9051 O 0 0 0 0 0 0 0 0 0 0 14
0.7221 0.1797 -3.8393 O 0 0 0 0 0 0 0 0 0 0 15
0.5309 -1.2194 1.7531 O 0 0 0 0 0 0 0 0 0 0 16
1.0907 0.5509 0.4890 O 0 0 0 0 0 0 0 0 0 0 17
-0.3032 -2.3025 -0.3452 H 0 0 0 0 0 0 0 0 0 0 18
1.2980 -1.9298 -0.9681 H 0 0 0 0 0 0 0 0 0 0 19
-0.6344 -1.4479 -2.5299 H 0 0 0 0 0 0 0 0 0 0 20
-3.4890 -0.0296 -0.5745 H 0 0 0 0 0 0 0 0 0 0 21
-2.7351 -1.6208 -0.9609 H 0 0 0 0 0 0 0 0 0 0 22
-2.1895 -0.7049 0.4489 H 0 0 0 0 0 0 0 0 0 0 23
1.3274 0.8344 -0.8323 H 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0

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18 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
14 24 0 0 0 0
17 24 0 0 0 0
M END
$$$$
2-acetylbutanedioicacid.sdf
COSMOTHERM 3D 0
25 22 0 0 0 0 0 0 0 0 V2000
-0.5714 3.0738 -2.0986 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.4355 2.2051 -1.6384 H 0 0 0 0 0 0 0 0 0 0 0 2
0.0875 3.0895 -2.8158 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0982 4.2162 0.2057 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.1095 3.9631 -0.7485 H 0 0 0 0 0 0 0 0 0 0 0 5
0.9230 4.7342 0.1746 H 0 0 0 0 0 0 0 0 0 0 0 6
0.1382 0.9189 0.7781 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2772 -0.3543 1.5908 C 0 0 0 0 0 0 0 0 0 0 0 8
0.1197 -1.6151 0.7333 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.2710 -1.8039 0.1162 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.4089 -2.3967 -0.9639 O 0 0 0 0 0 0 0 0 0 0 0 11
-2.4678 -1.3505 0.8925 C 0 0 0 0 0 0 0 0 0 0 0 12
1.3099 -1.7705 -0.2395 C 0 0 0 0 0 0 0 0 0 0 0 13
1.0862 -2.4419 -1.3729 O 0 0 0 0 0 0 0 0 0 0 0 14
2.4222 -1.3423 0.0347 O 0 0 0 0 0 0 0 0 0 0 0 15
0.4233 2.0097 1.4676 O 0 0 0 0 0 0 0 0 0 0 0 16
-0.2221 0.8985 -0.4078 O 0 0 0 0 0 0 0 0 0 0 0 17
-0.4618 -0.3302 2.4048 H 0 0 0 0 0 0 0 0 0 0 0 18
1.2610 -0.3554 2.0771 H 0 0 0 0 0 0 0 0 0 0 0 19
0.2112 -2.4819 1.4184 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.3819 -1.7256 0.4198 H 0 0 0 0 0 0 0 0 0 0 0 21
-2.4079 -1.6998 1.9341 H 0 0 0 0 0 0 0 0 0 0 0 22
-2.5051 -0.2508 0.9253 H 0 0 0 0 0 0 0 0 0 0 0 23
0.0767 -2.6027 -1.4289 H 0 0 0 0 0 0 0 0 0 0 0 24
0.3000 2.8929 0.9092 H 0 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
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21 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
24 14 0 0 0 0
16 25 0 0 0 0
M END
$$$$
2-chlorophenol-anion.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 V2000
3.0533 1.4364 0.5681 O 0 0 0 0 0 0 0 0 0 0 0 1
2.3141 0.8205 0.2741 H 0 0 0 0 0 0 0 0 0 0 0 2
2.6296 2.3107 0.6046 H 0 0 0 0 0 0 0 0 0 0 0 3
2.8373 -2.5587 -0.2786 O 0 0 0 0 0 0 0 0 0 0 0 4
2.2128 -1.7632 -0.2337 H 0 0 0 0 0 0 0 0 0 0 0 5
2.7416 -2.9910 0.5872 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.6690 -1.7928 0.0528 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.0497 -1.9299 0.1884 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.8860 -0.8037 0.2081 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.3078 0.4658 0.0821 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.9265 0.5924 -0.0540 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0269 -0.5205 -0.0757 C 0 0 0 0 0 0 0 0 0 0 0 12
-3.9670 -0.9036 0.3144 H 0 0 0 0 0 0 0 0 0 0 0 13
1.2692 -0.4027 -0.2092 O 0 0 0 0 0 0 0 0 0 0 0 14
-0.0268 -2.6768 0.0351 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.4799 -2.9303 0.2827 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.9313 1.3616 0.0878 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.2415 2.2321 -0.2278 Cl 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
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17 10 0 0 0 0
12 11 0 0 0 0

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14 12 0 0 0 0
11 18 0 0 0 0
M END
$$$$
2-chlorophenol.sdf
COSMOtherm 3D 0

19 17 0 0 0 0 0 0 0 0 V2000
-5.0646 -0.4542 0.7725 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.2985 -1.3542 0.4809 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.9043 0.0390 0.7336 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.1040 0.6966 -0.6908 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.8561 0.2595 -0.1910 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.3859 0.7158 -1.6227 H 0 0 0 0 0 0 0 0 0 0 0 6
1.2476 2.4063 0.1228 C 0 0 0 0 0 0 0 0 0 0 0 7
0.1202 1.6164 -0.1133 C 0 0 0 0 0 0 0 0 0 0 0 8
0.2170 0.2108 -0.1609 C 0 0 0 0 0 0 0 0 0 0 0 9
1.4919 -0.3597 0.0377 C 0 0 0 0 0 0 0 0 0 0 0 10
2.6207 0.4236 0.2739 C 0 0 0 0 0 0 0 0 0 0 0 11
2.5023 1.8173 0.3169 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.8422 -0.5990 -0.3879 O 0 0 0 0 0 0 0 0 0 0 0 13
1.6549 -2.1250 -0.0150 Cl 0 0 0 0 0 0 0 0 0 0 0 14
-1.7001 -0.0608 -0.5105 H 0 0 0 0 0 0 0 0 0 0 0 15
1.1408 3.4921 0.1539 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.8582 2.0768 -0.2638 H 0 0 0 0 0 0 0 0 0 0 0 17
3.5874 -0.0588 0.4221 H 0 0 0 0 0 0 0 0 0 0 0 18
3.3852 2.4303 0.5009 H 0 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
15 13 0 0 0 0
12 19 0 0 0 0
M END
$$$$
2-chloropropanoicacid-anion.sdf
COSMOtherm 3D 0

16 13 0 0 0 0 0 0 0 0 V2000
-4.6596 0.2006 -1.1768 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.0192 -0.0452 -0.4497 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.3932 1.0965 -1.4448 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.9520 -0.5851 0.7936 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.9791 -0.5265 0.4853 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.9855 0.0021 1.5690 H 0 0 0 0 0 0 0 0 0 0 0 6
2.6233 -0.6403 1.1760 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7955 0.3359 0.3502 C 0 0 0 0 0 0 0 0 0 0 0 8
0.2861 0.2289 0.6776 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0525 0.8646 1.7100 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.4569 -0.4993 -0.0543 O 0 0 0 0 0 0 0 0 0 0 0 11
2.1500 0.0553 -1.4589 Cl 0 0 0 0 0 0 0 0 0 0 0 12
3.6951 -0.5269 0.9673 H 0 0 0 0 0 0 0 0 0 0 0 13
2.4541 -0.4323 2.2430 H 0 0 0 0 0 0 0 0 0 0 0 14
2.3275 -1.6786 0.9707 H 0 0 0 0 0 0 0 0 0 0 0 15
2.1195 1.3687 0.5152 H 0 0 0 0 0 0 0 0 0 0 0 16

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 16 0 0 0 0
M END
$$$$
2-chloropropanoicacid.sdf
COSMOtherm 3D 0

17 14 0 0 0 0 0 0 0 0 V2000
-0.7472 -4.6021 0.1642 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.0291 -4.9398 -0.7059 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.5582 -4.2296 0.5561 H 0 0 0 0 0 0 0 0 0 0 0 3
1.3053 -2.8705 -0.0901 O 0 0 0 0 0 0 0 0 0 0 0 4
0.5260 -3.4910 0.0332 H 0 0 0 0 0 0 0 0 0 0 0 5
1.8029 -2.9013 0.7473 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.8500 2.0694 -0.3704 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.4330 1.5900 -0.5865 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1757 0.1690 -0.0687 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7095 -0.4833 -0.8200 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.7328 -0.2905 0.9224 O 0 0 0 0 0 0 0 0 0 0 0 11
0.7654 2.6744 0.3369 Cl 0 0 0 0 0 0 0 0 0 0 0 12
-1.9636 3.1067 -0.7095 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.5309 1.4375 -0.9624 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.1377 1.9932 0.6863 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.1143 1.6731 -1.6299 H 0 0 0 0 0 0 0 0 0 0 0 16
0.8937 -1.4407 -0.4463 H 0 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0

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6 4 0 0 0 0
 8 7 0 0 0 0
 13 7 0 0 0 0
 14 7 0 0 0 0
 15 7 0 0 0 0
 9 8 0 0 0 0
 12 8 0 0 0 0
 16 8 0 0 0 0
 10 9 0 0 0 0
 11 9 0 0 0 0
 10 17 0 0 0 0

M END

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2-hydroxypropanoicacid-anion.sdf

COSMOTHERM 3D 0

17 14 0 0 0 0 0 0 0 0 0 V2000
 -4.6815 -0.7525 0.3319 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -3.9195 -0.1632 0.0618 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -4.5741 -0.8634 1.2919 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 -2.6256 0.8269 -0.5174 O 0 0 0 0 0 0 0 0 0 0 0 0 4
 -1.7209 0.4115 -0.2889 H 0 0 0 0 0 0 0 0 0 0 0 0 5
 -2.6217 1.6967 -0.0813 H 0 0 0 0 0 0 0 0 0 0 0 0 6
 2.2965 -1.6074 -0.6287 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 2.0237 -0.4967 0.3859 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 0.7190 0.2775 0.0646 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 0.8439 1.5184 -0.1518 O 0 0 0 0 0 0 0 0 0 0 0 0 10
 -0.3635 -0.3921 0.0492 O 0 0 0 0 0 0 0 0 0 0 0 0 11
 3.1178 0.4373 0.4264 O 0 0 0 0 0 0 0 0 0 0 0 0 12
 3.2312 -2.1296 -0.3778 H 0 0 0 0 0 0 0 0 0 0 0 0 13
 1.4778 -2.3401 -0.6264 H 0 0 0 0 0 0 0 0 0 0 0 0 14
 2.3920 -1.1890 -1.6419 H 0 0 0 0 0 0 0 0 0 0 0 0 15
 1.8991 -0.9438 1.3893 H 0 0 0 0 0 0 0 0 0 0 0 0 16
 2.6596 1.2883 0.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 17

2 1 0 0 0 0

3 1 0 0 0 0

5 4 0 0 0 0

6 4 0 0 0 0

8 7 0 0 0 0

13 7 0 0 0 0

14 7 0 0 0 0

15 7 0 0 0 0

9 8 0 0 0 0

12 8 0 0 0 0

16 8 0 0 0 0

10 9 0 0 0 0

11 9 0 0 0 0

12 17 0 0 0 0

M END

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2-hydroxypropanoicacid.sdf

COSMOTHERM 3D 0

18 15 0 0 0 0 0 0 0 0 0 V2000
 -0.7805 0.9213 -3.9008 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -1.5951 0.4925 -4.2194 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -0.3737 1.2964 -4.7029 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 0.9074 -0.7137 -2.6025 O 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.2492 -0.1374 -3.0996 H 0 0 0 0 0 0 0 0 0 0 0 0 5
 0.6820 -1.6334 -2.8304 H 0 0 0 0 0 0 0 0 0 0 0 0 6
 0.8324 1.2947 2.3916 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 0.2196 -0.0826 2.1237 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 0.0032 -0.3331 0.6290 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 -1.1283 -0.5365 0.1796 O 0 0 0 0 0 0 0 0 0 0 0 0 10
 1.1144 -0.3085 -0.0878 O 0 0 0 0 0 0 0 0 0 0 0 0 11
 -1.0355 -0.2224 2.8010 O 0 0 0 0 0 0 0 0 0 0 0 0 12
 0.9408 1.4391 3.4749 H 0 0 0 0 0 0 0 0 0 0 0 0 13
 1.8253 1.3756 1.9286 H 0 0 0 0 0 0 0 0 0 0 0 0 14
 0.1861 2.0901 1.9934 H 0 0 0 0 0 0 0 0 0 0 0 0 15
 0.9105 -0.8647 2.4862 H 0 0 0 0 0 0 0 0 0 0 0 0 16
 0.9307 -0.4854 -1.1046 H 0 0 0 0 0 0 0 0 0 0 0 0 17
 -1.6873 -0.4008 2.0850 H 0 0 0 0 0 0 0 0 0 0 0 0 18

2 1 0 0 0 0

3 1 0 0 0 0

5 4 0 0 0 0

6 4 0 0 0 0

8 7 0 0 0 0

13 7 0 0 0 0

14 7 0 0 0 0

15 7 0 0 0 0

9 8 0 0 0 0

12 8 0 0 0 0

16 8 0 0 0 0

10 9 0 0 0 0

11 9 0 0 0 0

17 11 0 0 0 0

12 18 0 0 0 0

M END

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3,3-dimethylsuccinimide-anion.sdf

COSMOTHERM 3D 0

23 21 0 0 0 0 0 0 0 0 0 V2000
 -3.9266 0.6553 -0.0049 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -3.6720 -0.3029 -0.0079 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -3.0355 1.0974 0.0055 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 -2.7020 -1.8646 -0.0602 O 0 0 0 0 0 0 0 0 0 0 0 0 4
 -1.8271 -1.3357 -0.0143 H 0 0 0 0 0 0 0 0 0 0 0 0 5
 -2.7548 -2.3387 0.7882 H 0 0 0 0 0 0 0 0 0 0 0 0 6
 1.9131 0.2577 -0.0032 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 1.0530 1.5353 0.0168 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 0.8268 -0.8526 0.0063 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 -0.4481 -0.3369 0.0079 N 0 0 0 0 0 0 0 0 0 0 0 0 10
 -0.3863 1.0246 0.0115 C 0 0 0 0 0 0 0 0 0 0 0 0 11
 2.8050 0.1141 1.2426 C 0 0 0 0 0 0 0 0 0 0 0 0 12

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15 11 0 0 0 0
16 11 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
29 15 0 0 0 0
24 16 0 0 0 0
25 16 0 0 0 0
23 22 0 0 0 0
26 22 0 0 0 0
30 22 0 0 0 0
24 23 0 0 0 0
31 23 0 0 0 0
32 24 0 0 0 0
26 25 0 0 0 0
33 25 0 0 0 0
26 34 0 0 0 0
M END
$$$$
3,4-dichlorophenol-anion.sdf
COSMOtherm 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-2.5391 3.5846 0.0374 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6007 3.2062 0.0433 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.8513 3.4412 -0.8722 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8945 4.4879 -0.0815 O 0 0 0 0 0 0 0 0 0 0 0 4
1.1854 3.7675 -0.0307 H 0 0 0 0 0 0 0 0 0 0 0 5
2.3429 4.3290 -0.9296 H 0 0 0 0 0 0 0 0 0 0 0 6
1.8132 -0.4924 0.0458 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5538 0.8745 0.0744 C 0 0 0 0 0 0 0 0 0 0 0 8
0.2195 1.3820 0.0674 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.8288 0.4121 0.0352 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.5506 -0.9513 0.0076 C 0 0 0 0 0 0 0 0 0 0 0 11
0.7687 -1.4248 0.0122 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.0403 2.6685 0.0911 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.9159 -2.0867 -0.0331 Cl 0 0 0 0 0 0 0 0 0 0 0 14
1.1475 -3.1542 -0.0248 Cl 0 0 0 0 0 0 0 0 0 0 0 15
2.8435 -0.8518 0.0504 H 0 0 0 0 0 0 0 0 0 0 0 16
2.3848 1.5819 0.1038 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.8646 0.7538 0.0331 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 12 0 0 0 0
10 18 0 0 0 0
M END
$$$$
3,4-dichlorophenol.sdf
COSMOtherm 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-5.5639 0.7603 1.1710 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.1476 -0.0099 1.2991 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.1766 1.5024 1.0167 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.7667 0.4429 -0.8199 O 0 0 0 0 0 0 0 0 0 0 0 4
-4.4739 0.5480 -0.1176 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.2461 0.3399 -1.6615 H 0 0 0 0 0 0 0 0 0 0 0 6
0.8743 0.4669 -0.1176 C 0 0 0 0 0 0 0 0 0 0 0 7
1.8329 -0.5264 0.1210 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4250 -1.8644 0.1741 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0875 -2.2085 -0.0064 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.8754 -1.2097 -0.2455 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.4697 0.1373 -0.3014 C 0 0 0 0 0 0 0 0 0 0 0 12
3.5378 -0.1360 0.3565 Cl 0 0 0 0 0 0 0 0 0 0 0 13
2.1674 -2.6409 0.3597 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.2220 -3.2536 0.0375 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.1650 -1.5903 -0.4173 O 0 0 0 0 0 0 0 0 0 0 0 16
-1.2008 0.9229 -0.4879 H 0 0 0 0 0 0 0 0 0 0 0 17
1.3321 2.1701 -0.1957 Cl 0 0 0 0 0 0 0 0 0 0 0 18
-2.7740 -0.7862 -0.5710 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
16 11 0 0 0 0
17 12 0 0 0 0
16 19 0 0 0 0
M END
$$$$
3,5-dichlorophenol-anion.sdf
COSMOtherm 3D 0
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18 16 0 0 0 0 0 0 0 0 0 V2000
-3.7523 -0.0685 2.2669 O 0 0 0 0 0 0 0 0 0 0 1
-3.1928 -0.0387 1.4264 H 0 0 0 0 0 0 0 0 0 0 2
-3.6881 0.8300 2.6336 H 0 0 0 0 0 0 0 0 0 0 3
-3.7497 0.0186 -2.2761 O 0 0 0 0 0 0 0 0 0 0 4
-3.1900 0.0122 -1.4346 H 0 0 0 0 0 0 0 0 0 0 5
-3.5936 0.8960 -2.6654 H 0 0 0 0 0 0 0 0 0 0 6
1.0923 0.0049 1.1842 C 0 0 0 0 0 0 0 0 0 0 7
-0.2940 -0.0129 1.2198 C 0 0 0 0 0 0 0 0 0 0 8
-1.0394 -0.0268 -0.0018 C 0 0 0 0 0 0 0 0 0 0 9
-0.2897 -0.0251 -1.2212 C 0 0 0 0 0 0 0 0 0 0 10
1.0962 -0.0088 -1.1810 C 0 0 0 0 0 0 0 0 0 0 11
1.8413 0.0076 0.0029 C 0 0 0 0 0 0 0 0 0 0 12
-2.3482 -0.0410 -0.0040 O 0 0 0 0 0 0 0 0 0 0 13
1.9959 -0.0083 -2.7242 Cl 0 0 0 0 0 0 0 0 0 0 14
1.9862 0.0228 2.7302 Cl 0 0 0 0 0 0 0 0 0 0 15
-0.8313 -0.0178 2.1683 H 0 0 0 0 0 0 0 0 0 0 16
-0.8237 -0.0411 -2.1713 H 0 0 0 0 0 0 0 0 0 0 17
2.9286 0.0217 0.0047 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
8 7 0 0 0 0 0
12 7 0 0 0 0 0
15 7 0 0 0 0 0
9 8 0 0 0 0 0
16 8 0 0 0 0 0
10 9 0 0 0 0 0
13 9 0 0 0 0 0
11 10 0 0 0 0 0
17 10 0 0 0 0 0
12 11 0 0 0 0 0
14 11 0 0 0 0 0
12 18 0 0 0 0 0
M END
$$$$
3,5-dichlorophenol.sdf
COSMOtherm 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-5.5772 -0.7630 1.0927 O 0 0 0 0 0 0 0 0 0 0 1
-5.8509 -1.6984 1.0961 H 0 0 0 0 0 0 0 0 0 0 2
-6.4098 -0.2682 0.9840 H 0 0 0 0 0 0 0 0 0 0 3
-3.7406 -0.1736 -0.7947 O 0 0 0 0 0 0 0 0 0 0 4
-4.4539 -0.4098 -0.1285 H 0 0 0 0 0 0 0 0 0 0 5
-4.1425 -0.3133 -1.6707 H 0 0 0 0 0 0 0 0 0 0 6
-1.5602 -1.5950 -0.5431 O 0 0 0 0 0 0 0 0 0 0 7
-0.4623 -0.8366 -0.3239 C 0 0 0 0 0 0 0 0 0 0 8
0.7700 -1.5014 -0.1669 C 0 0 0 0 0 0 0 0 0 0 9
1.9146 -0.7450 0.0581 C 0 0 0 0 0 0 0 0 0 0 10
3.4644 -1.5860 0.2551 Cl 0 0 0 0 0 0 0 0 0 0 11
1.9049 0.6503 0.1371 C 0 0 0 0 0 0 0 0 0 0 12
0.6650 1.2712 -0.0236 C 0 0 0 0 0 0 0 0 0 0 13
0.5959 3.0420 0.0670 Cl 0 0 0 0 0 0 0 0 0 0 14
-0.5161 0.5705 -0.2513 C 0 0 0 0 0 0 0 0 0 0 15
-2.4013 -1.0216 -0.6391 H 0 0 0 0 0 0 0 0 0 0 16
0.8093 -2.5885 -0.2236 H 0 0 0 0 0 0 0 0 0 0 17
2.8139 1.2209 0.3140 H 0 0 0 0 0 0 0 0 0 0 18
-1.4653 1.0915 -0.3727 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
8 7 0 0 0 0 0
16 7 0 0 0 0 0
9 8 0 0 0 0 0
15 8 0 0 0 0 0
10 9 0 0 0 0 0
17 9 0 0 0 0 0
11 10 0 0 0 0 0
12 10 0 0 0 0 0
13 12 0 0 0 0 0
18 12 0 0 0 0 0
14 13 0 0 0 0 0
15 13 0 0 0 0 0
15 19 0 0 0 0 0
M END
$$$$
3-chlorophenol-anion.sdf
COSMOtherm 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-3.0378 0.0518 2.1427 O 0 0 0 0 0 0 0 0 0 0 1
-2.0289 0.0329 2.0461 H 0 0 0 0 0 0 0 0 0 0 2
-3.2933 0.9412 1.8442 H 0 0 0 0 0 0 0 0 0 0 3
0.9537 -0.0544 4.2751 O 0 0 0 0 0 0 0 0 0 0 4
0.4785 -0.0552 3.3798 H 0 0 0 0 0 0 0 0 0 0 5
1.4702 -0.8783 4.2766 H 0 0 0 0 0 0 0 0 0 0 6
2.2879 0.0935 -0.5240 C 0 0 0 0 0 0 0 0 0 0 7
1.6525 0.0664 0.7163 C 0 0 0 0 0 0 0 0 0 0 8
0.2298 0.0002 0.8203 C 0 0 0 0 0 0 0 0 0 0 9
-0.5029 -0.0372 -0.4080 C 0 0 0 0 0 0 0 0 0 0 10
0.1732 -0.0067 -1.6213 C 0 0 0 0 0 0 0 0 0 0 11
1.5641 0.0572 -1.7274 C 0 0 0 0 0 0 0 0 0 0 12
-0.3873 -0.0265 1.9814 O 0 0 0 0 0 0 0 0 0 0 13
-0.7928 -0.0534 -3.1322 Cl 0 0 0 0 0 0 0 0 0 0 14
3.3786 0.1447 -0.5668 H 0 0 0 0 0 0 0 0 0 0 15
2.2389 0.1006 1.6369 H 0 0 0 0 0 0 0 0 0 0 16
-1.5919 -0.0900 -0.3739 H 0 0 0 0 0 0 0 0 0 0 17
2.0613 0.0796 -2.6960 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0

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8 7 0 0 0 0
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M END

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3-chlorophenol.sdf
COSMOtherm 3D 0

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19 17 0 0 0 0 0 0 0 0 0 V2000
-0.7238 1.1120 -5.0254 O 0 0 0 0 0 0 0 0 0 0 1
-1.5795 0.7700 -5.3422 H 0 0 0 0 0 0 0 0 0 0 2
-0.2884 1.4532 -5.8279 H 0 0 0 0 0 0 0 0 0 0 3
0.8399 -0.6880 -3.7461 O 0 0 0 0 0 0 0 0 0 0 4
0.2306 -0.0590 -4.2338 H 0 0 0 0 0 0 0 0 0 0 5
0.5041 -1.5824 -3.9323 H 0 0 0 0 0 0 0 0 0 0 6
0.8682 0.0681 1.0114 C 0 0 0 0 0 0 0 0 0 0 7
-0.1197 0.0384 1.9914 C 0 0 0 0 0 0 0 0 0 0 8
-1.4557 -0.2529 1.7094 C 0 0 0 0 0 0 0 0 0 0 9
-1.7918 -0.5245 0.3774 C 0 0 0 0 0 0 0 0 0 0 10
-0.8303 -0.5051 -0.6354 C 0 0 0 0 0 0 0 0 0 0 11
0.5103 -0.2064 -0.3233 C 0 0 0 0 0 0 0 0 0 0 12
-2.2072 -0.2678 2.4975 H 0 0 0 0 0 0 0 0 0 0 13
1.4985 -0.1669 -1.2537 O 0 0 0 0 0 0 0 0 0 0 14
1.9049 0.2981 1.2566 H 0 0 0 0 0 0 0 0 0 0 15
0.3465 0.3877 3.6735 Cl 0 0 0 0 0 0 0 0 0 0 16
-2.8286 -0.7560 0.1272 H 0 0 0 0 0 0 0 0 0 0 17
-1.1122 -0.7210 -1.6668 H 0 0 0 0 0 0 0 0 0 0 18
1.1491 -0.3813 -2.1829 H 0 0 0 0 0 0 0 0 0 0 19

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
14 12 0 0 0 0
14 19 0 0 0 0

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M END

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3-chloropropanoicacid-anion.sdf
COSMOtherm 3D 0

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```

16 13 0 0 0 0 0 0 0 0 0 V2000
-5.3061 0.9499 -0.6704 O 0 0 0 0 0 0 0 0 0 0 1
-4.6227 0.3279 -0.2832 H 0 0 0 0 0 0 0 0 0 0 2
-4.9468 1.1936 -1.5405 H 0 0 0 0 0 0 0 0 0 0 3
-3.5091 -0.7365 0.4820 O 0 0 0 0 0 0 0 0 0 0 4
-2.5958 -0.2874 0.6147 H 0 0 0 0 0 0 0 0 0 0 5
-3.3055 -1.4922 -0.0975 H 0 0 0 0 0 0 0 0 0 0 6
2.2085 -0.4155 -0.3406 C 0 0 0 0 0 0 0 0 0 0 7
1.1573 0.4044 0.3789 C 0 0 0 0 0 0 0 0 0 0 8
-0.2579 -0.1987 0.2279 C 0 0 0 0 0 0 0 0 0 0 9
-0.4121 -1.2250 -0.4868 O 0 0 0 0 0 0 0 0 0 0 10
-1.1849 0.4185 0.8612 O 0 0 0 0 0 0 0 0 0 0 11
1.1328 1.4330 -0.0124 H 0 0 0 0 0 0 0 0 0 0 12
2.3045 -1.4272 0.0633 H 0 0 0 0 0 0 0 0 0 0 13
2.0432 -0.4607 -1.4203 H 0 0 0 0 0 0 0 0 0 0 14
3.8905 0.3454 -0.1393 Cl 0 0 0 0 0 0 0 0 0 0 15
1.3878 0.4789 1.4521 H 0 0 0 0 0 0 0 0 0 0 16

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 16 0 0 0 0

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M END

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3-chloropropanoicacid.sdf
COSMOtherm 3D 0

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```

17 14 0 0 0 0 0 0 0 0 0 V2000
-1.2779 -0.5624 -4.7637 O 0 0 0 0 0 0 0 0 0 0 1
-1.0874 -1.0765 -5.5696 H 0 0 0 0 0 0 0 0 0 0 2
-1.8706 0.1499 -5.0650 H 0 0 0 0 0 0 0 0 0 0 3
0.9917 0.2836 -3.5747 O 0 0 0 0 0 0 0 0 0 0 4
1.0911 1.2367 -3.7469 H 0 0 0 0 0 0 0 0 0 0 5
0.1356 0.0145 -4.0251 H 0 0 0 0 0 0 0 0 0 0 6
-0.5467 0.2883 2.1256 C 0 0 0 0 0 0 0 0 0 0 7
0.5348 -0.2391 1.2001 C 0 0 0 0 0 0 0 0 0 0 8
0.2877 0.1738 -0.2421 C 0 0 0 0 0 0 0 0 0 0 9
1.1991 -0.3363 -1.0741 O 0 0 0 0 0 0 0 0 0 0 10

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-0.6412    0.8976   -0.5962 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.5919   -1.3368    1.2425 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.1958   -0.2130    3.8613 C1   0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.5913    1.3804    2.1366 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.5331   -0.1228    1.8931 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
1.5244    0.1399    1.4966 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.0286   -0.0336   -2.0525 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
8 7 0 0 0 0 0
13 7 0 0 0 0 0
14 7 0 0 0 0 0
15 7 0 0 0 0 0
9 8 0 0 0 0 0
12 8 0 0 0 0 0
16 8 0 0 0 0 0
10 9 0 0 0 0 0
11 9 0 0 0 0 0
10 17 0 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid-anion.sdf
COSMOTHERM        3D                                0
27 27 0 0 0 0 0 0 0 0 0 0 V2000
-1.1184   -6.1568    1.9746 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.4957   -5.6966    1.3420 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.9429   -5.6438    1.9208 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.6873   -4.9458    0.3158 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.6459   -3.9328    0.3649 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5170   -5.1500   -0.6202 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.2070    4.7174    0.9120 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0892    3.9977    2.1002 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.2503    2.6261    2.0545 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.1225    1.9167    0.8264 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.1782    2.6466   -0.3815 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.3373    4.0612   -0.2970 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.2827    0.5110    0.7444 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
0.1536   -0.1755   -0.4527 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.1500    0.5618   -1.6546 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.3078    1.9414   -1.6029 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
0.3276   -1.6739   -0.5075 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
0.6054   -2.3018   -0.5568 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
0.1786   -2.2357   -1.6568 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.2831   -0.0929   -2.8333 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.1180   -1.0912   -2.5666 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.3325    5.8012    0.9575 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
0.1882    4.5323    3.0465 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
0.4784    2.0644    2.9637 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
-0.5647    4.6210   -1.2071 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
0.5113   -0.0579    1.6484 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
-0.5371    2.4842   -2.5227 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
8 7 0 0 0 0 0
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9 8 0 0 0 0 0
23 8 0 0 0 0 0
10 9 0 0 0 0 0
24 9 0 0 0 0 0
11 10 0 0 0 0 0
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12 11 0 0 0 0 0
16 11 0 0 0 0 0
25 12 0 0 0 0 0
14 13 0 0 0 0 0
26 13 0 0 0 0 0
15 14 0 0 0 0 0
17 14 0 0 0 0 0
16 15 0 0 0 0 0
20 15 0 0 0 0 0
18 17 0 0 0 0 0
19 17 0 0 0 0 0
21 19 0 0 0 0 0
21 20 0 0 0 0 0
16 27 0 0 0 0 0
M END
$$$$
3-hydroxy-2-naphtoicacid.sdf
COSMOTHERM        3D                                0
28 27 0 0 0 0 0 0 0 0 0 V2000
1.3273    6.1685   -1.2527 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
2.0151    5.6523   -1.7114 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.7656    6.4917   -0.4444 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.9002    4.7326   -0.8004 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0593    5.2700   -0.9281 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3036    5.0626    0.0225 H    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2554   -4.7637   -0.7463 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0247   -4.0970   -1.9800 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.1317   -2.7259   -2.0053 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.0647   -1.9643   -0.8024 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.1690   -2.6403    0.4509 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.3265   -4.0569    0.4383 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.2230   -0.5604   -0.7942 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.1612    0.1765    0.3841 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
0.0727   -0.5062    1.6320 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
0.2337   -1.8838    1.6458 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.3358    1.6466    0.3850 C    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.5380    2.2036   -0.7983 O    0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18

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|---------|---------|---------|---|---|---|---|---|---|---|---|---|---|---|---|----|
| -0.2969 | 2.3127 | 1.4449 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 19 |
| 0.1389 | 0.1798 | 2.8025 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 20 |
| -0.6633 | 3.2412 | -0.7156 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 21 |
| -0.0120 | 1.1481 | 2.5544 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 |
| 0.3775 | -5.8485 | -0.7382 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 23 |
| -0.0287 | -4.6740 | -2.9045 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 24 |
| -0.3098 | -2.2037 | -2.9483 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 |
| 0.5040 | -4.5766 | 1.3823 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 26 |
| -0.4007 | -0.0397 | -1.7363 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 27 |
| 0.4099 | -2.3855 | 2.5993 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 28 |

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|----|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 24 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 25 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 26 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 27 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | 14 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 17 | 14 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 20 | 15 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 17 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 17 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 21 | 18 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 22 | 20 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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3-hydroxybenzoicacid-anion.sdf

COSMOtherm

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|---------|---------|---------|---|---|---|---|---|---|---|---|---|---|---|---|----|---|-------|
| 21 | 19 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | V2000 |
| -3.3029 | -0.0016 | 2.5352 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | |
| -3.6548 | -0.7848 | 2.0748 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | | |
| -3.6554 | 0.7575 | 2.0364 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | | |
| -1.4745 | 0.0110 | -4.6012 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | | |
| -1.2672 | 0.0038 | -3.6102 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | | |
| -0.5891 | 0.0087 | -5.0051 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | | |
| 2.5258 | 0.0032 | 1.3520 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | | |
| 2.1182 | -0.0002 | 0.0131 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | | |
| 0.7493 | -0.0024 | -0.3009 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | | |
| -0.1979 | -0.0014 | 0.7346 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | | |
| 0.2123 | 0.0020 | 2.0780 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | | |
| 1.5849 | 0.0044 | 2.3853 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | | |
| 0.2944 | -0.0053 | -1.7592 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 | | |
| -0.6717 | 0.0033 | 3.1219 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 14 | | |
| -0.9702 | -0.0055 | -1.9676 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | | |
| 1.1824 | -0.0072 | -2.6578 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 16 | | |
| 3.5898 | 0.0049 | 1.5987 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 17 | | |
| 2.8468 | -0.0011 | -0.7980 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 18 | | |
| -1.2589 | -0.0035 | 0.4790 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 19 | | |
| 1.8971 | 0.0072 | 3.4313 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 20 | | |
| -1.6193 | 0.0024 | 2.7934 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 21 | | |

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|----|----|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 17 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 20 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 21 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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3-hydroxybenzoicacid.sdf

COSMOtherm

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|---------|---------|---------|---|---|---|---|---|---|---|---|---|---|---|---|----|---|-------|
| 22 | 20 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | V2000 |
| -4.5212 | -0.0025 | 1.4974 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | |
| -5.0165 | -0.7722 | 1.1618 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 | | |
| -5.0133 | 0.7703 | 1.1638 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 | | |
| 2.3231 | 0.0025 | 3.3906 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 | | |
| 1.8069 | -0.7546 | 3.7219 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 | | |
| 1.8543 | 0.7891 | 3.7238 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 | | |
| 1.5123 | 0.0003 | -2.4823 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 | | |
| 0.1513 | 0.0015 | -2.1646 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 | | |
| -0.2414 | 0.0004 | -0.8157 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 | | |
| 0.7258 | -0.0012 | 0.2038 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 | | |
| 2.0915 | -0.0022 | -0.1231 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 | | |
| 2.4803 | -0.0015 | -1.4758 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 | | |
| -1.7028 | 0.0010 | -0.4961 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 | | |
| 3.0756 | -0.0028 | 0.8195 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 14 | | |
| -1.9673 | -0.0020 | 0.8210 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 | | |
| -2.5836 | 0.0043 | -1.3576 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 16 | | |

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3 1.8267 0.0008 -3.5273 H 0 0 0 0 0 0 0 0 0 0 17
4 -0.6087 0.0031 -2.9455 H 0 0 0 0 0 0 0 0 0 0 18
5 0.4149 -0.0019 1.2485 H 0 0 0 0 0 0 0 0 0 0 19
6 3.5438 -0.0026 -1.7213 H 0 0 0 0 0 0 0 0 0 0 20
7 2.6930 -0.0023 1.7494 H 0 0 0 0 0 0 0 0 0 0 21
8 -2.9765 -0.0032 0.9765 H 0 0 0 0 0 0 0 0 0 0 22
9 2 1 0 0 0 0
10 3 1 0 0 0 0
11 5 4 0 0 0 0
12 6 4 0 0 0 0
13 8 7 0 0 0 0
14 12 7 0 0 0 0
15 17 7 0 0 0 0
16 9 8 0 0 0 0
17 18 8 0 0 0 0
18 10 9 0 0 0 0
19 13 9 0 0 0 0
20 11 10 0 0 0 0
21 19 10 0 0 0 0
22 12 11 0 0 0 0
23 14 11 0 0 0 0
24 20 12 0 0 0 0
25 15 13 0 0 0 0
26 16 13 0 0 0 0
27 21 14 0 0 0 0
28 15 22 0 0 0 0
29 M END
30 \$\$\$\$
31 4-(1,1-dimethylethyl)-benzoicacid-anion.sdf
32 COSMOtherm 3D 0
33 32 30 0 0 0 0 0 0 0 0 0 0 V2000
34 -6.7350 0.8454 1.4462 O 0 0 0 0 0 0 0 0 0 0 1
35 -6.1553 0.3456 0.7990 H 0 0 0 0 0 0 0 0 0 0 2
36 -6.3518 1.7386 1.4761 H 0 0 0 0 0 0 0 0 0 0 3
37 -5.2147 -0.6131 -0.2678 O 0 0 0 0 0 0 0 0 0 0 4
38 -4.2149 -0.5742 -0.0290 H 0 0 0 0 0 0 0 0 0 0 5
39 -5.2429 -0.2656 -1.1770 H 0 0 0 0 0 0 0 0 0 0 6
40 1.7939 0.3143 -1.2154 C 0 0 0 0 0 0 0 0 0 0 7
41 0.4114 0.2519 -1.4216 C 0 0 0 0 0 0 0 0 0 0 8
42 -0.4595 -0.1002 -0.3815 C 0 0 0 0 0 0 0 0 0 0 9
43 0.0973 -0.3877 0.8764 C 0 0 0 0 0 0 0 0 0 0 10
44 1.4759 -0.3218 1.0800 C 0 0 0 0 0 0 0 0 0 0 11
45 2.3604 0.0304 0.0396 C 0 0 0 0 0 0 0 0 0 0 12
46 -1.9608 -0.1633 -0.6171 C 0 0 0 0 0 0 0 0 0 0 13
47 3.8748 0.0903 0.3046 C 0 0 0 0 0 0 0 0 0 0 14
48 4.1580 1.1239 1.4213 C 0 0 0 0 0 0 0 0 0 0 15
49 4.6735 0.4981 -0.9471 C 0 0 0 0 0 0 0 0 0 0 16
50 4.3682 -1.3032 0.7641 C 0 0 0 0 0 0 0 0 0 0 17
51 -2.4047 0.1534 -1.7559 O 0 0 0 0 0 0 0 0 0 0 18
52 -2.6820 -0.5425 0.3765 O 0 0 0 0 0 0 0 0 0 0 19
53 2.4335 0.5912 -2.0536 H 0 0 0 0 0 0 0 0 0 0 20
54 -0.0089 0.4785 -2.4031 H 0 0 0 0 0 0 0 0 0 0 21
55 -0.5679 -0.6641 1.6961 H 0 0 0 0 0 0 0 0 0 0 22
56 1.8697 -0.5501 2.0728 H 0 0 0 0 0 0 0 0 0 0 23
57 5.2387 1.1711 1.6257 H 0 0 0 0 0 0 0 0 0 0 24
58 3.6489 0.8592 2.3592 H 0 0 0 0 0 0 0 0 0 0 25
59 3.8213 2.1279 1.1219 H 0 0 0 0 0 0 0 0 0 0 26
60 5.7459 0.5255 -0.7031 H 0 0 0 0 0 0 0 0 0 0 27
4.5375 -0.2177 -1.7716 H 0 0 0 0 0 0 0 0 0 0 28
4.3880 1.4977 -1.3072 H 0 0 0 0 0 0 0 0 0 0 29
5.4500 -1.2717 0.9659 H 0 0 0 0 0 0 0 0 0 0 30
4.1861 -2.0604 -0.0135 H 0 0 0 0 0 0 0 0 0 0 31
3.8628 -1.6310 1.6838 H 0 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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28 16 0 0 0 0
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30 17 0 0 0 0
31 17 0 0 0 0
17 32 0 0 0 0
61 M END
62 \$\$\$\$
63 4-(1,1-dimethylethyl)-benzoicacid.sdf
64 COSMOtherm 3D 0
65 33 31 0 0 0 0 0 0 0 0 0 0 V2000
66 -0.8276 6.4010 1.0394 O 0 0 0 0 0 0 0 0 0 0 1
67 -1.7158 6.3418 0.6434 H 0 0 0 0 0 0 0 0 0 0 2
68 -0.6669 7.3580 1.1296 H 0 0 0 0 0 0 0 0 0 0 3
69 1.1202 5.1466 -0.3488 O 0 0 0 0 0 0 0 0 0 0 4
70 0.3734 5.6260 0.1195 H 0 0 0 0 0 0 0 0 0 0 5

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1.0811 5.4460 -1.2746 H 0 0 0 0 0 0 0 0 0 6  
-1.2367 -1.6546 -0.2267 C 0 0 0 0 0 0 0 0 0 7  
-1.2439 -0.2628 -0.3431 C 0 0 0 0 0 0 0 0 0 8  
-0.0578 0.4730 -0.2041 C 0 0 0 0 0 0 0 0 0 9  
1.1391 -0.2206 0.0530 C 0 0 0 0 0 0 0 0 0 10  
1.1374 -1.6095 0.1639 C 0 0 0 0 0 0 0 0 0 11  
-0.0480 -2.3620 0.0284 C 0 0 0 0 0 0 0 0 0 12  
-0.1054 1.9595 -0.3380 C 0 0 0 0 0 0 0 0 0 13  
-0.0032 -3.8926 0.1579 C 0 0 0 0 0 0 0 0 0 14  
0.9349 -4.4660 -0.9321 C 0 0 0 0 0 0 0 0 0 15  
-1.3921 -4.5367 -0.0069 C 0 0 0 0 0 0 0 0 0 16  
0.5479 -4.2699 1.5546 C 0 0 0 0 0 0 0 0 0 17  
-1.1376 2.5800 -0.6051 O 0 0 0 0 0 0 0 0 0 18  
1.0786 2.5569 -0.1397 O 0 0 0 0 0 0 0 0 0 19  
-2.1791 -2.1899 -0.3391 H 0 0 0 0 0 0 0 0 0 20  
-2.1771 0.2661 -0.5429 H 0 0 0 0 0 0 0 0 0 21  
2.0720 0.3326 0.1641 H 0 0 0 0 0 0 0 0 0 22  
2.0836 -2.1167 0.3608 H 0 0 0 0 0 0 0 0 0 23  
0.9802 -5.5626 -0.8479 H 0 0 0 0 0 0 0 0 0 24  
1.9582 -4.0771 -0.8339 H 0 0 0 0 0 0 0 0 0 25  
0.5683 -4.2144 -1.9386 H 0 0 0 0 0 0 0 0 0 26  
-1.3015 -5.6276 0.0976 H 0 0 0 0 0 0 0 0 0 27  
-2.1004 -4.1859 0.7586 H 0 0 0 0 0 0 0 0 0 28  
-1.8245 -4.3322 -0.9980 H 0 0 0 0 0 0 0 0 0 29  
0.5899 -5.3650 1.6563 H 0 0 0 0 0 0 0 0 0 30  
-0.0989 -3.8757 2.3527 H 0 0 0 0 0 0 0 0 0 31  
1.5629 -3.8779 1.7123 H 0 0 0 0 0 0 0 0 0 32  
0.9924 3.5809 -0.2486 H 0 0 0 0 0 0 0 0 0 33  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
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8 7 0 0 0 0  
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27 16 0 0 0 0  
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30 17 0 0 0 0  
31 17 0 0 0 0  
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19 33 0 0 0 0  
M END  
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4-(1-methylethyl)-benzoicacid-anion.sdf  
COSMOTHERM 3D 0  
29 27 0 0 0 0 0 0 0 0 V2000  
-6.5218 0.7130 1.3576 O 0 0 0 0 0 0 0 0 0 1  
-5.9074 0.2996 0.6822 H 0 0 0 0 0 0 0 0 0 2  
-6.1668 1.6079 1.4940 H 0 0 0 0 0 0 0 0 0 3  
-4.9117 -0.5235 -0.4469 O 0 0 0 0 0 0 0 0 0 4  
-3.9233 -0.5310 -0.1625 H 0 0 0 0 0 0 0 0 0 5  
-4.8971 -0.0749 -1.3109 H 0 0 0 0 0 0 0 0 0 6  
1.7010 -0.4524 1.2747 C 0 0 0 0 0 0 0 0 0 7  
0.3325 -0.4845 0.9885 C 0 0 0 0 0 0 0 0 0 8  
-0.1450 -0.0918 -0.2717 C 0 0 0 0 0 0 0 0 0 9  
0.7870 0.3308 -1.2350 C 0 0 0 0 0 0 0 0 0 10  
2.1530 0.3574 -0.9482 C 0 0 0 0 0 0 0 0 0 11  
2.6375 -0.0331 0.3146 C 0 0 0 0 0 0 0 0 0 12  
-1.6306 -0.1191 -0.5984 C 0 0 0 0 0 0 0 0 0 13  
4.1242 -0.0090 0.6376 C 0 0 0 0 0 0 0 0 0 14  
4.9155 -0.9912 -0.2482 C 0 0 0 0 0 0 0 0 0 15  
4.7085 1.4133 0.5401 C 0 0 0 0 0 0 0 0 0 16  
-2.4114 -0.5740 0.3155 O 0 0 0 0 0 0 0 0 0 17  
-2.0051 0.2984 -1.7294 O 0 0 0 0 0 0 0 0 0 18  
2.0527 -0.7602 2.2633 H 0 0 0 0 0 0 0 0 0 19  
-0.3827 -0.8148 1.7435 H 0 0 0 0 0 0 0 0 0 20  
0.4210 0.6380 -2.2163 H 0 0 0 0 0 0 0 0 0 21  
2.8521 0.6878 -1.7200 H 0 0 0 0 0 0 0 0 0 22  
4.2290 -0.3431 1.6834 H 0 0 0 0 0 0 0 0 0 23  
5.9754 -1.0048 0.0471 H 0 0 0 0 0 0 0 0 0 24  
4.5221 -2.0145 -0.1602 H 0 0 0 0 0 0 0 0 0 25  
4.8651 -0.6976 -1.3079 H 0 0 0 0 0 0 0 0 0 26  
5.7682 1.4137 0.8366 H 0 0 0 0 0 0 0 0 0 27  
4.1693 2.1129 1.1956 H 0 0 0 0 0 0 0 0 0 28  
4.6485 1.7981 -0.4898 H 0 0 0 0 0 0 0 0 0 29  
2 1 0 0 0 0  
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0.4197 -0.6103 1.8467 H 0 0 0 0 0 0 0 0 0 0 0 20
1.1876 0.4637 -2.2395 H 0 0 0 0 0 0 0 0 0 0 0 21
3.6197 0.6332 -1.7533 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
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12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
17 14 0 0 0 0
18 14 0 0 0 0
11 22 0 0 0 0
M END
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4-aminobenzoicacid.sdf
COSMOTHERM 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
-1.3649 -4.3767 0.0482 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7811 -4.6750 -0.7800 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.3566 -3.3799 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2886 -4.1607 -0.0365 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3228 -4.4425 0.0053 H 0 0 0 0 0 0 0 0 0 0 0 5
1.7041 -4.5126 0.7714 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2460 2.5576 0.0019 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2082 1.1719 -0.0023 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0179 0.4730 -0.0037 C 0 0 0 0 0 0 0 0 0 0 0 9
1.2137 1.2239 0.0022 C 0 0 0 0 0 0 0 0 0 0 0 10
1.1889 2.6107 0.0091 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0441 3.3114 0.0073 C 0 0 0 0 0 0 0 0 0 0 0 12
0.0158 -1.0000 -0.0039 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.0738 4.6816 -0.0352 N 0 0 0 0 0 0 0 0 0 0 0 14
-1.0374 -1.6689 0.0235 O 0 0 0 0 0 0 0 0 0 0 0 15
1.2333 -1.5553 -0.0371 O 0 0 0 0 0 0 0 0 0 0 0 16
0.7715 5.1946 0.1973 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.9412 5.1576 0.1947 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.2049 3.0803 0.0018 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.1403 0.6047 -0.0030 H 0 0 0 0 0 0 0 0 0 0 0 20
2.1732 0.7062 0.0074 H 0 0 0 0 0 0 0 0 0 0 0 21
2.1241 3.1747 0.0170 H 0 0 0 0 0 0 0 0 0 0 0 22
1.1950 -2.5882 -0.0177 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
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6 4 0 0 0 0
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22 11 0 0 0 0
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17 14 0 0 0 0
18 14 0 0 0 0
16 23 0 0 0 0
M END
$$$$
4-bromobenzoicacid-anion.sdf
COSMOTHERM 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-6.9661 1.0452 1.4610 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.4447 0.4526 0.8438 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.5015 1.8988 1.4264 H 0 0 0 0 0 0 0 0 0 0 0 3
-5.6136 -0.6369 -0.1949 O 0 0 0 0 0 0 0 0 0 0 0 4
-4.6076 -0.6432 0.0073 H 0 0 0 0 0 0 0 0 0 0 0 5
-5.6582 -0.3197 -1.1144 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1006 -0.4309 1.0550 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.2804 -0.5039 0.8481 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.8483 -0.1478 -0.3853 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0028 0.2853 -1.4186 C 0 0 0 0 0 0 0 0 0 0 0 10
1.3807 0.3639 -1.2358 C 0 0 0 0 0 0 0 0 0 0 0 11
1.9119 0.0032 -0.0045 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.3545 -0.2247 -0.6100 C 0 0 0 0 0 0 0 0 0 0 0 13
3.8214 0.1076 0.2748 Br 0 0 0 0 0 0 0 0 0 0 0 14
-3.0533 -0.6731 0.3679 O 0 0 0 0 0 0 0 0 0 0 0 15
-2.8093 0.1496 -1.7247 O 0 0 0 0 0 0 0 0 0 0 0 16
1.5327 -0.7076 2.0167 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.9329 -0.8422 1.6539 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.4421 0.5630 -2.3778 H 0 0 0 0 0 0 0 0 0 0 0 19
2.0294 0.6993 -2.0451 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0

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17 7 0 0 0 0
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11 10 0 0 0 0
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12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-bromobenzoicacid.sdf
COSMOTHERM 3D 0
21 19 0 0 0 0 0 0 0 0 0 V2000
-0.1834 -1.5466 -6.8430 O 0 0 0 0 0 0 0 0 0 0 1
-0.0994 -1.4206 -7.8056 H 0 0 0 0 0 0 0 0 0 0 2
-0.9512 -2.1385 -6.7448 H 0 0 0 0 0 0 0 0 0 0 3
-0.5763 0.7906 -5.5368 O 0 0 0 0 0 0 0 0 0 0 4
-0.4182 -0.0686 -6.0326 H 0 0 0 0 0 0 0 0 0 0 5
0.1542 1.3797 -5.7981 H 0 0 0 0 0 0 0 0 0 0 6
1.2775 -0.0491 1.3465 C 0 0 0 0 0 0 0 0 0 0 7
1.3797 0.0857 -0.0382 C 0 0 0 0 0 0 0 0 0 0 8
0.2326 0.2598 -0.8296 C 0 0 0 0 0 0 0 0 0 0 9
-1.0296 0.3002 -0.2139 C 0 0 0 0 0 0 0 0 0 0 10
-1.1488 0.1687 1.1712 C 0 0 0 0 0 0 0 0 0 0 11
0.0096 -0.0055 1.9321 C 0 0 0 0 0 0 0 0 0 0 12
0.3959 0.3972 -2.3112 C 0 0 0 0 0 0 0 0 0 0 13
-0.1449 -0.1913 3.8422 Br 0 0 0 0 0 0 0 0 0 0 14
1.4973 0.3848 -2.8647 O 0 0 0 0 0 0 0 0 0 0 15
-0.7617 0.5287 -2.9685 O 0 0 0 0 0 0 0 0 0 0 16
2.1705 -0.1846 1.9558 H 0 0 0 0 0 0 0 0 0 0 17
2.3594 0.0562 -0.5163 H 0 0 0 0 0 0 0 0 0 0 18
-1.9266 0.4344 -0.8178 H 0 0 0 0 0 0 0 0 0 0 19
-2.1294 0.1998 1.6455 H 0 0 0 0 0 0 0 0 0 0 20
-0.5952 0.6202 -3.9881 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
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10 9 0 0 0 0
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15 13 0 0 0 0
16 13 0 0 0 0
16 21 0 0 0 0
M END
$$$$
4-butylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
32 30 0 0 0 0 0 0 0 0 0 V2000
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-6.7395 1.5003 1.2015 H 0 0 0 0 0 0 0 0 0 0 3
-5.4093 -1.0348 -0.0851 O 0 0 0 0 0 0 0 0 0 0 4
-4.4198 -0.8384 0.1188 H 0 0 0 0 0 0 0 0 0 0 5
-5.4802 -0.8748 -1.0430 H 0 0 0 0 0 0 0 0 0 0 6
1.1585 0.3852 1.1316 C 0 0 0 0 0 0 0 0 0 0 7
-0.1927 0.0822 0.9459 C 0 0 0 0 0 0 0 0 0 0 8
-0.7605 0.0913 -0.3389 C 0 0 0 0 0 0 0 0 0 0 9
0.0636 0.4102 -1.4306 C 0 0 0 0 0 0 0 0 0 0 10
1.4155 0.7076 -1.2434 C 0 0 0 0 0 0 0 0 0 0 11
1.9884 0.7021 0.0411 C 0 0 0 0 0 0 0 0 0 0 12
-2.2327 -0.2269 -0.5541 C 0 0 0 0 0 0 0 0 0 0 13
3.4592 0.9880 0.2391 C 0 0 0 0 0 0 0 0 0 0 14
4.3320 -0.2847 0.1874 C 0 0 0 0 0 0 0 0 0 0 15
5.8253 0.0029 0.3866 C 0 0 0 0 0 0 0 0 0 0 16
6.6909 -1.2619 0.3471 C 0 0 0 0 0 0 0 0 0 0 17
-2.9045 -0.5649 0.4879 O 0 0 0 0 0 0 0 0 0 0 18
-2.7012 -0.1439 -1.7233 O 0 0 0 0 0 0 0 0 0 0 19
1.5788 0.3822 2.1410 H 0 0 0 0 0 0 0 0 0 0 20
-0.8274 -0.1600 1.7998 H 0 0 0 0 0 0 0 0 0 0 21
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2.0386 0.9564 -2.1066 H 0 0 0 0 0 0 0 0 0 0 23
3.6108 1.4839 1.2119 H 0 0 0 0 0 0 0 0 0 0 24
3.8058 1.6896 -0.5370 H 0 0 0 0 0 0 0 0 0 0 25
4.1796 -0.7883 -0.7829 H 0 0 0 0 0 0 0 0 0 0 26
3.9863 -0.9909 0.9619 H 0 0 0 0 0 0 0 0 0 0 27
5.9682 0.5182 1.3519 H 0 0 0 0 0 0 0 0 0 0 28
6.1647 0.7077 -0.3917 H 0 0 0 0 0 0 0 0 0 0 29
7.7554 -1.0243 0.4921 H 0 0 0 0 0 0 0 0 0 0 30
6.5920 -1.7806 -0.6192 H 0 0 0 0 0 0 0 0 0 0 31
6.3949 -1.9694 1.1373 H 0 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0

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10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
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15 14 0 0 0 0
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16 15 0 0 0 0
26 15 0 0 0 0
27 15 0 0 0 0
17 16 0 0 0 0
28 16 0 0 0 0
29 16 0 0 0 0
30 17 0 0 0 0
31 17 0 0 0 0
17 32 0 0 0 0
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M END

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4-butylbenzoicacid.sdf
COSMOTHERM 3D 0

```
33 31 0 0 0 0 0 0 0 0 0 V2000
-1.7363 -6.4760 0.7640 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7376 -7.3981 1.0820 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.1564 -6.5196 -0.1139 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7551 -5.4234 0.7432 O 0 0 0 0 0 0 0 0 0 0 0 4
1.2654 -5.8776 0.0491 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.1636 -5.8241 0.7065 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.3475 1.3593 -1.3953 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.4591 -0.0294 -1.3312 C 0 0 0 0 0 0 0 0 0 0 0 8
0.2916 -0.7614 -0.3943 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1566 -0.0720 0.4744 C 0 0 0 0 0 0 0 0 0 0 0 10
1.2637 1.3173 0.4029 C 0 0 0 0 0 0 0 0 0 0 0 11
0.5154 2.0586 -0.5305 C 0 0 0 0 0 0 0 0 0 0 0 12
0.1515 -2.2476 -0.3614 C 0 0 0 0 0 0 0 0 0 0 0 13
0.6078 3.5655 -0.5751 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.3809 4.2559 0.3908 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.2881 5.7857 0.3474 C 0 0 0 0 0 0 0 0 0 0 0 16
-1.2670 6.4729 1.3062 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.5828 -2.8731 -1.1312 O 0 0 0 0 0 0 0 0 0 0 0 18
0.8972 -2.8380 0.5825 O 0 0 0 0 0 0 0 0 0 0 0 19
-0.9340 1.9136 -2.1323 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.1255 -0.5626 -2.0094 H 0 0 0 0 0 0 0 0 0 0 0 21
1.7486 -0.6277 1.2017 H 0 0 0 0 0 0 0 0 0 0 0 22
1.9454 1.8393 1.0791 H 0 0 0 0 0 0 0 0 0 0 0 23
0.4082 3.9158 -1.6005 H 0 0 0 0 0 0 0 0 0 0 0 24
1.6327 3.8790 -0.3191 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.1860 3.9042 1.4179 H 0 0 0 0 0 0 0 0 0 0 0 26
-1.4086 3.9406 0.1422 H 0 0 0 0 0 0 0 0 0 0 0 27
-0.4778 6.1298 -0.6839 H 0 0 0 0 0 0 0 0 0 0 0 28
0.7437 6.0918 0.5904 H 0 0 0 0 0 0 0 0 0 0 0 29
-1.1761 7.5684 1.2547 H 0 0 0 0 0 0 0 0 0 0 0 30
-1.0800 6.1700 2.3481 H 0 0 0 0 0 0 0 0 0 0 0 31
-2.3089 6.2108 1.0647 H 0 0 0 0 0 0 0 0 0 0 0 32
0.7693 -3.8636 0.5601 H 0 0 0 0 0 0 0 0 0 0 0 33
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
24 14 0 0 0 0
25 14 0 0 0 0
16 15 0 0 0 0
26 15 0 0 0 0
27 15 0 0 0 0
17 16 0 0 0 0
28 16 0 0 0 0
29 16 0 0 0 0
30 17 0 0 0 0
31 17 0 0 0 0
32 17 0 0 0 0
19 33 0 0 0 0
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M END

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4-carbamoylbenzoicacid-anion.sdf
COSMOTHERM 3D 0

```
24 22 0 0 0 0 0 0 0 0 0 V2000
-1.1115 6.4131 -1.2776 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.4983 5.8516 -0.7188 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.9962 6.0449 -1.1124 H 0 0 0 0 0 0 0 0 0 0 0 3
0.6479 4.9381 0.1815 O 0 0 0 0 0 0 0 0 0 0 0 4
0.5895 3.9389 -0.0424 H 0 0 0 0 0 0 0 0 0 0 0 5
0.4495 4.9715 1.1343 H 0 0 0 0 0 0 0 0 0 0 0 6
0.2015 -1.7451 -1.1737 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2975 -0.3704 -0.9589 C 0 0 0 0 0 0 0 0 0 0 0 8
```

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3 0.1570 0.1644 0.3324 C 0 0 0 0 0 0 0 0 0 0 0 9
4 -0.0815 -0.7112 1.4034 C 0 0 0 0 0 0 0 0 0 0 0 10
5 -0.1851 -2.0868 1.1928 C 0 0 0 0 0 0 0 0 0 0 0 11
6 -0.0486 -2.6188 -0.1020 C 0 0 0 0 0 0 0 0 0 0 0 12
7 0.2648 1.6666 0.5800 C 0 0 0 0 0 0 0 0 0 0 0 13
8 -0.1292 -4.0930 -0.3918 C 0 0 0 0 0 0 0 0 0 0 0 14
9 0.3980 -4.5835 -1.4091 O 0 0 0 0 0 0 0 0 0 0 0 15
10 -0.7990 -4.8554 0.5074 N 0 0 0 0 0 0 0 0 0 0 0 16
11 0.5283 2.3934 -0.4433 O 0 0 0 0 0 0 0 0 0 0 0 17
12 0.0924 2.0893 1.7552 O 0 0 0 0 0 0 0 0 0 0 0 18
13 -0.8812 -5.8556 0.3455 H 0 0 0 0 0 0 0 0 0 0 0 19
14 -1.3233 -4.4572 1.2795 H 0 0 0 0 0 0 0 0 0 0 0 20
15 0.3165 -2.1592 -2.1764 H 0 0 0 0 0 0 0 0 0 0 0 21
16 0.4846 0.3077 -1.7923 H 0 0 0 0 0 0 0 0 0 0 0 22
17 -0.1785 -0.2968 2.4077 H 0 0 0 0 0 0 0 0 0 0 0 23
18 -0.3457 -2.7417 2.0514 H 0 0 0 0 0 0 0 0 0 0 0 24

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
10 9 0 0 0 0
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11 10 0 0 0 0
23 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
17 13 0 0 0 0
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15 14 0 0 0 0
16 14 0 0 0 0
19 16 0 0 0 0
20 16 0 0 0 0
11 24 0 0 0 0

M END

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4-carbamoylbenzoicacid.sdf

COSMOTHERM 3D 0

25 23 0 0 0 0 0 0 0 0 0 V2000
-0.8195 -1.3390 -6.2495 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.5276 -1.3186 -7.1792 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.7880 -1.4362 -6.3026 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.1479 0.8839 -4.8699 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.3744 0.0612 -5.3999 H 0 0 0 0 0 0 0 0 0 0 0 5
0.7726 1.1010 -5.1028 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1567 -0.3674 2.0658 C 0 0 0 0 0 0 0 0 0 0 0 7
1.3548 -0.2678 0.6912 C 0 0 0 0 0 0 0 0 0 0 0 8
0.3088 0.1525 -0.1474 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.9387 0.4715 0.4139 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.1380 0.3644 1.7906 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0933 -0.0603 2.6294 C 0 0 0 0 0 0 0 0 0 0 0 12
0.5635 0.2591 -1.6209 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.2396 -0.1683 4.1258 C 0 0 0 0 0 0 0 0 0 0 0 14
0.7544 -0.1163 4.8739 O 0 0 0 0 0 0 0 0 0 0 0 15
-1.4978 -0.3161 4.6046 N 0 0 0 0 0 0 0 0 0 0 0 16
1.6660 0.0363 -2.1247 O 0 0 0 0 0 0 0 0 0 0 0 17
-0.5134 0.6193 -2.3254 O 0 0 0 0 0 0 0 0 0 0 0 18
-1.6396 -0.3977 5.6081 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.2994 -0.4694 4.0016 H 0 0 0 0 0 0 0 0 0 0 0 20
1.9683 -0.6868 2.7204 H 0 0 0 0 0 0 0 0 0 0 0 21
2.3226 -0.5131 0.2528 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.7513 0.8103 -0.2278 H 0 0 0 0 0 0 0 0 0 0 0 23
-2.1090 0.6421 2.2030 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.2854 0.6889 -3.3357 H 0 0 0 0 0 0 0 0 0 0 0 25

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
21 7 0 0 0 0
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22 8 0 0 0 0
10 9 0 0 0 0
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11 10 0 0 0 0
23 10 0 0 0 0
12 11 0 0 0 0
24 11 0 0 0 0
14 12 0 0 0 0
17 13 0 0 0 0
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15 14 0 0 0 0
16 14 0 0 0 0
19 16 0 0 0 0
20 16 0 0 0 0
18 25 0 0 0 0

M END

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4-chlorobenzoicacid-anion.sdf

COSMOTHERM 3D 0

20 18 0 0 0 0 0 0 0 0 0 V2000
-6.1498 0.9741 1.3241 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.5888 0.4039 0.7207 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.7084 1.8406 1.3187 H 0 0 0 0 0 0 0 0 0 0 0 3
-4.6808 -0.6624 -0.2759 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.6841 -0.6296 -0.0335 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.6994 -0.3617 -1.2019 H 0 0 0 0 0 0 0 0 0 0 0 6
1.9828 -0.3447 1.1982 C 0 0 0 0 0 0 0 0 0 0 0 7

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0.6103 -0.4306 0.9483 C 0 0 0 0 0 0 0 0 0 0 8
0.0825 -0.1159 -0.3141 C 0 0 0 0 0 0 0 0 0 0 9
0.9607 0.2894 -1.3315 C 0 0 0 0 0 0 0 0 0 0 10
2.3363 0.3811 -1.1047 C 0 0 0 0 0 0 0 0 0 0 11
2.8273 0.0613 0.1629 C 0 0 0 0 0 0 0 0 0 0 12
-1.4146 -0.2066 -0.5860 C 0 0 0 0 0 0 0 0 0 0 13
4.5731 0.1744 0.4665 Cl 0 0 0 0 0 0 0 0 0 0 14
-2.1460 -0.6090 0.3885 O 0 0 0 0 0 0 0 0 0 0 15
-1.8324 0.1133 -1.7320 O 0 0 0 0 0 0 0 0 0 0 16
2.3879 -0.5886 2.1805 H 0 0 0 0 0 0 0 0 0 0 17
-0.0679 -0.7460 1.7419 H 0 0 0 0 0 0 0 0 0 0 18
0.5525 0.5346 -2.3129 H 0 0 0 0 0 0 0 0 0 0 19
3.0141 0.6950 -1.8988 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
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18 8 0 0 0 0
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11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-chlorobenzoicacid.sdf
COSMOtherm 3D 0

21 19 0 0 0 0 0 0 0 0 0 0 V2000
-0.7679 5.8890 1.0494 O 0 0 0 0 0 0 0 0 0 0 1
-1.6677 5.8792 0.6757 H 0 0 0 0 0 0 0 0 0 0 2
-0.5623 6.8353 1.1593 H 0 0 0 0 0 0 0 0 0 0 3
1.0859 4.5945 -0.4194 O 0 0 0 0 0 0 0 0 0 0 4
0.3718 5.0894 0.0839 H 0 0 0 0 0 0 0 0 0 0 5
1.0046 4.8872 -1.3447 H 0 0 0 0 0 0 0 0 0 0 6
-1.2253 -2.2093 -0.1836 C 0 0 0 0 0 0 0 0 0 0 7
-1.2393 -0.8208 -0.3145 C 0 0 0 0 0 0 0 0 0 0 8
-0.0573 -0.0742 -0.1773 C 0 0 0 0 0 0 0 0 0 0 9
1.1500 -0.7400 0.0957 C 0 0 0 0 0 0 0 0 0 0 10
1.1808 -2.1292 0.2288 C 0 0 0 0 0 0 0 0 0 0 11
-0.0105 -2.8448 0.0866 C 0 0 0 0 0 0 0 0 0 0 12
-0.1243 1.4133 -0.3299 C 0 0 0 0 0 0 0 0 0 0 13
0.0197 -4.6064 0.2531 Cl 0 0 0 0 0 0 0 0 0 0 14
-1.1736 2.0133 -0.5723 O 0 0 0 0 0 0 0 0 0 0 15
1.0578 2.0204 -0.1792 O 0 0 0 0 0 0 0 0 0 0 16
-2.1427 -2.7877 -0.2903 H 0 0 0 0 0 0 0 0 0 0 17
-2.1761 -0.3043 -0.5259 H 0 0 0 0 0 0 0 0 0 0 18
2.0727 -0.1709 0.2046 H 0 0 0 0 0 0 0 0 0 0 19
2.1167 -2.6461 0.4397 H 0 0 0 0 0 0 0 0 0 0 20
0.9640 3.0464 -0.2968 H 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
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20 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
16 21 0 0 0 0
M END
$$$$
4-chlorophenol-anion.sdf
COSMOtherm 3D 0

18 16 0 0 0 0 0 0 0 0 0 0 V2000
-2.2519 -0.0568 3.6678 O 0 0 0 0 0 0 0 0 0 0 1
-1.4103 -0.0221 3.0998 H 0 0 0 0 0 0 0 0 0 0 2
-2.6309 0.8356 3.5925 H 0 0 0 0 0 0 0 0 0 0 3
2.2532 0.0215 3.6640 O 0 0 0 0 0 0 0 0 0 0 4
1.4104 0.0095 3.0968 H 0 0 0 0 0 0 0 0 0 0 5
2.7035 -0.8128 3.4475 H 0 0 0 0 0 0 0 0 0 0 6
-1.2155 -0.0173 -1.1923 C 0 0 0 0 0 0 0 0 0 0 7
-1.2132 -0.0105 0.2036 C 0 0 0 0 0 0 0 0 0 0 8
-0.0003 0.0138 0.9560 C 0 0 0 0 0 0 0 0 0 0 9
1.2123 0.0306 0.2027 C 0 0 0 0 0 0 0 0 0 0 10
1.2140 0.0254 -1.1933 C 0 0 0 0 0 0 0 0 0 0 11
-0.0009 0.0003 -1.8828 C 0 0 0 0 0 0 0 0 0 0 12
0.0001 0.0196 2.2742 O 0 0 0 0 0 0 0 0 0 0 13
-0.0015 -0.0085 -3.6702 Cl 0 0 0 0 0 0 0 0 0 0 14
-2.1604 -0.0357 -1.7386 H 0 0 0 0 0 0 0 0 0 0 15
-2.1625 -0.0264 0.7439 H 0 0 0 0 0 0 0 0 0 0 16
2.1623 0.0559 0.7415 H 0 0 0 0 0 0 0 0 0 0 17
2.1588 0.0398 -1.7400 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0

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8 7 0 0 0 0  
12 7 0 0 0 0  
15 7 0 0 0 0  
9 8 0 0 0 0  
16 8 0 0 0 0  
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13 9 0 0 0 0  
11 10 0 0 0 0  
17 10 0 0 0 0  
12 11 0 0 0 0  
14 12 0 0 0 0  
11 18 0 0 0 0  
M END  
$$$$  
4-chlorophenol.sdf  
COSMOtherm 3D 0  
19 17 0 0 0 0 0 0 0 0 0 V2000  
-1.7217 4.7271 0.8187 O 0 0 0 0 0 0 0 0 0 1  
-2.5087 4.1585 0.8985 H 0 0 0 0 0 0 0 0 0 2  
-2.0749 5.5958 0.5533 H 0 0 0 0 0 0 0 0 0 3  
0.2658 3.8327 -0.8041 O 0 0 0 0 0 0 0 0 0 4  
-0.5035 4.1447 -0.2433 H 0 0 0 0 0 0 0 0 0 5  
-0.0691 3.7923 -1.7173 H 0 0 0 0 0 0 0 0 0 6  
1.7447 -0.5877 0.4549 C 0 0 0 0 0 0 0 0 0 7  
1.1630 -1.8570 0.4527 C 0 0 0 0 0 0 0 0 0 8  
-0.1501 -2.0072 -0.0020 C 0 0 0 0 0 0 0 0 0 9  
-0.8861 -0.9111 -0.4525 C 0 0 0 0 0 0 0 0 0 10  
-0.2999 0.3591 -0.4482 C 0 0 0 0 0 0 0 0 0 11  
1.0216 0.5325 0.0075 C 0 0 0 0 0 0 0 0 0 12  
-0.8942 -3.6236 -0.0052 C1 0 0 0 0 0 0 0 0 0 13  
1.6418 1.7442 0.0387 O 0 0 0 0 0 0 0 0 0 14  
2.7696 -0.4560 0.8068 H 0 0 0 0 0 0 0 0 0 15  
1.7320 -2.7200 0.8018 H 0 0 0 0 0 0 0 0 0 16  
-1.9092 -1.0373 -0.8072 H 0 0 0 0 0 0 0 0 0 17  
-0.8749 1.2174 -0.8000 H 0 0 0 0 0 0 0 0 0 18  
1.0402 2.4831 -0.3057 H 0 0 0 0 0 0 0 0 0 19  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
8 7 0 0 0 0  
12 7 0 0 0 0  
15 7 0 0 0 0  
9 8 0 0 0 0  
16 8 0 0 0 0  
10 9 0 0 0 0  
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12 11 0 0 0 0  
18 11 0 0 0 0  
14 12 0 0 0 0  
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$$$$  
4-cyanobenzoicacid-anion.sdf  
COSMOtherm 3D 0  
21 19 0 0 0 0 0 0 0 0 0 V2000  
-6.1765 0.5578 1.4240 O 0 0 0 0 0 0 0 0 0 1  
-5.5352 0.1903 0.7488 H 0 0 0 0 0 0 0 0 0 2  
-5.8608 1.4619 1.5924 H 0 0 0 0 0 0 0 0 0 3  
-4.4793 -0.5604 -0.3852 O 0 0 0 0 0 0 0 0 0 4  
-3.4937 -0.4754 -0.1249 H 0 0 0 0 0 0 0 0 0 5  
-4.5277 -0.1442 -1.2639 H 0 0 0 0 0 0 0 0 0 6  
2.1389 -0.1456 1.2824 C 0 0 0 0 0 0 0 0 0 7  
0.7754 -0.1813 0.9993 C 0 0 0 0 0 0 0 0 0 8  
0.3089 -0.0282 -0.3166 C 0 0 0 0 0 0 0 0 0 9  
1.2360 0.1588 -1.3549 C 0 0 0 0 0 0 0 0 0 10  
2.6040 0.1856 -1.0958 C 0 0 0 0 0 0 0 0 0 11  
3.0606 0.0352 0.2303 C 0 0 0 0 0 0 0 0 0 12  
-1.1876 -0.0612 -0.6264 C 0 0 0 0 0 0 0 0 0 13  
4.4606 0.0645 0.5084 C 0 0 0 0 0 0 0 0 0 14  
5.6061 0.0874 0.7360 N 0 0 0 0 0 0 0 0 0 15  
-1.9559 -0.3961 0.3422 O 0 0 0 0 0 0 0 0 0 16  
-1.5546 0.2351 -1.7943 O 0 0 0 0 0 0 0 0 0 17  
2.4967 -0.2590 2.3060 H 0 0 0 0 0 0 0 0 0 18  
0.0525 -0.3286 1.8019 H 0 0 0 0 0 0 0 0 0 19  
0.8666 0.2814 -2.3734 H 0 0 0 0 0 0 0 0 0 20  
3.3204 0.3233 -1.9061 H 0 0 0 0 0 0 0 0 0 21  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
8 7 0 0 0 0  
12 7 0 0 0 0  
18 7 0 0 0 0  
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19 8 0 0 0 0  
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20 10 0 0 0 0  
12 11 0 0 0 0  
14 12 0 0 0 0  
16 13 0 0 0 0  
17 13 0 0 0 0  
15 14 0 0 0 0  
11 21 0 0 0 0  
M END  
$$$$  
4-cyanobenzoicacid.sdf  
COSMOtherm 3D 0
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22 20 0 0 0 0 0 0 0 0 0 V2000
-0.7978 5.7070 0.9726 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6819 5.6973 0.5629 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.5889 6.6535 1.0748 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1104 4.3838 -0.3881 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3738 4.8879 0.0734 H 0 0 0 0 0 0 0 0 0 0 0 5
1.0807 4.6674 -1.3193 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2330 -2.3921 -0.1552 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2433 -1.0064 -0.2797 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0539 -0.2700 -0.1537 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1567 -0.9366 0.1009 C 0 0 0 0 0 0 0 0 0 0 0 10
1.1834 -2.3233 0.2267 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0144 -3.0548 0.0982 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.1165 1.2245 -0.3026 C 0 0 0 0 0 0 0 0 0 0 0 13
0.0070 -4.4779 0.2243 C 0 0 0 0 0 0 0 0 0 0 0 14
0.0250 -5.6406 0.3262 N 0 0 0 0 0 0 0 0 0 0 0 15
-1.1649 1.8203 -0.5515 O 0 0 0 0 0 0 0 0 0 0 0 16
1.0640 1.8233 -0.1392 O 0 0 0 0 0 0 0 0 0 0 0 17
-2.1558 -2.9636 -0.2531 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.1777 -0.4808 -0.4771 H 0 0 0 0 0 0 0 0 0 0 0 19
2.0799 -0.3672 0.1995 H 0 0 0 0 0 0 0 0 0 0 0 20
2.1216 -2.8419 0.4226 H 0 0 0 0 0 0 0 0 0 0 0 21
0.9831 2.8544 -0.2592 H 0 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
8 7 0 0 0 0 0
12 7 0 0 0 0 0
18 7 0 0 0 0 0
9 8 0 0 0 0 0
19 8 0 0 0 0 0
10 9 0 0 0 0 0
13 9 0 0 0 0 0
11 10 0 0 0 0 0
20 10 0 0 0 0 0
12 11 0 0 0 0 0
21 11 0 0 0 0 0
14 12 0 0 0 0 0
16 13 0 0 0 0 0
17 13 0 0 0 0 0
15 14 0 0 0 0 0
17 22 0 0 0 0 0

M END
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4-dimethylaminobenzoicacid-anion.sdf
COSMOTHERM 3D 0

28 26 0 0 0 0 0 0 0 0 0 V2000
6.4089 1.3471 1.0142 O 0 0 0 0 0 0 0 0 0 0 0 1
5.8461 0.7293 0.4600 H 0 0 0 0 0 0 0 0 0 0 0 2
6.4603 0.9157 1.8842 H 0 0 0 0 0 0 0 0 0 0 0 3
4.9095 -0.2521 -0.5890 O 0 0 0 0 0 0 0 0 0 0 0 4
3.9092 0.0028 -0.5652 H 0 0 0 0 0 0 0 0 0 0 0 5
4.9077 -1.1845 -0.3079 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.7559 1.1663 -0.3041 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.3854 0.9360 -0.3831 C 0 0 0 0 0 0 0 0 0 0 0 8
0.1687 -0.3372 -0.1574 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.7213 -1.3793 0.1597 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.0951 -1.1750 0.2428 C 0 0 0 0 0 0 0 0 0 0 0 11
-2.6596 0.1090 -0.0010 C 0 0 0 0 0 0 0 0 0 0 0 12
1.6550 -0.5844 -0.2360 C 0 0 0 0 0 0 0 0 0 0 0 13
-4.0227 0.3168 0.0432 N 0 0 0 0 0 0 0 0 0 0 0 14
-4.9029 -0.7365 0.5419 C 0 0 0 0 0 0 0 0 0 0 0 15
-4.5523 1.6765 -0.0143 C 0 0 0 0 0 0 0 0 0 0 0 16
2.3967 0.4257 -0.5429 O 0 0 0 0 0 0 0 0 0 0 0 17
2.0941 -1.7480 -0.0027 O 0 0 0 0 0 0 0 0 0 0 0 18
-2.1307 2.1739 -0.4776 H 0 0 0 0 0 0 0 0 0 0 0 19
0.2850 1.7644 -0.6196 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.3123 -2.3736 0.3500 H 0 0 0 0 0 0 0 0 0 0 0 21
-2.7375 -2.0158 0.5007 H 0 0 0 0 0 0 0 0 0 0 0 22
-5.9420 -0.4101 0.4272 H 0 0 0 0 0 0 0 0 0 0 0 23
-4.7764 -1.6634 -0.0364 H 0 0 0 0 0 0 0 0 0 0 0 24
-4.7248 -0.9664 1.6086 H 0 0 0 0 0 0 0 0 0 0 0 25
-5.6463 1.6275 -0.0305 H 0 0 0 0 0 0 0 0 0 0 0 26
-4.2430 2.2875 0.8535 H 0 0 0 0 0 0 0 0 0 0 0 27
-4.2252 2.1894 -0.9308 H 0 0 0 0 0 0 0 0 0 0 0 28

2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
8 7 0 0 0 0 0
12 7 0 0 0 0 0
19 7 0 0 0 0 0
9 8 0 0 0 0 0
20 8 0 0 0 0 0
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11 10 0 0 0 0 0
21 10 0 0 0 0 0
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14 12 0 0 0 0 0
17 13 0 0 0 0 0
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15 14 0 0 0 0 0
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23 15 0 0 0 0 0
24 15 0 0 0 0 0
25 15 0 0 0 0 0
26 16 0 0 0 0 0
27 16 0 0 0 0 0
16 28 0 0 0 0 0

M END
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For Peer Review Only

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4-dimethylaminobenzoicacid.sdf
COSMOTHERM      3D      0

29 27 0 0 0 0 0 0 0 0 0 V2000
-0.8468 6.1367 0.9888 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.7219 6.1125 0.5611 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.6635 7.0862 1.1092 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1229 4.8714 -0.3739 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3694 5.3490 0.0825 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.0986 5.1753 -1.2987 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.2345 -1.9557 -0.1529 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2370 -0.5735 -0.2624 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.0474 0.1786 -0.1722 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.1590 -0.5235 0.0341 C 0 0 0 0 0 0 0 0 0 0 0 0 10
1.1832 -1.9065 0.1445 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.0174 -2.6713 0.0541 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.1045 1.6481 -0.2994 C 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.0030 -4.0353 0.1609 N 0 0 0 0 0 0 0 0 0 0 0 0 14
1.2553 -4.7478 0.3722 C 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.2465 -4.7979 0.0658 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-1.1502 2.2829 -0.4937 O 0 0 0 0 0 0 0 0 0 0 0 0 17
1.0951 2.2556 -0.1843 O 0 0 0 0 0 0 0 0 0 0 0 0 18
-2.1789 -2.4924 -0.2286 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-2.1809 -0.0491 -0.4217 H 0 0 0 0 0 0 0 0 0 0 0 0 20
2.0959 0.0297 0.1084 H 0 0 0 0 0 0 0 0 0 0 0 0 21
2.1384 -2.4049 0.3016 H 0 0 0 0 0 0 0 0 0 0 0 0 22
1.0479 -5.8207 0.4288 H 0 0 0 0 0 0 0 0 0 0 0 0 23
1.9619 -4.5764 -0.4560 H 0 0 0 0 0 0 0 0 0 0 0 0 24
1.7422 -4.4411 1.3125 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.0166 -5.8621 0.1755 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-1.9569 -4.5153 0.8597 H 0 0 0 0 0 0 0 0 0 0 0 0 27
-1.7391 -4.6507 -0.9093 H 0 0 0 0 0 0 0 0 0 0 0 0 28
0.9896 3.2711 -0.2813 H 0 0 0 0 0 0 0 0 0 0 0 0 29

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
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11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
23 15 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
26 16 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
18 29 0 0 0 0

M END
$$$$
4-ethylbenzoicacid-anion.sdf
COSMOTHERM      3D      0

26 24 0 0 0 0 0 0 0 0 V2000
-1.5479 -0.8893 5.9638 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.8534 -0.4119 5.4203 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.6264 -1.7622 5.5428 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.3346 0.4775 4.5598 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1083 0.5360 3.5584 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.1901 0.0125 4.5725 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1050 -0.3120 -2.4914 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.3298 -0.3384 -1.1126 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.3737 0.1711 -0.2184 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.8126 0.7091 -0.7451 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.0356 0.7337 -2.1244 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.0818 0.2232 -3.0233 C 0 0 0 0 0 0 0 0 0 0 0 0 12
0.6291 0.1427 1.2811 C 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.3423 0.2135 -4.5136 C 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.0537 -1.0694 -4.9845 C 0 0 0 0 0 0 0 0 0 0 0 0 15
1.7001 -0.3784 1.6992 O 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.2791 0.6613 2.0272 O 0 0 0 0 0 0 0 0 0 0 0 0 17
1.8656 -0.7076 -3.1702 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2.2553 -0.7527 -0.7090 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-1.5569 1.1137 -0.0576 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-1.9630 1.1622 -2.5136 H 0 0 0 0 0 0 0 0 0 0 0 0 21
0.6130 0.3151 -5.0516 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-0.9568 1.0868 -4.7827 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-1.2240 -1.0436 -6.0711 H 0 0 0 0 0 0 0 0 0 0 0 0 24
-2.0297 -1.1837 -4.4894 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-0.4515 -1.9610 -4.7554 H 0 0 0 0 0 0 0 0 0 0 0 0 26

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
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8 7 0 0 0 0
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12 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
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22 14 0 0 0 0
23 14 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
15 26 0 0 0 0

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M END

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4-ethylbenzoicacid.sdf
COSMOTHERM 3D

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0

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27 25 0 0 0 0 0 0 0 0 0 V2000
-0.6942 1.3292 5.7722 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.6350 1.2130 5.5468 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.5039 2.2594 5.5522 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.9874 -0.3650 4.4979 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7736 -1.2598 4.8171 H 0 0 0 0 0 0 0 0 0 0 0 0 5
0.3364 0.2454 4.9560 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.1548 -0.4374 -2.3732 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.2083 -0.5174 -0.9822 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.0476 -0.3253 -0.2129 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.1670 -0.0548 -0.8685 C 0 0 0 0 0 0 0 0 0 0 0 0 10
1.2126 0.0208 -2.2611 C 0 0 0 0 0 0 0 0 0 0 0 0 11
0.0553 -0.1671 -3.0386 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.1417 -0.4264 1.2741 C 0 0 0 0 0 0 0 0 0 0 0 0 13
0.1031 -0.0433 -4.5439 C 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.1269 1.4026 -5.0257 C 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.1883 -0.7041 1.8658 O 0 0 0 0 0 0 0 0 0 0 0 0 16
1.0162 -0.1872 1.9062 O 0 0 0 0 0 0 0 0 0 0 0 0 17
-2.0652 -0.5939 -2.9568 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-2.1505 -0.7332 -0.4762 H 0 0 0 0 0 0 0 0 0 0 0 0 19
2.0758 0.0901 -0.2843 H 0 0 0 0 0 0 0 0 0 0 0 0 20
2.1651 0.2236 -2.7565 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.6614 -0.6990 -4.9884 H 0 0 0 0 0 0 0 0 0 0 0 0 22
1.0809 -0.3945 -4.9078 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-0.0837 1.4554 -6.1234 H 0 0 0 0 0 0 0 0 0 0 0 0 24
0.6395 2.0802 -4.6212 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.1113 1.7734 -4.7046 H 0 0 0 0 0 0 0 0 0 0 0 0 26
0.8998 -0.2819 2.9284 H 0 0 0 0 0 0 0 0 0 0 0 0 27

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
22 14 0 0 0 0
23 14 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
26 15 0 0 0 0
17 27 0 0 0 0

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M END

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4-fluorobenzoicacid-anion.sdf
COSMOTHERM 3D

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20 18 0 0 0 0 0 0 0 0 0 V2000
-5.7199 0.9290 1.2087 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.1346 0.3762 0.6120 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.3306 1.8194 1.1743 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-4.1845 -0.6668 -0.3684 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-3.1979 -0.6385 -0.0846 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-4.1633 -0.3503 -1.2891 H 0 0 0 0 0 0 0 0 0 0 0 0 6
2.4160 -0.2667 1.3373 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.0533 -0.3728 1.0440 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.5654 -0.0951 -0.2440 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.4728 0.2938 -1.2435 C 0 0 0 0 0 0 0 0 0 0 0 0 10
2.8398 0.4033 -0.9750 C 0 0 0 0 0 0 0 0 0 0 0 0 11
3.2790 0.1200 0.3156 C 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.9195 -0.2080 -0.5628 C 0 0 0 0 0 0 0 0 0 0 0 0 13
4.6175 0.2254 0.5917 F 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.6778 -0.6170 0.3893 O 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.3071 0.1017 -1.7223 O 0 0 0 0 0 0 0 0 0 0 0 0 16
2.8050 -0.4772 2.3342 H 0 0 0 0 0 0 0 0 0 0 0 0 17
0.3504 -0.6748 1.8209 H 0 0 0 0 0 0 0 0 0 0 0 0 18
1.0925 0.5097 -2.2425 H 0 0 0 0 0 0 0 0 0 0 0 0 19
3.5526 0.7019 -1.7447 H 0 0 0 0 0 0 0 0 0 0 0 0 20

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0

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13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
11 20 0 0 0 0
M END
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4-fluorobenzoicacid.sdf
COSMOtherm          3D          0

21 19 0 0 0 0 0 0 0 0 0 0 V2000
-0.8236 5.4240 0.9369 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7013 5.4108 0.5138 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.6229 6.3714 1.0471 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1105 4.1141 -0.4125 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3682 4.6132 0.0429 H 0 0 0 0 0 0 0 0 0 0 0 5
1.0816 4.3956 -1.3443 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2278 -2.6809 -0.1127 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2355 -1.2941 -0.2592 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0478 -0.5519 -0.1361 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1595 -1.2195 0.1382 C 0 0 0 0 0 0 0 0 0 0 0 10
1.1853 -2.6069 0.2877 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0123 -3.3058 0.1582 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.1084 0.9324 -0.3058 C 0 0 0 0 0 0 0 0 0 0 0 13
0.0053 -4.6632 0.3025 F 0 0 0 0 0 0 0 0 0 0 0 14
-1.1519 1.5355 -0.5661 O 0 0 0 0 0 0 0 0 0 0 0 15
1.0745 1.5388 -0.1476 O 0 0 0 0 0 0 0 0 0 0 0 16
-2.1404 -3.2700 -0.2049 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.1696 -0.7735 -0.4718 H 0 0 0 0 0 0 0 0 0 0 0 18
2.0838 -0.6511 0.2352 H 0 0 0 0 0 0 0 0 0 0 0 19
2.1124 -3.1399 0.4996 H 0 0 0 0 0 0 0 0 0 0 0 20
0.9838 2.5623 -0.2763 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 13 0 0 0 0
16 13 0 0 0 0
16 21 0 0 0 0
M END
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4-hydroxybenzoicacid-anion.sdf
COSMOtherm          3D          0

21 19 0 0 0 0 0 0 0 0 0 0 V2000
-1.4572 0.0138 5.0810 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.0471 -0.7603 5.0367 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.0521 0.7828 5.0186 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.9993 0.0337 -5.3129 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.0115 0.0076 -4.2987 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.0468 0.0459 -5.5120 H 0 0 0 0 0 0 0 0 0 0 0 6
1.6701 0.0045 1.3340 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5270 -0.0001 -0.0523 C 0 0 0 0 0 0 0 0 0 0 0 8
0.2568 -0.0091 -0.6577 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.8724 -0.0134 0.1790 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.7476 -0.0084 1.5694 C 0 0 0 0 0 0 0 0 0 0 0 11
0.5300 0.0009 2.1594 C 0 0 0 0 0 0 0 0 0 0 0 12
0.1214 -0.0129 -2.1691 C 0 0 0 0 0 0 0 0 0 0 0 13
-1.0721 -0.0288 -2.6438 O 0 0 0 0 0 0 0 0 0 0 0 14
1.1775 -0.0003 -2.8658 O 0 0 0 0 0 0 0 0 0 0 0 15
0.7213 0.0065 3.5094 O 0 0 0 0 0 0 0 0 0 0 0 16
-0.1536 0.0057 4.0037 H 0 0 0 0 0 0 0 0 0 0 0 17
2.6594 0.0114 1.7965 H 0 0 0 0 0 0 0 0 0 0 0 18
2.4108 0.0032 -0.6930 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.8634 -0.0208 -0.2778 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.6377 -0.0114 2.2026 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
16 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
17 16 0 0 0 0
11 21 0 0 0 0
M END
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4-hydroxybenzoicacid.sdf
COSMOtherm          3D          0

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22 20 0 0 0 0 0 0 0 0 V2000
-5.2431 0.0177 1.1698 O 0 0 0 0 0 0 0 0 0 0 1
-5.6925 -0.7349 0.7429 H 0 0 0 0 0 0 0 0 0 0 2
-5.6544 0.8063 0.7703 H 0 0 0 0 0 0 0 0 0 0 3
4.8819 0.0178 1.6446 O 0 0 0 0 0 0 0 0 0 0 4
5.4734 0.7895 1.7146 H 0 0 0 0 0 0 0 0 0 0 5
5.4718 -0.7536 1.7287 H 0 0 0 0 0 0 0 0 0 0 6
1.4126 -0.0003 -1.6839 C 0 0 0 0 0 0 0 0 0 0 7
0.0272 -0.0018 -1.5873 C 0 0 0 0 0 0 0 0 0 0 8
-0.6127 -0.0074 -0.3317 C 0 0 0 0 0 0 0 0 0 0 9
0.1831 -0.0116 0.8304 C 0 0 0 0 0 0 0 0 0 0 10
1.5726 -0.0094 0.7464 C 0 0 0 0 0 0 0 0 0 0 11
2.2023 -0.0034 -0.5155 C 0 0 0 0 0 0 0 0 0 0 12
-2.0943 -0.0047 -0.2800 C 0 0 0 0 0 0 0 0 0 0 13
-2.5958 -0.0273 0.9715 O 0 0 0 0 0 0 0 0 0 0 14
-2.8148 0.0167 -1.2826 O 0 0 0 0 0 0 0 0 0 0 15
3.5490 -0.0008 -0.6645 O 0 0 0 0 0 0 0 0 0 0 16
-3.6129 -0.0146 0.9349 H 0 0 0 0 0 0 0 0 0 0 17
4.0213 0.0057 0.2291 H 0 0 0 0 0 0 0 0 0 0 18
1.9062 0.0036 -2.6572 H 0 0 0 0 0 0 0 0 0 0 19
-0.5823 0.0016 -2.4922 H 0 0 0 0 0 0 0 0 0 0 20
-0.2938 -0.0159 1.8107 H 0 0 0 0 0 0 0 0 0 0 21
2.1795 -0.0114 1.6534 H 0 0 0 0 0 0 0 0 0 0 22
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
16 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
17 14 0 0 0 0
18 16 0 0 0 0
11 22 0 0 0 0
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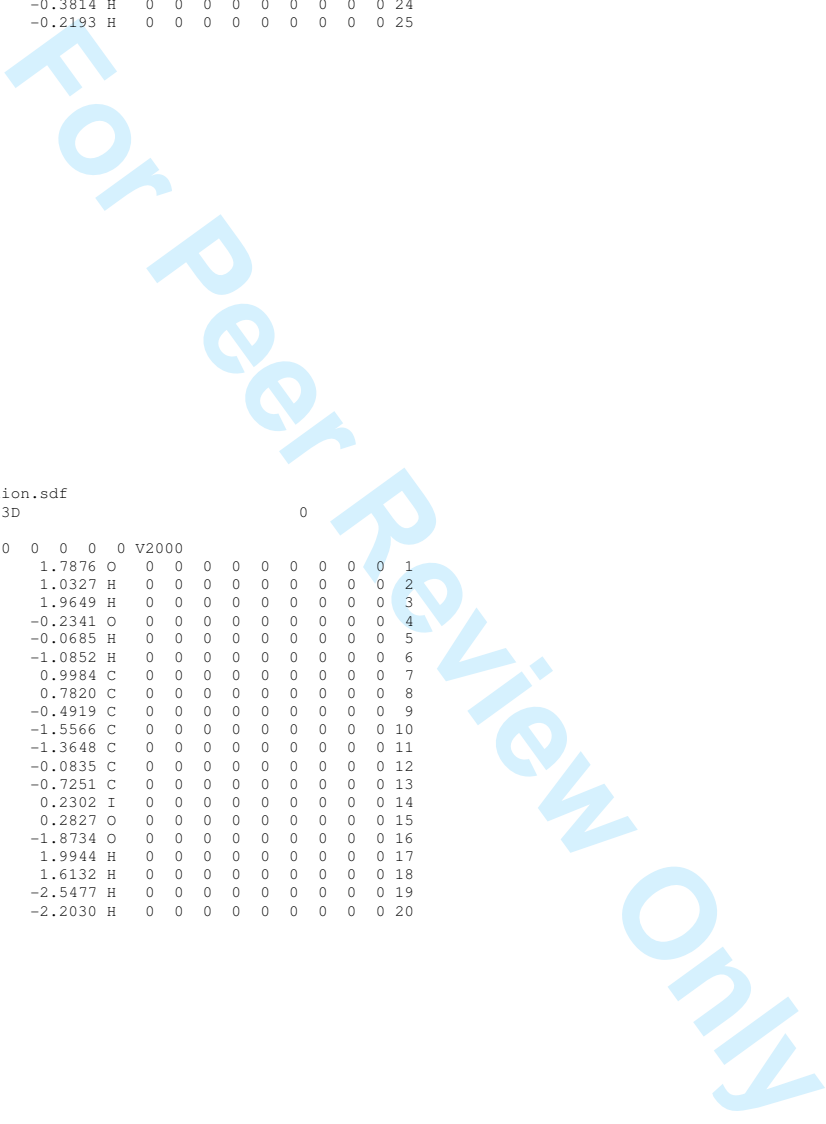
```
M END
$$$$
4-hydroxymethylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
24 22 0 0 0 0 0 0 0 0 V2000
-6.1330 0.7800 1.2803 O 0 0 0 0 0 0 0 0 0 0 1
-5.5373 0.2480 0.6749 H 0 0 0 0 0 0 0 0 0 0 2
-5.7408 1.6697 1.2872 H 0 0 0 0 0 0 0 0 0 0 3
-4.5624 -0.7614 -0.3156 O 0 0 0 0 0 0 0 0 0 0 4
-3.5716 -0.6768 -0.0571 H 0 0 0 0 0 0 0 0 0 0 5
-4.5815 -0.4655 -1.2431 H 0 0 0 0 0 0 0 0 0 0 6
2.0394 -0.0333 1.2774 C 0 0 0 0 0 0 0 0 0 0 7
0.6797 -0.2131 1.0104 C 0 0 0 0 0 0 0 0 0 0 8
0.1706 -0.0011 -0.2814 C 0 0 0 0 0 0 0 0 0 0 9
1.0548 0.3946 -1.2984 C 0 0 0 0 0 0 0 0 0 0 10
2.4142 0.5722 -1.0310 C 0 0 0 0 0 0 0 0 0 0 11
2.9242 0.3618 0.2607 C 0 0 0 0 0 0 0 0 0 0 12
-1.3125 -0.1835 -0.5827 C 0 0 0 0 0 0 0 0 0 0 13
4.3956 0.5213 0.5415 C 0 0 0 0 0 0 0 0 0 0 14
5.0483 -0.7553 0.3098 O 0 0 0 0 0 0 0 0 0 0 15
-2.0503 -0.5701 0.3943 O 0 0 0 0 0 0 0 0 0 0 16
-1.7186 0.0517 -1.7537 O 0 0 0 0 0 0 0 0 0 0 17
5.9973 -0.6253 0.4929 H 0 0 0 0 0 0 0 0 0 0 18
2.4207 -0.1954 2.2886 H 0 0 0 0 0 0 0 0 0 0 19
-0.0061 -0.5158 1.8028 H 0 0 0 0 0 0 0 0 0 0 20
0.6577 0.5651 -2.3002 H 0 0 0 0 0 0 0 0 0 0 21
3.0898 0.8842 -1.8313 H 0 0 0 0 0 0 0 0 0 0 22
4.5497 0.8370 1.5872 H 0 0 0 0 0 0 0 0 0 0 23
4.8273 1.2891 -0.1227 H 0 0 0 0 0 0 0 0 0 0 24
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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
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11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
23 14 0 0 0 0
18 15 0 0 0 0
14 24 0 0 0 0
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M END
$$$$
4-hydroxymethylbenzoicacid.sdf
COSMOTHERM 3D 0
25 23 0 0 0 0 0 0 0 0 V2000
-0.8166 -5.7453 1.2385 O 0 0 0 0 0 0 0 0 0 0 1
-0.6279 -6.6922 1.3702 H 0 0 0 0 0 0 0 0 0 0 2
-1.7155 -5.7286 0.8633 H 0 0 0 0 0 0 0 0 0 0 3
1.0497 -4.5252 -0.2799 O 0 0 0 0 0 0 0 0 0 0 4
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0.9554 -4.8517 -1.1925 H 0 0 0 0 0 0 0 0 0 0 0 0 5  
0.3331 -4.9894 0.2481 H 0 0 0 0 0 0 0 0 0 0 0 0 6  
-1.1493 2.3179 -0.4656 C 0 0 0 0 0 0 0 0 0 0 0 0 7  
-1.1919 0.9252 -0.5277 C 0 0 0 0 0 0 0 0 0 0 0 0 8  
-0.0276 0.1702 -0.3044 C 0 0 0 0 0 0 0 0 0 0 0 0 9  
1.1788 0.8335 -0.0193 C 0 0 0 0 0 0 0 0 0 0 0 0 10  
1.2142 2.2277 0.0395 C 0 0 0 0 0 0 0 0 0 0 0 0 11  
0.0535 2.9861 -0.1830 C 0 0 0 0 0 0 0 0 0 0 0 0 12  
-0.1090 -1.3224 -0.3924 C 0 0 0 0 0 0 0 0 0 0 0 0 13  
0.0899 4.4899 -0.0842 C 0 0 0 0 0 0 0 0 0 0 0 0 14  
-0.1902 4.8598 1.2900 O 0 0 0 0 0 0 0 0 0 0 0 0 15  
-1.1497 -1.9212 -0.6737 O 0 0 0 0 0 0 0 0 0 0 0 0 16  
1.0509 -1.9401 -0.1375 O 0 0 0 0 0 0 0 0 0 0 0 0 17  
-0.1799 5.8344 1.3288 H 0 0 0 0 0 0 0 0 0 0 0 0 18  
-2.0584 2.8965 -0.6450 H 0 0 0 0 0 0 0 0 0 0 0 0 19  
-2.1255 0.4079 -0.7531 H 0 0 0 0 0 0 0 0 0 0 0 0 20  
2.0871 0.2558 0.1498 H 0 0 0 0 0 0 0 0 0 0 0 0 21  
2.1566 2.7358 0.2549 H 0 0 0 0 0 0 0 0 0 0 0 0 22  
-0.6658 4.9306 -0.7557 H 0 0 0 0 0 0 0 0 0 0 0 0 23  
1.0836 4.8642 -0.3814 H 0 0 0 0 0 0 0 0 0 0 0 0 24  
0.9449 -2.9687 -0.2193 H 0 0 0 0 0 0 0 0 0 0 0 0 25  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
8 7 0 0 0 0  
12 7 0 0 0 0  
19 7 0 0 0 0  
9 8 0 0 0 0  
20 8 0 0 0 0  
10 9 0 0 0 0  
13 9 0 0 0 0  
11 10 0 0 0 0  
21 10 0 0 0 0  
12 11 0 0 0 0  
22 11 0 0 0 0  
14 12 0 0 0 0  
16 13 0 0 0 0  
17 13 0 0 0 0  
15 14 0 0 0 0  
23 14 0 0 0 0  
24 14 0 0 0 0  
18 15 0 0 0 0  
17 25 0 0 0 0  
M END  
$$$$  
4-iodobenzoicacid-anion.sdf  
COSMOtherm 3D 0  
20 17 0 0 0 0 0 0 0 0 V2000  
-7.8130 0.6164 1.7876 O 0 0 0 0 0 0 0 0 0 0 1  
-7.2635 0.2535 1.0327 H 0 0 0 0 0 0 0 0 0 0 2  
-7.4343 1.4943 1.9649 H 0 0 0 0 0 0 0 0 0 0 3  
-6.3675 -0.4873 -0.2341 O 0 0 0 0 0 0 0 0 0 0 4  
-5.3561 -0.4419 -0.0685 H 0 0 0 0 0 0 0 0 0 0 5  
-6.4914 -0.0316 -1.0852 H 0 0 0 0 0 0 0 0 0 0 6  
0.3522 -0.2771 0.9984 C 0 0 0 0 0 0 0 0 0 0 7  
-1.0295 -0.3071 0.7820 C 0 0 0 0 0 0 0 0 0 0 8  
-1.5689 -0.0710 -0.4919 C 0 0 0 0 0 0 0 0 0 0 9  
-0.6943 0.1954 -1.5566 C 0 0 0 0 0 0 0 0 0 0 10  
0.6906 0.2252 -1.3648 C 0 0 0 0 0 0 0 0 0 0 11  
1.1959 -0.0113 -0.0835 C 0 0 0 0 0 0 0 0 0 0 12  
-3.0757 -0.0968 -0.7251 C 0 0 0 0 0 0 0 0 0 0 13  
3.3161 0.0356 0.2302 I 0 0 0 0 0 0 0 0 0 0 14  
-3.8000 -0.4212 0.2827 O 0 0 0 0 0 0 0 0 0 0 15  
-3.5052 0.1969 -1.8734 O 0 0 0 0 0 0 0 0 0 0 16  
0.7555 -0.4589 1.9944 H 0 0 0 0 0 0 0 0 0 0 17  
-1.7042 -0.5157 1.6132 H 0 0 0 0 0 0 0 0 0 0 18  
-1.1107 0.3812 -2.5477 H 0 0 0 0 0 0 0 0 0 0 19  
1.3563 0.4307 -2.2030 H 0 0 0 0 0 0 0 0 0 0 20  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
8 7 0 0 0 0  
12 7 0 0 0 0  
17 7 0 0 0 0  
9 8 0 0 0 0  
18 8 0 0 0 0  
10 9 0 0 0 0  
13 9 0 0 0 0  
11 10 0 0 0 0  
19 10 0 0 0 0  
12 11 0 0 0 0  
15 13 0 0 0 0  
16 13 0 0 0 0  
11 20 0 0 0 0  
M END  
$$$$  
4-iodobenzoicacid.sdf  
COSMOtherm 3D 0  
21 18 0 0 0 0 0 0 0 0 V2000  
-0.0919 -1.5447 -7.5842 O 0 0 0 0 0 0 0 0 0 0 1  
-0.0551 -1.4210 -8.5507 H 0 0 0 0 0 0 0 0 0 0 2  
-0.7827 -2.2201 -7.4545 H 0 0 0 0 0 0 0 0 0 0 3  
-0.6872 0.7389 -6.2671 O 0 0 0 0 0 0 0 0 0 0 4  
-0.4465 -0.0963 -6.7708 H 0 0 0 0 0 0 0 0 0 0 5  
-0.0496 1.4147 -6.5593 H 0 0 0 0 0 0 0 0 0 0 6  
1.3120 0.0278 0.6022 C 0 0 0 0 0 0 0 0 0 0 7  
1.3954 0.1436 -0.7863 C 0 0 0 0 0 0 0 0 0 0 8  
0.2355 0.2696 -1.5678 C 0 0 0 0 0 0 0 0 0 0 9  
-1.0204 0.2789 -0.9385 C 0 0 0 0 0 0 0 0 0 0 10  
-1.1203 0.1662 0.4505 C 0 0 0 0 0 0 0 0 0 0 11  
0.0501 0.0421 1.2046 C 0 0 0 0 0 0 0 0 0 0 12
```



```

1
2
3      0.3776  0.3975  -3.0528 C  0  0  0  0  0  0  0  0  0  0  0  0  13
4     -0.0928 -0.1292   3.3314 I  0  0  0  0  0  0  0  0  0  0  0  0  14
5      1.4727  0.4291  -3.6180 O  0  0  0  0  0  0  0  0  0  0  0  0  15
6     -0.7914  0.4778  -3.6973 O  0  0  0  0  0  0  0  0  0  0  0  0  16
7      2.2189 -0.0712   1.1974 H  0  0  0  0  0  0  0  0  0  0  0  0  17
8      2.3708  0.1354  -1.2742 H  0  0  0  0  0  0  0  0  0  0  0  0  18
9     -1.9279  0.3773  -1.5337 H  0  0  0  0  0  0  0  0  0  0  0  0  19
10    -2.0992  0.1776   0.9291 H  0  0  0  0  0  0  0  0  0  0  0  0  20
11    -0.6441  0.5725  -4.7195 H  0  0  0  0  0  0  0  0  0  0  0  0  21
12    2  1  0  0  0  0
13    3  1  0  0  0  0
14    5  4  0  0  0  0
15    6  4  0  0  0  0
16    8  7  0  0  0  0
17    12  7  0  0  0  0
18    17  7  0  0  0  0
19    9  8  0  0  0  0
20    18  8  0  0  0  0
21    10  9  0  0  0  0
22    13  9  0  0  0  0
23    11  10  0  0  0  0
24    19  10  0  0  0  0
25    12  11  0  0  0  0
26    20  11  0  0  0  0
27    15  13  0  0  0  0
28    16  13  0  0  0  0
29    16  21  0  0  0  0
M   END
$$$
4-methoxybenzoicacid-anion.sdf
COSMOTHERM      3D          0
24 22 0 0 0 0 0 0 0 0 0 0 V2000
-6.2839  0.7418  1.1799 O  0  0  0  0  0  0  0  0  0  0  0  0  1
-5.6280  0.3013  0.5631 H  0  0  0  0  0  0  0  0  0  0  0  0  2
-5.9788  1.6629  1.2428 H  0  0  0  0  0  0  0  0  0  0  0  0  3
-4.5577  -0.5679  -0.4548 O  0  0  0  0  0  0  0  0  0  0  0  0  4
-3.5784  -0.4986  -0.1461 H  0  0  0  0  0  0  0  0  0  0  0  0  5
-4.5392  -0.2102  -1.3601 H  0  0  0  0  0  0  0  0  0  0  0  0  6
 1.9971  -0.2319  1.4190 C  0  0  0  0  0  0  0  0  0  0  0  0  7
 0.6431  -0.2808  1.1017 C  0  0  0  0  0  0  0  0  0  0  0  0  8
 0.1960  -0.0819  -0.2190 C  0  0  0  0  0  0  0  0  0  0  0  0  9
 1.1561  0.1654  -1.2105 C  0  0  0  0  0  0  0  0  0  0  0  0  10
 2.5223  0.2121  -0.9146 C  0  0  0  0  0  0  0  0  0  0  0  0  11
 2.9482  0.0145  -0.4100 C  0  0  0  0  0  0  0  0  0  0  0  0  12
-1.2786  -0.1323  -0.5707 C  0  0  0  0  0  0  0  0  0  0  0  0  13
 4.2564  0.0438  0.8151 O  0  0  0  0  0  0  0  0  0  0  0  0  14
 5.2654  0.2857  -0.1855 C  0  0  0  0  0  0  0  0  0  0  0  0  15
-2.0872  -0.4336  0.3836 O  0  0  0  0  0  0  0  0  0  0  0  0  16
-1.6251  0.1168  -1.7595 O  0  0  0  0  0  0  0  0  0  0  0  0  17
 2.3407  -0.3829  2.4441 H  0  0  0  0  0  0  0  0  0  0  0  0  18
-0.0931  -0.4746  1.8830 H  0  0  0  0  0  0  0  0  0  0  0  0  19
 0.8198  0.3216  -2.2368 H  0  0  0  0  0  0  0  0  0  0  0  0  20
 3.2392  0.4033  -1.7123 H  0  0  0  0  0  0  0  0  0  0  0  0  21
 6.2200  0.2657  0.3501 H  0  0  0  0  0  0  0  0  0  0  0  0  22
 5.2570  -0.5013  -0.9551 H  0  0  0  0  0  0  0  0  0  0  0  0  23
 5.1273  1.2701  -0.6581 H  0  0  0  0  0  0  0  0  0  0  0  0  24
25  2  1  0  0  0  0
26  3  1  0  0  0  0
27  5  4  0  0  0  0
28  6  4  0  0  0  0
29  8  7  0  0  0  0
30  12  7  0  0  0  0
31  18  7  0  0  0  0
32  9  8  0  0  0  0
33  19  8  0  0  0  0
34  10  9  0  0  0  0
35  13  9  0  0  0  0
36  11  10  0  0  0  0
37  20  10  0  0  0  0
38  12  11  0  0  0  0
39  21  11  0  0  0  0
40  14  12  0  0  0  0
41  16  13  0  0  0  0
42  17  13  0  0  0  0
43  15  14  0  0  0  0
44  22  15  0  0  0  0
45  23  15  0  0  0  0
46  15  24  0  0  0  0
M   END
$$$
4-methoxybenzoicacid.sdf
COSMOTHERM      3D          0
25 23 0 0 0 0 0 0 0 0 0 0 V2000
-0.4815  5.8579  1.1366 O  0  0  0  0  0  0  0  0  0  0  0  0  1
-1.4215  5.8608  0.8799 H  0  0  0  0  0  0  0  0  0  0  0  0  2
-0.2390  6.8012  1.1738 H  0  0  0  0  0  0  0  0  0  0  0  0  3
 1.1330  4.4578  -0.5183 O  0  0  0  0  0  0  0  0  0  0  0  0  4
 0.5043  4.9895  0.0545 H  0  0  0  0  0  0  0  0  0  0  0  0  5
 0.9528  4.7402  -1.4327 H  0  0  0  0  0  0  0  0  0  0  0  0  6
-1.4101  -2.2694  -0.1049 C  0  0  0  0  0  0  0  0  0  0  0  0  7
-1.3855  -0.8885  -0.2351 C  0  0  0  0  0  0  0  0  0  0  0  0  8
-0.1690  -0.1776  -0.1774 C  0  0  0  0  0  0  0  0  0  0  0  0  9
 1.0227  -0.8966  0.0147 C  0  0  0  0  0  0  0  0  0  0  0  0  10
 1.0144  -2.2864  0.1452 C  0  0  0  0  0  0  0  0  0  0  0  0  11
-0.2075  -2.9808  0.0858 C  0  0  0  0  0  0  0  0  0  0  0  0  12
-0.1892  1.3018  -0.3281 C  0  0  0  0  0  0  0  0  0  0  0  0  13
-0.3304  -4.3336  0.2010 O  0  0  0  0  0  0  0  0  0  0  0  0  14
 0.8707  -5.1116  0.3925 C  0  0  0  0  0  0  0  0  0  0  0  0  15
-1.2226  1.9486  -0.5252 O  0  0  0  0  0  0  0  0  0  0  0  0  16
 1.0225  1.8733  -0.2307 O  0  0  0  0  0  0  0  0  0  0  0  0  17
-2.3502  -2.8216  -0.1481 H  0  0  0  0  0  0  0  0  0  0  0  0  18
-2.3154  -0.3378  -0.3840 H  0  0  0  0  0  0  0  0  0  0  0  0  19
 1.9726  -0.3639  0.0617 H  0  0  0  0  0  0  0  0  0  0  0  0  20

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2
3 1.9548 -2.8157 0.2911 H 0 0 0 0 0 0 0 0 0 0 21
4 0.5366 -6.1519 0.4556 H 0 0 0 0 0 0 0 0 0 0 22
5 1.5565 -4.9927 -0.4591 H 0 0 0 0 0 0 0 0 0 0 23
6 1.3789 -4.8282 1.3262 H 0 0 0 0 0 0 0 0 0 0 24
7 0.9535 2.8944 -0.3563 H 0 0 0 0 0 0 0 0 0 0 25
8 2 1 0 0 0 0
9 3 1 0 0 0 0
10 5 4 0 0 0 0
11 6 4 0 0 0 0
12 8 7 0 0 0 0
13 12 7 0 0 0 0
14 18 7 0 0 0 0
15 9 8 0 0 0 0
16 19 8 0 0 0 0
17 10 9 0 0 0 0
18 13 9 0 0 0 0
19 11 10 0 0 0 0
20 20 10 0 0 0 0
21 12 11 0 0 0 0
22 21 11 0 0 0 0
23 14 12 0 0 0 0
24 16 13 0 0 0 0
25 17 13 0 0 0 0
26 15 14 0 0 0 0
27 22 15 0 0 0 0
28 23 15 0 0 0 0
29 24 15 0 0 0 0
30 17 25 0 0 0 0
31 M END
32 \$\$\$\$
33 4-methylaminobenzoicacid-anion.sdf
34 COSMOTHERM 3D 0
35
36 25 23 0 0 0 0 0 0 0 0 0 0 V2000
37 -6.1100 1.0797 1.0503 O 0 0 0 0 0 0 0 0 0 0 1
38 -5.5106 0.4878 0.5052 H 0 0 0 0 0 0 0 0 0 0 2
39 -5.7321 1.9697 0.9471 H 0 0 0 0 0 0 0 0 0 0 3
40 -4.5442 -0.6158 -0.3753 O 0 0 0 0 0 0 0 0 0 0 4
41 -3.5645 -0.5947 -0.0489 H 0 0 0 0 0 0 0 0 0 0 5
42 -4.4671 -0.3442 -1.3076 H 0 0 0 0 0 0 0 0 0 0 6
43 2.0273 -0.3246 1.4006 C 0 0 0 0 0 0 0 0 0 0 7
44 0.6711 -0.4038 1.1103 C 0 0 0 0 0 0 0 0 0 0 8
45 0.1801 -0.1644 -0.1900 C 0 0 0 0 0 0 0 0 0 0 9
46 1.1151 0.1599 -1.1876 C 0 0 0 0 0 0 0 0 0 0 10
47 2.4809 0.2433 -0.9185 C 0 0 0 0 0 0 0 0 0 0 11
48 2.9700 -0.0039 0.3884 C 0 0 0 0 0 0 0 0 0 0 12
49 -1.2927 -0.2473 -0.5089 C 0 0 0 0 0 0 0 0 0 0 13
50 4.3138 0.0291 0.6854 N 0 0 0 0 0 0 0 0 0 0 14
51 5.3152 0.5691 -0.2222 C 0 0 0 0 0 0 0 0 0 0 15
52 -2.0782 -0.5835 0.4573 O 0 0 0 0 0 0 0 0 0 0 16
53 -1.6785 0.0106 -1.6863 O 0 0 0 0 0 0 0 0 0 0 17
54 4.5502 0.0463 1.6731 H 0 0 0 0 0 0 0 0 0 0 18
55 2.3832 -0.5134 2.4169 H 0 0 0 0 0 0 0 0 0 0 19
56 -0.0393 -0.6519 1.9009 H 0 0 0 0 0 0 0 0 0 0 20
57 0.7508 0.3533 -2.1984 H 0 0 0 0 0 0 0 0 0 0 21
58 3.1728 0.4997 -1.7213 H 0 0 0 0 0 0 0 0 0 0 22
59 6.2909 0.5286 0.2750 H 0 0 0 0 0 0 0 0 0 0 23
60 5.3787 -0.0298 -1.1434 H 0 0 0 0 0 0 0 0 0 0 24
5.1104 1.6171 -0.5071 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
18 14 0 0 0 0
23 15 0 0 0 0
24 15 0 0 0 0
15 25 0 0 0 0
M END
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4-methylaminobenzoicacid.sdf
COSMOTHERM 3D 0
26 24 0 0 0 0 0 0 0 0 0 0 V2000
-0.6335 5.8145 1.0120 O 0 0 0 0 0 0 0 0 0 0 1
-1.5241 5.8219 0.6168 H 0 0 0 0 0 0 0 0 0 0 2
-0.4166 6.7573 1.1311 H 0 0 0 0 0 0 0 0 0 0 3
1.2281 4.4596 -0.4112 O 0 0 0 0 0 0 0 0 0 0 4
0.5169 4.9756 0.0712 H 0 0 0 0 0 0 0 0 0 0 5
1.1819 4.7586 -1.3368 H 0 0 0 0 0 0 0 0 0 0 6
-1.4305 -2.2512 -0.1350 C 0 0 0 0 0 0 0 0 0 0 7
-1.3776 -0.8736 -0.2502 C 0 0 0 0 0 0 0 0 0 0 8
-0.1515 -0.1749 -0.1675 C 0 0 0 0 0 0 0 0 0 0 9
1.0245 -0.9252 0.0369 C 0 0 0 0 0 0 0 0 0 0 10
0.9908 -2.3098 0.1533 C 0 0 0 0 0 0 0 0 0 0 11
-0.2431 -3.0102 0.0703 C 0 0 0 0 0 0 0 0 0 0 12
-0.1457 1.2955 -0.3007 C 0 0 0 0 0 0 0 0 0 0 13
-0.3120 -4.3670 0.1826 N 0 0 0 0 0 0 0 0 0 0 14
0.8345 -5.2388 0.3776 C 0 0 0 0 0 0 0 0 0 0 15
-1.1634 1.9746 -0.4933 O 0 0 0 0 0 0 0 0 0 0 16
1.0796 1.8519 -0.1926 O 0 0 0 0 0 0 0 0 0 0 17

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-1.2258 -4.8003 0.1018 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.3889 -2.7718 -0.2014 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.2969 -0.3072 -0.4082 H 0 0 0 0 0 0 0 0 0 0 0 20
1.9833 -0.4101 0.1042 H 0 0 0 0 0 0 0 0 0 0 0 21
1.9200 -2.8582 0.3092 H 0 0 0 0 0 0 0 0 0 0 0 22
0.4770 -6.2728 0.4321 H 0 0 0 0 0 0 0 0 0 0 0 23
1.5525 -5.1633 -0.4562 H 0 0 0 0 0 0 0 0 0 0 0 24
1.3680 -5.0075 1.3145 H 0 0 0 0 0 0 0 0 0 0 0 25
1.0188 2.8710 -0.3006 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
18 14 0 0 0 0
23 15 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
17 26 0 0 0 0
M END
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4-methylbenzoicacid-anion.sdf
COSMOtherm 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
-5.6243 0.9671 1.1706 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.0403 0.3924 0.5929 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.1729 1.8280 1.1919 H 0 0 0 0 0 0 0 0 0 0 0 3
-4.0990 -0.6815 -0.3581 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.1134 -0.6594 -0.0652 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.0620 -0.3720 -1.2809 H 0 0 0 0 0 0 0 0 0 0 0 6
2.5044 -0.2516 1.3302 C 0 0 0 0 0 0 0 0 0 0 0 7
1.1399 -0.3749 1.0541 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6382 -0.0981 -0.2282 C 0 0 0 0 0 0 0 0 0 0 0 9
1.5425 0.3059 -1.2241 C 0 0 0 0 0 0 0 0 0 0 0 10
2.9063 0.4256 -0.9474 C 0 0 0 0 0 0 0 0 0 0 0 11
3.4142 0.1465 0.3344 C 0 0 0 0 0 0 0 0 0 0 0 12
4.8916 0.2469 0.6239 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.8452 -0.2218 -0.5408 C 0 0 0 0 0 0 0 0 0 0 0 14
-1.5998 -0.6432 0.4103 O 0 0 0 0 0 0 0 0 0 0 0 15
-1.2437 0.0910 -1.6975 O 0 0 0 0 0 0 0 0 0 0 0 16
2.8722 -0.4654 2.3371 H 0 0 0 0 0 0 0 0 0 0 0 17
0.4442 -0.6844 1.8355 H 0 0 0 0 0 0 0 0 0 0 0 18
1.1579 0.5286 -2.2209 H 0 0 0 0 0 0 0 0 0 0 0 19
3.5916 0.7435 -1.7376 H 0 0 0 0 0 0 0 0 0 0 0 20
5.4006 -0.7046 0.3976 H 0 0 0 0 0 0 0 0 0 0 0 21
5.0790 0.4727 1.6828 H 0 0 0 0 0 0 0 0 0 0 0 22
5.3692 1.0244 0.0112 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
13 12 0 0 0 0
21 13 0 0 0 0
22 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
13 23 0 0 0 0
M END
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4-methylbenzoicacid.sdf
COSMOtherm 3D 0
24 22 0 0 0 0 0 0 0 0 0 V2000
-0.8344 5.3473 0.9272 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7070 5.3434 0.4937 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.6323 6.2921 1.0536 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1159 4.0434 -0.4119 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3691 4.5380 0.0395 H 0 0 0 0 0 0 0 0 0 0 0 5
1.0946 4.3322 -1.3416 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2127 -2.7621 -0.1057 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2305 -1.3766 -0.2597 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0468 -0.6299 -0.1301 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1534 -1.3034 0.1595 C 0 0 0 0 0 0 0 0 0 0 0 10
1.1631 -2.6903 0.3121 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0162 -3.4460 0.1793 C 0 0 0 0 0 0 0 0 0 0 0 12
0.0060 -4.9468 0.3128 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.1053 0.8524 -0.3011 C 0 0 0 0 0 0 0 0 0 0 0 14
-1.1483 1.4620 -0.5515 O 0 0 0 0 0 0 0 0 0 0 0 15
1.0819 1.4592 -0.1581 O 0 0 0 0 0 0 0 0 0 0 0 16

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 2
 3 -2.1428 -3.3264 -0.2056 H 0 0 0 0 0 0 0 0 0 0 0 17
 4 -2.1644 -0.8571 -0.4792 H 0 0 0 0 0 0 0 0 0 0 0 18
 5 2.0785 -0.7370 0.2680 H 0 0 0 0 0 0 0 0 0 0 0 19
 6 2.1030 -3.1980 0.5409 H 0 0 0 0 0 0 0 0 0 0 0 20
 7 0.2024 -5.4189 -0.6638 H 0 0 0 0 0 0 0 0 0 0 0 21
 8 -0.9574 -5.3320 0.6734 H 0 0 0 0 0 0 0 0 0 0 0 22
 9 0.7975 -5.2768 0.9995 H 0 0 0 0 0 0 0 0 0 0 0 23
 10 0.9876 2.4803 -0.2840 H 0 0 0 0 0 0 0 0 0 0 0 24
 11
 12 2 1 0 0 0 0
 13 3 1 0 0 0 0
 14 5 4 0 0 0 0
 15 6 4 0 0 0 0
 16 8 7 0 0 0 0
 17 12 7 0 0 0 0
 18 17 7 0 0 0 0
 19 9 8 0 0 0 0
 20 18 8 0 0 0 0
 21 10 9 0 0 0 0
 22 14 9 0 0 0 0
 23 11 10 0 0 0 0
 24 19 10 0 0 0 0
 25 12 11 0 0 0 0
 26 20 11 0 0 0 0
 27 13 12 0 0 0 0
 28 21 13 0 0 0 0
 29 22 13 0 0 0 0
 30 23 13 0 0 0 0
 31 15 14 0 0 0 0
 32 16 14 0 0 0 0
 33 16 24 0 0 0 0

M END

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4-nitrobenzoicacid-anion.sdf

COSMOtherm

3D

0

22 20 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
 -6.4162 0.9784 1.3881 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -5.8628 0.4204 0.7677 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -6.0119 1.8618 1.3460 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 -4.9617 -0.6345 -0.2556 O 0 0 0 0 0 0 0 0 0 0 0 0 4
 -3.9634 -0.5987 -0.0365 H 0 0 0 0 0 0 0 0 0 0 0 0 5
 -5.0068 -0.3416 -1.1831 H 0 0 0 0 0 0 0 0 0 0 0 0 6
 2.0816 0.2654 -1.1791 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 0.7091 0.1817 -1.4007 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 -0.1729 -0.1284 -0.3517 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 0.3429 -0.3551 0.9357 C 0 0 0 0 0 0 0 0 0 0 0 0 10
 1.7122 -0.2722 1.1806 C 0 0 0 0 0 0 0 0 0 0 0 0 11
 2.5634 0.0377 0.1146 C 0 0 0 0 0 0 0 0 0 0 0 0 12
 -1.6769 -0.2113 -0.6196 C 0 0 0 0 0 0 0 0 0 0 0 0 13
 4.0137 0.1278 0.3616 N 0 0 0 0 0 0 0 0 0 0 0 0 14
 4.4314 -0.0915 1.5108 O 0 0 0 0 0 0 0 0 0 0 0 0 15
 4.7566 0.4199 -0.5901 O 0 0 0 0 0 0 0 0 0 0 0 0 16
 -2.0850 0.0806 -1.7745 O 0 0 0 0 0 0 0 0 0 0 0 0 17
 -2.4047 -0.5761 0.3685 O 0 0 0 0 0 0 0 0 0 0 0 0 18
 2.7718 0.5028 -1.9869 H 0 0 0 0 0 0 0 0 0 0 0 0 19
 0.3010 0.3572 -2.3961 H 0 0 0 0 0 0 0 0 0 0 0 0 20
 -0.3450 -0.5969 1.7457 H 0 0 0 0 0 0 0 0 0 0 0 0 21
 2.1199 -0.4427 2.1756 H 0 0 0 0 0 0 0 0 0 0 0 0 22

M END

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4-nitrobenzoicacid.sdf

COSMOtherm

3D

0

23 21 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
 -0.6482 6.1465 1.1548 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -1.5720 6.2031 0.8501 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -0.3849 7.0730 1.3036 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 1.0305 4.8472 -0.4974 O 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.3751 5.3499 0.0759 H 0 0 0 0 0 0 0 0 0 0 0 0 5
 0.8489 5.1280 -1.4121 H 0 0 0 0 0 0 0 0 0 0 0 0 6
 -1.2389 -1.9461 -0.1433 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 -1.2669 -0.5597 -0.2682 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 -0.0793 0.1866 -0.1908 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 1.1474 -0.4680 0.0148 C 0 0 0 0 0 0 0 0 0 0 0 0 10
 1.1918 -1.8550 0.1404 C 0 0 0 0 0 0 0 0 0 0 0 0 11
 -0.0051 -2.5713 0.0587 C 0 0 0 0 0 0 0 0 0 0 0 0 12
 -0.1610 1.6814 -0.3389 C 0 0 0 0 0 0 0 0 0 0 0 0 13
 0.0345 -4.0447 0.1892 N 0 0 0 0 0 0 0 0 0 0 0 0 14
 1.1347 -4.5862 0.3738 O 0 0 0 0 0 0 0 0 0 0 0 0 15
 -1.0341 -4.6690 0.1074 O 0 0 0 0 0 0 0 0 0 0 0 0 16
 -1.2249 2.2652 -0.5449 O 0 0 0 0 0 0 0 0 0 0 0 0 17
 1.0192 2.2898 -0.2268 O 0 0 0 0 0 0 0 0 0 0 0 0 18
 -2.1521 -2.5356 -0.2017 H 0 0 0 0 0 0 0 0 0 0 0 0 19
 -2.2133 -0.0434 -0.4280 H 0 0 0 0 0 0 0 0 0 0 0 0 20
 2.0687 0.1092 0.0755 H 0 0 0 0 0 0 0 0 0 0 0 0 21

M END

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4-nitrobenzoicacid.sdf

COSMOtherm

3D

0

23 21 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
 -0.6482 6.1465 1.1548 O 0 0 0 0 0 0 0 0 0 0 0 0 1
 -1.5720 6.2031 0.8501 H 0 0 0 0 0 0 0 0 0 0 0 0 2
 -0.3849 7.0730 1.3036 H 0 0 0 0 0 0 0 0 0 0 0 0 3
 1.0305 4.8472 -0.4974 O 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.3751 5.3499 0.0759 H 0 0 0 0 0 0 0 0 0 0 0 0 5
 0.8489 5.1280 -1.4121 H 0 0 0 0 0 0 0 0 0 0 0 0 6
 -1.2389 -1.9461 -0.1433 C 0 0 0 0 0 0 0 0 0 0 0 0 7
 -1.2669 -0.5597 -0.2682 C 0 0 0 0 0 0 0 0 0 0 0 0 8
 -0.0793 0.1866 -0.1908 C 0 0 0 0 0 0 0 0 0 0 0 0 9
 1.1474 -0.4680 0.0148 C 0 0 0 0 0 0 0 0 0 0 0 0 10
 1.1918 -1.8550 0.1404 C 0 0 0 0 0 0 0 0 0 0 0 0 11
 -0.0051 -2.5713 0.0587 C 0 0 0 0 0 0 0 0 0 0 0 0 12
 -0.1610 1.6814 -0.3389 C 0 0 0 0 0 0 0 0 0 0 0 0 13
 0.0345 -4.0447 0.1892 N 0 0 0 0 0 0 0 0 0 0 0 0 14
 1.1347 -4.5862 0.3738 O 0 0 0 0 0 0 0 0 0 0 0 0 15
 -1.0341 -4.6690 0.1074 O 0 0 0 0 0 0 0 0 0 0 0 0 16
 -1.2249 2.2652 -0.5449 O 0 0 0 0 0 0 0 0 0 0 0 0 17
 1.0192 2.2898 -0.2268 O 0 0 0 0 0 0 0 0 0 0 0 0 18
 -2.1521 -2.5356 -0.2017 H 0 0 0 0 0 0 0 0 0 0 0 0 19
 -2.2133 -0.0434 -0.4280 H 0 0 0 0 0 0 0 0 0 0 0 0 20
 2.0687 0.1092 0.0755 H 0 0 0 0 0 0 0 0 0 0 0 0 21


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2
3       2.1347  -2.3754  0.2984 H  0  0  0  0  0  0  0  0  0  0  0  0  0  22
4       0.9243  3.3204 -0.3484 H  0  0  0  0  0  0  0  0  0  0  0  0  0  23
5       2  1  0  0  0  0  0
6       3  1  0  0  0  0  0
7       5  4  0  0  0  0  0
8       6  4  0  0  0  0  0
9       8  7  0  0  0  0  0
10      12  7  0  0  0  0  0
11      19  7  0  0  0  0  0
12      9  8  0  0  0  0  0
13      20  8  0  0  0  0  0
14      10  9  0  0  0  0  0
15      13  9  0  0  0  0  0
16      11 10  0  0  0  0  0
17      21 10  0  0  0  0  0
18      12 11  0  0  0  0  0
19      22 11  0  0  0  0  0
20      14 12  0  0  0  0  0
21      17 13  0  0  0  0  0
22      18 13  0  0  0  0  0
23      15 14  0  0  0  0  0
24      16 14  0  0  0  0  0
25      18 23  0  0  0  0  0
M  END
$$$$
4-phenylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
30 29 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.4495  7.2516 -1.2665 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-0.7315  6.7438 -0.7859 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-2.2756  6.8119 -1.0023 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
0.5742  5.9226 -0.0341 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
0.5323  4.9126 -0.2199 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
0.5043  5.9781  0.9357 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
0.1548 -0.8163 -1.0650 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
0.2600  0.5674 -0.9190 C  0  0  0  0  0  0  0  0  0  0  0  0  0  8
0.2584  1.1601  0.3542 C  0  0  0  0  0  0  0  0  0  0  0  0  0  9
0.1492  0.3249  1.4779 C  0  0  0  0  0  0  0  0  0  0  0  0  0 10
0.0445 -1.0587  1.3358 C  0  0  0  0  0  0  0  0  0  0  0  0  0 11
0.0445 -1.6596  0.0600 C  0  0  0  0  0  0  0  0  0  0  0  0  0 12
-0.0668 -3.1323 -0.0922 C  0  0  0  0  0  0  0  0  0  0  0  0  0 13
0.3733  2.6687  0.5247 C  0  0  0  0  0  0  0  0  0  0  0  0  0 14
-0.9528 -5.2823  0.6566 C  0  0  0  0  0  0  0  0  0  0  0  0  0 15
-0.8494 -3.8959  0.7981 C  0  0  0  0  0  0  0  0  0  0  0  0  0 16
0.6082 -3.8078 -1.1296 C  0  0  0  0  0  0  0  0  0  0  0  0  0 17
0.5052 -5.1945 -1.2707 C  0  0  0  0  0  0  0  0  0  0  0  0  0 18
-0.2760 -5.9389 -0.3785 C  0  0  0  0  0  0  0  0  0  0  0  0  0 19
0.4859  3.3592 -0.5525 O  0  0  0  0  0  0  0  0  0  0  0  0  0 20
0.3509  3.1422  1.6941 O  0  0  0  0  0  0  0  0  0  0  0  0  0 21
0.1339 -1.2481 -2.0676 H  0  0  0  0  0  0  0  0  0  0  0  0  0 22
0.3366  1.2087 -1.7983 H  0  0  0  0  0  0  0  0  0  0  0  0  0 23
0.1561  0.7790  2.4701 H  0  0  0  0  0  0  0  0  0  0  0  0  0 24
-0.0155 -1.6849  2.2282 H  0  0  0  0  0  0  0  0  0  0  0  0  0 25
-1.5711 -5.8514  1.3535 H  0  0  0  0  0  0  0  0  0  0  0  0  0 26
-1.4008 -3.3967  1.5971 H  0  0  0  0  0  0  0  0  0  0  0  0  0 27
1.2388 -3.2448 -1.8201 H  0  0  0  0  0  0  0  0  0  0  0  0  0 28
1.0438 -5.6966 -2.0767 H  0  0  0  0  0  0  0  0  0  0  0  0  0 29
-0.3561 -7.0219 -0.4884 H  0  0  0  0  0  0  0  0  0  0  0  0  0 30
2  1  0  0  0  0  0
3  1  0  0  0  0  0
4  0  0  0  0  0  0
5  4  0  0  0  0  0
6  4  0  0  0  0  0
7  0  0  0  0  0  0
8  7  0  0  0  0  0
12  7  0  0  0  0  0
22  7  0  0  0  0  0
9  8  0  0  0  0  0
23  8  0  0  0  0  0
10  9  0  0  0  0  0
14  9  0  0  0  0  0
11 10  0  0  0  0  0
24 10  0  0  0  0  0
12 11  0  0  0  0  0
25 11  0  0  0  0  0
13 12  0  0  0  0  0
16 13  0  0  0  0  0
17 13  0  0  0  0  0
20 14  0  0  0  0  0
21 14  0  0  0  0  0
16 15  0  0  0  0  0
19 15  0  0  0  0  0
26 15  0  0  0  0  0
27 16  0  0  0  0  0
18 17  0  0  0  0  0
28 17  0  0  0  0  0
19 18  0  0  0  0  0
29 18  0  0  0  0  0
19 30  0  0  0  0  0
M  END
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4-phenylbenzoicacid.sdf
COSMOTHERM 3D 0
31 30 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
1.2251  -0.5303  7.1083 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1.0328  -1.4855  7.0946 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
1.2854  -0.3101  8.0558 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-0.5859  1.0064  5.8236 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
0.0507  0.4026  6.3108 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-1.4737  0.7545  6.1346 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
0.0959  -1.2488 -0.9722 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
0.0172  -1.2842  0.4175 C  0  0  0  0  0  0  0  0  0  0  0  0  0  8
-0.1814 -0.1031  1.1528 C  0  0  0  0  0  0  0  0  0  0  0  0  0  9
-0.3009  1.1156  0.4619 C  0  0  0  0  0  0  0  0  0  0  0  0  0 10
-0.2255  1.1479 -0.9293 C  0  0  0  0  0  0  0  0  0  0  0  0  0 11

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24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
26 15 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
16 29 0 0 0 0

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M END
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4-propylbenzoicacid.sdf
COSMOtherm 3D 0

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30 28 0 0 0 0 0 0 0 0 V2000
-0.7980 6.3382 0.6286 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6332 6.3598 0.1273 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.5578 7.2764 0.7384 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1818 4.9056 -0.5206 O 0 0 0 0 0 0 0 0 0 0 0 4
0.4257 5.4453 -0.1414 H 0 0 0 0 0 0 0 0 0 0 0 5
1.2067 5.1215 -1.4698 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2883 -1.8234 0.1202 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2746 -0.4483 -0.1094 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0787 0.2811 0.0078 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1011 -0.3977 0.3617 C 0 0 0 0 0 0 0 0 0 0 0 10
1.0792 -1.7743 0.5888 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.1127 -2.5126 0.4720 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.1024 1.7525 -0.2467 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.1215 -4.0087 0.6751 C 0 0 0 0 0 0 0 0 0 0 0 14
0.1435 -4.7912 -0.6300 C 0 0 0 0 0 0 0 0 0 0 0 15
0.1434 -6.3081 -0.4160 C 0 0 0 0 0 0 0 0 0 0 0 16
-1.1228 2.3637 -0.5743 O 0 0 0 0 0 0 0 0 0 0 0 17
1.0884 2.3474 -0.0862 O 0 0 0 0 0 0 0 0 0 0 0 18
-2.2276 -2.3747 0.0315 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.1925 0.0769 -0.3780 H 0 0 0 0 0 0 0 0 0 0 0 20
2.0342 0.1569 0.4615 H 0 0 0 0 0 0 0 0 0 0 0 21
2.0030 -2.2870 0.8678 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.0961 -4.3198 1.0850 H 0 0 0 0 0 0 0 0 0 0 0 23
0.6451 -4.2840 1.4172 H 0 0 0 0 0 0 0 0 0 0 0 24
1.1120 -4.4721 -1.0489 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.6229 -4.5178 -1.3737 H 0 0 0 0 0 0 0 0 0 0 0 26
0.3297 -6.8418 -1.3595 H 0 0 0 0 0 0 0 0 0 0 0 27
-0.8244 -6.6533 -0.0204 H 0 0 0 0 0 0 0 0 0 0 0 28
0.9242 -6.6078 0.3000 H 0 0 0 0 0 0 0 0 0 0 0 29
1.0198 3.3595 -0.2830 H 0 0 0 0 0 0 0 0 0 0 0 30

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
12 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
15 14 0 0 0 0
23 14 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
26 15 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
29 16 0 0 0 0
18 30 0 0 0 0

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M END
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4-sulfamoylbenzoicacid-anion.sdf
COSMOtherm 3D 0

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```

25 23 0 0 0 0 0 0 0 0 V2000
-7.0507 0.8445 1.6226 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.5336 0.3535 0.9195 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.6293 1.7197 1.6672 H 0 0 0 0 0 0 0 0 0 0 0 3
-5.6892 -0.5945 -0.2448 O 0 0 0 0 0 0 0 0 0 0 0 4
-4.6810 -0.5783 -0.0649 H 0 0 0 0 0 0 0 0 0 0 0 5
-5.7749 -0.2188 -1.1389 H 0 0 0 0 0 0 0 0 0 0 0 6
1.0089 -0.3279 1.0636 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.3653 -0.4068 0.8288 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.8977 -0.1049 -0.4348 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0310 0.2785 -1.4707 C 0 0 0 0 0 0 0 0 0 0 0 10
1.3462 0.3617 -1.2584 C 0 0 0 0 0 0 0 0 0 0 0 11
1.8469 0.0530 0.0109 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.4037 -0.1801 -0.6875 C 0 0 0 0 0 0 0 0 0 0 0 13
3.6359 0.1488 0.2996 S 0 0 0 0 0 0 0 0 0 0 0 14
3.8591 0.3323 1.7641 O 0 0 0 0 0 0 0 0 0 0 0 15
4.2079 1.1246 -0.6745 O 0 0 0 0 0 0 0 0 0 0 0 16
4.3482 -1.3432 -0.0847 N 0 0 0 0 0 0 0 0 0 0 0 17
-3.1204 -0.5790 0.2962 O 0 0 0 0 0 0 0 0 0 0 0 18
-2.8285 0.1495 -1.8266 O 0 0 0 0 0 0 0 0 0 0 0 19
3.9785 -2.0923 0.5098 H 0 0 0 0 0 0 0 0 0 0 0 20
4.2067 -1.5747 -1.0736 H 0 0 0 0 0 0 0 0 0 0 0 21
1.4201 -0.5512 2.0482 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.0422 -0.6988 1.6319 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.4517 0.5188 -2.4475 H 0 0 0 0 0 0 0 0 0 0 0 24
2.0162 0.6686 -2.0618 H 0 0 0 0 0 0 0 0 0 0 0 25

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0

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6 4 0 0 0 0
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12 7 0 0 0 0
22 7 0 0 0 0
9 8 0 0 0 0
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11 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
11 25 0 0 0 0
M END
$$$$
4-sulfamoylbenzoicacid.sdf
COSMOTHERM 3D 0
26 24 0 0 0 0 0 0 0 0 0 V2000
-0.8280 6.7706 1.0794 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7122 6.7583 0.6701 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.6466 7.7155 1.2350 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1013 5.5688 -0.3622 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3589 6.0329 0.1311 H 0 0 0 0 0 0 0 0 0 0 0 5
1.0486 5.8909 -1.2798 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2339 -1.2051 -0.2264 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.2339 0.1827 -0.3606 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0428 0.9124 -0.2158 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1587 0.2410 0.0655 C 0 0 0 0 0 0 0 0 0 0 0 10
1.1743 -1.1483 0.2006 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0243 -1.8509 0.0482 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.0980 2.4072 -0.3610 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.0132 -3.6627 0.2140 S 0 0 0 0 0 0 0 0 0 0 0 14
-1.3791 -4.0903 0.6344 O 0 0 0 0 0 0 0 0 0 0 0 15
1.1792 -4.0389 1.0266 O 0 0 0 0 0 0 0 0 0 0 0 16
0.2343 -4.3556 -1.3107 N 0 0 0 0 0 0 0 0 0 0 0 17
-1.1428 3.0082 -0.6142 O 0 0 0 0 0 0 0 0 0 0 0 18
1.0828 3.0021 -0.1883 O 0 0 0 0 0 0 0 0 0 0 0 19
-0.5237 -4.1198 -1.9593 H 0 0 0 0 0 0 0 0 0 0 0 20
1.1412 -4.0827 -1.7031 H 0 0 0 0 0 0 0 0 0 0 0 21
-2.1593 -1.7722 -0.3272 H 0 0 0 0 0 0 0 0 0 0 0 22
-2.1630 0.7123 -0.5721 H 0 0 0 0 0 0 0 0 0 0 0 23
2.0825 0.8055 0.1854 H 0 0 0 0 0 0 0 0 0 0 0 24
2.1028 -1.6722 0.4277 H 0 0 0 0 0 0 0 0 0 0 0 25
0.9978 4.0355 -0.2878 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
22 7 0 0 0 0
9 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
25 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
19 26 0 0 0 0
M END
$$$$
4-trifluoromethylbenzoicacid-anion.sdf
COSMOTHERM 3D 0
23 21 0 0 0 0 0 0 0 0 V2000
-6.8334 0.9642 1.4738 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.3047 0.4017 0.8353 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.3955 1.8322 1.4526 H 0 0 0 0 0 0 0 0 0 0 0 3
-5.4442 -0.6600 -0.2116 O 0 0 0 0 0 0 0 0 0 0 0 4
-4.4371 -0.6191 -0.0237 H 0 0 0 0 0 0 0 0 0 0 0 5
-5.5214 -0.3663 -1.1366 H 0 0 0 0 0 0 0 0 0 0 0 6
1.2562 -0.3695 1.0841 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.1189 -0.4461 0.8578 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.6602 -0.1156 -0.3940 C 0 0 0 0 0 0 0 0 0 0 0 9
0.2033 0.2976 -1.4209 C 0 0 0 0 0 0 0 0 0 0 0 10
1.5796 0.3778 -1.2080 C 0 0 0 0 0 0 0 0 0 0 0 11
2.1056 0.0486 0.0502 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.1658 -0.1953 -0.6441 C 0 0 0 0 0 0 0 0 0 0 0 13
3.5934 0.0873 0.2685 C 0 0 0 0 0 0 0 0 0 0 0 14
4.2047 -1.0804 -0.1273 F 0 0 0 0 0 0 0 0 0 0 0 15
3.9308 0.2669 1.5790 F 0 0 0 0 0 0 0 0 0 0 0 16
4.2029 1.0881 -0.4351 F 0 0 0 0 0 0 0 0 0 0 0 17
-2.8810 -0.5989 0.3401 O 0 0 0 0 0 0 0 0 0 0 0 18
-2.5963 0.1348 -1.7813 O 0 0 0 0 0 0 0 0 0 0 0 19
1.6635 -0.6254 2.0626 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.7901 -0.7647 1.6556 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.2206 0.5567 -2.3916 H 0 0 0 0 0 0 0 0 0 0 0 22
2.2387 0.7035 -2.0136 H 0 0 0 0 0 0 0 0 0 0 0 23

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
11 23 0 0 0 0

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M END

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4-trifluoromethylbenzoicacid.sdf

COSMOTHERM

3D

0

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24 22 0 0 0 0 0 0 0 0 0 V2000
-1.3701 -5.6476 0.0630 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7761 -5.9650 -0.7636 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.4012 -4.6556 0.0098 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2723 -5.3791 -0.0001 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3076 -5.6735 0.0285 H 0 0 0 0 0 0 0 0 0 0 0 5
1.6799 -5.7143 0.8191 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.2141 1.3132 -0.0410 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.1907 -0.0799 -0.0357 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0326 -0.7687 -0.0299 C 0 0 0 0 0 0 0 0 0 0 0 9
1.2375 -0.0470 -0.0342 C 0 0 0 0 0 0 0 0 0 0 0 10
1.2201 1.3474 -0.0384 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0062 2.0250 -0.0453 C 0 0 0 0 0 0 0 0 0 0 0 12
0.0178 -2.2668 -0.0141 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.0289 3.5314 0.0075 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.0739 3.9925 1.3003 F 0 0 0 0 0 0 0 0 0 0 0 15
-1.1149 4.0613 -0.6256 F 0 0 0 0 0 0 0 0 0 0 0 16
1.0753 4.0927 -0.5621 F 0 0 0 0 0 0 0 0 0 0 0 17
-1.0457 -2.9035 0.0270 O 0 0 0 0 0 0 0 0 0 0 0 18
1.2233 -2.8164 -0.0457 O 0 0 0 0 0 0 0 0 0 0 0 19
-2.1680 1.8409 -0.0484 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.1233 -0.6439 -0.0352 H 0 0 0 0 0 0 0 0 0 0 0 21
2.1891 -0.5769 -0.0315 H 0 0 0 0 0 0 0 0 0 0 0 22
2.1587 1.9014 -0.0415 H 0 0 0 0 0 0 0 0 0 0 0 23
1.1954 -3.8654 -0.0076 H 0 0 0 0 0 0 0 0 0 0 0 24

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
19 24 0 0 0 0

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M END

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5-fluorouracil-anion.sdf

COSMOTHERM

3D

0

```

17 15 0 0 0 0 0 0 0 0 0 V2000
-1.4634 -0.6132 -4.5588 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.6911 -0.1839 -4.0891 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.1660 0.0585 -4.5371 H 0 0 0 0 0 0 0 0 0 0 0 3
0.7082 0.4673 -3.3102 O 0 0 0 0 0 0 0 0 0 0 0 4
0.6448 0.3714 -2.2909 H 0 0 0 0 0 0 0 0 0 0 0 5
0.7809 1.4239 -3.4727 H 0 0 0 0 0 0 0 0 0 0 0 6
1.4978 -0.0378 0.1959 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2133 -0.1724 1.5698 N 0 0 0 0 0 0 0 0 0 0 0 8
-0.0404 -0.1106 2.1881 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.0823 0.1157 1.2279 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.8089 0.2445 -0.1089 C 0 0 0 0 0 0 0 0 0 0 0 11
0.4380 0.1743 -0.6413 N 0 0 0 0 0 0 0 0 0 0 0 12
-0.1715 -0.2437 3.4225 O 0 0 0 0 0 0 0 0 0 0 0 13
2.6846 -0.1172 -0.1897 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.3680 0.1985 1.6958 F 0 0 0 0 0 0 0 0 0 0 0 15
2.0131 -0.3309 2.1851 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.6306 0.4142 -0.8112 H 0 0 0 0 0 0 0 0 0 0 0 17

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0

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3 10 9 0 0 0 0
4 13 9 0 0 0 0
5 11 10 0 0 0 0
6 15 10 0 0 0 0
7 12 11 0 0 0 0
8 11 17 0 0 0 0
9 M END
10 $$$$
11 5-fluorouracil.sdf
12 COSMOtherm 3D 0
13
14 18 16 0 0 0 0 0 0 0 0 0 V2000
15 -4.8889 0.9926 -0.1165 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
16 -5.4730 0.6068 0.5613 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
17 -5.4989 1.3242 -0.8005 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
18 -3.0587 -0.7593 -1.1039 O 0 0 0 0 0 0 0 0 0 0 0 0 0 4
19 -3.7602 -0.1531 -0.7265 H 0 0 0 0 0 0 0 0 0 0 0 0 0 5
20 -3.3850 -1.6627 -0.9459 H 0 0 0 0 0 0 0 0 0 0 0 0 0 6
21 -0.2060 -0.2433 1.1447 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
22 1.1430 0.0036 1.4009 N 0 0 0 0 0 0 0 0 0 0 0 0 0 8
23 2.1839 0.1665 0.4755 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
24 1.7203 0.0549 -0.8927 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
25 0.4182 -0.1834 -1.1912 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
26 -0.5157 -0.3262 -0.1998 N 0 0 0 0 0 0 0 0 0 0 0 0 0 12
27 3.3488 0.3795 0.8345 O 0 0 0 0 0 0 0 0 0 0 0 0 0 13
28 -1.0392 -0.3733 2.0454 O 0 0 0 0 0 0 0 0 0 0 0 0 0 14
29 2.6474 0.1973 -1.8728 F 0 0 0 0 0 0 0 0 0 0 0 0 0 15
30 1.4014 0.0704 2.3870 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
31 -1.5228 -0.5073 -0.4657 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
32 0.0614 -0.2708 -2.2165 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
33
34 2 1 0 0 0 0
35 3 1 0 0 0 0
36 5 4 0 0 0 0
37 6 4 0 0 0 0
38 8 7 0 0 0 0
39 12 7 0 0 0 0
40 14 7 0 0 0 0
41 9 8 0 0 0 0
42 16 8 0 0 0 0
43 10 9 0 0 0 0
44 13 9 0 0 0 0
45 11 10 0 0 0 0
46 15 10 0 0 0 0
47 12 11 0 0 0 0
48 17 12 0 0 0 0
49 11 18 0 0 0 0
50 M END
51 $$$$
52 5-iodo-2-hydroxybenzoicacid-anion.sdf
53 COSMOtherm 3D 0
54
55 21 19 0 0 0 0 0 0 0 0 V2000
56 -3.3919 0.8547 6.0064 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
57 -2.5722 0.3248 5.7924 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
58 -3.0940 1.7801 5.9880 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
59 -1.2228 -0.6954 5.4098 O 0 0 0 0 0 0 0 0 0 0 0 0 0 4
60 -0.9401 -0.5891 4.4411 H 0 0 0 0 0 0 0 0 0 0 0 0 0 5
61 -0.4268 -0.4705 5.9222 H 0 0 0 0 0 0 0 0 0 0 0 0 0 6
62 0.5587 0.0548 -1.2005 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
63 0.1411 -0.1116 0.1150 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
64 1.0765 -0.0583 1.1608 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
65 2.4485 0.1660 0.8593 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
66 2.8461 0.3304 -0.4810 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
67 1.9081 0.2758 -1.5099 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12
68 0.6363 -0.2357 2.5921 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13
69 1.5570 -0.1684 3.4909 O 0 0 0 0 0 0 0 0 0 0 0 0 0 14
70 -0.5892 -0.4373 2.8409 O 0 0 0 0 0 0 0 0 0 0 0 0 0 15
71 3.3730 0.2247 1.8412 O 0 0 0 0 0 0 0 0 0 0 0 0 0 16
72 -0.8834 -0.0258 -2.7896 I 0 0 0 0 0 0 0 0 0 0 0 0 0 17
73 2.7980 0.0721 2.7059 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
74 -0.9050 -0.2846 0.3689 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
75 3.9001 0.5014 -0.7066 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
76 2.2337 0.4063 -2.5422 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
77
78 2 1 0 0 0 0
79 3 1 0 0 0 0
80 5 4 0 0 0 0
81 6 4 0 0 0 0
82 8 7 0 0 0 0
83 12 7 0 0 0 0
84 9 8 0 0 0 0
85 19 8 0 0 0 0
86 10 9 0 0 0 0
87 13 9 0 0 0 0
88 11 10 0 0 0 0
89 16 10 0 0 0 0
90 12 11 0 0 0 0
91 20 11 0 0 0 0
92 14 13 0 0 0 0
93 15 13 0 0 0 0
94 18 14 0 0 0 0
95 18 16 0 0 0 0
96 12 21 0 0 0 0
97 M END
98 $$$$
99 5-iodo-2-hydroxybenzoicacid.sdf
100 COSMOtherm 3D 0
101
102 22 19 0 0 0 0 0 0 0 0 V2000
103 1.2575 -1.7159 -6.6209 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
104 1.1299 -1.0496 -7.3210 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
105 1.4577 -2.5394 -7.1029 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
106 -0.8158 -2.0121 -4.9498 O 0 0 0 0 0 0 0 0 0 0 0 0 0 4
107 -0.0658 -1.8808 -5.6075 H 0 0 0 0 0 0 0 0 0 0 0 0 0 5
108 -1.6199 -1.6910 -5.3963 H 0 0 0 0 0 0 0 0 0 0 0 0 0 6
109 0.0406 0.5465 1.2056 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7

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-0.1337 0.0017 -0.0586 C 0 0 0 0 0 0 0 0 0 0 0 8  
-0.1438 0.8431 -1.1896 C 0 0 0 0 0 0 0 0 0 0 0 9  
0.0230 2.2456 -1.0212 C 0 0 0 0 0 0 0 0 0 0 0 10  
0.2001 2.7696 0.2720 C 0 0 0 0 0 0 0 0 0 0 0 11  
0.2089 1.9296 1.3800 C 0 0 0 0 0 0 0 0 0 0 0 12  
-0.3268 0.2987 -2.5526 C 0 0 0 0 0 0 0 0 0 0 0 13  
-0.4632 -1.0132 -2.6349 O 0 0 0 0 0 0 0 0 0 0 0 14  
-0.3473 1.0488 -3.5557 O 0 0 0 0 0 0 0 0 0 0 0 15  
0.0173 3.0968 -2.0706 O 0 0 0 0 0 0 0 0 0 0 0 16  
0.0521 -0.7354 2.9195 I 0 0 0 0 0 0 0 0 0 0 0 17  
-0.6002 -1.3315 -3.6274 H 0 0 0 0 0 0 0 0 0 0 0 18  
-0.1260 2.5101 -2.8849 H 0 0 0 0 0 0 0 0 0 0 0 19  
-0.2662 -1.0696 -0.2026 H 0 0 0 0 0 0 0 0 0 0 0 20  
0.3294 3.8459 0.3942 H 0 0 0 0 0 0 0 0 0 0 0 21  
0.3468 2.3538 2.3744 H 0 0 0 0 0 0 0 0 0 0 0 22  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
8 7 0 0 0 0  
12 7 0 0 0 0  
9 8 0 0 0 0  
20 8 0 0 0 0  
10 9 0 0 0 0  
13 9 0 0 0 0  
11 10 0 0 0 0  
16 10 0 0 0 0  
12 11 0 0 0 0  
21 11 0 0 0 0  
14 13 0 0 0 0  
15 13 0 0 0 0  
18 14 0 0 0 0  
19 16 0 0 0 0  
12 22 0 0 0 0  
M END  
$$$$  
5-nitrouracil-anion.sdf  
COSMOTHERM 3D 0  
19 17 0 0 0 0 0 0 0 0 0 V2000  
-2.0359 -4.5691 -0.8592 O 0 0 0 0 0 0 0 0 0 0 0 1  
-1.2714 -4.2524 -0.3002 H 0 0 0 0 0 0 0 0 0 0 0 2  
-2.8266 -4.2307 -0.4057 H 0 0 0 0 0 0 0 0 0 0 0 3  
0.1341 -3.7581 0.6005 O 0 0 0 0 0 0 0 0 0 0 0 4  
0.3312 -2.7702 0.4946 H 0 0 0 0 0 0 0 0 0 0 0 5  
0.0110 -3.8922 1.5568 H 0 0 0 0 0 0 0 0 0 0 0 6  
-0.4546 -0.2290 0.2661 C 0 0 0 0 0 0 0 0 0 0 0 7  
-0.3848 1.1579 0.0649 C 0 0 0 0 0 0 0 0 0 0 0 8  
0.9087 1.7804 -0.1871 C 0 0 0 0 0 0 0 0 0 0 0 9  
1.9389 0.8258 -0.1829 N 0 0 0 0 0 0 0 0 0 0 0 10  
1.8428 -0.5522 0.0224 C 0 0 0 0 0 0 0 0 0 0 0 11  
0.5738 -1.0662 0.2526 N 0 0 0 0 0 0 0 0 0 0 0 12  
1.1812 2.9694 -0.3889 O 0 0 0 0 0 0 0 0 0 0 0 13  
2.8566 -1.2627 -0.0041 O 0 0 0 0 0 0 0 0 0 0 0 14  
-1.5931 1.9134 0.1143 N 0 0 0 0 0 0 0 0 0 0 0 15  
-1.4382 -0.6668 0.4511 H 0 0 0 0 0 0 0 0 0 0 0 16  
2.8768 1.1943 -0.3521 H 0 0 0 0 0 0 0 0 0 0 0 17  
-2.6734 1.3080 0.3444 O 0 0 0 0 0 0 0 0 0 0 0 18  
-1.5572 3.1495 -0.0697 O 0 0 0 0 0 0 0 0 0 0 0 19  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
8 7 0 0 0 0  
12 7 0 0 0 0  
16 7 0 0 0 0  
9 8 0 0 0 0  
15 8 0 0 0 0  
10 9 0 0 0 0  
13 9 0 0 0 0  
11 10 0 0 0 0  
17 10 0 0 0 0  
12 11 0 0 0 0  
14 11 0 0 0 0  
18 15 0 0 0 0  
15 19 0 0 0 0  
M END  
$$$$  
5-nitrouracil.sdf  
COSMOTHERM 3D 0  
20 18 0 0 0 0 0 0 0 0 0 V2000  
-5.3012 0.7287 0.9415 O 0 0 0 0 0 0 0 0 0 0 0 1  
-5.9765 0.1510 0.5416 H 0 0 0 0 0 0 0 0 0 0 0 2  
-5.7962 1.5191 1.2248 H 0 0 0 0 0 0 0 0 0 0 0 3  
-3.2571 1.3376 -0.7167 O 0 0 0 0 0 0 0 0 0 0 0 4  
-4.0418 1.1047 -0.1364 H 0 0 0 0 0 0 0 0 0 0 0 5  
-3.5794 1.2756 -1.6333 H 0 0 0 0 0 0 0 0 0 0 0 6  
0.1180 0.7932 -0.2004 C 0 0 0 0 0 0 0 0 0 0 0 7  
1.3847 0.2858 -0.0027 C 0 0 0 0 0 0 0 0 0 0 0 8  
1.5891 -1.1610 0.1126 C 0 0 0 0 0 0 0 0 0 0 0 9  
0.3757 -1.8707 -0.0050 N 0 0 0 0 0 0 0 0 0 0 0 10  
-0.9046 -1.3836 -0.2033 C 0 0 0 0 0 0 0 0 0 0 0 11  
-0.9668 0.0129 -0.2949 N 0 0 0 0 0 0 0 0 0 0 0 12  
2.6365 -1.7779 0.2903 O 0 0 0 0 0 0 0 0 0 0 0 13  
-1.8994 -2.0952 -0.2915 O 0 0 0 0 0 0 0 0 0 0 0 14  
2.4779 1.2262 0.0819 N 0 0 0 0 0 0 0 0 0 0 0 15  
-0.0438 1.8669 -0.2886 H 0 0 0 0 0 0 0 0 0 0 0 16  
0.4574 -2.8868 0.0678 H 0 0 0 0 0 0 0 0 0 0 0 17  
-1.9247 0.4640 -0.4626 H 0 0 0 0 0 0 0 0 0 0 0 18  
2.2134 2.4455 -0.0079 O 0 0 0 0 0 0 0 0 0 0 0 19  
3.6311 0.7944 0.2388 O 0 0 0 0 0 0 0 0 0 0 0 20  
2 1 0 0 0 0  
3 1 0 0 0 0  
5 4 0 0 0 0
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For Peer Review Only

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6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0

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M END

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aceticacid-anion.sdf

COSMOTHERM 3D

0

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13 10 0 0 0 0 0 0 0 0 V2000
-2.9319 -0.0699 1.2546 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.9830 0.0027 0.9219 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.4174 0.6151 0.7648 H 0 0 0 0 0 0 0 0 0 0 0 0 3
2.9232 -0.0055 1.1675 O 0 0 0 0 0 0 0 0 0 0 0 0 4
2.2943 -0.0129 0.3761 H 0 0 0 0 0 0 0 0 0 0 0 0 5
2.3184 0.0251 1.9288 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.9589 -0.0026 -1.7905 C 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0745 0.0095 -0.6630 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.3079 -0.0299 -0.9798 O 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.3528 0.0610 0.5372 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.4843 -0.0674 -0.0674 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.6427 -0.8537 -1.6578 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.5685 0.9120 -1.7425 H 0 0 0 0 0 0 0 0 0 0 0 0 13

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 13 0 0 0 0

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M END

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aceticacid.sdf

COSMOTHERM 3D

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14 11 0 0 0 0 0 0 0 0 V2000
-0.7176 0.5610 -3.3800 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.3312 -0.0617 -3.8115 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.2453 0.9858 -4.1196 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.0173 -0.5927 -1.6558 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3555 -0.2092 -2.3053 H 0 0 0 0 0 0 0 0 0 0 0 0 5
0.8859 -1.5570 -1.6870 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.1340 0.5762 2.8934 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.1399 -0.0384 1.5155 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9761 -0.8528 1.1258 O 0 0 0 0 0 0 0 0 0 0 0 0 9
0.8732 0.3971 0.7516 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.9576 0.1728 3.4910 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.8234 0.3708 3.3929 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.2343 1.6683 2.8163 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.8439 -0.0417 -0.1813 H 0 0 0 0 0 0 0 0 0 0 0 0 14

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
10 14 0 0 0 0

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M END

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acrylicacid-anion.sdf

COSMOTHERM 3D

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14 11 0 0 0 0 0 0 0 0 V2000
-4.1451 0.6031 -0.5848 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.3786 0.1853 -0.0923 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.9176 1.5474 -0.6318 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-2.1167 -0.6398 0.7314 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.2421 -0.6298 0.1897 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.8741 -0.1803 1.5550 H 0 0 0 0 0 0 0 0 0 0 0 0 6
3.5032 0.4413 -0.1521 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.3885 -0.0589 -0.7008 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.0561 -0.1057 0.0127 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.0985 -0.6435 -0.6618 O 0 0 0 0 0 0 0 0 0 0 0 0 10
0.9520 0.3616 1.1791 O 0 0 0 0 0 0 0 0 0 0 0 0 11
4.4525 0.4584 -0.6916 H 0 0 0 0 0 0 0 0 0 0 0 0 12
3.4866 0.8487 0.8620 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.4007 -0.4686 -1.7152 H 0 0 0 0 0 0 0 0 0 0 0 0 14

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0

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8 14 0 0 0 0
M END
$$$$
acrylicacid.sdf
COSMOTHERM      3D      0
15 12 0 0 0 0 0 0 0 0 0 V2000
-1.0253 3.6936 -0.4305 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6497 3.2243 -1.0135 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.7204 4.4508 -0.9632 H 0 0 0 0 0 0 0 0 0 0 0 3
1.0595 2.2055 0.4402 O 0 0 0 0 0 0 0 0 0 0 0 4
1.0587 2.2943 1.4101 H 0 0 0 0 0 0 0 0 0 0 0 5
0.2733 2.7405 0.1216 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.6712 -3.3932 -0.1364 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2227 -2.4433 -0.4394 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0998 -1.0525 0.0785 C 0 0 0 0 0 0 0 0 0 0 0 9
1.0972 -0.2666 -0.3588 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.8030 -0.6603 0.8188 O 0 0 0 0 0 0 0 0 0 0 0 11
-0.5710 -4.4092 -0.5200 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.5277 -3.1745 0.5052 H 0 0 0 0 0 0 0 0 0 0 0 13
1.0820 -2.6525 -1.0798 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9979 0.6948 0.0086 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 15 0 0 0 0
M END
$$$$
anthracene-9-carboxylicacid-anion.sdf
COSMOTHERM      3D      0
32 32 0 0 0 0 0 0 0 0 V2000
-6.2568 -0.0651 -0.7905 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.5670 0.5928 -0.4867 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.8732 0.4628 -1.3262 H 0 0 0 0 0 0 0 0 0 0 0 3
-4.3850 1.7484 0.0294 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.4387 1.4328 -0.1925 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.3829 1.8132 1.0010 H 0 0 0 0 0 0 0 0 0 0 0 6
3.4290 2.8049 -0.2605 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1125 3.3130 -0.0558 C 0 0 0 0 0 0 0 0 0 0 0 8
1.0456 2.4541 0.0828 C 0 0 0 0 0 0 0 0 0 0 0 9
1.2236 1.0341 0.0247 C 0 0 0 0 0 0 0 0 0 0 0 10
2.5639 0.5198 -0.1861 C 0 0 0 0 0 0 0 0 0 0 0 11
3.6454 1.4478 -0.3240 C 0 0 0 0 0 0 0 0 0 0 0 12
0.1443 0.1315 0.1697 C 0 0 0 0 0 0 0 0 0 0 0 13
0.3623 -1.2645 0.1041 C 0 0 0 0 0 0 0 0 0 0 0 14
1.7047 -1.7703 -0.1126 C 0 0 0 0 0 0 0 0 0 0 0 15
2.7702 -0.8670 -0.2486 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.7039 -2.2113 0.2382 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.4677 -3.5657 0.1681 C 0 0 0 0 0 0 0 0 0 0 0 18
0.8530 -4.0606 -0.0420 C 0 0 0 0 0 0 0 0 0 0 0 19
1.9064 -3.1863 -0.1782 C 0 0 0 0 0 0 0 0 0 0 0 20
-1.2598 0.6654 0.4278 C 0 0 0 0 0 0 0 0 0 0 0 21
-1.6239 0.7844 1.6263 O 0 0 0 0 0 0 0 0 0 0 0 22
-1.9530 0.9496 -0.6077 O 0 0 0 0 0 0 0 0 0 0 0 23
4.2641 3.4998 -0.3669 H 0 0 0 0 0 0 0 0 0 0 0 24
1.9540 4.3921 -0.0091 H 0 0 0 0 0 0 0 0 0 0 0 25
0.0417 2.8545 0.2371 H 0 0 0 0 0 0 0 0 0 0 0 26
4.6521 1.0531 -0.4806 H 0 0 0 0 0 0 0 0 0 0 0 27
3.7810 -1.2516 -0.4080 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.7190 -1.8439 0.3994 H 0 0 0 0 0 0 0 0 0 0 0 29
-1.2952 -4.2699 0.2724 H 0 0 0 0 0 0 0 0 0 0 0 30
1.0227 -5.1376 -0.0945 H 0 0 0 0 0 0 0 0 0 0 0 31
2.9203 -3.5601 -0.3404 H 0 0 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
24 7 0 0 0 0
9 8 0 0 0 0
25 8 0 0 0 0
10 9 0 0 0 0
26 9 0 0 0 0
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12 11 0 0 0 0
16 11 0 0 0 0
27 12 0 0 0 0
14 13 0 0 0 0
21 13 0 0 0 0
15 14 0 0 0 0
17 14 0 0 0 0
16 15 0 0 0 0
20 15 0 0 0 0
28 16 0 0 0 0
18 17 0 0 0 0
29 17 0 0 0 0
19 18 0 0 0 0
30 18 0 0 0 0
20 19 0 0 0 0
31 19 0 0 0 0
22 21 0 0 0 0
23 21 0 0 0 0
20 32 0 0 0 0
M END

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$$$$
anthracene-9-carboxylicacid.sdf
COSMOtherm          3D              0

33 33 0 0 0 0 0 0 0 0 0 0 V2000
-1.2258 -4.8980 -0.5371 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.2277 -5.2535 -1.4437 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.2284 -3.9098 -0.6410 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1303 -4.5912 0.6526 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.8823 -4.9581 0.1532 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.2982 -4.9047 0.1754 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1176 2.1808 -3.6705 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.1371 0.7562 -3.6827 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0967 0.0394 -2.5084 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.0311 0.7013 -1.2398 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0210 2.1513 -1.2307 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.0616 2.8570 -2.4750 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.0140 0.0087 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.0291 0.7031 1.2299 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.0597 2.1531 1.2174 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.0280 2.8342 -0.0073 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.0853 0.0434 2.5003 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.1489 0.7617 3.6727 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.1651 2.1862 3.6570 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.1220 2.8606 2.4599 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
0.0128 -1.4951 -0.0130 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.9295 -2.1408 -0.4939 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
1.0948 -2.0335 0.5293 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
0.1502 2.7295 -4.6131 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
0.1870 0.2283 -4.6368 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
0.1091 -1.0502 -2.5439 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
0.0518 3.9489 -2.4521 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
-0.0437 3.9270 -0.0085 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 28
-0.0727 -1.0459 2.5401 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29
-0.1914 0.2349 4.6277 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 30
-0.2146 2.7364 4.5981 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 31
-0.1407 3.9523 2.4340 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 32
1.0743 -3.0875 0.5378 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 33

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
24 7 0 0 0 0
9 8 0 0 0 0
25 8 0 0 0 0
10 9 0 0 0 0
26 9 0 0 0 0
11 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
16 11 0 0 0 0
27 12 0 0 0 0
14 13 0 0 0 0
21 13 0 0 0 0
15 14 0 0 0 0
17 14 0 0 0 0
16 15 0 0 0 0
20 15 0 0 0 0
28 16 0 0 0 0
18 17 0 0 0 0
29 17 0 0 0 0
19 18 0 0 0 0
30 18 0 0 0 0
20 19 0 0 0 0
31 19 0 0 0 0
32 20 0 0 0 0
22 21 0 0 0 0
23 21 0 0 0 0
23 33 0 0 0 0

M END
$$$$
benzoicacid-anion.sdf
COSMOtherm          3D              0

20 18 0 0 0 0 0 0 0 0 V2000
-5.2507 0.9145 0.9956 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.6333 0.3421 0.4517 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.8620 1.8045 0.9476 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-3.6291 -0.7256 -0.4436 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.6552 -0.6693 -0.1196 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-3.5737 -0.4436 -1.3740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
2.8819 -0.1451 1.5359 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5330 -0.2878 1.1937 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.1003 -0.0546 -0.1227 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.0459 0.3224 -1.0910 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.3959 0.4614 -0.7534 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
3.8173 0.2288 0.5625 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.3677 -0.2048 -0.5054 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.1615 -0.6100 0.4191 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.7096 0.0721 -1.6880 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
3.2056 -0.3262 2.5629 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
0.7972 -0.5812 1.9439 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
1.7047 0.5032 -2.1115 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
4.1215 0.7523 -1.5160 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
4.8706 0.3388 0.8281 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0

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17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
12 20 0 0 0 0
M END
$$$$
benzoicacid.sdf
COSMOtherm 3D 0
21 19 0 0 0 0 0 0 0 0 V2000
-0.8035 4.9122 0.9008 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.7008 4.8667 0.5237 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.6168 5.8665 0.9657 H 0 0 0 0 0 0 0 0 0 0 0 3
1.0878 3.5814 -0.4899 O 0 0 0 0 0 0 0 0 0 0 0 4
0.3600 4.0871 -0.0188 H 0 0 0 0 0 0 0 0 0 0 0 5
1.0141 3.8319 -1.4281 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1799 -3.1259 0.4030 C 0 0 0 0 0 0 0 0 0 0 0 7
1.1617 -1.7409 0.2184 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0462 -1.0849 -0.0797 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.2317 -1.8327 -0.1884 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.2106 -3.2162 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0045 -3.8652 0.2936 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.1101 0.3960 -0.2905 C 0 0 0 0 0 0 0 0 0 0 0 13
1.0684 1.0128 -0.1382 O 0 0 0 0 0 0 0 0 0 0 0 14
-1.1528 0.9888 -0.5772 O 0 0 0 0 0 0 0 0 0 0 0 15
2.1200 -3.6302 0.6327 H 0 0 0 0 0 0 0 0 0 0 0 16
2.0826 -1.1641 0.3034 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.1645 -1.3167 -0.4197 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.1345 -3.7907 -0.0869 H 0 0 0 0 0 0 0 0 0 0 0 19
0.0121 -4.9469 0.4384 H 0 0 0 0 0 0 0 0 0 0 0 20
0.9731 2.0302 -0.3011 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
20 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
14 21 0 0 0 0
M END
$$$$
boricacid-anion.sdf
COSMOtherm 3D 0
12 9 0 0 0 0 0 0 0 0 V2000
-2.5583 -0.0768 -1.1409 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.5314 -0.0077 -1.1310 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.8703 0.8015 -1.4206 H 0 0 0 0 0 0 0 0 0 0 0 3
2.5620 -0.0725 -1.1420 O 0 0 0 0 0 0 0 0 0 0 0 4
1.5353 0.0008 -1.1275 H 0 0 0 0 0 0 0 0 0 0 0 5
2.8790 0.8210 -1.3611 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0010 0.0160 0.6218 B 0 0 0 0 0 0 0 0 0 0 0 7
-1.1796 0.0036 1.4016 O 0 0 0 0 0 0 0 0 0 0 0 8
0.0021 0.0410 -0.7271 O 0 0 0 0 0 0 0 0 0 0 0 9
1.1738 -0.0070 1.4069 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.9436 0.0044 0.7800 H 0 0 0 0 0 0 0 0 0 0 0 11
1.9403 -0.0203 0.7889 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
10 12 0 0 0 0
M END
$$$$
boricacid.sdf
COSMOtherm 3D 0
13 10 0 0 0 0 0 0 0 0 V2000
-3.6721 -0.0008 0.6790 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.2466 -0.7742 0.5306 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.2511 0.7669 0.5192 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.4581 -0.0069 -0.8563 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.7226 -0.0043 -1.7932 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.3095 -0.0042 -0.3241 H 0 0 0 0 0 0 0 0 0 0 0 6
1.5365 0.0051 0.0647 B 0 0 0 0 0 0 0 0 0 0 0 7
2.8635 0.0549 0.4618 O 0 0 0 0 0 0 0 0 0 0 0 8
0.9045 1.2210 -0.1230 O 0 0 0 0 0 0 0 0 0 0 0 9
0.9130 -1.2175 -0.1227 O 0 0 0 0 0 0 0 0 0 0 0 10
3.2394 -0.8360 0.5716 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.0314 1.0614 -0.4071 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0253 -1.0695 -0.4074 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0

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6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
12 9 0 0 0 0
10 13 0 0 0 0
M END
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bromoaceticacid-anion.sdf
COSMOTHERM 3D 0
13 9 0 0 0 0 0 0 0 0 0 V2000
1.6525 -0.4721 4.9433 O 0 0 0 0 0 0 0 0 0 0 0 1
0.8962 -0.0792 4.4192 H 0 0 0 0 0 0 0 0 0 0 0 2
1.8136 -1.3363 4.5276 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3742 0.7087 3.5508 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.3003 0.5506 2.5461 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.2454 0.3458 3.7889 H 0 0 0 0 0 0 0 0 0 0 0 6
0.5840 0.0316 -2.1064 Br 0 0 0 0 0 0 0 0 0 0 0 7
-1.1373 -0.3308 -1.1480 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.1396 -0.0759 0.3675 C 0 0 0 0 0 0 0 0 0 0 0 9
-2.2598 -0.3324 0.8868 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.0952 0.3435 0.9516 O 0 0 0 0 0 0 0 0 0 0 0 11
-1.3616 -1.3815 -1.3563 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.8763 0.3078 -1.6417 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0
M END
$$$$
bromoaceticacid.sdf
COSMOTHERM 3D 0
14 10 0 0 0 0 0 0 0 0 V2000
-1.4283 -4.8120 0.5141 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.6518 -5.6884 0.1504 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.2207 -4.2707 0.3440 H 0 0 0 0 0 0 0 0 0 0 0 3
0.8735 -3.8164 -0.4469 O 0 0 0 0 0 0 0 0 0 0 0 4
0.8748 -3.8956 -1.4178 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.0128 -4.1837 -0.1443 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.2885 2.3278 0.0035 Br 0 0 0 0 0 0 0 0 0 0 0 7
0.9205 0.8587 0.4990 C 0 0 0 0 0 0 0 0 0 0 0 8
0.4940 -0.4897 -0.0688 C 0 0 0 0 0 0 0 0 0 0 0 9
1.3443 -1.4275 0.3496 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.4693 -0.6842 -0.7967 O 0 0 0 0 0 0 0 0 0 0 0 11
0.9438 0.8222 1.5926 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9140 1.1279 0.1256 H 0 0 0 0 0 0 0 0 0 0 0 13
1.0859 -2.3713 -0.0241 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 14 0 0 0 0
M END
$$$$
carbonicacid-anion.sdf
COSMOTHERM 3D 0
11 8 0 0 0 0 0 0 0 0 V2000
-3.8027 0.4365 -0.5538 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.0104 0.0842 -0.0546 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.6415 1.3931 -0.6205 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.6845 -0.6334 0.7910 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.8159 -0.5602 0.2607 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.5041 -0.1612 1.6224 H 0 0 0 0 0 0 0 0 0 0 0 6
1.4924 0.0360 -0.0193 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5343 0.5082 1.1396 O 0 0 0 0 0 0 0 0 0 0 0 8
2.6680 0.0810 -0.7904 O 0 0 0 0 0 0 0 0 0 0 0 9
0.5189 -0.4987 -0.6335 O 0 0 0 0 0 0 0 0 0 0 0 10
3.3471 0.5059 -0.2302 H 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 11 0 0 0 0
M END
$$$$
carbonicacid.sdf
COSMOTHERM 3D 0
12 9 0 0 0 0 0 0 0 0 V2000
-3.3851 0.0055 -0.3588 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5453 -0.7840 -0.9079 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5155 0.7584 -0.9644 H 0 0 0 0 0 0 0 0 0 0 0 3
3.3848 -0.0033 -0.3596 O 0 0 0 0 0 0 0 0 0 0 0 4
3.5763 0.8270 -0.8330 H 0 0 0 0 0 0 0 0 0 0 0 5
3.4780 -0.7001 -1.0349 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0003 -0.0022 0.1594 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0007 -0.0032 -1.0700 O 0 0 0 0 0 0 0 0 0 0 0 8
-1.0949 0.0025 0.9300 O 0 0 0 0 0 0 0 0 0 0 0 9

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1.0948 -0.0061 0.9310 O 0 0 0 0 0 0 0 0 0 0 10
-1.9290 0.0030 0.3436 H 0 0 0 0 0 0 0 0 0 0 11
1.9293 -0.0043 0.3452 H 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 9 0 0 0 0
10 12 0 0 0 0
M END
$$$$
chloroaceticacid-anion.sdf
COSMOTHERM 3D 0
13 10 0 0 0 0 0 0 0 0 0 V2000
-4.4049 0.4776 -1.2896 O 0 0 0 0 0 0 0 0 0 0 1
-3.7928 0.0802 -0.6055 H 0 0 0 0 0 0 0 0 0 0 2
-4.4878 1.4105 -1.0282 H 0 0 0 0 0 0 0 0 0 0 3
-2.7510 -0.7184 0.5229 O 0 0 0 0 0 0 0 0 0 0 4
-1.7644 -0.5671 0.3124 H 0 0 0 0 0 0 0 0 0 0 5
-2.8622 -0.3698 1.4249 H 0 0 0 0 0 0 0 0 0 0 6
2.6446 -0.0587 -1.0673 Cl 0 0 0 0 0 0 0 0 0 0 7
2.0078 0.3096 0.6211 C 0 0 0 0 0 0 0 0 0 0 8
0.5030 0.0707 0.8384 C 0 0 0 0 0 0 0 0 0 0 9
-0.2123 -0.3725 -0.1118 O 0 0 0 0 0 0 0 0 0 0 10
0.1318 0.3575 2.0081 O 0 0 0 0 0 0 0 0 0 0 11
2.2479 1.3608 0.8108 H 0 0 0 0 0 0 0 0 0 0 12
2.5851 -0.3221 1.3044 H 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0
M END
$$$$
chloroaceticacid.sdf
COSMOTHERM 3D 0
14 11 0 0 0 0 0 0 0 0 0 V2000
-1.2601 -4.0991 0.5078 O 0 0 0 0 0 0 0 0 0 0 1
-1.3871 -5.0035 0.1677 H 0 0 0 0 0 0 0 0 0 0 2
-2.0950 -3.6422 0.2985 H 0 0 0 0 0 0 0 0 0 0 3
0.9617 -2.9277 -0.4464 O 0 0 0 0 0 0 0 0 0 0 4
0.9743 -3.0106 -1.4168 H 0 0 0 0 0 0 0 0 0 0 5
0.1057 -3.3617 -0.1460 H 0 0 0 0 0 0 0 0 0 0 6
-0.5304 3.0050 0.0056 Cl 0 0 0 0 0 0 0 0 0 0 7
0.6783 1.7448 0.4845 C 0 0 0 0 0 0 0 0 0 0 8
0.3419 0.3617 -0.0640 C 0 0 0 0 0 0 0 0 0 0 9
1.2671 -0.5079 0.3392 O 0 0 0 0 0 0 0 0 0 0 10
-0.6243 0.0949 -0.7645 O 0 0 0 0 0 0 0 0 0 0 11
0.7086 1.7152 1.5790 H 0 0 0 0 0 0 0 0 0 0 12
1.6559 2.0660 0.1087 H 0 0 0 0 0 0 0 0 0 0 13
1.0701 -1.4700 -0.0226 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
10 14 0 0 0 0
M END
$$$$
cis-5-formyluracil-anion.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
-4.4743 0.3799 -0.2295 O 0 0 0 0 0 0 0 0 0 0 1
-4.1993 -0.5648 -0.1156 H 0 0 0 0 0 0 0 0 0 0 2
-3.6083 0.8468 -0.1272 H 0 0 0 0 0 0 0 0 0 0 3
-3.1464 -2.0688 0.0983 O 0 0 0 0 0 0 0 0 0 0 4
-2.3030 -1.5080 0.1007 H 0 0 0 0 0 0 0 0 0 0 5
-3.2287 -2.4031 1.0088 H 0 0 0 0 0 0 0 0 0 0 6
0.3154 -1.1317 -0.0077 C 0 0 0 0 0 0 0 0 0 0 7
1.5804 -0.5279 -0.0203 C 0 0 0 0 0 0 0 0 0 0 8
1.6368 0.9256 0.0199 C 0 0 0 0 0 0 0 0 0 0 9
0.3611 1.5141 0.0558 N 0 0 0 0 0 0 0 0 0 0 10
-0.8715 0.8639 0.0519 C 0 0 0 0 0 0 0 0 0 0 11
-0.8675 -0.5152 0.0267 N 0 0 0 0 0 0 0 0 0 0 12
2.6441 1.6483 0.0246 O 0 0 0 0 0 0 0 0 0 0 13
-1.9195 1.5436 0.0734 O 0 0 0 0 0 0 0 0 0 0 14
2.7382 -1.3932 -0.0631 C 0 0 0 0 0 0 0 0 0 0 15
0.2724 -2.2274 -0.0307 H 0 0 0 0 0 0 0 0 0 0 16
0.3358 2.5357 0.0771 H 0 0 0 0 0 0 0 0 0 0 17
3.9324 -1.0638 -0.0767 O 0 0 0 0 0 0 0 0 0 0 18
2.4690 -2.4786 -0.0861 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0

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15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 15 0 0 0 0
15 19 0 0 0 0
M END
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cis-5-formyluracil.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 V2000
-5.1383 -0.5699 1.0003 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.6866 -1.3385 1.2422 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.7765 0.0871 0.6679 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.1929 -1.2320 -0.7683 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.5394 -1.0854 -1.6662 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.9354 -0.9718 -0.1478 H 0 0 0 0 0 0 0 0 0 0 0 6
0.2445 -0.9937 -0.2394 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5579 -0.6287 -0.0158 C 0 0 0 0 0 0 0 0 0 0 0 8
1.8712 0.7943 0.1331 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7404 1.6302 0.0210 N 0 0 0 0 0 0 0 0 0 0 0 10
-0.5770 1.2663 -0.2059 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.7684 -0.1128 -0.3304 N 0 0 0 0 0 0 0 0 0 0 0 12
2.9785 1.2949 0.3364 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.4990 2.0737 -0.2915 O 0 0 0 0 0 0 0 0 0 0 0 14
2.5455 -1.6987 0.0549 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.0328 -2.0436 -0.3556 H 0 0 0 0 0 0 0 0 0 0 0 16
0.9128 2.6329 0.1176 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.7578 -0.4643 -0.5058 H 0 0 0 0 0 0 0 0 0 0 0 18
3.7565 -1.5773 0.2451 O 0 0 0 0 0 0 0 0 0 0 0 19
2.1007 -2.7136 -0.0856 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
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10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0

M END
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cyanoaceticacid-anion.sdf
COSMOtherm 3D 0
14 11 0 0 0 0 0 0 0 0 V2000
-4.2229 0.4596 -1.2793 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6001 0.0791 -0.5957 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.3134 1.3952 -1.0303 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.5394 -0.6940 0.5347 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.5559 -0.5390 0.3193 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.6489 -0.3449 1.4366 H 0 0 0 0 0 0 0 0 0 0 0 6
2.6399 0.0401 -0.8402 C 0 0 0 0 0 0 0 0 0 0 0 7
2.2580 0.2685 0.5403 C 0 0 0 0 0 0 0 0 0 0 0 8
0.7313 0.0665 0.8450 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0003 -0.3389 -0.1131 O 0 0 0 0 0 0 0 0 0 0 0 10
0.3854 0.3229 2.0213 O 0 0 0 0 0 0 0 0 0 0 0 11
2.9428 -0.1412 -1.9511 N 0 0 0 0 0 0 0 0 0 0 0 12
2.5405 1.2918 0.8290 H 0 0 0 0 0 0 0 0 0 0 0 13
2.8300 -0.4132 1.1884 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
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12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
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8 14 0 0 0 0

M END
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cyanoaceticacid.sdf
COSMOtherm 3D 0
15 12 0 0 0 0 0 0 0 0 V2000
1.2978 3.8757 -0.5318 O 0 0 0 0 0 0 0 0 0 0 0 1
2.1053 3.7973 0.0081 H 0 0 0 0 0 0 0 0 0 0 0 2
1.1862 4.8349 -0.6639 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.8984 2.7366 0.5031 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.0545 3.1717 0.1690 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.8766 2.8210 1.4731 H 0 0 0 0 0 0 0 0 0 0 0 6
0.2690 -2.9507 -0.1632 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7070 -1.9317 -0.5099 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3580 -0.5465 0.0575 C 0 0 0 0 0 0 0 0 0 0 0 9
0.6253 -0.3233 0.7514 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.2673 0.3463 -0.3103 O 0 0 0 0 0 0 0 0 0 0 0 11
1.0442 -3.7751 0.1063 N 0 0 0 0 0 0 0 0 0 0 0 12
-1.6983 -2.2328 -0.1370 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.7915 -1.8633 -1.6054 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.0434 1.3003 0.0689 H 0 0 0 0 0 0 0 0 0 0 0 15

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2 1 0 0 0 0
3 1 0 0 0 0
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6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
11 15 0 0 0 0

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M END

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dichloroaceticacid-anion.sdf

COSMOTHERM 3D

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13 10 0 0 0 0 0 0 0 0 0 V2000
-4.9776 0.9794 -0.7027 O 0 0 0 0 0 0 0 0 0 0 1
-4.3324 0.2755 -0.4069 H 0 0 0 0 0 0 0 0 0 0 2
-4.6393 1.8012 -0.3078 H 0 0 0 0 0 0 0 0 0 0 3
-3.2579 -1.0172 0.0208 O 0 0 0 0 0 0 0 0 0 0 4
-2.2871 -0.7375 -0.0742 H 0 0 0 0 0 0 0 0 0 0 5
-3.3537 -1.2552 0.9600 H 0 0 0 0 0 0 0 0 0 0 6
2.3029 -0.9671 -0.9289 Cl 0 0 0 0 0 0 0 0 0 0 7
1.5303 -0.0610 0.4547 C 0 0 0 0 0 0 0 0 0 0 8
0.0404 -0.4805 0.6320 C 0 0 0 0 0 0 0 0 0 0 9
-0.7362 -0.2699 -0.3456 O 0 0 0 0 0 0 0 0 0 0 10
-0.2196 -0.9877 1.7493 O 0 0 0 0 0 0 0 0 0 0 11
1.6679 1.7409 0.1920 Cl 0 0 0 0 0 0 0 0 0 0 12
2.1277 -0.2868 1.3389 H 0 0 0 0 0 0 0 0 0 0 13

```

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0

```

M END

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dichloroaceticacid.sdf

COSMOTHERM 3D

0

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14 12 0 0 0 0 0 0 0 0 0 V2000
-1.0981 -1.0396 3.4734 O 0 0 0 0 0 0 0 0 0 0 1
-0.8612 -1.9509 3.7236 H 0 0 0 0 0 0 0 0 0 0 2
-1.0971 -1.0285 2.4835 H 0 0 0 0 0 0 0 0 0 0 3
0.8806 0.7000 3.4195 O 0 0 0 0 0 0 0 0 0 0 4
0.1398 0.0383 3.6230 H 0 0 0 0 0 0 0 0 0 0 5
0.6568 1.5213 3.8946 H 0 0 0 0 0 0 0 0 0 0 6
1.3511 -0.7597 -1.8655 Cl 0 0 0 0 0 0 0 0 0 0 7
0.1916 0.4953 -1.2423 C 0 0 0 0 0 0 0 0 0 0 8
0.0408 0.2756 0.2755 C 0 0 0 0 0 0 0 0 0 0 9
-0.7605 -0.5319 0.7426 O 0 0 0 0 0 0 0 0 0 0 10
0.8826 1.0371 0.9333 O 0 0 0 0 0 0 0 0 0 0 11
-1.3958 0.3973 -2.0793 Cl 0 0 0 0 0 0 0 0 0 0 12
0.6277 1.4685 -1.4713 H 0 0 0 0 0 0 0 0 0 0 13
0.8493 0.8874 2.0040 H 0 0 0 0 0 0 0 0 0 0 14

```

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
4 14 0 0 0 0
11 14 0 0 0 0

```

M END

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dimethadione-anion.sdf

COSMOTHERM 3D

0

```

21 19 0 0 0 0 0 0 0 0 0 V2000
-3.8925 0.7602 -0.1031 O 0 0 0 0 0 0 0 0 0 0 1
-3.6721 -0.2057 -0.0592 H 0 0 0 0 0 0 0 0 0 0 2
-2.9979 1.1757 -0.0337 H 0 0 0 0 0 0 0 0 0 0 3
-2.7941 -1.8188 0.0056 O 0 0 0 0 0 0 0 0 0 0 4
-1.8894 -1.3589 0.0373 H 0 0 0 0 0 0 0 0 0 0 5
-2.9039 -2.2214 0.8847 H 0 0 0 0 0 0 0 0 0 0 6
1.8554 0.2152 -0.0113 C 0 0 0 0 0 0 0 0 0 0 7
0.8307 -0.9400 -0.0123 C 0 0 0 0 0 0 0 0 0 0 8
0.9756 1.3907 0.0282 O 0 0 0 0 0 0 0 0 0 0 9
-0.3324 0.9365 0.0442 C 0 0 0 0 0 0 0 0 0 0 10
-0.4316 -0.4250 0.0222 N 0 0 0 0 0 0 0 0 0 0 11
2.7235 0.1995 1.2439 C 0 0 0 0 0 0 0 0 0 0 12
2.6720 0.2456 -1.3004 C 0 0 0 0 0 0 0 0 0 0 13
1.1430 -2.1396 -0.0395 O 0 0 0 0 0 0 0 0 0 0 14
-1.2503 1.7681 0.0763 O 0 0 0 0 0 0 0 0 0 0 15
2.1050 0.2250 2.1518 H 0 0 0 0 0 0 0 0 0 0 16
3.3271 -0.7185 1.2593 H 0 0 0 0 0 0 0 0 0 0 17
3.4011 1.0650 1.2502 H 0 0 0 0 0 0 0 0 0 0 18
2.0172 0.3104 -2.1804 H 0 0 0 0 0 0 0 0 0 0 19
3.2684 -0.6741 -1.3766 H 0 0 0 0 0 0 0 0 0 0 20
3.3546 1.1071 -1.3003 H 0 0 0 0 0 0 0 0 0 0 21

```

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0

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9 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
16 12 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 13 0 0 0 0
20 13 0 0 0 0
13 21 0 0 0 0
M END
$$$$
dimethadione.sdf
COSMOTHERM 3D 0
22 20 0 0 0 0 0 0 0 0 V2000
-4.7085 0.0916 0.9286 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.1609 -0.7480 0.7282 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.4291 0.7436 1.0035 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.8444 0.7939 -0.9198 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.5563 0.5150 -0.2749 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.1480 0.4870 -1.7920 H 0 0 0 0 0 0 0 0 0 0 0 6
1.9779 0.0909 0.2014 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7269 0.9351 -0.0939 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4579 -1.2938 0.1129 O 0 0 0 0 0 0 0 0 0 0 0 9
0.1287 -1.2724 -0.1885 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.2978 0.0435 -0.3060 N 0 0 0 0 0 0 0 0 0 0 0 11
2.4908 0.3296 1.6172 C 0 0 0 0 0 0 0 0 0 0 0 12
3.0436 0.2819 -0.8722 C 0 0 0 0 0 0 0 0 0 0 0 13
0.6632 2.1575 -0.1315 O 0 0 0 0 0 0 0 0 0 0 0 14
-0.5400 -2.2811 -0.3227 O 0 0 0 0 0 0 0 0 0 0 0 15
-1.2985 0.3040 -0.5441 H 0 0 0 0 0 0 0 0 0 0 0 16
1.7051 0.1435 2.3616 H 0 0 0 0 0 0 0 0 0 0 0 17
2.8255 1.3713 1.7123 H 0 0 0 0 0 0 0 0 0 0 0 18
3.3427 -0.3325 1.8211 H 0 0 0 0 0 0 0 0 0 0 0 19
2.6472 0.0523 -1.8704 H 0 0 0 0 0 0 0 0 0 0 0 20
3.3868 1.3249 -0.8618 H 0 0 0 0 0 0 0 0 0 0 0 21
3.9011 -0.3725 -0.6669 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
16 11 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
13 22 0 0 0 0
M END
$$$$
ethanol-anion.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 V2000
-2.1617 -1.2703 -0.2007 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.2549 -0.8172 0.1017 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.2958 -0.9691 -1.1152 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2509 -1.1336 -0.2266 O 0 0 0 0 0 0 0 0 0 0 0 4
1.3206 -0.7377 0.0853 H 0 0 0 0 0 0 0 0 0 0 0 5
2.3973 -0.7624 -1.1130 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.1157 1.8634 -0.6841 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0111 1.1642 0.6804 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0203 -0.2394 0.5970 O 0 0 0 0 0 0 0 0 0 0 0 9
-0.1319 2.9610 -0.5755 H 0 0 0 0 0 0 0 0 0 0 0 10
0.7409 1.5967 -1.3236 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.0361 1.5576 -1.2064 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.8678 1.5034 1.3059 H 0 0 0 0 0 0 0 0 0 0 0 13
0.9009 1.5461 1.1934 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
9 2 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
8 14 0 0 0 0
M END
$$$$
ethanol.sdf
COSMOTHERM 3D 0
15 12 0 0 0 0 0 0 0 0 V2000
-0.9476 3.2338 -0.1529 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.6628 4.1626 -0.2295 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.5882 3.2390 0.5813 H 0 0 0 0 0 0 0 0 0 0 0 3
1.1687 1.5360 0.1937 O 0 0 0 0 0 0 0 0 0 0 0 4

```



```

1
2
3      1.4928    1.6437    1.1051 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    5
4      0.3955    2.1627    0.1166 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    6
5     -0.5730   -3.1000   -0.0145 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    7
6     -0.3860   -1.6347    0.3424 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    8
7      0.6816   -1.0909   -0.4540 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    9
8     -1.3890   -3.5376    0.5795 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    10
9     -0.8253   -3.2142   -1.0793 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    11
10      0.3443   -3.6724    0.1888 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    12
11     -0.1531   -1.5372    1.4194 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    13
12     -1.3261   -1.0812    0.1583 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    14
13      0.8110   -0.1395   -0.1890 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    15

```

```

2  1  0  0  0  0
3  1  0  0  0  0
5  4  0  0  0  0
6  4  0  0  0  0
8  7  0  0  0  0
10 7  0  0  0  0
11 7  0  0  0  0
12 7  0  0  0  0
9  8  0  0  0  0
13 8  0  0  0  0
14 8  0  0  0  0
9 15 0  0  0  0

```

```

M  END
$$$$
fluoroaceticacid-anion.sdf
COSMOTHERM          3D          0

```

```

13 10 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-4.0247    0.5671    0.9417 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    1
-3.3668    0.0990    0.3502 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    2
-3.7785    1.5060    0.8825 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    3
-2.2686   -0.8000   -0.6355 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    4
-1.3091   -0.6722   -0.3080 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    5
-2.2604   -0.4479   -1.5431 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    6
2.6663   -0.1240    1.2920 F    0    0    0    0    0    0    0    0    0    0    0    0    0    0    7
2.4104    0.3370   -0.0270 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    8
0.9728    0.0730   -0.4969 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    9
0.1787   -0.5234    0.2990 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    10
0.7229    0.4867   -1.6602 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    11
3.1161   -0.1738   -0.6982 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    12
2.6098    1.4182   -0.0444 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    13

```

```

2  1  0  0  0  0
3  1  0  0  0  0
5  4  0  0  0  0
6  4  0  0  0  0
8  7  0  0  0  0
9  8  0  0  0  0
12 8  0  0  0  0
10 9  0  0  0  0
11 9  0  0  0  0
8 13 0  0  0  0

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M  END
$$$$
fluoroaceticacid.sdf
COSMOTHERM          3D          0

```

```

14 11 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-0.9030   -0.5983   -3.9105 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    1
-0.5033   -0.8934   -4.7488 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    2
-1.6529   -0.0382   -4.1816 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    3
0.8964    0.6133   -2.3304 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    4
0.7261    1.5721   -2.3363 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    5
0.2046    0.2065   -2.9360 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    6
-0.5896   -0.0853    3.1947 F    0    0    0    0    0    0    0    0    0    0    0    0    0    0    7
0.3182   -0.6009    2.2584 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    8
0.1342    0.0827    0.9103 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    9
0.9860   -0.4126    0.0172 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    10
-0.6908    0.9643    0.7024 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    11
0.1419   -1.6814    2.1572 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    12
1.3407   -0.4289    2.6279 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    13
0.8814    0.0499   -0.9162 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    14

```

```

2  1  0  0  0  0
3  1  0  0  0  0
5  4  0  0  0  0
6  4  0  0  0  0
8  7  0  0  0  0
9  8  0  0  0  0
12 8  0  0  0  0
13 8  0  0  0  0
10 9  0  0  0  0
11 9  0  0  0  0
10 14 0  0  0  0

```

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M  END
$$$$
formicacid-anion.sdf
COSMOTHERM          3D          0

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```

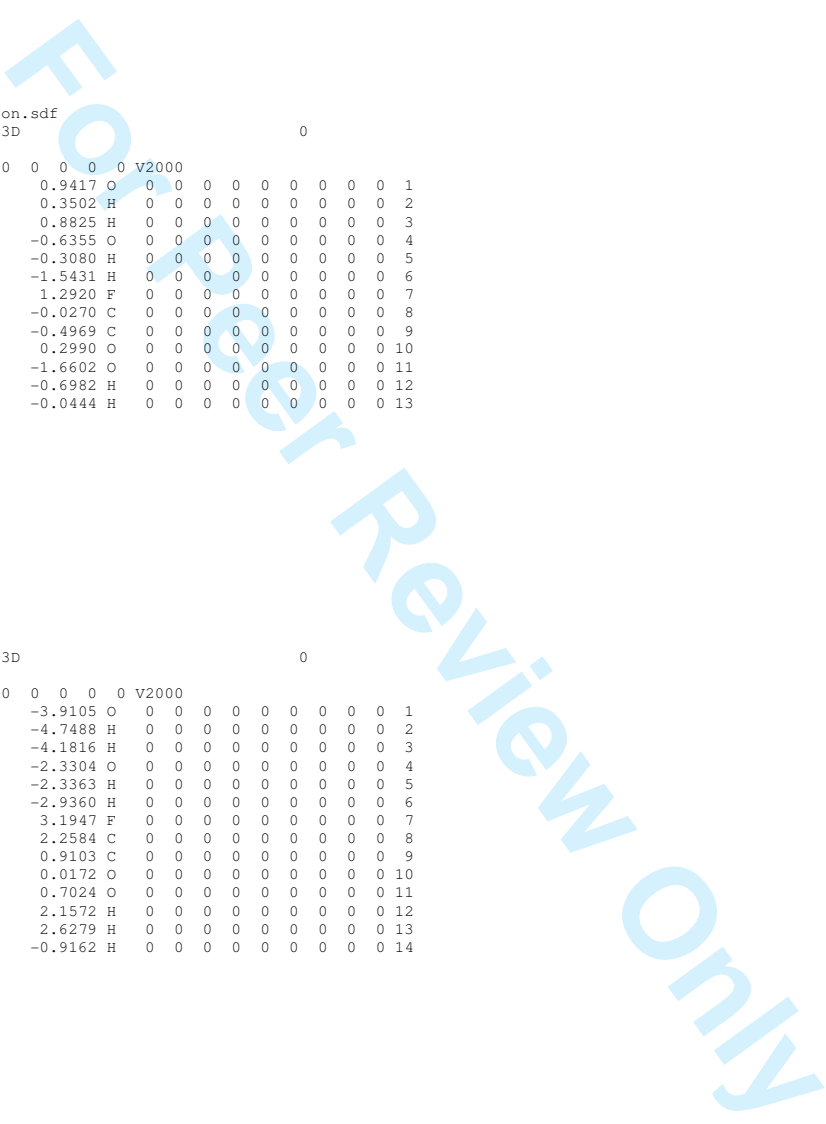
10 7 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-3.2783    0.5122   -0.1965 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    1
-2.4419    0.0481    0.0991 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    2
-3.1212    1.4508    0.0035 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    3
-1.0511   -0.8543    0.5715 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    4
-0.2388   -0.6313   -0.0121 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    5
-0.7706   -0.6063    1.4703 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    6
1.9879    0.2035   -0.3692 C    0    0    0    0    0    0    0    0    0    0    0    0    0    0    7
2.0686    0.4738    0.8537 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    8
1.0017   -0.3293   -0.9858 O    0    0    0    0    0    0    0    0    0    0    0    0    0    0    9
2.8708    0.4489   -1.0168 H    0    0    0    0    0    0    0    0    0    0    0    0    0    0    10

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2  1  0  0  0  0
3  1  0  0  0  0
5  4  0  0  0  0
6  4  0  0  0  0
8  7  0  0  0  0
9  7  0  0  0  0

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7 10 0 0 0 0
M  END
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formicacid.sdf
COSMOtherm      3D              0

11 8 0 0 0 0 0 0 0 0 0 V2000
-3.0716 -0.5713 -0.3489 O 0 0 0 0 0 0 0 0 0 0 1
-2.8136 -1.4068 -0.7796 H 0 0 0 0 0 0 0 0 0 0 2
-3.5079 -0.0583 -1.0539 H 0 0 0 0 0 0 0 0 0 0 3
-1.0579 0.8184 0.7750 O 0 0 0 0 0 0 0 0 0 0 4
-0.9560 0.4752 1.6806 H 0 0 0 0 0 0 0 0 0 0 5
-1.7907 0.2717 0.3577 H 0 0 0 0 0 0 0 0 0 0 6
2.0038 -0.1166 -0.3435 C 0 0 0 0 0 0 0 0 0 0 7
1.1317 0.8542 -0.5960 O 0 0 0 0 0 0 0 0 0 0 8
1.8644 -1.0157 0.4771 O 0 0 0 0 0 0 0 0 0 0 9
2.9030 -0.0155 -0.9810 H 0 0 0 0 0 0 0 0 0 0 10
0.2774 0.7644 -0.0071 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
8 11 0 0 0 0
M  END
$$$$
fumaricacid-anion.sdf
COSMOtherm      3D              0

17 14 0 0 0 0 0 0 0 0 0 V2000
-5.3168 -0.0065 0.1831 O 0 0 0 0 0 0 0 0 0 0 1
-5.4836 -0.4035 -0.6915 H 0 0 0 0 0 0 0 0 0 0 2
-5.7024 0.8871 0.1244 H 0 0 0 0 0 0 0 0 0 0 3
5.3716 0.0431 0.0689 O 0 0 0 0 0 0 0 0 0 0 4
4.4268 0.0276 -0.2879 H 0 0 0 0 0 0 0 0 0 0 5
5.2428 0.0251 1.0331 H 0 0 0 0 0 0 0 0 0 0 6
-0.4858 -0.0124 0.3631 C 0 0 0 0 0 0 0 0 0 0 7
0.5643 -0.0167 -0.4735 C 0 0 0 0 0 0 0 0 0 0 8
2.0035 -0.0174 -0.0001 C 0 0 0 0 0 0 0 0 0 0 9
-1.8879 -0.0043 -0.1228 C 0 0 0 0 0 0 0 0 0 0 10
-2.2256 -0.0142 -1.3077 O 0 0 0 0 0 0 0 0 0 0 11
-2.7688 0.0145 0.8958 O 0 0 0 0 0 0 0 0 0 0 12
2.8765 0.0106 -0.9402 O 0 0 0 0 0 0 0 0 0 0 13
2.2430 -0.0429 1.2374 O 0 0 0 0 0 0 0 0 0 0 14
-0.3262 -0.0120 1.4435 H 0 0 0 0 0 0 0 0 0 0 15
0.4004 -0.0152 -1.5549 H 0 0 0 0 0 0 0 0 0 0 16
-3.7240 0.0231 0.5341 H 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
12 17 0 0 0 0
M  END
$$$$
fumaricacid.sdf
COSMOtherm      3D              0

18 15 0 0 0 0 0 0 0 0 0 V2000
-5.3501 0.0220 0.1214 O 0 0 0 0 0 0 0 0 0 0 1
-5.6451 -0.7885 -0.3334 H 0 0 0 0 0 0 0 0 0 0 2
-5.5944 0.7478 -0.4820 H 0 0 0 0 0 0 0 0 0 0 3
5.3524 0.0227 -0.1246 O 0 0 0 0 0 0 0 0 0 0 4
5.6497 -0.7785 0.3445 H 0 0 0 0 0 0 0 0 0 0 5
5.5949 0.7595 0.4660 H 0 0 0 0 0 0 0 0 0 0 6
-0.5340 -0.0073 0.4072 C 0 0 0 0 0 0 0 0 0 0 7
0.5332 -0.0104 -0.4053 C 0 0 0 0 0 0 0 0 0 0 8
1.9234 -0.0075 0.1301 C 0 0 0 0 0 0 0 0 0 0 9
-1.9242 -0.0061 -0.1288 C 0 0 0 0 0 0 0 0 0 0 10
-2.2060 -0.0081 -1.3261 O 0 0 0 0 0 0 0 0 0 0 11
-2.8320 0.0010 0.8581 O 0 0 0 0 0 0 0 0 0 0 12
2.8303 -0.0003 -0.8578 O 0 0 0 0 0 0 0 0 0 0 13
2.2065 -0.0095 1.3270 O 0 0 0 0 0 0 0 0 0 0 14
-0.4104 -0.0057 1.4919 H 0 0 0 0 0 0 0 0 0 0 15
0.4093 -0.0126 -1.4903 H 0 0 0 0 0 0 0 0 0 0 16
-3.7831 0.0062 0.4736 H 0 0 0 0 0 0 0 0 0 0 17
3.7812 0.0025 -0.4745 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
17 12 0 0 0 0
13 18 0 0 0 0
M  END
$$$$
hypobromousacid-anion.sdf

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COSMOTHERM          3D                      0
      8 4 0 0 0 0 0 0 0 0 0 0 V2000
      -2.0240  2.1367  0.1899 O  0 0 0 0 0 0 0 0 0 0 1
      -1.4680  1.3230 -0.0857 H  0 0 0 0 0 0 0 0 0 0 2
      -1.7394  2.8418 -0.4159 H  0 0 0 0 0 0 0 0 0 0 3
      -2.0269 -2.1576  0.1009 O  0 0 0 0 0 0 0 0 0 0 4
      -1.4731 -1.3258 -0.1235 H  0 0 0 0 0 0 0 0 0 0 5
      -2.4677 -1.9359  0.9385 H  0 0 0 0 0 0 0 0 0 0 6
      -0.7103  0.0008 -0.5668 O  0 0 0 0 0 0 0 0 0 0 7
      1.0435 -0.0073  0.0513 Br 0 0 0 0 0 0 0 0 0 0 8
      2 1 0 0 0 0 0
      3 1 0 0 0 0 0
      5 4 0 0 0 0 0
      6 4 0 0 0 0 0
M  END
$$$$
hypobromousacid.sdf
COSMOTHERM          3D                      0
      9 5 0 0 0 0 0 0 0 0 0 0 V2000
      -4.1529 -0.5471  0.3376 O  0 0 0 0 0 0 0 0 0 0 1
      -4.7221 -0.6901 -0.4403 H  0 0 0 0 0 0 0 0 0 0 2
      -4.7471 -0.1580  1.0051 H  0 0 0 0 0 0 0 0 0 0 3
      -1.9916  1.0009 -0.1253 O  0 0 0 0 0 0 0 0 0 0 4
      -2.8208  0.4510  0.0070 H  0 0 0 0 0 0 0 0 0 0 5
      -2.2355  1.6976 -0.7604 H  0 0 0 0 0 0 0 0 0 0 6
      0.0216 -0.4076 -1.0105 O  0 0 0 0 0 0 0 0 0 0 7
      1.4187 -0.0276  0.1704 Br 0 0 0 0 0 0 0 0 0 0 8
      -0.7576  0.1545 -0.6487 H  0 0 0 0 0 0 0 0 0 0 9
      2 1 0 0 0 0 0
      3 1 0 0 0 0 0
      5 4 0 0 0 0 0
      6 4 0 0 0 0 0
      7 9 0 0 0 0 0
M  END
$$$$
hypochlorousacid-anion.sdf
COSMOTHERM          3D                      0
      8 5 0 0 0 0 0 0 0 0 0 0 V2000
      -1.5920 -0.1786  2.0263 O  0 0 0 0 0 0 0 0 0 0 1
      -0.9748  0.0847  1.2556 H  0 0 0 0 0 0 0 0 0 0 2
      -1.3511  0.4268  2.7479 H  0 0 0 0 0 0 0 0 0 0 3
      -1.3151 -0.0899 -2.2428 O  0 0 0 0 0 0 0 0 0 0 4
      -0.8062  0.1208 -1.3809 H  0 0 0 0 0 0 0 0 0 0 5
      -1.7848 -0.9192 -2.0508 H  0 0 0 0 0 0 0 0 0 0 6
      -0.1047  0.5536 -0.0102 O  0 0 0 0 0 0 0 0 0 0 7
      1.4990 -0.1205  0.0860 Cl 0 0 0 0 0 0 0 0 0 0 8
      2 1 0 0 0 0 0
      3 1 0 0 0 0 0
      5 4 0 0 0 0 0
      6 4 0 0 0 0 0
      7 8 0 0 0 0 0
M  END
$$$$
hypochlorousacid.sdf
COSMOTHERM          3D                      0
      9 6 0 0 0 0 0 0 0 0 0 0 V2000
      -3.3729 -0.5868  0.2226 O  0 0 0 0 0 0 0 0 0 0 1
      -3.6079 -1.0397 -0.6078 H  0 0 0 0 0 0 0 0 0 0 2
      -4.1861 -0.1155  0.4808 H  0 0 0 0 0 0 0 0 0 0 3
      -1.2244  1.0255  0.0316 O  0 0 0 0 0 0 0 0 0 0 4
      -2.0505  0.4548  0.0606 H  0 0 0 0 0 0 0 0 0 0 5
      -1.4464  1.7825 -0.5396 H  0 0 0 0 0 0 0 0 0 0 6
      0.8256 -0.2422 -0.9246 O  0 0 0 0 0 0 0 0 0 0 7
      2.0226 -0.1270  0.3349 Cl 0 0 0 0 0 0 0 0 0 0 8
      0.0186  0.2669 -0.5304 H  0 0 0 0 0 0 0 0 0 0 9
      2 1 0 0 0 0 0
      3 1 0 0 0 0 0
      5 4 0 0 0 0 0
      6 4 0 0 0 0 0
      8 7 0 0 0 0 0
      7 9 0 0 0 0 0
M  END
$$$$
hypoiodousacid-anion.sdf
COSMOTHERM          3D                      0
      8 4 0 0 0 0 0 0 0 0 0 0 V2000
      2.0639 -2.4777  0.1187 O  0 0 0 0 0 0 0 0 0 0 1
      1.2657 -1.8848 -0.1403 H  0 0 0 0 0 0 0 0 0 0 2
      1.8698 -2.7609  1.0282 H  0 0 0 0 0 0 0 0 0 0 3
      -2.0581 -2.4869  0.1216 O  0 0 0 0 0 0 0 0 0 0 4
      -1.2635 -1.8891 -0.1374 H  0 0 0 0 0 0 0 0 0 0 5
      -1.8323 -2.8190  1.0069 H  0 0 0 0 0 0 0 0 0 0 6
      -0.0012 -1.0804 -0.6338 O  0 0 0 0 0 0 0 0 0 0 7
      -0.0009  0.8364  0.0356 I  0 0 0 0 0 0 0 0 0 0 8
      2 1 0 0 0 0 0
      3 1 0 0 0 0 0
      5 4 0 0 0 0 0
      6 4 0 0 0 0 0
M  END
$$$$
hypoiodousacid.sdf
COSMOTHERM          3D                      0
      9 5 0 0 0 0 0 0 0 0 0 0 V2000
      -4.5893 -0.1138  0.7132 O  0 0 0 0 0 0 0 0 0 0 1
      -5.1147 -0.8519  0.3540 H  0 0 0 0 0 0 0 0 0 0 2
      -5.2353  0.6049  0.8394 H  0 0 0 0 0 0 0 0 0 0 3
      -2.5001  0.6175 -0.8413 O  0 0 0 0 0 0 0 0 0 0 4
      -3.3022  0.3375 -0.3086 H  0 0 0 0 0 0 0 0 0 0 5
      -2.7950  0.6296 -1.7692 H  0 0 0 0 0 0 0 0 0 0 6

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-0.4824 -1.0592 -0.5618 O 0 0 0 0 0 0 0 0 0 0 0 0 7
1.0952 0.0674 0.0992 I 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2478 -0.3927 -0.6600 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 9 0 0 0 0
M END
$$$$
hypophosphorousacid-anion.sdf
COSMOtherm 3D 0
11 8 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.2749 -2.0941 0.0517 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.3437 -1.0900 -0.0448 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.5930 -2.4510 -0.7961 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.5468 -1.8908 0.0906 O 0 0 0 0 0 0 0 0 0 0 0 0 4
1.5329 -0.9037 -0.0433 H 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5819 -2.1144 0.0761 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.3089 0.8484 -0.2797 O 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0793 1.3995 0.1483 P 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.3558 0.5642 -0.1704 O 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.0573 1.6788 1.5591 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.2533 2.7052 -0.4229 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
8 11 0 0 0 0
M END
$$$$
hypophosphorousacid.sdf
COSMOtherm 3D 0
12 9 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-3.6294 0.2901 0.6882 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.4726 -0.1838 0.5682 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.8380 1.2164 0.4687 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.6148 -0.7541 -0.7512 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.9324 -0.9284 -1.6554 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.3952 -0.3548 -0.2584 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.9564 -1.1818 -0.9301 H 0 0 0 0 0 0 0 0 0 0 0 0 7
1.7917 0.0072 -0.1585 P 0 0 0 0 0 0 0 0 0 0 0 0 8
2.8019 0.8979 -0.6131 H 0 0 0 0 0 0 0 0 0 0 0 0 9
1.8166 -0.2623 1.3448 O 0 0 0 0 0 0 0 0 0 0 0 0 10
0.4788 0.7372 -0.7743 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.3727 0.1433 -0.7655 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
11 12 0 0 0 0
M END
$$$$
iodoaceticacid-anion.sdf
COSMOtherm 3D 0
13 9 0 0 0 0 0 0 0 0 0 0 0 0 V2000
1.8087 5.3595 0.5575 O 0 0 0 0 0 0 0 0 0 0 0 0 1
1.0596 4.8864 0.0933 H 0 0 0 0 0 0 0 0 0 0 0 0 2
1.5142 5.4326 1.4814 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1800 4.0882 -0.8141 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2032 3.0839 -0.6383 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.0636 4.4000 -0.5502 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.3701 -1.7677 -0.0153 I 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.3919 -0.4782 0.3699 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2348 1.0202 0.0716 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.1517 1.4791 -0.4018 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.2834 1.6638 0.3498 O 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.6196 -0.6394 1.4278 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.1843 -0.9124 -0.2470 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 13 0 0 0 0
M END
$$$$
iodoaceticacid.sdf
COSMOtherm 3D 0
14 10 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-1.0963 4.4820 0.5820 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.4573 4.5938 1.4795 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.2847 3.5393 0.3371 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.4709 3.8353 0.4181 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.5640 4.2607 0.5417 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.9840 4.4438 -0.1440 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.0255 -1.7225 0.2037 I 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.4033 -0.1853 -1.3108 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.2067 1.1837 -0.7071 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.0532 1.5862 -0.7215 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.1624 1.8360 -0.2675 O 0 0 0 0 0 0 0 0 0 0 0 0 11
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2
3     -1.4430  -0.3479  -1.5973 H  0  0  0  0  0  0  0  0  0  0  12
4     0.2917  -0.3886  -2.1283 H  0  0  0  0  0  0  0  0  0  0  13
5     1.1879   2.5292  -0.2689 H  0  0  0  0  0  0  0  0  0  0  14
6     2  1  0  0  0  0  0
7     3  1  0  0  0  0  0
8     5  4  0  0  0  0  0
9     6  4  0  0  0  0  0
10    9  8  0  0  0  0  0
11   12  8  0  0  0  0  0
12   13  8  0  0  0  0  0
13   10  9  0  0  0  0  0
14   11  9  0  0  0  0  0
15   10 14  0  0  0  0  0
16 M  END
17 $$$$
18 maleicacid-anion.sdf
19 COSMOTHERM 3D 0
20
21 17 15 0 0 0 0 0 0 0 0 0 0 V2000
22 -5.5320 -0.0595 -0.8906 O 0 0 0 0 0 0 0 0 0 0 0 0 1
23 -4.7551 0.2234 -0.3311 H 0 0 0 0 0 0 0 0 0 0 0 0 2
24 -5.2534 0.1277 -1.8032 H 0 0 0 0 0 0 0 0 0 0 0 0 3
25 -3.4573 0.6821  0.7408 O 0 0 0 0 0 0 0 0 0 0 0 0 4
26 -2.6348 0.1140  0.6042 H 0 0 0 0 0 0 0 0 0 0 0 0 5
27 -3.1614 1.5933  0.5692 H 0 0 0 0 0 0 0 0 0 0 0 0 6
28 2.2582 -1.0935 -0.0804 C 0 0 0 0 0 0 0 0 0 0 0 0 7
29 0.9450 -1.3508  0.1004 C 0 0 0 0 0 0 0 0 0 0 0 0 8
30 3.0017  0.2041 -0.1890 C 0 0 0 0 0 0 0 0 0 0 0 0 9
31 -0.2184 -0.4102  0.2481 C 0 0 0 0 0 0 0 0 0 0 0 0 10
32 2.3362  1.3438 -0.1299 O 0 0 0 0 0 0 0 0 0 0 0 0 11
33 4.2328  0.1752 -0.3354 O 0 0 0 0 0 0 0 0 0 0 0 0 12
34 -1.3492 -0.9444  0.4182 O 0 0 0 0 0 0 0 0 0 0 0 0 13
35 -0.0332  0.8643  0.1977 O 0 0 0 0 0 0 0 0 0 0 0 0 14
36 2.9280 -1.9529 -0.1603 H 0 0 0 0 0 0 0 0 0 0 0 0 15
37 0.6481 -2.4012  0.1516 H 0 0 0 0 0 0 0 0 0 0 0 0 16
38 1.2518  1.1574  0.0164 H 0 0 0 0 0 0 0 0 0 0 0 0 17
39
40 2  1  0  0  0  0  0
41 3  1  0  0  0  0  0
42 5  4  0  0  0  0  0
43 6  4  0  0  0  0  0
44 8  7  0  0  0  0  0
45 9  7  0  0  0  0  0
46 15  7  0  0  0  0  0
47 10  8  0  0  0  0  0
48 16  8  0  0  0  0  0
49 11  9  0  0  0  0  0
50 12  9  0  0  0  0  0
51 13 10  0  0  0  0  0
52 14 10  0  0  0  0  0
53 11 17  0  0  0  0  0
54 14 17  0  0  0  0  0
55 M  END
56 $$$$
57 maleicacid.sdf
58 COSMOTHERM 3D 0
59
60 18 17 0 0 0 0 0 0 0 0 0 0 V2000
61 -1.4918 -4.3759  0.7998 O 0 0 0 0 0 0 0 0 0 0 0 0 1
62 -1.8234 -5.2489  0.5205 H 0 0 0 0 0 0 0 0 0 0 0 0 2
63 -2.2776 -3.7998  0.7798 H 0 0 0 0 0 0 0 0 0 0 0 0 3
64 0.5719 -3.5288 -0.6629 O 0 0 0 0 0 0 0 0 0 0 0 0 4
65 0.3344 -3.5624 -1.6071 H 0 0 0 0 0 0 0 0 0 0 0 0 5
66 -0.2442 -3.8398 -0.1573 H 0 0 0 0 0 0 0 0 0 0 0 0 6
67 1.3753  0.9963  0.4119 C 0 0 0 0 0 0 0 0 0 0 0 0 7
68 0.8769  2.2499  0.4397 C 0 0 0 0 0 0 0 0 0 0 0 0 8
69 0.7268 -0.2541 -0.0598 C 0 0 0 0 0 0 0 0 0 0 0 0 9
70 -0.4506  2.8129  0.0283 C 0 0 0 0 0 0 0 0 0 0 0 0 10
71 -0.4307 -0.3175 -0.5286 O 0 0 0 0 0 0 0 0 0 0 0 0 11
72 1.5047 -1.3060  0.0666 O 0 0 0 0 0 0 0 0 0 0 0 0 12
73 -0.6575  4.0193  0.1717 O 0 0 0 0 0 0 0 0 0 0 0 0 13
74 -1.3881  2.0164 -0.4841 O 0 0 0 0 0 0 0 0 0 0 0 0 14
75 2.3926  0.8530  0.7809 H 0 0 0 0 0 0 0 0 0 0 0 0 15
76 1.5323  3.0298  0.8318 H 0 0 0 0 0 0 0 0 0 0 0 0 16
77 1.0346 -2.2034 -0.2698 H 0 0 0 0 0 0 0 0 0 0 0 0 17
78 -1.0543  1.0349 -0.5322 H 0 0 0 0 0 0 0 0 0 0 0 0 18
79
80 2  1  0  0  0  0  0
81 3  1  0  0  0  0  0
82 5  4  0  0  0  0  0
83 6  4  0  0  0  0  0
84 17  4  0  0  0  0  0
85 8  7  0  0  0  0  0
86 9  7  0  0  0  0  0
87 15  7  0  0  0  0  0
88 10  8  0  0  0  0  0
89 16  8  0  0  0  0  0
90 11  9  0  0  0  0  0
91 12  9  0  0  0  0  0
92 13 10  0  0  0  0  0
93 14 10  0  0  0  0  0
94 17 12  0  0  0  0  0
95 11 18  0  0  0  0  0
96 14 18  0  0  0  0  0
97 M  END
98 $$$$
99 mandelicacid-anion.sdf
100 COSMOTHERM 3D 0
101
102 24 22 0 0 0 0 0 0 0 0 0 0 V2000
103 -2.5534 -4.5896 -0.3173 O 0 0 0 0 0 0 0 0 0 0 0 0 1
104 -1.5905 -4.3335 -0.2303 H 0 0 0 0 0 0 0 0 0 0 0 0 2
105 -2.9581 -3.8522 -0.8051 H 0 0 0 0 0 0 0 0 0 0 0 0 3
106 0.0816 -3.9628  0.0195 O 0 0 0 0 0 0 0 0 0 0 0 0 4
107 0.2152 -2.9851  0.2730 H 0 0 0 0 0 0 0 0 0 0 0 0 5
108 0.5992 -4.0778 -0.7967 H 0 0 0 0 0 0 0 0 0 0 0 0 6
109 -2.1092  2.9804 -0.3528 C 0 0 0 0 0 0 0 0 0 0 0 0 7

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0.0122  -1.6522  0.2832 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
-0.0025  -0.4962 -0.5195 O  0  0  0  0  0  0  0  0  0  0  0  0  0  8
-0.6527  -1.5679  1.1723 H  0  0  0  0  0  0  0  0  0  0  0  0  0  9
-0.3202  -2.5594 -0.2678 H  0  0  0  0  0  0  0  0  0  0  0  0  0  10
  1.0286  -1.8789  0.6725 H  0  0  0  0  0  0  0  0  0  0  0  0  0  11
2  1  0  0  0  0  0  0
3  1  0  0  0  0  0  0
8  2  0  0  0  0  0  0
5  4  0  0  0  0  0  0
6  4  0  0  0  0  0  0
8  5  0  0  0  0  0  0
8  7  0  0  0  0  0  0
9  7  0  0  0  0  0  0
10 7  0  0  0  0  0  0
7 11 0  0  0  0  0  0

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M  END
$$$$
methanol.sdf
COSMOtherm          3D                      0
12 9 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-2.6446  0.7126  0.1548 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-3.5414  0.3379  0.2246 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-2.7093  1.3537 -0.5761 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-0.7133 -1.1887 -0.2139 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
-0.7567 -1.4843 -1.1401 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-1.4388 -0.5086 -0.1233 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
  2.1603  0.8104 -0.3368 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
  1.7820 -0.2862  0.5048 O  0  0  0  0  0  0  0  0  0  0  0  0  0  8
  3.1612  1.1405 -0.0265 H  0  0  0  0  0  0  0  0  0  0  0  0  0  9
  1.4710  1.6681 -0.2398 H  0  0  0  0  0  0  0  0  0  0  0  0  0  10
  2.2078  0.5220 -1.4019 H  0  0  0  0  0  0  0  0  0  0  0  0  0  11
  0.8765 -0.5868  0.2206 H  0  0  0  0  0  0  0  0  0  0  0  0  0  12
2  1  0  0  0  0  0  0
3  1  0  0  0  0  0  0
5  4  0  0  0  0  0  0
6  4  0  0  0  0  0  0
8  7  0  0  0  0  0  0
9  7  0  0  0  0  0  0
10 7  0  0  0  0  0  0
11 7  0  0  0  0  0  0
8 12 0  0  0  0  0  0

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M  END
$$$$
methylthiouracil-anion.sdf
COSMOtherm          3D                      0
20 18 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-4.5520  0.8673  1.0900 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-3.9097  0.4665  0.4342 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-4.0861  0.8260  1.9424 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-2.8641 -0.1917 -0.7668 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
-1.9148  0.1464 -0.6299 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-2.7134 -1.1490 -0.6125 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
  0.3883 -0.8643 -0.0902 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
  1.7378 -0.8684  0.2021 N  0  0  0  0  0  0  0  0  0  0  0  0  0  8
  2.5625  0.2683  0.2758 C  0  0  0  0  0  0  0  0  0  0  0  0  0  9
  1.8614  1.4908  0.0146 C  0  0  0  0  0  0  0  0  0  0  0  0  0  10
  0.5108  1.4655 -0.2763 C  0  0  0  0  0  0  0  0  0  0  0  0  0  11
-0.2210  0.3085 -0.3309 N  0  0  0  0  0  0  0  0  0  0  0  0  0  12
  3.7756  0.1361  0.5482 O  0  0  0  0  0  0  0  0  0  0  0  0  0  13
-0.4468 -2.3825 -0.1304 S  0  0  0  0  0  0  0  0  0  0  0  0  0  14
  2.4183  2.4258  0.0498 H  0  0  0  0  0  0  0  0  0  0  0  0  0  15
  2.1795 -1.7717  0.3799 H  0  0  0  0  0  0  0  0  0  0  0  0  0  16
-0.2583  2.7261 -0.5581 C  0  0  0  0  0  0  0  0  0  0  0  0  0  17
-1.0923  2.8298  0.1525 H  0  0  0  0  0  0  0  0  0  0  0  0  0  18
  0.3812  3.6137 -0.4847 H  0  0  0  0  0  0  0  0  0  0  0  0  0  19
-0.6962  2.6869 -1.5671 H  0  0  0  0  0  0  0  0  0  0  0  0  0  20
2  1  0  0  0  0  0  0
3  1  0  0  0  0  0  0
5  4  0  0  0  0  0  0
6  4  0  0  0  0  0  0
8  7  0  0  0  0  0  0
12 7  0  0  0  0  0  0
14 7  0  0  0  0  0  0
9  8  0  0  0  0  0  0
16 8  0  0  0  0  0  0
10 9  0  0  0  0  0  0
13 9  0  0  0  0  0  0
11 10 0  0  0  0  0  0
15 10 0  0  0  0  0  0
12 11 0  0  0  0  0  0
17 11 0  0  0  0  0  0
18 17 0  0  0  0  0  0
19 17 0  0  0  0  0  0
17 20 0  0  0  0  0  0

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M  END
$$$$
methylthiouracil.sdf
COSMOtherm          3D                      0
21 19 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-4.6676  1.0172 -0.7490 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-4.3496  1.9383 -0.7447 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-5.4383  1.0268 -0.1526 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-2.7913 -0.8269  0.0031 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
-3.4683 -0.1320 -0.2361 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-2.5923 -0.6839  0.9554 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
  0.4055 -0.0810  0.9003 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
  1.7442  0.1910  0.9331 N  0  0  0  0  0  0  0  0  0  0  0  0  0  8
  2.6153  0.2780 -0.1796 C  0  0  0  0  0  0  0  0  0  0  0  0  0  9
  1.9682  0.0467 -1.4460 C  0  0  0  0  0  0  0  0  0  0  0  0  0  10
  0.6285 -0.2243 -1.5077 C  0  0  0  0  0  0  0  0  0  0  0  0  0  11
-0.1153 -0.2796 -0.3459 N  0  0  0  0  0  0  0  0  0  0  0  0  0  12
  3.8139  0.5332  0.0055 O  0  0  0  0  0  0  0  0  0  0  0  0  0  13

```

1
2
3 -0.5363 -0.1675 2.3161 S 0 0 0 0 0 0 0 0 0 14
4 2.5700 0.0933 -2.3505 H 0 0 0 0 0 0 0 0 0 15
5 2.1621 0.3446 1.8524 H 0 0 0 0 0 0 0 0 0 16
6 -1.1495 -0.4842 -0.3858 H 0 0 0 0 0 0 0 0 0 17
7 -0.1205 -0.4737 -2.7782 C 0 0 0 0 0 0 0 0 0 18
8 -0.9138 0.2769 -2.9127 H 0 0 0 0 0 0 0 0 0 19
9 0.5558 -0.4268 -3.6381 H 0 0 0 0 0 0 0 0 0 20
10 -0.5994 -1.4639 -2.7565 H 0 0 0 0 0 0 0 0 0 21
11 2 1 0 0 0 0
12 3 1 0 0 0 0
13 5 4 0 0 0 0
14 6 4 0 0 0 0
15 8 7 0 0 0 0
16 12 7 0 0 0 0
17 14 7 0 0 0 0
18 9 8 0 0 0 0
19 16 8 0 0 0 0
20 10 9 0 0 0 0
21 13 9 0 0 0 0
22 11 10 0 0 0 0
23 15 10 0 0 0 0
24 12 11 0 0 0 0
25 18 11 0 0 0 0
26 17 12 0 0 0 0
27 19 18 0 0 0 0
28 20 18 0 0 0 0
29 18 21 0 0 0 0
30 M END
31 \$\$\$
32 n-pentanoicacid-anion.sdf
33 COSMOTHERM 3D 0
34
35 22 19 0 0 0 0 0 0 0 0 0 V2000
36 -2.9306 -1.9272 0.0832 O 0 0 0 0 0 0 0 0 0 0 1
37 -1.9338 -1.8004 0.0198 H 0 0 0 0 0 0 0 0 0 0 2
38 -3.2889 -1.4340 -0.6741 H 0 0 0 0 0 0 0 0 0 0 3
39 1.3840 -3.8960 0.1301 O 0 0 0 0 0 0 0 0 0 0 4
40 0.7819 -3.0891 0.0683 H 0 0 0 0 0 0 0 0 0 0 5
41 2.2734 -3.5048 0.0788 H 0 0 0 0 0 0 0 0 0 0 6
42 0.3466 4.4869 0.1352 C 0 0 0 0 0 0 0 0 0 0 7
43 -0.4530 3.1901 -0.0357 C 0 0 0 0 0 0 0 0 0 0 8
44 0.4187 1.9297 0.0443 C 0 0 0 0 0 0 0 0 0 0 9
45 -0.3826 0.6374 -0.1223 C 0 0 0 0 0 0 0 0 0 0 10
46 0.4366 -0.6624 -0.0828 C 0 0 0 0 0 0 0 0 0 0 11
47 1.6902 -0.6240 -0.1191 O 0 0 0 0 0 0 0 0 0 0 12
48 -0.2514 -1.7591 -0.0235 O 0 0 0 0 0 0 0 0 0 0 13
49 -0.3027 5.3730 0.0734 H 0 0 0 0 0 0 0 0 0 0 14
50 0.8558 4.5125 1.1115 H 0 0 0 0 0 0 0 0 0 0 15
51 1.1182 4.5830 -0.6450 H 0 0 0 0 0 0 0 0 0 0 16
52 -0.9785 3.2066 -1.0063 H 0 0 0 0 0 0 0 0 0 0 17
53 -1.2401 3.1388 0.7369 H 0 0 0 0 0 0 0 0 0 0 18
54 0.9464 1.9106 1.0129 H 0 0 0 0 0 0 0 0 0 0 19
55 1.2040 1.9736 -0.7284 H 0 0 0 0 0 0 0 0 0 0 20
56 -0.9197 0.6481 -1.0877 H 0 0 0 0 0 0 0 0 0 0 21
57 -1.1685 0.5643 0.6479 H 0 0 0 0 0 0 0 0 0 0 22
58 2 1 0 0 0 0
59 3 1 0 0 0 0
60 5 4 0 0 0 0
61 6 4 0 0 0 0
62 8 7 0 0 0 0
63 14 7 0 0 0 0
64 15 7 0 0 0 0
65 16 7 0 0 0 0
66 9 8 0 0 0 0
67 17 8 0 0 0 0
68 18 8 0 0 0 0
69 10 9 0 0 0 0
70 19 9 0 0 0 0
71 20 9 0 0 0 0
72 11 10 0 0 0 0
73 21 10 0 0 0 0
74 12 11 0 0 0 0
75 13 11 0 0 0 0
76 10 22 0 0 0 0
77 M END
78 \$\$\$
79 n-pentanoicacid.sdf
80 COSMOTHERM 3D 0
81
82 23 20 0 0 0 0 0 0 0 0 0 V2000
83 -1.4234 -0.5616 -4.6492 O 0 0 0 0 0 0 0 0 0 0 1
84 -1.2167 -1.1904 -5.3647 H 0 0 0 0 0 0 0 0 0 0 2
85 -1.9819 0.1141 -5.0749 H 0 0 0 0 0 0 0 0 0 0 3
86 0.8426 0.4125 -3.5302 O 0 0 0 0 0 0 0 0 0 0 4
87 0.8381 1.3808 -3.6325 H 0 0 0 0 0 0 0 0 0 0 5
88 -0.0098 0.0941 -3.9524 H 0 0 0 0 0 0 0 0 0 0 6
89 -0.8521 0.0674 4.8261 C 0 0 0 0 0 0 0 0 0 0 7
90 0.1163 -0.3977 3.7332 C 0 0 0 0 0 0 0 0 0 0 8
91 -0.2646 0.1158 2.3383 C 0 0 0 0 0 0 0 0 0 0 9
92 0.7025 -0.3608 1.2544 C 0 0 0 0 0 0 0 0 0 0 10
93 0.3785 0.1362 -0.1407 C 0 0 0 0 0 0 0 0 0 0 11
94 -0.5397 0.9075 -0.4113 O 0 0 0 0 0 0 0 0 0 0 12
95 1.2185 -0.3595 -1.0646 O 0 0 0 0 0 0 0 0 0 0 13
96 -0.5530 -0.3107 5.8151 H 0 0 0 0 0 0 0 0 0 0 14
97 -0.8867 1.1665 4.8841 H 0 0 0 0 0 0 0 0 0 0 15
98 -1.8753 -0.2883 4.6270 H 0 0 0 0 0 0 0 0 0 0 16
99 0.1528 -1.5005 3.7175 H 0 0 0 0 0 0 0 0 0 0 17
100 1.1382 -0.0601 3.9775 H 0 0 0 0 0 0 0 0 0 0 18
101 -0.2922 1.2176 2.3461 H 0 0 0 0 0 0 0 0 0 0 19
102 -1.2860 -0.2165 2.0899 H 0 0 0 0 0 0 0 0 0 0 20
103 0.7398 -1.4622 1.2149 H 0 0 0 0 0 0 0 0 0 0 21
104 1.7340 -0.0416 1.4822 H 0 0 0 0 0 0 0 0 0 0 22
105 0.9852 -0.0007 -2.0022 H 0 0 0 0 0 0 0 0 0 0 23
106 2 1 0 0 0 0
107 3 1 0 0 0 0

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5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
10 9 0 0 0 0
19 9 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
13 23 0 0 0 0

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M END

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nitroaceticacid-anion.sdf

COSMOTHERM 3D

0

```

15 12 0 0 0 0 0 0 0 0 0 V2000
-4.4766 -0.3355 1.4496 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.9128 -0.0009 0.6957 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5251 -1.2962 1.3078 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.9446 0.7001 -0.5656 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.9593 0.5091 -0.4213 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.1490 0.3151 -1.4358 H 0 0 0 0 0 0 0 0 0 0 0 6
0.3333 -0.1523 -1.0344 C 0 0 0 0 0 0 0 0 0 0 0 7
1.8656 -0.3766 -0.7708 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3638 0.2897 -0.0745 O 0 0 0 0 0 0 0 0 0 0 0 9
-0.0214 -0.4493 -2.1964 O 0 0 0 0 0 0 0 0 0 0 0 10
2.2533 -0.0038 0.6191 N 0 0 0 0 0 0 0 0 0 0 0 11
2.5820 1.1722 0.8383 O 0 0 0 0 0 0 0 0 0 0 0 12
2.1674 -0.8725 1.5012 O 0 0 0 0 0 0 0 0 0 0 0 13
2.1060 -1.4357 -0.9050 H 0 0 0 0 0 0 0 0 0 0 0 14
2.4482 0.2507 -1.4524 H 0 0 0 0 0 0 0 0 0 0 0 15

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
8 15 0 0 0 0

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M END

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nitroaceticacid.sdf

COSMOTHERM 3D

0

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16 14 0 0 0 0 0 0 0 0 0 V2000
1.4238 4.2127 0.1637 O 0 0 0 0 0 0 0 0 0 0 0 1
1.3770 5.1668 0.3582 H 0 0 0 0 0 0 0 0 0 0 0 2
2.0406 4.1481 -0.5881 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.9991 3.1659 -0.2609 O 0 0 0 0 0 0 0 0 0 0 0 4
-1.2353 3.2805 -1.1991 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.0805 3.5667 -0.1534 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.4398 -0.1134 0.0394 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7106 -1.4870 0.6707 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.2509 0.7877 0.5653 O 0 0 0 0 0 0 0 0 0 0 0 9
0.4095 0.0799 -0.8195 O 0 0 0 0 0 0 0 0 0 0 0 10
0.2205 -2.5089 0.0823 N 0 0 0 0 0 0 0 0 0 0 0 11
1.3102 -2.6783 0.6396 O 0 0 0 0 0 0 0 0 0 0 0 12
-0.1441 -3.0930 -0.9430 O 0 0 0 0 0 0 0 0 0 0 0 13
-0.5307 -1.4545 1.7500 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.7359 -1.8095 0.4585 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.0853 1.7536 0.1614 H 0 0 0 0 0 0 0 0 0 0 0 16

```

```

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
4 16 0 0 0 0
9 16 0 0 0 0

```

M END

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nitromethane-anion.sdf

COSMOTHERM 3D

0

```

12 9 0 0 0 0 0 0 0 0 0 V2000
-3.6863 0.4711 -0.5248 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8901 0.0898 -0.0514 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5125 1.4271 -0.5613 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.5699 -0.6739 0.7442 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.7103 -0.6086 0.1948 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.3386 -0.2084 1.5677 H 0 0 0 0 0 0 0 0 0 0 0 6
2.7580 0.2315 -0.6599 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5786 0.0543 -0.0799 N 0 0 0 0 0 0 0 0 0 0 0 8
0.6056 -0.5628 -0.7395 O 0 0 0 0 0 0 0 0 0 0 0 9
1.3259 0.4623 1.1241 O 0 0 0 0 0 0 0 0 0 0 0 10
3.5305 0.7383 -0.0907 H 0 0 0 0 0 0 0 0 0 0 0 11
2.8923 -0.1364 -1.6715 H 0 0 0 0 0 0 0 0 0 0 0 12

```

2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 6 4 0 0 0 0
 8 7 0 0 0 0
 11 7 0 0 0 0
 9 8 0 0 0 0
 10 8 0 0 0 0
 7 12 0 0 0 0
 M END
 \$\$\$
 nitromethane.sdf
 COSMOTHERM 3D 0
 13 10 0 0 0 0 0 0 0 0 V2000
 -0.9268 3.4864 0.3990 O 0 0 0 0 0 0 0 0 0 0 0 1
 -0.1707 2.9020 0.1267 H 0 0 0 0 0 0 0 0 0 0 0 2
 -1.5665 3.4103 -0.3294 H 0 0 0 0 0 0 0 0 0 0 0 3
 1.2558 1.9142 -0.2648 O 0 0 0 0 0 0 0 0 0 0 0 4
 1.5552 2.0585 -1.1798 H 0 0 0 0 0 0 0 0 0 0 0 5
 1.0903 0.9447 -0.2016 H 0 0 0 0 0 0 0 0 0 0 0 6
 -0.2301 -2.9258 0.3826 C 0 0 0 0 0 0 0 0 0 0 0 7
 -0.0962 -1.4925 -0.0341 N 0 0 0 0 0 0 0 0 0 0 0 8
 -1.0414 -0.9694 -0.6238 O 0 0 0 0 0 0 0 0 0 0 0 9
 0.9642 -0.9029 0.2434 O 0 0 0 0 0 0 0 0 0 0 0 10
 0.7016 -3.2376 0.8570 H 0 0 0 0 0 0 0 0 0 0 0 11
 -1.0800 -2.9767 1.0723 H 0 0 0 0 0 0 0 0 0 0 0 12
 -0.4482 -3.5031 -0.5219 H 0 0 0 0 0 0 0 0 0 0 0 13
 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 6 4 0 0 0 0
 8 7 0 0 0 0
 11 7 0 0 0 0
 12 7 0 0 0 0
 9 8 0 0 0 0
 10 8 0 0 0 0
 7 13 0 0 0 0
 M END
 \$\$\$
 nitrousacid-anion.sdf
 COSMOTHERM 3D 0
 9 6 0 0 0 0 0 0 0 0 V2000
 -3.3778 0.3621 -0.2992 O 0 0 0 0 0 0 0 0 0 0 0 1
 -2.5144 0.0479 0.0940 H 0 0 0 0 0 0 0 0 0 0 0 2
 -3.1615 1.2174 -0.7082 H 0 0 0 0 0 0 0 0 0 0 0 3
 1.0076 -0.3769 -0.9351 O 0 0 0 0 0 0 0 0 0 0 0 4
 2.0871 0.1266 -0.4477 N 0 0 0 0 0 0 0 0 0 0 0 5
 2.0325 0.4720 0.7623 O 0 0 0 0 0 0 0 0 0 0 0 6
 -0.8178 -0.1437 1.6094 H 0 0 0 0 0 0 0 0 0 0 0 7
 -1.0641 -0.6080 0.7894 O 0 0 0 0 0 0 0 0 0 0 0 8
 -0.2579 -0.4864 0.1882 H 0 0 0 0 0 0 0 0 0 0 0 9
 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 6 5 0 0 0 0
 8 7 0 0 0 0
 8 9 0 0 0 0
 M END
 \$\$\$
 nitrousacid.sdf
 COSMOTHERM 3D 0
 10 7 0 0 0 0 0 0 0 0 V2000
 -3.0404 -0.9064 -0.1570 O 0 0 0 0 0 0 0 0 0 0 0 1
 -2.9357 -1.6373 -0.4792 H 0 0 0 0 0 0 0 0 0 0 0 2
 -3.9792 -0.6544 0.0847 H 0 0 0 0 0 0 0 0 0 0 0 3
 -1.3644 1.1540 -0.2311 O 0 0 0 0 0 0 0 0 0 0 0 4
 1.0556 0.6804 0.4947 O 0 0 0 0 0 0 0 0 0 0 0 5
 1.5279 -0.3469 -0.3148 N 0 0 0 0 0 0 0 0 0 0 0 6
 2.6595 -0.6488 -0.0489 O 0 0 0 0 0 0 0 0 0 0 0 7
 -2.0024 0.3817 -0.1415 H 0 0 0 0 0 0 0 0 0 0 0 8
 -1.4433 1.4605 -1.1521 H 0 0 0 0 0 0 0 0 0 0 0 9
 0.0775 0.8395 0.1620 H 0 0 0 0 0 0 0 0 0 0 0 10
 2 1 0 0 0 0
 3 1 0 0 0 0
 8 4 0 0 0 0
 9 4 0 0 0 0
 6 5 0 0 0 0
 7 6 0 0 0 0
 5 10 0 0 0 0
 M END
 \$\$\$
 oh.sdf
 COSMOTHERM 3D 0
 8 7 0 0 0 0 0 0 0 0 V2000
 -2.0395 0.4958 0.0398 O 0 0 0 0 0 0 0 0 0 0 0 1
 -1.1900 -0.1365 0.0119 H 0 0 0 0 0 0 0 0 0 0 0 2
 -1.7954 1.2616 -0.5065 H 0 0 0 0 0 0 0 0 0 0 0 3
 2.0375 0.4973 0.0475 O 0 0 0 0 0 0 0 0 0 0 0 4
 1.1890 -0.1346 0.0149 H 0 0 0 0 0 0 0 0 0 0 0 5
 1.8627 1.1794 -0.6223 H 0 0 0 0 0 0 0 0 0 0 0 6
 0.0004 -1.5224 -0.8081 H 0 0 0 0 0 0 0 0 0 0 0 7
 -0.0021 -1.0338 0.0330 O 0 0 0 0 0 0 0 0 0 0 0 8
 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
 6 4 0 0 0 0
 2 8 0 0 0 0
 5 8 0 0 0 0
 7 8 0 0 0 0
 M END
 \$\$\$

1
2
3 1.4751 3.4688 1.9699 H 0 0 0 0 0 0 0 0 0 0 42
4 -2.1337 -0.2476 -0.8026 H 0 0 0 0 0 0 0 0 0 0 43
5 -2.2291 -1.0004 0.7841 H 0 0 0 0 0 0 0 0 0 0 44
6 1.0631 -5.1557 -1.7112 H 0 0 0 0 0 0 0 0 0 0 45
7 1.3253 0.3184 -4.0072 H 0 0 0 0 0 0 0 0 0 0 46
8 2.5497 -1.7444 -4.7200 H 0 0 0 0 0 0 0 0 0 0 47
9 2.1801 -3.8793 -3.4919 H 0 0 0 0 0 0 0 0 0 0 48
10 -0.2101 0.2714 -2.0939 H 0 0 0 0 0 0 0 0 0 0 49
11 0.6668 5.9992 -0.1990 H 0 0 0 0 0 0 0 0 0 0 50
12 2 1 0 0 0 0
13 3 1 0 0 0 0
14 5 4 0 0 0 0
15 6 4 0 0 0 0
16 8 7 0 0 0 0
17 12 7 0 0 0 0
18 38 7 0 0 0 0
19 9 8 0 0 0 0
20 39 8 0 0 0 0
21 10 9 0 0 0 0
22 40 9 0 0 0 0
23 11 10 0 0 0 0
24 13 10 0 0 0 0
25 12 11 0 0 0 0
26 16 11 0 0 0 0
27 41 12 0 0 0 0
28 14 13 0 0 0 0
29 17 13 0 0 0 0
30 15 14 0 0 0 0
31 29 14 0 0 0 0
32 16 15 0 0 0 0
33 31 15 0 0 0 0
34 42 16 0 0 0 0
35 18 17 0 0 0 0
36 43 17 0 0 0 0
37 44 17 0 0 0 0
38 19 18 0 0 0 0
39 23 18 0 0 0 0
40 20 19 0 0 0 0
41 27 19 0 0 0 0
42 21 20 0 0 0 0
43 26 20 0 0 0 0
44 22 21 0 0 0 0
45 45 21 0 0 0 0
46 23 22 0 0 0 0
47 30 22 0 0 0 0
48 28 23 0 0 0 0
49 25 24 0 0 0 0
50 27 24 0 0 0 0
51 46 24 0 0 0 0
52 26 25 0 0 0 0
53 47 25 0 0 0 0
54 48 26 0 0 0 0
55 49 27 0 0 0 0
56 32 28 0 0 0 0
57 33 29 0 0 0 0
58 34 30 0 0 0 0
59 35 30 0 0 0 0
60 36 31 0 0 0 0
37 31 0 0 0 0
34 32 0 0 0 0
37 50 0 0 0 0
M END
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pamoicacid.sdf
COSMOtherm 3D 0
51 52 0 0 0 0 0 0 0 0 0 0 V2000
-2.8094 3.3617 5.8645 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6163 2.8778 6.1194 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1274 4.1152 5.3340 H 0 0 0 0 0 0 0 0 0 0 0 3
2.8310 3.3494 -5.8524 O 0 0 0 0 0 0 0 0 0 0 0 4
3.7114 2.9326 -5.8943 H 0 0 0 0 0 0 0 0 0 0 0 5
2.9829 4.2094 -5.4188 H 0 0 0 0 0 0 0 0 0 0 0 6
-4.2804 -1.3384 -3.0604 C 0 0 0 0 0 0 0 0 0 0 0 7
-4.0010 -2.0921 -1.8910 C 0 0 0 0 0 0 0 0 0 0 0 8
-2.7599 -2.0394 -1.2871 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.7056 -1.2334 -1.8145 C 0 0 0 0 0 0 0 0 0 0 0 10
-2.0004 -0.4685 -3.0071 C 0 0 0 0 0 0 0 0 0 0 0 11
-3.2948 -0.5416 -3.6015 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.4028 -1.1608 -1.2292 C 0 0 0 0 0 0 0 0 0 0 0 13
0.5753 -0.3800 -1.8535 C 0 0 0 0 0 0 0 0 0 0 0 14
0.2789 0.3951 -3.0292 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.9943 0.3353 -3.5803 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.0015 -1.9680 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 17
0.4003 -1.1625 1.2268 C 0 0 0 0 0 0 0 0 0 0 0 18
1.7031 -1.2369 1.8120 C 0 0 0 0 0 0 0 0 0 0 0 19
1.9984 -0.4739 3.0057 C 0 0 0 0 0 0 0 0 0 0 0 20
0.9930 0.3306 3.5794 C 0 0 0 0 0 0 0 0 0 0 0 21
-0.2801 0.3918 3.0286 C 0 0 0 0 0 0 0 0 0 0 0 22
-0.5773 -0.3825 1.8527 C 0 0 0 0 0 0 0 0 0 0 0 23
3.9982 -2.0968 1.8871 C 0 0 0 0 0 0 0 0 0 0 0 24
4.2779 -1.3452 3.0578 C 0 0 0 0 0 0 0 0 0 0 0 25
3.2927 -0.5487 3.6001 C 0 0 0 0 0 0 0 0 0 0 0 26
2.7570 -2.0428 1.2835 C 0 0 0 0 0 0 0 0 0 0 0 27
-1.8281 -0.3730 1.3277 O 0 0 0 0 0 0 0 0 0 0 0 28
1.8256 -0.3708 -1.3276 O 0 0 0 0 0 0 0 0 0 0 0 29
-1.3418 1.2168 3.6429 C 0 0 0 0 0 0 0 0 0 0 0 30
1.3418 1.2181 -3.6436 C 0 0 0 0 0 0 0 0 0 0 0 31
-2.3658 0.2460 1.9168 H 0 0 0 0 0 0 0 0 0 0 0 32
2.3641 0.2476 -1.9167 H 0 0 0 0 0 0 0 0 0 0 0 33
-2.5049 1.2583 3.1852 O 0 0 0 0 0 0 0 0 0 0 0 34
-0.9777 1.9129 4.7144 O 0 0 0 0 0 0 0 0 0 0 0 35
2.5049 1.2592 -3.1851 O 0 0 0 0 0 0 0 0 0 0 0 36
0.9802 1.9118 -4.7175 O 0 0 0 0 0 0 0 0 0 0 0 37
-5.2674 -1.3922 -3.5227 H 0 0 0 0 0 0 0 0 0 0 0 38

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-4.7815 -2.7214 -1.4584 H 0 0 0 0 0 0 0 0 0 0 0 0 0 39
-2.5948 -2.6214 -0.3823 H 0 0 0 0 0 0 0 0 0 0 0 0 0 40
-3.4860 0.0479 -4.5012 H 0 0 0 0 0 0 0 0 0 0 0 0 0 41
-1.2201 0.9158 -4.4755 H 0 0 0 0 0 0 0 0 0 0 0 0 0 42
0.8262 -2.6294 -0.2874 H 0 0 0 0 0 0 0 0 0 0 0 0 0 43
-0.8293 -2.6295 0.2831 H 0 0 0 0 0 0 0 0 0 0 0 0 0 44
1.2198 0.9107 4.4747 H 0 0 0 0 0 0 0 0 0 0 0 0 0 45
4.7783 -2.7258 1.4536 H 0 0 0 0 0 0 0 0 0 0 0 0 0 46
5.2649 -1.4000 3.5199 H 0 0 0 0 0 0 0 0 0 0 0 0 0 47
3.4842 0.0393 4.5008 H 0 0 0 0 0 0 0 0 0 0 0 0 0 48
2.5915 -2.6233 0.3777 H 0 0 0 0 0 0 0 0 0 0 0 0 0 49
-1.7693 2.4543 5.0883 H 0 0 0 0 0 0 0 0 0 0 0 0 0 50
1.7732 2.4538 -5.0885 H 0 0 0 0 0 0 0 0 0 0 0 0 0 51
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
38 7 0 0 0 0
9 8 0 0 0 0
39 8 0 0 0 0
10 9 0 0 0 0
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13 10 0 0 0 0
12 11 0 0 0 0
16 11 0 0 0 0
41 12 0 0 0 0
14 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
29 14 0 0 0 0
16 15 0 0 0 0
31 15 0 0 0 0
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25 24 0 0 0 0
27 24 0 0 0 0
46 24 0 0 0 0
26 25 0 0 0 0
47 25 0 0 0 0
48 26 0 0 0 0
49 27 0 0 0 0
32 28 0 0 0 0
33 29 0 0 0 0
34 30 0 0 0 0
35 30 0 0 0 0
36 31 0 0 0 0
37 31 0 0 0 0
50 35 0 0 0 0
37 51 0 0 0 0
M END

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$$$
pentachlorophenol-anion.sdf
COSMOTHERM 3D 0
18 16 0 0 0 0 0 0 0 0 0 V2000
-6.4443 -0.6273 -0.7586 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.7085 -0.3162 -0.1592 H 0 0 0 0 0 0 0 0 0 0 0 2
-6.4637 0.0249 -1.4797 H 0 0 0 0 0 0 0 0 0 0 0 3
-4.4569 0.1314 0.9626 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.5426 -0.1003 0.5983 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.4420 1.0949 1.0946 H 0 0 0 0 0 0 0 0 0 0 0 6
0.8500 1.3125 -0.0223 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.4973 0.9430 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9376 -0.4273 0.0196 C 0 0 0 0 0 0 0 0 0 0 0 9
0.1381 -1.3855 0.0131 C 0 0 0 0 0 0 0 0 0 0 0 10
1.4855 -1.0216 -0.0117 C 0 0 0 0 0 0 0 0 0 0 0 11
1.8605 0.3348 -0.0280 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.1667 -0.7845 0.0332 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.7593 2.1698 -0.0122 Cl 0 0 0 0 0 0 0 0 0 0 0 14
1.2953 3.0136 -0.0467 Cl 0 0 0 0 0 0 0 0 0 0 0 15
3.5543 0.7960 -0.0550 Cl 0 0 0 0 0 0 0 0 0 0 0 16
2.7328 -2.2610 -0.0201 Cl 0 0 0 0 0 0 0 0 0 0 0 17
-0.3349 -3.0779 0.0355 Cl 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
16 12 0 0 0 0
10 18 0 0 0 0

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For Peer Review Only

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-1.7947 3.6444 0.0272 H 0 0 0 0 0 0 0 0 0 0 0 18
1.1605 -1.2822 0.2872 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
18 12 0 0 0 0
13 19 0 0 0 0
M END
$$$$
phenytoin-anion.sdf
COSMOtherm 3D 0
36 36 0 0 0 0 0 0 0 0 0 0 V2000
-5.4473 0.7964 0.1170 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.2440 -0.1513 0.3244 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.5382 1.1936 0.0783 H 0 0 0 0 0 0 0 0 0 0 0 3
-4.3728 -1.7450 0.6320 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.4682 -1.2850 0.5390 H 0 0 0 0 0 0 0 0 0 0 0 5
-4.4349 -1.9916 1.5716 H 0 0 0 0 0 0 0 0 0 0 0 6
-2.0245 -0.3914 0.3048 N 0 0 0 0 0 0 0 0 0 0 0 7
-1.8958 0.9743 0.1245 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.7903 -0.9530 0.2571 C 0 0 0 0 0 0 0 0 0 0 0 9
0.3030 0.1686 0.0291 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.5659 1.3450 0.0833 N 0 0 0 0 0 0 0 0 0 0 0 11
0.9636 0.0635 -1.3538 C 0 0 0 0 0 0 0 0 0 0 0 12
1.3154 0.1143 1.1738 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.8377 1.7944 0.0286 O 0 0 0 0 0 0 0 0 0 0 0 14
-0.5144 -2.1552 0.3750 O 0 0 0 0 0 0 0 0 0 0 0 15
2.1647 0.9169 3.3090 C 0 0 0 0 0 0 0 0 0 0 0 16
1.2553 1.0127 2.2484 C 0 0 0 0 0 0 0 0 0 0 0 17
2.2984 -0.8907 1.1849 C 0 0 0 0 0 0 0 0 0 0 0 18
3.2016 -0.9909 2.2465 C 0 0 0 0 0 0 0 0 0 0 0 19
3.1400 -0.0853 3.3133 C 0 0 0 0 0 0 0 0 0 0 0 20
0.4300 -0.7373 -2.3758 C 0 0 0 0 0 0 0 0 0 0 0 21
1.0075 -0.7427 -3.6517 C 0 0 0 0 0 0 0 0 0 0 0 22
2.1240 0.0538 -3.9251 C 0 0 0 0 0 0 0 0 0 0 0 23
2.6621 0.8577 -2.9126 C 0 0 0 0 0 0 0 0 0 0 0 24
2.0885 0.8578 -1.6378 C 0 0 0 0 0 0 0 0 0 0 0 25
-0.2998 2.2304 -0.3420 H 0 0 0 0 0 0 0 0 0 0 0 26
2.1084 1.6300 4.1341 H 0 0 0 0 0 0 0 0 0 0 0 27
0.4931 1.7933 2.2504 H 0 0 0 0 0 0 0 0 0 0 0 28
2.3564 -1.5978 0.3562 H 0 0 0 0 0 0 0 0 0 0 0 29
3.9592 -1.7772 2.2392 H 0 0 0 0 0 0 0 0 0 0 0 30
3.8499 -0.1596 4.1394 H 0 0 0 0 0 0 0 0 0 0 0 31
-0.4368 -1.3703 -2.1813 H 0 0 0 0 0 0 0 0 0 0 0 32
0.5822 -1.3759 -4.4329 H 0 0 0 0 0 0 0 0 0 0 0 33
2.5744 0.0472 -4.9194 H 0 0 0 0 0 0 0 0 0 0 0 34
3.5340 1.4833 -3.1135 H 0 0 0 0 0 0 0 0 0 0 0 35
2.5224 1.4809 -0.8529 H 0 0 0 0 0 0 0 0 0 0 0 36
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
11 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
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21 12 0 0 0 0
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19 18 0 0 0 0
29 18 0 0 0 0
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30 19 0 0 0 0
31 20 0 0 0 0
22 21 0 0 0 0
32 21 0 0 0 0
23 22 0 0 0 0
33 22 0 0 0 0
24 23 0 0 0 0
34 23 0 0 0 0
25 24 0 0 0 0
35 24 0 0 0 0
25 36 0 0 0 0
M END
$$$$
phenytoin.sdf
COSMOtherm 3D 0
37 37 0 0 0 0 0 0 0 0 0 0 V2000
-0.5119 1.5234 5.8175 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.5187 2.4869 5.6728 H 0 0 0 0 0 0 0 0 0 0 0 2
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3 -0.4108 1.4267 6.7820 H 0 0 0 0 0 0 0 0 0 0 0 3
4 1.4251 0.1797 4.4472 O 0 0 0 0 0 0 0 0 0 0 0 4
5 0.7447 0.7091 4.9527 H 0 0 0 0 0 0 0 0 0 0 0 5
6 2.2444 0.7033 4.4958 H 0 0 0 0 0 0 0 0 0 0 0 6
7 0.7459 -0.4230 1.8472 N 0 0 0 0 0 0 0 0 0 0 0 7
8 0.8466 -1.7270 1.3234 C 0 0 0 0 0 0 0 0 0 0 0 8
9 0.3091 0.4817 0.9183 C 0 0 0 0 0 0 0 0 0 0 0 9
10 0.0436 -0.3164 -0.4052 C 0 0 0 0 0 0 0 0 0 0 0 10
11 0.3673 -1.6764 0.0448 N 0 0 0 0 0 0 0 0 0 0 0 11
12 0.9940 0.1022 -1.5375 C 0 0 0 0 0 0 0 0 0 0 0 12
13 -1.4368 -0.1492 -0.7740 C 0 0 0 0 0 0 0 0 0 0 0 13
14 1.2797 -2.7078 1.9279 O 0 0 0 0 0 0 0 0 0 0 0 14
15 0.1417 1.6839 1.0831 O 0 0 0 0 0 0 0 0 0 0 0 15
16 -3.7255 -0.9677 -0.8224 C 0 0 0 0 0 0 0 0 0 0 0 16
17 -2.3731 -1.1585 -0.5124 C 0 0 0 0 0 0 0 0 0 0 0 17
18 -1.8740 1.0606 -1.3395 C 0 0 0 0 0 0 0 0 0 0 0 18
19 -3.2250 1.2526 -1.6402 C 0 0 0 0 0 0 0 0 0 0 0 19
20 -4.1560 0.2377 -1.3850 C 0 0 0 0 0 0 0 0 0 0 0 20
21 2.1591 0.8452 -1.2961 C 0 0 0 0 0 0 0 0 0 0 0 21
22 3.0446 1.1345 -2.3409 C 0 0 0 0 0 0 0 0 0 0 0 22
23 2.7802 0.6793 -3.6363 C 0 0 0 0 0 0 0 0 0 0 0 23
24 1.6215 -0.0664 -3.8836 C 0 0 0 0 0 0 0 0 0 0 0 24
25 0.7331 -0.3487 -2.8425 C 0 0 0 0 0 0 0 0 0 0 0 25
26 1.0022 -0.1797 2.8426 H 0 0 0 0 0 0 0 0 0 0 0 26
27 0.5318 -2.4441 -0.6010 H 0 0 0 0 0 0 0 0 0 0 0 27
28 -4.4422 -1.7659 -0.6209 H 0 0 0 0 0 0 0 0 0 0 0 28
29 -2.0450 -2.0992 -0.0689 H 0 0 0 0 0 0 0 0 0 0 0 29
30 -1.1552 1.8537 -1.5483 H 0 0 0 0 0 0 0 0 0 0 0 30
31 -3.5514 2.1970 -2.0798 H 0 0 0 0 0 0 0 0 0 0 0 31
32 -5.2102 0.3864 -1.6260 H 0 0 0 0 0 0 0 0 0 0 0 32
33 2.3851 1.2129 -0.2943 H 0 0 0 0 0 0 0 0 0 0 0 33
34 3.9435 1.7194 -2.1381 H 0 0 0 0 0 0 0 0 0 0 0 34
35 3.4715 0.9061 -4.4499 H 0 0 0 0 0 0 0 0 0 0 0 35
36 1.4047 -0.4261 -4.8911 H 0 0 0 0 0 0 0 0 0 0 0 36
37 -0.1733 -0.9215 -3.0486 H 0 0 0 0 0 0 0 0 0 0 0 37
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45 M END
46 $$$$
47 phosphoricacid-anion.sdf
48 COSMOtherm 3D 0
49
50 13 10 0 0 0 0 0 0 0 0 0 0 V2000
51 -1.2640 0.0167 2.6381 O 0 0 0 0 0 0 0 0 0 0 0 1
52 -1.6098 -0.8197 2.9971 H 0 0 0 0 0 0 0 0 0 0 0 2
53 -1.3442 -0.0644 1.6314 H 0 0 0 0 0 0 0 0 0 0 0 3
54 1.3956 -0.0095 2.3952 O 0 0 0 0 0 0 0 0 0 0 0 4
55 0.4190 0.0339 2.6438 H 0 0 0 0 0 0 0 0 0 0 0 5
56 1.7632 0.8657 2.6113 H 0 0 0 0 0 0 0 0 0 0 0 6
57 -0.0963 -0.0763 -0.9626 P 0 0 0 0 0 0 0 0 0 0 0 7
58 0.2371 1.5324 -1.3060 O 0 0 0 0 0 0 0 0 0 0 0 8
59 -0.1665 -0.7891 -2.3097 O 0 0 0 0 0 0 0 0 0 0 0 9
60 1.2595 -0.6099 -0.1930 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.3076 -0.1054 0.0020 O 0 0 0 0 0 0 0 0 0 0 0 11
-0.0244 2.0957 -0.5529 H 0 0 0 0 0 0 0 0 0 0 0 12
1.3101 -0.3242 0.7807 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
10 13 0 0 0 0
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phosphoricacid.sdf
COSMOtherm 3D 0
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14 11 0 0 0 0 0 0 0 0 0 V2000
-3.0765 -1.3700 0.0373 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.1163 -2.3322 0.1889 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7748 -1.1925 -0.6197 H 0 0 0 0 0 0 0 0 0 0 0 3
3.0555 -1.4008 0.0185 O 0 0 0 0 0 0 0 0 0 0 0 4
3.8188 -1.1373 0.5650 H 0 0 0 0 0 0 0 0 0 0 0 5
3.4468 -1.7887 -0.7860 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0057 0.4872 0.0984 P 0 0 0 0 0 0 0 0 0 0 0 7
1.4742 0.5915 -0.5588 O 0 0 0 0 0 0 0 0 0 0 0 8
-0.6919 1.8916 -0.3828 O 0 0 0 0 0 0 0 0 0 0 0 9
-0.7448 -0.5986 -0.8259 O 0 0 0 0 0 0 0 0 0 0 0 10
-0.0458 0.2539 1.5942 O 0 0 0 0 0 0 0 0 0 0 0 11
2.0923 -0.1880 -0.3093 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5235 2.6057 0.2633 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.6549 -0.9004 -0.4596 H 0 0 0 0 0 0 0 0 0 0 0 14

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
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12 8 0 0 0 0
13 9 0 0 0 0
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M END

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phthalicacid-anion.sdf
COSMOTHERM 3D

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23 22 0 0 0 0 0 0 0 0 0 V2000
-1.4998 -0.0109 5.6900 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.6735 0.0069 5.1298 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.0968 0.6255 5.2607 H 0 0 0 0 0 0 0 0 0 0 0 3
0.8064 -0.0559 4.2083 O 0 0 0 0 0 0 0 0 0 0 0 4
0.6289 -0.3331 3.2535 H 0 0 0 0 0 0 0 0 0 0 0 5
1.2154 0.8247 4.1382 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0432 -2.6350 -2.0099 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.3214 -1.8497 -3.1318 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3620 -0.4635 -3.0015 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.1034 0.1858 -1.7784 C 0 0 0 0 0 0 0 0 0 0 0 10
0.1774 -0.6159 -0.6323 C 0 0 0 0 0 0 0 0 0 0 0 11
0.1868 -2.0163 -0.7828 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.1852 1.7062 -1.8646 C 0 0 0 0 0 0 0 0 0 0 0 13
0.4782 -0.1328 0.7832 C 0 0 0 0 0 0 0 0 0 0 0 14
0.4034 2.4349 -0.9389 O 0 0 0 0 0 0 0 0 0 0 0 15
-0.7641 2.2390 -2.8211 O 0 0 0 0 0 0 0 0 0 0 0 16
0.3036 -0.9437 1.7294 O 0 0 0 0 0 0 0 0 0 0 0 17
0.9386 1.0573 0.9661 O 0 0 0 0 0 0 0 0 0 0 0 18
-0.0097 -3.7230 -2.0868 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.5111 -2.3122 -4.1018 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.5963 0.1601 -3.8640 H 0 0 0 0 0 0 0 0 0 0 0 21
0.3837 -2.6186 0.1037 H 0 0 0 0 0 0 0 0 0 0 0 22
0.7354 1.8037 -0.0781 H 0 0 0 0 0 0 0 0 0 0 0 23

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
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10 9 0 0 0 0
21 9 0 0 0 0
11 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
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16 13 0 0 0 0
17 14 0 0 0 0
18 14 0 0 0 0
15 23 0 0 0 0
18 23 0 0 0 0

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M END

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phthalicacid.sdf
COSMOTHERM 3D

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24 24 0 0 0 0 0 0 0 0 0 V2000
-0.2796 -4.1921 1.2930 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.1520 -4.5616 1.5208 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.4093 -3.2148 1.2646 H 0 0 0 0 0 0 0 0 0 0 0 3
0.3092 -4.0920 -1.2743 O 0 0 0 0 0 0 0 0 0 0 0 4
0.1048 -4.3169 -0.3085 H 0 0 0 0 0 0 0 0 0 0 0 5
1.1727 -4.4962 -1.4777 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.2028 2.3271 -2.4063 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.1801 3.3112 -1.4168 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0646 2.9374 -0.0789 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0002 1.5914 0.3244 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.0290 0.5860 -0.6899 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.1159 0.9861 -2.0386 C 0 0 0 0 0 0 0 0 0 0 0 12
0.1425 1.4303 1.8319 C 0 0 0 0 0 0 0 0 0 0 0 13
0.0058 -0.8970 -0.4635 C 0 0 0 0 0 0 0 0 0 0 0 14
0.5483 2.3646 2.5215 O 0 0 0 0 0 0 0 0 0 0 0 15
-0.2242 0.2907 2.4162 O 0 0 0 0 0 0 0 0 0 0 0 16
-0.3540 -1.4329 0.6159 O 0 0 0 0 0 0 0 0 0 0 0 17
0.3977 -1.5966 -1.4945 O 0 0 0 0 0 0 0 0 0 0 0 18
-0.2848 2.5968 -3.4599 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.2444 4.3674 -1.6817 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.0201 3.7008 0.6967 H 0 0 0 0 0 0 0 0 0 0 0 21

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3 13 10 0 0 0 0
4 12 11 0 0 0 0
5 14 11 0 0 0 0
6 20 12 0 0 0 0
7 21 13 0 0 0 0
8 15 14 0 0 0 0
9 16 14 0 0 0 0
10 16 22 0 0 0 0
11 M END
12 $$$$
13 succinimide-anion.sdf
14 COSMOtherm 3D 0
15
16 17 15 0 0 0 0 0 0 0 0 V2000
17 -3.9456 -1.0950 0.0939 O 0 0 0 0 0 0 0 0 0 0 0 1
18 -3.3483 -0.2914 0.0405 H 0 0 0 0 0 0 0 0 0 0 0 2
19 -4.6745 -0.8156 0.6736 H 0 0 0 0 0 0 0 0 0 0 0 3
20 -2.3398 1.0978 -0.0551 O 0 0 0 0 0 0 0 0 0 0 0 4
21 -1.3455 0.8180 -0.0171 H 0 0 0 0 0 0 0 0 0 0 0 5
22 -2.4479 1.5024 -0.9338 H 0 0 0 0 0 0 0 0 0 0 0 6
23 2.3285 -0.5102 -0.7983 C 0 0 0 0 0 0 0 0 0 0 0 7
24 0.9302 0.0380 -1.1215 C 0 0 0 0 0 0 0 0 0 0 0 8
25 2.3753 -0.4880 0.7300 C 0 0 0 0 0 0 0 0 0 0 0 9
26 1.0020 0.0801 1.1227 C 0 0 0 0 0 0 0 0 0 0 0 10
27 0.2358 0.3497 0.0187 N 0 0 0 0 0 0 0 0 0 0 0 11
28 0.6431 0.2659 2.3004 O 0 0 0 0 0 0 0 0 0 0 0 12
29 0.4938 0.1804 -2.2789 O 0 0 0 0 0 0 0 0 0 0 0 13
30 3.0871 0.1287 -1.2730 H 0 0 0 0 0 0 0 0 0 0 0 14
31 2.4327 -1.5161 -1.2302 H 0 0 0 0 0 0 0 0 0 0 0 15
32 3.1664 0.1559 1.1404 H 0 0 0 0 0 0 0 0 0 0 0 16
33 2.4978 -1.4829 1.1824 H 0 0 0 0 0 0 0 0 0 0 0 17
34
35 2 1 0 0 0 0
36 3 1 0 0 0 0
37 5 4 0 0 0 0
38 6 4 0 0 0 0
39 8 7 0 0 0 0
40 9 7 0 0 0 0
41 14 7 0 0 0 0
42 15 7 0 0 0 0
43 11 8 0 0 0 0
44 13 8 0 0 0 0
45 10 9 0 0 0 0
46 16 9 0 0 0 0
47 11 10 0 0 0 0
48 12 10 0 0 0 0
49 9 17 0 0 0 0
50 M END
51 $$$$
52 succinimide.sdf
53 COSMOtherm 3D 0
54
55 18 16 0 0 0 0 0 0 0 0 V2000
56 -4.1741 -0.1825 0.8499 O 0 0 0 0 0 0 0 0 0 0 0 1
57 -4.7265 -0.9148 0.5214 H 0 0 0 0 0 0 0 0 0 0 0 2
58 -4.8126 0.5193 1.0728 H 0 0 0 0 0 0 0 0 0 0 0 3
59 -2.3001 0.7078 -0.9312 O 0 0 0 0 0 0 0 0 0 0 0 4
60 -3.0025 0.3545 -0.3150 H 0 0 0 0 0 0 0 0 0 0 0 5
61 -2.5349 0.3607 -1.8098 H 0 0 0 0 0 0 0 0 0 0 0 6
62 2.5824 0.4000 0.4111 C 0 0 0 0 0 0 0 0 0 0 0 7
63 1.2626 1.0820 0.0757 C 0 0 0 0 0 0 0 0 0 0 0 8
64 2.2971 -1.1032 0.2838 C 0 0 0 0 0 0 0 0 0 0 0 9
65 0.8309 -1.1938 -0.1183 C 0 0 0 0 0 0 0 0 0 0 0 10
66 0.3273 0.0969 -0.2111 N 0 0 0 0 0 0 0 0 0 0 0 11
67 0.1806 -2.2131 -0.3320 O 0 0 0 0 0 0 0 0 0 0 0 12
68 1.0341 2.2885 0.0539 O 0 0 0 0 0 0 0 0 0 0 0 13
69 2.8900 0.7016 1.4216 H 0 0 0 0 0 0 0 0 0 0 0 14
70 3.3527 0.7577 -0.2859 H 0 0 0 0 0 0 0 0 0 0 0 15
71 2.4412 -1.6551 1.2227 H 0 0 0 0 0 0 0 0 0 0 0 16
72 2.9060 -1.5994 -0.4843 H 0 0 0 0 0 0 0 0 0 0 0 17
73 -0.6689 0.3067 -0.4785 H 0 0 0 0 0 0 0 0 0 0 0 18
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75 2 1 0 0 0 0
76 3 1 0 0 0 0
77 5 4 0 0 0 0
78 6 4 0 0 0 0
79 8 7 0 0 0 0
80 9 7 0 0 0 0
81 14 7 0 0 0 0
82 15 7 0 0 0 0
83 11 8 0 0 0 0
84 13 8 0 0 0 0
85 10 9 0 0 0 0
86 16 9 0 0 0 0
87 17 9 0 0 0 0
88 11 10 0 0 0 0
89 12 10 0 0 0 0
90 11 18 0 0 0 0
91 M END
92 $$$$
93 sulfurousacid-anion.sdf
94 COSMOtherm 3D 0
95
96 11 8 0 0 0 0 0 0 0 0 V2000
97 -3.7682 -0.7281 0.1816 O 0 0 0 0 0 0 0 0 0 0 0 1
98 -3.0049 -0.1079 0.0388 H 0 0 0 0 0 0 0 0 0 0 0 2
99 -4.3877 -0.5182 -0.5380 H 0 0 0 0 0 0 0 0 0 0 0 3
100 -1.6171 0.9921 -0.0982 O 0 0 0 0 0 0 0 0 0 0 0 4
101 0.9773 0.9234 1.2004 O 0 0 0 0 0 0 0 0 0 0 0 5
102 1.5855 -0.0960 -0.1274 S 0 0 0 0 0 0 0 0 0 0 0 6
103 1.2205 -1.5194 0.3107 O 0 0 0 0 0 0 0 0 0 0 0 7
104 0.6494 0.3356 -1.3042 O 0 0 0 0 0 0 0 0 0 0 0 8
105 0.0010 1.0059 1.0385 H 0 0 0 0 0 0 0 0 0 0 0 9
106 -1.8788 1.8924 -0.3630 H 0 0 0 0 0 0 0 0 0 0 0 10
107 -0.8790 0.7246 -0.7334 H 0 0 0 0 0 0 0 0 0 0 0 11
108
109 2 1 0 0 0 0
110 3 1 0 0 0 0

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10 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
4 11 0 0 0 0
M END
$$$$
sulfurousacid.sdf
COSMOtherm 3D 0

12 9 0 0 0 0 0 0 0 0 0 V2000
-3.8880 0.2199 -0.0067 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-4.3854 0.0311 0.8100 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.4501 -0.1287 -0.7225 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.4335 -0.7797 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.4810 -1.7529 -0.0031 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.3883 -0.4435 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.5752 0.3524 0.0007 S 0 0 0 0 0 0 0 0 0 0 0 0 7
0.5006 0.5595 -1.2814 O 0 0 0 0 0 0 0 0 0 0 0 0 8
0.5097 0.5394 1.2932 O 0 0 0 0 0 0 0 0 0 0 0 0 9
1.9930 -1.0982 -0.0125 O 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.3066 -0.0138 -1.0755 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.3001 -0.0280 1.0835 H 0 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
9 12 0 0 0 0
M END
$$$$
tert-butanol-anion.sdf
COSMOtherm 3D 0

20 18 0 0 0 0 0 0 0 0 0 V2000
-0.8522 0.0089 3.2856 O 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0309 -0.0113 2.6918 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.5773 0.0383 2.6392 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.2693 -0.0961 1.8939 O 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7504 -0.5734 0.5361 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.5895 0.8131 1.7637 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0977 0.0182 -1.2269 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.0433 0.9770 -1.6194 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2273 0.7991 -0.5286 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.6392 -0.6933 -2.4730 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.6951 1.7604 -2.3107 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.0469 0.1163 -0.2578 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.1605 -1.2724 -2.9590 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.6348 1.5893 -1.1786 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.4547 1.4686 -0.7248 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.8553 0.4189 -2.1096 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-1.4482 -1.3860 -2.1959 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.8510 1.2687 0.3924 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-1.0358 0.0289 -3.2023 H 0 0 0 0 0 0 0 0 0 0 0 0 19
0.4039 -1.0077 -0.3536 O 0 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
4 2 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
11 8 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
12 9 0 0 0 0
14 9 0 0 0 0
18 9 0 0 0 0
13 10 0 0 0 0
17 10 0 0 0 0
19 10 0 0 0 0
5 20 0 0 0 0
7 20 0 0 0 0
M END
$$$$
tert-butanol.sdf
COSMOtherm 3D 0

21 18 0 0 0 0 0 0 0 0 0 V2000
-3.7549 -0.7955 0.0304 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.8311 -1.2542 -0.8255 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-4.6589 -0.4832 0.2167 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.9521 1.2682 0.0843 O 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.6088 0.5203 0.0089 H 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.0322 1.7616 -0.7505 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.4266 -0.1268 -0.0249 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.5150 0.5456 -1.4043 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.7626 -1.5084 -0.1403 C 0 0 0 0 0 0 0 0 0 0 0 0 9
2.8158 -0.2456 0.6094 C 0 0 0 0 0 0 0 0 0 0 0 0 10
2.1217 -0.0538 -2.0999 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.6815 -1.9767 0.8521 H 0 0 0 0 0 0 0 0 0 0 0 0 12
3.2765 0.7483 0.7127 H 0 0 0 0 0 0 0 0 0 0 0 0 13
1.3455 -2.1759 -0.7929 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.5118 0.6614 -1.8430 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.9716 1.5423 -1.3144 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.7436 -0.7023 1.6074 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.2484 -1.4171 -0.5652 H 0 0 0 0 0 0 0 0 0 0 0 0 18
3.4746 -0.8705 -0.0108 H 0 0 0 0 0 0 0 0 0 0 0 0 19
0.6553 0.7103 0.8773 O 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.2550 0.8326 0.4996 H 0 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0

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3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
20 7 0 0 0 0
11 8 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
12 9 0 0 0 0
14 9 0 0 0 0
18 9 0 0 0 0
13 10 0 0 0 0
17 10 0 0 0 0
19 10 0 0 0 0
20 21 0 0 0 0
M END
$$$$
thymine-anion.sdf
COSMOtherm 3D 0
20 18 0 0 0 0 0 0 0 0 0 V2000
-1.4276 -0.5927 4.5599 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.6691 -0.1679 4.0618 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.1384 0.0700 4.5325 H 0 0 0 0 0 0 0 0 0 0 0 3
0.6958 0.4844 3.2432 O 0 0 0 0 0 0 0 0 0 0 0 4
0.6193 0.3666 2.2198 H 0 0 0 0 0 0 0 0 0 0 0 5
0.7584 1.4449 3.3866 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.8426 0.2191 0.0712 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.1806 0.1144 -1.2641 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1046 -0.0934 -2.2010 C 0 0 0 0 0 0 0 0 0 0 0 9
1.1627 -0.1587 -1.6085 N 0 0 0 0 0 0 0 0 0 0 0 10
1.4615 -0.0446 -0.2419 C 0 0 0 0 0 0 0 0 0 0 0 11
0.4067 0.1471 0.6021 N 0 0 0 0 0 0 0 0 0 0 0 12
-0.2183 -0.2126 -3.4439 O 0 0 0 0 0 0 0 0 0 0 0 13
2.6548 -0.1232 0.1336 O 0 0 0 0 0 0 0 0 0 0 0 14
-2.5935 0.2030 -1.7675 C 0 0 0 0 0 0 0 0 0 0 0 15
-1.6405 0.3733 0.8069 H 0 0 0 0 0 0 0 0 0 0 0 16
1.9544 -0.3044 -2.2368 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.8937 -0.7152 -2.2977 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.7194 1.0338 -2.4801 H 0 0 0 0 0 0 0 0 0 0 0 19
-3.2928 0.3599 -0.9345 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 15 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M END
$$$$
thymine.sdf
COSMOtherm 3D 0
21 19 0 0 0 0 0 0 0 0 0 V2000
-4.0896 0.6265 -0.0341 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.4871 0.8845 -0.8848 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1816 1.0344 -0.0343 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.9755 -1.8287 -0.0091 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.5485 -1.0052 -0.0162 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.1871 -2.2833 0.8258 H 0 0 0 0 0 0 0 0 0 0 0 6
0.6492 -1.3379 -0.0034 C 0 0 0 0 0 0 0 0 0 0 0 7
1.9044 -0.8048 -0.0151 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0265 0.6459 -0.0032 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8010 1.3396 0.0175 N 0 0 0 0 0 0 0 0 0 0 0 10
-0.4697 0.7975 0.0314 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.4950 -0.5758 0.0167 N 0 0 0 0 0 0 0 0 0 0 0 12
3.0913 1.2815 -0.0102 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.4892 1.5139 0.0550 O 0 0 0 0 0 0 0 0 0 0 0 14
3.1509 -1.6391 -0.0364 C 0 0 0 0 0 0 0 0 0 0 0 15
0.4772 -2.4145 -0.0102 H 0 0 0 0 0 0 0 0 0 0 0 16
0.8531 2.3598 0.0277 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.4330 -1.0562 0.0349 H 0 0 0 0 0 0 0 0 0 0 0 18
3.7795 -1.4323 0.8431 H 0 0 0 0 0 0 0 0 0 0 0 19
3.7601 -1.4166 -0.9253 H 0 0 0 0 0 0 0 0 0 0 0 20
2.9037 -2.7084 -0.0430 H 0 0 0 0 0 0 0 0 0 0 0 21
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0

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20 15 0 0 0 0
15 21 0 0 0 0
M  END
$$$$
trans-5-formyluracil-anion.sdf
COSMOtherm      3D      0

19 17 0 0 0 0 0 0 0 0 V2000
1.6722 -4.3871 0.2923 O 0 0 0 0 0 0 0 0 0 0 0 1
0.7527 -4.0301 0.1286 H 0 0 0 0 0 0 0 0 0 0 0 2
1.9127 -4.0543 1.1735 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.8517 -3.4418 -0.1974 O 0 0 0 0 0 0 0 0 0 0 0 4
-0.8406 -2.4237 -0.1853 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.1432 -3.6758 -1.0965 H 0 0 0 0 0 0 0 0 0 0 0 6
0.5335 -0.1585 -0.1234 C 0 0 0 0 0 0 0 0 0 0 0 7
0.8042 1.2151 -0.0366 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.3202 2.1265 0.0810 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.5586 1.4709 0.0915 N 0 0 0 0 0 0 0 0 0 0 0 10
-1.7842 0.0928 0.0005 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.6727 -0.7267 -0.1105 N 0 0 0 0 0 0 0 0 0 0 0 12
-0.2739 3.3677 0.1685 O 0 0 0 0 0 0 0 0 0 0 0 13
-2.9441 -0.3493 0.0165 O 0 0 0 0 0 0 0 0 0 0 0 14
2.1551 1.7271 -0.0606 C 0 0 0 0 0 0 0 0 0 0 0 15
1.3822 -0.8460 -0.2060 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.3876 2.0620 0.1733 H 0 0 0 0 0 0 0 0 0 0 0 17
3.1884 1.0415 -0.1591 O 0 0 0 0 0 0 0 0 0 0 0 18
2.2335 2.8342 0.0172 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 15 0 0 0 0
15 19 0 0 0 0
M  END
$$$$
trans-5-formyluracil.sdf
COSMOtherm      3D      0

20 18 0 0 0 0 0 0 0 0 V2000
-5.0669 -0.4929 0.8925 O 0 0 0 0 0 0 0 0 0 0 0 1
-5.8675 -1.0385 0.7891 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.3682 0.4136 0.7006 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.0247 -1.3378 -0.6807 O 0 0 0 0 0 0 0 0 0 0 0 4
-3.3180 -1.2981 -1.6084 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.8024 -1.0086 -0.1408 H 0 0 0 0 0 0 0 0 0 0 0 6
0.4065 -0.9135 -0.1609 C 0 0 0 0 0 0 0 0 0 0 0 7
1.6933 -0.4598 0.0437 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9256 0.9793 0.1344 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7583 1.7516 -0.0046 N 0 0 0 0 0 0 0 0 0 0 0 10
-0.5369 1.3027 -0.2106 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.6510 -0.0900 -0.2815 N 0 0 0 0 0 0 0 0 0 0 0 12
3.0155 1.5337 0.3144 O 0 0 0 0 0 0 0 0 0 0 0 13
-1.5047 2.0508 -0.3211 O 0 0 0 0 0 0 0 0 0 0 0 14
2.8098 -1.3916 0.1663 C 0 0 0 0 0 0 0 0 0 0 0 15
0.1951 -1.9816 -0.2353 H 0 0 0 0 0 0 0 0 0 0 0 16
0.8738 2.7654 0.0515 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.6206 -0.4970 -0.4436 H 0 0 0 0 0 0 0 0 0 0 0 18
2.7105 -2.6217 0.1009 O 0 0 0 0 0 0 0 0 0 0 0 19
3.7990 -0.9134 0.3289 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
18 12 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M  END
$$$$
trichloroaceticacid-anion.sdf
COSMOtherm      3D      0

13 10 0 0 0 0 0 0 0 0 V2000
-5.5924 0.2214 -0.8335 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.8803 0.0480 -0.1555 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.3339 1.0637 -1.2452 H 0 0 0 0 0 0 0 0 0 0 0 3
-3.6752 -0.3549 1.0409 O 0 0 0 0 0 0 0 0 0 0 0 4
-2.7427 -0.2861 0.6606 H 0 0 0 0 0 0 0 0 0 0 0 5
-3.6934 0.2806 1.7776 H 0 0 0 0 0 0 0 0 0 0 0 6
1.4204 -1.6867 -0.6746 Cl 0 0 0 0 0 0 0 0 0 0 0 7
1.1345 0.0085 -0.0628 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.2828 0.0686 0.6862 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.2725 0.4219 1.8762 O 0 0 0 0 0 0 0 0 0 0 0 10
-1.2407 -0.2606 -0.0656 O 0 0 0 0 0 0 0 0 0 0 0 11

```

```

1
2
3      1.1093      1.1511      -1.4842 Cl  0  0  0  0  0  0  0  0  0  0  0  0  0  12
4      2.5204      0.4655      1.0074 Cl  0  0  0  0  0  0  0  0  0  0  0  0  0  13
5      2  1  0  0  0  0
6      3  1  0  0  0  0
7      5  4  0  0  0  0
8      6  4  0  0  0  0
9      8  7  0  0  0  0
10     9  8  0  0  0  0
11    12  8  0  0  0  0
12    10  9  0  0  0  0
13    11  9  0  0  0  0
14    8  13  0  0  0  0
M  END
$$$
trichloroaceticacid.sdf
COSMOTHERM      3D      0
14 12 0 0 0 0 0 0 0 0 0 V2000
0.9504  4.8833  -0.3752 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1.6564  4.9101  -0.2959 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
0.7410  5.8195  -0.5476 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-1.1964  3.4835  0.3072 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
-0.3698  4.0277  0.0952 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-1.4424  3.7007  1.2245 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
-1.3339  -1.8526  0.8689 Cl  0  0  0  0  0  0  0  0  0  0  0  0  0  7
0.0521  -1.0896  -0.0215 C  0  0  0  0  0  0  0  0  0  0  0  0  0  8
0.0746  0.4513  0.3094 C  0  0  0  0  0  0  0  0  0  0  0  0  0  9
1.0277  0.9581  0.8763 O  0  0  0  0  0  0  0  0  0  0  0  0  0  10
-1.0243  1.0324  -0.0979 O  0  0  0  0  0  0  0  0  0  0  0  0  0  11
-0.1709  -1.3163  -1.8070 Cl  0  0  0  0  0  0  0  0  0  0  0  0  0  12
1.5840  -1.8733  0.4863 Cl  0  0  0  0  0  0  0  0  0  0  0  0  0  13
-1.0321  2.0942  0.1203 H  0  0  0  0  0  0  0  0  0  0  0  0  0  14
2  1  0  0  0  0
3  1  0  0  0  0
5  4  0  0  0  0
6  4  0  0  0  0
8  7  0  0  0  0
9  8  0  0  0  0
12  8  0  0  0  0
13  8  0  0  0  0
10  9  0  0  0  0
11  9  0  0  0  0
4  14  0  0  0  0
11  14  0  0  0  0
M  END
$$$
uracil-anion.sdf
COSMOTHERM      3D      0
17 15 0 0 0 0 0 0 0 0 0 V2000
4.5904  0.6715  1.1155 O  0  0  0  0  0  0  0  0  0  0  0  0  0  1
3.9929  0.1942  0.4684 H  0  0  0  0  0  0  0  0  0  0  0  0  0  2
4.5697  0.1215  1.9171 H  0  0  0  0  0  0  0  0  0  0  0  0  0  3
3.0115  -0.5688  -0.7199 O  0  0  0  0  0  0  0  0  0  0  0  0  0  4
2.0038  -0.4443  -0.5443 H  0  0  0  0  0  0  0  0  0  0  0  0  0  5
3.1544  -1.5314  -0.7288 H  0  0  0  0  0  0  0  0  0  0  0  0  0  6
-0.0177  -0.3682  1.1153 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
-1.3202  -0.2489  1.5554 C  0  0  0  0  0  0  0  0  0  0  0  0  0  8
-2.3474  0.0557  0.6024 C  0  0  0  0  0  0  0  0  0  0  0  0  0  9
-1.8599  0.1972  -0.7055 N  0  0  0  0  0  0  0  0  0  0  0  0  0  10
-0.5257  0.0717  -1.1253 C  0  0  0  0  0  0  0  0  0  0  0  0  0  11
0.4052  -0.2207  -0.1646 N  0  0  0  0  0  0  0  0  0  0  0  0  0  12
-3.5723  0.1971  0.8292 O  0  0  0  0  0  0  0  0  0  0  0  0  0  13
-0.2476  0.2287  -2.3350 O  0  0  0  0  0  0  0  0  0  0  0  0  0  14
-1.5848  -0.3812  2.6027 H  0  0  0  0  0  0  0  0  0  0  0  0  0  15
0.7730  -0.6014  1.8357 H  0  0  0  0  0  0  0  0  0  0  0  0  0  16
-2.5449  0.4159  -1.4306 H  0  0  0  0  0  0  0  0  0  0  0  0  0  17
2  1  0  0  0  0
3  1  0  0  0  0
5  4  0  0  0  0
6  4  0  0  0  0
8  7  0  0  0  0
12  7  0  0  0  0
16  7  0  0  0  0
9  8  0  0  0  0
15  8  0  0  0  0
10  9  0  0  0  0
13  9  0  0  0  0
11  10  0  0  0  0
12  11  0  0  0  0
14  11  0  0  0  0
10  17  0  0  0  0
M  END
$$$
uracil.sdf
COSMOTHERM      3D      0
18 16 0 0 0 0 0 0 0 0 0 V2000
-4.6348  0.9766  0.2501 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-4.9546  0.6782  1.1209 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-5.4471  1.1105  -0.2716 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-2.8979  -0.7432  -0.9545 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
-3.5562  -0.1532  -0.4875 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-3.1881  -1.6528  -0.7644 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
0.5401  -0.0695  -1.4915 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
1.8769  0.1800  -1.4067 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
2.5119  0.2270  -0.1098 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
1.6307  -0.0061  0.9646 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0  10
0.2671  -0.2666  0.9004 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  11
-0.2398  -0.2840  -0.3885 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0  12
3.7138  0.4463  0.1147 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  13
-0.4244  -0.4636  1.9040 O  0  0  0  0  0  0  0  0  0  0  0  0  0  0  14
2.4779  0.3467  -2.2968 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  15
0.0141  -0.1139  -2.4451 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  16
2.0351  0.0153  1.9022 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  17

```



```

1
2
3      -1.2690  -0.4728  -0.5089 H  0  0  0  0  0  0  0  0  0  0  0  0  18
4      2  1  0  0  0  0
5      3  1  0  0  0  0
6      5  4  0  0  0  0
7      6  4  0  0  0  0
8      8  7  0  0  0  0
9     12  7  0  0  0  0
10    16  7  0  0  0  0
11    9  8  0  0  0  0
12   15  8  0  0  0  0
13   10  9  0  0  0  0
14   13  9  0  0  0  0
15   11 10  0  0  0  0
16   17 10  0  0  0  0
17   12 11  0  0  0  0
18   14 11  0  0  0  0
19   12 18  0  0  0  0
20 M  END
21 $$$$

```

S4 d) Bare Bases & Cations

1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
 COSMOTHERM 3D 0

```

33 35 0 0 0 0 0 0 0 0 0 V2000
34 -3.1559  0.5382  1.7695 C  0  0  0  0  0  0  0  0  0  0  0  0  0  1
35 -2.5277 -1.8007  0.1659 C  0  0  0  0  0  0  0  0  0  0  0  0  0  2
36 -2.0420 -3.0290 -0.2759 C  0  0  0  0  0  0  0  0  0  0  0  0  0  3
37 -0.7421 -3.1295 -0.7890 C  0  0  0  0  0  0  0  0  0  0  0  0  0  4
38  0.0639 -1.9958 -0.8327 C  0  0  0  0  0  0  0  0  0  0  0  0  0  5
39 -0.4028 -0.7375 -0.3972 C  0  0  0  0  0  0  0  0  0  0  0  0  0  6
40 -1.7307 -0.6423  0.0980 C  0  0  0  0  0  0  0  0  0  0  0  0  0  7
41  0.4987  0.4397 -0.4754 C  0  0  0  0  0  0  0  0  0  0  0  0  0  8
42 -2.2685  0.5788  0.5937 N  0  0  0  0  0  0  0  0  0  0  0  0  0  9
43  0.1203  1.6094 -0.8876 N  0  0  0  0  0  0  0  0  0  0  0  0  0 10
44 -1.2698  1.7572 -1.3165 C  0  0  0  0  0  0  0  0  0  0  0  0  0 11
45 -2.1806  1.7739 -0.0936 C  0  0  0  0  0  0  0  0  0  0  0  0  0 12
46  1.9278  0.2799 -0.0794 C  0  0  0  0  0  0  0  0  0  0  0  0  0 13
47  2.9241  1.0347 -0.7279 C  0  0  0  0  0  0  0  0  0  0  0  0  0 14
48  2.3026 -0.5833  0.9673 C  0  0  0  0  0  0  0  0  0  0  0  0  0 15
49  4.2607  0.9262 -0.3402 C  0  0  0  0  0  0  0  0  0  0  0  0  0 16
50  3.6399 -0.6800  1.3635 C  0  0  0  0  0  0  0  0  0  0  0  0  0 17
51  4.6230  0.0708  0.7091 C  0  0  0  0  0  0  0  0  0  0  0  0  0 18
52 -2.7774  2.7898  0.2833 O  0  0  0  0  0  0  0  0  0  0  0  0  0 19
53 -2.8299 -0.2684  2.4339 H  0  0  0  0  0  0  0  0  0  0  0  0  0 20
54 -3.0800  1.4991  2.2888 H  0  0  0  0  0  0  0  0  0  0  0  0  0 21
55 -4.2057  0.3793  1.4819 H  0  0  0  0  0  0  0  0  0  0  0  0  0 22
56 -3.5437 -1.7313  0.5535 H  0  0  0  0  0  0  0  0  0  0  0  0  0 23
57 -2.6850 -3.9091 -0.2273 H  0  0  0  0  0  0  0  0  0  0  0  0  0 24
58 -0.3608 -4.0869 -1.1462 H  0  0  0  0  0  0  0  0  0  0  0  0  0 25
59  1.0810 -2.0689 -1.2197 H  0  0  0  0  0  0  0  0  0  0  0  0  0 26
60 -1.5852  0.9450 -1.9975 H  0  0  0  0  0  0  0  0  0  0  0  0  0 27
61 -1.3894  2.7175 -1.8290 H  0  0  0  0  0  0  0  0  0  0  0  0  0 28
62  2.6365  1.6991 -1.5437 H  0  0  0  0  0  0  0  0  0  0  0  0  0 29
63  1.5422 -1.1684  1.4868 H  0  0  0  0  0  0  0  0  0  0  0  0  0 30
64  5.0249  1.5065 -0.8606 H  0  0  0  0  0  0  0  0  0  0  0  0  0 31
65  3.9137 -1.3437  2.1856 H  0  0  0  0  0  0  0  0  0  0  0  0  0 32
66  5.6682 -0.0122  1.0125 H  0  0  0  0  0  0  0  0  0  0  0  0  0 33

```

```

9  1  0  0  0  0
20 1  0  0  0  0
21 1  0  0  0  0
22 1  0  0  0  0
3  2  0  0  0  0
7  2  0  0  0  0
23 2  0  0  0  0
4  3  0  0  0  0
24 3  0  0  0  0
5  4  0  0  0  0
25 4  0  0  0  0
6  5  0  0  0  0
26 5  0  0  0  0
7  6  0  0  0  0
8  6  0  0  0  0
9  7  0  0  0  0
10 8  0  0  0  0
13 8  0  0  0  0
12 9  0  0  0  0
11 10 0  0  0  0
12 11 0  0  0  0
27 11 0  0  0  0
28 11 0  0  0  0
19 12 0  0  0  0
14 13 0  0  0  0
15 13 0  0  0  0
16 14 0  0  0  0
29 14 0  0  0  0
17 15 0  0  0  0
30 15 0  0  0  0
18 16 0  0  0  0
31 16 0  0  0  0
18 17 0  0  0  0
32 17 0  0  0  0
18 33 0  0  0  0

```

```

M  END
$$$$
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one_p1.sdf
COSMOTHERM 3D 0

```

```

34 36 0 0 0 0 0 0 0 0 0 V2000
35 -2.5140 -1.8206  0.0979 C  0  0  0  0  0  0  0  0  0  0  0  0  0  1

```


1
2
3 -4.1985 -1.5066 -1.9222 H 0 0 0 0 0 0 0 0 0 0 31
4 -5.7811 0.1549 -0.9421 H 0 0 0 0 0 0 0 0 0 0 32
5 -4.9341 1.8896 0.6394 H 0 0 0 0 0 0 0 0 0 0 33
6 2.0691 3.3864 0.6938 H 0 0 0 0 0 0 0 0 0 0 34
7 2 1 0 0 0 0
8 6 1 0 0 0 0
9 20 1 0 0 0 0
10 3 2 0 0 0 0
11 21 2 0 0 0 0
12 4 3 0 0 0 0
13 22 3 0 0 0 0
14 5 4 0 0 0 0
15 7 4 0 0 0 0
16 6 5 0 0 0 0
17 8 5 0 0 0 0
18 23 6 0 0 0 0
19 11 7 0 0 0 0
20 14 7 0 0 0 0
21 9 8 0 0 0 0
22 12 8 0 0 0 0
23 10 9 0 0 0 0
24 13 9 0 0 0 0
25 11 10 0 0 0 0
26 24 10 0 0 0 0
27 25 10 0 0 0 0
28 26 12 0 0 0 0
29 27 12 0 0 0 0
30 28 12 0 0 0 0
31 15 14 0 0 0 0
32 16 14 0 0 0 0
33 19 15 0 0 0 0
34 29 15 0 0 0 0
35 17 16 0 0 0 0
36 30 16 0 0 0 0
37 18 17 0 0 0 0
38 31 17 0 0 0 0
39 19 18 0 0 0 0
40 32 18 0 0 0 0
41 33 19 0 0 0 0
42 25 34 0 0 0 0
M END
\$\$\$\$
1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one_p1.sdf
COSMOtherm 3D 0
35 37 0 0 0 0 0 0 0 0 0 0 V2000
1.6473 -3.3298 0.6106 C 0 0 0 0 0 0 0 0 0 0 1
0.3329 -3.2493 1.0888 C 0 0 0 0 0 0 0 0 0 0 2
-0.3657 -2.0581 0.9605 C 0 0 0 0 0 0 0 0 0 0 3
0.2297 -0.9117 0.3792 C 0 0 0 0 0 0 0 0 0 0 4
1.5777 -0.9991 -0.0896 C 0 0 0 0 0 0 0 0 0 0 5
2.2554 -2.2230 0.0241 C 0 0 0 0 0 0 0 0 0 0 6
-0.5806 0.2961 0.2775 C 0 0 0 0 0 0 0 0 0 0 7
2.2425 0.0634 -0.7657 N 0 0 0 0 0 0 0 0 0 0 8
2.2815 1.3464 -0.3012 C 0 0 0 0 0 0 0 0 0 0 9
1.3875 1.6560 0.9185 C 0 0 0 0 0 0 0 0 0 0 10
-0.0096 1.4692 0.4657 N 0 0 0 0 0 0 0 0 0 0 11
3.1040 -0.2584 -1.9237 C 0 0 0 0 0 0 0 0 0 0 12
2.9379 2.2575 -0.8105 O 0 0 0 0 0 0 0 0 0 0 13
-2.0156 0.2550 -0.0173 C 0 0 0 0 0 0 0 0 0 0 14
-2.8860 1.2105 0.5506 C 0 0 0 0 0 0 0 0 0 0 15
-2.5268 -0.7121 -0.9087 C 0 0 0 0 0 0 0 0 0 0 16
-3.8823 -0.7105 -1.2335 C 0 0 0 0 0 0 0 0 0 0 17
-4.7406 0.2376 -0.6639 C 0 0 0 0 0 0 0 0 0 0 18
-4.2415 1.1938 0.2306 C 0 0 0 0 0 0 0 0 0 0 19
2.2090 -4.2601 0.7024 H 0 0 0 0 0 0 0 0 0 0 20
-0.1399 -4.1116 1.5585 H 0 0 0 0 0 0 0 0 0 0 21
-1.3844 -1.9821 1.3392 H 0 0 0 0 0 0 0 0 0 0 22
3.2787 -2.3022 -0.3399 H 0 0 0 0 0 0 0 0 0 0 23
1.5695 0.9476 1.7423 H 0 0 0 0 0 0 0 0 0 0 24
1.5771 2.9625 1.3348 O 0 0 0 0 0 0 0 0 0 0 25
2.6741 -1.1125 -2.4549 H 0 0 0 0 0 0 0 0 0 0 26
4.1292 -0.4885 -1.6045 H 0 0 0 0 0 0 0 0 0 0 27
3.1248 0.6158 -2.5823 H 0 0 0 0 0 0 0 0 0 0 28
-2.5111 1.9350 1.2756 H 0 0 0 0 0 0 0 0 0 0 29
-1.8566 -1.4379 -1.3696 H 0 0 0 0 0 0 0 0 0 0 30
-4.2699 -1.4493 -1.9359 H 0 0 0 0 0 0 0 0 0 0 31
-5.8026 0.2296 -0.9136 H 0 0 0 0 0 0 0 0 0 0 32
-4.9138 1.9202 0.6884 H 0 0 0 0 0 0 0 0 0 0 33
2.1025 3.3981 0.6193 H 0 0 0 0 0 0 0 0 0 0 34
-0.5319 2.3326 0.2879 H 0 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0
6 1 0 0 0 0
20 1 0 0 0 0
3 2 0 0 0 0
21 2 0 0 0 0
4 3 0 0 0 0
22 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
23 6 0 0 0 0
11 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
26 12 0 0 0 0
27 12 0 0 0 0
28 12 0 0 0 0

15 14 0 0 0 0
 16 14 0 0 0 0
 19 15 0 0 0 0
 29 15 0 0 0 0
 17 16 0 0 0 0
 30 16 0 0 0 0
 18 17 0 0 0 0
 31 17 0 0 0 0
 19 18 0 0 0 0
 32 18 0 0 0 0
 33 19 0 0 0 0
 34 25 0 0 0 0
 11 35 0 0 0 0

M END

\$\$\$\$

1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one.sdf

COSMOTHERM 3D 0

31 33 0 0 0 0 0 0 0 0 0 V2000
 0.5145 -3.2825 -0.9215 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
 -0.1408 -2.0552 -0.9137 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
 0.4201 -0.9208 -0.2872 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
 1.6892 -1.0618 0.3311 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 2.3275 -2.3139 0.3574 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 1.7462 -3.4150 -0.2641 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
 2.3246 0.0097 0.9993 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
 -0.3379 0.3568 -0.2491 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
 0.1958 1.5303 -0.3966 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
 1.6134 1.6188 -0.7086 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
 -1.8101 0.3044 -0.0162 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
 -2.6479 1.2608 -0.6206 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
 -2.3806 -0.6581 0.8378 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
 -4.0231 1.2506 -0.3811 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
 -4.5814 0.2931 0.4764 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
 -3.7559 -0.6572 1.0878 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
 2.3914 1.3046 0.5802 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
 3.0037 2.1900 1.1890 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
 1.9545 2.9130 -1.1531 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
 0.0651 -4.1381 -1.4269 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
 -1.1093 -1.9558 -1.4050 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
 3.2914 -2.4070 0.8609 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
 2.2600 -4.3772 -0.2455 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
 2.9356 -0.2308 1.7818 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
 1.8951 0.8973 -1.4980 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
 -2.2080 2.0044 -1.2867 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
 -1.7444 -1.3979 1.3254 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
 -4.6635 1.9887 -0.8674 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 28
 -5.6564 0.2871 0.6651 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29
 -4.1830 -1.4009 1.7629 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 30
 2.3465 3.3668 -0.3722 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 31

2 1 0 0 0 0
 6 1 0 0 0 0
 20 1 0 0 0 0
 3 2 0 0 0 0
 21 2 0 0 0 0
 4 3 0 0 0 0
 8 3 0 0 0 0
 5 4 0 0 0 0
 7 4 0 0 0 0
 6 5 0 0 0 0
 22 5 0 0 0 0
 23 6 0 0 0 0
 17 7 0 0 0 0
 24 7 0 0 0 0
 9 8 0 0 0 0
 11 8 0 0 0 0
 10 9 0 0 0 0
 17 10 0 0 0 0
 19 10 0 0 0 0
 25 10 0 0 0 0
 12 11 0 0 0 0
 13 11 0 0 0 0
 14 12 0 0 0 0
 26 12 0 0 0 0
 16 13 0 0 0 0
 27 13 0 0 0 0
 15 14 0 0 0 0
 28 14 0 0 0 0
 16 15 0 0 0 0
 29 15 0 0 0 0
 30 16 0 0 0 0
 18 17 0 0 0 0
 19 31 0 0 0 0

M END

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1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one_p1.sdf

COSMOTHERM 3D 0

32 34 0 0 0 0 0 0 0 0 0 V2000
 -3.3101 -0.4252 -0.8747 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
 -2.0811 0.2156 -0.8508 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
 -0.9402 -0.3940 -0.2697 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
 -1.0790 -1.7028 0.2850 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 -2.3414 -2.3165 0.2928 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 -3.4422 -1.6897 -0.2813 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
 -0.0328 -2.3972 0.9266 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
 0.2947 0.3760 -0.2033 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
 1.4605 -0.2324 -0.3137 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
 1.6497 -1.6491 -0.6964 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
 0.2944 1.8293 -0.0030 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
 1.2784 2.6302 -0.6222 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
 -0.6585 2.4283 0.8481 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
 1.3028 4.0043 -0.3938 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
 0.3602 4.5910 0.4608 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
 -0.6155 3.8018 1.0819 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16

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23 10 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
28 18 0 0 0 0
10 30 0 0 0 0
M END
$$$$
1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one_p2.sdf
COSMOTHERM 3D 0

31 33 0 0 0 0 0 0 0 0 0 V2000
2.1892 3.0098 -0.1068 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.9070 3.0900 -0.6731 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
0.1202 1.9512 -0.7423 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.5949 0.6945 -0.2863 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.9207 0.6170 0.2408 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.6849 1.7923 0.3450 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.3176 -0.4371 -0.3040 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
2.4905 -0.5592 0.7583 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.4522 -1.8301 0.2276 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.4905 -1.9870 -0.9493 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.1337 -1.6573 -0.5327 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
3.1395 -2.7462 0.6696 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.7569 -0.2784 -0.0596 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.6861 -1.0864 -0.7499 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.2168 0.6483 0.8996 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-3.5804 0.7508 1.1705 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-4.4969 -0.0513 0.4798 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-4.0484 -0.9659 -0.4818 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
2.8100 3.9030 -0.0274 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
0.5274 4.0400 -1.0486 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.8785 2.0056 -1.1740 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
3.6846 1.7319 0.7777 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
1.7945 -1.3193 -1.7701 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
-2.3467 -1.7749 -1.5258 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
-1.5032 1.2582 1.4538 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
-3.9292 1.4571 1.9249 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
-5.5640 0.0385 0.6883 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
-4.7637 -1.5775 -1.0328 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 28
1.5079 -3.0231 -1.2935 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29
3.2258 -0.4236 1.4556 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 30
-0.5072 -2.4414 -0.3954 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 31

2 1 0 0 0 0
6 1 0 0 0 0
19 1 0 0 0 0
3 2 0 0 0 0
20 2 0 0 0 0
4 3 0 0 0 0
21 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
22 6 0 0 0 0
11 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
30 8 0 0 0 0
10 9 0 0 0 0
12 9 0 0 0 0
11 10 0 0 0 0
23 10 0 0 0 0
29 10 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
18 14 0 0 0 0
24 14 0 0 0 0
16 15 0 0 0 0
25 15 0 0 0 0
17 16 0 0 0 0
26 16 0 0 0 0
18 17 0 0 0 0
27 17 0 0 0 0
28 18 0 0 0 0
11 31 0 0 0 0
M END
$$$$
1-methylindole-cation0.sdf
COSMOTHERM 3D 0

20 21 0 0 0 0 0 0 0 0 0 V2000
-2.1556 -1.1270 0.0657 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.5622 0.1959 -0.1619 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.6357 1.2459 -0.2123 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.2834 0.9406 -0.0289 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.0887 -0.3919 0.1966 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.8002 -1.4481 0.2536 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.5647 -0.4426 0.3564 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.9277 1.7585 -0.0136 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.9942 0.9767 0.2092 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2580 -1.3673 -0.6218 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.8989 -1.9239 0.1000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-3.6223 0.4108 -0.3025 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.9594 2.2721 -0.3872 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.4833 -2.4749 0.4354 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
0.9671 2.8353 -0.1596 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
3.0555 1.1836 0.2983 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16

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5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 10 0 0 0 0
19 10 0 0 0 0
10 20 0 0 0 0
M END
$$$$
1-methylindole.sdf
COSMOtherm 3D 0
19 20 0 0 0 0 0 0 0 0 V2000
1.4007 -2.4885 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.8514 -0.7865 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.9724 0.3481 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.1675 1.7446 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.0554 2.5850 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
1.2570 2.0575 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.4859 0.6809 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.3670 -0.1661 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.0522 -1.9113 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
0.2844 -1.5493 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
1.3705 -3.1238 -0.8959 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
2.3429 -1.9312 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
1.3703 -3.1240 0.8958 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.9379 -0.7771 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.1776 2.1606 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.1955 3.6678 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
2.1094 2.7393 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2.5038 0.2877 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-1.3268 -2.9628 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
10 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
10 8 0 0 0 0
10 9 0 0 0 0
9 19 0 0 0 0
M END
$$$$
1-methylpyrrole-cation0.sdf
COSMOtherm 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
-0.7328 1.3841 -0.1824 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
0.7327 1.3842 -0.1825 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.1730 0.1660 0.1693 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.0000 -0.7000 0.4220 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1730 0.1661 0.1693 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3612 2.2349 -0.4317 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.3612 2.2349 -0.4318 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.1601 -0.2646 0.2976 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0000 -1.9666 -0.4123 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.1601 -0.2647 0.2977 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0002 -0.9798 1.4184 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.8987 -2.5364 -0.1606 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.0010 -1.6722 -1.4656 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.8998 -2.5353 -0.1621 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
10 5 0 0 0 0
12 9 0 0 0 0
13 9 0 0 0 0
9 14 0 0 0 0
M END
$$$$
1-methylpyrrole-cation1.sdf
COSMOtherm 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
0.6199 1.5303 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.7391 1.4695 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
1.1642 0.1513 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0379 -0.6861 -0.0019 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.1051 0.0794 -0.0009 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.0033 -2.1517 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6

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1
2
3      1.2467   2.4187   0.0012 H   0 0 0 0 0 0 0 0 0 0 0 7
4     -1.4491   2.2912   0.0017 H   0 0 0 0 0 0 0 0 0 0 0 8
5     -2.1068  -0.3477  -0.0015 H   0 0 0 0 0 0 0 0 0 0 0 9
6      1.7792  -0.0742   0.8867 H   0 0 0 0 0 0 0 0 0 0 0 10
7      1.7790  -0.0723  -0.8888 H   0 0 0 0 0 0 0 0 0 0 0 11
8     -0.4683  -2.5292   0.9200 H   0 0 0 0 0 0 0 0 0 0 0 12
9      1.0410  -2.4743  -0.0387 H   0 0 0 0 0 0 0 0 0 0 0 13
10     -0.5393  -2.5343  -0.8748 H   0 0 0 0 0 0 0 0 0 0 0 14
11
12      2 1 0 0 0 0
13      3 1 0 0 0 0
14      7 1 0 0 0 0
15      5 2 0 0 0 0
16      8 2 0 0 0 0
17      4 3 0 0 0 0
18     10 3 0 0 0 0
19     11 3 0 0 0 0
20      5 4 0 0 0 0
21      6 4 0 0 0 0
22      9 5 0 0 0 0
23     12 6 0 0 0 0
24     13 6 0 0 0 0
25     6 14 0 0 0 0
26
27 M  END
28 $$$
29 1-methylpyrrole-cation2.sdf
30 COSMOTHERM      3D      0
31
32 14 14 0 0 0 0 0 0 0 0 0 V2000
33   0.7186   1.4840   0.0001 C   0 0 0 0 0 0 0 0 0 0 0 1
34  -0.7755   1.4249   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 2
35   1.1110   0.0612  -0.0001 C   0 0 0 0 0 0 0 0 0 0 0 3
36   0.0355  -0.6820   0.0000 N   0 0 0 0 0 0 0 0 0 0 0 4
37  -1.1451   0.1320   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 5
38   1.1407   2.0114  -0.8754 H   0 0 0 0 0 0 0 0 0 0 0 6
39   1.1405   2.0109   0.8759 H   0 0 0 0 0 0 0 0 0 0 0 7
40  -0.0135  -2.1469   0.0000 C   0 0 0 0 0 0 0 0 0 0 0 8
41  -1.4339   2.2880   0.0000 H   0 0 0 0 0 0 0 0 0 0 0 9
42   2.1106  -0.3669   0.0000 H   0 0 0 0 0 0 0 0 0 0 0 10
43  -2.1175  -0.3500   0.0001 H   0 0 0 0 0 0 0 0 0 0 0 11
44  -0.5490  -2.4817   0.8961 H   0 0 0 0 0 0 0 0 0 0 0 12
45   1.0080  -2.5369   0.0000 H   0 0 0 0 0 0 0 0 0 0 0 13
46  -0.5490  -2.4817  -0.8961 H   0 0 0 0 0 0 0 0 0 0 0 14
47
48      2 1 0 0 0 0
49      3 1 0 0 0 0
50      6 1 0 0 0 0
51      7 1 0 0 0 0
52      5 2 0 0 0 0
53      9 2 0 0 0 0
54      4 3 0 0 0 0
55     10 3 0 0 0 0
56      5 4 0 0 0 0
57      8 4 0 0 0 0
58     11 5 0 0 0 0
59     12 8 0 0 0 0
60     13 8 0 0 0 0
61     8 14 0 0 0 0
62
63 M  END
64 $$$
65 1-methylpyrrole.sdf
66 COSMOTHERM      3D      0
67
68 13 13 0 0 0 0 0 0 0 0 0 V2000
69  -0.7135   1.4603  -0.0135 C   0 0 0 0 0 0 0 0 0 0 0 1
70   0.7136   1.4602  -0.0135 C   0 0 0 0 0 0 0 0 0 0 0 2
71  -1.1240   0.1342   0.0110 C   0 0 0 0 0 0 0 0 0 0 0 3
72   0.0000  -0.6644   0.0317 N   0 0 0 0 0 0 0 0 0 0 0 4
73   1.1241   0.1340   0.0111 C   0 0 0 0 0 0 0 0 0 0 0 5
74   0.0000  -2.1239  -0.0245 C   0 0 0 0 0 0 0 0 0 0 0 6
75  -1.3679   2.3281  -0.0187 H   0 0 0 0 0 0 0 0 0 0 0 7
76   1.3681   2.3279  -0.0186 H   0 0 0 0 0 0 0 0 0 0 0 8
77  -2.1163  -0.3070   0.0199 H   0 0 0 0 0 0 0 0 0 0 0 9
78   2.1164  -0.3071   0.0198 H   0 0 0 0 0 0 0 0 0 0 0 10
79   0.0211  -2.4806  -1.0645 H   0 0 0 0 0 0 0 0 0 0 0 11
80  -0.9025  -2.5066   0.4665 H   0 0 0 0 0 0 0 0 0 0 0 12
81   0.8800  -2.5095   0.5040 H   0 0 0 0 0 0 0 0 0 0 0 13
82
83      2 1 0 0 0 0
84      3 1 0 0 0 0
85      7 1 0 0 0 0
86      5 2 0 0 0 0
87      8 2 0 0 0 0
88      4 3 0 0 0 0
89      9 3 0 0 0 0
90      5 4 0 0 0 0
91      6 4 0 0 0 0
92     10 5 0 0 0 0
93     11 6 0 0 0 0
94     12 6 0 0 0 0
95     6 13 0 0 0 0
96
97 M  END
98 $$$
99 2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine_new.sdf
100 COSMOTHERM      3D      0
101
102 34 36 0 0 0 0 0 0 0 0 0 V2000
103   0.9866   3.7460  -1.3608 H   0 0 0 0 0 0 0 0 0 0 0 1
104   1.2460   2.7785  -0.9292 C   0 0 0 0 0 0 0 0 0 0 0 2
105   0.3300   1.7264  -0.9514 C   0 0 0 0 0 0 0 0 0 0 0 3
106   0.6325   0.4629  -0.4126 C   0 0 0 0 0 0 0 0 0 0 0 4
107   1.9223   0.2397   0.1704 C   0 0 0 0 0 0 0 0 0 0 0 5
108   2.8235   1.3294   0.2122 C   0 0 0 0 0 0 0 0 0 0 0 6
109   2.4921   2.5729  -0.3263 C   0 0 0 0 0 0 0 0 0 0 0 7
110   2.2413  -0.9814   0.7815 N   0 0 0 0 0 0 0 0 0 0 0 8
111   2.1516  -2.2417   0.0094 C   0 0 0 0 0 0 0 0 0 0 0 9
112   1.1893  -2.1581  -1.1655 C   0 0 0 0 0 0 0 0 0 0 0 10
113  -0.1731  -1.8364  -0.7422 N   0 0 0 0 0 0 0 0 0 0 0 11

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1
2
3 -0.4075 -0.6018 -0.4296 C 0 0 0 0 0 0 0 0 0 0 0 0 12
4 -1.8089 -0.2387 -0.0603 C 0 0 0 0 0 0 0 0 0 0 0 0 13
5 -2.8904 -0.9137 -0.6586 C 0 0 0 0 0 0 0 0 0 0 0 0 14
6 -4.2048 -0.6119 -0.2967 C 0 0 0 0 0 0 0 0 0 0 0 0 15
7 -4.4612 0.3617 0.6784 C 0 0 0 0 0 0 0 0 0 0 0 0 16
8 -3.3938 1.0341 1.2844 C 0 0 0 0 0 0 0 0 0 0 0 0 17
9 -2.0776 0.7428 0.9121 C 0 0 0 0 0 0 0 0 0 0 0 0 18
10 3.3699 -1.0144 1.7096 C 0 0 0 0 0 0 0 0 0 0 0 0 19
11 -0.6563 1.8799 -1.3931 H 0 0 0 0 0 0 0 0 0 0 0 0 20
12 3.8096 1.1933 0.6545 H 0 0 0 0 0 0 0 0 0 0 0 0 21
13 3.2236 3.3828 -0.2860 H 0 0 0 0 0 0 0 0 0 0 0 0 22
14 1.8429 -3.0437 0.6983 H 0 0 0 0 0 0 0 0 0 0 0 0 23
15 3.1549 -2.5101 -0.3806 H 0 0 0 0 0 0 0 0 0 0 0 0 24
16 1.1808 -3.1385 -1.6628 H 0 0 0 0 0 0 0 0 0 0 0 0 25
17 1.5657 -1.4167 -1.8945 H 0 0 0 0 0 0 0 0 0 0 0 0 26
18 -2.6838 -1.6709 -1.4162 H 0 0 0 0 0 0 0 0 0 0 0 0 27
19 -5.0339 -1.1326 -0.7796 H 0 0 0 0 0 0 0 0 0 0 0 0 28
20 -5.4889 0.5968 0.9616 H 0 0 0 0 0 0 0 0 0 0 0 0 29
21 -3.5855 1.7886 2.0495 H 0 0 0 0 0 0 0 0 0 0 0 0 30
22 -1.2505 1.2692 1.3908 H 0 0 0 0 0 0 0 0 0 0 0 0 31
23 3.3076 -0.1793 2.4187 H 0 0 0 0 0 0 0 0 0 0 0 0 32
24 3.3175 -1.9530 2.2784 H 0 0 0 0 0 0 0 0 0 0 0 0 33
25 4.3532 -0.9812 1.2007 H 0 0 0 0 0 0 0 0 0 0 0 0 34
26
27 2 1 0 0 0 0 0
28 3 2 0 0 0 0 0
29 7 2 0 0 0 0 0
30 4 3 0 0 0 0 0
31 20 3 0 0 0 0 0
32 5 4 0 0 0 0 0
33 12 4 0 0 0 0 0
34 6 5 0 0 0 0 0
35 8 5 0 0 0 0 0
36 7 6 0 0 0 0 0
37 21 6 0 0 0 0 0
38 22 7 0 0 0 0 0
39 9 8 0 0 0 0 0
40 19 8 0 0 0 0 0
41 10 9 0 0 0 0 0
42 23 9 0 0 0 0 0
43 24 9 0 0 0 0 0
44 11 10 0 0 0 0 0
45 25 10 0 0 0 0 0
46 26 10 0 0 0 0 0
47 12 11 0 0 0 0 0
48 13 12 0 0 0 0 0
49 14 13 0 0 0 0 0
50 18 13 0 0 0 0 0
51 15 14 0 0 0 0 0
52 27 14 0 0 0 0 0
53 16 15 0 0 0 0 0
54 28 15 0 0 0 0 0
55 17 16 0 0 0 0 0
56 29 16 0 0 0 0 0
57 18 17 0 0 0 0 0
58 30 17 0 0 0 0 0
59 31 18 0 0 0 0 0
60 32 19 0 0 0 0 0
33 19 0 0 0 0 0
19 34 0 0 0 0 0
M END
$$$$
2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine_p1.sdf
COSMOtherm 3D 0
35 37 0 0 0 0 0 0 0 0 0 V2000
-2.3792 0.3792 -2.6518 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.0542 0.8148 -2.8345 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.1949 0.7795 -1.7536 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.6047 0.3405 -0.4627 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.9807 -0.0858 -0.2660 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.8215 -0.0604 -1.4152 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.4196 0.2997 0.5553 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.4843 -0.6189 0.9005 N 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.2106 -0.1117 2.2583 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.1746 0.9921 2.2885 C 0 0 0 0 0 0 0 0 0 0 0 0 10
0.1253 0.5147 1.8263 N 0 0 0 0 0 0 0 0 0 0 0 0 11
1.8334 0.0211 0.2364 C 0 0 0 0 0 0 0 0 0 0 0 0 12
2.8612 0.7183 0.9044 C 0 0 0 0 0 0 0 0 0 0 0 0 13
4.1976 0.4188 0.6379 C 0 0 0 0 0 0 0 0 0 0 0 0 14
4.5226 -0.5829 -0.2851 C 0 0 0 0 0 0 0 0 0 0 0 0 15
3.5069 -1.2836 -0.9472 C 0 0 0 0 0 0 0 0 0 0 0 0 16
2.1684 -0.9811 -0.6965 C 0 0 0 0 0 0 0 0 0 0 0 0 17
-3.7211 -1.4059 0.8646 C 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.0832 0.4053 -3.4856 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.7125 1.1794 -3.8030 H 0 0 0 0 0 0 0 0 0 0 0 0 20
0.8330 1.1208 -1.8728 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-3.8630 -0.3559 -1.3123 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-1.8911 -0.9455 2.9011 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-3.1539 0.2849 2.6745 H 0 0 0 0 0 0 0 0 0 0 0 0 24
-1.4812 1.8380 1.6558 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.0550 1.3514 3.3159 H 0 0 0 0 0 0 0 0 0 0 0 0 26
2.6148 1.5189 1.6041 H 0 0 0 0 0 0 0 0 0 0 0 0 27
4.9875 0.9761 1.1432 H 0 0 0 0 0 0 0 0 0 0 0 0 28
5.5687 -0.8167 -0.4892 H 0 0 0 0 0 0 0 0 0 0 0 0 29
3.7585 -2.0703 -1.6597 H 0 0 0 0 0 0 0 0 0 0 0 0 30
1.3781 -1.5388 -1.1996 H 0 0 0 0 0 0 0 0 0 0 0 0 31
-4.6236 -0.7707 0.8348 H 0 0 0 0 0 0 0 0 0 0 0 0 32
-3.7223 -2.0819 0.0022 H 0 0 0 0 0 0 0 0 0 0 0 0 33
-3.7590 -2.0145 1.7772 H 0 0 0 0 0 0 0 0 0 0 0 0 34
0.8496 0.3558 2.5272 H 0 0 0 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0 0
6 1 0 0 0 0 0
19 1 0 0 0 0 0
3 2 0 0 0 0 0
20 2 0 0 0 0 0
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4 3 0 0 0 0
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22 6 0 0 0 0
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26 10 0 0 0 0
13 12 0 0 0 0
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14 13 0 0 0 0
27 13 0 0 0 0
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28 14 0 0 0 0
16 15 0 0 0 0
29 15 0 0 0 0
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30 16 0 0 0 0
31 17 0 0 0 0
32 18 0 0 0 0
33 18 0 0 0 0
34 18 0 0 0 0
11 35 0 0 0 0
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M END

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2-aminopyridine.sdf

COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000

```
-2.2780 -0.0273 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.9128 -0.0281 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.3019 1.1823 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 3
1.0458 1.2052 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.8509 0.0680 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
1.2078 -1.1821 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.1778 -1.2433 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.7796 0.8539 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.8082 -0.8899 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
1.4975 2.2020 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
2.9372 0.1541 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
1.7914 -2.1048 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.7022 -2.2004 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0 0
8 1 0 0 0 0 0
9 1 0 0 0 0 0
3 2 0 0 0 0 0
7 2 0 0 0 0 0
4 3 0 0 0 0 0
5 4 0 0 0 0 0
10 4 0 0 0 0 0
6 5 0 0 0 0 0
11 5 0 0 0 0 0
7 6 0 0 0 0 0
12 6 0 0 0 0 0
7 13 0 0 0 0 0
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M END

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2-aminopyridine0.sdf

COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000

```
-1.0459 -1.2059 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.8505 -0.0683 -0.0035 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.2095 1.1817 0.0007 C 0 0 0 0 0 0 0 0 0 0 0 3
0.1773 1.2420 0.0038 C 0 0 0 0 0 0 0 0 0 0 0 4
0.9100 0.0286 0.0058 C 0 0 0 0 0 0 0 0 0 0 0 5
0.3019 -1.1802 0.0070 N 0 0 0 0 0 0 0 0 0 0 0 6
2.2875 0.0281 -0.0473 N 0 0 0 0 0 0 0 0 0 0 0 7
2.7413 -0.8423 0.2206 H 0 0 0 0 0 0 0 0 0 0 0 8
2.7710 0.8684 0.2572 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.4970 -2.2028 0.0007 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.9369 -0.1547 -0.0059 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.7937 2.1039 0.0030 H 0 0 0 0 0 0 0 0 0 0 0 12
0.7017 2.1991 0.0062 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0 0
6 1 0 0 0 0 0
10 1 0 0 0 0 0
3 2 0 0 0 0 0
11 2 0 0 0 0 0
4 3 0 0 0 0 0
12 3 0 0 0 0 0
5 4 0 0 0 0 0
6 5 0 0 0 0 0
7 5 0 0 0 0 0
8 7 0 0 0 0 0
9 7 0 0 0 0 0
4 13 0 0 0 0 0
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M END

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2-aminopyridine1.sdf

COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000

```
1.0458 -1.2052 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
1.8508 -0.0680 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
1.2079 1.1821 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
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-0.1778 1.2433 0.0001 C 0 0 0 0 0 0 0 0 0 0 4  
-0.9128 0.0281 0.0000 C 0 0 0 0 0 0 0 0 0 0 5  
-0.3019 -1.1822 0.0000 N 0 0 0 0 0 0 0 0 0 0 6  
-2.2780 0.0273 0.0001 N 0 0 0 0 0 0 0 0 0 0 7  
-2.7796 -0.8539 0.0003 H 0 0 0 0 0 0 0 0 0 0 8  
-2.8083 0.8899 -0.0013 H 0 0 0 0 0 0 0 0 0 0 9  
1.4975 -2.2021 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10  
2.9372 -0.1540 0.0000 H 0 0 0 0 0 0 0 0 0 0 11  
1.7915 2.1049 0.0000 H 0 0 0 0 0 0 0 0 0 0 12  
-0.7023 2.2004 0.0001 H 0 0 0 0 0 0 0 0 0 0 13
```

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2 1 0 0 0 0  
6 1 0 0 0 0  
10 1 0 0 0 0  
3 2 0 0 0 0  
11 2 0 0 0 0  
4 3 0 0 0 0  
12 3 0 0 0 0  
5 4 0 0 0 0  
6 5 0 0 0 0  
7 5 0 0 0 0  
8 7 0 0 0 0  
9 7 0 0 0 0  
4 13 0 0 0 0
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M END  
$$$$  
2-aminopyridine_p1.sdf  
COSMOtherm 3D 0
```

```
14 14 0 0 0 0 0 0 0 0 0 0 V2000  
1.1159 -1.1901 -0.0004 C 0 0 0 0 0 0 0 0 0 0 1  
1.8635 -0.0400 -0.0013 C 0 0 0 0 0 0 0 0 0 0 2  
1.1847 1.2013 0.0002 C 0 0 0 0 0 0 0 0 0 0 3  
-0.1935 1.2564 0.0012 C 0 0 0 0 0 0 0 0 0 0 4  
-0.9450 0.0541 0.0012 C 0 0 0 0 0 0 0 0 0 0 5  
-0.2476 -1.1213 0.0020 N 0 0 0 0 0 0 0 0 0 0 6  
-2.2836 0.0171 -0.0054 N 0 0 0 0 0 0 0 0 0 0 7  
-2.8155 0.8806 0.0188 H 0 0 0 0 0 0 0 0 0 0 8  
-2.8032 -0.8552 0.0180 H 0 0 0 0 0 0 0 0 0 0 9  
1.5319 -2.1948 -0.0009 H 0 0 0 0 0 0 0 0 0 0 10  
2.9495 -0.0969 -0.0031 H 0 0 0 0 0 0 0 0 0 0 11  
1.7560 2.1301 0.0004 H 0 0 0 0 0 0 0 0 0 0 12  
-0.7279 2.2054 0.0017 H 0 0 0 0 0 0 0 0 0 0 13  
-0.7698 -1.9989 0.0024 H 0 0 0 0 0 0 0 0 0 0 14
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2 1 0 0 0 0  
6 1 0 0 0 0  
10 1 0 0 0 0  
3 2 0 0 0 0  
11 2 0 0 0 0  
4 3 0 0 0 0  
12 3 0 0 0 0  
5 4 0 0 0 0  
13 4 0 0 0 0  
6 5 0 0 0 0  
7 5 0 0 0 0  
8 7 0 0 0 0  
9 7 0 0 0 0  
6 14 0 0 0 0
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M END  
$$$$  
2-aminothiazole.sdf  
COSMOtherm 3D 0
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```
10 10 0 0 0 0 0 0 0 0 0 V2000  
-0.8089 0.2133 0.0001 C 0 0 0 0 0 0 0 0 0 0 1  
-0.2024 1.3833 0.0001 N 0 0 0 0 0 0 0 0 0 0 2  
-2.1523 0.0406 -0.0001 N 0 0 0 0 0 0 0 0 0 0 3  
1.1730 1.2213 0.0000 C 0 0 0 0 0 0 0 0 0 0 4  
1.6497 -0.0562 -0.0001 C 0 0 0 0 0 0 0 0 0 0 5  
0.3012 -1.1909 0.0000 S 0 0 0 0 0 0 0 0 0 0 6  
-2.7582 0.8544 -0.0009 H 0 0 0 0 0 0 0 0 0 0 7  
-2.5777 -0.8783 0.0008 H 0 0 0 0 0 0 0 0 0 0 8  
1.8049 2.1093 0.0000 H 0 0 0 0 0 0 0 0 0 0 9  
2.6744 -0.4147 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10
```

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2 1 0 0 0 0  
3 1 0 0 0 0  
6 1 0 0 0 0  
4 2 0 0 0 0  
7 3 0 0 0 0  
8 3 0 0 0 0  
5 4 0 0 0 0  
9 4 0 0 0 0  
6 5 0 0 0 0  
5 10 0 0 0 0
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M END  
$$$$  
2-aminothiazole_p2.sdf  
COSMOtherm 3D 0
```

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11 11 0 0 0 0 0 0 0 0 0 V2000  
-2.1534 0.0692 -0.0008 N 0 0 0 0 0 0 0 0 0 0 1  
-0.8288 0.1635 0.0003 C 0 0 0 0 0 0 0 0 0 0 2  
-0.1401 1.3206 0.0002 N 0 0 0 0 0 0 0 0 0 0 3  
1.2458 1.1882 -0.0001 C 0 0 0 0 0 0 0 0 0 0 4  
1.6517 -0.0980 -0.0002 C 0 0 0 0 0 0 0 0 0 0 5  
0.2722 -1.1989 0.0001 S 0 0 0 0 0 0 0 0 0 0 6  
-2.7398 0.8998 0.0018 H 0 0 0 0 0 0 0 0 0 0 7  
-2.6171 -0.8340 0.0032 H 0 0 0 0 0 0 0 0 0 0 8  
1.8577 2.0849 -0.0001 H 0 0 0 0 0 0 0 0 0 0 9  
2.6605 -0.4954 -0.0005 H 0 0 0 0 0 0 0 0 0 0 10  
-0.6026 2.2303 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
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2 1 0 0 0 0  
7 1 0 0 0 0  
8 1 0 0 0 0  
3 2 0 0 0 0  
6 2 0 0 0 0
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4 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
3 11 0 0 0 0
M END
$$$$
2-methylimidazole.sdf
COSMOtherm 3D 0

12 12 0 0 0 0 0 0 0 0 V2000
-2.1570 0.0029 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6655 -0.0460 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.1269 1.0717 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 3
1.4490 0.6680 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4036 -0.7078 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0872 -1.1473 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.5447 0.5242 -0.8884 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.5512 -1.0201 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.5447 0.5253 0.8877 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.1970 2.0357 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
2.2676 1.3795 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
2.2357 -1.4064 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
5 12 0 0 0 0
M END
$$$$
2-methylimidazole_p2.sdf
COSMOtherm 3D 0

13 13 0 0 0 0 0 0 0 0 V2000
-2.1742 -0.0005 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6935 0.0008 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
0.1190 1.0751 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 3
1.4465 0.6818 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4457 -0.6839 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1170 -1.0736 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.5598 0.5151 -0.8904 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.5486 -1.0302 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.5598 0.5160 0.8900 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.2055 2.0401 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
2.2578 1.3986 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 11
2.2555 -1.4022 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.2115 -2.0374 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
6 13 0 0 0 0
M END
$$$$
2-methylindole-cation0.sdf
COSMOtherm 3D 0

20 21 0 0 0 0 0 0 0 0 V2000
-2.5979 -0.7246 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.6258 0.6777 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.4455 1.4338 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2236 0.7522 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2353 -0.6493 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.3783 -1.4239 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1699 -1.1103 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 7
1.1664 1.1990 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 8
2.0033 0.1440 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 9
1.3829 -1.6940 -0.8255 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.5325 -1.2860 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
-3.5884 1.1911 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.4789 2.5236 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.3451 -2.5132 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 14
1.4923 2.2364 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 15
3.4768 -0.0014 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 16
1.3828 -1.6942 0.8253 H 0 0 0 0 0 0 0 0 0 0 0 17
3.8269 -0.5509 0.8879 H 0 0 0 0 0 0 0 0 0 0 0 18
3.9400 0.9923 0.0013 H 0 0 0 0 0 0 0 0 0 0 0 19
3.8269 -0.5485 -0.8895 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0

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14 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
16 9 0 0 0 0
18 16 0 0 0 0
19 16 0 0 0 0
16 20 0 0 0 0
M END
$$$$
2-methylindole-cation1.sdf
COSMOtherm 3D 0
20 21 0 0 0 0 0 0 0 0 0 V2000
-2.5038 -0.7501 0.1576 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.5643 0.6881 0.1656 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.4320 1.4478 0.0374 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1783 0.7692 -0.1072 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.1405 -0.6937 -0.1071 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3281 -1.4547 0.0208 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1229 -1.0955 -0.2449 N 0 0 0 0 0 0 0 0 0 0 0 0 7
1.1124 1.2100 -0.2564 C 0 0 0 0 0 0 0 0 0 0 0 0 8
2.0275 0.0449 -0.3688 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.4296 -2.0648 -0.3006 H 0 0 0 0 0 0 0 0 0 0 0 0 10
3.1922 0.0094 0.6402 C 0 0 0 0 0 0 0 0 0 0 0 0 11
2.4507 0.0372 -1.3938 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.4388 -1.3028 0.2631 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-3.5377 1.1660 0.2775 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.4660 2.5372 0.0399 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.3057 -2.5438 0.0177 H 0 0 0 0 0 0 0 0 0 0 0 0 16
1.4588 2.2404 -0.3020 H 0 0 0 0 0 0 0 0 0 0 0 0 17
3.7924 -0.8940 0.4779 H 0 0 0 0 0 0 0 0 0 0 0 0 18
3.8291 0.8882 0.4844 H 0 0 0 0 0 0 0 0 0 0 0 0 19
2.8101 0.0153 1.6685 H 0 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
2-methylindole-cation2.sdf
COSMOtherm 3D 0
20 21 0 0 0 0 0 0 0 0 0 V2000
-2.5678 -0.7821 -0.0022 C 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.6381 0.6201 -0.0024 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.4779 1.4109 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.2445 0.7668 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2031 -0.6365 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3339 -1.4452 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1644 -1.0207 0.0045 N 0 0 0 0 0 0 0 0 0 0 0 0 7
1.1752 1.2665 0.0040 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.9834 0.0057 0.0033 C 0 0 0 0 0 0 0 0 0 0 0 0 9
1.4775 -1.9945 0.0054 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.4284 1.8773 0.8871 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.4331 1.8851 -0.8720 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.4877 -1.3678 -0.0040 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-3.6151 1.1055 -0.0038 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.5467 2.4993 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.2667 -2.5330 0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 16
3.4516 -0.1103 -0.0063 C 0 0 0 0 0 0 0 0 0 0 0 0 17
3.8445 0.3302 -0.9366 H 0 0 0 0 0 0 0 0 0 0 0 0 18
3.8762 0.4769 0.8216 H 0 0 0 0 0 0 0 0 0 0 0 0 19
3.7828 -1.1520 0.0702 H 0 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
4 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
12 8 0 0 0 0
17 9 0 0 0 0
18 17 0 0 0 0
19 17 0 0 0 0
17 20 0 0 0 0
M END

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2-methylindole.sdf
COSMOTHERM      3D      0

19 20 0 0 0 0 0 0 0 0 0 V2000
-1.4226 -1.4502 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6554 -2.6157 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7577 -2.5635 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
1.4348 -1.3417 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
0.6621 -0.1735 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7709 -0.1992 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.2098 1.1681 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0814 1.9716 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0539 3.4621 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 9
1.0406 1.1552 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 10
-2.5136 -1.5062 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.1525 -3.5880 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 12
1.3300 -3.4930 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 13
2.5257 -1.2997 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.2366 1.5246 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.4235 3.9046 0.8868 H 0 0 0 0 0 0 0 0 0 0 0 16
1.1098 3.7639 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.4243 3.9050 -0.8858 H 0 0 0 0 0 0 0 0 0 0 0 18
1.9983 1.4940 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 19

2 1 0 0 0 0 0
6 1 0 0 0 0 0
11 1 0 0 0 0 0
3 2 0 0 0 0 0
12 2 0 0 0 0 0
4 3 0 0 0 0 0
13 3 0 0 0 0 0
5 4 0 0 0 0 0
14 4 0 0 0 0 0
6 5 0 0 0 0 0
10 5 0 0 0 0 0
7 6 0 0 0 0 0
8 7 0 0 0 0 0
15 7 0 0 0 0 0
9 8 0 0 0 0 0
10 8 0 0 0 0 0
16 9 0 0 0 0 0
17 9 0 0 0 0 0
18 9 0 0 0 0 0
10 19 0 0 0 0 0

M END
$$$$
2-methylpyrrole-cation0.sdf
COSMOTHERM      3D      0

14 14 0 0 0 0 0 0 0 0 0 V2000
-1.4962 0.7071 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.1126 1.1814 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.5102 -0.6352 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.1071 -1.0975 0.0005 N 0 0 0 0 0 0 0 0 0 0 0 4
0.7374 0.1351 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.3770 1.3438 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 6
0.1883 2.2257 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.2959 -1.3823 -0.0008 H 0 0 0 0 0 0 0 0 0 0 0 8
0.0919 -1.6922 -0.8220 H 0 0 0 0 0 0 0 0 0 0 0 9
2.2128 -0.0005 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 10
0.0900 -1.6903 0.8249 H 0 0 0 0 0 0 0 0 0 0 0 11
2.5681 -0.5430 -0.8904 H 0 0 0 0 0 0 0 0 0 0 0 12
2.6669 0.9974 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 13
2.5691 -0.5460 0.8872 H 0 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0 0
3 1 0 0 0 0 0
6 1 0 0 0 0 0
5 2 0 0 0 0 0
7 2 0 0 0 0 0
4 3 0 0 0 0 0
8 3 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
11 4 0 0 0 0 0
10 5 0 0 0 0 0
12 10 0 0 0 0 0
13 10 0 0 0 0 0
10 14 0 0 0 0 0

M END
$$$$
2-methylpyrrole-cation1.sdf
COSMOTHERM      3D      0

14 14 0 0 0 0 0 0 0 0 0 V2000
-0.1921 -0.1715 1.1906 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.4150 0.1916 0.7185 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7343 -0.4376 0.0524 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.1315 -0.1667 -1.1008 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.3344 0.1808 -0.7178 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1684 -0.2583 -2.0714 H 0 0 0 0 0 0 0 0 0 0 0 6
0.1105 -0.2731 2.2303 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.3065 0.4479 1.2827 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.1166 0.4087 -1.4401 H 0 0 0 0 0 0 0 0 0 0 0 9
0.9863 -1.5148 0.0300 H 0 0 0 0 0 0 0 0 0 0 0 10
2.0334 0.3856 0.0299 C 0 0 0 0 0 0 0 0 0 0 0 11
2.6274 0.1337 0.9166 H 0 0 0 0 0 0 0 0 0 0 0 12
1.8111 1.4598 0.0382 H 0 0 0 0 0 0 0 0 0 0 0 13
2.6172 0.1389 -0.8653 H 0 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0 0
3 1 0 0 0 0 0
7 1 0 0 0 0 0
5 2 0 0 0 0 0
8 2 0 0 0 0 0
4 3 0 0 0 0 0
10 3 0 0 0 0 0
    
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11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
11 14 0 0 0 0
M END
$$$$
2-methylpyrrole-cation2.sdf
COSMOTHERM          3D          0

14 14 0 0 0 0 0 0 0 0 0 V2000
-0.1919  1.2050  0.0034 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.5597  0.5949 -0.0041 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
 0.7234  0.0283  0.0053 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0309 -1.0475  0.0037 N  0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.4222 -0.7428 -0.0029 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 0.0048  1.8551 -0.8670 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0052  1.8430  0.8854 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
 0.3326 -2.0030  0.0059 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.4907  1.1527 -0.0066 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
 2.1976  0.0181 -0.0037 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.1421 -1.5547 -0.0049 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
 2.5605  0.4533 -0.9485 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
 2.5823  0.6553  0.8056 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
 2.5997 -0.9959  0.1015 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 14

 2 1 0 0 0 0
 3 1 0 0 0 0
 6 1 0 0 0 0
 7 1 0 0 0 0
 5 2 0 0 0 0
 9 2 0 0 0 0
 4 3 0 0 0 0
10 3 0 0 0 0
 5 4 0 0 0 0
 8 4 0 0 0 0
11 5 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
10 14 0 0 0 0
M END
$$$$
2-methylpyrrole-cation3.sdf
COSMOTHERM          3D          0

14 14 0 0 0 0 0 0 0 0 0 V2000
-1.4475 -0.7307  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.0284 -1.0499 -0.0001 N  0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.4426  0.7537  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1589  1.1963  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.7147  0.0406  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 2.1970  0.0252  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.9416 -1.1611  0.8874 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
 0.3323 -2.0035 -0.0002 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.3511  1.3512 -0.0001 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
 0.1948  2.2233 -0.0001 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
 2.5713 -0.5052  0.8880 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
 2.5946  1.0448 -0.0027 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
 2.5715 -0.5103 -0.8848 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.9418 -1.1613 -0.8871 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 14

 2 1 0 0 0 0
 3 1 0 0 0 0
 7 1 0 0 0 0
 5 2 0 0 0 0
 8 2 0 0 0 0
 4 3 0 0 0 0
 9 3 0 0 0 0
 5 4 0 0 0 0
10 4 0 0 0 0
 6 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
 1 14 0 0 0 0
M END
$$$$
2-methylpyrrole-cation4.sdf
COSMOTHERM          3D          0

14 14 0 0 0 0 0 0 0 0 0 V2000
-1.3621 -0.7884  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.0867 -1.0606 -0.0001 N  0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.5232  0.6774  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.1147  1.1770 -0.0001 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 0.7304  0.1215 -0.0003 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 2.2114  0.0013  0.0002 C  0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
 0.2949 -2.0100 -0.0003 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.1169  1.0034  0.8747 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
 0.1693  2.2248 -0.0003 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
 2.5645 -0.5373  0.8923 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
 2.6633  0.9997 -0.0055 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
 2.5643 -0.5476 -0.8858 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.1233 -1.5649  0.0001 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.1171  1.0033 -0.8744 H  0 0 0 0 0 0 0 0 0 0 0 0 0 0 14

 2 1 0 0 0 0
 3 1 0 0 0 0
13 1 0 0 0 0
 5 2 0 0 0 0
 7 2 0 0 0 0
 4 3 0 0 0 0
 8 3 0 0 0 0
 5 4 0 0 0 0
 9 4 0 0 0 0
 6 5 0 0 0 0

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10 6 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
 3 14 0 0 0 0
M END
$$$$
2-methylpyrrole.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
 0.1624 -1.1720 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
 1.5031 -0.6733 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
 -0.7011 -0.0818 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
 0.0891 1.0512 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
 1.4267 0.7103 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
 -2.1950 -0.0100 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
 -0.2636 2.0039 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
 -0.1456 -2.2148 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 8
 2.4184 -1.2597 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
 2.1979 1.4742 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
 -2.5824 0.5172 0.8865 H 0 0 0 0 0 0 0 0 0 0 0 11
 -2.6169 -1.0233 0.0019 H 0 0 0 0 0 0 0 0 0 0 0 12
 -2.5824 0.5137 -0.8887 H 0 0 0 0 0 0 0 0 0 0 0 13
 2 1 0 0 0 0
 3 1 0 0 0 0
 8 1 0 0 0 0
 5 2 0 0 0 0
 9 2 0 0 0 0
 4 3 0 0 0 0
 6 3 0 0 0 0
 5 4 0 0 0 0
 7 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
 6 13 0 0 0 0
M END
$$$$
2-methylpyrrole0.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
 0.0000 1.1720 -0.1624 C 0 0 0 0 0 0 0 0 0 0 0 1
 0.0000 0.6733 -1.5031 C 0 0 0 0 0 0 0 0 0 0 0 2
 0.0000 0.0818 -0.7012 C 0 0 0 0 0 0 0 0 0 0 0 3
 0.0000 -1.0512 -0.0892 N 0 0 0 0 0 0 0 0 0 0 0 4
 0.0000 -0.7103 -1.4267 C 0 0 0 0 0 0 0 0 0 0 0 5
 0.0000 0.0100 2.1950 C 0 0 0 0 0 0 0 0 0 0 0 6
 -0.0001 -2.0039 0.2636 H 0 0 0 0 0 0 0 0 0 0 0 7
 -0.0001 2.2148 0.1456 H 0 0 0 0 0 0 0 0 0 0 0 8
 -0.0001 1.2597 -2.4184 H 0 0 0 0 0 0 0 0 0 0 0 9
 0.0000 -1.4742 -2.1979 H 0 0 0 0 0 0 0 0 0 0 0 10
 0.8883 -0.5143 2.5825 H 0 0 0 0 0 0 0 0 0 0 0 11
 -0.8869 -0.5166 2.5824 H 0 0 0 0 0 0 0 0 0 0 0 12
 -0.0014 1.0233 2.6169 H 0 0 0 0 0 0 0 0 0 0 0 13
 2 1 0 0 0 0
 3 1 0 0 0 0
 8 1 0 0 0 0
 5 2 0 0 0 0
 9 2 0 0 0 0
 4 3 0 0 0 0
 6 3 0 0 0 0
 5 4 0 0 0 0
 7 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
 6 13 0 0 0 0
M END
$$$$
2-methylpyrrole1.sdf
COSMOTHERM 3D 0

13 13 0 0 0 0 0 0 0 0 0 V2000
 -0.1687 1.1744 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 1
 -1.5057 0.6688 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 2
 0.7005 0.0872 -0.0006 C 0 0 0 0 0 0 0 0 0 0 0 3
 -0.0854 -1.0479 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 4
 -1.4243 -0.7155 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 5
 2.1970 0.0108 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 6
 0.2752 -1.9978 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 7
 0.1311 2.2197 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 8
 -2.4236 1.2513 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 9
 -2.1915 -1.4831 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
 2.5369 -1.0342 -0.0134 H 0 0 0 0 0 0 0 0 0 0 0 11
 2.6272 0.4880 0.8940 H 0 0 0 0 0 0 0 0 0 0 0 12
 2.6289 0.5123 -0.8788 H 0 0 0 0 0 0 0 0 0 0 0 13
 2 1 0 0 0 0
 3 1 0 0 0 0
 8 1 0 0 0 0
 5 2 0 0 0 0
 9 2 0 0 0 0
 4 3 0 0 0 0
 6 3 0 0 0 0
 5 4 0 0 0 0
 7 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
 6 13 0 0 0 0
M END
$$$$
3-aminopyridine.sdf
COSMOTHERM 3D 0

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13 13 0 0 0 0 0 0 0 0 0 0 V2000
-2.3249 -0.0284 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.9572 0.0159 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.1851 -1.1746 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1546 -1.1985 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 4
1.8161 -0.0225 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1486 1.2074 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2436 1.2354 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.8204 -0.9120 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.8772 0.8206 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.6941 -2.1443 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
2.9074 -0.0733 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
1.7172 2.1391 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.7841 2.1846 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
7 13 0 0 0 0
M END
$$$$
3-aminopyridine_p1.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 V2000
-2.3403 -0.0230 -0.0346 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.9807 0.0114 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.2265 -1.1784 0.0062 C 0 0 0 0 0 0 0 0 0 0 0 3
1.1195 -1.1169 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 4
1.8329 0.0292 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1322 1.2320 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2562 1.2316 0.0053 C 0 0 0 0 0 0 0 0 0 0 0 7
-2.8279 -0.8927 0.1567 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.8602 0.8264 0.1618 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.6700 -2.1712 0.0101 H 0 0 0 0 0 0 0 0 0 0 0 10
2.9150 -0.0622 -0.0082 H 0 0 0 0 0 0 0 0 0 0 0 11
1.6851 2.1698 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.8028 2.1758 0.0092 H 0 0 0 0 0 0 0 0 0 0 0 13
1.6294 -2.0028 0.0010 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
13 7 0 0 0 0
4 14 0 0 0 0
M END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine.sdf
COSMOTHERM 3D 0
35 37 0 0 0 0 0 0 0 0 V2000
-3.8018 -1.1222 -0.1384 C 0 0 0 0 0 0 0 0 0 0 0 1
-3.5153 0.1501 -0.6661 C 0 0 0 0 0 0 0 0 0 0 0 2
-2.1983 0.5832 -0.7209 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.1154 -0.2276 -0.2911 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.4091 -1.5355 0.2288 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.7688 -1.9329 0.3084 C 0 0 0 0 0 0 0 0 0 0 0 6
0.2261 0.3675 -0.3302 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2940 -0.3702 -0.6572 N 0 0 0 0 0 0 0 0 0 0 0 8
1.0852 -1.8004 -1.0280 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.4850 -2.4291 0.7505 N 0 0 0 0 0 0 0 0 0 0 0 10
0.7169 -2.5323 0.2399 C 0 0 0 0 0 0 0 0 0 0 0 11
0.4202 1.8015 -0.0137 C 0 0 0 0 0 0 0 0 0 0 0 12
1.6568 -3.2715 0.8730 N 0 0 0 0 0 0 0 0 0 0 0 13
-0.2315 2.3564 1.1052 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.0803 3.7096 1.4202 C 0 0 0 0 0 0 0 0 0 0 0 15
0.7106 4.5343 0.6125 C 0 0 0 0 0 0 0 0 0 0 0 16
1.3558 3.9942 -0.5081 C 0 0 0 0 0 0 0 0 0 0 0 17
1.2206 2.6390 -0.8159 C 0 0 0 0 0 0 0 0 0 0 0 18
2.9426 -3.7037 0.3266 C 0 0 0 0 0 0 0 0 0 0 0 19
2.5230 0.0323 -0.6226 O 0 0 0 0 0 0 0 0 0 0 0 20
1.3395 -3.7251 1.7280 H 0 0 0 0 0 0 0 0 0 0 0 21
-4.8339 -1.4725 -0.0755 H 0 0 0 0 0 0 0 0 0 0 0 22
-4.3183 0.7957 -1.0244 H 0 0 0 0 0 0 0 0 0 0 0 23
-1.9764 1.5755 -1.1163 H 0 0 0 0 0 0 0 0 0 0 0 24
-2.9770 -2.9161 0.7348 H 0 0 0 0 0 0 0 0 0 0 0 25
0.2619 -1.8687 -1.7515 H 0 0 0 0 0 0 0 0 0 0 0 26
2.0171 -2.1339 -1.4879 H 0 0 0 0 0 0 0 0 0 0 0 27
-0.8542 1.7193 1.7354 H 0 0 0 0 0 0 0 0 0 0 0 28
-0.5838 4.1201 2.2973 H 0 0 0 0 0 0 0 0 0 0 0 29
0.8253 5.5925 0.8542 H 0 0 0 0 0 0 0 0 0 0 0 30
1.9686 4.6334 -1.1465 H 0 0 0 0 0 0 0 0 0 0 0 31
1.7343 2.2256 -1.6832 H 0 0 0 0 0 0 0 0 0 0 0 32
3.4859 -4.2185 1.1259 H 0 0 0 0 0 0 0 0 0 0 0 33
2.8230 -4.4006 -0.5174 H 0 0 0 0 0 0 0 0 0 0 0 34
3.5470 -2.8455 0.0054 H 0 0 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0
6 1 0 0 0 0
22 1 0 0 0 0

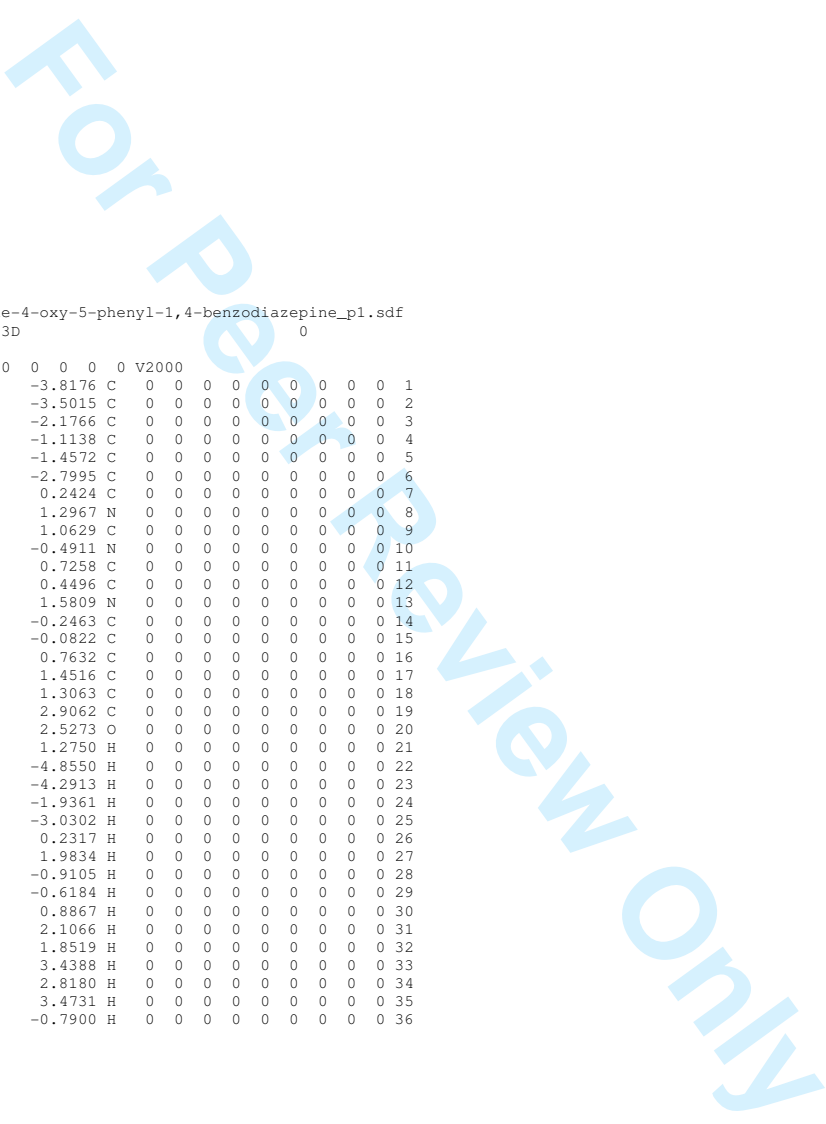
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23 2 0 0 0 0
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24 3 0 0 0 0
5 4 0 0 0 0
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25 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
11 9 0 0 0 0
26 9 0 0 0 0
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11 10 0 0 0 0
13 11 0 0 0 0
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18 12 0 0 0 0
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29 15 0 0 0 0
17 16 0 0 0 0
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18 17 0 0 0 0
31 17 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
34 19 0 0 0 0
19 35 0 0 0 0
M END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine_pl.sdf
COSMOTHERM 3D 0
36 38 0 0 0 0 0 0 0 0 0 V2000
1.0299 0.1384 -3.8176 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.2108 0.7111 -3.5015 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6226 0.7834 -2.1766 C 0 0 0 0 0 0 0 0 0 0 0 3
0.1842 0.3093 -1.1138 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4548 -0.2279 -1.4572 C 0 0 0 0 0 0 0 0 0 0 0 5
1.8552 -0.3258 -2.7995 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.3845 0.3261 0.2424 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3780 0.6358 1.2967 N 0 0 0 0 0 0 0 0 0 0 0 8
1.8117 1.0163 1.0629 C 0 0 0 0 0 0 0 0 0 0 0 9
2.3513 -0.7452 -0.4911 N 0 0 0 0 0 0 0 0 0 0 0 10
2.5661 -0.2273 0.7258 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.8133 0.0085 0.4496 C 0 0 0 0 0 0 0 0 0 0 0 12
3.3846 -0.8145 1.5809 N 0 0 0 0 0 0 0 0 0 0 0 13
-2.3851 -1.0758 -0.2463 C 0 0 0 0 0 0 0 0 0 0 0 14
-3.7357 -1.3914 -0.0822 C 0 0 0 0 0 0 0 0 0 0 0 15
-4.5397 -0.6186 0.7632 C 0 0 0 0 0 0 0 0 0 0 0 16
-3.9821 0.4667 1.4516 C 0 0 0 0 0 0 0 0 0 0 0 17
-2.6286 0.7754 1.3063 C 0 0 0 0 0 0 0 0 0 0 0 18
3.7690 -0.3108 2.9062 C 0 0 0 0 0 0 0 0 0 0 0 19
0.0094 0.6077 2.5273 O 0 0 0 0 0 0 0 0 0 0 0 20
3.8481 -1.6707 1.2750 H 0 0 0 0 0 0 0 0 0 0 0 21
1.3578 0.0649 -4.8550 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.8571 1.0951 -4.2913 H 0 0 0 0 0 0 0 0 0 0 0 23
-1.5949 1.2130 -1.9361 H 0 0 0 0 0 0 0 0 0 0 0 24
2.8287 -0.7615 -3.0302 H 0 0 0 0 0 0 0 0 0 0 0 25
1.8743 1.7311 0.2317 H 0 0 0 0 0 0 0 0 0 0 0 26
2.1569 1.4878 1.9834 H 0 0 0 0 0 0 0 0 0 0 0 27
-1.7652 -1.6799 -0.9105 H 0 0 0 0 0 0 0 0 0 0 0 28
-4.1607 -2.2415 -0.6184 H 0 0 0 0 0 0 0 0 0 0 0 29
-5.5967 -0.8610 0.8867 H 0 0 0 0 0 0 0 0 0 0 0 30
-4.6060 1.0774 2.1066 H 0 0 0 0 0 0 0 0 0 0 0 31
-2.2022 1.6160 1.8519 H 0 0 0 0 0 0 0 0 0 0 0 32
4.2496 -1.1362 3.4388 H 0 0 0 0 0 0 0 0 0 0 0 33
4.4793 0.5218 2.8180 H 0 0 0 0 0 0 0 0 0 0 0 34
2.8860 0.0034 3.4731 H 0 0 0 0 0 0 0 0 0 0 0 35
2.9323 -1.5313 -0.7900 H 0 0 0 0 0 0 0 0 0 0 0 36
2 1 0 0 0 0
6 1 0 0 0 0
22 1 0 0 0 0
3 2 0 0 0 0
23 2 0 0 0 0
4 3 0 0 0 0
24 3 0 0 0 0
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25 6 0 0 0 0
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21 13 0 0 0 0
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28 14 0 0 0 0
16 15 0 0 0 0
29 15 0 0 0 0

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17 16 0 0 0 0
30 16 0 0 0 0
18 17 0 0 0 0
31 17 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
34 19 0 0 0 0
35 19 0 0 0 0
10 36 0 0 0 0
M END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine_t_p1.sdf
COSMOTHERM      3D                    0

36 38 0 0 0 0 0 0 0 0 0 0 V2000
-3.8180 -0.1392 1.0263 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.5005 -0.7102 -0.2148 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.1751 -0.7823 -0.6251 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.1133 -0.3090 0.1835 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.4581 0.2269 1.4543 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.8008 0.3242 1.8532 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
 0.2433 -0.3245 -0.3842 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
 1.2973 -0.6336  0.3791 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
 1.0624 -1.0155  1.8118 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.4932  0.7439  2.3520 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
 0.7239  0.2268  2.5674 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
 0.4514 -0.0074 -1.8131 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
 1.5778  0.8136  3.3875 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.2457  1.0752 -2.3865 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.0823  1.3887 -3.7378 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
 0.7648  0.6165 -4.5404 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
 1.4545 -0.4672 -3.9811 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
 1.3093 -0.7742 -2.6271 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
 2.9028  0.3094  3.7732 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
 2.5282 -0.6039  0.0118 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-4.8557 -0.0660  1.3531 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-4.2897 -1.0930 -0.8627 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
-1.9335 -1.2108 -1.5976 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
-3.0326  0.7583  2.8272 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
 0.2315 -1.7308  1.8731 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
 1.9826 -1.4870  2.1578 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
-0.9108  1.6793 -1.7676 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 27
-0.6207  2.2367 -4.1643 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 28
 0.8880  0.8574 -5.5977 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 29
 2.1109 -1.0776 -4.6039 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 30
 1.8550 -1.6142 -2.1997 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 31
 3.4332  1.1330  4.2591 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 32
 2.8137 -0.5268  4.4791 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 33
 3.4725  0.0002  2.8902 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 34
-0.7934  1.5286  2.9341 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 35
 1.2710  1.6689  3.8524 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 36

 2 1 0 0 0 0 0
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21 1 0 0 0 0 0
 3 2 0 0 0 0 0
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14 12 0 0 0 0 0
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31 18 0 0 0 0 0
32 19 0 0 0 0 0
33 19 0 0 0 0 0
34 19 0 0 0 0 0
13 36 0 0 0 0 0
M END
$$$$
3-methylindole-cation0.sdf
COSMOTHERM      3D                    0

20 21 0 0 0 0 0 0 0 0 0 0 V2000
-2.5949 -0.0353  0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.0891  1.2732  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.7101  1.5234 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
 0.1596  0.4282 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3812 -0.8631 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.7333 -1.1455  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
 0.7437 -1.8235 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
 1.6289  0.3265  0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
 1.9645 -0.9779  0.0006 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
 0.7207 -2.4448 -0.8257 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10

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-3.6729 -0.1992 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.7847 -2.1133 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.3296 2.5452 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.1167 -2.1657 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 14
2.5647 1.4873 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 15
2.9212 -1.4894 0.0010 H 0 0 0 0 0 0 0 0 0 0 0 16
0.7193 -2.4460 0.8242 H 0 0 0 0 0 0 0 0 0 0 0 17
2.3970 2.1154 0.8877 H 0 0 0 0 0 0 0 0 0 0 0 18
2.3908 2.1203 -0.8830 H 0 0 0 0 0 0 0 0 0 0 0 19
3.6107 1.1584 -0.0045 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
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12 2 0 0 0 0
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13 3 0 0 0 0
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8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
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16 9 0 0 0 0
18 15 0 0 0 0
19 15 0 0 0 0
15 20 0 0 0 0
M END
$$$$
3-methylindole-cation1.sdf
COSMOtherm 3D 0
20 21 0 0 0 0 0 0 0 0 0 0 V2000
-2.5673 -0.0638 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.0756 1.2848 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7284 1.5474 0.0027 C 0 0 0 0 0 0 0 0 0 0 0 3
0.1765 0.4417 0.0021 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3433 -0.9170 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.7374 -1.1650 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6770 -1.7821 -0.0007 N 0 0 0 0 0 0 0 0 0 0 0 7
1.5620 0.3693 0.0024 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9389 -1.0705 0.0023 C 0 0 0 0 0 0 0 0 0 0 0 9
0.5973 -2.7960 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
2.5433 -1.3322 0.8892 H 0 0 0 0 0 0 0 0 0 0 0 11
2.5488 -1.3327 -0.8805 H 0 0 0 0 0 0 0 0 0 0 0 12
-3.6476 -0.2188 -0.0032 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.7954 2.1034 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.3493 2.5695 0.0047 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.1301 -2.1813 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 16
2.5513 1.4720 -0.0036 C 0 0 0 0 0 0 0 0 0 0 0 17
2.3673 2.1626 0.8337 H 0 0 0 0 0 0 0 0 0 0 0 18
2.4545 2.0655 -0.9271 H 0 0 0 0 0 0 0 0 0 0 0 19
3.5793 1.0982 0.0632 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
6 1 0 0 0 0
13 1 0 0 0 0
3 2 0 0 0 0
14 2 0 0 0 0
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16 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
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11 9 0 0 0 0
12 9 0 0 0 0
18 17 0 0 0 0
19 17 0 0 0 0
17 20 0 0 0 0
M END
$$$$
3-methylindole-cation2.sdf
COSMOtherm 3D 0
20 21 0 0 0 0 0 0 0 0 0 0 V2000
-2.5707 -0.1701 0.1669 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.1651 1.1574 -0.0478 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.8146 1.4905 -0.2367 C 0 0 0 0 0 0 0 0 0 0 0 3
0.1252 0.4647 -0.2034 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.3090 -0.8530 0.0173 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6388 -1.2144 0.2034 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8455 -1.6819 0.0098 N 0 0 0 0 0 0 0 0 0 0 0 7
1.6286 0.4471 -0.3692 C 0 0 0 0 0 0 0 0 0 0 0 8
1.9372 -1.0003 -0.1956 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8221 -2.6963 0.1450 H 0 0 0 0 0 0 0 0 0 0 0 10
2.4405 1.3738 0.5647 C 0 0 0 0 0 0 0 0 0 0 0 11
1.8992 0.6969 -1.4149 H 0 0 0 0 0 0 0 0 0 0 0 12
-3.6285 -0.3937 0.3086 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.9171 1.9472 -0.0690 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.5178 2.5262 -0.4060 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.9397 -2.2487 0.3690 H 0 0 0 0 0 0 0 0 0 0 0 16
2.9108 -1.4854 -0.2311 H 0 0 0 0 0 0 0 0 0 0 0 17
3.5150 1.2614 0.3738 H 0 0 0 0 0 0 0 0 0 0 0 18
2.1590 2.4155 0.3685 H 0 0 0 0 0 0 0 0 0 0 0 19
2.2351 1.1425 1.6174 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0

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6 1 0 0 0 0
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16 6 0 0 0 0
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18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
3-methylindole.sdf
COSMOTHERM 3D 0
19 20 0 0 0 0 0 0 0 0 0 V2000
-0.1901 -0.4240 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
0.6938 -1.5229 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
2.0688 -1.2878 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
2.5850 0.0294 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.7384 1.1393 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.3569 0.9005 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3090 -2.5451 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 7
2.7613 -2.1318 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 8
3.6661 0.1816 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1380 2.1553 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.6277 -0.2968 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.8922 1.0595 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.6308 -1.4112 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.7070 1.7787 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 14
-2.8458 1.5810 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.5203 -2.0580 0.8852 H 0 0 0 0 0 0 0 0 0 0 0 16
-3.6568 -1.0183 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.5195 -2.0587 -0.8847 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.6405 2.7915 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
14 6 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
14 12 0 0 0 0
15 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
14 19 0 0 0 0
M END
$$$$
3-methylpyrrole-cation0.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-1.1699 -0.0939 0.0004 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0302 0.7632 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.8087 -1.3850 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6662 -1.4411 -0.0007 N 0 0 0 0 0 0 0 0 0 0 0 4
1.1155 -0.0365 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.1942 0.2709 0.0014 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0034 2.2543 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.3576 -2.3200 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 8
1.0227 -1.9555 -0.8249 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1826 0.1577 0.0011 H 0 0 0 0 0 0 0 0 0 0 0 10
1.0239 -1.9583 0.8212 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5111 2.6262 -0.8997 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5567 2.6285 0.8694 H 0 0 0 0 0 0 0 0 0 0 0 13
1.0157 2.6752 0.0241 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
10 5 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
7 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation1.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000

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0.7564 0.0519 -0.0048 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.0388 1.1687 -0.0035 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.1347 -1.1507 -0.0036 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.4709 -0.5724 0.0034 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.4017 0.7393 0.0025 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.3314 -1.1180 0.0040 H 0 0 0 0 0 0 0 0 0 0 0 6
2.2373 -0.0298 0.0032 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2798 2.2070 -0.0056 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.3019 1.3515 0.0058 H 0 0 0 0 0 0 0 0 0 0 0 9
0.0100 -1.7927 0.8802 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0020 -1.7839 -0.8953 H 0 0 0 0 0 0 0 0 0 0 0 11
2.5980 -0.6823 -0.8064 H 0 0 0 0 0 0 0 0 0 0 0 12
2.6918 0.9619 -0.1027 H 0 0 0 0 0 0 0 0 0 0 0 13
2.5879 -0.4785 0.9468 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
8 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
11 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 5 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
7 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation2.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.0193 0.7566 -0.4119 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1951 -0.1421 -0.1510 C 0 0 0 0 0 0 0 0 0 0 0 2
1.1327 -0.1438 -0.1635 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6827 -1.3273 0.1501 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.7410 -1.3685 0.1689 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0120 0.9867 -1.4996 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0199 2.1030 0.3494 C 0 0 0 0 0 0 0 0 0 0 0 7
1.2745 -2.1371 0.3509 H 0 0 0 0 0 0 0 0 0 0 0 8
-2.2341 0.1638 -0.2291 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1964 0.0735 -0.2304 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.2425 -2.2987 0.4144 H 0 0 0 0 0 0 0 0 0 0 0 11
0.9236 2.6635 0.0806 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.8592 2.6967 0.0722 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0094 1.9339 1.4328 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
5 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
10 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
11 5 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
7 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation3.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
-0.0474 0.7697 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1459 -0.0428 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
1.0998 -0.1116 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.7246 -1.3661 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.7276 -1.4656 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0307 2.2621 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.1888 0.2658 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 7
2.1548 0.1591 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 8
1.3540 -2.1683 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.0710 -2.0251 0.8865 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5744 2.6256 0.8843 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.9731 2.7030 0.0032 H 0 0 0 0 0 0 0 0 0 0 0 12
0.5685 2.6256 -0.8880 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.0706 -2.0243 -0.8873 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
6 1 0 0 0 0
5 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
8 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
5 14 0 0 0 0
M END
$$$$
3-methylpyrrole-cation4.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 V2000
0.0392 -0.7597 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.1833 0.1180 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
1.1176 0.0613 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3

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0.6627    1.4052    0.0000 N    0  0  0  0  0  0  0  0  0  0  4
-0.6403    1.4900   -0.0002 C    0  0  0  0  0  0  0  0  0  0  5
0.0071   -2.2528   -0.0001 C    0  0  0  0  0  0  0  0  0  0  6
-1.8379   -0.0480   -0.8751 H    0  0  0  0  0  0  0  0  0  0  7
2.1844   -0.1370    0.0001 H    0  0  0  0  0  0  0  0  0  0  8
1.2921    2.2112   -0.0002 H    0  0  0  0  0  0  0  0  0  0  9
0.5200   -2.6572   -0.8851 H    0  0  0  0  0  0  0  0  0  0 10
-1.0241   -2.6259   -0.0015 H    0  0  0  0  0  0  0  0  0  0 11
0.5177   -2.6573    0.8863 H    0  0  0  0  0  0  0  0  0  0 12
-1.1645    2.4421   -0.0002 H    0  0  0  0  0  0  0  0  0  0 13
-1.8372   -0.0476    0.8759 H    0  0  0  0  0  0  0  0  0  0 14
2  1  0  0  0  0
3  1  0  0  0  0
6  1  0  0  0  0
5  2  0  0  0  0
7  2  0  0  0  0
4  3  0  0  0  0
8  3  0  0  0  0
5  4  0  0  0  0
9  4  0  0  0  0
13 5  0  0  0  0
10 6  0  0  0  0
11 6  0  0  0  0
12 6  0  0  0  0
2 14 0  0  0  0
M  END
$$$$
3-methylpyrrole.sdf
COSMOtherm           3D           0
13 13 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
-0.6511   -1.4106    0.0000 N    0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-1.1067   -0.1084    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-0.0016    0.7370    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
1.1545   -0.1072    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
0.7237   -1.4275    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
-0.0120    2.2425    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
-1.2446   -2.2344    0.0001 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
-2.1709    0.1086    0.0000 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
2.1907    0.2239   -0.0001 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
1.2735   -2.3634    0.0000 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 10
-0.5221    2.6524    0.8858 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 11
1.0138    2.6365   -0.0003 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 12
-0.5227    2.6526   -0.8853 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 13
2  1  0  0  0  0
5  1  0  0  0  0
7  1  0  0  0  0
3  2  0  0  0  0
8  2  0  0  0  0
4  3  0  0  0  0
6  3  0  0  0  0
5  4  0  0  0  0
9  4  0  0  0  0
10 5  0  0  0  0
11 6  0  0  0  0
12 6  0  0  0  0
6 13 0  0  0  0
M  END
$$$$
4-aminopyridine.sdf
COSMOtherm           3D           0
13 13 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1.1542    0.0003   -1.1441 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
-0.2346   -0.0064   -1.2036 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
-0.9780   -0.0057    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-0.2346   -0.0061    1.2035 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
1.1542    0.0001    1.1441 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
1.8756    0.0038    0.0000 N    0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
-2.3477    0.0416    0.0000 N    0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
-2.8390   -0.2004    0.8557 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
-2.8390   -0.1998   -0.8559 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
1.7308    0.0001   -2.0739 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 10
-0.7430   -0.0088   -2.1697 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 11
-0.7430   -0.0089    2.1697 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 12
1.7309   -0.0006    2.0738 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 13
2  1  0  0  0  0
6  1  0  0  0  0
10 1  0  0  0  0
3  2  0  0  0  0
11 2  0  0  0  0
4  3  0  0  0  0
7  3  0  0  0  0
5  4  0  0  0  0
12 4  0  0  0  0
6  5  0  0  0  0
8  7  0  0  0  0
9  7  0  0  0  0
5 13 0  0  0  0
M  END
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4-aminopyridine0.sdf
COSMOtherm           3D           0
13 13 0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
1.1441   -1.1542    0.0000 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
1.2036    0.2346    0.0059 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
0.0000    0.9781    0.0056 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
-1.2036    0.2346    0.0063 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
-1.1441   -1.1542   -0.0004 C    0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
0.0000   -1.8756   -0.0037 N    0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
0.0000    2.3475   -0.0411 N    0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
0.8561    2.8395    0.1979 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
-0.8559    2.8394    0.1989 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
2.0739   -1.7309    0.0009 H    0  0  0  0  0  0  0  0  0  0  0  0  0  0 10

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3 2.1698 0.7430 0.0087 H 0 0 0 0 0 0 0 0 0 0 0 11
4 -2.1697 0.7430 0.0090 H 0 0 0 0 0 0 0 0 0 0 0 12
5 -2.0739 -1.7309 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 13
6 2 1 0 0 0 0 0
7 6 1 0 0 0 0 0
8 10 1 0 0 0 0 0
9 3 2 0 0 0 0 0
10 11 2 0 0 0 0 0
11 4 3 0 0 0 0 0
12 7 3 0 0 0 0 0
13 5 4 0 0 0 0 0
14 12 4 0 0 0 0 0
15 6 5 0 0 0 0 0
16 8 7 0 0 0 0 0
17 9 7 0 0 0 0 0
18 5 13 0 0 0 0 0
19 M END
20 \$\$\$\$
21 4-aminopyridine1.sdf
22 COSMOTHERM 3D 0
23
24 13 13 0 0 0 0 0 0 0 0 0 0 V2000
25 1.1438 -1.1535 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 1
26 1.2044 0.2346 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 0 2
27 0.0000 0.9806 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
28 -1.2044 0.2346 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
29 -1.1438 -1.1535 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 5
30 0.0000 -1.8763 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 6
31 0.0000 2.3411 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 7
32 -0.8672 2.8657 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 8
33 0.8672 2.8657 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 9
34 2.0741 -1.7297 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 10
35 2.1709 0.7425 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 0 11
36 -2.1708 0.7425 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 12
37 -2.0741 -1.7296 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 13
38 2 1 0 0 0 0 0
39 6 1 0 0 0 0 0
40 10 1 0 0 0 0 0
41 3 2 0 0 0 0 0
42 11 2 0 0 0 0 0
43 4 3 0 0 0 0 0
44 7 3 0 0 0 0 0
45 5 4 0 0 0 0 0
46 12 4 0 0 0 0 0
47 6 5 0 0 0 0 0
48 8 7 0 0 0 0 0
49 9 7 0 0 0 0 0
50 5 13 0 0 0 0 0
51 M END
52 \$\$\$\$
53 4-aminopyridine_p1.sdf
54 COSMOTHERM 3D 0
55
56 14 14 0 0 0 0 0 0 0 0 0 0 V2000
57 1.1164 1.1870 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 1
58 -0.2543 1.2188 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 2
59 -0.9941 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
60 -0.2543 -1.2188 0.0002 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.1164 -1.1870 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.7811 0.0000 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 6
-2.3353 0.0000 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.8628 -0.8674 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.8628 0.8674 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 9
1.7307 2.0844 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.7677 2.1794 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.7676 -2.1794 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.7307 -2.0844 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2.8001 0.0000 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0 0
6 1 0 0 0 0 0
10 1 0 0 0 0 0
3 2 0 0 0 0 0
11 2 0 0 0 0 0
4 3 0 0 0 0 0
7 3 0 0 0 0 0
5 4 0 0 0 0 0
12 4 0 0 0 0 0
6 5 0 0 0 0 0
13 5 0 0 0 0 0
8 7 0 0 0 0 0
9 7 0 0 0 0 0
6 14 0 0 0 0 0
M END
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4-chloroaniline.sdf
COSMOTHERM 3D 0
14 14 0 0 0 0 0 0 0 0 0 0 V2000
2.6522 0.0000 0.0000 Cl 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.2149 -1.2135 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.9441 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.2149 1.2135 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.1800 1.2141 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.8701 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.1800 -1.2141 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-3.3165 0.0000 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.7509 -2.1650 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.7509 2.1650 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.7228 2.1600 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.7228 -2.1601 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-3.8401 -0.8666 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-3.8401 0.8666 -0.0009 H 0 0 0 0 0 0 0 0 0 0 0 0 14
6 1 0 0 0 0 0
3 2 0 0 0 0 0
7 2 0 0 0 0 0

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2
3 3.0993 -1.2023 0.9095 H 0 0 0 0 0 0 0 0 0 0 0 11
4 3.1221 -1.2109 -0.8924 H 0 0 0 0 0 0 0 0 0 0 0 12
5 -3.7215 0.4879 0.4846 H 0 0 0 0 0 0 0 0 0 0 0 13
6 -3.5165 -1.1504 0.4574 H 0 0 0 0 0 0 0 0 0 0 0 14
7 -1.9052 2.0711 0.0138 H 0 0 0 0 0 0 0 0 0 0 0 15
8 0.5675 2.3734 0.0041 H 0 0 0 0 0 0 0 0 0 0 0 16
9 1.0821 -1.9245 -0.0044 H 0 0 0 0 0 0 0 0 0 0 0 17
10 -1.3680 -2.2167 0.0064 H 0 0 0 0 0 0 0 0 0 0 0 18
11 -3.6194 -0.3076 -0.9635 H 0 0 0 0 0 0 0 0 0 0 0 19
12 9 1 0 0 0 0
13 10 1 0 0 0 0
14 11 1 0 0 0 0
15 12 1 0 0 0 0
16 3 2 0 0 0 0
17 13 2 0 0 0 0
18 14 2 0 0 0 0
19 4 3 0 0 0 0
20 8 3 0 0 0 0
21 5 4 0 0 0 0
22 15 4 0 0 0 0
23 6 5 0 0 0 0
24 16 5 0 0 0 0
25 7 6 0 0 0 0
26 9 6 0 0 0 0
27 8 7 0 0 0 0
28 17 7 0 0 0 0
29 18 8 0 0 0 0
30 2 19 0 0 0 0
31 M END
32 \$\$\$\$
33 4-methylpyridine.sdf
34 COSMOtherm 3D 0
35
36 14 14 0 0 0 0 0 0 0 0 0 V2000
37 -2.4802 -0.0024 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
38 -0.9755 -0.0045 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
39 -0.2412 1.1939 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
40 1.1529 1.1482 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
41 1.8670 0.0028 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 5
42 1.1603 -1.1443 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
43 -0.2361 -1.1964 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
44 -2.8703 0.5236 -0.8846 H 0 0 0 0 0 0 0 0 0 0 0 8
45 -2.8826 -1.0235 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
46 -2.8704 0.5238 0.8843 H 0 0 0 0 0 0 0 0 0 0 0 10
47 -0.7507 2.1599 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
48 1.7323 2.0759 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
49 1.7434 -2.0697 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 13
50 -0.7421 -2.1641 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 14
51 2 1 0 0 0 0
52 8 1 0 0 0 0
53 9 1 0 0 0 0
54 10 1 0 0 0 0
55 3 2 0 0 0 0
56 7 2 0 0 0 0
57 4 3 0 0 0 0
58 11 3 0 0 0 0
59 5 4 0 0 0 0
60 12 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
7 14 0 0 0 0
M END
\$\$\$\$
4-methylpyridine_pl.sdf
COSMOtherm 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
1.1284 0.0004 -1.1834 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.2553 -0.0015 -1.2078 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.9866 -0.0021 -0.0063 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.2632 -0.0015 1.2031 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1183 0.0003 1.1888 C 0 0 0 0 0 0 0 0 0 0 0 5
1.7733 0.0013 -0.0042 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.4839 0.0015 -0.0034 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7507 0.0006 -2.0752 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.7637 -0.0032 -2.1711 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.7784 -0.0032 2.1630 H 0 0 0 0 0 0 0 0 0 0 0 10
1.7349 0.0006 2.0845 H 0 0 0 0 0 0 0 0 0 0 0 11
2.7950 0.0018 0.0084 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.8689 -0.8420 0.5887 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.8908 -0.0604 -1.0191 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.8590 0.9213 0.4710 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
6 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
12 6 0 0 0 0
13 7 0 0 0 0
14 7 0 0 0 0
7 15 0 0 0 0
M END
\$\$\$\$
4-nitroaniline-cation1.sdf
COSMOtherm 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
0.0181 1.2242 0.0232 C 0 0 0 0 0 0 0 0 0 0 0 1

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1
2
3      0.0238      1.2219      1.4173 C      0 0 0 0 0 0 0 0 0 0 2
4      0.0054      0.0002      2.0861 C      0 0 0 0 0 0 0 0 0 0 3
5     -0.0145     -1.2225      1.4175 C      0 0 0 0 0 0 0 0 0 0 4
6     -0.0173     -1.2242      0.0239 C      0 0 0 0 0 0 0 0 0 0 5
7     -0.0018      0.0002     -0.6474 C      0 0 0 0 0 0 0 0 0 0 6
8     -0.0012      0.0001     -2.1295 N      0 0 0 0 0 0 0 0 0 0 7
9     -0.0072      0.0002      3.5603 N      0 0 0 0 0 0 0 0 0 0 8
10    -0.0404      1.0927     -2.7116 O      0 0 0 0 0 0 0 0 0 0 9
11     0.0381     -1.0930     -2.7110 O      0 0 0 0 0 0 0 0 0 0 10
12     0.5614     -0.7654      3.9503 H      0 0 0 0 0 0 0 0 0 0 11
13    -0.9615     -0.1100      3.9370 H      0 0 0 0 0 0 0 0 0 0 12
14     0.0342      2.1603     -0.5315 H      0 0 0 0 0 0 0 0 0 0 13
15     0.0439      2.1632      1.9671 H      0 0 0 0 0 0 0 0 0 0 14
16    -0.0259     -2.1637      1.9675 H      0 0 0 0 0 0 0 0 0 0 15
17    -0.0293     -2.1601     -0.5311 H      0 0 0 0 0 0 0 0 0 0 16
18     0.3672      0.8789      3.9454 H      0 0 0 0 0 0 0 0 0 0 17

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19      2 1 0 0 0 0
20      6 1 0 0 0 0
21     13 1 0 0 0 0
22      3 2 0 0 0 0
23     14 2 0 0 0 0
24      4 3 0 0 0 0
25      8 3 0 0 0 0
26      5 4 0 0 0 0
27     15 4 0 0 0 0
28      6 5 0 0 0 0
29     16 5 0 0 0 0
30      7 6 0 0 0 0
31      9 7 0 0 0 0
32     10 7 0 0 0 0
33     11 8 0 0 0 0
34     12 8 0 0 0 0
35      8 17 0 0 0 0

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M END

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4-nitroaniline1.sdf

COSMOtherm 3D 0

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36     16 16 0 0 0 0 0 0 0 0 0 V2000
37     -0.0573     -0.0207     -1.2179 C      0 0 0 0 0 0 0 0 0 0 1
38     -1.4319     -0.0241     -1.2199 C      0 0 0 0 0 0 0 0 0 0 2
39     -2.1502     -0.0077      0.0001 C      0 0 0 0 0 0 0 0 0 0 3
40     -1.4321     -0.0228      1.2198 C      0 0 0 0 0 0 0 0 0 0 4
41     -0.0574     -0.0201      1.2178 C      0 0 0 0 0 0 0 0 0 0 5
42      0.6764     -0.0045      0.0000 C      0 0 0 0 0 0 0 0 0 0 6
43     -3.4943      0.0813      0.0000 N      0 0 0 0 0 0 0 0 0 0 7
44      2.0256      0.0073     -0.0001 N      0 0 0 0 0 0 0 0 0 0 8
45      2.6590      0.0131      1.0948 O      0 0 0 0 0 0 0 0 0 0 9
46      2.6588      0.0153     -1.0946 O      0 0 0 0 0 0 0 0 0 0 10
47     -3.9805     -0.1796      0.8496 H      0 0 0 0 0 0 0 0 0 0 11
48     -3.9797     -0.1820     -0.8495 H      0 0 0 0 0 0 0 0 0 0 12
49      0.4783     -0.0300     -2.1636 H      0 0 0 0 0 0 0 0 0 0 13
50     -1.9693     -0.0380     -2.1671 H      0 0 0 0 0 0 0 0 0 0 14
51     -1.9696     -0.0353      2.1670 H      0 0 0 0 0 0 0 0 0 0 15
52      0.4784     -0.0289      2.1633 H      0 0 0 0 0 0 0 0 0 0 16

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53      2 1 0 0 0 0
54      6 1 0 0 0 0
55     13 1 0 0 0 0
56      3 2 0 0 0 0
57     14 2 0 0 0 0
58      4 3 0 0 0 0
59      7 3 0 0 0 0
60      5 4 0 0 0 0
61     15 4 0 0 0 0
62      6 5 0 0 0 0
63      8 6 0 0 0 0
64     11 7 0 0 0 0
65     12 7 0 0 0 0
66      9 8 0 0 0 0
67     10 8 0 0 0 0
68      5 16 0 0 0 0

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M END

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aniline-cation.sdf

COSMOtherm 3D 0

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69     15 15 0 0 0 0 0 0 0 0 0 V2000
70     -1.1972     -1.2132     -0.0012 C      0 0 0 0 0 0 0 0 0 0 1
71      0.2015     -1.2207      0.0049 C      0 0 0 0 0 0 0 0 0 0 2
72      0.8717      0.0000      0.0072 C      0 0 0 0 0 0 0 0 0 0 3
73      0.2015      1.2206      0.0052 C      0 0 0 0 0 0 0 0 0 0 4
74     -1.1972      1.2132     -0.0015 C      0 0 0 0 0 0 0 0 0 0 5
75     -1.8947      0.0000     -0.0052 C      0 0 0 0 0 0 0 0 0 0 6
76      2.3509      0.0000     -0.0069 N      0 0 0 0 0 0 0 0 0 0 7
77     -1.7390     -2.1597      0.0004 H      0 0 0 0 0 0 0 0 0 0 8
78      0.7549     -2.1612      0.0101 H      0 0 0 0 0 0 0 0 0 0 9
79      0.7549      2.1611      0.0102 H      0 0 0 0 0 0 0 0 0 0 10
80     -1.7389      2.1598     -0.0003 H      0 0 0 0 0 0 0 0 0 0 11
81     -2.9855      0.0001     -0.0078 H      0 0 0 0 0 0 0 0 0 0 12
82      2.7308      0.0028     -0.9655 H      0 0 0 0 0 0 0 0 0 0 13
83      2.7379     -0.8284     -0.4663 H      0 0 0 0 0 0 0 0 0 0 14
84      2.7380      0.8254      0.4715 H      0 0 0 0 0 0 0 0 0 0 15

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85      2 1 0 0 0 0
86      6 1 0 0 0 0
87      8 1 0 0 0 0
88      3 2 0 0 0 0
89      9 2 0 0 0 0
90      4 3 0 0 0 0
91      7 3 0 0 0 0
92      5 4 0 0 0 0
93     10 4 0 0 0 0
94      6 5 0 0 0 0
95     11 5 0 0 0 0
96     12 6 0 0 0 0
97     13 7 0 0 0 0

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12 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
5 16 0 0 0 0
M END
$$$$
clonidine-cation2.sdf
COSMOTHERM 3D 0
24 25 0 0 0 0 0 0 0 0 V2000
2.7823 0.9918 0.5509 C 0 0 0 0 0 0 0 0 0 0 0 1
1.5195 1.1167 -0.0268 C 0 0 0 0 0 0 0 0 0 0 0 2
0.7357 -0.0120 -0.3359 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2745 -1.2831 -0.0544 C 0 0 0 0 0 0 0 0 0 0 0 4
2.5327 -1.4268 0.5294 C 0 0 0 0 0 0 0 0 0 0 0 5
3.2786 -0.2843 0.8265 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8910 2.7212 -0.3805 C1 0 0 0 0 0 0 0 0 0 0 0 7
0.3468 -2.7219 -0.4560 C1 0 0 0 0 0 0 0 0 0 0 0 8
-0.5396 0.1298 -0.9530 N 0 0 0 0 0 0 0 0 0 0 0 9
-1.6941 0.1355 -0.2665 C 0 0 0 0 0 0 0 0 0 0 0 10
-3.9581 0.0522 0.1724 C 0 0 0 0 0 0 0 0 0 0 0 11
-3.1839 0.2225 1.4955 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.9010 0.3159 -0.8278 N 0 0 0 0 0 0 0 0 0 0 0 13
-1.7943 -0.0351 1.0609 N 0 0 0 0 0 0 0 0 0 0 0 14
-3.0556 0.1638 -1.8214 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.0012 0.0900 1.6849 H 0 0 0 0 0 0 0 0 0 0 0 16
3.3682 1.8811 0.7796 H 0 0 0 0 0 0 0 0 0 0 0 17
2.9261 -2.4206 0.7385 H 0 0 0 0 0 0 0 0 0 0 0 18
4.2650 -0.3899 1.2792 H 0 0 0 0 0 0 0 0 0 0 0 19
-4.3441 -0.9704 0.0519 H 0 0 0 0 0 0 0 0 0 0 0 20
-4.7789 0.7686 0.0684 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.2690 1.2440 1.8935 H 0 0 0 0 0 0 0 0 0 0 0 22
-3.4903 -0.4967 2.2615 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.5835 0.2607 -1.9627 H 0 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 6 0 0 0 0
10 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
22 12 0 0 0 0
23 12 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
9 24 0 0 0 0
M END
$$$$
clonidine.sdf
COSMOTHERM 3D 0
23 24 0 0 0 0 0 0 0 0 V2000
-0.6414 -2.8298 0.8595 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.3588 -1.6195 0.2590 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.0669 -1.8560 -1.0702 N 0 0 0 0 0 0 0 0 0 0 0 3
-0.5395 2.9761 -0.4990 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.9229 1.7267 -0.0170 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0027 0.6961 0.3045 C 0 0 0 0 0 0 0 0 0 0 0 6
1.3593 1.0382 0.0978 C 0 0 0 0 0 0 0 0 0 0 0 7
1.7742 2.2785 -0.3850 C 0 0 0 0 0 0 0 0 0 0 0 8
0.8182 3.2524 -0.6836 C 0 0 0 0 0 0 0 0 0 0 0 9
2.6036 -0.1604 0.5041 C1 0 0 0 0 0 0 0 0 0 0 0 10
-2.6498 1.4001 0.2048 C1 0 0 0 0 0 0 0 0 0 0 0 11
-0.4203 -0.4855 0.8978 N 0 0 0 0 0 0 0 0 0 0 0 12
-0.8022 -3.8672 -0.1730 C 0 0 0 0 0 0 0 0 0 0 0 13
0.0846 -3.3044 -1.2950 C 0 0 0 0 0 0 0 0 0 0 0 14
-1.2746 -2.8158 1.6559 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5515 -1.2106 -1.5555 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.2973 3.7250 -0.7290 H 0 0 0 0 0 0 0 0 0 0 0 17
2.8370 2.4809 -0.5177 H 0 0 0 0 0 0 0 0 0 0 0 18
1.1310 4.2272 -1.0583 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.8523 -3.9480 -0.5007 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.4604 -4.8451 0.1849 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.2616 -3.5916 -2.2945 H 0 0 0 0 0 0 0 0 0 0 0 22
1.1338 -3.6198 -1.1701 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
13 1 0 0 0 0
15 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
14 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0

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8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
18 8 0 0 0 0
19 9 0 0 0 0
14 13 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
22 14 0 0 0 0
14 23 0 0 0 0
M END
$$$$
clonidine0.sdf
COSMOtherm 3D 0
23 24 0 0 0 0 0 0 0 0 0 V2000
-1.7913 0.3793 -2.2634 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.3625 -0.0997 -1.0264 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0037 -0.2996 -0.6967 C 0 0 0 0 0 0 0 0 0 0 0 3
0.9122 0.0194 -1.7386 C 0 0 0 0 0 0 0 0 0 0 0 4
0.5146 0.4970 -2.9853 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8463 0.6780 -3.2479 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.5943 -0.5089 0.1842 C1 0 0 0 0 0 0 0 0 0 0 0 7
2.6429 -0.1973 -1.4299 C1 0 0 0 0 0 0 0 0 0 0 0 8
0.4381 -0.8875 0.4814 N 0 0 0 0 0 0 0 0 0 0 0 9
0.3717 -0.2549 1.6186 C 0 0 0 0 0 0 0 0 0 0 0 10
0.8241 0.1742 3.8651 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.0887 1.2812 3.3149 C 0 0 0 0 0 0 0 0 0 0 0 12
0.6745 -0.8561 2.8237 N 0 0 0 0 0 0 0 0 0 0 0 13
0.0576 1.0676 1.8642 N 0 0 0 0 0 0 0 0 0 0 0 14
1.3220 -1.6407 2.8005 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.5746 1.5446 1.2261 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.8566 0.5069 -2.4557 H 0 0 0 0 0 0 0 0 0 0 0 17
1.2640 0.7260 -3.7428 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.1701 1.0493 -4.2204 H 0 0 0 0 0 0 0 0 0 0 0 19
1.8683 0.5218 3.9384 H 0 0 0 0 0 0 0 0 0 0 0 20
0.4976 -0.1952 4.8440 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.1330 1.1327 3.6363 H 0 0 0 0 0 0 0 0 0 0 0 22
0.2386 2.2860 3.6056 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 6 0 0 0 0
10 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
20 11 0 0 0 0
21 11 0 0 0 0
14 12 0 0 0 0
22 12 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
12 23 0 0 0 0
M END
$$$$
clonidine1.sdf
COSMOtherm 3D 0
23 24 0 0 0 0 0 0 0 0 0 V2000
1.7883 0.3817 2.2655 C 0 0 0 0 0 0 0 0 0 0 0 1
1.3620 -0.1001 1.0286 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.0036 -0.3005 0.6965 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.9140 0.0185 1.7367 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.5190 0.4982 2.9833 C 0 0 0 0 0 0 0 0 0 0 0 5
0.8413 0.6802 3.2481 C 0 0 0 0 0 0 0 0 0 0 0 6
2.5959 -0.5090 -0.1798 C1 0 0 0 0 0 0 0 0 0 0 0 7
-2.6441 -0.1992 1.4249 C1 0 0 0 0 0 0 0 0 0 0 0 8
-0.4349 -0.8894 -0.4822 N 0 0 0 0 0 0 0 0 0 0 0 9
-0.3698 -0.2557 -1.6189 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.8202 0.1748 -3.8656 C 0 0 0 0 0 0 0 0 0 0 0 11
0.0880 1.2843 -3.3125 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.6693 -0.8562 -2.8251 N 0 0 0 0 0 0 0 0 0 0 0 13
-0.0587 1.0680 -1.8624 N 0 0 0 0 0 0 0 0 0 0 0 14
-1.3147 -1.6426 -2.8037 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5717 1.5456 -1.2229 H 0 0 0 0 0 0 0 0 0 0 0 16
2.8531 0.5101 2.4595 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.2697 0.7276 3.7393 H 0 0 0 0 0 0 0 0 0 0 0 18
1.1631 1.0535 4.2206 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.8653 0.5190 -3.9410 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.4903 -0.1925 -4.8441 H 0 0 0 0 0 0 0 0 0 0 0 21
1.1332 1.1405 -3.6333 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.2429 2.2883 -3.6021 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
6 1 0 0 0 0
17 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
4 3 0 0 0 0
9 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 6 0 0 0 0
10 9 0 0 0 0
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3 13 10 0 0 0 0
4 14 10 0 0 0 0
5 12 11 0 0 0 0
6 13 11 0 0 0 0
7 20 11 0 0 0 0
8 21 11 0 0 0 0
9 14 12 0 0 0 0
10 22 12 0 0 0 0
11 15 13 0 0 0 0
12 16 14 0 0 0 0
13 12 23 0 0 0 0
14 M END
15 $$$
16 clonidine_pl.sdf
17 COSMOTHERM 3D 0
18
19 24 25 0 0 0 0 0 0 0 0 0 V2000
20 -2.6479 -0.0153 0.5329 C1 0 0 0 0 0 0 0 0 0 0 0 0 1
21 -0.6424 -3.2432 -0.7885 C 0 0 0 0 0 0 0 0 0 0 0 0 2
22 -1.6704 -2.3535 -0.4699 C 0 0 0 0 0 0 0 0 0 0 0 0 3
23 -1.3491 -1.1188 0.0927 C 0 0 0 0 0 0 0 0 0 0 0 0 4
24 -0.0111 -0.7396 0.3201 C 0 0 0 0 0 0 0 0 0 0 0 0 5
25 0.9978 -1.6653 -0.0103 C 0 0 0 0 0 0 0 0 0 0 0 0 6
26 0.6943 -2.9092 -0.5615 C 0 0 0 0 0 0 0 0 0 0 0 0 7
27 2.6795 -1.2394 0.2783 C1 0 0 0 0 0 0 0 0 0 0 0 0 8
28 0.3155 0.5107 0.9153 N 0 0 0 0 0 0 0 0 0 0 0 0 9
29 0.2889 1.6795 0.2526 C 0 0 0 0 0 0 0 0 0 0 0 0 10
30 0.4971 2.8740 0.8308 N 0 0 0 0 0 0 0 0 0 0 0 0 11
31 0.0619 1.8106 -1.0634 N 0 0 0 0 0 0 0 0 0 0 0 0 12
32 0.6350 3.9114 -0.2141 C 0 0 0 0 0 0 0 0 0 0 0 0 13
33 -0.0744 3.2420 -1.4076 C 0 0 0 0 0 0 0 0 0 0 0 0 14
34 -0.8875 -4.2128 -1.2228 H 0 0 0 0 0 0 0 0 0 0 0 0 15
35 -2.7128 -2.6205 -0.6381 H 0 0 0 0 0 0 0 0 0 0 0 0 16
36 1.4940 -3.6066 -0.8070 H 0 0 0 0 0 0 0 0 0 0 0 0 17
37 0.9580 2.9585 1.7334 H 0 0 0 0 0 0 0 0 0 0 0 0 18
38 -0.3551 1.0728 -1.6245 H 0 0 0 0 0 0 0 0 0 0 0 0 19
39 1.6985 4.0984 -0.4220 H 0 0 0 0 0 0 0 0 0 0 0 0 20
40 0.1516 4.8424 0.0973 H 0 0 0 0 0 0 0 0 0 0 0 0 21
41 0.4097 3.4578 -2.3651 H 0 0 0 0 0 0 0 0 0 0 0 0 22
42 -1.1377 3.5171 -1.4614 H 0 0 0 0 0 0 0 0 0 0 0 0 23
43 0.6007 0.5239 1.8934 H 0 0 0 0 0 0 0 0 0 0 0 0 24
44 4 1 0 0 0 0
45 3 2 0 0 0 0
46 7 2 0 0 0 0
47 15 2 0 0 0 0
48 4 3 0 0 0 0
49 16 3 0 0 0 0
50 5 4 0 0 0 0
51 6 5 0 0 0 0
52 9 5 0 0 0 0
53 7 6 0 0 0 0
54 8 6 0 0 0 0
55 17 7 0 0 0 0
56 10 9 0 0 0 0
57 11 10 0 0 0 0
58 12 10 0 0 0 0
59 13 11 0 0 0 0
60 18 11 0 0 0 0
14 12 0 0 0 0
19 12 0 0 0 0
14 13 0 0 0 0
20 13 0 0 0 0
21 13 0 0 0 0
22 14 0 0 0 0
23 14 0 0 0 0
9 24 0 0 0 0
M END
$$$
clonidine_t_p3.sdf
COSMOTHERM 3D 0
24 25 0 0 0 0 0 0 0 0 0 V2000
0.2266 -3.1852 -1.4946 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0496 -3.9584 -0.1723 C 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.0338 -1.7954 -1.0617 N 0 0 0 0 0 0 0 0 0 0 0 0 3
2.7209 0.8916 0.3820 C1 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.2840 3.2789 -0.8267 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.9919 2.7821 -0.5519 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.1166 1.5200 0.0275 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0121 0.7353 0.3342 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2831 1.2753 0.0549 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.4267 2.5326 -0.5309 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-2.7220 0.3475 0.4561 C1 0 0 0 0 0 0 0 0 0 0 0 0 11
0.1292 -0.5399 0.9519 N 0 0 0 0 0 0 0 0 0 0 0 0 12
0.1353 -1.6947 0.2659 C 0 0 0 0 0 0 0 0 0 0 0 0 13
0.3141 -2.9015 0.8280 N 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.4884 -3.4922 -2.2642 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.2503 -3.2700 -1.8869 H 0 0 0 0 0 0 0 0 0 0 0 0 16
0.7627 -4.7818 -0.0657 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.9748 -4.3404 -0.0545 H 0 0 0 0 0 0 0 0 0 0 0 0 18
0.0945 -1.0027 -1.6856 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.3894 4.2648 -1.2802 H 0 0 0 0 0 0 0 0 0 0 0 0 20
1.8812 3.3682 -0.7795 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-2.4205 2.9261 -0.7398 H 0 0 0 0 0 0 0 0 0 0 0 0 22
0.2606 -0.5830 1.9615 H 0 0 0 0 0 0 0 0 0 0 0 0 23
0.1615 -3.0559 1.8216 H 0 0 0 0 0 0 0 0 0 0 0 0 24
2 1 0 0 0 0
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18 2 0 0 0 0
13 3 0 0 0 0
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18 5 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
6 20 0 0 0 0
M END
$$$$
debrisoquine.sdf
COSMOTHERM 3D 0
26 27 0 0 0 0 0 0 0 0 0 V2000
-0.3155 -3.3905 -0.6126 C 0 0 0 0 0 0 0 0 0 0 0 1
0.9954 -3.2267 -0.1453 C 0 0 0 0 0 0 0 0 0 0 0 2
1.3990 -1.9875 0.3573 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5122 -0.8985 0.3957 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8079 -1.0606 -0.0703 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2035 -2.3130 -0.5724 C 0 0 0 0 0 0 0 0 0 0 0 6
0.9814 0.4263 0.9789 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.7866 0.0970 -0.0308 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.3228 1.1946 0.9342 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0835 1.5422 0.6803 N 0 0 0 0 0 0 0 0 0 0 0 10
0.4490 2.4409 -0.3154 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.5118 3.4082 -0.6136 N 0 0 0 0 0 0 0 0 0 0 0 12
1.6042 2.3415 -0.9147 N 0 0 0 0 0 0 0 0 0 0 0 13
-0.6437 -4.3551 -1.0048 H 0 0 0 0 0 0 0 0 0 0 0 14
1.6988 -4.0612 -0.1735 H 0 0 0 0 0 0 0 0 0 0 0 15
2.4212 -1.8577 0.7235 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.2286 -2.4412 -0.9306 H 0 0 0 0 0 0 0 0 0 0 0 17
1.9754 0.6810 0.5943 H 0 0 0 0 0 0 0 0 0 0 0 18
1.0574 0.3305 2.0768 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.7849 -0.2632 0.2631 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.8956 0.5291 -1.0404 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.3853 0.8389 1.9743 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.9678 2.0758 0.8596 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.1499 4.1870 -1.1598 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.0876 3.7329 0.1611 H 0 0 0 0 0 0 0 0 0 0 0 25
1.7486 3.1609 -1.5153 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
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3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
17 6 0 0 0 0
10 7 0 0 0 0
18 7 0 0 0 0
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9 8 0 0 0 0
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21 8 0 0 0 0
10 9 0 0 0 0
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11 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
24 12 0 0 0 0
25 12 0 0 0 0
13 26 0 0 0 0
M END
$$$$
debrisoquine_a.sdf
COSMOTHERM 3D 0
26 27 0 0 0 0 0 0 0 0 0 V2000
-0.3158 -3.3907 -0.6122 C 0 0 0 0 0 0 0 0 0 0 0 1
0.9952 -3.2269 -0.1450 C 0 0 0 0 0 0 0 0 0 0 0 2
1.3989 -1.9876 0.3573 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5123 -0.8985 0.3954 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8078 -1.0606 -0.0705 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.2037 -2.3130 -0.5723 C 0 0 0 0 0 0 0 0 0 0 0 6
0.9816 0.4261 0.9784 C 0 0 0 0 0 0 0 0 0 0 0 7
-1.7862 0.0973 -0.0313 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.3227 1.1945 0.9342 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0837 1.5423 0.6806 N 0 0 0 0 0 0 0 0 0 0 0 10
0.4489 2.4410 -0.3153 C 0 0 0 0 0 0 0 0 0 0 0 11
-0.5116 3.4087 -0.6126 N 0 0 0 0 0 0 0 0 0 0 0 12
1.6037 2.3412 -0.9154 N 0 0 0 0 0 0 0 0 0 0 0 13
-0.6441 -4.3553 -1.0041 H 0 0 0 0 0 0 0 0 0 0 0 14
1.6985 -4.0615 -0.1730 H 0 0 0 0 0 0 0 0 0 0 0 15
2.4212 -1.8578 0.7234 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.2288 -2.4412 -0.9302 H 0 0 0 0 0 0 0 0 0 0 0 17
1.9754 0.6808 0.5935 H 0 0 0 0 0 0 0 0 0 0 0 18
1.0581 0.3301 2.0763 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.7849 -0.2627 0.2619 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.8945 0.5297 -1.0409 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.3852 0.8382 1.9741 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.9677 2.0757 0.8600 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.1497 4.1878 -1.1584 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.0872 3.7330 0.1625 H 0 0 0 0 0 0 0 0 0 0 0 25
1.7481 3.1608 -1.5158 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
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17 6 0 0 0 0
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11 10 0 0 0 0
12 11 0 0 0 0
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24 12 0 0 0 0
25 12 0 0 0 0
13 26 0 0 0 0

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M END

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debrisoquine_a_p2.sdf
COSMOtherm 3D 0

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27 28 0 0 0 0 0 0 0 0 0 V2000
-0.1971 -3.5846 -0.4254 C 0 0 0 0 0 0 0 0 0 0 1
1.1205 -3.3048 -0.0393 C 0 0 0 0 0 0 0 0 0 0 2
1.4740 -2.0019 0.3156 C 0 0 0 0 0 0 0 0 0 0 3
0.5245 -0.9679 0.2854 C 0 0 0 0 0 0 0 0 0 0 4
-0.7999 -1.2433 -0.0981 C 0 0 0 0 0 0 0 0 0 0 5
-1.1436 -2.5588 -0.4542 C 0 0 0 0 0 0 0 0 0 0 6
0.9480 0.4233 0.7167 C 0 0 0 0 0 0 0 0 0 0 7
-1.8334 -0.1388 -0.1458 C 0 0 0 0 0 0 0 0 0 0 8
-1.4179 1.0861 0.6726 C 0 0 0 0 0 0 0 0 0 0 9
-0.0316 1.4515 0.3330 N 0 0 0 0 0 0 0 0 0 0 10
0.3177 2.6416 -0.1852 C 0 0 0 0 0 0 0 0 0 0 11
-0.5515 3.6685 -0.1955 N 0 0 0 0 0 0 0 0 0 0 12
1.5458 2.8371 -0.7037 N 0 0 0 0 0 0 0 0 0 0 13
-0.4844 -4.6002 -0.7038 H 0 0 0 0 0 0 0 0 0 0 14
1.8687 -4.0990 -0.0152 H 0 0 0 0 0 0 0 0 0 0 15
2.5012 -1.7805 0.6168 H 0 0 0 0 0 0 0 0 0 0 16
-2.1723 -2.7767 -0.7521 H 0 0 0 0 0 0 0 0 0 0 17
1.9338 0.6606 0.3049 H 0 0 0 0 0 0 0 0 0 0 18
1.0524 0.4556 1.8162 H 0 0 0 0 0 0 0 0 0 0 19
-2.7990 -0.5056 0.2329 H 0 0 0 0 0 0 0 0 0 0 20
-2.0015 0.1679 -1.1915 H 0 0 0 0 0 0 0 0 0 0 21
-1.4601 0.8746 1.7524 H 0 0 0 0 0 0 0 0 0 0 22
-2.0952 1.9189 0.4648 H 0 0 0 0 0 0 0 0 0 0 23
-0.3021 4.5281 -0.6742 H 0 0 0 0 0 0 0 0 0 0 24
-1.2941 3.7348 0.4923 H 0 0 0 0 0 0 0 0 0 0 25
1.8012 3.7632 -1.0320 H 0 0 0 0 0 0 0 0 0 0 26
2.0735 2.0655 -1.0977 H 0 0 0 0 0 0 0 0 0 0 27

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2 1 0 0 0 0
6 1 0 0 0 0
14 1 0 0 0 0
3 2 0 0 0 0
15 2 0 0 0 0
4 3 0 0 0 0
16 3 0 0 0 0
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7 4 0 0 0 0
6 5 0 0 0 0
8 5 0 0 0 0
17 6 0 0 0 0
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21 8 0 0 0 0
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24 12 0 0 0 0
25 12 0 0 0 0
26 13 0 0 0 0
13 27 0 0 0 0

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M END

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debrisoquine_p2.sdf
COSMOtherm 3D 0

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27 28 0 0 0 0 0 0 0 0 0 V2000
-1.1679 -2.5717 0.3303 C 0 0 0 0 0 0 0 0 0 0 1
-0.7914 -1.2492 0.0383 C 0 0 0 0 0 0 0 0 0 0 2
0.5664 -0.9637 -0.1920 C 0 0 0 0 0 0 0 0 0 0 3
1.5156 -1.9977 -0.1353 C 0 0 0 0 0 0 0 0 0 0 4
1.1296 -3.3068 0.1563 C 0 0 0 0 0 0 0 0 0 0 5
-0.2212 -3.5954 0.3922 C 0 0 0 0 0 0 0 0 0 0 6
-1.8308 -0.1500 -0.0301 C 0 0 0 0 0 0 0 0 0 0 7
-1.3170 1.0363 -0.8414 C 0 0 0 0 0 0 0 0 0 0 8
1.0595 0.4393 -0.5108 C 0 0 0 0 0 0 0 0 0 0 9
0.0061 1.4475 -0.3417 N 0 0 0 0 0 0 0 0 0 0 10
0.2561 2.6597 0.1798 C 0 0 0 0 0 0 0 0 0 0 11
-0.7528 3.4708 0.5516 N 0 0 0 0 0 0 0 0 0 0 12
1.5229 3.0846 0.3381 N 0 0 0 0 0 0 0 0 0 0 13
-2.2233 -2.7955 0.5053 H 0 0 0 0 0 0 0 0 0 0 14
2.5692 -1.7706 -0.3177 H 0 0 0 0 0 0 0 0 0 0 15
1.8788 -4.0992 0.1999 H 0 0 0 0 0 0 0 0 0 0 16
-0.5342 -4.6161 0.6192 H 0 0 0 0 0 0 0 0 0 0 17
-2.0987 0.1830 0.9867 H 0 0 0 0 0 0 0 0 0 0 18
-2.7542 -0.5298 -0.4915 H 0 0 0 0 0 0 0 0 0 0 19
-2.0065 1.8855 -0.8157 H 0 0 0 0 0 0 0 0 0 0 20

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|---------|--------|---------|---|---|---|---|---|---|---|---|---|---|----|
| -1.1900 | 0.7504 | -1.8978 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 21 |
| 1.4461 | 0.4776 | -1.5442 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 |
| 1.8906 | 0.6836 | 0.1636 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 23 |
| -0.5419 | 4.4119 | 0.8688 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 24 |
| -1.6464 | 3.0903 | 0.8449 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 |
| 1.7009 | 3.9592 | 0.8220 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 26 |
| 2.2677 | 2.7401 | -0.2589 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 27 |

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|----|----|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 17 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 20 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 21 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 22 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 10 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 11 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 24 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 25 | 12 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 26 | 13 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

M END

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di-iso-butylamine-cation.sdf
COSMOTHERM 3D

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|----|------|---------|---------|---|---|---|---|---|---|---|---|---|---|---|---|---|-------|----|
| 29 | 28 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | V2000 | 1 |
| 3 | 7526 | 0.8082 | 0.1114 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| 2 | 5264 | -0.0069 | -0.3282 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 2 |
| 2 | 6291 | -1.4645 | 0.1446 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 3 |
| 1 | 2686 | 0.6881 | 0.2010 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 4 |
| 0 | 0001 | 0.0368 | -0.2980 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 5 |
| -1 | 2692 | 0.6903 | 0.1965 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 6 |
| -2 | 5261 | -0.0098 | -0.3279 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 7 |
| -3 | 7534 | 0.8077 | 0.1041 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 8 |
| -2 | 6281 | -1.4634 | 0.1568 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 9 |
| 4 | 6711 | 0.3580 | -0.2900 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 10 |
| 3 | 6967 | 1.8460 | -0.2477 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 11 |
| 3 | 8378 | 0.8285 | 1.2090 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 12 |
| 2 | 4827 | 0.0080 | -1.4313 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 13 |
| 3 | 5589 | -1.9186 | -0.2255 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 14 |
| 1 | 8033 | -2.0925 | -0.2238 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 15 |
| 2 | 6382 | -1.5202 | 1.2445 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 16 |
| 1 | 2215 | 1.7338 | -0.1257 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 17 |
| 1 | 2235 | 0.6550 | 1.2978 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 18 |
| -0 | 0013 | -0.9565 | -0.0260 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 19 |
| -1 | 2231 | 1.7338 | -0.1375 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 20 |
| -1 | 2238 | 0.6650 | 1.2934 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 21 |
| -2 | 4816 | -0.0037 | -1.4310 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 22 |
| -4 | 6710 | 0.3549 | -0.2965 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 23 |
| -3 | 6970 | 1.8434 | -0.2613 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 24 |
| -3 | 8409 | 0.8347 | 1.2014 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 25 |
| -3 | 5552 | -1.9227 | -0.2138 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 26 |
| -1 | 7993 | -2.0932 | -0.2019 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 27 |
| -2 | 6423 | -1.5094 | 1.2571 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 28 |
| 0 | 0019 | 0.0522 | -1.3275 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 29 |

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|----|----|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 17 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 20 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 21 | 6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 22 | 7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 23 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 24 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 25 | 8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 26 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 27 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 28 | 9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 29 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

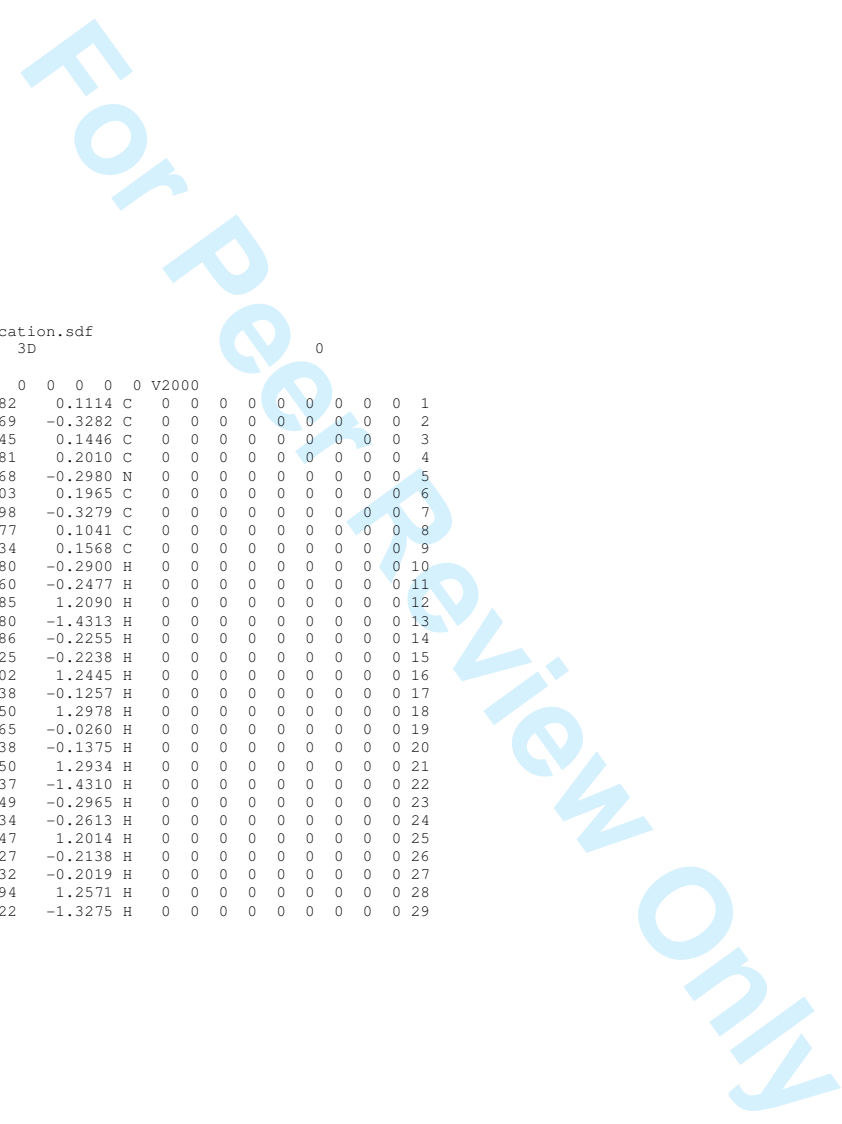
M END

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di-iso-butylamine.sdf
COSMOTHERM 3D

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|----|------|--------|--------|---|---|---|---|---|---|---|---|---|---|---|---|---|-------|---|
| 28 | 27 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | V2000 | 1 |
| 3 | 7305 | 0.8321 | 0.0829 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |



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2
3 2.5079 0.0022 -0.3357 C 0 0 0 0 0 0 0 0 0 0 2
4 2.6500 -1.4534 0.1342 C 0 0 0 0 0 0 0 0 0 0 3
5 1.2229 0.6590 0.1920 C 0 0 0 0 0 0 0 0 0 0 4
6 0.0000 -0.0057 -0.2836 N 0 0 0 0 0 0 0 0 0 0 5
7 -1.2231 0.6594 0.1907 C 0 0 0 0 0 0 0 0 0 0 6
8 -2.5080 0.0015 -0.3361 C 0 0 0 0 0 0 0 0 0 0 7
9 -3.7305 0.8320 0.0817 C 0 0 0 0 0 0 0 0 0 0 8
10 -2.6497 -1.4532 0.1367 C 0 0 0 0 0 0 0 0 0 0 9
11 4.6570 0.4016 -0.3251 H 0 0 0 0 0 0 0 0 0 0 10
12 3.6535 1.8704 -0.2743 H 0 0 0 0 0 0 0 0 0 0 11
13 3.8296 0.8591 1.1803 H 0 0 0 0 0 0 0 0 0 0 12
14 2.4470 0.0057 -1.4386 H 0 0 0 0 0 0 0 0 0 0 13
15 3.5914 -1.8915 -0.2303 H 0 0 0 0 0 0 0 0 0 0 14
16 1.8323 -2.0915 -0.2333 H 0 0 0 0 0 0 0 0 0 0 15
17 2.6578 -1.5089 1.2356 H 0 0 0 0 0 0 0 0 0 0 16
18 1.1867 1.7048 -0.1564 H 0 0 0 0 0 0 0 0 0 0 17
19 1.2712 0.6983 1.3042 H 0 0 0 0 0 0 0 0 0 0 18
20 -0.0004 -0.9664 0.0694 H 0 0 0 0 0 0 0 0 0 0 19
21 -1.1872 1.7046 -0.1593 H 0 0 0 0 0 0 0 0 0 0 20
22 -1.2716 0.7005 1.3029 H 0 0 0 0 0 0 0 0 0 0 21
23 -2.4472 0.0028 -1.4390 H 0 0 0 0 0 0 0 0 0 0 22
24 -4.6582 0.3953 -0.3170 H 0 0 0 0 0 0 0 0 0 0 23
25 -3.6582 1.8671 -0.2855 H 0 0 0 0 0 0 0 0 0 0 24
26 -3.8235 0.8690 1.1794 H 0 0 0 0 0 0 0 0 0 0 25
27 -3.5900 -1.8929 -0.2286 H 0 0 0 0 0 0 0 0 0 0 26
28 -1.8306 -2.0912 -0.2279 H 0 0 0 0 0 0 0 0 0 0 27
29 -2.6595 -1.5066 1.2381 H 0 0 0 0 0 0 0 0 0 0 28
30 2 1 0 0 0 0
31 10 1 0 0 0 0
32 11 1 0 0 0 0
33 12 1 0 0 0 0
34 3 2 0 0 0 0
35 4 2 0 0 0 0
36 13 2 0 0 0 0
37 14 3 0 0 0 0
38 15 3 0 0 0 0
39 16 3 0 0 0 0
40 5 4 0 0 0 0
41 17 4 0 0 0 0
42 18 4 0 0 0 0
43 6 5 0 0 0 0
44 19 5 0 0 0 0
45 7 6 0 0 0 0
46 20 6 0 0 0 0
47 21 6 0 0 0 0
48 8 7 0 0 0 0
49 9 7 0 0 0 0
50 22 7 0 0 0 0
51 23 8 0 0 0 0
52 24 8 0 0 0 0
53 25 8 0 0 0 0
54 26 9 0 0 0 0
55 27 9 0 0 0 0
56 9 28 0 0 0 0
57 M END
58 \$\$\$
59 di-iso-propylamine-cation.sdf
60 COSMOTHERM 3D 0
23 22 0 0 0 0 0 0 0 0 0 0 V2000
0.0000 -0.0002 -0.6037 N 0 0 0 0 0 0 0 0 0 0 0 1
1.2963 -0.2243 0.1752 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.2963 0.2242 0.1751 C 0 0 0 0 0 0 0 0 0 0 0 3
-2.3847 0.5771 -0.8353 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.6277 -1.0058 1.0099 C 0 0 0 0 0 0 0 0 0 0 0 5
1.6277 1.0058 1.0100 C 0 0 0 0 0 0 0 0 0 0 0 6
2.3847 -0.5769 -0.8353 C 0 0 0 0 0 0 0 0 0 0 0 7
0.1412 0.8073 -1.2292 H 0 0 0 0 0 0 0 0 0 0 0 8
1.0997 -1.0889 0.8213 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.0994 1.0888 0.8211 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.3118 0.8102 -0.2959 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.1102 1.4581 -1.4328 H 0 0 0 0 0 0 0 0 0 0 0 12
-2.5862 -0.2652 -1.5136 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.5776 -0.8283 1.5311 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.8668 -1.2163 1.7723 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.7506 -1.8948 0.3730 H 0 0 0 0 0 0 0 0 0 0 0 16
2.5766 0.8276 1.5325 H 0 0 0 0 0 0 0 0 0 0 0 17
0.8659 1.2172 1.7713 H 0 0 0 0 0 0 0 0 0 0 0 18
1.7521 1.8945 0.3730 H 0 0 0 0 0 0 0 0 0 0 0 19
3.3132 -0.8053 -0.2963 H 0 0 0 0 0 0 0 0 0 0 0 20
2.1122 -1.4606 -1.4299 H 0 0 0 0 0 0 0 0 0 0 0 21
2.5828 0.2639 -1.5164 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.1411 -0.8078 -1.2288 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
1 23 0 0 0 0

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23 17 0 0 0 0
24 17 0 0 0 0
25 17 0 0 0 0
26 20 0 0 0 0
27 20 0 0 0 0
28 20 0 0 0 0
  2 29 0 0 0 0

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M END

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di-n-butylamine.sdf

COSMOTHERM 3D 0

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28 27 0 0 0 0 0 0 0 0 0 V2000
  1.2254 -0.0132 0.5100 C 0 0 0 0 0 0 0 0 0 0 1
  0.0000 -0.0702 -0.3018 N 0 0 0 0 0 0 0 0 0 0 2
 -1.2254 -0.0132 0.5099 C 0 0 0 0 0 0 0 0 0 0 3
  2.4814 -0.0266 -0.3624 C 0 0 0 0 0 0 0 0 0 0 4
  1.2290 -0.8929 1.1768 H 0 0 0 0 0 0 0 0 0 0 5
  1.2450 0.8826 1.1701 H 0 0 0 0 0 0 0 0 0 0 6
  0.0000 0.7377 -0.9342 H 0 0 0 0 0 0 0 0 0 0 7
 -1.2294 -0.8935 1.1761 H 0 0 0 0 0 0 0 0 0 0 8
 -1.2446 0.8820 1.1708 H 0 0 0 0 0 0 0 0 0 0 9
 -2.4814 -0.0254 -0.3625 C 0 0 0 0 0 0 0 0 0 0 10
  3.7820 0.0326 0.4492 C 0 0 0 0 0 0 0 0 0 0 11
  2.4477 0.8326 -1.0568 H 0 0 0 0 0 0 0 0 0 0 12
  2.4734 -0.9361 -0.9872 H 0 0 0 0 0 0 0 0 0 0 13
 -3.7820 0.0317 0.4492 C 0 0 0 0 0 0 0 0 0 0 14
 -2.4481 0.8350 -1.0554 H 0 0 0 0 0 0 0 0 0 0 15
 -2.4730 -0.9339 -0.9888 H 0 0 0 0 0 0 0 0 0 0 16
  5.0386 0.0138 -0.4279 C 0 0 0 0 0 0 0 0 0 0 17
  3.8109 -0.8190 1.1509 H 0 0 0 0 0 0 0 0 0 0 18
  3.7816 0.9441 1.0711 H 0 0 0 0 0 0 0 0 0 0 19
 -5.0386 0.0139 -0.4278 C 0 0 0 0 0 0 0 0 0 0 20
 -3.8105 -0.8212 1.1493 H 0 0 0 0 0 0 0 0 0 0 21
 -3.7820 0.9422 1.0727 H 0 0 0 0 0 0 0 0 0 0 22
  5.9542 0.0575 0.1805 H 0 0 0 0 0 0 0 0 0 0 23
  5.0542 0.8725 -1.1175 H 0 0 0 0 0 0 0 0 0 0 24
  5.0842 -0.9031 -1.0362 H 0 0 0 0 0 0 0 0 0 0 25
 -5.9542 0.0576 0.1805 H 0 0 0 0 0 0 0 0 0 0 26
 -5.0539 0.8730 -1.1170 H 0 0 0 0 0 0 0 0 0 0 27
 -5.0846 -0.9027 -1.0367 H 0 0 0 0 0 0 0 0 0 0 28

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2 1 0 0 0 0

4 1 0 0 0 0

5 1 0 0 0 0

6 1 0 0 0 0

3 2 0 0 0 0

7 2 0 0 0 0

8 3 0 0 0 0

9 3 0 0 0 0

10 3 0 0 0 0

11 4 0 0 0 0

12 4 0 0 0 0

13 4 0 0 0 0

14 10 0 0 0 0

15 10 0 0 0 0

16 10 0 0 0 0

17 11 0 0 0 0

18 11 0 0 0 0

19 11 0 0 0 0

20 14 0 0 0 0

21 14 0 0 0 0

22 14 0 0 0 0

23 17 0 0 0 0

24 17 0 0 0 0

25 17 0 0 0 0

26 20 0 0 0 0

27 20 0 0 0 0

20 28 0 0 0 0

M END

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di-n-propylamine-cation.sdf

COSMOTHERM 3D 0

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23 22 0 0 0 0 0 0 0 0 0 V2000
  1.2701 0.0005 -0.3947 C 0 0 0 0 0 0 0 0 0 0 1
  0.0000 0.0006 0.4196 N 0 0 0 0 0 0 0 0 0 0 2
 -1.2701 0.0005 -0.3947 C 0 0 0 0 0 0 0 0 0 0 3
  2.5021 -0.0006 0.5026 C 0 0 0 0 0 0 0 0 0 0 4
  1.2295 -0.8921 -1.0319 H 0 0 0 0 0 0 0 0 0 0 5
  1.2304 0.8937 -1.0312 H 0 0 0 0 0 0 0 0 0 0 6
  0.0000 0.8206 1.0430 H 0 0 0 0 0 0 0 0 0 0 7
 -1.2298 -0.8922 -1.0317 H 0 0 0 0 0 0 0 0 0 0 8
 -1.2301 0.8935 -1.0314 H 0 0 0 0 0 0 0 0 0 0 9
 -2.5021 0.0002 0.5026 C 0 0 0 0 0 0 0 0 0 0 10
  3.7917 -0.0003 -0.3262 C 0 0 0 0 0 0 0 0 0 0 11
  2.4785 0.8857 1.1569 H 0 0 0 0 0 0 0 0 0 0 12
  2.4778 -0.8882 1.1552 H 0 0 0 0 0 0 0 0 0 0 13
 -3.7917 -0.0008 -0.3261 C 0 0 0 0 0 0 0 0 0 0 14
 -2.4786 0.8873 1.1558 H 0 0 0 0 0 0 0 0 0 0 15
 -2.4777 -0.8866 1.1562 H 0 0 0 0 0 0 0 0 0 0 16
  4.6706 -0.0031 0.3325 H 0 0 0 0 0 0 0 0 0 0 17
  3.8509 -0.8892 -0.9715 H 0 0 0 0 0 0 0 0 0 0 18
  3.8532 0.8916 -0.9671 H 0 0 0 0 0 0 0 0 0 0 19
 -4.6706 -0.0001 0.3326 H 0 0 0 0 0 0 0 0 0 0 20
 -3.8520 -0.8919 -0.9683 H 0 0 0 0 0 0 0 0 0 0 21
 -3.8522 0.8889 -0.9703 H 0 0 0 0 0 0 0 0 0 0 22
  0.0000 -0.8194 1.0430 H 0 0 0 0 0 0 0 0 0 0 23

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2 1 0 0 0 0

4 1 0 0 0 0

5 1 0 0 0 0

6 1 0 0 0 0

3 2 0 0 0 0

7 2 0 0 0 0

8 3 0 0 0 0

9 3 0 0 0 0

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10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
17 11 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
20 14 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
2 23 0 0 0 0
M END
$$$$
di-n-propylamine.sdf
COSMOTHERM 3D 0
22 21 0 0 0 0 0 0 0 0 V2000
1.2255 0.0141 -0.3703 C 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0586 0.4414 N 0 0 0 0 0 0 0 0 0 0 0 2
-1.2255 0.0134 -0.3703 C 0 0 0 0 0 0 0 0 0 0 0 3
2.4820 0.0181 0.5018 C 0 0 0 0 0 0 0 0 0 0 0 4
1.2288 0.9023 -1.0260 H 0 0 0 0 0 0 0 0 0 0 0 5
1.2478 -0.8730 -1.0423 H 0 0 0 0 0 0 0 0 0 0 0 6
0.0003 -0.7581 1.0623 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.2295 0.9018 -1.0256 H 0 0 0 0 0 0 0 0 0 0 0 8
-1.2472 -0.8735 -1.0427 H 0 0 0 0 0 0 0 0 0 0 0 9
-2.4820 0.0161 0.5018 C 0 0 0 0 0 0 0 0 0 0 0 10
3.7744 -0.0313 -0.3202 C 0 0 0 0 0 0 0 0 0 0 0 11
2.4468 -0.8483 1.1853 H 0 0 0 0 0 0 0 0 0 0 0 12
2.4713 0.9194 1.1363 H 0 0 0 0 0 0 0 0 0 0 0 13
-3.7744 -0.0299 -0.3203 C 0 0 0 0 0 0 0 0 0 0 0 14
-2.4475 -0.8518 1.1834 H 0 0 0 0 0 0 0 0 0 0 0 15
-2.4705 0.9160 1.1384 H 0 0 0 0 0 0 0 0 0 0 0 16
4.6606 -0.0251 0.3307 H 0 0 0 0 0 0 0 0 0 0 0 17
3.8503 0.8353 -0.9956 H 0 0 0 0 0 0 0 0 0 0 0 18
3.8200 -0.9417 -0.9378 H 0 0 0 0 0 0 0 0 0 0 0 19
-4.6606 -0.0258 0.3308 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.8501 0.8392 -0.9924 H 0 0 0 0 0 0 0 0 0 0 0 21
-3.8204 -0.9380 -0.9412 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
17 11 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
20 14 0 0 0 0
21 14 0 0 0 0
14 22 0 0 0 0
M END
$$$$
di-sec-butylamine-cation.sdf
COSMOTHERM 3D 0
29 28 0 0 0 0 0 0 0 0 V2000
-0.0212 0.6220 -0.5114 N 0 0 0 0 0 0 0 0 0 0 0 1
1.3787 0.4070 0.0707 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.1996 -0.0229 0.2194 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.4818 0.7540 1.4985 C 0 0 0 0 0 0 0 0 0 0 0 4
-2.3812 -0.0737 -0.7572 C 0 0 0 0 0 0 0 0 0 0 0 5
2.2783 1.5244 -0.4468 C 0 0 0 0 0 0 0 0 0 0 0 6
1.8577 -1.0022 -0.2928 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.2008 1.6352 -0.5735 H 0 0 0 0 0 0 0 0 0 0 0 8
1.2573 0.4962 1.1585 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8723 -1.0455 0.4531 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.8022 1.7824 1.2709 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.2901 0.2613 2.0527 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.6094 0.7917 2.1641 H 0 0 0 0 0 0 0 0 0 0 0 13
-2.0395 -0.5387 -1.6964 H 0 0 0 0 0 0 0 0 0 0 0 14
-3.5755 -0.8657 -0.2141 C 0 0 0 0 0 0 0 0 0 0 0 15
-2.6909 0.9559 -1.0027 H 0 0 0 0 0 0 0 0 0 0 0 16
3.2793 1.4255 -0.0094 H 0 0 0 0 0 0 0 0 0 0 0 17
1.8902 2.5135 -0.1643 H 0 0 0 0 0 0 0 0 0 0 0 18
2.3771 1.4784 -1.5414 H 0 0 0 0 0 0 0 0 0 0 0 19
3.1388 -1.4043 0.4473 C 0 0 0 0 0 0 0 0 0 0 0 20
1.0684 -1.7306 -0.0515 H 0 0 0 0 0 0 0 0 0 0 0 21
2.0186 -1.0514 -1.3831 H 0 0 0 0 0 0 0 0 0 0 0 22
-4.3592 -0.9365 -0.9807 H 0 0 0 0 0 0 0 0 0 0 0 23
-4.0182 -0.3865 0.6697 H 0 0 0 0 0 0 0 0 0 0 0 24
-3.2803 -1.8891 0.0613 H 0 0 0 0 0 0 0 0 0 0 0 25
3.4142 -2.4355 0.1885 H 0 0 0 0 0 0 0 0 0 0 0 26
3.9870 -0.7577 0.1829 H 0 0 0 0 0 0 0 0 0 0 0 27
2.9978 -1.3562 1.5373 H 0 0 0 0 0 0 0 0 0 0 0 28
-0.0162 0.2881 -1.4875 H 0 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0

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5 3 0 0 0 0
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18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
23 15 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
26 20 0 0 0 0
27 20 0 0 0 0
28 20 0 0 0 0
1 29 0 0 0 0
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M END
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di-sec-butylamine.sdf
COSMOtherm 3D 0

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28 27 0 0 0 0 0 0 0 0 V2000
-0.0130 0.6223 -0.5377 N 0 0 0 0 0 0 0 0 0 0 1
1.3284 0.4125 0.0522 C 0 0 0 0 0 0 0 0 0 0 2
-1.1469 -0.0029 0.1839 C 0 0 0 0 0 0 0 0 0 0 3
-1.4850 0.7107 1.5043 C 0 0 0 0 0 0 0 0 0 0 4
-2.3555 -0.0710 -0.7664 C 0 0 0 0 0 0 0 0 0 0 5
2.2506 1.5376 -0.4260 C 0 0 0 0 0 0 0 0 0 0 6
1.8657 -0.9774 -0.3390 C 0 0 0 0 0 0 0 0 0 0 7
-0.1902 1.6316 -0.5823 H 0 0 0 0 0 0 0 0 0 0 8
1.2883 0.4552 1.1621 H 0 0 0 0 0 0 0 0 0 0 9
-0.8449 -1.0393 0.4134 H 0 0 0 0 0 0 0 0 0 0 10
-1.8552 1.7298 1.3021 H 0 0 0 0 0 0 0 0 0 0 11
-2.2601 0.1755 2.0723 H 0 0 0 0 0 0 0 0 0 0 12
-0.6000 0.7910 2.1525 H 0 0 0 0 0 0 0 0 0 0 13
-2.0114 -0.5303 -1.7065 H 0 0 0 0 0 0 0 0 0 0 14
-3.5580 -0.8513 -0.2220 C 0 0 0 0 0 0 0 0 0 0 15
-2.6638 0.9600 -1.0179 H 0 0 0 0 0 0 0 0 0 0 16
3.2714 1.4101 -0.0411 H 0 0 0 0 0 0 0 0 0 0 17
1.8854 2.5189 -0.0856 H 0 0 0 0 0 0 0 0 0 0 18
2.2968 1.5500 -1.5268 H 0 0 0 0 0 0 0 0 0 0 19
3.1049 -1.4154 0.4508 C 0 0 0 0 0 0 0 0 0 0 20
1.0668 -1.7207 -0.1859 H 0 0 0 0 0 0 0 0 0 0 21
2.0825 -0.9728 -1.4211 H 0 0 0 0 0 0 0 0 0 0 22
-4.3523 -0.9239 -0.9796 H 0 0 0 0 0 0 0 0 0 0 23
-3.9937 -0.3723 0.6667 H 0 0 0 0 0 0 0 0 0 0 24
-3.2697 -1.8772 0.0573 H 0 0 0 0 0 0 0 0 0 0 25
3.4207 -2.4270 0.1566 H 0 0 0 0 0 0 0 0 0 0 26
3.9597 -0.7430 0.2842 H 0 0 0 0 0 0 0 0 0 0 27
2.8993 -1.4320 1.5329 H 0 0 0 0 0 0 0 0 0 0 28
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2 1 0 0 0 0
3 1 0 0 0 0
8 1 0 0 0 0
6 2 0 0 0 0
7 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
23 15 0 0 0 0
24 15 0 0 0 0
25 15 0 0 0 0
26 20 0 0 0 0
27 20 0 0 0 0
20 28 0 0 0 0
```

M END
\$\$\$\$

diethylamine-cation.sdf
COSMOtherm 3D 0

```
17 16 0 0 0 0 0 0 0 0 V2000
1.2712 -0.0047 0.5410 C 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0005 -0.2740 N 0 0 0 0 0 0 0 0 0 0 2
-1.2712 0.0047 0.5410 C 0 0 0 0 0 0 0 0 0 0 3
2.4951 0.0019 -0.3587 C 0 0 0 0 0 0 0 0 0 0 4
1.2278 0.8832 1.1829 H 0 0 0 0 0 0 0 0 0 0 5
1.2281 -0.9010 1.1710 H 0 0 0 0 0 0 0 0 0 0 6
-0.0030 -0.8190 -0.8980 H 0 0 0 0 0 0 0 0 0 0 7
-1.2286 0.9008 1.1714 H 0 0 0 0 0 0 0 0 0 0 8
-1.2273 -0.8835 1.1826 H 0 0 0 0 0 0 0 0 0 0 9
-2.4951 -0.0024 -0.3587 C 0 0 0 0 0 0 0 0 0 0 10
3.3966 -0.0049 0.2678 H 0 0 0 0 0 0 0 0 0 0 11
2.5251 -0.8870 -1.0047 H 0 0 0 0 0 0 0 0 0 0 12
2.5270 0.9025 -0.9882 H 0 0 0 0 0 0 0 0 0 0 13
-3.3966 0.0022 0.2678 H 0 0 0 0 0 0 0 0 0 0 14
-2.5256 -0.9020 -0.9896 H 0 0 0 0 0 0 0 0 0 0 15
-2.5264 0.8874 -1.0034 H 0 0 0 0 0 0 0 0 0 0 16
0.0030 0.8205 -0.8972 H 0 0 0 0 0 0 0 0 0 0 17
```

```
2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
2 17 0 0 0 0
```

M END

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diethylamine.sdf

COSMOtherm

3D

0

```
16 15 0 0 0 0 0 0 0 0 V2000
  1.2259  0.0167 -0.5183 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
  0.0000 -0.0716  0.2905 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
 -1.2259  0.0155 -0.5184 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
  2.4739 -0.0083  0.3599 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
  1.2359 -0.8448 -1.2070 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
  1.2361  0.9283 -1.1548 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
 -0.0004  0.7097  0.9557 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
 -1.2362 -0.8473 -1.2056 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
 -1.2362  0.9260 -1.1565 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
 -2.4739 -0.0077  0.3600 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 10
  3.3837  0.0363 -0.2560 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 11
  2.4922  0.8537  1.0454 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 12
  2.5100 -0.9267  0.9644 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 13
 -3.3837  0.0341 -0.2560 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 14
 -2.4927  0.8565  1.0427 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 15
 -2.5092 -0.9242  0.9674 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 16
  2  1  0  0  0  0
  4  1  0  0  0  0
  5  1  0  0  0  0
  6  1  0  0  0  0
  3  2  0  0  0  0
  7  2  0  0  0  0
  8  3  0  0  0  0
  9  3  0  0  0  0
 10  3  0  0  0  0
 11  4  0  0  0  0
 12  4  0  0  0  0
 13  4  0  0  0  0
 14 10  0  0  0  0
 15 10  0  0  0  0
 10 16  0  0  0  0
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M END

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dimethyl-iso-butylamine-cation.sdf

COSMOtherm

3D

0

```
23 22 0 0 0 0 0 0 0 0 V2000
  1.2294 -0.1796 -0.1110 N  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  1
  1.6111  1.0226 -0.9252 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  2
  2.3634 -0.6124  0.7741 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  3
 -0.0366  0.0366  0.7004 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  4
 -1.2990  0.2467 -0.1408 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  5
 -2.4785  0.4545  0.8240 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  6
 -1.5607 -0.9268 -1.0968 C  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  7
  2.5202  0.7841 -1.4856 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  8
  0.8002  1.2659 -1.6169 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  9
  1.7910  1.8562 -0.2384 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 10
  2.0689 -1.5275  1.2972 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 11
  2.5653  0.1905  1.4900 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 12
  3.2417 -0.7974  0.1483 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 13
  0.1666  0.8981  1.3495 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 14
 -0.1435 -0.8586  1.3288 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 15
 -1.1863  1.1710 -0.7303 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 16
 -3.3982  0.6557  0.2574 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 17
 -2.3009  1.3042  1.4988 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 18
 -2.6478 -0.4433  1.4386 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 19
 -2.5011 -0.7678 -1.6424 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 20
 -0.7730 -1.0448 -1.8584 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 21
 -1.6451 -1.8745 -0.5422 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 22
  1.0446 -0.9516 -0.7667 H  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0 23
  2  1  0  0  0  0
  3  1  0  0  0  0
  4  1  0  0  0  0
  8  2  0  0  0  0
  9  2  0  0  0  0
 10  2  0  0  0  0
 11  3  0  0  0  0
 12  3  0  0  0  0
 13  3  0  0  0  0
  5  4  0  0  0  0
 14  4  0  0  0  0
 15  4  0  0  0  0
  6  5  0  0  0  0
  7  5  0  0  0  0
 16  5  0  0  0  0
 17  6  0  0  0  0
 18  6  0  0  0  0
 19  6  0  0  0  0
 20  7  0  0  0  0
 21  7  0  0  0  0
 22  7  0  0  0  0
  1 23  0  0  0  0
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$$$$
dimethyl-iso-butylamine.sdf
COSMOtherm          3D              0

22 21 0 0 0 0 0 0 0 0 0 0 V2000
  1.2288 -0.1570 0.1768 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
  1.6285 -0.7790 -1.0875 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
  2.3258 0.6573 0.7050 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
  0.0141 0.6583 0.0280 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 -1.2770 -0.1351 -0.2402 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 -2.4442 0.8425 -0.4454 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
 -1.5761 -1.1306 0.8883 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
  2.5377 -1.3771 -0.9319 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
  0.8415 -1.4508 -1.4547 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
  1.8401 -0.0265 -1.8809 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
  2.0400 1.0849 1.6769 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
  2.6042 1.4959 0.0267 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
  3.2174 0.0305 0.8512 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
  0.1498 1.4131 -0.7829 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
 -0.1187 1.2223 0.9671 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
 -1.1515 -0.7023 -1.1789 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
 -3.3749 0.3014 -0.6726 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
 -2.2458 1.5382 -1.2749 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
 -2.6183 1.4416 0.4636 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
 -2.4768 -1.7223 0.6649 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
 -0.7351 -1.8216 1.0405 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
 -1.7490 -0.5969 1.8377 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22

  2 1 0 0 0 0
  3 1 0 0 0 0
  4 1 0 0 0 0
  8 2 0 0 0 0
  9 2 0 0 0 0
 10 2 0 0 0 0
 11 3 0 0 0 0
 12 3 0 0 0 0
 13 3 0 0 0 0
  5 4 0 0 0 0
 14 4 0 0 0 0
 15 4 0 0 0 0
  6 5 0 0 0 0
  7 5 0 0 0 0
 16 5 0 0 0 0
 17 6 0 0 0 0
 18 6 0 0 0 0
 19 6 0 0 0 0
 20 7 0 0 0 0
 21 7 0 0 0 0
  7 22 0 0 0 0

M  END
$$$$

```

```

dimethyl-iso-propylamine-cation.sdf
COSMOtherm          3D              0

20 19 0 0 0 0 0 0 0 0 V2000
  0.6794 -0.0013 0.2861 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
  1.4703 -1.2293 -0.0709 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
  1.4680 1.2306 -0.0630 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
 -0.7319 -0.0013 -0.3377 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 -1.4873 1.2631 0.0652 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 -1.4897 -1.2619 0.0729 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
  2.4676 -1.1304 0.3678 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
  0.9768 -2.1148 0.3348 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
  1.5386 -1.2893 -1.1622 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
  2.4676 1.1274 0.3696 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
  0.9763 2.1115 0.3548 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
  1.5304 1.3018 -1.1539 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
 -0.5428 -0.0046 -1.4205 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
 -2.5064 1.1940 -0.3363 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
 -1.0382 2.1780 -0.3382 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
 -1.5635 1.3503 1.1596 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
 -2.5083 -1.1941 -0.3300 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
 -1.0417 -2.1803 -0.3235 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
 -1.5670 -1.3412 1.1679 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
  0.5521 -0.0047 1.3085 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20

  2 1 0 0 0 0
  3 1 0 0 0 0
  4 1 0 0 0 0
  7 2 0 0 0 0
  8 2 0 0 0 0
  9 2 0 0 0 0
 10 3 0 0 0 0
 11 3 0 0 0 0
 12 3 0 0 0 0
  5 4 0 0 0 0
  6 4 0 0 0 0
 13 4 0 0 0 0
 14 5 0 0 0 0
 15 5 0 0 0 0
 16 5 0 0 0 0
 17 6 0 0 0 0
 18 6 0 0 0 0
 19 6 0 0 0 0
  1 20 0 0 0 0

M  END
$$$$

```

```

dimethyl-iso-propylamine.sdf
COSMOtherm          3D              0

19 18 0 0 0 0 0 0 0 0 V2000
  0.6711 -0.0003 0.3162 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
  1.4477 -1.1939 -0.0461 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
  1.4473 1.1939 -0.0448 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
 -0.6737 -0.0003 -0.3167 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
 -1.4724 1.2525 0.0696 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
 -1.4733 -1.2520 0.0709 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6

```

1
2
3 2.4460 -1.1229 0.4072 H 0 0 0 0 0 0 0 0 0 0 7
4 0.9718 -2.1051 0.3349 H 0 0 0 0 0 0 0 0 0 0 8
5 1.5773 -1.3009 -1.1468 H 0 0 0 0 0 0 0 0 0 0 9
6 2.4455 1.1230 0.4089 H 0 0 0 0 0 0 0 0 0 0 10
7 0.9708 2.1045 0.3366 H 0 0 0 0 0 0 0 0 0 0 11
8 1.5775 1.3019 -1.1453 H 0 0 0 0 0 0 0 0 0 0 12
9 -0.5464 -0.0010 -1.4253 H 0 0 0 0 0 0 0 0 0 0 13
10 -2.4905 1.1789 -0.3377 H 0 0 0 0 0 0 0 0 0 0 14
11 -1.0296 2.1777 -0.3207 H 0 0 0 0 0 0 0 0 0 0 15
12 -1.5464 1.3376 1.1653 H 0 0 0 0 0 0 0 0 0 0 16
13 -2.4903 -1.1796 -0.3395 H 0 0 0 0 0 0 0 0 0 0 17
14 -1.0293 -2.1782 -0.3156 H 0 0 0 0 0 0 0 0 0 0 18
15 -1.5502 -1.3340 1.1667 H 0 0 0 0 0 0 0 0 0 0 19
16 2 1 0 0 0 0
17 3 1 0 0 0 0
18 4 1 0 0 0 0
19 7 2 0 0 0 0
20 8 2 0 0 0 0
21 9 2 0 0 0 0
22 10 3 0 0 0 0
23 11 3 0 0 0 0
24 12 3 0 0 0 0
25 5 4 0 0 0 0
26 6 4 0 0 0 0
27 13 4 0 0 0 0
28 14 5 0 0 0 0
29 15 5 0 0 0 0
30 16 5 0 0 0 0
31 17 6 0 0 0 0
32 18 6 0 0 0 0
33 6 19 0 0 0 0
M END
\$\$\$\$
dimethyl-n-butylamine-cation.sdf
COSMOtherm 3D 0
23 22 0 0 0 0 0 0 0 0 0 0 V2000
2.7371 0.8985 -0.0533 C 0 0 0 0 0 0 0 0 0 0 1
1.5838 -0.0294 -0.3071 N 0 0 0 0 0 0 0 0 0 0 2
0.2913 0.5529 0.2370 C 0 0 0 0 0 0 0 0 0 0 3
1.8741 -1.4029 0.2257 C 0 0 0 0 0 0 0 0 0 0 4
3.6360 0.4691 -0.5057 H 0 0 0 0 0 0 0 0 0 0 5
2.5106 1.8695 -0.5041 H 0 0 0 0 0 0 0 0 0 0 6
2.8651 0.9988 1.0295 H 0 0 0 0 0 0 0 0 0 0 7
0.2527 1.5845 -0.1361 H 0 0 0 0 0 0 0 0 0 0 8
-0.9492 -0.2200 -0.1931 C 0 0 0 0 0 0 0 0 0 0 9
0.4060 0.5789 1.3288 H 0 0 0 0 0 0 0 0 0 0 10
2.8205 -1.7457 -0.2030 H 0 0 0 0 0 0 0 0 0 0 11
1.0675 -2.0817 -0.0638 H 0 0 0 0 0 0 0 0 0 0 12
1.9489 -1.3371 1.3163 H 0 0 0 0 0 0 0 0 0 0 13
-2.2287 0.4986 0.2651 C 0 0 0 0 0 0 0 0 0 0 14
-0.9393 -1.2362 0.2285 H 0 0 0 0 0 0 0 0 0 0 15
-0.9575 -0.3188 -1.2917 H 0 0 0 0 0 0 0 0 0 0 16
-3.5000 -0.2488 -0.1491 C 0 0 0 0 0 0 0 0 0 0 17
-2.2434 1.5175 -0.1549 H 0 0 0 0 0 0 0 0 0 0 18
-2.2067 0.6122 1.3614 H 0 0 0 0 0 0 0 0 0 0 19
-4.3993 0.2832 0.1934 H 0 0 0 0 0 0 0 0 0 0 20
-3.5238 -1.2614 0.2817 H 0 0 0 0 0 0 0 0 0 0 21
-3.5637 -0.3473 -1.2436 H 0 0 0 0 0 0 0 0 0 0 22
1.4741 -0.1098 -1.3274 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
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14 9 0 0 0 0
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17 14 0 0 0 0
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19 14 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
22 17 0 0 0 0
2 23 0 0 0 0
M END
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dimethyl-n-butylamine.sdf
COSMOtherm 3D 0
22 21 0 0 0 0 0 0 0 0 0 0 V2000
2.7135 0.8694 -0.0625 C 0 0 0 0 0 0 0 0 0 0 1
1.5898 -0.0312 -0.3367 N 0 0 0 0 0 0 0 0 0 0 2
0.3437 0.5301 0.2123 C 0 0 0 0 0 0 0 0 0 0 3
1.8750 -1.3648 0.2020 C 0 0 0 0 0 0 0 0 0 0 4
3.6311 0.4675 -0.5156 H 0 0 0 0 0 0 0 0 0 0 5
2.5154 1.8586 -0.5000 H 0 0 0 0 0 0 0 0 0 0 6
2.8986 1.0037 1.0271 H 0 0 0 0 0 0 0 0 0 0 7
0.2783 1.5739 -0.1360 H 0 0 0 0 0 0 0 0 0 0 8
-0.9251 -0.2111 -0.2167 C 0 0 0 0 0 0 0 0 0 0 9
0.3906 0.5684 1.3267 H 0 0 0 0 0 0 0 0 0 0 10
2.8194 -1.7360 -0.2206 H 0 0 0 0 0 0 0 0 0 0 11
1.0813 -2.0718 -0.0718 H 0 0 0 0 0 0 0 0 0 0 12
1.9703 -1.3607 1.3117 H 0 0 0 0 0 0 0 0 0 0 13
-2.2020 0.5000 0.2532 C 0 0 0 0 0 0 0 0 0 0 14
-0.9232 -1.2378 0.1840 H 0 0 0 0 0 0 0 0 0 0 15
-0.9319 -0.2992 -1.3167 H 0 0 0 0 0 0 0 0 0 0 16
-3.4823 -0.2510 -0.1281 C 0 0 0 0 0 0 0 0 0 0 17

1
2
3 -2.2296 1.5169 -0.1739 H 0 0 0 0 0 0 0 0 0 0 0 0 18
4 -2.1644 0.6276 1.3486 H 0 0 0 0 0 0 0 0 0 0 0 0 19
5 -4.3797 0.2864 0.2132 H 0 0 0 0 0 0 0 0 0 0 0 0 20
6 -3.5015 -1.2553 0.3228 H 0 0 0 0 0 0 0 0 0 0 0 0 21
7 -3.5607 -0.3740 -1.2197 H 0 0 0 0 0 0 0 0 0 0 0 0 22
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dimethyl-n-propylamine-cation.sdf
COSMOtherm                    3D                                                 0
20 19 0 0 0 0 0 0 0 0 0 0 0 V2000
2.0832   1.0286   0.0244 C   0 0 0 0 0 0 0 0 0 0 0 1
1.0250   0.0112   -0.2915 N   0 0 0 0 0 0 0 0 0 0 0 2
-0.3302   0.4589   0.2277 C   0 0 0 0 0 0 0 0 0 0 0 3
1.4210   -1.3474   0.2106 C   0 0 0 0 0 0 0 0 0 0 0 4
3.0350   0.6818   -0.3893 H   0 0 0 0 0 0 0 0 0 0 0 5
1.7966   1.9831   -0.4274 H   0 0 0 0 0 0 0 0 0 0 0 6
2.1526   1.1251   1.1129 H   0 0 0 0 0 0 0 0 0 0 0 7
-0.4313   1.5096   -0.0737 H   0 0 0 0 0 0 0 0 0 0 0 8
-1.4890   -0.3667   -0.3194 C   0 0 0 0 0 0 0 0 0 0 0 9
-0.2679   0.4128   1.3232 H   0 0 0 0 0 0 0 0 0 0 0 10
2.3877   -1.6097   -0.2299 H   0 0 0 0 0 0 0 0 0 0 0 11
0.6654   -2.0786   -0.0882 H   0 0 0 0 0 0 0 0 0 0 0 12
1.4983   -1.2980   1.3019 H   0 0 0 0 0 0 0 0 0 0 0 13
-2.8303   0.2151   0.1464 C   0 0 0 0 0 0 0 0 0 0 0 14
-1.4112   -1.4119   0.0133 H   0 0 0 0 0 0 0 0 0 0 0 15
-1.4461   -0.3678   -1.4206 H   0 0 0 0 0 0 0 0 0 0 0 16
-3.6635   -0.3772   -0.2550 H   0 0 0 0 0 0 0 0 0 0 0 17
-2.9561   1.2530   -0.1957 H   0 0 0 0 0 0 0 0 0 0 0 18
-2.9078   0.2064   1.2436 H   0 0 0 0 0 0 0 0 0 0 0 19
0.9522   -0.0473   -1.3166 H   0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
17 14 0 0 0 0
18 14 0 0 0 0
19 14 0 0 0 0
2 20 0 0 0 0
M   END
$$$$
dimethyl-n-propylamine.sdf
COSMOtherm                    3D                                                 0
19 18 0 0 0 0 0 0 0 0 0 0 V2000
2.0628   0.9940   0.0103 C   0 0 0 0 0 0 0 0 0 0 0 1
1.0283   0.0113   -0.3254 N   0 0 0 0 0 0 0 0 0 0 0 2
-0.2781   0.4508   0.1930 C   0 0 0 0 0 0 0 0 0 0 0 3
1.4067   -1.3091   0.1881 C   0 0 0 0 0 0 0 0 0 0 0 4
3.0253   0.6825   -0.4206 H   0 0 0 0 0 0 0 0 0 0 0 5
1.7967   1.9751   -0.4089 H   0 0 0 0 0 0 0 0 0 0 0 6
2.2007   1.1130   1.1087 H   0 0 0 0 0 0 0 0 0 0 0 7
-0.4156   1.4986   -0.1206 H   0 0 0 0 0 0 0 0 0 0 0 8
-1.4670   -0.3709   -0.3135 C   0 0 0 0 0 0 0 0 0 0 0 9
-0.2773   0.4498   1.3092 H   0 0 0 0 0 0 0 0 0 0 0 10
2.3925   -1.5881   -0.2102 H   0 0 0 0 0 0 0 0 0 0 0 11
0.6848   -2.0715   -0.1317 H   0 0 0 0 0 0 0 0 0 0 0 12
1.4645   -1.3292   1.3001 H   0 0 0 0 0 0 0 0 0 0 0 13
-2.8056   0.2195   0.1462 C   0 0 0 0 0 0 0 0 0 0 0 14
-1.3905   -1.4107   0.0408 H   0 0 0 0 0 0 0 0 0 0 0 15
-1.4282   -0.4064   -1.4147 H   0 0 0 0 0 0 0 0 0 0 0 16
-3.6502   -0.3892   -0.2075 H   0 0 0 0 0 0 0 0 0 0 0 17
-2.9438   1.2421   -0.2383 H   0 0 0 0 0 0 0 0 0 0 0 18
-2.8643   0.2652   1.2448 H   0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
5 1 0 0 0 0
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7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0

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19 6 0 0 0 0
20 15 0 0 0 0
21 15 0 0 0 0
15 22 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine-cation.sdf
COSMOtherm 3D 0

23 22 0 0 0 0 0 0 0 0 0 V2000
1.5905 -1.2243 -0.0043 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.8265 0.0035 0.4073 N 0 0 0 0 0 0 0 0 0 0 0 0 2
1.5941 1.2284 -0.0061 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.6863 -0.0018 -0.0240 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.2932 1.3429 0.3930 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3676 -1.1368 0.7504 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.7897 -0.2127 -1.5343 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.5590 -1.2006 0.5043 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.0416 -2.1209 0.2922 H 0 0 0 0 0 0 0 0 0 0 0 0 9
1.7387 -1.2018 -1.0875 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.6238 1.1096 0.3455 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.1501 2.1142 0.4522 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.5803 1.3070 -1.0971 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.3814 1.2810 0.2629 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.9335 2.1758 -0.2241 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.0967 1.5666 1.4520 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.4434 -1.1034 0.5349 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.0063 -2.1300 0.4565 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-1.2402 -1.0145 1.8366 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-1.8490 -0.1364 -1.8139 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.4374 -1.2054 -1.8424 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.2460 0.5553 -2.1012 H 0 0 0 0 0 0 0 0 0 0 0 0 22
0.8011 0.0050 1.4369 H 0 0 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
11 3 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
2 23 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine.sdf
COSMOtherm 3D 0

22 21 0 0 0 0 0 0 0 0 0 V2000
1.5723 -1.1946 0.0173 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.8227 0.0009 0.4211 N 0 0 0 0 0 0 0 0 0 0 0 0 2
1.5766 1.1925 0.0151 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.6202 -0.0010 -0.0046 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.2877 1.2963 0.4910 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.3336 -1.1827 0.6808 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.8002 -0.1114 -1.5366 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.5632 -1.1660 0.4938 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.0689 -2.1085 0.3545 H 0 0 0 0 0 0 0 0 0 0 0 0 9
1.7334 -1.2714 -1.0794 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2.5935 1.1177 0.4271 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.1220 2.1047 0.4189 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.6740 1.3088 -1.0862 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.3764 1.2218 0.3590 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.9493 2.1808 -0.0659 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.0795 1.4553 1.5599 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.4128 -1.1329 0.4759 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.9779 -2.1566 0.3182 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-1.1847 -1.1411 1.7703 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-1.8678 -0.0587 -1.7966 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.4105 -1.0645 -1.9226 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.2890 0.7085 -2.0626 H 0 0 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
11 3 0 0 0 0
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13 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
7 22 0 0 0 0
M END

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dimethylamine-cation.sdf
COSMOTHERM 3D 0

11 10 0 0 0 0 0 0 0 0 0 V2000
1.2556 0.0000 -0.2861 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0000 0.5299 N 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.2556 0.0000 -0.2861 C 0 0 0 0 0 0 0 0 0 0 0 0 3
2.1129 -0.0009 0.3934 H 0 0 0 0 0 0 0 0 0 0 0 0 4
1.2614 -0.8988 -0.9100 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.2623 0.8997 -0.9088 H 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.0001 0.8178 1.1531 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.1128 0.0014 0.3935 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2626 -0.8998 -0.9086 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.2612 0.8986 -0.9102 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0001 -0.8177 1.1532 H 0 0 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
2 11 0 0 0 0

M END
\$\$\$\$
dimethylamine.sdf
COSMOTHERM 3D 0

10 9 0 0 0 0 0 0 0 0 0 V2000
1.2168 0.0159 -0.2573 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 -0.0882 0.5567 N 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.2168 0.0159 -0.2573 C 0 0 0 0 0 0 0 0 0 0 0 0 3
2.1018 0.0109 0.3942 H 0 0 0 0 0 0 0 0 0 0 0 0 4
1.2859 -0.8543 -0.9284 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.2527 0.9295 -0.8875 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.0000 0.6739 1.2394 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.1018 0.0106 0.3943 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2858 -0.8541 -0.9286 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.2529 0.9296 -0.8873 H 0 0 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
4 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
7 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
3 10 0 0 0 0

M END
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dimethylethylamine-cation.sdf
COSMOTHERM 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
1.6899 0.8096 -0.0063 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.4590 -0.0005 -0.2935 N 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.7718 0.6486 0.3187 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.6416 -1.4260 0.1394 C 0 0 0 0 0 0 0 0 0 0 0 0 4
2.5434 0.3342 -0.4992 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.5414 1.8216 -0.3951 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.8401 0.8335 1.0780 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.7299 1.7015 0.0143 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.0701 0.0032 -0.1335 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.6334 0.5918 1.4060 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.5370 -1.8224 -0.3487 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.2332 -2.0099 -0.1586 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.7608 -1.4400 1.2280 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.9033 0.5960 0.2674 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.1855 -1.0232 0.2370 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.1571 0.0032 -1.2295 H 0 0 0 0 0 0 0 0 0 0 0 0 16
0.3236 -0.0019 -1.3139 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
2 17 0 0 0 0

M END
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dimethylethylamine.sdf
COSMOTHERM 3D 0

16 15 0 0 0 0 0 0 0 0 0 V2000
1.6571 0.7843 -0.0278 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.4542 0.0010 -0.3233 N 0 0 0 0 0 0 0 0 0 0 0 0 2
-0.7258 0.6265 0.2987 C 0 0 0 0 0 0 0 0 0 0 0 0 3
0.6378 -1.3846 0.1174 C 0 0 0 0 0 0 0 0 0 0 0 0 4
2.5247 0.3400 -0.5365 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.5316 1.8140 -0.3924 H 0 0 0 0 0 0 0 0 0 0 0 0 6
1.8830 0.8282 1.0616 H 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.7135 1.6901 0.0134 H 0 0 0 0 0 0 0 0 0 0 0 0 8
-2.0533 0.0084 -0.1372 C 0 0 0 0 0 0 0 0 0 0 0 0 9

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-0.6444 0.5937 1.4106 H 0 0 0 0 0 0 0 0 0 0 10
1.5290 -1.8084 -0.3668 H 0 0 0 0 0 0 0 0 0 0 11
-0.2257 -1.9997 -0.1671 H 0 0 0 0 0 0 0 0 0 0 12
0.7730 -1.4635 1.2203 H 0 0 0 0 0 0 0 0 0 0 13
-2.8888 0.5958 0.2708 H 0 0 0 0 0 0 0 0 0 0 14
-2.1718 -1.0240 0.2209 H 0 0 0 0 0 0 0 0 0 0 15
-2.1393 0.0056 -1.2342 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
9 16 0 0 0 0
M END
$$$$
ethylamine-cation.sdf
COSMOTHERM 3D 0
11 10 0 0 0 0 0 0 0 0 V2000
1.3011 0.0000 -0.2769 C 0 0 0 0 0 0 0 0 0 0 1
0.0590 0.0000 0.5959 C 0 0 0 0 0 0 0 0 0 0 2
-1.1924 0.0000 -0.2466 N 0 0 0 0 0 0 0 0 0 0 3
-2.0411 0.0126 0.3332 H 0 0 0 0 0 0 0 0 0 0 4
-1.2464 -0.8343 -0.8457 H 0 0 0 0 0 0 0 0 0 0 5
2.1896 -0.0024 0.3681 H 0 0 0 0 0 0 0 0 0 0 6
1.3442 -0.8932 -0.9164 H 0 0 0 0 0 0 0 0 0 0 7
1.3461 0.8959 -0.9124 H 0 0 0 0 0 0 0 0 0 0 8
0.0015 0.8915 1.2303 H 0 0 0 0 0 0 0 0 0 0 9
0.0010 -0.8907 1.2315 H 0 0 0 0 0 0 0 0 0 0 10
-1.2340 0.8221 -0.8634 H 0 0 0 0 0 0 0 0 0 0 11
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
10 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
3 11 0 0 0 0
M END
$$$$
ethylamine.sdf
COSMOTHERM 3D 0
10 9 0 0 0 0 0 0 0 0 V2000
1.2758 0.0160 -0.2572 C 0 0 0 0 0 0 0 0 0 0 1
-0.0054 -0.0334 0.5710 C 0 0 0 0 0 0 0 0 0 0 2
-1.1983 0.0724 -0.2982 N 0 0 0 0 0 0 0 0 0 0 3
-2.0440 0.0061 0.2757 H 0 0 0 0 0 0 0 0 0 0 4
-1.2295 -0.7435 -0.9182 H 0 0 0 0 0 0 0 0 0 0 5
2.1629 -0.0340 0.3910 H 0 0 0 0 0 0 0 0 0 0 6
1.3258 -0.8337 -0.9566 H 0 0 0 0 0 0 0 0 0 0 7
1.3284 0.9447 -0.8451 H 0 0 0 0 0 0 0 0 0 0 8
-0.0263 0.8158 1.2724 H 0 0 0 0 0 0 0 0 0 0 9
-0.0048 -0.9545 1.1863 H 0 0 0 0 0 0 0 0 0 0 10
2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
9 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
2 10 0 0 0 0
M END
$$$$
guanidine_a.sdf
COSMOTHERM 3D 0
9 8 0 0 0 0 0 0 0 0 V2000
-0.7948 -1.0826 -0.0500 N 0 0 0 0 0 0 0 0 0 0 1
0.0866 -0.0108 0.0019 C 0 0 0 0 0 0 0 0 0 0 2
-0.5356 1.2292 0.0530 N 0 0 0 0 0 0 0 0 0 0 3
1.3855 -0.0876 -0.0063 N 0 0 0 0 0 0 0 0 0 0 4
-0.3975 -1.9865 0.1941 H 0 0 0 0 0 0 0 0 0 0 5
-1.7164 -0.9376 0.3590 H 0 0 0 0 0 0 0 0 0 0 6
-1.4443 1.2969 -0.4012 H 0 0 0 0 0 0 0 0 0 0 7
0.0796 2.0051 -0.1819 H 0 0 0 0 0 0 0 0 0 0 8
1.6800 -1.0689 0.0535 H 0 0 0 0 0 0 0 0 0 0 9
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
4 9 0 0 0 0
M END
$$$$
guanidine_a_p2.sdf
COSMOTHERM 3D 0
10 9 0 0 0 0 0 0 0 0 V2000
-1.3381 -0.0340 0.0073 N 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0001 -0.0014 C 0 0 0 0 0 0 0 0 0 0 2
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3      0.6396   1.1760   0.0081 N   0 0 0 0 0 0 0 0 0 0 0 3
4      0.6986  -1.1420  -0.0096 N   0 0 0 0 0 0 0 0 0 0 0 4
5     -1.8388  -0.9153  -0.0270 H   0 0 0 0 0 0 0 0 0 0 0 5
6     -1.8833   0.8196  -0.0447 H   0 0 0 0 0 0 0 0 0 0 0 6
7      0.1272   2.0497  -0.0438 H   0 0 0 0 0 0 0 0 0 0 0 7
8      1.6517   1.2206  -0.0366 H   0 0 0 0 0 0 0 0 0 0 0 8
9      0.2309  -2.0407   0.0406 H   0 0 0 0 0 0 0 0 0 0 0 9
10     1.7112  -1.1352   0.0468 H   0 0 0 0 0 0 0 0 0 0 0 10
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M  END
$$$$
h2o.sdf
COSMOtherm      3D      0
3 2 0 0 0 0 0 0 0 0 0 0 V2000
0.0000 0.0000 0.0674 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.7649 0.0000 -0.5349 H 0 0 0 0 0 0 0 0 0 0 0 2
0.7648 0.0000 -0.5349 H 0 0 0 0 0 0 0 0 0 0 0 3
2 1 0 0 0 0 0
1 3 0 0 0 0 0
M  END
$$$$
hydroxyimidazo(2,3-a)isoindol_e-cation.sdf
COSMOtherm      3D      0
27 29 0 0 0 0 0 0 0 0 0 0 V2000
0.9004 0.2373 4.0032 C 0 0 0 0 0 0 0 0 0 0 0 1
1.8771 0.2080 2.9717 C 0 0 0 0 0 0 0 0 0 0 0 2
1.5273 0.0809 1.6351 C 0 0 0 0 0 0 0 0 0 0 0 3
0.1576 -0.0307 1.3023 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8330 0.0166 2.3529 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.4488 0.1463 3.7080 C 0 0 0 0 0 0 0 0 0 0 0 6
-2.0990 -0.0817 1.7379 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.5569 -0.1578 0.0747 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.9083 -0.1707 0.4067 N 0 0 0 0 0 0 0 0 0 0 0 9
-0.1086 -0.2589 -1.2648 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.0732 -0.1020 -3.5923 C 0 0 0 0 0 0 0 0 0 0 0 11
1.2662 -0.6599 -3.0856 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.8971 -0.1915 -2.3676 N 0 0 0 0 0 0 0 0 0 0 0 13
1.1705 -0.4552 -1.6335 N 0 0 0 0 0 0 0 0 0 0 0 14
0.1075 1.2411 -4.0169 O 0 0 0 0 0 0 0 0 0 0 0 15
1.2249 0.3381 5.0398 H 0 0 0 0 0 0 0 0 0 0 0 16
2.9314 0.2944 3.2393 H 0 0 0 0 0 0 0 0 0 0 0 17
2.3087 0.0816 0.8744 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.2028 0.1799 4.4961 H 0 0 0 0 0 0 0 0 0 0 0 19
-3.0974 -0.1049 2.1627 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.6722 -0.2969 -0.2550 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.5235 -0.7057 -4.3885 H 0 0 0 0 0 0 0 0 0 0 0 22
2.1124 -0.1117 -3.5147 H 0 0 0 0 0 0 0 0 0 0 0 23
1.3633 -1.7306 -3.3133 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.8170 0.2422 -2.3494 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.6516 1.4939 -4.5749 H 0 0 0 0 0 0 0 0 0 0 0 26
1.8606 -0.8492 -1.0012 H 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0 0
6 1 0 0 0 0 0
16 1 0 0 0 0 0
3 2 0 0 0 0 0
17 2 0 0 0 0 0
4 3 0 0 0 0 0
18 3 0 0 0 0 0
5 4 0 0 0 0 0
8 4 0 0 0 0 0
6 5 0 0 0 0 0
7 5 0 0 0 0 0
19 6 0 0 0 0 0
9 7 0 0 0 0 0
20 7 0 0 0 0 0
9 8 0 0 0 0 0
10 8 0 0 0 0 0
21 9 0 0 0 0 0
13 10 0 0 0 0 0
14 10 0 0 0 0 0
12 11 0 0 0 0 0
13 11 0 0 0 0 0
15 11 0 0 0 0 0
22 11 0 0 0 0 0
14 12 0 0 0 0 0
23 12 0 0 0 0 0
24 12 0 0 0 0 0
25 13 0 0 0 0 0
26 15 0 0 0 0 0
14 27 0 0 0 0 0
M  END
$$$$
hydroxyimidazo(2,3-a)isoindol_e0.sdf
COSMOtherm      3D      0
26 28 0 0 0 0 0 0 0 0 0 0 V2000
-3.8960 1.0816 -0.0210 C 0 0 0 0 0 0 0 0 0 0 0 1
-2.8081 1.9677 0.2320 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.5002 1.5168 0.2814 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.2410 0.1370 0.0700 C 0 0 0 0 0 0 0 0 0 0 0 4
-2.3554 -0.7659 -0.1715 C 0 0 0 0 0 0 0 0 0 0 0 5
-3.6836 -0.2702 -0.2186 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.8189 -2.0580 -0.3140 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0657 -0.6539 0.0569 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.4724 -1.9532 -0.1693 N 0 0 0 0 0 0 0 0 0 0 0 9

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2
3 1.3381 -0.3641 0.2443 C 0 0 0 0 0 0 0 0 0 0 10
4 3.2651 0.8925 0.1683 C 0 0 0 0 0 0 0 0 0 0 11
5 3.5266 -0.5727 0.5715 C 0 0 0 0 0 0 0 0 0 0 12
6 1.8073 0.9514 0.3241 N 0 0 0 0 0 0 0 0 0 0 13
7 2.2483 -1.2888 0.3959 N 0 0 0 0 0 0 0 0 0 0 14
8 3.6912 1.0843 -1.1922 O 0 0 0 0 0 0 0 0 0 0 15
9 -4.9107 1.4827 -0.0515 H 0 0 0 0 0 0 0 0 0 0 16
10 -3.0159 3.0269 0.3958 H 0 0 0 0 0 0 0 0 0 0 17
11 -0.6939 2.2202 0.4959 H 0 0 0 0 0 0 0 0 0 0 18
12 -4.5195 -0.9480 -0.4030 H 0 0 0 0 0 0 0 0 0 0 19
13 -2.2927 -3.0138 -0.5114 H 0 0 0 0 0 0 0 0 0 0 20
14 0.1865 -2.7290 -0.2206 H 0 0 0 0 0 0 0 0 0 0 21
15 3.7541 1.6344 0.8137 H 0 0 0 0 0 0 0 0 0 0 22
16 4.3248 -1.0093 -0.0459 H 0 0 0 0 0 0 0 0 0 0 23
17 3.8453 -0.6305 1.6257 H 0 0 0 0 0 0 0 0 0 0 24
18 1.3131 1.6880 -0.1777 H 0 0 0 0 0 0 0 0 0 0 25
19 3.7199 2.0430 -1.3674 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
19 6 0 0 0 0
9 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
21 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
23 12 0 0 0 0
24 12 0 0 0 0
25 13 0 0 0 0
15 26 0 0 0 0
M END
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hydroxyimidazo(2,3-a)isoindol_e1.sdf
COSMOTHERM 3D 0
26 28 0 0 0 0 0 0 0 0 0 V2000
-3.9905 0.8721 0.2787 C 0 0 0 0 0 0 0 0 0 0 1
-2.9721 1.8674 0.1972 C 0 0 0 0 0 0 0 0 0 0 2
-1.6390 1.5300 0.0325 C 0 0 0 0 0 0 0 0 0 0 3
-1.2909 0.1585 -0.0558 C 0 0 0 0 0 0 0 0 0 0 4
-2.3270 -0.8540 0.0329 C 0 0 0 0 0 0 0 0 0 0 5
-3.6839 -0.4744 0.1998 C 0 0 0 0 0 0 0 0 0 0 6
-1.6927 -2.1042 -0.0738 C 0 0 0 0 0 0 0 0 0 0 7
-0.0579 -0.5200 -0.2082 C 0 0 0 0 0 0 0 0 0 0 8
-0.3582 -1.8706 -0.2066 N 0 0 0 0 0 0 0 0 0 0 9
1.2929 -0.0206 -0.3202 C 0 0 0 0 0 0 0 0 0 0 10
3.5844 -0.0664 -0.0703 C 0 0 0 0 0 0 0 0 0 0 11
3.0694 1.2853 -0.6019 C 0 0 0 0 0 0 0 0 0 0 12
2.3911 -0.8990 -0.2662 N 0 0 0 0 0 0 0 0 0 0 13
1.5968 1.2309 -0.5322 N 0 0 0 0 0 0 0 0 0 0 14
3.9398 0.0855 1.3154 O 0 0 0 0 0 0 0 0 0 0 15
-5.0285 1.1847 0.4067 H 0 0 0 0 0 0 0 0 0 0 16
-3.2559 2.9194 0.2670 H 0 0 0 0 0 0 0 0 0 0 17
-0.8638 2.2941 -0.0341 H 0 0 0 0 0 0 0 0 0 0 18
-4.4669 -1.2325 0.2657 H 0 0 0 0 0 0 0 0 0 0 19
-2.0873 -3.1147 -0.0736 H 0 0 0 0 0 0 0 0 0 0 20
0.3231 -2.6135 -0.3476 H 0 0 0 0 0 0 0 0 0 0 21
4.4385 -0.4776 -0.6249 H 0 0 0 0 0 0 0 0 0 0 22
3.4728 2.1173 -0.0069 H 0 0 0 0 0 0 0 0 0 0 23
3.3873 1.4344 -1.6475 H 0 0 0 0 0 0 0 0 0 0 24
2.3276 -1.7351 0.3152 H 0 0 0 0 0 0 0 0 0 0 25
4.4521 -0.6993 1.5840 H 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
6 1 0 0 0 0
16 1 0 0 0 0
3 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
5 4 0 0 0 0
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19 6 0 0 0 0
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25 13 0 0 0 0
15 26 0 0 0 0

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M END
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hydroxyimidazo(2,3-a)isoindol_e2.sdf
COSMOtherm            3D            0
26 28 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-4.1010 -0.7457 0.0277 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.1290 -1.7891 -0.0146 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.7716 -1.5158 -0.0251 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.3507 -0.1625 0.0070 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.3399 0.8994 0.0433 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-3.7236 0.5847 0.0558 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.6382 2.1181 0.0547 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.0781 0.4565 -0.0036 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.3105 1.8205 0.0186 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.2535 -0.0991 -0.0738 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.5536 -0.0843 -0.4072 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
2.9913 -1.4916 -0.0533 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
2.3373 0.7249 -0.4128 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
1.5489 -1.3374 0.2094 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
4.5390 0.4064 0.5143 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-5.1605 -1.0085 0.0370 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.4693 -2.8262 -0.0383 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.0322 -2.3173 -0.0493 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-4.4720 1.3794 0.0850 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-1.9817 3.1464 0.0955 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
0.4252 2.5231 0.0630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
4.0594 -0.0485 -1.3795 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
3.1512 -2.2095 -0.8736 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
3.5083 -1.8938 0.8329 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
2.2289 1.4268 -1.1422 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
4.1454 0.3914 1.4084 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
 2 1 0 0 0 0 0
 6 1 0 0 0 0 0
16 1 0 0 0 0 0
 3 2 0 0 0 0 0
17 2 0 0 0 0 0
 4 3 0 0 0 0 0
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19 6 0 0 0 0 0
 9 7 0 0 0 0 0
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21 9 0 0 0 0 0
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13 11 0 0 0 0 0
15 11 0 0 0 0 0
22 11 0 0 0 0 0
14 12 0 0 0 0 0
23 12 0 0 0 0 0
24 12 0 0 0 0 0
25 13 0 0 0 0 0
15 26 0 0 0 0 0
M END
$$$$
hydroxyimidazo(2,3-a)isoindol_e3.sdf
COSMOtherm            3D            0
26 28 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
-3.8441 1.2247 0.0422 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.6952 2.0679 -0.0066 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.4128 1.5475 -0.0368 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.2449 0.1380 -0.0253 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-2.4181 -0.7182 0.0406 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-3.7184 -0.1521 0.0678 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.9599 -2.0479 0.0661 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.1161 -0.7174 -0.0371 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.6029 -2.0074 0.0211 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
1.3102 -0.4881 -0.0821 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
3.2791 0.7003 -0.3945 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
3.5159 -0.8005 -0.0475 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
1.8209 0.7799 -0.3618 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2.1945 -1.4161 0.1660 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
3.9034 1.6211 0.5104 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-4.8358 1.6804 0.0631 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.8346 3.1507 -0.0134 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.5525 2.2179 -0.0581 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-4.5999 -0.7946 0.1142 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-2.4956 -2.9905 0.1035 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
0.0095 -2.8220 0.0264 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 21
3.6729 0.9884 -1.3773 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 22
4.0552 -1.3237 -0.8524 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 23
4.1346 -0.8805 0.8618 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 24
1.3454 1.3822 -1.0295 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 25
3.5956 1.4071 1.4128 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 26
 2 1 0 0 0 0 0
 6 1 0 0 0 0 0
16 1 0 0 0 0 0
 3 2 0 0 0 0 0
17 2 0 0 0 0 0
 4 3 0 0 0 0 0
18 3 0 0 0 0 0
 5 4 0 0 0 0 0
 8 4 0 0 0 0 0
 6 5 0 0 0 0 0
 7 5 0 0 0 0 0
19 6 0 0 0 0 0
 9 7 0 0 0 0 0

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20 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
21 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 11 0 0 0 0
22 11 0 0 0 0
14 12 0 0 0 0
23 12 0 0 0 0
24 12 0 0 0 0
25 13 0 0 0 0
15 26 0 0 0 0

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M END

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imidazo-(2,3-b)-thioxazole_b-cation1.sdf

COSMOTHERM 3D 0

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18 19 0 0 0 0 0 0 0 0 0 V2000
3.1474 0.2861 0.6727 C 0 0 0 0 0 0 0 0 0 0 0 0 1
1.7392 0.2360 1.1207 N 0 0 0 0 0 0 0 0 0 0 0 0 2
3.0564 -0.3060 -0.7545 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.6033 -0.2502 -1.0222 N 0 0 0 0 0 0 0 0 0 0 0 0 4
0.9200 -0.0105 0.0981 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.6315 -0.2097 1.1747 N 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.2745 -0.2280 1.3476 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.9389 0.0093 -0.0833 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.5847 0.2110 -1.1676 S 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.5223 -0.0192 0.2063 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.4885 1.3301 0.6701 H 0 0 0 0 0 0 0 0 0 0 0 0 11
3.7863 -0.3039 1.3379 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.4271 0.6756 1.9825 H 0 0 0 0 0 0 0 0 0 0 0 0 13
3.3914 -1.3512 -0.7931 H 0 0 0 0 0 0 0 0 0 0 0 0 14
3.6086 0.2808 -1.4959 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.8622 -0.4250 2.3364 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.9547 0.0813 -0.4683 H 0 0 0 0 0 0 0 0 0 0 0 0 17
1.1874 -0.6914 -1.8388 H 0 0 0 0 0 0 0 0 0 0 0 0 18

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2 1 0 0 0 0

3 1 0 0 0 0

11 1 0 0 0 0

12 1 0 0 0 0

5 2 0 0 0 0

13 2 0 0 0 0

4 3 0 0 0 0

14 3 0 0 0 0

15 3 0 0 0 0

5 4 0 0 0 0

10 5 0 0 0 0

7 6 0 0 0 0

8 6 0 0 0 0

10 7 0 0 0 0

16 7 0 0 0 0

9 8 0 0 0 0

17 8 0 0 0 0

10 9 0 0 0 0

4 18 0 0 0 0

M END

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imidazo-(2,3-b)-thioxazole_b.sdf

COSMOTHERM 3D 0

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17 18 0 0 0 0 0 0 0 0 0 V2000
3.0440 0.7249 -0.3622 C 0 0 0 0 0 0 0 0 0 0 0 0 1
1.6115 1.0503 -0.1741 N 0 0 0 0 0 0 0 0 0 0 0 0 2
3.1096 -0.6878 0.2711 C 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7128 -1.1909 0.2911 N 0 0 0 0 0 0 0 0 0 0 0 0 4
0.9616 -0.1654 0.0230 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-2.6451 -1.1464 -0.2095 N 0 0 0 0 0 0 0 0 0 0 0 0 6
-1.2864 -1.3535 -0.2230 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-2.9235 0.1184 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.5315 1.1620 0.2024 S 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.4988 -0.2401 -0.0205 C 0 0 0 0 0 0 0 0 0 0 0 0 10
3.2971 0.7077 -1.4345 H 0 0 0 0 0 0 0 0 0 0 0 0 11
3.6880 1.4548 0.1438 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.1959 1.7072 -0.8339 H 0 0 0 0 0 0 0 0 0 0 0 0 13
3.4799 -0.6441 1.3094 H 0 0 0 0 0 0 0 0 0 0 0 0 14
3.7630 -1.3753 -0.2829 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-0.8932 -2.3534 -0.3971 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-3.9291 0.5313 0.0577 H 0 0 0 0 0 0 0 0 0 0 0 0 17

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2 1 0 0 0 0

3 1 0 0 0 0

11 1 0 0 0 0

12 1 0 0 0 0

5 2 0 0 0 0

13 2 0 0 0 0

4 3 0 0 0 0

14 3 0 0 0 0

15 3 0 0 0 0

5 4 0 0 0 0

10 5 0 0 0 0

7 6 0 0 0 0

8 6 0 0 0 0

10 7 0 0 0 0

16 7 0 0 0 0

9 8 0 0 0 0

10 9 0 0 0 0

8 17 0 0 0 0

M END

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imidazole-cation.sdf

COSMOTHERM 3D 0

10 10 0 0 0 0 0 0 0 0 0 V2000

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-0.9778    0.6844    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 1
 0.3480    1.0767    0.0000 N    0 0 0 0 0 0 0 0 0 0 0 2
-0.9779   -0.6842    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 3
 0.3477   -1.0767    0.0000 N    0 0 0 0 0 0 0 0 0 0 0 4
 1.1436   -0.0001    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 5
-1.7895    1.4006    0.0002 H    0 0 0 0 0 0 0 0 0 0 0 6
-1.7898   -1.4002   -0.0001 H    0 0 0 0 0 0 0 0 0 0 0 7
 2.2266   -0.0003    0.0002 H    0 0 0 0 0 0 0 0 0 0 0 8
 0.6814   -2.0391    0.0001 H    0 0 0 0 0 0 0 0 0 0 0 9
 0.6818    2.0389   -0.0002 H    0 0 0 0 0 0 0 0 0 0 0 10
 2 1 0 0 0 0
 3 1 0 0 0 0
 6 1 0 0 0 0
 5 2 0 0 0 0
 4 3 0 0 0 0
 7 3 0 0 0 0
 5 4 0 0 0 0
 9 4 0 0 0 0
 8 5 0 0 0 0
 2 10 0 0 0 0
M  END
$$$$
imidazole.sdf
COSMOtherm           3D           0
 9 9 0 0 0 0 0 0 0 0 0 0 0 V2000
-0.9869    0.6303    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 1
 0.2879    1.1767    0.0000 N    0 0 0 0 0 0 0 0 0 0 0 2
-0.9196   -0.7471    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 3
 0.4282   -1.0439    0.0000 N    0 0 0 0 0 0 0 0 0 0 0 4
 1.1148    0.1348    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 5
-1.8741    1.2574    0.0000 H    0 0 0 0 0 0 0 0 0 0 0 6
-1.6790   -1.5213   -0.0001 H    0 0 0 0 0 0 0 0 0 0 0 7
 2.2001    0.1779    0.0000 H    0 0 0 0 0 0 0 0 0 0 0 8
 0.8360   -1.9758   -0.0002 H    0 0 0 0 0 0 0 0 0 0 0 9
 2 1 0 0 0 0
 3 1 0 0 0 0
 6 1 0 0 0 0
 5 2 0 0 0 0
 4 3 0 0 0 0
 7 3 0 0 0 0
 5 4 0 0 0 0
 8 5 0 0 0 0
 4 9 0 0 0 0
M  END
$$$$
indole-cation0.sdf
COSMOtherm           3D           0
17 18 0 0 0 0 0 0 0 0 0 0 0 V2000
-2.1686   -0.7238    0.0004 C    0 0 0 0 0 0 0 0 0 0 0 1
-2.1977    0.6790    0.0001 C    0 0 0 0 0 0 0 0 0 0 0 2
-1.0181    1.4347   -0.0003 C    0 0 0 0 0 0 0 0 0 0 0 3
 0.2022    0.7511   -0.0003 C    0 0 0 0 0 0 0 0 0 0 0 4
 0.1934   -0.6510   -0.0004 C    0 0 0 0 0 0 0 0 0 0 0 5
-0.9506   -1.4248    0.0002 C    0 0 0 0 0 0 0 0 0 0 0 6
 1.5998   -1.1121   -0.0005 N    0 0 0 0 0 0 0 0 0 0 0 7
 1.5941    1.1987    0.0002 C    0 0 0 0 0 0 0 0 0 0 0 8
 2.4112    0.1349    0.0007 C    0 0 0 0 0 0 0 0 0 0 0 9
 1.8179   -1.6948   -0.8259 H    0 0 0 0 0 0 0 0 0 0 0 10
-3.1037   -1.2845    0.0010 H    0 0 0 0 0 0 0 0 0 0 0 11
-3.1607    1.1917    0.0003 H    0 0 0 0 0 0 0 0 0 0 0 12
-1.0497    2.5244   -0.0006 H    0 0 0 0 0 0 0 0 0 0 0 13
-0.9192   -2.5140    0.0006 H    0 0 0 0 0 0 0 0 0 0 0 14
 1.9256    2.2341    0.0005 H    0 0 0 0 0 0 0 0 0 0 0 15
 3.4902    0.0265    0.0012 H    0 0 0 0 0 0 0 0 0 0 0 16
 1.8173   -1.6970    0.8236 H    0 0 0 0 0 0 0 0 0 0 0 17
 2 1 0 0 0 0
 6 1 0 0 0 0
11 1 0 0 0 0
 3 2 0 0 0 0
12 2 0 0 0 0
 4 3 0 0 0 0
13 3 0 0 0 0
 5 4 0 0 0 0
 8 4 0 0 0 0
 6 5 0 0 0 0
 7 5 0 0 0 0
14 6 0 0 0 0
 9 7 0 0 0 0
10 7 0 0 0 0
 9 8 0 0 0 0
15 8 0 0 0 0
16 9 0 0 0 0
 7 17 0 0 0 0
M  END
$$$$
indole-cation1.sdf
COSMOtherm           3D           0
17 18 0 0 0 0 0 0 0 0 0 0 0 V2000
-2.1259   -0.7537   -0.0001 C    0 0 0 0 0 0 0 0 0 0 0 1
-2.1898    0.6838    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 2
-1.0517    1.4462    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 3
 0.2114    0.7707    0.0001 C    0 0 0 0 0 0 0 0 0 0 0 4
 0.2520   -0.6919    0.0001 C    0 0 0 0 0 0 0 0 0 0 0 5
-0.9405   -1.4555    0.0000 C    0 0 0 0 0 0 0 0 0 0 0 6
 1.5247   -1.0922    0.0001 N    0 0 0 0 0 0 0 0 0 0 0 7
 1.5110    1.2162    0.0001 C    0 0 0 0 0 0 0 0 0 0 0 8
 2.4185    0.0496   -0.0001 C    0 0 0 0 0 0 0 0 0 0 0 9
 1.8425   -2.0590    0.0000 H    0 0 0 0 0 0 0 0 0 0 0 10
 3.0829    0.0355    0.8831 H    0 0 0 0 0 0 0 0 0 0 0 11
 3.0821    0.0353   -0.8840 H    0 0 0 0 0 0 0 0 0 0 0 12
-3.0655   -1.3086   -0.0002 H    0 0 0 0 0 0 0 0 0 0 0 13
-3.1704    1.1600    0.0001 H    0 0 0 0 0 0 0 0 0 0 0 14

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14 13 0 0 0 0 0 0 0 0 0 V2000
  0.0008  0.0746  0.3767 C  0 0 0 0 0 0 0 0 0 0 0 1
 -0.0135 -1.3717 -0.0933 N  0 0 0 0 0 0 0 0 0 0 0 2
  1.2843  0.7340 -0.1113 C  0 0 0 0 0 0 0 0 0 0 0 3
 -1.2696  0.7589 -0.1113 C  0 0 0 0 0 0 0 0 0 0 0 4
 -0.8517 -1.8696  0.2342 H  0 0 0 0 0 0 0 0 0 0 0 5
  0.8032 -1.8923  0.2528 H  0 0 0 0 0 0 0 0 0 0 0 6
 -0.0001  0.0085  1.4724 H  0 0 0 0 0 0 0 0 0 0 0 7
  2.1750  0.1982  0.2462 H  0 0 0 0 0 0 0 0 0 0 0 8
  1.3292  1.7607  0.2742 H  0 0 0 0 0 0 0 0 0 0 0 9
  1.3134  0.7800 -1.2101 H  0 0 0 0 0 0 0 0 0 0 0 10
 -2.1705  0.2426  0.2495 H  0 0 0 0 0 0 0 0 0 0 0 11
 -1.2928  1.7874  0.2711 H  0 0 0 0 0 0 0 0 0 0 0 12
 -1.3000  0.8022 -1.2102 H  0 0 0 0 0 0 0 0 0 0 0 13
 -0.0027 -1.4348 -1.1209 H  0 0 0 0 0 0 0 0 0 0 0 14
  2 1 0 0 0 0 0
  3 1 0 0 0 0 0
  4 1 0 0 0 0 0
  7 1 0 0 0 0 0
  5 2 0 0 0 0 0
  6 2 0 0 0 0 0
  8 3 0 0 0 0 0
  9 3 0 0 0 0 0
 10 3 0 0 0 0 0
 11 4 0 0 0 0 0
 12 4 0 0 0 0 0
 13 4 0 0 0 0 0
  2 14 0 0 0 0 0
```

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M  END
$$$$
iso-propylamine.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
  0.0002  0.0080  0.3648 C  0 0 0 0 0 0 0 0 0 0 0 1
 -0.0031 -1.3751 -0.1702 N  0 0 0 0 0 0 0 0 0 0 0 2
  1.2685  0.7231 -0.1049 C  0 0 0 0 0 0 0 0 0 0 0 3
 -1.2649  0.7291 -0.1046 C  0 0 0 0 0 0 0 0 0 0 0 4
 -0.8227 -1.8736  0.1910 H  0 0 0 0 0 0 0 0 0 0 0 5
  0.8074 -1.8817  0.1999 H  0 0 0 0 0 0 0 0 0 0 0 6
  0.0001  0.0086  1.4741 H  0 0 0 0 0 0 0 0 0 0 0 7
  2.1717  0.1927  0.2351 H  0 0 0 0 0 0 0 0 0 0 0 8
  1.3093  1.7472  0.2939 H  0 0 0 0 0 0 0 0 0 0 0 9
  1.2954  0.7759 -1.2047 H  0 0 0 0 0 0 0 0 0 0 0 10
 -2.1707  0.2054  0.2386 H  0 0 0 0 0 0 0 0 0 0 0 11
 -1.2990  1.7548  0.2911 H  0 0 0 0 0 0 0 0 0 0 0 12
 -1.2936  0.7790 -1.2045 H  0 0 0 0 0 0 0 0 0 0 0 13
  2 1 0 0 0 0 0
  3 1 0 0 0 0 0
  4 1 0 0 0 0 0
  7 1 0 0 0 0 0
  5 2 0 0 0 0 0
  6 2 0 0 0 0 0
  8 3 0 0 0 0 0
  9 3 0 0 0 0 0
 10 3 0 0 0 0 0
 11 4 0 0 0 0 0
 12 4 0 0 0 0 0
  4 13 0 0 0 0 0
```

```
M  END
$$$$
isoquinoline.sdf
COSMOTHERM 3D 0
17 18 0 0 0 0 0 0 0 0 0 V2000
 -1.4145 -1.2319  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 1
 -0.6949 -0.0067  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 2
  0.7395 -0.0248  0.0000 C  0 0 0 0 0 0 0 0 0 0 0 3
  1.4112 -1.2778 -0.0001 C  0 0 0 0 0 0 0 0 0 0 0 4
  0.6858 -2.4545 -0.0001 C  0 0 0 0 0 0 0 0 0 0 0 5
 -0.7339 -2.4344  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 6
  1.4065  1.2295  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 7
  0.6661  2.3934  0.0001 C  0 0 0 0 0 0 0 0 0 0 0 8
 -1.3409  1.2613 -0.0001 C  0 0 0 0 0 0 0 0 0 0 0 9
 -0.7037  2.4251 -0.0001 N  0 0 0 0 0 0 0 0 0 0 0 10
 -2.5065 -1.2083  0.0001 H  0 0 0 0 0 0 0 0 0 0 0 11
  2.5030 -1.2971  0.0000 H  0 0 0 0 0 0 0 0 0 0 0 12
  1.2068 -3.4137 -0.0002 H  0 0 0 0 0 0 0 0 0 0 0 13
 -1.2848 -3.3763  0.0001 H  0 0 0 0 0 0 0 0 0 0 0 14
  2.4975  1.2703  0.0001 H  0 0 0 0 0 0 0 0 0 0 0 15
  1.1605  3.3676  0.0001 H  0 0 0 0 0 0 0 0 0 0 0 16
 -2.4359  1.2978 -0.0002 H  0 0 0 0 0 0 0 0 0 0 0 17
  2 1 0 0 0 0 0
  6 1 0 0 0 0 0
 11 1 0 0 0 0 0
  3 2 0 0 0 0 0
  9 2 0 0 0 0 0
  4 3 0 0 0 0 0
  7 3 0 0 0 0 0
  5 4 0 0 0 0 0
 12 4 0 0 0 0 0
  6 5 0 0 0 0 0
 13 5 0 0 0 0 0
 14 6 0 0 0 0 0
  8 7 0 0 0 0 0
 15 7 0 0 0 0 0
 10 8 0 0 0 0 0
 16 8 0 0 0 0 0
 10 9 0 0 0 0 0
  9 17 0 0 0 0 0
M  END
$$$$
isoquinoline_p1.sdf
COSMOTHERM 3D 0
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18 19 0 0 0 0 0 0 0 0 0 V2000
-2.3422 -0.6622 -0.0003 N 0 0 0 0 0 0 0 0 0 0 1
-2.3854 0.7092 0.0002 C 0 0 0 0 0 0 0 0 0 0 2
-1.2133 1.4185 0.0004 C 0 0 0 0 0 0 0 0 0 0 3
0.0359 0.7403 0.0001 C 0 0 0 0 0 0 0 0 0 0 4
0.0321 -0.7002 0.0001 C 0 0 0 0 0 0 0 0 0 0 5
-1.2061 -1.3642 -0.0002 C 0 0 0 0 0 0 0 0 0 0 6
1.2806 1.4171 -0.0003 C 0 0 0 0 0 0 0 0 0 0 7
2.4598 0.6946 -0.0003 C 0 0 0 0 0 0 0 0 0 0 8
1.2594 -1.4180 0.0003 C 0 0 0 0 0 0 0 0 0 0 9
2.4518 -0.7247 0.0001 C 0 0 0 0 0 0 0 0 0 0 10
-3.3757 1.1563 0.0003 H 0 0 0 0 0 0 0 0 0 0 11
-1.2483 2.5074 0.0006 H 0 0 0 0 0 0 0 0 0 0 12
-1.2981 -2.4489 -0.0007 H 0 0 0 0 0 0 0 0 0 0 13
1.2946 2.5078 -0.0006 H 0 0 0 0 0 0 0 0 0 0 14
3.4153 1.2212 -0.0006 H 0 0 0 0 0 0 0 0 0 0 15
1.2415 -2.5086 0.0004 H 0 0 0 0 0 0 0 0 0 0 16
3.3980 -1.2666 0.0004 H 0 0 0 0 0 0 0 0 0 0 17
-3.2280 -1.1720 -0.0009 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0 0
6 1 0 0 0 0 0
3 2 0 0 0 0 0
11 2 0 0 0 0 0
4 3 0 0 0 0 0
12 3 0 0 0 0 0
5 4 0 0 0 0 0
7 4 0 0 0 0 0
6 5 0 0 0 0 0
9 5 0 0 0 0 0
13 6 0 0 0 0 0
8 7 0 0 0 0 0
14 7 0 0 0 0 0
10 8 0 0 0 0 0
15 8 0 0 0 0 0
10 9 0 0 0 0 0
16 9 0 0 0 0 0
17 10 0 0 0 0 0
1 18 0 0 0 0 0
M END
$$$$
melamine.sdf
COSMOtherm 3D 0
15 15 0 0 0 0 0 0 0 0 0 V2000
1.2183 0.6718 0.0062 N 0 0 0 0 0 0 0 0 0 0 1
1.1212 -0.6772 0.0037 C 0 0 0 0 0 0 0 0 0 0 2
-0.0279 -1.3913 0.0066 N 0 0 0 0 0 0 0 0 0 0 3
-1.1469 -0.6323 0.0045 C 0 0 0 0 0 0 0 0 0 0 4
-1.1906 0.7191 0.0072 N 0 0 0 0 0 0 0 0 0 0 5
0.0261 1.3097 0.0040 C 0 0 0 0 0 0 0 0 0 0 6
0.0528 2.6675 -0.0315 N 0 0 0 0 0 0 0 0 0 0 7
-2.3363 -1.2876 -0.0319 N 0 0 0 0 0 0 0 0 0 0 8
2.2835 -1.3796 -0.0311 N 0 0 0 0 0 0 0 0 0 0 9
-0.8071 3.1756 0.1483 H 0 0 0 0 0 0 0 0 0 0 10
0.9322 3.1415 0.1474 H 0 0 0 0 0 0 0 0 0 0 11
-2.3469 -2.2862 0.1476 H 0 0 0 0 0 0 0 0 0 0 12
-3.1866 -0.7635 0.1477 H 0 0 0 0 0 0 0 0 0 0 13
3.1535 -0.8892 0.1479 H 0 0 0 0 0 0 0 0 0 0 14
2.2542 -2.3781 0.1483 H 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0 0
6 1 0 0 0 0 0
3 2 0 0 0 0 0
9 2 0 0 0 0 0
4 3 0 0 0 0 0
5 4 0 0 0 0 0
8 4 0 0 0 0 0
6 5 0 0 0 0 0
7 6 0 0 0 0 0
10 7 0 0 0 0 0
11 7 0 0 0 0 0
12 8 0 0 0 0 0
13 8 0 0 0 0 0
14 9 0 0 0 0 0
9 15 0 0 0 0 0
M END
$$$$
melamine_p2.sdf
COSMOtherm 3D 0
16 16 0 0 0 0 0 0 0 0 0 V2000
-1.2123 -0.7058 -0.0001 N 0 0 0 0 0 0 0 0 0 0 1
-1.1903 0.6213 -0.0003 C 0 0 0 0 0 0 0 0 0 0 2
-0.0003 1.3180 -0.0006 N 0 0 0 0 0 0 0 0 0 0 3
1.1900 0.6219 -0.0003 C 0 0 0 0 0 0 0 0 0 0 4
1.2127 -0.7052 0.0002 N 0 0 0 0 0 0 0 0 0 0 5
0.0004 -1.3198 -0.0001 C 0 0 0 0 0 0 0 0 0 0 6
0.0007 -2.6581 0.0004 N 0 0 0 0 0 0 0 0 0 0 7
-2.3244 1.3239 0.0013 N 0 0 0 0 0 0 0 0 0 0 8
2.3237 1.3251 0.0011 N 0 0 0 0 0 0 0 0 0 0 9
0.8774 -3.1692 -0.0022 H 0 0 0 0 0 0 0 0 0 0 10
-0.8756 -3.1698 -0.0035 H 0 0 0 0 0 0 0 0 0 0 11
-3.2098 0.8266 -0.0031 H 0 0 0 0 0 0 0 0 0 0 12
-2.3379 2.3389 -0.0048 H 0 0 0 0 0 0 0 0 0 0 13
2.3364 2.3402 -0.0054 H 0 0 0 0 0 0 0 0 0 0 14
3.2094 0.8284 -0.0032 H 0 0 0 0 0 0 0 0 0 0 15
-0.0005 2.3377 -0.0010 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0 0
6 1 0 0 0 0 0
3 2 0 0 0 0 0
8 2 0 0 0 0 0
4 3 0 0 0 0 0
5 4 0 0 0 0 0
9 4 0 0 0 0 0
6 5 0 0 0 0 0

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7 6 0 0 0 0
10 7 0 0 0 0
11 7 0 0 0 0
12 8 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
3 16 0 0 0 0
M END
$$$$
methylamine-cation.sdf
COSMOtherm 3D 0

8 7 0 0 0 0 0 0 0 0 0 V2000
0.7980 0.0000 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.6985 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 2
-1.0778 0.4774 0.8272 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.0780 -0.9550 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 4
1.1435 -0.5207 -0.8970 H 0 0 0 0 0 0 0 0 0 0 0 5
1.1435 1.0372 -0.0024 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1435 -0.5166 0.8994 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.0780 0.4778 -0.8269 H 0 0 0 0 0 0 0 0 0 0 0 8
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
2 8 0 0 0 0
M END
$$$$
methylamine.sdf
COSMOtherm 3D 0

7 6 0 0 0 0 0 0 0 0 0 V2000
0.7456 -0.0001 -0.0133 C 0 0 0 0 0 0 0 0 0 0 0 1
-0.7283 -0.0001 0.0751 N 0 0 0 0 0 0 0 0 0 0 0 2
-1.0989 -0.8135 -0.4232 H 0 0 0 0 0 0 0 0 0 0 0 3
-1.0970 0.8146 -0.4227 H 0 0 0 0 0 0 0 0 0 0 0 4
1.1415 0.8889 0.4982 H 0 0 0 0 0 0 0 0 0 0 0 5
1.1427 -0.8837 0.5066 H 0 0 0 0 0 0 0 0 0 0 0 6
1.1468 -0.0047 -1.0441 H 0 0 0 0 0 0 0 0 0 0 0 7
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
1 7 0 0 0 0
M END
$$$$
methylguanidine.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
-0.6504 -0.6692 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 1
0.0778 0.4923 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6786 1.6457 0.0005 N 0 0 0 0 0 0 0 0 0 0 0 3
1.3865 0.4454 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0255 -1.9799 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6620 -0.6167 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.2214 2.5488 -0.0029 H 0 0 0 0 0 0 0 0 0 0 0 7
-1.6922 1.6312 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 8
1.7615 1.4004 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8189 -2.7366 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 10
0.6058 -2.1288 -0.8901 H 0 0 0 0 0 0 0 0 0 0 0 11
0.6051 -2.1292 0.8904 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
5 12 0 0 0 0
M END
$$$$
methylguanidine_a.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
-0.6610 -0.6699 -0.0903 N 0 0 0 0 0 0 0 0 0 0 0 1
0.0855 0.4897 -0.0139 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6839 1.6484 0.0833 N 0 0 0 0 0 0 0 0 0 0 0 3
1.3858 0.5751 -0.0155 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0347 -1.9794 0.0440 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6155 -0.6037 0.2553 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.5733 1.6306 -0.4132 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.1522 2.4933 -0.1164 H 0 0 0 0 0 0 0 0 0 0 0 8
1.8080 -0.3582 0.0252 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8142 -2.7442 -0.0458 H 0 0 0 0 0 0 0 0 0 0 0 10
0.6940 -2.1435 -0.7629 H 0 0 0 0 0 0 0 0 0 0 0 11
0.4781 -2.1116 1.0130 H 0 0 0 0 0 0 0 0 0 0 0 12
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
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4 2 0 0 0 0
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8 3 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0

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5 12 0 0 0 0
M END
$$$$
methylguanidine_a_p2.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 0 V2000
-0.6695 -0.6749 -0.0045 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.0029 0.4848 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.6781 1.6487 0.0299 N 0 0 0 0 0 0 0 0 0 0 0 3
1.3377 0.4923 -0.0194 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0297 -1.9884 0.0017 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.6840 -0.6353 0.0081 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.6757 1.6593 -0.1577 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.1831 2.5225 -0.1181 H 0 0 0 0 0 0 0 0 0 0 0 8
1.8669 -0.3621 0.1171 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8199 -2.7443 -0.0086 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5982 -2.1285 -0.8899 H 0 0 0 0 0 0 0 0 0 0 0 11
0.5773 -2.1338 0.9074 H 0 0 0 0 0 0 0 0 0 0 0 12
1.8478 1.3656 0.0611 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
7 3 0 0 0 0
8 3 0 0 0 0
9 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
4 13 0 0 0 0
M END
$$$$
methylguanidine_p2.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 0 V2000
-0.6250 -0.6987 0.0008 N 0 0 0 0 0 0 0 0 0 0 0 1
-0.0111 -2.0235 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 2
-1.6414 -0.6741 -0.0019 H 0 0 0 0 0 0 0 0 0 0 0 3
1.0808 -1.9560 0.0027 H 0 0 0 0 0 0 0 0 0 0 0 4
-0.3217 -2.5801 0.8936 H 0 0 0 0 0 0 0 0 0 0 0 5
-0.3174 -2.5768 -0.8980 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.0011 0.4858 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.7348 1.6116 -0.0009 N 0 0 0 0 0 0 0 0 0 0 0 8
-0.2926 2.5239 -0.0012 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.7482 1.5787 0.0050 H 0 0 0 0 0 0 0 0 0 0 0 10
1.3357 0.5808 0.0016 N 0 0 0 0 0 0 0 0 0 0 0 11
1.7885 1.4881 -0.0041 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9332 -0.2366 -0.0101 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
7 1 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
6 2 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
12 11 0 0 0 0
11 13 0 0 0 0
M END
$$$$
methylguanidine_t.sdf
COSMOtherm 3D 0

12 11 0 0 0 0 0 0 0 0 0 V2000
0.0582 -1.9380 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
0.7703 -0.6643 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 2
0.0386 0.4167 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6491 1.6502 -0.0006 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.3355 0.4486 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 5
0.7896 -2.7581 0.0008 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.5864 -2.0809 0.8909 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.5845 -2.0813 -0.8924 H 0 0 0 0 0 0 0 0 0 0 0 8
0.1248 2.5158 0.0043 H 0 0 0 0 0 0 0 0 0 0 0 9
1.6604 1.6919 0.0015 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.8551 1.3184 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.8679 -0.4117 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
3 2 0 0 0 0
4 3 0 0 0 0
5 3 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 5 0 0 0 0
5 12 0 0 0 0
M END
$$$$
methylguanidine_t_p2.sdf
COSMOtherm 3D 0

13 12 0 0 0 0 0 0 0 0 0 V2000
0.0292 -1.9881 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
0.6698 -0.6755 0.0003 N 0 0 0 0 0 0 0 0 0 0 0 2
0.0032 0.4859 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6767 1.6467 -0.0003 N 0 0 0 0 0 0 0 0 0 0 0 4
-1.3368 0.4930 0.0004 N 0 0 0 0 0 0 0 0 0 0 0 5
0.8191 -2.7446 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 6
-0.5888 -2.1315 0.8983 H 0 0 0 0 0 0 0 0 0 0 0 7

```

```

1
2
3      -0.5875    -2.1317    -0.8994 H   0  0  0  0  0  0  0  0  0  0  0  8
4      0.1881     2.5352    -0.0004 H   0  0  0  0  0  0  0  0  0  0  0  9
5      1.6905     1.6648     0.0019 H   0  0  0  0  0  0  0  0  0  0  0 10
6     -1.8540     1.3654    -0.0009 H   0  0  0  0  0  0  0  0  0  0  0 11
7     -1.8718    -0.3678    -0.0023 H   0  0  0  0  0  0  0  0  0  0  0 12
8      1.6843    -0.6363    -0.0014 H   0  0  0  0  0  0  0  0  0  0  0 13
9
10     2  1  0  0  0  0
11     6  1  0  0  0  0
12     7  1  0  0  0  0
13     8  1  0  0  0  0
14     3  2  0  0  0  0
15     4  3  0  0  0  0
16     5  3  0  0  0  0
17     9  4  0  0  0  0
18    10  4  0  0  0  0
19    11  5  0  0  0  0
20    12  5  0  0  0  0
21    2 13  0  0  0  0

```

M END

\$\$\$\$

n-butylamine-cation.sdf
COSMOtherm 3D

0

```

17 16 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
18     2.6046    0.0002   -0.3317 C   0  0  0  0  0  0  0  0  0  0  0  0  1
19     1.3307    0.0000    0.5192 C   0  0  0  0  0  0  0  0  0  0  0  0  2
20     0.0526   -0.0004   -0.3317 C   0  0  0  0  0  0  0  0  0  0  0  0  3
21    -1.1973   -0.0001    0.5378 C   0  0  0  0  0  0  0  0  0  0  0  0  4
22    -2.4473    0.0002   -0.3038 N   0  0  0  0  0  0  0  0  0  0  0  0  5
23    -3.2958    0.0054    0.2767 H   0  0  0  0  0  0  0  0  0  0  0  0  6
24    -2.4984   -0.8306   -0.9081 H   0  0  0  0  0  0  0  0  0  0  0  0  7
25     3.5030    0.0016    0.3022 H   0  0  0  0  0  0  0  0  0  0  0  0  8
26     2.6509   -0.8900   -0.9778 H   0  0  0  0  0  0  0  0  0  0  0  0  9
27     2.6494    0.8890   -0.9797 H   0  0  0  0  0  0  0  0  0  0  0  0 10
28     1.3264    0.8837    1.1789 H   0  0  0  0  0  0  0  0  0  0  0  0 11
29     1.3269   -0.8832    1.1794 H   0  0  0  0  0  0  0  0  0  0  0  0 12
30     0.0451   -0.8882   -0.9863 H   0  0  0  0  0  0  0  0  0  0  0  0 13
31     0.0450    0.8871   -0.9868 H   0  0  0  0  0  0  0  0  0  0  0  0 14
32    -1.2523    0.8919    1.1733 H   0  0  0  0  0  0  0  0  0  0  0  0 15
33    -1.2529   -0.8917    1.1738 H   0  0  0  0  0  0  0  0  0  0  0  0 16
34    -2.4930    0.8262   -0.9150 H   0  0  0  0  0  0  0  0  0  0  0  0 17

```

```

35     2  1  0  0  0  0
36     8  1  0  0  0  0
37     9  1  0  0  0  0
38    10  1  0  0  0  0
39     3  2  0  0  0  0
40    11  2  0  0  0  0
41    12  2  0  0  0  0
42     4  3  0  0  0  0
43    13  3  0  0  0  0
44    14  3  0  0  0  0
45     5  4  0  0  0  0
46    15  4  0  0  0  0
47    16  4  0  0  0  0
48     6  5  0  0  0  0
49     7  5  0  0  0  0
50    5 17  0  0  0  0

```

M END

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n-butylamine.sdf
COSMOtherm 3D

0

```

16 15 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
17     2.5761    0.0047   -0.3223 C   0  0  0  0  0  0  0  0  0  0  0  0  1
18     1.2946   -0.0251    0.5179 C   0  0  0  0  0  0  0  0  0  0  0  0  2
19     0.0164    0.0326   -0.3284 C   0  0  0  0  0  0  0  0  0  0  0  0  3
20    -1.2629   -0.0080    0.5082 C   0  0  0  0  0  0  0  0  0  0  0  0  4
21    -2.4656    0.0520   -0.3511 N   0  0  0  0  0  0  0  0  0  0  0  0  5
22    -3.3034    0.0201    0.2372 H   0  0  0  0  0  0  0  0  0  0  0  0  6
23    -2.5073   -0.7985   -0.9220 H   0  0  0  0  0  0  0  0  0  0  0  0  7
24     3.4738   -0.0398    0.3121 H   0  0  0  0  0  0  0  0  0  0  0  0  8
25     2.6152   -0.8494   -1.0167 H   0  0  0  0  0  0  0  0  0  0  0  0  9
26     2.6359    0.9257   -0.9230 H   0  0  0  0  0  0  0  0  0  0  0  0 10
27     1.2993    0.8218    1.2259 H   0  0  0  0  0  0  0  0  0  0  0  0 11
28     1.2811   -0.9406    1.1339 H   0  0  0  0  0  0  0  0  0  0  0  0 12
29     0.0105   -0.8175   -1.0354 H   0  0  0  0  0  0  0  0  0  0  0  0 13
30     0.0150    0.9505   -0.9414 H   0  0  0  0  0  0  0  0  0  0  0  0 14
31    -1.2876    0.8641    1.1822 H   0  0  0  0  0  0  0  0  0  0  0  0 15
32    -1.2410   -0.9091    1.1538 H   0  0  0  0  0  0  0  0  0  0  0  0 16

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33     2  1  0  0  0  0
34     8  1  0  0  0  0
35     9  1  0  0  0  0
36    10  1  0  0  0  0
37     3  2  0  0  0  0
38    11  2  0  0  0  0
39    12  2  0  0  0  0
40     4  3  0  0  0  0
41    13  3  0  0  0  0
42    14  3  0  0  0  0
43     5  4  0  0  0  0
44    15  4  0  0  0  0
45     6  5  0  0  0  0
46     7  5  0  0  0  0
47    4 16  0  0  0  0

```

M END

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n-heptylamine-cation.sdf
COSMOtherm 3D

0

```

26 25 0 0 0 0 0 0 0 0 0 0 0 0 0 0 V2000
27     3.2538    0.0006   -0.5336 C   0  0  0  0  0  0  0  0  0  0  0  0  1
28     1.9982   -0.0010    0.3478 C   0  0  0  0  0  0  0  0  0  0  0  0  2
29     0.6878   -0.0007   -0.4493 C   0  0  0  0  0  0  0  0  0  0  0  0  3
30    -0.5614   -0.0017    0.4405 C   0  0  0  0  0  0  0  0  0  0  0  0  4
31    -1.8697   -0.0013   -0.3628 C   0  0  0  0  0  0  0  0  0  0  0  0  5

```


23 22 0 0 0 0 0 0 0 0 0 V2000
 3.9012 -0.0004 0.3550 C 0 0 0 0 0 0 0 0 0 0 1
 2.6224 -0.0003 -0.4898 C 0 0 0 0 0 0 0 0 0 0 2
 1.3409 0.0002 0.3536 C 0 0 0 0 0 0 0 0 0 0 3
 0.0601 0.0008 -0.4902 C 0 0 0 0 0 0 0 0 0 0 4
 -1.2180 0.0007 0.3603 C 0 0 0 0 0 0 0 0 0 0 5
 -2.4661 -0.0004 -0.5120 C 0 0 0 0 0 0 0 0 0 0 6
 -3.7182 -0.0004 0.3267 N 0 0 0 0 0 0 0 0 0 0 7
 -4.5652 -0.0027 -0.2560 H 0 0 0 0 0 0 0 0 0 0 8
 -3.7693 0.8291 0.9327 H 0 0 0 0 0 0 0 0 0 0 9
 4.8013 -0.0026 -0.2775 H 0 0 0 0 0 0 0 0 0 0 10
 3.9497 0.8896 1.0020 H 0 0 0 0 0 0 0 0 0 0 11
 3.9475 -0.8882 1.0051 H 0 0 0 0 0 0 0 0 0 0 12
 2.6185 -0.8833 -1.1521 H 0 0 0 0 0 0 0 0 0 0 13
 2.6190 0.8822 -1.1528 H 0 0 0 0 0 0 0 0 0 0 14
 1.3416 0.8840 1.0162 H 0 0 0 0 0 0 0 0 0 0 15
 1.3408 -0.8838 1.0160 H 0 0 0 0 0 0 0 0 0 0 16
 0.0578 -0.8834 -1.1509 H 0 0 0 0 0 0 0 0 0 0 17
 0.0582 0.8854 -1.1504 H 0 0 0 0 0 0 0 0 0 0 18
 -1.2276 0.8887 1.0144 H 0 0 0 0 0 0 0 0 0 0 19
 -1.2267 -0.8867 1.0153 H 0 0 0 0 0 0 0 0 0 0 20
 -2.5196 -0.8927 -1.1472 H 0 0 0 0 0 0 0 0 0 0 21
 -2.5203 0.8910 -1.1483 H 0 0 0 0 0 0 0 0 0 0 22
 -3.7671 -0.8278 0.9358 H 0 0 0 0 0 0 0 0 0 0 23

2 1 0 0 0 0
 10 1 0 0 0 0
 11 1 0 0 0 0
 12 1 0 0 0 0
 3 2 0 0 0 0
 13 2 0 0 0 0
 14 2 0 0 0 0
 4 3 0 0 0 0
 15 3 0 0 0 0
 16 3 0 0 0 0
 5 4 0 0 0 0
 17 4 0 0 0 0
 18 4 0 0 0 0
 6 5 0 0 0 0
 19 5 0 0 0 0
 20 5 0 0 0 0
 7 6 0 0 0 0
 21 6 0 0 0 0
 22 6 0 0 0 0
 8 7 0 0 0 0
 9 7 0 0 0 0
 7 23 0 0 0 0

M END
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n-hexylamine.sdf
 COSMOtherm 3D 0

22 21 0 0 0 0 0 0 0 0 0 V2000
 3.8687 -0.0078 -0.3493 C 0 0 0 0 0 0 0 0 0 0 1
 2.5877 -0.0264 0.4919 C 0 0 0 0 0 0 0 0 0 0 2
 1.3070 0.0258 -0.3514 C 0 0 0 0 0 0 0 0 0 0 3
 0.0207 0.0014 0.4840 C 0 0 0 0 0 0 0 0 0 0 4
 -1.2600 0.0421 -0.3590 C 0 0 0 0 0 0 0 0 0 0 5
 -2.5355 -0.0058 0.4834 C 0 0 0 0 0 0 0 0 0 0 6
 -3.7422 0.0306 -0.3715 N 0 0 0 0 0 0 0 0 0 0 7
 -4.5770 -0.0053 0.2209 H 0 0 0 0 0 0 0 0 0 0 8
 -3.7759 -0.8266 -0.9328 H 0 0 0 0 0 0 0 0 0 0 9
 4.7678 -0.0484 0.2836 H 0 0 0 0 0 0 0 0 0 0 10
 3.9050 -0.8682 -1.0362 H 0 0 0 0 0 0 0 0 0 0 11
 3.9299 0.9075 -0.9589 H 0 0 0 0 0 0 0 0 0 0 12
 2.5947 0.8271 1.1923 H 0 0 0 0 0 0 0 0 0 0 13
 2.5710 -0.9360 1.1170 H 0 0 0 0 0 0 0 0 0 0 14
 1.3006 -0.8275 -1.0538 H 0 0 0 0 0 0 0 0 0 0 15
 1.3203 0.9374 -0.9755 H 0 0 0 0 0 0 0 0 0 0 16
 0.0250 0.8577 1.1824 H 0 0 0 0 0 0 0 0 0 0 17
 0.0149 -0.9077 1.1116 H 0 0 0 0 0 0 0 0 0 0 18
 -1.2615 -0.8126 -1.0601 H 0 0 0 0 0 0 0 0 0 0 19
 -1.2737 0.9560 -0.9775 H 0 0 0 0 0 0 0 0 0 0 20
 -2.5687 0.8722 1.1493 H 0 0 0 0 0 0 0 0 0 0 21
 -2.4995 -0.9004 1.1375 H 0 0 0 0 0 0 0 0 0 0 22

2 1 0 0 0 0
 10 1 0 0 0 0
 11 1 0 0 0 0
 12 1 0 0 0 0
 3 2 0 0 0 0
 13 2 0 0 0 0
 14 2 0 0 0 0
 4 3 0 0 0 0
 15 3 0 0 0 0
 16 3 0 0 0 0
 5 4 0 0 0 0
 17 4 0 0 0 0
 18 4 0 0 0 0
 6 5 0 0 0 0
 19 5 0 0 0 0
 20 5 0 0 0 0
 7 6 0 0 0 0
 21 6 0 0 0 0
 8 7 0 0 0 0
 9 7 0 0 0 0
 6 22 0 0 0 0

M END
 \$\$\$

n-octylamine-cation.sdf
 COSMOtherm 3D 0

29 28 0 0 0 0 0 0 0 0 0 V2000
 2.6318 0.0002 0.3668 C 0 0 0 0 0 0 0 0 0 0 1
 1.3458 0.0014 -0.4692 C 0 0 0 0 0 0 0 0 0 0 2
 0.0645 0.0016 0.3742 C 0 0 0 0 0 0 0 0 0 0 3

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-1.2151 0.0015 -0.4715 C 0 0 0 0 0 0 0 0 0 0 4
-2.4950 0.0016 0.3762 C 0 0 0 0 0 0 0 0 0 0 5
-3.7408 -0.0020 -0.4994 C 0 0 0 0 0 0 0 0 0 0 6
-4.9952 -0.0014 0.3357 N 0 0 0 0 0 0 0 0 0 0 7
-5.8406 -0.0041 -0.2495 H 0 0 0 0 0 0 0 0 0 0 8
-5.0481 0.8286 0.9409 H 0 0 0 0 0 0 0 0 0 0 9
 3.9132 -0.0007 -0.4770 C 0 0 0 0 0 0 0 0 0 0 10
 2.6356 0.8837 1.0306 H 0 0 0 0 0 0 0 0 0 0 11
 2.6342 -0.8836 1.0301 H 0 0 0 0 0 0 0 0 0 0 12
 1.3432 -0.8818 -1.1331 H 0 0 0 0 0 0 0 0 0 0 13
 1.3441 0.8853 -1.1323 H 0 0 0 0 0 0 0 0 0 0 14
 0.0632 0.8858 1.0361 H 0 0 0 0 0 0 0 0 0 0 15
 0.0632 -0.8827 1.0361 H 0 0 0 0 0 0 0 0 0 0 16
 -1.2158 -0.8830 -1.1319 H 0 0 0 0 0 0 0 0 0 0 17
 -1.2161 0.8857 -1.1322 H 0 0 0 0 0 0 0 0 0 0 18
 -2.5071 0.8906 1.0289 H 0 0 0 0 0 0 0 0 0 0 19
 -2.5047 -0.8854 1.0318 H 0 0 0 0 0 0 0 0 0 0 20
 -3.7918 -0.8954 -1.1333 H 0 0 0 0 0 0 0 0 0 0 21
 -3.7938 0.8884 -1.1374 H 0 0 0 0 0 0 0 0 0 0 22
 5.1936 -0.0018 0.3656 C 0 0 0 0 0 0 0 0 0 0 23
 3.9083 -0.8833 -1.1401 H 0 0 0 0 0 0 0 0 0 0 24
 3.9098 0.8819 -1.1401 H 0 0 0 0 0 0 0 0 0 0 25
 6.0935 -0.0037 -0.2674 H 0 0 0 0 0 0 0 0 0 0 26
 5.2430 0.8874 1.0137 H 0 0 0 0 0 0 0 0 0 0 27
 5.2404 -0.8901 1.0152 H 0 0 0 0 0 0 0 0 0 0 28
 -5.0458 -0.8283 0.9453 H 0 0 0 0 0 0 0 0 0 0 29
 2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
 3 2 0 0 0 0
13 2 0 0 0 0
14 2 0 0 0 0
 4 3 0 0 0 0
15 3 0 0 0 0
16 3 0 0 0 0
 5 4 0 0 0 0
17 4 0 0 0 0
18 4 0 0 0 0
 6 5 0 0 0 0
19 5 0 0 0 0
20 5 0 0 0 0
 7 6 0 0 0 0
21 6 0 0 0 0
22 6 0 0 0 0
 8 7 0 0 0 0
 9 7 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
26 23 0 0 0 0
27 23 0 0 0 0
28 23 0 0 0 0
 7 29 0 0 0 0
M END
$$$$
n-octylamine.sdf
COSMOtherm 3D 0
28 27 0 0 0 0 0 0 0 0 0 0 v2000
 2.5962 0.0167 -0.3646 C 0 0 0 0 0 0 0 0 0 0 0 1
 1.3088 0.0016 0.4690 C 0 0 0 0 0 0 0 0 0 0 0 2
 0.0272 0.0423 -0.3733 C 0 0 0 0 0 0 0 0 0 0 0 3
 -1.2571 0.0151 0.4653 C 0 0 0 0 0 0 0 0 0 0 0 4
 -2.5401 0.0395 -0.3749 C 0 0 0 0 0 0 0 0 0 0 0 5
 -3.8129 -0.0118 0.4715 C 0 0 0 0 0 0 0 0 0 0 0 6
 -5.0222 0.0107 -0.3798 N 0 0 0 0 0 0 0 0 0 0 0 7
 -5.8550 -0.0248 0.2154 H 0 0 0 0 0 0 0 0 0 0 0 8
 -5.0529 -0.8509 -0.9344 H 0 0 0 0 0 0 0 0 0 0 0 9
 3.8770 -0.0330 0.4788 C 0 0 0 0 0 0 0 0 0 0 0 10
 2.5884 -0.8407 -1.0621 H 0 0 0 0 0 0 0 0 0 0 0 11
 2.6122 0.9245 -0.9946 H 0 0 0 0 0 0 0 0 0 0 0 12
 1.3152 0.8616 1.1632 H 0 0 0 0 0 0 0 0 0 0 0 13
 1.2973 -0.9040 1.1020 H 0 0 0 0 0 0 0 0 0 0 0 14
 0.0234 -0.8151 -1.0705 H 0 0 0 0 0 0 0 0 0 0 0 15
 0.0332 0.9505 -1.0023 H 0 0 0 0 0 0 0 0 0 0 0 16
 -1.2577 0.8767 1.1572 H 0 0 0 0 0 0 0 0 0 0 0 17
 -1.2546 -0.8892 1.0999 H 0 0 0 0 0 0 0 0 0 0 0 18
 -2.5366 -0.8205 -1.0695 H 0 0 0 0 0 0 0 0 0 0 0 19
 -2.5625 0.9487 -1.0001 H 0 0 0 0 0 0 0 0 0 0 0 20
 -3.8500 0.8695 1.1329 H 0 0 0 0 0 0 0 0 0 0 0 21
 -3.7686 -0.9027 1.1302 H 0 0 0 0 0 0 0 0 0 0 0 22
 5.1582 -0.0179 -0.3624 C 0 0 0 0 0 0 0 0 0 0 0 23
 3.8844 0.8231 1.1759 H 0 0 0 0 0 0 0 0 0 0 0 24
 3.8601 -0.9402 1.1074 H 0 0 0 0 0 0 0 0 0 0 0 25
 6.0574 -0.0564 0.2705 H 0 0 0 0 0 0 0 0 0 0 0 26
 5.1943 -0.8807 -1.0462 H 0 0 0 0 0 0 0 0 0 0 0 27
 5.2196 0.8952 -0.9753 H 0 0 0 0 0 0 0 0 0 0 0 28
 2 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
12 1 0 0 0 0
 3 2 0 0 0 0
13 2 0 0 0 0
14 2 0 0 0 0
 4 3 0 0 0 0
15 3 0 0 0 0
16 3 0 0 0 0
 5 4 0 0 0 0
17 4 0 0 0 0
18 4 0 0 0 0
 6 5 0 0 0 0
19 5 0 0 0 0
20 5 0 0 0 0
 7 6 0 0 0 0
```

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1
2
3
4 21 6 0 0 0 0
5 22 6 0 0 0 0
6 8 7 0 0 0 0
7 9 7 0 0 0 0
8 23 10 0 0 0 0
9 24 10 0 0 0 0
10 25 10 0 0 0 0
11 26 23 0 0 0 0
12 27 23 0 0 0 0
13 23 28 0 0 0 0
14 M END
15 $$$$
16 n-pentylamine-cation.sdf
17 COSMOTHERM 3D 0
18
19 20 19 0 0 0 0 0 0 0 0 V2000
21 3.2728 0.0009 0.2228 C 0 0 0 0 0 0 0 0 0 0 0 1
22 1.9469 -0.0002 -0.5457 C 0 0 0 0 0 0 0 0 0 0 0 2
23 0.7220 -0.0008 0.3777 C 0 0 0 0 0 0 0 0 0 0 0 3
24 -0.6076 -0.0009 -0.3895 C 0 0 0 0 0 0 0 0 0 0 0 4
25 -1.7981 -0.0003 0.5596 C 0 0 0 0 0 0 0 0 0 0 0 5
26 -3.1007 0.0009 -0.1984 N 0 0 0 0 0 0 0 0 0 0 0 6
27 -3.9091 0.0036 0.4368 H 0 0 0 0 0 0 0 0 0 0 0 7
28 -3.1908 -0.8282 -0.8003 H 0 0 0 0 0 0 0 0 0 0 0 8
29 4.1331 0.0006 -0.4627 H 0 0 0 0 0 0 0 0 0 0 0 9
30 3.3579 0.8906 0.8662 H 0 0 0 0 0 0 0 0 0 0 0 10
31 3.3584 -0.8874 0.8678 H 0 0 0 0 0 0 0 0 0 0 0 11
32 1.9028 -0.8833 -1.2057 H 0 0 0 0 0 0 0 0 0 0 0 12
33 1.9016 0.8826 -1.2061 H 0 0 0 0 0 0 0 0 0 0 0 13
34 0.7629 0.8834 1.0373 H 0 0 0 0 0 0 0 0 0 0 0 14
35 0.7634 -0.8852 1.0370 H 0 0 0 0 0 0 0 0 0 0 0 15
36 -0.6586 -0.8887 -1.0420 H 0 0 0 0 0 0 0 0 0 0 0 16
37 -0.6583 0.8865 -1.0425 H 0 0 0 0 0 0 0 0 0 0 0 17
38 -1.8111 0.8915 1.1977 H 0 0 0 0 0 0 0 0 0 0 0 18
39 -1.8125 -0.8923 1.1974 H 0 0 0 0 0 0 0 0 0 0 0 19
40 -3.1874 0.8286 -0.8028 H 0 0 0 0 0 0 0 0 0 0 0 20
41
42 2 1 0 0 0 0
43 9 1 0 0 0 0
44 10 1 0 0 0 0
45 11 1 0 0 0 0
46 3 2 0 0 0 0
47 12 2 0 0 0 0
48 13 2 0 0 0 0
49 4 3 0 0 0 0
50 14 3 0 0 0 0
51 15 3 0 0 0 0
52 5 4 0 0 0 0
53 16 4 0 0 0 0
54 17 4 0 0 0 0
55 6 5 0 0 0 0
56 18 5 0 0 0 0
57 19 5 0 0 0 0
58 7 6 0 0 0 0
59 8 6 0 0 0 0
60 6 20 0 0 0 0
M END
$$$$
n-pentylamine.sdf
COSMOTHERM 3D 0
19 18 0 0 0 0 0 0 0 0 V2000
3.2401 -0.0309 0.2271 C 0 0 0 0 0 0 0 0 0 0 0 1
1.9152 0.0218 -0.5417 C 0 0 0 0 0 0 0 0 0 0 0 2
0.6845 0.0003 0.3739 C 0 0 0 0 0 0 0 0 0 0 0 3
-0.6473 0.0406 -0.3857 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.8670 0.0006 -0.5359 C 0 0 0 0 0 0 0 0 0 0 0 5
-3.1250 0.0290 -0.2419 N 0 0 0 0 0 0 0 0 0 0 0 6
-3.9208 -0.0036 0.4021 H 0 0 0 0 0 0 0 0 0 0 0 7
-3.1920 -0.8322 -0.7939 H 0 0 0 0 0 0 0 0 0 0 0 8
4.1034 -0.0142 -0.4548 H 0 0 0 0 0 0 0 0 0 0 0 9
3.3375 0.8277 0.9101 H 0 0 0 0 0 0 0 0 0 0 0 10
3.3103 -0.9479 0.8331 H 0 0 0 0 0 0 0 0 0 0 0 11
1.8603 -0.8315 -1.2399 H 0 0 0 0 0 0 0 0 0 0 0 12
1.8868 0.9318 -1.1657 H 0 0 0 0 0 0 0 0 0 0 0 13
0.7354 0.8578 1.0691 H 0 0 0 0 0 0 0 0 0 0 0 14
0.7189 -0.9075 1.0027 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.6957 -0.8179 -1.0804 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.6978 0.9511 -1.0072 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.8585 0.8847 1.1945 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.7892 -0.8880 1.1944 H 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
13 2 0 0 0 0
4 3 0 0 0 0
14 3 0 0 0 0
15 3 0 0 0 0
5 4 0 0 0 0
16 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 19 0 0 0 0
M END
$$$$
n-propylamine-cation.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 V2000
1.9973 -0.0002 0.1345 C 0 0 0 0 0 0 0 0 0 0 0 1

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0.6126 0.0002 -0.5230 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.4934 0.0002 0.5243 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.8560 -0.0002 -0.1195 N 0 0 0 0 0 0 0 0 0 0 0 4
-2.6070 0.0078 0.5826 H 0 0 0 0 0 0 0 0 0 0 0 5
-1.9985 -0.8325 -0.7067 H 0 0 0 0 0 0 0 0 0 0 0 6
2.7861 0.0016 -0.6301 H 0 0 0 0 0 0 0 0 0 0 0 7
2.1383 0.8888 0.7667 H 0 0 0 0 0 0 0 0 0 0 0 8
2.1392 -0.8913 0.7636 H 0 0 0 0 0 0 0 0 0 0 0 9
0.5042 -0.8859 -1.1688 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5044 0.8870 -1.1678 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4516 0.8924 1.1606 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.4514 -0.8913 1.1615 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.9927 0.8242 -0.7191 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
4 14 0 0 0 0
M END
$$$$
n-propylamine.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
1.9655 -0.0207 0.1392 C 0 0 0 0 0 0 0 0 0 0 0 1
0.5809 0.0402 -0.5150 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.5582 -0.0114 0.5042 C 0 0 0 0 0 0 0 0 0 0 0 3
-1.8767 0.0498 -0.1633 N 0 0 0 0 0 0 0 0 0 0 0 4
-2.6160 0.0224 0.5451 H 0 0 0 0 0 0 0 0 0 0 0 5
-2.0067 -0.8018 -0.7188 H 0 0 0 0 0 0 0 0 0 0 0 6
2.7653 0.0170 -0.6147 H 0 0 0 0 0 0 0 0 0 0 0 7
2.1172 0.8238 0.8294 H 0 0 0 0 0 0 0 0 0 0 0 8
2.0933 -0.9501 0.7157 H 0 0 0 0 0 0 0 0 0 0 0 9
0.4679 -0.8025 -1.2193 H 0 0 0 0 0 0 0 0 0 0 0 10
0.4830 0.9623 -1.1116 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4821 0.8562 1.1802 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.4350 -0.9163 1.1331 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
7 1 0 0 0 0
8 1 0 0 0 0
9 1 0 0 0 0
3 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
3 13 0 0 0 0
M END
$$$$
neo-pentylamine-cation.sdf
COSMOTHERM 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
1.6474 -0.0100 -0.9834 C 0 0 0 0 0 0 0 0 0 0 0 1
0.4710 0.0000 0.0128 C 0 0 0 0 0 0 0 0 0 0 0 2
0.5434 1.2704 0.8824 C 0 0 0 0 0 0 0 0 0 0 0 3
0.5355 -1.2592 0.8990 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8093 -0.0014 -0.8412 C 0 0 0 0 0 0 0 0 0 0 0 5
-2.0732 0.0002 -0.0194 N 0 0 0 0 0 0 0 0 0 0 0 6
-2.9072 -0.0021 -0.6208 H 0 0 0 0 0 0 0 0 0 0 0 7
-2.1407 0.8311 0.5833 H 0 0 0 0 0 0 0 0 0 0 0 8
2.6021 -0.0044 -0.4382 H 0 0 0 0 0 0 0 0 0 0 0 9
1.6239 -0.9085 -1.6187 H 0 0 0 0 0 0 0 0 0 0 0 10
1.6239 0.8754 -1.6368 H 0 0 0 0 0 0 0 0 0 0 0 11
1.4972 1.2970 1.4286 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.2562 1.3097 1.6397 H 0 0 0 0 0 0 0 0 0 0 0 13
0.4790 2.1795 0.2658 H 0 0 0 0 0 0 0 0 0 0 0 14
1.4924 -1.2885 1.4398 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.2594 -1.2798 1.6619 H 0 0 0 0 0 0 0 0 0 0 0 16
0.4582 -2.1760 0.2953 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.8599 -0.8950 -1.4754 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.8596 0.8892 -1.4795 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.1392 -0.8275 0.5879 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
5 2 0 0 0 0
12 3 0 0 0 0
13 3 0 0 0 0
14 3 0 0 0 0
15 4 0 0 0 0
16 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
6 20 0 0 0 0
M END
$$$$
neo-pentylamine.sdf
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0.4800 -0.8244 3.2021 H 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
17 8 0 0 0 0
7 18 0 0 0 0
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M END
$$$$
p-toluidine.sdf
COSMOtherm 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
-2.9502 0.0012 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.4387 -0.0022 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
-0.7030 1.1978 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
0.6920 1.2093 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4255 -0.0011 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.7028 -1.1988 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6949 -1.2104 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 7
2.8031 0.0024 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 8
-3.3560 0.5166 -0.8852 H 0 0 0 0 0 0 0 0 0 0 0 9
-3.3469 -1.0236 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 10
-3.3561 0.5169 0.8849 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.2345 2.1538 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 12
1.2294 2.1612 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2350 -2.1542 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 14
1.2318 -2.1624 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 15
3.3240 0.8704 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 16
3.3286 -0.8628 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
9 1 0 0 0 0
10 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
6 2 0 0 0 0
4 3 0 0 0 0
12 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
15 7 0 0 0 0
16 8 0 0 0 0
8 17 0 0 0 0
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M END
$$$$
p-toluidine0.sdf
COSMOtherm 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
-1.1983 -0.7030 0.0108 C 0 0 0 0 0 0 0 0 0 0 0 1
-1.2099 0.6933 0.0029 C 0 0 0 0 0 0 0 0 0 0 0 2
0.0000 1.4253 -0.0040 C 0 0 0 0 0 0 0 0 0 0 0 3
1.2099 0.6933 0.0027 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1983 -0.7030 0.0110 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0001 -1.4387 0.0119 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0000 2.8030 -0.0102 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0001 -2.9497 -0.0181 C 0 0 0 0 0 0 0 0 0 0 0 8
0.8667 3.3261 -0.0122 H 0 0 0 0 0 0 0 0 0 0 0 9
-0.8666 3.3262 -0.0106 H 0 0 0 0 0 0 0 0 0 0 0 10
-2.1540 -1.2348 0.0188 H 0 0 0 0 0 0 0 0 0 0 0 11
-2.1617 1.2306 0.0061 H 0 0 0 0 0 0 0 0 0 0 0 12
2.1617 1.2306 0.0062 H 0 0 0 0 0 0 0 0 0 0 0 13
2.1539 -1.2349 0.0190 H 0 0 0 0 0 0 0 0 0 0 0 14
0.0030 -3.3355 -1.0515 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.8913 -3.3606 0.4777 H 0 0 0 0 0 0 0 0 0 0 0 16
0.8886 -3.3606 0.4827 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
6 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
12 2 0 0 0 0
4 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
8 6 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
15 8 0 0 0 0
16 8 0 0 0 0
8 17 0 0 0 0
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M END
$$$$
p-toluidine1.sdf
COSMOtherm 3D 0
17 17 0 0 0 0 0 0 0 0 0 V2000
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2
3 -1.1992 -0.7042 0.0137 C 0 0 0 0 0 0 0 0 0 0 0 1
4 -1.2083 0.6928 0.0116 C 0 0 0 0 0 0 0 0 0 0 0 2
5 0.0000 1.4200 0.0037 C 0 0 0 0 0 0 0 0 0 0 0 3
6 1.2083 0.6927 0.0111 C 0 0 0 0 0 0 0 0 0 0 0 4
7 1.1992 -0.7043 0.0135 C 0 0 0 0 0 0 0 0 0 0 0 5
8 -0.0001 -1.4379 0.0110 C 0 0 0 0 0 0 0 0 0 0 0 6
9 0.0001 2.8173 -0.0731 N 0 0 0 0 0 0 0 0 0 0 0 7
10 0.0000 -2.9484 -0.0237 C 0 0 0 0 0 0 0 0 0 0 0 8
11 0.8402 3.2684 0.2843 H 0 0 0 0 0 0 0 0 0 0 0 9
12 -0.8407 3.2678 0.2834 H 0 0 0 0 0 0 0 0 0 0 0 10
13 -2.1541 -1.2370 0.0194 H 0 0 0 0 0 0 0 0 0 0 0 11
14 -2.1597 1.2309 0.0173 H 0 0 0 0 0 0 0 0 0 0 0 12
15 2.1597 1.2308 0.0167 H 0 0 0 0 0 0 0 0 0 0 0 13
16 2.1541 -1.2369 0.0238 H 0 0 0 0 0 0 0 0 0 0 0 14
17 0.0095 -3.3283 -1.0591 H 0 0 0 0 0 0 0 0 0 0 0 15
18 -0.8948 -3.3610 0.4640 H 0 0 0 0 0 0 0 0 0 0 0 16
19 0.8856 -3.3615 0.4802 H 0 0 0 0 0 0 0 0 0 0 0 17
20
21 2 1 0 0 0 0
22 6 1 0 0 0 0
23 11 1 0 0 0 0
24 3 2 0 0 0 0
25 12 2 0 0 0 0
26 4 3 0 0 0 0
27 7 3 0 0 0 0
28 5 4 0 0 0 0
29 13 4 0 0 0 0
30 6 5 0 0 0 0
31 14 5 0 0 0 0
32 8 6 0 0 0 0
33 9 7 0 0 0 0
34 10 7 0 0 0 0
35 15 8 0 0 0 0
36 16 8 0 0 0 0
37 8 17 0 0 0 0
38
39 M END
40 $$$
41 pyrazine.sdf
42 COSMOTHERM 3D 0
43
44 10 10 0 0 0 0 0 0 0 0 0 V2000
45 -0.6993 -1.1404 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
46 -1.4124 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 2
47 0.6993 -1.1403 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
48 1.4124 0.0000 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 4
49 0.6993 1.1404 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
50 -0.6993 -1.1403 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
51 -1.2578 -2.0795 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 7
52 1.2579 -2.0794 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 8
53 1.2578 2.0795 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
54 -1.2579 2.0794 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
55
56 2 1 0 0 0 0
57 3 1 0 0 0 0
58 7 1 0 0 0 0
59 6 2 0 0 0 0
60 4 3 0 0 0 0
61 8 3 0 0 0 0
62 5 4 0 0 0 0
63 6 5 0 0 0 0
64 9 5 0 0 0 0
65 6 10 0 0 0 0
66
67 M END
68 $$$
69 pyrazine_pl.sdf
70 COSMOTHERM 3D 0
71
72 11 11 0 0 0 0 0 0 0 0 0 V2000
73 -0.6741 -1.1789 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
74 -1.3234 0.0001 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 2
75 -0.6739 1.1790 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
76 0.7190 1.1489 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
77 1.4139 -0.0001 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 5
78 0.7188 -1.1490 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 6
79 -2.3481 0.0001 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 7
80 -1.2719 -2.0869 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 8
81 -1.2716 2.0870 0.0003 H 0 0 0 0 0 0 0 0 0 0 0 9
82 1.2817 2.0825 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 10
83 1.2813 -2.0827 0.0002 H 0 0 0 0 0 0 0 0 0 0 0 11
84
85 2 1 0 0 0 0
86 6 1 0 0 0 0
87 8 1 0 0 0 0
88 3 2 0 0 0 0
89 7 2 0 0 0 0
90 4 3 0 0 0 0
91 9 3 0 0 0 0
92 5 4 0 0 0 0
93 10 4 0 0 0 0
94 6 5 0 0 0 0
95 6 11 0 0 0 0
96
97 M END
98 $$$
99 pyrazole.sdf
100 COSMOTHERM 3D 0
101
102 9 9 0 0 0 0 0 0 0 0 0 V2000
103 0.5469 -1.0998 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
104 1.1477 0.1797 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
105 0.2287 1.1628 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 3
106 -0.9595 0.5043 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
107 -0.8197 -0.8472 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
108 1.0343 -2.0693 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 6
109 2.2047 0.4349 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
110 -1.8268 1.0343 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 8
111 -1.6821 -1.5064 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
112
113 2 1 0 0 0 0
114 5 1 0 0 0 0

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3      6 1 0 0 0 0
4      3 2 0 0 0 0
5      7 2 0 0 0 0
6      4 3 0 0 0 0
7      5 4 0 0 0 0
8      8 4 0 0 0 0
9      5 9 0 0 0 0
10 M END
11 $$$$
12 pyrazole_p2.sdf
13 COSMOTHERM      3D      0
14
15 10 10 0 0 0 0 0 0 0 0 0 V2000
16 -0.3985 -1.1151 -0.0001 C 0 0 0 0 0 0 0 0 0 0 0 1
17 -1.2372 0.0010 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
18 -0.3968 1.1157 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
19 0.8736 0.6733 -0.0001 N 0 0 0 0 0 0 0 0 0 0 0 4
20 0.8726 -0.6746 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 5
21 -0.6116 -2.1785 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 6
22 -2.3204 0.0019 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
23 -0.6082 2.1794 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 8
24 1.7464 -1.1993 0.0004 H 0 0 0 0 0 0 0 0 0 0 0 9
25 1.7483 1.1965 -0.0004 H 0 0 0 0 0 0 0 0 0 0 0 10
26
27 2 1 0 0 0 0
28 5 1 0 0 0 0
29 6 1 0 0 0 0
30 3 2 0 0 0 0
31 7 2 0 0 0 0
32 4 3 0 0 0 0
33 8 3 0 0 0 0
34 5 4 0 0 0 0
35 9 5 0 0 0 0
36 4 10 0 0 0 0
37 M END
38 $$$$
39 pyridine.sdf
40 COSMOTHERM      3D      0
41
42 11 11 0 0 0 0 0 0 0 0 0 V2000
43 -1.1501 -0.6948 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
44 -1.2019 0.7023 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
45 -0.0001 1.4160 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 3
46 1.2018 0.7025 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
47 1.1502 -0.6946 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
48 0.0001 -1.3983 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 6
49 -2.0729 -1.2817 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
50 -2.1649 1.2148 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 8
51 -0.0001 2.5072 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 9
52 2.1647 1.2151 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 10
53 2.0730 -1.2814 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 11
54
55 2 1 0 0 0 0
56 6 1 0 0 0 0
57 7 1 0 0 0 0
58 3 2 0 0 0 0
59 8 2 0 0 0 0
60 4 3 0 0 0 0
61 9 3 0 0 0 0
62 5 4 0 0 0 0
63 10 4 0 0 0 0
64 6 5 0 0 0 0
65 5 11 0 0 0 0
66 M END
67 $$$$
68 pyridine_p1.sdf
69 COSMOTHERM      3D      0
70
71 12 12 0 0 0 0 0 0 0 0 0 V2000
72 -1.2112 -0.7187 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
73 -1.1899 0.6674 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 2
74 0.0000 1.3094 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 3
75 1.1899 0.6674 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 4
76 1.2112 -0.7187 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
77 0.0000 -1.4188 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
78 -2.1677 -1.2380 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 7
79 -2.0793 1.2929 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 8
80 2.0793 1.2929 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 9
81 2.1677 -1.2379 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 10
82 0.0000 -2.5088 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 11
83 -0.0001 2.3319 -0.0003 H 0 0 0 0 0 0 0 0 0 0 0 12
84
85 2 1 0 0 0 0
86 6 1 0 0 0 0
87 7 1 0 0 0 0
88 3 2 0 0 0 0
89 8 2 0 0 0 0
90 4 3 0 0 0 0
91 5 4 0 0 0 0
92 9 4 0 0 0 0
93 6 5 0 0 0 0
94 10 5 0 0 0 0
95 11 6 0 0 0 0
96 3 12 0 0 0 0
97 M END
98 $$$$
99 pyrimidine.sdf
100 COSMOTHERM      3D      0
101
102 10 10 0 0 0 0 0 0 0 0 0 V2000
103 -0.6564 -1.1881 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 1
104 0.6912 -1.2024 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 2
105 1.2903 0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 3
106 0.6910 1.2025 0.0000 N 0 0 0 0 0 0 0 0 0 0 0 4
107 -0.6566 1.1880 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 5
108 -1.3873 -0.0001 0.0000 C 0 0 0 0 0 0 0 0 0 0 0 6
109 -1.1562 -2.1601 0.0001 H 0 0 0 0 0 0 0 0 0 0 0 7
110 2.3839 0.0002 0.0000 H 0 0 0 0 0 0 0 0 0 0 0 8

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-1.1566 2.1600 0.0000 H 0 0 0 0 0 0 0 0 0 0 9  
-2.4769 -0.0002 0.0000 H 0 0 0 0 0 0 0 0 0 0 10  
2 1 0 0 0 0  
6 1 0 0 0 0  
7 1 0 0 0 0  
3 2 0 0 0 0  
4 3 0 0 0 0  
8 3 0 0 0 0  
5 4 0 0 0 0  
6 5 0 0 0 0  
9 5 0 0 0 0  
6 10 0 0 0 0
```

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M END  
$$$$  
pyrimidine_p1.sdf  
COSMOTHERM 3D 0  
11 11 0 0 0 0 0 0 0 0 0 V2000  
-0.7982 -1.1061 0.0000 C 0 0 0 0 0 0 0 0 0 0 1  
-1.3940 0.1580 0.0000 C 0 0 0 0 0 0 0 0 0 0 2  
-0.5567 1.2603 0.0000 C 0 0 0 0 0 0 0 0 0 0 3  
0.7766 1.0443 0.0000 N 0 0 0 0 0 0 0 0 0 0 4  
1.2964 -0.2050 0.0000 C 0 0 0 0 0 0 0 0 0 0 5  
0.5393 -1.2892 0.0000 N 0 0 0 0 0 0 0 0 0 0 6  
-1.4091 -2.0104 0.0000 H 0 0 0 0 0 0 0 0 0 0 7  
-2.4747 0.2819 -0.0001 H 0 0 0 0 0 0 0 0 0 0 8  
-0.8916 2.2951 0.0000 H 0 0 0 0 0 0 0 0 0 0 9  
2.3827 -0.2851 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10  
1.4162 1.8440 0.0000 H 0 0 0 0 0 0 0 0 0 0 11  
2 1 0 0 0 0  
6 1 0 0 0 0  
7 1 0 0 0 0  
3 2 0 0 0 0  
8 2 0 0 0 0  
4 3 0 0 0 0  
9 3 0 0 0 0  
5 4 0 0 0 0  
6 5 0 0 0 0  
10 5 0 0 0 0  
4 11 0 0 0 0
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M END  
$$$$  
pyrrole-cation0.sdf  
COSMOTHERM 3D 0  
11 11 0 0 0 0 0 0 0 0 0 V2000  
-0.7253 1.0037 0.0000 C 0 0 0 0 0 0 0 0 0 0 1  
0.7402 0.9928 0.0000 C 0 0 0 0 0 0 0 0 0 0 2  
-1.1784 -0.2604 0.0000 C 0 0 0 0 0 0 0 0 0 0 3  
-0.0087 -1.1603 0.0000 N 0 0 0 0 0 0 0 0 0 0 4  
1.1744 -0.2781 0.0000 C 0 0 0 0 0 0 0 0 0 0 5  
-1.3458 1.8956 0.0001 H 0 0 0 0 0 0 0 0 0 0 6  
1.3740 1.8752 -0.0001 H 0 0 0 0 0 0 0 0 0 0 7  
-2.1671 -0.7054 0.0001 H 0 0 0 0 0 0 0 0 0 0 8  
-0.0134 -1.7885 -0.8228 H 0 0 0 0 0 0 0 0 0 0 9  
2.1564 -0.7379 -0.0001 H 0 0 0 0 0 0 0 0 0 0 10  
-0.0133 -1.7886 0.8228 H 0 0 0 0 0 0 0 0 0 0 11  
2 1 0 0 0 0  
3 1 0 0 0 0  
6 1 0 0 0 0  
5 2 0 0 0 0  
7 2 0 0 0 0  
4 3 0 0 0 0  
8 3 0 0 0 0  
5 4 0 0 0 0  
9 4 0 0 0 0  
10 5 0 0 0 0  
4 11 0 0 0 0
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M END  
$$$$  
pyrrole-cation1.sdf  
COSMOTHERM 3D 0  
11 11 0 0 0 0 0 0 0 0 0 V2000  
0.6758 0.0000 1.0240 C 0 0 0 0 0 0 0 0 0 0 1  
-0.6860 0.0000 1.0408 C 0 0 0 0 0 0 0 0 0 0 2  
1.1485 0.0000 -0.3821 C 0 0 0 0 0 0 0 0 0 0 3  
-0.0964 0.0000 -1.1364 N 0 0 0 0 0 0 0 0 0 0 4  
-1.1277 0.0000 -0.3272 C 0 0 0 0 0 0 0 0 0 0 5  
-0.1477 0.0000 -2.1547 H 0 0 0 0 0 0 0 0 0 0 6  
1.3497 -0.0001 1.8772 H 0 0 0 0 0 0 0 0 0 0 7  
-1.3478 0.0000 1.9014 H 0 0 0 0 0 0 0 0 0 0 8  
-2.1472 -0.0002 -0.7087 H 0 0 0 0 0 0 0 0 0 0 9  
1.7534 -0.8866 -0.6379 H 0 0 0 0 0 0 0 0 0 0 10  
1.7535 0.8863 -0.6382 H 0 0 0 0 0 0 0 0 0 0 11  
2 1 0 0 0 0  
3 1 0 0 0 0  
7 1 0 0 0 0  
5 2 0 0 0 0  
8 2 0 0 0 0  
4 3 0 0 0 0  
10 3 0 0 0 0  
5 4 0 0 0 0  
6 4 0 0 0 0  
9 5 0 0 0 0  
3 11 0 0 0 0
```

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M END  
$$$$  
pyrrole-cation2.sdf  
COSMOTHERM 3D 0  
11 11 0 0 0 0 0 0 0 0 0 V2000  
1.0729 0.6260 0.0000 C 0 0 0 0 0 0 0 0 0 0 1  
-0.3101 1.1955 0.0000 C 0 0 0 0 0 0 0 0 0 0 2  
0.8423 -0.8313 0.0000 C 0 0 0 0 0 0 0 0 0 0 3
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2
3      -0.4462  -1.0429  0.0000 N  0  0  0  0  0  0  0  0  0  0  4
4      -1.1876  0.1728  0.0000 C  0  0  0  0  0  0  0  0  0  0  5
5       1.6792  0.9284  -0.8742 H  0  0  0  0  0  0  0  0  0  0  6
6       1.6795  0.9285  0.8740 H  0  0  0  0  0  0  0  0  0  0  7
7      -0.8798  -1.9693  -0.0001 H  0  0  0  0  0  0  0  0  0  0  8
8      -0.5474  2.2546  0.0000 H  0  0  0  0  0  0  0  0  0  0  9
9       1.5657  -1.6427  0.0002 H  0  0  0  0  0  0  0  0  0  0 10
10      -2.2717  0.1347  -0.0001 H  0  0  0  0  0  0  0  0  0  0 11
11
12      2  1  0  0  0  0
13      3  1  0  0  0  0
14      6  1  0  0  0  0
15      7  1  0  0  0  0
16      5  2  0  0  0  0
17      9  2  0  0  0  0
18      4  3  0  0  0  0
19     10  3  0  0  0  0
20      5  4  0  0  0  0
21      8  4  0  0  0  0
22     5 11  0  0  0  0
23
24 M  END
25 $$$
26 pyrrole.sdf
27 COSMOTHERM      3D      0
28
29 10 10 0 0 0 0 0 0 0 0 0 0 V2000
30 -0.9895  -0.7145  0.0000 C  0  0  0  0  0  0  0  0  0  0  1
31 -0.9895  0.7146  0.0000 C  0  0  0  0  0  0  0  0  0  0  2
32  0.3351  1.1286  0.0000 C  0  0  0  0  0  0  0  0  0  0  3
33  1.1240  0.0000  0.0000 N  0  0  0  0  0  0  0  0  0  0  4
34  0.3351  -1.1286  0.0000 C  0  0  0  0  0  0  0  0  0  0  5
35 -1.8588  -1.3668  0.0000 H  0  0  0  0  0  0  0  0  0  0  6
36 -1.8588  1.3669  0.0000 H  0  0  0  0  0  0  0  0  0  0  7
37  0.7775  2.1198  0.0000 H  0  0  0  0  0  0  0  0  0  0  8
38  2.1396  -0.0001  -0.0001 H  0  0  0  0  0  0  0  0  0  0  9
39  0.7774  -2.1198  0.0000 H  0  0  0  0  0  0  0  0  0  0 10
40
41      2  1  0  0  0  0
42      5  1  0  0  0  0
43      6  1  0  0  0  0
44      3  2  0  0  0  0
45      7  2  0  0  0  0
46      4  3  0  0  0  0
47      8  3  0  0  0  0
48      5  4  0  0  0  0
49      9  4  0  0  0  0
50     5 10  0  0  0  0
51
52 M  END
53 $$$
54 quinoline.sdf
55 COSMOTHERM      3D      0
56
57 17 18 0 0 0 0 0 0 0 0 0 0 V2000
58  0.0244  -0.6934  -0.0001 C  0  0  0  0  0  0  0  0  0  0  1
59  1.1994  -1.4043  0.0000 N  0  0  0  0  0  0  0  0  0  0  2
60  2.3361  -0.7179  0.0001 C  0  0  0  0  0  0  0  0  0  0  3
61  2.4131  0.6978  0.0000 C  0  0  0  0  0  0  0  0  0  0  4
62  1.2426  1.4273  -0.0001 C  0  0  0  0  0  0  0  0  0  0  5
63 -0.0024  0.7446  0.0000 C  0  0  0  0  0  0  0  0  0  0  6
64 -1.2057  -1.4049  -0.0001 C  0  0  0  0  0  0  0  0  0  0  7
65 -2.4084  -0.7235  0.0000 C  0  0  0  0  0  0  0  0  0  0  8
66 -2.4351  0.6951  0.0001 C  0  0  0  0  0  0  0  0  0  0  9
67 -1.2559  1.4156  0.0001 C  0  0  0  0  0  0  0  0  0  0 10
68  3.2575  -1.3082  0.0003 H  0  0  0  0  0  0  0  0  0  0 11
69  3.3880  1.1866  0.0000 H  0  0  0  0  0  0  0  0  0  0 12
70  1.2580  2.5195  -0.0002 H  0  0  0  0  0  0  0  0  0  0 13
71 -1.1709  -2.4959  -0.0001 H  0  0  0  0  0  0  0  0  0  0 14
72 -3.3482  -1.2785  -0.0001 H  0  0  0  0  0  0  0  0  0  0 15
73 -3.3942  1.2157  0.0002 H  0  0  0  0  0  0  0  0  0  0 16
74 -1.2705  2.5079  0.0001 H  0  0  0  0  0  0  0  0  0  0 17
75
76      2  1  0  0  0  0
77      6  1  0  0  0  0
78      7  1  0  0  0  0
79      3  2  0  0  0  0
80      4  3  0  0  0  0
81     11  3  0  0  0  0
82      5  4  0  0  0  0
83     12  4  0  0  0  0
84      6  5  0  0  0  0
85     13  5  0  0  0  0
86     10  6  0  0  0  0
87      8  7  0  0  0  0
88     14  7  0  0  0  0
89      9  8  0  0  0  0
90     15  8  0  0  0  0
91     10  9  0  0  0  0
92     16  9  0  0  0  0
93     10 17  0  0  0  0
94
95 M  END
96 $$$
97 quinoline_pl.sdf
98 COSMOTHERM      3D      0
99
100 18 19 0 0 0 0 0 0 0 0 0 0 V2000
101 -1.4219  -1.2739  0.0003 C  0  0  0  0  0  0  0  0  0  0  1
102 -0.6955  -2.4478  0.0000 C  0  0  0  0  0  0  0  0  0  0  2
103  0.7222  -2.4193  -0.0002 C  0  0  0  0  0  0  0  0  0  0  3
104  1.4124  -1.2207  -0.0002 C  0  0  0  0  0  0  0  0  0  0  4
105  0.6782  -0.0185  0.0002 C  0  0  0  0  0  0  0  0  0  0  5
106 -0.7525  -0.0208  0.0002 C  0  0  0  0  0  0  0  0  0  0  6
107 -1.4294  1.2233  -0.0002 C  0  0  0  0  0  0  0  0  0  0  7
108 -0.7213  2.4140  -0.0003 C  0  0  0  0  0  0  0  0  0  0  8
109  0.6766  2.3763  0.0000 C  0  0  0  0  0  0  0  0  0  0  9
110  1.3166  1.2013  0.0003 N  0  0  0  0  0  0  0  0  0  0 10
111 -2.5125  -1.2872  0.0003 H  0  0  0  0  0  0  0  0  0  0 11
112 -1.2113  -3.4084  0.0000 H  0  0  0  0  0  0  0  0  0  0 12
113  1.2777  -3.3577  -0.0006 H  0  0  0  0  0  0  0  0  0  0 13

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1
2
3 2.5029 -1.1936 -0.0005 H 0 0 0 0 0 0 0 0 0 14
4 -2.5206 1.2333 -0.0005 H 0 0 0 0 0 0 0 0 0 15
5 -1.2250 3.3783 -0.0006 H 0 0 0 0 0 0 0 0 0 16
6 1.3006 3.2674 0.0000 H 0 0 0 0 0 0 0 0 0 17
7 2.3395 1.2050 0.0004 H 0 0 0 0 0 0 0 0 0 18
8
9 2 1 0 0 0 0
10 6 1 0 0 0 0
11 11 1 0 0 0 0
12 3 2 0 0 0 0
13 12 2 0 0 0 0
14 4 3 0 0 0 0
15 13 3 0 0 0 0
16 5 4 0 0 0 0
17 14 4 0 0 0 0
18 6 5 0 0 0 0
19 10 5 0 0 0 0
20 7 6 0 0 0 0
21 8 7 0 0 0 0
22 15 7 0 0 0 0
23 9 8 0 0 0 0
24 16 8 0 0 0 0
25 10 9 0 0 0 0
26 17 9 0 0 0 0
27 10 18 0 0 0 0
28 M END
29 \$\$\$
30 sec-butylamine-cation.sdf
31 COSMOTHERM 3D 0
32
33 17 16 0 0 0 0 0 0 0 0 0 0 V2000
34 0.4666 0.0762 0.3399 C 0 0 0 0 0 0 0 0 0 1
35 1.7549 0.8090 -0.0110 C 0 0 0 0 0 0 0 0 0 2
36 0.5951 -1.3689 -0.1180 N 0 0 0 0 0 0 0 0 0 3
37 -0.7844 0.6996 -0.2826 C 0 0 0 0 0 0 0 0 0 4
38 -2.1013 0.0227 0.1126 C 0 0 0 0 0 0 0 0 0 5
39 1.3881 -1.8400 0.3364 H 0 0 0 0 0 0 0 0 0 6
40 -0.2461 -1.9190 0.1015 H 0 0 0 0 0 0 0 0 0 7
41 0.3493 0.0108 1.4304 H 0 0 0 0 0 0 0 0 0 8
42 2.6315 0.3216 0.4386 H 0 0 0 0 0 0 0 0 0 9
43 1.7025 1.8346 0.3759 H 0 0 0 0 0 0 0 0 0 10
44 1.8977 0.8605 -1.1007 H 0 0 0 0 0 0 0 0 0 11
45 -0.7984 1.7505 0.0425 H 0 0 0 0 0 0 0 0 0 12
46 -0.6714 0.7169 -1.3796 H 0 0 0 0 0 0 0 0 0 13
47 -2.9544 0.5850 -0.2908 H 0 0 0 0 0 0 0 0 0 14
48 -2.1847 -1.0022 -0.2812 H 0 0 0 0 0 0 0 0 0 15
49 -2.2138 -0.0213 1.2063 H 0 0 0 0 0 0 0 0 0 16
50 0.7464 -1.4300 -1.1345 H 0 0 0 0 0 0 0 0 0 17
51
52 2 1 0 0 0 0
53 3 1 0 0 0 0
54 4 1 0 0 0 0
55 8 1 0 0 0 0
56 9 2 0 0 0 0
57 10 2 0 0 0 0
58 11 2 0 0 0 0
59 6 3 0 0 0 0
60 7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
3 17 0 0 0 0
M END
\$\$\$
sec-butylamine.sdf
COSMOTHERM 3D 0
16 15 0 0 0 0 0 0 0 0 V2000
0.4785 0.0085 0.3293 C 0 0 0 0 0 0 0 0 0 1
1.7562 0.7776 -0.0113 C 0 0 0 0 0 0 0 0 0 2
0.5980 -1.3732 -0.1943 N 0 0 0 0 0 0 0 0 0 3
-0.7620 0.6916 -0.2647 C 0 0 0 0 0 0 0 0 0 4
-2.0912 0.0231 0.1055 C 0 0 0 0 0 0 0 0 0 5
1.4078 -1.8264 0.2401 H 0 0 0 0 0 0 0 0 0 6
-0.2109 -1.9263 0.1035 H 0 0 0 0 0 0 0 0 0 7
0.3613 0.0102 1.4340 H 0 0 0 0 0 0 0 0 0 8
2.6417 0.2851 0.4196 H 0 0 0 0 0 0 0 0 0 9
1.7133 1.8018 0.3870 H 0 0 0 0 0 0 0 0 0 10
1.8933 0.8334 -1.1028 H 0 0 0 0 0 0 0 0 0 11
-0.7716 1.7370 0.0852 H 0 0 0 0 0 0 0 0 0 12
-0.6505 0.7249 -1.3625 H 0 0 0 0 0 0 0 0 0 13
-2.9442 0.6047 -0.2741 H 0 0 0 0 0 0 0 0 0 14
-2.1758 -0.9886 -0.3199 H 0 0 0 0 0 0 0 0 0 15
-2.2033 -0.0584 1.1984 H 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
4 1 0 0 0 0
8 1 0 0 0 0
9 2 0 0 0 0
10 2 0 0 0 0
11 2 0 0 0 0
6 3 0 0 0 0
7 3 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 5 0 0 0 0
15 5 0 0 0 0
5 16 0 0 0 0
M END
\$\$\$
tert-butylamine-cation.sdf
COSMOTHERM 3D 0

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2
3 2.3844 1.3664 1.3815 H 0 0 0 0 0 0 0 0 0 0 0 29
4 3.0388 2.2231 -0.0195 H 0 0 0 0 0 0 0 0 0 0 0 30
5 1.2834 1.2641 -1.4910 H 0 0 0 0 0 0 0 0 0 0 0 31
6 0.5396 2.1042 -0.1136 H 0 0 0 0 0 0 0 0 0 0 0 32
7 -0.9769 -1.0473 -1.2319 H 0 0 0 0 0 0 0 0 0 0 0 33
8 2 1 0 0 0 0 0
9 6 1 0 0 0 0 0
10 12 1 0 0 0 0 0
11 3 2 0 0 0 0 0
12 4 2 0 0 0 0 0
13 5 2 0 0 0 0 0
14 13 3 0 0 0 0 0
15 14 3 0 0 0 0 0
16 15 3 0 0 0 0 0
17 16 4 0 0 0 0 0
18 17 4 0 0 0 0 0
19 18 4 0 0 0 0 0
20 19 5 0 0 0 0 0
21 20 5 0 0 0 0 0
22 21 5 0 0 0 0 0
23 7 6 0 0 0 0 0
24 11 6 0 0 0 0 0
25 22 6 0 0 0 0 0
26 8 7 0 0 0 0 0
27 23 7 0 0 0 0 0
28 24 7 0 0 0 0 0
29 9 8 0 0 0 0 0
30 25 8 0 0 0 0 0
31 26 8 0 0 0 0 0
32 10 9 0 0 0 0 0
33 27 9 0 0 0 0 0
34 28 9 0 0 0 0 0
35 11 10 0 0 0 0 0
36 29 10 0 0 0 0 0
37 30 10 0 0 0 0 0
38 31 11 0 0 0 0 0
39 32 11 0 0 0 0 0
40 1 33 0 0 0 0 0
41 M END
42 \$\$\$\$
43 tert-butylcyclohexylamine.sdf
44 COSMOTHERM 3D 0
45
46 32 32 0 0 0 0 0 0 0 0 0 0 V2000
47 -0.9160 0.7367 -0.1926 N 0 0 0 0 0 0 0 0 0 0 0 1
48 -2.1679 -0.0504 0.0069 C 0 0 0 0 0 0 0 0 0 0 0 2
49 -2.3372 -1.1680 -1.0486 C 0 0 0 0 0 0 0 0 0 0 0 3
50 -3.3283 0.9497 -0.1289 C 0 0 0 0 0 0 0 0 0 0 0 4
51 -2.1850 -0.6607 1.4174 C 0 0 0 0 0 0 0 0 0 0 0 5
52 0.3826 0.0281 -0.0908 C 0 0 0 0 0 0 0 0 0 0 0 6
53 1.2667 0.3521 -1.3079 C 0 0 0 0 0 0 0 0 0 0 0 7
54 2.6518 -0.3077 -1.2191 C 0 0 0 0 0 0 0 0 0 0 0 8
55 3.3698 0.0511 0.0901 C 0 0 0 0 0 0 0 0 0 0 0 9
56 2.4949 -0.2794 1.3085 C 0 0 0 0 0 0 0 0 0 0 0 10
57 1.1211 0.4019 1.2090 C 0 0 0 0 0 0 0 0 0 0 0 11
58 -0.9781 1.1584 -1.1245 H 0 0 0 0 0 0 0 0 0 0 0 12
59 -3.2712 -1.7272 -0.8852 H 0 0 0 0 0 0 0 0 0 0 0 13
60 -1.5071 -1.8893 -1.0079 H 0 0 0 0 0 0 0 0 0 0 0 14
-2.3695 -0.7385 -2.0619 H 0 0 0 0 0 0 0 0 0 0 0 15
-3.2525 1.7354 0.6375 H 0 0 0 0 0 0 0 0 0 0 0 16
-3.3145 1.4324 -1.1192 H 0 0 0 0 0 0 0 0 0 0 0 17
-4.2971 0.4412 -0.0151 H 0 0 0 0 0 0 0 0 0 0 0 18
-3.1389 -1.1805 1.5902 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.0717 0.1227 2.1811 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.3772 -1.3947 1.5533 H 0 0 0 0 0 0 0 0 0 0 0 21
0.2205 -1.0674 -0.0841 H 0 0 0 0 0 0 0 0 0 0 0 22
1.3854 1.4498 -1.3691 H 0 0 0 0 0 0 0 0 0 0 0 23
0.7518 0.0338 -2.2298 H 0 0 0 0 0 0 0 0 0 0 0 24
2.5328 -1.4040 -1.2779 H 0 0 0 0 0 0 0 0 0 0 0 25
3.2633 -0.0121 -2.0867 H 0 0 0 0 0 0 0 0 0 0 0 26
3.6015 1.1313 0.0937 H 0 0 0 0 0 0 0 0 0 0 0 27
4.3331 -0.4797 0.1528 H 0 0 0 0 0 0 0 0 0 0 0 28
2.3574 -1.3739 1.3704 H 0 0 0 0 0 0 0 0 0 0 0 29
3.0008 0.0251 2.2388 H 0 0 0 0 0 0 0 0 0 0 0 30
1.2475 1.4989 1.2234 H 0 0 0 0 0 0 0 0 0 0 0 31
0.4972 0.1437 2.0785 H 0 0 0 0 0 0 0 0 0 0 0 32
2 1 0 0 0 0 0
6 1 0 0 0 0 0
12 1 0 0 0 0 0
3 2 0 0 0 0 0
4 2 0 0 0 0 0
5 2 0 0 0 0 0
13 3 0 0 0 0 0
14 3 0 0 0 0 0
15 3 0 0 0 0 0
16 4 0 0 0 0 0
17 4 0 0 0 0 0
18 4 0 0 0 0 0
19 5 0 0 0 0 0
20 5 0 0 0 0 0
21 5 0 0 0 0 0
7 6 0 0 0 0 0
11 6 0 0 0 0 0
22 6 0 0 0 0 0
8 7 0 0 0 0 0
23 7 0 0 0 0 0
24 7 0 0 0 0 0
9 8 0 0 0 0 0
25 8 0 0 0 0 0
26 8 0 0 0 0 0
10 9 0 0 0 0 0
27 9 0 0 0 0 0
28 9 0 0 0 0 0
11 10 0 0 0 0 0
29 10 0 0 0 0 0

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30 10 0 0 0 0
31 11 0 0 0 0
11 32 0 0 0 0

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M END

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tetrahydrozoline-cation2.sdf

COSMOtherm 3D

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32 34 0 0 0 0 0 0 0 0 0 V2000
  3.0694 -0.1025 1.8534 C 0 0 0 0 0 0 0 0 0 0 0 1
  1.8934 0.4494 2.3770 C 0 0 0 0 0 0 0 0 0 0 0 2
  0.8030 0.6650 1.5338 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.8571 0.3274 0.1688 C 0 0 0 0 0 0 0 0 0 0 0 4
  2.0450 -0.2126 -0.3655 C 0 0 0 0 0 0 0 0 0 0 0 5
  3.1374 -0.4210 0.4965 C 0 0 0 0 0 0 0 0 0 0 0 6
 -0.3517 0.6267 -0.7219 C 0 0 0 0 0 0 0 0 0 0 0 7
 -0.2533 -0.0070 -2.1376 C 0 0 0 0 0 0 0 0 0 0 0 8
  1.1541 0.1817 -2.7044 C 0 0 0 0 0 0 0 0 0 0 0 9
  2.1724 -0.5603 -1.8354 C 0 0 0 0 0 0 0 0 0 0 0 10
 -1.6462 0.1946 -0.0978 C 0 0 0 0 0 0 0 0 0 0 0 11
 -3.2183 -1.0660 1.0572 C 0 0 0 0 0 0 0 0 0 0 0 12
 -1.8425 -0.9620 0.5267 N 0 0 0 0 0 0 0 0 0 0 0 13
 -2.7730 0.8919 -0.1682 N 0 0 0 0 0 0 0 0 0 0 0 14
 -3.9225 0.1239 0.3550 C 0 0 0 0 0 0 0 0 0 0 0 15
 -1.0827 -1.5723 0.8151 H 0 0 0 0 0 0 0 0 0 0 0 16
  3.9327 -0.2733 2.4992 H 0 0 0 0 0 0 0 0 0 0 0 17
  1.8289 0.7173 3.4328 H 0 0 0 0 0 0 0 0 0 0 0 18
 -0.1080 1.1089 1.9437 H 0 0 0 0 0 0 0 0 0 0 0 19
  4.0602 -0.8364 0.0837 H 0 0 0 0 0 0 0 0 0 0 0 20
 -0.4192 1.7198 -0.8492 H 0 0 0 0 0 0 0 0 0 0 0 21
 -0.4802 -1.0834 -2.0775 H 0 0 0 0 0 0 0 0 0 0 0 22
 -1.0116 0.4518 -2.7874 H 0 0 0 0 0 0 0 0 0 0 0 23
  1.4003 1.2558 -2.7454 H 0 0 0 0 0 0 0 0 0 0 0 24
  1.1893 -0.1966 -3.7364 H 0 0 0 0 0 0 0 0 0 0 0 25
  2.0298 -1.6486 -1.9611 H 0 0 0 0 0 0 0 0 0 0 0 26
  3.1993 -0.3478 -2.1694 H 0 0 0 0 0 0 0 0 0 0 0 27
 -3.6613 -2.0327 0.7962 H 0 0 0 0 0 0 0 0 0 0 0 28
 -3.2014 -0.9579 2.1502 H 0 0 0 0 0 0 0 0 0 0 0 29
 -4.5144 0.7355 1.0438 H 0 0 0 0 0 0 0 0 0 0 0 30
 -4.5573 -0.2013 -0.4804 H 0 0 0 0 0 0 0 0 0 0 0 31
 -2.8641 1.7593 -0.6899 H 0 0 0 0 0 0 0 0 0 0 0 32

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  2 1 0 0 0 0
  6 1 0 0 0 0
 17 1 0 0 0 0
  3 2 0 0 0 0
 18 2 0 0 0 0
  4 3 0 0 0 0
 19 3 0 0 0 0
  5 4 0 0 0 0
  7 4 0 0 0 0
  6 5 0 0 0 0
 10 5 0 0 0 0
 20 6 0 0 0 0
  8 7 0 0 0 0
 11 7 0 0 0 0
 21 7 0 0 0 0
  9 8 0 0 0 0
 22 8 0 0 0 0
 23 8 0 0 0 0
 10 9 0 0 0 0
 24 9 0 0 0 0
 25 9 0 0 0 0
 26 10 0 0 0 0
 27 10 0 0 0 0
 13 11 0 0 0 0
 14 11 0 0 0 0
 13 12 0 0 0 0
 15 12 0 0 0 0
 28 12 0 0 0 0
 29 12 0 0 0 0
 16 13 0 0 0 0
 15 14 0 0 0 0
 30 15 0 0 0 0
 31 15 0 0 0 0
 14 32 0 0 0 0

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M END

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tetrahydrozoline-cation3.sdf

COSMOtherm 3D

0

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32 34 0 0 0 0 0 0 0 0 0 V2000
  3.0626 -0.1063 1.8598 C 0 0 0 0 0 0 0 0 0 0 0 1
  1.8861 0.4472 2.3804 C 0 0 0 0 0 0 0 0 0 0 0 2
  0.7984 0.6652 1.5343 C 0 0 0 0 0 0 0 0 0 0 0 3
  0.8562 0.3285 0.1692 C 0 0 0 0 0 0 0 0 0 0 0 4
  2.0447 -0.2127 -0.3623 C 0 0 0 0 0 0 0 0 0 0 0 5
  3.1339 -0.4245 0.5030 C 0 0 0 0 0 0 0 0 0 0 0 6
 -0.3508 0.6299 -0.7237 C 0 0 0 0 0 0 0 0 0 0 0 7
 -0.2487 -0.0005 -2.1405 C 0 0 0 0 0 0 0 0 0 0 0 8
  1.1607 0.1875 -2.7025 C 0 0 0 0 0 0 0 0 0 0 0 9
  2.1754 -0.5583 -1.8324 C 0 0 0 0 0 0 0 0 0 0 0 10
 -1.6453 0.1947 -0.1014 C 0 0 0 0 0 0 0 0 0 0 0 11
 -3.2195 -1.0820 1.0341 C 0 0 0 0 0 0 0 0 0 0 0 12
 -1.8452 -0.9730 0.5012 N 0 0 0 0 0 0 0 0 0 0 0 13
 -2.7673 0.9010 -0.1495 N 0 0 0 0 0 0 0 0 0 0 0 14
 -3.9185 0.1327 0.3693 C 0 0 0 0 0 0 0 0 0 0 0 15
 -1.0885 -1.5967 0.7685 H 0 0 0 0 0 0 0 0 0 0 0 16
  3.9234 -0.2799 2.5081 H 0 0 0 0 0 0 0 0 0 0 0 17
  1.8190 0.7144 3.4362 H 0 0 0 0 0 0 0 0 0 0 0 18
 -0.1135 1.1094 1.9419 H 0 0 0 0 0 0 0 0 0 0 0 19
  4.0573 -0.8407 0.0925 H 0 0 0 0 0 0 0 0 0 0 0 20
 -0.4184 1.7232 -0.8480 H 0 0 0 0 0 0 0 0 0 0 0 21
 -0.4772 -1.0768 -2.0840 H 0 0 0 0 0 0 0 0 0 0 0 22
 -1.0046 0.4607 -2.7915 H 0 0 0 0 0 0 0 0 0 0 0 23
  1.4087 1.2612 -2.7402 H 0 0 0 0 0 0 0 0 0 0 0 24

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2
3 1.1984 -0.1884 -3.7353 H 0 0 0 0 0 0 0 0 0 0 25
4 2.0308 -1.6461 -1.9604 H 0 0 0 0 0 0 0 0 0 0 26
5 3.2035 -0.3471 -2.1633 H 0 0 0 0 0 0 0 0 0 0 27
6 -3.6704 -2.0376 0.7468 H 0 0 0 0 0 0 0 0 0 0 28
7 -3.1979 -1.0060 2.1297 H 0 0 0 0 0 0 0 0 0 0 29
8 -4.4947 0.7338 1.0803 H 0 0 0 0 0 0 0 0 0 0 30
9 -4.5674 -0.1647 -0.4654 H 0 0 0 0 0 0 0 0 0 0 31
10 -2.8551 1.7812 -0.6497 H 0 0 0 0 0 0 0 0 0 0 32
11 2 1 0 0 0 0
12 6 1 0 0 0 0
13 17 1 0 0 0 0
14 3 2 0 0 0 0
15 18 2 0 0 0 0
16 4 3 0 0 0 0
17 19 3 0 0 0 0
18 5 4 0 0 0 0
19 7 4 0 0 0 0
20 6 5 0 0 0 0
21 10 5 0 0 0 0
22 20 6 0 0 0 0
23 8 7 0 0 0 0
24 11 7 0 0 0 0
25 21 7 0 0 0 0
26 9 8 0 0 0 0
27 22 8 0 0 0 0
28 23 8 0 0 0 0
29 10 9 0 0 0 0
30 24 9 0 0 0 0
31 25 9 0 0 0 0
32 26 10 0 0 0 0
33 27 10 0 0 0 0
34 13 11 0 0 0 0
35 14 11 0 0 0 0
36 13 12 0 0 0 0
37 15 12 0 0 0 0
38 28 12 0 0 0 0
39 29 12 0 0 0 0
40 16 13 0 0 0 0
41 15 14 0 0 0 0
42 30 15 0 0 0 0
43 31 15 0 0 0 0
44 14 32 0 0 0 0
45 M END
46 \$\$\$
47 tetrahydrozoline.sdf
48 COSMOTHERM 3D 0
49
50 31 33 0 0 0 0 0 0 0 0 0 0 V2000
51 -0.6581 1.5436 0.9871 N 0 0 0 0 0 0 0 0 0 0 1
52 -1.1160 2.9269 1.2888 C 0 0 0 0 0 0 0 0 0 0 2
53 -0.5134 3.8181 0.1762 C 0 0 0 0 0 0 0 0 0 0 3
54 -0.2837 2.8047 -0.8737 N 0 0 0 0 0 0 0 0 0 0 4
55 0.6122 -1.8403 0.2494 C 0 0 0 0 0 0 0 0 0 0 5
56 -0.1730 -0.9394 -0.4968 C 0 0 0 0 0 0 0 0 0 0 6
57 0.3772 0.3952 -0.9835 C 0 0 0 0 0 0 0 0 0 0 7
58 1.9265 0.4391 -0.9401 C 0 0 0 0 0 0 0 0 0 0 8
59 2.4502 -0.0787 0.4017 C 0 0 0 0 0 0 0 0 0 0 9
60 2.0639 -1.5496 0.5855 C 0 0 0 0 0 0 0 0 0 0 10
-0.2048 1.5729 -0.2262 C 0 0 0 0 0 0 0 0 0 0 11
0.0388 -3.0589 0.6611 C 0 0 0 0 0 0 0 0 0 0 12
-1.2787 -3.3909 0.3426 C 0 0 0 0 0 0 0 0 0 0 13
-2.0548 -2.4965 -0.4078 C 0 0 0 0 0 0 0 0 0 0 14
-1.4981 -1.2847 -0.8182 C 0 0 0 0 0 0 0 0 0 0 15
-0.8024 3.2316 2.2960 H 0 0 0 0 0 0 0 0 0 0 16
-2.2196 2.9501 1.2629 H 0 0 0 0 0 0 0 0 0 0 17
0.4371 4.2821 0.4919 H 0 0 0 0 0 0 0 0 0 0 18
-1.1957 4.6063 -0.1668 H 0 0 0 0 0 0 0 0 0 0 19
0.3949 3.0124 -1.6050 H 0 0 0 0 0 0 0 0 0 0 20
0.0647 0.5242 -2.0337 H 0 0 0 0 0 0 0 0 0 0 21
2.2781 1.4637 -1.1341 H 0 0 0 0 0 0 0 0 0 0 22
2.3164 -0.1900 -1.7571 H 0 0 0 0 0 0 0 0 0 0 23
2.0239 0.5271 1.2182 H 0 0 0 0 0 0 0 0 0 0 24
3.5438 0.0316 0.4552 H 0 0 0 0 0 0 0 0 0 0 25
2.2739 -1.8812 1.6146 H 0 0 0 0 0 0 0 0 0 0 26
2.7017 -2.1732 -0.0671 H 0 0 0 0 0 0 0 0 0 0 27
0.6467 -3.7575 1.2427 H 0 0 0 0 0 0 0 0 0 0 28
-1.6990 -4.3427 0.6739 H 0 0 0 0 0 0 0 0 0 0 29
-3.0850 -2.7444 -0.6708 H 0 0 0 0 0 0 0 0 0 0 30
-2.1004 -0.5848 -1.4041 H 0 0 0 0 0 0 0 0 0 0 31
2 1 0 0 0 0
11 1 0 0 0 0
3 2 0 0 0 0
16 2 0 0 0 0
17 2 0 0 0 0
4 3 0 0 0 0
18 3 0 0 0 0
19 3 0 0 0 0
11 4 0 0 0 0
20 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
24 9 0 0 0 0
25 9 0 0 0 0
26 10 0 0 0 0
27 10 0 0 0 0


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2
3 21 7 0 0 0 0
4 22 7 0 0 0 0
5 23 8 0 0 0 0
6 24 8 0 0 0 0
7 25 8 0 0 0 0
8 26 16 0 0 0 0
9 27 16 0 0 0 0
10 28 16 0 0 0 0
11 29 22 0 0 0 0
12 30 22 0 0 0 0
13 31 22 0 0 0 0
14 3 32 0 0 0 0
15 M END
16 $$$$
17 tri-n-propylamine.sdf
18 COSMOTHERM 3D 0
19
20 31 30 0 0 0 0 0 0 0 0 V2000
21 2.5169 0.6977 -0.4412 C 0 0 0 0 0 0 0 0 0 0 1
22 1.2164 0.9080 -0.3413 C 0 0 0 0 0 0 0 0 0 0 2
23 0.0041 0.4473 -0.3581 N 0 0 0 0 0 0 0 0 0 0 3
24 -1.2046 0.9202 0.3396 C 0 0 0 0 0 0 0 0 0 0 4
25 -2.5076 0.7095 -0.4384 C 0 0 0 0 0 0 0 0 0 0 5
26 -0.0030 -1.0005 -0.6487 C 0 0 0 0 0 0 0 0 0 0 6
27 -0.0165 -1.9733 0.5472 C 0 0 0 0 0 0 0 0 0 0 7
28 3.7084 1.3811 0.2407 C 0 0 0 0 0 0 0 0 0 0 8
29 2.7318 -0.3774 -0.5472 H 0 0 0 0 0 0 0 0 0 0 9
30 2.3849 1.0966 -1.4606 H 0 0 0 0 0 0 0 0 0 0 10
31 1.0874 1.9896 0.5142 H 0 0 0 0 0 0 0 0 0 0 11
32 1.3208 0.4467 1.3491 H 0 0 0 0 0 0 0 0 0 0 12
33 -1.0696 2.0024 0.5033 H 0 0 0 0 0 0 0 0 0 0 13
34 -1.3095 0.4676 1.3514 H 0 0 0 0 0 0 0 0 0 0 14
35 -2.7294 -0.3653 -0.5320 H 0 0 0 0 0 0 0 0 0 0 15
36 -3.6935 1.4080 0.2379 C 0 0 0 0 0 0 0 0 0 0 16
37 -2.3751 1.0962 -1.4625 H 0 0 0 0 0 0 0 0 0 0 17
38 0.8766 -1.2189 -1.2740 H 0 0 0 0 0 0 0 0 0 0 18
39 -0.8775 -1.2083 -1.2847 H 0 0 0 0 0 0 0 0 0 0 19
40 -0.9031 -1.7856 1.1739 H 0 0 0 0 0 0 0 0 0 0 20
41 0.8624 -1.7942 1.1872 H 0 0 0 0 0 0 0 0 0 0 21
42 -0.0202 -3.4339 0.0808 C 0 0 0 0 0 0 0 0 0 0 22
43 4.6392 1.2074 -0.3184 H 0 0 0 0 0 0 0 0 0 0 23
44 3.5569 2.4694 0.3116 H 0 0 0 0 0 0 0 0 0 0 24
45 3.8565 0.9976 1.2624 H 0 0 0 0 0 0 0 0 0 0 25
46 -4.6268 1.2323 -0.3164 H 0 0 0 0 0 0 0 0 0 0 26
47 -3.5360 2.4963 0.2946 H 0 0 0 0 0 0 0 0 0 0 27
48 -3.8409 1.0383 1.2648 H 0 0 0 0 0 0 0 0 0 0 28
49 -0.0323 -4.1288 0.9335 H 0 0 0 0 0 0 0 0 0 0 29
50 0.8726 -3.6605 -0.5229 H 0 0 0 0 0 0 0 0 0 0 30
51 -0.9038 -3.6505 -0.5399 H 0 0 0 0 0 0 0 0 0 0 31
52
53 2 1 0 0 0 0
54 8 1 0 0 0 0
55 9 1 0 0 0 0
56 10 1 0 0 0 0
57 3 2 0 0 0 0
58 11 2 0 0 0 0
59 12 2 0 0 0 0
60 4 3 0 0 0 0
6 3 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
22 7 0 0 0 0
23 8 0 0 0 0
24 8 0 0 0 0
25 8 0 0 0 0
26 16 0 0 0 0
27 16 0 0 0 0
28 16 0 0 0 0
29 22 0 0 0 0
30 22 0 0 0 0
22 31 0 0 0 0
M END
$$$$
triethylamine-cation.sdf
COSMOTHERM 3D 0
23 22 0 0 0 0 0 0 0 0 V2000
2.5323 0.5836 -0.2812 C 0 0 0 0 0 0 0 0 0 0 1
1.2514 0.7976 0.5080 C 0 0 0 0 0 0 0 0 0 0 2
0.0029 0.3797 -0.2523 N 0 0 0 0 0 0 0 0 0 0 3
-1.2432 0.8082 0.5058 C 0 0 0 0 0 0 0 0 0 0 4
-2.5254 0.5967 -0.2821 C 0 0 0 0 0 0 0 0 0 0 5
-0.0028 -1.0861 -0.6666 C 0 0 0 0 0 0 0 0 0 0 6
-0.0150 -2.0607 0.4971 C 0 0 0 0 0 0 0 0 0 0 7
3.3592 1.0347 0.2837 H 0 0 0 0 0 0 0 0 0 0 8
2.7717 -0.4776 -0.4267 H 0 0 0 0 0 0 0 0 0 0 9
2.4878 1.0792 -1.2616 H 0 0 0 0 0 0 0 0 0 0 10
1.1072 1.8604 0.7366 H 0 0 0 0 0 0 0 0 0 0 11
1.2469 0.2423 1.4527 H 0 0 0 0 0 0 0 0 0 0 12
-1.0932 1.8715 0.7287 H 0 0 0 0 0 0 0 0 0 0 13
-1.2416 0.2578 1.4533 H 0 0 0 0 0 0 0 0 0 0 14
-3.3495 1.0564 0.2798 H 0 0 0 0 0 0 0 0 0 0 15
-2.7707 -0.4640 -0.4207 H 0 0 0 0 0 0 0 0 0 0 16
-2.4781 1.0857 -1.2657 H 0 0 0 0 0 0 0 0 0 0 17
0.8820 -1.2227 -1.2981 H 0 0 0 0 0 0 0 0 0 0 18
-0.8820 -1.2127 -1.3082 H 0 0 0 0 0 0 0 0 0 0 19
-0.0159 -3.0769 0.0803 H 0 0 0 0 0 0 0 0 0 0 20

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13 4 0 0 0 0
2 14 0 0 0 0
M END
$$$$
trimethylamine.sdf
COSMOtherm 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
0.7878 1.1467 -0.0906 C 0 0 0 0 0 0 0 0 0 0 0 0 1
0.0000 0.0000 0.3668 N 0 0 0 0 0 0 0 0 0 0 0 0 2
0.5992 -1.2556 -0.0906 C 0 0 0 0 0 0 0 0 0 0 0 0 3
-1.3871 0.1089 -0.0906 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.3467 2.0787 0.2909 H 0 0 0 0 0 0 0 0 0 0 0 0 5
1.8162 1.0688 0.2906 H 0 0 0 0 0 0 0 0 0 0 0 0 6
0.8350 1.2152 -1.2013 H 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0177 -2.1073 0.2905 H 0 0 0 0 0 0 0 0 0 0 0 0 8
1.6270 -1.3393 0.2908 H 0 0 0 0 0 0 0 0 0 0 0 0 9
0.6352 -1.3306 -1.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.9736 -0.7393 0.2908 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.8338 1.0385 0.2904 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.4700 0.1152 -1.2010 H 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
5 1 0 0 0 0
6 1 0 0 0 0
7 1 0 0 0 0
3 2 0 0 0 0
4 2 0 0 0 0
8 3 0 0 0 0
9 3 0 0 0 0
10 3 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
4 13 0 0 0 0
M END
$$$$

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S4 e) Mono-solvated Bases & Cations

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1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOtherm 3D 0
36 37 0 0 0 0 0 0 0 0 0 V2000
-3.6952 1.7533 -0.3767 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.8296 1.2610 -0.4899 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.5129 2.4029 0.3236 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.5794 -3.2399 1.7782 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.7270 -2.8586 0.0630 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.9816 -2.5173 -0.4357 C 0 0 0 0 0 0 0 0 0 0 0 0 6
3.2167 -1.2289 -0.9331 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.1913 -0.2898 -0.9046 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.9077 -0.6088 -0.4116 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.6730 -1.9257 0.0693 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.1425 0.4362 -0.4108 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.5751 -2.3205 0.6262 N 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.3749 0.2083 -0.7507 N 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.7290 -1.1397 -1.1920 C 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.7887 -2.0718 0.0135 C 0 0 0 0 0 0 0 0 0 0 0 0 15
0.2259 1.8250 -0.0195 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.3767 2.9240 -0.6610 C 0 0 0 0 0 0 0 0 0 0 0 0 17
1.1534 2.0616 1.0130 C 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.0624 4.2281 -0.2740 C 0 0 0 0 0 0 0 0 0 0 0 0 19
1.4568 3.3677 1.4065 C 0 0 0 0 0 0 0 0 0 0 0 0 20
0.8527 4.4539 0.7625 C 0 0 0 0 0 0 0 0 0 0 0 0 21
-2.8462 -2.5506 0.4370 O 0 0 0 0 0 0 0 0 0 0 0 0 22
0.2970 -3.0346 2.4008 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-1.4928 -3.0606 2.3545 H 0 0 0 0 0 0 0 0 0 0 0 0 24
-0.5692 -4.2920 1.4582 H 0 0 0 0 0 0 0 0 0 0 0 0 25
1.5537 -3.8666 0.4386 H 0 0 0 0 0 0 0 0 0 0 0 0 26
3.7767 -3.2644 -0.4435 H 0 0 0 0 0 0 0 0 0 0 0 0 27
4.1947 -0.9599 -1.3338 H 0 0 0 0 0 0 0 0 0 0 0 0 28
2.3696 0.7188 -1.2794 H 0 0 0 0 0 0 0 0 0 0 0 0 29
-1.0061 -1.5329 -1.9293 H 0 0 0 0 0 0 0 0 0 0 0 0 30
-2.7252 -1.1202 -1.6455 H 0 0 0 0 0 0 0 0 0 0 0 0 31
-1.0846 2.7462 -1.4712 H 0 0 0 0 0 0 0 0 0 0 0 0 32
1.6246 1.2198 1.5226 H 0 0 0 0 0 0 0 0 0 0 0 0 33
-0.5262 5.0724 -0.7871 H 0 0 0 0 0 0 0 0 0 0 0 0 34
2.1668 3.5374 2.2177 H 0 0 0 0 0 0 0 0 0 0 0 0 35
1.0970 5.4739 1.0643 H 0 0 0 0 0 0 0 0 0 0 0 0 36
2 1 0 0 0 0
3 1 0 0 0 0
12 4 0 0 0 0
23 4 0 0 0 0
24 4 0 0 0 0
25 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
26 5 0 0 0 0
7 6 0 0 0 0
27 6 0 0 0 0
8 7 0 0 0 0
28 7 0 0 0 0
9 8 0 0 0 0
29 8 0 0 0 0
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16 11 0 0 0 0
15 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0

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30 14 0 0 0 0
31 14 0 0 0 0
22 15 0 0 0 0
17 16 0 0 0 0
18 16 0 0 0 0
19 17 0 0 0 0
32 17 0 0 0 0
20 18 0 0 0 0
33 18 0 0 0 0
21 19 0 0 0 0
34 19 0 0 0 0
21 20 0 0 0 0
35 20 0 0 0 0
21 36 0 0 0 0
M END
$$$$
1,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepin-2-one-cation.sdf
COSMOTHERM 3D 0
37 38 0 0 0 0 0 0 0 0 0 V2000
-3.6426 -0.2738 -1.5991 O 0 0 0 0 0 0 0 0 0 0 1
-3.9990 -1.0038 -2.1372 H 0 0 0 0 0 0 0 0 0 0 2
-3.7093 0.5123 -2.1710 H 0 0 0 0 0 0 0 0 0 0 3
1.7804 0.0243 2.8210 C 0 0 0 0 0 0 0 0 0 0 4
-0.4914 1.7163 3.3295 C 0 0 0 0 0 0 0 0 0 0 5
-0.5268 0.5995 2.3641 N 0 0 0 0 0 0 0 0 0 0 6
-1.7559 0.0027 2.1552 C 0 0 0 0 0 0 0 0 0 0 7
-2.7842 0.3927 2.7070 O 0 0 0 0 0 0 0 0 0 0 8
-1.7474 -1.1599 1.1639 C 0 0 0 0 0 0 0 0 0 0 9
-1.3448 -0.6757 -0.1505 N 0 0 0 0 0 0 0 0 0 0 10
-0.1040 -0.3618 -0.4572 C 0 0 0 0 0 0 0 0 0 0 11
0.7040 0.0502 1.9165 C 0 0 0 0 0 0 0 0 0 0 12
0.9275 -0.3858 0.5737 C 0 0 0 0 0 0 0 0 0 0 13
3.0338 -0.4433 2.4370 C 0 0 0 0 0 0 0 0 0 0 14
3.2566 -0.8886 1.1270 C 0 0 0 0 0 0 0 0 0 0 15
2.2171 -0.8444 0.2098 C 0 0 0 0 0 0 0 0 0 0 16
0.2093 -0.0100 -1.8497 C 0 0 0 0 0 0 0 0 0 0 17
1.1430 1.0106 -2.1268 C 0 0 0 0 0 0 0 0 0 0 18
1.4075 1.3750 -3.4466 C 0 0 0 0 0 0 0 0 0 0 19
0.7622 0.7160 -4.5002 C 0 0 0 0 0 0 0 0 0 0 20
-0.1549 -0.3087 -4.2331 C 0 0 0 0 0 0 0 0 0 0 21
-0.4371 -0.6695 -2.9165 C 0 0 0 0 0 0 0 0 0 0 22
1.6255 0.3614 3.8448 H 0 0 0 0 0 0 0 0 0 0 23
-0.4523 1.3530 4.3659 H 0 0 0 0 0 0 0 0 0 0 24
0.3828 2.3389 3.1176 H 0 0 0 0 0 0 0 0 0 0 25
-1.4053 2.3044 3.1988 H 0 0 0 0 0 0 0 0 0 0 26
-2.7592 -1.5660 1.0910 H 0 0 0 0 0 0 0 0 0 0 27
-1.0581 -1.9492 1.4991 H 0 0 0 0 0 0 0 0 0 0 28
3.8411 -0.4679 3.1701 H 0 0 0 0 0 0 0 0 0 0 29
4.2346 -1.2650 0.8277 H 0 0 0 0 0 0 0 0 0 0 30
2.3774 -1.1928 -0.8102 H 0 0 0 0 0 0 0 0 0 0 31
1.6350 1.5348 -1.3072 H 0 0 0 0 0 0 0 0 0 0 32
2.1184 2.1758 -3.6540 H 0 0 0 0 0 0 0 0 0 0 33
0.9789 0.9965 -5.5321 H 0 0 0 0 0 0 0 0 0 0 34
-0.6429 -0.8351 -5.0543 H 0 0 0 0 0 0 0 0 0 0 35
-1.1272 -1.4892 -2.7141 H 0 0 0 0 0 0 0 0 0 0 36
-2.1280 -0.5262 -0.8408 H 0 0 0 0 0 0 0 0 0 0 37
2 1 0 0 0 0
3 1 0 0 0 0
12 4 0 0 0 0
14 4 0 0 0 0
23 4 0 0 0 0
6 5 0 0 0 0
24 5 0 0 0 0
25 5 0 0 0 0
26 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 9 0 0 0 0
27 9 0 0 0 0
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13 11 0 0 0 0
17 11 0 0 0 0
13 12 0 0 0 0
16 13 0 0 0 0
15 14 0 0 0 0
29 14 0 0 0 0
16 15 0 0 0 0
30 15 0 0 0 0
31 16 0 0 0 0
18 17 0 0 0 0
22 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
20 19 0 0 0 0
33 19 0 0 0 0
21 20 0 0 0 0
34 20 0 0 0 0
22 21 0 0 0 0
35 21 0 0 0 0
36 22 0 0 0 0
10 37 0 0 0 0
M END
$$$$
1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOTHERM 3D 0
37 38 0 0 0 0 0 0 0 0 0 V2000
-3.6233 0.2305 -1.5383 O 0 0 0 0 0 0 0 0 0 0 1
-2.7994 -0.0815 -1.0710 H 0 0 0 0 0 0 0 0 0 0 2
-3.2911 0.7969 -2.2561 H 0 0 0 0 0 0 0 0 0 0 3
3.3277 -0.5131 2.1869 C 0 0 0 0 0 0 0 0 0 0 4

```

```
1
2
3 3.4105 -1.0596 0.8997 C 0 0 0 0 0 0 0 0 0 0 0 5
4 2.3097 -0.9834 0.0526 C 0 0 0 0 0 0 0 0 0 0 0 6
5 1.0962 -0.3938 0.4676 C 0 0 0 0 0 0 0 0 0 0 0 7
6 1.0178 0.1366 1.7840 C 0 0 0 0 0 0 0 0 0 0 0 8
7 2.1462 0.0828 2.6214 C 0 0 0 0 0 0 0 0 0 0 0 9
8 -0.0426 -0.3433 -0.4804 C 0 0 0 0 0 0 0 0 0 0 0 10
9 -0.1506 0.7939 2.2704 N 0 0 0 0 0 0 0 0 0 0 0 11
10 -1.4075 0.2794 2.1192 C 0 0 0 0 0 0 0 0 0 0 0 12
11 -1.5243 -0.9866 1.2510 C 0 0 0 0 0 0 0 0 0 0 0 13
12 -1.2705 -0.5804 -0.1284 N 0 0 0 0 0 0 0 0 0 0 0 14
13 0.0037 1.9866 3.1258 C 0 0 0 0 0 0 0 0 0 0 0 15
14 -2.4264 0.7938 2.5996 O 0 0 0 0 0 0 0 0 0 0 0 16
15 0.2242 -0.0178 -1.9076 C 0 0 0 0 0 0 0 0 0 0 0 17
16 -0.5238 -0.6412 -2.9247 C 0 0 0 0 0 0 0 0 0 0 0 18
17 1.2002 0.9333 -2.2615 C 0 0 0 0 0 0 0 0 0 0 0 19
18 1.4106 1.2653 -3.6024 C 0 0 0 0 0 0 0 0 0 0 0 20
19 0.6633 0.6393 -4.6068 C 0 0 0 0 0 0 0 0 0 0 0 21
20 -0.3019 -0.3167 -4.2643 C 0 0 0 0 0 0 0 0 0 0 0 22
21 4.1846 -0.5582 2.8605 H 0 0 0 0 0 0 0 0 0 0 0 23
22 4.3304 -1.5360 0.5593 H 0 0 0 0 0 0 0 0 0 0 0 24
23 2.3709 -1.3968 -0.9545 H 0 0 0 0 0 0 0 0 0 0 0 25
24 2.0892 0.4976 3.6271 H 0 0 0 0 0 0 0 0 0 0 0 26
25 -0.7936 -1.7475 1.5774 H 0 0 0 0 0 0 0 0 0 0 0 27
26 -2.8171 -1.5249 1.3871 O 0 0 0 0 0 0 0 0 0 0 0 28
27 0.8871 2.5448 2.8000 H 0 0 0 0 0 0 0 0 0 0 0 29
28 0.1076 1.7093 4.1841 H 0 0 0 0 0 0 0 0 0 0 0 30
29 -0.8899 2.6079 3.0100 H 0 0 0 0 0 0 0 0 0 0 0 31
30 -1.2687 -1.3912 -2.6564 H 0 0 0 0 0 0 0 0 0 0 0 32
31 1.7831 1.4288 -1.4837 H 0 0 0 0 0 0 0 0 0 0 0 33
32 2.1602 2.0144 -3.8628 H 0 0 0 0 0 0 0 0 0 0 0 34
33 0.8352 0.8920 -5.6546 H 0 0 0 0 0 0 0 0 0 0 0 35
34 -0.8778 -0.8161 -5.0452 H 0 0 0 0 0 0 0 0 0 0 0 36
35 -3.3694 -0.7924 1.7471 H 0 0 0 0 0 0 0 0 0 0 0 37
36
37 2 1 0 0 0 0
38 3 1 0 0 0 0
39 5 4 0 0 0 0
40 9 4 0 0 0 0
41 23 4 0 0 0 0
42 6 5 0 0 0 0
43 24 5 0 0 0 0
44 7 6 0 0 0 0
45 25 6 0 0 0 0
46 8 7 0 0 0 0
47 10 7 0 0 0 0
48 9 8 0 0 0 0
49 11 8 0 0 0 0
50 26 9 0 0 0 0
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31 15 0 0 0 0
32 18 17 0 0 0 0
33 19 17 0 0 0 0
34 22 18 0 0 0 0
35 32 18 0 0 0 0
36 20 19 0 0 0 0
37 33 19 0 0 0 0
38 21 20 0 0 0 0
39 34 20 0 0 0 0
40 22 21 0 0 0 0
41 35 21 0 0 0 0
42 36 22 0 0 0 0
43 28 37 0 0 0 0
M END
$$$$
1,3-dihydro-3-hydroxy-1-methyl-5-phenyl-1,4-benzodiazepin-2-one-cation.sdf
COSMOtherm 3D 0
38 39 0 0 0 0 0 0 0 0 0 0 V2000
-3.5131 0.2785 -1.3959 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.0854 -0.4027 -1.7936 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4378 0.9697 -2.0788 H 0 0 0 0 0 0 0 0 0 0 0 3
3.3716 -0.5273 2.0958 C 0 0 0 0 0 0 0 0 0 0 0 4
3.4393 -1.0276 0.7888 C 0 0 0 0 0 0 0 0 0 0 0 5
2.3249 -0.9381 -0.0331 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1096 -0.3781 0.4297 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0449 0.1115 1.7710 C 0 0 0 0 0 0 0 0 0 0 0 8
2.1937 0.0399 2.5753 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0092 -0.3002 -0.5074 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.1028 0.7595 2.3116 N 0 0 0 0 0 0 0 0 0 0 0 11
-1.3666 0.2522 2.2126 C 0 0 0 0 0 0 0 0 0 0 0 12
-1.5325 -0.9750 1.2934 C 0 0 0 0 0 0 0 0 0 0 0 13
-1.2352 -0.5101 -0.0783 N 0 0 0 0 0 0 0 0 0 0 0 14
0.0896 1.9253 3.2003 C 0 0 0 0 0 0 0 0 0 0 0 15
-2.3602 0.7338 2.7633 O 0 0 0 0 0 0 0 0 0 0 0 16
0.2024 -0.0024 -1.9302 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.5868 -0.6345 -2.9146 C 0 0 0 0 0 0 0 0 0 0 0 18
1.1819 0.9354 -2.3193 C 0 0 0 0 0 0 0 0 0 0 0 19
1.3517 1.2472 -3.6677 C 0 0 0 0 0 0 0 0 0 0 0 20
0.5666 0.6145 -4.6392 C 0 0 0 0 0 0 0 0 0 0 0 21
-0.3977 -0.3287 -4.2611 C 0 0 0 0 0 0 0 0 0 0 0 22
4.2404 -0.5871 2.7522 H 0 0 0 0 0 0 0 0 0 0 0 23
4.3573 -1.4821 0.4166 H 0 0 0 0 0 0 0 0 0 0 0 24
2.3656 -1.3280 -1.0496 H 0 0 0 0 0 0 0 0 0 0 0 25
2.1566 0.4194 3.5952 H 0 0 0 0 0 0 0 0 0 0 0 26
-0.8079 -1.7649 1.5471 H 0 0 0 0 0 0 0 0 0 0 0 27
-2.8297 -1.4605 1.3682 O 0 0 0 0 0 0 0 0 0 0 0 28
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1
2
3 0.9703 2.4815 2.8655 H 0 0 0 0 0 0 0 0 0 0 0 0 0 29
4 0.2155 1.6125 4.2454 H 0 0 0 0 0 0 0 0 0 0 0 0 0 30
5 -0.7996 2.5588 3.1236 H 0 0 0 0 0 0 0 0 0 0 0 0 0 31
6 -1.3160 -1.3920 -2.6257 H 0 0 0 0 0 0 0 0 0 0 0 0 0 32
7 1.7841 1.4394 -1.5630 H 0 0 0 0 0 0 0 0 0 0 0 0 0 33
8 2.0988 1.9855 -3.9614 H 0 0 0 0 0 0 0 0 0 0 0 0 0 34
9 0.7098 0.8525 -5.6944 H 0 0 0 0 0 0 0 0 0 0 0 0 0 35
10 -0.9956 -0.8355 -5.0196 H 0 0 0 0 0 0 0 0 0 0 0 0 0 36
11 -3.3520 -0.7634 1.8341 H 0 0 0 0 0 0 0 0 0 0 0 0 0 37
12 -2.0800 -0.2818 -0.6776 H 0 0 0 0 0 0 0 0 0 0 0 0 0 38
13 2 1 0 0 0 0
14 3 1 0 0 0 0
15 5 4 0 0 0 0
16 9 4 0 0 0 0
17 23 4 0 0 0 0
18 6 5 0 0 0 0
19 24 5 0 0 0 0
20 7 6 0 0 0 0
21 25 6 0 0 0 0
22 8 7 0 0 0 0
23 10 7 0 0 0 0
24 9 8 0 0 0 0
25 11 8 0 0 0 0
26 26 9 0 0 0 0
27 14 10 0 0 0 0
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29 12 11 0 0 0 0
30 15 11 0 0 0 0
31 13 12 0 0 0 0
32 16 12 0 0 0 0
33 14 13 0 0 0 0
34 27 13 0 0 0 0
35 28 13 0 0 0 0
36 29 15 0 0 0 0
37 30 15 0 0 0 0
38 31 15 0 0 0 0
39 18 17 0 0 0 0
40 19 17 0 0 0 0
41 22 18 0 0 0 0
42 32 18 0 0 0 0
43 20 19 0 0 0 0
44 33 19 0 0 0 0
45 21 20 0 0 0 0
46 34 20 0 0 0 0
47 22 21 0 0 0 0
48 35 21 0 0 0 0
49 36 22 0 0 0 0
50 37 28 0 0 0 0
51 14 38 0 0 0 0
52 M END
53 \$\$\$\$
54 1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one.sdf
55 COSMOTHERM 3D 0
56 34 35 0 0 0 0 0 0 0 0 0 V2000
57 -1.3958 3.5854 0.3743 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
58 -0.9016 2.7816 0.0509 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
59 -2.1555 3.2188 0.8591 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
60 1.0534 -3.4544 -0.8153 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
0.2389 -2.3279 -0.8516 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.6436 -1.1033 -0.2751 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.9205 -1.0466 0.3434 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
2.7194 -2.2008 0.4163 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
2.2913 -3.3933 -0.1587 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.4082 0.1230 0.9684 N 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.2855 0.0518 -0.2778 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.0845 1.2849 -0.4562 N 0 0 0 0 0 0 0 0 0 0 0 0 0 12
1.4786 1.5624 -0.7847 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.7361 -0.2036 -0.0542 C 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-2.6978 0.5456 -0.7581 C 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-2.1670 -1.1648 0.8798 C 0 0 0 0 0 0 0 0 0 0 0 0 0 16
-4.0597 0.3390 -0.5300 C 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-4.4797 -0.6103 0.4106 C 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.5303 -1.3585 1.1165 C 0 0 0 0 0 0 0 0 0 0 0 0 0 19
2.3011 1.3999 0.5052 C 0 0 0 0 0 0 0 0 0 0 0 0 0 20
2.7980 2.3795 1.0717 O 0 0 0 0 0 0 0 0 0 0 0 0 0 21
1.6293 2.8728 -1.2733 O 0 0 0 0 0 0 0 0 0 0 0 0 0 22
0.7235 -4.3821 -1.2837 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
-0.7345 -2.3781 -1.3402 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24
3.6862 -2.1451 0.9197 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25
2.9293 -4.2764 -0.1041 H 0 0 0 0 0 0 0 0 0 0 0 0 0 26
3.0528 -0.0073 1.7503 H 0 0 0 0 0 0 0 0 0 0 0 0 0 27
1.8459 0.8566 -1.5521 H 0 0 0 0 0 0 0 0 0 0 0 0 0 28
-2.3683 1.2792 -1.4950 H 0 0 0 0 0 0 0 0 0 0 0 0 0 29
-1.4327 -1.7478 1.4377 H 0 0 0 0 0 0 0 0 0 0 0 0 0 30
-4.7967 0.9155 -1.0917 H 0 0 0 0 0 0 0 0 0 0 0 0 0 31
-5.5445 -0.7692 0.5894 H 0 0 0 0 0 0 0 0 0 0 0 0 0 32
-3.8515 -2.0958 1.8542 H 0 0 0 0 0 0 0 0 0 0 0 0 0 33
1.9751 3.4020 -0.5183 H 0 0 0 0 0 0 0 0 0 0 0 0 0 34
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
23 4 0 0 0 0
6 5 0 0 0 0
24 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
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10 7 0 0 0 0
9 8 0 0 0 0
25 8 0 0 0 0
26 9 0 0 0 0
20 10 0 0 0 0
27 10 0 0 0 0

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12 11 0 0 0 0
14 11 0 0 0 0
13 12 0 0 0 0
20 13 0 0 0 0
22 13 0 0 0 0
28 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
17 15 0 0 0 0
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19 16 0 0 0 0
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18 17 0 0 0 0
31 17 0 0 0 0
19 18 0 0 0 0
32 18 0 0 0 0
33 19 0 0 0 0
21 20 0 0 0 0
22 34 0 0 0 0

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M END

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1,3-dihydro-3-hydroxy-5-phenyl-1,4-benzodiazepin-2-one-cation.sdf
COSMOTHERM 3D 0

35 36 0 0 0 0 0 0 0 0 0 V2000

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-3.4973 -0.4119 -1.2084 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.3989 -1.0856 -1.9056 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.0827 0.2639 -1.5958 H 0 0 0 0 0 0 0 0 0 0 0 3
3.4965 0.7857 0.9172 C 0 0 0 0 0 0 0 0 0 0 0 4
2.3507 0.8126 0.1363 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1277 0.2646 0.5975 C 0 0 0 0 0 0 0 0 0 0 0 6
1.0944 -0.3119 1.9034 C 0 0 0 0 0 0 0 0 0 0 0 7
2.2749 -0.3739 2.6610 C 0 0 0 0 0 0 0 0 0 0 0 8
3.4600 0.1700 2.1776 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.0502 -0.9207 2.4588 N 0 0 0 0 0 0 0 0 0 0 0 10
-0.0125 0.2391 -0.3143 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.2399 0.3833 0.1408 N 0 0 0 0 0 0 0 0 0 0 0 12
-1.5522 0.7779 1.5306 C 0 0 0 0 0 0 0 0 0 0 0 13
0.1742 0.0403 -1.7592 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.6355 0.7377 -2.6805 C 0 0 0 0 0 0 0 0 0 0 0 15
1.1441 -0.8681 -2.2324 C 0 0 0 0 0 0 0 0 0 0 0 16
-0.4749 0.5264 -4.0489 C 0 0 0 0 0 0 0 0 0 0 0 17
0.4798 -0.3881 -4.5113 C 0 0 0 0 0 0 0 0 0 0 0 18
1.2850 -1.0854 -3.6024 C 0 0 0 0 0 0 0 0 0 0 0 19
-1.3342 -0.4689 2.4100 C 0 0 0 0 0 0 0 0 0 0 0 20
-2.2832 -0.9984 2.9883 O 0 0 0 0 0 0 0 0 0 0 0 21
-2.8640 1.2172 1.6254 O 0 0 0 0 0 0 0 0 0 0 0 22
4.4197 1.2315 0.5473 H 0 0 0 0 0 0 0 0 0 0 0 23
2.3743 1.2792 -0.8480 H 0 0 0 0 0 0 0 0 0 0 0 24
2.2455 -0.8458 3.6442 H 0 0 0 0 0 0 0 0 0 0 0 25
4.3602 0.1234 2.7914 H 0 0 0 0 0 0 0 0 0 0 0 26
0.1195 -1.6699 3.1334 H 0 0 0 0 0 0 0 0 0 0 0 27
-0.8512 1.5792 1.8173 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.3584 1.4723 -2.3240 H 0 0 0 0 0 0 0 0 0 0 0 29
1.7607 -1.4243 -1.5258 H 0 0 0 0 0 0 0 0 0 0 0 30
-1.0892 1.0834 -4.7575 H 0 0 0 0 0 0 0 0 0 0 0 31
0.6003 -0.5532 -5.5831 H 0 0 0 0 0 0 0 0 0 0 0 32
2.0245 -1.8020 -3.9622 H 0 0 0 0 0 0 0 0 0 0 0 33
-3.3647 0.4965 2.0764 H 0 0 0 0 0 0 0 0 0 0 0 34
-2.0802 0.1606 -0.4670 H 0 0 0 0 0 0 0 0 0 0 0 35

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
23 4 0 0 0 0
6 5 0 0 0 0
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7 6 0 0 0 0
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8 7 0 0 0 0
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20 10 0 0 0 0
27 10 0 0 0 0
12 11 0 0 0 0
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13 12 0 0 0 0
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15 14 0 0 0 0
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29 15 0 0 0 0
19 16 0 0 0 0
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32 18 0 0 0 0
33 19 0 0 0 0
21 20 0 0 0 0
34 22 0 0 0 0
12 35 0 0 0 0

M END

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1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one.sdf
COSMOTHERM 3D 0

33 34 0 0 0 0 0 0 0 0 0 V2000

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-1.7446 -3.6345 -0.1202 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.1984 -2.8103 -0.2830 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.4296 -3.3492 0.5085 H 0 0 0 0 0 0 0 0 0 0 0 3

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2.7947 2.8635 -0.1177 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.5638 3.1311 -0.7351 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.6028 2.1287 -0.8102 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.8462 0.8295 -0.3117 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.1150 0.5609 0.2659 C 0 0 0 0 0 0 0 0 0 0 0 0 8
3.0657 1.5921 0.3779 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.2349 -0.1835 -0.3449 C 0 0 0 0 0 0 0 0 0 0 0 0 10
2.4506 -0.6968 0.8068 N 0 0 0 0 0 0 0 0 0 0 0 0 11
2.1913 -1.9325 0.2583 C 0 0 0 0 0 0 0 0 0 0 0 0 12
1.2893 -1.8983 -0.9702 C 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.0498 -1.4432 -0.6010 N 0 0 0 0 0 0 0 0 0 0 0 0 14
2.6533 -2.9676 0.7461 O 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.6296 0.2581 -0.0569 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.7081 -0.3116 -0.7601 C 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.8939 1.2183 0.9384 C 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.2090 1.5859 1.2355 C 0 0 0 0 0 0 0 0 0 0 0 0 19
-4.2748 1.0150 0.5300 C 0 0 0 0 0 0 0 0 0 0 0 0 20
-4.0204 0.0680 -0.4704 C 0 0 0 0 0 0 0 0 0 0 0 0 21
3.5495 3.6467 -0.0323 H 0 0 0 0 0 0 0 0 0 0 0 0 22
1.3544 4.1212 -1.1414 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-0.3648 2.3395 -1.2669 H 0 0 0 0 0 0 0 0 0 0 0 0 24
4.0267 1.3764 0.8488 H 0 0 0 0 0 0 0 0 0 0 0 0 25
1.7482 -1.2389 -1.7297 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-2.5072 -1.0454 -1.5412 H 0 0 0 0 0 0 0 0 0 0 0 0 27
-1.0685 1.6634 1.4960 H 0 0 0 0 0 0 0 0 0 0 0 0 28
-3.4015 2.3199 2.0198 H 0 0 0 0 0 0 0 0 0 0 0 0 29
-5.3011 1.3096 0.7563 H 0 0 0 0 0 0 0 0 0 0 0 0 30
-4.8476 -0.3709 -1.0309 H 0 0 0 0 0 0 0 0 0 0 0 0 31
3.1571 -0.6993 1.5448 H 0 0 0 0 0 0 0 0 0 0 0 0 32
1.2272 -2.9150 -1.3716 H 0 0 0 0 0 0 0 0 0 0 0 0 33

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
22 4 0 0 0 0
6 5 0 0 0 0
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8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
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32 11 0 0 0 0
13 12 0 0 0 0
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26 13 0 0 0 0
17 16 0 0 0 0
18 16 0 0 0 0
21 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
20 19 0 0 0 0
29 19 0 0 0 0
21 20 0 0 0 0
30 20 0 0 0 0
31 21 0 0 0 0
13 33 0 0 0 0
M END
$$$$
1,3-dihydro-5-phenyl-1,4-benzodiazepin-2-one_p2.sdf
COSMOTHERM 3D 0

34 35 0 0 0 0 0 0 0 0 0 V2000
-1.5533 -0.0560 3.6077 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.1893 -0.7270 3.9149 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.0426 0.7860 3.6436 H 0 0 0 0 0 0 0 0 0 0 0 0 3
2.7034 -0.1288 -2.9427 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.4442 -0.6968 -3.1918 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5094 -0.7566 -2.1699 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.8080 -0.2919 -0.8642 C 0 0 0 0 0 0 0 0 0 0 0 0 7
2.1095 0.2372 -0.6124 C 0 0 0 0 0 0 0 0 0 0 0 0 8
3.0280 0.3330 -1.6724 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.2527 -0.2997 0.1354 C 0 0 0 0 0 0 0 0 0 0 0 0 10
2.5116 0.7630 0.6279 N 0 0 0 0 0 0 0 0 0 0 0 0 11
2.2917 0.2410 1.8831 C 0 0 0 0 0 0 0 0 0 0 0 0 12
1.3200 -0.9376 1.9074 C 0 0 0 0 0 0 0 0 0 0 0 0 13
0.0150 -0.5249 1.4054 N 0 0 0 0 0 0 0 0 0 0 0 0 14
2.8378 0.6934 2.8862 O 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.6532 -0.0468 -0.2397 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.6971 -0.7633 0.3826 C 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.9622 0.9366 -1.2027 C 0 0 0 0 0 0 0 0 0 0 0 0 18
-3.2925 1.2084 -1.5202 C 0 0 0 0 0 0 0 0 0 0 0 0 19
-4.3236 0.4921 -0.8997 C 0 0 0 0 0 0 0 0 0 0 0 0 20
-4.0236 -0.4966 0.0460 C 0 0 0 0 0 0 0 0 0 0 0 0 21
3.4403 -0.0557 -3.7435 H 0 0 0 0 0 0 0 0 0 0 0 0 22
1.1969 -1.0794 -4.1818 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-0.4743 -1.1860 -2.3578 H 0 0 0 0 0 0 0 0 0 0 0 0 24
4.0102 0.7676 -1.4793 H 0 0 0 0 0 0 0 0 0 0 0 0 25
1.7155 -1.7572 1.2878 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-2.4657 -1.5555 1.0954 H 0 0 0 0 0 0 0 0 0 0 0 0 27
-1.1614 1.5062 -1.6747 H 0 0 0 0 0 0 0 0 0 0 0 0 28
-3.5258 1.9820 -2.2528 H 0 0 0 0 0 0 0 0 0 0 0 0 29
-5.3630 0.7002 -1.1580 H 0 0 0 0 0 0 0 0 0 0 0 0 30
-4.8256 -1.0676 0.5152 H 0 0 0 0 0 0 0 0 0 0 0 0 31
1.2034 -1.2827 2.9376 H 0 0 0 0 0 0 0 0 0 0 0 0 32
3.2589 1.4597 0.5923 H 0 0 0 0 0 0 0 0 0 0 0 0 33
-0.7197 -0.3608 2.1439 H 0 0 0 0 0 0 0 0 0 0 0 0 34

2 1 0 0 0 0

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3 1 0 0 0 0
5 4 0 0 0 0
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6 5 0 0 0 0
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11 8 0 0 0 0
25 9 0 0 0 0
14 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
33 11 0 0 0 0
13 12 0 0 0 0
15 12 0 0 0 0
14 13 0 0 0 0
26 13 0 0 0 0
32 13 0 0 0 0
17 16 0 0 0 0
18 16 0 0 0 0
21 17 0 0 0 0
27 17 0 0 0 0
19 18 0 0 0 0
28 18 0 0 0 0
20 19 0 0 0 0
29 19 0 0 0 0
21 20 0 0 0 0
30 20 0 0 0 0
31 21 0 0 0 0
14 34 0 0 0 0
M END
$$$$
1-methylindole-cation0.sdf
COSMOTHERM 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
1.2462 0.2039 -0.6915 O 0 0 0 0 0 0 0 0 0 0 0 1
0.3770 -0.2263 -0.5874 H 0 0 0 0 0 0 0 0 0 0 0 2
1.0583 1.1596 -0.6363 H 0 0 0 0 0 0 0 0 0 0 0 3
4.8260 -3.2872 -1.1738 C 0 0 0 0 0 0 0 0 0 0 0 4
6.0932 -2.6874 -1.2319 C 0 0 0 0 0 0 0 0 0 0 0 5
6.3569 -1.4766 -0.5788 C 0 0 0 0 0 0 0 0 0 0 0 6
5.3180 -0.8746 0.1400 C 0 0 0 0 0 0 0 0 0 0 0 7
4.0610 -1.4991 0.1807 C 0 0 0 0 0 0 0 0 0 0 0 8
3.7739 -2.6928 -0.4576 C 0 0 0 0 0 0 0 0 0 0 0 9
3.1442 -0.6562 0.9727 N 0 0 0 0 0 0 0 0 0 0 0 10
5.2292 0.3579 0.9185 C 0 0 0 0 0 0 0 0 0 0 0 11
3.9832 0.4832 1.4056 C 0 0 0 0 0 0 0 0 0 0 0 12
2.4629 -1.3631 2.1189 C 0 0 0 0 0 0 0 0 0 0 0 13
4.6487 -4.2298 -1.6923 H 0 0 0 0 0 0 0 0 0 0 0 14
6.8884 -3.1749 -1.7976 H 0 0 0 0 0 0 0 0 0 0 0 15
7.3436 -1.0151 -0.6305 H 0 0 0 0 0 0 0 0 0 0 0 16
2.7898 -3.1597 -0.4153 H 0 0 0 0 0 0 0 0 0 0 0 17
6.0374 1.0665 1.0827 H 0 0 0 0 0 0 0 0 0 0 0 18
3.5164 1.2429 2.0240 H 0 0 0 0 0 0 0 0 0 0 0 19
2.3555 -0.2791 0.3144 H 0 0 0 0 0 0 0 0 0 0 0 20
1.8532 -2.1755 1.7116 H 0 0 0 0 0 0 0 0 0 0 0 21
1.8256 -0.6372 2.6333 H 0 0 0 0 0 0 0 0 0 0 0 22
3.2290 -1.7545 2.7951 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
17 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
19 12 0 0 0 0
21 13 0 0 0 0
22 13 0 0 0 0
13 23 0 0 0 0
M END
$$$$
1-methylindole-cation1.sdf
COSMOTHERM 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
0.4865 -0.1995 0.2488 O 0 0 0 0 0 0 0 0 0 0 0 1
0.1818 -0.8389 -0.4203 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.1009 0.5679 0.1255 H 0 0 0 0 0 0 0 0 0 0 0 3
5.5162 4.4930 0.6148 C 0 0 0 0 0 0 0 0 0 0 0 4
6.1017 3.7036 1.6644 C 0 0 0 0 0 0 0 0 0 0 0 5
5.8064 2.3720 1.8021 C 0 0 0 0 0 0 0 0 0 0 0 6
4.8972 1.7814 0.8672 C 0 0 0 0 0 0 0 0 0 0 0 7
4.3160 2.6008 -0.1929 C 0 0 0 0 0 0 0 0 0 0 0 8
4.6338 3.9776 -0.3094 C 0 0 0 0 0 0 0 0 0 0 0 9
3.5029 1.8509 -0.9459 N 0 0 0 0 0 0 0 0 0 0 0 10
4.3950 0.5088 0.7232 C 0 0 0 0 0 0 0 0 0 0 0 11
3.4708 0.4917 -0.4231 C 0 0 0 0 0 0 0 0 0 0 0 12
2.7162 2.2989 -2.0908 C 0 0 0 0 0 0 0 0 0 0 0 13

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2.4244 0.2257 -0.1213 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
3.7551 -0.2414 -1.1988 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
5.7860 5.5485 0.5536 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
6.7904 4.1882 2.3566 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
6.2426 1.7666 2.5972 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
4.2041 4.5988 -1.0946 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
4.6098 -0.3645 1.3357 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
2.0817 3.1483 -1.8055 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
2.0801 1.4724 -2.4218 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
3.3774 2.5949 -2.9165 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 12 0 0 0 0
21 13 0 0 0 0
22 13 0 0 0 0
13 23 0 0 0 0
M END
$$$$
1-methylindole-cation2.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
-4.6216 -0.0057 0.4272 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-5.0079 -0.7734 -0.0311 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-5.0240 0.7613 -0.0183 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
2.9023 -0.0028 -0.8996 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
3.1677 -0.0028 0.4793 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
2.1300 -0.0009 1.4238 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.8184 0.0009 0.9576 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.5801 0.0007 -0.4259 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
1.5883 -0.0009 -1.3843 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.8384 0.0027 -0.6256 N 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.5159 0.0033 1.6506 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.4739 0.0042 0.5178 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.4626 0.0027 -1.9517 C 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.6862 0.8826 2.2966 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.6891 -0.8747 2.2976 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
3.7312 -0.0040 -1.6080 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
4.2030 -0.0043 0.8228 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
2.3490 -0.0009 2.4921 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
1.3788 -0.0007 -2.4538 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-2.5714 0.0052 0.5537 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-1.1422 0.8989 -2.4964 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-2.5491 0.0048 -1.8277 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
-1.1454 -0.8955 -2.4949 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 13 0 0 0 0
22 13 0 0 0 0
13 23 0 0 0 0
M END
$$$$
1-methylindole.sdf
COSMOtherm 3D 0
22 22 0 0 0 0 0 0 0 0 0 V2000
-1.4013 -2.2633 2.2413 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.6263 -1.7545 1.9164 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.0889 -2.6554 3.0760 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.3507 2.5359 1.3727 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.2120 -0.7753 1.0433 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.6653 -0.6084 -0.2764 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.6554 -1.3924 -1.4478 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0064 -0.9052 -2.5817 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.6375 0.3544 -2.5729 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.6459 1.1564 -1.4304 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0085 0.6648 -0.2912 C 0 0 0 0 0 0 0 0 0 0 0 0 0 11
0.8839 0.3639 1.7574 C 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.1584 1.2322 0.9641 N 0 0 0 0 0 0 0 0 0 0 0 0 0 13
0.1655 3.3443 0.8351 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14

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1
2
3 -1.4299 2.6039 1.1771 H 0 0 0 0 0 0 0 0 0 0 0 0 15
4 -0.1795 2.6583 2.4475 H 0 0 0 0 0 0 0 0 0 0 0 0 16
5 1.8080 -1.6064 1.4104 H 0 0 0 0 0 0 0 0 0 0 0 0 17
6 1.1478 -2.3669 -1.4655 H 0 0 0 0 0 0 0 0 0 0 0 0 18
7 -0.0074 -1.5034 -3.4946 H 0 0 0 0 0 0 0 0 0 0 0 0 19
8 -1.1382 0.7072 -3.4764 H 0 0 0 0 0 0 0 0 0 0 0 0 20
9 -1.1437 2.1275 -1.4299 H 0 0 0 0 0 0 0 0 0 0 0 0 21
10 1.1161 0.6349 2.7841 H 0 0 0 0 0 0 0 0 0 0 0 0 22
11 2 1 0 0 0 0
12 3 1 0 0 0 0
13 4 0 0 0 0 0
14 4 0 0 0 0 0
15 4 0 0 0 0 0
16 4 0 0 0 0 0
17 6 5 0 0 0 0
18 12 5 0 0 0 0
19 17 5 0 0 0 0
20 7 6 0 0 0 0
21 11 6 0 0 0 0
22 8 7 0 0 0 0
23 18 7 0 0 0 0
24 9 8 0 0 0 0
25 19 8 0 0 0 0
26 10 9 0 0 0 0
27 20 9 0 0 0 0
28 11 10 0 0 0 0
29 21 10 0 0 0 0
30 13 11 0 0 0 0
31 13 12 0 0 0 0
32 12 22 0 0 0 0
33 M END
34 $$$$
35 1-methylpyrrole-cation0.sdf
36 COSMOtherm 3D 0
37
38 17 16 0 0 0 0 0 0 0 0 0 V2000
39 -2.4045 -0.0292 1.1089 O 0 0 0 0 0 0 0 0 0 0 0 0 1
40 -3.1849 -0.4535 0.7060 H 0 0 0 0 0 0 0 0 0 0 0 0 2
41 -2.7165 0.8473 1.4020 H 0 0 0 0 0 0 0 0 0 0 0 0 3
42 1.6966 0.7229 0.5710 C 0 0 0 0 0 0 0 0 0 0 0 0 4
43 1.6886 -0.7392 0.5668 C 0 0 0 0 0 0 0 0 0 0 0 0 5
44 0.5706 1.1641 -0.0205 C 0 0 0 0 0 0 0 0 0 0 0 0 6
45 -0.2397 0.0053 -0.4126 N 0 0 0 0 0 0 0 0 0 0 0 0 7
46 0.5586 -1.1641 -0.0289 C 0 0 0 0 0 0 0 0 0 0 0 0 8
47 2.4825 1.3490 0.9850 H 0 0 0 0 0 0 0 0 0 0 0 0 9
48 2.4677 -1.3764 0.9765 H 0 0 0 0 0 0 0 0 0 0 0 0 10
49 0.1861 2.1575 -0.2252 H 0 0 0 0 0 0 0 0 0 0 0 0 11
50 -0.6851 0.0132 -1.8547 C 0 0 0 0 0 0 0 0 0 0 0 0 12
51 0.1626 -2.1517 -0.2384 H 0 0 0 0 0 0 0 0 0 0 0 0 13
52 -1.1569 0.0085 0.2062 H 0 0 0 0 0 0 0 0 0 0 0 0 14
53 -1.2863 -0.8839 -2.0314 H 0 0 0 0 0 0 0 0 0 0 0 0 15
54 0.2015 0.0173 -2.4960 H 0 0 0 0 0 0 0 0 0 0 0 0 16
55 -1.2874 0.9114 -2.0205 H 0 0 0 0 0 0 0 0 0 0 0 0 17
56 2 1 0 0 0 0
57 3 1 0 0 0 0
58 5 4 0 0 0 0
59 6 4 0 0 0 0
60 9 4 0 0 0 0
61 8 5 0 0 0 0
62 10 5 0 0 0 0
63 7 6 0 0 0 0
64 11 6 0 0 0 0
65 8 7 0 0 0 0
66 12 7 0 0 0 0
67 14 7 0 0 0 0
68 13 8 0 0 0 0
69 15 12 0 0 0 0
70 16 12 0 0 0 0
71 12 17 0 0 0 0
72 M END
73 $$$$
74 1-methylpyrrole-cation1.sdf
75 COSMOtherm 3D 0
76
77 17 16 0 0 0 0 0 0 0 0 0 V2000
78 -3.3810 -0.0118 0.5310 O 0 0 0 0 0 0 0 0 0 0 0 0 1
79 -3.7804 -0.7405 0.0228 H 0 0 0 0 0 0 0 0 0 0 0 0 2
80 -3.7953 0.7876 0.1592 H 0 0 0 0 0 0 0 0 0 0 0 0 3
81 2.0049 -0.0064 0.9686 C 0 0 0 0 0 0 0 0 0 0 0 0 4
82 0.7705 0.0055 1.5375 C 0 0 0 0 0 0 0 0 0 0 0 0 5
83 1.8562 -0.0088 -0.5085 C 0 0 0 0 0 0 0 0 0 0 0 0 6
84 0.4025 0.0026 -0.6969 N 0 0 0 0 0 0 0 0 0 0 0 0 7
85 -0.1983 0.0121 0.4714 C 0 0 0 0 0 0 0 0 0 0 0 0 8
86 -0.2347 0.0055 -2.0113 C 0 0 0 0 0 0 0 0 0 0 0 0 9
87 2.9698 -0.0136 1.4699 H 0 0 0 0 0 0 0 0 0 0 0 0 10
88 0.5191 0.0108 2.5940 H 0 0 0 0 0 0 0 0 0 0 0 0 11
89 -1.2939 0.0193 0.5412 H 0 0 0 0 0 0 0 0 0 0 0 0 12
90 2.2919 -0.9017 -0.9866 H 0 0 0 0 0 0 0 0 0 0 0 0 13
91 2.3073 0.8739 -0.9916 H 0 0 0 0 0 0 0 0 0 0 0 0 14
92 0.0545 -0.8999 -2.5594 H 0 0 0 0 0 0 0 0 0 0 0 0 15
93 0.0901 0.8913 -2.5715 H 0 0 0 0 0 0 0 0 0 0 0 0 16
94 -1.3204 0.0287 -1.8764 H 0 0 0 0 0 0 0 0 0 0 0 0 17
95 2 1 0 0 0 0
96 3 1 0 0 0 0
97 5 4 0 0 0 0
98 6 4 0 0 0 0
99 10 4 0 0 0 0
100 8 5 0 0 0 0
101 11 5 0 0 0 0
102 7 6 0 0 0 0
103 13 6 0 0 0 0
104 14 6 0 0 0 0
105 8 7 0 0 0 0
106 9 7 0 0 0 0
107 12 8 0 0 0 0
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15 9 0 0 0 0
16 9 0 0 0 0
9 17 0 0 0 0

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M END

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1-methylpyrrole-cation2.sdf

COSMOTHERM 3D 0

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17 16 0 0 0 0 0 0 0 0 0 V2000
-3.3699 0.0024 0.5250 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.7638 -0.8037 0.1459 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7876 0.7257 0.0241 H 0 0 0 0 0 0 0 0 0 0 0 3
0.8005 0.0031 1.5424 C 0 0 0 0 0 0 0 0 0 0 0 4
2.0981 -0.0023 0.7987 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.2105 0.0040 0.4647 C 0 0 0 0 0 0 0 0 0 0 0 6
0.4030 0.0007 -0.6912 N 0 0 0 0 0 0 0 0 0 0 0 7
1.8265 -0.0037 -0.5181 C 0 0 0 0 0 0 0 0 0 0 0 8
0.6689 -0.8704 2.2073 H 0 0 0 0 0 0 0 0 0 0 0 9
0.6738 0.8803 2.2034 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.2337 0.0007 -2.0117 C 0 0 0 0 0 0 0 0 0 0 0 11
3.0819 -0.0049 1.2582 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.3052 0.0086 0.5382 H 0 0 0 0 0 0 0 0 0 0 0 13
2.4651 -0.0072 -1.3957 H 0 0 0 0 0 0 0 0 0 0 0 14
0.0866 0.8948 -2.5596 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.3195 0.0049 -1.8813 H 0 0 0 0 0 0 0 0 0 0 0 16
0.0801 -0.8976 -2.5565 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
9 4 0 0 0 0 0
10 4 0 0 0 0 0
8 5 0 0 0 0 0
12 5 0 0 0 0 0
7 6 0 0 0 0 0
13 6 0 0 0 0 0
8 7 0 0 0 0 0
11 7 0 0 0 0 0
14 8 0 0 0 0 0
15 11 0 0 0 0 0
16 11 0 0 0 0 0
11 17 0 0 0 0 0

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M END

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1-methylpyrrole.sdf

COSMOTHERM 3D 0

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16 15 0 0 0 0 0 0 0 0 0 V2000
-2.7239 -1.1023 0.3805 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.7295 -1.8131 -0.2846 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.0259 -0.4877 0.0628 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3490 1.4611 0.4504 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6113 0.9852 -0.8716 C 0 0 0 0 0 0 0 0 0 0 0 5
0.7114 0.7190 0.9498 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1044 -0.1792 -0.0203 N 0 0 0 0 0 0 0 0 0 0 0 7
0.3031 -0.0308 -1.1295 C 0 0 0 0 0 0 0 0 0 0 0 8
2.1284 -1.2082 0.1476 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.8666 2.2622 0.9712 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.3526 1.3656 -1.5698 H 0 0 0 0 0 0 0 0 0 0 0 11
1.2181 0.7528 1.9095 H 0 0 0 0 0 0 0 0 0 0 0 12
0.4524 -0.6492 -2.0095 H 0 0 0 0 0 0 0 0 0 0 0 13
1.6956 -2.1322 0.5565 H 0 0 0 0 0 0 0 0 0 0 0 14
2.9027 -0.8411 0.8312 H 0 0 0 0 0 0 0 0 0 0 0 15
2.5874 -1.4255 -0.8242 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0 0
3 1 0 0 0 0 0
5 4 0 0 0 0 0
6 4 0 0 0 0 0
10 4 0 0 0 0 0
8 5 0 0 0 0 0
11 5 0 0 0 0 0
7 6 0 0 0 0 0
12 6 0 0 0 0 0
8 7 0 0 0 0 0
9 7 0 0 0 0 0
13 8 0 0 0 0 0
14 9 0 0 0 0 0
15 9 0 0 0 0 0
9 16 0 0 0 0 0

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M END

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2,3-dihydro-1-methyl-5-phenyl-1,4-benzodiazepine_new.sdf

COSMOTHERM 3D 0

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37 38 0 0 0 0 0 0 0 0 0 V2000
-2.1123 -3.6017 -0.1734 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.5060 -2.8126 -0.3282 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.7501 -3.2898 0.4914 H 0 0 0 0 0 0 0 0 0 0 0 3
1.6521 3.7835 -1.4585 H 0 0 0 0 0 0 0 0 0 0 0 4
1.7763 2.8003 -1.0032 C 0 0 0 0 0 0 0 0 0 0 0 5
0.7185 1.8925 -0.9834 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8461 0.6109 -0.4154 C 0 0 0 0 0 0 0 0 0 0 0 7
2.1004 0.2178 0.1578 C 0 0 0 0 0 0 0 0 0 0 0 8
3.1486 1.1683 0.1573 C 0 0 0 0 0 0 0 0 0 0 0 9
2.9903 2.4315 -0.4117 C 0 0 0 0 0 0 0 0 0 0 0 10
2.2528 -1.0166 0.8031 N 0 0 0 0 0 0 0 0 0 0 0 11
1.9693 -2.2759 0.0786 C 0 0 0 0 0 0 0 0 0 0 0 12
1.0021 -2.0936 -1.0797 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.2860 -1.5513 -0.6456 N 0 0 0 0 0 0 0 0 0 0 0 14
-0.3397 -0.2816 -0.3848 C 0 0 0 0 0 0 0 0 0 0 0 15
-1.6660 0.3009 -0.0291 C 0 0 0 0 0 0 0 0 0 0 0 16
-2.8385 -0.1794 -0.6426 C 0 0 0 0 0 0 0 0 0 0 0 17
-4.0870 0.3364 -0.2885 C 0 0 0 0 0 0 0 0 0 0 0 18
-4.1845 1.3350 0.6891 C 0 0 0 0 0 0 0 0 0 0 0 19
-3.0249 1.8186 1.3063 C 0 0 0 0 0 0 0 0 0 0 0 20

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23 5 0 0 0 0
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11 8 0 0 0 0
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27 12 0 0 0 0
14 13 0 0 0 0
28 13 0 0 0 0
29 13 0 0 0 0
16 15 0 0 0 0
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20 19 0 0 0 0
33 19 0 0 0 0
34 20 0 0 0 0
35 21 0 0 0 0
36 21 0 0 0 0
37 21 0 0 0 0
14 38 0 0 0 0
M END
$$$$
2-aminopyridine0.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.1787 0.7279 0.0496 O 0 0 0 0 0 0 0 0 0 0 1
-2.1731 0.7593 -0.0068 H 0 0 0 0 0 0 0 0 0 0 2
-3.3753 0.8918 0.9883 H 0 0 0 0 0 0 0 0 0 0 3
0.5287 1.4578 -0.0791 C 0 0 0 0 0 0 0 0 0 0 4
1.8899 1.1872 0.0067 C 0 0 0 0 0 0 0 0 0 0 5
2.2841 -0.1601 0.0871 C 0 0 0 0 0 0 0 0 0 0 6
1.3253 -1.1622 0.0709 C 0 0 0 0 0 0 0 0 0 0 7
-0.0400 -0.7970 -0.0276 C 0 0 0 0 0 0 0 0 0 0 8
-0.4227 0.5014 -0.0968 N 0 0 0 0 0 0 0 0 0 0 9
-1.0349 -1.7410 -0.1125 N 0 0 0 0 0 0 0 0 0 0 10
-1.9868 -1.4145 0.0520 H 0 0 0 0 0 0 0 0 0 0 11
-0.8328 -2.6780 0.2235 H 0 0 0 0 0 0 0 0 0 0 12
0.1628 2.4860 -0.1362 H 0 0 0 0 0 0 0 0 0 0 13
2.6172 1.9980 0.0166 H 0 0 0 0 0 0 0 0 0 0 14
3.3408 -0.4223 0.1627 H 0 0 0 0 0 0 0 0 0 0 15
1.6050 -2.2147 0.1294 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
7 16 0 0 0 0
M END
$$$$
2-aminopyridine1.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.2025 -0.1015 -0.7335 O 0 0 0 0 0 0 0 0 0 0 1
-2.1987 -0.0183 -0.7201 H 0 0 0 0 0 0 0 0 0 0 2
-3.5222 0.8162 -0.6877 H 0 0 0 0 0 0 0 0 0 0 3
0.4760 0.0355 -1.4565 C 0 0 0 0 0 0 0 0 0 0 4
1.8481 0.0020 -1.2339 C 0 0 0 0 0 0 0 0 0 0 5
2.2923 -0.0355 0.0995 C 0 0 0 0 0 0 0 0 0 0 6
1.3692 -0.0321 1.1346 C 0 0 0 0 0 0 0 0 0 0 7
-0.0109 0.0086 0.8171 C 0 0 0 0 0 0 0 0 0 0 8
-0.4418 0.0370 -0.4674 N 0 0 0 0 0 0 0 0 0 0 9
-0.9730 0.0721 1.7960 N 0 0 0 0 0 0 0 0 0 0 10
-1.9267 -0.1472 1.5124 H 0 0 0 0 0 0 0 0 0 0 11
-0.7209 -0.2316 2.7319 H 0 0 0 0 0 0 0 0 0 0 12
0.0728 0.0595 -2.4721 H 0 0 0 0 0 0 0 0 0 0 13
2.5462 0.0009 -2.0701 H 0 0 0 0 0 0 0 0 0 0 14
3.3597 -0.0688 0.3252 H 0 0 0 0 0 0 0 0 0 0 15
1.6877 -0.0595 2.1774 H 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
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14 4 0 0 0 0
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15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
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11 7 0 0 0 0
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12 10 0 0 0 0
13 10 0 0 0 0
20 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
19 12 0 0 0 0
21 19 0 0 0 0
22 19 0 0 0 0
19 23 0 0 0 0
M END
$$$$
2-methylindole-cation1.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
-3.0723 -0.1149 -2.1235 O 0 0 0 0 0 0 0 0 0 0 1
-3.0625 -0.8501 -2.7630 H 0 0 0 0 0 0 0 0 0 0 2
-3.1223 0.6891 -2.6716 H 0 0 0 0 0 0 0 0 0 0 3
2.3194 0.1988 -1.4919 C 0 0 0 0 0 0 0 0 0 0 4
3.0229 0.1156 -0.2375 C 0 0 0 0 0 0 0 0 0 0 5
2.3522 -0.0507 0.9446 C 0 0 0 0 0 0 0 0 0 0 6
0.9222 -0.1412 0.9016 C 0 0 0 0 0 0 0 0 0 0 7
0.2246 -0.0515 -0.3836 C 0 0 0 0 0 0 0 0 0 0 8
0.9495 0.1169 -1.5929 C 0 0 0 0 0 0 0 0 0 0 9
-1.0872 -0.1571 -0.1881 N 0 0 0 0 0 0 0 0 0 0 10
-0.0359 -0.3026 1.8698 C 0 0 0 0 0 0 0 0 0 0 11
-1.3790 -0.3367 1.2322 C 0 0 0 0 0 0 0 0 0 0 12
-1.8203 -0.1385 -0.9388 H 0 0 0 0 0 0 0 0 0 0 13
-2.4023 0.6799 1.7749 C 0 0 0 0 0 0 0 0 0 0 14
-1.7947 -1.3561 1.3699 H 0 0 0 0 0 0 0 0 0 0 15
2.9078 0.3312 -2.4014 H 0 0 0 0 0 0 0 0 0 0 16
4.1105 0.1881 -0.2472 H 0 0 0 0 0 0 0 0 0 0 17
2.8758 -0.1163 1.8986 H 0 0 0 0 0 0 0 0 0 0 18
0.4397 0.1824 -2.5536 H 0 0 0 0 0 0 0 0 0 0 19
0.1157 -0.4065 2.9423 H 0 0 0 0 0 0 0 0 0 0 20
-3.3503 0.5771 1.2331 H 0 0 0 0 0 0 0 0 0 0 21
-2.5821 0.4788 2.8380 H 0 0 0 0 0 0 0 0 0 0 22
-2.0252 1.7036 1.6592 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
14 12 0 0 0 0
15 12 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
14 23 0 0 0 0
M END
$$$$
2-methylindole-cation2.sdf
COSMOtherm 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
-2.9036 0.0044 -2.2117 O 0 0 0 0 0 0 0 0 0 0 1
-2.8905 -0.7612 -2.8148 H 0 0 0 0 0 0 0 0 0 0 2
-2.8973 0.7848 -2.7956 H 0 0 0 0 0 0 0 0 0 0 3
2.4642 -0.0021 -1.3987 C 0 0 0 0 0 0 0 0 0 0 4
3.0703 0.0017 -0.1328 C 0 0 0 0 0 0 0 0 0 0 5
2.3038 0.0038 1.0439 C 0 0 0 0 0 0 0 0 0 0 6
0.9175 0.0016 0.9252 C 0 0 0 0 0 0 0 0 0 0 7
0.3337 -0.0019 -0.3526 C 0 0 0 0 0 0 0 0 0 0 8
1.0696 -0.0043 -1.5333 C 0 0 0 0 0 0 0 0 0 0 9
-1.0778 -0.0032 -0.1902 N 0 0 0 0 0 0 0 0 0 0 10
-0.1999 0.0020 1.9327 C 0 0 0 0 0 0 0 0 0 0 11
-1.4290 -0.0011 1.0740 C 0 0 0 0 0 0 0 0 0 0 12
-1.7652 -0.0034 -1.0007 H 0 0 0 0 0 0 0 0 0 0 13
-0.1999 0.8831 2.5963 H 0 0 0 0 0 0 0 0 0 0 14
-0.1976 -0.8769 2.5991 H 0 0 0 0 0 0 0 0 0 0 15
3.0865 -0.0039 -2.2944 H 0 0 0 0 0 0 0 0 0 0 16
4.1589 0.0030 -0.0615 H 0 0 0 0 0 0 0 0 0 0 17
2.7872 0.0063 2.0218 H 0 0 0 0 0 0 0 0 0 0 18
0.5911 -0.0070 -2.5129 H 0 0 0 0 0 0 0 0 0 0 19
-2.8284 -0.0030 1.5422 C 0 0 0 0 0 0 0 0 0 0 20
-3.0038 -0.8866 2.1751 H 0 0 0 0 0 0 0 0 0 0 21
-3.0058 0.8776 2.1785 H 0 0 0 0 0 0 0 0 0 0 22
-3.5405 -0.0026 0.7095 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0

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6 5 0 0 0 0
17 5 0 0 0 0
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18 6 0 0 0 0
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19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 20 0 0 0 0
22 20 0 0 0 0
20 23 0 0 0 0
M END
$$$$
2-methylindole.sdf
COSMOtherm 3D 0
22 22 0 0 0 0 0 0 0 0 0 V2000
-3.0510 -2.2527 0.0235 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.9347 -2.9000 0.7422 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0829 -2.7954 -0.7848 H 0 0 0 0 0 0 0 0 0 0 0 3
2.3322 1.0011 0.0123 C 0 0 0 0 0 0 0 0 0 0 0 4
3.0682 -0.1851 0.0061 C 0 0 0 0 0 0 0 0 0 0 0 5
2.4261 -1.4445 -0.0072 C 0 0 0 0 0 0 0 0 0 0 0 6
1.0325 -1.5448 -0.0150 C 0 0 0 0 0 0 0 0 0 0 0 7
0.2940 -0.3536 -0.0086 C 0 0 0 0 0 0 0 0 0 0 0 8
0.9237 0.9348 0.0052 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.1349 1.9060 0.0094 C 0 0 0 0 0 0 0 0 0 0 0 10
-1.3359 1.2151 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 11
-2.7379 1.7307 -0.0089 C 0 0 0 0 0 0 0 0 0 0 0 12
-1.0722 -0.1470 -0.0146 N 0 0 0 0 0 0 0 0 0 0 0 13
2.8416 1.9677 0.0227 H 0 0 0 0 0 0 0 0 0 0 0 14
4.1594 -0.1427 0.0111 H 0 0 0 0 0 0 0 0 0 0 0 15
3.0284 -2.3550 -0.0119 H 0 0 0 0 0 0 0 0 0 0 0 16
0.5380 -2.5181 -0.0256 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.0326 2.9883 0.0192 H 0 0 0 0 0 0 0 0 0 0 0 18
-3.2702 1.4416 -0.9291 H 0 0 0 0 0 0 0 0 0 0 0 19
-3.3178 1.3380 0.8409 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.7380 2.8260 0.0541 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.7863 -0.8950 -0.0088 H 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
19 12 0 0 0 0
20 12 0 0 0 0
21 12 0 0 0 0
13 22 0 0 0 0
M END
$$$$
2-methylpyrrole-cation0.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-2.6590 0.4143 -0.4713 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.2414 -0.0140 -1.1262 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.6620 1.3602 -0.7096 H 0 0 0 0 0 0 0 0 0 0 0 3
1.6220 0.3213 -1.1109 C 0 0 0 0 0 0 0 0 0 0 0 4
1.5638 0.5509 0.3296 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5606 -0.4194 -1.4817 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2539 -0.6730 -0.2889 N 0 0 0 0 0 0 0 0 0 0 0 7
0.4670 -0.0498 0.8432 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3992 0.6882 -1.7762 H 0 0 0 0 0 0 0 0 0 0 0 9
2.2921 1.1172 0.9045 H 0 0 0 0 0 0 0 0 0 0 0 10
0.2238 -0.8114 -2.4350 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4149 -1.6815 -0.1393 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0925 -0.1596 2.2129 C 0 0 0 0 0 0 0 0 0 0 0 13
-1.2582 -0.2228 -0.4003 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.1810 -1.2104 2.5299 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5656 0.3601 2.9193 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.0954 0.2905 2.2791 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
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13 8 0 0 0 0
15 13 0 0 0 0

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6 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
4 17 0 0 0 0
M END
$$$$
2-methylpyrrole-cation4.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 V2000
-3.0040 -0.4190 0.0159 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.3964 -1.0518 0.6449 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4136 -0.6353 -0.8418 H 0 0 0 0 0 0 0 0 0 0 0 3
0.4695 -1.4531 -0.0051 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.2833 -0.3892 -0.0048 N 0 0 0 0 0 0 0 0 0 0 0 5
1.8872 -1.0392 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 6
1.8000 0.4530 0.0033 C 0 0 0 0 0 0 0 0 0 0 0 7
0.4976 0.8174 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1812 2.1408 0.0022 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.3477 -0.4101 -0.0061 H 0 0 0 0 0 0 0 0 0 0 0 10
2.4193 -1.4568 -0.8753 H 0 0 0 0 0 0 0 0 0 0 0 11
2.6544 1.1231 0.0074 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.8164 2.2618 -0.8879 H 0 0 0 0 0 0 0 0 0 0 0 13
0.5668 2.9420 0.0065 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.8218 2.2572 0.8890 H 0 0 0 0 0 0 0 0 0 0 0 15
0.0568 -2.4595 -0.0091 H 0 0 0 0 0 0 0 0 0 0 0 16
2.4149 -1.4612 0.8750 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
16 4 0 0 0 0
8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 9 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
6 17 0 0 0 0
M END
$$$$
2-methylpyrrole.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 V2000
-3.1515 0.0009 0.4699 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5751 -0.7676 0.0472 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5727 0.7694 0.0446 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8655 0.0011 -0.3578 C 0 0 0 0 0 0 0 0 0 0 0 4
1.8749 0.0008 1.0723 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5376 -0.0003 -0.7750 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2450 -0.0015 0.3622 N 0 0 0 0 0 0 0 0 0 0 0 7
0.5520 -0.0008 1.4887 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0562 -0.0004 -2.1487 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.2777 -0.0016 0.3688 H 0 0 0 0 0 0 0 0 0 0 0 10
2.7310 0.0021 -1.0164 H 0 0 0 0 0 0 0 0 0 0 0 11
2.7476 0.0015 1.7207 H 0 0 0 0 0 0 0 0 0 0 0 12
0.1153 -0.0016 2.4829 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.6864 -0.8865 -2.3265 H 0 0 0 0 0 0 0 0 0 0 0 14
0.7433 -0.0026 -2.9010 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.6830 0.8878 -2.3282 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
11 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
9 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
9 16 0 0 0 0
M END
$$$$
2-methylpyrrole_90.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 V2000
-3.1515 0.0009 0.4699 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5751 -0.7676 0.0472 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5727 0.7694 0.0446 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8655 0.0011 -0.3578 C 0 0 0 0 0 0 0 0 0 0 0 4
1.8749 0.0008 1.0723 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5376 -0.0003 -0.7750 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2450 -0.0015 0.3622 N 0 0 0 0 0 0 0 0 0 0 0 7
0.5520 -0.0008 1.4887 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.0562 -0.0004 -2.1487 C 0 0 0 0 0 0 0 0 0 0 0 9

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3 -1.2777 -0.0016 0.3688 H 0 0 0 0 0 0 0 0 0 0 10
4 2.7310 0.0021 -1.0164 H 0 0 0 0 0 0 0 0 0 0 11
5 2.7476 0.0015 1.7207 H 0 0 0 0 0 0 0 0 0 0 12
6 0.1153 -0.0016 2.4829 H 0 0 0 0 0 0 0 0 0 0 13
7 -0.6864 -0.8865 -2.3265 H 0 0 0 0 0 0 0 0 0 0 14
8 0.7433 -0.0026 -2.9010 H 0 0 0 0 0 0 0 0 0 0 15
9 -0.6830 0.8878 -2.3282 H 0 0 0 0 0 0 0 0 0 0 16
10 2 1 0 0 0 0
11 3 1 0 0 0 0
12 5 4 0 0 0 0
13 6 4 0 0 0 0
14 11 4 0 0 0 0
15 8 5 0 0 0 0
16 12 5 0 0 0 0
17 7 6 0 0 0 0
18 9 6 0 0 0 0
19 8 7 0 0 0 0
20 10 7 0 0 0 0
21 13 8 0 0 0 0
22 14 9 0 0 0 0
23 15 9 0 0 0 0
24 9 16 0 0 0 0
M END
$$$$
3-aminopyridine.sdf
COSMOtherm 3D 0
16 15 0 0 0 0 0 0 0 0 0 V2000
-3.6378 0.6632 -0.0544 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.6709 0.3789 -0.0212 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.8323 0.9639 0.8499 H 0 0 0 0 0 0 0 0 0 0 0 3
2.2989 1.5481 -0.0048 N 0 0 0 0 0 0 0 0 0 0 0 4
1.3698 0.5464 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.0178 0.8346 -0.0024 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.9676 -0.1109 -0.0016 N 0 0 0 0 0 0 0 0 0 0 0 7
-0.6045 -1.4102 0.0020 C 0 0 0 0 0 0 0 0 0 0 0 8
0.7407 -1.7933 0.0038 C 0 0 0 0 0 0 0 0 0 0 0 9
1.7351 -0.8194 0.0029 C 0 0 0 0 0 0 0 0 0 0 0 10
2.0202 2.5218 0.0202 H 0 0 0 0 0 0 0 0 0 0 0 11
3.2907 1.3426 0.0152 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.3590 1.8739 -0.0056 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.4114 -2.1453 0.0039 H 0 0 0 0 0 0 0 0 0 0 0 14
1.0076 -2.8512 0.0066 H 0 0 0 0 0 0 0 0 0 0 0 15
2.7903 -1.1000 0.0045 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
15 9 0 0 0 0
10 16 0 0 0 0
M END
$$$$
3-aminopyridine-cation.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-3.5120 -0.0007 0.7133 O 0 0 0 0 0 0 0 0 0 0 0 1
-4.0281 -0.7757 0.4250 H 0 0 0 0 0 0 0 0 0 0 0 2
-4.0343 0.7683 0.4202 H 0 0 0 0 0 0 0 0 0 0 0 3
2.3385 0.0386 1.5211 N 0 0 0 0 0 0 0 0 0 0 0 4
1.3876 -0.0065 0.5446 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0162 -0.0057 0.8681 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.9110 0.0014 -0.1076 N 0 0 0 0 0 0 0 0 0 0 0 7
-0.6145 0.0052 -1.4237 C 0 0 0 0 0 0 0 0 0 0 0 8
0.7260 -0.0003 -1.8017 C 0 0 0 0 0 0 0 0 0 0 0 9
1.7218 -0.0070 -0.8334 C 0 0 0 0 0 0 0 0 0 0 0 10
2.0768 -0.1743 2.4791 H 0 0 0 0 0 0 0 0 0 0 0 11
3.2990 -0.1816 1.2753 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.3517 -0.0093 1.8922 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.4500 0.0105 -2.1188 H 0 0 0 0 0 0 0 0 0 0 0 14
0.9834 -0.0012 -2.8597 H 0 0 0 0 0 0 0 0 0 0 0 15
2.7722 -0.0122 -1.1282 H 0 0 0 0 0 0 0 0 0 0 0 16
-1.9315 0.0013 0.1819 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
10 9 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
7 17 0 0 0 0
M END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine.sdf
COSMOtherm 3D 0
38 39 0 0 0 0 0 0 0 0 0 V2000
-2.3433 0.3376 -4.0730 O 0 0 0 0 0 0 0 0 0 0 0 1
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-1.6066  0.5395  -3.4197  H  0  0  0  0  0  0  0  0  0  0  2
-2.0160  0.6666  -4.9286  H  0  0  0  0  0  0  0  0  0  0  3
  0.5356  3.7225  -0.9611  C  0  0  0  0  0  0  0  0  0  0  4
  0.9173  3.4758  0.3694  C  0  0  0  0  0  0  0  0  0  0  5
  0.8888  2.1767  0.8571  C  0  0  0  0  0  0  0  0  0  0  6
  0.5164  1.0728  0.0472  C  0  0  0  0  0  0  0  0  0  0  7
  0.1569  1.3261  -1.3192  C  0  0  0  0  0  0  0  0  0  0  8
  0.1555  2.6669  -1.7774  C  0  0  0  0  0  0  0  0  0  0  9
  0.4403  -0.2434  0.6958  C  0  0  0  0  0  0  0  0  0  0  10
  0.8221  -1.3482  0.0434  N  0  0  0  0  0  0  0  0  0  0  11
  1.3718  -1.2063  -1.3372  C  0  0  0  0  0  0  0  0  0  0  12
-0.2785  0.3701  -2.2305  N  0  0  0  0  0  0  0  0  0  0  13
  0.2138  -0.8500  -2.2344  C  0  0  0  0  0  0  0  0  0  0  14
-0.0666  -0.3668  2.0810  C  0  0  0  0  0  0  0  0  0  0  15
-0.3440  -1.7958  -3.0185  N  0  0  0  0  0  0  0  0  0  0  16
-1.2012  0.3735  2.4691  C  0  0  0  0  0  0  0  0  0  0  17
-1.6984  0.2869  3.7719  C  0  0  0  0  0  0  0  0  0  0  18
-1.0608  -0.5276  4.7143  C  0  0  0  0  0  0  0  0  0  0  19
  0.0739  -1.2601  4.3419  C  0  0  0  0  0  0  0  0  0  0  20
  0.5637  -1.1896  3.0364  C  0  0  0  0  0  0  0  0  0  0  21
  0.2061  -3.1173  -3.3159  C  0  0  0  0  0  0  0  0  0  0  22
  0.7034  -2.5588  0.4810  O  0  0  0  0  0  0  0  0  0  0  23
-1.1346  -1.4726  -3.5854  H  0  0  0  0  0  0  0  0  0  0  24
  0.5379  4.7403  -1.3553  H  0  0  0  0  0  0  0  0  0  0  25
  1.2267  4.2962  1.0184  H  0  0  0  0  0  0  0  0  0  0  26
  1.1685  1.9863  1.8942  H  0  0  0  0  0  0  0  0  0  0  27
-0.1491  2.8460  -2.8100  H  0  0  0  0  0  0  0  0  0  0  28
  2.1173  -0.4000  -1.3497  H  0  0  0  0  0  0  0  0  0  0  29
  1.8472  -2.1597  -1.5747  H  0  0  0  0  0  0  0  0  0  0  30
-1.7007  1.0145  1.7410  H  0  0  0  0  0  0  0  0  0  0  31
-2.5852  0.8588  4.0508  H  0  0  0  0  0  0  0  0  0  0  32
-1.4457  -0.5930  5.7336  H  0  0  0  0  0  0  0  0  0  0  33
  0.5807  -1.8919  5.0738  H  0  0  0  0  0  0  0  0  0  0  34
  1.4399  -1.7716  2.7538  H  0  0  0  0  0  0  0  0  0  0  35
-0.5537  -3.6748  -3.8735  H  0  0  0  0  0  0  0  0  0  0  36
  1.1168  -3.0577  -3.9313  H  0  0  0  0  0  0  0  0  0  0  37
  0.4256  -3.6726  -2.3952  H  0  0  0  0  0  0  0  0  0  0  38

  2  1  0  0  0  0
  3  1  0  0  0  0
  5  4  0  0  0  0
  9  4  0  0  0  0
25  4  0  0  0  0
  6  5  0  0  0  0
26  5  0  0  0  0
  7  6  0  0  0  0
27  6  0  0  0  0
  8  7  0  0  0  0
10  7  0  0  0  0
  9  8  0  0  0  0
13  8  0  0  0  0
28  9  0  0  0  0
11 10  0  0  0  0
15 10  0  0  0  0
12 11  0  0  0  0
23 11  0  0  0  0
14 12  0  0  0  0
29 12  0  0  0  0
30 12  0  0  0  0
14 13  0  0  0  0
16 14  0  0  0  0
17 15  0  0  0  0
21 15  0  0  0  0
22 16  0  0  0  0
24 16  0  0  0  0
18 17  0  0  0  0
31 17  0  0  0  0
19 18  0  0  0  0
32 18  0  0  0  0
20 19  0  0  0  0
33 19  0  0  0  0
21 20  0  0  0  0
34 20  0  0  0  0
35 21  0  0  0  0
36 22  0  0  0  0
37 22  0  0  0  0
22 38  0  0  0  0

M  END
$$$$
3-hydro-2-methylamine-4-oxy-5-phenyl-1,4-benzodiazepine-cation.sdf
COSMOTHERM 3D 0
39 40 0 0 0 0 0 0 0 0 V2000
-4.2172  0.2359  2.1508  O  0  0  0  0  0  0  0  0  0  0  1
-5.1005  0.6325  2.0413  H  0  0  0  0  0  0  0  0  0  0  2
-4.0375  0.2649  3.1082  H  0  0  0  0  0  0  0  0  0  0  3
-0.8211  3.7614  -0.4850  C  0  0  0  0  0  0  0  0  0  0  4
  0.4864  3.4755  -0.9049  C  0  0  0  0  0  0  0  0  0  0  5
  0.9406  2.1625  -0.9057  C  0  0  0  0  0  0  0  0  0  0  6
  0.1138  1.0826  -0.5109  C  0  0  0  0  0  0  0  0  0  0  7
-1.2225  1.3916  -0.1327  C  0  0  0  0  0  0  0  0  0  0  8
-1.6662  2.7250  -0.1050  C  0  0  0  0  0  0  0  0  0  0  9
  0.7216  -0.2546  -0.4284  C  0  0  0  0  0  0  0  0  0  0  10
  0.0338  -1.3404  -0.7985  N  0  0  0  0  0  0  0  0  0  0  11
-1.3454  -1.1642  -1.3627  C  0  0  0  0  0  0  0  0  0  0  12
-2.1455  0.4097  0.2885  N  0  0  0  0  0  0  0  0  0  0  13
-2.2620  -0.8195  -0.2343  C  0  0  0  0  0  0  0  0  0  0  14
  2.1036  -0.4095  0.0732  C  0  0  0  0  0  0  0  0  0  0  15
-3.1398  -1.6742  0.2645  N  0  0  0  0  0  0  0  0  0  0  16
  2.5180  0.3404  1.1924  C  0  0  0  0  0  0  0  0  0  0  17
  3.8200  0.2233  1.6839  C  0  0  0  0  0  0  0  0  0  0  18
  4.7338  -0.6296  1.0551  C  0  0  0  0  0  0  0  0  0  0  19
  4.3347  -1.3707  -0.0645  C  0  0  0  0  0  0  0  0  0  0  20
  3.0291  -1.2721  -0.5485  C  0  0  0  0  0  0  0  0  0  0  21
-3.4366  -3.0150  -0.2502  C  0  0  0  0  0  0  0  0  0  0  22
  0.4321  -2.5580  -0.6880  O  0  0  0  0  0  0  0  0  0  0  23

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24 4 0 0 0 0
6 5 0 0 0 0
25 5 0 0 0 0
7 6 0 0 0 0
26 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
27 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
14 12 0 0 0 0
28 12 0 0 0 0
29 12 0 0 0 0
14 13 0 0 0 0
38 13 0 0 0 0
16 14 0 0 0 0
17 15 0 0 0 0
21 15 0 0 0 0
22 16 0 0 0 0
18 17 0 0 0 0
30 17 0 0 0 0
19 18 0 0 0 0
31 18 0 0 0 0
20 19 0 0 0 0
32 19 0 0 0 0
21 20 0 0 0 0
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34 21 0 0 0 0
35 22 0 0 0 0
36 22 0 0 0 0
37 22 0 0 0 0
16 39 0 0 0 0

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M END

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3-methylindole-cation0.sdf

COSMOtherm 3D 0

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23 23 0 0 0 0 0 0 0 0 0 V2000
1.4088 0.2248 -0.5581 O 0 0 0 0 0 0 0 0 0 0 1
0.5021 -0.0947 -0.7229 H 0 0 0 0 0 0 0 0 0 0 2
1.3007 1.1602 -0.3040 H 0 0 0 0 0 0 0 0 0 0 3
4.5367 -3.6329 -1.2507 C 0 0 0 0 0 0 0 0 0 0 4
5.8553 -3.2897 -0.9131 C 0 0 0 0 0 0 0 0 0 0 5
6.1299 -2.3282 0.0685 C 0 0 0 0 0 0 0 0 0 0 6
5.0504 -1.7114 0.7112 C 0 0 0 0 0 0 0 0 0 0 7
3.7454 -2.0756 0.3494 C 0 0 0 0 0 0 0 0 0 0 8
3.4438 -3.0205 -0.6152 C 0 0 0 0 0 0 0 0 0 0 9
2.8080 -1.2683 1.1442 N 0 0 0 0 0 0 0 0 0 0 10
4.9721 -0.6855 1.7625 C 0 0 0 0 0 0 0 0 0 0 11
3.6690 -0.4419 2.0132 C 0 0 0 0 0 0 0 0 0 0 12
2.1647 -1.8528 1.7002 H 0 0 0 0 0 0 0 0 0 0 13
4.3528 -4.3863 -2.0171 H 0 0 0 0 0 0 0 0 0 0 14
6.6827 -3.7822 -1.4260 H 0 0 0 0 0 0 0 0 0 0 15
7.1589 -2.0707 0.3228 H 0 0 0 0 0 0 0 0 0 0 16
2.4175 -3.2832 -0.8724 H 0 0 0 0 0 0 0 0 0 0 17
6.1460 -0.0453 2.4247 C 0 0 0 0 0 0 0 0 0 0 18
3.1817 0.2295 2.7128 H 0 0 0 0 0 0 0 0 0 0 19
2.1826 -0.6442 0.4955 H 0 0 0 0 0 0 0 0 0 0 20
6.7817 0.4609 1.6823 H 0 0 0 0 0 0 0 0 0 0 21
6.7690 -0.8052 2.9208 H 0 0 0 0 0 0 0 0 0 0 22
5.8301 0.6904 3.1740 H 0 0 0 0 0 0 0 0 0 0 23

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2 1 0 0 0 0

3 1 0 0 0 0

5 4 0 0 0 0

9 4 0 0 0 0

14 4 0 0 0 0

6 5 0 0 0 0

15 5 0 0 0 0

7 6 0 0 0 0

16 6 0 0 0 0

8 7 0 0 0 0

11 7 0 0 0 0

9 8 0 0 0 0

10 8 0 0 0 0

17 9 0 0 0 0

12 10 0 0 0 0

13 10 0 0 0 0

20 10 0 0 0 0

12 11 0 0 0 0

18 11 0 0 0 0

19 12 0 0 0 0

21 18 0 0 0 0

22 18 0 0 0 0

18 23 0 0 0 0

M END

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3-methylindole-cation1.sdf

COSMOtherm 3D 0

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23 23 0 0 0 0 0 0 0 0 0 V2000
0.8175 0.0068 -0.2490 O 0 0 0 0 0 0 0 0 0 0 1
0.3335 -0.7595 0.1086 H 0 0 0 0 0 0 0 0 0 0 2
0.3367 0.7838 0.0895 H 0 0 0 0 0 0 0 0 0 0 3
4.9342 -0.0407 3.4195 C 0 0 0 0 0 0 0 0 0 0 4
6.3305 -0.0700 3.0818 C 0 0 0 0 0 0 0 0 0 0 5
6.7425 -0.0813 1.7728 C 0 0 0 0 0 0 0 0 0 0 6
5.7454 -0.0620 0.7486 C 0 0 0 0 0 0 0 0 0 0 7
4.3345 -0.0320 1.1104 C 0 0 0 0 0 0 0 0 0 0 8
3.9344 -0.0221 2.4720 C 0 0 0 0 0 0 0 0 0 0 9
3.5827 -0.0164 0.0072 N 0 0 0 0 0 0 0 0 0 0 10
5.8264 -0.0625 -0.6354 C 0 0 0 0 0 0 0 0 0 0 11

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3 4.4347 -0.0389 -1.1649 C 0 0 0 0 0 0 0 0 0 0 12
4 2.5374 -0.0029 -0.0304 H 0 0 0 0 0 0 0 0 0 0 13
5 4.2295 -0.9264 -1.7901 H 0 0 0 0 0 0 0 0 0 0 14
6 4.2572 0.8407 -1.8090 H 0 0 0 0 0 0 0 0 0 0 15
7 4.6601 -0.0334 4.4759 H 0 0 0 0 0 0 0 0 0 0 16
8 7.0628 -0.0838 3.8893 H 0 0 0 0 0 0 0 0 0 0 17
9 7.8010 -0.1036 1.5117 H 0 0 0 0 0 0 0 0 0 0 18
10 2.8815 -0.0005 2.7508 H 0 0 0 0 0 0 0 0 0 0 19
11 7.0294 -0.0652 -1.5013 C 0 0 0 0 0 0 0 0 0 0 20
12 7.7552 -0.8217 -1.1687 H 0 0 0 0 0 0 0 0 0 0 21
13 7.5379 0.9120 -1.4403 H 0 0 0 0 0 0 0 0 0 0 22
14 6.7734 -0.2492 -2.5515 H 0 0 0 0 0 0 0 0 0 0 23
15 2 1 0 0 0 0
16 3 1 0 0 0 0
17 5 4 0 0 0 0
18 9 4 0 0 0 0
19 16 4 0 0 0 0
20 6 5 0 0 0 0
21 17 5 0 0 0 0
22 7 6 0 0 0 0
23 18 6 0 0 0 0
24 8 7 0 0 0 0
25 11 7 0 0 0 0
26 9 8 0 0 0 0
27 10 8 0 0 0 0
28 19 9 0 0 0 0
29 12 10 0 0 0 0
30 13 10 0 0 0 0
31 12 11 0 0 0 0
32 20 11 0 0 0 0
33 14 12 0 0 0 0
34 15 12 0 0 0 0
35 21 20 0 0 0 0
36 22 20 0 0 0 0
37 20 23 0 0 0 0
M END
\$\$\$\$
3-methylindole-cation2.sdf
COSMOTHERM 3D 0
23 23 0 0 0 0 0 0 0 0 0 V2000
1.2525 -0.4529 -0.8008 O 0 0 0 0 0 0 0 0 0 0 1
0.6379 -1.1429 -0.4899 H 0 0 0 0 0 0 0 0 0 0 2
0.6974 0.1644 -1.3118 H 0 0 0 0 0 0 0 0 0 0 3
6.3816 0.3414 0.4727 C 0 0 0 0 0 0 0 0 0 0 4
6.8243 1.0293 1.6141 C 0 0 0 0 0 0 0 0 0 0 5
5.9186 1.5731 2.5389 C 0 0 0 0 0 0 0 0 0 0 6
4.5574 1.4162 2.2957 C 0 0 0 0 0 0 0 0 0 0 7
4.1401 0.7253 1.1450 C 0 0 0 0 0 0 0 0 0 0 8
5.0155 0.1739 0.2143 C 0 0 0 0 0 0 0 0 0 0 9
2.7177 0.7147 1.1362 N 0 0 0 0 0 0 0 0 0 0 10
3.3243 1.8562 3.0522 C 0 0 0 0 0 0 0 0 0 0 11
2.2351 1.3350 2.1745 C 0 0 0 0 0 0 0 0 0 0 12
2.1200 0.2545 0.3763 H 0 0 0 0 0 0 0 0 0 0 13
3.2048 3.3670 3.3574 C 0 0 0 0 0 0 0 0 0 0 14
3.2466 1.3072 4.0114 H 0 0 0 0 0 0 0 0 0 0 15
7.1115 -0.0695 -0.2254 H 0 0 0 0 0 0 0 0 0 0 16
7.8956 1.1425 1.7863 H 0 0 0 0 0 0 0 0 0 0 17
6.2803 2.1017 3.4219 H 0 0 0 0 0 0 0 0 0 0 18
4.6614 -0.3597 -0.6677 H 0 0 0 0 0 0 0 0 0 0 19
1.1621 1.4272 2.3344 H 0 0 0 0 0 0 0 0 0 0 20
2.2584 3.5795 3.8707 H 0 0 0 0 0 0 0 0 0 0 21
4.0310 3.6696 4.0124 H 0 0 0 0 0 0 0 0 0 0 22
3.2516 3.9553 2.4324 H 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
19 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
20 12 0 0 0 0
21 14 0 0 0 0
22 14 0 0 0 0
14 23 0 0 0 0
M END
\$\$\$\$
3-methylindole.sdf
COSMOTHERM 3D 0
22 22 0 0 0 0 0 0 0 0 0 V2000
-4.0948 0.0052 -0.5293 O 0 0 0 0 0 0 0 0 0 0 1
-4.3574 -0.7628 -1.0677 H 0 0 0 0 0 0 0 0 0 0 2
-4.3486 0.7751 -1.0692 H 0 0 0 0 0 0 0 0 0 0 3
0.9313 0.0001 0.3719 C 0 0 0 0 0 0 0 0 0 0 4
2.2160 0.0026 -0.2101 C 0 0 0 0 0 0 0 0 0 0 5
2.3309 0.0025 -1.6005 C 0 0 0 0 0 0 0 0 0 0 6
1.1836 -0.0004 -2.4287 C 0 0 0 0 0 0 0 0 0 0 7
-0.1019 -0.0030 -1.8849 C 0 0 0 0 0 0 0 0 0 0 8
-0.2175 -0.0028 -0.4866 C 0 0 0 0 0 0 0 0 0 0 9
3.1103 0.0048 0.4172 H 0 0 0 0 0 0 0 0 0 0 10
3.3210 0.0048 -2.0613 H 0 0 0 0 0 0 0 0 0 0 11
1.3057 -0.0005 -3.5136 H 0 0 0 0 0 0 0 0 0 0 12

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9 7 0 0 0 0
12 8 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
10 17 0 0 0 0
M END
$$$$
3-methylpyrrole-cation2.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
0.6594 0.2895 -0.6696 O 0 0 0 0 0 0 0 0 0 0 0 1
0.1119 -0.3142 -1.2047 H 0 0 0 0 0 0 0 0 0 0 0 2
0.0195 0.8590 -0.2043 H 0 0 0 0 0 0 0 0 0 0 0 3
3.3615 -2.2364 2.6033 C 0 0 0 0 0 0 0 0 0 0 0 4
4.4315 -1.5289 1.8212 C 0 0 0 0 0 0 0 0 0 0 0 5
2.1210 -1.7475 1.9489 C 0 0 0 0 0 0 0 0 0 0 0 6
2.4320 -0.9436 0.9708 N 0 0 0 0 0 0 0 0 0 0 0 7
3.8446 -0.7859 0.8634 C 0 0 0 0 0 0 0 0 0 0 0 8
3.4157 -3.3224 2.3701 H 0 0 0 0 0 0 0 0 0 0 0 9
3.4000 -2.0871 4.1415 C 0 0 0 0 0 0 0 0 0 0 0 10
1.7249 -0.4692 0.3298 H 0 0 0 0 0 0 0 0 0 0 0 11
5.4975 -1.6268 2.0048 H 0 0 0 0 0 0 0 0 0 0 0 12
1.0900 -1.9981 2.1896 H 0 0 0 0 0 0 0 0 0 0 0 13
4.2528 -0.1442 0.0893 H 0 0 0 0 0 0 0 0 0 0 0 14
2.5658 -2.6351 4.5967 H 0 0 0 0 0 0 0 0 0 0 0 15
4.3420 -2.5016 4.5204 H 0 0 0 0 0 0 0 0 0 0 0 16
3.3343 -1.0305 4.4293 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
14 8 0 0 0 0
15 10 0 0 0 0
16 10 0 0 0 0
10 17 0 0 0 0
M END

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3-methylpyrrole-cation3.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-0.4357 0.0030 3.4680 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.8860 -0.7997 3.7886 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.9981 0.7390 3.7712 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.1922 -0.0004 -1.4806 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1529 0.0001 -1.2473 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8207 0.0001 -0.1746 C 0 0 0 0 0 0 0 0 0 0 0 6
0.0701 0.0012 0.7835 N 0 0 0 0 0 0 0 0 0 0 0 7
1.4115 0.0013 0.2140 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.9334 -0.0013 -2.7784 C 0 0 0 0 0 0 0 0 0 0 0 9
1.9463 -0.0001 -1.9914 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.8874 -0.0007 0.0482 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.1432 0.0011 1.8201 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9713 -0.8843 0.5595 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.5827 -0.8857 -2.8583 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.2365 -0.0047 -3.6250 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.5781 0.8862 -2.8619 H 0 0 0 0 0 0 0 0 0 0 0 16
1.9709 0.8876 0.5582 H 0 0 0 0 0 0 0 0 0 0 0 17
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
15 9 0 0 0 0
16 9 0 0 0 0
8 17 0 0 0 0
M END

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$$$$
3-methylpyrrole-cation4.sdf
COSMOtherm 3D 0
17 16 0 0 0 0 0 0 0 0 0 V2000
-3.4628 0.4141 -0.0012 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.7790 0.9214 -0.7711 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7874 0.9095 0.7730 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4422 0.2532 -0.0007 C 0 0 0 0 0 0 0 0 0 0 0 4
1.1686 -1.2279 -0.0018 C 0 0 0 0 0 0 0 0 0 0 0 5
0.2407 0.8778 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.7928 -0.0977 0.0022 N 0 0 0 0 0 0 0 0 0 0 0 7
-0.3084 -1.3089 0.0011 C 0 0 0 0 0 0 0 0 0 0 0 8
2.7998 0.8634 0.0006 C 0 0 0 0 0 0 0 0 0 0 0 9
1.5895 -1.7501 -0.8802 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.0198 1.9315 0.0006 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.8300 0.1386 0.0047 H 0 0 0 0 0 0 0 0 0 0 0 12
2.7441 1.9588 -0.0199 H 0 0 0 0 0 0 0 0 0 0 0 13
3.3809 0.5252 -0.8712 H 0 0 0 0 0 0 0 0 0 0 0 14
3.3627 0.5587 0.8967 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.9419 -2.1926 0.0020 H 0 0 0 0 0 0 0 0 0 0 0 16

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3 3.2225 0.0231 0.0052 C 0 0 0 0 0 0 0 0 0 0 4
4 1.7186 0.0037 0.0006 C 0 0 0 0 0 0 0 0 0 0 5
5 0.9721 1.1951 0.0014 C 0 0 0 0 0 0 0 0 0 0 6
6 -0.4198 1.1371 -0.0017 C 0 0 0 0 0 0 0 0 0 0 7
7 -1.1118 -0.0212 -0.0068 N 0 0 0 0 0 0 0 0 0 0 8
8 -0.4011 -1.1652 -0.0079 C 0 0 0 0 0 0 0 0 0 0 9
9 0.9940 -1.1979 -0.0046 C 0 0 0 0 0 0 0 0 0 0 10
10 3.6025 0.5452 0.8964 H 0 0 0 0 0 0 0 0 0 0 11
11 3.6373 -0.9927 -0.0038 H 0 0 0 0 0 0 0 0 0 0 12
12 3.6084 0.5640 -0.8720 H 0 0 0 0 0 0 0 0 0 0 13
13 1.4712 2.1660 0.0052 H 0 0 0 0 0 0 0 0 0 0 14
14 -1.0145 2.0539 0.0003 H 0 0 0 0 0 0 0 0 0 0 15
15 -0.9786 -2.0929 -0.0119 H 0 0 0 0 0 0 0 0 0 0 16
16 1.5114 -2.1590 -0.0053 H 0 0 0 0 0 0 0 0 0 0 17
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M END
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4-methylpyridine-cation.sdf
COSMOtherm 3D 0
18 17 0 0 0 0 0 0 0 0 0 V2000
-3.7695 -0.0586 0.0092 O 0 0 0 0 0 0 0 0 0 0 1
-4.1810 0.2255 -0.8275 H 0 0 0 0 0 0 0 0 0 0 2
-4.2034 0.4805 0.6956 H 0 0 0 0 0 0 0 0 0 0 3
-0.4038 -1.1692 0.0028 C 0 0 0 0 0 0 0 0 0 0 4
0.9809 -1.2055 -0.0037 C 0 0 0 0 0 0 0 0 0 0 5
1.7195 -0.0085 -0.0075 C 0 0 0 0 0 0 0 0 0 0 6
1.0017 1.2034 -0.0079 C 0 0 0 0 0 0 0 0 0 0 7
-0.3816 1.1920 -0.0009 C 0 0 0 0 0 0 0 0 0 0 8
-1.0495 0.0168 0.0047 N 0 0 0 0 0 0 0 0 0 0 9
3.2176 -0.0155 0.0060 C 0 0 0 0 0 0 0 0 0 0 10
-1.0260 -2.0621 0.0044 H 0 0 0 0 0 0 0 0 0 0 11
1.4840 -2.1719 -0.0078 H 0 0 0 0 0 0 0 0 0 0 12
1.5218 2.1609 -0.0155 H 0 0 0 0 0 0 0 0 0 0 13
-0.9876 2.0959 -0.0010 H 0 0 0 0 0 0 0 0 0 0 14
-2.1106 0.0250 0.0064 H 0 0 0 0 0 0 0 0 0 0 15
3.6202 0.7133 -0.7112 H 0 0 0 0 0 0 0 0 0 0 16
3.6189 -1.0095 -0.2243 H 0 0 0 0 0 0 0 0 0 0 17
3.5826 0.2794 1.0028 H 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
17 10 0 0 0 0
10 18 0 0 0 0
M END
$$$$
4-nitroaniline-cation1.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 V2000
-1.3645 4.2122 -0.4517 O 0 0 0 0 0 0 0 0 0 0 1
-1.2480 4.7864 -1.2315 H 0 0 0 0 0 0 0 0 0 0 2
-1.7344 4.7970 0.2357 H 0 0 0 0 0 0 0 0 0 0 3
-0.0340 -0.5776 1.2644 C 0 0 0 0 0 0 0 0 0 0 4
0.2390 0.7854 1.3632 C 0 0 0 0 0 0 0 0 0 0 5
0.5918 1.4922 0.2134 C 0 0 0 0 0 0 0 0 0 0 6
0.6786 0.8771 -1.0367 C 0 0 0 0 0 0 0 0 0 0 7
0.4041 -0.4846 -1.1415 C 0 0 0 0 0 0 0 0 0 0 8
0.0527 -1.1890 0.0124 C 0 0 0 0 0 0 0 0 0 0 9
-0.2320 -2.6365 -0.0950 N 0 0 0 0 0 0 0 0 0 0 10
0.8474 2.9311 0.3128 N 0 0 0 0 0 0 0 0 0 0 11
-0.4979 -3.2577 0.9441 O 0 0 0 0 0 0 0 0 0 0 12
-0.1911 -3.1575 -1.2189 O 0 0 0 0 0 0 0 0 0 0 13
1.6342 3.2187 -0.2848 H 0 0 0 0 0 0 0 0 0 0 14
1.0929 3.2048 1.2734 H 0 0 0 0 0 0 0 0 0 0 15
-0.3068 -1.1555 2.1451 H 0 0 0 0 0 0 0 0 0 0 16
0.1802 1.2867 2.3298 H 0 0 0 0 0 0 0 0 0 0 17
0.9609 1.4474 -1.9219 H 0 0 0 0 0 0 0 0 0 0 18
0.4668 -0.9926 -2.1017 H 0 0 0 0 0 0 0 0 0 0 19
-0.0263 3.5135 0.0154 H 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0

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11 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
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12 10 0 0 0 0
13 10 0 0 0 0
14 11 0 0 0 0
15 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
4-nitroaniline1.sdf
COSMOtherm 3D 0

19 18 0 0 0 0 0 0 0 0 0 V2000
-1.0217 0.0017 4.9205 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.5558 -0.8099 4.9918 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.6792 0.7200 4.8989 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.3461 0.0056 -0.8656 C 0 0 0 0 0 0 0 0 0 0 0 0 4
1.6665 0.0069 0.4769 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.6441 0.0019 1.4715 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.7167 -0.0044 1.0423 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.0338 -0.0039 -0.3011 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.0058 0.0001 -1.2660 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.9522 0.0023 2.7864 N 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.3367 -0.0008 -2.6607 N 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.5459 0.0135 -3.0015 O 0 0 0 0 0 0 0 0 0 0 0 0 12
0.5915 -0.0165 -3.5079 O 0 0 0 0 0 0 0 0 0 0 0 0 13
0.2233 0.0021 3.5151 H 0 0 0 0 0 0 0 0 0 0 0 0 14
1.9231 0.0084 3.0834 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2.1306 0.0098 -1.6208 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.7125 0.0124 0.7878 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.5115 -0.0093 1.7899 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-2.0741 -0.0084 -0.6226 H 0 0 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
16 4 0 0 0 0
6 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
11 9 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
8 19 0 0 0 0
M END
$$$$
aniline-cation.sdf
COSMOtherm 3D 0

18 17 0 0 0 0 0 0 0 0 0 V2000
-0.9194 -0.3289 -3.2766 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-0.5812 -0.9004 -3.9908 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.3774 0.3981 -3.7378 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.4874 1.0331 1.8729 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.0025 1.2827 0.5862 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.4900 0.2156 -0.1660 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.5032 -1.0890 0.3271 C 0 0 0 0 0 0 0 0 0 0 0 0 7
0.0115 -1.3259 1.6143 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.4831 -0.2680 2.3867 C 0 0 0 0 0 0 0 0 0 0 0 0 9
0.9804 0.4670 -1.5304 N 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.8706 1.8601 2.4717 H 0 0 0 0 0 0 0 0 0 0 0 0 11
0.0041 2.2954 0.1783 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.8962 -1.9075 -0.2779 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.0203 -2.3408 2.0138 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.8610 -0.4585 3.3922 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.8495 -0.0493 -1.7224 H 0 0 0 0 0 0 0 0 0 0 0 0 16
1.1970 1.4620 -1.6724 H 0 0 0 0 0 0 0 0 0 0 0 0 17
0.2566 0.1775 -2.2779 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
13 7 0 0 0 0
9 8 0 0 0 0
14 8 0 0 0 0
15 9 0 0 0 0
16 10 0 0 0 0
17 10 0 0 0 0
10 18 0 0 0 0
M END
$$$$
aniline.sdf
COSMOtherm 3D 0

17 16 0 0 0 0 0 0 0 0 0 V2000
-3.4772 0.9917 -0.0927 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.7842 0.2776 -0.0125 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.4177 1.4813 0.7459 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7135 0.2509 -1.2279 C 0 0 0 0 0 0 0 0 0 0 0 0 4

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2
3 0.4379 -0.3194 -1.1983 C 0 0 0 0 0 0 0 0 0 0 5
4 -0.1963 -0.5777 0.0315 C 0 0 0 0 0 0 0 0 0 0 6
5 0.4742 -0.2532 1.2257 C 0 0 0 0 0 0 0 0 0 0 7
6 1.7494 0.3175 1.1858 C 0 0 0 0 0 0 0 0 0 0 8
7 2.3798 0.5743 -0.0386 C 0 0 0 0 0 0 0 0 0 0 9
8 -1.5133 -1.0891 0.0649 N 0 0 0 0 0 0 0 0 0 0 10
9 2.1912 0.4400 -2.1914 H 0 0 0 0 0 0 0 0 0 0 11
10 -0.0732 -0.5692 -2.1310 H 0 0 0 0 0 0 0 0 0 0 12
11 -0.0081 -0.4520 2.1858 H 0 0 0 0 0 0 0 0 0 0 13
12 2.2557 0.5577 2.1230 H 0 0 0 0 0 0 0 0 0 0 14
13 3.3762 1.0178 -0.0655 H 0 0 0 0 0 0 0 0 0 0 15
14 -1.7275 -1.6034 0.9204 H 0 0 0 0 0 0 0 0 0 0 16
15 -1.7446 -1.6669 -0.7447 H 0 0 0 0 0 0 0 0 0 0 17
16 2 1 0 0 0 0
17 3 1 0 0 0 0
18 5 4 0 0 0 0
19 9 4 0 0 0 0
20 11 4 0 0 0 0
21 6 5 0 0 0 0
22 12 5 0 0 0 0
23 7 6 0 0 0 0
24 10 6 0 0 0 0
25 8 7 0 0 0 0
26 13 7 0 0 0 0
27 9 8 0 0 0 0
28 14 8 0 0 0 0
29 15 9 0 0 0 0
30 16 10 0 0 0 0
31 10 17 0 0 0 0
32 M END
33 \$\$\$\$
34 benzimidazole.sdf
35 COSMOTHERM 3D 0
36 18 18 0 0 0 0 0 0 0 0 0 V2000
37 -3.7844 1.1119 -0.0707 O 0 0 0 0 0 0 0 0 0 0 1
38 -2.9237 0.5993 -0.0261 H 0 0 0 0 0 0 0 0 0 0 2
39 -3.8689 1.5177 0.8092 H 0 0 0 0 0 0 0 0 0 0 3
40 2.2409 -0.6270 -0.0113 C 0 0 0 0 0 0 0 0 0 0 4
41 0.8601 -0.8534 -0.0019 C 0 0 0 0 0 0 0 0 0 0 5
42 -0.0860 0.2076 0.0088 C 0 0 0 0 0 0 0 0 0 0 6
43 0.3517 1.5410 0.0104 C 0 0 0 0 0 0 0 0 0 0 7
44 1.7278 1.7723 0.0013 C 0 0 0 0 0 0 0 0 0 0 8
45 2.6564 0.7062 -0.0090 C 0 0 0 0 0 0 0 0 0 0 9
46 -1.3781 -0.3182 0.0174 N 0 0 0 0 0 0 0 0 0 0 10
47 0.0956 -2.0091 -0.0004 N 0 0 0 0 0 0 0 0 0 0 11
48 -1.2177 -1.6339 0.0110 C 0 0 0 0 0 0 0 0 0 0 12
49 2.9586 -1.4482 -0.0198 H 0 0 0 0 0 0 0 0 0 0 13
50 -0.3639 2.3646 0.0179 H 0 0 0 0 0 0 0 0 0 0 14
51 2.0988 2.7986 0.0025 H 0 0 0 0 0 0 0 0 0 0 15
52 3.7243 0.9306 -0.0160 H 0 0 0 0 0 0 0 0 0 0 16
53 0.4365 -2.9672 -0.0057 H 0 0 0 0 0 0 0 0 0 0 17
54 -2.0214 -2.3653 0.0146 H 0 0 0 0 0 0 0 0 0 0 18
55 2 1 0 0 0 0
56 3 1 0 0 0 0
57 5 4 0 0 0 0
58 9 4 0 0 0 0
59 13 4 0 0 0 0
60 6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
14 7 0 0 0 0
9 8 0 0 0 0
15 8 0 0 0 0
16 9 0 0 0 0
12 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
12 18 0 0 0 0
M END
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benzimidazole-cation.sdf
COSMOTHERM 3D 0
19 19 0 0 0 0 0 0 0 0 0 V2000
-3.7170 0.0009 -1.0375 O 0 0 0 0 0 0 0 0 0 0 1
-3.9078 -0.7689 -1.6039 H 0 0 0 0 0 0 0 0 0 0 2
-3.9155 0.7769 -1.5926 H 0 0 0 0 0 0 0 0 0 0 3
-1.2673 -0.0008 1.5890 C 0 0 0 0 0 0 0 0 0 0 4
-1.3327 -0.0014 0.2548 N 0 0 0 0 0 0 0 0 0 0 5
-0.0364 -0.0008 -0.2579 C 0 0 0 0 0 0 0 0 0 0 6
0.8358 -0.0005 0.8545 C 0 0 0 0 0 0 0 0 0 0 7
0.0153 0.0006 1.9795 N 0 0 0 0 0 0 0 0 0 0 8
0.4503 -0.0002 -1.5690 C 0 0 0 0 0 0 0 0 0 0 9
1.8365 -0.0006 -1.7180 C 0 0 0 0 0 0 0 0 0 0 10
2.7067 0.0004 -0.6044 C 0 0 0 0 0 0 0 0 0 0 11
2.2251 0.0015 0.7041 C 0 0 0 0 0 0 0 0 0 0 12
-2.1178 -0.0008 2.2616 H 0 0 0 0 0 0 0 0 0 0 13
-2.2358 0.0000 -0.2996 H 0 0 0 0 0 0 0 0 0 0 14
-0.2191 -0.0004 -2.4286 H 0 0 0 0 0 0 0 0 0 0 15
2.2621 -0.0001 -2.7221 H 0 0 0 0 0 0 0 0 0 0 16
3.7841 0.0022 -0.7733 H 0 0 0 0 0 0 0 0 0 0 17
2.8938 0.0028 1.5643 H 0 0 0 0 0 0 0 0 0 0 18
0.3190 -0.0010 2.9515 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
14 5 0 0 0 0
7 6 0 0 0 0
9 6 0 0 0 0

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8 7 0 0 0 0
12 7 0 0 0 0
10 9 0 0 0 0
15 9 0 0 0 0
11 10 0 0 0 0
16 10 0 0 0 0
12 11 0 0 0 0
17 11 0 0 0 0
18 12 0 0 0 0
8 19 0 0 0 0
M END
$$$$
clonidine-cation2.sdf
COSMOtherm 3D 0
27 27 0 0 0 0 0 0 0 0 0 V2000
1.8027 -1.9601 2.4012 O 0 0 0 0 0 0 0 0 0 0 0 1
1.8325 -1.6945 3.3384 H 0 0 0 0 0 0 0 0 0 0 0 2
1.7088 -2.9297 2.4184 H 0 0 0 0 0 0 0 0 0 0 0 3
-2.6505 1.6329 -0.0583 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.3378 1.3127 0.2870 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8399 -0.0010 0.1692 C 0 0 0 0 0 0 0 0 0 0 0 6
-1.7333 -0.9926 -0.2840 C 0 0 0 0 0 0 0 0 0 0 0 7
-3.0548 -0.6965 -0.6141 C 0 0 0 0 0 0 0 0 0 0 0 8
-3.5034 0.6215 -0.5045 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.2865 2.5852 0.9040 Cl 0 0 0 0 0 0 0 0 0 0 0 10
-1.1642 -2.6522 -0.4315 Cl 0 0 0 0 0 0 0 0 0 0 0 11
0.4874 -0.3341 0.5391 N 0 0 0 0 0 0 0 0 0 0 0 12
1.5747 0.0058 -0.1736 C 0 0 0 0 0 0 0 0 0 0 0 13
3.7745 0.0016 -0.8620 C 0 0 0 0 0 0 0 0 0 0 0 14
2.9643 0.9787 -1.7387 C 0 0 0 0 0 0 0 0 0 0 0 15
2.8265 -0.2620 0.2385 N 0 0 0 0 0 0 0 0 0 0 0 16
1.5779 0.6241 -1.3664 N 0 0 0 0 0 0 0 0 0 0 0 17
2.9807 -0.9616 0.9697 H 0 0 0 0 0 0 0 0 0 0 0 18
0.7714 1.1243 -1.7293 H 0 0 0 0 0 0 0 0 0 0 0 19
-3.0036 2.6585 0.0402 H 0 0 0 0 0 0 0 0 0 0 0 20
-3.7206 -1.4866 -0.9586 H 0 0 0 0 0 0 0 0 0 0 0 21
-4.5336 0.8635 -0.7666 H 0 0 0 0 0 0 0 0 0 0 0 22
4.0064 -0.9311 -1.3977 H 0 0 0 0 0 0 0 0 0 0 0 23
4.7004 0.4452 -0.4824 H 0 0 0 0 0 0 0 0 0 0 0 24
3.1692 2.0283 -1.4814 H 0 0 0 0 0 0 0 0 0 0 0 25
3.1290 0.8249 -2.8097 H 0 0 0 0 0 0 0 0 0 0 0 26
0.6673 -0.9771 1.3349 H 0 0 0 0 0 0 0 0 0 0 0 27
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
20 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
9 8 0 0 0 0
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13 12 0 0 0 0
16 13 0 0 0 0
17 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
23 14 0 0 0 0
24 14 0 0 0 0
17 15 0 0 0 0
25 15 0 0 0 0
26 15 0 0 0 0
18 16 0 0 0 0
19 17 0 0 0 0
12 27 0 0 0 0
M END
$$$$
clonidine.sdf
COSMOtherm 3D 0
26 26 0 0 0 0 0 0 0 0 0 V2000
-2.2157 2.4338 1.3631 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.5941 1.7934 0.9011 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1023 2.0588 1.2213 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3167 0.3478 2.8317 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.0339 -0.1052 1.5653 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5724 -1.3349 1.6623 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.5847 -0.6395 -3.0386 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.9176 -0.3132 -1.7255 C 0 0 0 0 0 0 0 0 0 0 0 8
0.0274 0.1485 -0.7760 C 0 0 0 0 0 0 0 0 0 0 0 9
1.3536 0.2655 -1.2634 C 0 0 0 0 0 0 0 0 0 0 0 10
1.7183 -0.0597 -2.5693 C 0 0 0 0 0 0 0 0 0 0 0 11
0.7420 -0.5127 -3.4597 C 0 0 0 0 0 0 0 0 0 0 0 12
2.6075 0.8817 -0.1719 Cl 0 0 0 0 0 0 0 0 0 0 0 13
-2.6030 -0.4876 -1.2128 Cl 0 0 0 0 0 0 0 0 0 0 0 14
-0.3683 0.5677 0.4912 N 0 0 0 0 0 0 0 0 0 0 0 15
-0.1294 -0.7461 3.7990 C 0 0 0 0 0 0 0 0 0 0 0 16
0.9152 -1.6085 3.0705 C 0 0 0 0 0 0 0 0 0 0 0 17
-1.0953 1.0015 2.9273 H 0 0 0 0 0 0 0 0 0 0 0 18
1.1985 -1.6406 0.9219 H 0 0 0 0 0 0 0 0 0 0 0 19
-1.3561 -0.9912 -3.7233 H 0 0 0 0 0 0 0 0 0 0 0 20
2.7545 0.0527 -2.8871 H 0 0 0 0 0 0 0 0 0 0 0 21
1.0147 -0.7644 -4.4847 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.0671 -1.3049 3.9559 H 0 0 0 0 0 0 0 0 0 0 0 23
0.2317 -0.3705 4.7629 H 0 0 0 0 0 0 0 0 0 0 0 24
0.8209 -2.6754 3.3014 H 0 0 0 0 0 0 0 0 0 0 0 25
1.9404 -1.2757 3.3004 H 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0

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16 4 0 0 0 0
18 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
17 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
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11 10 0 0 0 0
13 10 0 0 0 0
12 11 0 0 0 0
21 11 0 0 0 0
22 12 0 0 0 0
17 16 0 0 0 0
23 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
17 26 0 0 0 0
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M END

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clonidine-cation.sdf
COSMOTHERM 3D 0

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27 27 0 0 0 0 0 0 0 0 0 V2000
-1.7823 2.3939 -1.9839 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.6918 2.3996 -2.9540 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.8014 3.3341 -1.7285 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.2524 0.9052 2.5799 Cl 0 0 0 0 0 0 0 0 0 0 0 0 4
3.4986 -0.4944 0.6585 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.6315 -0.0499 1.6585 C 0 0 0 0 0 0 0 0 0 0 0 0 6
1.3213 0.2890 1.3213 C 0 0 0 0 0 0 0 0 0 0 0 0 7
0.8397 0.1660 0.0018 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.7474 -0.2846 -0.9778 C 0 0 0 0 0 0 0 0 0 0 0 0 9
3.0664 -0.6087 -0.6646 C 0 0 0 0 0 0 0 0 0 0 0 0 10
1.1989 -0.4382 -2.6437 Cl 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.4843 0.5308 -0.3484 N 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.5749 -0.1765 -0.0093 C 0 0 0 0 0 0 0 0 0 0 0 0 13
-2.8243 0.2388 -0.2828 N 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.5844 -1.3676 0.6129 N 0 0 0 0 0 0 0 0 0 0 0 0 15
-3.7782 -0.8553 -0.0145 C 0 0 0 0 0 0 0 0 0 0 0 0 16
-2.9733 -1.7310 0.9680 C 0 0 0 0 0 0 0 0 0 0 0 0 17
4.5269 -0.7518 0.9135 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2.9712 0.0522 2.6884 H 0 0 0 0 0 0 0 0 0 0 0 0 19
3.7431 -0.9520 -1.4459 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-2.9753 0.9700 -0.9830 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.7817 -1.7292 1.1201 H 0 0 0 0 0 0 0 0 0 0 0 0 22
-4.0116 -1.3947 -0.9447 H 0 0 0 0 0 0 0 0 0 0 0 0 23
-4.7027 -0.4686 0.4260 H 0 0 0 0 0 0 0 0 0 0 0 0 24
-3.1433 -2.8019 0.8194 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-3.1780 -1.4671 2.0160 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-0.6590 1.3256 -0.9944 H 0 0 0 0 0 0 0 0 0 0 0 0 27
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2 1 0 0 0 0
3 1 0 0 0 0
7 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
10 9 0 0 0 0
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20 10 0 0 0 0
13 12 0 0 0 0
14 13 0 0 0 0
15 13 0 0 0 0
16 14 0 0 0 0
21 14 0 0 0 0
17 15 0 0 0 0
22 15 0 0 0 0
17 16 0 0 0 0
23 16 0 0 0 0
24 16 0 0 0 0
25 17 0 0 0 0
26 17 0 0 0 0
12 27 0 0 0 0
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M END

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clonidine_t_p3.sdf
COSMOTHERM 3D 0

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27 27 0 0 0 0 0 0 0 0 0 V2000
-2.4431 1.8145 1.8993 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.4633 1.7240 2.8692 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.3796 1.8275 1.6304 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7686 2.9508 -0.9573 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.8684 3.7714 -0.0109 C 0 0 0 0 0 0 0 0 0 0 0 0 5
1.3801 1.5689 -0.6042 N 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.8934 -0.3148 -2.5923 Cl 0 0 0 0 0 0 0 0 0 0 0 0 7
0.5153 -3.5059 -0.5874 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0689 -2.6662 -1.6097 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.2816 -1.3513 -1.3055 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.1718 -0.8390 0.0035 C 0 0 0 0 0 0 0 0 0 0 0 0 11
0.2802 -1.7196 1.0067 C 0 0 0 0 0 0 0 0 0 0 0 0 12
0.6189 -3.0424 0.7260 C 0 0 0 0 0 0 0 0 0 0 0 0 13
0.4183 -1.1320 2.6605 Cl 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.5474 0.4909 0.3193 N 0 0 0 0 0 0 0 0 0 0 0 0 15
0.1743 1.5737 -0.0137 C 0 0 0 0 0 0 0 0 0 0 0 0 16
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1.7285 0.0694 -1.2808 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.6660 -1.1297 0.0598 N 0 0 0 0 0 0 0 0 0 0 0 10
-1.9406 -1.7243 -0.7292 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.9280 -1.6530 0.9018 H 0 0 0 0 0 0 0 0 0 0 0 12
1.7197 1.8670 -0.0711 H 0 0 0 0 0 0 0 0 0 0 0 13
3.2664 1.0071 -0.0565 H 0 0 0 0 0 0 0 0 0 0 0 14
2.2993 -0.7997 1.3453 H 0 0 0 0 0 0 0 0 0 0 0 15
2.0287 0.7609 2.1316 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.3156 0.8266 1.2838 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.0386 -0.6720 2.1898 H 0 0 0 0 0 0 0 0 0 0 0 18
0.3284 -1.9065 0.0705 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.3416 0.7349 -1.3197 H 0 0 0 0 0 0 0 0 0 0 0 20
-0.0751 -0.8222 -2.1247 H 0 0 0 0 0 0 0 0 0 0 0 21
2.2778 -0.8876 -1.3175 H 0 0 0 0 0 0 0 0 0 0 0 22
1.9889 0.6167 -2.2006 H 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
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16 5 0 0 0 0
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19 7 0 0 0 0
9 8 0 0 0 0
20 8 0 0 0 0
21 8 0 0 0 0
22 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
9 23 0 0 0 0
M END
$$$$
debrisoquine.sdf
COSMOtherm 3D 0
29 29 0 0 0 0 0 0 0 0 0 0 V2000
-3.3937 0.4642 -0.5125 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.5893 0.4496 -1.1302 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0508 0.8217 0.3247 H 0 0 0 0 0 0 0 0 0 0 0 3
0.3096 0.6626 3.4125 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.8309 -0.1217 3.1977 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.0193 -0.7404 1.9596 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0855 -0.5809 0.9237 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0649 0.2046 1.1360 C 0 0 0 0 0 0 0 0 0 0 0 8
1.2447 0.8205 2.3867 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.3040 -1.2953 -0.4008 C 0 0 0 0 0 0 0 0 0 0 0 10
2.0865 0.3990 0.0318 C 0 0 0 0 0 0 0 0 0 0 0 11
1.9256 -0.6376 -1.0868 C 0 0 0 0 0 0 0 0 0 0 0 12
0.5110 -0.7449 -1.4852 N 0 0 0 0 0 0 0 0 0 0 0 13
-0.0587 0.1477 -2.3756 C 0 0 0 0 0 0 0 0 0 0 0 14
0.8152 0.6962 -3.3060 N 0 0 0 0 0 0 0 0 0 0 0 15
-1.3317 0.4502 -2.3173 N 0 0 0 0 0 0 0 0 0 0 0 16
0.4711 1.1471 4.3775 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.5689 -0.2512 3.9918 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.9078 -1.3537 1.7882 H 0 0 0 0 0 0 0 0 0 0 0 19
2.1383 1.4272 2.5565 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.3594 -1.2535 -0.6908 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.0356 -2.3603 -0.2888 H 0 0 0 0 0 0 0 0 0 0 0 22
3.1056 0.3455 0.4457 H 0 0 0 0 0 0 0 0 0 0 0 23
1.9788 1.4101 -0.3973 H 0 0 0 0 0 0 0 0 0 0 0 24
2.2336 -1.6332 -0.7334 H 0 0 0 0 0 0 0 0 0 0 0 25
2.5628 -0.3929 -1.9429 H 0 0 0 0 0 0 0 0 0 0 0 26
0.3602 1.1841 -4.0744 H 0 0 0 0 0 0 0 0 0 0 0 27
1.5768 0.1031 -3.6305 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.6017 1.0123 -3.1301 H 0 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
11 8 0 0 0 0
20 9 0 0 0 0
13 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
24 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
16 29 0 0 0 0
M END
$$$$
debrisoquine_a.sdf
COSMOtherm 3D 0

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29 29 0 0 0 0 0 0 0 0 0 V2000
-3.0390 -0.0050 -0.7814 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.4539 -0.8002 -0.5493 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.4706 0.7652 -0.5984 H 0 0 0 0 0 0 0 0 0 0 0 3
0.3613 3.3672 -0.6303 C 0 0 0 0 0 0 0 0 0 0 0 4
-0.6758 3.2120 0.2984 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.8492 1.9819 0.9391 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.0035 0.8955 0.6571 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0449 1.0500 -0.2713 C 0 0 0 0 0 0 0 0 0 0 0 8
1.2104 2.2928 -0.9066 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.2059 -0.4234 1.3858 C 0 0 0 0 0 0 0 0 0 0 0 10
1.9737 -0.1059 -0.5916 C 0 0 0 0 0 0 0 0 0 0 0 11
1.8874 -1.2226 0.4564 C 0 0 0 0 0 0 0 0 0 0 0 12
0.4787 -1.5447 0.7417 N 0 0 0 0 0 0 0 0 0 0 0 13
-0.2436 -2.4075 -0.0648 C 0 0 0 0 0 0 0 0 0 0 0 14
0.4953 -3.4272 -0.6467 N 0 0 0 0 0 0 0 0 0 0 0 15
-1.5281 -2.2391 -0.2574 N 0 0 0 0 0 0 0 0 0 0 0 16
0.5086 4.3235 -1.1357 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.3446 4.0449 0.5235 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.6519 1.8595 1.6714 H 0 0 0 0 0 0 0 0 0 0 0 19
2.0243 2.4173 -1.6258 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.2726 -0.6627 1.4643 H 0 0 0 0 0 0 0 0 0 0 0 21
0.1885 -0.3351 2.4133 H 0 0 0 0 0 0 0 0 0 0 0 22
3.0115 0.2545 -0.6671 H 0 0 0 0 0 0 0 0 0 0 0 23
1.7169 -0.5215 -1.5813 H 0 0 0 0 0 0 0 0 0 0 0 24
2.3423 -0.8979 1.4045 H 0 0 0 0 0 0 0 0 0 0 0 25
2.4336 -2.1106 0.1229 H 0 0 0 0 0 0 0 0 0 0 0 26
-0.0608 -4.1553 -1.0886 H 0 0 0 0 0 0 0 0 0 0 0 27
1.2703 -3.8066 -0.1062 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.9243 -3.0472 -0.7479 H 0 0 0 0 0 0 0 0 0 0 0 29

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
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18 5 0 0 0 0
7 6 0 0 0 0
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8 7 0 0 0 0
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13 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
12 11 0 0 0 0
23 11 0 0 0 0
24 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
16 29 0 0 0 0

M END
$$$$
debrisoquine_a_p2.sdf
COSMOTHERM 3D 0

30 30 0 0 0 0 0 0 0 0 0 V2000
-2.8379 0.9930 -2.8225 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6348 0.4333 -2.8559 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.9169 1.5657 -3.6070 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.2267 -0.2292 3.8879 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.3420 -0.7982 3.2612 C 0 0 0 0 0 0 0 0 0 0 0 5
-1.4745 -0.7253 1.8700 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.4992 -0.0728 1.1057 C 0 0 0 0 0 0 0 0 0 0 0 7
0.6216 0.4999 1.7317 C 0 0 0 0 0 0 0 0 0 0 0 8
0.7559 0.4100 3.1231 C 0 0 0 0 0 0 0 0 0 0 0 9
-0.6489 0.0855 -0.3876 C 0 0 0 0 0 0 0 0 0 0 0 10
1.6374 1.1542 0.8332 C 0 0 0 0 0 0 0 0 0 0 0 11
1.9071 0.2734 -0.3897 C 0 0 0 0 0 0 0 0 0 0 0 12
0.6465 -0.0444 -1.0969 N 0 0 0 0 0 0 0 0 0 0 0 13
0.6753 -0.4473 -2.3788 C 0 0 0 0 0 0 0 0 0 0 0 14
1.8608 -0.7487 -2.9553 N 0 0 0 0 0 0 0 0 0 0 0 15
-0.4530 -0.5434 -3.1017 N 0 0 0 0 0 0 0 0 0 0 0 16
-0.1176 -0.2910 4.9723 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.1047 -1.3062 3.8541 H 0 0 0 0 0 0 0 0 0 0 0 18
-2.3397 -1.1766 1.3784 H 0 0 0 0 0 0 0 0 0 0 0 19
1.6333 0.8433 3.6089 H 0 0 0 0 0 0 0 0 0 0 0 20
-1.0885 1.0721 -0.6170 H 0 0 0 0 0 0 0 0 0 0 0 21
-1.3340 -0.6779 -0.7795 H 0 0 0 0 0 0 0 0 0 0 0 22
2.5866 1.3221 1.3597 H 0 0 0 0 0 0 0 0 0 0 0 23
1.2750 2.1402 0.4957 H 0 0 0 0 0 0 0 0 0 0 0 24
2.3996 -0.6595 -0.0683 H 0 0 0 0 0 0 0 0 0 0 0 25
2.5732 0.7945 -1.0912 H 0 0 0 0 0 0 0 0 0 0 0 26
1.8700 -1.0435 -3.9270 H 0 0 0 0 0 0 0 0 0 0 0 27
2.6323 -1.0864 -2.3880 H 0 0 0 0 0 0 0 0 0 0 0 28
-0.3876 -0.9316 -4.0382 H 0 0 0 0 0 0 0 0 0 0 0 29
-1.3007 0.0215 -2.9049 H 0 0 0 0 0 0 0 0 0 0 0 30

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
18 5 0 0 0 0
7 6 0 0 0 0
19 6 0 0 0 0

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8 7 0 0 0 0
10 7 0 0 0 0
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24 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
29 16 0 0 0 0
16 30 0 0 0 0
M END
$$$$
debrisoquine_p2.sdf
COSMOTHERM 3D 0

30 30 0 0 0 0 0 0 0 0 0 V2000
-5.3329 0.7293 -0.5254 O 0 0 0 0 0 0 0 0 0 0 0 1
-6.1068 0.1406 -0.5842 H 0 0 0 0 0 0 0 0 0 0 0 2
-5.6819 1.6247 -0.6848 H 0 0 0 0 0 0 0 0 0 0 0 3
3.1833 0.5324 0.9989 C 0 0 0 0 0 0 0 0 0 0 0 4
1.8590 0.1344 0.7455 C 0 0 0 0 0 0 0 0 0 0 0 5
1.4918 -0.2101 -0.5676 C 0 0 0 0 0 0 0 0 0 0 0 6
2.4479 -0.1567 -1.5956 C 0 0 0 0 0 0 0 0 0 0 0 7
3.7589 0.2418 -1.3320 C 0 0 0 0 0 0 0 0 0 0 0 8
4.1288 0.5903 -0.0260 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8439 0.0718 1.8667 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.3085 -0.8605 1.5059 C 0 0 0 0 0 0 0 0 0 0 0 11
0.0819 -0.6498 -0.9289 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.8551 -0.4923 0.1893 N 0 0 0 0 0 0 0 0 0 0 0 13
-2.1413 -0.1527 -0.0095 C 0 0 0 0 0 0 0 0 0 0 0 14
-2.9561 0.1407 1.0245 N 0 0 0 0 0 0 0 0 0 0 0 15
-2.6541 -0.0929 -1.2540 N 0 0 0 0 0 0 0 0 0 0 0 16
3.4711 0.7949 2.0201 H 0 0 0 0 0 0 0 0 0 0 0 17
2.1573 -0.4278 -2.6139 H 0 0 0 0 0 0 0 0 0 0 0 18
4.4898 0.2815 -2.1415 H 0 0 0 0 0 0 0 0 0 0 0 19
5.1523 0.9010 0.1914 H 0 0 0 0 0 0 0 0 0 0 0 20
0.4510 1.0799 2.0805 H 0 0 0 0 0 0 0 0 0 0 0 21
1.3217 -0.2844 2.7912 H 0 0 0 0 0 0 0 0 0 0 0 22
-1.1006 -0.8426 2.2606 H 0 0 0 0 0 0 0 0 0 0 0 23
0.0486 -1.9008 1.4354 H 0 0 0 0 0 0 0 0 0 0 0 24
0.0914 -1.7025 -1.2630 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.2710 -0.0381 -1.7698 H 0 0 0 0 0 0 0 0 0 0 0 26
-3.9189 0.4122 0.7919 H 0 0 0 0 0 0 0 0 0 0 0 27
-2.5736 0.5027 1.8918 H 0 0 0 0 0 0 0 0 0 0 0 28
-3.6386 0.1871 -1.3412 H 0 0 0 0 0 0 0 0 0 0 0 29
-2.2638 -0.6592 -2.0001 H 0 0 0 0 0 0 0 0 0 0 0 30

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
17 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
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12 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
11 10 0 0 0 0
21 10 0 0 0 0
22 10 0 0 0 0
13 11 0 0 0 0
23 11 0 0 0 0
24 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
15 14 0 0 0 0
16 14 0 0 0 0
27 15 0 0 0 0
28 15 0 0 0 0
29 16 0 0 0 0
16 30 0 0 0 0
M END
$$$$
di-iso-butylamine-cation.sdf
COSMOTHERM 3D 0

32 30 0 0 0 0 0 0 0 0 0 V2000
-2.4904 0.0684 -0.6627 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.2283 0.1954 -0.0393 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.7771 -0.6687 -1.2319 H 0 0 0 0 0 0 0 0 0 0 0 3
1.2532 3.6910 -0.2243 C 0 0 0 0 0 0 0 0 0 0 0 4
0.5186 2.5003 0.4124 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.9681 2.8159 0.6252 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7587 1.2629 -0.4600 C 0 0 0 0 0 0 0 0 0 0 0 7
0.1842 -0.0011 0.1383 N 0 0 0 0 0 0 0 0 0 0 0 8
0.7611 -1.2697 -0.4485 C 0 0 0 0 0 0 0 0 0 0 0 9
0.4889 -2.5064 0.4158 C 0 0 0 0 0 0 0 0 0 0 0 10
1.2758 -3.6902 -0.1696 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.0028 -2.8444 0.5426 C 0 0 0 0 0 0 0 0 0 0 0 12

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
19 13 0 0 0 0
5 20 0 0 0 0

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M END

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diethylamine.sdf

COSMOTHERM 3D

0

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19 17 0 0 0 0 0 0 0 0 0 V2000
-2.4197 0.0798 -0.0748 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.4092 -0.0328 -0.0391 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.5526 0.9671 -0.4501 H 0 0 0 0 0 0 0 0 0 0 0 3
0.9245 0.3815 -1.2014 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3344 -0.2104 0.0180 N 0 0 0 0 0 0 0 0 0 0 0 5
0.8648 0.3898 1.2599 C 0 0 0 0 0 0 0 0 0 0 0 6
0.4372 -0.3320 -2.4590 C 0 0 0 0 0 0 0 0 0 0 0 7
0.6313 1.4434 -1.2290 H 0 0 0 0 0 0 0 0 0 0 0 8
2.0313 0.3567 -1.1564 H 0 0 0 0 0 0 0 0 0 0 0 9
0.5555 -1.2127 0.0263 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5621 1.4493 1.2713 H 0 0 0 0 0 0 0 0 0 0 0 11
1.9729 0.3734 1.2642 H 0 0 0 0 0 0 0 0 0 0 0 12
0.3281 -0.3241 2.4971 C 0 0 0 0 0 0 0 0 0 0 0 13
0.8698 0.1333 -3.3561 H 0 0 0 0 0 0 0 0 0 0 0 14
0.7356 -1.3917 -2.4532 H 0 0 0 0 0 0 0 0 0 0 0 15
-0.6585 -0.2845 -2.5395 H 0 0 0 0 0 0 0 0 0 0 0 16
0.7217 0.1442 3.4104 H 0 0 0 0 0 0 0 0 0 0 0 17
0.6309 -1.3825 2.5055 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.7702 -0.2798 2.5326 H 0 0 0 0 0 0 0 0 0 0 0 19

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 13 0 0 0 0
18 13 0 0 0 0
13 19 0 0 0 0

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M END

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dimethyl-iso-butylamine-cation.sdf

COSMOTHERM 3D

0

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26 24 0 0 0 0 0 0 0 0 0 V2000
-1.8809 0.2729 2.1334 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.4047 -0.5181 2.3558 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.5334 0.9092 1.7892 H 0 0 0 0 0 0 0 0 0 0 0 3
0.5848 -0.0270 0.8766 N 0 0 0 0 0 0 0 0 0 0 0 4
0.9713 -1.4680 1.0099 C 0 0 0 0 0 0 0 0 0 0 0 5
1.3776 0.8235 1.8260 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7353 0.4977 -0.5377 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0392 -0.2629 -1.6190 C 0 0 0 0 0 0 0 0 0 0 0 8
0.3027 0.3783 -2.9751 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.5551 -0.2690 -1.3804 C 0 0 0 0 0 0 0 0 0 0 0 10
0.8772 -1.7557 2.0620 H 0 0 0 0 0 0 0 0 0 0 0 11
0.3063 -2.0844 0.3983 H 0 0 0 0 0 0 0 0 0 0 0 12
2.0091 -1.5868 0.6787 H 0 0 0 0 0 0 0 0 0 0 0 13
1.0468 1.8613 1.7286 H 0 0 0 0 0 0 0 0 0 0 0 14
2.4400 0.7382 1.5725 H 0 0 0 0 0 0 0 0 0 0 0 15
1.2021 0.4660 2.8457 H 0 0 0 0 0 0 0 0 0 0 0 16
1.8135 0.4790 -0.7491 H 0 0 0 0 0 0 0 0 0 0 0 17
0.4093 1.5467 -0.5022 H 0 0 0 0 0 0 0 0 0 0 0 18
0.3226 -1.3034 -1.6473 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.1955 -0.1687 -3.7877 H 0 0 0 0 0 0 0 0 0 0 0 20
1.3853 0.3631 -3.1681 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.0381 1.4248 -3.0129 H 0 0 0 0 0 0 0 0 0 0 0 22
-2.0652 -0.7871 -2.2048 H 0 0 0 0 0 0 0 0 0 0 0 23
-1.8374 -0.7829 -0.4497 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.9479 0.7592 -1.3330 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.4215 0.0625 1.1859 H 0 0 0 0 0 0 0 0 0 0 0 26

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
11 5 0 0 0 0
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13 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0

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8 7 0 0 0 0
9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
4 23 0 0 0 0

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M END
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dimethyl-iso-propylamine.sdf
COSMOtherm 3D 0

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22 20 0 0 0 0 0 0 0 0 0 V2000
-2.0223 -0.1972 1.6354 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.3685 -0.1031 0.8635 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.1600 0.7131 1.9490 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3056 0.0265 -0.5381 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.6807 1.2690 -1.2396 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.6142 -1.1228 -1.4106 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1313 0.0393 -0.1207 C 0 0 0 0 0 0 0 0 0 0 0 7
1.5196 -1.2687 0.5799 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4286 1.2272 0.8045 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.7242 1.1895 -1.5712 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.6036 2.1330 -0.5699 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.0440 1.4522 -2.1287 H 0 0 0 0 0 0 0 0 0 0 0 12
-1.6565 -1.0437 -1.7466 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.5058 -2.0669 -0.8646 H 0 0 0 0 0 0 0 0 0 0 0 14
0.0396 -1.1524 -2.3056 H 0 0 0 0 0 0 0 0 0 0 0 15
1.7528 0.1433 -1.0371 H 0 0 0 0 0 0 0 0 0 0 0 16
2.5534 -1.1916 0.9445 H 0 0 0 0 0 0 0 0 0 0 0 17
1.4712 -2.1396 -0.0859 H 0 0 0 0 0 0 0 0 0 0 0 18
0.8645 -1.4530 1.4453 H 0 0 0 0 0 0 0 0 0 0 0 19
2.4677 1.1639 1.1563 H 0 0 0 0 0 0 0 0 0 0 0 20
1.3106 2.1975 0.3055 H 0 0 0 0 0 0 0 0 0 0 0 21
0.7685 1.2038 1.6854 H 0 0 0 0 0 0 0 0 0 0 0 22

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
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13 6 0 0 0 0
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15 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
9 22 0 0 0 0

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M END
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dimethyl-n-butylamine-cation.sdf
COSMOtherm 3D 0

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26 24 0 0 0 0 0 0 0 0 0 V2000
-2.3073 -0.0874 1.8174 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.7885 -0.8790 1.5149 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.8614 0.6612 1.5308 H 0 0 0 0 0 0 0 0 0 0 0 3
1.0157 -0.8509 2.3666 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4180 0.0214 1.3040 N 0 0 0 0 0 0 0 0 0 0 0 5
0.7360 -0.5229 -0.0727 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8464 1.4460 1.4814 C 0 0 0 0 0 0 0 0 0 0 0 7
0.7328 -0.4547 3.3471 H 0 0 0 0 0 0 0 0 0 0 0 8
0.6303 -1.8684 2.2456 H 0 0 0 0 0 0 0 0 0 0 0 9
2.1056 -0.8439 2.2571 H 0 0 0 0 0 0 0 0 0 0 0 10
0.4279 -1.5769 -0.0538 H 0 0 0 0 0 0 0 0 0 0 0 11
0.0343 0.2192 -1.2054 C 0 0 0 0 0 0 0 0 0 0 0 12
1.8293 -0.4859 -0.1783 H 0 0 0 0 0 0 0 0 0 0 0 13
0.6024 1.7566 2.5024 H 0 0 0 0 0 0 0 0 0 0 0 14
0.3139 2.0787 0.7661 H 0 0 0 0 0 0 0 0 0 0 0 15
1.9277 1.5118 1.3151 H 0 0 0 0 0 0 0 0 0 0 0 16
0.2601 -0.4922 -2.5491 C 0 0 0 0 0 0 0 0 0 0 0 17
0.4084 1.2514 -1.2801 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.0475 0.2767 -0.9985 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.4020 0.2414 -3.7198 C 0 0 0 0 0 0 0 0 0 0 0 20
-0.1316 -1.5205 -2.4853 H 0 0 0 0 0 0 0 0 0 0 0 21
1.3436 -0.5810 -2.7341 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.2265 -0.2883 -4.6673 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.0025 1.2617 -3.8258 H 0 0 0 0 0 0 0 0 0 0 0 24
-1.4904 0.3201 -3.5750 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.6336 -0.0144 1.4289 H 0 0 0 0 0 0 0 0 0 0 0 26

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 12 0 0 0 0

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16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
22 17 0 0 0 0
5 23 0 0 0 0
M END
$$$$
dimethyl-n-propylamine.sdf
COSMOtherm 3D 0
22 20 0 0 0 0 0 0 0 0 V2000
-2.1982 -0.1277 1.5878 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.2380 -0.0725 1.2573 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.5764 0.7431 1.3757 H 0 0 0 0 0 0 0 0 0 0 0 0 3
1.1621 -0.9576 1.6330 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.4427 -0.0151 0.7600 N 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5793 -0.4269 -0.6557 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.9339 1.3542 0.9863 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.0167 -0.6706 2.6835 H 0 0 0 0 0 0 0 0 0 0 0 0 8
0.7653 -1.9717 1.4889 H 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2507 -0.9721 1.4224 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.3213 -1.4967 -0.7033 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.3207 0.3443 -1.6245 C 0 0 0 0 0 0 0 0 0 0 0 0 12
1.6401 -0.3366 -0.9765 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.8243 1.6081 2.0494 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.3483 2.0739 0.4010 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2.0022 1.4601 0.7081 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.2239 -0.2101 -3.0505 C 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.0479 1.4109 -1.6326 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-1.3614 0.2833 -1.2664 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.8709 0.3535 -3.7378 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.5310 -1.2666 -3.0896 H 0 0 0 0 0 0 0 0 0 0 0 0 21
0.8063 -0.1458 -3.4341 H 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
19 12 0 0 0 0
20 17 0 0 0 0
21 17 0 0 0 0
17 22 0 0 0 0
M END
$$$$
dimethyl-sec-butylamine-cation.sdf
COSMOtherm 3D 0
26 24 0 0 0 0 0 0 0 0 V2000
-1.7263 -2.0925 0.5418 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-1.7437 -2.7917 -0.1370 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-2.6268 -2.0960 0.9149 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.8199 0.4144 -0.2831 N 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.7298 1.3964 0.3942 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-1.0121 0.5168 -1.7685 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.6614 0.5646 0.1178 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.4490 -0.6804 -0.3260 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.8037 0.8121 1.6177 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-2.7405 1.2499 -0.0006 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.7291 1.2204 1.4724 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.3871 2.4128 0.1713 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-2.0617 0.3055 -1.9962 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.3741 -0.2066 -2.2817 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.7565 1.5347 -2.0832 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.0059 1.4469 -0.4435 H 0 0 0 0 0 0 0 0 0 0 0 0 16
1.1204 -1.0095 -1.3215 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.9616 -0.4309 -0.3825 C 0 0 0 0 0 0 0 0 0 0 0 0 18
1.2276 -1.5052 0.3702 H 0 0 0 0 0 0 0 0 0 0 0 0 19
1.8719 0.8114 1.8688 H 0 0 0 0 0 0 0 0 0 0 0 0 20
0.3983 1.7812 1.9308 H 0 0 0 0 0 0 0 0 0 0 0 0 21
0.3253 0.0124 2.2028 H 0 0 0 0 0 0 0 0 0 0 0 0 22
3.4808 -1.3393 -0.7178 H 0 0 0 0 0 0 0 0 0 0 0 0 23
3.3738 -0.1570 0.5988 H 0 0 0 0 0 0 0 0 0 0 0 0 24
3.2020 0.3762 -1.0905 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.1361 -0.5513 0.0148 H 0 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
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15 6 0 0 0 0
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20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 18 0 0 0 0
24 18 0 0 0 0
25 18 0 0 0 0
4 26 0 0 0 0
M END
$$$$
dimethyl-sec-butylamine.sdf
COSMOtherm 3D 0
25 23 0 0 0 0 0 0 0 0 V2000
2.0780 -1.8077 0.6067 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
1.1979 -1.4148 0.2853 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
2.7576 -1.2685 0.1671 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.3686 -0.8310 -0.2756 N 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-1.3774 -1.7204 0.3309 C 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4146 -1.0172 -1.7391 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.5596 0.6073 0.0975 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.6713 1.4431 -0.3149 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.8231 0.7723 1.5987 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.1938 -2.7462 -0.0161 H 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.2988 -1.7130 1.4235 H 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-2.4104 -1.4373 0.0445 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.2459 -2.0769 -1.9718 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
0.3674 -0.4339 -2.2379 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-1.3967 -0.7178 -2.1583 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.4445 0.9902 -0.4582 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.0300 1.1224 -1.3029 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
0.4000 2.9516 -0.3714 C 0 0 0 0 0 0 0 0 0 0 0 0 0 18
1.4875 1.2322 0.3964 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
-1.7984 0.3746 1.9064 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
-0.8108 1.8391 1.8586 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.0368 0.2723 2.1856 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
1.2986 3.4940 -0.6995 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
0.1088 3.3594 0.6076 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24
-0.4077 3.1808 -1.0838 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
10 5 0 0 0 0
11 5 0 0 0 0
12 5 0 0 0 0
13 6 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
16 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 18 0 0 0 0
24 18 0 0 0 0
18 25 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine-cation.sdf
COSMOtherm 3D 0
26 24 0 0 0 0 0 0 0 0 V2000
-2.6947 0.0177 0.8570 O 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.2957 -0.7298 0.6839 H 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.2556 0.8080 0.7539 H 0 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.3618 1.2116 -1.4980 C 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3108 0.0016 -0.6121 N 0 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.4083 -1.2341 -1.4580 C 0 0 0 0 0 0 0 0 0 0 0 0 0 6
0.8784 -0.0002 0.4060 C 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.8150 -1.3124 1.1996 C 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.6689 1.1844 1.3602 C 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.2078 0.1251 -0.3411 C 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.3212 1.2006 -2.0259 H 0 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.2872 2.1202 -0.8962 H 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.4558 1.1666 -2.2241 H 0 0 0 0 0 0 0 0 0 0 0 0 0 13
-1.2626 -1.1125 -2.1321 H 0 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.5682 -2.1077 -0.8222 H 0 0 0 0 0 0 0 0 0 0 0 0 0 15
0.5074 -1.3509 -2.0458 H 0 0 0 0 0 0 0 0 0 0 0 0 0 16
1.5393 -1.2507 2.0226 H 0 0 0 0 0 0 0 0 0 0 0 0 0 17
1.0817 -2.1850 0.5902 H 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.1789 -1.4719 1.6429 H 0 0 0 0 0 0 0 0 0 0 0 0 0 19
1.4368 1.1347 2.1438 H 0 0 0 0 0 0 0 0 0 0 0 0 0 20
0.7761 2.1558 0.8615 H 0 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.3141 1.1375 1.8505 H 0 0 0 0 0 0 0 0 0 0 0 0 0 22
3.0199 0.0666 0.3964 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
2.3035 1.0873 -0.8611 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24
2.3614 -0.6897 -1.0617 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.1897 0.0234 -0.0247 H 0 0 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0

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9 7 0 0 0 0
10 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
25 10 0 0 0 0
5 26 0 0 0 0
M END
$$$$
dimethyl-tert-butylamine.sdf
COSMOTHERM 3D 0
25 23 0 0 0 0 0 0 0 0 0 V2000
-2.7239 -0.0870 -0.8895 O 0 0 0 0 0 0 0 0 0 0 1
-1.8341 -0.0470 -0.3972 H 0 0 0 0 0 0 0 0 0 0 2
-2.9288 0.8408 -1.0980 H 0 0 0 0 0 0 0 0 0 0 3
-0.4497 -1.1757 1.4474 C 0 0 0 0 0 0 0 0 0 0 4
-0.3594 -0.0008 0.5598 N 0 0 0 0 0 0 0 0 0 0 5
-0.5027 1.2192 1.3773 C 0 0 0 0 0 0 0 0 0 0 6
0.8559 -0.0015 -0.3447 C 0 0 0 0 0 0 0 0 0 0 7
0.7991 1.2464 -1.2462 C 0 0 0 0 0 0 0 0 0 0 8
0.7915 -1.2450 -1.2519 C 0 0 0 0 0 0 0 0 0 0 9
2.1840 -0.0058 0.4408 C 0 0 0 0 0 0 0 0 0 0 10
-1.4148 -1.1407 1.9716 H 0 0 0 0 0 0 0 0 0 0 11
-0.4147 -2.1056 0.8691 H 0 0 0 0 0 0 0 0 0 0 12
0.3501 -1.2033 2.2121 H 0 0 0 0 0 0 0 0 0 0 13
-1.4424 1.1472 1.9424 H 0 0 0 0 0 0 0 0 0 0 14
-0.5601 2.1105 0.7426 H 0 0 0 0 0 0 0 0 0 0 15
0.3200 1.3539 2.1052 H 0 0 0 0 0 0 0 0 0 0 16
1.5630 1.1624 -2.0322 H 0 0 0 0 0 0 0 0 0 0 17
0.9990 2.1737 -0.6924 H 0 0 0 0 0 0 0 0 0 0 18
-0.1836 1.3322 -1.7333 H 0 0 0 0 0 0 0 0 0 0 19
1.5905 -1.1879 -2.0050 H 0 0 0 0 0 0 0 0 0 0 20
0.9360 -2.1802 -0.6943 H 0 0 0 0 0 0 0 0 0 0 21
-0.1739 -1.2941 -1.7767 H 0 0 0 0 0 0 0 0 0 0 22
3.0294 0.0219 -0.2622 H 0 0 0 0 0 0 0 0 0 0 23
2.2928 -0.9121 1.0539 H 0 0 0 0 0 0 0 0 0 0 24
2.2726 0.8714 1.0983 H 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
10 7 0 0 0 0
17 8 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
10 25 0 0 0 0
M END
$$$$
dimethylamine-cation.sdf
COSMOTHERM 3D 0
14 12 0 0 0 0 0 0 0 0 0 V2000
2.1938 -0.0026 -0.1109 O 0 0 0 0 0 0 0 0 0 0 1
2.6814 -0.7814 0.2143 H 0 0 0 0 0 0 0 0 0 0 2
2.6869 0.7580 0.2475 H 0 0 0 0 0 0 0 0 0 0 3
-1.0662 1.2544 -0.1830 C 0 0 0 0 0 0 0 0 0 0 4
-0.5225 -0.0002 0.4215 N 0 0 0 0 0 0 0 0 0 0 5
-1.0776 -1.2500 -0.1824 C 0 0 0 0 0 0 0 0 0 0 6
-0.6124 2.1129 0.3220 H 0 0 0 0 0 0 0 0 0 0 7
-0.8142 1.2649 -1.2480 H 0 0 0 0 0 0 0 0 0 0 8
-2.1530 1.2715 -0.0514 H 0 0 0 0 0 0 0 0 0 0 9
-0.7141 0.0009 1.4309 H 0 0 0 0 0 0 0 0 0 0 10
-0.6320 -2.1124 0.3231 H 0 0 0 0 0 0 0 0 0 0 11
-0.8252 -1.2639 -1.2475 H 0 0 0 0 0 0 0 0 0 0 12
-2.1644 -1.2561 -0.0516 H 0 0 0 0 0 0 0 0 0 0 13
0.5333 -0.0041 0.3181 H 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
7 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
5 14 0 0 0 0
M END
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dimethylamine.sdf
COSMOTHERM 3D 0
13 11 0 0 0 0 0 0 0 0 0 V2000
-2.2579 0.0129 0.0035 O 0 0 0 0 0 0 0 0 0 0 1
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16 7 0 0 0 0
17 12 0 0 0 0
18 12 0 0 0 0
12 19 0 0 0 0
M END
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ethylamine-cation.sdf
COSMOtherm 3D 0

14 12 0 0 0 0 0 0 0 0 0 V2000
-2.3013 0.0579 -0.3158 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.4642 -0.5444 -1.0644 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.4905 0.9467 -0.6675 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4879 -0.1765 -1.0412 C 0 0 0 0 0 0 0 0 0 0 0 4
1.2615 0.4106 0.3421 C 0 0 0 0 0 0 0 0 0 0 0 5
0.1047 -0.2611 1.0335 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.0375 0.1229 1.9756 H 0 0 0 0 0 0 0 0 0 0 0 7
0.2751 -1.2682 1.1468 H 0 0 0 0 0 0 0 0 0 0 0 8
2.3441 0.3272 -1.5088 H 0 0 0 0 0 0 0 0 0 0 0 9
1.7140 -1.2512 -0.9887 H 0 0 0 0 0 0 0 0 0 0 0 10
0.6129 -0.0303 -1.6899 H 0 0 0 0 0 0 0 0 0 0 0 11
1.0198 1.4789 0.2975 H 0 0 0 0 0 0 0 0 0 0 0 12
2.1376 0.2792 0.9875 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.7998 -0.1412 0.4940 H 0 0 0 0 0 0 0 0 0 0 0 14

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
13 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
6 14 0 0 0 0
M END
$$$$
ethylamine.sdf
COSMOtherm 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-2.3162 0.3514 0.1253 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.4362 -0.1324 -0.0385 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.3691 1.0057 -0.5925 H 0 0 0 0 0 0 0 0 0 0 0 3
1.4519 1.0325 -0.1578 C 0 0 0 0 0 0 0 0 0 0 0 4
1.2252 -0.3749 0.3862 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0571 -1.0126 -0.2689 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.0680 -1.9618 0.0956 H 0 0 0 0 0 0 0 0 0 0 0 7
0.2480 -1.1258 -1.2698 H 0 0 0 0 0 0 0 0 0 0 0 8
2.3052 1.5088 0.3457 H 0 0 0 0 0 0 0 0 0 0 0 9
1.6694 1.0083 -1.2371 H 0 0 0 0 0 0 0 0 0 0 0 10
0.5631 1.6613 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 11
1.0146 -0.3312 1.4655 H 0 0 0 0 0 0 0 0 0 0 0 12
2.1436 -0.9757 0.2597 H 0 0 0 0 0 0 0 0 0 0 0 13

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
5 13 0 0 0 0
M END
$$$$
guanidine_a.sdf
COSMOtherm 3D 0

12 10 0 0 0 0 0 0 0 0 0 V2000
-2.7623 -0.1144 -0.0128 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.8265 -0.0146 -0.4001 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0212 0.7905 0.2325 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1109 -0.1222 -0.3647 N 0 0 0 0 0 0 0 0 0 0 0 4
0.7760 0.0238 -0.0488 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4993 0.0855 1.3036 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.2014 0.0944 -0.9124 N 0 0 0 0 0 0 0 0 0 0 0 7
2.3720 0.0900 -1.3240 H 0 0 0 0 0 0 0 0 0 0 0 8
2.7918 0.2004 0.3197 H 0 0 0 0 0 0 0 0 0 0 0 9
1.1460 -0.3915 1.9279 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.4789 -0.0745 1.5373 H 0 0 0 0 0 0 0 0 0 0 0 11
0.1420 0.1312 -1.8761 H 0 0 0 0 0 0 0 0 0 0 0 12

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
7 12 0 0 0 0
M END
$$$$
guanidine_a_p2.sdf
COSMOtherm 3D 0

13 11 0 0 0 0 0 0 0 0 0 V2000
-2.5414 0.0064 0.0002 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.1398 -0.7618 -0.0216 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1286 0.7834 0.0188 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1277 0.0154 0.0002 N 0 0 0 0 0 0 0 0 0 0 0 4
0.7873 -0.0026 0.0001 C 0 0 0 0 0 0 0 0 0 0 0 5
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16 5 0 0 0 0
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17 6 0 0 0 0
18 6 0 0 0 0
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13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
20 11 0 0 0 0
13 12 0 0 0 0
7 21 0 0 0 0
M END
$$$$
imidazo-(2,3-b)-thioxazole_b.sdf
COSMOTHERM 3D 0

20 20 0 0 0 0 0 0 0 0 V2000
-3.2274 -1.7469 0.2047 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.2208 -1.7171 0.1851 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.4712 -1.2515 1.0054 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
1.7649 -2.6115 -0.2912 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
1.7429 -1.1514 -0.0457 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
0.3183 -2.9995 0.1032 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.4566 -1.7352 0.0588 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.4127 -0.7693 -0.0338 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
-1.2688 2.5596 -0.3487 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.1872 1.1891 -0.3913 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.1191 3.0860 0.0015 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
1.1628 1.9352 0.3122 S 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
0.0378 0.6429 -0.0698 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
1.9738 -2.8177 -1.3529 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 14
2.5257 -3.1061 0.3246 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 15
2.4079 -0.5750 -0.5592 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 16
0.2752 -3.4022 1.1288 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 17
-0.1221 -3.7490 -0.5676 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 18
-2.0620 0.6025 -0.6690 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 19
0.0675 4.1531 0.1093 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
8 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
13 10 0 0 0 0
19 10 0 0 0 0
12 11 0 0 0 0
13 12 0 0 0 0
11 20 0 0 0 0
M END
$$$$
imidazole-cation.sdf
COSMOTHERM 3D 0

13 12 0 0 0 0 0 0 0 0 V2000
-3.0497 0.0014 -0.0593 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.4650 -0.7808 0.3480 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.4666 0.7619 0.3856 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.4820 -0.0005 1.1468 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3294 -0.0002 0.0268 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
1.7775 -0.0002 0.7025 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.7146 0.0003 -0.6781 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.4329 0.0004 -1.0728 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8
0.0771 -0.0007 2.1511 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 9
2.7199 -0.0005 1.2354 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 10
0.0850 0.0009 -2.0986 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 11
2.5138 0.0006 -1.3090 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 12
-1.3881 0.0005 0.0272 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
8 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
11 8 0 0 0 0
5 13 0 0 0 0
M END
$$$$
imidazole.sdf
COSMOTHERM 3D 0

12 11 0 0 0 0 0 0 0 0 V2000
-3.1604 -0.0441 0.0048 O 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.1542 -0.0284 0.0025 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.4155 0.8941 0.0270 H 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 3
0.4514 -0.0083 -1.1154 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.3795 -0.0233 -0.0065 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 5
1.7688 0.0142 -0.7141 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 6
1.7310 0.0127 0.6659 N 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 7
0.4268 -0.0098 1.0524 C 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 8

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3 -0.1817 1.7774 -0.7935 H 0 0 0 0 0 0 0 0 0 0 8
4 -0.1794 1.7475 0.8553 H 0 0 0 0 0 0 0 0 0 0 9
5 1.9357 1.0003 0.0048 H 0 0 0 0 0 0 0 0 0 0 10
6 1.1101 0.0665 2.1709 H 0 0 0 0 0 0 0 0 0 0 11
7 2.0553 -1.1486 1.2840 H 0 0 0 0 0 0 0 0 0 0 12
8 0.2790 -1.2560 1.2987 H 0 0 0 0 0 0 0 0 0 0 13
9 1.0666 0.1184 -2.1742 H 0 0 0 0 0 0 0 0 0 0 14
10 2.0528 -1.0987 -1.3377 H 0 0 0 0 0 0 0 0 0 0 15
11 0.2795 -1.2406 -1.3190 H 0 0 0 0 0 0 0 0 0 0 16
12 -1.0389 0.5652 0.0103 H 0 0 0 0 0 0 0 0 0 0 17
13 2 1 0 0 0 0 0
14 3 1 0 0 0 0 0
15 5 4 0 0 0 0 0
16 6 4 0 0 0 0 0
17 7 4 0 0 0 0 0
18 10 4 0 0 0 0 0
19 8 5 0 0 0 0 0
20 9 5 0 0 0 0 0
21 11 6 0 0 0 0 0
22 12 6 0 0 0 0 0
23 13 6 0 0 0 0 0
24 14 7 0 0 0 0 0
25 15 7 0 0 0 0 0
26 16 7 0 0 0 0 0
27 5 17 0 0 0 0 0
M END
$$$$
iso-propylamine.sdf
COSMOtherm 3D 0
16 14 0 0 0 0 0 0 0 0 0 0 V2000
21 -2.5499 -0.3909 0.0580 O 0 0 0 0 0 0 0 0 0 0 1
22 -1.6797 0.1313 0.0436 H 0 0 0 0 0 0 0 0 0 0 2
23 -2.7706 -0.5172 -0.8809 H 0 0 0 0 0 0 0 0 0 0 3
24 1.0628 0.3248 -0.0018 C 0 0 0 0 0 0 0 0 0 0 4
25 -0.2046 1.1021 0.0542 N 0 0 0 0 0 0 0 0 0 0 5
26 1.1548 -0.5689 1.2362 C 0 0 0 0 0 0 0 0 0 0 6
27 1.0929 -0.4864 -1.2981 C 0 0 0 0 0 0 0 0 0 0 7
28 -0.2434 1.7508 -0.7389 H 0 0 0 0 0 0 0 0 0 0 8
29 -0.2074 1.6931 0.8919 H 0 0 0 0 0 0 0 0 0 0 9
30 1.9325 1.0097 0.0000 H 0 0 0 0 0 0 0 0 0 0 10
31 1.1273 0.0291 2.1600 H 0 0 0 0 0 0 0 0 0 0 11
32 2.0942 -1.1398 1.2316 H 0 0 0 0 0 0 0 0 0 0 12
33 0.3143 -1.2800 1.2628 H 0 0 0 0 0 0 0 0 0 0 13
34 1.0355 0.1704 -2.1796 H 0 0 0 0 0 0 0 0 0 0 14
35 2.0237 -1.0670 -1.3697 H 0 0 0 0 0 0 0 0 0 0 15
36 0.2429 -1.1856 -1.3347 H 0 0 0 0 0 0 0 0 0 0 16
37 2 1 0 0 0 0 0
38 3 1 0 0 0 0 0
39 5 4 0 0 0 0 0
40 6 4 0 0 0 0 0
41 7 4 0 0 0 0 0
42 10 4 0 0 0 0 0
43 8 5 0 0 0 0 0
44 9 5 0 0 0 0 0
45 11 6 0 0 0 0 0
46 12 6 0 0 0 0 0
47 13 6 0 0 0 0 0
48 14 7 0 0 0 0 0
49 15 7 0 0 0 0 0
50 7 16 0 0 0 0 0
M END
$$$$
isoquinoline.sdf
COSMOtherm 3D 0
20 20 0 0 0 0 0 0 0 0 0 V2000
41 -4.5752 -0.0313 0.6928 O 0 0 0 0 0 0 0 0 0 0 1
42 -3.6081 -0.0241 0.4179 H 0 0 0 0 0 0 0 0 0 0 2
43 -4.8022 0.9092 0.7930 H 0 0 0 0 0 0 0 0 0 0 3
44 1.4498 -0.0051 1.5949 C 0 0 0 0 0 0 0 0 0 0 4
45 0.4560 -0.0068 0.5793 C 0 0 0 0 0 0 0 0 0 0 5
46 0.8480 0.0017 -0.8016 C 0 0 0 0 0 0 0 0 0 0 6
47 2.2326 0.0115 -1.1222 C 0 0 0 0 0 0 0 0 0 0 7
48 3.1783 0.0135 -0.1140 C 0 0 0 0 0 0 0 0 0 0 8
49 2.7878 0.0049 1.2511 C 0 0 0 0 0 0 0 0 0 0 9
50 -0.1861 0.0002 -1.7758 C 0 0 0 0 0 0 0 0 0 0 10
51 -1.5033 -0.0106 -1.3706 C 0 0 0 0 0 0 0 0 0 0 11
52 -0.9342 -0.0179 0.8727 C 0 0 0 0 0 0 0 0 0 0 12
53 -1.8833 -0.0206 -0.0548 N 0 0 0 0 0 0 0 0 0 0 13
54 1.1418 -0.0119 2.6426 H 0 0 0 0 0 0 0 0 0 0 14
55 2.5364 0.0180 -2.1708 H 0 0 0 0 0 0 0 0 0 0 15
56 4.2403 0.0211 -0.3658 H 0 0 0 0 0 0 0 0 0 0 16
57 3.5532 0.0064 2.0287 H 0 0 0 0 0 0 0 0 0 0 17
58 0.0615 0.0066 -2.8388 H 0 0 0 0 0 0 0 0 0 0 18
59 -2.3172 -0.0123 -2.0981 H 0 0 0 0 0 0 0 0 0 0 19
60 -1.2632 -0.0255 1.9166 H 0 0 0 0 0 0 0 0 0 0 20
61 2 1 0 0 0 0 0
62 3 1 0 0 0 0 0
63 5 4 0 0 0 0 0
64 9 4 0 0 0 0 0
65 14 4 0 0 0 0 0
66 6 5 0 0 0 0 0
67 12 5 0 0 0 0 0
68 7 6 0 0 0 0 0
69 10 6 0 0 0 0 0
70 8 7 0 0 0 0 0
71 15 7 0 0 0 0 0
72 9 8 0 0 0 0 0
73 16 8 0 0 0 0 0
74 17 9 0 0 0 0 0
75 11 10 0 0 0 0 0
76 18 10 0 0 0 0 0
77 13 11 0 0 0 0 0
78 19 11 0 0 0 0 0

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3 1.7994 -0.2799 0.0009 C 0 0 0 0 0 0 0 0 0 0 9
4 3.1101 -0.5583 0.0022 N 0 0 0 0 0 0 0 0 0 0 10
5 -1.2845 -1.9836 -0.0022 N 0 0 0 0 0 0 0 0 0 0 11
6 -0.2987 2.5466 0.0011 N 0 0 0 0 0 0 0 0 0 0 12
7 3.7921 0.1929 0.0033 H 0 0 0 0 0 0 0 0 0 0 13
8 3.4280 -1.5218 0.0032 H 0 0 0 0 0 0 0 0 0 0 14
9 -1.0019 -2.9584 0.0019 H 0 0 0 0 0 0 0 0 0 0 15
10 -2.2758 -1.7369 -0.0013 H 0 0 0 0 0 0 0 0 0 0 16
11 -1.2877 2.7741 -0.0138 H 0 0 0 0 0 0 0 0 0 0 17
12 0.3749 3.3060 -0.0050 H 0 0 0 0 0 0 0 0 0 0 18
13 -1.8150 0.4467 -0.0025 H 0 0 0 0 0 0 0 0 0 0 19
14 2 1 0 0 0 0
15 3 1 0 0 0 0
16 5 4 0 0 0 0
17 9 4 0 0 0 0
18 6 5 0 0 0 0
19 11 5 0 0 0 0
20 7 6 0 0 0 0
21 8 7 0 0 0 0
22 12 7 0 0 0 0
23 9 8 0 0 0 0
24 10 9 0 0 0 0
25 13 10 0 0 0 0
26 14 10 0 0 0 0
27 15 11 0 0 0 0
28 16 11 0 0 0 0
29 17 12 0 0 0 0
30 18 12 0 0 0 0
31 6 19 0 0 0 0
32 M END
33 \$\$\$\$
34 methylamine-cation.sdf
35 COSMOTHERM 3D 0
36 11 9 0 0 0 0 0 0 0 0 0 V2000
37 -1.9574 -0.0969 0.0132 O 0 0 0 0 0 0 0 0 0 0 1
38 -2.1513 -0.8167 0.6411 H 0 0 0 0 0 0 0 0 0 0 2
39 -2.2761 -0.4296 -0.8456 H 0 0 0 0 0 0 0 0 0 0 3
40 1.5798 -0.5592 -0.0096 C 0 0 0 0 0 0 0 0 0 0 4
41 0.7100 0.6558 0.0080 N 0 0 0 0 0 0 0 0 0 0 5
42 0.8932 1.2582 -0.8032 H 0 0 0 0 0 0 0 0 0 0 6
43 0.8808 1.2245 0.8458 H 0 0 0 0 0 0 0 0 0 0 7
44 1.3437 -1.1687 0.8673 H 0 0 0 0 0 0 0 0 0 0 8
45 1.3756 -1.1206 -0.9257 H 0 0 0 0 0 0 0 0 0 0 9
46 2.6286 -0.2495 -0.0173 H 0 0 0 0 0 0 0 0 0 0 10
47 -0.3168 0.3910 -0.0035 H 0 0 0 0 0 0 0 0 0 0 11
48 2 1 0 0 0 0
49 3 1 0 0 0 0
50 5 4 0 0 0 0
51 8 4 0 0 0 0
52 9 4 0 0 0 0
53 10 4 0 0 0 0
54 6 5 0 0 0 0
55 7 5 0 0 0 0
56 5 11 0 0 0 0
57 M END
58 \$\$\$\$
59 methylamine.sdf
60 COSMOTHERM 3D 0
61 10 8 0 0 0 0 0 0 0 0 V2000
62 -1.9905 -0.0602 -0.1540 O 0 0 0 0 0 0 0 0 0 0 1
63 -1.0166 -0.0134 0.1408 H 0 0 0 0 0 0 0 0 0 0 2
64 -2.2154 0.8543 -0.3973 H 0 0 0 0 0 0 0 0 0 0 3
65 1.5747 -0.0062 -0.5143 C 0 0 0 0 0 0 0 0 0 0 4
66 0.6472 0.0122 0.6378 N 0 0 0 0 0 0 0 0 0 0 5
67 0.8250 0.8418 1.2106 H 0 0 0 0 0 0 0 0 0 0 6
68 0.8371 -0.7886 1.2467 H 0 0 0 0 0 0 0 0 0 0 7
69 1.3913 -0.9094 -1.1117 H 0 0 0 0 0 0 0 0 0 0 8
70 1.3768 0.8658 -1.1520 H 0 0 0 0 0 0 0 0 0 0 9
71 2.6394 0.0089 -0.2265 H 0 0 0 0 0 0 0 0 0 0 10
72 2 1 0 0 0 0
73 3 1 0 0 0 0
74 5 4 0 0 0 0
75 8 4 0 0 0 0
76 9 4 0 0 0 0
77 6 5 0 0 0 0
78 7 5 0 0 0 0
79 4 10 0 0 0 0
80 M END
81 \$\$\$\$
82 methylguanidine.sdf
83 COSMOTHERM 3D 0
84 15 13 0 0 0 0 0 0 0 0 V2000
85 -2.9373 -0.5458 -0.0587 O 0 0 0 0 0 0 0 0 0 0 1
86 -1.9286 -0.6173 0.0141 H 0 0 0 0 0 0 0 0 0 0 2
87 -3.0881 0.1492 -0.7214 H 0 0 0 0 0 0 0 0 0 0 3
88 0.9401 1.0381 0.0610 N 0 0 0 0 0 0 0 0 0 0 4
89 0.8927 -0.3320 0.0394 C 0 0 0 0 0 0 0 0 0 0 5
90 2.1201 -0.9471 -0.1832 N 0 0 0 0 0 0 0 0 0 0 6
91 -0.2393 -0.9704 0.1918 N 0 0 0 0 0 0 0 0 0 0 7
92 -0.2727 1.8451 0.0088 C 0 0 0 0 0 0 0 0 0 0 8
93 1.7723 1.4612 -0.3404 H 0 0 0 0 0 0 0 0 0 0 9
94 2.1686 -1.9221 0.1042 H 0 0 0 0 0 0 0 0 0 0 10
95 2.9454 -0.4246 0.1079 H 0 0 0 0 0 0 0 0 0 0 11
96 -0.0799 -1.9824 0.2147 H 0 0 0 0 0 0 0 0 0 0 12
97 0.0080 2.8962 0.1424 H 0 0 0 0 0 0 0 0 0 0 13
98 -0.8080 1.7392 -0.9502 H 0 0 0 0 0 0 0 0 0 0 14
99 -0.9529 1.5554 0.8193 H 0 0 0 0 0 0 0 0 0 0 15
100 2 1 0 0 0 0
101 3 1 0 0 0 0
102 5 4 0 0 0 0
103 8 4 0 0 0 0
104 9 4 0 0 0 0

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6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
8 15 0 0 0 0
M END
$$$$
methylguanidine_a.sdf
COSMOTHERM 3D 0
15 13 0 0 0 0 0 0 0 0 V2000
-3.1365 -0.4868 0.0980 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.1347 -0.6502 0.0176 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4346 -0.3531 -0.8182 H 0 0 0 0 0 0 0 0 0 0 0 3
1.6711 0.3347 0.1015 N 0 0 0 0 0 0 0 0 0 0 0 4
0.3051 0.3088 -0.0088 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.2993 1.5563 -0.0874 N 0 0 0 0 0 0 0 0 0 0 0 6
-0.4371 -0.7678 -0.0611 N 0 0 0 0 0 0 0 0 0 0 0 7
2.4771 -0.8744 -0.0129 C 0 0 0 0 0 0 0 0 0 0 0 8
2.1299 1.2077 -0.1449 H 0 0 0 0 0 0 0 0 0 0 0 9
0.1629 2.3112 0.4162 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.3030 1.5288 0.0874 H 0 0 0 0 0 0 0 0 0 0 0 11
0.1203 -1.6242 -0.1069 H 0 0 0 0 0 0 0 0 0 0 0 12
3.5267 -0.6034 0.1448 H 0 0 0 0 0 0 0 0 0 0 0 13
2.1955 -1.6018 0.7621 H 0 0 0 0 0 0 0 0 0 0 0 14
2.3825 -1.3552 -1.0017 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
8 15 0 0 0 0
M END
$$$$
methylguanidine_a_p2.sdf
COSMOTHERM 3D 0
16 14 0 0 0 0 0 0 0 0 V2000
-2.6771 -0.2274 -0.0472 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.2134 -0.4016 -0.8414 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.2773 -0.3862 0.7034 H 0 0 0 0 0 0 0 0 0 0 0 3
0.1584 -0.7409 0.0347 N 0 0 0 0 0 0 0 0 0 0 0 4
0.5650 0.5331 0.0076 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.3503 1.5187 0.0972 N 0 0 0 0 0 0 0 0 0 0 0 6
1.8697 0.8341 -0.0858 N 0 0 0 0 0 0 0 0 0 0 0 7
1.0590 -1.8880 0.0214 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.8590 -0.8889 0.0272 H 0 0 0 0 0 0 0 0 0 0 0 9
-1.3380 1.2574 0.0154 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.0884 2.4682 -0.1476 H 0 0 0 0 0 0 0 0 0 0 0 11
2.5790 0.1097 -0.0659 H 0 0 0 0 0 0 0 0 0 0 0 12
0.4502 -2.7940 0.0950 H 0 0 0 0 0 0 0 0 0 0 0 13
1.6409 -1.9371 -0.9116 H 0 0 0 0 0 0 0 0 0 0 0 14
1.7470 -1.8654 0.8799 H 0 0 0 0 0 0 0 0 0 0 0 15
2.1861 1.7933 0.0080 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
10 6 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
7 16 0 0 0 0
M END
$$$$
methylguanidine_p2.sdf
COSMOTHERM 3D 0
16 14 0 0 0 0 0 0 0 0 V2000
-2.8995 -0.5713 -0.1202 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.1864 -0.3855 -1.0324 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4080 0.0555 0.4250 H 0 0 0 0 0 0 0 0 0 0 0 3
0.8883 1.0506 -0.1003 N 0 0 0 0 0 0 0 0 0 0 0 4
-0.3290 1.8265 0.1178 C 0 0 0 0 0 0 0 0 0 0 0 5
1.7238 1.5473 -0.3940 H 0 0 0 0 0 0 0 0 0 0 0 6
-1.0625 1.6697 -0.6860 H 0 0 0 0 0 0 0 0 0 0 0 7
-0.7856 1.5663 1.0829 H 0 0 0 0 0 0 0 0 0 0 0 8
-0.0511 2.8845 0.1382 H 0 0 0 0 0 0 0 0 0 0 0 9
0.9720 -0.2818 0.0111 C 0 0 0 0 0 0 0 0 0 0 0 10
2.1725 -0.8780 -0.1419 N 0 0 0 0 0 0 0 0 0 0 0 11
2.2571 -1.8806 -0.0094 H 0 0 0 0 0 0 0 0 0 0 0 12
3.0247 -0.3355 -0.0415 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.1149 -1.0189 0.2699 N 0 0 0 0 0 0 0 0 0 0 0 14
-0.0052 -2.0221 0.3824 H 0 0 0 0 0 0 0 0 0 0 0 15
-1.0814 -0.6785 0.1226 H 0 0 0 0 0 0 0 0 0 0 0 16
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0

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7 5 0 0 0 0
8 5 0 0 0 0
9 5 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
12 11 0 0 0 0
13 11 0 0 0 0
15 14 0 0 0 0
14 16 0 0 0 0
M END
\$\$\$\$
methylguanidine_t.sdf
COSMOtherm 3D 0

| Atom | X | Y | Z | Element | Charge | Occupancy | Disorder | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|------|---------|---------|---------|---------|--------|-----------|----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 15 | 13 | 0 | 0 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | -2.7457 | -0.1051 | -0.1285 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | -1.7898 | -0.0336 | 0.2286 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | -3.0345 | 0.8175 | -0.2382 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | 0.4076 | 0.0365 | 1.9650 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | -0.1477 | 0.0281 | 0.6149 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0.6779 | 0.0070 | -0.3943 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 0.1802 | 0.1136 | -1.6869 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 2.0466 | -0.1132 | -0.3005 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | -0.4150 | 0.1274 | 2.6859 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 0.9560 | -0.8935 | 2.2046 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | 1.0947 | 0.8860 | 2.1415 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 0.6990 | -0.3905 | -2.4041 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | -0.8250 | -0.0555 | -1.7417 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 2.6024 | 0.2179 | -1.0854 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | 2.4676 | 0.0784 | 0.6042 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
14 8 0 0 0 0
8 15 0 0 0 0
M END
\$\$\$\$
methylguanidine_t_p2.sdf
COSMOtherm 3D 0

| Atom | X | Y | Z | Element | Charge | Occupancy | Disorder | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|------|---------|---------|---------|---------|--------|-----------|----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 16 | 14 | 0 | 0 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | -2.9205 | -0.0019 | 0.5632 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | -3.3293 | -0.8743 | 0.4220 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | -3.3523 | 0.5744 | -0.0920 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | -0.3478 | 0.0334 | -1.8100 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.9008 | -0.0488 | -1.0574 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0.9846 | -0.0082 | 0.2798 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 2.1986 | 0.0187 | 0.8643 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | -0.1170 | 0.0360 | 1.0361 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | -0.1018 | -0.0483 | -2.8727 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | -1.0260 | -0.7901 | -1.5471 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | -0.8564 | 0.9937 | -1.6394 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | 2.2844 | -0.1030 | 1.8676 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | 3.0389 | -0.1129 | 0.3115 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | -0.0211 | 0.0551 | 2.0463 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | -1.0814 | 0.0147 | 0.6653 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 1.7710 | -0.0625 | -1.5801 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
11 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
8 6 0 0 0 0
12 7 0 0 0 0
13 7 0 0 0 0
14 8 0 0 0 0
15 8 0 0 0 0
5 16 0 0 0 0
M END
\$\$\$\$
n-butylamine-cation.sdf
COSMOtherm 3D 0

| Atom | X | Y | Z | Element | Charge | Occupancy | Disorder | U ₁₁ | U ₂₂ | U ₃₃ | U ₁₂ | U ₁₃ | U ₂₃ |
|------|---------|---------|---------|---------|--------|-----------|----------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 20 | 18 | 0 | 0 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 1 | -1.3036 | 0.1207 | 2.9363 | O | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 2 | -2.0105 | -0.5279 | 2.7651 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3 | -1.7274 | 0.9885 | 2.8076 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4 | -0.9142 | -0.1954 | -3.0163 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0.1530 | 0.3639 | -2.0699 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6 | 0.0915 | -0.2652 | -0.6706 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7 | 1.1534 | 0.3185 | 0.2537 | C | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8 | 1.1005 | -0.3119 | 1.6188 | N | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9 | 1.8321 | 0.0699 | 2.2305 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10 | 1.2593 | -1.3257 | 1.5648 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11 | -0.8452 | 0.2705 | -4.0099 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 12 | -0.8001 | -1.2826 | -3.1458 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 13 | -1.9268 | -0.0082 | -2.6271 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 14 | 0.0324 | 1.4562 | -1.9812 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 15 | 1.1545 | 0.1948 | -2.4996 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 16 | 0.2331 | -1.3561 | -0.7502 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 17 | -0.9083 | -0.1004 | -0.2353 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 18 | 1.0126 | 1.3965 | 0.4004 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 19 | 2.1641 | 0.1498 | -0.1382 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 20 | 0.1659 | -0.1512 | 2.0931 | H | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

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17 6 0 0 0 0
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18 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
8 20 0 0 0 0
M END
$$$$
n-butylamine.sdf
COSMOTHERM 3D 0
19 17 0 0 0 0 0 0 0 0 0 V2000
1.3689 -2.9093 -0.1854 O 0 0 0 0 0 0 0 0 0 0 1
0.4930 -2.4341 0.0206 H 0 0 0 0 0 0 0 0 0 0 2
1.9715 -2.6228 0.5222 H 0 0 0 0 0 0 0 0 0 0 3
0.8944 2.9876 0.1905 C 0 0 0 0 0 0 0 0 0 0 4
-0.1688 2.0329 -0.3637 C 0 0 0 0 0 0 0 0 0 0 5
-0.0981 0.6308 0.2545 C 0 0 0 0 0 0 0 0 0 0 6
-1.1650 -0.3178 -0.2923 C 0 0 0 0 0 0 0 0 0 0 7
-1.0469 -1.6655 0.3150 N 0 0 0 0 0 0 0 0 0 0 8
-1.7805 -2.2759 -0.0575 H 0 0 0 0 0 0 0 0 0 0 9
-1.2289 -1.6017 1.3217 H 0 0 0 0 0 0 0 0 0 0 10
0.8348 3.9762 -0.2884 H 0 0 0 0 0 0 0 0 0 0 11
0.7712 3.1324 1.2752 H 0 0 0 0 0 0 0 0 0 0 12
1.9084 2.5933 0.0202 H 0 0 0 0 0 0 0 0 0 0 13
-0.0551 1.9509 -1.4581 H 0 0 0 0 0 0 0 0 0 0 14
-1.1721 2.4583 -0.1896 H 0 0 0 0 0 0 0 0 0 0 15
-0.2115 0.7092 1.3505 H 0 0 0 0 0 0 0 0 0 0 16
0.8982 0.1927 0.0717 H 0 0 0 0 0 0 0 0 0 0 17
-1.0385 -0.4317 -1.3804 H 0 0 0 0 0 0 0 0 0 0 18
-2.1667 0.1209 -0.1269 H 0 0 0 0 0 0 0 0 0 0 19
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
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15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
17 6 0 0 0 0
8 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0
M END
$$$$
n-heptylamine-cation.sdf
COSMOTHERM 3D 0
29 27 0 0 0 0 0 0 0 0 0 V2000
-1.7848 -0.1888 4.3958 O 0 0 0 0 0 0 0 0 0 0 1
-2.0781 -1.1158 4.3306 H 0 0 0 0 0 0 0 0 0 0 2
-2.4740 0.3221 3.9338 H 0 0 0 0 0 0 0 0 0 0 3
-0.5953 0.3770 -3.8375 C 0 0 0 0 0 0 0 0 0 0 4
0.1851 -0.2628 -2.6813 C 0 0 0 0 0 0 0 0 0 0 5
-0.1288 0.3533 -1.3121 C 0 0 0 0 0 0 0 0 0 0 6
0.6609 -0.2889 -0.1639 C 0 0 0 0 0 0 0 0 0 0 7
0.3429 0.3296 1.2044 C 0 0 0 0 0 0 0 0 0 0 8
1.1587 -0.3219 2.3151 C 0 0 0 0 0 0 0 0 0 0 9
0.8505 0.2897 3.6543 N 0 0 0 0 0 0 0 0 0 0 10
1.4484 -0.1087 4.3886 H 0 0 0 0 0 0 0 0 0 0 11
-0.1583 0.1284 3.9362 H 0 0 0 0 0 0 0 0 0 0 12
-0.2749 -0.2469 -5.2004 C 0 0 0 0 0 0 0 0 0 0 13
-1.6771 0.2878 -3.6365 H 0 0 0 0 0 0 0 0 0 0 14
-0.3766 1.4584 -3.8663 H 0 0 0 0 0 0 0 0 0 0 15
1.2680 -0.1726 -2.8814 H 0 0 0 0 0 0 0 0 0 0 16
-0.0329 -1.3454 -2.6524 H 0 0 0 0 0 0 0 0 0 0 17
-1.2101 0.2584 -1.1084 H 0 0 0 0 0 0 0 0 0 0 18
0.0870 1.4358 -1.3407 H 0 0 0 0 0 0 0 0 0 0 19
1.7417 -0.1905 -0.3650 H 0 0 0 0 0 0 0 0 0 0 20
0.4462 -1.3710 -0.1335 H 0 0 0 0 0 0 0 0 0 0 21
-0.7326 0.2170 1.4199 H 0 0 0 0 0 0 0 0 0 0 22
0.5567 1.4114 1.1805 H 0 0 0 0 0 0 0 0 0 0 23
2.2357 -0.1976 2.1464 H 0 0 0 0 0 0 0 0 0 0 24
0.9411 -1.3936 2.4027 H 0 0 0 0 0 0 0 0 0 0 25
-0.8486 0.2314 -6.0084 H 0 0 0 0 0 0 0 0 0 0 26
0.7945 -0.1425 -5.4423 H 0 0 0 0 0 0 0 0 0 0 27
-0.5148 -1.3218 -5.2108 H 0 0 0 0 0 0 0 0 0 0 28
1.0248 1.3027 3.6485 H 0 0 0 0 0 0 0 0 0 0 29
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
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16 5 0 0 0 0
17 5 0 0 0 0
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18 6 0 0 0 0
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8 7 0 0 0 0
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25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
26 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
10 29 0 0 0 0
M END
$$$$
n-heptylamine.sdf
COSMOtherm 3D 0
28 26 0 0 0 0 0 0 0 0 0 V2000
-1.8357 -0.2676 -4.3924 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.8844 -0.0394 -4.1133 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.3808 0.4242 -3.9798 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.6195 0.3486 3.8005 C 0 0 0 0 0 0 0 0 0 0 0 4
0.2064 -0.2473 2.6525 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.1395 0.3358 1.2766 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6889 -0.2626 0.1319 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3325 0.3121 -1.2449 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1713 -0.2854 -2.3751 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7812 0.2806 -3.6888 N 0 0 0 0 0 0 0 0 0 0 0 10
1.3713 -0.1182 -4.4251 H 0 0 0 0 0 0 0 0 0 0 0 11
0.9748 1.2872 -3.6972 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.2613 -0.2369 5.1712 C 0 0 0 0 0 0 0 0 0 0 0 13
-0.4763 1.4429 3.8186 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.6919 0.1829 3.5981 H 0 0 0 0 0 0 0 0 0 0 0 15
0.0600 -1.3423 2.6316 H 0 0 0 0 0 0 0 0 0 0 0 16
1.2801 -0.0853 2.8567 H 0 0 0 0 0 0 0 0 0 0 0 17
0.0071 1.4305 1.2975 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.2128 0.1730 1.0722 H 0 0 0 0 0 0 0 0 0 0 0 19
0.5485 -1.3580 0.1164 H 0 0 0 0 0 0 0 0 0 0 0 20
1.7615 -0.0918 0.3324 H 0 0 0 0 0 0 0 0 0 0 0 21
0.4731 1.4077 -1.2318 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.7350 0.1332 -1.4587 H 0 0 0 0 0 0 0 0 0 0 0 23
1.0101 -1.3739 -2.4218 H 0 0 0 0 0 0 0 0 0 0 0 24
2.2445 -0.1255 -2.1608 H 0 0 0 0 0 0 0 0 0 0 0 25
-0.8734 0.2051 5.9716 H 0 0 0 0 0 0 0 0 0 0 0 26
-0.4209 -1.3266 5.1910 H 0 0 0 0 0 0 0 0 0 0 0 27
0.7960 -0.0512 5.4170 H 0 0 0 0 0 0 0 0 0 0 0 28
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
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10 9 0 0 0 0
24 9 0 0 0 0
25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
26 13 0 0 0 0
27 13 0 0 0 0
13 28 0 0 0 0
M END
$$$$
n-hexylamine-cation.sdf
COSMOtherm 3D 0
26 24 0 0 0 0 0 0 0 0 0 V2000
-1.7287 0.2071 -3.7423 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.2914 -0.5721 -3.9039 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.7896 0.7274 -4.5643 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.7365 -0.2228 4.4406 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0749 0.3898 3.2934 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.2007 -0.2727 1.9376 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6136 0.3358 0.7886 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3272 -0.3248 -0.5667 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1667 0.2932 -1.6794 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8829 -0.3542 -3.0074 N 0 0 0 0 0 0 0 0 0 0 0 10
1.5016 0.0161 -3.7390 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.1194 -0.1900 -3.3183 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5194 0.2755 5.3970 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.8182 -0.1325 4.2542 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.5074 -1.2932 4.5610 H 0 0 0 0 0 0 0 0 0 0 0 15
1.1519 0.3122 3.5214 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.1468 1.4682 3.2203 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.2773 -0.1907 1.7052 H 0 0 0 0 0 0 0 0 0 0 0 18
0.0189 -1.3526 2.0082 H 0 0 0 0 0 0 0 0 0 0 0 19
1.6894 0.2448 1.0174 H 0 0 0 0 0 0 0 0 0 0 0 20
0.3993 1.4162 0.7205 H 0 0 0 0 0 0 0 0 0 0 0 21
-0.7429 -0.2197 -0.8095 H 0 0 0 0 0 0 0 0 0 0 0 22

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0.5406 -1.4052 -0.5052 H 0 0 0 0 0 0 0 0 0 0 0 0 0 23
2.2397 0.1707 -1.4857 H 0 0 0 0 0 0 0 0 0 0 0 0 0 24
0.9556 1.3629 -1.8012 H 0 0 0 0 0 0 0 0 0 0 0 0 0 25
1.0469 -1.3679 -2.9681 H 0 0 0 0 0 0 0 0 0 0 0 0 0 26
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
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18 6 0 0 0 0
19 6 0 0 0 0
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20 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
24 9 0 0 0 0
25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
10 26 0 0 0 0
M END
$$$$
n-hexylamine.sdf
COSMOTHERM 3D 0
25 23 0 0 0 0 0 0 0 0 0 V2000
-1.7758 -0.2420 -3.8114 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.8328 -0.0080 -3.5098 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.3323 0.4561 -3.4254 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.7583 0.1983 4.4017 C 0 0 0 0 0 0 0 0 0 0 0 4
0.1195 -0.3499 3.2708 C 0 0 0 0 0 0 0 0 0 0 0 5
-0.2208 0.2435 1.8975 C 0 0 0 0 0 0 0 0 0 0 0 6
0.6534 -0.3009 0.7601 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3109 0.2939 -0.6115 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1947 -0.2496 -1.7346 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8171 0.3346 -3.0440 N 0 0 0 0 0 0 0 0 0 0 0 10
1.4326 -0.0324 -3.7761 H 0 0 0 0 0 0 0 0 0 0 0 11
0.9840 1.3459 -3.0268 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.4899 -0.2459 5.3719 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.6512 1.2907 4.4930 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.8228 -0.0174 4.2181 H 0 0 0 0 0 0 0 0 0 0 0 15
0.0178 -1.4480 3.2252 H 0 0 0 0 0 0 0 0 0 0 0 16
1.1807 -0.1493 3.4978 H 0 0 0 0 0 0 0 0 0 0 0 17
-0.1180 1.3425 1.9415 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.2829 0.0431 1.6689 H 0 0 0 0 0 0 0 0 0 0 0 19
0.5501 -1.3997 0.7167 H 0 0 0 0 0 0 0 0 0 0 0 20
1.7147 -0.0998 0.9901 H 0 0 0 0 0 0 0 0 0 0 0 21
0.4154 1.3929 -0.5700 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.7448 0.0863 -0.8553 H 0 0 0 0 0 0 0 0 0 0 0 23
1.0701 -1.3413 -1.8099 H 0 0 0 0 0 0 0 0 0 0 0 24
2.2570 -0.0607 -1.4913 H 0 0 0 0 0 0 0 0 0 0 0 25
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
6 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
7 6 0 0 0 0
18 6 0 0 0 0
19 6 0 0 0 0
8 7 0 0 0 0
20 7 0 0 0 0
21 7 0 0 0 0
9 8 0 0 0 0
22 8 0 0 0 0
23 8 0 0 0 0
10 9 0 0 0 0
24 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
9 25 0 0 0 0
M END
$$$$
n-octylamine-cation.sdf
COSMOTHERM 3D 0
32 30 0 0 0 0 0 0 0 0 0 V2000
-1.9226 -4.9259 -0.2235 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.2177 -4.7328 -1.1319 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.6042 -4.5282 0.3479 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.3277 3.2564 0.2666 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4065 2.0480 -0.3288 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0119 0.7111 0.3119 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7590 -0.4881 -0.2860 C 0 0 0 0 0 0 0 0 0 0 0 7
0.3527 -1.8272 0.3451 C 0 0 0 0 0 0 0 0 0 0 0 8
1.1266 -2.9893 -0.2666 C 0 0 0 0 0 0 0 0 0 0 0 9
0.7240 -4.3022 0.3477 N 0 0 0 0 0 0 0 0 0 0 0 10
1.2902 -5.0736 -0.0259 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.2939 -4.5281 0.1590 H 0 0 0 0 0 0 0 0 0 0 0 12
0.0571 4.5910 -0.3854 C 0 0 0 0 0 0 0 0 0 0 0 13
-1.4178 3.1057 0.1672 H 0 0 0 0 0 0 0 0 0 0 0 14
-0.1226 3.3097 1.3509 H 0 0 0 0 0 0 0 0 0 0 0 15
1.4960 2.1955 -0.2202 H 0 0 0 0 0 0 0 0 0 0 0 16
0.2090 2.0018 -1.4146 H 0 0 0 0 0 0 0 0 0 0 0 17

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-1.0755    0.5576    0.1959 H    0    0    0    0    0    0    0    0    0    0    18
 0.2045    0.7552    1.3983 H    0    0    0    0    0    0    0    0    0    0    19
 1.8454   -0.3407   -0.1594 H    0    0    0    0    0    0    0    0    0    0    20
 0.5739   -0.5278   -1.3733 H    0    0    0    0    0    0    0    0    0    0    21
-0.7291   -1.9885    0.2052 H    0    0    0    0    0    0    0    0    0    0    22
 0.5376   -1.7962    1.4320 H    0    0    0    0    0    0    0    0    0    0    23
 2.2066   -2.8794   -0.1084 H    0    0    0    0    0    0    0    0    0    0    24
 0.9392   -3.0770   -1.3441 H    0    0    0    0    0    0    0    0    0    0    25
-0.6774    5.7940    0.2174 C    0    0    0    0    0    0    0    0    0    0    26
 1.1467    4.7391   -0.2892 H    0    0    0    0    0    0    0    0    0    0    27
-0.1507    4.5372   -1.4680 H    0    0    0    0    0    0    0    0    0    0    28
-0.3809    6.7340   -0.2715 H    0    0    0    0    0    0    0    0    0    0    29
-1.7682    5.6888    0.1064 H    0    0    0    0    0    0    0    0    0    0    30
-0.4605    5.8932    1.2926 H    0    0    0    0    0    0    0    0    0    0    31
 0.8680   -4.2958    1.3653 H    0    0    0    0    0    0    0    0    0    0    32
 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
15 4 0 0 0 0
 6 5 0 0 0 0
16 5 0 0 0 0
17 5 0 0 0 0
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18 6 0 0 0 0
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25 9 0 0 0 0
11 10 0 0 0 0
12 10 0 0 0 0
26 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
29 26 0 0 0 0
30 26 0 0 0 0
31 26 0 0 0 0
10 32 0 0 0 0
M END
$$$$
n-octylamine.sdf
COSMOTHERM          3D          0
31 29 0 0 0 0 0 0 0 0 0 V2000
-1.9624   -0.2928   -4.9311 O    0    0    0    0    0    0    0    0    0    0    1
-1.0072   -0.0398   -4.6883 H    0    0    0    0    0    0    0    0    0    0    2
-2.5079    0.3928   -4.5086 H    0    0    0    0    0    0    0    0    0    0    3
-0.3750    0.2079    3.2171 C    0    0    0    0    0    0    0    0    0    0    4
 0.4541   -0.2834    2.0236 C    0    0    0    0    0    0    0    0    0    0    5
-0.0405    0.2444    0.6702 C    0    0    0    0    0    0    0    0    0    0    6
 0.7898   -0.2533   -0.5202 C    0    0    0    0    0    0    0    0    0    0    7
 0.3113    0.2944   -1.8710 C    0    0    0    0    0    0    0    0    0    0    8
 1.1461   -0.2121   -3.0478 C    0    0    0    0    0    0    0    0    0    0    9
 0.6586    0.3471   -4.3318 N    0    0    0    0    0    0    0    0    0    0    10
 1.2377   -0.0017   -5.1015 H    0    0    0    0    0    0    0    0    0    0    11
 0.7887    1.3638   -4.3305 H    0    0    0    0    0    0    0    0    0    0    12
 0.1302   -0.3064    4.5720 C    0    0    0    0    0    0    0    0    0    0    13
-0.3782    1.3127    3.2281 H    0    0    0    0    0    0    0    0    0    0    14
-1.4274   -0.1002    3.0817 H    0    0    0    0    0    0    0    0    0    0    15
 0.4483   -1.3879    2.0070 H    0    0    0    0    0    0    0    0    0    0    16
 1.5079    0.0159    2.1661 H    0    0    0    0    0    0    0    0    0    0    17
-0.0290    1.3489    0.6849 H    0    0    0    0    0    0    0    0    0    0    18
-1.0953   -0.0502    0.5267 H    0    0    0    0    0    0    0    0    0    0    19
 0.7644   -1.3572   -0.5445 H    0    0    0    0    0    0    0    0    0    0    20
 1.8469    0.0273   -0.3673 H    0    0    0    0    0    0    0    0    0    0    21
 0.3494    1.3982   -1.8506 H    0    0    0    0    0    0    0    0    0    0    22
-0.7440    0.0181   -2.0352 H    0    0    0    0    0    0    0    0    0    0    23
 1.0699   -1.3089   -3.1129 H    0    0    0    0    0    0    0    0    0    0    24
 2.2114    0.0288   -2.8736 H    0    0    0    0    0    0    0    0    0    0    25
-0.7030    0.1914    5.7583 C    0    0    0    0    0    0    0    0    0    0    26
 0.1330   -1.4101    4.5611 H    0    0    0    0    0    0    0    0    0    0    27
 1.1818    0.0013    4.7056 H    0    0    0    0    0    0    0    0    0    0    28
-0.3172   -0.1953    6.7135 H    0    0    0    0    0    0    0    0    0    0    29
-0.6946    1.2913    5.8150 H    0    0    0    0    0    0    0    0    0    0    30
-1.7529   -0.1285    5.6675 H    0    0    0    0    0    0    0    0    0    0    31
 2 1 0 0 0 0
 3 1 0 0 0 0
 5 4 0 0 0 0
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12 10 0 0 0 0

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26 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
29 26 0 0 0 0
30 26 0 0 0 0
26 31 0 0 0 0
M END
$$$$
n-pentylamine-cation.sdf
COSMOtherm 3D 0
23 21 0 0 0 0 0 0 0 0 0 V2000
-1.4802 0.1347 3.4282 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.2034 -0.4255 3.0927 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-1.8329 1.0423 3.3915 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.4255 0.2035 -3.8838 C 0 0 0 0 0 0 0 0 0 0 0 0 4
-0.5724 -0.3896 -2.4787 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.3622 0.2653 -1.4532 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.2205 -0.3286 -0.0454 C 0 0 0 0 0 0 0 0 0 0 0 0 7
1.1661 0.3429 0.9435 C 0 0 0 0 0 0 0 0 0 0 0 0 8
1.0349 -0.2526 2.3190 N 0 0 0 0 0 0 0 0 0 0 0 0 9
1.7043 0.1736 2.9713 H 0 0 0 0 0 0 0 0 0 0 0 0 10
1.2338 -1.2608 2.3075 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-1.1049 -0.2847 -4.5980 H 0 0 0 0 0 0 0 0 0 0 0 0 12
-0.6545 1.2806 -3.8859 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.6019 0.0803 -4.2610 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.3698 -1.4735 -2.5121 H 0 0 0 0 0 0 0 0 0 0 0 0 15
-1.6162 -0.2808 -2.1383 H 0 0 0 0 0 0 0 0 0 0 0 0 16
0.1584 1.3492 -1.4149 H 0 0 0 0 0 0 0 0 0 0 0 0 17
1.4073 0.1565 -1.7913 H 0 0 0 0 0 0 0 0 0 0 0 0 18
0.4324 -1.4104 -0.0774 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-0.8197 -0.2130 0.3018 H 0 0 0 0 0 0 0 0 0 0 0 0 20
0.9525 1.4142 1.0440 H 0 0 0 0 0 0 0 0 0 0 0 0 21
2.2139 0.2237 0.6411 H 0 0 0 0 0 0 0 0 0 0 0 0 22
0.0625 -0.1135 2.7175 H 0 0 0 0 0 0 0 0 0 0 0 0 23
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
19 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
22 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
9 23 0 0 0 0
M END
$$$$
n-pentylamine.sdf
COSMOtherm 3D 0
22 20 0 0 0 0 0 0 0 0 0 V2000
1.5564 -3.3717 -0.2059 O 0 0 0 0 0 0 0 0 0 0 0 0 1
0.6290 -2.9940 -0.0242 H 0 0 0 0 0 0 0 0 0 0 0 0 2
2.1170 -2.9775 0.4842 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.3989 3.8482 -0.1921 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.5807 2.4321 0.3647 C 0 0 0 0 0 0 0 0 0 0 0 0 5
-0.3890 1.4128 -0.2480 C 0 0 0 0 0 0 0 0 0 0 0 0 6
-0.2107 -0.0069 0.3029 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-1.1894 -1.0113 -0.3065 C 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.9794 -2.3696 0.2498 N 0 0 0 0 0 0 0 0 0 0 0 0 9
-1.6527 -3.0201 -0.1664 H 0 0 0 0 0 0 0 0 0 0 0 0 10
-1.1903 -2.3624 1.2529 H 0 0 0 0 0 0 0 0 0 0 0 0 11
1.1062 4.5555 0.2666 H 0 0 0 0 0 0 0 0 0 0 0 0 12
0.5620 3.8706 -1.2813 H 0 0 0 0 0 0 0 0 0 0 0 0 13
-0.6195 4.2218 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 0 14
0.4455 2.4462 1.4600 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.6171 2.0962 0.1873 H 0 0 0 0 0 0 0 0 0 0 0 0 16
-0.2551 1.3992 -1.3444 H 0 0 0 0 0 0 0 0 0 0 0 0 17
-1.4265 1.7473 -0.0687 H 0 0 0 0 0 0 0 0 0 0 0 0 18
-0.3455 0.0069 1.3994 H 0 0 0 0 0 0 0 0 0 0 0 0 19
0.8203 -0.3534 0.1162 H 0 0 0 0 0 0 0 0 0 0 0 0 20
-1.0327 -1.0707 -1.3951 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-2.2252 -0.6579 -0.1471 H 0 0 0 0 0 0 0 0 0 0 0 0 22
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
16 5 0 0 0 0
7 6 0 0 0 0
17 6 0 0 0 0
18 6 0 0 0 0
8 7 0 0 0 0
19 7 0 0 0 0
20 7 0 0 0 0
9 8 0 0 0 0
21 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
8 22 0 0 0 0
M END
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17 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
20 11 0 0 0 0
10 21 0 0 0 0
M END
$$$$
p-toluidine.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
0.1002 1.3000 -3.7656 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.8257 1.5460 -3.9342 H 0 0 0 0 0 0 0 0 0 0 0 2
0.0381 0.4944 -3.1768 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0270 0.6835 3.4364 C 0 0 0 0 0 0 0 0 0 0 0 4
0.0060 0.2214 1.9982 C 0 0 0 0 0 0 0 0 0 0 0 5
1.1996 -0.0318 1.2975 C 0 0 0 0 0 0 0 0 0 0 0 6
1.1918 -0.4566 -0.0326 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0247 -0.6458 -0.7145 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.2003 0.0266 1.3063 C 0 0 0 0 0 0 0 0 0 0 0 9
-1.2239 -0.3989 -0.0263 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.0347 -1.0068 -2.0840 N 0 0 0 0 0 0 0 0 0 0 0 11
0.5306 1.6577 3.5391 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.9918 0.7893 3.8335 H 0 0 0 0 0 0 0 0 0 0 0 13
0.5683 -0.0266 4.0807 H 0 0 0 0 0 0 0 0 0 0 0 14
2.1595 0.1031 1.8027 H 0 0 0 0 0 0 0 0 0 0 0 15
2.1356 -0.6439 -0.5504 H 0 0 0 0 0 0 0 0 0 0 0 16
-2.1482 0.2064 1.8198 H 0 0 0 0 0 0 0 0 0 0 0 17
-2.1799 -0.5430 -0.5354 H 0 0 0 0 0 0 0 0 0 0 0 18
0.7798 -1.5580 -2.3593 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.8829 -1.5025 -2.3628 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
9 5 0 0 0 0
7 6 0 0 0 0
15 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
10 8 0 0 0 0
11 8 0 0 0 0
10 9 0 0 0 0
17 9 0 0 0 0
18 10 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
p-toluidine0.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-1.2986 0.1085 -3.7746 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.5119 -0.8113 -4.0086 H 0 0 0 0 0 0 0 0 0 0 0 2
-0.4972 0.0341 -3.1825 H 0 0 0 0 0 0 0 0 0 0 0 3
0.0451 1.1999 1.3012 C 0 0 0 0 0 0 0 0 0 0 0 4
0.4649 1.1894 -0.0319 C 0 0 0 0 0 0 0 0 0 0 0 5
0.6429 -0.0277 -0.7129 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3939 -1.2261 -0.0212 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0251 -1.1999 1.3120 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.2132 0.0098 2.0029 C 0 0 0 0 0 0 0 0 0 0 0 9
0.9999 -0.0436 -2.0835 N 0 0 0 0 0 0 0 0 0 0 0 10
-0.6985 0.0308 3.4332 C 0 0 0 0 0 0 0 0 0 0 0 11
1.4923 -0.8943 -2.3605 H 0 0 0 0 0 0 0 0 0 0 0 12
1.5532 0.7681 -2.3626 H 0 0 0 0 0 0 0 0 0 0 0 13
-0.0777 2.1603 1.8083 H 0 0 0 0 0 0 0 0 0 0 0 14
0.6604 2.1321 -0.5489 H 0 0 0 0 0 0 0 0 0 0 0 15
0.5337 -2.1833 -0.5295 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.2045 -2.1467 1.8278 H 0 0 0 0 0 0 0 0 0 0 0 17
-1.7996 0.0628 3.4818 H 0 0 0 0 0 0 0 0 0 0 0 18
-0.3240 0.9135 3.9707 H 0 0 0 0 0 0 0 0 0 0 0 19
-0.3755 -0.8668 3.9795 H 0 0 0 0 0 0 0 0 0 0 0 20
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
10 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
9 8 0 0 0 0
17 8 0 0 0 0
11 9 0 0 0 0
12 10 0 0 0 0
13 10 0 0 0 0
18 11 0 0 0 0
19 11 0 0 0 0
11 20 0 0 0 0
M END
$$$$
p-toluidine1.sdf
COSMOtherm 3D 0
20 19 0 0 0 0 0 0 0 0 0 V2000
-3.7656 -1.3067 0.0814 O 0 0 0 0 0 0 0 0 0 0 0 1

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3      -3.1790  -0.4993   0.0237 H   0 0 0 0 0 0 0 0 0 0 0 2
4      -4.0171  -1.4867  -0.8409 H   0 0 0 0 0 0 0 0 0 0 0 3
5      1.3026   0.0271   1.1997 C   0 0 0 0 0 0 0 0 0 0 0 4
6      -0.0302   0.4475   1.1991 C   0 0 0 0 0 0 0 0 0 0 0 5
7      -0.7141   0.6455  -0.0136 C   0 0 0 0 0 0 0 0 0 0 0 6
8      -0.0248   0.4151  -1.2171 C   0 0 0 0 0 0 0 0 0 0 0 7
9      1.3079  -0.0058  -1.2005 C   0 0 0 0 0 0 0 0 0 0 0 8
10     2.0014  -0.2134   0.0042 C   0 0 0 0 0 0 0 0 0 0 0 9
11     -2.0844  1.0027  -0.0206 N   0 0 0 0 0 0 0 0 0 0 0 10
12     3.4312  -0.7007   0.0146 C   0 0 0 0 0 0 0 0 0 0 0 11
13     -2.3623  1.5108  -0.8616 H   0 0 0 0 0 0 0 0 0 0 0 12
14     -2.3630  1.5408   0.8014 H   0 0 0 0 0 0 0 0 0 0 0 13
15     1.8116  -0.1114   2.1570 H   0 0 0 0 0 0 0 0 0 0 0 14
16     -0.5448   0.6289   2.1458 H   0 0 0 0 0 0 0 0 0 0 0 15
17     -0.5352   0.5705  -2.1708 H   0 0 0 0 0 0 0 0 0 0 0 16
18     1.8213  -0.1699  -2.1513 H   0 0 0 0 0 0 0 0 0 0 0 17
19     3.4787  -1.8022   0.0292 H   0 0 0 0 0 0 0 0 0 0 0 18
20     3.9707  -0.3408   0.9022 H   0 0 0 0 0 0 0 0 0 0 0 19
21     3.9758  -0.3638  -0.8788 H   0 0 0 0 0 0 0 0 0 0 0 20
22     2 1 0 0 0 0 0
23     3 1 0 0 0 0 0
24     5 4 0 0 0 0 0
25     9 4 0 0 0 0 0
26     14 4 0 0 0 0 0
27     6 5 0 0 0 0 0
28     15 5 0 0 0 0 0
29     7 6 0 0 0 0 0
30     10 6 0 0 0 0 0
31     8 7 0 0 0 0 0
32     16 7 0 0 0 0 0
33     9 8 0 0 0 0 0
34     17 8 0 0 0 0 0
35     11 9 0 0 0 0 0
36     12 10 0 0 0 0 0
37     13 10 0 0 0 0 0
38     18 11 0 0 0 0 0
39     19 11 0 0 0 0 0
40     11 20 0 0 0 0 0
41 M END
42 $$$$
43 pyrazine.sdf
44 COSMOTHERM 3D 0
45
46     13 12 0 0 0 0 0 0 0 0 0 0 V2000
47     -3.4665  -0.0478  -0.0042 O   0 0 0 0 0 0 0 0 0 0 0 1
48     -2.4676  -0.0340   0.0043 H   0 0 0 0 0 0 0 0 0 0 0 2
49     -3.7188   0.8897   0.0535 H   0 0 0 0 0 0 0 0 0 0 0 3
50     1.4739   0.0036   1.1381 C   0 0 0 0 0 0 0 0 0 0 0 4
51     2.1789   0.0100  -0.0067 N   0 0 0 0 0 0 0 0 0 0 0 5
52     0.0759  -0.0075   1.1483 C   0 0 0 0 0 0 0 0 0 0 0 6
53     -0.6340  -0.0121   0.0069 N   0 0 0 0 0 0 0 0 0 0 0 7
54     0.0650  -0.0062  -1.1413 C   0 0 0 0 0 0 0 0 0 0 0 8
55     1.4628   0.0050  -1.1446 C   0 0 0 0 0 0 0 0 0 0 0 9
56     2.0372   0.0071   2.0738 H   0 0 0 0 0 0 0 0 0 0 0 10
57     -0.4821  -0.0126   2.0866 H   0 0 0 0 0 0 0 0 0 0 0 11
58     -0.5019  -0.0103  -2.0743 H   0 0 0 0 0 0 0 0 0 0 0 12
59     2.0171   0.0096  -2.0857 H   0 0 0 0 0 0 0 0 0 0 0 13
60     2 1 0 0 0 0 0
61     3 1 0 0 0 0 0
62     5 4 0 0 0 0 0
63     6 4 0 0 0 0 0
64     10 4 0 0 0 0 0
65     9 5 0 0 0 0 0
66     7 6 0 0 0 0 0
67     11 6 0 0 0 0 0
68     8 7 0 0 0 0 0
69     9 8 0 0 0 0 0
70     12 8 0 0 0 0 0
71     9 13 0 0 0 0 0
72 M END
73 $$$$
74 pyrazine-cation.sdf
75 COSMOTHERM 3D 0
76
77     14 13 0 0 0 0 0 0 0 0 0 0 V2000
78     -3.2535   0.0515   0.0028 O   0 0 0 0 0 0 0 0 0 0 0 1
79     -3.6709  -0.3104   0.8063 H   0 0 0 0 0 0 0 0 0 0 0 2
80     -3.6985  -0.3974  -0.7395 H   0 0 0 0 0 0 0 0 0 0 0 3
81     0.0369   1.1570  -0.0051 C   0 0 0 0 0 0 0 0 0 0 0 4
82     -0.5974  -0.0292  -0.0084 N   0 0 0 0 0 0 0 0 0 0 0 5
83     0.0855  -1.1880  -0.0044 C   0 0 0 0 0 0 0 0 0 0 0 6
84     1.4782  -1.1341   0.0033 C   0 0 0 0 0 0 0 0 0 0 0 7
85     2.1514   0.0282   0.0064 N   0 0 0 0 0 0 0 0 0 0 0 8
86     1.4307   1.1614   0.0006 C   0 0 0 0 0 0 0 0 0 0 0 9
87     -1.6778  -0.0455  -0.0121 H   0 0 0 0 0 0 0 0 0 0 0 10
88     -0.5737   2.0575  -0.0077 H   0 0 0 0 0 0 0 0 0 0 0 11
89     -0.4858  -2.1139  -0.0074 H   0 0 0 0 0 0 0 0 0 0 0 12
90     2.0598  -2.0562   0.0072 H   0 0 0 0 0 0 0 0 0 0 0 13
91     1.9735   2.1069   0.0031 H   0 0 0 0 0 0 0 0 0 0 0 14
92     2 1 0 0 0 0 0
93     3 1 0 0 0 0 0
94     5 4 0 0 0 0 0
95     9 4 0 0 0 0 0
96     11 4 0 0 0 0 0
97     6 5 0 0 0 0 0
98     10 5 0 0 0 0 0
99     7 6 0 0 0 0 0
100    12 6 0 0 0 0 0
101    8 7 0 0 0 0 0
102    13 7 0 0 0 0 0
103    9 8 0 0 0 0 0
104    9 14 0 0 0 0 0
105 M END
106 $$$$
107 pyrazole.sdf

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2.0158 2.1518 0.0047 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.5110 2.0965 -0.0019 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5661 -2.0602 -0.0067 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9589 -2.1823 0.0009 H 0 0 0 0 0 0 0 0 0 0 0 13
3.2600 -0.0319 0.0064 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.6322 0.0305 -0.0065 H 0 0 0 0 0 0 0 0 0 0 0 15
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
14 9 0 0 0 0
6 15 0 0 0 0
M END
$$$$
pyrimidine.sdf
COSMOtherm 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
-3.4437 -0.0635 -0.0158 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.4456 -0.0214 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.7230 0.8679 0.0117 H 0 0 0 0 0 0 0 0 0 0 0 3
2.1191 -0.0047 -0.0414 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4422 -0.0010 -1.2070 N 0 0 0 0 0 0 0 0 0 0 0 5
0.1049 0.0056 -1.1102 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6138 0.0093 0.0254 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0811 0.0047 1.1798 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4744 -0.0018 1.1957 C 0 0 0 0 0 0 0 0 0 0 0 9
3.2096 -0.0103 -0.1099 H 0 0 0 0 0 0 0 0 0 0 0 10
-0.4597 0.0091 -2.0459 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5016 0.0069 2.1036 H 0 0 0 0 0 0 0 0 0 0 0 12
2.0333 -0.0051 2.1308 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
11 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
12 8 0 0 0 0
9 13 0 0 0 0
M END
$$$$
pyrimidine-cation.sdf
COSMOtherm 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.2426 -0.0636 -0.0007 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.6753 0.3787 -0.7542 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.6684 0.3114 0.7922 H 0 0 0 0 0 0 0 0 0 0 0 3
2.0974 -0.0533 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 4
1.4717 1.1959 0.0010 C 0 0 0 0 0 0 0 0 0 0 0 5
0.0865 1.2148 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.5773 0.0398 -0.0022 N 0 0 0 0 0 0 0 0 0 0 0 7
0.0907 -1.1343 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 8
1.4137 -1.2168 0.0001 N 0 0 0 0 0 0 0 0 0 0 0 9
3.1860 -0.1325 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 10
2.0428 2.1219 0.0023 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.5131 2.1235 -0.0005 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.5116 -2.0427 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.6549 0.0316 -0.0028 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
12 6 0 0 0 0
8 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
7 14 0 0 0 0
M END
$$$$
pyrrole-cation0.sdf
COSMOtherm 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-2.6041 0.0101 0.4602 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.0592 -0.8531 0.4655 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.2471 0.6318 0.0700 H 0 0 0 0 0 0 0 0 0 0 0 3
1.5369 0.7370 0.4344 C 0 0 0 0 0 0 0 0 0 0 0 4
1.5485 -0.7243 0.4312 C 0 0 0 0 0 0 0 0 0 0 0 5
0.4751 1.1657 -0.2759 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2692 -0.0054 -0.7396 N 0 0 0 0 0 0 0 0 0 0 0 7
0.4929 -1.1669 -0.2799 C 0 0 0 0 0 0 0 0 0 0 0 8
2.2651 1.3730 0.9304 H 0 0 0 0 0 0 0 0 0 0 0 9
2.2875 -1.3507 0.9235 H 0 0 0 0 0 0 0 0 0 0 0 10
0.0998 2.1530 -0.5224 H 0 0 0 0 0 0 0 0 0 0 0 11
-0.4145 -0.0058 -1.7618 H 0 0 0 0 0 0 0 0 0 0 0 12
0.1350 -2.1588 -0.5336 H 0 0 0 0 0 0 0 0 0 0 0 13
-1.2922 -0.0131 -0.2895 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0

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3 1 0 0 0 0
4 4 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
7 4 0 0 0 0
8 5 0 0 0 0
9 5 0 0 0 0
10 5 0 0 0 0
11 6 0 0 0 0
12 7 0 0 0 0
13 8 0 0 0 0
14 7 14 0 0 0 0
M END
$$$$
pyrrole-cation1.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.0547 -0.0450 0.0199 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4484 -0.0111 -0.8712 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4901 0.6769 0.5091 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8833 -0.6195 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 4
1.8266 0.7402 -0.0089 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5013 -1.1625 0.0094 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.3255 0.0376 0.0073 N 0 0 0 0 0 0 0 0 0 0 0 7
0.4333 1.1047 -0.0045 C 0 0 0 0 0 0 0 0 0 0 0 8
-1.3837 0.0340 0.0071 H 0 0 0 0 0 0 0 0 0 0 0 9
2.7711 -1.2471 -0.0021 H 0 0 0 0 0 0 0 0 0 0 0 10
2.6504 1.4475 -0.0175 H 0 0 0 0 0 0 0 0 0 0 0 11
0.0050 2.1058 -0.0090 H 0 0 0 0 0 0 0 0 0 0 0 12
0.2855 -1.7775 0.8995 H 0 0 0 0 0 0 0 0 0 0 0 13
0.2753 -1.7867 -0.8717 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
11 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
9 7 0 0 0 0
12 8 0 0 0 0
6 14 0 0 0 0
M END
$$$$
pyrrole-cation2.sdf
COSMOTHERM 3D 0
14 13 0 0 0 0 0 0 0 0 0 V2000
-3.0354 0.0436 -0.0056 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.4467 -0.2946 0.8108 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.4554 -0.4630 -0.7247 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8228 0.7342 -0.0008 C 0 0 0 0 0 0 0 0 0 0 0 4
1.7899 -0.7614 0.0013 C 0 0 0 0 0 0 0 0 0 0 0 5
0.3911 1.1000 -0.0019 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.3255 0.0094 -0.0002 N 0 0 0 0 0 0 0 0 0 0 0 7
0.4997 -1.1514 0.0021 C 0 0 0 0 0 0 0 0 0 0 0 8
2.3417 1.1690 0.8736 H 0 0 0 0 0 0 0 0 0 0 0 9
2.3423 1.1669 -0.8759 H 0 0 0 0 0 0 0 0 0 0 0 10
-1.3908 -0.0170 -0.0013 H 0 0 0 0 0 0 0 0 0 0 0 11
2.6645 -1.4045 0.0030 H 0 0 0 0 0 0 0 0 0 0 0 12
-0.0556 2.0916 -0.0041 H 0 0 0 0 0 0 0 0 0 0 0 13
0.0390 -2.1340 0.0036 H 0 0 0 0 0 0 0 0 0 0 0 14
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
6 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
8 5 0 0 0 0
12 5 0 0 0 0
7 6 0 0 0 0
13 6 0 0 0 0
8 7 0 0 0 0
11 7 0 0 0 0
8 14 0 0 0 0
M END
$$$$
pyrrole.sdf
COSMOTHERM 3D 0
13 12 0 0 0 0 0 0 0 0 0 V2000
-3.1605 0.0125 0.0535 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.5334 -0.8583 -0.1739 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5513 0.6172 -0.6028 H 0 0 0 0 0 0 0 0 0 0 0 3
1.8445 -0.0065 -0.7257 C 0 0 0 0 0 0 0 0 0 0 0 4
1.8594 -0.0011 0.7028 C 0 0 0 0 0 0 0 0 0 0 0 5
0.5370 0.0064 1.1279 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.2675 0.0058 0.0107 N 0 0 0 0 0 0 0 0 0 0 0 7
0.5135 -0.0021 -1.1228 C 0 0 0 0 0 0 0 0 0 0 0 8
2.7066 -0.0130 -1.3877 H 0 0 0 0 0 0 0 0 0 0 0 9
2.7352 -0.0025 1.3468 H 0 0 0 0 0 0 0 0 0 0 0 10
0.1089 0.0123 2.1257 H 0 0 0 0 0 0 0 0 0 0 0 11
-1.3011 0.0083 0.0182 H 0 0 0 0 0 0 0 0 0 0 0 12
0.0645 -0.0044 -2.1115 H 0 0 0 0 0 0 0 0 0 0 0 13
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
10 5 0 0 0 0
7 6 0 0 0 0

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11 6 0 0 0 0
8 7 0 0 0 0
12 7 0 0 0 0
8 13 0 0 0 0

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M END

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quinoline.sdf
COSMOTHERM 3D 0

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20 20 0 0 0 0 0 0 0 0 0 V2000
-3.4690 1.7152 -0.0583 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.7048 1.0658 -0.0173 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.5114 2.0931 0.8371 H 0 0 0 0 0 0 0 0 0 0 0 3
-0.0379 0.2273 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 4
-1.3609 -0.1421 0.0038 N 0 0 0 0 0 0 0 0 0 0 0 5
-1.6564 -1.4374 0.0043 C 0 0 0 0 0 0 0 0 0 0 0 6
-0.6842 -2.4659 0.0019 C 0 0 0 0 0 0 0 0 0 0 0 7
0.6514 -2.1193 -0.0003 C 0 0 0 0 0 0 0 0 0 0 0 8
1.0182 -0.7478 -0.0002 C 0 0 0 0 0 0 0 0 0 0 0 9
0.2933 1.6082 0.0009 C 0 0 0 0 0 0 0 0 0 0 0 10
1.6171 2.0060 -0.0005 C 0 0 0 0 0 0 0 0 0 0 0 11
2.6616 1.0459 -0.0015 C 0 0 0 0 0 0 0 0 0 0 0 12
2.3691 -0.3044 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.7199 -1.6913 0.0070 H 0 0 0 0 0 0 0 0 0 0 0 14
-1.0018 -3.5086 0.0019 H 0 0 0 0 0 0 0 0 0 0 0 15
1.4311 -2.8844 -0.0021 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.5176 2.3388 -0.0002 H 0 0 0 0 0 0 0 0 0 0 0 17
1.8645 3.0689 -0.0007 H 0 0 0 0 0 0 0 0 0 0 0 18
3.7001 1.3805 -0.0023 H 0 0 0 0 0 0 0 0 0 0 0 19
3.1687 -1.0484 -0.0027 H 0 0 0 0 0 0 0 0 0 0 0 20

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 6 0 0 0 0
14 6 0 0 0 0
8 7 0 0 0 0
15 7 0 0 0 0
9 8 0 0 0 0
16 8 0 0 0 0
13 9 0 0 0 0
11 10 0 0 0 0
17 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
13 12 0 0 0 0
19 12 0 0 0 0
13 20 0 0 0 0

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M END

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quinoline-cation.sdf
COSMOTHERM 3D 0

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21 21 0 0 0 0 0 0 0 0 0 V2000
-3.2512 1.7780 0.0135 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.9725 1.6523 0.6570 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.6997 1.9148 -0.8412 H 0 0 0 0 0 0 0 0 0 0 0 3
2.3653 -0.3586 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 4
2.6872 0.9840 0.0016 C 0 0 0 0 0 0 0 0 0 0 0 5
1.6678 1.9697 0.0014 C 0 0 0 0 0 0 0 0 0 0 0 6
0.3311 1.6146 0.0003 C 0 0 0 0 0 0 0 0 0 0 0 7
-0.0093 0.2449 -0.0023 C 0 0 0 0 0 0 0 0 0 0 0 8
1.0042 -0.7665 -0.0013 C 0 0 0 0 0 0 0 0 0 0 0 9
0.5998 -2.1248 -0.0004 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.7436 -2.4594 -0.0011 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.6997 -1.4360 -0.0016 C 0 0 0 0 0 0 0 0 0 0 0 12
-1.3265 -0.1531 -0.0012 N 0 0 0 0 0 0 0 0 0 0 0 13
3.1436 -1.1232 0.0017 H 0 0 0 0 0 0 0 0 0 0 0 14
3.7324 1.2946 0.0033 H 0 0 0 0 0 0 0 0 0 0 0 15
1.9423 3.0251 0.0030 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.4553 2.3702 0.0023 H 0 0 0 0 0 0 0 0 0 0 0 17
1.3620 -2.9060 0.0021 H 0 0 0 0 0 0 0 0 0 0 0 18
-1.0737 -3.4962 -0.0001 H 0 0 0 0 0 0 0 0 0 0 0 19
-2.7714 -1.6285 -0.0017 H 0 0 0 0 0 0 0 0 0 0 0 20
-2.0826 0.5924 -0.0010 H 0 0 0 0 0 0 0 0 0 0 0 21

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
15 5 0 0 0 0
7 6 0 0 0 0
16 6 0 0 0 0
8 7 0 0 0 0
17 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
10 9 0 0 0 0
11 10 0 0 0 0
18 10 0 0 0 0
12 11 0 0 0 0
19 11 0 0 0 0
13 12 0 0 0 0
20 12 0 0 0 0
13 21 0 0 0 0

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M END

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sec-butylamine-cation.sdf
COSMOTHERM 3D 0

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20 18 0 0 0 0 0 0 0 0 0 V2000
-2.5056 0.4073 0.9056 O 0 0 0 0 0 0 0 0 0 0 0 1

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-2.6773    0.3192    1.8609 H    0 0 0 0 0 0 0 0 0 0 0 2
-3.3654    0.2216    0.4860 H    0 0 0 0 0 0 0 0 0 0 0 3
 0.5942   -0.2765   -0.7790 C    0 0 0 0 0 0 0 0 0 0 0 4
-0.0817    0.4322   -1.9477 C    0 0 0 0 0 0 0 0 0 0 0 5
-0.4309   -1.1524   -0.0818 N    0 0 0 0 0 0 0 0 0 0 0 6
 1.2249    0.6846    0.2322 C    0 0 0 0 0 0 0 0 0 0 0 7
 1.9820    0.0042    1.3790 C    0 0 0 0 0 0 0 0 0 0 0 8
-0.8163   -1.8527   -0.7277 H    0 0 0 0 0 0 0 0 0 0 0 9
-0.0080   -1.6773    0.6938 H    0 0 0 0 0 0 0 0 0 0 0 10
 1.3586   -0.9725   -1.1534 H    0 0 0 0 0 0 0 0 0 0 0 11
-0.5600   -0.2849   -2.6302 H    0 0 0 0 0 0 0 0 0 0 0 12
 0.6727    0.9892   -2.5189 H    0 0 0 0 0 0 0 0 0 0 0 13
-0.8407    1.1462   -1.5957 H    0 0 0 0 0 0 0 0 0 0 0 14
 1.9191    1.3208   -0.3374 H    0 0 0 0 0 0 0 0 0 0 0 15
 0.4451    1.3568    0.6278 H    0 0 0 0 0 0 0 0 0 0 0 16
 2.4847    0.7563    2.0027 H    0 0 0 0 0 0 0 0 0 0 0 17
 1.3171   -0.5668    2.0463 H    0 0 0 0 0 0 0 0 0 0 0 18
 2.7500   -0.6844    0.9956 H    0 0 0 0 0 0 0 0 0 0 0 19
-1.2426   -0.5864    0.3039 H    0 0 0 0 0 0 0 0 0 0 0 20
 2 1 0 0 0 0 0
 3 1 0 0 0 0 0
 5 4 0 0 0 0 0
 6 4 0 0 0 0 0
 7 4 0 0 0 0 0
11 4 0 0 0 0 0
12 5 0 0 0 0 0
13 5 0 0 0 0 0
14 5 0 0 0 0 0
 9 6 0 0 0 0 0
10 6 0 0 0 0 0
 8 7 0 0 0 0 0
15 7 0 0 0 0 0
16 7 0 0 0 0 0
17 8 0 0 0 0 0
18 8 0 0 0 0 0
19 8 0 0 0 0 0
 6 20 0 0 0 0 0
M END
$$$$
sec-butylamine.sdf
COSMOtherm          3D          0
19 17 0 0 0 0 0 0 0 0 0 0 V2000
-2.6012   -0.9728    0.3938 O    0 0 0 0 0 0 0 0 0 0 0 1
-1.8215   -0.5798   -0.1233 H    0 0 0 0 0 0 0 0 0 0 0 2
-3.2525   -0.2515    0.4336 H    0 0 0 0 0 0 0 0 0 0 0 3
 0.5784    0.7544   -0.3142 C    0 0 0 0 0 0 0 0 0 0 0 4
-0.0337    1.9538    0.4113 C    0 0 0 0 0 0 0 0 0 0 0 5
-0.4899    0.0670   -1.0882 N    0 0 0 0 0 0 0 0 0 0 0 6
 1.2331   -0.2287    0.6660 C    0 0 0 0 0 0 0 0 0 0 0 7
 1.9557   -1.4049   -0.0020 C    0 0 0 0 0 0 0 0 0 0 0 8
-0.8898    0.7226   -1.7675 H    0 0 0 0 0 0 0 0 0 0 0 9
-0.0837   -0.6881   -1.6488 H    0 0 0 0 0 0 0 0 0 0 0 10
 1.3672    1.1259   -0.9982 H    0 0 0 0 0 0 0 0 0 0 0 11
-0.4949    2.6550   -0.3010 H    0 0 0 0 0 0 0 0 0 0 0 12
 0.7374    2.5013    0.9721 H    0 0 0 0 0 0 0 0 0 0 0 13
-0.8096    1.6235    1.1189 H    0 0 0 0 0 0 0 0 0 0 0 14
 1.9532    0.3392    1.2768 H    0 0 0 0 0 0 0 0 0 0 0 15
 0.4581   -0.6038    1.3561 H    0 0 0 0 0 0 0 0 0 0 0 16
 2.4647   -2.0283    0.7474 H    0 0 0 0 0 0 0 0 0 0 0 17
 1.2615   -2.0616   -0.5486 H    0 0 0 0 0 0 0 0 0 0 0 18
 2.7169   -1.0505   -0.7147 H    0 0 0 0 0 0 0 0 0 0 0 19
 2 1 0 0 0 0 0
 3 1 0 0 0 0 0
 5 4 0 0 0 0 0
 6 4 0 0 0 0 0
 7 4 0 0 0 0 0
11 4 0 0 0 0 0
12 5 0 0 0 0 0
13 5 0 0 0 0 0
14 5 0 0 0 0 0
 9 6 0 0 0 0 0
10 6 0 0 0 0 0
 8 7 0 0 0 0 0
15 7 0 0 0 0 0
16 7 0 0 0 0 0
17 8 0 0 0 0 0
18 8 0 0 0 0 0
 8 19 0 0 0 0 0
M END
$$$$
tert-butylamine-cation.sdf
COSMOtherm          3D          0
20 18 0 0 0 0 0 0 0 0 0 0 V2000
-2.8548    0.0010    0.0347 O    0 0 0 0 0 0 0 0 0 0 0 1
-3.3787   -0.7799   -0.2221 H    0 0 0 0 0 0 0 0 0 0 0 2
-3.4030    0.7606   -0.2347 H    0 0 0 0 0 0 0 0 0 0 0 3
 2.1301    0.0061   -0.6321 C    0 0 0 0 0 0 0 0 0 0 0 4
 0.7611   -0.0017    0.0538 C    0 0 0 0 0 0 0 0 0 0 0 5
 0.5557    1.2451    0.9189 C    0 0 0 0 0 0 0 0 0 0 0 6
 0.5368   -1.2896    0.8514 C    0 0 0 0 0 0 0 0 0 0 0 7
-0.2985    0.0354   -1.0476 N    0 0 0 0 0 0 0 0 0 0 0 8
-1.2865    0.0235   -0.6566 H    0 0 0 0 0 0 0 0 0 0 0 9
-0.1998   -0.7698   -1.6795 H    0 0 0 0 0 0 0 0 0 0 0 10
 2.2552   -0.8716   -1.2831 H    0 0 0 0 0 0 0 0 0 0 0 11
 2.2692    0.9158   -1.2347 H    0 0 0 0 0 0 0 0 0 0 0 12
 2.9199   -0.0210    0.1305 H    0 0 0 0 0 0 0 0 0 0 0 13
-0.4424    1.2524    1.3792 H    0 0 0 0 0 0 0 0 0 0 0 14
 0.6814    2.1646    0.3286 H    0 0 0 0 0 0 0 0 0 0 0 15
 1.3025    1.2536    1.7239 H    0 0 0 0 0 0 0 0 0 0 0 16
-0.4579   -1.3023    1.3190 H    0 0 0 0 0 0 0 0 0 0 0 17
 0.6397   -2.1779    0.2112 H    0 0 0 0 0 0 0 0 0 0 0 18
 1.2890   -1.3568    1.6484 H    0 0 0 0 0 0 0 0 0 0 0 19
-0.1982    0.8792   -1.6265 H    0 0 0 0 0 0 0 0 0 0 0 20

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
19 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
8 20 0 0 0 0

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M END

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tert-butylamine.sdf

COSMOTHERM 3D 0

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19 17 0 0 0 0 0 0 0 0 0 V2000
-2.9674 -0.0574 0.0093 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-2.0076 -0.0630 0.3412 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.1629 0.8819 -0.1509 H 0 0 0 0 0 0 0 0 0 0 0 0 3
0.5937 -1.1746 -0.9956 C 0 0 0 0 0 0 0 0 0 0 0 0 4
0.7309 0.0027 -0.0190 C 0 0 0 0 0 0 0 0 0 0 0 0 5
0.5422 1.3364 -0.7572 C 0 0 0 0 0 0 0 0 0 0 0 0 6
2.1107 -0.0336 0.6661 C 0 0 0 0 0 0 0 0 0 0 0 0 7
-0.3704 -0.1149 0.9845 N 0 0 0 0 0 0 0 0 0 0 0 0 8
-0.2771 0.6380 1.6756 H 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.2526 -0.9856 1.5146 H 0 0 0 0 0 0 0 0 0 0 0 0 10
0.6892 -2.1356 -0.4664 H 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.3853 -1.1519 -1.4960 H 0 0 0 0 0 0 0 0 0 0 0 0 12
1.3789 -1.1324 -1.7643 H 0 0 0 0 0 0 0 0 0 0 0 0 13
0.6205 2.1854 -0.0601 H 0 0 0 0 0 0 0 0 0 0 0 0 14
-0.4451 1.3757 -1.2403 H 0 0 0 0 0 0 0 0 0 0 0 0 15
1.3126 1.4627 -1.5312 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.2107 0.7955 1.3840 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.2488 -0.9794 1.2128 H 0 0 0 0 0 0 0 0 0 0 0 0 18
2.9230 0.0558 -0.0715 H 0 0 0 0 0 0 0 0 0 0 0 0 19

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
11 4 0 0 0 0
12 4 0 0 0 0
13 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
8 5 0 0 0 0
14 6 0 0 0 0
15 6 0 0 0 0
16 6 0 0 0 0
17 7 0 0 0 0
18 7 0 0 0 0
9 8 0 0 0 0
10 8 0 0 0 0
7 19 0 0 0 0

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M END

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tert-butylcyclohexylamine-cation.sdf

COSMOTHERM 3D 0

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36 35 0 0 0 0 0 0 0 0 0 V2000
-2.8269 1.1312 -0.7075 O 0 0 0 0 0 0 0 0 0 0 0 0 1
-3.3907 1.1957 0.0845 H 0 0 0 0 0 0 0 0 0 0 0 0 2
-3.1605 1.8269 -1.3028 H 0 0 0 0 0 0 0 0 0 0 0 0 3
-0.0254 0.8387 -0.5273 N 0 0 0 0 0 0 0 0 0 0 0 0 4
0.6057 2.0559 0.1867 C 0 0 0 0 0 0 0 0 0 0 0 0 5
2.1257 1.9840 0.0155 C 0 0 0 0 0 0 0 0 0 0 0 0 6
0.0411 3.2912 -0.5264 C 0 0 0 0 0 0 0 0 0 0 0 0 7
0.1955 2.0375 1.6601 C 0 0 0 0 0 0 0 0 0 0 0 0 8
0.3149 -0.5627 -0.0168 C 0 0 0 0 0 0 0 0 0 0 0 0 9
-0.8615 -1.1730 0.7509 C 0 0 0 0 0 0 0 0 0 0 0 0 10
-0.5016 -2.5881 1.2345 C 0 0 0 0 0 0 0 0 0 0 0 0 11
-0.0742 -3.4896 0.0679 C 0 0 0 0 0 0 0 0 0 0 0 0 12
1.0822 -2.8628 -0.7232 C 0 0 0 0 0 0 0 0 0 0 0 0 13
0.7355 -1.4429 -1.1991 C 0 0 0 0 0 0 0 0 0 0 0 0 14
0.2714 0.8961 -1.5117 H 0 0 0 0 0 0 0 0 0 0 0 0 15
2.5741 2.8784 0.4679 H 0 0 0 0 0 0 0 0 0 0 0 0 16
2.5640 1.1084 0.5132 H 0 0 0 0 0 0 0 0 0 0 0 0 17
2.4068 1.9675 -1.0479 H 0 0 0 0 0 0 0 0 0 0 0 0 18
0.4772 4.1944 -0.0797 H 0 0 0 0 0 0 0 0 0 0 0 0 19
-1.0511 3.3523 -0.4191 H 0 0 0 0 0 0 0 0 0 0 0 0 20
0.2941 3.2864 -1.5969 H 0 0 0 0 0 0 0 0 0 0 0 0 21
-0.8974 2.0635 1.7757 H 0 0 0 0 0 0 0 0 0 0 0 0 22
0.5910 1.1599 2.1894 H 0 0 0 0 0 0 0 0 0 0 0 0 23
0.6063 2.9312 2.1484 H 0 0 0 0 0 0 0 0 0 0 0 0 24
1.1697 -0.4428 0.6633 H 0 0 0 0 0 0 0 0 0 0 0 0 25
-1.7381 -1.2255 0.0838 H 0 0 0 0 0 0 0 0 0 0 0 0 26
-1.1378 -0.5372 1.6054 H 0 0 0 0 0 0 0 0 0 0 0 0 27
0.3187 -2.5235 1.9705 H 0 0 0 0 0 0 0 0 0 0 0 0 28
-1.3650 -3.0202 1.7618 H 0 0 0 0 0 0 0 0 0 0 0 0 29
-0.9345 -3.6469 -0.6058 H 0 0 0 0 0 0 0 0 0 0 0 0 30
0.2199 -4.4814 0.4441 H 0 0 0 0 0 0 0 0 0 0 0 0 31
1.9829 -2.8214 -0.0868 H 0 0 0 0 0 0 0 0 0 0 0 0 32
1.3399 -3.4843 -1.5939 H 0 0 0 0 0 0 0 0 0 0 0 0 33
-0.0948 -1.4896 -1.9255 H 0 0 0 0 0 0 0 0 0 0 0 0 34
1.5983 -0.9914 -1.7147 H 0 0 0 0 0 0 0 0 0 0 0 0 35
-1.0740 0.9682 -0.5453 H 0 0 0 0 0 0 0 0 0 0 0 0 36

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0

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34 14 0 0 0 0
14 35 0 0 0 0
M END

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tetrahydrozoline-cation2.sdf
COSMOtherm 3D 0

```

```

35 36 0 0 0 0 0 0 0 0 V2000
-3.0467 0.3542 -0.4084 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8612 0.2818 -0.9384 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.1617 1.1749 0.1034 H 0 0 0 0 0 0 0 0 0 0 0 3
0.2010 1.9286 3.0281 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7194 2.3907 1.8122 C 0 0 0 0 0 0 0 0 0 0 0 5
0.8957 1.4946 0.7570 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5508 0.1378 0.8868 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0352 -0.3335 2.1111 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1291 0.5797 3.1682 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8193 -0.8228 -0.2787 C 0 0 0 0 0 0 0 0 0 0 0 10
0.1081 -2.1898 -0.1210 C 0 0 0 0 0 0 0 0 0 0 0 11
0.3149 -2.7236 1.2970 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.3455 -1.7875 2.3127 C 0 0 0 0 0 0 0 0 0 0 0 13
0.4717 -0.2131 -1.6070 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.7081 0.7983 -3.3206 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.7366 0.1897 -1.9727 N 0 0 0 0 0 0 0 0 0 0 0 16
1.3569 -0.0435 -2.5861 N 0 0 0 0 0 0 0 0 0 0 0 17
0.7086 0.4241 -3.8275 C 0 0 0 0 0 0 0 0 0 0 0 18
-1.5656 0.2515 -1.3418 H 0 0 0 0 0 0 0 0 0 0 0 19
0.0637 2.6152 3.8655 H 0 0 0 0 0 0 0 0 0 0 0 20
0.9918 3.4404 1.6889 H 0 0 0 0 0 0 0 0 0 0 0 21
1.3129 1.8580 -0.1859 H 0 0 0 0 0 0 0 0 0 0 0 22
-0.5214 0.2148 4.1209 H 0 0 0 0 0 0 0 0 0 0 0 23
1.9050 -1.0153 -0.3071 H 0 0 0 0 0 0 0 0 0 0 0 24
-0.9699 -2.0727 -0.3139 H 0 0 0 0 0 0 0 0 0 0 0 25
0.5025 -2.8879 -0.8731 H 0 0 0 0 0 0 0 0 0 0 0 26
1.3937 -2.8140 1.5079 H 0 0 0 0 0 0 0 0 0 0 0 27
-0.1138 -3.7332 1.3806 H 0 0 0 0 0 0 0 0 0 0 0 28
-1.4430 -1.8807 2.2274 H 0 0 0 0 0 0 0 0 0 0 0 29
-0.0942 -2.0890 3.3409 H 0 0 0 0 0 0 0 0 0 0 0 30
-1.5033 0.3831 -3.9497 H 0 0 0 0 0 0 0 0 0 0 0 31
-0.8482 1.8854 -3.2391 H 0 0 0 0 0 0 0 0 0 0 0 32
1.2487 1.2783 -4.2494 H 0 0 0 0 0 0 0 0 0 0 0 33
0.6895 -0.3915 -4.5636 H 0 0 0 0 0 0 0 0 0 0 0 34
2.3137 -0.3817 -2.5401 H 0 0 0 0 0 0 0 0 0 0 0 35

```

```

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
20 4 0 0 0 0
6 5 0 0 0 0
21 5 0 0 0 0
7 6 0 0 0 0
22 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
23 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
25 11 0 0 0 0
26 11 0 0 0 0
13 12 0 0 0 0
27 12 0 0 0 0
28 12 0 0 0 0
29 13 0 0 0 0
30 13 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
16 15 0 0 0 0
18 15 0 0 0 0
31 15 0 0 0 0
32 15 0 0 0 0
19 16 0 0 0 0
18 17 0 0 0 0
33 18 0 0 0 0
34 18 0 0 0 0
17 35 0 0 0 0

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M END
$$$$
tetrahydrozoline-cation3.sdf
COSMOtherm 3D 0

```

```

35 36 0 0 0 0 0 0 0 0 V2000
-3.0142 0.4468 -0.3537 O 0 0 0 0 0 0 0 0 0 0 0 1
-3.8306 0.4936 -0.8838 H 0 0 0 0 0 0 0 0 0 0 0 2
-3.0520 1.2376 0.2133 H 0 0 0 0 0 0 0 0 0 0 0 3
0.2427 1.9205 3.0210 C 0 0 0 0 0 0 0 0 0 0 0 4
0.7684 2.3726 1.8045 C 0 0 0 0 0 0 0 0 0 0 0 5
0.9262 1.4731 0.7491 C 0 0 0 0 0 0 0 0 0 0 0 6
0.5598 0.1220 0.8809 C 0 0 0 0 0 0 0 0 0 0 0 7
0.0374 -0.3395 2.1064 C 0 0 0 0 0 0 0 0 0 0 0 8
-0.1108 0.5779 3.1626 C 0 0 0 0 0 0 0 0 0 0 0 9
0.8027 -0.8425 -0.2864 C 0 0 0 0 0 0 0 0 0 0 0 10
0.0593 -2.1922 -0.1270 C 0 0 0 0 0 0 0 0 0 0 0 11
0.2637 -2.7346 1.2883 C 0 0 0 0 0 0 0 0 0 0 0 12
-0.3681 -1.7863 2.3110 C 0 0 0 0 0 0 0 0 0 0 0 13
0.4610 -0.2243 -1.6122 C 0 0 0 0 0 0 0 0 0 0 0 14
-0.7082 0.8176 -3.3146 C 0 0 0 0 0 0 0 0 0 0 0 15
-0.7389 0.2136 -1.9648 N 0 0 0 0 0 0 0 0 0 0 0 16
1.3409 -0.0801 -2.6007 N 0 0 0 0 0 0 0 0 0 0 0 17
0.6907 0.3988 -3.8371 C 0 0 0 0 0 0 0 0 0 0 0 18
-1.5555 0.3000 -1.3210 H 0 0 0 0 0 0 0 0 0 0 0 19
0.1165 2.6104 3.8576 H 0 0 0 0 0 0 0 0 0 0 0 20

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1
2
3 1.0578 3.4175 1.6797 H 0 0 0 0 0 0 0 0 0 0 21
4 1.3502 1.8285 -0.1939 H 0 0 0 0 0 0 0 0 0 0 22
5 -0.5099 0.2210 4.1157 H 0 0 0 0 0 0 0 0 0 0 23
6 1.8833 -1.0601 -0.3199 H 0 0 0 0 0 0 0 0 0 0 24
7 -1.0168 -2.0484 -0.3126 H 0 0 0 0 0 0 0 0 0 0 25
8 0.4315 -2.8979 -0.8834 H 0 0 0 0 0 0 0 0 0 0 26
9 1.3419 -2.8493 1.4904 H 0 0 0 0 0 0 0 0 0 0 27
10 -0.1864 -3.7345 1.3726 H 0 0 0 0 0 0 0 0 0 0 28
11 -1.4680 -1.8583 2.2369 H 0 0 0 0 0 0 0 0 0 0 29
12 -0.1122 -2.0929 3.3366 H 0 0 0 0 0 0 0 0 0 0 30
13 -1.5236 0.4263 -3.9329 H 0 0 0 0 0 0 0 0 0 0 31
14 -0.8128 1.9087 -3.2335 H 0 0 0 0 0 0 0 0 0 0 32
15 1.2506 1.2340 -4.2713 H 0 0 0 0 0 0 0 0 0 0 33
16 0.6374 -0.4202 -4.5676 H 0 0 0 0 0 0 0 0 0 0 34
17 2.2832 -0.4585 -2.5686 H 0 0 0 0 0 0 0 0 0 0 35
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
9 4 0 0 0 0
20 4 0 0 0 0
6 5 0 0 0 0
21 5 0 0 0 0
7 6 0 0 0 0
22 6 0 0 0 0
8 7 0 0 0 0
10 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0
23 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
25 11 0 0 0 0
26 11 0 0 0 0
13 12 0 0 0 0
27 12 0 0 0 0
28 12 0 0 0 0
29 13 0 0 0 0
30 13 0 0 0 0
16 14 0 0 0 0
17 14 0 0 0 0
16 15 0 0 0 0
18 15 0 0 0 0
31 15 0 0 0 0
32 15 0 0 0 0
19 16 0 0 0 0
18 17 0 0 0 0
33 18 0 0 0 0
34 18 0 0 0 0
17 35 0 0 0 0
M END
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tetrahydrozoline.sdf
COSMOTHERM 3D 0
34 35 0 0 0 0 0 0 0 0 0 V2000
-0.4967 -1.7169 -2.1863 O 0 0 0 0 0 0 0 0 0 0 1
0.2268 -1.3392 -1.5882 H 0 0 0 0 0 0 0 0 0 0 2
-1.3169 -1.3619 -1.7977 H 0 0 0 0 0 0 0 0 0 0 3
1.5639 -0.7632 -0.6151 N 0 0 0 0 0 0 0 0 0 0 4
2.9208 -1.3446 -0.7914 C 0 0 0 0 0 0 0 0 0 0 5
3.8450 -0.5003 0.1189 C 0 0 0 0 0 0 0 0 0 0 6
2.8514 0.0570 1.0575 N 0 0 0 0 0 0 0 0 0 0 7
-1.7986 0.6962 -0.1807 C 0 0 0 0 0 0 0 0 0 0 8
-0.8819 0.1656 0.7487 C 0 0 0 0 0 0 0 0 0 0 9
0.4724 0.8159 1.0019 C 0 0 0 0 0 0 0 0 0 0 10
0.5341 2.2721 0.4728 C 0 0 0 0 0 0 0 0 0 0 11
-0.0328 2.3669 -0.9449 C 0 0 0 0 0 0 0 0 0 0 12
-1.5122 1.9715 -0.9502 C 0 0 0 0 0 0 0 0 0 0 13
1.6189 0.0038 0.4329 C 0 0 0 0 0 0 0 0 0 0 14
-3.0252 0.0309 -0.3768 C 0 0 0 0 0 0 0 0 0 0 15
-3.3507 -1.1252 0.3352 C 0 0 0 0 0 0 0 0 0 0 16
-2.4426 -1.6402 1.2700 C 0 0 0 0 0 0 0 0 0 0 17
-1.2221 -0.9943 1.4670 C 0 0 0 0 0 0 0 0 0 0 18
3.2225 -1.3201 -1.8463 H 0 0 0 0 0 0 0 0 0 0 19
2.9002 -2.4004 -0.4718 H 0 0 0 0 0 0 0 0 0 0 20
4.3504 0.3053 -0.4399 H 0 0 0 0 0 0 0 0 0 0 21
4.6011 -1.0984 0.6422 H 0 0 0 0 0 0 0 0 0 0 22
3.0942 0.8740 1.6145 H 0 0 0 0 0 0 0 0 0 0 23
0.6332 0.8445 2.0923 H 0 0 0 0 0 0 0 0 0 0 24
1.5707 2.6394 0.5114 H 0 0 0 0 0 0 0 0 0 0 25
-0.0544 2.9114 1.1508 H 0 0 0 0 0 0 0 0 0 0 26
0.5350 1.6989 -1.6128 H 0 0 0 0 0 0 0 0 0 0 27
0.0836 3.3888 -1.3353 H 0 0 0 0 0 0 0 0 0 0 28
-1.8850 1.8663 -1.9807 H 0 0 0 0 0 0 0 0 0 0 29
-2.1048 2.7880 -0.4982 H 0 0 0 0 0 0 0 0 0 0 30
-3.7351 0.4364 -1.1029 H 0 0 0 0 0 0 0 0 0 0 31
-4.3074 -1.6224 0.1634 H 0 0 0 0 0 0 0 0 0 0 32
-2.6855 -2.5396 1.8390 H 0 0 0 0 0 0 0 0 0 0 33
-0.5098 -1.3960 2.1928 H 0 0 0 0 0 0 0 0 0 0 34
2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
14 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
20 5 0 0 0 0
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21 6 0 0 0 0
22 6 0 0 0 0
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23 7 0 0 0 0
9 8 0 0 0 0
13 8 0 0 0 0

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15 8 0 0 0 0
10 9 0 0 0 0
18 9 0 0 0 0
11 10 0 0 0 0
14 10 0 0 0 0
24 10 0 0 0 0
12 11 0 0 0 0
25 11 0 0 0 0
26 11 0 0 0 0
13 12 0 0 0 0
27 12 0 0 0 0
28 12 0 0 0 0
29 13 0 0 0 0
30 13 0 0 0 0
16 15 0 0 0 0
31 15 0 0 0 0
17 16 0 0 0 0
32 16 0 0 0 0
18 17 0 0 0 0
33 17 0 0 0 0
18 34 0 0 0 0

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M END

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tetrahydrozoline_p2.sdf

COSMOtherm

0

```

35 36 0 0 0 0 0 0 0 0 0 V2000
-1.0162 -2.0946 3.9019 O 0 0 0 0 0 0 0 0 0 0 0 1
-0.8552 -3.0160 3.6294 H 0 0 0 0 0 0 0 0 0 0 0 2
-1.9856 -2.0231 3.9666 H 0 0 0 0 0 0 0 0 0 0 0 3
0.3036 0.1814 1.2406 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3989 -0.1108 2.5289 N 0 0 0 0 0 0 0 0 0 0 0 5
1.2105 0.8965 3.2456 C 0 0 0 0 0 0 0 0 0 0 0 6
1.8383 1.7069 2.0811 C 0 0 0 0 0 0 0 0 0 0 0 7
1.0357 1.2489 0.9279 N 0 0 0 0 0 0 0 0 0 0 0 8
-0.5669 -0.5766 0.2717 C 0 0 0 0 0 0 0 0 0 0 0 9
0.0006 -0.5305 -1.1454 C 0 0 0 0 0 0 0 0 0 0 0 10
-0.6097 0.2334 -2.1604 C 0 0 0 0 0 0 0 0 0 0 0 11
-1.8901 1.0112 -1.9230 C 0 0 0 0 0 0 0 0 0 0 0 12
-2.2029 1.2409 -0.4412 C 0 0 0 0 0 0 0 0 0 0 0 13
-2.0290 -0.0586 0.3470 C 0 0 0 0 0 0 0 0 0 0 0 14
1.1586 -1.2763 -1.4335 C 0 0 0 0 0 0 0 0 0 0 0 15
1.7227 -1.2682 -2.7089 C 0 0 0 0 0 0 0 0 0 0 0 16
1.1249 -0.5038 -3.7201 C 0 0 0 0 0 0 0 0 0 0 0 17
-0.0264 0.2331 -3.4421 C 0 0 0 0 0 0 0 0 0 0 0 18
-0.1566 -0.8549 3.0031 H 0 0 0 0 0 0 0 0 0 0 0 19
1.9625 0.4099 3.8762 H 0 0 0 0 0 0 0 0 0 0 0 20
0.5579 1.5160 3.8760 H 0 0 0 0 0 0 0 0 0 0 0 21
2.8958 1.4577 1.9175 H 0 0 0 0 0 0 0 0 0 0 0 22
1.7396 2.7892 2.2167 H 0 0 0 0 0 0 0 0 0 0 0 23
-0.5571 -1.6215 0.6187 H 0 0 0 0 0 0 0 0 0 0 0 24
-2.7224 0.4488 -2.3829 H 0 0 0 0 0 0 0 0 0 0 0 25
-1.8399 1.9691 -2.4624 H 0 0 0 0 0 0 0 0 0 0 0 26
-3.2330 1.6099 -0.3298 H 0 0 0 0 0 0 0 0 0 0 0 27
-1.5440 2.0235 -0.0299 H 0 0 0 0 0 0 0 0 0 0 0 28
-2.6756 -0.8415 -0.0794 H 0 0 0 0 0 0 0 0 0 0 0 29
-2.3273 0.0667 1.3974 H 0 0 0 0 0 0 0 0 0 0 0 30
1.6183 -1.8738 -0.6418 H 0 0 0 0 0 0 0 0 0 0 0 31
2.6200 -1.8543 -2.9148 H 0 0 0 0 0 0 0 0 0 0 0 32
1.5568 -0.4841 -4.7225 H 0 0 0 0 0 0 0 0 0 0 0 33
-0.4935 0.8253 -4.2332 H 0 0 0 0 0 0 0 0 0 0 0 34
1.2259 1.5207 -0.0328 H 0 0 0 0 0 0 0 0 0 0 0 35

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2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
6 5 0 0 0 0
19 5 0 0 0 0
7 6 0 0 0 0
20 6 0 0 0 0
21 6 0 0 0 0
8 7 0 0 0 0
22 7 0 0 0 0
23 7 0 0 0 0
10 9 0 0 0 0
14 9 0 0 0 0
24 9 0 0 0 0
11 10 0 0 0 0
15 10 0 0 0 0
12 11 0 0 0 0
18 11 0 0 0 0
13 12 0 0 0 0
25 12 0 0 0 0
26 12 0 0 0 0
14 13 0 0 0 0
27 13 0 0 0 0
28 13 0 0 0 0
29 14 0 0 0 0
30 14 0 0 0 0
16 15 0 0 0 0
31 15 0 0 0 0
17 16 0 0 0 0
32 16 0 0 0 0
18 17 0 0 0 0
33 17 0 0 0 0
34 18 0 0 0 0
8 35 0 0 0 0

```

M END

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tetrahydrozoline_t_p2.sdf

COSMOtherm

3D

0

```

35 36 0 0 0 0 0 0 0 0 0 V2000
-2.9312 -0.9333 0.3366 O 0 0 0 0 0 0 0 0 0 0 0 1

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```

1
2
3 27 11 0 0 0 0
4 28 11 0 0 0 0
5 29 19 0 0 0 0
6 30 19 0 0 0 0
7 31 19 0 0 0 0
8 32 25 0 0 0 0
9 33 25 0 0 0 0
10 25 34 0 0 0 0
11 M END
12 $$$$
13 triethylamine-cation.sdf
14 COSMOtherm 3D 0
15
16 26 24 0 0 0 0 0 0 0 0 0 V2000
17 0.0593 -0.7412 -2.6475 O 0 0 0 0 0 0 0 0 0 0 0 1
18 0.2544 -1.6840 -2.7985 H 0 0 0 0 0 0 0 0 0 0 0 2
19 0.6327 -0.2681 -3.2778 H 0 0 0 0 0 0 0 0 0 0 0 3
20 2.5361 0.2823 -0.0242 C 0 0 0 0 0 0 0 0 0 0 0 4
21 1.2300 1.0338 0.1831 C 0 0 0 0 0 0 0 0 0 0 0 5
22 -0.0041 0.1712 -0.0018 N 0 0 0 0 0 0 0 0 0 0 0 6
23 -1.2504 1.0290 0.1025 C 0 0 0 0 0 0 0 0 0 0 0 7
24 -2.5357 0.2755 -0.2036 C 0 0 0 0 0 0 0 0 0 0 0 8
25 -0.0303 -1.0579 0.8877 C 0 0 0 0 0 0 0 0 0 0 0 9
26 -0.0723 -0.7540 2.3762 C 0 0 0 0 0 0 0 0 0 0 0 10
27 3.3567 1.0123 -0.0033 H 0 0 0 0 0 0 0 0 0 0 0 11
28 2.7304 -0.4555 0.7645 H 0 0 0 0 0 0 0 0 0 0 0 12
29 2.5628 -0.2237 -0.9997 H 0 0 0 0 0 0 0 0 0 0 0 13
30 1.1282 1.8459 -0.5480 H 0 0 0 0 0 0 0 0 0 0 0 14
31 1.1684 1.4769 1.1849 H 0 0 0 0 0 0 0 0 0 0 0 15
32 -1.1002 1.8467 -0.6137 H 0 0 0 0 0 0 0 0 0 0 0 16
33 -1.2608 1.4641 1.1096 H 0 0 0 0 0 0 0 0 0 0 0 17
34 -3.3582 1.0031 -0.2341 H 0 0 0 0 0 0 0 0 0 0 0 18
35 -2.7826 -0.4699 0.5629 H 0 0 0 0 0 0 0 0 0 0 0 19
36 -2.4910 -0.2201 -1.1838 H 0 0 0 0 0 0 0 0 0 0 0 20
37 0.8591 -1.6422 0.6249 H 0 0 0 0 0 0 0 0 0 0 0 21
38 -0.9043 -1.6410 0.5752 H 0 0 0 0 0 0 0 0 0 0 0 22
39 -0.0854 -1.7098 2.9168 H 0 0 0 0 0 0 0 0 0 0 0 23
40 -0.9740 -0.1980 2.6658 H 0 0 0 0 0 0 0 0 0 0 0 24
41 0.8100 -0.1948 2.7150 H 0 0 0 0 0 0 0 0 0 0 0 25
42 0.0303 -0.1919 -0.9940 H 0 0 0 0 0 0 0 0 0 0 0 26
43
44 2 1 0 0 0 0
45 3 1 0 0 0 0
46 5 4 0 0 0 0
47 11 4 0 0 0 0
48 12 4 0 0 0 0
49 13 4 0 0 0 0
50 6 5 0 0 0 0
51 14 5 0 0 0 0
52 15 5 0 0 0 0
53 7 6 0 0 0 0
54 9 6 0 0 0 0
55 8 7 0 0 0 0
56 16 7 0 0 0 0
57 17 7 0 0 0 0
58 18 8 0 0 0 0
59 19 8 0 0 0 0
60 20 8 0 0 0 0
10 9 0 0 0 0
11 9 0 0 0 0
12 9 0 0 0 0
13 10 0 0 0 0
14 10 0 0 0 0
15 10 0 0 0 0
16 6 26 0 0 0 0
17 M END
18 $$$$
19 triethylamine.sdf
20 COSMOtherm 3D 0
21
22 25 23 0 0 0 0 0 0 0 0 0 V2000
23 0.0434 -0.8594 -2.6092 O 0 0 0 0 0 0 0 0 0 0 0 1
24 0.0260 -0.4827 -1.6640 H 0 0 0 0 0 0 0 0 0 0 0 2
25 0.1234 -0.0755 -3.1794 H 0 0 0 0 0 0 0 0 0 0 0 3
26 2.5205 0.2663 -0.1288 C 0 0 0 0 0 0 0 0 0 0 0 4
27 1.2068 1.0075 0.1135 C 0 0 0 0 0 0 0 0 0 0 0 5
28 -0.0015 0.1583 -0.0261 N 0 0 0 0 0 0 0 0 0 0 0 6
29 -1.2148 1.0053 0.0772 C 0 0 0 0 0 0 0 0 0 0 0 7
30 -2.5190 0.2631 -0.2088 C 0 0 0 0 0 0 0 0 0 0 0 8
31 -0.0142 -1.0061 0.8956 C 0 0 0 0 0 0 0 0 0 0 0 9
32 -0.0348 -0.6978 2.3996 C 0 0 0 0 0 0 0 0 0 0 0 10
33 3.3473 0.9908 -0.1564 H 0 0 0 0 0 0 0 0 0 0 0 11
34 2.7462 -0.4595 0.6646 H 0 0 0 0 0 0 0 0 0 0 0 12
35 2.4995 -0.2660 -1.0912 H 0 0 0 0 0 0 0 0 0 0 0 13
36 1.1042 1.8132 -0.6303 H 0 0 0 0 0 0 0 0 0 0 0 14
37 1.2306 1.5022 1.1054 H 0 0 0 0 0 0 0 0 0 0 0 15
38 -1.0899 1.8131 -0.6608 H 0 0 0 0 0 0 0 0 0 0 0 16
39 -1.2709 1.4972 1.0692 H 0 0 0 0 0 0 0 0 0 0 0 17
40 -3.3458 0.9863 -0.2580 H 0 0 0 0 0 0 0 0 0 0 0 18
41 -2.7674 -0.4673 0.5736 H 0 0 0 0 0 0 0 0 0 0 0 19
42 -2.4680 -0.2639 -1.1731 H 0 0 0 0 0 0 0 0 0 0 0 20
43 0.8663 -1.6186 0.6565 H 0 0 0 0 0 0 0 0 0 0 0 21
44 -0.8879 -1.6186 0.6325 H 0 0 0 0 0 0 0 0 0 0 0 22
45 -0.0435 -1.6419 2.9635 H 0 0 0 0 0 0 0 0 0 0 0 23
46 -0.9281 -0.1273 2.6925 H 0 0 0 0 0 0 0 0 0 0 0 24
47 0.8513 -0.1293 2.7170 H 0 0 0 0 0 0 0 0 0 0 0 25
48
49 2 1 0 0 0 0
50 3 1 0 0 0 0
51 5 4 0 0 0 0
52 11 4 0 0 0 0
53 12 4 0 0 0 0
54 13 4 0 0 0 0
55 6 5 0 0 0 0
56 14 5 0 0 0 0
57 15 5 0 0 0 0
58 7 6 0 0 0 0

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9 6 0 0 0 0
8 7 0 0 0 0
16 7 0 0 0 0
17 7 0 0 0 0
18 8 0 0 0 0
19 8 0 0 0 0
20 8 0 0 0 0
10 9 0 0 0 0
21 9 0 0 0 0
22 9 0 0 0 0
23 10 0 0 0 0
24 10 0 0 0 0
10 25 0 0 0 0

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M END

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trimethylamine-cation.sdf

COSMOTHERM 3D

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17 15 0 0 0 0 0 0 0 0 0 V2000
-2.3746 -0.0344 0.0064 O 0 0 0 0 0 0 0 0 0 0 0 1
-2.8028 0.3592 -0.7758 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.8002 0.4059 0.7647 H 0 0 0 0 0 0 0 0 0 0 0 3
0.8378 0.2976 -1.3989 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3917 0.0041 0.0009 N 0 0 0 0 0 0 0 0 0 0 0 5
0.8694 1.0509 0.9583 C 0 0 0 0 0 0 0 0 0 0 0 6
0.8115 -1.3674 0.4336 C 0 0 0 0 0 0 0 0 0 0 0 7
0.4264 -0.4660 -2.0671 H 0 0 0 0 0 0 0 0 0 0 0 8
0.4699 1.2880 -1.6853 H 0 0 0 0 0 0 0 0 0 0 0 9
1.9329 0.2778 -1.4320 H 0 0 0 0 0 0 0 0 0 0 0 10
0.4848 0.8186 1.9569 H 0 0 0 0 0 0 0 0 0 0 0 11
0.4978 2.0265 0.6288 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9650 1.0475 0.9669 H 0 0 0 0 0 0 0 0 0 0 0 13
0.4225 -1.5535 1.4399 H 0 0 0 0 0 0 0 0 0 0 0 14
0.4028 -2.0990 -0.2708 H 0 0 0 0 0 0 0 0 0 0 0 15
1.9063 -1.4167 0.4368 H 0 0 0 0 0 0 0 0 0 0 0 16
-0.6690 0.0260 0.0064 H 0 0 0 0 0 0 0 0 0 0 0 17

```

```

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
16 7 0 0 0 0
5 17 0 0 0 0

```

M END

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trimethylamine.sdf

COSMOTHERM 3D

0

```

16 14 0 0 0 0 0 0 0 0 0 V2000
-2.4073 -0.0778 0.0107 O 0 0 0 0 0 0 0 0 0 0 0 1
-1.3910 -0.0362 0.0110 H 0 0 0 0 0 0 0 0 0 0 0 2
-2.6880 0.8530 -0.0121 H 0 0 0 0 0 0 0 0 0 0 0 3
0.8204 0.3267 1.3578 C 0 0 0 0 0 0 0 0 0 0 0 4
0.3550 -0.0013 0.0015 N 0 0 0 0 0 0 0 0 0 0 0 5
0.8384 -1.3284 -0.4105 C 0 0 0 0 0 0 0 0 0 0 0 6
0.7774 1.0293 -0.9593 C 0 0 0 0 0 0 0 0 0 0 0 7
0.4196 1.3043 1.6589 H 0 0 0 0 0 0 0 0 0 0 0 8
0.4602 -0.4328 2.0652 H 0 0 0 0 0 0 0 0 0 0 0 9
1.9271 0.3670 1.4178 H 0 0 0 0 0 0 0 0 0 0 0 10
0.4490 -1.5690 -1.4092 H 0 0 0 0 0 0 0 0 0 0 0 11
0.4807 -2.0876 0.2984 H 0 0 0 0 0 0 0 0 0 0 0 12
1.9459 -1.3730 -0.4447 H 0 0 0 0 0 0 0 0 0 0 0 13
0.3863 0.7857 -1.9568 H 0 0 0 0 0 0 0 0 0 0 0 14
0.3758 2.0053 -0.6537 H 0 0 0 0 0 0 0 0 0 0 0 15
1.8814 1.1084 -1.0238 H 0 0 0 0 0 0 0 0 0 0 0 16

```

```

2 1 0 0 0 0
3 1 0 0 0 0
5 4 0 0 0 0
8 4 0 0 0 0
9 4 0 0 0 0
10 4 0 0 0 0
6 5 0 0 0 0
7 5 0 0 0 0
11 6 0 0 0 0
12 6 0 0 0 0
13 6 0 0 0 0
14 7 0 0 0 0
15 7 0 0 0 0
7 16 0 0 0 0

```

M END

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