



HAL
open science

(SI) Band Gap Tuning in Nanodiamonds: First Principle Computational Studies

Peter R Schreiner, Andrey A Fokin

► **To cite this version:**

Peter R Schreiner, Andrey A Fokin. (SI) Band Gap Tuning in Nanodiamonds: First Principle Computational Studies. *Molecular Physics*, 2009, 107 (08-12), pp.823-830. 10.1080/00268970802649625 . hal-00513243

HAL Id: hal-00513243

<https://hal.science/hal-00513243v1>

Submitted on 1 Sep 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



(SI) Band Gap Tuning in Nanodiamonds: First Principle Computational Studies

Journal:	<i>Molecular Physics</i>
Manuscript ID:	TMPH-2008-0322.R1
Manuscript Type:	Special Issue Paper - Fritz Schaefer
Date Submitted by the Author:	23-Nov-2008
Complete List of Authors:	Schreiner, Peter; Justus-Liebig-University, Institute of Organic Chemistry Fokin, Andrey; Kiev Polytechnic Institute, Department of Organic Chemistry
Keywords:	nanodiamonds, density functional theory, band gap, doping



Band Gap Tuning in Nanodiamonds: First Principle Computational Studies[§]

Andrey A. Fokin^{a,b*} and Peter R. Schreiner^{b*}

^aDepartment of Organic Chemistry, Kiev Polytechnic Institute, pr. Pobedy 37, 03056 Kiev, Ukraine and ^bInstitute of Organic Chemistry, Justus-Liebig University, Heinrich-Buff-Ring 58, D-35392 Giessen, Germany

(Received...)

We present a density functional theory study on changes in band gap effects of nanodiamonds (hydrogen terminated diamond-like molecules, diamondoids) depending on size, shape, and the incorporation of heteroatom functionalities. Strong quantum confinement effects were identified at particle sizes from 0.5 to at least 2 nm, when the band gaps of **these** nanodiamonds are reduced to 6.7 eV. Octahedral and tetrahedral nanodiamonds show the same trends in band gap narrowing, and it is the dimension rather than the shape/morphology of the nanodiamonds that alters the band gaps. Band gap tuning through external (by C–H bond substitution) or internal (by replacing CH or CH₂ moieties) doping is non-additive for the same dopant. Push-pull doping, with electron donating and electron withdrawing groups is most effective and reduces the band **gaps** of diamondoids to that of bulk diamond. Further reductions down to 1–2 eV are conceivable with charged external substituents. The combination of increasing the size of the nanodiamond and push-pull doping are likely to make these materials highly valuable for semiconductor applications.

Keywords: Diamondoids; DFT methods; electronic gaps; nanodiamonds

1. Introduction

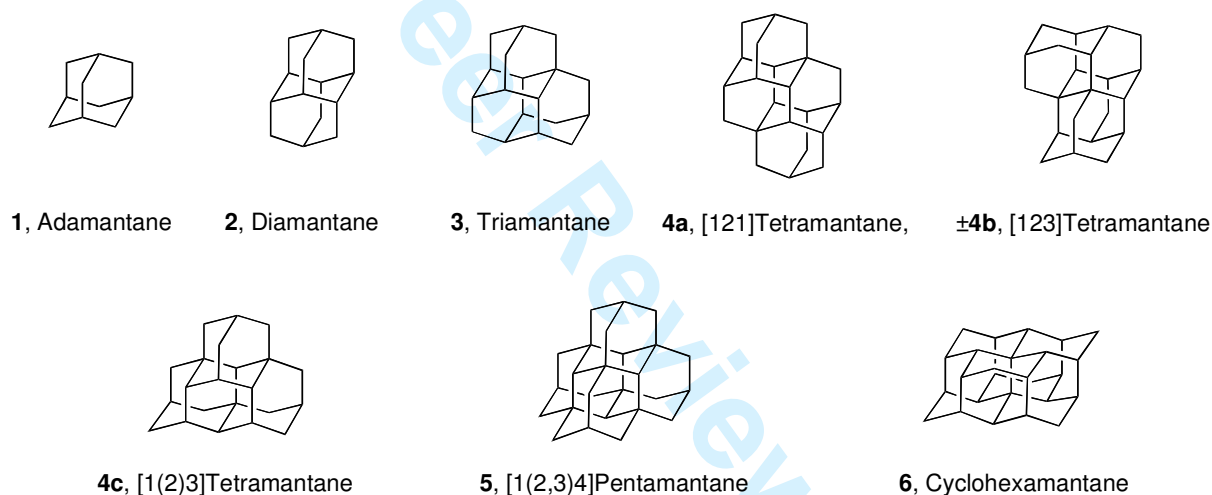
Nanodiamonds are nm-sized single-molecule diamond-like hydrocarbons (so-called *diamondoids*) that nicely close the gap between chemistry, physics, and the material sciences (for the first representatives of this series of molecules see Scheme 1).^[1, 2] They represent the long underrated world of sp³ carbon materials that have complementary properties to the nowadays ubiquitous fullerenes and carbon nanotubes.^[3] The physics community uses the term “nanodiamond” in singular form for the constituents of a variety of systems ranging from interstellar dusts and meteorites, carbonaceous residues of detonations to diamond-like films.^[4] The combination of strength, hardness, semiconductivity (upon doping), electron field emission,^[5] and unique optical properties make diamond-like materials particularly promising for discovering unusual properties at the borderline between chemistry and physics and for designing novel materials.

For a long time the chemistry of diamondoids was associated only with adamantane C₁₀H₁₆

[§] Functionalized Nanodiamonds, part 16. For part 15, see: C. Sinkel, S. Agarwal, N. A. Fokina, P. R. Schreiner *Macromol. Chem. Phys.* **2008**, 209, submitted

* Corresponding authors: aaf@xtf.ntu-kpi.kiev.ua and prs@org.chemie.uni-giessen.de

(1),^[6] whose derivatives have found an incredible number of highly practical applications;^[7] 1, diamantane (2),^[8] triamantane (3),^[9] and [121]tetramantane (4)^[10] have also been synthesized chemically. Despite some recent experimental progress,^[11-13] much of the chemistry of higher diamondoids (those with isomeric structure, i.e., starting with tetramantane, 4) remains largely unexplored as sizeable quantities of these hydrocarbons became readily available from natural sources only recently.^[14] Diamondoids were found in substantial amounts in petroleum cuts^[15] and natural gas condensates.^[16] The big advantage of diamondoids is that they are, in contrast to detonation and CVD nanodiamond, “knowable,” i.e., they are physically and chemically well characterized and are all structurally homogeneous.^[1] Chemical purity and homogeneity is a *conditione sine qua non* for using carbon materials for applications and as a test bed for sp³ nanomaterials.



Scheme 1. First members in the series of diamondoid hydrocarbons (nanodiamonds) with numbering of carbon atoms.

A particular promising scientific road is the ability to selectively replace diamondoid C–H bonds with a large variety of substituents.^[11, 12, 17] Moreover, it is also likely to be possible to substitute methylene groups (–CH₂–) with heteroatom functionalities (O, S, NH, etc.), which constitutes a rational synthetic approach to selectively doping diamond materials. As doped diamond shows unique properties such as pronounced semiconductivity, fluorescence shifts, deep coloration,^[18] it would be highly desirable to prepare materials with such properties in a predictable and reproducible fashion. At the same time, computational assessments^[19] of the properties to be expected will provide valuable guidelines as to which dopants and which diamondoid types are most promising for particular (mostly semiconductor) applications.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

Herein we examine computationally three different approaches for *band gap tuning* of diamondoids, as the band gap of such materials (including undoped bulk diamond) is just too high to be useful for semiconductor applications. The first approach is based on the enlargement and changing of the shapes/morphologies of the particles themselves to probe quantum confinement effects.^[20, 21] Second, we examine the effect of “external doping” based on C–H bond substitutions with various functional groups. Finally, we present an analysis of “interstitial” or internal doping by incorporating heteroatom functionalities of one or more CH or CH₂ fragments.

2. Computational Methods

All computations were performed with the GAUSSIAN03 program suite^[22] employing analytical first and second energy derivatives. Harmonic vibrational frequencies were computed to characterize stationary points. We used the B3LYP^[23] functional for comparison with earlier results and the B3PW91^[24] functional because it is more trustworthy for large molecules than many other popular DFT methods.^[25] We utilized 6-31G(d) and 6-31G(d,p) basis sets for all computations.^[26]

3. Results and Discussion

Size/shape dependence of the band gap. Previous attempts to examine size effects of diamond nanoclusters on the band gap are rather controversial as the results are sensitive to the theoretical method employed. GGA and TDLDA computations^[27] give band gaps for large diamond clusters that are lower than for bulk diamond (5.5 eV) and quantum confinement effects were considered negligible for diamond particles larger than 1 nm. Diffusion Monte-Carlo computations^[28] predict larger band gaps and confirmed the size dependence for quantum confinement. However, these results are not supported by tight-binding simulations^[29] for which the effects disappear for particles larger than 2.5 nm. Our conclusion is that some computational approaches simply are not able to reproduce quantitatively the orbital energies in nanodiamonds and are therefore unsuitable to study these materials. This conclusion is confirmed by the enormous discrepancies in reported band gap values ranging from 0.74 eV to 9.3 eV for adamantane (for a detailed discussion see ref.^[30]). In general, periodic plane-wave DFT approaches underestimate the band gaps in nanodiamond materials substantially. For instance, **recent plane-wave** pseudopotential computations reveal a 7.9 eV band gap in [121]tetramantane,^[31] whereas our computed B3PW91/6-31G(d,p) value is 8.6 eV (we will argue below that this is likely to be much closer

to experiment). A new study on the direct band gaps of the crystals of lower diamondoids utilizing plane waves and periodic boundary conditions also notes that such approaches (here with GGA and LDA combinations for the correlation and exchange potentials) underestimate the true band gaps of these materials.^[32] However, these periodic methods qualitatively confirmed^[28] the very important experimental observation that the unoccupied states in carbon nanoparticles, in contrast to their silicon or germanium counterparts, do not show quantum confinement effects.^[20]

The first nonperiodic, i. e., molecular DFT (B3LYP) computations on small^[33] as well as large^[34] diamond nanoclusters including vibrational frequency computations covered nanocarbon particles with up to 286 carbon atoms. Despite the use of moderately sized basis sets [6-21G for C and 6-31G(d,p) for H]^[34] reasonable results were obtained: The band gap of bulk diamond was not reached even for the 3 nm particle $C_{969}H_{324}$ that has a band gap of 6.6 eV. However, only octahedral diamondoids were studied leaving the question of the influence of the shape (morphology) of the particle on the band gap unanswered.

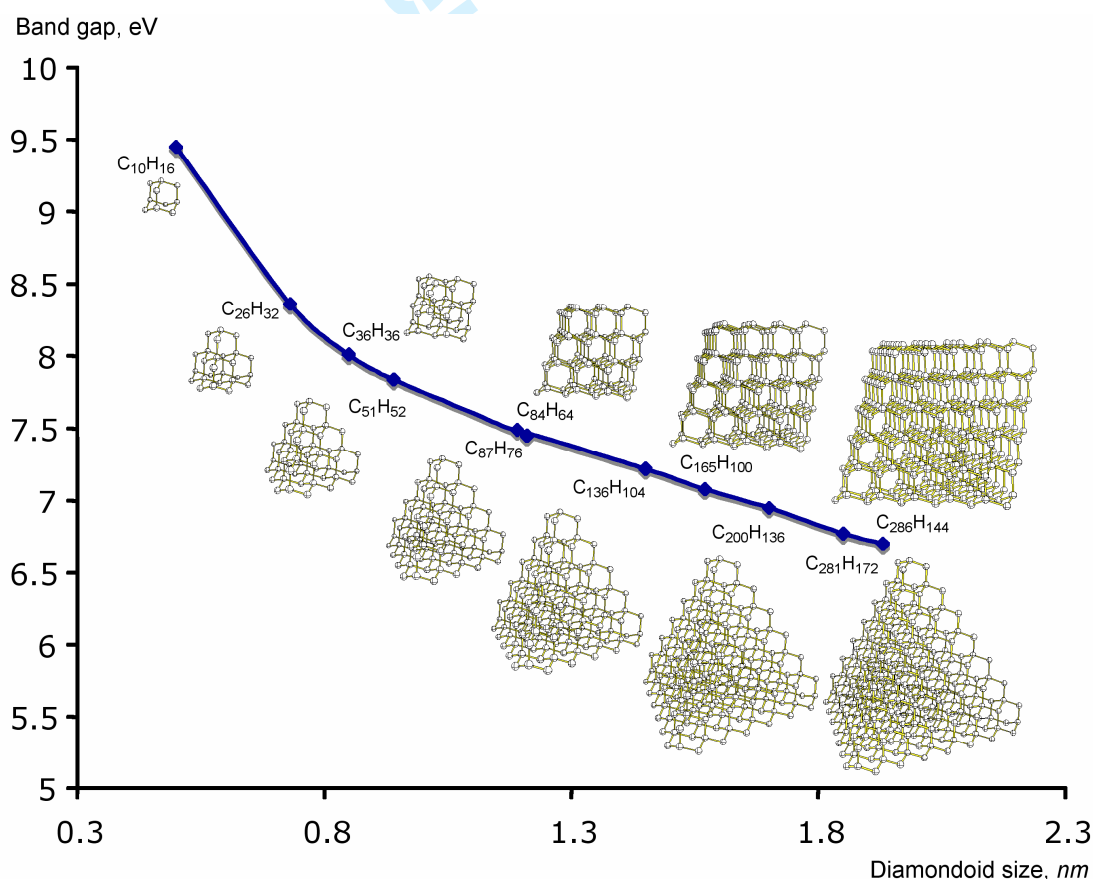


Figure 1. The dependence of the band gap of hydrogen-terminated nanodiamonds on particle size [B3LYP/6-31G(d), the surface hydrogens are omitted for clarity].

Earlier we predicted^[11] that the ionization potentials of diamondoids only slightly depend on the shape of the molecules but instead are mostly determined by the dimensions of the

1
2
3
4 particles. Recently these B3LYP/6-31G(d) computations were confirmed experimentally by
5 total-ion-yield spectroscopy of diamondoids.^[35] We now fully optimized at the B3LYP/6-
6 31(d) level a number of *tetrahedral* hydrogen-terminated diamondoids from up to C₂₈₁H₁₇₂
7 and plotted these together with the data for the previously computed^[34] *octahedral*
8 nanodiamonds (Figure 1). The results clearly demonstrate **that the** band gap rapidly decreases
9 with increasing size, but even at ca. 2 nm it only reaches 6.7 eV; this is still much larger than
10 that of bulk diamond (5.5 eV). **Even though the computed value for bulk diamond is not**
11 **available at this level,** *strong* quantum confinement effects still are expected for diamondoids
12 above 2 nm in size. At the same time the trends in band gap changes are independent of the
13 particle shapes – both tetrahedral and octahedral particles fit onto the same curve nicely
14 (Figure 1).
15
16
17
18
19
20
21
22
23

24 **Substitutional (external) doping.** Many attempts to prepare functionalized nanodiamond
25 led to inseparable inhomogeneous mixtures.^[36] These difficulties make precise tuning of the
26 electronic properties of functionalized detonation or CVD nanodiamond rather difficult. As
27 outlined above, functionalized diamondoids (nanodiamonds) represent chemically and
28 physically homogeneous materials with well-defined electronic properties. For instance, our
29 recent experimental studies have shown that diamondoid thiols^[37] form highly structured self-
30 assembled monolayers on metal surfaces.^[38] **We also found experimentally that**
31 **[121]tetramantane-6-thiol** (4) on gold and silver surfaces behaves as a high quantum yield
32 monochromatic electron emitter.^[37] Thus, diamondoids offer unique opportunities to study
33 the relationships between the substitution pattern and the properties of nanodiamond
34 particles,^[35, 39] and, in contrast to previous attempts with traditional bulk nanodiamond, allow
35 the fine tuning of these properties of diamond at the nanolevel.
36
37
38
39
40
41
42
43
44

45 We computed the band gaps for a number of preparatively available mono- and
46 disubstituted diamantanes as a model for “external” doping by substitution (Table 1). The
47 difference between the B3PW91 and B3LYP results is negligible in the present case. Thus,
48 the band gap of unsubstituted diamantane C₁₄H₂₀ is 9.0 eV (entry 7) at B3PW91/6-31G(d,p),
49 which is only slightly larger than the previously computed B3LYP/6-31G(d) value of 8.8
50 eV.^[11] The B3PW91 adiabatic ionization potential (8.4 eV) of diamantane is the same as that
51 at B3LYP (8.4 eV);^[40] the vertical ionization potential computed at B3PW91 (8.9 eV) is
52 identical to the available experimental value.^[41]
53
54
55
56
57
58
59
60

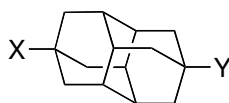
Substitution with alkyl, perfluoroalkyl groups as well as with fluorine increases the band
gap in diamantane derivatives (entries 1–6) mostly due to stabilization of the occupied states

(the HOMOs are downshifted by up to 0.03 au). While fluorination of nanodiamond was considered as very promising for several applications,^[4] we conclude, however, that the undesired insulating properties of nanodiamond materials will only increase after fluorination of the surface.

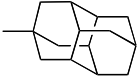
Remarkably, the band gap of bis-diadamantyl (entry 10) narrows only slightly relative to that of **2** (8.8 vs 9.0 eV) despite a doubling of the dimensions of the molecule to 0.8 nm; a band gap of ca 8 eV may have been expected for a diamondoid of that size from Figure 1. We also computed the dimer of **4** and found that the band gap in this ca 1.8 nm structure is 8.4 eV, close to that of the parent monomeric hydrocarbon (8.6 eV). These observations allow us to predict that agglomeration of nanodiamond particles, despite a formal increase in size, will show only little quantum confinement effects. This may limit electronic applications of traditional nanodiamond, which consists of conglomerates, whose separation represents a formidable challenge.^[42]

A substantial decrease of the band gap of **2** was achieved through incorporation of amino-, nitro-, and phenyl-functionalities. The substitution effects are not additive (compare, for instance, the mono- and dinitroderivatives, entries 19 and 21). The most electron-withdrawing group dominates the electronic properties of the substituted diamondoids. With nitro substitution the band gap of **2** can be reduced to ca. 6 eV (entry 19–21). Outstanding semiconductor properties may be expected for the highly polarized betaine structure of the formal bis-apical amino acid derivative of **2** (entry 22).

Table 1. The computed HOMO/LUMO energies and energy separations for 4,9-disubstituted diamantanes (B3PW91/6-31G(d,p)).



#	X	Y	HOMO, au	LUMO, au	HOMO–LUMO gap, kcal/mol	HOMO–LUMO gap, eV
1	CF ₃	CF ₃	-0.28682	0.06085	218.2	9.5
2	CH ₃	CF ₃	-0.27507	0.06753	215.0	9.3
3	CH ₃	CH ₃	-0.26302	0.07463	211.9	9.2
4	CH ₃	F	-0.27167	0.06354	210.3	9.1
5	H	CH ₃	-0.26067	0.07362	209.8	9.1
6	F	F	-0.27928	0.05393	209.1	9.1

7	H	H	-0.25845	0.07273	207.8	9.0
8	CN	CN	-0.29816	0.03153	206.9	9.0
9	CH ₃	CN	-0.28111	0.04421	204.1	8.8
10	H		-0.25030	0.07344	203.1	8.8
11	OH	OH	-0.25278	0.06555	199.7	8.7
12	CH ₃	NH ₂	-0.22692	0.07326	188.4	8.2
13	NH ₂	NH ₂	-0.22738	0.07220	187.9	8.1
14	CH=CH ₂	F	-0.25199	0.01364	166.7	7.2
15	H	NH ₃ ⁺	-0.39239	-0.13090	164.1	7.1
16	NH ₂	COOH	-0.23055	0.01143	151.8	6.6
17	Ph	CN	-0.24506	-0.00602	150.0	6.5
18	Ph	F	-0.24084	-0.00212	149.8	6.5
19	NO ₂	NO ₂	-0.29143	-0.06691	140.9	6.1
20	CH ₃	NO ₂	-0.27895	-0.05669	139.5	6.0
21	H	NO ₂	-0.27789	-0.05655	138.9	6.0
22	NH ₃ ⁺	COO ⁻	-0.11669	-0.05125	41.1	1.8

Interstitial (internal) doping. The semiconductor properties of natural bulk diamond are determined by trace amounts of nitrogen (type I) or boron (type II) impurities. Modeling these effects by placing the dopant atom in the center of spherical diamond nanocrystals largely leads to unstable structures.^[43] In contrast, substitutional internal doping in diamondoid does give rise to stable molecules.^[33] We first computed the band gap for the parent heteroadamantanes (Table 2) with oxygen, nitrogen as well as sulfur as n-, and boron as p-dopants. While the HOMO of n-doped structures (entries 2–4) mostly describe the n-electrons of the heteroatom, the empty *p*-orbital of boron interacts strongly with the diamondoid LUMOs. Remarkably, interstitial doping dramatically reduces the band gap down to about 7 eV for the sulfur (entry 3) and boron (entry 6) derivatives.

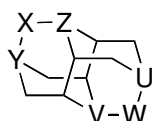
Table 2. The computed HOMO/LUMO energies and gaps for doped adamantanes [B3PW91/6-31G(d,p)].

#	X	Y	HOMO, au	LUMO, au	HOMO–LUMO gap,	
					kcal/mol	gap, eV
1	CH	CH ₂	-0.27293	0.07434	217.9	9.4
2	O	CH ₂	-0.23266	0.07550	193.4	8.4
3	S	CH ₂	-0.21058	0.04023	157.4	6.8

4	CH ₂	N	-0.19592	0.07653	171.0	7.4
6	CH ₂	B	-0.25846	-0.00370	159.9	6.9

Several questions arise: *i*) how does such internal doping influence the band gap for larger diamond particles, *ii*) are these effects additive and do they depend on the position of the dopant, and *iii*) to what extent do conducting and valence bands shrink upon enlarging the particles, *i. e.*, what is the degree of mixing of the carbon and heteroatom orbitals. To answer these questions we fully optimized a number of diamantane (**2**) and triamantane (**3**) derivatives at B3PW91/6-31G(d,p). Internal doping of two different CH positions of the cage of **2** (entries 2 and 3) reduces the band gap almost equally relative to the undoped molecule (entry 1); the substitution of the CH₂ moieties reduces the band gap to a lesser extent (entry 4). Importantly, double doping virtually provides no additional effect as compared to the incorporation of only one dopant (entry 5 vs 3); this will make the preparation of such molecules less challenging. In agreement with data for the adamantane derivatives, doping with oxygen (entries 6 and 7) is less effective, while sulfur (entries 8–10) and boron (entries 11 and 12) incorporation is more effective than *N*-doping. The most pronounced effect was found for push-pull doping with boron and nitrogen that reduces the band gap of **2** (entries 13 and 14) to that of bulk diamond.

Table 3. The computed HOMO/LUMO energies and gaps for doped diamantanes [B3PW91/6-31G(d,p)].

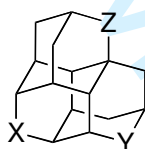


#	X	Y	Z	W	U	V	HOMO, au	LUMO, au	HOMO– LUMO gap, kcal/mol	HOMO– LUMO gap, eV
1	CH ₂	CH	CH	CH ₂	CH ₂	CH	-0.25845	0.07273	207.8	9.0
2	CH ₂	N	CH	CH ₂	CH ₂	CH	-0.19597	0.07607	170.7	7.4
3	CH ₂	CH	N	CH ₂	CH ₂	CH	-0.19390	0.07402	168.1	7.3
4	NH	CH	CH	CH ₂	CH ₂	CH	-0.20722	0.07141	174.8	7.6
5	CH ₂	N	CH	CH ₂	N	CH	-0.18617	0.08200	168.3	7.3

6	O	CH	CH	CH ₂	CH ₂	CH	-0.23035	0.07181	189.6	8.2
7	O	CH	CH	O	CH ₂	CH	-0.23064	0.07515	191.9	8.3
8	S	CH	CH	CH ₂	CH ₂	CH	-0.21083	0.03945	157.0	6.8
9	S	CH	CH	S	CH ₂	CH	-0.20946	0.03453	153.1	6.6
10	O	CH	CH	S	CH ₂	CH	-0.21510	0.03586	157.5	6.8
11	CH ₂	B	CH	CH ₂	CH ₂	CH	-0.25684	-0.00512	157.9	6.8
12	CH ₂	B	CH	CH ₂	B	CH	-0.26093	-0.00909	158.0	6.8
13	CH ₂	N	CH	CH ₂	B	CH	-0.20185	-0.00854	121.3	5.3
14	CH ₂	CH ₂	N	CH ₂	CH ₂	B	-0.20237	-0.00605	123.2	5.3

The trends found for our diamantane model are nicely reflected in the series of doped triamantanes (Table 4). The position of the dopant has a negligible influence of the HOMO-LUMO gaps. Narrowing of the gap is determined only by the nature of the dopant, rather than by the size of the cage. This is due to the dominant contributions of the atomic orbitals of the dopant into the HOMOs and the LUMOs.

Table 4. The computed HOMO/LUMO energies and gaps for doped diamantanes [B3PW91/6-31G(d,p)].



X	Y	Z	HOMO, au	LUMO, au	HOMO-LUMO gap, kcal/mol	HOMO-LUMO gap, eV
CH ₂	CH ₂	CH ₂	-0.24929	0.07140	201.2	8.7
O	CH ₂	CH ₂	-0.22779	0.07126	187.6	8.1
S	CH ₂	CH ₂	-0.20821	0.04330	157.8	6.8
CH ₂	O	CH ₂	-0.22813	0.07111	187.8	8.1
CH ₂	S	CH ₂	-0.20885	0.04143	157.0	6.8
CH ₂	CH ₂	O	-0.22821	0.07202	188.4	8.2
CH ₂	CH ₂	S	-0.20865	0.03907	155.4	6.7

At the same time, increasing the size of the particle increases the densities of both the occupied and the unoccupied states, i. e., we observe the transition of discrete molecular

orbital levels to band structures as the diamondoids become larger. The energies of the frontier and related molecular orbitals for six representative *S*-doped hydrocarbons are depicted in Fig. 2. While the densities of the unoccupied states increase only slightly the density of the valence bands increases considerably. That is, large doped nanodiamonds will behave as semiconductors, analogous to doped bulk diamond.

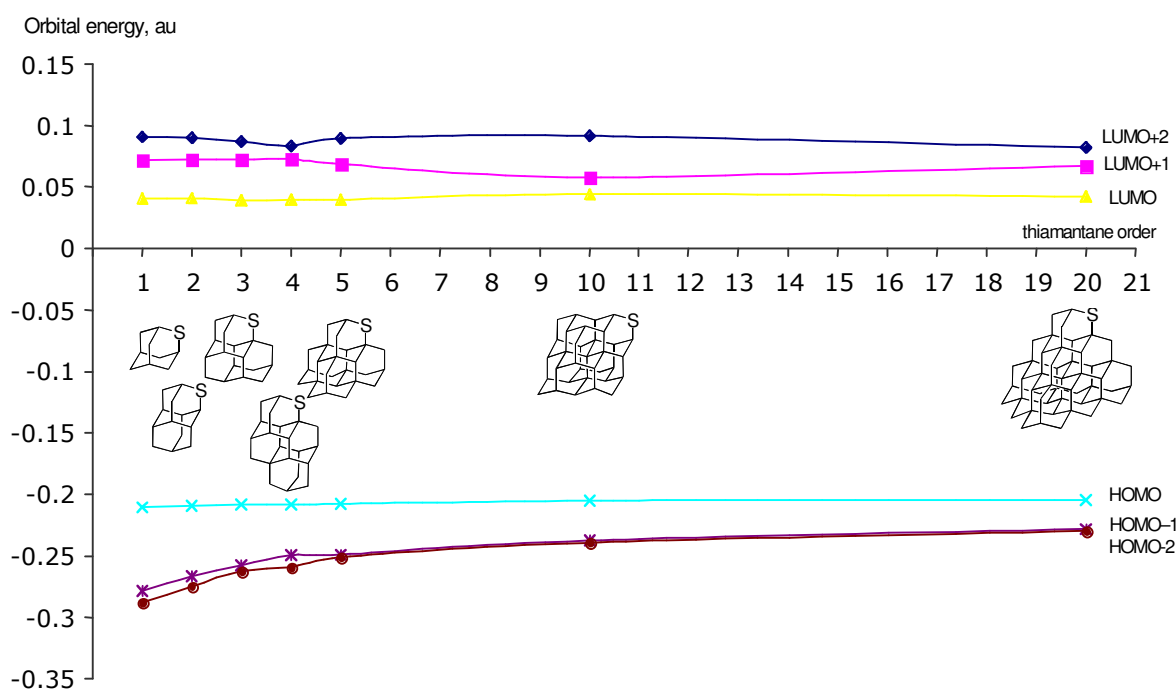


Figure 2. Changes in the densities of the unoccupied and occupied states with increasing size of *S*-doped nanodiamonds [*thiamantanes*, at B3PW91/6-31G(d,p)].

4. Conclusions

Well-defined nanodiamonds display strong quantum confinement effects at particle sizes from 0.5 to at least 2 nm, when their band gaps are reduced to 6.7 eV, which is likely to be still much wider than that of bulk diamond. Octahedral and tetrahedral nanodiamonds show the same trends in band gap narrowing, and it is the dimension rather than the shape/morphology of the nanodiamonds that affects the band gaps. Clustering of diamondoids apparently does not lead to substantial additive band-gap lowering as shown for the diamondoid dimers; this is also evident from most recent computations on diamondoid crystals.^[32]

1
2
3 Band gap tuning through external (by C–H bond substitution) or internal (by replacing CH
4 or CH₂ moieties) doping is non-additive for the same dopant. However, push-pull doping,
5 with electron donating and electron withdrawing groups is most effective and reduces the
6 band gap of diamondoids to that of bulk diamond. Further reductions down to 1–2 eV are
7 conceivable with charged external substituents. The combination of increasing the size of the
8 nanodiamond and push-pull doping are likely to make these materials highly valuable for
9 semiconductor applications. Experimental work in this direction is currently underway in our
10 laboratories.
11
12
13
14
15
16
17
18
19

20 Acknowledgments

21 This paper is dedicated to Fritz Schaefer for his many valuable contributions to computational
22 as well as theoretical chemistry, and on the occasion of his 65th birthday. We thank Trevor
23 M. Willey, Jeremy E. P. Dahl, and Robert M. K. Carlson for fruitful discussions. This work
24 was supported by the Deutsche Forschungsgemeinschaft, the Ministry of Science and
25 Education of Ukraine, Ukrainian Basic Research Fund, and the Fonds der Chemischen
26 Industrie. We thank the CSC Frankfurt for computational resources.
27
28
29
30
31

32 References

- 33 [1] J. E. Dahl, S. G. Liu, R. M. K. Carlson, *Science* **299**, 96 (2003).
34 [2] a) A. P. Marchand, *Science* **299**, 52 (2003); b) H. Hopf, *Angew. Chem. Int. Ed.* **42**,
35 2000 (2003).
36 [3] A. S. Barnard, S. P. Russo, I. K. Snook, *J. Chem. Phys.* **118**, 5094 (2003).
37 [4] M. Baidarakova, A. Vul', *J. Phys. D: Appl. Phys.* **40**, 6300 (2007).
38 [5] W. P. Kang, J. L. Davidson, Y. M. Wong, K. Holmes, *Diam. Relat. Mater.* **13**, 975
39 (2004).
40 [6] P. v. R. Schleyer, *J. Am. Chem. Soc.* **79**, 3292 (1957).
41 [7] a) J. G. Henkel, J. T. Hane, *J. Med. Chem.* **25**, 51 (1982); b) Y. N. Klimochkin, M. V.
42 Leonova, I. R. Korzhev, I. K. Moiseyev, G. V. Vladyko, L. V. Korobchenko, Y. I.
43 Boreko, S. N. Nikolayeva, *Khim. Farm. Zh.* **26**, 58 (1992); c) W. J. Hoekstra, J. B.
44 Press, M. P. Bonner, P. Angrade-Gordon, P. M. Keane, K. A. Durkin, D. C. Liotta, K.
45 H. Mayo, *Bioorg. Chem. Lett.* **4**, 1361 (1994); d) Y. I. Bagrii, *Petroleum Chem.* **35**,
46 205 (1995); e) J. Kornhuber, G. Quack, W. Danysz, K. Jellinger, W. Danielczyk, W.
47 Gsell, P. Riederer, *Neuropharmacology* **34**, 713 (1995); f) Y. Kuroda, H. Ueda, H.
48 Nozawa, H. Ogoshi, *Tetrahedron Lett.* **38**, 7901 (1997); g) D. Gully, B. Labeuw, R.
49 Boigegrain, F. OuryDonat, A. Bachy, M. Poncelet, R. Steinberg, M. F. SuaudChagny,
50 V. Santucci, N. Vita, F. Pecceu, C. LabbeJullie, P. Kitabgi, P. Soubrie, G. LeFur, J. P.
51 Maffrand, *J. Pharm. Exper. Therap.* **280**, 802 (1997); h) K. Kitagawa, N. Mizobuchi,
52 T. Hama, T. Hibi, R. Konishi, S. Futaki, *Chem. Pharm. Bull.* **45**, 1782 (1997); i) D.
53 Ranganathan, V. Haridas, K. P. Madhusudanan, R. Roy, R. Nagaraj, G. B. John, *J.*
54 *Am. Chem. Soc.* **119**, 11578 (1997); j) S. Samnick, S. Ametamey, M. R. Gold, P. A.
55 Schubiger, *J. Label. Comp. Radiopharm.* **39**, 241 (1997); k) E. A. Blokhina, I. A.
56 Sukhotina, A. Y. Bespalov, *Eur. J. Pharm.* **406**, 227 (2000); l) J. Kotlinska, G. Biala,
57 *Pol. J. Pharm.* **52**, 179 (2000); m) M. A. Rogawski, *Amino Acids* **19**, 133 (2000); n)

- 1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
- F. G. Costa, R. Frussa, L. F. Felicio, *Eur. J. Pharm.* **428**, 97 (2001); o) J. M. Kelly, G. Quack, M. M. Miles, *Antimicrob. Agents Chemother.* **45**, 1360 (2001); p) I. S. Morozov, I. A. Ivanova, T. A. Lukicheva, *Khim. Farm. Zhurn.* **35**, 235 (2001); r) A. Baxter, J. Bent, K. Bowers, M. Braddock, S. Brough, M. Fagura, M. Lawson, T. McNally, M. Mortimore, M. Robertson, R. Weaver, W. P., *Bioorg. Med. Chem. Lett.* **13**, 4047 (2003).
- [8] T. Courtney, D. E. Johnston, M. A. McKervery, J. J. Rooney, *J. Chem. Soc., Perkin Trans. 1* 2691 (1972).
- [9] a) V. Z. Williams, P. v. R. Schleyer, G. J. Gleicher, L. B. Rodewald, *J. Am. Chem. Soc.* **88**, 3862 (1966); b) F. S. Hollowood, M. A. McKervery, R. Hamilton, J. J. Rooney, *J. Org. Chem.* **45**, 4954 (1980).
- [10] a) W. Burns, M. A. McKervery, T. R. B. Mitchell, J. J. Rooney, *J. Am. Chem. Soc.* **100**, 906 (1978); b) W. Burns, T. R. B. Mitchell, M. A. McKervery, J. J. Rooney, G. Ferguson, P. Roberts, *J. Chem. Soc. Chem. Comm.* 893 (1976).
- [11] A. A. Fokin, B. A. Tkachenko, P. A. Gunchenko, D. V. Gusev, P. R. Schreiner, *Chem. Eur. J.* **11**, 7091 (2005).
- [12] a) P. R. Schreiner, N. A. Fokina, B. A. Tkachenko, H. Hausmann, M. Serafin, J. E. P. Dahl, S. G. Liu, R. M. K. Carlson, A. A. Fokin, *J. Org. Chem.* **71**, 6709 (2006); b) B. A. Tkachenko, N. A. Fokina, L. V. Chernish, J. E. P. Dahl, S. G. Liu, R. M. K. Carlson, A. A. Fokin, P. R. Schreiner, *Org. Lett.* **8**, 1767 (2006); c) A. A. Fokin, E. D. Butova, L. V. Chernish, N. A. Fokina, J. E. P. Dahl, R. M. K. Carlson, P. R. Schreiner, *Org. Lett.* **9**, 2541 (2007); d) N. A. Fokina, B. A. Tkachenko, A. Merz, M. Serafin, J. E. P. Dahl, R. M. K. Carlson, A. A. Fokin, P. R. Schreiner, *Eur. J. Org. Chem.* 4738 (2007).
- [13] H. Schwertfeger, A. A. Fokin, P. R. Schreiner, *Angew. Chem. Int. Ed.* **47**, 1022 (2008).
- [14] M. Schoell, R. M. K. Carlson, *Nature* **399**, 15 (1999).
- [15] R. Lin, Z. A. Wilk, *Fuel* **74**, 1512 (1995).
- [16] J. E. Dahl, J. M. Moldowan, K. E. Peters, G. E. Claypool, M. A. Rooney, G. E. Michael, M. R. Mello, M. L. Kohnen, *Nature* **399**, 54 (1999).
- [17] A. A. Fokin, P. R. Schreiner, N. A. Fokina, B. A. Tkachenko, H. Hausmann, M. Serafin, J. E. P. Dahl, S. G. Liu, R. M. K. Carlson, *J. Org. Chem.* **71**, 8532 (2006).
- [18] a) A. S. Barnard, S. P. Russo, I. K. Snook, *J. Phys. Chem. B* **109**, 11991 (2005); b) A. V. G. Chizmeshya, C. Ritter, J. Tolle, C. Cook, J. Menendez, J. Kouvetakis, *Chem. Mater.* **18**, 6266 (2006); c) H. Uetsuka, D. Shin, N. Tokuda, K. Saeki, C. E. Nebel, *Langmuir* **23**, 3466 (2007).
- [19] M. Shen, H. F. Schaefer, C. Liang, J. H. Lii, N. L. Allinger, P. v. R. Schleyer, *J. Am. Chem. Soc.* **114**, 497 (1992).
- [20] T. M. Willey, C. Bostedt, T. van Buuren, J. E. Dahl, S. G. Liu, R. M. K. Carlson, L. J. Terminello, T. Möller, *Phys. Rev. Lett.* **95**, 113401 (2005).
- [21] T. M. Willey, C. Bostedt, T. van Buuren, J. E. Dahl, S. G. Liu, R. M. K. Carlson, R. W. Meulenberg, E. J. Nelson, L. J. Terminello, *Phys. Rev.* **74**, 205432 (2006).
- [22] M. J. Frisch, et., al., Gaussian, Inc., Pittsburgh PA, 2004.
- [23] a) A. D. Becke, *Phys. Rev. A* **38**, 3098 (1988); b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B* **37**, 785 (1988).
- [24] J. P. Perdew, Y. Wang, *Phys. Rev. B* **23**, 5048 (1992).
- [25] a) P. R. Schreiner, A. A. Fokin, R. A. Pascal, A. de Meijere, *Org. Lett.* **8**, 3635 (2006); b) P. R. Schreiner, *Angew. Chem. Int. Ed.* **23**, 4217 (2007).
- [26] P. C. Hariharan, J. A. Pople, *Theoret. Chim. Acta* **28**, 213 (1973).

- 1
2
3
4 [27] a) J. Y. Raty, G. Galli, C. Bostedt, T. W. van Buuren, L. J. Terminello, *Phys. Rev. Lett.* **90**, 0374011 (2003); b) B. Wen, J. Zhao, T. Li, *Chem. Phys. Lett.* **441**, 318 (2007).
- 6
7 [28] N. D. Drummond, A. J. Williamson, R. J. Needs, G. Galli, *Phys. Rev. Lett.* **95**, 096801 (2005).
- 9
10 [29] D. A. Areshkin, O. A. Shenderova, S. P. Adiga, D. W. Brenner, *Diam. Relat. Mater.* **13**, 1826 (2004).
- 11
12 [30] T. M. Willey, C. Bostedt, T. van Buuren, J. E. Dahl, S. G. Liu, R. M. K. Carlson, R. W. Meulenber, E. J. Nelson, L. J. Terminello, *Phys. Rev.* **74**, 205432 (2006).
- 13
14 [31] Y. Wang, E. Kioupakis, X. Liu, D. Wegner, R. Yamachika, J. E. Dahl, R. M. K. Carlson, S. G. Louie, M. F. Crommie, *Nat. Mater.* **7**, 38 (2008).
- 15
16 [32] T. Sasagawa, Z.-x. Shen, *J. Appl. Phys.* **104**, 073704 (2008).
- 17
18 [33] G. C. McIntosh, M. Yoon, S. Berber, D. Tománek, *Phys. Rev. B* **70**, 045401 (2004).
- 19
20 [34] M. Linnolahti, A. J. Karttunen, T. A. Pakkanen, *J. Phys. Chem.* **111**, 18118 (2007).
- 21
22 [35] K. Lenzke, L. Landt, M. Hoener, H. Thomas, J. E. Dahl, S. G. Liu, R. M. K. Carlson, T. Möller, C. Bostedt, *J. Chem. Phys.* **127**, 084320 (2007).
- 23
24 [36] a) A. Kruger, *Angew. Chem. Int. Ed.* **45**, 6426 (2006); b) A. Kruger, Y. Liang, G. Jarre, J. Stegk, *J. Mater. Chem.* **16**, 2322 (2006); c) L. Li, J. L. Davidson, C. M. Lukehart, *Carbon* **44**, 2308 (2006); d) V. N. Khabasheskua, J. L. F. Margravea, E. V. Barrera, *Diam. Relat. Mater.* **14**, 859 (2005); e) Y. Liu, Z. Gu, J. L. Margrave, V. N. Khabashesku, *Chem. Mater.* **16**, 3924 (2004).
- 26
27
28 [37] W. L. Yang, J. D. Fabbri, T. M. Willey, J. R. I. Lee, J. E. Dahl, R. M. K. Carlson, P. R. Schreiner, A. A. Fokin, B. A. Tkachenko, N. A. Fokina, W. Meevasana, N. Mannella, K. Tanaka, X. J. Zhou, T. van Buuren, M. A. Kelly, Z. Hussain, N. A. Melosh, Z.-x. Shen, *Science* **316**, 1460 (2007).
- 29
30
31 [38] T. M. Willey, J. D. Fabbri, J. R. I. Lee, P. R. Schreiner, A. A. Fokin, B. A. Tkachenko, N. A. Fokina, J. E. P. Dahl, R. M. K. Carlson, A. L. Vance, W. Yang, L. J. Terminello, T. v. Buuren, N. A. Melosh, *J. Am. Chem. Soc.* **130**, 10536 (2008).
- 33
34 [39] P.-H. Chung, E. Perevedentseva, C.-L. Cheng, *Surf. Sci.* **601**, 3866 (2007).
- 35
36 [40] a) A. J. Lu, B. C. Pan, J. G. Han, *Phys. Rev. B.* **72**, 035447 (erratum: 209901) (2005); b) A. A. Fokin, B. A. Tkachenko, P. A. Gunchenko, D. V. Gusev, P. R. Schreiner, *Chem. Eur. J.* **11**, 7091 (2005).
- 37
38
39 [41] M. J. S. Dewar, S. D. Worley, *J. Chem. Phys.* **50**, 654 (1969).
- 40
41 [42] A. Kruger, F. Kataoka, M. Ozawa, T. Fujino, Y. Suzuki, A. E. Aleksenskii, A. Y. Vul', E. Osawa, *Carbon* **43**, 1722 (2005).
- 42
43 [43] a) A. S. Barnard, S. P. Russo, I. K. Snook, *J. Phys. Chem. B.* **109**, 11991 (2005); b) A. S. Barnard, S. P. Russo, I. K. Snook, *J. Chem. Phys.* **118**, 10725 (2003).
- 44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

SUPPLEMENTARY INFORMATION

Band Gap Tuning in Nanodiamonds: First Principle Computational Studies

Andrey A. Fokin^{a,b*} and Peter R. Schreiner^{b*}

^aDepartment of Organic Chemistry, Kiev Polytechnic Institute, pr. Pobedy 37, 03056 Kiev, Ukraine and ^bInstitute of Organic Chemistry, Justus-Liebig University, Heinrich-Buff-Ring 58, D-35392 Giessen, Germany

Table 1s. The XYZ-coordinates of optimized molecular geometries and absolute energies in au.

C ₁₀ H ₁₆ , B3LYP/6-31G*, E=-390.72601				C ₂₆ H ₃₂ , B3LYP/6-31G*, E=-1010.13421			
C	0.892683	0.892683	0.892683	C	0.885156	0.885156	0.885156
C	-0.892683	-0.892683	0.892683	C	-0.885156	-0.885156	0.885156
C	-0.892683	0.892683	-0.892683	C	-0.885156	0.885156	-0.885156
C	0.892683	-0.892683	-0.892683	C	0.885156	-0.885156	-0.885156
C	0.000000	0.000000	1.781020	C	0.000000	1.805160	0.000000
C	0.000000	1.781020	0.000000	C	0.000000	-1.805160	0.000000
C	1.781020	0.000000	0.000000	C	0.000000	0.000000	-1.805160
C	-1.781020	0.000000	0.000000	C	0.000000	0.000000	1.805160
C	0.000000	-1.781020	0.000000	C	-1.805160	0.000000	0.000000
C	0.000000	0.000000	-1.781020	C	1.805160	0.000000	0.000000
H	-0.623944	0.623944	2.436301	C	0.898953	2.674657	-0.898953
H	0.623944	-0.623944	2.436301	C	-0.898953	-2.674657	-0.898953
H	0.623944	2.436301	-0.623944	C	-0.898953	2.674657	0.898953
H	-0.623944	2.436301	0.623944	C	0.898953	-2.674657	0.898953
H	2.436301	-0.623944	0.623944	C	-0.898953	-0.898953	-2.674657
H	2.436301	0.623944	-0.623944	C	0.898953	0.898953	-2.674657
H	-2.436301	-0.623944	-0.623944	C	0.898953	-0.898953	2.674657
H	-2.436301	0.623944	0.623944	C	-0.898953	0.898953	2.674657
H	-0.623944	-0.623944	-2.436301	C	-2.674657	0.898953	0.898953
H	0.623944	0.623944	-2.436301	C	2.674657	-0.898953	0.898953
H	-0.623944	-2.436301	-0.623944	C	2.674657	0.898953	-0.898953
H	0.623944	-2.436301	0.623944	C	-2.674657	-0.898953	-0.898953
H	1.526783	1.526783	1.526783	H	1.521811	1.521811	1.521811
H	-1.526783	-1.526783	1.526783	H	-1.521811	-1.521811	1.521811
H	-1.526783	1.526783	-1.526783	H	-1.521811	1.521811	-1.521811
H	1.526783	-1.526783	-1.526783	H	1.521811	-1.521811	-1.521811
				H	-1.521717	3.331308	0.273708
				H	1.521717	-3.331308	0.273708
				H	1.521717	3.331308	-0.273708
				H	-1.521717	-3.331308	-0.273708
				H	0.273708	1.521717	-3.331308
				H	-0.273708	-1.521717	-3.331308
				H	-0.273708	1.521717	3.331308
				H	0.273708	-1.521717	3.331308
				H	-3.331308	-0.273708	-1.521717
				H	3.331308	0.273708	-1.521717
				H	3.331308	-0.273708	1.521717
				H	-3.331308	0.273708	1.521717
				H	-0.273708	3.331308	1.521717
				H	0.273708	-3.331308	1.521717
				H	0.273708	3.331308	-1.521717
				H	-0.273708	-3.331308	-1.521717
				H	1.521717	0.273708	-3.331308
				H	-1.521717	-0.273708	-3.331308
				H	-1.521717	0.273708	3.331308
				H	1.521717	-0.273708	3.331308
				H	-3.331308	-1.521717	-0.273708
				H	3.331308	1.521717	-0.273708
				H	3.331308	-1.521717	0.273708

* Corresponding authors: aaf@xtf.ntu-kpi.kiev.ua and prs@org.chemie.uni-giessen.de

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

H	-3.331308	1.521717	0.273708
C	1.789780	-1.789780	1.789780
C	-1.789780	1.789780	1.789780
C	-1.789780	-1.789780	-1.789780
C	1.789780	1.789780	-1.789780
H	2.423846	-2.423846	2.423846
H	-2.423846	2.423846	2.423846
H	-2.423846	-2.423846	-2.423846
H	2.423846	2.423846	-2.423846

C₅₁H₅₂, B3LYP/6-31G*, E=- -1974.9449

C	-0.898555	-0.898555	0.898555
C	0.898555	0.898555	0.898555
C	0.898555	-0.898555	-0.898555
C	-0.898555	0.898555	-0.898555
C	-0.898297	0.898297	2.700887
C	0.898297	-0.898297	2.700887
C	0.898297	0.898297	-2.700887
C	-0.898297	-0.898297	-2.700887
C	-0.898297	2.700887	0.898297
C	0.898297	-2.700887	0.898297
C	0.898297	2.700887	-0.898297
C	-0.898297	-2.700887	-0.898297
C	-2.700887	0.898297	0.898297
C	2.700887	-0.898297	0.898297
C	2.700887	0.898297	-0.898297
C	-2.700887	-0.898297	-0.898297
C	-1.782104	0.014063	1.782104
C	1.782104	-0.014063	1.782104
C	1.782104	0.014063	-1.782104
C	-1.782104	-0.014063	-1.782104
C	-0.014063	1.782104	1.782104
C	0.014063	-1.782104	1.782104
C	0.014063	1.782104	-1.782104
C	-0.014063	-1.782104	-1.782104
C	-1.782104	1.782104	0.014063
C	1.782104	-1.782104	0.014063
C	1.782104	1.782104	-0.014063
C	-1.782104	-1.782104	-0.014063
C	0.000000	0.000000	0.000000
C	0.000000	3.566813	0.000000
C	0.000000	-3.566813	0.000000
C	-3.566813	0.000000	0.000000
C	3.566813	0.000000	0.000000
C	0.000000	0.000000	3.566813
C	0.000000	0.000000	-3.566813
H	2.417040	2.417040	0.625854
H	-2.417040	-2.417040	0.625854
H	-2.417040	2.417040	-0.625854
H	2.417040	-2.417040	-0.625854
H	-2.417040	0.625854	-2.417040
H	2.417040	-0.625854	-2.417040
H	2.417040	0.625854	2.417040
H	-2.417040	-0.625854	2.417040
H	-0.625854	2.417040	-2.417040
H	0.625854	-2.417040	-2.417040
H	0.625854	2.417040	2.417040
H	-0.625854	-2.417040	2.417040
C	-3.572596	1.796460	1.796460
C	3.572596	-1.796460	1.796460
C	3.572596	1.796460	-1.796460
C	-3.572596	-1.796460	-1.796460
C	-1.796460	3.572596	1.796460
C	1.796460	-3.572596	1.796460
C	1.796460	3.572596	-1.796460
C	-1.796460	-3.572596	-1.796460
C	-1.796460	1.796460	3.572596
C	1.796460	-1.796460	3.572596
C	1.796460	1.796460	-3.572596
C	-1.796460	-1.796460	-3.572596

C₈₇H₇₆, B3LYP/6-31G*, E=- 3361.41152

C	0.000000	0.000000	0.000000
C	1.795873	1.795873	0.000973
C	-1.795873	-1.795873	0.000973
C	-1.795873	1.795873	-0.000973
C	1.795873	-1.795873	-0.000973
C	1.795873	-0.000973	-1.795873
C	-1.795873	0.000973	-1.795873
C	-1.795873	-0.000973	1.795873
C	1.795873	0.000973	1.795873
C	-0.000973	1.795873	-1.795873
C	0.000973	-1.795873	-1.795873
C	0.000973	1.795873	1.795873
C	-0.000973	-1.795873	1.795873
C	1.795528	1.795528	-3.598365
C	-1.795528	-1.795528	-3.598365
C	-1.795528	1.795528	3.598365
C	1.795528	-1.795528	3.598365
C	0.000000	0.000000	-3.595288
C	0.000000	0.000000	3.595288
C	0.000000	3.595288	0.000000
C	0.000000	-3.595288	0.000000
C	1.795528	3.598365	-1.795528
C	-1.795527	-3.598365	-1.795528
C	-1.795528	3.598365	1.795528
C	1.795528	-3.598365	1.795528
C	3.595288	0.000000	0.000000
C	-3.595288	0.000000	0.000000
C	3.598365	1.795528	-1.795528
C	-3.598365	-1.795528	-1.795528
C	-3.598365	1.795528	1.795528
C	3.598365	-1.795527	1.795527
C	-0.896703	0.896703	0.896703
C	0.896703	-0.896703	0.896703
C	0.896703	0.896703	-0.896703
C	-0.896703	-0.896703	-0.896703
C	2.676780	0.883388	0.883388
C	-2.676780	-0.883388	0.883388
C	-2.676780	0.883388	-0.883388
C	2.676780	-0.883388	-0.883388
C	2.678989	0.911107	-2.678989
C	-2.678989	-0.911107	-2.678989
C	-2.678989	0.911107	2.678989
C	2.678989	-0.911107	2.678989
C	-0.883388	0.883388	-2.676780
C	0.883388	-0.883388	-2.676780
C	0.883388	0.883388	2.676780
C	-0.883388	-0.883388	2.676780
C	0.883388	2.676780	0.883388
C	-0.883388	-2.676780	0.883388
C	-0.883388	2.676780	-0.883388
C	0.883388	-2.676780	-0.883388
C	0.911107	2.678989	-2.678989
C	-0.911107	-2.678989	-2.678989
C	-0.911107	2.678989	2.678989
C	0.911107	-2.678989	2.678989
C	2.678989	2.678989	-0.911107
C	-2.678989	-2.678989	-0.911107
C	-2.678989	2.678989	0.911107
C	2.678989	-2.678989	0.911107

1								
2								
3	H	-0.624047	4.224135	-0.624047	C	0.897087	4.461957	-0.897087
4	H	0.624047	-4.224135	-0.624047	C	-0.897087	-4.461957	-0.897087
5	H	0.624047	4.224135	0.624047	C	-0.897087	4.461957	0.897087
6	H	-0.624047	-4.224135	0.624047	C	0.897087	-4.461957	0.897087
7	H	-4.224135	0.624047	-0.624047	C	4.461957	0.897087	-0.897087
8	H	4.224135	-0.624047	-0.624047	C	-4.461957	-0.897087	-0.897087
9	H	4.224135	0.624047	0.624047	C	-4.461957	0.897087	0.897087
10	H	-4.224135	-0.624047	0.624047	C	4.461957	-0.897087	0.897087
11	H	0.624047	0.624047	4.224135	C	0.897087	0.897087	-4.461957
12	H	-0.624047	-0.624047	4.224135	C	-0.897087	-0.897087	-4.461957
13	H	0.624047	-0.624047	-4.224135	C	-0.897087	0.897087	4.461957
14	H	-1.170512	4.228595	2.418574	H	3.314241	3.314241	-0.271068
15	H	1.170512	-4.228595	2.418574	H	-3.314241	-3.314241	-0.271068
16	H	1.170512	4.228595	-2.418574	H	-3.314241	3.314241	0.271068
17	H	-1.170512	-4.228595	-2.418574	H	3.314241	-3.314241	0.271068
18	H	-2.418574	4.228595	1.170512	H	-1.521359	3.311759	-1.521359
19	H	2.418574	-4.228595	1.170512	H	1.521359	-3.311759	-1.521359
20	H	2.418574	4.228595	-1.170512	H	1.521359	3.311759	1.521359
21	H	-2.418574	-4.228595	-1.170512	H	-1.521359	-3.311759	-1.521359
22	H	-4.228595	1.170512	2.418574	H	3.311759	1.521359	-1.521359
23	H	4.228595	-1.170512	2.418574	H	-3.311759	-1.521359	1.521359
24	H	4.228595	1.170512	-2.418574	H	-3.311759	-1.521359	1.521359
25	H	-4.228595	-1.170512	-2.418574	H	3.311759	1.521359	-1.521359
26	H	-4.228595	2.418574	1.170512	H	-1.521359	1.521359	-3.311759
27	H	4.228595	-2.418574	1.170512	H	1.521359	-1.521359	-3.311759
28	H	4.228595	2.418574	-1.170512	H	1.521359	1.521359	3.311759
29	H	-4.228595	-2.418574	-1.170512	H	-1.521359	-1.521359	3.311759
30	H	-1.170512	2.418574	4.228595	H	3.314241	0.271068	-3.314241
31	H	1.170512	-2.418574	4.228595	H	-3.314241	-0.271068	-3.314241
32	H	1.170512	2.418574	-4.228595	H	-3.314241	0.271068	3.314241
33	H	-1.170512	-2.418574	-4.228595	H	3.314241	-0.271068	3.314241
34	C	-2.687543	2.687543	2.687543	H	0.271068	3.314241	-3.314241
35	C	2.687543	-2.687543	2.687543	H	-0.271068	-3.314241	-3.314241
36	C	2.687543	2.687543	-2.687543	H	-0.271068	3.314241	3.314241
37	C	-2.687543	-2.687543	-2.687543	H	0.271068	-3.314241	3.314241
38	H	-2.418574	1.170512	4.228595	C	4.469088	2.693421	-2.693421
39	H	2.418574	-1.170512	4.228595	C	-4.469088	-2.693421	-2.693421
40	H	2.418574	1.170512	-4.228595	C	-4.469088	2.693421	2.693421
41	H	-2.418574	-1.170512	-4.228595	C	4.469088	-2.693421	-2.693421
42	H	3.321597	3.321597	-3.321597	C	2.693421	4.469088	-2.693421
43	H	-3.321597	-3.321597	-3.321597	C	-2.693421	-4.469088	-2.693421
44	H	-3.321597	3.321597	3.321597	C	-2.693421	4.469088	2.693421
45	H	3.321597	-3.321597	3.321597	C	2.693421	-4.469088	2.693421
46					C	2.693421	2.693421	-4.469088
47					C	-2.693421	-2.693421	-4.469088
48					C	-2.693421	2.693421	4.469088
49					C	2.693421	-2.693421	4.469088
50					H	0.272628	5.120610	-1.520127
51					H	-0.272628	-5.120610	-1.520127
52					H	-0.272628	5.120610	1.520127
53					H	0.272628	-5.120610	1.520127
54					H	1.520127	5.120610	-0.272628
55					H	-1.520127	-5.120610	-0.272628
56					H	-1.520127	5.120610	0.272628
57					H	1.520127	-5.120610	0.272628
58					H	5.120610	0.272628	-1.520127
59					H	-5.120610	-0.272628	-1.520127
60					H	-5.120610	0.272628	1.520127
					H	5.120610	-0.272628	1.520127
					H	5.120610	1.520127	-0.272628
					H	-5.120610	-1.520127	-0.272628
					H	-5.120610	1.520127	0.272628
					H	5.120610	-1.520127	0.272628
					H	0.272628	1.520127	-5.120610
					H	-0.272628	-1.520127	-5.120610
					H	-0.272628	1.520127	5.120610
					H	0.272628	-1.520127	5.120610
					H	1.520127	0.272628	-5.120610
					H	-1.520127	-0.272628	-5.120610
					H	-1.520127	0.272628	5.120610

1	C	2.692251	2.692251	4.495115	6	0.001160	3.587468	1.794783
2	C	-2.692251	-2.692251	4.495115	6	0.883075	4.468310	0.883075
3	C	-2.692251	2.692251	-4.495115	6	1.794783	3.587468	0.001160
4	C	2.692251	-2.692251	-4.495115	6	2.675094	2.675094	0.882102
5	C	2.692251	4.495115	2.692251	6	3.587468	1.794783	0.001160
6	C	-2.692251	-4.495115	2.692251	6	4.469175	2.676885	-0.910585
7	C	-2.692251	4.495115	-2.692251	6	3.589277	3.589277	-1.792922
8	C	2.692251	-4.495115	-2.692251	6	2.676885	4.469175	-0.910585
9	C	4.491543	0.897138	0.897138	6	1.793894	5.387827	-1.793894
10	C	-4.491543	-0.897138	0.897138	6	0.910585	4.469175	-2.676885
11	C	-4.491543	0.897138	-0.897138	6	1.792922	3.589277	-3.589277
12	C	4.491543	-0.897138	-0.897138	6	2.690072	2.690072	-2.690072
13	C	4.495115	2.692251	2.692251	6	3.589277	1.792922	-3.589277
14	C	-4.495115	-2.692251	2.692251	6	2.676885	0.910585	-4.469175
15	C	-4.495115	2.692251	-2.692251	6	1.793894	1.793894	-5.387827
16	C	4.495115	-2.692251	-2.692251	6	0.910585	2.676885	-4.469175
17	C	0.000000	1.791840	0.000000	6	-0.001160	1.794783	-3.587468
18	C	0.000000	-1.791840	0.000000	6	-0.882102	2.675094	-2.675094
19	C	0.000000	0.000000	1.791840	6	-1.794053	1.794053	-1.794053
20	C	0.000000	0.000000	-1.791840	6	-0.895472	0.895472	-0.895472
21	C	1.791840	0.000000	0.000000	6	0.000000	0.000000	-1.792011
22	C	-1.791840	0.000000	0.000000	6	0.895472	-0.895472	-0.895472
23	C	1.793491	1.793491	1.793491	6	1.794053	-1.794053	-1.794053
24	C	-1.793491	-1.793491	1.793491	6	2.675094	-0.882102	-2.675094
25	C	-1.793491	1.793491	-1.793491	6	3.587468	-0.001160	-1.794783
26	C	1.793491	-1.793491	-1.793491	6	4.469175	0.910585	-2.676885
27	C	1.780210	3.572648	0.013943	6	5.387827	1.793894	-1.793894
28	C	-1.780210	-3.572648	0.013943	6	6.253308	0.896782	-0.896782
29	C	-1.780210	3.572648	-0.013943	1	6.911662	0.272674	-1.520400
30	C	1.780210	-3.572648	-0.013943	1	6.911662	1.520400	-0.272674
31	C	1.780210	0.013943	3.572648	6	5.387019	0.000000	0.000000
32	C	-1.780210	-0.013943	3.572648	6	4.468310	0.883075	0.883075
33	C	-1.780210	0.013943	-3.572648	6	3.587468	0.001160	1.794783
34	C	1.780210	-0.013943	-3.572648	6	4.469175	-0.910585	2.676885
35	C	0.013943	3.572648	1.780210	6	3.589277	-1.792922	3.589277
36	C	-0.013943	-3.572648	1.780210	6	2.676885	-0.910585	4.469175
37	C	-0.013943	3.572648	-1.780210	6	1.793894	-1.793894	5.387827
38	C	0.013943	-3.572648	-1.780210	6	0.896782	-0.896782	6.253308
39	C	0.013943	1.780210	3.572648	6	0.000000	0.000000	5.387019
40	C	-0.013943	-1.780210	3.572648	6	-0.896782	0.896782	6.253308
41	C	-0.013943	1.780210	-3.572648	6	-1.793894	1.793894	5.387827
42	C	0.013943	-1.780210	-3.572648	6	-0.910585	2.676885	4.469175
43	C	1.778736	-1.778736	1.778736	6	0.001160	1.794783	3.587468
44	C	-1.778736	1.778736	1.778736	6	-0.896596	0.896596	2.687853
45	C	-1.778736	-1.778736	-1.778736	6	-1.794783	-0.001160	3.587468
46	C	1.778736	1.778736	-1.778736	6	-2.676885	0.910585	4.469175
47	C	1.808047	3.575724	3.575724	6	-3.589277	1.792922	3.589277
48	C	-1.808047	-3.575724	3.575724	6	-4.469175	0.910585	2.676885
49	C	-1.808047	3.575724	-3.575724	6	-5.387827	1.793894	1.793894
50	C	1.808047	-3.575724	-3.575724	6	-4.469175	2.676885	0.910585
51	C	3.572648	1.780210	0.013943	6	-3.587468	1.794783	-0.001160
52	C	-3.572648	-1.780210	0.013943	6	-4.468310	0.883075	-0.883075
53	C	-3.572648	1.780210	-0.013943	6	-3.587468	0.001160	-1.794783
54	C	3.572648	-1.780210	-0.013943	6	-2.675094	0.882102	-2.675094
55	C	3.572648	0.013943	1.780210	6	-1.794783	0.001160	-3.587468
56	C	-3.572648	-0.013943	1.780210	6	-2.676885	-0.910585	-4.469175
57	C	-3.572648	0.013943	-1.780210	6	-1.793894	-1.793894	-5.387827
58	C	3.572648	-0.013943	-1.780210	6	-0.910585	-2.676885	-4.469175
59	C	3.575724	1.808047	3.575724	1	-0.271610	-3.314221	-5.103817
60	C	-3.575724	-1.808047	3.575724	6	-1.792922	-3.589277	-3.589277
	C	-3.575724	1.808047	-3.575724	6	-0.910585	-4.469175	-2.676885
	C	3.575724	-1.808047	-3.575724	6	0.001160	-3.587468	-1.794783
	C	3.575724	3.575724	1.808047	6	0.882102	-2.675094	-2.675094
	C	-3.575724	-3.575724	1.808047	6	0.001160	-1.794783	-3.587468
	C	-3.575724	3.575724	-1.808047	6	0.883075	-0.883075	-4.468310
	C	3.575724	-3.575724	-1.808047	6	1.794783	-0.001160	-3.587468
	C	5.358325	1.794044	1.794044	6	0.896596	0.896596	-2.687853
	C	-5.358325	-1.794044	1.794044	6	0.000000	0.000000	-5.387019
	C	-5.358325	1.794044	-1.794044	6	-0.883075	0.883075	-4.468310
	C	5.358325	-1.794044	-1.794044	1	-1.521319	1.521319	-5.102823
	C	5.356459	0.000000	0.000000	6	-0.896782	-0.896782	-6.253308

1	C	-5.356459	0.000000	0.000000	1	-0.272674	-1.520400	-6.911662
2	C	1.794044	5.358325	1.794044	1	-1.520400	-0.272674	-6.911662
3	C	-1.794044	-5.358325	1.794044	6	0.896782	0.896782	-6.253308
4	C	-1.794044	5.358325	-1.794044	1	1.520400	0.272674	-6.911662
5	C	1.794044	-5.358325	-1.794044	1	0.272674	1.520400	-6.911662
6	C	1.794044	1.794044	5.358325	1	1.521319	-1.521319	-5.102823
7	C	-1.794044	-1.794044	5.358325	6	-0.896596	-0.896596	-2.687853
8	C	-1.794044	1.794044	-5.358325	1	1.519903	-3.311870	-3.311870
9	C	1.794044	-1.794044	-5.358325	6	0.883075	-4.468310	-0.883075
10	C	0.000000	5.356459	0.000000	6	1.794783	-3.587468	-0.001160
11	C	0.000000	-5.356459	0.000000	6	2.676885	-4.469175	0.910585
12	C	0.000000	0.000000	5.356459	6	1.793894	-5.387827	1.793894
13	C	0.000000	0.000000	-5.356459	6	2.690652	-6.255059	2.690652
14	H	4.210835	4.210835	1.167888	6	3.589189	-5.391877	3.589189
15	H	-4.210835	-4.210835	1.167888	6	4.472447	-4.472447	2.704829
16	H	-4.210835	4.210835	-1.167888	6	5.391877	-3.589189	3.589189
17	H	4.210835	-4.210835	-1.167888	6	6.255059	-2.690652	2.690652
18	H	4.210835	1.167888	4.210835	6	5.387827	-1.793894	1.793894
19	H	-4.210835	-1.167888	4.210835	6	4.469175	-2.676885	0.910585
20	H	4.210835	1.167888	-4.210835	6	3.589277	-3.589277	1.792922
21	H	4.210835	-1.167888	-4.210835	6	2.690072	-2.690072	2.690072
22	H	-2.417367	4.207573	0.624829	6	1.792922	-3.589277	3.589277
23	H	2.417367	-4.207573	0.624829	6	0.910585	-4.469175	2.676885
24	H	2.417367	4.207573	-0.624828	6	-0.001160	-3.587468	1.794783
25	H	-2.417367	-4.207573	-0.624828	6	-0.883075	-4.468310	0.883075
26	H	-2.417367	0.624829	4.207573	6	-1.794783	-3.587468	0.001160
27	H	2.417367	-0.624828	4.207573	6	-2.676885	-4.469175	-0.910585
28	H	2.417367	0.624828	-4.207573	6	-3.589277	-3.589277	-1.792922
29	H	-2.417367	-0.624829	-4.207573	6	-4.469175	-2.676885	-0.910585
30	H	4.207573	-2.417367	0.624829	6	-5.387827	-1.793894	-1.793894
31	H	-4.207573	2.417367	0.624829	6	-4.469175	-0.910585	-2.676885
32	H	-4.207573	-2.417367	-0.624829	6	-3.589277	-1.792922	-3.589277
33	H	4.207573	2.417367	-0.624829	6	-2.690072	-2.690072	-2.690072
34	H	4.207573	0.624829	-2.417367	6	-4.472447	-2.704829	-4.472447
35	H	-4.207573	-0.624828	-2.417367	6	-5.391877	-3.589189	-3.589189
36	H	-4.207573	0.624829	2.417367	6	-4.472447	-4.472447	-2.704829
37	H	4.207573	-0.624828	2.417367	6	-3.589189	-5.391877	-3.589189
38	H	-2.415802	2.415802	2.415802	6	-2.690652	-6.255059	-2.690652
39	H	2.415802	-2.415802	2.415802	6	-1.793894	-5.387827	-1.793894
40	H	2.415802	2.415802	-2.415802	6	-0.896782	-6.253308	-0.896782
41	H	-2.415802	-2.415802	-2.415802	6	0.000000	-5.387019	0.000000
42	H	-0.624829	4.207573	2.417367	6	0.896782	-6.253308	0.896782
43	H	0.624828	-4.207573	2.417367	1	1.520400	-6.911662	0.272674
44	H	0.624829	4.207573	-2.417367	1	0.272674	-6.911662	1.520400
45	H	-0.624828	-4.207573	-2.417367	1	-0.272674	-6.911662	-1.520400
46	H	-0.624829	2.417367	4.207573	1	-1.520400	-6.911662	-0.272674
47	H	0.624829	-2.417367	4.207573	1	-2.065823	-6.913573	-3.313438
48	H	0.624828	2.417367	-4.207573	1	-3.313438	-6.913573	-2.065823
49	H	-0.624828	-2.417367	-4.207573	6	-2.704829	-4.472447	-4.472447
50	H	1.167888	4.210835	4.210835	6	-3.589189	-3.589189	-5.391877
51	H	-1.167888	-4.210835	4.210835	6	-4.487031	-4.487031	-6.262723
52	H	-1.167888	4.210835	-4.210835	6	-5.378061	-5.378061	-5.378061
53	H	1.167888	-4.210835	-4.210835	6	-6.262723	-4.487031	-4.487031
54	C	3.590209	5.365781	3.590209	1	-6.919385	-3.861222	-5.109127
55	C	-3.590209	-5.365781	3.590209	1	-6.919385	-5.109127	-3.861222
56	C	-3.590209	5.365781	-3.590209	6	-4.487031	-6.262723	-4.487031
57	C	3.590209	-5.365781	-3.590209	1	-3.861222	-6.919385	-5.109127
58	C	3.590209	3.590209	5.365781	1	-5.109127	-6.919385	-3.861222
59	C	-3.590209	-3.590209	5.365781	1	-6.012014	-6.012014	-6.012014
60	C	-3.590209	3.590209	-5.365781	1	-3.861222	-5.109127	-6.919385
	C	3.590209	-3.590209	-5.365781	1	-5.109127	-3.861222	-6.919385
	C	5.365781	3.590209	3.590209	6	-2.690652	-2.690652	-6.255059
	C	-5.365781	-3.590209	3.590209	1	-2.065823	-3.313438	-6.913573
	C	-5.365781	3.590209	-3.590209	1	-3.313438	-2.065823	-6.913573
	C	5.365781	-3.590209	-3.590209	1	-2.064503	-5.107540	-5.107540
	H	6.017083	1.169217	2.416627	1	-5.107540	-5.107540	-2.064503
	H	-6.017083	-1.169217	2.416627	6	-6.255059	-2.690652	-2.690652
	H	-6.017083	1.169217	-2.416627	1	-6.913573	-3.313438	-2.065823
	H	6.017083	-1.169217	-2.416627	1	-6.913573	-2.065823	-3.313438
	H	6.017083	2.416627	1.169217	1	-5.107540	-2.064503	-5.107540
	H	-6.017083	-2.416627	1.169217	1	-5.103817	-0.271610	-3.314221

1	H	-6.017083	2.416627	-1.169217	6	-6.253308	-0.896782	-0.896782
2	H	6.017083	-2.416627	-1.169217	6	-5.387019	0.000000	0.000000
3	H	6.015824	0.623539	-0.623539	6	-4.468310	-0.883075	0.883075
4	H	-6.015824	-0.623539	-0.623539	6	-3.587468	-0.001160	1.794783
5	H	-6.015824	0.623539	0.623539	6	-2.675094	-0.882102	2.675094
6	H	6.015824	-0.623539	0.623539	1	-3.311870	-1.519903	3.311870
7	H	1.169217	6.017083	2.416627	1	-5.102823	-1.521319	1.521319
8	H	-1.169217	-6.017083	2.416627	6	-6.253308	0.896782	0.896782
9	H	-1.169217	6.017083	-2.416627	1	-6.911662	0.272674	1.520400
10	H	1.169217	-6.017083	-2.416627	1	-6.911662	1.520400	0.272674
11	H	1.169217	2.416627	6.017083	1	-6.911662	-1.520400	-0.272674
12	H	-1.169217	-2.416627	6.017083	1	-6.911662	-0.272674	-1.520400
13	H	-1.169217	2.416627	-6.017083	1	-5.103817	-3.314221	-0.271610
14	H	1.169217	-2.416627	-6.017083	1	-3.314221	-5.103817	-0.271610
15	H	0.623539	6.015824	-0.623539	1	-1.521319	-5.102823	1.521319
16	H	-0.623539	-6.015824	-0.623539	1	0.271610	-5.103817	3.314221
17	H	-0.623539	6.015824	0.623539	6	2.704829	-4.472447	4.472447
18	H	0.623539	-6.015824	0.623539	6	3.589189	-3.589189	5.391877
19	H	0.623539	-0.623539	6.015824	6	4.472447	-2.704829	4.472447
20	H	-0.623539	0.623539	6.015824	1	5.107540	-2.064503	5.107540
21	H	-0.623539	-0.623539	-6.015824	6	2.690652	-2.690652	6.255059
22	H	0.623539	0.623539	-6.015824	1	3.313438	-2.065823	6.913573
23	H	2.416627	6.017083	1.169217	1	2.065823	-3.313438	6.913573
24	H	-2.416627	-6.017083	1.169217	6	4.487031	-4.487031	6.262723
25	H	-2.416627	6.017083	-1.169217	1	5.109127	-3.861222	6.919385
26	H	2.416627	-6.017083	-1.169217	1	3.861222	-5.109127	6.919385
27	H	2.416627	1.169217	6.017083	6	5.378061	-5.378061	5.378061
28	H	-2.416627	-1.169217	6.017083	6	4.487031	-6.262723	4.487031
29	H	-2.416627	1.169217	-6.017083	1	5.109127	-6.919385	3.861222
30	H	2.416627	-1.169217	-6.017083	1	3.861222	-6.919385	5.109127
31	H	6.022343	2.964396	4.212371	6	6.262723	-4.487031	4.487031
32	H	-6.022343	-2.964396	4.212371	1	6.919385	-5.109127	3.861222
33	H	-6.022343	2.964396	-4.212371	1	6.919385	-3.861222	5.109127
34	H	6.022343	-2.964396	-4.212371	1	6.012014	-6.012014	6.012014
35	H	6.022343	4.212371	2.964396	1	2.064503	-5.107540	5.107540
36	H	-6.022343	-4.212371	2.964396	6	0.910585	-2.676885	4.469175
37	H	-6.022343	4.212371	-2.964396	1	0.271610	-3.314221	5.103817
38	H	6.022343	-4.212371	-2.964396	6	3.587468	-1.794783	-0.001160
39	H	2.964396	6.022343	4.212371	6	2.675094	-2.675094	-0.882102
40	H	-2.964396	-6.022343	4.212371	1	3.311870	-3.311870	-1.519903
41	H	-2.964396	6.022343	-4.212371	6	4.468310	-0.883075	-0.883075
42	H	2.964396	-6.022343	-4.212371	1	5.102823	-1.521319	-1.521319
43	H	2.964396	4.212371	6.022343	1	5.103817	-3.314221	0.271610
44	H	-2.964396	-4.212371	6.022343	6	6.253308	-0.896782	0.896782
45	H	-2.964396	4.212371	-6.022343	1	6.911662	-1.520400	0.272674
46	H	2.964396	-4.212371	-6.022343	1	6.911662	-0.272674	1.520400
47	H	4.212371	6.022343	2.964396	1	6.913573	-2.065823	3.313438
48	H	-4.212371	-6.022343	2.964396	1	6.913573	-3.313438	2.065823
49	H	-4.212371	6.022343	-2.964396	1	5.107540	-5.107540	2.064503
50	H	4.212371	-6.022343	-2.964396	1	3.313438	-6.913573	2.065823
51	H	4.212371	2.964396	6.022343	1	2.065823	-6.913573	3.313438
52	H	-4.212371	-2.964396	6.022343	1	3.314221	-5.103817	0.271610
53	H	-4.212371	2.964396	-6.022343	1	1.521319	-5.102823	-1.521319
54	H	4.212371	-2.964396	-6.022343	1	-0.271610	-5.103817	-3.314221
55	C	4.481212	4.481212	4.481212	1	-3.314221	-0.271610	-5.103817
56	C	-4.481212	-4.481212	4.481212	1	-3.311870	1.519903	-3.311870
57	C	-4.481212	4.481212	-4.481212	1	-5.102823	1.521319	-1.521319
58	C	4.481212	-4.481212	-4.481212	6	-2.675094	2.675094	-0.882102
59	H	5.115108	5.115108	5.115108	1	-3.311870	3.311870	-1.519903
60	H	-5.115108	-5.115108	5.115108	1	-5.103817	3.314221	0.271610
	H	-5.115108	5.115108	-5.115108	6	-6.255059	2.690652	2.690652
	H	5.115108	-5.115108	-5.115108	6	-5.391877	3.589189	3.589189
					6	-4.472447	2.704829	4.472447
					6	-3.589189	3.589189	5.391877
					6	-2.690652	2.690652	6.255059
					1	-3.313438	2.065823	6.913573
					1	-2.065823	3.313438	6.913573
					6	-2.704829	4.472447	4.472447
					6	-3.589189	5.391877	3.589189
					6	-4.472447	4.472447	2.704829
					1	-5.107540	5.107540	2.064503

1				
2				
3				
4				
5				
6				
7				
8				
9				
10				
11				
12				
13				
14				
15				
16				
17				
18				
19				
20				
21				
22				
23				
24				
25				
26				
27				
28				
29				
30				
31				
32				
33				
34				
35				
36				
37				
38				
39				
40				
41				
42				
43				
44				
45				
46				
47				
48				
49				
50				
51				
52				
53				
54				
55				
56				
57				
58				
59				
60				

		1	5.103817	0.271610	-3.314221
		1	3.311870	-1.519903	-3.311870
		1	-1.519903	3.311870	-3.311870
		1	0.271610	3.314221	-5.103817
		1	3.314221	0.271610	-5.103817
		1	0.271610	5.103817	-3.314221
		1	3.314221	5.103817	-0.271610
		1	5.103817	3.314221	-0.271610
		1	3.311870	3.311870	1.519903
		1	1.521319	5.102823	1.521319
		1	-0.271610	5.103817	3.314221
		1	-3.314221	5.103817	0.271610
		1	-1.521319	5.102823	-1.521319
		1	-3.311870	-3.311870	1.519903
		1	3.311870	1.519903	3.311870
		1	-1.519903	-3.311870	3.311870
C ₂₈₁ H ₁₇₂ , B3LYP/6-31G*, E=-10812.77944		C ₁₆ H ₁₈ F ₆ RB3PW91/6-31G(d,p) E=-1219.26501			
6	.895651	-.895651	.895651		
6	-.000933	-1.791447	1.791447		
6	-.896445	-.896445	2.688001		
6	.000000	.000000	3.583331		
6	.896445	.896445	2.688001		
6	.000933	1.791447	1.791447		
6	-.895651	.895651	.895651		
6	.000000	.000000	.000000		
6	-.895651	-.895651	-.895651		
6	-1.791447	.000933	-1.791447		
6	-2.688001	.896445	-.896445		
6	-1.791447	1.791447	-.000933		
6	-2.690143	2.690143	.897329		
6	-1.778288	3.570707	1.778288		
6	-.897329	2.690143	2.690143		
6	.014493	3.571353	3.571353		
6	.895492	2.691319	4.483739		
6	1.793125	1.793125	3.584108		
6	2.689589	2.689589	2.689589		
6	1.793125	3.584108	1.793125		
6	.896445	2.688001	.896445		
6	.000000	3.583331	.000000		
6	-.896445	2.688001	-.896445		
6	-.000933	1.791447	-1.791447		
6	.895651	.895651	-.895651		
6	1.791447	-.000933	-1.791447		
6	2.688001	-.896445	-.896445		
6	1.791447	-1.791447	-.000933		
6	2.690143	-2.690143	.897329		
6	1.778288	-3.570707	1.778288		
6	.897329	-2.690143	2.690143		
6	-.014493	-3.571353	3.571353		
6	-.895492	-2.691319	4.483739		
6	-1.793125	-1.793125	3.584108		
6	-2.689589	-2.689589	2.689589		
6	-1.793125	-3.584108	1.793125		
6	-.896445	-2.688001	.896445		
6	.000000	-3.583331	.000000		
6	.896445	-2.688001	-.896445		
6	.000933	-1.791447	-1.791447		
6	.896445	-.896445	-2.688001		
6	1.793125	-1.793125	-3.584108		
6	2.689589	-2.689589	-2.689589		
6	1.793125	-3.584108	-1.793125		
6	2.691319	-4.483739	-.895492		
6	3.571353	-3.571353	-.014493		
6	4.483739	-2.691319	-.895492		
6	3.584108	-1.793125	-1.793125		
6	4.483739	-.895492	-2.691319		
6	5.364275	-.013632	-1.779684		
6	6.283029	-.896714	-.896714		
		H	0.000000	2.482353	0.088825
		H	-2.149781	-1.241177	0.088825
		H	2.149781	1.241177	-0.088825
		H	0.000000	-2.482353	-0.088825
		H	2.149781	-1.241177	0.088825
		H	-2.149781	1.241177	-0.088825
		H	-1.272863	1.753580	2.179419
		H	-2.155076	0.225542	2.179419
		H	2.155076	-0.225542	-2.179419
		H	1.272863	-1.753580	-2.179419
		H	2.155076	0.225542	2.179419
		H	0.882213	-1.979122	2.179419
		H	-0.882213	1.979122	-2.179419
		H	-2.155076	-0.225542	-2.179419
		H	-0.882213	-1.979122	2.179419
		H	1.272863	1.753580	2.179419
		H	-1.272863	-1.753580	-2.179419
		H	0.882213	1.979122	-2.179419
		C	0.000000	1.448158	-1.802672
		C	-1.254141	-0.724079	-1.802672
		C	1.254141	0.724079	1.802672
		C	0.000000	-1.448158	1.802672
		C	1.254141	-0.724079	-1.802672
		C	-1.254141	0.724079	1.802672
		C	0.000000	0.000000	-2.327847
		C	0.000000	0.000000	2.327847
		C	-1.250488	-0.721969	-0.270833
		C	0.000000	1.443939	-0.270833
		C	0.000000	-1.443939	0.270833
		C	1.250488	0.721969	0.270833
		C	1.250488	-0.721969	-0.270833
		C	-1.250488	0.721969	0.270833
		C	0.000000	0.000000	-3.848513
		C	0.000000	0.000000	3.848513
		F	0.000000	-1.252479	-4.353466
		F	1.084678	0.626239	-4.353466
		F	-1.084678	-0.626239	4.353466
		F	0.000000	1.252479	4.353466
		F	-1.084678	0.626239	-4.353466
		F	1.084678	-0.626239	4.353466

6	5.364275	-1.779684	-.013632
6	4.483095	-.897859	.897859
6	3.570707	-1.778288	1.778288
6	2.690143	-.897329	2.690143
6	1.791447	.000933	1.791447
6	2.688001	.896445	.896445
6	1.791447	1.791447	.000933
6	2.690143	2.690143	-.897329
6	3.570707	1.778288	-1.778288
6	2.690143	.897329	-2.690143
6	3.571353	-.014493	-3.571353
6	2.691319	-.895492	-4.483739
6	1.779684	-.013632	-5.364275
1	2.417710	.624890	-5.998738
6	.896714	-.896714	-6.283029
6	1.793351	-1.793351	-7.149529
1	1.169178	-2.416799	-7.808066
1	2.416799	-1.169178	-7.808066
6	2.690484	-2.690484	-6.284278
6	3.573443	-1.807168	-5.365621
6	4.485861	-2.689542	-4.485861
6	3.586660	-3.586660	-3.586660
6	4.485861	-4.485861	-2.689542
6	5.365621	-3.573443	-1.807168
6	6.284278	-2.690484	-2.690484
6	5.365621	-1.807168	-3.573443
1	6.000259	-1.168087	-4.210681
6	7.149529	-1.793351	-1.793351
1	7.808066	-1.169178	-2.416799
1	7.808066	-2.416799	-1.169178
6	7.151577	-3.587211	-3.587211
1	7.810266	-2.962409	-4.209917
1	7.810266	-4.209917	-2.962409
6	6.288559	-4.485789	-4.485789
6	5.369100	-5.369100	-3.601434
1	6.004194	-6.004194	-2.961112
6	4.485789	-6.288559	-4.485789
6	3.601434	-5.369100	-5.369100
6	2.689542	-4.485861	-4.485861
6	1.807168	-5.365621	-3.573443
6	.895492	-4.483739	-2.691319
6	.014493	-3.571353	-3.571353
6	.895492	-2.691319	-4.483739
6	.013632	-1.779684	-5.364275
6	-.897859	-.897859	-4.483095
6	-1.778288	-1.778288	-3.570707
6	-.897329	-2.690143	-2.690143
6	-1.778288	-3.570707	-1.778288
6	-.897859	-4.483095	-.897859
6	-1.779684	-5.364275	.013632
6	-2.691319	-4.483739	.895492
6	-3.571353	-3.571353	.014493
6	-4.483739	-2.691319	.895492
6	-5.365621	-3.573443	1.807168
6	-4.485861	-4.485861	2.689542
6	-5.369100	-5.369100	3.601434
6	-4.485789	-6.288559	4.485789
6	-5.383621	-7.159334	5.383621
6	-6.274579	-6.274579	6.274579
6	-7.159334	-5.383621	5.383621
6	-6.288559	-4.485789	4.485789
6	-7.151577	-3.587211	3.587211
6	-6.284278	-2.690484	2.690484
6	-5.365621	-1.807168	3.573443
6	-4.485861	-2.689542	4.485861
6	-3.573443	-1.807168	5.365621
6	-2.690484	-2.690484	6.284278
6	-1.807168	-3.573443	5.365621
6	-2.689542	-4.485861	4.485861
6	-1.807168	-5.365621	3.573443
6	-.895492	-4.483739	2.691319

6	-.013632	-5.364275	1.779684
6	.897859	-4.483095	.897859
6	1.779684	-5.364275	-.013632
6	.896714	-6.283029	-.896714
6	1.793351	-7.149529	-1.793351
6	2.690484	-6.284278	-2.690484
6	3.573443	-5.365621	-1.807168
1	4.210681	-6.000259	-1.168087
6	3.587211	-7.151577	-3.587211
1	2.962409	-7.810266	-4.209917
1	4.209917	-7.810266	-2.962409
1	1.169178	-7.808066	-2.416799
1	2.416799	-7.808066	-1.169178
6	.013632	-5.364275	-1.779684
1	-.624890	-5.998738	-2.417710
6	.000000	-7.148945	.000000
6	-.896714	-6.283029	.896714
6	-1.793351	-7.149529	1.793351
1	-2.416799	-7.808066	1.169178
1	-1.169178	-7.808066	2.416799
6	-2.690484	-6.284278	2.690484
6	-3.573443	-5.365621	1.807168
1	-4.210681	-6.000259	1.168087
6	-3.587211	-7.151577	3.587211
1	-4.209917	-7.810266	2.962409
1	-2.962409	-7.810266	4.209917
1	-.623818	-7.807467	-.623818
1	.623818	-7.807467	.623818
1	2.417710	-5.998738	.624890
1	.624890	-5.998738	2.417710
1	-1.168087	-6.000259	4.210681
6	-3.586660	-3.586660	3.586660
6	-3.601434	-5.369100	5.369100
1	-2.961112	-6.004194	6.004194
6	-4.485789	-4.485789	6.288559
6	-5.369100	-3.601434	5.369100
1	-6.004194	-2.961112	6.004194
6	-3.587211	-3.587211	7.151577
1	-2.962409	-4.209917	7.810266
1	-4.209917	-2.962409	7.810266
6	-5.383621	-5.383621	7.159334
1	-4.758027	-6.005813	7.816194
1	-6.005813	-4.758027	7.816194
1	-1.168087	-4.210681	6.000259
6	-1.793351	-1.793351	7.149529
6	-.896714	-.896714	6.283029
6	-1.779684	-.013632	5.364275
6	-2.691319	-.895492	4.483739
6	-3.571353	-.014493	3.571353
6	-2.690143	.897329	2.690143
6	-1.791447	-.000933	1.791447
6	-2.688001	-.896445	.896445
6	-3.584108	-1.793125	1.793125
6	-4.483739	-.895492	2.691319
6	-5.364275	-.013632	1.779684
6	-4.483095	.897859	.897859
6	-5.364275	1.779684	-.013632
6	-4.483739	2.691319	-.895492
6	-3.584108	1.793125	-1.793125
6	-2.689589	2.689589	-2.689589
6	-1.793125	1.793125	-3.584108
6	-.896445	.896445	-2.688001
6	.000000	.000000	-3.583331
6	.897859	.897859	-4.483095
6	1.778288	1.778288	-3.570707
6	.897329	2.690143	-2.690143
6	-.014493	3.571353	-3.571353
6	-.895492	4.483739	-2.691319
6	-1.793125	3.584108	-1.793125
6	-2.691319	4.483739	-.895492
6	-3.573443	5.365621	-1.807168

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

6	-4.485861	4.485861	-2.689542
6	-3.586660	3.586660	-3.586660
6	-4.485861	2.689542	-4.485861
6	-5.369100	3.601434	-5.369100
6	-6.288559	4.485789	-4.485789
6	-7.151577	3.587211	-3.587211
6	-6.284278	2.690484	-2.690484
6	-5.365621	1.807168	-3.573443
6	-4.483739	.895492	-2.691319
6	-5.364275	.013632	-1.779684
6	-6.283029	.896714	-.896714
6	-7.148945	.000000	.000000
6	-6.283029	-.896714	.896714
6	-5.364275	-1.779684	.013632
6	-4.483095	-.897859	-.897859
6	-3.570707	-1.778288	-1.778288
6	-2.690143	-.897329	-2.690143
6	-3.571353	.014493	-3.571353
6	-2.691319	.895492	-4.483739
6	-1.779684	.013632	-5.364275
6	-.896714	.896714	-6.283029
6	-.013632	1.779684	-5.364275
6	-.895492	2.691319	-4.483739
6	-1.807168	3.573443	-5.365621
6	-2.689542	4.485861	-4.485861
6	-1.807168	5.365621	-3.573443
6	-2.690484	6.284278	-2.690484
6	-1.793351	7.149529	-1.793351
6	-.896714	6.283029	-.896714
6	-.013632	5.364275	-1.779684
6	.897859	4.483095	-.897859
6	1.779684	5.364275	.013632
6	2.691319	4.483739	.895492
6	3.573443	5.365621	1.807168
6	4.485861	4.485861	2.689542
6	5.365621	3.573443	1.807168
6	6.284278	2.690484	2.690484
6	5.365621	1.807168	3.573443
6	4.483739	.895492	2.691319
6	3.571353	.014493	3.571353
6	2.691319	.895492	4.483739
6	1.779684	.013632	5.364275
6	.897859	-.897859	4.483095
6	-.013632	-1.779684	5.364275
1	.624890	-2.417710	5.998738
6	1.778288	-1.778288	3.570707
1	2.415747	-2.415747	4.207200
6	.896714	.896714	6.283029
6	1.793351	1.793351	7.149529
6	2.690484	2.690484	6.284278
6	1.807168	3.573443	5.365621
6	2.689542	4.485861	4.485861
6	1.807168	5.365621	3.573443
6	.895492	4.483739	2.691319
6	.013632	5.364275	1.779684
6	-.897859	4.483095	.897859
6	-1.779684	5.364275	-.013632
1	-2.417710	5.998738	.624890
6	.896714	6.283029	.896714
6	1.793351	7.149529	1.793351
6	2.690484	6.284278	2.690484
6	3.587211	7.151577	3.587211
6	4.485789	6.288559	4.485789
6	3.601434	5.369100	5.369100
6	4.485789	4.485789	6.288559
6	5.369100	3.601434	5.369100
6	4.485861	2.689542	4.485861
6	3.573443	1.807168	5.365621
1	4.210681	1.168087	6.000259
6	3.586660	3.586660	3.586660
6	6.288559	4.485789	4.485789

6	5.369100	5.369100	3.601434
1	6.004194	6.004194	2.961112
6	7.159334	5.383621	5.383621
6	6.274579	6.274579	6.274579
6	5.383621	5.383621	7.159334
1	6.005813	4.758027	7.816194
1	4.758027	6.005813	7.816194
6	5.383621	7.159334	5.383621
1	6.005813	7.816194	4.758027
1	4.758027	7.816194	6.005813
1	6.908586	6.908586	6.908586
1	7.816194	6.005813	4.758027
1	7.816194	4.758027	6.005813
6	7.151577	3.587211	3.587211
1	7.810266	4.209917	2.962409
1	7.810266	2.962409	4.209917
1	6.004194	2.961112	6.004194
6	3.587211	3.587211	7.151577
1	2.962409	4.209917	7.810266
1	4.209917	2.962409	7.810266
1	2.961112	6.004194	6.004194
1	4.209917	7.810266	2.962409
1	2.962409	7.810266	4.209917
1	2.416799	7.808066	1.169178
1	1.169178	7.808066	2.416799
6	.000000	7.148945	.000000
1	.623818	7.807467	-.623818
1	-.623818	7.807467	.623818
1	-.624890	5.998738	2.417710
1	1.168087	6.000259	4.210681
1	1.168087	4.210681	6.000259
1	1.169178	2.416799	7.808066
1	2.416799	1.169178	7.808066
6	.013632	1.779684	5.364275
6	-.897859	.897859	4.483095
6	-1.778288	1.778288	3.570707
1	-2.415747	2.415747	4.207200
1	-.624890	2.417710	5.998738
6	.000000	.000000	7.148945
1	-.623818	.623818	7.807467
1	.623818	-.623818	7.807467
1	2.417710	-.624890	5.998738
1	4.207982	-.623617	4.207982
6	5.364275	.013632	1.779684
6	6.283029	.896714	.896714
6	5.364275	1.779684	.013632
6	4.483739	2.691319	.895492
6	3.571353	3.571353	.014493
1	4.207982	4.207982	-.623617
6	3.584108	1.793125	1.793125
6	4.483095	.897859	-.897859
6	3.583331	.000000	.000000
1	5.998738	2.417710	-.624890
6	7.149529	1.793351	1.793351
1	7.808066	2.416799	1.169178
1	7.808066	1.169178	2.416799
6	7.148945	.000000	.000000
1	7.807467	.623818	-.623818
1	7.807467	-.623818	.623818
1	5.998738	-.624890	2.417710
1	6.000259	1.168087	4.210681
1	6.000259	4.210681	1.168087
1	4.210681	6.000259	1.168087
1	2.417710	5.998738	-.624890
6	1.778288	3.570707	-1.778288
1	2.415747	4.207200	-2.415747
1	.624890	5.998738	-2.417710
1	-1.169178	7.808066	-2.416799
1	-2.416799	7.808066	-1.169178
6	-3.587211	7.151577	-3.587211
6	-4.485789	6.288559	-4.485789

1			
2			
3			
4	6	-3.601434	5.369100
5	6	-4.485789	4.485789
6	6	-3.587211	3.587211
7	6	-2.690484	2.690484
8	6	-1.793351	1.793351
9	1	-2.416799	1.169178
10	1	-1.169178	2.416799
11	6	-3.573443	1.807168
12	1	-4.210681	1.168087
13	1	-4.209917	2.962409
14	1	-2.962409	4.209917
15	6	-5.383621	5.383621
16	1	-6.005813	4.758027
17	1	-4.758027	6.005813
18	6	-6.274579	6.274579
19	6	-7.159334	5.383621
20	1	-7.816194	6.005813
21	1	-7.816194	4.758027
22	1	-6.908586	6.908586
23	6	-5.383621	7.159334
24	1	-6.005813	7.816194
25	1	-4.758027	7.816194
26	1	-2.961112	6.004194
27	6	-5.369100	5.369100
28	1	-6.004194	6.004194
29	1	-2.962409	7.810266
30	1	-4.209917	7.810266
31	1	-1.168087	6.000259
32	1	-1.168087	4.210681
33	1	.624890	2.417710
34	6	.000000	.000000
35	1	-.623818	-.623818
36	1	.623818	.623818
37	1	-2.417710	-.624890
38	1	-4.207982	-.623617
39	6	-2.690143	-2.690143
40	6	-1.791447	-1.791447
41	1	-4.207200	-2.415747
42	6	-3.583331	.000000
43	1	-5.998738	-2.417710
44	6	-7.149529	-1.793351
45	1	-7.808066	-2.416799
46	1	-7.808066	-1.169178
47	1	-7.807467	-.623818
48	1	-7.807467	.623818
49	6	-7.149529	1.793351
50	1	-7.808066	1.169178
51	1	-7.808066	2.416799
52	1	-5.998738	-.624890
53	1	-6.000259	1.168087
54	6	-5.365621	3.573443
55	1	-6.000259	4.210681
56	1	-7.810266	2.962409
57	1	-7.810266	4.209917
58	1	-6.004194	2.961112
59	1	-4.210681	6.000259
60	6	-3.571353	3.571353
	1	-4.207982	4.207982
	1	.623617	4.207982
	1	2.415747	2.415747
	1	-5.998738	2.417710
	6	-3.570707	1.778288
	1	-4.207200	2.415747
	1	-5.998738	.624890
	1	-4.207982	.623617
	1	-2.417710	.624890
	1	-1.169178	-2.416799
	1	-2.416799	-1.169178
	1	-4.210681	-1.168087
	1	-6.000259	-1.168087
	1	-7.810266	-4.209917

1	1	-7.810266	-2.962409	4.209917				
2	1	-7.816194	-6.005813	4.758027				
3	1	-7.816194	-4.758027	6.005813				
4	1	-6.908586	-6.908586	6.908586				
5	1	-6.005813	-7.816194	4.758027				
6	1	-4.758027	-7.816194	6.005813				
7	1	-6.004194	-6.004194	2.961112				
8	1	-6.000259	-4.210681	1.168087				
9	1	-4.207982	-4.207982	-.623617				
10	1	-2.417710	-5.998738	-.624890				
11	1	-2.415747	-4.207200	-2.415747				
12	1	-2.415747	-2.415747	-4.207200				
13	1	-.624890	-2.417710	-5.998738				
14	6	1.807168	-3.573443	-5.365621				
15	1	1.168087	-4.210681	-6.000259				
16	1	-.623617	-4.207982	-4.207982				
17	1	1.168087	-6.000259	-4.210681				
18	1	2.961112	-6.004194	-6.004194				
19	6	4.485789	-4.485789	-6.288559				
20	6	5.369100	-3.601434	-5.369100				
21	1	6.004194	-2.961112	-6.004194				
22	6	5.383621	-5.383621	-7.159334				
23	1	4.758027	-6.005813	-7.816194				
24	6	6.274579	-6.274579	-6.274579				
25	6	7.159334	-5.383621	-5.383621				
26	1	7.816194	-6.005813	-4.758027				
27	1	7.816194	-4.758027	-6.005813				
28	1	6.908586	-6.908586	-6.908586				
29	6	5.383621	-7.159334	-5.383621				
30	1	6.005813	-7.816194	-4.758027				
31	1	4.758027	-7.816194	-6.005813				
32	1	6.005813	-4.758027	-7.816194				
33	6	3.587211	-3.587211	-7.151577				
34	1	2.962409	-4.209917	-7.810266				
35	1	4.209917	-2.962409	-7.810266				
36	1	6.000259	-4.210681	-1.168087				
37	1	4.210681	-1.168087	-6.000259				
38	1	4.207982	.623617	-4.207982				
39	1	4.207200	2.415747	-2.415747				
40	1	4.207200	-2.415747	2.415747				
41	1	5.998738	-2.417710	.624890				
42	1	5.998738	.624890	-2.417710				
43	1	4.207982	-4.207982	.623617				
44	1	.623617	-4.207982	4.207982				
45	1	2.415747	-4.207200	2.415747				
46	1	-.623617	4.207982	4.207982				
47	1	-2.415747	4.207200	2.415747				
48	1	-2.415747	4.207200	2.415747				
49	$C_{16}H_{21}F_3$ RB3PW91\6-31G(d,p) E=-921.649850				$C_{16}H_{24}$ RB3PW91\6-31G(d,p) E=-624.03403			
50	H	2.149454	-1.240988	0.814014	H	0.000000	2.481770	0.091848
51	H	0.000000	2.481976	0.814014	H	-2.149276	-1.240885	0.091848
52	H	-2.149454	-1.240988	0.814014	H	2.149276	1.240885	-0.091848
53	H	2.153935	0.225381	2.905335	H	0.000000	-2.481770	-0.091848
54	H	1.272153	1.752672	2.905335	H	2.149276	-1.240885	0.091848
55	H	-1.272153	1.752672	2.905335	H	-2.149276	1.240885	-0.091848
56	H	0.881782	-1.978053	2.905335	H	-1.271452	1.752638	2.180685
57	H	-0.881782	-1.978053	2.905335	H	-2.153555	0.224791	2.180685
58	H	-2.153935	0.225381	2.905335	H	2.153555	-0.224791	-2.180685
59	C	1.254182	-0.724102	-1.077510	H	1.271452	-1.752638	-2.180685
60	C	0.000000	1.448204	-1.077510	H	-0.882103	-1.977429	2.180685
	C	-1.254182	-0.724102	-1.077510	H	1.271452	1.752638	2.180685
	C	0.000000	0.000000	-1.602543	H	-1.271452	-1.752638	-2.180685
	C	0.000000	1.443151	0.454782	H	0.882103	1.977429	-2.180685
	C	1.249806	-0.721576	0.454782	H	2.153555	0.224791	2.180685
	C	-1.249806	-0.721576	0.454782	H	0.882103	-1.977429	2.180685
	H	2.154829	-0.224990	-1.454461	H	-0.882103	1.977429	-2.180685
	H	0.882567	1.978632	-1.454461	H	-2.153555	-0.224791	-2.180685
	H	-0.882567	1.978632	-1.454461	C	0.000000	1.440266	-1.804043
	H	1.272262	-1.753641	-1.454461	C	-1.247307	-0.720133	-1.804043
	H	-1.272262	-1.753641	-1.454461	C	1.247307	0.720133	1.804043

1						
2						
3						
4						
5						
6						
7						
8						
9						
10						
11						
12						
13						
14						
15						
16						
17						
18						
19						
20						
21						
22						
23						
24						
25						
26						
27						
28						
29						
30						
31						
32						
33						
34						
35						
36						
37						
38						
39						
40						
41						
42						
43						
44						
45						
46						
47						
48						
49						
50						
51						
52						
53						
54						
55						
56						
57						
58						
59						
60						
	H -2.154829	-0.224990	-1.454461	C 0.000000	-1.440266	1.804043
	C 1.247483	0.720235	2.529114	C 1.247307	-0.720133	-1.804043
	C -1.247483	0.720235	2.529114	C -1.247307	0.720133	1.804043
	C 0.000000	-1.440469	2.529114	C 0.000000	0.000000	-2.349217
	C 0.000000	-1.444457	0.996826	C 0.000000	0.000000	2.349217
	C -1.250936	0.722228	0.996826	C -1.250248	-0.721831	-0.271490
	C 1.250936	0.722228	0.996826	C 0.000000	1.443662	-0.271490
	H 0.000000	-2.482016	0.632815	C 0.000000	-1.443662	0.271490
	H -2.149489	1.241008	0.632815	C 1.250248	0.721831	0.271490
	H 2.149489	1.241008	0.632815	C 1.250248	-0.721831	-0.271490
	C 0.000000	0.000000	3.074306	C -1.250248	0.721831	0.271490
	C 0.000000	0.000000	4.601354	C 0.000000	0.000000	-3.875821
	C 0.000000	0.000000	-3.122939	C 0.000000	0.000000	3.875821
	H -0.885595	-0.511299	4.996524	H 0.885591	-0.511296	4.271424
	H 0.885595	-0.511299	4.996524	H -0.885591	0.511296	-4.271424
	H 0.000000	1.022597	4.996524	H 0.000000	1.022592	4.271424
	F -1.084595	0.626191	-3.629415	H -0.885591	-0.511296	4.271424
	F 0.000000	-1.252383	-3.629415	H 0.885591	0.511296	-4.271424
	F 1.084595	0.626191	-3.629415	H 0.000000	-1.022592	-4.271424
	C ₁₅ H ₂₁ FRB3PW91\6-31G(d,p) E=- 683.93162			C ₁₅ H ₂₂ RB3PW91\6-31G(d,p) E=- 584.72880		
	H -1.242314	2.151030	0.165870	H -2.150308	1.241481	-0.195893
	H -1.242314	-2.151030	0.165870	H 0.000000	-2.482961	-0.195893
	H 2.483529	0.000000	0.167804	H 2.150308	1.241481	-0.195893
	H -1.978252	0.881502	2.256507	H -2.153575	-0.224802	1.887468
	H -1.978252	-0.881502	2.256507	H -1.271472	-1.752650	1.887468
	H 1.752282	1.272520	2.256677	H 0.882103	1.977452	1.887468
	H 1.752282	-1.272520	2.256677	H 2.153575	-0.224802	1.887468
	H 0.224483	-2.153549	2.256631	H 1.271472	-1.752650	1.887468
	H 0.224483	2.153549	2.256631	H -0.882103	1.977452	1.887468
	C -0.721291	1.248854	-1.729725	C -1.251790	0.722721	-2.097640
	C -0.721291	-1.248854	-1.729725	C 0.000000	-1.445443	-2.097640
	C 1.442453	0.000000	-1.727865	C 1.251790	0.722721	-2.097640
	C 0.000398	0.000000	-2.224563	C 0.000000	0.000000	-2.615511
	C -0.723574	-1.251922	-0.194641	C 0.000000	-1.446412	-0.563692
	C -0.723574	1.251922	-0.194641	C -1.252630	0.723206	-0.563692
	C 1.445620	0.000000	-0.193064	C 1.252630	0.723206	-0.563692
	H -1.746469	1.256121	-2.120261	H -2.157138	0.226370	-2.472692
	H -1.746469	-1.256121	-2.120261	H -0.882527	-1.981322	-2.472692
	H 1.961733	0.884077	-2.118243	H 1.274612	1.754951	-2.472692
	H 1.961733	-0.884077	-2.118243	H 2.157138	0.226370	-2.472692
	H -0.214707	-2.140679	-2.119012	H 0.882527	-1.981322	-2.472692
	H -0.214707	2.140679	-2.119012	H -1.274612	1.754951	-2.472692
	C -1.440443	0.000000	1.879823	C -1.247306	-0.720132	1.510734
	C 0.719876	1.247434	1.880401	C 0.000000	1.440264	1.510734
	C 0.719876	-1.247434	1.880401	C 1.247306	-0.720132	1.510734
	C 0.721892	1.251126	0.347644	C 0.000000	1.444134	-0.022180
	C 0.721892	-1.251126	0.347644	C 1.250656	-0.722067	-0.022180
	C -1.445514	0.000000	0.346826	C -1.250656	-0.722067	-0.022180
	F 0.001385	0.000000	-3.624892	H 0.000000	2.482677	-0.384489
	H 1.240572	2.150138	-0.015006	H 2.150062	-1.241339	-0.384489
	H 1.240572	-2.150138	-0.015006	H -2.150062	-1.241339	-0.384489
	H -2.483753	0.000000	-0.014898	C 0.000000	0.000000	2.055824
	C -0.000046	0.000000	2.425316	C 0.000000	0.000000	3.583065
	C 0.001496	0.000000	3.952199	H 0.885655	0.511333	3.978387
	H 1.024867	0.000000	4.345629	H 0.000000	-1.022666	3.978387
	H -0.509225	-0.885682	4.348036	H -0.885655	0.511333	3.978387
	H -0.509225	0.885682	4.348036	H 0.000000	0.000000	-3.712908
	C ₁₄ H ₁₈ F ₂ RB3PW91\6-31G(d,p) E=-743.82873			C ₁₄ H ₂₀ RB3PW91\6-31G(d,p) E=-545.42352		
	H 0.000000	2.484639	0.090363	H 0.000000	2.483635	0.096658
	H 2.151760	-1.242319	0.090363	H -1.274501	1.754770	2.179600
	H -2.151760	1.242319	-0.090363	C 0.000000	1.445319	-1.804141
	H 0.000000	-2.484639	-0.090363	C -1.251683	-0.722660	-1.804141
	H -2.151760	-1.242319	0.090363	C 0.000000	0.000000	-2.321989
	H 2.151760	1.242319	-0.090363	C -1.252901	-0.723363	-0.270235
	H -1.256631	1.746057	2.195545	C 0.000000	1.446725	-0.270235
	H 0.883814	-1.961302	2.195545	H -0.882425	1.981135	-2.179600
	H -0.883814	1.961302	-2.195545	H -2.156926	-0.226365	-2.179600
	H 1.256631	-1.746057	-2.195545	C -1.251683	0.722660	1.804141

H	2.140445	0.215245	2.195545	H	1.274501	1.754770	2.179600
H	1.256631	1.746057	2.195545	C	1.252901	0.723363	0.270235
H	-1.256631	-1.746057	-2.195545	C	-1.252901	0.723363	0.270235
H	-2.140445	-0.215245	-2.195545	H	0.882425	1.981135	-2.179600
H	-0.883814	-1.961302	2.195545	H	-1.274501	-1.754770	-2.179600
H	-2.140445	0.215245	2.195545	H	0.000000	0.000000	-3.419716
H	2.140445	-0.215245	-2.195545	H	-2.150891	-1.241818	0.096658
H	0.883814	1.961302	-2.195545	H	2.150891	1.241818	-0.096658
C	0.000000	1.442048	-1.805315	C	0.000000	-1.446725	0.270235
C	1.248850	-0.721024	-1.805315	C	0.000000	0.000000	2.321989
C	-1.248850	0.721024	1.805315	C	0.000000	-1.445319	1.804141
C	0.000000	-1.442048	1.805315	C	1.251683	0.722660	1.804141
C	-1.248850	-0.721024	-1.805315	H	-0.882425	-1.981135	2.179600
C	1.248850	0.721024	1.805315	H	-2.156926	0.226365	2.179600
C	0.000000	0.000000	-2.301025	H	2.156926	-0.226365	-2.179600
C	0.000000	0.000000	2.301025	H	0.882425	-1.981135	2.179600
C	-1.253060	-0.723454	-0.270212	H	2.156926	0.226365	2.179600
C	1.253060	0.723454	0.270212	C	1.252901	-0.723363	-0.270235
C	0.000000	1.446909	-0.270212	H	0.000000	-2.483635	-0.096658
C	1.253060	-0.723454	-0.270212	H	0.000000	0.000000	3.419716
C	-1.253060	0.723454	0.270212	C	1.251683	-0.722660	-1.804141
C	0.000000	-1.446909	0.270212	H	2.150891	-1.241818	0.096658
F	0.000000	0.000000	-3.699950	H	1.274501	-1.754770	-2.179600
F	0.000000	0.000000	3.699950	H	-2.150891	1.241818	-0.096658
$C_{16}H_{18}N_2$ RB3PW91\6-31G(d,p) E=-729.82155				$C_{16}H_{21}N$ RB3PW91\6-31G(d,p) E=-676.92868			
H	0.000000	2.483432	0.089915	H	2.150001	1.241304	-0.261075
H	-2.150715	-1.241716	0.089915	H	-2.150001	1.241304	-0.261075
H	2.150715	1.241716	-0.089915	H	0.000000	-2.482607	-0.261075
H	0.000000	-2.483432	-0.089915	H	2.153797	-0.225447	-2.351197
H	2.150715	-1.241716	0.089915	H	-2.153797	-0.225447	-2.351197
H	-2.150715	1.241716	-0.089915	H	-0.881656	1.977966	-2.351197
H	-1.276377	1.755416	2.181664	H	0.881656	1.977966	-2.351197
H	-2.158423	0.227667	2.181664	H	-1.272141	-1.752519	-2.351197
H	2.158423	-0.227667	-2.181664	H	1.272141	-1.752519	-2.351197
H	1.276377	-1.755416	-2.181664	C	1.259398	0.727114	1.630285
H	2.158423	0.227667	2.181664	C	-1.259398	0.727114	1.630285
H	0.882047	-1.983083	2.181664	C	0.000000	-1.454228	1.630285
H	-0.882047	1.983083	-2.181664	C	0.000000	0.000000	2.158086
H	-2.158423	-0.227667	-2.181664	C	0.000000	-1.443890	0.098364
H	-0.882047	-1.983083	2.181664	C	1.250445	0.721945	0.098364
H	1.276377	1.755416	2.181664	C	-1.250445	0.721945	0.098364
H	-1.276377	-1.755416	-2.181664	H	2.158279	0.227206	2.010926
H	0.882047	1.983083	-2.181664	H	-2.158279	0.227206	2.010926
C	0.000000	1.453879	-1.801961	H	-1.275906	1.755522	2.010926
C	-1.259096	-0.726940	-1.801961	H	1.275906	1.755522	2.010926
C	1.259096	0.726940	1.801961	H	-0.882373	-1.982728	2.010926
C	0.000000	-1.453879	1.801961	H	0.882373	-1.982728	2.010926
C	1.259096	-0.726940	-1.801961	C	1.247450	-0.720215	-1.974964
C	-1.259096	0.726940	1.801961	C	-1.247450	-0.720215	-1.974964
C	0.000000	0.000000	-2.329200	C	0.000000	1.440431	-1.974964
C	0.000000	0.000000	2.329200	C	0.000000	1.445009	-0.442656
C	-1.251576	-0.722598	-0.269798	C	-1.251415	-0.722505	-0.442656
C	0.000000	1.445196	-0.269798	C	1.251415	-0.722505	-0.442656
C	0.000000	-1.445196	0.269798	C	0.000000	0.000000	3.623979
C	1.251576	0.722598	0.269798	H	0.000000	2.482814	-0.079464
C	1.251576	-0.722598	-0.269798	H	-2.150180	-1.241407	-0.079464
C	-1.251576	0.722598	0.269798	H	2.150180	-1.241407	-0.079464
C	0.000000	0.000000	-3.795294	C	0.000000	0.000000	-2.520024
C	0.000000	0.000000	3.795294	C	0.000000	0.000000	-4.047106
N	0.000000	0.000000	-4.957115	N	0.000000	0.000000	4.785947
N	0.000000	0.000000	4.957115	H	-0.885557	0.511277	-4.442180
				H	0.885557	0.511277	-4.442180
				H	0.000000	-1.022553	-4.442180
$C_{28}H_{38}$ RB3PW91\6-31G(d,p) E=-1089.63243				$C_{14}H_{20}O_2$ RB3PW91\6-31G(d,p) E=-695.80434			
H	-2.147348	-1.239772	3.255188	H	1.241037	0.098085	2.150849
H	0.000000	2.479544	3.255188	H	1.241037	0.098085	-2.150849
H	0.000000	-2.479544	-3.255188	H	-1.241037	-0.098085	2.150849
				H	-1.241037	-0.098085	-2.150849

1								
2								
3								
4	H	2.147348	1.239772	-3.255188	H -2.483587	0.078600	0.000000	
5	H	2.147348	-1.239772	3.255188	H	2.483587	-0.078600	0.000000
6	H	-2.147348	1.239772	-3.255188	H	1.955355	2.204101	0.882237
7	H	-2.148711	1.240559	3.076971	H	1.955355	2.204101	-0.882237
8	H	2.148711	-1.240559	-3.076971	H	-1.955355	-2.204101	0.882237
9	H	0.000000	-2.481118	3.076971	H	-1.955355	-2.204101	-0.882237
10	H	2.148711	1.240559	3.076971	H	-1.757994	2.177447	-1.263958
11	H	-2.148711	-1.240559	-3.076971	H	-1.757994	2.177447	1.263958
12	H	0.000000	2.481118	-3.076971	H	1.757994	-2.177447	-1.263958
13	H	-0.882299	-1.981536	5.354864	H	1.757994	-2.177447	1.263958
14	H	1.274911	1.754861	5.354864	H	-0.223768	2.193274	2.142639
15	H	-1.274911	-1.754861	-5.354864	H	-0.223768	2.193274	-2.142639
16	H	0.882299	1.981536	-5.354864	H	0.223768	-2.193274	2.142639
17	H	2.157210	0.226674	5.354864	H	0.223768	-2.193274	-2.142639
18	H	0.882299	-1.981536	5.354864	C	0.724272	-1.800848	1.248660
19	H	-0.882299	1.981536	-5.354864	C	0.724272	-1.800848	-1.248660
20	H	-2.157210	-0.226674	-5.354864	C	-0.724272	1.800848	1.248660
21	H	-1.274911	1.754861	5.354864	C	-0.724272	1.800848	-1.248660
22	H	-2.157210	0.226674	5.354864	C	-1.435091	-1.811026	0.000000
23	H	2.157210	-0.226674	-5.354864	C	1.435091	1.811026	0.000000
24	H	1.274911	-1.754861	-5.354864	C	0.004366	-2.326763	0.000000
25	H	-0.880664	1.988156	1.015697	C	-0.004366	2.326763	0.000000
26	H	-2.162126	-0.231401	1.015697	C	0.724272	-0.267153	-1.252243
27	H	2.162126	0.231401	-1.015697	C	0.724272	-0.267153	1.252243
28	H	0.880664	-1.988156	-1.015697	C	-0.724272	0.267153	-1.252243
29	H	-1.281462	-1.756755	1.015697	C	-0.724272	0.267153	1.252243
30	H	0.880664	1.988156	1.015697	C	-1.443772	-0.277971	0.000000
31	H	-0.880664	-1.988156	-1.015697	C	1.443772	0.277971	0.000000
32	H	1.281462	1.756755	-1.015697	O	0.070055	-3.747121	0.000000
33	H	2.162126	-0.231401	1.015697	O	0.070055	3.747121	0.000000
34	H	1.281462	-1.756755	1.015697	H	0.835435	-4.081550	0.000000
35	H	-1.281462	1.756755	-1.015697	H	-0.835435	4.081550	0.000000
36	H	-2.162126	0.231401	-1.015697				
37	C	-1.244697	-0.718626	1.367725				
38	C	0.000000	1.437252	1.367725				
39	C	0.000000	-1.437252	-1.367725				
40	C	1.244697	0.718626	-1.367725				
41	C	1.244697	-0.718626	1.367725				
42	C	-1.244697	0.718626	-1.367725				
43	C	-1.251606	0.722615	4.979736				
44	C	1.251606	-0.722615	-4.979736				
45	C	0.000000	-1.445230	4.979736				
46	C	1.251606	0.722615	4.979736				
47	C	-1.251606	-0.722615	-4.979736				
48	C	0.000000	1.445230	-4.979736				
49	C	0.000000	0.000000	0.792245				
50	C	0.000000	0.000000	-0.792245				
51	C	0.000000	0.000000	5.498840				
52	C	0.000000	0.000000	-5.498840				
53	C	1.245019	-0.718812	2.901896				
54	C	-1.245019	0.718812	-2.901896				
55	C	0.000000	1.437624	2.901896				
56	C	-1.245019	-0.718812	2.901896				
57	C	1.245019	0.718812	-2.901896				
58	C	0.000000	-1.437624	-2.901896				
59	C	1.251461	0.722531	3.446362				
60	C	0.000000	-1.445063	3.446362				
	C	0.000000	1.445063	-3.446362				
	C	-1.251461	-0.722531	-3.446362				
	C	-1.251461	0.722531	3.446362				
	C	1.251461	-0.722531	-3.446362				
	H	0.000000	0.000000	6.596482				
	H	0.000000	0.000000	-6.596482				
	C ₁₅ H ₂₃ N RB3PW91\6-31G(d,p) E=-640.06121				C ₁₄ H ₂₂ N ₂ RB3PW91\6-31G(d,p) E=-656.08833			
	H	-1.240438	0.081528	2.149243	H	1.241338	-0.087302	2.149308
	H	-1.240438	0.081528	-2.149243	H	1.241338	-0.087302	-2.149308
	H	2.483748	0.083248	0.000000	H	-1.241338	0.087302	2.149308
	H	0.225087	2.170932	2.153334	H	-1.241338	0.087302	-2.149308
	H	0.225087	2.170932	-2.153334	H	-2.482986	-0.099593	0.000000

1	H	-1.976166	2.172104	-0.881696	H	2.482986	0.099593	0.000000
2	H	-1.976166	2.172104	0.881696	H	-0.221229	-2.184567	2.149731
3	H	1.753647	2.171231	-1.272721	H	-0.221229	-2.184567	-2.149731
4	H	1.753647	2.171231	1.272721	H	0.221229	2.184567	2.149731
5	C	-0.726684	-1.813667	1.245881	H	0.221229	2.184567	-2.149731
6	C	-0.726684	-1.813667	-1.245881	H	1.974269	-2.179361	-0.883118
7	C	1.435482	-1.812105	0.000000	H	1.974269	-2.179361	0.883118
8	C	-0.009070	-2.352841	0.000000	H	-1.974269	2.179361	-0.883118
9	C	1.445341	-0.279153	0.000000	H	-1.974269	2.179361	0.883118
10	C	-0.721851	-0.281293	1.250057	H	-1.746441	-2.197539	-1.260546
11	C	-0.721851	-0.281293	-1.250057	H	-1.746441	-2.197539	1.260546
12	H	-0.227764	-2.193429	2.149800	H	1.746441	2.197539	-1.260546
13	H	-0.227764	-2.193429	-2.149800	H	1.746441	2.197539	1.260546
14	H	-1.752877	-2.201254	-1.260017	C	0.721629	1.806404	1.246091
15	H	-1.752877	-2.201254	1.260017	C	0.721629	1.806404	-1.246091
16	H	1.968164	-2.194305	-0.883216	C	-0.721629	-1.806404	1.246091
17	H	1.968164	-2.194305	0.883216	C	-0.721629	-1.806404	-1.246091
18	C	0.721178	1.794639	1.247448	C	-1.440104	1.799073	0.000000
19	C	0.721178	1.794639	-1.247448	C	-1.440104	-1.799073	0.000000
20	C	-1.438638	1.795003	0.000000	C	0.002505	2.343240	0.000000
21	C	-1.443555	0.262399	0.000000	C	-0.002505	-2.343240	0.000000
22	C	0.722492	0.262003	-1.250326	C	-1.446112	0.265859	0.000000
23	C	0.722492	0.262003	1.250326	C	1.446112	-0.265859	0.000000
24	N	-0.099211	-3.812754	0.000000	C	0.721629	0.273965	1.250189
25	H	-2.481624	-0.099884	0.000000	C	0.721629	0.273965	-1.250189
26	H	1.241399	-0.101028	-2.149599	C	-0.721629	-0.273965	1.250189
27	H	1.241399	-0.101028	2.149599	C	-0.721629	-0.273965	-1.250189
28	C	0.001692	2.340272	0.000000	N	0.089308	3.803773	0.000000
29	C	0.003698	3.867317	0.000000	N	-0.089308	-3.803773	0.000000
30	H	-0.507075	4.263342	-0.885591	H	-0.404829	4.168714	-0.812295
31	H	-0.507075	4.263342	0.885591	H	-0.404829	4.168714	0.812295
32	H	1.027016	4.260941	0.000000	H	0.404829	-4.168714	-0.812295
33	H	0.393034	-4.179396	-0.812501	H	0.404829	-4.168714	0.812295
34	H	0.393034	-4.179396	0.812501				
35	C ₁₆ H ₂₁ F RB3PW91\6-31G(d,p) E=-721.98753				C ₁₄ H ₂₂ N(1+) RB3PW91\6-31G(d,p) E=-601.14291			
36	H	1.290962	0.258032	2.151206	H	-2.152684	-1.242853	-0.396011
37	H	1.290962	0.258032	-2.151206	H	2.152684	-1.242853	-0.396011
38	H	-2.425250	-0.002638	0.000000	H	0.000000	2.485706	-0.396011
39	H	-0.025935	-1.931037	2.155121	H	-2.158710	0.229945	-2.491104
40	H	-0.025935	-1.931037	-2.155121	H	2.158710	0.229945	-2.491104
41	H	2.171352	-1.773649	-0.881803	H	1.278493	1.754525	-2.491104
42	H	2.171352	-1.773649	0.881803	H	-1.278493	1.754525	-2.491104
43	H	-1.547965	-2.036978	-1.277551	H	0.880217	-1.984470	-2.491104
44	H	-1.547965	-2.036978	1.277551	H	-0.880217	-1.984470	-2.491104
45	C	0.638113	2.112829	1.248864	C	-1.256946	-0.725698	1.488564
46	C	0.638113	2.112829	-1.248864	C	1.256946	-0.725698	1.488564
47	C	-1.519271	1.961552	0.000000	C	0.000000	1.451396	1.488564
48	C	-0.115720	2.565596	0.000000	C	0.000000	0.000000	1.966016
49	C	-1.415048	0.430115	0.000000	C	0.000000	1.445203	-0.049430
50	C	0.748435	0.582117	1.252238	C	1.251583	-0.722602	-0.049430
51	C	0.748435	0.582117	-1.252238	C	-1.251583	-0.722602	-0.049430
52	H	0.104916	2.466445	2.140134	H	-2.158072	-0.220436	1.863423
53	H	0.104916	2.466445	-2.140134	H	2.158072	-0.220436	1.863423
54	H	1.632433	2.576358	-1.257134	H	0.888133	1.979163	1.863423
55	H	1.632433	2.576358	1.257134	H	-0.888133	1.979163	1.863423
56	H	-2.064400	2.314880	-0.884056	H	1.269939	-1.758727	1.863423
57	H	-2.064400	2.314880	0.884056	H	-1.269939	-1.758727	1.863423
58	C	-0.546879	-1.588287	1.251392	C	-1.252301	0.723016	-2.118976
59	C	-0.546879	-1.588287	-1.251392	C	1.252301	0.723016	-2.118976
60	C	1.609405	-1.435428	0.000000	C	0.000000	-1.446033	-2.118976
	C	1.505967	0.092413	0.000000	C	0.000000	-1.450653	-0.584880
	C	-0.655150	-0.059470	-1.250732	C	-1.256303	0.725327	-0.584880
	C	-0.655150	-0.059470	1.250732	C	1.256303	0.725327	-0.584880
	H	2.516584	0.525329	0.000000	N	0.000000	0.000000	3.502570
	H	-1.197829	0.265429	-2.150085	H	0.000000	-2.487762	-0.220237
	H	-1.197829	0.265429	2.150085	H	-2.154465	1.243881	-0.220237
	C	0.211671	-2.084672	0.000000	H	2.154465	1.243881	-0.220237
	C	0.341354	-3.595492	0.000000	C	0.000000	0.000000	-2.634888
	C	-0.665391	-4.469149	0.000000	H	0.828818	0.478518	3.868497
	F	-0.213264	3.953187	0.000000	H	-0.828818	0.478518	3.868497

H	1.360784	-3.984962	0.000000	H	0.000000	-0.957036	3.868497
H	-1.707607	-4.157210	0.000000	H	0.000000	0.000000	-3.730415
H	-0.484230	-5.540047	0.000000				
C ₁₅ H ₂₁ NO ₂ RB3PW91\6-31G(d,p) E=-789.25454				C ₂₁ H ₂₃ N RB3PW91\6-31G(d,p) E=-868.58858			
H	-1.241501	-0.392463	2.149315	H	1.281485	-0.955185	2.149455
H	-1.241501	-0.392463	-2.149315	H	1.281485	-0.955185	-2.149455
H	2.482762	-0.395126	0.000000	H	-2.441423	-0.952611	0.000000
H	0.228873	1.689972	2.158126	H	2.014401	1.129047	0.882561
H	0.228873	1.689972	-2.158126	H	2.014401	1.129047	-0.882561
H	-1.986531	1.697878	-0.879370	H	-1.713771	1.125133	1.291743
H	-1.986531	1.697878	0.879370	H	-1.713771	1.125133	-1.291743
H	1.750773	1.703457	-1.262401	H	-0.180921	1.135917	-2.155461
H	1.750773	1.703457	1.262401	H	-0.180921	1.135917	2.155461
C	-0.730396	-2.288625	1.245845	C	0.768485	-2.847024	1.258270
C	-0.730396	-2.288625	-1.245845	C	0.768485	-2.847024	-1.258270
C	1.431972	-2.289748	0.000000	C	-1.413843	-2.844847	0.000000
C	-0.013326	-2.828873	0.000000	C	0.039803	-3.374343	0.000000
C	1.444679	-0.756934	0.000000	C	0.761933	-1.315026	-1.250346
C	-0.723700	-0.756392	1.250287	C	0.761933	-1.315026	1.250346
C	-0.723700	-0.756392	-1.250287	C	-1.402982	-1.312807	0.000000
H	-0.232276	-2.668689	2.149905	H	1.797200	-3.226888	1.272808
H	-0.232276	-2.668689	-2.149905	H	1.797200	-3.226888	-1.272808
H	-1.757133	-2.674446	-1.260097	H	-1.942832	-3.225270	0.882199
H	-1.757133	-2.674446	1.260097	H	-1.942832	-3.225270	-0.882199
H	1.964495	-2.672104	-0.883066	H	0.270226	-3.227408	-2.158108
H	1.964495	-2.672104	0.883066	H	0.270226	-3.227408	2.158108
C	0.725889	1.315787	1.253022	C	1.472633	0.763732	0.000000
C	0.725889	1.315787	-1.253022	C	-0.680807	0.758601	1.253788
C	-1.449891	1.322001	0.000000	C	-0.680807	0.758601	-1.253788
C	-1.444233	-0.211765	0.000000	C	-0.680807	-0.773427	1.251079
C	0.721431	-0.215591	-1.249567	C	-0.680807	-0.773427	-1.251079
C	0.721431	-0.215591	1.249567	C	1.478765	-0.769506	0.000000
N	-0.105816	-4.288031	0.000000	C	0.038719	-4.840173	0.000000
H	-2.482471	-0.572257	0.000000	H	-1.200344	-1.135058	2.150116
H	1.240817	-0.575423	-2.149466	H	-1.200344	-1.135058	-2.150116
H	1.240817	-0.575423	2.149466	H	2.520154	-1.121946	0.000000
C	-0.006305	1.849269	0.000000	C	0.034245	1.317153	0.000000
C	0.105192	3.363259	0.000000	C	-0.017488	2.844771	0.000000
O	1.155772	3.968868	0.000000	C	1.131916	3.643455	0.000000
H	0.384751	-4.656574	-0.812523	C	1.047698	5.036339	0.000000
H	0.384751	-4.656574	0.812523	C	-0.191965	5.667131	0.000000
O	-1.083818	4.004199	0.000000	C	-1.258739	3.500794	0.000000
H	-0.866956	4.950444	0.000000	C	-1.348728	4.888955	0.000000
				H	2.115038	3.184850	0.000000
				H	1.959915	5.627061	0.000000
				H	-0.258626	6.751399	0.000000
				H	-2.177433	2.919825	0.000000
				H	-2.326111	5.364175	0.000000
				N	0.038819	-6.002105	0.000000

C ₂₀ H ₂₃ F RB3PW91\6-31G(d,p) E=-875.59164				C ₁₄ H ₁₈ N ₂ O ₄ RB3PW91\6-31G(d,p) E=-954.27746			
H	1.284871	-1.140510	2.150633	H	-1.243044	0.083403	2.150980
H	1.284871	-1.140510	-2.150633	H	-1.243044	0.083403	-2.150980
H	-2.439987	-1.139361	0.000000	H	1.243044	-0.083403	2.150980
H	2.015274	0.944406	0.882592	H	1.243044	-0.083403	-2.150980
H	2.015274	0.944406	-0.882592	H	2.482983	0.091360	0.000000
H	-1.711852	0.938177	1.292965	H	-2.482983	-0.091360	0.000000
H	-1.711852	0.938177	-1.292965	H	0.218014	2.184418	2.151768
H	-0.178168	0.949285	-2.155075	H	0.218014	2.184418	-2.151768
H	-0.178168	0.949285	2.155075	H	-0.218014	-2.184418	2.151768
C	0.765847	-3.036772	1.248021	H	-0.218014	-2.184418	-2.151768
C	0.765847	-3.036772	-1.248021	H	-1.983480	2.185269	-0.879393
C	-1.398459	-3.035235	0.000000	H	-1.983480	2.185269	0.879393
C	0.043573	-3.532210	0.000000	H	1.983480	-2.185269	-0.879393
C	0.765847	-1.502189	-1.252125	H	1.983480	-2.185269	0.879393
C	0.765847	-1.502189	1.252125	H	1.743858	2.197044	-1.255380
C	-1.402117	-1.500841	0.000000	H	1.743858	2.197044	1.255380
H	1.791124	-3.427002	1.254063	H	-1.743858	-2.197044	-1.255380
H	1.791124	-3.427002	-1.254063	H	-1.743858	-2.197044	1.255380
H	-1.917497	-3.426317	0.883879	C	-0.722079	-1.804804	1.254201
H	-1.917497	-3.426317	-0.883879	C	-0.722079	-1.804804	-1.254201
H	0.260780	-3.427158	-2.140166	C	0.722079	1.804804	1.254201
H	0.260780	-3.427158	2.140166	C	0.722079	1.804804	-1.254201
C	1.474003	0.578198	0.000000	C	1.454746	-1.802940	0.000000
C	-0.678941	0.571466	1.253994	C	-1.454746	1.802940	0.000000
C	-0.678941	0.571466	-1.253994	C	0.011679	-2.299169	0.000000
C	-0.678089	-0.960652	1.250951	C	-0.011679	2.299169	0.000000
C	-0.678089	-0.960652	-1.250951	C	1.445271	-0.267614	0.000000
C	1.481098	-0.955383	0.000000	C	-1.445271	0.267614	0.000000
F	0.042384	-4.931955	0.000000	C	-0.722079	-0.271713	1.251535
H	-1.197597	-1.322092	2.150008	C	-0.722079	-0.271713	-1.251535
H	-1.197597	-1.322092	-2.150008	C	0.722079	0.271713	1.251535
H	2.522855	-1.306530	0.000000	C	0.722079	0.271713	-1.251535
C	0.035166	1.130553	0.000000	N	-0.035830	-3.820932	0.000000
C	-0.018679	2.657956	0.000000	N	0.035830	3.820932	0.000000
C	1.129334	3.458663	0.000000	O	-1.147014	-4.334005	0.000000
C	1.043069	4.851479	0.000000	O	1.147014	4.334005	0.000000
C	-0.197474	5.480554	0.000000	O	1.019548	-4.437089	0.000000
C	-1.260847	3.312491	0.000000	O	-1.019548	4.437089	0.000000
C	-1.353020	4.700483	0.000000				
H	2.112942	3.001071	0.000000				
H	1.954439	5.443606	0.000000				
H	-0.265761	6.564767	0.000000				
H	-2.178441	2.729829	0.000000				
H	-2.331208	5.174169	0.000000				
C ₁₅ H ₂₁ NO ₂ RB3PW91\6-31G(d,p) E=-789.15688				C ₁₄ H ₁₉ NO ₂ RB3PW91\6-31G(d,p) E=-749.85162			
H	-0.936328	-0.964342	2.150234	H	-1.206235	-0.864128	2.150680
H	-0.936328	-0.964342	-2.150234	H	-1.206235	-0.864128	-2.150680
H	0.372628	2.521632	0.000000	H	0.098986	2.624082	0.000000
H	-2.382876	1.144211	2.153441	H	-2.653491	1.244997	2.157262
H	-2.382876	1.144211	-2.153441	H	-2.653491	1.244997	-2.157262
H	-3.156770	-0.917372	-0.881414	H	-3.427024	-0.823851	-0.881599
H	-3.156770	-0.917372	0.881414	H	-3.427024	-0.823851	0.881599
H	-1.846855	2.574407	-1.272640	H	-2.118912	2.675769	-1.275664
H	-1.846855	2.574407	1.272640	H	-2.118912	2.675769	1.275664
C	1.014406	-1.143363	1.254028	C	0.744442	-1.040539	1.254028
C	1.014406	-1.143363	-1.254028	C	0.744442	-1.040539	-1.254028
C	1.781680	0.892168	0.000000	C	1.509371	0.995931	0.000000
C	1.737099	-0.632535	0.000000	C	1.466132	-0.528714	0.000000
C	0.340520	1.423460	0.000000	C	0.067668	1.525891	0.000000
C	-0.421082	-0.601885	1.249951	C	-0.691780	-0.500844	1.250269
C	-0.421082	-0.601885	-1.249951	C	-0.691780	-0.500844	-1.250269
H	1.547824	-0.804239	2.151195	H	1.277458	-0.700988	2.151313
H	1.547824	-0.804239	-2.151195	H	1.277458	-0.700988	-2.151313
H	1.022251	-2.238006	-1.255606	H	0.753465	-2.135229	-1.255658
H	1.022251	-2.238006	1.255606	H	0.753465	-2.135229	1.255658
H	2.326073	1.251105	-0.879933	H	2.053393	1.355536	-0.879947
H	2.326073	1.251105	0.879933	H	2.053393	1.355536	0.879947
C	-1.857582	1.475889	1.246877	C	-2.129446	1.578015	1.251436

C	-1.857582	1.475889	-1.246877	C	-2.129446	1.578015	-1.251436
C	-2.615821	-0.545540	0.000000	C	-2.888319	-0.451585	0.000000
C	-1.182277	-1.088936	0.000000	C	-1.452105	-0.991283	0.000000
C	-0.421082	0.939881	-1.250829	C	-0.691780	1.041860	-1.253124
C	-0.421082	0.939881	1.250829	C	-0.691780	1.041860	1.253124
H	-1.207913	-2.187809	0.000000	H	-1.471575	-2.090310	0.000000
H	0.100737	1.298221	-2.149647	H	-0.166250	1.398319	-2.150538
H	0.100737	1.298221	2.149647	H	-0.166250	1.398319	2.150538
C	-2.621414	0.993784	0.000000	C	-2.868180	1.083189	0.000000
C	-4.052164	1.527700	0.000000	N	2.875102	-1.106654	0.000000
N	3.144715	-1.212259	0.000000	O	2.968681	-2.327495	0.000000
O	3.236474	-2.433309	0.000000	O	3.823017	-0.334687	0.000000
O	4.093707	-0.441649	0.000000	H	-3.896140	1.466934	0.000000
H	-4.601449	1.186515	-0.885263				
H	-4.601449	1.186515	0.885263				
H	-4.066040	2.623790	0.000000				
C ₁₅ H ₂₁ NO ₂ (betaine form) RB3PW91\6-31G(d,p) E=-789.14845				C ₁₀ H ₁₆ RB3PW91\6-31G(d,p) E=-390.61847			
H	0.124565	1.289515	2.150182	C	0.889016	0.889016	0.889016
H	0.124565	1.289515	-2.150182	C	-0.889016	-0.889016	0.889016
H	-1.167420	-2.202941	0.000000	C	-0.889016	0.889016	-0.889016
H	1.577646	-0.803358	2.149222	C	0.889016	-0.889016	-0.889016
H	1.577646	-0.803358	-2.149222	C	0.000000	0.000000	1.774011
H	2.363495	1.253789	-0.873140	C	0.000000	1.774011	0.000000
H	2.363495	1.253789	0.873140	C	1.774011	0.000000	0.000000
H	1.092890	-2.233816	-1.241298	C	-1.774011	0.000000	0.000000
H	1.092890	-2.233816	1.241298	C	0.000000	-1.774011	0.000000
C	-1.826793	1.461338	1.256590	C	0.000000	0.000000	-1.774011
C	-1.826793	1.461338	-1.256590	H	-0.623686	0.623686	2.428542
C	-2.581401	-0.579386	0.000000	H	0.623686	-0.623686	2.428542
C	-2.519015	0.944333	0.000000	H	0.623686	2.428542	-0.623686
C	-1.135093	-1.106940	0.000000	H	-0.623686	2.428542	0.623686
C	-0.383452	0.924454	1.249365	H	2.428542	-0.623686	0.623686
C	-0.383452	0.924454	-1.249365	H	2.428542	0.623686	-0.623686
H	-2.358566	1.113183	2.154860	H	-2.428542	-0.623686	-0.623686
H	-2.358566	1.113183	-2.154860	H	-2.428542	0.623686	0.623686
H	-1.825448	2.561584	-1.266298	H	-0.623686	-0.623686	-2.428542
H	-1.825448	2.561584	1.266298	H	0.623686	0.623686	-2.428542
H	-3.118796	-0.938910	-0.890370	H	-0.623686	-2.428542	-0.623686
H	-3.118796	-0.938910	0.890370	H	0.623686	-2.428542	0.623686
C	1.059254	-1.138837	1.240742	H	1.522839	1.522839	1.522839
C	1.059254	-1.138837	-1.240742	H	-1.522839	-1.522839	1.522839
C	1.812842	0.886973	0.000000	H	-1.522839	1.522839	-1.522839
C	0.373040	1.424136	0.000000	H	1.522839	-1.522839	-1.522839
C	-0.383452	-0.618645	-1.254992				
C	-0.383452	-0.618645	1.254992				
N	-3.964868	1.477231	0.000000				
H	0.374543	2.526779	0.000000				
H	-0.914429	-0.974944	-2.153368				
H	-0.914429	-0.974944	2.153368				
C	1.810026	-0.640281	0.000000				
C	3.270167	-1.259787	0.000000				
O	3.270784	-2.511995	0.000000				
H	-4.467630	1.151166	-0.830248				
H	-4.467630	1.151166	0.830248				
O	4.204204	-0.432506	0.000000				
H	-3.970496	2.501130	0.000000				
C ₉ H ₁₄ O RB3PW91\6-31G(d,p) E=-426.49393				C ₉ H ₁₄ S RB3PW91\6-31G(d,p) E=-749.45268			
H	-2.158152	0.000000	-1.510468	H	-2.151650	0.000000	-1.717236
H	2.158152	0.000000	-1.510468	H	2.151650	0.000000	-1.717236
H	-2.148155	1.249282	0.669675	H	-2.153908	1.298918	0.418638
H	-2.148155	-1.249282	0.669675	H	-2.153908	-1.298918	0.418638
H	2.148155	-1.249282	0.669675	H	2.153908	-1.298918	0.418638
H	2.148155	1.249282	0.669675	H	2.153908	1.298918	0.418638
H	1.263438	-2.162571	-0.562078	H	1.300818	-2.153221	-0.872896
H	1.263438	2.162571	-0.562078	H	1.300818	2.153221	-0.872896
H	-1.263438	2.162571	-0.562078	H	-1.300818	2.153221	-0.872896
H	-1.263438	-2.162571	-0.562078	H	-1.300818	-2.153221	-0.872896
C	-1.256819	-1.239292	0.031305	C	-1.262514	-1.270880	-0.217756
C	-1.256819	1.239292	0.031305	C	-1.262514	1.270880	-0.217756

C	1.256819	1.239292	0.031305	C	1.262514	1.270880	-0.217756
C	1.256819	-1.239292	0.031305	C	1.262514	-1.270880	-0.217756
O	0.000000	0.000000	1.701721	S	0.000000	0.000000	1.894650
C	0.000000	-1.190222	0.906014	C	0.000000	-1.353722	0.649918
C	0.000000	1.190222	0.906014	C	0.000000	1.353722	0.649918
C	0.000000	0.000000	-1.758445	C	0.000000	0.000000	-1.972579
C	1.262092	0.000000	-0.877452	C	1.254563	0.000000	-1.085026
C	-1.262092	0.000000	-0.877452	C	-1.254563	0.000000	-1.085026
H	0.000000	-2.012273	1.630065	H	0.000000	-2.278102	1.237113
H	0.000000	2.012273	1.630065	H	0.000000	2.278102	1.237113
H	0.000000	0.881759	-2.413370	H	0.000000	0.881882	-2.627112
H	0.000000	-0.881759	-2.413370	H	0.000000	-0.881882	-2.627112
C ₉ H ₁₅ N RB3PW91\6-31G(d,p) E=-406.62791				C ₉ H ₁₅ B RB3PW91\6-31G(d,p) E=-376.74748			
C	0.328914	1.408485	-0.494519	C	0.280009	1.439275	-0.455999
C	1.046044	-0.990355	-0.513218	C	1.107059	-0.961647	-0.455751
N	0.015263	-0.007287	1.529011	B	-0.001003	-0.000126	1.405138
C	-1.389753	-0.410927	-0.485439	C	-1.386209	-0.477222	-0.457026
C	1.379543	0.419943	-1.027789	C	1.373852	0.472681	-0.945798
C	0.331830	1.340421	1.043462	C	0.292840	1.513420	1.114077
C	-1.064665	1.000348	-1.001464	C	-1.095501	0.952745	-0.947072
C	1.014571	-0.956113	1.025950	C	1.163112	-1.011224	1.114402
C	-0.345695	-1.404755	-1.020999	C	-0.276299	-1.424785	-0.947429
C	-1.315462	-0.399879	1.051841	C	-1.458324	-0.503038	1.112877
H	2.382000	0.717662	-0.690796	H	2.355678	0.810923	-0.590531
H	1.394211	0.432592	-2.125927	H	1.411917	0.485602	-2.043343
H	-0.402531	2.040749	1.462727	H	-0.478436	2.216882	1.447623
H	1.315570	1.626738	1.438607	H	1.270568	1.878163	1.448760
H	-1.093521	1.021041	-2.099252	H	-1.124135	0.978106	-2.044690
H	-1.820725	1.715367	-0.648935	H	-1.879892	1.634215	-0.593733
H	0.780756	-1.950477	1.429165	H	0.989804	-2.040482	1.448478
H	1.996172	-0.668082	1.425260	H	2.157880	-0.695635	1.449131
H	-1.547840	-1.394027	1.456036	H	-1.682455	-1.522813	1.446017
H	-2.052677	0.299440	1.468001	H	-2.263702	0.160851	1.447077
H	-0.583967	-2.422186	-0.681564	H	-0.474206	-2.445234	-0.595051
H	-0.361956	-1.422270	-2.119097	H	-0.282830	-1.461700	-2.045071
H	0.567902	2.428927	-0.822379	H	0.474653	2.440493	-0.864014
H	1.804064	-1.707826	-0.854336	H	1.877023	-1.630404	-0.863984
H	-2.396254	-0.709652	-0.807529	H	-2.350085	-0.809570	-0.866047
4-C ₁₃ H ₁₉ N RB3PW91\6-31G(d,p) E=-561.43457				1-C ₁₃ H ₁₉ N RB3PW91\6-31G(d,p) E=-561.43710			
H	-0.000345	-2.484693	0.103491	H	-1.281647	0.129630	2.075554
H	2.151980	1.242048	0.103491	H	-1.281647	0.129630	-2.075554
H	-2.151635	1.242646	0.103491	H	2.492341	0.105498	0.000000
H	-2.155953	-1.244053	-0.048895	H	1.227306	-0.086177	-2.155994
H	2.155358	-1.245083	-0.048895	H	1.227306	-0.086177	2.155994
H	0.000595	2.489137	-0.048895	H	0.201795	2.180421	2.158147
H	1.195073	-1.711986	2.221278	H	0.201795	2.180421	-2.158147
H	0.885087	1.890956	2.221278	H	-1.772392	-2.142838	-1.249257
H	-2.080160	-0.178970	2.221278	H	-1.772392	-2.142838	1.249257
H	-2.157380	0.226232	-2.172807	H	1.723409	2.213804	1.263133
H	0.882768	-1.981462	-2.172807	H	1.723409	2.213804	-1.263133
H	1.274612	1.755230	-2.172807	H	-0.251291	-2.139481	-2.157822
H	2.079983	-0.180828	2.221644	H	-0.251291	-2.139481	2.157822
H	-0.883390	1.891732	2.221644	H	-2.020179	2.019038	-0.883567
H	-1.196593	-1.710904	2.221644	H	-2.020179	2.019038	0.883567
H	-1.275267	1.755085	-2.173172	H	1.981057	-2.171936	0.881898
H	-0.882314	-1.981956	-2.173172	H	1.981057	-2.171936	-0.881898
H	2.157582	0.226872	-2.173172	C	-0.735606	-1.786812	1.238236
C	0.000000	-1.445787	-1.797804	C	-0.735606	-1.786812	-1.238236
C	1.252088	0.722893	-1.797804	C	-1.457589	1.688630	0.000000
C	-1.252088	0.722893	-1.797804	C	1.445615	-1.794689	0.000000
C	-1.195489	-0.689588	1.817795	C	0.699988	1.814641	-1.249572
C	1.194945	-0.690529	1.817795	C	0.699988	1.814641	1.249572
C	0.000543	1.380118	1.817795	C	-0.000951	-2.314891	0.000000
C	0.000000	0.000000	-2.315628	C	-0.046653	2.301677	0.000000
N	0.000000	0.000000	2.310339	C	1.454633	-0.259084	0.000000
C	1.253884	0.723835	-0.264749	C	0.724502	0.281106	-1.249737
C	-1.253802	0.723978	-0.264749	C	0.724502	0.281106	1.249737
C	-0.000082	-1.447813	-0.264749	C	-0.723688	-0.258139	1.211344
C	0.000202	1.440045	0.282533	C	-0.723688	-0.258139	-1.211344

C	-1.247217	-0.719848	0.282533	N	-1.420247	0.223566	0.000000
C	1.247015	-0.720197	0.282533	H	-0.002399	-3.412184	0.000000
H	0.000000	0.000000	-3.413190	H	-0.117025	3.397388	0.000000
C ₁₂ H ₁₈ N ₂ RB3PW91\6-31G(d,p) E=-577.44550				C ₁₃ H ₁₈ O RB3PW91\6-31G(d,p) E=-581.30087			
H	0.000000	2.490862	0.055193	H	-1.188393	0.384606	2.155061
H	-2.157150	1.245431	-0.055193	H	-1.188393	0.384606	-2.155061
H	-2.157150	-1.245431	0.055193	H	1.208498	-0.340351	2.140154
H	2.157150	1.245431	-0.055193	H	1.208498	-0.340351	-2.140154
H	2.157150	-1.245431	0.055193	H	2.316567	-0.873025	0.000000
H	0.000000	-2.490862	-0.055193	H	-2.273044	1.011250	0.000000
H	-1.195922	1.711602	2.215365	H	-2.628733	-1.293463	0.882083
H	-0.884330	1.891500	-2.215365	H	-2.628733	-1.293463	-0.882083
H	-0.884330	-1.891500	2.215365	H	0.858776	-2.654070	1.262482
H	2.080252	-0.179898	-2.215365	H	0.858776	-2.654070	-1.262482
H	2.080252	0.179898	2.215365	H	-0.756609	2.701993	1.257968
H	-1.195922	-1.711602	-2.215365	H	-0.756609	2.701993	-1.257968
H	0.884330	-1.891500	2.215365	H	-0.557836	-2.105895	-2.157889
H	1.195922	-1.711602	-2.215365	H	-0.557836	-2.105895	2.157889
H	1.195922	1.711602	2.215365	H	0.647368	2.090588	-2.146381
H	-2.080252	-0.179898	-2.215365	H	0.647368	2.090588	2.146381
H	-2.080252	0.179898	2.215365	C	0.031028	1.937327	1.252531
H	0.884330	1.891500	-2.215365	C	0.031028	1.937327	-1.252531
C	0.000000	1.380391	-1.811617	C	0.031028	-1.931918	1.247226
C	-1.195454	0.690196	1.811617	C	0.031028	-1.931918	-1.247226
C	-1.195454	-0.690196	-1.811617	O	1.934080	1.103029	0.000000
C	1.195454	0.690196	1.811617	C	-1.993043	-1.137629	0.000000
C	1.195454	-0.690196	-1.811617	C	0.895917	2.087932	0.000000
C	0.000000	-1.380391	1.811617	C	-0.836911	-2.148751	0.000000
N	0.000000	0.000000	-2.301748	C	-0.570891	0.528625	-1.256873
N	0.000000	0.000000	2.301748	C	-0.570891	0.528625	1.256873
C	-1.248590	-0.720874	-0.277176	C	0.577470	-0.499569	-1.255804
C	1.248590	0.720874	0.277176	C	0.577470	-0.499569	1.255804
C	1.248590	-0.720874	-0.277176	C	1.425865	-0.232438	0.000000
C	0.000000	-1.441747	0.277176	C	-1.439683	0.293752	0.000000
C	0.000000	1.441747	-0.277176	H	1.419345	3.050037	0.000000
C	-1.248590	0.720874	0.277176	H	-1.238144	-3.170095	0.000000
C ₁₃ H ₁₈ S RB3PW91\6-31G(d,p) E=-904.25850				C ₁₃ H ₁₉ B RB3PW91\6-31G(d,p) E=-531.55185			
H	-1.335907	-0.272623	2.148662	H	2.150985	1.242374	-0.166218
H	-1.335907	-0.272623	-2.148662	H	0.000435	-2.483995	-0.166218
H	1.142690	-0.048098	2.146760	H	-2.151420	1.241621	-0.166218
H	1.142690	-0.048098	-2.146760	H	0.000223	2.483717	0.079987
H	2.390689	-0.304764	0.000000	H	2.150850	-1.242052	0.079987
H	-2.589742	-0.084669	0.000000	H	-2.151074	-1.241665	0.079987
H	-2.074228	-2.354888	0.882094	H	2.250854	-0.268493	-2.220969
H	-2.074228	-2.354888	-0.882094	H	-1.357949	-1.815050	-2.220969
H	1.655557	-2.329737	1.287367	H	-0.892905	2.083543	-2.220969
H	1.655557	-2.329737	-1.287367	H	-1.274689	1.755297	2.111810
H	-1.955864	1.948474	1.304973	H	2.157476	0.226265	2.111810
H	-1.955864	1.948474	-1.304973	H	-0.882787	-1.981561	2.111810
H	0.121151	-2.329470	-2.158061	H	1.361881	-1.811824	-2.223288
H	0.121151	-2.329470	2.158061	H	-2.250026	-0.273511	-2.223288
H	-0.407020	2.044827	-2.152059	H	0.888145	2.085335	-2.223288
H	-0.407020	2.044827	2.152059	H	-2.157171	0.228778	2.113337
C	-0.900487	1.641671	1.260812	H	1.276713	1.753775	2.113337
C	-0.900487	1.641671	-1.260812	H	0.880457	-1.982554	2.113337
C	0.622505	-1.958291	1.254079	C	1.252492	0.722505	1.736667
C	0.622505	-1.958291	-1.254079	C	-0.000538	-1.445942	1.736667
S	1.542535	1.901409	0.000000	C	-1.251954	0.723437	1.736667
C	-1.540286	-1.976314	0.000000	C	-0.001447	1.538071	-1.890945
C	-0.263574	2.234498	0.000000	C	1.332732	-0.767782	-1.890945
C	-0.091977	-2.482710	0.000000	C	-1.331285	-0.770289	-1.890945
C	-0.830913	0.107743	-1.249019	C	0.000000	0.000000	2.253928
C	-0.830913	0.107743	1.249019	B	0.000000	0.000000	-2.186192
C	0.622505	-0.420377	-1.255426	C	0.000310	-1.447908	0.200558
C	0.622505	-0.420377	1.255426	C	-1.254080	0.723685	0.200558
C	1.362318	0.077506	0.000000	C	1.253770	0.724222	0.200558
C	-1.550183	-0.443746	0.000000	C	-1.265312	-0.730528	-0.325617
H	-0.354896	3.325710	0.000000	C	0.000000	1.461056	-0.325617

H	-0.080496	-3.580149	0.000000	C	1.265312	-0.730528	-0.325617
				H	0.000000	0.000000	3.351497
4,9-C ₁₂ H ₁₈ B ₂ RB3PW91\6-31G(d,p) E=-517.67973				4,9-C ₁₂ H ₁₈ B _N RB3PW91\6-31G(d,p) E=-547.56273			
H	0.000000	2.483829	0.153075	H	0.114962	1.278171	2.136374
H	-2.151059	1.241914	-0.153075	H	-0.086461	-1.208983	2.170883
H	-2.151059	-1.241914	0.153075	H	0.118337	-2.489407	0.038267
H	2.151059	1.241914	-0.153075	H	-0.085644	2.485139	-0.038284
H	2.151059	-1.241914	0.153075	H	0.118271	1.211936	-2.174451
H	0.000000	-2.483829	-0.153075	H	-0.083801	-1.274973	-2.133239
H	-1.361934	1.813842	2.153576	H	2.213839	-0.235565	2.255633
H	-0.889866	2.086390	-2.153576	H	-2.157081	0.214170	2.076086
H	-0.889866	-2.086390	2.153576	H	2.215549	-1.834747	-1.330941
H	2.251800	-0.272548	-2.153576	H	-2.155030	1.691657	-1.224411
H	2.251800	0.272548	2.153576	H	2.215252	2.070863	-0.922143
H	-1.361934	-1.813842	-2.153576	H	-2.154919	-1.908360	-0.852042
H	0.889866	-2.086390	2.153576	H	2.215832	-0.306564	-2.246088
H	1.361934	-1.813842	-2.153576	H	-2.153065	0.148276	-2.083642
H	1.361934	1.813842	2.153576	H	2.214759	2.098503	0.859199
H	-2.251800	-0.272548	-2.153576	H	-2.152747	-1.877845	0.913970
H	-2.251800	0.272548	2.153576	H	2.214796	-1.791932	1.389086
H	0.889866	2.086390	-2.153576	H	-2.156585	1.729381	1.168266
C	0.000000	1.540430	-1.820602	C	-1.752649	0.708700	1.183312
C	-1.334051	0.770215	1.820602	C	1.884161	-0.747927	1.344475
C	-1.334051	-0.770215	-1.820602	C	-1.750388	-1.380879	0.021580
C	1.334051	0.770215	1.820602	C	1.884859	1.538064	-0.022993
C	1.334051	-0.770215	-1.820602	C	-1.750195	0.671401	-1.206628
C	0.000000	-1.540430	1.820602	C	1.885477	-0.789614	-1.319338
B	0.000000	0.000000	-2.116158	N	-2.241846	-0.000711	-0.001089
B	0.000000	0.000000	2.116158	B	2.180840	0.000151	0.000738
C	-1.267029	-0.731520	-0.255058	C	-0.212289	-1.441149	0.021756
C	1.267029	0.731520	0.255058	C	0.319711	1.462099	-0.022071
C	1.267029	-0.731520	-0.255058	C	-0.212289	0.701477	-1.258744
C	0.000000	-1.463040	0.255058	C	0.320904	-0.750026	-1.254651
C	0.000000	1.463040	-0.255058	C	-0.214484	0.739794	1.236389
C	-1.267029	0.731520	0.255058	C	0.319259	-0.711190	1.277146
1,6-C ₁₂ H ₁₈ B _N RB3PW91\6-31G(d,p) E=-547.56671				C ₁₈ H ₂₄ RB3PW91\6-31G(d,p) E=-700.23078			
H	1.241362	-0.053483	2.240387	C	1.250555	1.274410	0.695332
H	1.241362	-0.053483	-2.240387	C	-1.250555	1.274410	0.695332
H	-1.245257	0.149724	2.069746	C	-1.250555	-1.274410	0.695332
H	-1.245257	0.149724	-2.069746	C	1.250555	-1.274410	0.695332
H	-0.212287	-2.126927	2.156759	C	0.000000	0.000000	2.476548
H	-0.212287	-2.126927	-2.156759	C	0.000000	1.254099	1.597543
H	0.232228	2.235662	2.154029	C	0.000000	-1.254099	1.597543
H	0.232228	2.235662	-2.154029	C	1.249379	0.000000	-0.170742
H	-1.746728	-2.116586	-1.275157	C	-1.249379	0.000000	-0.170742
H	-1.746728	-2.116586	1.275157	C	1.251795	-2.524304	-0.193173
H	1.767128	2.268246	-1.293004	C	-1.251795	-2.524304	-0.193173
H	1.767128	2.268246	1.293004	C	-1.251795	2.524304	-0.193173
H	1.996164	-2.353413	-0.889774	C	1.251795	2.524304	-0.193173
H	1.996164	-2.353413	0.889774	H	0.881867	-1.261850	-2.614905
H	-1.956057	2.037783	-0.883838	H	-0.881867	-1.261850	-2.614905
H	-1.956057	2.037783	0.883838	H	-0.881867	1.261850	-2.614905
C	0.753425	1.847723	1.265319	H	0.881867	1.261850	-2.614905
C	0.753425	1.847723	-1.265319	C	0.000000	0.000000	-1.091810
C	-0.705225	-1.776280	1.241858	H	-0.881853	0.000000	3.132148
C	-0.705225	-1.776280	-1.241858	H	0.881853	0.000000	3.132148
C	-1.393154	1.709508	0.000000	H	0.000000	-2.151495	2.233319
C	1.510521	-1.936117	0.000000	H	0.000000	2.151495	2.233319
C	0.018138	2.316259	0.000000	C	0.000000	-2.526660	-1.081910
C	-0.005225	-2.347315	0.000000	C	0.000000	2.526660	-1.081910
N	-1.354359	0.244531	0.000000	C	0.000000	-1.266781	-1.957825
B	1.331645	-0.378224	0.000000	C	0.000000	1.266781	-1.957825
C	0.805016	0.313368	-1.302657	H	-1.275454	-3.428644	0.429881
C	0.805016	0.313368	1.302657	H	1.275454	-3.428644	0.429881
C	-0.683873	-0.245325	-1.210402	H	1.275454	3.428644	0.429881
C	-0.683873	-0.245325	1.210402	H	-1.275454	3.428644	0.429881
H	-0.059352	3.411731	0.000000	H	-2.157076	-2.541838	-0.815111
H	-0.059352	3.411731	0.000000	H	2.157076	-2.541838	-0.815111
H	-0.085250	-3.442167	0.000000	H	2.157076	2.541838	-0.815111

		H	-2.157076	2.541838	-0.815111			
		H	-2.149131	-1.272231	1.329809			
		H	2.149131	-1.272231	1.329809			
		H	2.149131	1.272231	1.329809			
		H	-2.149131	1.272231	1.329809			
		H	0.000000	-3.419769	-1.720239			
		H	0.000000	3.419769	-1.720239			
		H	-2.148957	0.000000	-0.807096			
		H	2.148957	0.000000	-0.807096			
	16-C ₁₇ H ₂₂ O RB3PW91\6-31G(d,p) E=-736.11067				16-C ₁₇ H ₂₂ S RB3PW91\6-31G(d,p) E=-1059.06576			
	C	-0.705891	1.267516	1.250659	C	-0.645336	1.449973	1.250270
	C	-0.705891	1.267516	-1.250659	C	-0.645336	1.449973	-1.250270
	C	-0.687144	-1.291095	-1.255334	C	-0.955725	-1.070532	-1.246143
	C	-0.687144	-1.291095	1.255334	C	-0.955725	-1.070532	1.246143
	C	-2.471813	-0.030692	0.000000	C	-2.574210	0.415518	0.000000
	C	-1.607467	1.237201	0.000000	C	-1.542108	1.544085	0.000000
	C	-1.585175	-1.283000	0.000000	C	-1.851959	-0.932146	0.000000
	C	0.155772	-0.006224	1.255322	C	0.074935	0.080391	1.248631
	C	0.155772	-0.006224	-1.255322	C	0.074935	0.080391	-1.248631
	C	0.268774	-2.488889	-1.250642	C	-0.297122	-2.456650	1.262738
	C	0.268774	-2.488889	1.250642	C	-0.297122	-2.456650	-1.262738
	C	0.201474	2.504398	-1.248159	C	0.372699	2.596972	-1.255469
	C	0.201474	2.504398	1.248159	C	0.372699	2.596972	1.255469
	H	2.611677	1.180532	-0.883003	H	2.638835	1.087824	-0.883343
	H	2.611677	1.180532	0.883003	H	2.638835	1.087824	0.883343
	C	1.055903	-0.015504	0.000000	C	0.984498	0.011194	0.000000
	H	-3.127588	-0.036063	-0.881547	H	-3.223575	0.495352	-0.882492
	H	-3.127588	-0.036063	0.881547	H	-3.223575	0.495352	0.882492
	H	-2.216031	-2.183489	0.000000	H	-2.590026	-1.747237	0.000000
	H	-2.256190	2.124707	0.000000	H	-2.054229	2.516991	0.000000
	C	1.145947	-2.400696	0.000000	C	0.539170	-2.683376	0.000000
	C	1.096808	2.485138	0.000000	C	1.250588	2.510307	0.000000
	O	1.890581	-1.177450	0.000000	S	1.974289	-1.542463	0.000000
	C	1.960783	1.211717	0.000000	C	1.991657	1.168271	0.000000
	H	-0.284897	-3.436761	-1.251093	H	-1.084312	-3.223276	-1.313928
	H	-0.284897	-3.436761	1.251093	H	-1.084312	-3.223276	1.313928
	H	-0.405518	3.419537	1.260689	H	-0.152160	3.561299	1.286411
	H	-0.405518	3.419537	-1.260689	H	-0.152160	3.561299	-1.286411
	H	0.900056	-2.473721	-2.147133	H	0.332015	-2.577057	-2.151729
	H	0.900056	-2.473721	2.147133	H	0.332015	-2.577057	2.151729
	H	0.816667	2.516600	2.157696	H	0.997999	2.544417	2.156698
	H	0.816667	2.516600	-2.157696	H	0.997999	2.544417	-2.156698
	H	-1.320581	-1.314481	-2.153683	H	-1.578842	-0.968437	-2.146627
	H	-1.320581	-1.314481	2.153683	H	-1.578842	-0.968437	2.146627
	H	-1.338981	1.272856	2.149993	H	-1.275289	1.511051	2.149819
	H	-1.338981	1.272856	-2.149993	H	-1.275289	1.511051	-2.149819
	H	1.904098	-3.191238	0.000000	H	0.971495	-3.689662	0.000000
	H	1.750510	3.366428	0.000000	H	1.981395	3.329022	0.000000
	H	0.812779	-0.003631	-2.137397	H	0.707085	0.001481	-2.144390
	H	0.812779	-0.003631	2.137397	H	0.707085	0.001481	2.144390
	5-C ₁₇ H ₂₂ O RB3PW91\6-31G(d,p) E=-736.10846				5-C ₁₇ H ₂₂ S RB3PW91\6-31G(d,p) E=-1059.06527			
	C	1.254209	1.259598	0.705500	C	1.254069	1.289542	0.531948
	C	-1.254209	1.259598	0.705500	C	-1.254069	1.289542	0.531948
	C	-1.254209	-1.259598	0.705500	C	-1.254069	-1.289542	0.531948
	C	1.254209	-1.259598	0.705500	C	1.254069	-1.289542	0.531948
	O	0.000000	0.000000	2.378932	S	0.000000	0.000000	2.660489
	C	0.000000	1.190285	1.590450	C	0.000000	1.342469	1.422481
	C	0.000000	-1.190285	1.590450	C	0.000000	-1.342469	1.422481
	C	1.255464	0.000000	-0.175026	C	1.243387	0.000000	-0.317620
	C	-1.255464	0.000000	-0.175026	C	-1.243387	0.000000	-0.317620
	C	1.246395	-2.524141	-0.160461	C	1.257071	-2.525423	-0.382536
	C	-1.246395	-2.524141	-0.160461	C	-1.257071	-2.525423	-0.382536
	C	-1.246395	2.524141	-0.160461	C	-1.257071	2.525423	-0.382536
	C	1.246395	2.524141	-0.160461	C	1.257071	2.525423	-0.382536
	H	0.882018	-1.276572	-2.601734	H	0.881847	-1.243670	-2.781155
	H	-0.882018	-1.276572	-2.601734	H	-0.881847	-1.243670	-2.781155
	H	-0.882018	1.276572	-2.601734	H	-0.881847	1.243670	-2.781155
	H	0.882018	1.276572	-2.601734	H	0.881847	1.243670	-2.781155
	C	0.000000	0.000000	-1.089153	C	0.000000	0.000000	-1.246053

1								
2								
3								
4	H	0.000000	-2.011579	2.317571	H	0.000000	-2.269715	2.008555
5	H	0.000000	2.011579	2.317571	H	0.000000	2.269715	2.008555
6	C	0.000000	-2.527725	-1.056415	C	0.000000	-2.524659	-1.264087
7	C	0.000000	2.527725	-1.056415	C	0.000000	2.524659	-1.264087
8	C	0.000000	-1.273939	-1.945194	C	0.000000	-1.258074	-2.124584
9	C	0.000000	1.273939	-1.945194	C	0.000000	1.258074	-2.124584
10	H	-1.257409	-3.421221	0.473386	H	-1.297120	-3.438418	0.226489
11	H	1.257409	-3.421221	0.473386	H	1.297120	-3.438418	0.226489
12	H	1.257409	3.421221	0.473386	H	1.297120	3.438418	0.226489
13	H	-1.257409	3.421221	0.473386	H	-1.297120	3.438418	0.226489
14	H	-2.158246	-2.556494	-0.771675	H	-2.158159	-2.522878	-1.010727
15	H	2.158246	-2.556494	-0.771675	H	2.158159	-2.522878	-1.010727
16	H	2.158246	2.556494	-0.771675	H	2.158159	2.522878	-1.010727
17	H	-2.158246	2.556494	-0.771675	H	-2.158159	2.522878	-1.010727
18	H	-2.138673	-1.248565	1.356197	H	-2.145516	-1.294574	1.171587
19	H	2.138673	-1.248565	1.356197	H	2.145516	-1.294574	1.171587
20	H	2.138673	1.248565	1.356197	H	2.145516	1.294574	1.171587
21	H	-2.138673	1.248565	1.356197	H	-2.145516	1.294574	1.171587
22	H	0.000000	-3.425508	-1.687663	H	0.000000	-3.412380	-1.909293
23	H	0.000000	3.425508	-1.687663	H	0.000000	3.412380	-1.909293
24	H	-2.152890	0.000000	-0.813876	H	-2.147279	0.000000	-0.947487
25	H	2.152890	0.000000	-0.813876	H	2.147279	0.000000	-0.947487
26	8-C ₁₇ H ₂₂ O RB3PW91\6-31G(d,p) E=-736.10786				8-C ₁₇ H ₂₂ S RB3PW91\6-31G(d,p) E=-1059.06580			
27	C	1.306585	0.688777	1.234880	C	0.956714	0.735087	1.426669
28	C	1.283805	0.638163	-1.239422	C	1.160026	0.800052	-1.083154
29	C	-1.266646	0.694470	-1.246946	C	-1.346736	0.682574	-1.295669
30	C	-1.239514	0.715656	1.255490	C	-1.582836	0.657300	1.191521
31	C	0.041285	2.469588	-0.035990	C	-0.253964	2.491926	0.089478
32	C	1.284495	1.577094	-0.022982	C	1.029250	1.654488	0.188953
33	C	-1.222404	1.605826	-0.004508	C	-1.472630	1.573012	-0.042711
34	C	0.023990	-0.167816	1.251898	C	-0.286055	-0.166418	1.301032
35	C	-0.007574	-0.192179	-1.246003	C	-0.046922	-0.146359	-1.187886
36	C	-2.501121	-0.156305	1.276415	C	-2.795571	-0.272576	1.068203
37	C	-2.525295	-0.182273	-1.228735	C	-2.561667	-0.243555	-1.423305
38	O	2.432939	-0.209305	-1.235367	S	2.742920	-0.119913	-1.119822
39	C	2.554749	-0.198219	1.188248	C	2.216164	-0.127215	1.591694
40	H	-1.274953	-2.599683	0.920842	H	-1.423002	-2.645817	0.795829
41	H	-1.291393	-2.617636	-0.843432	H	-1.258212	-2.624353	-0.960840
42	H	1.243251	-2.604917	-0.922297	H	1.258915	-2.580632	-0.670634
43	H	1.310105	-2.616798	0.846691	H	1.008461	-2.587538	1.079697
44	C	-0.006885	-1.099933	0.009294	C	-0.132917	-1.075117	0.054574
45	H	0.039129	3.105858	-0.931884	H	-0.194051	3.167035	-0.775013
46	H	0.061929	3.144851	0.830223	H	-0.354958	3.125843	0.980953
47	H	-2.111579	2.252420	0.000141	H	-2.385380	2.180270	-0.125144
48	H	2.194764	2.189974	-0.055048	H	1.903510	2.311971	0.270033
49	C	-2.527685	-1.057620	0.033407	C	-2.650998	-1.146004	-0.185643
50	C	2.488107	-1.051135	-0.079725	C	2.390657	-1.079093	0.404423
51	C	-1.280811	-1.952516	0.031871	C	-1.368105	-1.979853	-0.077186
52	C	1.260077	-1.960961	-0.033622	C	1.134986	-1.931576	0.204588
53	H	-3.422948	0.450071	-1.251822	H	-3.478651	0.352383	-1.525848
54	H	-3.396581	0.479158	1.302161	H	-3.718926	0.319631	1.013135
55	H	3.460973	0.418680	1.170793	H	3.105474	0.504086	1.697544
56	H	-2.556341	-0.813146	-2.127165	H	-2.474703	-0.853825	-2.332188
57	H	-2.519031	-0.769008	2.187874	H	-2.875965	-0.904753	1.962896
58	H	2.610819	-0.845695	2.072869	H	2.125333	-0.720557	2.513276
59	H	-1.266566	1.321105	-2.150884	H	-1.279996	1.324293	-2.186389
60	H	-1.220728	1.358770	2.147584	H	-1.684983	1.279956	2.092418
	H	1.326261	1.324277	2.131906	H	0.846263	1.369077	2.318384
	H	1.363734	1.219474	-2.166600	H	1.192302	1.451462	-1.965412
	H	-3.430106	-1.682257	0.047974	H	-3.517621	-1.813740	-0.274152
	H	3.403803	-1.639466	-0.202781	H	3.267657	-1.718425	0.550597
	H	-0.003972	-0.829298	-2.142489	H	0.064328	-0.767032	-2.087993
	H	0.024985	-0.795995	2.156866	H	-0.348885	-0.810760	2.192518
	C ₂₁ H ₂₆ S RB3PW91\6-31G(d,p) E=-1213.87305				C ₂₅ H ₃₀ S RB3PW91\6-31G(d,p) E=-1368.68334			
	C	-0.300059	0.868433	1.244901	C	-1.513941	-0.310736	0.000000
	C	-0.300059	0.868433	-1.244901	C	0.426605	0.649458	1.248868
	C	0.164855	-0.605032	1.245668	C	0.426605	0.649458	-1.248868
	C	0.164855	-0.605032	-1.245668	C	0.666157	-1.506429	0.000000
	C	-0.654295	-3.036926	-1.262854	C	-0.864504	-1.713665	0.000000

1										
2										
3										
4	C	-0.654295	-3.036926	1.262854	C	-1.115573	0.478224	-1.267760		
5	C	0.405045	3.295146	-1.253750	C	-1.115573	0.478224	1.267760		
6	C	0.405045	3.295146	1.253750	C	0.901810	1.425068	0.000000		
7	S	1.743967	-2.541742	0.000000	C	1.112018	-0.746387	1.271165		
8	C	-1.643442	2.606897	0.000000	C	1.112018	-0.746387	-1.271165		
9	C	-1.052429	-1.554909	-1.246701	C	-1.281920	-2.471632	-1.266326		
10	C	-1.052429	-1.554909	1.246701	C	-1.281920	-2.471632	1.266326		
11	C	0.893770	1.841699	-1.251251	C	-1.838192	1.834360	-1.259713		
12	C	0.893770	1.841699	1.251251	C	-1.838192	1.834360	1.259713		
13	C	-1.909758	-1.260891	0.000000	C	-1.522755	-0.318270	2.515565		
14	C	1.751084	1.568831	0.000000	C	-1.522755	-0.318270	-2.515565		
15	C	-2.379651	0.191446	0.000000	C	2.428251	1.567378	0.000000		
16	C	2.241192	0.121122	0.000000	C	2.636515	-0.578474	1.253125		
17	C	-1.182627	1.142859	0.000000	C	2.636515	-0.578474	-1.253125		
18	C	1.049351	-0.838625	0.000000	S	0.232433	3.137473	0.000000		
19	C	0.129414	-3.408083	0.000000	C	0.663464	-1.519848	2.517302		
20	C	-0.441568	3.557571	0.000000	C	0.663464	-1.519848	-2.517302		
21	H	-2.273131	2.791531	0.882098	H	0.733687	1.209593	2.145366		
22	H	-2.273131	2.791531	-0.882098	H	0.733687	1.209593	-2.145366		
23	H	-0.907235	1.041325	-2.147971	H	1.153355	-2.496578	0.000000		
24	H	-0.907235	1.041325	2.147971	H	-0.825386	-3.471683	1.263471		
25	H	0.772377	-0.790562	-2.142853	H	-0.825386	-3.471683	-1.263471		
26	H	0.772377	-0.790562	2.142853	H	-1.241748	0.243070	-3.417873		
27	H	2.864364	-0.072386	0.883196	H	-1.241748	0.243070	3.417873		
28	H	2.864364	-0.072386	-0.883196	H	-1.569074	2.412733	2.151692		
29	H	-3.005554	0.388176	0.882359	H	-1.569074	2.412733	-2.151692		
30	H	-3.005554	0.388176	-0.882359	H	0.986025	-0.981670	3.419903		
31	H	-1.566998	-3.648907	1.310828	H	0.986025	-0.981670	-3.419903		
32	H	-1.566998	-3.648907	-1.310828	H	1.162733	-2.499115	-2.537371		
33	H	1.264821	3.978117	1.282740	H	1.162733	-2.499115	2.537371		
34	H	1.264821	3.978117	-1.282740	H	-2.371023	-2.621465	-1.262631		
35	H	-2.783220	-1.929322	0.000000	H	-2.371023	-2.621465	1.262631		
36	H	2.618150	2.244924	0.000000	H	-2.922295	1.649059	-1.308157		
37	H	-1.646753	-1.341282	2.147034	H	-2.922295	1.649059	1.308157		
38	H	-1.646753	-1.341282	-2.147034	H	-2.616670	-0.424446	2.536403		
39	H	1.500694	1.654345	2.148971	H	-2.616670	-0.424446	-2.536403		
40	H	1.500694	1.654345	-2.148971	H	2.740229	2.139959	0.883287		
41	H	0.374559	-4.475496	0.000000	H	2.740229	2.139959	-0.883287		
42	H	-0.791078	4.598040	0.000000	H	3.112458	-1.568806	1.285086		
43	H	-0.058831	-3.270700	2.152327	H	3.112458	-1.568806	-1.285086		
44	H	-0.058831	-3.270700	-2.152327	H	2.959681	-0.042247	-2.156554		
45	H	-0.188000	3.491357	2.157221	H	2.959681	-0.042247	2.156554		
46	H	-0.188000	3.491357	-2.157221	C	-1.528144	2.643377	0.000000		
47					C	-0.857676	-1.698505	2.520442		
48					C	-0.857676	-1.698505	-2.520442		
49					C	3.080197	0.182554	0.000000		
50					H	-2.092835	3.582101	0.000000		
51					H	-1.163623	-2.252502	3.417422		
52					H	-1.163623	-2.252502	-3.417422		
53					H	4.172106	0.294050	0.000000		
54					H	-2.610325	-0.436511	0.000000		
55	C ₃₄ H ₃₄ S RB3PW91\6-31G(d,p) E=-1713.98966					C ₅₀ H ₅₀ S RB3PW91\6-31G(d,p) E=-2333.22784				
56	C	-1.267414	0.000000	0.782964	C	1.261655	0.000000	0.834229		
57	C	1.267414	0.000000	0.782964	C	-1.261655	0.000000	0.834229		
58	C	0.000000	1.270253	-1.024531	C	0.000000	1.261738	-0.971601		
59	C	0.000000	-1.270253	-1.024531	C	0.000000	-1.261738	-0.971601		
60	C	-1.271580	-2.526083	0.744243	C	0.000000	-1.360824	2.608264		
	C	-1.271580	2.526083	0.744243	C	0.000000	1.360824	2.608264		
	C	1.271580	2.526083	0.744243	C	-1.265484	0.000000	-2.767733		
	C	1.271580	-2.526083	0.744243	C	1.265484	0.000000	-2.767733		
	C	2.518525	1.265308	-1.008255	C	-1.270786	-2.548738	0.797303		
	C	2.518525	-1.265308	-1.008255	C	-1.270786	2.548738	0.797303		
	C	-2.518525	-1.265308	-1.008255	C	1.270786	2.548738	0.797303		
	C	-2.518525	1.265308	-1.008255	C	1.270786	-2.548738	0.797303		
	C	0.000000	-1.333546	2.538691	C	-2.534932	-1.265501	-0.971051		
	C	0.000000	1.333546	2.538691	C	-2.534932	1.265501	-0.971051		
	C	1.249626	0.000000	-2.802987	C	2.534932	1.265501	-0.971051		
	C	-1.249626	0.000000	-2.802987	C	2.534932	-1.265501	-0.971051		
	C	-1.252409	-1.281844	1.653131	C	1.247556	-1.287383	1.702346		
	C	-1.252409	1.281844	1.653131	C	1.247556	1.287383	1.702346		

1	C	1.252409	1.281844	1.653131	C	-1.247556	1.287383	1.702346
2	C	1.252409	-1.281844	1.653131	C	-1.247556	-1.287383	1.702346
3	C	1.269349	1.245834	-1.904286	C	-1.264657	1.240970	-1.850271
4	C	1.269349	-1.245834	-1.904286	C	-1.264657	-1.240970	-1.850271
5	C	-1.269349	1.245834	-1.904286	C	1.264657	-1.240970	-1.850271
6	C	-1.269349	-1.245834	-1.904286	C	1.264657	1.240970	-1.850271
7	C	0.000000	-2.520631	-0.120566	C	0.000000	-2.511637	-0.079727
8	C	0.000000	2.520631	-0.120566	C	0.000000	2.511637	-0.079727
9	C	2.515032	0.000000	-0.133594	C	-2.508396	0.000000	-0.082409
10	C	-2.515032	0.000000	-0.133594	C	2.508396	0.000000	-0.082409
11	C	0.000000	0.000000	-0.120157	C	0.000000	0.000000	-0.067084
12	C	2.522513	-2.520568	-0.135453	C	-2.514230	-2.512452	-0.090225
13	C	2.522513	2.520568	-0.135453	C	-2.514230	2.512452	-0.090225
14	C	-2.522513	2.520568	-0.135453	C	2.514230	2.512452	-0.090225
15	C	-2.522513	-2.520568	-0.135453	C	2.514230	-2.512452	-0.090225
16	S	0.000000	0.000000	3.784065	S	0.000000	0.000000	3.820789
17	C	0.000000	0.000000	-3.686053	C	0.000000	0.000000	-3.628150
18	H	1.267528	-2.146924	-2.538704	H	-3.409450	0.000000	0.554571
19	H	1.267528	2.146924	-2.538704	H	3.409450	0.000000	0.554571
20	H	-1.267528	2.146924	-2.538704	H	0.000000	-3.402958	-0.730580
21	H	-1.267528	-2.146924	-2.538704	H	0.000000	3.402958	-0.730580
22	H	2.144244	-1.283231	2.295732	H	1.261006	-2.144789	-2.483922
23	H	2.144244	1.283231	2.295732	H	1.261006	2.144789	-2.483922
24	H	-2.144244	1.283231	2.295732	H	-1.261006	2.144789	-2.483922
25	H	-2.144244	-1.283231	2.295732	H	-1.261006	-2.144789	-2.483922
26	H	3.414188	0.000000	0.502903	H	-2.143285	1.291032	2.342486
27	H	-3.414188	0.000000	0.502903	H	-2.143285	-1.291032	2.342486
28	H	0.000000	-3.414801	-0.764090	H	2.143285	-1.291032	2.342486
29	H	0.000000	3.414801	-0.764090	H	2.143285	1.291032	2.342486
30	H	0.000000	-2.265432	3.118206	C	1.255056	-3.823549	1.651150
31	H	0.000000	2.265432	3.118206	C	1.255056	3.823549	1.651150
32	H	2.150105	0.000000	-3.434920	C	-1.255056	3.823549	1.651150
33	H	-2.150105	0.000000	-3.434920	C	-1.255056	-3.823549	1.651150
34	H	1.269654	-3.424615	1.378661	C	-3.781036	1.247290	-1.866137
35	H	1.269654	3.424615	1.378661	C	-3.781036	-1.247290	-1.866137
36	H	-1.269654	3.424615	1.378661	C	3.781036	-1.247290	-1.866137
37	H	-1.269654	-3.424615	1.378661	C	3.781036	1.247290	-1.866137
38	H	3.415065	-1.252584	-1.645310	C	0.000000	-2.648092	3.443064
39	H	3.415065	1.252584	-1.645310	C	0.000000	2.648092	3.443064
40	H	-3.415065	1.252584	-1.645310	C	-2.530117	0.000000	-3.635521
41	H	-3.415065	-1.252584	-1.645310	C	-2.530117	0.000000	-3.635521
42	H	3.424206	-2.545276	0.491147	H	-2.542610	-3.412458	-0.722760
43	H	3.424206	2.545276	0.491147	H	-2.542610	3.412458	-0.722760
44	H	-3.424206	2.545276	0.491147	H	2.542610	3.412458	-0.722760
45	H	-3.424206	-2.545276	0.491147	H	2.542610	-3.412458	-0.722760
46	H	2.546114	-3.420243	-0.765208	H	-3.417177	-2.540775	0.537947
47	H	2.546114	3.420243	-0.765208	H	-3.417177	2.540775	0.537947
48	H	-2.546114	3.420243	-0.765208	H	3.417177	2.540775	0.537947
49	H	-2.546114	-3.420243	-0.765208	H	3.417177	-2.540775	0.537947
50	H	0.000000	-0.882076	-4.341058	H	0.000000	-0.882153	-4.286242
51	H	0.000000	0.882076	-4.341058	H	0.000000	0.882153	-4.286242
52					H	-2.156134	-3.860026	2.279548
53					H	-2.156134	3.860026	2.279548
54					H	2.156134	3.860026	2.279548
55					H	2.156134	-3.860026	2.279548
56					H	-3.799108	-2.156328	-2.484075
57					H	-3.799108	2.156328	-2.484075
58					H	3.799108	2.156328	-2.484075
59					H	3.799108	-2.156328	-2.484075
60					H	-1.293831	-4.700080	0.989206
					H	-1.293831	4.700080	0.989206
					H	1.293831	4.700080	0.989206
					H	1.293831	-4.700080	0.989206
					H	-4.684032	-1.271724	-1.239735
					H	-4.684032	1.271724	-1.239735
					H	4.684032	1.271724	-1.239735
					H	4.684032	-1.271724	-1.239735
					H	-0.882992	-2.654109	4.095824
					H	-0.882992	2.654109	4.095824
					H	0.882992	2.654109	4.095824
					H	0.882992	-2.654109	4.095824

	H	-2.525196	-0.882158	-4.291707
	H	-2.525196	0.882158	-4.291707
	H	2.525196	0.882158	-4.291707
	H	2.525196	-0.882158	-4.291707
	C	0.000000	-3.870097	2.526498
	C	0.000000	3.870097	2.526498
	C	-3.785706	0.000000	-2.755697
	C	3.785706	0.000000	-2.755697
	H	-4.681756	0.000000	-3.389949
	H	4.681756	0.000000	-3.389949
	H	0.000000	-4.785355	3.132383
	H	0.000000	4.785355	3.132383

For Peer Review Only