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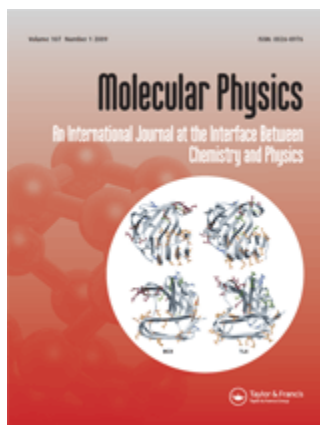
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Tetrahedranes. A Theoretical Study of Singlet E4H4 Molecules (E = C to Pb and B to Tl)

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Tetrahedranes. A Theoretical Study of Singlet E_4H_4 Molecules ($E = C - Pb$ and $B - Tl$)

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(Received)

ABSTRACT

Quantum chemical calculations using DFT (B3LYP) and ab initio (CCSD(T)) methods have been carried out to elucidate the E_4H_4 singlet potential energy hypersurface for the group-13 and group-14 elements. The results show that there are numerous E_4H_4 energy minima for the compounds of group-13 and group-14 elements. This holds particularly for the heavier atoms. The classical T_d tetrahedron structure is energetically more favourable for the group-13 compounds E_4H_4 where the tetrahedron isomers are energy minima for all elements E except for thallium. The tetrahedranes Al_4H_4 **1Al** and Ga_4H_4 **1Ga** are the global energy minima on the singlet PES while **1B** is slightly less stable than the singly hydrogen-bridged planar form **12B** which has a rhombic B_4 core. The lowest-lying energy minima for In_4H_4 and Tl_4H_4 are tetrahedranes where the E_4 core is face-bridged by the hydrogen atoms. The classical T_d tetrahedron structure of the group-14 elements is only for carbon and silicon an energy minimum at B3LYP/def2-TZVPP. The latter form of Si_4H_4 is a third-order saddle point at BP86/def2-TZVPP and MP2/def2-TZVPP. The global energy minimum form for C_4H_4 is the vinylideneacetylene isomer **27C** which is -63.7 kcal/mol lower in energy than the tetrahedrane. The most stable isomers of Si_4H_4 and Ge_4H_4 at CCSD(T)/def2-QZVPP are the singly hydrogen edge-bridged tetrahedrane structures **18E** which are more than 40 kcal/mol lower in energy than the classical tetrahedrane. The B3LYP/def2-TZVPP calculations predict that tetrahedrane structure with edge-bridging hydrogen atoms **3Ge** is slightly more stable than **18Ge**. The former isomer is calculated as global energy minimum on the singlet PES of Sn_4H_4 and Pb_4H_4 .

1. INTRODUCTION

The synthesis of hydrocarbons which have the shape of platonic solid geometries belongs to the classic challenges in hydrocarbon chemistry. [1,2] There are five platonic solids, icosahedron, octahedron, tetrahedron, hexahedron (cube) and dodecahedron. Because of the valence restrictions of carbon only the latter three may become synthesized as hydrocarbons. Cubane (C_8H_8) has been isolated in 1964 [3] while the synthesis of dodecahedrane ($C_{20}H_{20}$) was achieved in 1981. [4] The smallest platonic hydrocarbon tetrahedrane could until now only become synthesized as substituted derivative C_4R_4 where $R = t$ -butyl. [5] The parent system C_4H_4 has been the subject of numerous theoretical studies. [6]

Tetrahedrane structures E_4R_4 with bulky substituents could also become synthesized for the heavier group-14 elements silicon [7] and germanium [8] while tetrastannatetrahedranes and tetraplumbatetrahedranes are still waiting to be prepared. Theoretical studies of the heavier group-14 homologues E_4R_4 where $E = Si - Pb$ have also been published. [9,10] Ab initio calculations at the Hartree-Fock (HF) level and DFT calculations using B3LYP predict that the tetrahedrane structures of C_4H_4 and Si_4H_4 are minima on the potential energy surface (PES) while the heavier homologues of tetrahedrane E_4H_4 where $E = Ge - Pb$ are third-order saddle points. [9] However, MP2 calculations suggest that tetrasilatetrahedrane is a second-order saddle point while all other tetrahedranes E_4H_4 where $E = C, Ge - Pb$ are energy minima. [9] Tetrahedrane structures have also been synthesized for substituted derivatives of the group-13 elements E_4R_4 where $E = B - In$ and $R = t$ -Bu, $Si(t$ -Bu) $_3$, $C(SiMe_3)_3$, $Si(SiMe_3)_3$, or $Si(GeMe_3)_3$. [11] A thallium compound $Tl_4[C(SiMe_3)_3]_4$ has also become isolated but the x-ray structure analysis showed that it has a distorted tetrahedron structure where the Tl-Tl-distances vary between 3.335 and 3.575 Å. [12] The only group-13 tetrahedrane compound which could become isolated without a bulky substituent is B_4Cl_4 . [13] Very few theoretical studies have been published about the PES of E_4H_4 where $E = B - Tl$. [10,14]

In this work we report about quantum chemical calculations using DFT and ab initio methods of the singlet potential energy surfaces of group-13 and group-14 species E_4H_4 where $E = B - Tl$ and $E = C - Pb$. The starting point of our study is the tetrahedrane structure of E_4H_4 . However, we systematically searched for other energy minima on the singlet PES

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3 with the goal to identify the global energy minimum for each species. We found more than
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5 40 different structures which are energy minima on at least one of the E_4H_4 PES. The
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7 complexity of the systems made it impractical to locate the transition states for
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9 interconversion of the minima. However, the results give an overview of the energetically
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11 lowest lying structures and particularly the global energy minimum for each E_4H_4 species. We
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13 also optimized the geometries of several substituted tetrahedranes E_4R_4 which are
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15 experimentally known.
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18 2. COMPUTATIONAL METHODS

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21 For all geometry optimizations of the E_4H_4 structures the gradient corrected hybrid
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23 density functional B3LYP [15] as implemented [16] in the Gaussian 03 program [17] was
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25 employed in conjunction with a triple zeta quality basis set with two sets of polarization
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27 functions (def2-TZVPP) [18]. The nature of the stationary point (minimum, transition state or
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29 higher order saddle point) was clarified by calculating the harmonic vibrational frequencies.
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31 For low lying transition states, intrinsic reaction coordinate (IRC) [19] calculations were
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33 performed in order to identify the minima connected to the transition states. In case of small
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35 imaginary modes, the verification was done by dynamic reaction path (DRP) [20] calculations
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37 using the frog module of the TURBOMOLE program [21]. The geometries of the parent
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39 tetrahedranes E_4H_4 have also been optimized using coupled-cluster theory at the CCSD(T)
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41 [22] level as implemented in the Molpro 2006.1 program [23] with a quadruple-zeta basis set
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43 with two sets of polarization functions (def2-QZVPP) [18]. Single-point energy calculations
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45 have been performed for selected E_4H_4 species at CCSD(T)/def2-QZVPP using B3LYP/def2-
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47 TZVPP optimized geometries.

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49 The substituted E_4R_4 tetrahedrane structures were optimized using the gradient
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51 corrected density functional BP86 [24] via an interface to TURBOMOLE for the energy and
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53 gradient calculations using the resolution of the identity (RI) approximation [26], and
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55 Gaussian 03 for the geometry optimization.
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3. RESULTS AND DISCUSSION

3.1. Substituted tetrahedranes E_4R_4 (E = B – Tl; C – Pb)

We optimized the geometries of the substituted group-13 tetrahedranes $B_4(t\text{-butyl})_4$, $Al_4[Si(t\text{-butyl})_3]_4$, $E_4[C(SiMe_3)_3]_4$ (E = Ga, In, Tl) and the group-14 tetrahedranes (E = Si, Ge, Sn, Pb) at RI-BP86/def2-TZVPP. The geometries of the latter compounds have been determined with x-ray structure analysis, except for $Sn_4[Si(t\text{-butyl})_3]_4$ and $Pb_4[Si(t\text{-butyl})_3]_4$ which have not been synthesized until now. Table 1 shows the calculated and experimental E-E and E-R distances.

Table 1

The optimizations of the E_4R_4 species were carried out with local T_d symmetry restriction of the E_4 core. Table 1 shows that the calculated E-E and E-R distances of the group-13 compounds where E = B – In are in reasonable agreement with the experimental values. The experimentally observed bond lengths in the solid state are shorter than the calculated data particularly for the heavier species Al – In. This can be explained with the effect of intermolecular interactions which yield a bond shortening that is more pronounced when the bonds are weaker. [28] The x-ray structure analysis of $Tl_4[C(SiMe_3)_3]_4$ reveals a significantly distorted tetrahedron core where the Tl-Tl distances vary between 3.322 – 3.638 Å. [12] A geometry optimization of $Tl_4[C(SiMe_3)_3]_4$ without symmetry restriction gave a structure which has Tl-Tl distances in the range of 3.436 – 3.687 Å and Tl-C distances between 2.434 – 2.462 Å. This agrees quite well with the experimental values. The calculated values for the group-14 tetrahedranes $C_4(t\text{-butyl})_4$, $Si_4[Si(t\text{-butyl})_3]_4$ and $Ge_4[Si(t\text{-butyl})_3]_4$ also agree quite well with the experimental values. [5,7,8] The differences between the slightly shorter distances which are calculated at the RI-BP86/def2-TZVPP level and the experimental data are at least partly due to solid state effects.

3.2. Parent tetrahedranes E_4H_4 ($E = B - Tl; C - Pb$)

Table 2

Table 2 shows the calculated E-E and E-H distances of the T_d structures of the group-13 and group-14 tetrahedranes E_4H_4 ($E = B - Tl$ and $C - Pb$) at RI-BP86/def2-TZVPP, B3LYP/def2-TZVPP and CCSD(T)/def2-QZVPP. The theoretically predicted bond lengths using DFT are in very good agreement with the highly accurate ab initio values. This is gratifying because the large number of structures which is discussed below could only become optimized at B3LYP/def2-TZVPP while the substituted systems were optimized at RI-BP86/def2-TZVPP.

While the geometries are very similar, there is a remarkable difference between the DFT results at RI-BP86/def2-TZVPP and B3LYP/def2-TZVPP for the silicon tetrahedrane Si_4H_4 . The calculation of the vibrational frequencies showed that the B3LYP/def2-TZVPP optimized structure is a minimum ($i = 0$) while the RI-BP86/def2-TZVPP optimized form has a degenerate imaginary mode ($i = 2$). It has already been noted before that the nature of the optimized tetrahedrane structure of Si_4H_4 depends on the level of theory. Jemmis and coworkers reported that Si_4H_4 (T_d) is a minimum at HF and B3LYP but it has two imaginary modes at MP2. [9f].

3.3. Potential energy surfaces of Group-13 Compounds E_4H_4 ($E = B - Tl$)

We made an extensive search for energy minima on the E_4H_4 singlet PES in order to locate not only local minima but also in order to find the global energy minima. We optimized numerous structures with and without symmetry constraints and calculated the vibrational frequencies in order to see if the species are energy minima. Whenever we found a transition state ($i = 1$) or higher order saddle point ($i > 2$) we located the associated energy minima. This procedure gave rise to 48 different structures which are shown in Figure 1.

Figure 1

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3 Many structures which are shown in Figure 1 are not relevant for the discussion in this
4 paper which focuses on find low-lying energy minima on the E_4H_4 singlet PES. They may be
5 helpful for future studies where pathways for rearrangement of the E_4H_4 isomers may be
6 important. The calculated relative energies at B3LYP/def2-TZVPP of the group-13
7 structures are shown in table 3. The bond lengths of the energetically lowest lying isomers
8 are given in figure 2.
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15 The red entries in table 3 denote the global energy minima on the E_4H_4 singlet PES
16 calculated at B3LYP/def2-TZVPP. The "classical" [26] tetrahedrane structures of aluminium
17 **1Al** and gallium **1Ga** are predicted to be the lowest lying isomers of the Al_4H_4 and Ga_4H_4
18 species. The classical tetrahedrane forms of B_4H_4 and In_4H_4 are also energy minima but the
19 calculations show that there are energetically more stable isomers. The planar structures **12B**
20 and **14B** are 11.7 and 4.7 kcal/mol lower in energy than **1B** and the former structure is
21 predicted as global minimum on the B_4H_4 singlet PES. The global energy minimum for In_4H_4
22 is the quadruply hydrogen bridged **2In** which has also T_d symmetry. It can be considered as
23 "nonclassical" [26] tetrahedrane. The hydrogen atoms in **2In** are on top of each In_3 plane
24 where each hydrogen bridges three indium atoms. The isomer **2E** is also the global energy
25 minimum for $E = Tl$ while it is an energetically higher lying local minimum for $E = Al$ and E
26 = Ga (Table 3). The structure **2B**, however, is a saddle point with eight imaginary frequencies
27 which is 310.2 kcal/mol higher in energy than **1B**. This demonstrates once more that
28 chemical bonding of the elements of the first octal row is very different from the heavier
29 homologues. The reasons for this are well understood. [27] The B3LYP/def2-TZVPP
30 calculations of the indium compounds suggest that there are seven other isomers (**5In**, **6In**,
31 **21In**, **23In**, **29In**, **31In**, **34In**, **36In**, **38In**, **45In**,) lower in energy than **1In**.
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46 Figure 2, Table 3
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49 The quadruply hydrogen face-bridged structure **2Tl** is 62.7 kcal/mol lower in energy
50 than the tetrahedrane **1Tl** which has three imaginary frequencies and thus, is not a minimum
51 on the PES (Table 3). There are five other energy minima which are more stable than **1Tl**,
52 that is **11Tl**, **17Tl**, **21Tl**, **34Tl**, and **39Tl**. The second lowest-lying isomer **34Tl** has a very
53 interesting pseudo-tetrahedral structure where the four thallium atoms are connected to each
54 other through four hydrogen bonds (Figure 2).
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Table 4

Table 4 gives the relative energies of the energy minima structures at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. The ab initio data conform that the tetrahedrane structures **1Al** and **1Ga** are the global energy minima on the Al_4H_4 and Ga_4H_4 singlet PES, structures **2In** and **2Tl** are the most stable structures of In_4H_4 and Tl_4H_4 and **12B** is the energetically lowest lying singlet species for B_4H_4 . However, there are significant changes in the energy differences between the isomers when one goes from B3LYP/def2-TZVPP to CCSD(T)/def2-QZVPP. The ab initio calculations predicted that the planar form **12B** is only 5.7 kcal/mol lower in energy than the tetrahedrane **1B** while **14B** is even slightly less stable than **1B**. Overall, the tetrahedrane structures **1E** are calculated at the ab initio level to be more stable relative to the other isomers of all elements E compared with the DFT values. It is gratifying that both methods predict the same structures as global minima on the group-13 E_4H_4 singlet PES.

3.4. Potential energy surfaces of Group-14 Compounds E_4H_4 (E = C – Pb)

The relative energies of the group-14 structures E_4H_4 are shown in table 5. There are significant differences in the relative energies compared to the group-13 species (Table 4).

Table 5

The classical tetrahedran form **1E** is a minimum at the B3LYP/def2-TZVPP level only for E = C, Si while it is a third-order saddle point for E = Ge, Sn, Pb. As noted before, the T_d form **1Si** is a second-order saddle point at BP86/def2-TZVPP and MP2/def2-TZVPP. For all group-14 E_4H_4 species holds that there are several energy minima which are much lower in energy than the classical tetrahedrane form **1E**. The calculated energies in Table 5 show that there are seven C_4H_4 carbon isomers which are more stable than **1C**. The global energy minimum form is the vinylideneacetylene isomer **27C** (-63.7 kcal/mol) which is slightly lower in energy than the cummulene **40C** (-60.4 kcal/mol). The other energy minima **16C** (-7.1 kcal/mol), **20C** (-24.5 kcal/mol), **18C** (-8.8 kcal/mol), **24C** (-27.5 kcal/mol) and **44C** (-16.0 kcal/mol) are clearly less stable than **27C**.

The global energy minimum structure for Si_4H_4 is the singly hydrogen edge-bridged tetrahedrane structure **18Si** which is 46.8 kcal/mol lower in energy than **1Si**. There are six other local minima on the Si_4H_4 PES which possess a distorted tetrahedrane Si_4 core and which are lower in energy than **1Si**. They are in descending order **44Si** (-41.7 kcal/mol), **8Si** (-31.0 kcal/mol), **10Si** (-29.2 kcal/mol), **16Si** (-26.3 kcal/mol), **9Si** (-25.2 kcal/mol) and **3Si** (-24.3 kcal/mol).

The global energy minimum for the heavier group-14 systems E_4H_4 where $\text{E} = \text{Ge}, \text{Sn}, \text{Pb}$ is the quadruply hydrogen edge-bridged tetrahedrane structure **3E** which is for all three elements much lower in energy than **1E**. The energy difference between the classical tetrahedrane form and **3E** is 67.2 kcal/mol for $\text{E} = \text{Ge}$, 88.8 kcal/mol for $\text{E} = \text{Sn}$ and 125.1 kcal/mol for $\text{E} = \text{Pb}$. However, there are several other isomeric forms of the latter species which have a distorted E_4 core that are close in energy to **3E**. For the germanium compounds there are four isomers **4Ge** (-61.8 kcal/mol), **8Ge** (-64.1 kcal/mol), **18Ge** (-65.5 kcal/mol) and **44Ge** (-60.9 kcal/mol) which are < 10 kcal/mol less stable than **3Ge**. The tin isomers **4Sn** (-83.9 kcal/mol) and **8Sn** (-78.9 kcal/mol) are also within a range of 10 kcal/mol of the global energy minimum **3Sn**. The lead structure **4Pb** (-120.7 kcal/mol) is only 4.4 kcal/mol higher in energy than **3Pb** (Table 5). Altogether, we located 12 energy minima for Ge_4H_4 and Sn_4H_4 and 11 energy minima for Ge_4H_4 at B3LYP/def2-TZVPP.

Table 6

Table 6 gives the relative energies of the group-14 isomers of E_4H_4 which are calculated at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. The ab initio data give the same global energy minima as the DFT values except for the germanium system Ge_4H_4 . The energetically lowest lying form at CCSD(T)/def2-QZVPP is **18Ge** while the calculations at B3LYP/def2-TZVPP predict that **3Ge** is the global energy form. However, the energy difference between **18Ge** and **3Ge** at both levels of theory is very small. The ab initio calculations suggest that **18Ge** is 1.7 kcal/mol lower in energy than the second lowest-lying isomer **3Ge** while the DFT calculations give the same energy difference but in favor of **3Ge** (Table 5). Note that the CCSD(T)/def2-QZVPP calculation predict that **44Ge** is another isomer which is only slightly less stable by 3.2 kcal/mol than **18Ge**. The energy difference between **18Ge** and **44Ge** at B3LYP/def2-TZVPP is 4.6 kcal/mol. Generally, the calculated

energy differences between the isomers of E_4H_4 at CCSD(T)/def2-QZVPP (Table 6) are not very different from the B3LYP/def2-TZVPP values (Table 5).

4. SUMMARY

The calculations which are presented in this work show that there are numerous energy minima on the singlet PES for E_4H_4 of the elements of groups 13 and 14. This holds particularly for the heavier atoms. The classical T_d tetrahedron structure is energetically more favourable for the group-13 compounds E_4H_4 where the tetrahedron isomers are energy minima for all elements E except for thallium. The tetrahedranes Al_4H_4 **1A** and Ga_4H_4 **1Ga** are the global energy minima on the singlet PES while **1B** is slightly less stable than the singly hydrogen-bridged planar form **12B** which has a rhombic B_4 core. The lowest-lying energy minima for In_4H_4 and Tl_4H_4 are tetrahedranes where the E_4 core is face-bridged by the hydrogen atoms. The classical T_d tetrahedron structure of the group-14 elements is only for carbon and silicon an energy minimum at B3LYP/def2-TZVPP. The latter form of Si_4H_4 is a third-order saddle point at BP86/def2-TZVPP and MP2/def2-TZVPP. The global energy minimum form for C_4H_4 is the vinylideneacetylene isomer **27C** which is -63.7 kcal/mol lower in energy than the tetrahedrane. The most stable isomers of Si_4H_4 and Ge_4H_4 at CCSD(T)/def2-QZVPP are the singly hydrogen edge-bridged tetrahedrane structures **18E** which are more than 40 kcal/mol lower in energy than the classical tetrahedrane. The B3LYP/def2-TZVPP calculations predict that tetrahedrane structure with edge-bridging hydrogen atoms **3Ge** is slightly more stable than **18Ge**. The former isomer is calculated as global energy minimum on the singlet PES of Sn_4H_4 and Pb_4H_4 .

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Figure Captions

Figure 1. Optimized E₄H₄ structures at B3LYP/def2-TZVPP.

Figure 2. Selected calculated bond lengths and angles (in Ångstroms and degrees) of the energetically lowest-lying E₄H₄ structures at B3LYP/def2-TZVPP.

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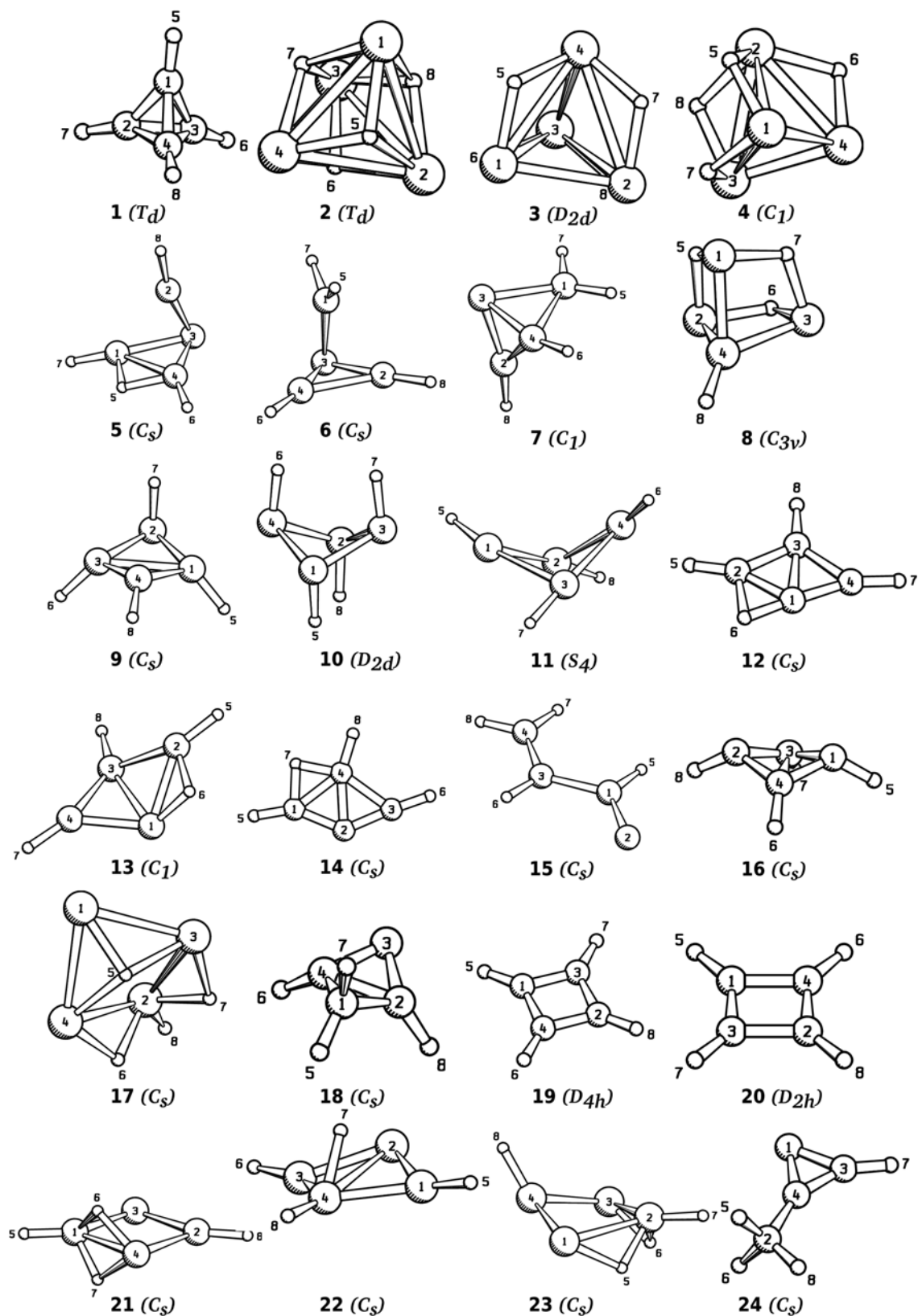


Figure 1

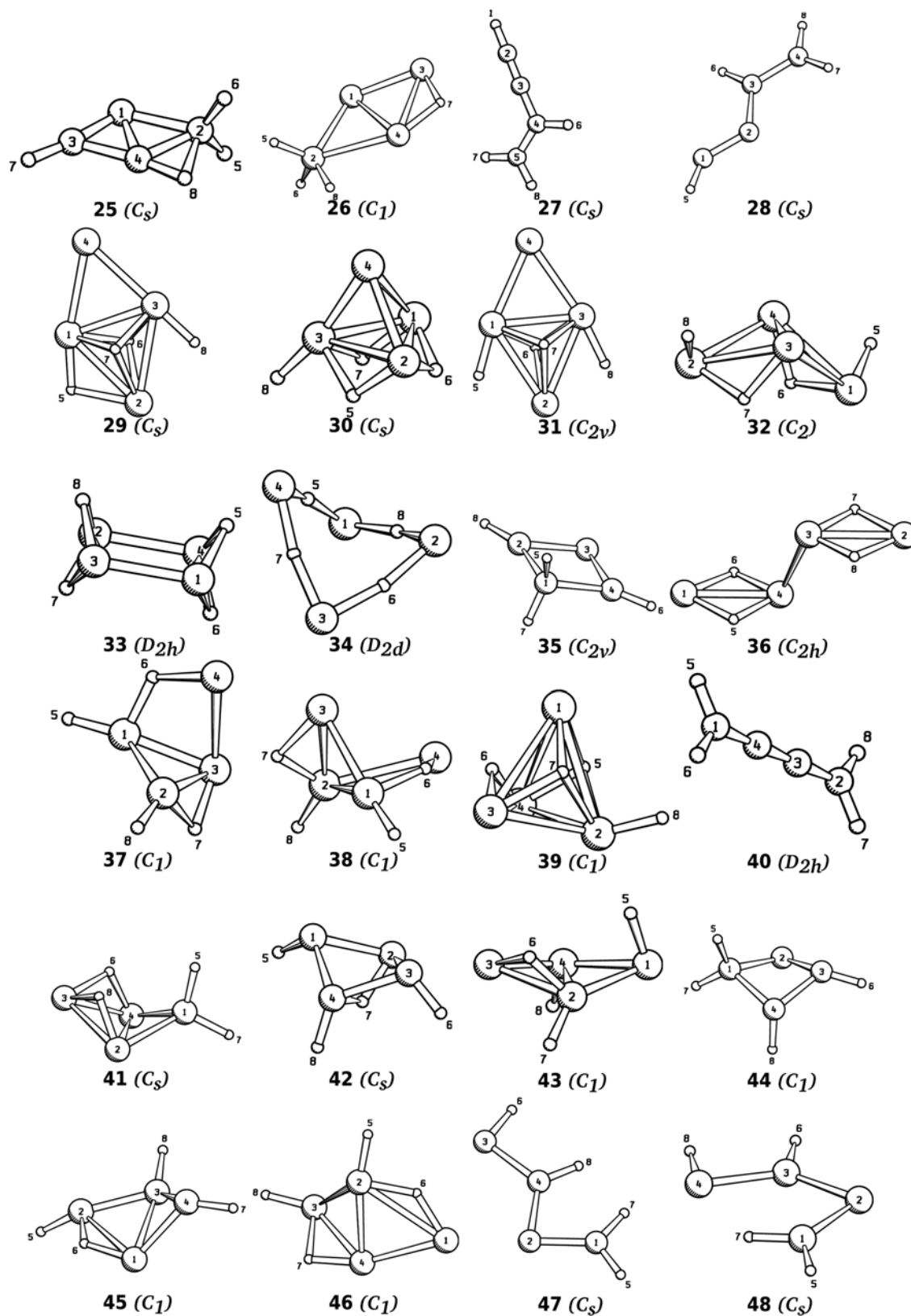


Figure 1 (continued)

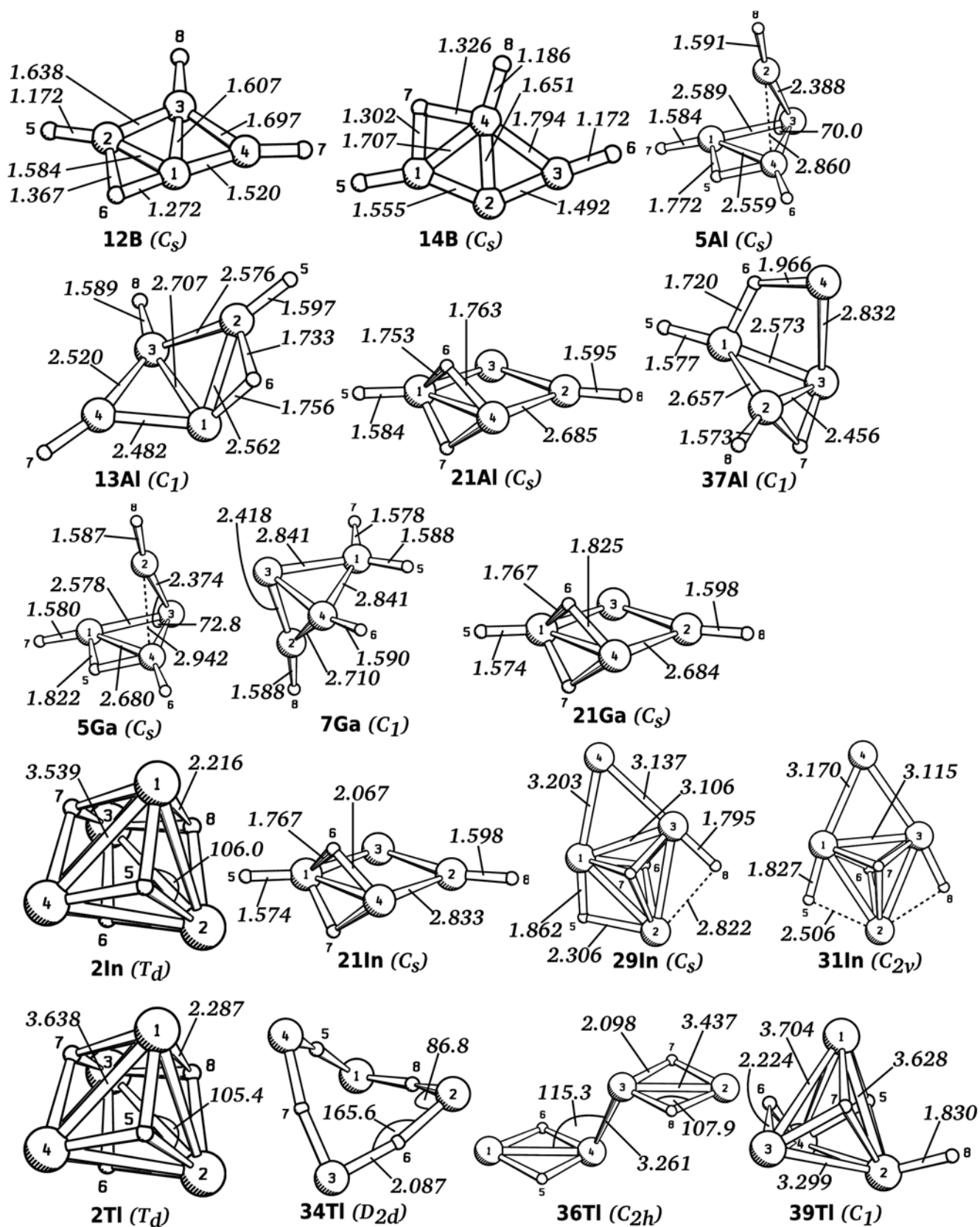


Figure 2

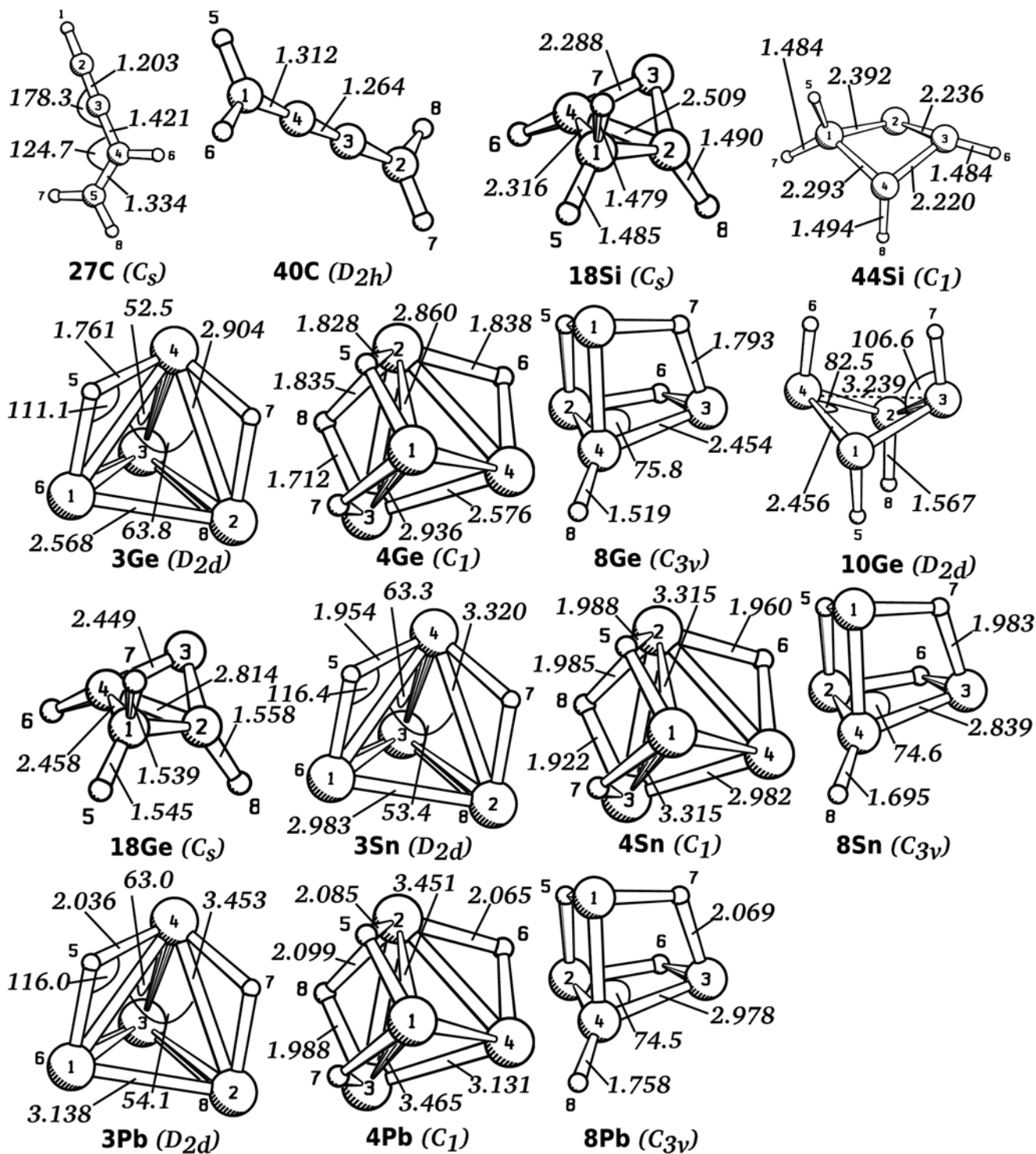


Figure 2 (continued)

Table 1. Calculated E_4R_4 bond lengths [\AA] for $E = B - Tl$ and $C - Pb$ at RI-BP86/def2-TZVPP .

structure	$d(E-E)_{\text{calc}}$	$d(E-R)_{\text{calc}}$	$d(E-E)_{\text{exp}}$	$d(E-R)_{\text{exp}}$
$B_4(t\text{-Bu})_4$	1.699	1.582	1.699 – 1.714 ^a	1.570 – 1.576 ^a
$Al_4[\text{Si}(t\text{-Bu})_3]_4$	2.627	2.534	2.600 – 2.612 ^b	2.467 – 2.501 ^b
$Ga_4[\text{C}(\text{SiMe}_3)_3]_4$	2.751	2.116	2.678 – 2.702 ^c	2.06 – 2.11 ^c
$In_4[\text{C}(\text{SiMe}_3)_3]_4$	3.098	2.317	2.989 – 3.013 ^e	2.24 – 2.26 ^d
$Tl_4[\text{C}(\text{SiMe}_3)_3]_4$	3.411	2.448	3.322 – 3.638 ^f	2.33 – 2.38 ^f
$C_4(t\text{-Bu})_4$	1.499	1.503	1.480 – 1.487 ^g	1.480 - 1.503 ^g
$Si_4[\text{Si}(t\text{-Bu})_3]_4$	2.362	2.400	2.315 – 2.320 ^h	2.355 – 2.365 ^h
$Ge_4[\text{Si}(t\text{-Bu})_3]_4$	2.508	2.440	2.431 – 2.447 ⁱ	2.378 – 2.385 ⁱ
$Sn_4[\text{Si}(t\text{-Bu})_3]_4$	2.891	2.642	-	-
$Pb_4[\text{Si}(t\text{-Bu})_3]_4$	3.076	2.738	-	-

Experimental values were taken from a) ref. 29, b) ref. 30, c) ref. 31, d) ref. 32, e) ref. 12, f) ref. 5, g) ref. 7, h) ref. 8

Table 2. Calculated E₄H₄ bond lengths [Å] of the tetrahedrane structures **1E** at RI-BP86/def2-TZVPP, B3LYP/def2-TZVPP and CCSD(T)/def2-QZVPP.

	RI-BP86/def2-TZVPP		B3LYP/def2-TZVPP		CCSD(T)/def2-QZVPP	
	d(E-E)	d(E-H)	d(E-E)	d(E-H)	d(E-E)	d(E-H)
1B	1.684	1.191	1.676	1.181	1.685	1.183
1Al	2.597	1.603	2.591	1.590	2.592	1.590
1Ga	2.556	1.586	2.568	1.582	2.604	1.596
1In	2.944	1.765	2.962	1.763	2.984	1.775
1Tl	3.133	1.836	3.194	1.843	3.155	1.847
1C	1.483	1.076	1.474	1.068	1.480	1.069
1Si	2.324	1.483	2.316	1.472	2.317	1.472
1Ge	2.471	1.540	2.469	1.531	2.478	1.533
1Sn	2.881	1.726	2.879	1.715	2.877	1.718
1Pb	3.126	1.820	3.143	1.813	3.100	1.810

Table 3. Calculated E_4H_4 energies in kcal/mol for all group-13 elements at B3LYP/def2-TZVPP relative to **1E**. All values in kcal/mol. The values for the global energy minima are given in red.

	B	Al	Ga	In	Tl
1 T_d	0.0	0.0	0.0	0.0	0.0 (i = 3)
2 T_d	310.2 (i = 8)	34.3	7.9	-26.6	-62.7
3 D_{2d}	150.3 (i = 2)	47.5 (i = 3)	→ 34Ga	→ 34In	→ 34Tl
4 C_I	→ 12B	→ 29Al	→ 29Ga	→ 2In	→ 2Tl
5 C_s	→ 14B	5.5	4.8	-3.5	rearr.
6 C_s	25.5 (i = 1)	11.7 (i = 1)	3.7 (i = 1)	-3.7	-17.0 (i = 2)
7 C_I	n/c	n/c	3.4	n/c	n/c
8 C_{3v}	135.5 (i = 3)	35.7	23.5 (i = 2)	-6.1 (i = 2)	rearr.
9 C_s	→ 12B	→ 11Al	→ 22Ga	→ 23In	→ 23Tl
10 D_{2d}	45.8	→ 1Al	→ 11Ga	18.6 (i=1)	-5.3 (i = 3)
11 S_4	→ 1B	33.4	23.9	10.9 (i=1)	-13.5
12 C_s	-11.7	16.1 (i = 1)	6.8 (i = 1)	4.3 (i = 1)	1.5 (i = 1)
13 C_I	n/c	14.4	5.9	-1.7	n/c
14 C_s	-4.7	14.7 (i = 1)	9.1 (i = 1)	10.7 (i = 2)	rearr.
16 C_s	→ 19B	→ 1Al	→ 1Ga	→ 1In	→ 17Tl
17 C_s	n/c	n/c	n/c	n/c	-33.8
18 C_s	49.9 (i = 1)	→ 6Al	→ 35Ga	→ 6In	→ 6Tl
19 D_{4h}	0.6 (i = 3)	34.1 (i = 1)	25.7 (i = 3)	17.1 (i = 1)	18.2 (i = 1)

1							
2							
3							
4	20	D_{2h}	36.8 (i = 2)	44.6 (i = 3)	→ 19Ga	→ 19In	31.0 (i = 4)
5							
6	21	C_s	→ 35B	13.4	0.3	-13.4	-30.3
7							
8	22	C_s	→ 14B	24.0 (i = 1)	14.4 (i=2)	5.4 (i = 2)	-5.6 (i = 2)
9							
10	23	C_s	→ 12B	18.1	6.6	-5.7	-24.2 (i = 1)
11							
12	24	C_s	→ 25B	→ 25Al	27.4 (i = 1)	9.2	-9.4 (i = 1)
13							
14	25	C_s	38.1	29.4 (i = 1)	n/c	n/c	n/c
15							
16	27	C_s	→ 12B	→ 14Al	→ 14Ga	→ 12In	→ 28Tl
17							
18	29	C_s	rearr.	21.8	5.9	-17.1	→ 31Tl
19							
20	31	C_{2v}	→ 12B	22.4 (i = 1)	→ 29Ga	-17.1	rearr.
21							
22	32	C_2	→ 12B	→ 33Al	→ 33Ga	→ 36In	→ 2Tl
23							
24	33	D_{2h}	n/c	20.2	17.7 (i = 2)	n/c	n/c
25							
26	34	D_{2d}	298.7 (i = 3)	47.9 (i = 3)	18.4 (i = 3)	-16.6	-52.0
27							
28	35	C_{2v}	41.7 (i = 2)	31.8 (i = 1)	13.9	5.3 (i = 2)	-5.6 (i = 2)
29							
30	36	C_{2h}	130.3	22.1	8.3	-15.1	-43.9 (i=1)
31							
32	37	C_1	→ 12B	15.2	6.5	→ 38In	→ 38Tl
33							
34	38	C_1	n/c	n/c	n/c	-8.2	n/c
35							
36	39	C_1	n/c	n/c	n/c	n/c	-47.8
37							
38	40	D_{2h}	37.0	42.1 (i = 1)	26.2 (i = 1)	22.4 (i = 1)	21.2 (i = 1)
39							
40	45	C_1	n/c	n/c	5.9	-1.7	n/c
41							
42	46	C_1	n/c	n/c	n/c	n/c	-25.9 (i=1)
43							
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53	n/c: not calculated						
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55	rearr.: rearranges into another structure type						
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Table 4: Relative energies of group-13 E_4H_4 isomers at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. All values in kcal/mol. The values for the global energy minima are given in red.

	B	Al	Ga	In	Tl
1 T_d	0.0	0.0	0.0	0.0	0.0
2 T_d	n/c	41.8	19.5	-13.2	-58.7
5 C_s	n/c	6.2	6.5	1.4	n/c
6 C_s	n/c	n/c	n/c	1.5	n/c
7 C_1	n/c	n/c	6.9	n/c	n/c
8 C_{3v}	n/c	40.1	n/c	n/c	n/c
11 S_4	n/c	39.0	27.5	n/c	n/c
12 C_s	-5.7	n/c	n/c	n/c	n/c
13 C_1	n/c	18.0	11.7	7.0	n/c
14 C_s	0.9	n/c	n/c	n/c	n/c
17 C_s	n/c	n/c	n/c	n/c	-28.2
21 C_s	n/c	19.6	8.3	-3.3	-25.0
22 C_s	n/c	n/c	19.0	n/c	n/c
23 C_s	n/c	22.6	14.9	5.4	n/c
24 C_s	n/c	n/c	n/c	22.7	n/c
29 C_s	n/c	29.2	15.5	-5.8	n/c
31 C_{2v}	n/c	n/c	n/c	-5.8	n/c
33 D_{2h}	n/c	22.0	n/c	n/c	n/c
34 D_{2d}	n/c	n/c	n/c	4.6	-41.3
35 C_{2v}	n/c	n/c	22.4	n/c	n/c
36 C_{2h}	n/c	30.7	19.3	1.5	-35.1
37 C_1	n/c	19.5	12.8	n/c	n/c
38 C_1	n/c	n/c	n/c	1.6	n/c
39 C_1	n/c	n/c	n/c	n/c	-43.5
45 C_1	n/c	n/c	11.7	7.0	n/c

n/c: not calculated

Table 5. Calculated E_4H_4 energies in kcal/mol for all group-14 elements at B3LYP/def2-TZVPP relative to **1E**. All values in kcal/mol. The values for the global energy minima are given in red.

	C	Si	Ge	Sn	Pb
1 T_d	0.0	0.0	0.0 (i = 3)	0.0 (i = 3)	0.0 (i = 3)
2 T_d	298.8 (i = 8)	37.0	-13.0	-47.0	-88.1
3 D_{2d}	129.9 (i = 6)	-24.3	-67.2	-88.8	-125.1
4 C_1	→ 24C	→ 8Si	-61.8	-83.9	-120.7 (i = 1)
8 C_{3v}	91.5 (i = 3)	-31.0	-64.1	-78.9	-104.8
9 C_s	→ 16C	-25.2	-46.2	-52.3	→ 23Pb
10 D_{2d}	→ 1C	-29.2	-56.0	-62.1	-83.2
11 S_4	→ 20C	→ 10Si	26.4 (i = 7)	→ 10Sn	→ 32Pb
12 C_s	→ 20C	29.7 (i = 3)	12.1 (i = 3)	-0.9 (i = 4)	→ 4Pb
14 C_s	→ 27C	→ 15Si	→ 47Ge	→ 48Sn	rearr.
15 C_s	nc	0.3 (i = 1)	n/c	n/c	n/c
16 C_s	-7.1	-26.3	-44.8	→ 17Sn	→ 17Pb
17 C_s	n/c	n/c	n/c	-53.0	-80.0
18 C_s	-8.8	-46.8	-65.5	-67.8	→ 4Pb
19 D_{4h}	10.7 (i = 2)	81.8 (i = 6)	26.4 (i = 7)	-7.0 (i = 6)	-46.7 (i = 6)
20 D_{2h}	-24.5	-4.3 (i = 3)	-13.9 (i = 3)	-6.5 (i = 4)	→ 19Pb
21 C_s	→ 35C	→ 35Si	-28.8 (i = 1)	-46.8	-71.5
22 C_s	→ 44C	→ 42Si	→ 42Ge	→ 18Sn	→ 4Pb
23 C_s	→ 20C	-10.6 (i = 1)	→ 43Ge	-48.9 (i = 2)	-85.6

24	C_s	-27.5	-35.5 (i = 1)	-53.6 (i = 1)	-53.2 (i = 1)	→ 25Pb
26	C_I	n/c	n/c	n/c	n/c	-90.2
27	C_s	-63.7	→ 28Si	→ 28Ge	rearr.	rearr.
28	C_s	n/c	7.6 (i = 2)	-14.8 (i = 2)	n/c	n/c
29	C_s	→ 18C	→ 24Si	→ 30Ge	→ 41Sn	→ 41Pb
30	C_s	n/c	n/c	-56.1	n/c	n/c
31	C_{2v}	→ 35C	rearr.	rearr.	rearr.	rearr.
32	C_2	→ 44C	-8.9 (i = 1)	-44.6 (i=1)	-63.8	-98.7 (i=1)
34	D_{2d}	rearr.	→ 3Si	→ 3Ge	→ 3Sn	→ 3Pb
35	C_{2v}	16.5 (i = 1)	-40.6 (i = 1)	-57.9 (i = 1)	-60.3 (i = 1)	-71.6 (i = 1)
40	D_{2h}	-60.4	19.2 (i = 3)	8.1 (i = 3)	18.0 (i = 3)	31.8 (i = 1)
41	C_s	n/c	n/c	n/c	-44.9	-77.2 (i = 1)
42	C_s	n/c	11.9 (i = 2)	-20.5 (i = 2)	n/c	n/c
43	C_I	n/c	n/c	-47.8	n/c	n/c
44	C_I	-16.0	-41.7	-60.9	-62.0	→ 3Pb
47	C_s	n/c	n/c	-26.2 (i = 2)	n/c	n/c
48	C_s	n/c	n/c	n/c	-41.8 (i = 2)	n/c

n/c: not calculated

rearr.: rearranges into different structure type

Table 6: Relative energies of group-14 E₄H₄ isomers at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. All values in kcal/mol. The values for the global energy minima are given in red.

	C	Si	Ge	Sn	Pb
1 T _d	0.00	0.0	0.0	0.0	0.0
2 T _d	n/c	n/c	n/c	-35.9	n/c
3 D _{2d}	n/c	-21.2	-54.9	-74.1	-120.1
4 C ₁	n/c	n/c	-50.1	-69.4	-115.8
8 C _{3v}	n/c	-28.5	-53.9	-67.2	-101.7
9 C _s	n/c	-20.7	-36.4	-40.3	n/c
10 D _{2d}	n/c	-28.1	-48.2	-52.1	n/c
16 C _s	n/c	-22.5	-36.0	n/c	n/c
17 C _s	n/c	n/c	n/c	-40.6	n/c
18 C _s	n/c	-43.7	-56.6	-57.2	n/c
20 D _{2h}	-27.1	n/c	n/c	n/c	n/c
21 C _s	n/c	n/c	n/c	-35.8	n/c
24 C _s	-24.7	n/c	n/c	n/c	n/c
27 C _s	-60.6	n/c	n/c	n/c	n/c
30 C _s	n/c	n/c	-46.8	n/c	n/c
32 C ₂	n/c	n/c	-31.9	-48.4	-92.2
40 D _{2h}	-52.3	n/c	n/c	n/c	n/c
41 C _s	n/c	n/c	n/c	-30.0	n/c
43 C ₁	n/c	n/c	-36.7	n/c	n/c
44 C ₁	n/c	-38.8	-53.4	-53.1	n/c

n/c: not calculated

Supporting Information for:

**Tetrahedranes. A Theoretical Study of Singlet E₄H₄ Molecules (E = C – Pb
and B – Tl)**

By **ROBIN HAUNSCHILD** and **GERNOT FRENKING***

Table S1: Energies and coordinates of the calculated molecules

10B:

8

E(RB+HF-LYP) = -101.673657527

B	0.76573700	-0.76584500	-0.33330400
B	-0.76573700	0.76584500	-0.33330400
B	0.76584500	0.76573700	0.33330400
B	-0.76584500	-0.76573700	0.33330400
H	1.24654900	-1.22606800	-1.31433600
H	-1.22606800	-1.24654900	1.31433600
H	1.22606800	1.24654900	1.31433600
H	-1.24654900	1.22606800	-1.31433600

10Ge:

8

E(RB+HF-LYP) = -8310.59744785

Ge	0.00000000	1.61962200	0.44331600
Ge	0.00000000	-1.61962200	0.44331600
Ge	1.61962200	0.00000000	-0.44331600
Ge	-1.61962200	0.00000000	-0.44331600
H	0.00000000	1.44532100	2.00044900
H	-1.44532100	0.00000000	-2.00044900
H	1.44532100	0.00000000	-2.00044900
H	0.00000000	-1.44532100	2.00044900

10In:

8

E(RB+HF-LYP) = -763.202705902

In	0.00000000	2.07492700	0.40629400
In	0.00000000	-2.07492700	0.40629400
In	2.07492700	0.00000000	-0.40629400
In	-2.07492700	0.00000000	-0.40629400
H	0.00000000	2.79941800	2.03099600
H	-2.79941800	0.00000000	-2.03099600
H	2.79941800	0.00000000	-2.03099600

1
2
3 H 0.00000000 -2.79941800 2.03099600
4
5
6 10Pb:
7
8 8
9 E(RB+HF-LYP) = -774.193121064
10 Pb 0.00000000 1.99765500 0.51578600
11 Pb 0.00000000 -1.99765500 0.51578600
12 Pb 1.99765500 0.00000000 -0.51578600
13 Pb -1.99765500 0.00000000 -0.51578600
14 H 0.00000000 1.73090200 2.32859800
15 H -1.73090200 0.00000000 -2.32859800
16 H 1.73090200 0.00000000 -2.32859800
17 H 0.00000000 -1.73090200 2.32859800
18
19
20 10Si:
21 8
22 E(RB+HF-LYP) = -1160.39076157
23 Si 0.00000000 1.51939300 0.41838700
24 Si 0.00000000 -1.51939300 0.41838700
25 Si 1.51939300 0.00000000 -0.41838700
26 Si -1.51939300 0.00000000 -0.41838700
27 H 0.00000000 1.45563300 1.91157500
28 H -1.45563300 0.00000000 -1.91157500
29 H 1.45563300 0.00000000 -1.91157500
30 H 0.00000000 -1.45563300 1.91157500
31
32
33
34 10Sn:
35 8
36 E(RB+HF-LYP) = -859.940543098
37 Sn 0.00000000 1.89001700 0.49089200
38 Sn 0.00000000 -1.89001700 0.49089200
39 Sn 1.89001700 0.00000000 -0.49089200
40 Sn -1.89001700 0.00000000 -0.49089200
41 H 0.00000000 1.66233500 2.22979300
42 H -1.66233500 0.00000000 -2.22979300
43 H 1.66233500 0.00000000 -2.22979300
44 H 0.00000000 -1.66233500 2.22979300
45
46
47
48 10Tl:
49 8
50 E(RB+HF-LYP) = -692.683692501
51 Tl 0.00000000 2.15545200 0.60503900
52 Tl 0.00000000 -2.15545200 0.60503900
53 Tl 2.15408800 0.00000000 -0.60507200
54 Tl -2.15408800 0.00000000 -0.60507200
55 H 0.00000000 2.61112600 2.39771000
56 H -2.62219100 0.00000000 -2.39509900
57 H 2.62219100 0.00000000 -2.39509900
58 H 0.00000000 -2.61112600 2.39771000
59
60

11Al:

1
2
3
4 8
5 E(RB+HF-LYP) = -972.150787518
6 Al 0.00000000 1.82716700 0.26769900
7 Al 0.00000000 -1.82716700 0.26769900
8 Al 1.82716700 0.00000000 -0.26769900
9 Al -1.82716700 0.00000000 -0.26769900
10 H 0.00000000 3.20822200 1.05797400
11 H -3.20822200 0.00000000 -1.05797400
12 H 3.20822200 0.00000000 -1.05797400
13 H 0.00000000 -3.20822200 1.05797400
14

15
16 11Ga:

17 8
18 E(RB+HF-LYP) = -7701.98523261
19 Ga 0.00000000 1.76297300 0.29387000
20 Ga 0.00000000 -1.76297300 0.29387000
21 Ga 1.76297300 0.00000000 -0.29387000
22 Ga -1.76297300 0.00000000 -0.29387000
23 H 0.00000000 3.07970500 1.16584800
24 H -3.07970500 0.00000000 -1.16584800
25 H 3.07970500 0.00000000 -1.16584800
26 H 0.00000000 -3.07970500 1.16584800
27
28
29

30 11Ge:

31 8
32 E(RB+HF-LYP) = -8310.46625246
33 Ge 0.00000000 1.84854900 0.18829800
34 Ge 0.00000000 -1.84854900 0.18829800
35 Ge 1.84854900 0.00000000 -0.18829800
36 Ge -1.84854900 0.00000000 -0.18829800
37 H 0.00000000 3.44721700 0.61536900
38 H -3.44721700 0.00000000 -0.61536900
39 H 3.44721700 0.00000000 -0.61536900
40 H 0.00000000 -3.44721700 0.61536900
41
42
43
44

45 11In:

46 8
47 E(RB+HF-LYP) = -763.214864629
48 In -1.38074200 1.38074200 0.64863200
49 In -1.38074200 -1.38074200 -0.64863200
50 In 1.38074200 -1.38074200 0.64863200
51 In 1.38074200 1.38074200 -0.64863200
52 H -1.31435700 2.89431400 1.58250500
53 H 1.31435700 -2.89431400 1.58250500
54 H -2.89431400 -1.31435700 -1.58250500
55 H 2.89431400 1.31435700 -1.58250500
56
57
58

59 11Tl:

60 8
E(RB+HF-LYP) = -692.696834121
Tl -1.52323700 -1.52323700 0.61006900

1				
2				
3	TI	-1.52323700	1.52323700	-0.61006900
4	TI	1.52323700	-1.52323700	-0.61006900
5				
6	TI	1.52323700	1.52323700	0.61006900
7	H	-3.12568400	-1.27424100	1.49886300
8	H	3.12568400	1.27424100	1.49886300
9	H	1.27424100	-3.12568400	-1.49886300
10	H	-1.27424100	3.12568400	-1.49886300
11				

12Al:

8

E(RB+HF-LYP) = -972.178229668

16	Al	0.11606800	-1.39362900	0.00000000
17	Al	-2.06552100	-0.11352200	0.00000000
18	Al	0.00000000	1.36188700	0.00000000
19	Al	2.10373800	0.09269100	0.00000000
20	H	-3.63939300	-0.10026500	0.00000000
21	H	-1.56947500	-1.78045500	0.00000000
22	H	3.62209500	-0.32799900	0.00000000
23	H	-0.41893100	2.89216800	0.00000000
24				
25				

12B:

8

E(RB+HF-LYP) = -101.765371951

30	B	0.00000000	0.78077900	0.00000000
31	B	-1.34178400	-0.06174900	0.00000000
32	B	0.10934600	-0.82245100	0.00000000
33	B	1.42430700	0.24961100	0.00000000
34	H	-2.50059400	-0.23961200	0.00000000
35	H	-1.16441100	1.29359500	0.00000000
36	H	2.59630700	0.21647000	0.00000000
37	H	0.10935500	-2.00140400	0.00000000
38				
39				

12Ga:

8

E(RB+HF-LYP) = -7702.01257832

44	Ga	-0.09329800	-1.52958700	0.00000000
45	Ga	2.04500900	0.08025000	0.00000000
46	Ga	0.00000000	1.34117100	0.00000000
47	Ga	-2.01283200	0.08023100	0.00000000
48	H	3.60297300	0.14561000	0.00000000
49	H	1.67507600	-1.62111200	0.00000000
50	H	-3.43284600	-0.55987200	0.00000000
51	H	0.04953300	2.90136200	0.00000000
52				
53				

12Ge:

8

E(RB+HF-LYP) = -8310.48894881

58	Ge	2.07640000	-0.09500400	0.00000000
59	Ge	-0.20622600	-1.65679200	0.00000000
60	Ge	-1.79712500	0.23709100	0.00000000
	Ge	0.00000000	1.56805300	0.00000000

H	-0.38824900	-3.18920000	0.00000000
H	1.39045700	-1.65778600	0.00000000
H	-0.02065900	3.11755800	0.00000000
H	-3.31911200	0.02229800	0.00000000

12In:

8

E(RB+HF-LYP) = -763.225471654

In	-0.07453900	-1.81446000	0.00000000
In	2.33604200	0.16628800	0.00000000
In	0.00000000	1.52210900	0.00000000
In	-2.30263100	0.10348000	0.00000000
H	4.04966800	0.31620200	0.00000000
H	1.93605400	-1.67548800	0.00000000
H	-3.79561200	-0.76841400	0.00000000
H	-0.17481500	3.23426400	0.00000000

12Si:

8

E(RB+HF-LYP) = -1160.29688745

Si	2.01031300	-0.04496500	0.00000000
Si	-0.05753900	-1.28535900	0.00000000
Si	-1.84663000	0.17196800	0.00000000
Si	0.00000000	1.25631700	0.00000000
H	-0.16797600	-2.77302900	0.00000000
H	1.57976900	-1.52738600	0.00000000
H	0.42291600	2.68848900	0.00000000
H	-3.32072800	0.24047500	0.00000000

12Sn:

8

E(RB+HF-LYP) = -859.843041061

Sn	2.41013900	-0.11577200	0.00000000
Sn	-0.24111400	-1.92765800	0.00000000
Sn	-2.11266500	0.26928700	0.00000000
Sn	0.00000000	1.81911700	0.00000000
H	-0.25295800	-3.65533500	0.00000000
H	1.53770800	-1.81207300	0.00000000
H	-0.37154200	3.51577000	0.00000000
H	-3.73119300	-0.29707300	0.00000000

12Tl:

8

E(RB+HF-LYP) = -692.672857918

Tl	0.00342800	-1.90453400	0.00000000
Tl	-2.42038600	0.26901400	0.00000000
Tl	0.00000000	1.53349700	0.00000000
Tl	2.43690700	0.08166400	0.00000000
H	-4.04224200	0.85692900	0.00000000
H	-2.20593300	-1.55580100	0.00000000
H	3.98955800	-0.79803600	0.00000000

1				
2				
3	H	0.64272600	3.14597400	0.00000000
4				
5				
6	13Al:			
7	8			
8	E(RB+HF-LYP) =	-972.180964053		
9	Al	-0.05544600	-1.33049400	0.52459300
10	Al	1.95339800	-0.03562000	-0.39707800
11	Al	-0.06426100	1.37165100	0.36900900
12	Al	-1.97512400	-0.07004800	-0.41739100
13	H	3.52059200	-0.07224000	-0.58835800
14	H	1.48611300	-1.69603400	-0.23226500
15	H	-3.52240000	-0.29508400	-0.65595000
16	H	0.35431400	2.90199400	0.44785200
17				
18				
19				
20	13Ga:			
21	8			
22	E(RB+HF-LYP) =	-7702.01403854		
23	Ga	-0.20288300	1.50919400	0.23923700
24	Ga	2.04100400	0.01841600	-0.24735800
25	Ga	0.08114400	-1.34491600	0.27599200
26	Ga	-1.97855600	-0.15556900	-0.25735400
27	H	3.58340400	0.26401700	-0.09738500
28	H	1.45261400	1.68341600	-0.34660800
29	H	-3.50107100	0.09980800	0.02374200
30	H	0.30305800	-2.88809900	0.09422600
31				
32				
33				
34	13In:			
35	8			
36	E(RB+HF-LYP) =	-763.234939018		
37	In	0.40537700	1.75174500	0.35875600
38	In	-2.42335700	0.08928300	-0.37267100
39	In	-0.21692300	-1.51360800	0.46023600
40	In	2.27495300	-0.30526400	-0.43713300
41	H	-3.97456700	0.89562900	-0.19104000
42	H	-1.33630400	1.75784200	-0.55762000
43	H	3.90303300	-0.54264600	0.20250600
44	H	-0.55465100	-3.19647100	0.09597100
45				
46				
47				
48	14Al:			
49	8			
50	E(RB+HF-LYP) =	-972.180478976		
51	Al	2.06288100	0.06854000	0.00000000
52	Al	0.00000000	1.39171100	0.00000000
53	Al	-2.08422100	0.27873100	0.00000000
54	Al	-0.07919200	-1.40039200	0.00000000
55	H	3.63036700	0.15905000	0.00000000
56	H	-3.63180600	-0.02666100	0.00000000
57	H	1.65955100	-1.57326900	0.00000000
58	H	-0.35119300	-2.96078500	0.00000000
59				
60				

14B:

1
2
3
4 8
5 E(RB+HF-LYP) = -101.754093641
6 B -1.35068500 -0.24224400 0.00000000
7 B 0.08220700 -0.84653900 0.00000000
8 B 1.45119700 -0.25231300 0.00000000
9 B 0.00000000 0.80230700 0.00000000
10 H -2.51231800 -0.43893400 0.00000000
11 H 2.55680500 0.13638300 0.00000000
12 H -1.30121900 1.05876900 0.00000000
13 H 0.34313500 1.93772700 0.00000000
14

15
16 14Ga:

17 8
18 E(RB+HF-LYP) = -7702.00884906
19 Ga 2.00968700 0.09071300 0.00000000
20 Ga 0.00000000 1.37980300 0.00000000
21 Ga -1.97671100 0.15382600 0.00000000
22 Ga -0.07930200 -1.47553700 0.00000000
23 H 3.56186600 0.12136200 0.00000000
24 H -3.51271500 -0.10097900 0.00000000
25 H 1.67041500 -1.60396000 0.00000000
26 H -0.28346200 -3.02937700 0.00000000
27
28
29

30 14In:

31 8
32 E(RB+HF-LYP) = -763.215262054
33 In -2.27218900 0.09906700 0.00000000
34 In 0.00000000 1.63924500 0.00000000
35 In 2.20598100 0.08951300 0.00000000
36 In 0.09443100 -1.71818500 0.00000000
37 H -3.97551200 -0.14640400 0.00000000
38 H 3.92313000 0.00000000 0.00000000
39 H -1.77757800 -1.82061600 0.00000000
40 H 0.44702300 -3.40900000 0.00000000
41
42
43
44

45 15Si:

46 8
47 E(RB+HF-LYP) = -1160.34371743
48 Si -0.16573500 -1.20567200 0.00000000
49 Si -2.05745000 -2.35148800 0.00000000
50 Si 0.00000000 1.06604300 0.00000000
51 Si 1.86539100 2.13462200 0.00000000
52 H 1.15561700 -1.88532600 0.00000000
53 H -1.25920100 1.83896200 0.00000000
54 H 3.15948200 1.43080900 0.00000000
55 H 1.95322100 3.60648400 0.00000000
56
57
58

59 16C:

60 8
E(RB+HF-LYP) = -154.711848828
C 0.57576100 0.99246100 0.00000000

1				
2				
3	C	-0.07877700	-1.14472000	0.00000000
4	C	-0.07877700	0.02411900	0.82446500
5	C	-0.07877700	0.02411900	-0.82446500
6	C	-0.07877700	0.02411900	-0.82446500
7	H	0.38668600	2.05529000	0.00000000
8	H	-0.79612800	0.24392000	-1.60983500
9	H	-0.79612800	0.24392000	1.60983500
10	H	-0.83100400	-1.91900200	0.00000000
11				
12				
13	16Ge:			
14	8			
15	E(RB+HF-LYP) =	-8310.57971449		
16	Ge	0.24901200	-2.02457100	0.00000000
17	Ge	-0.84271600	1.68017200	0.00000000
18	Ge	0.24901200	0.12985700	1.38718800
19	Ge	0.24901200	0.12985700	-1.38718800
20	Ge	0.24901200	0.12985700	-1.38718800
21	H	1.85057100	-1.87520000	0.00000000
22	H	1.09253900	0.68251500	-2.57249800
23	H	1.09253900	0.68251500	2.57249800
24	H	1.09253900	0.68251500	2.57249800
25	H	-0.97386200	3.22012100	0.00000000
26				
27	16Si:			
28	8			
29	E(RB+HF-LYP) =	-1160.38620187		
30	Si	0.24721300	-1.89743700	0.00000000
31	Si	-0.93606000	1.51491300	0.00000000
32	Si	-0.93606000	1.51491300	0.00000000
33	Si	0.24721300	0.11413300	1.25160800
34	Si	0.24721300	0.11413300	-1.25160800
35	H	1.77402200	-1.88553600	0.00000000
36	H	1.05885600	0.53316100	-2.42734000
37	H	1.05885600	0.53316100	-2.42734000
38	H	1.05885600	0.53316100	2.42734000
39	H	-1.16982900	2.97883300	0.00000000
40				
41	17Pb:			
42	8			
43	E(RB+HF-LYP) =	-774.187889467		
44	Pb	0.43335000	2.56099700	0.00000000
45	Pb	0.43335000	2.56099700	0.00000000
46	Pb	-0.11976300	-2.63511300	0.00000000
47	Pb	-0.11976300	-2.63511300	0.00000000
48	Pb	-0.11976300	0.04220900	1.68248700
49	Pb	-0.11976300	0.04220900	-1.68248700
50	H	-1.11228900	1.14111000	0.00000000
51	H	-1.49395000	0.37959900	-2.84726500
52	H	-1.49395000	0.37959900	-2.84726500
53	H	-1.49395000	0.37959900	2.84726500
54	H	-1.97293500	-2.74498500	0.00000000
55				
56	17Sn:			
57	8			
58	E(RB+HF-LYP) =	-859.926053347		
59	Sn	0.71115300	2.34314900	0.00000000
60	Sn	-0.19784300	-2.44614900	0.00000000
	Sn	-0.19784300	-2.44614900	0.00000000
	Sn	-0.19784300	0.05593600	1.57022200
	Sn	-0.19784300	0.05593600	-1.57022200

H	-1.02517100	1.33928500	0.00000000
H	-1.44339800	0.42067000	-2.74509000
H	-1.44339800	0.42067000	2.74509000
H	-1.96926200	-2.62420100	0.00000000

17Tl:

8

E(RB+HF-LYP) = -692.729132789

Tl	1.39266300	1.93765900	0.00000000
Tl	-0.44410500	-2.21084800	0.00000000
Tl	-0.44410500	0.16936500	2.05067500
Tl	-0.44410500	0.16936500	-2.05067500
H	-0.65900900	1.32383200	0.00000000
H	-1.67668600	-1.34220000	-1.48105900
H	-1.67668600	-1.34220000	1.48105900
H	-0.87574300	-3.94817900	0.00000000

18B:

8

E(RB+HF-LYP) = -101.667176072

B	0.00008400	1.26111100	0.00000000
B	0.00008400	-0.33581300	0.86219500
B	-0.00033900	-1.54350900	0.00000000
B	0.00008400	-0.33581300	-0.86219500
H	-1.03784200	1.83443800	0.00000000
H	0.00015100	0.55059500	-1.67893200
H	1.03797800	1.83449500	0.00000000
H	0.00015100	0.55059500	1.67893200

18C:

8

E(RB+HF-LYP) = -154.714616683

C	0.57285000	0.92145300	0.00000000
C	-0.19577100	-0.08503600	0.79909000
C	-0.19577100	-1.26034400	0.00000000
C	-0.19577100	-0.08503600	-0.79909000
H	0.25543800	1.96324400	0.00000000
H	-0.90825300	0.14682900	-1.58279400
H	1.64784700	0.79688100	0.00000000
H	-0.90825300	0.14682900	1.58279400

18Ge:

8

E(RB+HF-LYP) = -8310.61270979

Ge	0.52654300	1.87584000	0.00000000
Ge	-0.16369200	-0.01781400	1.40710200
Ge	-0.16369200	-2.02213700	0.00000000
Ge	-0.16369200	-0.01781400	-1.40710200
H	-0.18214700	3.24849300	0.00000000
H	-1.50115500	0.23880000	-2.16374000
H	2.04946700	2.09555000	0.00000000

1				
2				
3	H	-1.50115500	0.23880000	2.16374000
4				
5				
6	18Si:			
7	8			
8	E(RB+HF-LYP) =	-1160.41887853		
9	Si	-0.16937900	1.80509700	0.00000000
10	Si	-0.16937900	-0.14203300	1.25470400
11	Si	0.69332800	-1.84914700	0.00000000
12	Si	-0.16937900	-0.14203300	-1.25470400
13	H	-1.32352200	2.73995000	0.00000000
14	H	-1.18244000	-0.35885900	-2.32609600
15	H	1.09573400	2.57137600	0.00000000
16	H	-1.18244000	-0.35885900	2.32609600
17				
18				
19				
20	18Sn:			
21	8			
22	E(RB+HF-LYP) =	-859.949753719		
23	Sn	0.45749600	2.20632000	0.00000000
24	Sn	-0.13977000	-0.01137500	1.68696600
25	Sn	-0.13977000	-2.31674400	0.00000000
26	Sn	-0.13977000	-0.01137500	-1.68696600
27	H	-0.39164400	3.70772600	0.00000000
28	H	-1.82470200	0.17127700	-2.12839000
29	H	2.13170300	2.60840100	0.00000000
30	H	-1.82470200	0.17127700	2.12839000
31				
32				
33				
34	19Al:			
35	8			
36	E(RB+HF-LYP) =	-972.149572720		
37	Al	0.00000000	1.33114000	1.33114400
38	Al	0.00000000	-1.33114000	-1.33114400
39	Al	0.00000000	-1.33114000	1.33114400
40	Al	0.00000000	1.33114000	-1.33114400
41	H	0.00000000	2.45812800	2.45819600
42	H	0.00000000	2.45812800	-2.45819600
43	H	0.00000000	-2.45812800	2.45819600
44	H	0.00000000	-2.45812800	-2.45819600
45				
46				
47				
48	19B:			
49	8			
50	E(RB+HF-LYP) =	-101.745763189		
51	B	0.00000000	0.00000000	1.39630200
52	B	0.00000000	0.00000000	-1.39630200
53	B	0.00000000	0.79358800	0.00000000
54	B	0.00000000	-0.79358800	0.00000000
55	H	0.00000000	0.00000000	2.56776600
56	H	0.00000000	-1.97278400	0.00000000
57	H	0.00000000	1.97278400	0.00000000
58	H	0.00000000	0.00000000	-2.56776600
59				
60				

19C:

1
2
3
4 8
5 E(RB+HF-LYP) = -154.683574125
6 C 0.00000000 0.00000000 1.06536600
7 C 0.00000000 0.00000000 -1.06536600
8 C 0.00000000 0.96001600 0.00000000
9 C 0.00000000 -0.96001600 0.00000000
10 H 0.00000000 0.00000000 2.13461700
11 H 0.00000000 -2.04887000 0.00000000
12 H 0.00000000 2.04887000 0.00000000
13 H 0.00000000 0.00000000 -2.13461700
14

15
16 19Ga:

17 8
18 E(RB+HF-LYP) = -7701.98246619
19 Ga 0.00000000 1.29739400 1.29740200
20 Ga 0.00000000 -1.29739400 -1.29740200
21 Ga 0.00000000 1.29739400 -1.29740200
22 Ga 0.00000000 -1.29739400 1.29740200
23 H 0.00000000 2.41794800 2.41787400
24 H 0.00000000 -2.41794800 2.41787400
25 H 0.00000000 2.41794800 -2.41787400
26 H 0.00000000 -2.41794800 -2.41787400
27
28
29

30 19Ge:

31 8
32 E(RB+HF-LYP) = -8310.46622305
33 Ge 0.00000000 1.87812200 0.00000000
34 Ge 0.00000000 -1.87812200 0.00000000
35 Ge 1.87812200 0.00000000 0.00000000
36 Ge -1.87812200 0.00000000 0.00000000
37 H 0.00000000 3.53388600 0.00000000
38 H -3.53388600 0.00000000 0.00000000
39 H 3.53388600 0.00000000 0.00000000
40 H 0.00000000 -3.53388600 0.00000000
41
42
43
44

45 19In:

46 8
47 E(RB+HF-LYP) = -763.204994188
48 In 0.00000000 2.06556600 0.00000000
49 In 0.00000000 -2.06556600 0.00000000
50 In 2.06556600 0.00000000 0.00000000
51 In -2.06556600 0.00000000 0.00000000
52 H 0.00000000 3.81749300 0.00000000
53 H -3.81749300 0.00000000 0.00000000
54 H 3.81749300 0.00000000 0.00000000
55 H 0.00000000 -3.81749300 0.00000000
56
57
58

59 19Pb:

60 8
E(RB+HF-LYP) = -774.134888878
Pb 0.00000000 1.56211100 1.56213500

1				
2				
3	Pb	0.00000000	-1.56211100	-1.56213500
4	Pb	0.00000000	1.56211100	-1.56213500
5				
6	Pb	0.00000000	-1.56211100	1.56213500
7	H	0.00000000	2.89447300	2.89470200
8	H	0.00000000	-2.89447300	2.89470200
9	H	0.00000000	2.89447300	-2.89470200
10	H	0.00000000	-2.89447300	-2.89470200
11				
12				
13	19Si:			
14	8			
15	E(RB+HF-LYP) =	-1160.21381713		
16	Si	0.00000000	1.79891500	0.00000000
17	Si	0.00000000	-1.79891500	0.00000000
18	Si	1.79891500	0.00000000	0.00000000
19	Si	-1.79891500	0.00000000	0.00000000
20	H	0.00000000	3.38359700	0.00000000
21	H	-3.38359700	0.00000000	0.00000000
22	H	3.38359700	0.00000000	0.00000000
23	H	0.00000000	-3.38359700	0.00000000
24				
25				
26				
27	19Sn:			
28	8			
29	E(RB+HF-LYP) =	-859.852856650		
30	Sn	0.00000000	2.13638300	0.00000000
31	Sn	0.00000000	-2.13638300	0.00000000
32	Sn	2.13638300	0.00000000	0.00000000
33	Sn	-2.13638300	0.00000000	0.00000000
34	H	0.00000000	3.95757300	0.00000000
35	H	-3.95757300	0.00000000	0.00000000
36	H	3.95757300	0.00000000	0.00000000
37	H	0.00000000	-3.95757300	0.00000000
38				
39				
40				
41	19Tl:			
42	8			
43	E(RB+HF-LYP) =	-692.646212833		
44	Tl	0.00000000	2.11021100	0.00000000
45	Tl	0.00000000	-2.11021100	0.00000000
46	Tl	2.11021100	0.00000000	0.00000000
47	Tl	-2.11021100	0.00000000	0.00000000
48	H	0.00000000	3.89231700	0.00000000
49	H	-3.89231700	0.00000000	0.00000000
50	H	3.89231700	0.00000000	0.00000000
51	H	0.00000000	-3.89231700	0.00000000
52				
53				
54				
55	1Al:			
56	8			
57	E(RB+HF-LYP) =	-972.203952060		
58	Al	0.91592800	0.91592800	0.91592800
59	Al	-0.91592800	-0.91592800	0.91592800
60	Al	-0.91592800	0.91592800	-0.91592800
	Al	0.91592800	-0.91592800	-0.91592800

1
2
3 H 1.83411100 1.83411100 1.83411100
4 H -1.83411100 1.83411100 -1.83411100
5 H -1.83411100 -1.83411100 1.83411100
6 H 1.83411100 -1.83411100 -1.83411100
7
8

9 1B:

10 8

11 E(RB+HF-LYP) = -101.746668796

12 B 0.59249800 0.59249800 0.59249800
13 B -0.59249800 -0.59249800 0.59249800
14 B -0.59249800 0.59249800 -0.59249800
15 B 0.59249800 -0.59249800 -0.59249800
16 H 1.27420000 1.27420000 1.27420000
17 H -1.27420000 1.27420000 -1.27420000
18 H -1.27420000 -1.27420000 1.27420000
19 H 1.27420000 -1.27420000 -1.27420000
20
21
22

23 1C:

24 8

25 E(RB+HF-LYP) = -154.700564766

26 C 0.52123400 0.52123400 0.52123400
27 C -0.52123400 -0.52123400 0.52123400
28 C -0.52123400 0.52123400 -0.52123400
29 C 0.52123400 -0.52123400 -0.52123400
30 H 1.13794000 1.13794000 1.13794000
31 H -1.13794000 1.13794000 -1.13794000
32 H -1.13794000 -1.13794000 1.13794000
33 H 1.13794000 -1.13794000 -1.13794000
34
35
36

37 1Ga:

38 8

39 E(RB+HF-LYP) = -7702.02337014

40 Ga 0.90807300 0.90807300 0.90807300
41 Ga -0.90807300 -0.90807300 0.90807300
42 Ga -0.90807300 0.90807300 -0.90807300
43 Ga 0.90807300 -0.90807300 -0.90807300
44 H 1.82119600 1.82119600 1.82119600
45 H -1.82119600 1.82119600 -1.82119600
46 H -1.82119600 -1.82119600 1.82119600
47 H 1.82119600 -1.82119600 -1.82119600
48
49
50

51 1Ge:

52 8

53 E(RB+HF-LYP) = -8310.50829308

54 Ge 0.87289300 0.87289300 0.87289300
55 Ge -0.87289300 -0.87289300 0.87289300
56 Ge -0.87289300 0.87289300 -0.87289300
57 Ge 0.87289300 -0.87289300 -0.87289300
58 H 1.75663200 1.75663200 1.75663200
59 H -1.75663200 1.75663200 -1.75663200
60 H -1.75663200 -1.75663200 1.75663200

1
2
3 H 1.75663200 -1.75663200 -1.75663200
4
5
6 1In:
7
8
9 E(RB+HF-LYP) = -763.232284688
10 In 1.04717200 1.04717200 1.04717200
11 In -1.04717200 -1.04717200 1.04717200
12 In -1.04717200 1.04717200 -1.04717200
13 In 1.04717200 -1.04717200 -1.04717200
14 H 2.06498800 2.06498800 2.06498800
15 H -2.06498800 2.06498800 -2.06498800
16 H -2.06498800 -2.06498800 2.06498800
17 H 2.06498800 -2.06498800 -2.06498800
18
19
20 1Pb:
21
22 8
23 E(RB+HF-LYP) = -774.060473026
24 Pb 1.11103100 1.11103100 1.11103100
25 Pb -1.11103100 -1.11103100 1.11103100
26 Pb -1.11103100 1.11103100 -1.11103100
27 Pb 1.11103100 -1.11103100 -1.11103100
28 H 2.15788100 2.15788100 2.15788100
29 H -2.15788100 2.15788100 -2.15788100
30 H -2.15788100 -2.15788100 2.15788100
31 H 2.15788100 -2.15788100 -2.15788100
32
33
34 1Si:
35
36 8
37 E(RB+HF-LYP) = -1160.34422852
38 Si 0.81881800 0.81881800 0.81881800
39 Si -0.81881800 -0.81881800 0.81881800
40 Si -0.81881800 0.81881800 -0.81881800
41 Si 0.81881800 -0.81881800 -0.81881800
42 H 1.66878200 1.66878200 1.66878200
43 H -1.66878200 1.66878200 -1.66878200
44 H -1.66878200 -1.66878200 1.66878200
45 H 1.66878200 -1.66878200 -1.66878200
46
47
48 1Sn:
49
50 8
51 E(RB+HF-LYP) = -859.841665923
52 Sn 1.01791000 1.01791000 1.01791000
53 Sn -1.01791000 -1.01791000 1.01791000
54 Sn -1.01791000 1.01791000 -1.01791000
55 Sn 1.01791000 -1.01791000 -1.01791000
56 H 2.00803100 2.00803100 2.00803100
57 H -2.00803100 2.00803100 -2.00803100
58 H -2.00803100 -2.00803100 2.00803100
59 H 2.00803100 -2.00803100 -2.00803100
60

1Tl:

1
2
3
4 8
5 E(RB+HF-LYP) = -692.675261786
6 TI 1.12921300 1.12921300 1.12921300
7 TI -1.12921300 -1.12921300 1.12921300
8 TI -1.12921300 1.12921300 -1.12921300
9 TI 1.12921300 -1.12921300 -1.12921300
10 H 2.19311300 2.19311300 2.19311300
11 H -2.19311300 2.19311300 -2.19311300
12 H -2.19311300 -2.19311300 2.19311300
13 H 2.19311300 -2.19311300 -2.19311300
14

15
16 20Al:

17 8
18 E(RB+HF-LYP) = -972.132956259
19 Al 0.00000000 1.81266500 0.00000000
20 Al 0.00000000 -1.81266500 0.00000000
21 Al -1.81266500 0.00000000 0.00000000
22 Al 1.81266500 0.00000000 0.00000000
23 H 0.00000000 3.40605100 0.00000000
24 H 3.40605100 0.00000000 0.00000000
25 H -3.40605100 0.00000000 0.00000000
26 H 0.00000000 -3.40605100 0.00000000
27
28
29

30 20B:

31 8
32 E(RB+HF-LYP) = -101.688051651
33 B 0.00000000 0.95497500 0.74695800
34 B 0.00000000 -0.95497500 -0.74695800
35 B 0.00000000 0.95497500 -0.74695800
36 B 0.00000000 -0.95497500 0.74695800
37 H 0.00000000 1.16965900 1.89874400
38 H 0.00000000 -1.16965900 1.89874400
39 H 0.00000000 1.16965900 -1.89874400
40 H 0.00000000 -1.16965900 -1.89874400
41
42
43
44

45 20C:

46 8
47 E(RB+HF-LYP) = -154.739553668
48 C -0.78703000 0.66466000 -0.00001100
49 C 0.78703000 -0.66466000 0.00001100
50 C -0.78703000 -0.66466000 -0.00002000
51 C 0.78703000 0.66466000 0.00001400
52 H -1.54901100 1.42864000 -0.00003300
53 H 1.54901100 1.42864100 0.00006600
54 H -1.54901100 -1.42864100 -0.00000200
55 H 1.54901100 -1.42864000 0.00000900
56
57
58

59 20Ge:

60 8
E(RB+HF-LYP) = -8310.53047289
Ge 0.00000000 1.11602100 1.24727000

1				
2				
3	Ge	0.00000000	-1.11602100	-1.24727000
4	Ge	0.00000000	1.11602100	-1.24727000
5	Ge	0.00000000	-1.11602100	1.24727000
6	H	0.00000000	2.24645200	2.27634000
7	H	0.00000000	-2.24645200	2.27634000
8	H	0.00000000	2.24645200	-2.27634000
9	H	0.00000000	-2.24645200	-2.27634000
10				
11				
12	20Si:			
13	8			
14	E(RB+HF-LYP) =	-1160.35099338		
15	Si	0.00000000	1.06567700	1.18922700
16	Si	0.00000000	-1.06567700	-1.18922700
17	Si	0.00000000	1.06567700	-1.18922700
18	Si	0.00000000	-1.06567700	1.18922700
19	H	0.00000000	2.15736700	2.18156300
20	H	0.00000000	-2.15736700	2.18156300
21	H	0.00000000	2.15736700	-2.18156300
22	H	0.00000000	-2.15736700	-2.18156300
23				
24				
25				
26				
27	20Sn:			
28	8			
29	E(RB+HF-LYP) =	-859.852057062		
30	Sn	0.00000000	1.29151600	1.42586800
31	Sn	0.00000000	-1.29151600	-1.42586800
32	Sn	0.00000000	1.29151600	-1.42586800
33	Sn	0.00000000	-1.29151600	1.42586800
34	H	0.00000000	2.55379000	2.56491600
35	H	0.00000000	-2.55379000	2.56491600
36	H	0.00000000	2.55379000	-2.56491600
37	H	0.00000000	-2.55379000	-2.56491600
38				
39				
40				
41	20Tl:			
42	8			
43	E(RB+HF-LYP) =	-692.625793586		
44	Tl	0.00000000	2.05878900	0.00000000
45	Tl	0.00000000	-2.05878900	0.00000000
46	Tl	-2.05878900	0.00000000	0.00000000
47	Tl	2.05878900	0.00000000	0.00000000
48	H	0.00000000	3.84355800	0.00000000
49	H	3.84355800	0.00000000	0.00000000
50	H	-3.84355800	0.00000000	0.00000000
51	H	0.00000000	-3.84355800	0.00000000
52				
53				
54				
55	21Al:			
56	8			
57	E(RB+HF-LYP) =	-972.182568865		
58	Al	0.00000000	1.82635000	0.00000000
59	Al	0.09838800	-1.92320100	0.00000000
60	Al	1.93525900	0.00000000	0.00000000
	Al	-1.83326700	-0.05860500	0.00000000

1				
2				
3	H	-0.16238300	3.40226300	0.00000000
4	H	-1.13506100	1.10556600	1.12509200
5	H	-1.13506100	1.10556600	-1.12509200
6	H	-0.17244500	-3.49536500	0.00000000
7				
8				

21Ga:

8

E(RB+HF-LYP) = -7702.02292378

13	Ga	-1.87895900	0.03300000	0.00000000
14	Ga	1.91655400	0.05377900	0.00000000
15	Ga	0.00000000	1.85755000	0.00000000
16	Ga	0.03643400	-1.86126400	0.00000000
17	H	-3.44685800	-0.10702800	0.00000000
18	H	-1.16648000	-1.10702900	1.14686800
19	H	-1.16648000	-1.10702900	-1.14686800
20	H	3.48491900	-0.25395400	0.00000000
21				
22				

21Ge:

8

E(RB+HF-LYP) = -8310.55424394

27	Ge	-0.21298600	-1.39207600	0.00000000
28	Ge	0.00000000	1.37034600	0.00000000
29	Ge	-2.07992700	0.19061500	0.00000000
30	Ge	2.19801900	-0.10122200	0.00000000
31	H	0.05831700	-2.93970200	0.00000000
32	H	1.38230300	-1.07166400	1.09229900
33	H	1.38230300	-1.07166400	-1.09229900
34	H	0.21368500	2.91779900	0.00000000
35				
36				

21In:

8

E(RB+HF-LYP) = -763.253678344

41	In	-2.14173200	0.04637600	0.00000000
42	In	2.19326500	0.03131100	0.00000000
43	In	0.00000000	2.11948700	0.00000000
44	In	0.00000000	-2.13500600	0.00000000
45	H	-3.87151700	-0.18127900	0.00000000
46	H	-1.33343800	-1.24774700	1.23697600
47	H	-1.33343800	-1.24774700	-1.23697600
48	H	3.92730000	-0.36943500	0.00000000
49				
50				

21Pb:

8

E(RB+HF-LYP) = -774.174448734

55	Pb	-0.19399600	-1.82956600	0.00000000
56	Pb	0.00000000	1.70634400	0.00000000
57	Pb	-2.47745400	0.22650000	0.00000000
58	Pb	2.62850100	-0.07551700	0.00000000
59	H	0.49461600	-3.52353600	0.00000000
60	H	1.44859300	-1.13640600	1.20816400
	H	1.44859300	-1.13640600	-1.20816400

1
2
3 H 0.13007300 3.51990900 0.00000000
4
5
6 21Sn:
7
8
9 E(RB+HF-LYP) = -859.916281800
10 Sn -0.19699100 -1.66511100 0.00000000
11 Sn 0.00000000 1.60448300 0.00000000
12 Sn -2.37606900 0.21045300 0.00000000
13 Sn 2.50714000 -0.10304500 0.00000000
14 H 0.26267800 -3.35712400 0.00000000
15 H 1.41785900 -1.15876600 1.16035200
16 H 1.41785900 -1.15876600 -1.16035200
17 H 0.19762000 3.33568000 0.00000000
18
19
20 21Tl:
21
22
23 E(RB+HF-LYP) = -692.723575098
24 Tl -2.28566800 0.11601200 0.00000000
25 Tl 2.36458300 -0.04628900 0.00000000
26 Tl 0.00000000 2.13379900 0.00000000
27 Tl -0.04529800 -2.16249500 0.00000000
28 H -4.01540100 -0.29063200 0.00000000
29 H -1.42240400 -1.25385000 1.26725300
30 H -1.42240400 -1.25385000 -1.26725300
31 H 4.13716000 -0.52486000 0.00000000
32
33
34 22Al:
35
36
37 E(RB+HF-LYP) = -972.165639588
38 Al 0.23504800 0.00000000 2.04625900
39 Al 0.23504800 1.47106500 0.00000000
40 Al 0.23504800 0.00000000 -2.04625900
41 Al -0.53451200 -1.33006900 0.00000000
42 H 0.25540900 0.10098000 3.62508700
43 H 0.25540900 0.10098000 -3.62508700
44 H -1.31328700 0.35226000 0.00000000
45 H -1.41573700 -2.64388900 0.00000000
46
47
48 22Ga:
49
50
51 E(RB+HF-LYP) = -7702.00040653
52 Ga 0.15608800 -0.01808000 1.99240400
53 Ga 0.15608800 1.50185800 0.00000000
54 Ga 0.15608800 -0.01808000 -1.99240400
55 Ga -0.39405100 -1.38466900 0.00000000
56 H 0.03730300 0.13470400 3.54739500
57 H 0.03730300 0.13470400 -3.54739500
58 H -1.44492400 0.06338900 0.00000000
59 H -0.93033800 -2.84469800 0.00000000
60

22In:

1
2
3 8
4 E(RB+HF-LYP) = -763.223624684
5 In 2.24647500 0.00000000 -0.02344800
6 In 0.00000000 0.00000000 1.98294500
7 In -2.24647500 0.00000000 -0.02344800
8 In 0.00000000 0.00000000 -1.84150700
9 H 3.98036300 0.00000000 0.21820300
10 H -3.98036300 0.00000000 0.21820300
11 H 0.00000000 -1.57596200 -2.53626100
12 H 0.00000000 1.57596200 -2.53626100
13
14

15
16 22Tl:

17 8
18 E(RB+HF-LYP) = -692.684202831
19 Tl 2.31743600 0.00000000 -0.03098500
20 Tl 0.00000000 0.00000000 2.08174500
21 Tl -2.31743600 0.00000000 -0.03098500
22 Tl 0.00000000 0.00000000 -1.96536900
23 H 4.11340100 0.00000000 0.09786800
24 H -4.11340100 0.00000000 0.09786800
25 H 0.00000000 -1.65149200 -2.30216000
26 H 0.00000000 1.65149200 -2.30216000
27
28
29

30 23Al:

31 8
32 E(RB+HF-LYP) = -972.175190507
33 Al -0.37467600 0.05526500 2.04152200
34 Al 0.63896800 -1.39030800 0.00000000
35 Al -0.37467600 0.05526500 -2.04152200
36 Al 0.00000000 1.50667000 0.00000000
37 H -0.50909600 -1.53435600 1.29001900
38 H -0.50909600 -1.53435600 -1.29001900
39 H 1.53213000 -2.69632200 0.00000000
40 H 0.93492500 2.78755000 0.00000000
41
42
43
44

45 23Ga:

46 8
47 E(RB+HF-LYP) = -7702.01286271
48 Ga 0.19375100 -0.14432600 1.97459200
49 Ga 0.19375100 1.67750100 0.00000000
50 Ga 0.19375100 -0.14432600 -1.97459200
51 Ga -0.59663400 -1.50250100 0.00000000
52 H 1.25135500 1.19001300 1.30203300
53 H 1.25135500 1.19001300 -1.30203300
54 H 0.04594900 3.24294100 0.00000000
55 H -2.07185100 -2.09974600 0.00000000
56
57
58

59 23In:

60 8
E(RB+HF-LYP) = -763.241317970
In 0.21411600 -0.11188500 2.25593100

1				
2				
3	In	0.21411600	1.93658100	0.00000000
4	In	0.21411600	-0.11188500	-2.25593100
5				
6	In	-0.65728700	-1.79127000	0.00000000
7	H	1.38478800	1.31312900	1.43933400
8	H	1.38478800	1.31312900	-1.43933400
9	H	0.26642700	3.68120300	0.00000000
10	H	-2.30396500	-2.46293900	0.00000000
11				
12				
13	23Pb:			
14	8			
15	E(RB+HF-LYP) =	-774.196949559		
16	Pb	-0.52326400	-0.14871200	1.92118100
17	Pb	-0.52326400	2.15109700	0.00000000
18	Pb	-0.52326400	-0.14871200	-1.92118100
19	Pb	1.52288800	-1.85689200	0.00000000
20	H	1.41944700	-0.35226600	1.41072800
21	H	1.41944700	-0.35226600	-1.41072800
22	H	-2.32924600	2.56663800	0.00000000
23	H	3.33641200	-1.59817500	0.00000000
24				
25				
26				
27	23Si:			
28	8			
29	E(RB+HF-LYP) =	-1160.36107393		
30	Si	0.13524900	-0.06068100	2.02812800
31	Si	0.13524900	1.11971800	0.00000000
32	Si	0.13524900	-0.06068100	-2.02812800
33	Si	-0.49010200	-1.13399500	0.00000000
34	H	1.41766800	0.40043200	1.17078700
35	H	1.41766800	0.40043200	-1.17078700
36	H	0.28647300	2.59179000	0.00000000
37	H	-1.94082600	-1.49372300	0.00000000
38				
39				
40				
41	23Sn:			
42	8			
43	E(RB+HF-LYP) =	-859.919594460		
44	Sn	-0.22865300	-0.09940100	2.48655800
45	Sn	0.68981800	-1.27979100	0.00000000
46	Sn	-0.22865300	-0.09940100	-2.48655800
47	Sn	-0.22865300	1.53269100	0.00000000
48	H	-1.21122700	-1.21480200	1.36961700
49	H	-1.21122700	-1.21480200	-1.36961700
50	H	1.12165700	-2.94970800	0.00000000
51	H	1.10781700	2.67441000	0.00000000
52				
53				
54				
55	23Tl:			
56	8			
57	E(RB+HF-LYP) =	-692.713838881		
58	Tl	-0.10980900	0.01519500	2.17022500
59	Tl	-0.10980900	-2.32153500	0.00000000
60	Tl	-0.10980900	0.01519500	-2.17022500
	Tl	0.33859500	2.24584400	0.00000000

H	-1.01672800	1.72496100	1.54606900
H	-1.01672800	1.72496100	-1.54606900
H	0.97082400	-3.81886100	0.00000000
H	0.32008400	4.03833400	0.00000000

24C:

8

E(RB+HF-LYP) = -154.744302845

C	-0.21172100	-1.36488700	0.00000000
C	-0.69978400	1.35351400	0.00000000
C	1.04327400	-0.72926700	0.00000000
C	-0.03493600	0.04074000	0.00000000
H	-1.34840200	1.42528000	-0.87535800
H	-1.34840200	1.42528000	0.87535800
H	2.11654200	-0.83995700	0.00000000
H	0.00000000	2.18789800	0.00000000

24Ga:

8

E(RB+HF-LYP) = -7701.97969785

Ga	0.53504200	-2.03862600	0.00000000
Ga	1.35232000	2.73831000	0.00000000
Ga	-1.90227000	-1.25543400	0.00000000
Ga	0.00000000	0.34089600	0.00000000
H	2.05611300	2.83617400	1.38793100
H	2.05611300	2.83617400	-1.38793100
H	-3.39387500	-1.76635700	0.00000000
H	-0.25621900	2.75448900	0.00000000

24Ge:

8

E(RB+HF-LYP) = -8310.59368679

Ge	1.67141300	-1.46354000	0.00000000
Ge	-0.77323100	2.68762200	0.00000000
Ge	-0.74730200	-1.79871100	0.00000000
Ge	0.00000000	0.35741000	0.00000000
H	-0.22463500	3.39184500	1.25308000
H	-0.22463500	3.39184500	-1.25308000
H	-2.07022500	-2.59806800	0.00000000
H	-2.30864900	2.76536700	0.00000000

24In:

8

E(RB+HF-LYP) = -763.217633138

In	1.86088600	-1.90401000	0.00000000
In	-0.79482700	3.68780300	0.00000000
In	-0.95721700	-2.76876500	0.00000000
In	0.00000000	0.80690600	0.00000000
H	-0.04599100	4.18222300	1.49599000
H	-0.04599100	4.18222300	-1.49599000
H	-2.71959000	-3.06441900	0.00000000

1				
2				
3	H	-2.52168600	3.42519400	0.00000000
4				
5				
6	24Si:			
7	8			
8	E(RB+HF-LYP) =	-1160.40074551		
9	Si	1.45806400	-1.56581500	0.00000000
10	Si	-0.38523500	2.56498700	0.00000000
11	Si	-0.82705900	-1.72308700	0.00000000
12	Si	0.00000000	0.24802800	0.00000000
13	H	0.24192600	3.15056300	1.20770600
14	H	0.24192600	3.15056300	-1.20770600
15	H	-2.09075300	-2.50698800	0.00000000
16	H	-1.83387200	2.86827800	0.00000000
17				
18				
19				
20	24Sn:			
21	8			
22	E(RB+HF-LYP) =	-859.926365461		
23	Sn	1.87321300	-1.69746900	0.00000000
24	Sn	-0.82820000	3.14369900	0.00000000
25	Sn	-0.93565500	-2.05816400	0.00000000
26	Sn	0.00000000	0.44441900	0.00000000
27	H	-0.21535700	3.93893500	1.39135600
28	H	-0.21535700	3.93893500	-1.39135600
29	H	-2.50040400	-2.78710700	0.00000000
30	H	-2.53680100	3.28497700	0.00000000
31				
32				
33				
34	24Tl:			
35	8			
36	E(RB+HF-LYP) =	-692.690287828		
37	Tl	1.50605600	-2.32871800	0.00000000
38	Tl	0.06557000	3.93983600	0.00000000
39	Tl	-1.53412000	-2.57651500	0.00000000
40	Tl	0.00000000	0.83932700	0.00000000
41	H	0.96960300	4.04713200	1.50489300
42	H	0.96960300	4.04713200	-1.50489300
43	H	-3.32877900	-2.17270200	0.00000000
44	H	-1.64844200	4.29012600	0.00000000
45				
46				
47				
48	25Al:			
49	8			
50	E(RB+HF-LYP) =	-972.157148870		
51	Al	-0.29379600	-1.24961000	0.00000000
52	Al	2.28275300	-0.10194300	0.00000000
53	Al	-2.29189600	0.06208100	0.00000000
54	Al	0.00000000	1.16143600	0.00000000
55	H	3.02065000	-0.26897200	1.38423700
56	H	3.02065000	-0.26897200	-1.38423700
57	H	-3.77458900	0.59757500	0.00000000
58	H	1.67150300	1.60483300	0.00000000
59				
60				

25B:

1
2
3
4 8
5 E(RB+HF-LYP) = -101.685883565
6 B -0.39988500 -0.79240100 0.00000000
7 B 1.45969400 -0.22981700 0.00000000
8 B -1.57592900 0.12187100 0.00000000
9 B 0.00000000 0.66236300 0.00000000
10 H 2.04630100 -0.37426000 1.02354100
11 H 2.04630100 -0.37426000 -1.02354100
12 H -2.60754300 0.68250900 0.00000000
13 H 1.09554800 1.25593500 0.00000000
14

15
16 26Pb:

17 8
18 E(RB+HF-LYP) = -774.204281208
19
20 Pb 0.00000000 1.41175900 0.00000000
21 Pb -2.79997800 0.18590000 0.00000000
22 Pb 2.69806100 0.13908200 0.00000000
23 Pb 0.20184000 -1.71599000 0.00000000
24 H -3.65422600 0.83399000 1.42597500
25 H -3.65422600 0.83399000 -1.42597500
26 H 2.27775700 -1.80165900 0.00000000
27 H -3.16301200 -1.56782800 0.00000000
28
29

30 27C:

31 8
32 E(RB+HF-LYP) = -154.802131169
33
34 H -0.86197700 2.83736800 0.00000000
35 C -0.45514100 1.85674600 0.00000000
36 C 0.00000000 0.74308300 0.00000000
37 C 0.57646900 -0.55526700 0.00000000
38 C -0.11883400 -1.69404700 0.00000000
39 H 1.66124400 -0.59130700 0.00000000
40 H -1.20021800 -1.69929600 0.00000000
41 H 0.38598400 -2.64985400 0.00000000
42
43

44 28Ge:

45 8
46 E(RB+HF-LYP) = -8310.53179155
47
48 Ge -1.98994500 -2.25055300 0.00000000
49 Ge 0.02224200 -1.28433700 0.00000000
50 Ge 0.00000000 1.13538600 0.00000000
51 Ge 1.92354300 2.28621000 0.00000000
52 H -2.53536100 -3.70482400 0.00000000
53 H -1.30960300 1.93442200 0.00000000
54 H 3.27891100 1.58288300 0.00000000
55 H 1.97915300 3.81290200 0.00000000
56
57

58 28Si:

59 8
60 E(RB+HF-LYP) = -1160.33207094
Si -1.94089500 -2.16318400 0.00000000

1				
2				
3	Si	-0.06091900	-1.22253500	0.00000000
4	Si	0.00000000	1.06995400	0.00000000
5	Si	1.89302300	2.08658100	0.00000000
6	H	-2.43007700	-3.56924900	0.00000000
7	H	-1.23815600	1.87543600	0.00000000
8	H	3.16812500	1.34764000	0.00000000
9	H	2.02317300	3.55475900	0.00000000
10				
11				
12	29Al:			
13	8			
14	E(RB+HF-LYP) =	-972.169149691		
15	Al	0.00000000	1.25097000	0.00000000
16	Al	2.52384200	-0.03322600	0.00000000
17	Al	-0.21274700	-1.32814300	0.00000000
18	Al	-2.62418800	0.19303300	0.00000000
19	H	1.64941500	1.66345700	0.00000000
20	H	0.75650300	-0.13278700	1.02957500
21	H	0.75650300	-0.13278700	-1.02957500
22	H	0.90779000	-2.47212900	0.00000000
23				
24	29Ga:			
25	8			
26	E(RB+HF-LYP) =	-7702.01398562		
27	Ga	-0.01272700	1.33369400	-0.01297400
28	Ga	2.59307700	-0.01308200	0.00000000
29	Ga	-0.15573500	-1.35785900	0.01320400
30	Ga	-2.56164700	0.06478600	0.00000000
31	H	1.63501200	1.77301800	-0.01743400
32	H	0.77400500	-0.10230700	1.06864800
33	H	0.77377000	-0.12306100	-1.06665500
34	H	1.06520400	-2.40138100	0.02320100
35				
36	29In:			
37	8			
38	E(RB+HF-LYP) =	-763.259478149		
39	In	0.00000000	1.55296000	-0.01500400
40	In	2.85509500	-0.02665700	0.00000000
41	In	-0.12167600	-1.55095500	0.01499000
42	In	-2.82700000	0.03638200	0.00000000
43	H	1.79518300	2.02169800	-0.01931200
44	H	0.83710000	-0.05706000	1.15551500
45	H	0.83734800	-0.07936200	-1.15398700
46	H	1.42655800	-2.46004200	0.02394400
47				
48	2Al:			
49	8			
50	E(RB+HF-LYP) =	-972.149295766		
51	Al	1.10130800	-1.10130800	1.10130800
52	Al	1.10130800	1.10130800	-1.10130800
53	Al	-1.10130800	-1.10130800	-1.10130800
54	Al	-1.10130800	1.10130800	1.10130800

1				
2				
3	H	0.81712300	0.81712300	0.81712300
4	H	-0.81712300	-0.81712300	0.81712300
5	H	0.81712300	-0.81712300	-0.81712300
6	H	-0.81712300	0.81712300	-0.81712300
7				
8				

2B:

8

E(RB+HF-LYP) = -101.252374030

11				
12				
13	B	0.81795600	-0.81795600	0.81795600
14	B	0.81795600	0.81795600	-0.81795600
15	B	-0.81795600	-0.81795600	-0.81795600
16	B	-0.81795600	0.81795600	0.81795600
17	H	0.74051500	0.74051500	0.74051500
18	H	-0.74051500	-0.74051500	0.74051500
19	H	0.74051500	-0.74051500	-0.74051500
20	H	-0.74051500	0.74051500	-0.74051500
21				
22				

2C:

8

E(RB+HF-LYP) = -154.224429611

23				
24				
25				
26				
27	C	0.61522000	0.61522000	0.61522000
28	C	-0.61522000	-0.61522000	0.61522000
29	C	-0.61522000	0.61522000	-0.61522000
30	C	0.61522000	-0.61522000	-0.61522000
31	H	0.76341700	-0.76341700	0.76341700
32	H	0.76341700	0.76341700	-0.76341700
33	H	-0.76341700	0.76341700	0.76341700
34	H	-0.76341700	-0.76341700	-0.76341700
35				
36				

2Ga:

8

E(RB+HF-LYP) = -7702.01076676

37				
38				
39				
40				
41	Ga	1.13227100	-1.13227100	1.13227100
42	Ga	1.13227100	1.13227100	-1.13227100
43	Ga	-1.13227100	-1.13227100	-1.13227100
44	Ga	-1.13227100	1.13227100	1.13227100
45	H	0.84241300	0.84241300	0.84241300
46	H	-0.84241300	-0.84241300	0.84241300
47	H	0.84241300	-0.84241300	-0.84241300
48	H	-0.84241300	0.84241300	-0.84241300
49				
50				

2Ge:

8

E(RB+HF-LYP) = -8310.52902422

51				
52				
53				
54				
55	Ge	1.02166300	-1.02166300	1.02166300
56	Ge	1.02166300	1.02166300	-1.02166300
57	Ge	-1.02166300	-1.02166300	-1.02166300
58	Ge	-1.02166300	1.02166300	1.02166300
59	H	0.82672100	0.82672100	0.82672100
60	H	-0.82672100	-0.82672100	0.82672100
	H	0.82672100	-0.82672100	-0.82672100

1
2
3 H -0.82672100 0.82672100 -0.82672100
4
5
6 2In:
7
8
9 E(RB+HF-LYP) = -763.274648770
10 In 1.25111300 -1.25111300 1.25111300
11 In 1.25111300 1.25111300 -1.25111300
12 In -1.25111300 -1.25111300 -1.25111300
13 In -1.25111300 1.25111300 1.25111300
14 H 0.91255100 0.91255100 0.91255100
15 H -0.91255100 -0.91255100 0.91255100
16 H 0.91255100 -0.91255100 -0.91255100
17 H -0.91255100 0.91255100 -0.91255100
18
19
20 2Pb:
21
22 8
23 E(RB+HF-LYP) = -774.200788937
24 Pb 1.20434000 -1.20434000 1.20434000
25 Pb 1.20434000 1.20434000 -1.20434000
26 Pb -1.20434000 -1.20434000 -1.20434000
27 Pb -1.20434000 1.20434000 1.20434000
28 H 0.92120100 0.92120100 0.92120100
29 H -0.92120100 -0.92120100 0.92120100
30 H 0.92120100 -0.92120100 -0.92120100
31 H -0.92120100 0.92120100 -0.92120100
32
33
34 2Si:
35
36 8
37 E(RB+HF-LYP) = -1160.28532570
38 Si 0.95536300 -0.95536300 0.95536300
39 Si 0.95536300 0.95536300 -0.95536300
40 Si -0.95536300 -0.95536300 -0.95536300
41 Si -0.95536300 0.95536300 0.95536300
42 H 0.79485500 0.79485500 0.79485500
43 H -0.79485500 -0.79485500 0.79485500
44 H 0.79485500 -0.79485500 -0.79485500
45 H -0.79485500 0.79485500 -0.79485500
46
47
48 2Sn:
49
50 8
51 E(RB+HF-LYP) = -859.916580679
52 Sn 1.15305000 1.15305000 -1.15305000
53 Sn 1.15305000 -1.15305000 1.15305000
54 Sn -1.15305000 -1.15305000 -1.15305000
55 Sn -1.15305000 1.15305000 1.15305000
56 H 0.88610700 0.88610700 0.88610700
57 H -0.88610700 -0.88610700 0.88610700
58 H -0.88610700 0.88610700 -0.88610700
59 H 0.88610700 -0.88610700 -0.88610700
60

2Tl:

1
2
3 8
4 E(RB+HF-LYP) = -692.775226789
5
6 Tl 1.28628300 1.28628300 -1.28628300
7 Tl 1.28628300 -1.28628300 1.28628300
8 Tl -1.28628300 -1.28628300 -1.28628300
9 Tl -1.28628300 1.28628300 1.28628300
10 H 0.95036800 0.95036800 0.95036800
11 H -0.95036800 -0.95036800 0.95036800
12 H -0.95036800 0.95036800 -0.95036800
13 H 0.95036800 -0.95036800 -0.95036800
14

15
16 30Ge:

17 8
18 E(RB+HF-LYP) = -8310.59762962
19
20 Ge 0.45589500 -0.84227300 1.45944900
21 Ge 0.45589500 -0.84227300 -1.45944900
22 Ge 0.45589500 1.45389900 0.00000000
23 Ge -1.55091600 0.16852600 0.00000000
24 H 1.50593500 0.48184600 -1.26554200
25 H 1.27822500 -1.49625100 0.00000000
26 H 1.50593500 0.48184600 1.26554200
27 H 1.57333500 2.52044100 0.00000000
28
29

30 31Al:

31 8
32 E(RB+HF-LYP) = -972.168199820
33
34 Al 0.00000000 1.30965000 0.08843600
35 Al 0.00000000 0.00000000 -2.47903900
36 Al 0.00000000 -1.30965000 0.08843600
37 Al 0.00000000 0.00000000 2.63072600
38 H 0.00000000 1.96291600 -1.42283200
39 H 1.03171100 0.00000000 -0.71280200
40 H -1.03171100 0.00000000 -0.71280200
41 H 0.00000000 -1.96291600 -1.42283200
42
43

44 31In:

45 8
46 E(RB+HF-LYP) = -763.259469595
47
48 In 0.00000000 1.55768100 -0.06103400
49 In 0.00000000 0.00000000 2.84394500
50 In 0.00000000 -1.55768100 -0.06103400
51 In 0.00000000 0.00000000 -2.82241700
52 H 0.00000000 2.20252300 1.64791400
53 H -1.15733800 0.00000000 0.81532100
54 H 1.15733800 0.00000000 0.81532100
55 H 0.00000000 -2.20252300 1.64791400
56
57

58 32Ge:

59 8
60 E(RB+HF-LYP) = -8310.57934692
Ge -1.84607000 0.08432600 0.57701600

1				
2				
3	Ge	1.84175200	-0.08603400	0.58971200
4	Ge	-0.19628300	-1.39030300	-0.60651900
5	Ge	0.20074700	1.39213000	-0.60119100
6				
7	H	-2.86226700	0.90393900	-0.28698000
8	H	-0.86115000	1.42680100	0.93585800
9	H	0.85484000	-1.43222300	0.93315500
10	H	2.86391900	-0.90230600	-0.27057400
11				
12				
13	32Pb:			
14	8			
15	E(RB+HF-LYP) =	-774.217752892		
16	Pb	-0.99101300	2.19589400	0.68870700
17	Pb	0.99101300	-2.19589400	0.68870700
18	Pb	-1.44980800	-0.72938400	-0.69768900
19	Pb	1.44980800	0.72938400	-0.69768900
20	H	0.00000000	3.30017300	-0.43556500
21	H	0.88097900	1.45515600	1.13120500
22	H	-0.88097900	-1.45515600	1.13120500
23	H	0.00000000	-3.30017300	-0.43556500
24				
25				
26				
27	32Si:			
28	8			
29	E(RB+HF-LYP) =	-1160.35847650		
30	Si	-1.69275800	-0.02921700	0.51453200
31	Si	1.68911300	0.02663900	0.52202700
32	Si	-0.10986700	-1.32468700	-0.57451700
33	Si	0.11371700	1.32777000	-0.56733200
34	H	-2.85946600	0.53330500	-0.22169600
35	H	-0.93216100	1.30075600	0.95171100
36	H	0.92352800	-1.30737300	0.94438200
37	H	2.86523300	-0.53374700	-0.20033500
38				
39				
40				
41	32Sn:			
42	8			
43	E(RB+HF-LYP) =	-859.943319160		
44	Sn	1.26062100	1.78788900	0.69211700
45	Sn	-1.26062100	-1.78788900	0.69211700
46	Sn	-1.26062100	0.94615300	-0.70517500
47	Sn	1.26062100	-0.94615300	-0.70517500
48	H	2.68266100	1.88235400	-0.35079100
49	H	1.75453800	-0.06765300	1.00371400
50	H	-1.75453800	0.06765300	1.00371400
51	H	-2.68266100	-1.88235400	-0.35079100
52				
53				
54				
55	33Al:			
56	8			
57	E(RB+HF-LYP) =	-972.171756720		
58	Al	0.00000000	-1.25235100	-1.29536300
59	Al	0.00000000	1.25235100	1.29536300
60	Al	0.00000000	-1.25235100	1.29536300
	Al	0.00000000	1.25235100	-1.29536300

1				
2				
3	H	1.13565600	0.00000000	-1.78949300
4	H	-1.13565600	0.00000000	-1.78949300
5	H	-1.13565600	0.00000000	1.78949300
6	H	1.13565600	0.00000000	1.78949300
7				
8				

33Ga:

8

E(RB+HF-LYP) = -7701.99523390

11				
12				
13	Ga	-1.27483500	1.26375600	0.00000000
14	Ga	1.27483500	-1.26375600	0.00000000
15	Ga	1.27483500	1.26375600	0.00000000
16	Ga	-1.27483500	-1.26375600	0.00000000
17	H	-1.78078800	0.00000000	1.16678800
18	H	-1.78078800	0.00000000	-1.16678800
19	H	1.78078800	0.00000000	-1.16678800
20	H	1.78078800	0.00000000	1.16678800
21				
22				

34Al:

8

E(RB+HF-LYP) = -972.127643150

23				
24				
25				
26				
27	Al	0.00000000	2.07626800	1.03656600
28	Al	-2.07626800	0.00000000	-1.03656600
29	Al	0.00000000	-2.07626800	1.03656600
30	Al	2.07626800	0.00000000	-1.03656600
31	H	1.19837900	1.19837900	0.00000000
32	H	-1.19837900	-1.19837900	0.00000000
33	H	1.19837900	-1.19837900	0.00000000
34	H	-1.19837900	1.19837900	0.00000000
35				
36				

34B:

8

E(RB+HF-LYP) = -101.270634815

37				
38				
39				
40				
41	B	0.00000000	1.59775500	0.75389500
42	B	-1.59775500	0.00000000	-0.75389500
43	B	0.00000000	-1.59775500	0.75389500
44	B	1.59775500	0.00000000	-0.75389500
45	H	1.03397100	1.03397100	0.00000000
46	H	-1.03397100	-1.03397100	0.00000000
47	H	1.03397100	-1.03397100	0.00000000
48	H	-1.03397100	1.03397100	0.00000000
49				
50				

34Ga:

8

E(RB+HF-LYP) = -7701.99412324

51				
52				
53				
54				
55	Ga	0.00000000	2.16796300	1.00297800
56	Ga	-2.16796300	0.00000000	-1.00297800
57	Ga	0.00000000	-2.16796300	1.00297800
58	Ga	2.16796300	0.00000000	-1.00297800
59	H	1.24576400	1.24576400	0.00000000
60	H	-1.24576400	-1.24576400	0.00000000
	H	1.24576400	-1.24576400	0.00000000

1				
2				
3	H	-1.24576400	1.24576400	0.00000000
4				
5				
6	34In:			
7	8			
8	E(RB+HF-LYP) =	-763.258709475		
9	In	0.00000000	2.41125500	1.07325700
10	In	-2.41125500	0.00000000	-1.07325700
11	In	0.00000000	-2.41125500	1.07325700
12	In	2.41125500	0.00000000	-1.07325700
13	H	1.36508100	1.36508100	0.00000000
14	H	-1.36508100	-1.36508100	0.00000000
15	H	1.36508100	-1.36508100	0.00000000
16	H	-1.36508100	1.36508100	0.00000000
17				
18				
19				
20	34Tl:			
21	8			
22	E(RB+HF-LYP) =	-692.758133506		
23	Tl	0.00000000	2.49746600	1.08161900
24	Tl	-2.49746600	0.00000000	-1.08161900
25	Tl	0.00000000	-2.49746600	1.08161900
26	Tl	2.49746600	0.00000000	-1.08161900
27	H	1.43420600	1.43420600	0.00000000
28	H	-1.43420600	-1.43420600	0.00000000
29	H	1.43420600	-1.43420600	0.00000000
30	H	-1.43420600	1.43420600	0.00000000
31				
32				
33				
34	35Al:			
35	8			
36	E(RB+HF-LYP) =	-972.153227703		
37	Al	0.00000000	0.00000000	-1.61353200
38	Al	0.00000000	2.03545900	0.07319700
39	Al	0.00000000	0.00000000	1.77987000
40	Al	0.00000000	-2.03545900	0.07319700
41	H	-1.42543800	0.00000000	-2.32407400
42	H	0.00000000	-3.60813100	0.29131800
43	H	1.42543800	0.00000000	-2.32407400
44	H	0.00000000	3.60813100	0.29131800
45				
46				
47				
48	35B:			
49	8			
50	E(RB+HF-LYP) =	-101.680291307		
51	B	0.00000000	0.00000000	-0.79705300
52	B	0.00000000	1.38944700	0.18114000
53	B	0.00000000	0.00000000	0.98817800
54	B	0.00000000	-1.38944700	0.18114000
55	H	-1.00252700	0.00000000	-1.48549600
56	H	0.00000000	-2.56097800	0.10198200
57	H	1.00252700	0.00000000	-1.48549600
58	H	0.00000000	2.56097800	0.10198200
59				
60				

35C:

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2
3
4 8
5 E(RB+HF-LYP) = -154.674331368
6 C 0.00000000 0.00000000 -1.04046500
7 C 0.00000000 0.94033700 0.16170800
8 C 0.00000000 -0.94033700 0.16170800
9 C 0.00000000 0.00000000 1.21762900
10 H -0.88816700 0.00000000 -1.67839200
11 H 0.00000000 -2.03329900 0.17673300
12 H 0.88816700 0.00000000 -1.67839200
13 H 0.00000000 2.03329900 0.17673300
14

15
16 35Ga:

17 8
18 E(RB+HF-LYP) = -7702.00118532
19
20 Ga 0.00000000 0.00000000 -1.59299200
21 Ga 1.98652500 0.00000000 0.00000000
22 Ga 0.00000000 0.00000000 1.73421900
23 Ga -1.98652500 0.00000000 0.00000000
24 H 0.00000000 1.41149800 -2.27619700
25 H -3.55325500 0.00000000 0.19128500
26 H 0.00000000 -1.41149800 -2.27619700
27 H 3.55325500 0.00000000 0.19128500
28
29

30 35Ge:

31 8
32 E(RB+HF-LYP) = -8310.60053427
33
34 Ge 0.00000000 0.00000000 -1.92464500
35 Ge 0.00000000 1.46194600 0.05754500
36 Ge 0.00000000 0.00000000 1.99035000
37 Ge 0.00000000 -1.46194600 0.05754500
38 H -1.24490900 0.00000000 -2.84502900
39 H 0.00000000 -3.02233800 -0.04770300
40 H 1.24490900 0.00000000 -2.84502900
41 H 0.00000000 3.02233800 -0.04770300
42
43
44

45 35In:

46 8
47 E(RB+HF-LYP) = -763.223769847
48 In 0.00000000 0.00000000 -1.83985700
49 In 0.00000000 2.24734400 -0.02461800
50 In 0.00000000 0.00000000 1.98354800
51 In 0.00000000 -2.24734400 -0.02461800
52 H -1.57520500 0.00000000 -2.53591800
53 H 0.00000000 -3.98054000 0.22176900
54 H 1.57520500 0.00000000 -2.53591800
55 H 0.00000000 3.98054000 0.22176900
56
57
58

59 35Pb:

60 8
E(RB+HF-LYP) = -774.174526381
Pb 0.00000000 0.00000000 2.35069900

1				
2				
3	Pb	0.00000000	1.82616800	-0.05307200
4	Pb	0.00000000	0.00000000	-2.33490400
5	Pb	0.00000000	-1.82616800	-0.05307200
6	H	1.39972400	0.00000000	3.48807600
7	H	0.00000000	-3.62705700	0.21628200
8	H	-1.39972400	0.00000000	3.48807600
9	H	0.00000000	3.62705700	0.21628200
10				
11				
12	35Si:			
13	8			
14	E(RB+HF-LYP) =	-1160.40887537		
15	Si	0.00000000	0.00000000	-1.79479500
16	Si	0.00000000	1.33729100	0.10780400
17	Si	0.00000000	0.00000000	1.95056900
18	Si	0.00000000	-1.33729100	0.10780400
19	H	-1.20085800	0.00000000	-2.67119100
20	H	0.00000000	-2.83567000	0.07152600
21	H	1.20085800	0.00000000	-2.67119100
22	H	0.00000000	2.83567000	0.07152600
23				
24	35Sn:			
25	8			
26	E(RB+HF-LYP) =	-859.937757302		
27	Sn	0.00000000	0.00000000	-2.23253600
28	Sn	0.00000000	1.69631500	0.04821800
29	Sn	0.00000000	0.00000000	2.27236300
30	Sn	0.00000000	-1.69631500	0.04821800
31	H	-1.37341900	0.00000000	-3.28097200
32	H	0.00000000	-3.43325200	-0.12560900
33	H	1.37341900	0.00000000	-3.28097200
34	H	0.00000000	3.43325200	-0.12560900
35				
36	35Tl:			
37	8			
38	E(RB+HF-LYP) =	-692.684202654		
39	Tl	0.00000000	0.00000000	-1.96478500
40	Tl	0.00000000	2.31814800	-0.03166700
41	Tl	0.00000000	0.00000000	2.08255600
42	Tl	0.00000000	-2.31814800	-0.03166700
43	H	-1.65143100	0.00000000	-2.30041400
44	H	0.00000000	-4.11417800	0.09566000
45	H	1.65143100	0.00000000	-2.30041400
46	H	0.00000000	4.11417800	0.09566000
47				
48	36Al:			
49	8			
50	E(RB+HF-LYP) =	-972.168785473		
51	Al	-0.97625800	-2.61405200	0.00000000
52	Al	0.97625800	2.61405200	0.00000000
53	Al	-0.97625800	0.79053800	0.00000000
54	Al	0.97625800	-0.79053800	0.00000000

H	0.41504300	-1.92815100	1.11995700
H	0.41504300	-1.92815100	-1.11995700
H	-0.41504300	1.92815100	-1.11995700
H	-0.41504300	1.92815100	1.11995700

36B:

8

E(RB+HF-LYP) = -101.539032777

B	-0.38413600	0.68964900	0.00000000
B	0.38413600	-0.68964900	0.00000000
B	-0.38413600	-2.12902800	0.00000000
B	0.38413600	2.12902800	0.00000000
H	0.69097900	-1.39563100	0.96840800
H	0.69097900	-1.39563100	-0.96840800
H	-0.69097900	1.39563100	-0.96840800
H	-0.69097900	1.39563100	0.96840800

36Ga:

8

E(RB+HF-LYP) = -7702.01010636

Ga	-0.97595400	-2.71724100	0.00000000
Ga	0.97595400	2.71724100	0.00000000
Ga	-0.97595400	0.78023900	0.00000000
Ga	0.97595400	-0.78023900	0.00000000
H	0.44341500	-1.95174500	1.14436700
H	0.44341500	-1.95174500	-1.14436700
H	-0.44341500	1.95174500	-1.14436700
H	-0.44341500	1.95174500	1.14436700

36In:

8

E(RB+HF-LYP) = -763.256377697

In	-1.40235300	3.76011100	0.00000000
In	1.40235300	-3.76011100	0.00000000
In	1.40235300	-0.48165200	0.00000000
In	-1.40235300	0.48165200	0.00000000
H	-1.48855300	2.05896000	1.21084800
H	-1.48855300	2.05896000	-1.21084800
H	1.48855300	-2.05896000	-1.21084800
H	1.48855300	-2.05896000	1.21084800

36Tl:

8

E(RB+HF-LYP) = -692.745196596

Tl	-0.89502000	-4.29781600	0.00000000
Tl	0.89502000	4.29781600	0.00000000
Tl	-0.89502000	1.36318400	0.00000000
Tl	0.89502000	-1.36318400	0.00000000
H	0.04810200	-2.81834600	1.25127400
H	0.04810200	-2.81834600	-1.25127400
H	-0.04810200	2.81834600	-1.25127400

1				
2				
3	H	-0.04810200	2.81834600	1.25127400
4				
5				
6	37Al:			
7	8			
8	E(RB+HF-LYP) =	-972.179716665		
9	Al	0.16523000	1.62121200	0.07311000
10	Al	1.35255600	-0.64719600	-0.76505500
11	Al	0.17749200	-0.58171900	1.36527800
12	Al	-1.93935300	-0.56666000	-0.55762600
13	H	0.38909500	3.16925700	-0.17662900
14	H	-1.43331200	1.26910700	-0.35548800
15	H	1.77469100	-1.09292800	0.85570500
16	H	2.44249900	-1.07871300	-1.82778100
17				
18				
19				
20	37Ga:			
21	8			
22	E(RB+HF-LYP) =	-7702.01309274		
23	Ga	0.50661900	1.57876300	0.05777900
24	Ga	1.33743400	-0.79223100	-0.80562500
25	Ga	0.08638600	-0.63453800	1.30173700
26	Ga	-2.05737300	-0.21904200	-0.50155900
27	H	0.91128300	3.04964300	-0.33996300
28	H	-1.17207600	1.52656600	-0.31391600
29	H	1.71644800	-1.28919700	0.83579000
30	H	2.47930800	-1.20855700	-1.80423300
31				
32				
33				
34	38In:			
35	8			
36	E(RB+HF-LYP) =	-763.245353074		
37	In	0.66943600	1.67792700	-0.72618700
38	In	0.04629000	-1.50552800	-1.00740600
39	In	1.58331700	-0.36594200	1.22775400
40	In	-2.32396000	0.17579200	0.59172500
41	H	0.42437600	3.18123800	-1.61905400
42	H	-1.02096300	1.74297300	0.34303900
43	H	1.88360000	-1.56684400	-0.47245100
44	H	-0.06612100	-2.48754300	-2.45994900
45				
46				
47				
48	39Tl:			
49	8			
50	E(RB+HF-LYP) =	-692.751453235		
51	Tl	0.00000000	1.86362100	-1.35617300
52	Tl	0.15164900	0.34495800	1.93541000
53	Tl	-1.98969000	-1.02168500	-0.17008200
54	Tl	1.82703500	-1.22739200	-0.43142000
55	H	1.45386900	0.92468800	0.07496200
56	H	-0.12753300	-0.67116900	-1.33433500
57	H	-1.32375700	1.07385400	0.26530200
58	H	0.29666200	1.95287900	2.79758000
59				
60				

3Al:

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8
E(RB+HF-LYP) = -972.128291939
Al 0.00000000 1.45267700 1.35832700
Al -1.45267700 0.00000000 -1.35832700
Al 0.00000000 -1.45267700 1.35832700
Al 1.45267700 0.00000000 -1.35832700
H 1.20123000 1.20123000 0.00000000
H -1.20123000 -1.20123000 0.00000000
H 1.20123000 -1.20123000 0.00000000
H -1.20123000 1.20123000 0.00000000

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3B:

8
E(RB+HF-LYP) = -101.507236311
B 0.00000000 0.78703600 0.68121000
B -0.78703600 0.00000000 -0.68121000
B 0.00000000 -0.78703600 0.68121000
B 0.78703600 0.00000000 -0.68121000
H 1.12901700 1.12901700 0.00000000
H -1.12901700 -1.12901700 0.00000000
H 1.12901700 -1.12901700 0.00000000
H -1.12901700 1.12901700 0.00000000

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3C:

8
E(RB+HF-LYP) = -154.493568425
C 0.00000000 0.70993700 0.75773000
C -0.70993700 0.00000000 -0.75773000
C 0.00000000 -0.70993700 0.75773000
C 0.70993700 0.00000000 -0.75773000
H 1.01462300 1.01462300 0.00000000
H -1.01462300 -1.01462300 0.00000000
H 1.01462300 -1.01462300 0.00000000
H -1.01462300 1.01462300 0.00000000

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3Ge:

8
E(RB+HF-LYP) = -8310.61531413
Ge 0.00000000 1.28420600 1.13321300
Ge -1.28420600 0.00000000 -1.13321300
Ge 0.00000000 -1.28420600 1.13321300
Ge 1.28420600 0.00000000 -1.13321300
H 1.34696800 1.34696800 0.00000000
H -1.34696800 -1.34696800 0.00000000
H 1.34696800 -1.34696800 0.00000000
H -1.34696800 1.34696800 0.00000000

59
60

3Pb:

8
E(RB+HF-LYP) = -774.259793208
Pb 0.00000000 1.56913100 1.32273000

1				
2				
3	Pb	0.00000000	-1.56913100	1.32273000
4	Pb	-1.56913100	0.00000000	-1.32273000
5	Pb	1.56913100	0.00000000	-1.32273000
6	Pb	1.56913100	0.00000000	-1.32273000
7	H	1.54754000	1.54754000	0.00000000
8	H	-1.54754000	1.54754000	0.00000000
9	H	1.54754000	-1.54754000	0.00000000
10	H	-1.54754000	-1.54754000	0.00000000
11				
12				
13	3Si:			
14	8			
15	E(RB+HF-LYP) =	-1160.38290960		
16	Si	0.00000000	1.19718700	1.05993600
17	Si	-1.19718700	0.00000000	-1.05993600
18	Si	0.00000000	-1.19718700	1.05993600
19	Si	1.19718700	0.00000000	-1.05993600
20	Si	1.19718700	0.00000000	-1.05993600
21	H	1.29438900	1.29438900	0.00000000
22	H	-1.29438900	-1.29438900	0.00000000
23	H	1.29438900	-1.29438900	0.00000000
24	H	-1.29438900	1.29438900	0.00000000
25	H	-1.29438900	1.29438900	0.00000000
26				
27	3Sn:			
28	8			
29	E(RB+HF-LYP) =	-859.983172356		
30	Sn	0.00000000	1.49130900	1.28190700
31	Sn	-1.49130900	0.00000000	-1.28190700
32	Sn	0.00000000	-1.49130900	1.28190700
33	Sn	1.49130900	0.00000000	-1.28190700
34	Sn	1.49130900	0.00000000	-1.28190700
35	H	1.47405400	1.47405400	0.00000000
36	H	-1.47405400	-1.47405400	0.00000000
37	H	1.47405400	-1.47405400	0.00000000
38	H	-1.47405400	1.47405400	0.00000000
39	H	-1.47405400	1.47405400	0.00000000
40				
41	40Al:			
42	8			
43	E(RB+HF-LYP) =	-972.136858091		
44	Al	0.00000000	0.00000000	1.22102400
45	Al	0.00000000	0.00000000	-1.22102400
46	Al	0.00000000	0.00000000	-3.73625100
47	Al	0.00000000	0.00000000	-3.73625100
48	H	0.00000000	-1.37544500	-4.51871000
49	H	0.00000000	1.37544500	-4.51871000
50	H	0.00000000	1.37544500	-4.51871000
51	H	0.00000000	-1.37544500	4.51871000
52	H	0.00000000	-1.37544500	4.51871000
53	H	0.00000000	-1.37544500	4.51871000
54				
55	40B:			
56	8			
57	E(RB+HF-LYP) =	-101.687637643		
58	B	0.00000000	0.00000000	2.36362500
59	B	0.00000000	0.00000000	-2.36362500
60	B	0.00000000	0.00000000	-0.78043400
	B	0.00000000	0.00000000	0.78043400

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2				
3	H	0.00000000	1.01781800	2.98735500
4	H	0.00000000	-1.01781800	2.98735500
5	H	0.00000000	-1.01781800	-2.98735500
6	H	0.00000000	1.01781800	-2.98735500
7				
8				

40C:

8

E(RB+HF-LYP) = -154.796772661

13	C	0.00000000	0.00000000	1.94411700
14	C	0.00000000	0.00000000	-1.94411700
15	C	0.00000000	0.00000000	-0.63200400
16	C	0.00000000	0.00000000	0.63200400
17	H	0.00000000	0.92475900	2.50871300
18	H	0.00000000	-0.92475900	2.50871300
19	H	0.00000000	-0.92475900	-2.50871300
20	H	0.00000000	0.92475900	-2.50871300
21				
22				

40Ga:

8

E(RB+HF-LYP) = -7701.98168355

27	Ga	0.00000000	0.00000000	1.18472800
28	Ga	0.00000000	0.00000000	-1.18472800
29	Ga	0.00000000	0.00000000	-3.59720200
30	H	0.00000000	-1.37296300	-4.35267000
31	H	0.00000000	1.37296300	-4.35267000
32	Ga	0.00000000	0.00000000	3.59720200
33	H	0.00000000	1.37296300	4.35267000
34	H	0.00000000	-1.37296300	4.35267000
35				
36				

40Ge:

8

E(RB+HF-LYP) = -8310.49534834

41	Ge	0.00000000	0.00000000	1.08137900
42	Ge	0.00000000	0.00000000	-1.08137900
43	Ge	0.00000000	0.00000000	-3.29931100
44	H	0.00000000	-1.32009300	-4.05459000
45	H	0.00000000	1.32009300	-4.05459000
46	Ge	0.00000000	0.00000000	3.29931100
47	H	0.00000000	1.32009300	4.05459000
48	H	0.00000000	-1.32009300	4.05459000
49				
50				

40In:

8

E(RB+HF-LYP) = -763.196597258

55	In	0.00000000	0.00000000	1.34987500
56	In	0.00000000	0.00000000	-1.34987500
57	In	0.00000000	0.00000000	-4.08919000
58	H	0.00000000	-1.52535300	-4.90372500
59	H	0.00000000	1.52535300	-4.90372500
60	In	0.00000000	0.00000000	4.08919000
	H	0.00000000	1.52535300	4.90372500

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2				
3	H	0.00000000	-1.52535300	4.90372500
4				
5				
6	40Pb:			
7	8			
8	E(RB+HF-LYP) =	-774.009731566		
9	Pb	0.00000000	0.00000000	1.32837100
10	Pb	0.00000000	0.00000000	-1.32837100
11	Pb	0.00000000	0.00000000	-4.04628200
12	H	0.00000000	-1.58988400	-4.72565000
13	H	0.00000000	1.58988400	-4.72565000
14	Pb	0.00000000	0.00000000	4.04628200
15	H	0.00000000	1.58988400	4.72565000
16	H	0.00000000	-1.58988400	4.72565000
17				
18				
19				
20	40Si:			
21	8			
22	E(RB+HF-LYP) =	-1160.31356146		
23	Si	0.00000000	0.00000000	1.03802200
24	Si	0.00000000	0.00000000	-1.03802200
25	Si	0.00000000	0.00000000	-3.16372100
26	H	0.00000000	-1.25638800	-3.92662100
27	H	0.00000000	1.25638800	-3.92662100
28	Si	0.00000000	0.00000000	3.16372100
29	H	0.00000000	1.25638800	3.92662100
30	H	0.00000000	-1.25638800	3.92662100
31				
32				
33				
34	40Sn:			
35	8			
36	E(RB+HF-LYP) =	-859.812928932		
37	Sn	0.00000000	0.00000000	1.25642400
38	Sn	0.00000000	0.00000000	-1.25642400
39	Sn	0.00000000	0.00000000	-3.82326400
40	H	0.00000000	-1.47651100	-4.64749000
41	H	0.00000000	1.47651100	-4.64749000
42	Sn	0.00000000	0.00000000	3.82326400
43	H	0.00000000	1.47651100	4.64749000
44	H	0.00000000	-1.47651100	4.64749000
45				
46				
47				
48	40Tl:			
49	8			
50	E(RB+HF-LYP) =	-692.641548519		
51	Tl	0.00000000	0.00000000	1.40388600
52	Tl	0.00000000	0.00000000	-1.40388600
53	Tl	0.00000000	0.00000000	-4.23532300
54	H	0.00000000	-1.60328200	-4.88535600
55	H	0.00000000	1.60328200	-4.88535600
56	Tl	0.00000000	0.00000000	4.23532300
57	H	0.00000000	1.60328200	4.88535600
58	H	0.00000000	-1.60328200	4.88535600
59				
60				

41Pb:

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4 8
5 E(RB+HF-LYP) = -774.183546018
6 Pb 0.39701600 1.43735000 -0.03075100
7 Pb 3.22203600 -0.29187700 0.01806300
8 Pb -1.01059000 -1.63968800 0.00000000
9 Pb -2.70237100 0.50091400 0.01299700
10 H 3.82627600 1.47100500 -0.03839200
11 H 1.70888100 0.35321700 1.20655400
12 H 1.69229800 0.27979400 -1.19843500
13 H 0.47314300 -2.65333800 -0.01895600

14
15
16 41Sn:

17 8
18 E(RB+HF-LYP) = -859.913148097
19 Sn 0.00000000 1.38574700 0.00000000
20 Sn 3.05694900 0.54927800 0.00000000
21 Sn -0.56416600 -1.76092700 0.00000000
22 Sn -2.63658800 -0.20010800 0.00000000
23 H 3.15586900 2.32975700 0.00000000
24 H 1.50454000 0.70073800 1.15678800
25 H 1.50454000 0.70073800 -1.15678800
26 H 1.02529500 -2.43071500 0.00000000

27
28
29
30 42Ge:

31 8
32 E(RB+HF-LYP) = -8310.54091381
33 Ge 0.39264600 -0.19430400 1.86881900
34 Ge 0.39264600 1.56330000 0.00000000
35 Ge 0.39264600 -0.19430400 -1.86881900
36 Ge -1.02554600 -1.16686400 0.00000000
37 H -0.60941200 0.13321400 3.03230000
38 H -0.60941200 0.13321400 -3.03230000
39 H -1.06340100 0.59097600 0.00000000
40 H -2.59427300 -1.10792300 0.00000000

41
42
43
44 42Si:

45 8
46 E(RB+HF-LYP) = -1160.32525806
47 Si 0.40446700 -0.18341400 1.72570800
48 Si 0.40446700 1.48629800 0.00000000
49 Si 0.40446700 -0.18341400 -1.72570800
50 Si -0.90646400 -1.09442700 0.00000000
51 H -0.43939000 0.13959400 2.91870800
52 H -0.43939000 0.13959400 -2.91870800
53 H -1.01743000 0.56331900 0.00000000
54 H -2.40091000 -1.19310700 0.00000000

55
56
57
58 43Ge:

59 8
60 E(RB+HF-LYP) = -8310.58447627
Ge 2.18119900 -0.12043600 -0.18796800

1				
2				
3	Ge	0.12299200	1.32018300	0.21455100
4	Ge	-2.15730600	0.00000000	-0.23857500
5	Ge	-0.14015400	-1.26745100	0.20581300
6				
7	H	1.72429200	-0.06388200	-1.71484400
8	H	-1.02585400	1.42889000	-0.97793000
9	H	-0.46484800	2.31544900	1.24706400
10	H	-0.44899300	-1.80749000	1.64345000
11				
12	44C:			
13	8			
14				
15	E(RB+HF-LYP) =	-154.726103194		
16	C	-1.08697200	-0.08978400	-0.13872300
17	C	0.15738500	-0.91669300	0.33674100
18	C	1.08539500	-0.06049900	-0.18194400
19	C	0.02994800	0.85440000	0.01302400
20	H	-1.35599500	-0.35505600	-1.15259000
21	H	2.15541800	-0.01992100	-0.28547900
22	H	-1.94861200	-0.01252200	0.52011800
23	H	0.03465600	1.66295300	0.74336500
24				
25				
26				
27	44Ge:			
28	8			
29				
30	E(RB+HF-LYP) =	-8310.60533355		
31	Ge	-1.74503400	0.13213700	0.29408600
32	Ge	0.21207900	1.60013300	-0.35262700
33	Ge	1.68998400	-0.10808800	0.36062300
34	Ge	-0.08912700	-1.55068700	-0.28823700
35	H	-2.19706700	0.10003400	1.76500000
36	H	3.17072400	-0.46839400	0.09681300
37	H	-2.99740100	0.22782800	-0.60312300
38	H	-0.14917000	-2.21132300	-1.70175700
39				
40				
41	44Si:			
42	8			
43				
44	E(RB+HF-LYP) =	-1160.41062445		
45	Si	-1.62230700	0.08143800	0.28536700
46	Si	0.15427700	1.52554800	-0.40641600
47	Si	1.58811900	0.00000000	0.36741400
48	Si	0.00000000	-1.43933000	-0.24703600
49	H	-2.04259400	0.09796900	1.70402500
50	H	3.06075700	-0.19023100	0.35210700
51	H	-2.82811500	0.12244700	-0.57855700
52	H	0.00000000	-2.29963500	-1.46817300
53				
54				
55	44Sn:			
56	8			
57				
58	E(RB+HF-LYP) =	-859.940458914		
59	Sn	2.05795100	0.13412400	-0.35419100
60	Sn	-0.20015100	1.79834600	0.40095100
	Sn	-2.02156800	-0.11046400	-0.41646000
	Sn	0.10791000	-1.77242900	0.35052400

H	2.59584700	0.14531300	-1.98674000
H	-3.53183900	-0.57559200	0.29882200
H	3.47256200	0.22029800	0.62364400
H	0.25631400	-2.26887900	2.02304900

45Ga:

8

E(RB+HF-LYP) = -7702.01403854

Ga	-0.20288300	1.50919400	0.23923700
Ga	2.04100400	0.01841600	-0.24735800
Ga	0.08114400	-1.34491600	0.27599200
Ga	-1.97855600	-0.15556900	-0.25735400
H	3.58340400	0.26401700	-0.09738500
H	1.45261400	1.68341600	-0.34660800
H	-3.50107100	0.09980800	0.02374200
H	0.30305800	-2.88809900	0.09422600

45In:

8

E(RB+HF-LYP) = -763.234939071

In	-0.40536400	1.75204000	0.35855700
In	2.42329000	0.08910300	-0.37260500
In	0.21682600	-1.51350600	0.46029300
In	-2.27480700	-0.30549600	-0.43705300
H	3.97507900	0.89433300	-0.19110900
H	1.33704400	1.75813800	-0.55644800
H	-3.90319700	-0.54114800	0.20241100
H	0.55370000	-3.19626500	0.09473100

46Tl:

8

E(RB+HF-LYP) = -692.716535453

Tl	-2.94358900	-0.12941400	-0.39437600
Tl	0.23739000	1.78103500	0.33820200
Tl	2.65592900	-0.28812700	-0.48209900
Tl	-0.00872500	-1.40672600	0.53147600
H	0.26877600	3.49764200	-0.27097700
H	-1.65339400	1.44567700	-0.56838700
H	1.78586600	-1.40766100	1.31045100
H	4.37730800	-0.03388100	0.07950400

47Ge:

8

E(RB+HF-LYP) = -8310.55009168

Ge	2.07629700	-1.65129800	0.00000000
Ge	-0.33352400	-1.59213100	0.00000000
Ge	-1.94659100	2.40054000	0.00000000
Ge	0.00000000	0.79114900	0.00000000
H	2.95953300	-2.94033000	0.00000000
H	-0.96557100	3.66311600	0.00000000
H	3.09429900	-0.47826700	0.00000000

1				
2				
3	H	1.43391300	1.41115200	0.00000000
4				
5				
6	48Sn:			
7	8			
8	E(RB+HF-LYP) =	-859.908253021		
9	Sn	0.52737400	-2.13323700	0.00000000
10	Sn	2.38266100	-0.05711300	0.00000000
11	Sn	0.00000000	1.39702600	0.00000000
12	Sn	-2.84512600	0.79764200	0.00000000
13	H	0.79540400	-3.85488400	0.00000000
14	H	0.30478700	3.12170500	0.00000000
15	H	-1.20479600	-2.04162100	0.00000000
16	H	-3.14088500	2.55888500	0.00000000
17				
18				
19				
20	4Ge:			
21	8			
22	E(RB+HF-LYP) =	-8310.60680180		
23	Ge	-1.55522900	-0.20907800	-0.72204700
24	Ge	0.38853700	1.70845500	0.12913800
25	Ge	1.31100200	-0.84547300	-0.72845300
26	Ge	-0.15961900	-0.72776500	1.38274500
27	H	-1.02824400	1.40514900	-0.98468700
28	H	0.17550300	0.87810700	1.75503000
29	H	-0.17904000	-0.74895400	-1.71902100
30	H	1.52165900	0.82927100	-1.01559900
31				
32				
33				
34	4Pb:			
35	8			
36	E(RB+HF-LYP) =	-774.252771367		
37	Pb	0.95080200	-1.59496400	-0.89985900
38	Pb	-2.10075700	-0.37954400	0.15950000
39	Pb	0.31332100	1.81108700	-0.91976500
40	Pb	0.87128100	0.17074700	1.68780400
41	H	-1.03803200	-1.68885300	-1.06628900
42	H	-1.05284500	-0.24533300	1.93329400
43	H	0.81844200	0.13194600	-2.02185700
44	H	-1.56860300	1.20156800	-1.11494500
45				
46				
47				
48	4Sn:			
49	8			
50	E(RB+HF-LYP) =	-859.975313181		
51	Sn	-0.59296100	1.66756700	-0.85993000
52	Sn	2.06410200	-0.03640800	0.15234400
53	Sn	-0.65549500	-1.64723400	-0.85740500
54	Sn	-0.87215700	0.01743600	1.60740500
55	H	1.30139300	1.38915100	-1.00386400
56	H	1.02764100	-0.03064300	1.81556200
57	H	-0.75371700	0.01125000	-1.93780500
58	H	1.25023100	-1.43779400	-0.99464500
59				
60				

5Al:

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8
E(RB+HF-LYP) = -972.195134389
Al -0.55901700 -0.79382400 1.28453700
Al 1.63575500 0.51365300 0.00000000
Al -0.55901700 1.45425500 0.00000000
Al -0.55901700 -0.79382400 -1.28453700
H -0.85955400 -1.97663000 0.00000000
H -0.90925900 -1.64530100 -2.57404400
H -0.90925900 -1.64530100 2.57404400
H 3.21491100 0.32384200 0.00000000

5Ga:
8
E(RB+HF-LYP) = -7702.01574645
Ga 0.98440300 1.34308800 -0.24896200
Ga -1.58680700 0.00000000 -0.73327500
Ga -0.49655900 0.00000000 1.37535900
Ga 0.99273900 -1.33716900 -0.25383600
H 2.06495400 0.00000000 -0.85732300
H 1.90622700 -2.52918400 -0.74342800
H 1.88878300 2.54333100 -0.73553200
H -2.56704800 0.00000000 -1.98156800

5In:
8
E(RB+HF-LYP) = -763.237905149
In -0.65098700 -0.98664000 1.59967800
In 1.94738500 0.53015700 0.00000000
In -0.65098700 1.57681900 0.00000000
In -0.65098700 -0.98664000 -1.59967800
H -1.14462400 -2.11851300 0.00000000
H -1.10424900 -2.19110100 -2.80135200
H -1.10424900 -2.19110100 2.80135200
H 3.62637400 -0.05045000 0.00000000

6Al:
8
E(RB+HF-LYP) = -972.185239325
Al -1.76790800 0.22584000 0.00000000
Al 0.68169400 -0.69443300 1.32872000
Al 0.68169400 1.38726200 0.00000000
Al 0.68169400 -0.69443300 -1.32872000
H -2.61858000 -1.12453800 0.00000000
H 0.83486600 -1.66859700 -2.57940700
H -2.65442200 1.54665800 0.00000000
H 0.83486600 -1.66859700 2.57940700

6B:
8
E(RB+HF-LYP) = -101.706071196
B -1.11792500 0.71442100 0.00000000

1				
2				
3	B	0.52149900	-0.58725400	0.88305900
4	B	0.52149900	0.64196300	0.00000000
5	B	0.52149900	-0.58725400	-0.88305900
6	B	0.52149900	-0.58725400	-0.88305900
7	H	-2.04074600	-0.02867100	0.00000000
8	H	0.58508200	-1.38488800	-1.74468100
9	H	-1.36227500	1.88907100	0.00000000
10	H	0.58508200	-1.38488800	1.74468100
11				
12				
13	6Ga:			
14	8			
15	E(RB+HF-LYP) =	-7702.01742096		
16	Ga	-1.82250600	0.15585200	0.00000000
17	Ga	0.64975700	-0.70920800	1.33174200
18	Ga	0.64975700	1.36617700	0.00000000
19	Ga	0.64975700	-0.70920800	-1.33174200
20	Ga	0.64975700	-0.70920800	-1.33174200
21	H	-2.69062900	-1.17207700	0.00000000
22	H	0.72364200	-1.76013600	-2.52231900
23	H	-2.68634600	1.48034000	0.00000000
24	H	0.72364200	-1.76013600	2.52231900
25				
26				
27	6In:			
28	8			
29	E(RB+HF-LYP) =	-763.238145315		
30	In	-2.07188200	0.09558100	0.00000000
31	In	0.72314400	-0.81583700	1.54434200
32	In	0.72314400	1.61828200	0.00000000
33	In	0.72314400	-0.81583700	-1.54434200
34	In	0.72314400	-0.81583700	-1.54434200
35	H	-3.02880600	-1.37929200	0.00000000
36	H	0.66419400	-2.08923700	-2.77536300
37	H	-3.07944900	1.53049900	0.00000000
38	H	0.66419400	-2.08923700	2.77536300
39				
40				
41	6Tl:			
42	8			
43	E(RB+HF-LYP) =	-692.702383246		
44	Tl	-2.14684100	0.07375300	0.00000000
45	Tl	0.73902500	-0.86455200	1.70597600
46	Tl	0.73902500	1.71050000	0.00000000
47	Tl	0.73902500	-0.86455200	-1.70597600
48	Tl	0.73902500	-0.86455200	-1.70597600
49	H	-3.21546800	-1.36562400	0.00000000
50	H	0.35247100	-2.32471900	-2.74845800
51	H	-3.17844900	1.54803300	0.00000000
52	H	0.35247100	-2.32471900	2.74845800
53				
54				
55	7Ga:			
56	8			
57	E(RB+HF-LYP) =	-7702.01795942		
58	Ga	-1.73603100	-0.52789000	-0.33748900
59	Ga	1.35441700	-0.78094600	-0.73046900
60	Ga	0.32821500	-0.28304700	1.40188800
	Ga	0.15288200	1.59017700	-0.20136700

H	-2.58063700	0.33991900	-1.36526900
H	-0.31359700	2.89958100	-0.97332000
H	-2.46682400	-1.84790400	0.12604500
H	2.27705000	-1.33871700	-1.89693600

8Al:

8

E(RB+HF-LYP) = -972.147102069

Al	1.36218500	-0.96794000	-0.67350900
Al	-1.56395600	-0.89387900	-0.04364500
Al	-0.12062600	1.62537600	-0.75089600
Al	0.33178200	0.24299300	1.51117800
H	-0.25095500	-1.62244100	-0.97434900
H	0.66621300	0.47778000	3.03393700
H	0.95569400	0.49868400	-1.57374100
H	-1.49296200	0.56081500	-1.04650200

8B:

8

E(RB+HF-LYP) = -101.530780690

B	0.00000000	0.94551100	-0.35396400
B	-0.81883600	-0.47275500	-0.35396400
B	0.81883600	-0.47275500	-0.35396400
B	0.00000000	0.00000000	1.14173600
H	-1.22989600	0.71008100	-0.90437200
H	0.00000000	-1.42016200	-0.90437200
H	1.22989600	0.71008100	-0.90437200
H	0.00000000	0.00000000	2.31389700

8C:

8

E(RB+HF-LYP) = -154.554715649

C	0.00000000	1.01572400	-0.22999100
C	-0.87964300	-0.50786200	-0.22999100
C	0.87964300	-0.50786200	-0.22999100
C	0.00000000	0.00000000	0.82281200
H	-1.02241300	0.59029000	-0.89796500
H	0.00000000	-1.18058100	-0.89796500
H	1.02241300	0.59029000	-0.89796500
H	0.00000000	0.00000000	1.89685600

8Ga:

8

E(RB+HF-LYP) = -7701.98593128

Ga	0.00000000	1.92830700	-0.56138000
Ga	-1.66996300	-0.96415300	-0.56138000
Ga	1.66996300	-0.96415300	-0.56138000
Ga	0.00000000	0.00000000	1.68065400
H	-1.29000400	0.74478400	-1.06173800
H	0.00000000	-1.48956800	-1.06173800
H	1.29000400	0.74478400	-1.06173800

1				
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3	H	0.00000000	0.00000000	3.29323400
4				
5				
6	8Ge:			
7	8			
8	E(RB+HF-LYP) =	-8310.61039069		
9	Ge	0.00000000	1.74065700	-0.42557900
10	Ge	-1.50745300	-0.87032900	-0.42557900
11	Ge	1.50745300	-0.87032900	-0.42557900
12	Ge	0.00000000	0.00000000	1.30452400
13	H	-1.21349900	0.70061400	-1.23739100
14	H	0.00000000	-1.40122800	-1.23739100
15	H	1.21349900	0.70061400	-1.23739100
16	H	0.00000000	0.00000000	2.82304800
17				
18				
19				
20	8In:			
21	8			
22	E(RB+HF-LYP) =	-763.242034450		
23	In	0.00000000	2.20544200	-0.69788700
24	In	-1.90996900	-1.10272100	-0.69788700
25	In	1.90996900	-1.10272100	-0.69788700
26	In	0.00000000	0.00000000	2.08042400
27	H	-1.39872700	0.80755500	-1.08002000
28	H	0.00000000	-1.61511100	-1.08002000
29	H	1.39872700	0.80755500	-1.08002000
30	H	0.00000000	0.00000000	3.88871000
31				
32				
33				
34	8Pb:			
35	8			
36	E(RB+HF-LYP) =	-774.227457792		
37	Pb	0.00000000	2.08134400	-0.52997700
38	Pb	-1.80249700	-1.04067200	-0.52997700
39	Pb	1.80249700	-1.04067200	-0.52997700
40	Pb	0.00000000	0.00000000	1.59993200
41	H	-1.36625800	0.78880900	-1.39262000
42	H	0.00000000	-1.57761800	-1.39262000
43	H	1.36625800	0.78880900	-1.39262000
44	H	0.00000000	0.00000000	3.35788100
45				
46				
47				
48	8Si:			
49	8			
50	E(RB+HF-LYP) =	-1160.39360685		
51	Si	0.00000000	1.61249200	-0.39625900
52	Si	-1.39645900	-0.80624600	-0.39625900
53	Si	1.39645900	-0.80624600	-0.39625900
54	Si	0.00000000	0.00000000	1.25013000
55	H	-1.17665700	0.67934300	-1.19184100
56	H	0.00000000	-1.35868700	-1.19184100
57	H	1.17665700	0.67934300	-1.19184100
58	H	0.00000000	0.00000000	2.71660200
59				
60				

8Sn:

1
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3 8
4 E(RB+HF-LYP) = -859.967357364
5 Sn 0.00000000 1.98739200 -0.50280900
6 Sn 1.72113200 -0.99369600 -0.50280900
7 Sn -1.72113200 -0.99369600 -0.50280900
8 Sn 0.00000000 0.00000000 1.52433800
9 H 1.31383700 0.75854400 -1.33820900
10 H 0.00000000 0.00000000 3.21902800
11 H -1.31383700 0.75854400 -1.33820900
12 H 0.00000000 -1.51708800 -1.33820900
13
14

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16 9Ge:

17 8
18 E(RB+HF-LYP) = -8310.58187564
19 Ge -0.15434100 0.00000000 1.43339000
20 Ge 0.51454500 -1.96654200 0.00000000
21 Ge -0.15434100 0.00000000 -1.43339000
22 Ge -0.15434100 1.90192400 0.00000000
23 H -1.30284800 0.05038000 2.48823300
24 H -1.30284800 0.05038000 -2.48823300
25 H 2.06441000 -1.64825800 0.00000000
26 H -1.10740800 3.13603400 0.00000000
27
28
29

30 9Si:

31 8
32 E(RB+HF-LYP) = -1160.38446343
33 Si -0.14187300 -0.01610500 1.30414500
34 Si 0.51807600 -1.85681100 0.00000000
35 Si -0.14187300 -0.01610500 -1.30414500
36 Si -0.14187300 1.81036200 0.00000000
37 H -1.09092400 -0.07050500 2.45571600
38 H -1.09092400 -0.07050500 -2.45571600
39 H 2.01495300 -1.69664200 0.00000000
40 H -1.12752000 2.93887800 0.00000000
41
42
43

44 9Sn:

45 8
46 E(RB+HF-LYP) = -859.925047028
47 Sn -0.11106800 0.04315300 1.75946900
48 Sn -0.11106800 -2.29367100 0.00000000
49 Sn -0.11106800 0.04315300 -1.75946900
50 Sn 0.36978600 2.15195100 0.00000000
51 H -1.62812900 0.65243900 2.40062500
52 H -1.62812900 0.65243900 -2.40062500
53 H 1.65940700 -2.32424600 0.00000000
54 H -0.23228700 3.79002500 0.00000000
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3 **Tetrahedranes. A Theoretical Study of Singlet E₄H₄ Molecules**
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6 **(E = C – Pb and B – Tl)**
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11 **By ROBIN HAUNSCHILD and GERNOT FRENKING***
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ABSTRACT

Quantum chemical calculations using DFT (B3LYP) and ab initio (CCSD(T)) methods have been carried out to elucidate the E_4H_4 singlet potential energy hypersurface for the group-13 and group-14 elements. The results show that there are numerous E_4H_4 energy minima for the compounds of group-13 and group-14 elements. This holds particularly for the heavier atoms. The classical T_d tetrahedron structure is energetically more favourable for the group-13 compounds E_4H_4 where the tetrahedron isomers are energy minima for all elements E except for thallium. The tetrahedranes Al_4H_4 **1Al** and Ga_4H_4 **1Ga** are the global energy minima on the singlet PES while **1B** is slightly less stable than the singly hydrogen-bridged planar form **12B** which has a rhombic B_4 core. The lowest-lying energy minima for In_4H_4 and Tl_4H_4 are tetrahedranes where the E_4 core is face-bridged by the hydrogen atoms. The classical T_d tetrahedron structure of the group-14 elements is only for carbon and silicon an energy minimum at B3LYP/def2-TZVPP. The latter form of Si_4H_4 is a third-order saddle point at BP86/def2-TZVPP and MP2/def2-TZVPP. The global energy minimum form for C_4H_4 is the vinylideneacetylene isomer **27C** which is -63.7 kcal/mol lower in energy than the tetrahedrane. The most stable isomers of Si_4H_4 and Ge_4H_4 at CCSD(T)/def2-QZVPP are the singly hydrogen edge-bridged tetrahedrane structures **18E** which are more than 40 kcal/mol lower in energy than the classical tetrahedrane. The B3LYP/def2-TZVPP calculations predict that tetrahedrane structure with edge-bridging hydrogen atoms **3Ge** is slightly more stable than **18Ge**. The former isomer is calculated as the global energy minimum on the singlet PES of Sn_4H_4 and Pb_4H_4 .

1. INTRODUCTION

The synthesis of hydrocarbons which have the shape of platonic solid geometries belongs to the classic challenges in hydrocarbon chemistry. [1,2] There are five platonic solids, icosahedron, octahedron, tetrahedron, hexahedron (cube) and dodecahedron. Because of the valence restrictions of carbon only the latter three may become synthesized as hydrocarbons. Cubane (C_8H_8) has been isolated in 1964 [3] while the synthesis of dodecahedrane ($C_{20}H_{20}$) was achieved in 1981. [4] The smallest platonic hydrocarbon tetrahedrane could until now only become synthesized as substituted derivative C_4R_4 where $R = t$ -butyl. [5] The parent system C_4H_4 has been the subject of numerous theoretical studies. [6]

Tetrahedrane structures E_4R_4 with bulky substituents could also become synthesized for the heavier group-14 elements silicon [7] and germanium [8] while tetrastannatetrahedranes and tetraplumbatetrahedranes are still waiting to be prepared. Theoretical studies of the heavier group-14 homologues E_4R_4 where $E = Si - Pb$ have also been published. [9,10] Ab initio calculations at the Hartree-Fock (HF) level and DFT calculations using B3LYP predict that the tetrahedrane structures of C_4H_4 and Si_4H_4 are minima on the potential energy surface (PES) while the heavier homologues of tetrahedrane E_4H_4 where $E = Ge - Pb$ are third-order saddle points. [9] However, MP2 calculations suggest that tetrasilatetrahedrane is a second-order saddle point while all other tetrahedranes E_4H_4 where $E = C, Ge - Pb$ are energy minima. [9] Tetrahedrane structures have also been synthesized for substituted derivatives of the group-13 elements E_4R_4 where $E = B - In$ and $R = t$ -Bu, $Si(t$ -Bu) $_3$, $C(SiMe_3)_3$, $Si(SiMe_3)_3$, or $Si(GeMe_3)_3$. [11] A thallium compound $Tl_4[C(SiMe_3)_3]_4$ has also become isolated but the x-ray structure analysis showed that it has a distorted tetrahedron structure where the Tl-Tl-distances vary between 3.335 and 3.575 Å. [12] The only group-13 tetrahedrane compound which could become isolated without a bulky substituent is B_4Cl_4 . [13] Very few theoretical studies have been published about the PES of E_4H_4 where $E = B - Tl$. [10,14]

In this work we report about quantum chemical calculations using DFT and ab initio methods of the singlet potential energy surfaces of group-13 and group-14 species E_4H_4 where $E = B - Tl$ and $E = C - Pb$. The starting point of our study is the tetrahedrane structure of E_4H_4 . However, we systematically searched for other energy minima on the singlet PES with

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3 the goal to identify the global energy minimum for each species. To this end we used every
4 equilibrium structures which was found for a particular element E as starting point for
5 geometry optimizations of the other E_4H_4 species. We found more than 40 different structures
6 which are energy minima on at least one of the E_4H_4 PES. The complexity of the systems
7 made it impractical to locate the transition states for interconversion of the minima. However,
8 the results give an overview of the energetically lowest lying structures and particularly the
9 global energy minimum for each E_4H_4 species. We also optimized the geometries of several
10 substituted tetrahedranes E_4R_4 which are experimentally known.
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20 2. COMPUTATIONAL METHODS

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22 For all geometry optimizations of the E_4H_4 structures the gradient corrected hybrid
23 density functional B3LYP [15] as implemented [16] in the Gaussian 03 program [17] was
24 employed in conjunction with a triple zeta quality basis set with two sets of polarization
25 functions (def2-TZVPP) [18]. The nature of the stationary point (minimum, transition state or
26 higher order saddle point) was clarified by calculating the harmonic vibrational frequencies.
27 For low lying transition states, intrinsic reaction coordinate (IRC) [19] calculations were
28 performed in order to identify the minima connected to the transition states. In the case of
29 small imaginary modes, the verification was done by dynamic reaction path (DRP) [20]
30 calculations using the frog module of the TURBOMOLE program [21]. The geometries of the
31 parent tetrahedranes E_4H_4 have also been optimized using coupled-cluster theory at the
32 CCSD(T) [22] level as implemented in the Molpro 2006.1 program [23] with a quadruple-
33 zeta basis set with two sets of polarization functions (def2-QZVPP) [18]. Single-point energy
34 calculations have been performed for selected E_4H_4 species at CCSD(T)/def2-QZVPP using
35 B3LYP/def2-TZVPP optimized geometries.
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48 The substituted E_4R_4 tetrahedrane structures were optimized using the gradient
49 corrected density functional BP86 [24] via an interface to TURBOMOLE for the energy and
50 gradient calculations using the resolution of the identity (RI) approximation [26], and
51 Gaussian 03 for the geometry optimization.
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3. RESULTS AND DISCUSSION

3.1. Substituted tetrahedranes E_4R_4 (E = B – Tl; C – Pb)

We optimized the geometries of the substituted group-13 tetrahedranes $B_4(t\text{-butyl})_4$, $Al_4[Si(t\text{-butyl})_3]_4$, $E_4[C(SiMe_3)_3]_4$ (E = Ga, In, Tl) and the group-14 tetrahedranes (E = Si, Ge, Sn, Pb) at RI-BP86/def2-TZVPP. The geometries of the latter compounds have been determined with x-ray structure analysis, except for $Sn_4[Si(t\text{-butyl})_3]_4$ and $Pb_4[Si(t\text{-butyl})_3]_4$ which have not been synthesized until now. Table 1 shows the calculated and experimental E-E and E-R distances.

Table 1

The optimizations of the E_4R_4 species were carried out with local T_d symmetry restriction of the E_4 core. Table 1 shows that the calculated E-E and E-R distances of the group-13 compounds where E = B – In are in reasonable agreement with the experimental values. The experimentally observed bond lengths in the solid state are shorter than the calculated data particularly for the heavier species Al – In. This can be explained with the effect of intermolecular interactions which yield a bond shortening that is more pronounced when the bonds are weaker. [28] The x-ray structure analysis of $Tl_4[C(SiMe_3)_3]_4$ reveals a significantly distorted tetrahedron core where the Tl-Tl distances vary between 3.322 – 3.638 Å. [12] A geometry optimization of $Tl_4[C(SiMe_3)_3]_4$ without symmetry restriction gave a structure which has Tl-Tl distances in the range of 3.436 – 3.687 Å and Tl-C distances between 2.434 – 2.462 Å. This agrees quite well with the experimental values. The calculated values for the group-14 tetrahedranes $C_4(t\text{-butyl})_4$, $Si_4[Si(t\text{-butyl})_3]_4$ and $Ge_4[Si(t\text{-butyl})_3]_4$ also agree quite well with the experimental values. [5,7,8] The differences between the slightly shorter distances which are calculated at the RI-BP86/def2-TZVPP level and the experimental data are at least partly due to solid state effects.

3.2. Parent tetrahedranes E_4H_4 ($E = B - Tl; C - Pb$)

Table 2

Table 2 shows the calculated E-E and E-H distances of the T_d structures of the group-13 and group-14 tetrahedranes E_4H_4 ($E = B - Tl$ and $C - Pb$) at RI-BP86/def2-TZVPP, B3LYP/def2-TZVPP and CCSD(T)/def2-QZVPP. The theoretically predicted bond lengths using DFT are in very good agreement with the highly accurate ab initio values. This is gratifying because the large number of structures which is discussed below could only become optimized at B3LYP/def2-TZVPP while the substituted systems were optimized at RI-BP86/def2-TZVPP.

While the geometries are very similar, there is a remarkable difference between the DFT results at RI-BP86/def2-TZVPP and B3LYP/def2-TZVPP for the silicon tetrahedrane Si_4H_4 . The calculation of the vibrational frequencies showed that the B3LYP/def2-TZVPP optimized structure is a minimum ($i = 0$) while the RI-BP86/def2-TZVPP optimized form has a degenerate imaginary mode ($i = 2$). It has already been noted before that the nature of the optimized tetrahedrane structure of Si_4H_4 depends on the level of theory. Jemmis and coworkers reported that Si_4H_4 (T_d) is a minimum at HF and B3LYP but it has two imaginary modes at MP2. [9f].

3.3. Potential energy surfaces of Group-13 Compounds E_4H_4 ($E = B - Tl$)

We made an extensive search for energy minima on the E_4H_4 singlet PES in order to locate not only local minima but also in order to find the global energy minima. We optimized numerous structures with and without symmetry constraints and calculated the vibrational frequencies in order to see if the species are energy minima. Whenever we found a transition state ($i = 1$) or higher order saddle point ($i > 2$) we located the associated energy minima. This procedure gave rise to 48 different structures which are shown in Figure 1.

Figure 1

Many structures which are shown in Figure 1 are not relevant for the discussion in this paper which focuses on finding low-lying energy minima on the E_4H_4 singlet PES. They may be helpful for future studies where pathways for rearrangement of the E_4H_4 isomers may be important. The calculated relative energies at B3LYP/def2-TZVPP of the group-13 structures are shown in table 3. The bond lengths of the energetically lowest lying isomers are given in figure 2.

The red entries in table 3 denote the global energy minima on the E_4H_4 singlet PES calculated at B3LYP/def2-TZVPP. The "classical" [26] tetrahedrane structures of aluminium **1Al** and gallium **1Ga** are predicted to be the lowest lying isomers of the Al_4H_4 and Ga_4H_4 species. The classical tetrahedrane forms of B_4H_4 and In_4H_4 are also energy minima but the calculations show that there are energetically more stable isomers. The planar structures **12B** and **14B** are 11.7 and 4.7 kcal/mol lower in energy than **1B** and the former structure is predicted as the global minimum on the B_4H_4 singlet PES. The global energy minimum for In_4H_4 is the quadruply hydrogen bridged **2In** which has also T_d symmetry. It can be considered as "nonclassical" [26] tetrahedrane. The hydrogen atoms in **2In** are on top of each In_3 plane where each hydrogen bridges three indium atoms. The isomer **2E** is also the global energy minimum for $E = Tl$ while it is an energetically higher lying local minimum for $E = Al$ and $E = Ga$ (Table 3). The structure **2B**, however, is a saddle point with eight imaginary frequencies which is 310.2 kcal/mol higher in energy than **1B**. This demonstrates once more that chemical bonding of the elements of the first octal row is very different from the heavier homologues. The reasons for this are well understood. [27] The B3LYP/def2-TZVPP calculations of the indium compounds suggest that there are seven other isomers (**5In**, **6In**, **21In**, **23In**, **29In**, **31In**, **34In**, **36In**, **38In**, **45In**,) lower in energy than **1In**.

Figure 2, Table 3

The quadruply hydrogen face-bridged structure **2Tl** is 62.7 kcal/mol lower in energy than the tetrahedrane **1Tl** which has three imaginary frequencies and thus, is not a minimum on the PES (Table 3). There are five other energy minima which are more stable than **1Tl**, that

is **11Tl**, **17Tl**, **21Tl**, **34Tl**, and **39Tl**. The second lowest-lying isomer **34Tl** has a very interesting pseudo-tetrahedral structure where the four thallium atoms are connected to each other through four hydrogen bonds (Figure 2).

Table 4

Table 4 gives the relative energies of the energy minima structures at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. The ab initio data conform that the tetrahedrane structures **1Al** and **1Ga** are the global energy minima on the Al_4H_4 and Ga_4H_4 singlet PES, structures **2In** and **2Tl** are the most stable structures of In_4H_4 and Tl_4H_4 and **12B** is the energetically lowest lying singlet species for B_4H_4 . However, there are significant changes in the energy differences between the isomers when one goes from B3LYP/def2-TZVPP to CCSD(T)/def2-QZVPP. The ab initio calculations predicted that the planar form **12B** is only 5.7 kcal/mol lower in energy than the tetrahedrane **1B** while **14B** is even slightly less stable than **1B**. Overall, the tetrahedrane structures **1E** are calculated at the ab initio level to be more stable relative to the other isomers of all elements E compared with the DFT values. It is gratifying that both methods predict the same structures as global minima on the group-13 E_4H_4 singlet PES.

3.4. Potential energy surfaces of Group-14 Compounds E_4H_4 (E = C – Pb)

The relative energies of the group-14 structures E_4H_4 are shown in table 5. There are significant differences in the relative energies compared to the group-13 species (Table 4).

Table 5

The classical tetrahedran form **1E** is a minimum at the B3LYP/def2-TZVPP level only for E = C, Si while it is a third-order saddle point for E = Ge, Sn, Pb. As noted before, the T_d form **1Si** is a second-order saddle point at BP86/def2-TZVPP and MP2/def2-TZVPP. For all group-14 E_4H_4 species holds that there are several energy minima which are much lower in energy than the classical tetrahedrane form **1E**. The calculated energies in Table 5 show that there are seven C_4H_4 carbon isomers which are more stable than **1C**. The global energy minimum form is the vinylideneacetylene isomer **27C** (-63.7 kcal/mol) which is slightly lower

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3 in energy than the cummulene **40C** (-60.4 kcal/mol). The other energy minima **16C** (-7.1
4 kcal/mol), **20C** (-24.5 kcal/mol), **18C** (-8.8 kcal/mol), **24C** (-27.5 kcal/mol) and **44C** (-16.0
5 kcal/mol) are clearly less stable than **27C**.
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10 The global energy minimum structure for Si_4H_4 is the singly hydrogen edge-bridged
11 tetrahedrane structure **18Si** which is 46.8 kcal/mol lower in energy than **1Si**. There are six
12 other local minima on the Si_4H_4 PES which possess a distorted tetrahedrane Si_4 core and
13 which are lower in energy than **1Si**. They are in descending order **44Si** (-41.7 kcal/mol), **8Si**
14 (-31.0 kcal/mol), **10Si** (-29.2 kcal/mol), **16Si** (-26.3 kcal/mol), **9Si** (-25.2 kcal/mol) and **3Si** (-
15 24.3 kcal/mol).
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22 The global energy minimum for the heavier group-14 systems E_4H_4 where $\text{E} = \text{Ge}, \text{Sn},$
23 **Pb** is the quadruply hydrogen edge-bridged tetrahedrane structure **3E** which is for all three
24 elements much lower in energy than **1E**. The energy difference between the classical
25 tetrahedrane form and **3E** is 67.2 kcal/mol for $\text{E} = \text{Ge}$, 88.8 kcal/mol for $\text{E} = \text{Sn}$ and 125.1
26 kcal/mol for $\text{E} = \text{Pb}$. However, there are several other isomeric forms of the latter species
27 which have a distorted E_4 core that are close in energy to **3E**. For the germanium compounds
28 there are four isomers **4Ge** (-61.8 kcal/mol), **8Ge** (-64.1 kcal/mol), **18Ge** (-65.5 kcal/mol) and
29 **44Ge** (-60.9 kcal/mol) which are < 10 kcal/mol less stable than **3Ge**. The tin isomers **4Sn** (-
30 83.9 kcal/mol) and **8Sn** (-78.9 kcal/mol) are also within a range of 10 kcal/mol of the global
31 energy minimum **3Sn**. The lead structure **4Pb** (-120.7 kcal/mol) is only 4.4 kcal/mol higher in
32 energy than **3Pb** (Table 5). Altogether, we located 12 energy minima for Ge_4H_4 and Sn_4H_4
33 and 11 energy minima for Ge_4H_4 at B3LYP/def2-TZVPP.
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Table 6

Table 6 gives the relative energies of the group-14 isomers of E_4H_4 which are
calculated at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. The ab initio data give the same
global energy minima as the DFT values except for the germanium system Ge_4H_4 . The
energetically lowest lying form at CCSD(T)/def2-QZVPP is **18Ge** while the calculations at
B3LYP/def2-TZVPP predict that **3Ge** is the global energy form. However, the energy
difference between **18Ge** and **3Ge** at both levels of theory is very small. The ab initio

calculations suggest that **18Ge** is 1.7 kcal/mol lower in energy than the second lowest-lying isomer **3Ge** while the DFT calculations give the same energy difference but in favor of **3Ge** (Table 5). Note that the CCSD(T)/def2-QZVPP calculations predict that **44Ge** is another isomer which is only slightly less stable by 3.2 kcal/mol than **18Ge**. The energy difference between **18Ge** and **44Ge** at B3LYP/def2-TZVPP is 4.6 kcal/mol. Generally, the calculated energy differences between the isomers of E_4H_4 at CCSD(T)/def2-QZVPP (Table 6) are not very different from the B3LYP/def2-TZVPP values (Table 5).

4. SUMMARY

The calculations which are presented in this work show that there are numerous energy minima on the singlet PES for E_4H_4 of the elements of groups 13 and 14. This holds particularly for the heavier atoms. The classical T_d tetrahedron structure is energetically more favourable for the group-13 compounds E_4H_4 where the tetrahedron isomers are energy minima for all elements E except for thallium. The tetrahedranes Al_4H_4 **1Al** and Ga_4H_4 **1Ga** are the global energy minima on the singlet PES while **1B** is slightly less stable than the singly hydrogen-bridged planar form **12B** which has a rhombic B_4 core. The lowest-lying energy minima for In_4H_4 and Tl_4H_4 are tetrahedranes where the E_4 core is face-bridged by the hydrogen atoms. The classical T_d tetrahedron structure of the group-14 elements is only for carbon and silicon an energy minimum at B3LYP/def2-TZVPP. The latter form of Si_4H_4 is a third-order saddle point at BP86/def2-TZVPP and MP2/def2-TZVPP. The global energy minimum form for C_4H_4 is the vinylideneacetylene isomer **27C** which is -63.7 kcal/mol lower in energy than the tetrahedrane. The most stable isomers of Si_4H_4 and Ge_4H_4 at CCSD(T)/def2-QZVPP are the singly hydrogen edge-bridged tetrahedrane structures **18E** which are more than 40 kcal/mol lower in energy than the classical tetrahedrane. The B3LYP/def2-TZVPP calculations predict that the tetrahedrane structure with edge-bridging hydrogen atoms **3Ge** is slightly more stable than **18Ge**. The former isomer is calculated as the global energy minimum on the singlet PES of Sn_4H_4 and Pb_4H_4 .

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39 [26] The classical tetrahedrane structure of E₄H₄ **1E** has T_d symmetry where each
40 hydrogen atom is terminally bonded to an atom E. Nonclassical tetrahedranes have one or more
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3 hydrogen atoms which are bridging two or three atoms E. Examples are structure **2E** which has
4 also T_d symmetry but the hydrogen atoms are face-bridging between three atoms E. Other
5 nonclassical tetrahedrane-type structures are **3E**, **4E**, **5E**, **7E**, **14E** where the E_4 core does not have
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Figure Captions

Figure 1. Optimized E₄H₄ structures at B3LYP/def2-TZVPP.

Figure 2. Selected calculated bond lengths and angles (in Ångstroms and degrees) of the energetically lowest-lying E₄H₄ structures at B3LYP/def2-TZVPP.

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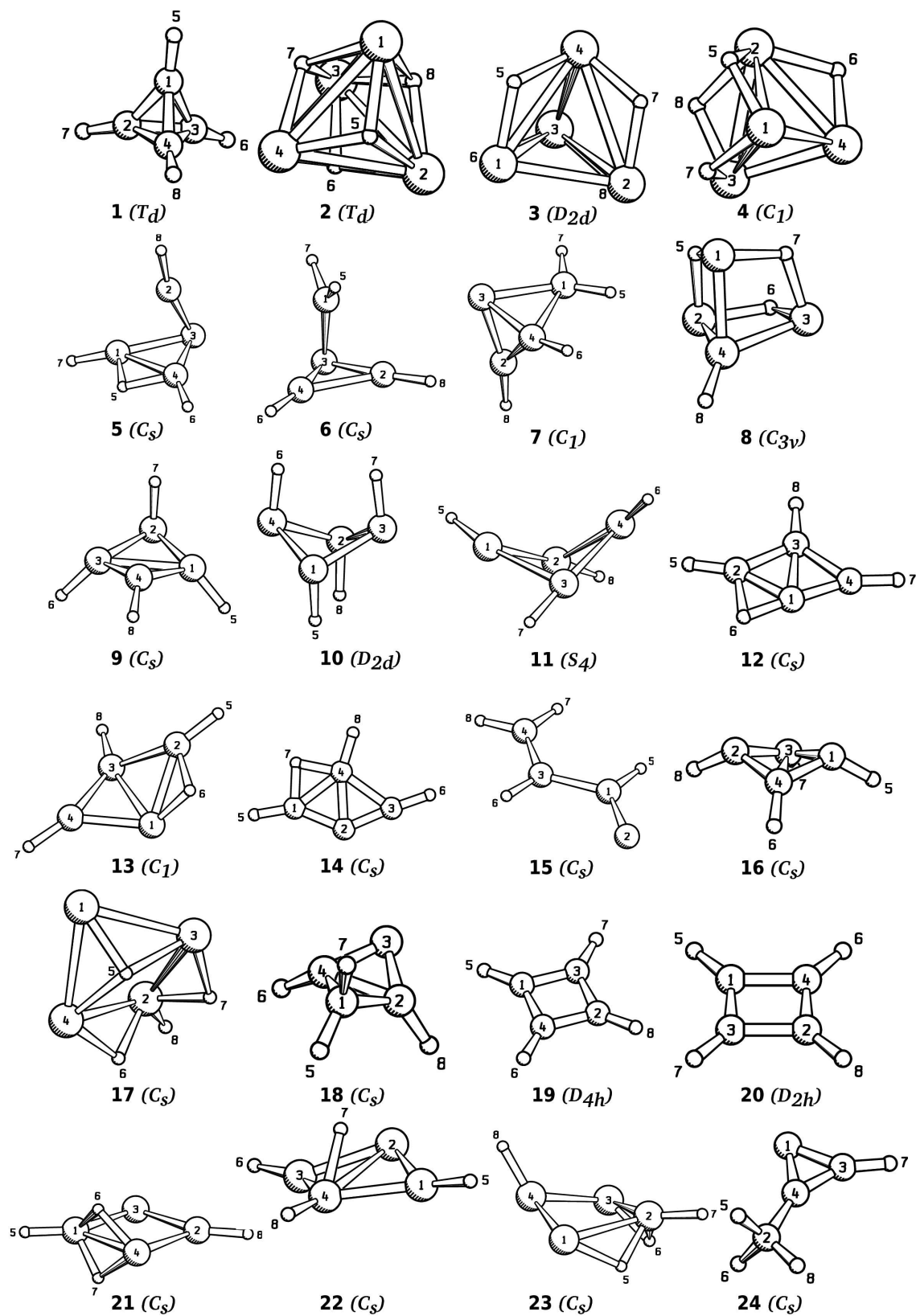


Figure 1

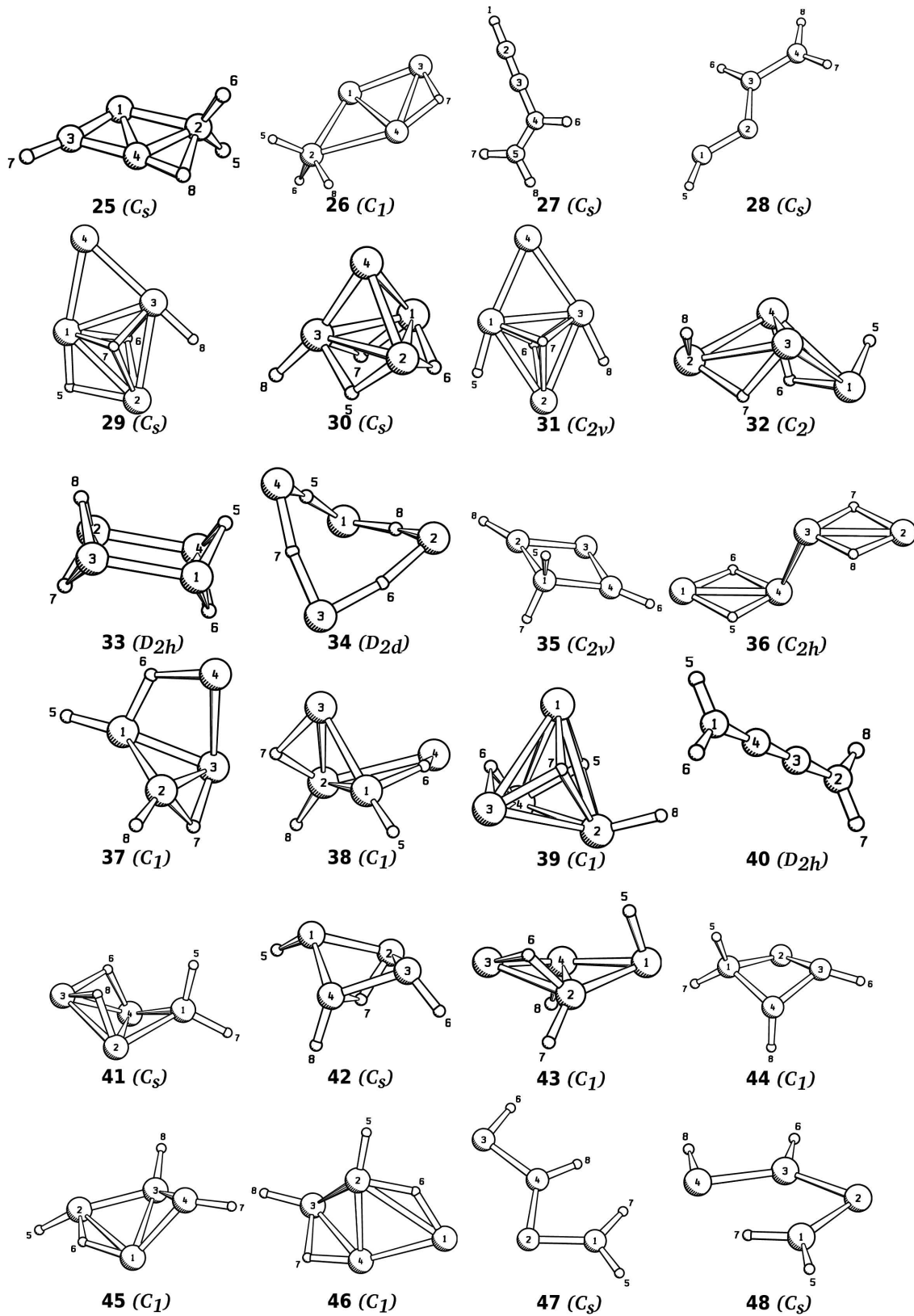


Figure 1 (continued)

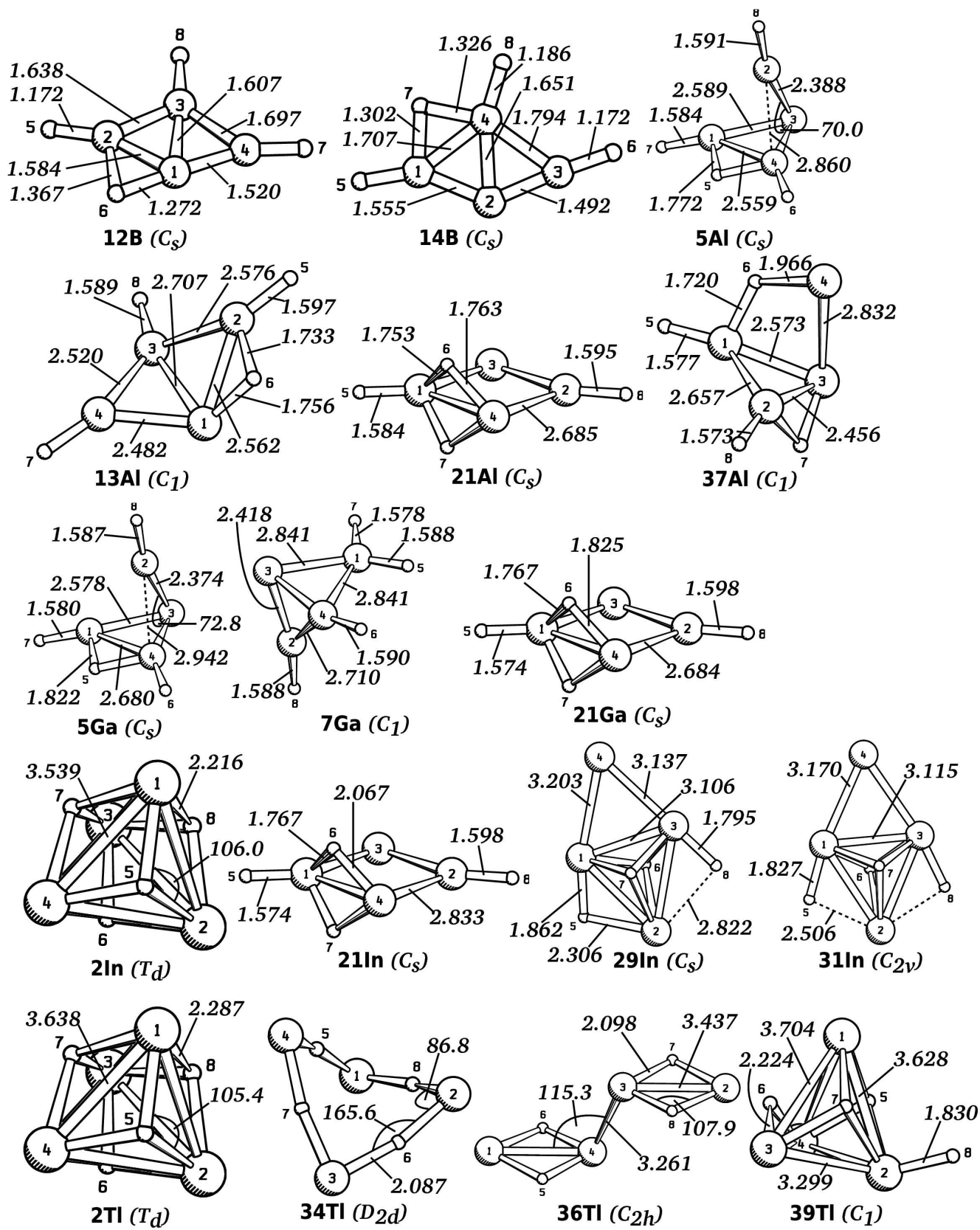


Figure 2

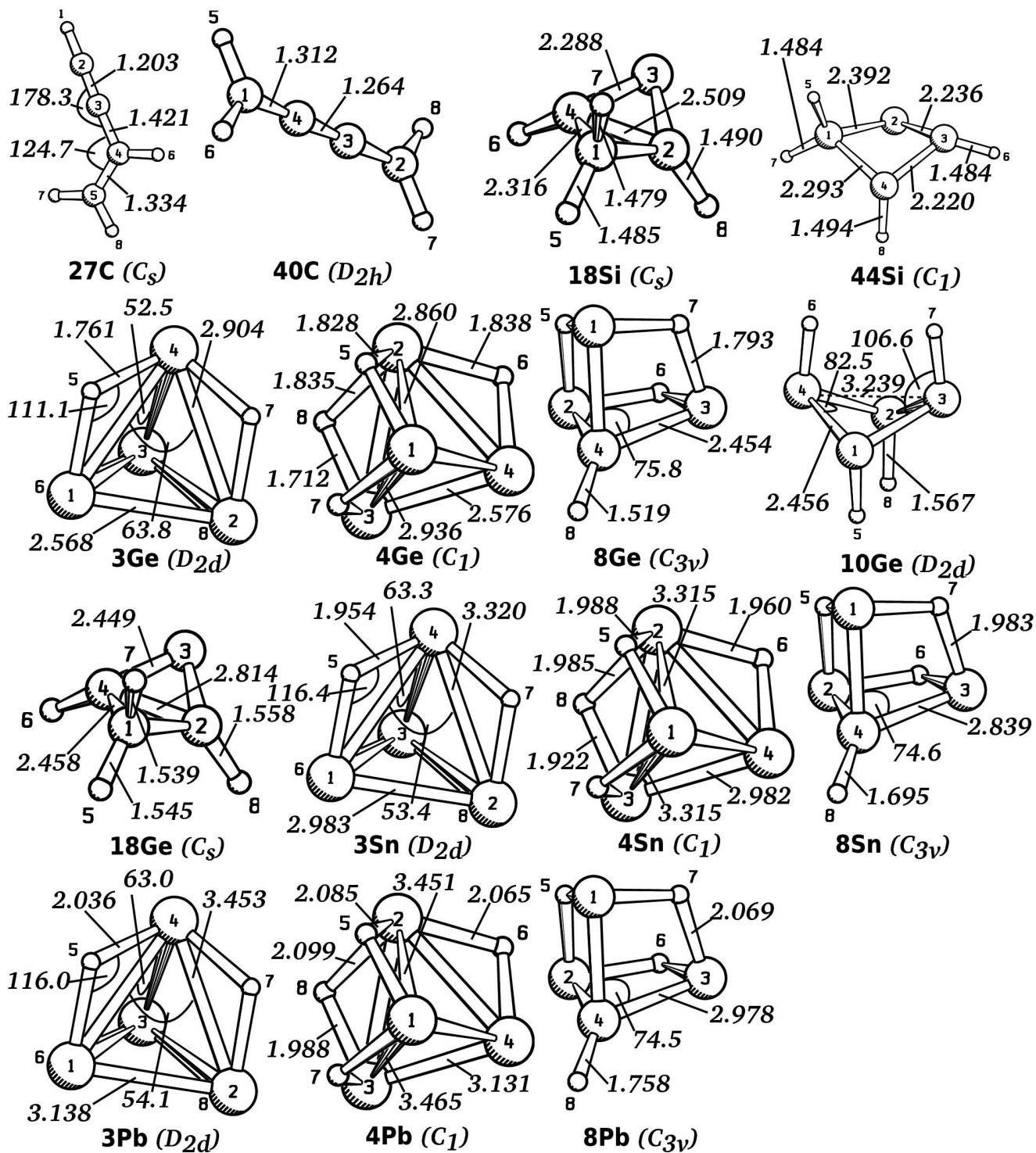


Figure 2 (continued)

Table 1. Calculated E_4R_4 bond lengths [\AA] for $E = B - Tl$ and $C - Pb$ at RI-BP86/def2-TZVPP .

structure	$d(E-E)_{\text{calc}}$	$d(E-R)_{\text{calc}}$	$d(E-E)_{\text{exp}}$	$d(E-R)_{\text{exp}}$
$B_4(t\text{-Bu})_4$	1.699	1.582	1.699 – 1.714 ^a	1.570 – 1.576 ^a
$Al_4[\text{Si}(t\text{-Bu})_3]_4$	2.627	2.534	2.600 – 2.612 ^b	2.467 – 2.501 ^b
$Ga_4[\text{C}(\text{SiMe}_3)_3]_4$	2.751	2.116	2.678 – 2.702 ^c	2.06 – 2.11 ^c
$In_4[\text{C}(\text{SiMe}_3)_3]_4$	3.098	2.317	2.989 – 3.013 ^e	2.24 – 2.26 ^d
$Tl_4[\text{C}(\text{SiMe}_3)_3]_4$	3.411	2.448	3.322 – 3.638 ^f	2.33 – 2.38 ^f
$C_4(t\text{-Bu})_4$	1.499	1.503	1.480 – 1.487 ^g	1.480 - 1.503 ^g
$Si_4[\text{Si}(t\text{-Bu})_3]_4$	2.362	2.400	2.315 – 2.320 ^h	2.355 – 2.365 ^h
$Ge_4[\text{Si}(t\text{-Bu})_3]_4$	2.508	2.440	2.431 – 2.447 ⁱ	2.378 – 2.385 ⁱ
$Sn_4[\text{Si}(t\text{-Bu})_3]_4$	2.891	2.642	-	-
$Pb_4[\text{Si}(t\text{-Bu})_3]_4$	3.076	2.738	-	-

Experimental values were taken from a) ref. 29, b) ref. 30, c) ref. 31, d) ref. 32, e) ref. 12, f) ref. 5, g) ref. 7, h) ref. 8

Table 2. Calculated E₄H₄ bond lengths [Å] of the tetrahedrane structures **1E** at RI-BP86/def2-TZVPP, B3LYP/def2-TZVPP and CCSD(T)/def2-QZVPP.

	RI-BP86/def2-TZVPP		B3LYP/def2-TZVPP		CCSD(T)/def2-QZVPP	
	d(E-E)	d(E-H)	d(E-E)	d(E-H)	d(E-E)	d(E-H)
1B	1.684	1.191	1.676	1.181	1.685	1.183
1Al	2.597	1.603	2.591	1.590	2.592	1.590
1Ga	2.556	1.586	2.568	1.582	2.604	1.596
1In	2.944	1.765	2.962	1.763	2.984	1.775
1Tl	3.133	1.836	3.194	1.843	3.155	1.847
1C	1.483	1.076	1.474	1.068	1.480	1.069
1Si	2.324	1.483	2.316	1.472	2.317	1.472
1Ge	2.471	1.540	2.469	1.531	2.478	1.533
1Sn	2.881	1.726	2.879	1.715	2.877	1.718
1Pb	3.126	1.820	3.143	1.813	3.100	1.810

Table 3. Calculated E_4H_4 energies in kcal/mol for all group-13 elements at B3LYP/def2-TZVPP relative to **1E**. All values in kcal/mol. The values for the global energy minima are given in red.

	B	Al	Ga	In	Tl
1 T_d	0.0	0.0	0.0	0.0	0.0 (i = 3)
2 T_d	310.2 (i = 8)	34.3	7.9	-26.6	-62.7
3 D_{2d}	150.3 (i = 2)	47.5 (i = 3)	→ 34Ga	→ 34In	→ 34Tl
4 C_I	→ 12B	→ 29Al	→ 29Ga	→ 2In	→ 2Tl
5 C_s	→ 14B	5.5	4.8	-3.5	rearr.
6 C_s	25.5 (i = 1)	11.7 (i = 1)	3.7 (i = 1)	-3.7	-17.0 (i = 2)
7 C_I	n/c	n/c	3.4	n/c	n/c
8 C_{3v}	135.5 (i = 3)	35.7	23.5 (i = 2)	-6.1 (i = 2)	rearr.
9 C_s	→ 12B	→ 11Al	→ 22Ga	→ 23In	→ 23Tl
10 D_{2d}	45.8	→ 1Al	→ 11Ga	18.6 (i=1)	-5.3 (i = 3)
11 S_4	→ 1B	33.4	23.9	10.9 (i=1)	-13.5
12 C_s	-11.7	16.1 (i = 1)	6.8 (i = 1)	4.3 (i = 1)	1.5 (i = 1)
13 C_I	n/c	14.4	5.9	-1.7	n/c
14 C_s	-4.7	14.7 (i = 1)	9.1 (i = 1)	10.7 (i = 2)	rearr.
16 C_s	→ 19B	→ 1Al	→ 1Ga	→ 1In	→ 17Tl
17 C_s	n/c	n/c	n/c	n/c	-33.8
18 C_s	49.9 (i = 1)	→ 6Al	→ 35Ga	→ 6In	→ 6Tl
19 D_{4h}	0.6 (i = 3)	34.1 (i = 1)	25.7 (i = 3)	17.1 (i = 1)	18.2 (i = 1)

1							
2							
3							
4	20	D_{2h}	36.8 (i = 2)	44.6 (i = 3)	→ 19Ga	→ 19In	31.0 (i = 4)
5							
6	21	C_s	→ 35B	13.4	0.3	-13.4	-30.3
7							
8							
9	22	C_s	→ 14B	24.0 (i = 1)	14.4 (i=2)	5.4 (i = 2)	-5.6 (i = 2)
10							
11	23	C_s	→ 12B	18.1	6.6	-5.7	-24.2 (i = 1)
12							
13	24	C_s	→ 25B	→ 25Al	27.4 (i = 1)	9.2	-9.4 (i = 1)
14							
15							
16	25	C_s	38.1	29.4 (i = 1)	n/c	n/c	n/c
17							
18							
19	27	C_s	→ 12B	→ 14Al	→ 14Ga	→ 12In	→ 28Tl
20							
21	29	C_s	rearr.	21.8	5.9	-17.1	→ 31Tl
22							
23							
24	31	C_{2v}	→ 12B	22.4 (i = 1)	→ 29Ga	-17.1	rearr.
25							
26	32	C_2	→ 12B	→ 33Al	→ 33Ga	→ 36In	→ 2Tl
27							
28							
29	33	D_{2h}	n/c	20.2	17.7 (i = 2)	n/c	n/c
30							
31	34	D_{2d}	298.7 (i = 3)	47.9 (i = 3)	18.4 (i = 3)	-16.6	-52.0
32							
33							
34	35	C_{2v}	41.7 (i = 2)	31.8 (i = 1)	13.9	5.3 (i = 2)	-5.6 (i = 2)
35							
36	36	C_{2h}	130.3	22.1	8.3	-15.1	-43.9 (i=1)
37							
38							
39	37	C_1	→ 12B	15.2	6.5	→ 38In	→ 38Tl
40							
41	38	C_1	n/c	n/c	n/c	-8.2	n/c
42							
43							
44	39	C_1	n/c	n/c	n/c	n/c	-47.8
45							
46	40	D_{2h}	37.0	42.1 (i = 1)	26.2 (i = 1)	22.4 (i = 1)	21.2 (i = 1)
47							
48							
49	45	C_1	n/c	n/c	5.9	-1.7	n/c
50							
51	46	C_1	n/c	n/c	n/c	n/c	-25.9 (i=1)
52							
53							
54	n/c: not calculated						
55							
56	rearr.: rearranges into another structure type						
57							
58							
59							
60							

Table 4: Relative energies of group-13 E_4H_4 isomers at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. All values in kcal/mol. The values for the global energy minima are given in red.

	B	Al	Ga	In	Tl
1 T_d	0.0	0.0	0.0	0.0	0.0
2 T_d	n/c	41.8	19.5	-13.2	-58.7
5 C_s	n/c	6.2	6.5	1.4	n/c
6 C_s	n/c	n/c	n/c	1.5	n/c
7 C_1	n/c	n/c	6.9	n/c	n/c
8 C_{3v}	n/c	40.1	n/c	n/c	n/c
11 S_4	n/c	39.0	27.5	n/c	n/c
12 C_s	-5.7	n/c	n/c	n/c	n/c
13 C_1	n/c	18.0	11.7	7.0	n/c
14 C_s	0.9	n/c	n/c	n/c	n/c
17 C_s	n/c	n/c	n/c	n/c	-28.2
21 C_s	n/c	19.6	8.3	-3.3	-25.0
22 C_s	n/c	n/c	19.0	n/c	n/c
23 C_s	n/c	22.6	14.9	5.4	n/c
24 C_s	n/c	n/c	n/c	22.7	n/c
29 C_s	n/c	29.2	15.5	-5.8	n/c
31 C_{2v}	n/c	n/c	n/c	-5.8	n/c
33 D_{2h}	n/c	22.0	n/c	n/c	n/c
34 D_{2d}	n/c	n/c	n/c	4.6	-41.3
35 C_{2v}	n/c	n/c	22.4	n/c	n/c
36 C_{2h}	n/c	30.7	19.3	1.5	-35.1
37 C_1	n/c	19.5	12.8	n/c	n/c
38 C_1	n/c	n/c	n/c	1.6	n/c
39 C_1	n/c	n/c	n/c	n/c	-43.5
45 C_1	n/c	n/c	11.7	7.0	n/c

n/c: not calculated

Table 5. Calculated E_4H_4 energies in kcal/mol for all group-14 elements at B3LYP/def2-TZVPP relative to **1E**. All values in kcal/mol. The values for the global energy minima are given in red.

	C	Si	Ge	Sn	Pb
1 T_d	0.0	0.0	0.0 (i = 3)	0.0 (i = 3)	0.0 (i = 3)
2 T_d	298.8 (i = 8)	37.0	-13.0	-47.0	-88.1
3 D_{2d}	129.9 (i = 6)	-24.3	-67.2	-88.8	-125.1
4 C_I	→ 24C	→ 8Si	-61.8	-83.9	-120.7 (i = 1)
8 C_{3v}	91.5 (i = 3)	-31.0	-64.1	-78.9	-104.8
9 C_s	→ 16C	-25.2	-46.2	-52.3	→ 23Pb
10 D_{2d}	→ 1C	-29.2	-56.0	-62.1	-83.2
11 S_4	→ 20C	→ 10Si	26.4 (i = 7)	→ 10Sn	→ 32Pb
12 C_s	→ 20C	29.7 (i = 3)	12.1 (i = 3)	-0.9 (i = 4)	→ 4Pb
14 C_s	→ 27C	→ 15Si	→ 47Ge	→ 48Sn	rearr.
15 C_s	nc	0.3 (i = 1)	n/c	n/c	n/c
16 C_s	-7.1	-26.3	-44.8	→ 17Sn	→ 17Pb
17 C_s	n/c	n/c	n/c	-53.0	-80.0
18 C_s	-8.8	-46.8	-65.5	-67.8	→ 4Pb
19 D_{4h}	10.7 (i = 2)	81.8 (i = 6)	26.4 (i = 7)	-7.0 (i = 6)	-46.7 (i = 6)
20 D_{2h}	-24.5	-4.3 (i = 3)	-13.9 (i = 3)	-6.5 (i = 4)	→ 19Pb
21 C_s	→ 35C	→ 35Si	-28.8 (i = 1)	-46.8	-71.5
22 C_s	→ 44C	→ 42Si	→ 42Ge	→ 18Sn	→ 4Pb

23	C_s	→ 20C	-10.6 (i = 1)	→ 43Ge	-48.9 (i = 2)	-85.6
24	C_s	-27.5	-35.5 (i = 1)	-53.6 (i = 1)	-53.2 (i = 1)	→ 25Pb
26	C_I	n/c	n/c	n/c	n/c	-90.2
27	C_s	-63.7	→ 28Si	→ 28Ge	rearr.	rearr.
28	C_s	n/c	7.6 (i = 2)	-14.8 (i = 2)	n/c	n/c
29	C_s	→ 18C	→ 24Si	→ 30Ge	→ 41Sn	→ 41Pb
30	C_s	n/c	n/c	-56.1	n/c	n/c
31	C_{2v}	→ 35C	rearr.	rearr.	rearr.	rearr.
32	C_2	→ 44C	-8.9 (i = 1)	-44.6 (i=1)	-63.8	-98.7 (i=1)
34	D_{2d}	rearr.	→ 3Si	→ 3Ge	→ 3Sn	→ 3Pb
35	C_{2v}	16.5 (i = 1)	-40.6 (i = 1)	-57.9 (i = 1)	-60.3 (i = 1)	-71.6 (i = 1)
40	D_{2h}	-60.4	19.2 (i = 3)	8.1 (i = 3)	18.0 (i = 3)	31.8 (i = 1)
41	C_s	n/c	n/c	n/c	-44.9	-77.2 (i = 1)
42	C_s	n/c	11.9 (i = 2)	-20.5 (i = 2)	n/c	n/c
43	C_I	n/c	n/c	-47.8	n/c	n/c
44	C_I	-16.0	-41.7	-60.9	-62.0	→ 3Pb
47	C_s	n/c	n/c	-26.2 (i = 2)	n/c	n/c
48	C_s	n/c	n/c	n/c	-41.8 (i = 2)	n/c

n/c: not calculated

rearr.: rearranges into different structure type

Table 6: Relative energies of group-14 E₄H₄ isomers at CCSD(T)/def2-QZVPP//B3LYP/def2-TZVPP. All values in kcal/mol. The values for the global energy minima are given in red.

	C	Si	Ge	Sn	Pb
1 T _d	0.00	0.0	0.0	0.0	0.0
2 T _d	n/c	n/c	n/c	-35.9	n/c
3 D _{2d}	n/c	-21.2	-54.9	-74.1	-120.1
4 C ₁	n/c	n/c	-50.1	-69.4	-115.8
8 C _{3v}	n/c	-28.5	-53.9	-67.2	-101.7
9 C _s	n/c	-20.7	-36.4	-40.3	n/c
10 D _{2d}	n/c	-28.1	-48.2	-52.1	n/c
16 C _s	n/c	-22.5	-36.0	n/c	n/c
17 C _s	n/c	n/c	n/c	-40.6	n/c
18 C _s	n/c	-43.7	-56.6	-57.2	n/c
20 D _{2h}	-27.1	n/c	n/c	n/c	n/c
21 C _s	n/c	n/c	n/c	-35.8	n/c
24 C _s	-24.7	n/c	n/c	n/c	n/c
27 C _s	-60.6	n/c	n/c	n/c	n/c
30 C _s	n/c	n/c	-46.8	n/c	n/c
32 C ₂	n/c	n/c	-31.9	-48.4	-92.2
40 D _{2h}	-52.3	n/c	n/c	n/c	n/c
41 C _s	n/c	n/c	n/c	-30.0	n/c
43 C ₁	n/c	n/c	-36.7	n/c	n/c
44 C ₁	n/c	-38.8	-53.4	-53.1	n/c

n/c: not calculated

Supporting Information for:

**Tetrahedranes. A Theoretical Study of Singlet E₄H₄ Molecules (E = C – Pb
and B – Tl)**

By **ROBIN HAUNSCHILD** and **GERNOT FRENKING***

Table S1: Energies and coordinates of the calculated molecules

10B:

8

E(RB+HF-LYP) = -101.673657527

B	0.76573700	-0.76584500	-0.33330400
B	-0.76573700	0.76584500	-0.33330400
B	0.76584500	0.76573700	0.33330400
B	-0.76584500	-0.76573700	0.33330400
H	1.24654900	-1.22606800	-1.31433600
H	-1.22606800	-1.24654900	1.31433600
H	1.22606800	1.24654900	1.31433600
H	-1.24654900	1.22606800	-1.31433600

10Ge:

8

E(RB+HF-LYP) = -8310.59744785

Ge	0.00000000	1.61962200	0.44331600
Ge	0.00000000	-1.61962200	0.44331600
Ge	1.61962200	0.00000000	-0.44331600
Ge	-1.61962200	0.00000000	-0.44331600
H	0.00000000	1.44532100	2.00044900
H	-1.44532100	0.00000000	-2.00044900
H	1.44532100	0.00000000	-2.00044900
H	0.00000000	-1.44532100	2.00044900

10In:

8

E(RB+HF-LYP) = -763.202705902

In	0.00000000	2.07492700	0.40629400
In	0.00000000	-2.07492700	0.40629400
In	2.07492700	0.00000000	-0.40629400
In	-2.07492700	0.00000000	-0.40629400
H	0.00000000	2.79941800	2.03099600
H	-2.79941800	0.00000000	-2.03099600
H	2.79941800	0.00000000	-2.03099600

1
2
3 H 0.00000000 -2.79941800 2.03099600
4
5
6 10Pb:
7
8 8
9 E(RB+HF-LYP) = -774.193121064
10 Pb 0.00000000 1.99765500 0.51578600
11 Pb 0.00000000 -1.99765500 0.51578600
12 Pb 1.99765500 0.00000000 -0.51578600
13 Pb -1.99765500 0.00000000 -0.51578600
14 H 0.00000000 1.73090200 2.32859800
15 H -1.73090200 0.00000000 -2.32859800
16 H 1.73090200 0.00000000 -2.32859800
17 H 0.00000000 -1.73090200 2.32859800
18
19
20 10Si:
21 8
22 E(RB+HF-LYP) = -1160.39076157
23 Si 0.00000000 1.51939300 0.41838700
24 Si 0.00000000 -1.51939300 0.41838700
25 Si 1.51939300 0.00000000 -0.41838700
26 Si -1.51939300 0.00000000 -0.41838700
27 H 0.00000000 1.45563300 1.91157500
28 H -1.45563300 0.00000000 -1.91157500
29 H 1.45563300 0.00000000 -1.91157500
30 H 0.00000000 -1.45563300 1.91157500
31
32
33
34 10Sn:
35 8
36 E(RB+HF-LYP) = -859.940543098
37 Sn 0.00000000 1.89001700 0.49089200
38 Sn 0.00000000 -1.89001700 0.49089200
39 Sn 1.89001700 0.00000000 -0.49089200
40 Sn -1.89001700 0.00000000 -0.49089200
41 H 0.00000000 1.66233500 2.22979300
42 H -1.66233500 0.00000000 -2.22979300
43 H 1.66233500 0.00000000 -2.22979300
44 H 0.00000000 -1.66233500 2.22979300
45
46
47
48 10Tl:
49 8
50 E(RB+HF-LYP) = -692.683692501
51 Tl 0.00000000 2.15545200 0.60503900
52 Tl 0.00000000 -2.15545200 0.60503900
53 Tl 2.15408800 0.00000000 -0.60507200
54 Tl -2.15408800 0.00000000 -0.60507200
55 H 0.00000000 2.61112600 2.39771000
56 H -2.62219100 0.00000000 -2.39509900
57 H 2.62219100 0.00000000 -2.39509900
58 H 0.00000000 -2.61112600 2.39771000
59
60

11Al:

1
2
3
4 8
5 E(RB+HF-LYP) = -972.150787518
6 Al 0.00000000 1.82716700 0.26769900
7 Al 0.00000000 -1.82716700 0.26769900
8 Al 1.82716700 0.00000000 -0.26769900
9 Al -1.82716700 0.00000000 -0.26769900
10 H 0.00000000 3.20822200 1.05797400
11 H -3.20822200 0.00000000 -1.05797400
12 H 3.20822200 0.00000000 -1.05797400
13 H 0.00000000 -3.20822200 1.05797400
14

15
16 11Ga:

17 8
18 E(RB+HF-LYP) = -7701.98523261
19 Ga 0.00000000 1.76297300 0.29387000
20 Ga 0.00000000 -1.76297300 0.29387000
21 Ga 1.76297300 0.00000000 -0.29387000
22 Ga -1.76297300 0.00000000 -0.29387000
23 H 0.00000000 3.07970500 1.16584800
24 H -3.07970500 0.00000000 -1.16584800
25 H 3.07970500 0.00000000 -1.16584800
26 H 0.00000000 -3.07970500 1.16584800
27
28
29

30 11Ge:

31 8
32 E(RB+HF-LYP) = -8310.46625246
33 Ge 0.00000000 1.84854900 0.18829800
34 Ge 0.00000000 -1.84854900 0.18829800
35 Ge 1.84854900 0.00000000 -0.18829800
36 Ge -1.84854900 0.00000000 -0.18829800
37 H 0.00000000 3.44721700 0.61536900
38 H -3.44721700 0.00000000 -0.61536900
39 H 3.44721700 0.00000000 -0.61536900
40 H 0.00000000 -3.44721700 0.61536900
41
42
43
44

45 11In:

46 8
47 E(RB+HF-LYP) = -763.214864629
48 In -1.38074200 1.38074200 0.64863200
49 In -1.38074200 -1.38074200 -0.64863200
50 In 1.38074200 -1.38074200 0.64863200
51 In 1.38074200 1.38074200 -0.64863200
52 H -1.31435700 2.89431400 1.58250500
53 H 1.31435700 -2.89431400 1.58250500
54 H -2.89431400 -1.31435700 -1.58250500
55 H 2.89431400 1.31435700 -1.58250500
56
57
58

59 11Tl:

60 8
E(RB+HF-LYP) = -692.696834121
Tl -1.52323700 -1.52323700 0.61006900

1				
2				
3	TI	-1.52323700	1.52323700	-0.61006900
4	TI	1.52323700	-1.52323700	-0.61006900
5				
6	TI	1.52323700	1.52323700	0.61006900
7	H	-3.12568400	-1.27424100	1.49886300
8	H	3.12568400	1.27424100	1.49886300
9	H	1.27424100	-3.12568400	-1.49886300
10	H	-1.27424100	3.12568400	-1.49886300
11				

12Al:

8

E(RB+HF-LYP) = -972.178229668

16	Al	0.11606800	-1.39362900	0.00000000
17	Al	-2.06552100	-0.11352200	0.00000000
18	Al	0.00000000	1.36188700	0.00000000
19	Al	2.10373800	0.09269100	0.00000000
20	H	-3.63939300	-0.10026500	0.00000000
21	H	-1.56947500	-1.78045500	0.00000000
22	H	3.62209500	-0.32799900	0.00000000
23	H	-0.41893100	2.89216800	0.00000000
24				
25				

12B:

8

E(RB+HF-LYP) = -101.765371951

30	B	0.00000000	0.78077900	0.00000000
31	B	-1.34178400	-0.06174900	0.00000000
32	B	0.10934600	-0.82245100	0.00000000
33	B	1.42430700	0.24961100	0.00000000
34	H	-2.50059400	-0.23961200	0.00000000
35	H	-1.16441100	1.29359500	0.00000000
36	H	2.59630700	0.21647000	0.00000000
37	H	0.10935500	-2.00140400	0.00000000
38				
39				

12Ga:

8

E(RB+HF-LYP) = -7702.01257832

44	Ga	-0.09329800	-1.52958700	0.00000000
45	Ga	2.04500900	0.08025000	0.00000000
46	Ga	0.00000000	1.34117100	0.00000000
47	Ga	-2.01283200	0.08023100	0.00000000
48	H	3.60297300	0.14561000	0.00000000
49	H	1.67507600	-1.62111200	0.00000000
50	H	-3.43284600	-0.55987200	0.00000000
51	H	0.04953300	2.90136200	0.00000000
52				
53				

12Ge:

8

E(RB+HF-LYP) = -8310.48894881

59	Ge	2.07640000	-0.09500400	0.00000000
60	Ge	-0.20622600	-1.65679200	0.00000000
	Ge	-1.79712500	0.23709100	0.00000000
	Ge	0.00000000	1.56805300	0.00000000

H	-0.38824900	-3.18920000	0.00000000
H	1.39045700	-1.65778600	0.00000000
H	-0.02065900	3.11755800	0.00000000
H	-3.31911200	0.02229800	0.00000000

12In:

8

E(RB+HF-LYP) = -763.225471654

In	-0.07453900	-1.81446000	0.00000000
In	2.33604200	0.16628800	0.00000000
In	0.00000000	1.52210900	0.00000000
In	-2.30263100	0.10348000	0.00000000
H	4.04966800	0.31620200	0.00000000
H	1.93605400	-1.67548800	0.00000000
H	-3.79561200	-0.76841400	0.00000000
H	-0.17481500	3.23426400	0.00000000

12Si:

8

E(RB+HF-LYP) = -1160.29688745

Si	2.01031300	-0.04496500	0.00000000
Si	-0.05753900	-1.28535900	0.00000000
Si	-1.84663000	0.17196800	0.00000000
Si	0.00000000	1.25631700	0.00000000
H	-0.16797600	-2.77302900	0.00000000
H	1.57976900	-1.52738600	0.00000000
H	0.42291600	2.68848900	0.00000000
H	-3.32072800	0.24047500	0.00000000

12Sn:

8

E(RB+HF-LYP) = -859.843041061

Sn	2.41013900	-0.11577200	0.00000000
Sn	-0.24111400	-1.92765800	0.00000000
Sn	-2.11266500	0.26928700	0.00000000
Sn	0.00000000	1.81911700	0.00000000
H	-0.25295800	-3.65533500	0.00000000
H	1.53770800	-1.81207300	0.00000000
H	-0.37154200	3.51577000	0.00000000
H	-3.73119300	-0.29707300	0.00000000

12Tl:

8

E(RB+HF-LYP) = -692.672857918

Tl	0.00342800	-1.90453400	0.00000000
Tl	-2.42038600	0.26901400	0.00000000
Tl	0.00000000	1.53349700	0.00000000
Tl	2.43690700	0.08166400	0.00000000
H	-4.04224200	0.85692900	0.00000000
H	-2.20593300	-1.55580100	0.00000000
H	3.98955800	-0.79803600	0.00000000

1
2
3 H 0.64272600 3.14597400 0.00000000
4
5
6 13Al:
7
8
9 E(RB+HF-LYP) = -972.180964053
10 Al -0.05544600 -1.33049400 0.52459300
11 Al 1.95339800 -0.03562000 -0.39707800
12 Al -0.06426100 1.37165100 0.36900900
13 Al -1.97512400 -0.07004800 -0.41739100
14 H 3.52059200 -0.07224000 -0.58835800
15 H 1.48611300 -1.69603400 -0.23226500
16 H -3.52240000 -0.29508400 -0.65595000
17 H 0.35431400 2.90199400 0.44785200
18
19
20 13Ga:
21
22 8
23 E(RB+HF-LYP) = -7702.01403854
24 Ga -0.20288300 1.50919400 0.23923700
25 Ga 2.04100400 0.01841600 -0.24735800
26 Ga 0.08114400 -1.34491600 0.27599200
27 Ga -1.97855600 -0.15556900 -0.25735400
28 H 3.58340400 0.26401700 -0.09738500
29 H 1.45261400 1.68341600 -0.34660800
30 H -3.50107100 0.09980800 0.02374200
31 H 0.30305800 -2.88809900 0.09422600
32
33
34 13In:
35
36 8
37 E(RB+HF-LYP) = -763.234939018
38 In 0.40537700 1.75174500 0.35875600
39 In -2.42335700 0.08928300 -0.37267100
40 In -0.21692300 -1.51360800 0.46023600
41 In 2.27495300 -0.30526400 -0.43713300
42 H -3.97456700 0.89562900 -0.19104000
43 H -1.33630400 1.75784200 -0.55762000
44 H 3.90303300 -0.54264600 0.20250600
45 H -0.55465100 -3.19647100 0.09597100
46
47
48 14Al:
49
50 8
51 E(RB+HF-LYP) = -972.180478976
52 Al 2.06288100 0.06854000 0.00000000
53 Al 0.00000000 1.39171100 0.00000000
54 Al -2.08422100 0.27873100 0.00000000
55 Al -0.07919200 -1.40039200 0.00000000
56 H 3.63036700 0.15905000 0.00000000
57 H -3.63180600 -0.02666100 0.00000000
58 H 1.65955100 -1.57326900 0.00000000
59 H -0.35119300 -2.96078500 0.00000000
60

14B:

1
2
3
4 8
5 E(RB+HF-LYP) = -101.754093641
6 B -1.35068500 -0.24224400 0.00000000
7 B 0.08220700 -0.84653900 0.00000000
8 B 1.45119700 -0.25231300 0.00000000
9 B 0.00000000 0.80230700 0.00000000
10 H -2.51231800 -0.43893400 0.00000000
11 H 2.55680500 0.13638300 0.00000000
12 H -1.30121900 1.05876900 0.00000000
13 H 0.34313500 1.93772700 0.00000000
14

15
16 14Ga:

17 8
18 E(RB+HF-LYP) = -7702.00884906
19 Ga 2.00968700 0.09071300 0.00000000
20 Ga 0.00000000 1.37980300 0.00000000
21 Ga -1.97671100 0.15382600 0.00000000
22 Ga -0.07930200 -1.47553700 0.00000000
23 H 3.56186600 0.12136200 0.00000000
24 H -3.51271500 -0.10097900 0.00000000
25 H 1.67041500 -1.60396000 0.00000000
26 H -0.28346200 -3.02937700 0.00000000
27
28
29

30 14In:

31 8
32 E(RB+HF-LYP) = -763.215262054
33 In -2.27218900 0.09906700 0.00000000
34 In 0.00000000 1.63924500 0.00000000
35 In 2.20598100 0.08951300 0.00000000
36 In 0.09443100 -1.71818500 0.00000000
37 H -3.97551200 -0.14640400 0.00000000
38 H 3.92313000 0.00000000 0.00000000
39 H -1.77757800 -1.82061600 0.00000000
40 H 0.44702300 -3.40900000 0.00000000
41
42
43
44

45 15Si:

46 8
47 E(RB+HF-LYP) = -1160.34371743
48 Si -0.16573500 -1.20567200 0.00000000
49 Si -2.05745000 -2.35148800 0.00000000
50 Si 0.00000000 1.06604300 0.00000000
51 Si 1.86539100 2.13462200 0.00000000
52 H 1.15561700 -1.88532600 0.00000000
53 H -1.25920100 1.83896200 0.00000000
54 H 3.15948200 1.43080900 0.00000000
55 H 1.95322100 3.60648400 0.00000000
56
57
58

59 16C:

60 8
E(RB+HF-LYP) = -154.711848828
C 0.57576100 0.99246100 0.00000000

1				
2				
3	C	-0.07877700	-1.14472000	0.00000000
4	C	-0.07877700	0.02411900	0.82446500
5	C	-0.07877700	0.02411900	-0.82446500
6	C	-0.07877700	0.02411900	-0.82446500
7	H	0.38668600	2.05529000	0.00000000
8	H	-0.79612800	0.24392000	-1.60983500
9	H	-0.79612800	0.24392000	1.60983500
10	H	-0.83100400	-1.91900200	0.00000000
11				
12				
13	16Ge:			
14	8			
15	E(RB+HF-LYP) =	-8310.57971449		
16	Ge	0.24901200	-2.02457100	0.00000000
17	Ge	-0.84271600	1.68017200	0.00000000
18	Ge	0.24901200	0.12985700	1.38718800
19	Ge	0.24901200	0.12985700	-1.38718800
20	Ge	0.24901200	0.12985700	-1.38718800
21	H	1.85057100	-1.87520000	0.00000000
22	H	1.09253900	0.68251500	-2.57249800
23	H	1.09253900	0.68251500	2.57249800
24	H	1.09253900	0.68251500	2.57249800
25	H	-0.97386200	3.22012100	0.00000000
26				
27	16Si:			
28	8			
29	E(RB+HF-LYP) =	-1160.38620187		
30	Si	0.24721300	-1.89743700	0.00000000
31	Si	-0.93606000	1.51491300	0.00000000
32	Si	-0.93606000	1.51491300	0.00000000
33	Si	0.24721300	0.11413300	1.25160800
34	Si	0.24721300	0.11413300	-1.25160800
35	H	1.77402200	-1.88553600	0.00000000
36	H	1.05885600	0.53316100	-2.42734000
37	H	1.05885600	0.53316100	-2.42734000
38	H	1.05885600	0.53316100	2.42734000
39	H	-1.16982900	2.97883300	0.00000000
40				
41	17Pb:			
42	8			
43	E(RB+HF-LYP) =	-774.187889467		
44	Pb	0.43335000	2.56099700	0.00000000
45	Pb	0.43335000	2.56099700	0.00000000
46	Pb	-0.11976300	-2.63511300	0.00000000
47	Pb	-0.11976300	-2.63511300	0.00000000
48	Pb	-0.11976300	0.04220900	1.68248700
49	Pb	-0.11976300	0.04220900	-1.68248700
50	H	-1.11228900	1.14111000	0.00000000
51	H	-1.49395000	0.37959900	-2.84726500
52	H	-1.49395000	0.37959900	-2.84726500
53	H	-1.49395000	0.37959900	2.84726500
54	H	-1.97293500	-2.74498500	0.00000000
55				
56	17Sn:			
57	8			
58	E(RB+HF-LYP) =	-859.926053347		
59	Sn	0.71115300	2.34314900	0.00000000
60	Sn	-0.19784300	-2.44614900	0.00000000
	Sn	-0.19784300	-2.44614900	0.00000000
	Sn	-0.19784300	0.05593600	1.57022200
	Sn	-0.19784300	0.05593600	-1.57022200

H	-1.02517100	1.33928500	0.00000000
H	-1.44339800	0.42067000	-2.74509000
H	-1.44339800	0.42067000	2.74509000
H	-1.96926200	-2.62420100	0.00000000

17Tl:

8

E(RB+HF-LYP) = -692.729132789

Tl	1.39266300	1.93765900	0.00000000
Tl	-0.44410500	-2.21084800	0.00000000
Tl	-0.44410500	0.16936500	2.05067500
Tl	-0.44410500	0.16936500	-2.05067500
H	-0.65900900	1.32383200	0.00000000
H	-1.67668600	-1.34220000	-1.48105900
H	-1.67668600	-1.34220000	1.48105900
H	-0.87574300	-3.94817900	0.00000000

18B:

8

E(RB+HF-LYP) = -101.667176072

B	0.00008400	1.26111100	0.00000000
B	0.00008400	-0.33581300	0.86219500
B	-0.00033900	-1.54350900	0.00000000
B	0.00008400	-0.33581300	-0.86219500
H	-1.03784200	1.83443800	0.00000000
H	0.00015100	0.55059500	-1.67893200
H	1.03797800	1.83449500	0.00000000
H	0.00015100	0.55059500	1.67893200

18C:

8

E(RB+HF-LYP) = -154.714616683

C	0.57285000	0.92145300	0.00000000
C	-0.19577100	-0.08503600	0.79909000
C	-0.19577100	-1.26034400	0.00000000
C	-0.19577100	-0.08503600	-0.79909000
H	0.25543800	1.96324400	0.00000000
H	-0.90825300	0.14682900	-1.58279400
H	1.64784700	0.79688100	0.00000000
H	-0.90825300	0.14682900	1.58279400

18Ge:

8

E(RB+HF-LYP) = -8310.61270979

Ge	0.52654300	1.87584000	0.00000000
Ge	-0.16369200	-0.01781400	1.40710200
Ge	-0.16369200	-2.02213700	0.00000000
Ge	-0.16369200	-0.01781400	-1.40710200
H	-0.18214700	3.24849300	0.00000000
H	-1.50115500	0.23880000	-2.16374000
H	2.04946700	2.09555000	0.00000000

1
2
3 H -1.50115500 0.23880000 2.16374000
4
5
6 18Si:
7
8
9 E(RB+HF-LYP) = -1160.41887853
10 Si -0.16937900 1.80509700 0.00000000
11 Si -0.16937900 -0.14203300 1.25470400
12 Si 0.69332800 -1.84914700 0.00000000
13 Si -0.16937900 -0.14203300 -1.25470400
14 H -1.32352200 2.73995000 0.00000000
15 H -1.18244000 -0.35885900 -2.32609600
16 H 1.09573400 2.57137600 0.00000000
17 H -1.18244000 -0.35885900 2.32609600
18
19
20 18Sn:
21
22
23 E(RB+HF-LYP) = -859.949753719
24 Sn 0.45749600 2.20632000 0.00000000
25 Sn -0.13977000 -0.01137500 1.68696600
26 Sn -0.13977000 -2.31674400 0.00000000
27 Sn -0.13977000 -0.01137500 -1.68696600
28 H -0.39164400 3.70772600 0.00000000
29 H -1.82470200 0.17127700 -2.12839000
30 H 2.13170300 2.60840100 0.00000000
31 H -1.82470200 0.17127700 2.12839000
32
33
34 19Al:
35
36
37 E(RB+HF-LYP) = -972.149572720
38 Al 0.00000000 1.33114000 1.33114400
39 Al 0.00000000 -1.33114000 -1.33114400
40 Al 0.00000000 -1.33114000 1.33114400
41 Al 0.00000000 1.33114000 -1.33114400
42 H 0.00000000 2.45812800 2.45819600
43 H 0.00000000 2.45812800 -2.45819600
44 H 0.00000000 -2.45812800 2.45819600
45 H 0.00000000 -2.45812800 -2.45819600
46
47
48 19B:
49
50
51 E(RB+HF-LYP) = -101.745763189
52 B 0.00000000 0.00000000 1.39630200
53 B 0.00000000 0.00000000 -1.39630200
54 B 0.00000000 0.79358800 0.00000000
55 B 0.00000000 -0.79358800 0.00000000
56 H 0.00000000 0.00000000 2.56776600
57 H 0.00000000 -1.97278400 0.00000000
58 H 0.00000000 1.97278400 0.00000000
59 H 0.00000000 0.00000000 -2.56776600
60

19C:

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8
E(RB+HF-LYP) = -154.683574125
C 0.00000000 0.00000000 1.06536600
C 0.00000000 0.00000000 -1.06536600
C 0.00000000 0.96001600 0.00000000
C 0.00000000 -0.96001600 0.00000000
H 0.00000000 0.00000000 2.13461700
H 0.00000000 -2.04887000 0.00000000
H 0.00000000 2.04887000 0.00000000
H 0.00000000 0.00000000 -2.13461700

19Ga:
8
E(RB+HF-LYP) = -7701.98246619
Ga 0.00000000 1.29739400 1.29740200
Ga 0.00000000 -1.29739400 -1.29740200
Ga 0.00000000 1.29739400 -1.29740200
Ga 0.00000000 -1.29739400 1.29740200
H 0.00000000 2.41794800 2.41787400
H 0.00000000 -2.41794800 2.41787400
H 0.00000000 2.41794800 -2.41787400
H 0.00000000 -2.41794800 -2.41787400

19Ge:
8
E(RB+HF-LYP) = -8310.46622305
Ge 0.00000000 1.87812200 0.00000000
Ge 0.00000000 -1.87812200 0.00000000
Ge 1.87812200 0.00000000 0.00000000
Ge -1.87812200 0.00000000 0.00000000
H 0.00000000 3.53388600 0.00000000
H -3.53388600 0.00000000 0.00000000
H 3.53388600 0.00000000 0.00000000
H 0.00000000 -3.53388600 0.00000000

19In:
8
E(RB+HF-LYP) = -763.204994188
In 0.00000000 2.06556600 0.00000000
In 0.00000000 -2.06556600 0.00000000
In 2.06556600 0.00000000 0.00000000
In -2.06556600 0.00000000 0.00000000
H 0.00000000 3.81749300 0.00000000
H -3.81749300 0.00000000 0.00000000
H 3.81749300 0.00000000 0.00000000
H 0.00000000 -3.81749300 0.00000000

19Pb:
8
E(RB+HF-LYP) = -774.134888878
Pb 0.00000000 1.56211100 1.56213500

1				
2				
3	Pb	0.00000000	-1.56211100	-1.56213500
4	Pb	0.00000000	1.56211100	-1.56213500
5				
6	Pb	0.00000000	-1.56211100	1.56213500
7	H	0.00000000	2.89447300	2.89470200
8	H	0.00000000	-2.89447300	2.89470200
9	H	0.00000000	2.89447300	-2.89470200
10	H	0.00000000	-2.89447300	-2.89470200
11				
12				
13	19Si:			
14	8			
15	E(RB+HF-LYP) =	-1160.21381713		
16	Si	0.00000000	1.79891500	0.00000000
17	Si	0.00000000	-1.79891500	0.00000000
18	Si	1.79891500	0.00000000	0.00000000
19	Si	-1.79891500	0.00000000	0.00000000
20	H	0.00000000	3.38359700	0.00000000
21	H	-3.38359700	0.00000000	0.00000000
22	H	3.38359700	0.00000000	0.00000000
23	H	0.00000000	-3.38359700	0.00000000
24				
25				
26				
27	19Sn:			
28	8			
29	E(RB+HF-LYP) =	-859.852856650		
30	Sn	0.00000000	2.13638300	0.00000000
31	Sn	0.00000000	-2.13638300	0.00000000
32	Sn	2.13638300	0.00000000	0.00000000
33	Sn	-2.13638300	0.00000000	0.00000000
34	H	0.00000000	3.95757300	0.00000000
35	H	-3.95757300	0.00000000	0.00000000
36	H	3.95757300	0.00000000	0.00000000
37	H	0.00000000	-3.95757300	0.00000000
38				
39				
40				
41	19Tl:			
42	8			
43	E(RB+HF-LYP) =	-692.646212833		
44	Tl	0.00000000	2.11021100	0.00000000
45	Tl	0.00000000	-2.11021100	0.00000000
46	Tl	2.11021100	0.00000000	0.00000000
47	Tl	-2.11021100	0.00000000	0.00000000
48	H	0.00000000	3.89231700	0.00000000
49	H	-3.89231700	0.00000000	0.00000000
50	H	3.89231700	0.00000000	0.00000000
51	H	0.00000000	-3.89231700	0.00000000
52				
53				
54				
55	1Al:			
56	8			
57	E(RB+HF-LYP) =	-972.203952060		
58	Al	0.91592800	0.91592800	0.91592800
59	Al	-0.91592800	-0.91592800	0.91592800
60	Al	-0.91592800	0.91592800	-0.91592800
	Al	0.91592800	-0.91592800	-0.91592800

1
2
3 H 1.83411100 1.83411100 1.83411100
4 H -1.83411100 1.83411100 -1.83411100
5 H -1.83411100 -1.83411100 1.83411100
6 H 1.83411100 -1.83411100 -1.83411100
7
8

9 1B:

10 8

11 E(RB+HF-LYP) = -101.746668796

12 B 0.59249800 0.59249800 0.59249800
13 B -0.59249800 -0.59249800 0.59249800
14 B -0.59249800 0.59249800 -0.59249800
15 B 0.59249800 -0.59249800 -0.59249800
16 H 1.27420000 1.27420000 1.27420000
17 H -1.27420000 1.27420000 -1.27420000
18 H -1.27420000 -1.27420000 1.27420000
19 H 1.27420000 -1.27420000 -1.27420000
20
21
22

23 1C:

24 8

25 E(RB+HF-LYP) = -154.700564766

26 C 0.52123400 0.52123400 0.52123400
27 C -0.52123400 -0.52123400 0.52123400
28 C -0.52123400 0.52123400 -0.52123400
29 C 0.52123400 -0.52123400 -0.52123400
30 H 1.13794000 1.13794000 1.13794000
31 H -1.13794000 1.13794000 -1.13794000
32 H -1.13794000 -1.13794000 1.13794000
33 H 1.13794000 -1.13794000 -1.13794000
34
35
36

37 1Ga:

38 8

39 E(RB+HF-LYP) = -7702.02337014

40 Ga 0.90807300 0.90807300 0.90807300
41 Ga -0.90807300 -0.90807300 0.90807300
42 Ga -0.90807300 0.90807300 -0.90807300
43 Ga 0.90807300 -0.90807300 -0.90807300
44 H 1.82119600 1.82119600 1.82119600
45 H -1.82119600 1.82119600 -1.82119600
46 H -1.82119600 -1.82119600 1.82119600
47 H 1.82119600 -1.82119600 -1.82119600
48
49
50

51 1Ge:

52 8

53 E(RB+HF-LYP) = -8310.50829308

54 Ge 0.87289300 0.87289300 0.87289300
55 Ge -0.87289300 -0.87289300 0.87289300
56 Ge -0.87289300 0.87289300 -0.87289300
57 Ge 0.87289300 -0.87289300 -0.87289300
58 H 1.75663200 1.75663200 1.75663200
59 H -1.75663200 1.75663200 -1.75663200
60 H -1.75663200 -1.75663200 1.75663200

1
2
3 H 1.75663200 -1.75663200 -1.75663200
4
5
6 1In:
7
8
9 E(RB+HF-LYP) = -763.232284688
10 In 1.04717200 1.04717200 1.04717200
11 In -1.04717200 -1.04717200 1.04717200
12 In -1.04717200 1.04717200 -1.04717200
13 In 1.04717200 -1.04717200 -1.04717200
14 H 2.06498800 2.06498800 2.06498800
15 H -2.06498800 2.06498800 -2.06498800
16 H -2.06498800 -2.06498800 2.06498800
17 H 2.06498800 -2.06498800 -2.06498800
18
19 1Pb:
20
21 8
22 E(RB+HF-LYP) = -774.060473026
23 Pb 1.11103100 1.11103100 1.11103100
24 Pb -1.11103100 -1.11103100 1.11103100
25 Pb -1.11103100 1.11103100 -1.11103100
26 Pb 1.11103100 -1.11103100 -1.11103100
27 H 2.15788100 2.15788100 2.15788100
28 H -2.15788100 2.15788100 -2.15788100
29 H -2.15788100 -2.15788100 2.15788100
30 H 2.15788100 -2.15788100 -2.15788100
31
32
33 1Si:
34
35 8
36 E(RB+HF-LYP) = -1160.34422852
37 Si 0.81881800 0.81881800 0.81881800
38 Si -0.81881800 -0.81881800 0.81881800
39 Si -0.81881800 0.81881800 -0.81881800
40 Si 0.81881800 -0.81881800 -0.81881800
41 H 1.66878200 1.66878200 1.66878200
42 H -1.66878200 1.66878200 -1.66878200
43 H -1.66878200 -1.66878200 1.66878200
44 H 1.66878200 -1.66878200 -1.66878200
45
46
47 1Sn:
48
49 8
50 E(RB+HF-LYP) = -859.841665923
51 Sn 1.01791000 1.01791000 1.01791000
52 Sn -1.01791000 -1.01791000 1.01791000
53 Sn -1.01791000 1.01791000 -1.01791000
54 Sn 1.01791000 -1.01791000 -1.01791000
55 H 2.00803100 2.00803100 2.00803100
56 H -2.00803100 2.00803100 -2.00803100
57 H -2.00803100 -2.00803100 2.00803100
58 H 2.00803100 -2.00803100 -2.00803100
59
60

1Tl:

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4 8
5 E(RB+HF-LYP) = -692.675261786
6 TI 1.12921300 1.12921300 1.12921300
7 TI -1.12921300 -1.12921300 1.12921300
8 TI -1.12921300 1.12921300 -1.12921300
9 TI 1.12921300 -1.12921300 -1.12921300
10 H 2.19311300 2.19311300 2.19311300
11 H -2.19311300 2.19311300 -2.19311300
12 H -2.19311300 -2.19311300 2.19311300
13 H 2.19311300 -2.19311300 -2.19311300
14

15
16 20Al:

17 8
18 E(RB+HF-LYP) = -972.132956259
19 Al 0.00000000 1.81266500 0.00000000
20 Al 0.00000000 -1.81266500 0.00000000
21 Al -1.81266500 0.00000000 0.00000000
22 Al 1.81266500 0.00000000 0.00000000
23 H 0.00000000 3.40605100 0.00000000
24 H 3.40605100 0.00000000 0.00000000
25 H -3.40605100 0.00000000 0.00000000
26 H 0.00000000 -3.40605100 0.00000000
27
28
29

30 20B:

31 8
32 E(RB+HF-LYP) = -101.688051651
33 B 0.00000000 0.95497500 0.74695800
34 B 0.00000000 -0.95497500 -0.74695800
35 B 0.00000000 0.95497500 -0.74695800
36 B 0.00000000 -0.95497500 0.74695800
37 H 0.00000000 1.16965900 1.89874400
38 H 0.00000000 -1.16965900 1.89874400
39 H 0.00000000 1.16965900 -1.89874400
40 H 0.00000000 -1.16965900 -1.89874400
41
42
43

44 20C:

45 8
46 E(RB+HF-LYP) = -154.739553668
47 C -0.78703000 0.66466000 -0.00001100
48 C 0.78703000 -0.66466000 0.00001100
49 C -0.78703000 -0.66466000 -0.00002000
50 C 0.78703000 0.66466000 0.00001400
51 H -1.54901100 1.42864000 -0.00003300
52 H 1.54901100 1.42864100 0.00006600
53 H -1.54901100 -1.42864100 -0.00000200
54 H 1.54901100 -1.42864000 0.00000900
55
56
57

58 20Ge:

59 8
60 E(RB+HF-LYP) = -8310.53047289
Ge 0.00000000 1.11602100 1.24727000

1				
2				
3	Ge	0.00000000	-1.11602100	-1.24727000
4	Ge	0.00000000	1.11602100	-1.24727000
5	Ge	0.00000000	-1.11602100	1.24727000
6	H	0.00000000	2.24645200	2.27634000
7	H	0.00000000	-2.24645200	2.27634000
8	H	0.00000000	2.24645200	-2.27634000
9	H	0.00000000	-2.24645200	-2.27634000
10				
11				
12	20Si:			
13	8			
14	E(RB+HF-LYP) =	-1160.35099338		
15	Si	0.00000000	1.06567700	1.18922700
16	Si	0.00000000	-1.06567700	-1.18922700
17	Si	0.00000000	1.06567700	-1.18922700
18	Si	0.00000000	-1.06567700	1.18922700
19	H	0.00000000	2.15736700	2.18156300
20	H	0.00000000	-2.15736700	2.18156300
21	H	0.00000000	2.15736700	-2.18156300
22	H	0.00000000	-2.15736700	-2.18156300
23				
24				
25				
26				
27	20Sn:			
28	8			
29	E(RB+HF-LYP) =	-859.852057062		
30	Sn	0.00000000	1.29151600	1.42586800
31	Sn	0.00000000	-1.29151600	-1.42586800
32	Sn	0.00000000	1.29151600	-1.42586800
33	Sn	0.00000000	-1.29151600	1.42586800
34	H	0.00000000	2.55379000	2.56491600
35	H	0.00000000	-2.55379000	2.56491600
36	H	0.00000000	2.55379000	-2.56491600
37	H	0.00000000	-2.55379000	-2.56491600
38				
39				
40				
41	20Tl:			
42	8			
43	E(RB+HF-LYP) =	-692.625793586		
44	Tl	0.00000000	2.05878900	0.00000000
45	Tl	0.00000000	-2.05878900	0.00000000
46	Tl	-2.05878900	0.00000000	0.00000000
47	Tl	2.05878900	0.00000000	0.00000000
48	H	0.00000000	3.84355800	0.00000000
49	H	3.84355800	0.00000000	0.00000000
50	H	-3.84355800	0.00000000	0.00000000
51	H	0.00000000	-3.84355800	0.00000000
52				
53				
54				
55	21Al:			
56	8			
57	E(RB+HF-LYP) =	-972.182568865		
58	Al	0.00000000	1.82635000	0.00000000
59	Al	0.09838800	-1.92320100	0.00000000
60	Al	1.93525900	0.00000000	0.00000000
	Al	-1.83326700	-0.05860500	0.00000000

1				
2				
3	H	-0.16238300	3.40226300	0.00000000
4	H	-1.13506100	1.10556600	1.12509200
5	H	-1.13506100	1.10556600	-1.12509200
6	H	-0.17244500	-3.49536500	0.00000000
7				
8				

21Ga:

8

E(RB+HF-LYP) = -7702.02292378

11				
12				
13	Ga	-1.87895900	0.03300000	0.00000000
14	Ga	1.91655400	0.05377900	0.00000000
15	Ga	0.00000000	1.85755000	0.00000000
16	Ga	0.03643400	-1.86126400	0.00000000
17	H	-3.44685800	-0.10702800	0.00000000
18	H	-1.16648000	-1.10702900	1.14686800
19	H	-1.16648000	-1.10702900	-1.14686800
20	H	3.48491900	-0.25395400	0.00000000
21				
22				

21Ge:

8

E(RB+HF-LYP) = -8310.55424394

23				
24				
25				
26				
27	Ge	-0.21298600	-1.39207600	0.00000000
28	Ge	0.00000000	1.37034600	0.00000000
29	Ge	-2.07992700	0.19061500	0.00000000
30	Ge	2.19801900	-0.10122200	0.00000000
31	H	0.05831700	-2.93970200	0.00000000
32	H	1.38230300	-1.07166400	1.09229900
33	H	1.38230300	-1.07166400	-1.09229900
34	H	0.21368500	2.91779900	0.00000000
35				
36				

21In:

8

E(RB+HF-LYP) = -763.253678344

37				
38				
39				
40				
41	In	-2.14173200	0.04637600	0.00000000
42	In	2.19326500	0.03131100	0.00000000
43	In	0.00000000	2.11948700	0.00000000
44	In	0.00000000	-2.13500600	0.00000000
45	H	-3.87151700	-0.18127900	0.00000000
46	H	-1.33343800	-1.24774700	1.23697600
47	H	-1.33343800	-1.24774700	-1.23697600
48	H	3.92730000	-0.36943500	0.00000000
49				
50				

21Pb:

8

E(RB+HF-LYP) = -774.174448734

51				
52				
53				
54				
55	Pb	-0.19399600	-1.82956600	0.00000000
56	Pb	0.00000000	1.70634400	0.00000000
57	Pb	-2.47745400	0.22650000	0.00000000
58	Pb	2.62850100	-0.07551700	0.00000000
59	H	0.49461600	-3.52353600	0.00000000
60	H	1.44859300	-1.13640600	1.20816400
	H	1.44859300	-1.13640600	-1.20816400

1
2
3 H 0.13007300 3.51990900 0.00000000
4
5
6 21Sn:
7
8
9 E(RB+HF-LYP) = -859.916281800
10 Sn -0.19699100 -1.66511100 0.00000000
11 Sn 0.00000000 1.60448300 0.00000000
12 Sn -2.37606900 0.21045300 0.00000000
13 Sn 2.50714000 -0.10304500 0.00000000
14 H 0.26267800 -3.35712400 0.00000000
15 H 1.41785900 -1.15876600 1.16035200
16 H 1.41785900 -1.15876600 -1.16035200
17 H 0.19762000 3.33568000 0.00000000
18
19
20 21Tl:
21
22
23 E(RB+HF-LYP) = -692.723575098
24 Tl -2.28566800 0.11601200 0.00000000
25 Tl 2.36458300 -0.04628900 0.00000000
26 Tl 0.00000000 2.13379900 0.00000000
27 Tl -0.04529800 -2.16249500 0.00000000
28 H -4.01540100 -0.29063200 0.00000000
29 H -1.42240400 -1.25385000 1.26725300
30 H -1.42240400 -1.25385000 -1.26725300
31 H 4.13716000 -0.52486000 0.00000000
32
33
34 22Al:
35
36
37 E(RB+HF-LYP) = -972.165639588
38 Al 0.23504800 0.00000000 2.04625900
39 Al 0.23504800 1.47106500 0.00000000
40 Al 0.23504800 0.00000000 -2.04625900
41 Al -0.53451200 -1.33006900 0.00000000
42 H 0.25540900 0.10098000 3.62508700
43 H 0.25540900 0.10098000 -3.62508700
44 H -1.31328700 0.35226000 0.00000000
45 H -1.41573700 -2.64388900 0.00000000
46
47
48 22Ga:
49
50
51 E(RB+HF-LYP) = -7702.00040653
52 Ga 0.15608800 -0.01808000 1.99240400
53 Ga 0.15608800 1.50185800 0.00000000
54 Ga 0.15608800 -0.01808000 -1.99240400
55 Ga -0.39405100 -1.38466900 0.00000000
56 H 0.03730300 0.13470400 3.54739500
57 H 0.03730300 0.13470400 -3.54739500
58 H -1.44492400 0.06338900 0.00000000
59 H -0.93033800 -2.84469800 0.00000000
60

22In:

1
2
3
4 8
5 E(RB+HF-LYP) = -763.223624684
6 In 2.24647500 0.00000000 -0.02344800
7 In 0.00000000 0.00000000 1.98294500
8 In -2.24647500 0.00000000 -0.02344800
9 In 0.00000000 0.00000000 -1.84150700
10 H 3.98036300 0.00000000 0.21820300
11 H -3.98036300 0.00000000 0.21820300
12 H 0.00000000 -1.57596200 -2.53626100
13 H 0.00000000 1.57596200 -2.53626100
14

15
16 22Tl:

17 8
18 E(RB+HF-LYP) = -692.684202831
19
20 Tl 2.31743600 0.00000000 -0.03098500
21 Tl 0.00000000 0.00000000 2.08174500
22 Tl -2.31743600 0.00000000 -0.03098500
23 Tl 0.00000000 0.00000000 -1.96536900
24 H 4.11340100 0.00000000 0.09786800
25 H -4.11340100 0.00000000 0.09786800
26 H 0.00000000 -1.65149200 -2.30216000
27 H 0.00000000 1.65149200 -2.30216000
28
29

30 23Al:

31 8
32 E(RB+HF-LYP) = -972.175190507
33
34 Al -0.37467600 0.05526500 2.04152200
35 Al 0.63896800 -1.39030800 0.00000000
36 Al -0.37467600 0.05526500 -2.04152200
37 Al 0.00000000 1.50667000 0.00000000
38 H -0.50909600 -1.53435600 1.29001900
39 H -0.50909600 -1.53435600 -1.29001900
40 H 1.53213000 -2.69632200 0.00000000
41 H 0.93492500 2.78755000 0.00000000
42
43

44 23Ga:

45 8
46 E(RB+HF-LYP) = -7702.01286271
47
48 Ga 0.19375100 -0.14432600 1.97459200
49 Ga 0.19375100 1.67750100 0.00000000
50 Ga 0.19375100 -0.14432600 -1.97459200
51 Ga -0.59663400 -1.50250100 0.00000000
52 H 1.25135500 1.19001300 1.30203300
53 H 1.25135500 1.19001300 -1.30203300
54 H 0.04594900 3.24294100 0.00000000
55 H -2.07185100 -2.09974600 0.00000000
56
57

58 23In:

59 8
60 E(RB+HF-LYP) = -763.241317970
In 0.21411600 -0.11188500 2.25593100

1				
2				
3	In	0.21411600	1.93658100	0.00000000
4	In	0.21411600	-0.11188500	-2.25593100
5				
6	In	-0.65728700	-1.79127000	0.00000000
7	H	1.38478800	1.31312900	1.43933400
8	H	1.38478800	1.31312900	-1.43933400
9	H	0.26642700	3.68120300	0.00000000
10	H	-2.30396500	-2.46293900	0.00000000
11				
12	23Pb:			
13	8			
14				
15	E(RB+HF-LYP) =	-774.196949559		
16	Pb	-0.52326400	-0.14871200	1.92118100
17	Pb	-0.52326400	2.15109700	0.00000000
18	Pb	-0.52326400	-0.14871200	-1.92118100
19	Pb	1.52288800	-1.85689200	0.00000000
20	H	1.41944700	-0.35226600	1.41072800
21	H	1.41944700	-0.35226600	-1.41072800
22	H	-2.32924600	2.56663800	0.00000000
23	H	3.33641200	-1.59817500	0.00000000
24				
25				
26				
27	23Si:			
28	8			
29				
30	E(RB+HF-LYP) =	-1160.36107393		
31	Si	0.13524900	-0.06068100	2.02812800
32	Si	0.13524900	1.11971800	0.00000000
33	Si	0.13524900	-0.06068100	-2.02812800
34	Si	-0.49010200	-1.13399500	0.00000000
35	H	1.41766800	0.40043200	1.17078700
36	H	1.41766800	0.40043200	-1.17078700
37	H	0.28647300	2.59179000	0.00000000
38	H	-1.94082600	-1.49372300	0.00000000
39				
40				
41	23Sn:			
42	8			
43				
44	E(RB+HF-LYP) =	-859.919594460		
45	Sn	-0.22865300	-0.09940100	2.48655800
46	Sn	0.68981800	-1.27979100	0.00000000
47	Sn	-0.22865300	-0.09940100	-2.48655800
48	Sn	-0.22865300	1.53269100	0.00000000
49	H	-1.21122700	-1.21480200	1.36961700
50	H	-1.21122700	-1.21480200	-1.36961700
51	H	1.12165700	-2.94970800	0.00000000
52	H	1.10781700	2.67441000	0.00000000
53				
54				
55	23Tl:			
56	8			
57				
58	E(RB+HF-LYP) =	-692.713838881		
59	Tl	-0.10980900	0.01519500	2.17022500
60	Tl	-0.10980900	-2.32153500	0.00000000
	Tl	-0.10980900	0.01519500	-2.17022500
	Tl	0.33859500	2.24584400	0.00000000

H	-1.01672800	1.72496100	1.54606900
H	-1.01672800	1.72496100	-1.54606900
H	0.97082400	-3.81886100	0.00000000
H	0.32008400	4.03833400	0.00000000

24C:

8

E(RB+HF-LYP) = -154.744302845

C	-0.21172100	-1.36488700	0.00000000
C	-0.69978400	1.35351400	0.00000000
C	1.04327400	-0.72926700	0.00000000
C	-0.03493600	0.04074000	0.00000000
H	-1.34840200	1.42528000	-0.87535800
H	-1.34840200	1.42528000	0.87535800
H	2.11654200	-0.83995700	0.00000000
H	0.00000000	2.18789800	0.00000000

24Ga:

8

E(RB+HF-LYP) = -7701.97969785

Ga	0.53504200	-2.03862600	0.00000000
Ga	1.35232000	2.73831000	0.00000000
Ga	-1.90227000	-1.25543400	0.00000000
Ga	0.00000000	0.34089600	0.00000000
H	2.05611300	2.83617400	1.38793100
H	2.05611300	2.83617400	-1.38793100
H	-3.39387500	-1.76635700	0.00000000
H	-0.25621900	2.75448900	0.00000000

24Ge:

8

E(RB+HF-LYP) = -8310.59368679

Ge	1.67141300	-1.46354000	0.00000000
Ge	-0.77323100	2.68762200	0.00000000
Ge	-0.74730200	-1.79871100	0.00000000
Ge	0.00000000	0.35741000	0.00000000
H	-0.22463500	3.39184500	1.25308000
H	-0.22463500	3.39184500	-1.25308000
H	-2.07022500	-2.59806800	0.00000000
H	-2.30864900	2.76536700	0.00000000

24In:

8

E(RB+HF-LYP) = -763.217633138

In	1.86088600	-1.90401000	0.00000000
In	-0.79482700	3.68780300	0.00000000
In	-0.95721700	-2.76876500	0.00000000
In	0.00000000	0.80690600	0.00000000
H	-0.04599100	4.18222300	1.49599000
H	-0.04599100	4.18222300	-1.49599000
H	-2.71959000	-3.06441900	0.00000000

1
2
3 H -2.52168600 3.42519400 0.00000000
4
5
6 24Si:
7
8
9 E(RB+HF-LYP) = -1160.40074551
10 Si 1.45806400 -1.56581500 0.00000000
11 Si -0.38523500 2.56498700 0.00000000
12 Si -0.82705900 -1.72308700 0.00000000
13 Si 0.00000000 0.24802800 0.00000000
14 H 0.24192600 3.15056300 1.20770600
15 H 0.24192600 3.15056300 -1.20770600
16 H -2.09075300 -2.50698800 0.00000000
17 H -1.83387200 2.86827800 0.00000000
18
19
20 24Sn:
21
22
23 E(RB+HF-LYP) = -859.926365461
24 Sn 1.87321300 -1.69746900 0.00000000
25 Sn -0.82820000 3.14369900 0.00000000
26 Sn -0.93565500 -2.05816400 0.00000000
27 Sn 0.00000000 0.44441900 0.00000000
28 H -0.21535700 3.93893500 1.39135600
29 H -0.21535700 3.93893500 -1.39135600
30 H -2.50040400 -2.78710700 0.00000000
31 H -2.53680100 3.28497700 0.00000000
32
33
34 24Tl:
35
36
37 E(RB+HF-LYP) = -692.690287828
38 Tl 1.50605600 -2.32871800 0.00000000
39 Tl 0.06557000 3.93983600 0.00000000
40 Tl -1.53412000 -2.57651500 0.00000000
41 Tl 0.00000000 0.83932700 0.00000000
42 H 0.96960300 4.04713200 1.50489300
43 H 0.96960300 4.04713200 -1.50489300
44 H -3.32877900 -2.17270200 0.00000000
45 H -1.64844200 4.29012600 0.00000000
46
47
48 25Al:
49
50
51 E(RB+HF-LYP) = -972.157148870
52 Al -0.29379600 -1.24961000 0.00000000
53 Al 2.28275300 -0.10194300 0.00000000
54 Al -2.29189600 0.06208100 0.00000000
55 Al 0.00000000 1.16143600 0.00000000
56 H 3.02065000 -0.26897200 1.38423700
57 H 3.02065000 -0.26897200 -1.38423700
58 H -3.77458900 0.59757500 0.00000000
59 H 1.67150300 1.60483300 0.00000000
60

25B:

1
2
3
4 8
5 E(RB+HF-LYP) = -101.685883565
6 B -0.39988500 -0.79240100 0.00000000
7 B 1.45969400 -0.22981700 0.00000000
8 B -1.57592900 0.12187100 0.00000000
9 B 0.00000000 0.66236300 0.00000000
10 H 2.04630100 -0.37426000 1.02354100
11 H 2.04630100 -0.37426000 -1.02354100
12 H -2.60754300 0.68250900 0.00000000
13 H 1.09554800 1.25593500 0.00000000
14

15
16 26Pb:

17 8
18 E(RB+HF-LYP) = -774.204281208
19
20 Pb 0.00000000 1.41175900 0.00000000
21 Pb -2.79997800 0.18590000 0.00000000
22 Pb 2.69806100 0.13908200 0.00000000
23 Pb 0.20184000 -1.71599000 0.00000000
24 H -3.65422600 0.83399000 1.42597500
25 H -3.65422600 0.83399000 -1.42597500
26 H 2.27775700 -1.80165900 0.00000000
27 H -3.16301200 -1.56782800 0.00000000
28
29

30 27C:

31 8
32 E(RB+HF-LYP) = -154.802131169
33
34 H -0.86197700 2.83736800 0.00000000
35 C -0.45514100 1.85674600 0.00000000
36 C 0.00000000 0.74308300 0.00000000
37 C 0.57646900 -0.55526700 0.00000000
38 C -0.11883400 -1.69404700 0.00000000
39 H 1.66124400 -0.59130700 0.00000000
40 H -1.20021800 -1.69929600 0.00000000
41 H 0.38598400 -2.64985400 0.00000000
42
43

44 28Ge:

45 8
46 E(RB+HF-LYP) = -8310.53179155
47
48 Ge -1.98994500 -2.25055300 0.00000000
49 Ge 0.02224200 -1.28433700 0.00000000
50 Ge 0.00000000 1.13538600 0.00000000
51 Ge 1.92354300 2.28621000 0.00000000
52 H -2.53536100 -3.70482400 0.00000000
53 H -1.30960300 1.93442200 0.00000000
54 H 3.27891100 1.58288300 0.00000000
55 H 1.97915300 3.81290200 0.00000000
56
57

58 28Si:

59 8
60 E(RB+HF-LYP) = -1160.33207094
Si -1.94089500 -2.16318400 0.00000000

1
2
3 Si -0.06091900 -1.22253500 0.00000000
4 Si 0.00000000 1.06995400 0.00000000
5 Si 1.89302300 2.08658100 0.00000000
6 H -2.43007700 -3.56924900 0.00000000
7 H -1.23815600 1.87543600 0.00000000
8 H 3.16812500 1.34764000 0.00000000
9 H 2.02317300 3.55475900 0.00000000
10
11
12 29Al:
13 8
14 E(RB+HF-LYP) = -972.169149691
15 Al 0.00000000 1.25097000 0.00000000
16 Al 2.52384200 -0.03322600 0.00000000
17 Al -0.21274700 -1.32814300 0.00000000
18 Al -2.62418800 0.19303300 0.00000000
19 H 1.64941500 1.66345700 0.00000000
20 H 0.75650300 -0.13278700 1.02957500
21 H 0.75650300 -0.13278700 -1.02957500
22 H 0.90779000 -2.47212900 0.00000000
23
24
25
26 29Ga:
27 8
28 E(RB+HF-LYP) = -7702.01398562
29 Ga -0.01272700 1.33369400 -0.01297400
30 Ga 2.59307700 -0.01308200 0.00000000
31 Ga -0.15573500 -1.35785900 0.01320400
32 Ga -2.56164700 0.06478600 0.00000000
33 H 1.63501200 1.77301800 -0.01743400
34 H 0.77400500 -0.10230700 1.06864800
35 H 0.77377000 -0.12306100 -1.06665500
36 H 1.06520400 -2.40138100 0.02320100
37
38
39
40
41 29In:
42 8
43 E(RB+HF-LYP) = -763.259478149
44 In 0.00000000 1.55296000 -0.01500400
45 In 2.85509500 -0.02665700 0.00000000
46 In -0.12167600 -1.55095500 0.01499000
47 In -2.82700000 0.03638200 0.00000000
48 H 1.79518300 2.02169800 -0.01931200
49 H 0.83710000 -0.05706000 1.15551500
50 H 0.83734800 -0.07936200 -1.15398700
51 H 1.42655800 -2.46004200 0.02394400
52
53
54
55 2Al:
56 8
57 E(RB+HF-LYP) = -972.149295766
58 Al 1.10130800 -1.10130800 1.10130800
59 Al 1.10130800 1.10130800 -1.10130800
60 Al -1.10130800 -1.10130800 -1.10130800
Al -1.10130800 1.10130800 1.10130800

1
2
3 H 0.81712300 0.81712300 0.81712300
4 H -0.81712300 -0.81712300 0.81712300
5 H 0.81712300 -0.81712300 -0.81712300
6 H -0.81712300 0.81712300 -0.81712300
7
8

9 2B:

10 8

11 E(RB+HF-LYP) = -101.252374030

12 B 0.81795600 -0.81795600 0.81795600
13 B 0.81795600 0.81795600 -0.81795600
14 B -0.81795600 -0.81795600 -0.81795600
15 B -0.81795600 0.81795600 0.81795600
16 H 0.74051500 0.74051500 0.74051500
17 H -0.74051500 -0.74051500 0.74051500
18 H 0.74051500 -0.74051500 -0.74051500
19 H -0.74051500 0.74051500 -0.74051500
20
21
22

23 2C:

24 8

25 E(RB+HF-LYP) = -154.224429611

26 C 0.61522000 0.61522000 0.61522000
27 C -0.61522000 -0.61522000 0.61522000
28 C -0.61522000 0.61522000 -0.61522000
29 C 0.61522000 -0.61522000 -0.61522000
30 H 0.76341700 -0.76341700 0.76341700
31 H 0.76341700 0.76341700 -0.76341700
32 H -0.76341700 0.76341700 0.76341700
33 H -0.76341700 -0.76341700 -0.76341700
34
35
36

37 2Ga:

38 8

39 E(RB+HF-LYP) = -7702.01076676

40 Ga 1.13227100 -1.13227100 1.13227100
41 Ga 1.13227100 1.13227100 -1.13227100
42 Ga -1.13227100 -1.13227100 -1.13227100
43 Ga -1.13227100 1.13227100 1.13227100
44 H 0.84241300 0.84241300 0.84241300
45 H -0.84241300 -0.84241300 0.84241300
46 H 0.84241300 -0.84241300 -0.84241300
47 H -0.84241300 0.84241300 -0.84241300
48
49
50

51 2Ge:

52 8

53 E(RB+HF-LYP) = -8310.52902422

54 Ge 1.02166300 -1.02166300 1.02166300
55 Ge 1.02166300 1.02166300 -1.02166300
56 Ge -1.02166300 -1.02166300 -1.02166300
57 Ge -1.02166300 1.02166300 1.02166300
58 H 0.82672100 0.82672100 0.82672100
59 H -0.82672100 -0.82672100 0.82672100
60 H 0.82672100 -0.82672100 -0.82672100

1
2
3 H -0.82672100 0.82672100 -0.82672100
4
5
6 2In:
7
8
9 E(RB+HF-LYP) = -763.274648770
10 In 1.25111300 -1.25111300 1.25111300
11 In 1.25111300 1.25111300 -1.25111300
12 In -1.25111300 -1.25111300 -1.25111300
13 In -1.25111300 1.25111300 1.25111300
14 H 0.91255100 0.91255100 0.91255100
15 H -0.91255100 -0.91255100 0.91255100
16 H 0.91255100 -0.91255100 -0.91255100
17 H -0.91255100 0.91255100 -0.91255100
18
19
20 2Pb:
21
22 8
23 E(RB+HF-LYP) = -774.200788937
24 Pb 1.20434000 -1.20434000 1.20434000
25 Pb 1.20434000 1.20434000 -1.20434000
26 Pb -1.20434000 -1.20434000 -1.20434000
27 Pb -1.20434000 1.20434000 1.20434000
28 H 0.92120100 0.92120100 0.92120100
29 H -0.92120100 -0.92120100 0.92120100
30 H 0.92120100 -0.92120100 -0.92120100
31 H -0.92120100 0.92120100 -0.92120100
32
33
34 2Si:
35
36 8
37 E(RB+HF-LYP) = -1160.28532570
38 Si 0.95536300 -0.95536300 0.95536300
39 Si 0.95536300 0.95536300 -0.95536300
40 Si -0.95536300 -0.95536300 -0.95536300
41 Si -0.95536300 0.95536300 0.95536300
42 H 0.79485500 0.79485500 0.79485500
43 H -0.79485500 -0.79485500 0.79485500
44 H 0.79485500 -0.79485500 -0.79485500
45 H -0.79485500 0.79485500 -0.79485500
46
47
48 2Sn:
49
50 8
51 E(RB+HF-LYP) = -859.916580679
52 Sn 1.15305000 1.15305000 -1.15305000
53 Sn 1.15305000 -1.15305000 1.15305000
54 Sn -1.15305000 -1.15305000 -1.15305000
55 Sn -1.15305000 1.15305000 1.15305000
56 H 0.88610700 0.88610700 0.88610700
57 H -0.88610700 -0.88610700 0.88610700
58 H -0.88610700 0.88610700 -0.88610700
59 H 0.88610700 -0.88610700 -0.88610700
60

2Tl:

1
2
3
4 8
5 E(RB+HF-LYP) = -692.775226789
6 Tl 1.28628300 1.28628300 -1.28628300
7 Tl 1.28628300 -1.28628300 1.28628300
8 Tl -1.28628300 -1.28628300 -1.28628300
9 Tl -1.28628300 1.28628300 1.28628300
10 H 0.95036800 0.95036800 0.95036800
11 H -0.95036800 -0.95036800 0.95036800
12 H -0.95036800 0.95036800 -0.95036800
13 H 0.95036800 -0.95036800 -0.95036800
14

15
16 30Ge:

17 8
18 E(RB+HF-LYP) = -8310.59762962
19 Ge 0.45589500 -0.84227300 1.45944900
20 Ge 0.45589500 -0.84227300 -1.45944900
21 Ge 0.45589500 1.45389900 0.00000000
22 Ge -1.55091600 0.16852600 0.00000000
23 H 1.50593500 0.48184600 -1.26554200
24 H 1.27822500 -1.49625100 0.00000000
25 H 1.50593500 0.48184600 1.26554200
26 H 1.57333500 2.52044100 0.00000000
27
28
29

30 31Al:

31 8
32 E(RB+HF-LYP) = -972.168199820
33 Al 0.00000000 1.30965000 0.08843600
34 Al 0.00000000 0.00000000 -2.47903900
35 Al 0.00000000 -1.30965000 0.08843600
36 Al 0.00000000 0.00000000 2.63072600
37 H 0.00000000 1.96291600 -1.42283200
38 H 1.03171100 0.00000000 -0.71280200
39 H -1.03171100 0.00000000 -0.71280200
40 H 0.00000000 -1.96291600 -1.42283200
41
42
43

44 31In:

45 8
46 E(RB+HF-LYP) = -763.259469595
47 In 0.00000000 1.55768100 -0.06103400
48 In 0.00000000 0.00000000 2.84394500
49 In 0.00000000 -1.55768100 -0.06103400
50 In 0.00000000 0.00000000 -2.82241700
51 H 0.00000000 2.20252300 1.64791400
52 H -1.15733800 0.00000000 0.81532100
53 H 1.15733800 0.00000000 0.81532100
54 H 0.00000000 -2.20252300 1.64791400
55
56
57
58

59 32Ge:

60 8
E(RB+HF-LYP) = -8310.57934692
Ge -1.84607000 0.08432600 0.57701600

1				
2				
3	Ge	1.84175200	-0.08603400	0.58971200
4	Ge	-0.19628300	-1.39030300	-0.60651900
5	Ge	0.20074700	1.39213000	-0.60119100
6				
7	H	-2.86226700	0.90393900	-0.28698000
8	H	-0.86115000	1.42680100	0.93585800
9	H	0.85484000	-1.43222300	0.93315500
10	H	2.86391900	-0.90230600	-0.27057400
11				
12				
13	32Pb:			
14	8			
15	E(RB+HF-LYP) =	-774.217752892		
16	Pb	-0.99101300	2.19589400	0.68870700
17	Pb	0.99101300	-2.19589400	0.68870700
18	Pb	-1.44980800	-0.72938400	-0.69768900
19	Pb	1.44980800	0.72938400	-0.69768900
20	H	0.00000000	3.30017300	-0.43556500
21	H	0.88097900	1.45515600	1.13120500
22	H	-0.88097900	-1.45515600	1.13120500
23	H	0.00000000	-3.30017300	-0.43556500
24				
25				
26				
27	32Si:			
28	8			
29	E(RB+HF-LYP) =	-1160.35847650		
30	Si	-1.69275800	-0.02921700	0.51453200
31	Si	1.68911300	0.02663900	0.52202700
32	Si	-0.10986700	-1.32468700	-0.57451700
33	Si	0.11371700	1.32777000	-0.56733200
34	H	-2.85946600	0.53330500	-0.22169600
35	H	-0.93216100	1.30075600	0.95171100
36	H	0.92352800	-1.30737300	0.94438200
37	H	2.86523300	-0.53374700	-0.20033500
38				
39				
40				
41	32Sn:			
42	8			
43	E(RB+HF-LYP) =	-859.943319160		
44	Sn	1.26062100	1.78788900	0.69211700
45	Sn	-1.26062100	-1.78788900	0.69211700
46	Sn	-1.26062100	0.94615300	-0.70517500
47	Sn	1.26062100	-0.94615300	-0.70517500
48	H	2.68266100	1.88235400	-0.35079100
49	H	1.75453800	-0.06765300	1.00371400
50	H	-1.75453800	0.06765300	1.00371400
51	H	-2.68266100	-1.88235400	-0.35079100
52				
53				
54				
55	33Al:			
56	8			
57	E(RB+HF-LYP) =	-972.171756720		
58	Al	0.00000000	-1.25235100	-1.29536300
59	Al	0.00000000	1.25235100	1.29536300
60	Al	0.00000000	-1.25235100	1.29536300
	Al	0.00000000	1.25235100	-1.29536300

1				
2				
3	H	1.13565600	0.00000000	-1.78949300
4	H	-1.13565600	0.00000000	-1.78949300
5	H	-1.13565600	0.00000000	1.78949300
6	H	1.13565600	0.00000000	1.78949300
7				
8				

33Ga:

8

E(RB+HF-LYP) = -7701.99523390

11				
12				
13	Ga	-1.27483500	1.26375600	0.00000000
14	Ga	1.27483500	-1.26375600	0.00000000
15	Ga	1.27483500	1.26375600	0.00000000
16	Ga	-1.27483500	-1.26375600	0.00000000
17	H	-1.78078800	0.00000000	1.16678800
18	H	-1.78078800	0.00000000	-1.16678800
19	H	1.78078800	0.00000000	-1.16678800
20	H	1.78078800	0.00000000	1.16678800
21				
22				

34Al:

8

E(RB+HF-LYP) = -972.127643150

23				
24				
25				
26				
27	Al	0.00000000	2.07626800	1.03656600
28	Al	-2.07626800	0.00000000	-1.03656600
29	Al	0.00000000	-2.07626800	1.03656600
30	Al	2.07626800	0.00000000	-1.03656600
31	H	1.19837900	1.19837900	0.00000000
32	H	-1.19837900	-1.19837900	0.00000000
33	H	1.19837900	-1.19837900	0.00000000
34	H	-1.19837900	1.19837900	0.00000000
35				
36				

34B:

8

E(RB+HF-LYP) = -101.270634815

37				
38				
39				
40				
41	B	0.00000000	1.59775500	0.75389500
42	B	-1.59775500	0.00000000	-0.75389500
43	B	0.00000000	-1.59775500	0.75389500
44	B	1.59775500	0.00000000	-0.75389500
45	H	1.03397100	1.03397100	0.00000000
46	H	-1.03397100	-1.03397100	0.00000000
47	H	1.03397100	-1.03397100	0.00000000
48	H	-1.03397100	1.03397100	0.00000000
49				
50				

34Ga:

8

E(RB+HF-LYP) = -7701.99412324

51				
52				
53				
54				
55	Ga	0.00000000	2.16796300	1.00297800
56	Ga	-2.16796300	0.00000000	-1.00297800
57	Ga	0.00000000	-2.16796300	1.00297800
58	Ga	2.16796300	0.00000000	-1.00297800
59	H	1.24576400	1.24576400	0.00000000
60	H	-1.24576400	-1.24576400	0.00000000
	H	1.24576400	-1.24576400	0.00000000

1
2
3 H -1.24576400 1.24576400 0.00000000
4
5
6 34In:
7
8
9 E(RB+HF-LYP) = -763.258709475
10 In 0.00000000 2.41125500 1.07325700
11 In -2.41125500 0.00000000 -1.07325700
12 In 0.00000000 -2.41125500 1.07325700
13 In 2.41125500 0.00000000 -1.07325700
14 H 1.36508100 1.36508100 0.00000000
15 H -1.36508100 -1.36508100 0.00000000
16 H 1.36508100 -1.36508100 0.00000000
17 H -1.36508100 1.36508100 0.00000000
18
19
20 34Tl:
21
22
23 E(RB+HF-LYP) = -692.758133506
24 Tl 0.00000000 2.49746600 1.08161900
25 Tl -2.49746600 0.00000000 -1.08161900
26 Tl 0.00000000 -2.49746600 1.08161900
27 Tl 2.49746600 0.00000000 -1.08161900
28 H 1.43420600 1.43420600 0.00000000
29 H -1.43420600 -1.43420600 0.00000000
30 H 1.43420600 -1.43420600 0.00000000
31 H -1.43420600 1.43420600 0.00000000
32
33
34 35Al:
35
36
37 E(RB+HF-LYP) = -972.153227703
38 Al 0.00000000 0.00000000 -1.61353200
39 Al 0.00000000 2.03545900 0.07319700
40 Al 0.00000000 0.00000000 1.77987000
41 Al 0.00000000 -2.03545900 0.07319700
42 H -1.42543800 0.00000000 -2.32407400
43 H 0.00000000 -3.60813100 0.29131800
44 H 1.42543800 0.00000000 -2.32407400
45 H 0.00000000 3.60813100 0.29131800
46
47
48 35B:
49
50
51 E(RB+HF-LYP) = -101.680291307
52 B 0.00000000 0.00000000 -0.79705300
53 B 0.00000000 1.38944700 0.18114000
54 B 0.00000000 0.00000000 0.98817800
55 B 0.00000000 -1.38944700 0.18114000
56 H -1.00252700 0.00000000 -1.48549600
57 H 0.00000000 -2.56097800 0.10198200
58 H 1.00252700 0.00000000 -1.48549600
59 H 0.00000000 2.56097800 0.10198200
60

35C:

1
2
3
4 8
5 E(RB+HF-LYP) = -154.674331368
6 C 0.00000000 0.00000000 -1.04046500
7 C 0.00000000 0.94033700 0.16170800
8 C 0.00000000 -0.94033700 0.16170800
9 C 0.00000000 0.00000000 1.21762900
10 H -0.88816700 0.00000000 -1.67839200
11 H 0.00000000 -2.03329900 0.17673300
12 H 0.88816700 0.00000000 -1.67839200
13 H 0.00000000 2.03329900 0.17673300
14

15
16 35Ga:

17 8
18 E(RB+HF-LYP) = -7702.00118532
19
20 Ga 0.00000000 0.00000000 -1.59299200
21 Ga 1.98652500 0.00000000 0.00000000
22 Ga 0.00000000 0.00000000 1.73421900
23 Ga -1.98652500 0.00000000 0.00000000
24 H 0.00000000 1.41149800 -2.27619700
25 H -3.55325500 0.00000000 0.19128500
26 H 0.00000000 -1.41149800 -2.27619700
27 H 3.55325500 0.00000000 0.19128500
28
29

30 35Ge:

31 8
32 E(RB+HF-LYP) = -8310.60053427
33
34 Ge 0.00000000 0.00000000 -1.92464500
35 Ge 0.00000000 1.46194600 0.05754500
36 Ge 0.00000000 0.00000000 1.99035000
37 Ge 0.00000000 -1.46194600 0.05754500
38 H -1.24490900 0.00000000 -2.84502900
39 H 0.00000000 -3.02233800 -0.04770300
40 H 1.24490900 0.00000000 -2.84502900
41 H 0.00000000 3.02233800 -0.04770300
42
43

44 35In:

45 8
46 E(RB+HF-LYP) = -763.223769847
47
48 In 0.00000000 0.00000000 -1.83985700
49 In 0.00000000 2.24734400 -0.02461800
50 In 0.00000000 0.00000000 1.98354800
51 In 0.00000000 -2.24734400 -0.02461800
52 H -1.57520500 0.00000000 -2.53591800
53 H 0.00000000 -3.98054000 0.22176900
54 H 1.57520500 0.00000000 -2.53591800
55 H 0.00000000 3.98054000 0.22176900
56
57

58 35Pb:

59 8
60 E(RB+HF-LYP) = -774.174526381
Pb 0.00000000 0.00000000 2.35069900

1				
2				
3	Pb	0.00000000	1.82616800	-0.05307200
4	Pb	0.00000000	0.00000000	-2.33490400
5	Pb	0.00000000	-1.82616800	-0.05307200
6	H	1.39972400	0.00000000	3.48807600
7	H	0.00000000	-3.62705700	0.21628200
8	H	-1.39972400	0.00000000	3.48807600
9	H	0.00000000	3.62705700	0.21628200
10				
11				
12	35Si:			
13	8			
14	E(RB+HF-LYP) =	-1160.40887537		
15	Si	0.00000000	0.00000000	-1.79479500
16	Si	0.00000000	1.33729100	0.10780400
17	Si	0.00000000	0.00000000	1.95056900
18	Si	0.00000000	-1.33729100	0.10780400
19	H	-1.20085800	0.00000000	-2.67119100
20	H	0.00000000	-2.83567000	0.07152600
21	H	1.20085800	0.00000000	-2.67119100
22	H	0.00000000	2.83567000	0.07152600
23				
24	35Sn:			
25	8			
26	E(RB+HF-LYP) =	-859.937757302		
27	Sn	0.00000000	0.00000000	-2.23253600
28	Sn	0.00000000	1.69631500	0.04821800
29	Sn	0.00000000	0.00000000	2.27236300
30	Sn	0.00000000	-1.69631500	0.04821800
31	H	-1.37341900	0.00000000	-3.28097200
32	H	0.00000000	-3.43325200	-0.12560900
33	H	1.37341900	0.00000000	-3.28097200
34	H	0.00000000	3.43325200	-0.12560900
35				
36	35Tl:			
37	8			
38	E(RB+HF-LYP) =	-692.684202654		
39	Tl	0.00000000	0.00000000	-1.96478500
40	Tl	0.00000000	2.31814800	-0.03166700
41	Tl	0.00000000	0.00000000	2.08255600
42	Tl	0.00000000	-2.31814800	-0.03166700
43	H	-1.65143100	0.00000000	-2.30041400
44	H	0.00000000	-4.11417800	0.09566000
45	H	1.65143100	0.00000000	-2.30041400
46	H	0.00000000	4.11417800	0.09566000
47				
48	36Al:			
49	8			
50	E(RB+HF-LYP) =	-972.168785473		
51	Al	-0.97625800	-2.61405200	0.00000000
52	Al	0.97625800	2.61405200	0.00000000
53	Al	-0.97625800	0.79053800	0.00000000
54	Al	0.97625800	-0.79053800	0.00000000

H	0.41504300	-1.92815100	1.11995700
H	0.41504300	-1.92815100	-1.11995700
H	-0.41504300	1.92815100	-1.11995700
H	-0.41504300	1.92815100	1.11995700

36B:

8

E(RB+HF-LYP) = -101.539032777

B	-0.38413600	0.68964900	0.00000000
B	0.38413600	-0.68964900	0.00000000
B	-0.38413600	-2.12902800	0.00000000
B	0.38413600	2.12902800	0.00000000
H	0.69097900	-1.39563100	0.96840800
H	0.69097900	-1.39563100	-0.96840800
H	-0.69097900	1.39563100	-0.96840800
H	-0.69097900	1.39563100	0.96840800

36Ga:

8

E(RB+HF-LYP) = -7702.01010636

Ga	-0.97595400	-2.71724100	0.00000000
Ga	0.97595400	2.71724100	0.00000000
Ga	-0.97595400	0.78023900	0.00000000
Ga	0.97595400	-0.78023900	0.00000000
H	0.44341500	-1.95174500	1.14436700
H	0.44341500	-1.95174500	-1.14436700
H	-0.44341500	1.95174500	-1.14436700
H	-0.44341500	1.95174500	1.14436700

36In:

8

E(RB+HF-LYP) = -763.256377697

In	-1.40235300	3.76011100	0.00000000
In	1.40235300	-3.76011100	0.00000000
In	1.40235300	-0.48165200	0.00000000
In	-1.40235300	0.48165200	0.00000000
H	-1.48855300	2.05896000	1.21084800
H	-1.48855300	2.05896000	-1.21084800
H	1.48855300	-2.05896000	-1.21084800
H	1.48855300	-2.05896000	1.21084800

36Tl:

8

E(RB+HF-LYP) = -692.745196596

Tl	-0.89502000	-4.29781600	0.00000000
Tl	0.89502000	4.29781600	0.00000000
Tl	-0.89502000	1.36318400	0.00000000
Tl	0.89502000	-1.36318400	0.00000000
H	0.04810200	-2.81834600	1.25127400
H	0.04810200	-2.81834600	-1.25127400
H	-0.04810200	2.81834600	-1.25127400

1
2
3 H -0.04810200 2.81834600 1.25127400
4
5
6 37Al:
7
8
9 E(RB+HF-LYP) = -972.179716665
10 Al 0.16523000 1.62121200 0.07311000
11 Al 1.35255600 -0.64719600 -0.76505500
12 Al 0.17749200 -0.58171900 1.36527800
13 Al -1.93935300 -0.56666000 -0.55762600
14 H 0.38909500 3.16925700 -0.17662900
15 H -1.43331200 1.26910700 -0.35548800
16 H 1.77469100 -1.09292800 0.85570500
17 H 2.44249900 -1.07871300 -1.82778100
18
19
20 37Ga:
21
22
23 E(RB+HF-LYP) = -7702.01309274
24 Ga 0.50661900 1.57876300 0.05777900
25 Ga 1.33743400 -0.79223100 -0.80562500
26 Ga 0.08638600 -0.63453800 1.30173700
27 Ga -2.05737300 -0.21904200 -0.50155900
28 H 0.91128300 3.04964300 -0.33996300
29 H -1.17207600 1.52656600 -0.31391600
30 H 1.71644800 -1.28919700 0.83579000
31 H 2.47930800 -1.20855700 -1.80423300
32
33
34 38In:
35
36
37 E(RB+HF-LYP) = -763.245353074
38 In 0.66943600 1.67792700 -0.72618700
39 In 0.04629000 -1.50552800 -1.00740600
40 In 1.58331700 -0.36594200 1.22775400
41 In -2.32396000 0.17579200 0.59172500
42 H 0.42437600 3.18123800 -1.61905400
43 H -1.02096300 1.74297300 0.34303900
44 H 1.88360000 -1.56684400 -0.47245100
45 H -0.06612100 -2.48754300 -2.45994900
46
47
48 39Tl:
49
50
51 E(RB+HF-LYP) = -692.751453235
52 Tl 0.00000000 1.86362100 -1.35617300
53 Tl 0.15164900 0.34495800 1.93541000
54 Tl -1.98969000 -1.02168500 -0.17008200
55 Tl 1.82703500 -1.22739200 -0.43142000
56 H 1.45386900 0.92468800 0.07496200
57 H -0.12753300 -0.67116900 -1.33433500
58 H -1.32375700 1.07385400 0.26530200
59 H 0.29666200 1.95287900 2.79758000
60

3Al:

1
2
3
4 8
5 E(RB+HF-LYP) = -972.128291939
6 Al 0.00000000 1.45267700 1.35832700
7 Al -1.45267700 0.00000000 -1.35832700
8 Al 0.00000000 -1.45267700 1.35832700
9 Al 1.45267700 0.00000000 -1.35832700
10 H 1.20123000 1.20123000 0.00000000
11 H -1.20123000 -1.20123000 0.00000000
12 H 1.20123000 -1.20123000 0.00000000
13 H -1.20123000 1.20123000 0.00000000
14

15
16 3B:

17 8
18 E(RB+HF-LYP) = -101.507236311
19 B 0.00000000 0.78703600 0.68121000
20 B -0.78703600 0.00000000 -0.68121000
21 B 0.00000000 -0.78703600 0.68121000
22 B 0.78703600 0.00000000 -0.68121000
23 H 1.12901700 1.12901700 0.00000000
24 H -1.12901700 -1.12901700 0.00000000
25 H 1.12901700 -1.12901700 0.00000000
26 H -1.12901700 1.12901700 0.00000000
27
28
29

30 3C:

31 8
32 E(RB+HF-LYP) = -154.493568425
33 C 0.00000000 0.70993700 0.75773000
34 C -0.70993700 0.00000000 -0.75773000
35 C 0.00000000 -0.70993700 0.75773000
36 C 0.70993700 0.00000000 -0.75773000
37 H 1.01462300 1.01462300 0.00000000
38 H -1.01462300 -1.01462300 0.00000000
39 H 1.01462300 -1.01462300 0.00000000
40 H -1.01462300 1.01462300 0.00000000
41
42
43

44 3Ge:

45 8
46 E(RB+HF-LYP) = -8310.61531413
47 Ge 0.00000000 1.28420600 1.13321300
48 Ge -1.28420600 0.00000000 -1.13321300
49 Ge 0.00000000 -1.28420600 1.13321300
50 Ge 1.28420600 0.00000000 -1.13321300
51 H 1.34696800 1.34696800 0.00000000
52 H -1.34696800 -1.34696800 0.00000000
53 H 1.34696800 -1.34696800 0.00000000
54 H -1.34696800 1.34696800 0.00000000
55
56
57
58

59 3Pb:

60 8
E(RB+HF-LYP) = -774.259793208
Pb 0.00000000 1.56913100 1.32273000

1				
2				
3	Pb	0.00000000	-1.56913100	1.32273000
4	Pb	-1.56913100	0.00000000	-1.32273000
5	Pb	1.56913100	0.00000000	-1.32273000
6	Pb	1.56913100	0.00000000	-1.32273000
7	H	1.54754000	1.54754000	0.00000000
8	H	-1.54754000	1.54754000	0.00000000
9	H	1.54754000	-1.54754000	0.00000000
10	H	-1.54754000	-1.54754000	0.00000000
11				
12				
13	3Si:			
14	8			
15	E(RB+HF-LYP) =	-1160.38290960		
16	Si	0.00000000	1.19718700	1.05993600
17	Si	-1.19718700	0.00000000	-1.05993600
18	Si	0.00000000	-1.19718700	1.05993600
19	Si	1.19718700	0.00000000	-1.05993600
20	Si	1.19718700	0.00000000	-1.05993600
21	H	1.29438900	1.29438900	0.00000000
22	H	-1.29438900	-1.29438900	0.00000000
23	H	1.29438900	-1.29438900	0.00000000
24	H	-1.29438900	1.29438900	0.00000000
25	H	-1.29438900	1.29438900	0.00000000
26				
27	3Sn:			
28	8			
29	E(RB+HF-LYP) =	-859.983172356		
30	Sn	0.00000000	1.49130900	1.28190700
31	Sn	-1.49130900	0.00000000	-1.28190700
32	Sn	0.00000000	-1.49130900	1.28190700
33	Sn	1.49130900	0.00000000	-1.28190700
34	Sn	1.49130900	0.00000000	-1.28190700
35	H	1.47405400	1.47405400	0.00000000
36	H	-1.47405400	-1.47405400	0.00000000
37	H	1.47405400	-1.47405400	0.00000000
38	H	-1.47405400	1.47405400	0.00000000
39	H	-1.47405400	1.47405400	0.00000000
40				
41	40Al:			
42	8			
43	E(RB+HF-LYP) =	-972.136858091		
44	Al	0.00000000	0.00000000	1.22102400
45	Al	0.00000000	0.00000000	-1.22102400
46	Al	0.00000000	0.00000000	-3.73625100
47	Al	0.00000000	0.00000000	-3.73625100
48	H	0.00000000	-1.37544500	-4.51871000
49	H	0.00000000	1.37544500	-4.51871000
50	H	0.00000000	1.37544500	-4.51871000
51	H	0.00000000	-1.37544500	4.51871000
52	H	0.00000000	-1.37544500	4.51871000
53	H	0.00000000	-1.37544500	4.51871000
54				
55	40B:			
56	8			
57	E(RB+HF-LYP) =	-101.687637643		
58	B	0.00000000	0.00000000	2.36362500
59	B	0.00000000	0.00000000	-2.36362500
60	B	0.00000000	0.00000000	-0.78043400
	B	0.00000000	0.00000000	0.78043400

1				
2				
3	H	0.00000000	1.01781800	2.98735500
4	H	0.00000000	-1.01781800	2.98735500
5	H	0.00000000	-1.01781800	-2.98735500
6	H	0.00000000	1.01781800	-2.98735500
7				
8				

40C:

8

E(RB+HF-LYP) = -154.796772661

13	C	0.00000000	0.00000000	1.94411700
14	C	0.00000000	0.00000000	-1.94411700
15	C	0.00000000	0.00000000	-0.63200400
16	C	0.00000000	0.00000000	0.63200400
17	H	0.00000000	0.92475900	2.50871300
18	H	0.00000000	-0.92475900	2.50871300
19	H	0.00000000	-0.92475900	-2.50871300
20	H	0.00000000	0.92475900	-2.50871300
21				
22				

40Ga:

8

E(RB+HF-LYP) = -7701.98168355

27	Ga	0.00000000	0.00000000	1.18472800
28	Ga	0.00000000	0.00000000	-1.18472800
29	Ga	0.00000000	0.00000000	-3.59720200
30	H	0.00000000	-1.37296300	-4.35267000
31	H	0.00000000	1.37296300	-4.35267000
32	Ga	0.00000000	0.00000000	3.59720200
33	H	0.00000000	1.37296300	4.35267000
34	H	0.00000000	-1.37296300	4.35267000
35				
36				

40Ge:

8

E(RB+HF-LYP) = -8310.49534834

41	Ge	0.00000000	0.00000000	1.08137900
42	Ge	0.00000000	0.00000000	-1.08137900
43	Ge	0.00000000	0.00000000	-3.29931100
44	H	0.00000000	-1.32009300	-4.05459000
45	H	0.00000000	1.32009300	-4.05459000
46	Ge	0.00000000	0.00000000	3.29931100
47	H	0.00000000	1.32009300	4.05459000
48	H	0.00000000	-1.32009300	4.05459000
49				
50				

40In:

8

E(RB+HF-LYP) = -763.196597258

55	In	0.00000000	0.00000000	1.34987500
56	In	0.00000000	0.00000000	-1.34987500
57	In	0.00000000	0.00000000	-4.08919000
58	H	0.00000000	-1.52535300	-4.90372500
59	H	0.00000000	1.52535300	-4.90372500
60	In	0.00000000	0.00000000	4.08919000
	H	0.00000000	1.52535300	4.90372500

1
2
3 H 0.00000000 -1.52535300 4.90372500
4
5
6 40Pb:
7
8 8
9 E(RB+HF-LYP) = -774.009731566
10 Pb 0.00000000 0.00000000 1.32837100
11 Pb 0.00000000 0.00000000 -1.32837100
12 Pb 0.00000000 0.00000000 -4.04628200
13 H 0.00000000 -1.58988400 -4.72565000
14 H 0.00000000 1.58988400 -4.72565000
15 Pb 0.00000000 0.00000000 4.04628200
16 H 0.00000000 1.58988400 4.72565000
17 H 0.00000000 -1.58988400 4.72565000
18
19
20 40Si:
21 8
22 E(RB+HF-LYP) = -1160.31356146
23 Si 0.00000000 0.00000000 1.03802200
24 Si 0.00000000 0.00000000 -1.03802200
25 Si 0.00000000 0.00000000 -3.16372100
26 H 0.00000000 -1.25638800 -3.92662100
27 H 0.00000000 1.25638800 -3.92662100
28 Si 0.00000000 0.00000000 3.16372100
29 H 0.00000000 1.25638800 3.92662100
30 H 0.00000000 -1.25638800 3.92662100
31
32
33
34 40Sn:
35 8
36 E(RB+HF-LYP) = -859.812928932
37 Sn 0.00000000 0.00000000 1.25642400
38 Sn 0.00000000 0.00000000 -1.25642400
39 Sn 0.00000000 0.00000000 -3.82326400
40 H 0.00000000 -1.47651100 -4.64749000
41 H 0.00000000 1.47651100 -4.64749000
42 Sn 0.00000000 0.00000000 3.82326400
43 H 0.00000000 1.47651100 4.64749000
44 H 0.00000000 -1.47651100 4.64749000
45
46
47
48 40Tl:
49 8
50 E(RB+HF-LYP) = -692.641548519
51 Tl 0.00000000 0.00000000 1.40388600
52 Tl 0.00000000 0.00000000 -1.40388600
53 Tl 0.00000000 0.00000000 -4.23532300
54 H 0.00000000 -1.60328200 -4.88535600
55 H 0.00000000 1.60328200 -4.88535600
56 Tl 0.00000000 0.00000000 4.23532300
57 H 0.00000000 1.60328200 4.88535600
58 H 0.00000000 -1.60328200 4.88535600
59
60

41Pb:

1
2
3
4 8
5 E(RB+HF-LYP) = -774.183546018
6 Pb 0.39701600 1.43735000 -0.03075100
7 Pb 3.22203600 -0.29187700 0.01806300
8 Pb -1.01059000 -1.63968800 0.00000000
9 Pb -2.70237100 0.50091400 0.01299700
10 H 3.82627600 1.47100500 -0.03839200
11 H 1.70888100 0.35321700 1.20655400
12 H 1.69229800 0.27979400 -1.19843500
13 H 0.47314300 -2.65333800 -0.01895600

14
15
16 41Sn:

17 8
18 E(RB+HF-LYP) = -859.913148097
19 Sn 0.00000000 1.38574700 0.00000000
20 Sn 3.05694900 0.54927800 0.00000000
21 Sn -0.56416600 -1.76092700 0.00000000
22 Sn -2.63658800 -0.20010800 0.00000000
23 H 3.15586900 2.32975700 0.00000000
24 H 1.50454000 0.70073800 1.15678800
25 H 1.50454000 0.70073800 -1.15678800
26 H 1.02529500 -2.43071500 0.00000000

27
28
29
30 42Ge:

31 8
32 E(RB+HF-LYP) = -8310.54091381
33 Ge 0.39264600 -0.19430400 1.86881900
34 Ge 0.39264600 1.56330000 0.00000000
35 Ge 0.39264600 -0.19430400 -1.86881900
36 Ge -1.02554600 -1.16686400 0.00000000
37 H -0.60941200 0.13321400 3.03230000
38 H -0.60941200 0.13321400 -3.03230000
39 H -1.06340100 0.59097600 0.00000000
40 H -2.59427300 -1.10792300 0.00000000

41
42
43
44 42Si:

45 8
46 E(RB+HF-LYP) = -1160.32525806
47 Si 0.40446700 -0.18341400 1.72570800
48 Si 0.40446700 1.48629800 0.00000000
49 Si 0.40446700 -0.18341400 -1.72570800
50 Si -0.90646400 -1.09442700 0.00000000
51 H -0.43939000 0.13959400 2.91870800
52 H -0.43939000 0.13959400 -2.91870800
53 H -1.01743000 0.56331900 0.00000000
54 H -2.40091000 -1.19310700 0.00000000

55
56
57
58 43Ge:

59 8
60 E(RB+HF-LYP) = -8310.58447627
Ge 2.18119900 -0.12043600 -0.18796800

1				
2				
3	Ge	0.12299200	1.32018300	0.21455100
4	Ge	-2.15730600	0.00000000	-0.23857500
5	Ge	-0.14015400	-1.26745100	0.20581300
6	Ge	-0.14015400	-1.26745100	0.20581300
7	H	1.72429200	-0.06388200	-1.71484400
8	H	-1.02585400	1.42889000	-0.97793000
9	H	-0.46484800	2.31544900	1.24706400
10	H	-0.44899300	-1.80749000	1.64345000
11				
12				
13	44C:			
14	8			
15	E(RB+HF-LYP) =	-154.726103194		
16	C	-1.08697200	-0.08978400	-0.13872300
17	C	0.15738500	-0.91669300	0.33674100
18	C	1.08539500	-0.06049900	-0.18194400
19	C	1.08539500	-0.06049900	-0.18194400
20	C	0.02994800	0.85440000	0.01302400
21	H	-1.35599500	-0.35505600	-1.15259000
22	H	2.15541800	-0.01992100	-0.28547900
23	H	-1.94861200	-0.01252200	0.52011800
24	H	-1.94861200	-0.01252200	0.52011800
25	H	0.03465600	1.66295300	0.74336500
26				
27	44Ge:			
28	8			
29	E(RB+HF-LYP) =	-8310.60533355		
30	Ge	-1.74503400	0.13213700	0.29408600
31	Ge	0.21207900	1.60013300	-0.35262700
32	Ge	0.21207900	1.60013300	-0.35262700
33	Ge	1.68998400	-0.10808800	0.36062300
34	Ge	-0.08912700	-1.55068700	-0.28823700
35	H	-2.19706700	0.10003400	1.76500000
36	H	3.17072400	-0.46839400	0.09681300
37	H	-2.99740100	0.22782800	-0.60312300
38	H	-2.99740100	0.22782800	-0.60312300
39	H	-0.14917000	-2.21132300	-1.70175700
40				
41	44Si:			
42	8			
43	E(RB+HF-LYP) =	-1160.41062445		
44	Si	-1.62230700	0.08143800	0.28536700
45	Si	-1.62230700	0.08143800	0.28536700
46	Si	0.15427700	1.52554800	-0.40641600
47	Si	1.58811900	0.00000000	0.36741400
48	Si	0.00000000	-1.43933000	-0.24703600
49	H	-2.04259400	0.09796900	1.70402500
50	H	-2.04259400	0.09796900	1.70402500
51	H	3.06075700	-0.19023100	0.35210700
52	H	-2.82811500	0.12244700	-0.57855700
53	H	0.00000000	-2.29963500	-1.46817300
54				
55	44Sn:			
56	8			
57	E(RB+HF-LYP) =	-859.940458914		
58	Sn	2.05795100	0.13412400	-0.35419100
59	Sn	-0.20015100	1.79834600	0.40095100
60	Sn	-2.02156800	-0.11046400	-0.41646000
	Sn	0.10791000	-1.77242900	0.35052400

1				
2				
3	H	2.59584700	0.14531300	-1.98674000
4	H	-3.53183900	-0.57559200	0.29882200
5	H	3.47256200	0.22029800	0.62364400
6	H	0.25631400	-2.26887900	2.02304900
7				
8				

45Ga:

8

E(RB+HF-LYP) = -7702.01403854

10				
11				
12				
13	Ga	-0.20288300	1.50919400	0.23923700
14	Ga	2.04100400	0.01841600	-0.24735800
15	Ga	0.08114400	-1.34491600	0.27599200
16	Ga	-1.97855600	-0.15556900	-0.25735400
17	H	3.58340400	0.26401700	-0.09738500
18	H	1.45261400	1.68341600	-0.34660800
19	H	-3.50107100	0.09980800	0.02374200
20	H	0.30305800	-2.88809900	0.09422600
21				
22				

45In:

8

E(RB+HF-LYP) = -763.234939071

23				
24				
25				
26				
27	In	-0.40536400	1.75204000	0.35855700
28	In	2.42329000	0.08910300	-0.37260500
29	In	0.21682600	-1.51350600	0.46029300
30	In	-2.27480700	-0.30549600	-0.43705300
31	H	3.97507900	0.89433300	-0.19110900
32	H	1.33704400	1.75813800	-0.55644800
33	H	-3.90319700	-0.54114800	0.20241100
34	H	0.55370000	-3.19626500	0.09473100
35				
36				

46Tl:

8

E(RB+HF-LYP) = -692.716535453

37				
38				
39				
40				
41	Tl	-2.94358900	-0.12941400	-0.39437600
42	Tl	0.23739000	1.78103500	0.33820200
43	Tl	2.65592900	-0.28812700	-0.48209900
44	Tl	-0.00872500	-1.40672600	0.53147600
45	H	0.26877600	3.49764200	-0.27097700
46	H	-1.65339400	1.44567700	-0.56838700
47	H	1.78586600	-1.40766100	1.31045100
48	H	4.37730800	-0.03388100	0.07950400
49				
50				

47Ge:

8

E(RB+HF-LYP) = -8310.55009168

51				
52				
53				
54				
55	Ge	2.07629700	-1.65129800	0.00000000
56	Ge	-0.33352400	-1.59213100	0.00000000
57	Ge	-1.94659100	2.40054000	0.00000000
58	Ge	0.00000000	0.79114900	0.00000000
59	H	2.95953300	-2.94033000	0.00000000
60	H	-0.96557100	3.66311600	0.00000000
	H	3.09429900	-0.47826700	0.00000000

1
2
3 H 1.43391300 1.41115200 0.00000000
4
5
6 48Sn:
7
8
9 E(RB+HF-LYP) = -859.908253021
10 Sn 0.52737400 -2.13323700 0.00000000
11 Sn 2.38266100 -0.05711300 0.00000000
12 Sn 0.00000000 1.39702600 0.00000000
13 Sn -2.84512600 0.79764200 0.00000000
14 H 0.79540400 -3.85488400 0.00000000
15 H 0.30478700 3.12170500 0.00000000
16 H -1.20479600 -2.04162100 0.00000000
17 H -3.14088500 2.55888500 0.00000000
18
19
20 4Ge:
21
22
23 E(RB+HF-LYP) = -8310.60680180
24 Ge -1.55522900 -0.20907800 -0.72204700
25 Ge 0.38853700 1.70845500 0.12913800
26 Ge 1.31100200 -0.84547300 -0.72845300
27 Ge -0.15961900 -0.72776500 1.38274500
28 H -1.02824400 1.40514900 -0.98468700
29 H 0.17550300 0.87810700 1.75503000
30 H -0.17904000 -0.74895400 -1.71902100
31 H 1.52165900 0.82927100 -1.01559900
32
33
34 4Pb:
35
36
37 E(RB+HF-LYP) = -774.252771367
38 Pb 0.95080200 -1.59496400 -0.89985900
39 Pb -2.10075700 -0.37954400 0.15950000
40 Pb 0.31332100 1.81108700 -0.91976500
41 Pb 0.87128100 0.17074700 1.68780400
42 H -1.03803200 -1.68885300 -1.06628900
43 H -1.05284500 -0.24533300 1.93329400
44 H 0.81844200 0.13194600 -2.02185700
45 H -1.56860300 1.20156800 -1.11494500
46
47
48 4Sn:
49
50
51 E(RB+HF-LYP) = -859.975313181
52 Sn -0.59296100 1.66756700 -0.85993000
53 Sn 2.06410200 -0.03640800 0.15234400
54 Sn -0.65549500 -1.64723400 -0.85740500
55 Sn -0.87215700 0.01743600 1.60740500
56 H 1.30139300 1.38915100 -1.00386400
57 H 1.02764100 -0.03064300 1.81556200
58 H -0.75371700 0.01125000 -1.93780500
59 H 1.25023100 -1.43779400 -0.99464500
60

5Al:

1
2
3
4 8
5 E(RB+HF-LYP) = -972.195134389
6 Al -0.55901700 -0.79382400 1.28453700
7 Al 1.63575500 0.51365300 0.00000000
8 Al -0.55901700 1.45425500 0.00000000
9 Al -0.55901700 -0.79382400 -1.28453700
10 H -0.85955400 -1.97663000 0.00000000
11 H -0.90925900 -1.64530100 -2.57404400
12 H -0.90925900 -1.64530100 2.57404400
13 H 3.21491100 0.32384200 0.00000000
14

15
16 5Ga:

17 8
18 E(RB+HF-LYP) = -7702.01574645
19 Ga 0.98440300 1.34308800 -0.24896200
20 Ga -1.58680700 0.00000000 -0.73327500
21 Ga -0.49655900 0.00000000 1.37535900
22 Ga 0.99273900 -1.33716900 -0.25383600
23 H 2.06495400 0.00000000 -0.85732300
24 H 1.90622700 -2.52918400 -0.74342800
25 H 1.88878300 2.54333100 -0.73553200
26 H -2.56704800 0.00000000 -1.98156800
27
28
29

30 5In:

31 8
32 E(RB+HF-LYP) = -763.237905149
33 In -0.65098700 -0.98664000 1.59967800
34 In 1.94738500 0.53015700 0.00000000
35 In -0.65098700 1.57681900 0.00000000
36 In -0.65098700 -0.98664000 -1.59967800
37 H -1.14462400 -2.11851300 0.00000000
38 H -1.10424900 -2.19110100 -2.80135200
39 H -1.10424900 -2.19110100 2.80135200
40 H 3.62637400 -0.05045000 0.00000000
41
42
43

44 6Al:

45 8
46 E(RB+HF-LYP) = -972.185239325
47 Al -1.76790800 0.22584000 0.00000000
48 Al 0.68169400 -0.69443300 1.32872000
49 Al 0.68169400 1.38726200 0.00000000
50 Al 0.68169400 -0.69443300 -1.32872000
51 H -2.61858000 -1.12453800 0.00000000
52 H 0.83486600 -1.66859700 -2.57940700
53 H -2.65442200 1.54665800 0.00000000
54 H 0.83486600 -1.66859700 2.57940700
55
56
57

58 6B:

59 8
60 E(RB+HF-LYP) = -101.706071196
B -1.11792500 0.71442100 0.00000000

1
2
3 B 0.52149900 -0.58725400 0.88305900
4 B 0.52149900 0.64196300 0.00000000
5
6 B 0.52149900 -0.58725400 -0.88305900
7 H -2.04074600 -0.02867100 0.00000000
8 H 0.58508200 -1.38488800 -1.74468100
9 H -1.36227500 1.88907100 0.00000000
10 H 0.58508200 -1.38488800 1.74468100
11
12
13 6Ga:
14 8
15 E(RB+HF-LYP) = -7702.01742096
16 Ga -1.82250600 0.15585200 0.00000000
17 Ga 0.64975700 -0.70920800 1.33174200
18 Ga 0.64975700 1.36617700 0.00000000
19 Ga 0.64975700 -0.70920800 -1.33174200
20 H -2.69062900 -1.17207700 0.00000000
21 H 0.72364200 -1.76013600 -2.52231900
22 H -2.68634600 1.48034000 0.00000000
23 H 0.72364200 -1.76013600 2.52231900
24
25
26
27 6In:
28 8
29 E(RB+HF-LYP) = -763.238145315
30 In -2.07188200 0.09558100 0.00000000
31 In 0.72314400 -0.81583700 1.54434200
32 In 0.72314400 1.61828200 0.00000000
33 In 0.72314400 -0.81583700 -1.54434200
34 H -3.02880600 -1.37929200 0.00000000
35 H 0.66419400 -2.08923700 -2.77536300
36 H -3.07944900 1.53049900 0.00000000
37 H 0.66419400 -2.08923700 2.77536300
38
39
40
41 6Tl:
42 8
43 E(RB+HF-LYP) = -692.702383246
44 Tl -2.14684100 0.07375300 0.00000000
45 Tl 0.73902500 -0.86455200 1.70597600
46 Tl 0.73902500 1.71050000 0.00000000
47 Tl 0.73902500 -0.86455200 -1.70597600
48 H -3.21546800 -1.36562400 0.00000000
49 H 0.35247100 -2.32471900 -2.74845800
50 H -3.17844900 1.54803300 0.00000000
51 H 0.35247100 -2.32471900 2.74845800
52
53
54
55 7Ga:
56 8
57 E(RB+HF-LYP) = -7702.01795942
58 Ga -1.73603100 -0.52789000 -0.33748900
59 Ga 1.35441700 -0.78094600 -0.73046900
60 Ga 0.32821500 -0.28304700 1.40188800
Ga 0.15288200 1.59017700 -0.20136700

H	-2.58063700	0.33991900	-1.36526900
H	-0.31359700	2.89958100	-0.97332000
H	-2.46682400	-1.84790400	0.12604500
H	2.27705000	-1.33871700	-1.89693600

8Al:

8

E(RB+HF-LYP) = -972.147102069

Al	1.36218500	-0.96794000	-0.67350900
Al	-1.56395600	-0.89387900	-0.04364500
Al	-0.12062600	1.62537600	-0.75089600
Al	0.33178200	0.24299300	1.51117800
H	-0.25095500	-1.62244100	-0.97434900
H	0.66621300	0.47778000	3.03393700
H	0.95569400	0.49868400	-1.57374100
H	-1.49296200	0.56081500	-1.04650200

8B:

8

E(RB+HF-LYP) = -101.530780690

B	0.00000000	0.94551100	-0.35396400
B	-0.81883600	-0.47275500	-0.35396400
B	0.81883600	-0.47275500	-0.35396400
B	0.00000000	0.00000000	1.14173600
H	-1.22989600	0.71008100	-0.90437200
H	0.00000000	-1.42016200	-0.90437200
H	1.22989600	0.71008100	-0.90437200
H	0.00000000	0.00000000	2.31389700

8C:

8

E(RB+HF-LYP) = -154.554715649

C	0.00000000	1.01572400	-0.22999100
C	-0.87964300	-0.50786200	-0.22999100
C	0.87964300	-0.50786200	-0.22999100
C	0.00000000	0.00000000	0.82281200
H	-1.02241300	0.59029000	-0.89796500
H	0.00000000	-1.18058100	-0.89796500
H	1.02241300	0.59029000	-0.89796500
H	0.00000000	0.00000000	1.89685600

8Ga:

8

E(RB+HF-LYP) = -7701.98593128

Ga	0.00000000	1.92830700	-0.56138000
Ga	-1.66996300	-0.96415300	-0.56138000
Ga	1.66996300	-0.96415300	-0.56138000
Ga	0.00000000	0.00000000	1.68065400
H	-1.29000400	0.74478400	-1.06173800
H	0.00000000	-1.48956800	-1.06173800
H	1.29000400	0.74478400	-1.06173800

1				
2				
3	H	0.00000000	0.00000000	3.29323400
4				
5				
6	8Ge:			
7	8			
8	E(RB+HF-LYP) =	-8310.61039069		
9	Ge	0.00000000	1.74065700	-0.42557900
10	Ge	-1.50745300	-0.87032900	-0.42557900
11	Ge	1.50745300	-0.87032900	-0.42557900
12	Ge	0.00000000	0.00000000	1.30452400
13	H	-1.21349900	0.70061400	-1.23739100
14	H	0.00000000	-1.40122800	-1.23739100
15	H	1.21349900	0.70061400	-1.23739100
16	H	0.00000000	0.00000000	2.82304800
17				
18				
19				
20	8In:			
21	8			
22	E(RB+HF-LYP) =	-763.242034450		
23	In	0.00000000	2.20544200	-0.69788700
24	In	-1.90996900	-1.10272100	-0.69788700
25	In	1.90996900	-1.10272100	-0.69788700
26	In	0.00000000	0.00000000	2.08042400
27	H	-1.39872700	0.80755500	-1.08002000
28	H	0.00000000	-1.61511100	-1.08002000
29	H	1.39872700	0.80755500	-1.08002000
30	H	0.00000000	0.00000000	3.88871000
31				
32				
33				
34	8Pb:			
35	8			
36	E(RB+HF-LYP) =	-774.227457792		
37	Pb	0.00000000	2.08134400	-0.52997700
38	Pb	-1.80249700	-1.04067200	-0.52997700
39	Pb	1.80249700	-1.04067200	-0.52997700
40	Pb	0.00000000	0.00000000	1.59993200
41	H	-1.36625800	0.78880900	-1.39262000
42	H	0.00000000	-1.57761800	-1.39262000
43	H	1.36625800	0.78880900	-1.39262000
44	H	0.00000000	0.00000000	3.35788100
45				
46				
47				
48	8Si:			
49	8			
50	E(RB+HF-LYP) =	-1160.39360685		
51	Si	0.00000000	1.61249200	-0.39625900
52	Si	-1.39645900	-0.80624600	-0.39625900
53	Si	1.39645900	-0.80624600	-0.39625900
54	Si	0.00000000	0.00000000	1.25013000
55	H	-1.17665700	0.67934300	-1.19184100
56	H	0.00000000	-1.35868700	-1.19184100
57	H	1.17665700	0.67934300	-1.19184100
58	H	0.00000000	0.00000000	2.71660200
59				
60				

8Sn:

1
2
3 8
4 E(RB+HF-LYP) = -859.967357364
5 Sn 0.00000000 1.98739200 -0.50280900
6 Sn 1.72113200 -0.99369600 -0.50280900
7 Sn -1.72113200 -0.99369600 -0.50280900
8 Sn 0.00000000 0.00000000 1.52433800
9 H 1.31383700 0.75854400 -1.33820900
10 H 0.00000000 0.00000000 3.21902800
11 H -1.31383700 0.75854400 -1.33820900
12 H 0.00000000 -1.51708800 -1.33820900
13
14

15
16 9Ge:

17 8
18 E(RB+HF-LYP) = -8310.58187564
19 Ge -0.15434100 0.00000000 1.43339000
20 Ge 0.51454500 -1.96654200 0.00000000
21 Ge -0.15434100 0.00000000 -1.43339000
22 Ge -0.15434100 1.90192400 0.00000000
23 H -1.30284800 0.05038000 2.48823300
24 H -1.30284800 0.05038000 -2.48823300
25 H 2.06441000 -1.64825800 0.00000000
26 H -1.10740800 3.13603400 0.00000000
27
28
29

30 9Si:

31 8
32 E(RB+HF-LYP) = -1160.38446343
33 Si -0.14187300 -0.01610500 1.30414500
34 Si 0.51807600 -1.85681100 0.00000000
35 Si -0.14187300 -0.01610500 -1.30414500
36 Si -0.14187300 1.81036200 0.00000000
37 H -1.09092400 -0.07050500 2.45571600
38 H -1.09092400 -0.07050500 -2.45571600
39 H 2.01495300 -1.69664200 0.00000000
40 H -1.12752000 2.93887800 0.00000000
41
42
43

44 9Sn:

45 8
46 E(RB+HF-LYP) = -859.925047028
47 Sn -0.11106800 0.04315300 1.75946900
48 Sn -0.11106800 -2.29367100 0.00000000
49 Sn -0.11106800 0.04315300 -1.75946900
50 Sn 0.36978600 2.15195100 0.00000000
51 H -1.62812900 0.65243900 2.40062500
52 H -1.62812900 0.65243900 -2.40062500
53 H 1.65940700 -2.32424600 0.00000000
54 H -0.23228700 3.79002500 0.00000000
55
56
57
58
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