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

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

2. COMPUTATIONAL METHODS

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

The substituted E_4R_4 tetrahedrane structures were optimized using the gradient corrected density functional BP86 [24] via an interface to TURBOMOLE for the energy and gradient calculations using the resolution of the identity (RI) approximation [26], and 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 find 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 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 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 **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 .

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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.

Figure 1

Figure 1 (continued)

Figure 2

Figure 2 (continued)

Table 1. Calculated E_4R_4 bond lengths [$\text{\AA}$] 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	$1.699 - 1.714^a$	$1.570 - 1.576^a$
$Al_4[Si(t\text{-Bu})_3]_4$	2.627	2.534	$2.600 - 2.612^b$	$2.467 - 2.501^b$
$Ga_4[C(SiMe_3)_3]_4$	2.751	2.116	$2.678 - 2.702^c$	$2.06 - 2.11^c$
$In_4[C(SiMe_3)_3]_4$	3.098	2.317	$2.989 - 3.013^e$	$2.24 - 2.26^d$
$Tl_4[C(SiMe_3)_3]_4$	3.411	2.448	$3.322 - 3.638^f$	$2.33 - 2.38^f$
$C_4(t\text{-Bu})_4$	1.499	1.503	$1.480 - 1.487^g$	$1.480 - 1.503^g$
$Si_4[Si(t\text{-Bu})_3]_4$	2.362	2.400	$2.315 - 2.320^h$	$2.355 - 2.365^h$
$Ge_4[Si(t\text{-Bu})_3]_4$	2.508	2.440	$2.431 - 2.447^i$	$2.378 - 2.385^i$
$Sn_4[Si(t\text{-Bu})_3]_4$	2.891	2.642	-	-
$Pb_4[Si(t\text{-Bu})_3]_4$	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)

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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)
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n/c: not calculated

rearr.: rearranges into another structure type

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_I	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_I	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_I	n/c	n/c	n/c	1.6	n/c
39 C_I	n/c	n/c	n/c	n/c	-43.5
45 C_I	n/c	n/c	11.7	7.0	n/c

n/c: not calculated

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Table 5. Calculated E₄H₄ 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

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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 _I	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 _I	n/c	n/c	-36.7	n/c	n/c
44 C _I	n/c	-38.8	-53.4	-53.1	n/c
n/c: not calculated					

Supporting Information for:

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

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

Table S1: Energies and coordinates of the calculated molecules

10B:

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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:

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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

H 0.00000000 -2.79941800 2.03099600

10Pb:

8

E(RB+HF-LYP) = -774.193121064

Pb 0.00000000 1.99765500 0.51578600

Pb 0.00000000 -1.99765500 0.51578600

Pb 1.99765500 0.00000000 -0.51578600

Pb -1.99765500 0.00000000 -0.51578600

H 0.00000000 1.73090200 2.32859800

H -1.73090200 0.00000000 -2.32859800

H 1.73090200 0.00000000 -2.32859800

H 0.00000000 -1.73090200 2.32859800

10Si:

8

E(RB+HF-LYP) = -1160.39076157

Si 0.00000000 1.51939300 0.41838700

Si 0.00000000 -1.51939300 0.41838700

Si 1.51939300 0.00000000 -0.41838700

Si -1.51939300 0.00000000 -0.41838700

H 0.00000000 1.45563300 1.91157500

H -1.45563300 0.00000000 -1.91157500

H 1.45563300 0.00000000 -1.91157500

H 0.00000000 -1.45563300 1.91157500

10Sn:

8

E(RB+HF-LYP) = -859.940543098

Sn 0.00000000 1.89001700 0.49089200

Sn 0.00000000 -1.89001700 0.49089200

Sn 1.89001700 0.00000000 -0.49089200

Sn -1.89001700 0.00000000 -0.49089200

H 0.00000000 1.66233500 2.22979300

H -1.66233500 0.00000000 -2.22979300

H 1.66233500 0.00000000 -2.22979300

H 0.00000000 -1.66233500 2.22979300

10Tl:

8

E(RB+HF-LYP) = -692.683692501

Tl 0.00000000 2.15545200 0.60503900

Tl 0.00000000 -2.15545200 0.60503900

Tl 2.15408800 0.00000000 -0.60507200

Tl -2.15408800 0.00000000 -0.60507200

H 0.00000000 2.61112600 2.39771000

H -2.62219100 0.00000000 -2.39509900

H 2.62219100 0.00000000 -2.39509900

H 0.00000000 -2.61112600 2.39771000

11Al:

8
 E(RB+HF-LYP) = -972.150787518
 Al 0.00000000 1.82716700 0.26769900
 Al 0.00000000 -1.82716700 0.26769900
 Al 1.82716700 0.00000000 -0.26769900
 Al -1.82716700 0.00000000 -0.26769900
 H 0.00000000 3.20822200 1.05797400
 H -3.20822200 0.00000000 -1.05797400
 H 3.20822200 0.00000000 -1.05797400
 H 0.00000000 -3.20822200 1.05797400

11Ga:
 8
 E(RB+HF-LYP) = -7701.98523261
 Ga 0.00000000 1.76297300 0.29387000
 Ga 0.00000000 -1.76297300 0.29387000
 Ga 1.76297300 0.00000000 -0.29387000
 Ga -1.76297300 0.00000000 -0.29387000
 H 0.00000000 3.07970500 1.16584800
 H -3.07970500 0.00000000 -1.16584800
 H 3.07970500 0.00000000 -1.16584800
 H 0.00000000 -3.07970500 1.16584800

11Ge:
 8
 E(RB+HF-LYP) = -8310.46625246
 Ge 0.00000000 1.84854900 0.18829800
 Ge 0.00000000 -1.84854900 0.18829800
 Ge 1.84854900 0.00000000 -0.18829800
 Ge -1.84854900 0.00000000 -0.18829800
 H 0.00000000 3.44721700 0.61536900
 H -3.44721700 0.00000000 -0.61536900
 H 3.44721700 0.00000000 -0.61536900
 H 0.00000000 -3.44721700 0.61536900

11In:
 8
 E(RB+HF-LYP) = -763.214864629
 In -1.38074200 1.38074200 0.64863200
 In -1.38074200 -1.38074200 -0.64863200
 In 1.38074200 -1.38074200 0.64863200
 In 1.38074200 1.38074200 -0.64863200
 H -1.31435700 2.89431400 1.58250500
 H 1.31435700 -2.89431400 1.58250500
 H -2.89431400 -1.31435700 -1.58250500
 H 2.89431400 1.31435700 -1.58250500

11Tl:
 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	TI	1.52323700	1.52323700	0.61006900
6				
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				
12	12Al:			
13	8			
14	E(RB+HF-LYP) =	-972.178229668		
15	Al	0.11606800	-1.39362900	0.00000000
16	Al	-2.06552100	-0.11352200	0.00000000
17	Al	0.00000000	1.36188700	0.00000000
18	Al	2.10373800	0.09269100	0.00000000
19	H	-3.63939300	-0.10026500	0.00000000
20	H	-1.56947500	-1.78045500	0.00000000
21	H	3.62209500	-0.32799900	0.00000000
22	H	-0.41893100	2.89216800	0.00000000
23				
24	12B:			
25	8			
26	E(RB+HF-LYP) =	-101.765371951		
27	B	0.00000000	0.78077900	0.00000000
28	B	-1.34178400	-0.06174900	0.00000000
29	B	0.10934600	-0.82245100	0.00000000
30	B	1.42430700	0.24961100	0.00000000
31	H	-2.50059400	-0.23961200	0.00000000
32	H	-1.16441100	1.29359500	0.00000000
33	H	2.59630700	0.21647000	0.00000000
34	H	0.10935500	-2.00140400	0.00000000
35				
36	12Ga:			
37	8			
38	E(RB+HF-LYP) =	-7702.01257832		
39	Ga	-0.09329800	-1.52958700	0.00000000
40	Ga	2.04500900	0.08025000	0.00000000
41	Ga	0.00000000	1.34117100	0.00000000
42	Ga	-2.01283200	0.08023100	0.00000000
43	H	3.60297300	0.14561000	0.00000000
44	H	1.67507600	-1.62111200	0.00000000
45	H	-3.43284600	-0.55987200	0.00000000
46	H	0.04953300	2.90136200	0.00000000
47				
48	12Ge:			
49	8			
50	E(RB+HF-LYP) =	-8310.48894881		
51	Ge	2.07640000	-0.09500400	0.00000000
52	Ge	-0.20622600	-1.65679200	0.00000000
53	Ge	-1.79712500	0.23709100	0.00000000
54	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

H 0.64272600 3.14597400 0.00000000

13Al:

8

E(RB+HF-LYP) = -972.180964053

Al	-0.05544600	-1.33049400	0.52459300
Al	1.95339800	-0.03562000	-0.39707800
Al	-0.06426100	1.37165100	0.36900900
Al	-1.97512400	-0.07004800	-0.41739100
H	3.52059200	-0.07224000	-0.58835800
H	1.48611300	-1.69603400	-0.23226500
H	-3.52240000	-0.29508400	-0.65595000
H	0.35431400	2.90199400	0.44785200

13Ga:

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

13In:

8

E(RB+HF-LYP) = -763.234939018

In	0.40537700	1.75174500	0.35875600
In	-2.42335700	0.08928300	-0.37267100
In	-0.21692300	-1.51360800	0.46023600
In	2.27495300	-0.30526400	-0.43713300
H	-3.97456700	0.89562900	-0.19104000
H	-1.33630400	1.75784200	-0.55762000
H	3.90303300	-0.54264600	0.20250600
H	-0.55465100	-3.19647100	0.09597100

14Al:

8

E(RB+HF-LYP) = -972.180478976

Al	2.06288100	0.06854000	0.00000000
Al	0.00000000	1.39171100	0.00000000
Al	-2.08422100	0.27873100	0.00000000
Al	-0.07919200	-1.40039200	0.00000000
H	3.63036700	0.15905000	0.00000000
H	-3.63180600	-0.02666100	0.00000000
H	1.65955100	-1.57326900	0.00000000
H	-0.35119300	-2.96078500	0.00000000

14B:

8
 E(RB+HF-LYP) = -101.754093641
 B -1.35068500 -0.24224400 0.00000000
 B 0.08220700 -0.84653900 0.00000000
 B 1.45119700 -0.25231300 0.00000000
 B 0.00000000 0.80230700 0.00000000
 H -2.51231800 -0.43893400 0.00000000
 H 2.55680500 0.13638300 0.00000000
 H -1.30121900 1.05876900 0.00000000
 H 0.34313500 1.93772700 0.00000000

14Ga:
 8
 E(RB+HF-LYP) = -7702.00884906
 Ga 2.00968700 0.09071300 0.00000000
 Ga 0.00000000 1.37980300 0.00000000
 Ga -1.97671100 0.15382600 0.00000000
 Ga -0.07930200 -1.47553700 0.00000000
 H 3.56186600 0.12136200 0.00000000
 H -3.51271500 -0.10097900 0.00000000
 H 1.67041500 -1.60396000 0.00000000
 H -0.28346200 -3.02937700 0.00000000

14In:
 8
 E(RB+HF-LYP) = -763.215262054
 In -2.27218900 0.09906700 0.00000000
 In 0.00000000 1.63924500 0.00000000
 In 2.20598100 0.08951300 0.00000000
 In 0.09443100 -1.71818500 0.00000000
 H -3.97551200 -0.14640400 0.00000000
 H 3.92313000 0.00000000 0.00000000
 H -1.77757800 -1.82061600 0.00000000
 H 0.44702300 -3.40900000 0.00000000

15Si:
 8
 E(RB+HF-LYP) = -1160.34371743
 Si -0.16573500 -1.20567200 0.00000000
 Si -2.05745000 -2.35148800 0.00000000
 Si 0.00000000 1.06604300 0.00000000
 Si 1.86539100 2.13462200 0.00000000
 H 1.15561700 -1.88532600 0.00000000
 H -1.25920100 1.83896200 0.00000000
 H 3.15948200 1.43080900 0.00000000
 H 1.95322100 3.60648400 0.00000000

16C:
 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				
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	16Ge:			
13	8			
14	E(RB+HF-LYP) =	-8310.57971449		
15	Ge	0.24901200	-2.02457100	0.00000000
16	Ge	-0.84271600	1.68017200	0.00000000
17	Ge	0.24901200	0.12985700	1.38718800
18	Ge	0.24901200	0.12985700	-1.38718800
19	H	1.85057100	-1.87520000	0.00000000
20	H	1.09253900	0.68251500	-2.57249800
21	H	1.09253900	0.68251500	2.57249800
22	H	-0.97386200	3.22012100	0.00000000
23				
24	16Si:			
25	8			
26	E(RB+HF-LYP) =	-1160.38620187		
27	Si	0.24721300	-1.89743700	0.00000000
28	Si	-0.93606000	1.51491300	0.00000000
29	Si	0.24721300	0.11413300	1.25160800
30	Si	0.24721300	0.11413300	-1.25160800
31	H	1.77402200	-1.88553600	0.00000000
32	H	1.05885600	0.53316100	-2.42734000
33	H	1.05885600	0.53316100	2.42734000
34	H	-1.16982900	2.97883300	0.00000000
35				
36	17Pb:			
37	8			
38	E(RB+HF-LYP) =	-774.187889467		
39	Pb	0.43335000	2.56099700	0.00000000
40	Pb	-0.11976300	-2.63511300	0.00000000
41	Pb	-0.11976300	0.04220900	1.68248700
42	Pb	-0.11976300	0.04220900	-1.68248700
43	H	-1.11228900	1.14111000	0.00000000
44	H	-1.49395000	0.37959900	-2.84726500
45	H	-1.49395000	0.37959900	2.84726500
46	H	-1.97293500	-2.74498500	0.00000000
47				
48	17Sn:			
49	8			
50	E(RB+HF-LYP) =	-859.926053347		
51	Sn	0.71115300	2.34314900	0.00000000
52	Sn	-0.19784300	-2.44614900	0.00000000
53	Sn	-0.19784300	0.05593600	1.57022200
54	Sn	-0.19784300	0.05593600	-1.57022200

60

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

H -1.50115500 0.23880000 2.16374000

18Si:

8

E(RB+HF-LYP) = -1160.41887853

Si -0.16937900 1.80509700 0.00000000

Si -0.16937900 -0.14203300 1.25470400

Si 0.69332800 -1.84914700 0.00000000

Si -0.16937900 -0.14203300 -1.25470400

H -1.32352200 2.73995000 0.00000000

H -1.18244000 -0.35885900 -2.32609600

H 1.09573400 2.57137600 0.00000000

H -1.18244000 -0.35885900 2.32609600

18Sn:

8

E(RB+HF-LYP) = -859.949753719

Sn 0.45749600 2.20632000 0.00000000

Sn -0.13977000 -0.01137500 1.68696600

Sn -0.13977000 -2.31674400 0.00000000

Sn -0.13977000 -0.01137500 -1.68696600

H -0.39164400 3.70772600 0.00000000

H -1.82470200 0.17127700 -2.12839000

H 2.13170300 2.60840100 0.00000000

H -1.82470200 0.17127700 2.12839000

19Al:

8

E(RB+HF-LYP) = -972.149572720

Al 0.00000000 1.33114000 1.33114400

Al 0.00000000 -1.33114000 -1.33114400

Al 0.00000000 -1.33114000 1.33114400

Al 0.00000000 1.33114000 -1.33114400

H 0.00000000 2.45812800 2.45819600

H 0.00000000 2.45812800 -2.45819600

H 0.00000000 -2.45812800 2.45819600

H 0.00000000 -2.45812800 -2.45819600

19B:

8

E(RB+HF-LYP) = -101.745763189

B 0.00000000 0.00000000 1.39630200

B 0.00000000 0.00000000 -1.39630200

B 0.00000000 0.79358800 0.00000000

B 0.00000000 -0.79358800 0.00000000

H 0.00000000 0.00000000 2.56776600

H 0.00000000 -1.97278400 0.00000000

H 0.00000000 1.97278400 0.00000000

H 0.00000000 0.00000000 -2.56776600

19C:

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

60

H	1.83411100	1.83411100	1.83411100
H	-1.83411100	1.83411100	-1.83411100
H	-1.83411100	-1.83411100	1.83411100
H	1.83411100	-1.83411100	-1.83411100

1B:

8

E(RB+HF-LYP) = -101.746668796

B	0.59249800	0.59249800	0.59249800
B	-0.59249800	-0.59249800	0.59249800
B	-0.59249800	0.59249800	-0.59249800
B	0.59249800	-0.59249800	-0.59249800
H	1.27420000	1.27420000	1.27420000
H	-1.27420000	1.27420000	-1.27420000
H	-1.27420000	-1.27420000	1.27420000
H	1.27420000	-1.27420000	-1.27420000

1C:

8

E(RB+HF-LYP) = -154.700564766

C	0.52123400	0.52123400	0.52123400
C	-0.52123400	-0.52123400	0.52123400
C	-0.52123400	0.52123400	-0.52123400
C	0.52123400	-0.52123400	-0.52123400
H	1.13794000	1.13794000	1.13794000
H	-1.13794000	1.13794000	-1.13794000
H	-1.13794000	-1.13794000	1.13794000
H	1.13794000	-1.13794000	-1.13794000

1Ga:

8

E(RB+HF-LYP) = -7702.02337014

Ga	0.90807300	0.90807300	0.90807300
Ga	-0.90807300	-0.90807300	0.90807300
Ga	-0.90807300	0.90807300	-0.90807300
Ga	0.90807300	-0.90807300	-0.90807300
H	1.82119600	1.82119600	1.82119600
H	-1.82119600	1.82119600	-1.82119600
H	-1.82119600	-1.82119600	1.82119600
H	1.82119600	-1.82119600	-1.82119600

1Ge:

8

E(RB+HF-LYP) = -8310.50829308

Ge	0.87289300	0.87289300	0.87289300
Ge	-0.87289300	-0.87289300	0.87289300
Ge	-0.87289300	0.87289300	-0.87289300
Ge	0.87289300	-0.87289300	-0.87289300
H	1.75663200	1.75663200	1.75663200
H	-1.75663200	1.75663200	-1.75663200
H	-1.75663200	-1.75663200	1.75663200

H 1.75663200 -1.75663200 -1.75663200

1In:

8

E(RB+HF-LYP) = -763.232284688

In 1.04717200 1.04717200 1.04717200

In -1.04717200 -1.04717200 1.04717200

In -1.04717200 1.04717200 -1.04717200

In 1.04717200 -1.04717200 -1.04717200

H 2.06498800 2.06498800 2.06498800

H -2.06498800 2.06498800 -2.06498800

H -2.06498800 -2.06498800 2.06498800

H 2.06498800 -2.06498800 -2.06498800

1Pb:

8

E(RB+HF-LYP) = -774.060473026

Pb 1.11103100 1.11103100 1.11103100

Pb -1.11103100 -1.11103100 1.11103100

Pb -1.11103100 1.11103100 -1.11103100

Pb 1.11103100 -1.11103100 -1.11103100

H 2.15788100 2.15788100 2.15788100

H -2.15788100 2.15788100 -2.15788100

H -2.15788100 -2.15788100 2.15788100

H 2.15788100 -2.15788100 -2.15788100

1Si:

8

E(RB+HF-LYP) = -1160.34422852

Si 0.81881800 0.81881800 0.81881800

Si -0.81881800 -0.81881800 0.81881800

Si -0.81881800 0.81881800 -0.81881800

Si 0.81881800 -0.81881800 -0.81881800

H 1.66878200 1.66878200 1.66878200

H -1.66878200 1.66878200 -1.66878200

H -1.66878200 -1.66878200 1.66878200

H 1.66878200 -1.66878200 -1.66878200

1Sn:

8

E(RB+HF-LYP) = -859.841665923

Sn 1.01791000 1.01791000 1.01791000

Sn -1.01791000 -1.01791000 1.01791000

Sn -1.01791000 1.01791000 -1.01791000

Sn 1.01791000 -1.01791000 -1.01791000

H 2.00803100 2.00803100 2.00803100

H -2.00803100 2.00803100 -2.00803100

H -2.00803100 -2.00803100 2.00803100

H 2.00803100 -2.00803100 -2.00803100

1Tl:

8
 E(RB+HF-LYP) = -692.675261786
 Ti 1.12921300 1.12921300 1.12921300
 Ti -1.12921300 -1.12921300 1.12921300
 Ti -1.12921300 1.12921300 -1.12921300
 Ti 1.12921300 -1.12921300 -1.12921300
 H 2.19311300 2.19311300 2.19311300
 H -2.19311300 2.19311300 -2.19311300
 H -2.19311300 -2.19311300 2.19311300
 H 2.19311300 -2.19311300 -2.19311300

20Al:

8
 E(RB+HF-LYP) = -972.132956259
 Al 0.00000000 1.81266500 0.00000000
 Al 0.00000000 -1.81266500 0.00000000
 Al -1.81266500 0.00000000 0.00000000
 Al 1.81266500 0.00000000 0.00000000
 H 0.00000000 3.40605100 0.00000000
 H 3.40605100 0.00000000 0.00000000
 H -3.40605100 0.00000000 0.00000000
 H 0.00000000 -3.40605100 0.00000000

20B:

8
 E(RB+HF-LYP) = -101.688051651
 B 0.00000000 0.95497500 0.74695800
 B 0.00000000 -0.95497500 -0.74695800
 B 0.00000000 0.95497500 -0.74695800
 B 0.00000000 -0.95497500 0.74695800
 H 0.00000000 1.16965900 1.89874400
 H 0.00000000 -1.16965900 1.89874400
 H 0.00000000 1.16965900 -1.89874400
 H 0.00000000 -1.16965900 -1.89874400

20C:

8
 E(RB+HF-LYP) = -154.739553668
 C -0.78703000 0.66466000 -0.00001100
 C 0.78703000 -0.66466000 0.00001100
 C -0.78703000 -0.66466000 -0.00002000
 C 0.78703000 0.66466000 0.00001400
 H -1.54901100 1.42864000 -0.00003300
 H 1.54901100 1.42864100 0.00006600
 H -1.54901100 -1.42864100 -0.00000200
 H 1.54901100 -1.42864000 0.00000900

20Ge:

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	20Sn:			
25	8			
26	E(RB+HF-LYP) =	-859.852057062		
27	Sn	0.00000000	1.29151600	1.42586800
28	Sn	0.00000000	-1.29151600	-1.42586800
29	Sn	0.00000000	1.29151600	-1.42586800
30	Sn	0.00000000	-1.29151600	1.42586800
31	H	0.00000000	2.55379000	2.56491600
32	H	0.00000000	-2.55379000	2.56491600
33	H	0.00000000	2.55379000	-2.56491600
34	H	0.00000000	-2.55379000	-2.56491600
35				
36	20Tl:			
37	8			
38	E(RB+HF-LYP) =	-692.625793586		
39	Tl	0.00000000	2.05878900	0.00000000
40	Tl	0.00000000	-2.05878900	0.00000000
41	Tl	-2.05878900	0.00000000	0.00000000
42	Tl	2.05878900	0.00000000	0.00000000
43	H	0.00000000	3.84355800	0.00000000
44	H	3.84355800	0.00000000	0.00000000
45	H	-3.84355800	0.00000000	0.00000000
46	H	0.00000000	-3.84355800	0.00000000
47				
48	21Al:			
49	8			
50	E(RB+HF-LYP) =	-972.182568865		
51	Al	0.00000000	1.82635000	0.00000000
52	Al	0.09838800	-1.92320100	0.00000000
53	Al	1.93525900	0.00000000	0.00000000
54	Al	-1.83326700	-0.05860500	0.00000000

H	-0.16238300	3.40226300	0.00000000
H	-1.13506100	1.10556600	1.12509200
H	-1.13506100	1.10556600	-1.12509200
H	-0.17244500	-3.49536500	0.00000000

21Ga:

8

E(RB+HF-LYP) = -7702.02292378

Ga	-1.87895900	0.03300000	0.00000000
Ga	1.91655400	0.05377900	0.00000000
Ga	0.00000000	1.85755000	0.00000000
Ga	0.03643400	-1.86126400	0.00000000
H	-3.44685800	-0.10702800	0.00000000
H	-1.16648000	-1.10702900	1.14686800
H	-1.16648000	-1.10702900	-1.14686800
H	3.48491900	-0.25395400	0.00000000

21Ge:

8

E(RB+HF-LYP) = -8310.55424394

Ge	-0.21298600	-1.39207600	0.00000000
Ge	0.00000000	1.37034600	0.00000000
Ge	-2.07992700	0.19061500	0.00000000
Ge	2.19801900	-0.10122200	0.00000000
H	0.05831700	-2.93970200	0.00000000
H	1.38230300	-1.07166400	1.09229900
H	1.38230300	-1.07166400	-1.09229900
H	0.21368500	2.91779900	0.00000000

21In:

8

E(RB+HF-LYP) = -763.253678344

In	-2.14173200	0.04637600	0.00000000
In	2.19326500	0.03131100	0.00000000
In	0.00000000	2.11948700	0.00000000
In	0.00000000	-2.13500600	0.00000000
H	-3.87151700	-0.18127900	0.00000000
H	-1.33343800	-1.24774700	1.23697600
H	-1.33343800	-1.24774700	-1.23697600
H	3.92730000	-0.36943500	0.00000000

21Pb:

8

E(RB+HF-LYP) = -774.174448734

Pb	-0.19399600	-1.82956600	0.00000000
Pb	0.00000000	1.70634400	0.00000000
Pb	-2.47745400	0.22650000	0.00000000
Pb	2.62850100	-0.07551700	0.00000000
H	0.49461600	-3.52353600	0.00000000
H	1.44859300	-1.13640600	1.20816400
H	1.44859300	-1.13640600	-1.20816400

H 0.13007300 3.51990900 0.00000000

21Sn:

8

E(RB+HF-LYP) = -859.916281800

Sn -0.19699100 -1.66511100 0.00000000

Sn 0.00000000 1.60448300 0.00000000

Sn -2.37606900 0.21045300 0.00000000

Sn 2.50714000 -0.10304500 0.00000000

H 0.26267800 -3.35712400 0.00000000

H 1.41785900 -1.15876600 1.16035200

H 1.41785900 -1.15876600 -1.16035200

H 0.19762000 3.33568000 0.00000000

21Tl:

8

E(RB+HF-LYP) = -692.723575098

Tl -2.28566800 0.11601200 0.00000000

Tl 2.36458300 -0.04628900 0.00000000

Tl 0.00000000 2.13379900 0.00000000

Tl -0.04529800 -2.16249500 0.00000000

H -4.01540100 -0.29063200 0.00000000

H -1.42240400 -1.25385000 1.26725300

H -1.42240400 -1.25385000 -1.26725300

H 4.13716000 -0.52486000 0.00000000

22Al:

8

E(RB+HF-LYP) = -972.165639588

Al 0.23504800 0.00000000 2.04625900

Al 0.23504800 1.47106500 0.00000000

Al 0.23504800 0.00000000 -2.04625900

Al -0.53451200 -1.33006900 0.00000000

H 0.25540900 0.10098000 3.62508700

H 0.25540900 0.10098000 -3.62508700

H -1.31328700 0.35226000 0.00000000

H -1.41573700 -2.64388900 0.00000000

22Ga:

8

E(RB+HF-LYP) = -7702.00040653

Ga 0.15608800 -0.01808000 1.99240400

Ga 0.15608800 1.50185800 0.00000000

Ga 0.15608800 -0.01808000 -1.99240400

Ga -0.39405100 -1.38466900 0.00000000

H 0.03730300 0.13470400 3.54739500

H 0.03730300 0.13470400 -3.54739500

H -1.44492400 0.06338900 0.00000000

H -0.93033800 -2.84469800 0.00000000

22In:

8
 E(RB+HF-LYP) = -763.223624684
 In 2.24647500 0.00000000 -0.02344800
 In 0.00000000 0.00000000 1.98294500
 In -2.24647500 0.00000000 -0.02344800
 In 0.00000000 0.00000000 -1.84150700
 H 3.98036300 0.00000000 0.21820300
 H -3.98036300 0.00000000 0.21820300
 H 0.00000000 -1.57596200 -2.53626100
 H 0.00000000 1.57596200 -2.53626100

22Tl:

8
 E(RB+HF-LYP) = -692.684202831
 Tl 2.31743600 0.00000000 -0.03098500
 Tl 0.00000000 0.00000000 2.08174500
 Tl -2.31743600 0.00000000 -0.03098500
 Tl 0.00000000 0.00000000 -1.96536900
 H 4.11340100 0.00000000 0.09786800
 H -4.11340100 0.00000000 0.09786800
 H 0.00000000 -1.65149200 -2.30216000
 H 0.00000000 1.65149200 -2.30216000

23Al:

8
 E(RB+HF-LYP) = -972.175190507
 Al -0.37467600 0.05526500 2.04152200
 Al 0.63896800 -1.39030800 0.00000000
 Al -0.37467600 0.05526500 -2.04152200
 Al 0.00000000 1.50667000 0.00000000
 H -0.50909600 -1.53435600 1.29001900
 H -0.50909600 -1.53435600 -1.29001900
 H 1.53213000 -2.69632200 0.00000000
 H 0.93492500 2.78755000 0.00000000

23Ga:

8
 E(RB+HF-LYP) = -7702.01286271
 Ga 0.19375100 -0.14432600 1.97459200
 Ga 0.19375100 1.67750100 0.00000000
 Ga 0.19375100 -0.14432600 -1.97459200
 Ga -0.59663400 -1.50250100 0.00000000
 H 1.25135500 1.19001300 1.30203300
 H 1.25135500 1.19001300 -1.30203300
 H 0.04594900 3.24294100 0.00000000
 H -2.07185100 -2.09974600 0.00000000

23In:

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

In	0.21411600	1.93658100	0.00000000
In	0.21411600	-0.11188500	-2.25593100
In	-0.65728700	-1.79127000	0.00000000
H	1.38478800	1.31312900	1.43933400
H	1.38478800	1.31312900	-1.43933400
H	0.26642700	3.68120300	0.00000000
H	-2.30396500	-2.46293900	0.00000000

23Pb:

8

E(RB+HF-LYP) = -774.196949559

Pb	-0.52326400	-0.14871200	1.92118100
Pb	-0.52326400	2.15109700	0.00000000
Pb	-0.52326400	-0.14871200	-1.92118100
Pb	1.52288800	-1.85689200	0.00000000
H	1.41944700	-0.35226600	1.41072800
H	1.41944700	-0.35226600	-1.41072800
H	-2.32924600	2.56663800	0.00000000
H	3.33641200	-1.59817500	0.00000000

23Si:

8

E(RB+HF-LYP) = -1160.36107393

Si	0.13524900	-0.06068100	2.02812800
Si	0.13524900	1.11971800	0.00000000
Si	0.13524900	-0.06068100	-2.02812800
Si	-0.49010200	-1.13399500	0.00000000
H	1.41766800	0.40043200	1.17078700
H	1.41766800	0.40043200	-1.17078700
H	0.28647300	2.59179000	0.00000000
H	-1.94082600	-1.49372300	0.00000000

23Sn:

8

E(RB+HF-LYP) = -859.919594460

Sn	-0.22865300	-0.09940100	2.48655800
Sn	0.68981800	-1.27979100	0.00000000
Sn	-0.22865300	-0.09940100	-2.48655800
Sn	-0.22865300	1.53269100	0.00000000
H	-1.21122700	-1.21480200	1.36961700
H	-1.21122700	-1.21480200	-1.36961700
H	1.12165700	-2.94970800	0.00000000
H	1.10781700	2.67441000	0.00000000

23Tl:

8

E(RB+HF-LYP) = -692.713838881

Tl	-0.10980900	0.01519500	2.17022500
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

H	-2.52168600	3.42519400	0.00000000
24Si:			
8			
E(RB+HF-LYP) = -1160.40074551			
Si	1.45806400	-1.56581500	0.00000000
Si	-0.38523500	2.56498700	0.00000000
Si	-0.82705900	-1.72308700	0.00000000
Si	0.00000000	0.24802800	0.00000000
H	0.24192600	3.15056300	1.20770600
H	0.24192600	3.15056300	-1.20770600
H	-2.09075300	-2.50698800	0.00000000
H	-1.83387200	2.86827800	0.00000000
24Sn:			
8			
E(RB+HF-LYP) = -859.926365461			
Sn	1.87321300	-1.69746900	0.00000000
Sn	-0.82820000	3.14369900	0.00000000
Sn	-0.93565500	-2.05816400	0.00000000
Sn	0.00000000	0.44441900	0.00000000
H	-0.21535700	3.93893500	1.39135600
H	-0.21535700	3.93893500	-1.39135600
H	-2.50040400	-2.78710700	0.00000000
H	-2.53680100	3.28497700	0.00000000
24Tl:			
8			
E(RB+HF-LYP) = -692.690287828			
Tl	1.50605600	-2.32871800	0.00000000
Tl	0.06557000	3.93983600	0.00000000
Tl	-1.53412000	-2.57651500	0.00000000
Tl	0.00000000	0.83932700	0.00000000
H	0.96960300	4.04713200	1.50489300
H	0.96960300	4.04713200	-1.50489300
H	-3.32877900	-2.17270200	0.00000000
H	-1.64844200	4.29012600	0.00000000
25Al:			
8			
E(RB+HF-LYP) = -972.157148870			
Al	-0.29379600	-1.24961000	0.00000000
Al	2.28275300	-0.10194300	0.00000000
Al	-2.29189600	0.06208100	0.00000000
Al	0.00000000	1.16143600	0.00000000
H	3.02065000	-0.26897200	1.38423700
H	3.02065000	-0.26897200	-1.38423700
H	-3.77458900	0.59757500	0.00000000
H	1.67150300	1.60483300	0.00000000
25B:			

8
 E(RB+HF-LYP) = -101.685883565
 B -0.39988500 -0.79240100 0.00000000
 B 1.45969400 -0.22981700 0.00000000
 B -1.57592900 0.12187100 0.00000000
 B 0.00000000 0.66236300 0.00000000
 H 2.04630100 -0.37426000 1.02354100
 H 2.04630100 -0.37426000 -1.02354100
 H -2.60754300 0.68250900 0.00000000
 H 1.09554800 1.25593500 0.00000000

26Pb:

8
 E(RB+HF-LYP) = -774.204281208
 Pb 0.00000000 1.41175900 0.00000000
 Pb -2.79997800 0.18590000 0.00000000
 Pb 2.69806100 0.13908200 0.00000000
 Pb 0.20184000 -1.71599000 0.00000000
 H -3.65422600 0.83399000 1.42597500
 H -3.65422600 0.83399000 -1.42597500
 H 2.27775700 -1.80165900 0.00000000
 H -3.16301200 -1.56782800 0.00000000

27C:

8
 E(RB+HF-LYP) = -154.802131169
 H -0.86197700 2.83736800 0.00000000
 C -0.45514100 1.85674600 0.00000000
 C 0.00000000 0.74308300 0.00000000
 C 0.57646900 -0.55526700 0.00000000
 C -0.11883400 -1.69404700 0.00000000
 H 1.66124400 -0.59130700 0.00000000
 H -1.20021800 -1.69929600 0.00000000
 H 0.38598400 -2.64985400 0.00000000

28Ge:

8
 E(RB+HF-LYP) = -8310.53179155
 Ge -1.98994500 -2.25055300 0.00000000
 Ge 0.02224200 -1.28433700 0.00000000
 Ge 0.00000000 1.13538600 0.00000000
 Ge 1.92354300 2.28621000 0.00000000
 H -2.53536100 -3.70482400 0.00000000
 H -1.30960300 1.93442200 0.00000000
 H 3.27891100 1.58288300 0.00000000
 H 1.97915300 3.81290200 0.00000000

28Si:

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

Si	-0.06091900	-1.22253500	0.00000000
Si	0.00000000	1.06995400	0.00000000
Si	1.89302300	2.08658100	0.00000000
H	-2.43007700	-3.56924900	0.00000000
H	-1.23815600	1.87543600	0.00000000
H	3.16812500	1.34764000	0.00000000
H	2.02317300	3.55475900	0.00000000

29Al:

8

E(RB+HF-LYP) = -972.169149691

Al	0.00000000	1.25097000	0.00000000
Al	2.52384200	-0.03322600	0.00000000
Al	-0.21274700	-1.32814300	0.00000000
Al	-2.62418800	0.19303300	0.00000000
H	1.64941500	1.66345700	0.00000000
H	0.75650300	-0.13278700	1.02957500
H	0.75650300	-0.13278700	-1.02957500
H	0.90779000	-2.47212900	0.00000000

29Ga:

8

E(RB+HF-LYP) = -7702.01398562

Ga	-0.01272700	1.33369400	-0.01297400
Ga	2.59307700	-0.01308200	0.00000000
Ga	-0.15573500	-1.35785900	0.01320400
Ga	-2.56164700	0.06478600	0.00000000
H	1.63501200	1.77301800	-0.01743400
H	0.77400500	-0.10230700	1.06864800
H	0.77377000	-0.12306100	-1.06665500
H	1.06520400	-2.40138100	0.02320100

29In:

8

E(RB+HF-LYP) = -763.259478149

In	0.00000000	1.55296000	-0.01500400
In	2.85509500	-0.02665700	0.00000000
In	-0.12167600	-1.55095500	0.01499000
In	-2.82700000	0.03638200	0.00000000
H	1.79518300	2.02169800	-0.01931200
H	0.83710000	-0.05706000	1.15551500
H	0.83734800	-0.07936200	-1.15398700
H	1.42655800	-2.46004200	0.02394400

2Al:

8

E(RB+HF-LYP) = -972.149295766

Al	1.10130800	-1.10130800	1.10130800
Al	1.10130800	1.10130800	-1.10130800
Al	-1.10130800	-1.10130800	-1.10130800
Al	-1.10130800	1.10130800	1.10130800

H	0.81712300	0.81712300	0.81712300
H	-0.81712300	-0.81712300	0.81712300
H	0.81712300	-0.81712300	-0.81712300
H	-0.81712300	0.81712300	-0.81712300

2B:

8

E(RB+HF-LYP) = -101.252374030

B	0.81795600	-0.81795600	0.81795600
B	0.81795600	0.81795600	-0.81795600
B	-0.81795600	-0.81795600	-0.81795600
B	-0.81795600	0.81795600	0.81795600
H	0.74051500	0.74051500	0.74051500
H	-0.74051500	-0.74051500	0.74051500
H	0.74051500	-0.74051500	-0.74051500
H	-0.74051500	0.74051500	-0.74051500

2C:

8

E(RB+HF-LYP) = -154.224429611

C	0.61522000	0.61522000	0.61522000
C	-0.61522000	-0.61522000	0.61522000
C	-0.61522000	0.61522000	-0.61522000
C	0.61522000	-0.61522000	-0.61522000
H	0.76341700	-0.76341700	0.76341700
H	0.76341700	0.76341700	-0.76341700
H	-0.76341700	0.76341700	0.76341700
H	-0.76341700	-0.76341700	-0.76341700

2Ga:

8

E(RB+HF-LYP) = -7702.01076676

Ga	1.13227100	-1.13227100	1.13227100
Ga	1.13227100	1.13227100	-1.13227100
Ga	-1.13227100	-1.13227100	-1.13227100
Ga	-1.13227100	1.13227100	1.13227100
H	0.84241300	0.84241300	0.84241300
H	-0.84241300	-0.84241300	0.84241300
H	0.84241300	-0.84241300	-0.84241300
H	-0.84241300	0.84241300	-0.84241300

2Ge:

8

E(RB+HF-LYP) = -8310.52902422

Ge	1.02166300	-1.02166300	1.02166300
Ge	1.02166300	1.02166300	-1.02166300
Ge	-1.02166300	-1.02166300	-1.02166300
Ge	-1.02166300	1.02166300	1.02166300
H	0.82672100	0.82672100	0.82672100
H	-0.82672100	-0.82672100	0.82672100
H	0.82672100	-0.82672100	-0.82672100

H -0.82672100 0.82672100 -0.82672100

2In:

8

E(RB+HF-LYP) = -763.274648770

In 1.25111300 -1.25111300 1.25111300

In 1.25111300 1.25111300 -1.25111300

In -1.25111300 -1.25111300 -1.25111300

In -1.25111300 1.25111300 1.25111300

H 0.91255100 0.91255100 0.91255100

H -0.91255100 -0.91255100 0.91255100

H 0.91255100 -0.91255100 -0.91255100

H -0.91255100 0.91255100 -0.91255100

2Pb:

8

E(RB+HF-LYP) = -774.200788937

Pb 1.20434000 -1.20434000 1.20434000

Pb 1.20434000 1.20434000 -1.20434000

Pb -1.20434000 -1.20434000 -1.20434000

Pb -1.20434000 1.20434000 1.20434000

H 0.92120100 0.92120100 0.92120100

H -0.92120100 -0.92120100 0.92120100

H 0.92120100 -0.92120100 -0.92120100

H -0.92120100 0.92120100 -0.92120100

2Si:

8

E(RB+HF-LYP) = -1160.28532570

Si 0.95536300 -0.95536300 0.95536300

Si 0.95536300 0.95536300 -0.95536300

Si -0.95536300 -0.95536300 -0.95536300

Si -0.95536300 0.95536300 0.95536300

H 0.79485500 0.79485500 0.79485500

H -0.79485500 -0.79485500 0.79485500

H 0.79485500 -0.79485500 -0.79485500

H -0.79485500 0.79485500 -0.79485500

2Sn:

8

E(RB+HF-LYP) = -859.916580679

Sn 1.15305000 1.15305000 -1.15305000

Sn 1.15305000 -1.15305000 1.15305000

Sn -1.15305000 -1.15305000 -1.15305000

Sn -1.15305000 1.15305000 1.15305000

H 0.88610700 0.88610700 0.88610700

H -0.88610700 -0.88610700 0.88610700

H -0.88610700 0.88610700 -0.88610700

H 0.88610700 -0.88610700 -0.88610700

2Tl:

8
 $E(\text{RB+HF-LYP}) = -692.775226789$

Tl	1.28628300	1.28628300	-1.28628300
Tl	1.28628300	-1.28628300	1.28628300
Tl	-1.28628300	-1.28628300	-1.28628300
Tl	-1.28628300	1.28628300	1.28628300
H	0.95036800	0.95036800	0.95036800
H	-0.95036800	-0.95036800	0.95036800
H	-0.95036800	0.95036800	-0.95036800
H	0.95036800	-0.95036800	-0.95036800

30Ge:
8
 $E(\text{RB+HF-LYP}) = -8310.59762962$

Ge	0.45589500	-0.84227300	1.45944900
Ge	0.45589500	-0.84227300	-1.45944900
Ge	0.45589500	1.45389900	0.00000000
Ge	-1.55091600	0.16852600	0.00000000
H	1.50593500	0.48184600	-1.26554200
H	1.27822500	-1.49625100	0.00000000
H	1.50593500	0.48184600	1.26554200
H	1.57333500	2.52044100	0.00000000

31Al:
8
 $E(\text{RB+HF-LYP}) = -972.168199820$

Al	0.00000000	1.30965000	0.08843600
Al	0.00000000	0.00000000	-2.47903900
Al	0.00000000	-1.30965000	0.08843600
Al	0.00000000	0.00000000	2.63072600
H	0.00000000	1.96291600	-1.42283200
H	1.03171100	0.00000000	-0.71280200
H	-1.03171100	0.00000000	-0.71280200
H	0.00000000	-1.96291600	-1.42283200

31In:
8
 $E(\text{RB+HF-LYP}) = -763.259469595$

In	0.00000000	1.55768100	-0.06103400
In	0.00000000	0.00000000	2.84394500
In	0.00000000	-1.55768100	-0.06103400
In	0.00000000	0.00000000	-2.82241700
H	0.00000000	2.20252300	1.64791400
H	-1.15733800	0.00000000	0.81532100
H	1.15733800	0.00000000	0.81532100
H	0.00000000	-2.20252300	1.64791400

32Ge:
8
 $E(\text{RB+HF-LYP}) = -8310.57934692$

Ge	-1.84607000	0.08432600	0.57701600
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Ge	1.84175200	-0.08603400	0.58971200
Ge	-0.19628300	-1.39030300	-0.60651900
Ge	0.20074700	1.39213000	-0.60119100
H	-2.86226700	0.90393900	-0.28698000
H	-0.86115000	1.42680100	0.93585800
H	0.85484000	-1.43222300	0.93315500
H	2.86391900	-0.90230600	-0.27057400
32Pb:			
8			
E(RB+HF-LYP) = -774.217752892			
Pb	-0.99101300	2.19589400	0.68870700
Pb	0.99101300	-2.19589400	0.68870700
Pb	-1.44980800	-0.72938400	-0.69768900
Pb	1.44980800	0.72938400	-0.69768900
H	0.00000000	3.30017300	-0.43556500
H	0.88097900	1.45515600	1.13120500
H	-0.88097900	-1.45515600	1.13120500
H	0.00000000	-3.30017300	-0.43556500
32Si:			
8			
E(RB+HF-LYP) = -1160.35847650			
Si	-1.69275800	-0.02921700	0.51453200
Si	1.68911300	0.02663900	0.52202700
Si	-0.10986700	-1.32468700	-0.57451700
Si	0.11371700	1.32777000	-0.56733200
H	-2.85946600	0.53330500	-0.22169600
H	-0.93216100	1.30075600	0.95171100
H	0.92352800	-1.30737300	0.94438200
H	2.86523300	-0.53374700	-0.20033500
32Sn:			
8			
E(RB+HF-LYP) = -859.943319160			
Sn	1.26062100	1.78788900	0.69211700
Sn	-1.26062100	-1.78788900	0.69211700
Sn	-1.26062100	0.94615300	-0.70517500
Sn	1.26062100	-0.94615300	-0.70517500
H	2.68266100	1.88235400	-0.35079100
H	1.75453800	-0.06765300	1.00371400
H	-1.75453800	0.06765300	1.00371400
H	-2.68266100	-1.88235400	-0.35079100
33Al:			
8			
E(RB+HF-LYP) = -972.171756720			
Al	0.00000000	-1.25235100	-1.29536300
Al	0.00000000	1.25235100	1.29536300
Al	0.00000000	-1.25235100	1.29536300
Al	0.00000000	1.25235100	-1.29536300

H	1.13565600	0.00000000	-1.78949300
H	-1.13565600	0.00000000	-1.78949300
H	-1.13565600	0.00000000	1.78949300
H	1.13565600	0.00000000	1.78949300

33Ga:

8

E(RB+HF-LYP) = -7701.99523390

Ga	-1.27483500	1.26375600	0.00000000
Ga	1.27483500	-1.26375600	0.00000000
Ga	1.27483500	1.26375600	0.00000000
Ga	-1.27483500	-1.26375600	0.00000000
H	-1.78078800	0.00000000	1.16678800
H	-1.78078800	0.00000000	-1.16678800
H	1.78078800	0.00000000	-1.16678800
H	1.78078800	0.00000000	1.16678800

34Al:

8

E(RB+HF-LYP) = -972.127643150

Al	0.00000000	2.07626800	1.03656600
Al	-2.07626800	0.00000000	-1.03656600
Al	0.00000000	-2.07626800	1.03656600
Al	2.07626800	0.00000000	-1.03656600
H	1.19837900	1.19837900	0.00000000
H	-1.19837900	-1.19837900	0.00000000
H	1.19837900	-1.19837900	0.00000000
H	-1.19837900	1.19837900	0.00000000

34B:

8

E(RB+HF-LYP) = -101.270634815

B	0.00000000	1.59775500	0.75389500
B	-1.59775500	0.00000000	-0.75389500
B	0.00000000	-1.59775500	0.75389500
B	1.59775500	0.00000000	-0.75389500
H	1.03397100	1.03397100	0.00000000
H	-1.03397100	-1.03397100	0.00000000
H	1.03397100	-1.03397100	0.00000000
H	-1.03397100	1.03397100	0.00000000

34Ga:

8

E(RB+HF-LYP) = -7701.99412324

Ga	0.00000000	2.16796300	1.00297800
Ga	-2.16796300	0.00000000	-1.00297800
Ga	0.00000000	-2.16796300	1.00297800
Ga	2.16796300	0.00000000	-1.00297800
H	1.24576400	1.24576400	0.00000000
H	-1.24576400	-1.24576400	0.00000000
H	1.24576400	-1.24576400	0.00000000

H -1.24576400 1.24576400 0.00000000

34In:

8

E(RB+HF-LYP) = -763.258709475

In 0.00000000 2.41125500 1.07325700

In -2.41125500 0.00000000 -1.07325700

In 0.00000000 -2.41125500 1.07325700

In 2.41125500 0.00000000 -1.07325700

H 1.36508100 1.36508100 0.00000000

H -1.36508100 -1.36508100 0.00000000

H 1.36508100 -1.36508100 0.00000000

H -1.36508100 1.36508100 0.00000000

34Tl:

8

E(RB+HF-LYP) = -692.758133506

Tl 0.00000000 2.49746600 1.08161900

Tl -2.49746600 0.00000000 -1.08161900

Tl 0.00000000 -2.49746600 1.08161900

Tl 2.49746600 0.00000000 -1.08161900

H 1.43420600 1.43420600 0.00000000

H -1.43420600 -1.43420600 0.00000000

H 1.43420600 -1.43420600 0.00000000

H -1.43420600 1.43420600 0.00000000

35Al:

8

E(RB+HF-LYP) = -972.153227703

Al 0.00000000 0.00000000 -1.61353200

Al 0.00000000 2.03545900 0.07319700

Al 0.00000000 0.00000000 1.77987000

Al 0.00000000 -2.03545900 0.07319700

H -1.42543800 0.00000000 -2.32407400

H 0.00000000 -3.60813100 0.29131800

H 1.42543800 0.00000000 -2.32407400

H 0.00000000 3.60813100 0.29131800

35B:

8

E(RB+HF-LYP) = -101.680291307

B 0.00000000 0.00000000 -0.79705300

B 0.00000000 1.38944700 0.18114000

B 0.00000000 0.00000000 0.98817800

B 0.00000000 -1.38944700 0.18114000

H -1.00252700 0.00000000 -1.48549600

H 0.00000000 -2.56097800 0.10198200

H 1.00252700 0.00000000 -1.48549600

H 0.00000000 2.56097800 0.10198200

35C:

8
 E(RB+HF-LYP) = -154.674331368

C	0.00000000	0.00000000	-1.04046500
C	0.00000000	0.94033700	0.16170800
C	0.00000000	-0.94033700	0.16170800
C	0.00000000	0.00000000	1.21762900
H	-0.88816700	0.00000000	-1.67839200
H	0.00000000	-2.03329900	0.17673300
H	0.88816700	0.00000000	-1.67839200
H	0.00000000	2.03329900	0.17673300

35Ga:
 8
 E(RB+HF-LYP) = -7702.00118532

Ga	0.00000000	0.00000000	-1.59299200
Ga	1.98652500	0.00000000	0.00000000
Ga	0.00000000	0.00000000	1.73421900
Ga	-1.98652500	0.00000000	0.00000000
H	0.00000000	1.41149800	-2.27619700
H	-3.55325500	0.00000000	0.19128500
H	0.00000000	-1.41149800	-2.27619700
H	3.55325500	0.00000000	0.19128500

35Ge:
 8
 E(RB+HF-LYP) = -8310.60053427

Ge	0.00000000	0.00000000	-1.92464500
Ge	0.00000000	1.46194600	0.05754500
Ge	0.00000000	0.00000000	1.99035000
Ge	0.00000000	-1.46194600	0.05754500
H	-1.24490900	0.00000000	-2.84502900
H	0.00000000	-3.02233800	-0.04770300
H	1.24490900	0.00000000	-2.84502900
H	0.00000000	3.02233800	-0.04770300

35In:
 8
 E(RB+HF-LYP) = -763.223769847

In	0.00000000	0.00000000	-1.83985700
In	0.00000000	2.24734400	-0.02461800
In	0.00000000	0.00000000	1.98354800
In	0.00000000	-2.24734400	-0.02461800
H	-1.57520500	0.00000000	-2.53591800
H	0.00000000	-3.98054000	0.22176900
H	1.57520500	0.00000000	-2.53591800
H	0.00000000	3.98054000	0.22176900

35Pb:
 8
 E(RB+HF-LYP) = -774.174526381

Pb	0.00000000	0.00000000	2.35069900
----	------------	------------	------------

Pb	0.00000000	1.82616800	-0.05307200
Pb	0.00000000	0.00000000	-2.33490400
Pb	0.00000000	-1.82616800	-0.05307200
H	1.39972400	0.00000000	3.48807600
H	0.00000000	-3.62705700	0.21628200
H	-1.39972400	0.00000000	3.48807600
H	0.00000000	3.62705700	0.21628200

35Si:

8

E(RB+HF-LYP) = -1160.40887537

Si	0.00000000	0.00000000	-1.79479500
Si	0.00000000	1.33729100	0.10780400
Si	0.00000000	0.00000000	1.95056900
Si	0.00000000	-1.33729100	0.10780400
H	-1.20085800	0.00000000	-2.67119100
H	0.00000000	-2.83567000	0.07152600
H	1.20085800	0.00000000	-2.67119100
H	0.00000000	2.83567000	0.07152600

35Sn:

8

E(RB+HF-LYP) = -859.937757302

Sn	0.00000000	0.00000000	-2.23253600
Sn	0.00000000	1.69631500	0.04821800
Sn	0.00000000	0.00000000	2.27236300
Sn	0.00000000	-1.69631500	0.04821800
H	-1.37341900	0.00000000	-3.28097200
H	0.00000000	-3.43325200	-0.12560900
H	1.37341900	0.00000000	-3.28097200
H	0.00000000	3.43325200	-0.12560900

35Tl:

8

E(RB+HF-LYP) = -692.684202654

Tl	0.00000000	0.00000000	-1.96478500
Tl	0.00000000	2.31814800	-0.03166700
Tl	0.00000000	0.00000000	2.08255600
Tl	0.00000000	-2.31814800	-0.03166700
H	-1.65143100	0.00000000	-2.30041400
H	0.00000000	-4.11417800	0.09566000
H	1.65143100	0.00000000	-2.30041400
H	0.00000000	4.11417800	0.09566000

36Al:

8

E(RB+HF-LYP) = -972.168785473

Al	-0.97625800	-2.61405200	0.00000000
Al	0.97625800	2.61405200	0.00000000
Al	-0.97625800	0.79053800	0.00000000
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

H -0.04810200 2.81834600 1.25127400

37Al:

8

E(RB+HF-LYP) = -972.179716665

Al 0.16523000 1.62121200 0.07311000

Al 1.35255600 -0.64719600 -0.76505500

Al 0.17749200 -0.58171900 1.36527800

Al -1.93935300 -0.56666000 -0.55762600

H 0.38909500 3.16925700 -0.17662900

H -1.43331200 1.26910700 -0.35548800

H 1.77469100 -1.09292800 0.85570500

H 2.44249900 -1.07871300 -1.82778100

37Ga:

8

E(RB+HF-LYP) = -7702.01309274

Ga 0.50661900 1.57876300 0.05777900

Ga 1.33743400 -0.79223100 -0.80562500

Ga 0.08638600 -0.63453800 1.30173700

Ga -2.05737300 -0.21904200 -0.50155900

H 0.91128300 3.04964300 -0.33996300

H -1.17207600 1.52656600 -0.31391600

H 1.71644800 -1.28919700 0.83579000

H 2.47930800 -1.20855700 -1.80423300

38In:

8

E(RB+HF-LYP) = -763.245353074

In 0.66943600 1.67792700 -0.72618700

In 0.04629000 -1.50552800 -1.00740600

In 1.58331700 -0.36594200 1.22775400

In -2.32396000 0.17579200 0.59172500

H 0.42437600 3.18123800 -1.61905400

H -1.02096300 1.74297300 0.34303900

H 1.88360000 -1.56684400 -0.47245100

H -0.06612100 -2.48754300 -2.45994900

39Tl:

8

E(RB+HF-LYP) = -692.751453235

Tl 0.00000000 1.86362100 -1.35617300

Tl 0.15164900 0.34495800 1.93541000

Tl -1.98969000 -1.02168500 -0.17008200

Tl 1.82703500 -1.22739200 -0.43142000

H 1.45386900 0.92468800 0.07496200

H -0.12753300 -0.67116900 -1.33433500

H -1.32375700 1.07385400 0.26530200

H 0.29666200 1.95287900 2.79758000

3Al:

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

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

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

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

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				
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	3Si:			
13	8			
14	E(RB+HF-LYP) =	-1160.38290960		
15	Si	0.00000000	1.19718700	1.05993600
16	Si	-1.19718700	0.00000000	-1.05993600
17	Si	0.00000000	-1.19718700	1.05993600
18	Si	1.19718700	0.00000000	-1.05993600
19	H	1.29438900	1.29438900	0.00000000
20	H	-1.29438900	-1.29438900	0.00000000
21	H	1.29438900	-1.29438900	0.00000000
22	H	-1.29438900	1.29438900	0.00000000
23				
24	3Sn:			
25	8			
26	E(RB+HF-LYP) =	-859.983172356		
27	Sn	0.00000000	1.49130900	1.28190700
28	Sn	-1.49130900	0.00000000	-1.28190700
29	Sn	0.00000000	-1.49130900	1.28190700
30	Sn	1.49130900	0.00000000	-1.28190700
31	H	1.47405400	1.47405400	0.00000000
32	H	-1.47405400	-1.47405400	0.00000000
33	H	1.47405400	-1.47405400	0.00000000
34	H	-1.47405400	1.47405400	0.00000000
35				
36	40Al:			
37	8			
38	E(RB+HF-LYP) =	-972.136858091		
39	Al	0.00000000	0.00000000	1.22102400
40	Al	0.00000000	0.00000000	-1.22102400
41	Al	0.00000000	0.00000000	-3.73625100
42	H	0.00000000	-1.37544500	-4.51871000
43	H	0.00000000	1.37544500	-4.51871000
44	Al	0.00000000	0.00000000	3.73625100
45	H	0.00000000	1.37544500	4.51871000
46	H	0.00000000	-1.37544500	4.51871000
47				
48	40B:			
49	8			
50	E(RB+HF-LYP) =	-101.687637643		
51	B	0.00000000	0.00000000	2.36362500
52	B	0.00000000	0.00000000	-2.36362500
53	B	0.00000000	0.00000000	-0.78043400
54	B	0.00000000	0.00000000	0.78043400

60

H	0.00000000	1.01781800	2.98735500
H	0.00000000	-1.01781800	2.98735500
H	0.00000000	-1.01781800	-2.98735500
H	0.00000000	1.01781800	-2.98735500

40C:

8

E(RB+HF-LYP) = -154.796772661

C	0.00000000	0.00000000	1.94411700
C	0.00000000	0.00000000	-1.94411700
C	0.00000000	0.00000000	-0.63200400
C	0.00000000	0.00000000	0.63200400
H	0.00000000	0.92475900	2.50871300
H	0.00000000	-0.92475900	2.50871300
H	0.00000000	-0.92475900	-2.50871300
H	0.00000000	0.92475900	-2.50871300

40Ga:

8

E(RB+HF-LYP) = -7701.98168355

Ga	0.00000000	0.00000000	1.18472800
Ga	0.00000000	0.00000000	-1.18472800
Ga	0.00000000	0.00000000	-3.59720200
H	0.00000000	-1.37296300	-4.35267000
H	0.00000000	1.37296300	-4.35267000
Ga	0.00000000	0.00000000	3.59720200
H	0.00000000	1.37296300	4.35267000
H	0.00000000	-1.37296300	4.35267000

40Ge:

8

E(RB+HF-LYP) = -8310.49534834

Ge	0.00000000	0.00000000	1.08137900
Ge	0.00000000	0.00000000	-1.08137900
Ge	0.00000000	0.00000000	-3.29931100
H	0.00000000	-1.32009300	-4.05459000
H	0.00000000	1.32009300	-4.05459000
Ge	0.00000000	0.00000000	3.29931100
H	0.00000000	1.32009300	4.05459000
H	0.00000000	-1.32009300	4.05459000

40In:

8

E(RB+HF-LYP) = -763.196597258

In	0.00000000	0.00000000	1.34987500
In	0.00000000	0.00000000	-1.34987500
In	0.00000000	0.00000000	-4.08919000
H	0.00000000	-1.52535300	-4.90372500
H	0.00000000	1.52535300	-4.90372500
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	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				
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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:

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

41Sn:
 8
 E(RB+HF-LYP) = -859.913148097
 Sn 0.00000000 1.38574700 0.00000000
 Sn 3.05694900 0.54927800 0.00000000
 Sn -0.56416600 -1.76092700 0.00000000
 Sn -2.63658800 -0.20010800 0.00000000
 H 3.15586900 2.32975700 0.00000000
 H 1.50454000 0.70073800 1.15678800
 H 1.50454000 0.70073800 -1.15678800
 H 1.02529500 -2.43071500 0.00000000

42Ge:
 8
 E(RB+HF-LYP) = -8310.54091381
 Ge 0.39264600 -0.19430400 1.86881900
 Ge 0.39264600 1.56330000 0.00000000
 Ge 0.39264600 -0.19430400 -1.86881900
 Ge -1.02554600 -1.16686400 0.00000000
 H -0.60941200 0.13321400 3.03230000
 H -0.60941200 0.13321400 -3.03230000
 H -1.06340100 0.59097600 0.00000000
 H -2.59427300 -1.10792300 0.00000000

42Si:
 8
 E(RB+HF-LYP) = -1160.32525806
 Si 0.40446700 -0.18341400 1.72570800
 Si 0.40446700 1.48629800 0.00000000
 Si 0.40446700 -0.18341400 -1.72570800
 Si -0.90646400 -1.09442700 0.00000000
 H -0.43939000 0.13959400 2.91870800
 H -0.43939000 0.13959400 -2.91870800
 H -1.01743000 0.56331900 0.00000000
 H -2.40091000 -1.19310700 0.00000000

43Ge:
 8
 E(RB+HF-LYP) = -8310.58447627
 Ge 2.18119900 -0.12043600 -0.18796800

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Ge	0.12299200	1.32018300	0.21455100
Ge	-2.15730600	0.00000000	-0.23857500
Ge	-0.14015400	-1.26745100	0.20581300
H	1.72429200	-0.06388200	-1.71484400
H	-1.02585400	1.42889000	-0.97793000
H	-0.46484800	2.31544900	1.24706400
H	-0.44899300	-1.80749000	1.64345000
44C:			
8			
E(RB+HF-LYP) = -154.726103194			
C	-1.08697200	-0.08978400	-0.13872300
C	0.15738500	-0.91669300	0.33674100
C	1.08539500	-0.06049900	-0.18194400
C	0.02994800	0.85440000	0.01302400
H	-1.35599500	-0.35505600	-1.15259000
H	2.15541800	-0.01992100	-0.28547900
H	-1.94861200	-0.01252200	0.52011800
H	0.03465600	1.66295300	0.74336500
44Ge:			
8			
E(RB+HF-LYP) = -8310.60533355			
Ge	-1.74503400	0.13213700	0.29408600
Ge	0.21207900	1.60013300	-0.35262700
Ge	1.68998400	-0.10808800	0.36062300
Ge	-0.08912700	-1.55068700	-0.28823700
H	-2.19706700	0.10003400	1.76500000
H	3.17072400	-0.46839400	0.09681300
H	-2.99740100	0.22782800	-0.60312300
H	-0.14917000	-2.21132300	-1.70175700
44Si:			
8			
E(RB+HF-LYP) = -1160.41062445			
Si	-1.62230700	0.08143800	0.28536700
Si	0.15427700	1.52554800	-0.40641600
Si	1.58811900	0.00000000	0.36741400
Si	0.00000000	-1.43933000	-0.24703600
H	-2.04259400	0.09796900	1.70402500
H	3.06075700	-0.19023100	0.35210700
H	-2.82811500	0.12244700	-0.57855700
H	0.00000000	-2.29963500	-1.46817300
44Sn:			
8			
E(RB+HF-LYP) = -859.940458914			
Sn	2.05795100	0.13412400	-0.35419100
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

H 1.43391300 1.41115200 0.00000000

48Sn:

8

E(RB+HF-LYP) = -859.908253021

Sn 0.52737400 -2.13323700 0.00000000

Sn 2.38266100 -0.05711300 0.00000000

Sn 0.00000000 1.39702600 0.00000000

Sn -2.84512600 0.79764200 0.00000000

H 0.79540400 -3.85488400 0.00000000

H 0.30478700 3.12170500 0.00000000

H -1.20479600 -2.04162100 0.00000000

H -3.14088500 2.55888500 0.00000000

4Ge:

8

E(RB+HF-LYP) = -8310.60680180

Ge -1.55522900 -0.20907800 -0.72204700

Ge 0.38853700 1.70845500 0.12913800

Ge 1.31100200 -0.84547300 -0.72845300

Ge -0.15961900 -0.72776500 1.38274500

H -1.02824400 1.40514900 -0.98468700

H 0.17550300 0.87810700 1.75503000

H -0.17904000 -0.74895400 -1.71902100

H 1.52165900 0.82927100 -1.01559900

4Pb:

8

E(RB+HF-LYP) = -774.252771367

Pb 0.95080200 -1.59496400 -0.89985900

Pb -2.10075700 -0.37954400 0.15950000

Pb 0.31332100 1.81108700 -0.91976500

Pb 0.87128100 0.17074700 1.68780400

H -1.03803200 -1.68885300 -1.06628900

H -1.05284500 -0.24533300 1.93329400

H 0.81844200 0.13194600 -2.02185700

H -1.56860300 1.20156800 -1.11494500

4Sn:

8

E(RB+HF-LYP) = -859.975313181

Sn -0.59296100 1.66756700 -0.85993000

Sn 2.06410200 -0.03640800 0.15234400

Sn -0.65549500 -1.64723400 -0.85740500

Sn -0.87215700 0.01743600 1.60740500

H 1.30139300 1.38915100 -1.00386400

H 1.02764100 -0.03064300 1.81556200

H -0.75371700 0.01125000 -1.93780500

H 1.25023100 -1.43779400 -0.99464500

5Al:

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

B	0.52149900	-0.58725400	0.88305900
B	0.52149900	0.64196300	0.00000000
B	0.52149900	-0.58725400	-0.88305900
H	-2.04074600	-0.02867100	0.00000000
H	0.58508200	-1.38488800	-1.74468100
H	-1.36227500	1.88907100	0.00000000
H	0.58508200	-1.38488800	1.74468100

6Ga:

8

E(RB+HF-LYP) = -7702.01742096

Ga	-1.82250600	0.15585200	0.00000000
Ga	0.64975700	-0.70920800	1.33174200
Ga	0.64975700	1.36617700	0.00000000
Ga	0.64975700	-0.70920800	-1.33174200
H	-2.69062900	-1.17207700	0.00000000
H	0.72364200	-1.76013600	-2.52231900
H	-2.68634600	1.48034000	0.00000000
H	0.72364200	-1.76013600	2.52231900

6In:

8

E(RB+HF-LYP) = -763.238145315

In	-2.07188200	0.09558100	0.00000000
In	0.72314400	-0.81583700	1.54434200
In	0.72314400	1.61828200	0.00000000
In	0.72314400	-0.81583700	-1.54434200
H	-3.02880600	-1.37929200	0.00000000
H	0.66419400	-2.08923700	-2.77536300
H	-3.07944900	1.53049900	0.00000000
H	0.66419400	-2.08923700	2.77536300

6Tl:

8

E(RB+HF-LYP) = -692.702383246

Tl	-2.14684100	0.07375300	0.00000000
Tl	0.73902500	-0.86455200	1.70597600
Tl	0.73902500	1.71050000	0.00000000
Tl	0.73902500	-0.86455200	-1.70597600
H	-3.21546800	-1.36562400	0.00000000
H	0.35247100	-2.32471900	-2.74845800
H	-3.17844900	1.54803300	0.00000000
H	0.35247100	-2.32471900	2.74845800

7Ga:

8

E(RB+HF-LYP) = -7702.01795942

Ga	-1.73603100	-0.52789000	-0.33748900
Ga	1.35441700	-0.78094600	-0.73046900
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

H	0.00000000	0.00000000	3.29323400
8Ge:			
8			
E(RB+HF-LYP) = -8310.61039069			
Ge	0.00000000	1.74065700	-0.42557900
Ge	-1.50745300	-0.87032900	-0.42557900
Ge	1.50745300	-0.87032900	-0.42557900
Ge	0.00000000	0.00000000	1.30452400
H	-1.21349900	0.70061400	-1.23739100
H	0.00000000	-1.40122800	-1.23739100
H	1.21349900	0.70061400	-1.23739100
H	0.00000000	0.00000000	2.82304800
8In:			
8			
E(RB+HF-LYP) = -763.242034450			
In	0.00000000	2.20544200	-0.69788700
In	-1.90996900	-1.10272100	-0.69788700
In	1.90996900	-1.10272100	-0.69788700
In	0.00000000	0.00000000	2.08042400
H	-1.39872700	0.80755500	-1.08002000
H	0.00000000	-1.61511100	-1.08002000
H	1.39872700	0.80755500	-1.08002000
H	0.00000000	0.00000000	3.88871000
8Pb:			
8			
E(RB+HF-LYP) = -774.227457792			
Pb	0.00000000	2.08134400	-0.52997700
Pb	-1.80249700	-1.04067200	-0.52997700
Pb	1.80249700	-1.04067200	-0.52997700
Pb	0.00000000	0.00000000	1.59993200
H	-1.36625800	0.78880900	-1.39262000
H	0.00000000	-1.57761800	-1.39262000
H	1.36625800	0.78880900	-1.39262000
H	0.00000000	0.00000000	3.35788100
8Si:			
8			
E(RB+HF-LYP) = -1160.39360685			
Si	0.00000000	1.61249200	-0.39625900
Si	-1.39645900	-0.80624600	-0.39625900
Si	1.39645900	-0.80624600	-0.39625900
Si	0.00000000	0.00000000	1.25013000
H	-1.17665700	0.67934300	-1.19184100
H	0.00000000	-1.35868700	-1.19184100
H	1.17665700	0.67934300	-1.19184100
H	0.00000000	0.00000000	2.71660200
8Sn:			

8
 E(RB+HF-LYP) = -859.967357364
 Sn 0.00000000 1.98739200 -0.50280900
 Sn 1.72113200 -0.99369600 -0.50280900
 Sn -1.72113200 -0.99369600 -0.50280900
 Sn 0.00000000 0.00000000 1.52433800
 H 1.31383700 0.75854400 -1.33820900
 H 0.00000000 0.00000000 3.21902800
 H -1.31383700 0.75854400 -1.33820900
 H 0.00000000 -1.51708800 -1.33820900

9Ge:

8
 E(RB+HF-LYP) = -8310.58187564
 Ge -0.15434100 0.00000000 1.43339000
 Ge 0.51454500 -1.96654200 0.00000000
 Ge -0.15434100 0.00000000 -1.43339000
 Ge -0.15434100 1.90192400 0.00000000
 H -1.30284800 0.05038000 2.48823300
 H -1.30284800 0.05038000 -2.48823300
 H 2.06441000 -1.64825800 0.00000000
 H -1.10740800 3.13603400 0.00000000

9Si:

8
 E(RB+HF-LYP) = -1160.38446343
 Si -0.14187300 -0.01610500 1.30414500
 Si 0.51807600 -1.85681100 0.00000000
 Si -0.14187300 -0.01610500 -1.30414500
 Si -0.14187300 1.81036200 0.00000000
 H -1.09092400 -0.07050500 2.45571600
 H -1.09092400 -0.07050500 -2.45571600
 H 2.01495300 -1.69664200 0.00000000
 H -1.12752000 2.93887800 0.00000000

9Sn:

8
 E(RB+HF-LYP) = -859.925047028
 Sn -0.11106800 0.04315300 1.75946900
 Sn -0.11106800 -2.29367100 0.00000000
 Sn -0.11106800 0.04315300 -1.75946900
 Sn 0.36978600 2.15195100 0.00000000
 H -1.62812900 0.65243900 2.40062500
 H -1.62812900 0.65243900 -2.40062500
 H 1.65940700 -2.32424600 0.00000000
 H -0.23228700 3.79002500 0.00000000

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

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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

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

2. COMPUTATIONAL METHODS

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

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

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 tetrahdrane 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 tetrahdrane 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

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 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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hydrogen atoms which are bridging two or three atoms E. Examples are structure **2E** which has also T_d symmetry but the hydrogen atoms are face-bridging between three atoms E. Other nonclassical tetrahedrane-type structures are **3E**, **4E**, **5E**, **7E**, **14E** where the E_4 core does not have T_d symmetry.

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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.

Figure 1

Figure 1 (continued)

Figure 2

Figure 2 (continued)

Table 1. Calculated E_4R_4 bond lengths [$\text{\AA}$] 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
$Al_4[Si(t\text{-Bu})_3]_4$	2.627	2.534	2.600 – 2.612 ^b	2.467 – 2.501 ^b
$Ga_4[C(SiMe_3)_3]_4$	2.751	2.116	2.678 – 2.702 ^c	2.06 – 2.11 ^c
$In_4[C(SiMe_3)_3]_4$	3.098	2.317	2.989 – 3.013 ^c	2.24 – 2.26 ^d
$Tl_4[C(SiMe_3)_3]_4$	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
$Si_4[Si(t\text{-Bu})_3]_4$	2.362	2.400	2.315 – 2.320 ^h	2.355 – 2.365 ^h
$Ge_4[Si(t\text{-Bu})_3]_4$	2.508	2.440	2.431 – 2.447 ⁱ	2.378 – 2.385 ⁱ
$Sn_4[Si(t\text{-Bu})_3]_4$	2.891	2.642	-	-
$Pb_4[Si(t\text{-Bu})_3]_4$	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)

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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)
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n/c: not calculated

rearr.: rearranges into another structure type

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_I	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_I	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_I	n/c	n/c	n/c	1.6	n/c
39 C_I	n/c	n/c	n/c	n/c	-43.5
45 C_I	n/c	n/c	11.7	7.0	n/c

n/c: not calculated

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Table 5. Calculated E₄H₄ 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

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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 E_4H_4 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

H 0.00000000 -2.79941800 2.03099600

10Pb:

8

E(RB+HF-LYP) = -774.193121064

Pb 0.00000000 1.99765500 0.51578600

Pb 0.00000000 -1.99765500 0.51578600

Pb 1.99765500 0.00000000 -0.51578600

Pb -1.99765500 0.00000000 -0.51578600

H 0.00000000 1.73090200 2.32859800

H -1.73090200 0.00000000 -2.32859800

H 1.73090200 0.00000000 -2.32859800

H 0.00000000 -1.73090200 2.32859800

10Si:

8

E(RB+HF-LYP) = -1160.39076157

Si 0.00000000 1.51939300 0.41838700

Si 0.00000000 -1.51939300 0.41838700

Si 1.51939300 0.00000000 -0.41838700

Si -1.51939300 0.00000000 -0.41838700

H 0.00000000 1.45563300 1.91157500

H -1.45563300 0.00000000 -1.91157500

H 1.45563300 0.00000000 -1.91157500

H 0.00000000 -1.45563300 1.91157500

10Sn:

8

E(RB+HF-LYP) = -859.940543098

Sn 0.00000000 1.89001700 0.49089200

Sn 0.00000000 -1.89001700 0.49089200

Sn 1.89001700 0.00000000 -0.49089200

Sn -1.89001700 0.00000000 -0.49089200

H 0.00000000 1.66233500 2.22979300

H -1.66233500 0.00000000 -2.22979300

H 1.66233500 0.00000000 -2.22979300

H 0.00000000 -1.66233500 2.22979300

10Tl:

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E(RB+HF-LYP) = -692.683692501

Tl 0.00000000 2.15545200 0.60503900

Tl 0.00000000 -2.15545200 0.60503900

Tl 2.15408800 0.00000000 -0.60507200

Tl -2.15408800 0.00000000 -0.60507200

H 0.00000000 2.61112600 2.39771000

H -2.62219100 0.00000000 -2.39509900

H 2.62219100 0.00000000 -2.39509900

H 0.00000000 -2.61112600 2.39771000

11Al:

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 E(RB+HF-LYP) = -972.150787518
 Al 0.00000000 1.82716700 0.26769900
 Al 0.00000000 -1.82716700 0.26769900
 Al 1.82716700 0.00000000 -0.26769900
 Al -1.82716700 0.00000000 -0.26769900
 H 0.00000000 3.20822200 1.05797400
 H -3.20822200 0.00000000 -1.05797400
 H 3.20822200 0.00000000 -1.05797400
 H 0.00000000 -3.20822200 1.05797400

11Ga:
 8
 E(RB+HF-LYP) = -7701.98523261
 Ga 0.00000000 1.76297300 0.29387000
 Ga 0.00000000 -1.76297300 0.29387000
 Ga 1.76297300 0.00000000 -0.29387000
 Ga -1.76297300 0.00000000 -0.29387000
 H 0.00000000 3.07970500 1.16584800
 H -3.07970500 0.00000000 -1.16584800
 H 3.07970500 0.00000000 -1.16584800
 H 0.00000000 -3.07970500 1.16584800

11Ge:
 8
 E(RB+HF-LYP) = -8310.46625246
 Ge 0.00000000 1.84854900 0.18829800
 Ge 0.00000000 -1.84854900 0.18829800
 Ge 1.84854900 0.00000000 -0.18829800
 Ge -1.84854900 0.00000000 -0.18829800
 H 0.00000000 3.44721700 0.61536900
 H -3.44721700 0.00000000 -0.61536900
 H 3.44721700 0.00000000 -0.61536900
 H 0.00000000 -3.44721700 0.61536900

11In:
 8
 E(RB+HF-LYP) = -763.214864629
 In -1.38074200 1.38074200 0.64863200
 In -1.38074200 -1.38074200 -0.64863200
 In 1.38074200 -1.38074200 0.64863200
 In 1.38074200 1.38074200 -0.64863200
 H -1.31435700 2.89431400 1.58250500
 H 1.31435700 -2.89431400 1.58250500
 H -2.89431400 -1.31435700 -1.58250500
 H 2.89431400 1.31435700 -1.58250500

11Tl:
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 E(RB+HF-LYP) = -692.696834121
 Tl -1.52323700 -1.52323700 0.61006900

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3	TI	-1.52323700	1.52323700	-0.61006900
4	TI	1.52323700	-1.52323700	-0.61006900
5	TI	1.52323700	1.52323700	0.61006900
6				
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:

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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				
21	H	-3.63939300	-0.10026500	0.00000000
22	H	-1.56947500	-1.78045500	0.00000000
23	H	3.62209500	-0.32799900	0.00000000
24	H	-0.41893100	2.89216800	0.00000000
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				
35	H	-2.50059400	-0.23961200	0.00000000
36	H	-1.16441100	1.29359500	0.00000000
37	H	2.59630700	0.21647000	0.00000000
38	H	0.10935500	-2.00140400	0.00000000
39				

12Ga:

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E(RB+HF-LYP) = -7702.01257832

45	Ga	-0.09329800	-1.52958700	0.00000000
46	Ga	2.04500900	0.08025000	0.00000000
47	Ga	0.00000000	1.34117100	0.00000000
48	Ga	-2.01283200	0.08023100	0.00000000
49				
50	H	3.60297300	0.14561000	0.00000000
51	H	1.67507600	-1.62111200	0.00000000
52	H	-3.43284600	-0.55987200	0.00000000
53	H	0.04953300	2.90136200	0.00000000
54				

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

H 0.64272600 3.14597400 0.00000000

13Al:

8

E(RB+HF-LYP) = -972.180964053

Al	-0.05544600	-1.33049400	0.52459300
Al	1.95339800	-0.03562000	-0.39707800
Al	-0.06426100	1.37165100	0.36900900
Al	-1.97512400	-0.07004800	-0.41739100
H	3.52059200	-0.07224000	-0.58835800
H	1.48611300	-1.69603400	-0.23226500
H	-3.52240000	-0.29508400	-0.65595000
H	0.35431400	2.90199400	0.44785200

13Ga:

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

13In:

8

E(RB+HF-LYP) = -763.234939018

In	0.40537700	1.75174500	0.35875600
In	-2.42335700	0.08928300	-0.37267100
In	-0.21692300	-1.51360800	0.46023600
In	2.27495300	-0.30526400	-0.43713300
H	-3.97456700	0.89562900	-0.19104000
H	-1.33630400	1.75784200	-0.55762000
H	3.90303300	-0.54264600	0.20250600
H	-0.55465100	-3.19647100	0.09597100

14Al:

8

E(RB+HF-LYP) = -972.180478976

Al	2.06288100	0.06854000	0.00000000
Al	0.00000000	1.39171100	0.00000000
Al	-2.08422100	0.27873100	0.00000000
Al	-0.07919200	-1.40039200	0.00000000
H	3.63036700	0.15905000	0.00000000
H	-3.63180600	-0.02666100	0.00000000
H	1.65955100	-1.57326900	0.00000000
H	-0.35119300	-2.96078500	0.00000000

14B:

8
 E(RB+HF-LYP) = -101.754093641
 B -1.35068500 -0.24224400 0.00000000
 B 0.08220700 -0.84653900 0.00000000
 B 1.45119700 -0.25231300 0.00000000
 B 0.00000000 0.80230700 0.00000000
 H -2.51231800 -0.43893400 0.00000000
 H 2.55680500 0.13638300 0.00000000
 H -1.30121900 1.05876900 0.00000000
 H 0.34313500 1.93772700 0.00000000

14Ga:
 8
 E(RB+HF-LYP) = -7702.00884906
 Ga 2.00968700 0.09071300 0.00000000
 Ga 0.00000000 1.37980300 0.00000000
 Ga -1.97671100 0.15382600 0.00000000
 Ga -0.07930200 -1.47553700 0.00000000
 H 3.56186600 0.12136200 0.00000000
 H -3.51271500 -0.10097900 0.00000000
 H 1.67041500 -1.60396000 0.00000000
 H -0.28346200 -3.02937700 0.00000000

14In:
 8
 E(RB+HF-LYP) = -763.215262054
 In -2.27218900 0.09906700 0.00000000
 In 0.00000000 1.63924500 0.00000000
 In 2.20598100 0.08951300 0.00000000
 In 0.09443100 -1.71818500 0.00000000
 H -3.97551200 -0.14640400 0.00000000
 H 3.92313000 0.00000000 0.00000000
 H -1.77757800 -1.82061600 0.00000000
 H 0.44702300 -3.40900000 0.00000000

15Si:
 8
 E(RB+HF-LYP) = -1160.34371743
 Si -0.16573500 -1.20567200 0.00000000
 Si -2.05745000 -2.35148800 0.00000000
 Si 0.00000000 1.06604300 0.00000000
 Si 1.86539100 2.13462200 0.00000000
 H 1.15561700 -1.88532600 0.00000000
 H -1.25920100 1.83896200 0.00000000
 H 3.15948200 1.43080900 0.00000000
 H 1.95322100 3.60648400 0.00000000

16C:
 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				
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	16Ge:			
13	8			
14	E(RB+HF-LYP) = -8310.57971449			
15	Ge	0.24901200	-2.02457100	0.00000000
16	Ge	-0.84271600	1.68017200	0.00000000
17	Ge	0.24901200	0.12985700	1.38718800
18	Ge	0.24901200	0.12985700	-1.38718800
19	H	1.85057100	-1.87520000	0.00000000
20	H	1.09253900	0.68251500	-2.57249800
21	H	1.09253900	0.68251500	2.57249800
22	H	-0.97386200	3.22012100	0.00000000
23				
24	16Si:			
25	8			
26	E(RB+HF-LYP) = -1160.38620187			
27	Si	0.24721300	-1.89743700	0.00000000
28	Si	-0.93606000	1.51491300	0.00000000
29	Si	0.24721300	0.11413300	1.25160800
30	Si	0.24721300	0.11413300	-1.25160800
31	H	1.77402200	-1.88553600	0.00000000
32	H	1.05885600	0.53316100	-2.42734000
33	H	1.05885600	0.53316100	2.42734000
34	H	-1.16982900	2.97883300	0.00000000
35				
36	17Pb:			
37	8			
38	E(RB+HF-LYP) = -774.187889467			
39	Pb	0.43335000	2.56099700	0.00000000
40	Pb	-0.11976300	-2.63511300	0.00000000
41	Pb	-0.11976300	0.04220900	1.68248700
42	Pb	-0.11976300	0.04220900	-1.68248700
43	H	-1.11228900	1.14111000	0.00000000
44	H	-1.49395000	0.37959900	-2.84726500
45	H	-1.49395000	0.37959900	2.84726500
46	H	-1.97293500	-2.74498500	0.00000000
47				
48	17Sn:			
49	8			
50	E(RB+HF-LYP) = -859.926053347			
51	Sn	0.71115300	2.34314900	0.00000000
52	Sn	-0.19784300	-2.44614900	0.00000000
53	Sn	-0.19784300	0.05593600	1.57022200
54	Sn	-0.19784300	0.05593600	-1.57022200

60

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

H -1.50115500 0.23880000 2.16374000

18Si:

8

E(RB+HF-LYP) = -1160.41887853

Si -0.16937900 1.80509700 0.00000000

Si -0.16937900 -0.14203300 1.25470400

Si 0.69332800 -1.84914700 0.00000000

Si -0.16937900 -0.14203300 -1.25470400

H -1.32352200 2.73995000 0.00000000

H -1.18244000 -0.35885900 -2.32609600

H 1.09573400 2.57137600 0.00000000

H -1.18244000 -0.35885900 2.32609600

18Sn:

8

E(RB+HF-LYP) = -859.949753719

Sn 0.45749600 2.20632000 0.00000000

Sn -0.13977000 -0.01137500 1.68696600

Sn -0.13977000 -2.31674400 0.00000000

Sn -0.13977000 -0.01137500 -1.68696600

H -0.39164400 3.70772600 0.00000000

H -1.82470200 0.17127700 -2.12839000

H 2.13170300 2.60840100 0.00000000

H -1.82470200 0.17127700 2.12839000

19Al:

8

E(RB+HF-LYP) = -972.149572720

Al 0.00000000 1.33114000 1.33114400

Al 0.00000000 -1.33114000 -1.33114400

Al 0.00000000 -1.33114000 1.33114400

Al 0.00000000 1.33114000 -1.33114400

H 0.00000000 2.45812800 2.45819600

H 0.00000000 2.45812800 -2.45819600

H 0.00000000 -2.45812800 2.45819600

H 0.00000000 -2.45812800 -2.45819600

19B:

8

E(RB+HF-LYP) = -101.745763189

B 0.00000000 0.00000000 1.39630200

B 0.00000000 0.00000000 -1.39630200

B 0.00000000 0.79358800 0.00000000

B 0.00000000 -0.79358800 0.00000000

H 0.00000000 0.00000000 2.56776600

H 0.00000000 -1.97278400 0.00000000

H 0.00000000 1.97278400 0.00000000

H 0.00000000 0.00000000 -2.56776600

19C:

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

60

H	1.83411100	1.83411100	1.83411100
H	-1.83411100	1.83411100	-1.83411100
H	-1.83411100	-1.83411100	1.83411100
H	1.83411100	-1.83411100	-1.83411100

1B:

8

E(RB+HF-LYP) = -101.746668796

B	0.59249800	0.59249800	0.59249800
B	-0.59249800	-0.59249800	0.59249800
B	-0.59249800	0.59249800	-0.59249800
B	0.59249800	-0.59249800	-0.59249800
H	1.27420000	1.27420000	1.27420000
H	-1.27420000	1.27420000	-1.27420000
H	-1.27420000	-1.27420000	1.27420000
H	1.27420000	-1.27420000	-1.27420000

1C:

8

E(RB+HF-LYP) = -154.700564766

C	0.52123400	0.52123400	0.52123400
C	-0.52123400	-0.52123400	0.52123400
C	-0.52123400	0.52123400	-0.52123400
C	0.52123400	-0.52123400	-0.52123400
H	1.13794000	1.13794000	1.13794000
H	-1.13794000	1.13794000	-1.13794000
H	-1.13794000	-1.13794000	1.13794000
H	1.13794000	-1.13794000	-1.13794000

1Ga:

8

E(RB+HF-LYP) = -7702.02337014

Ga	0.90807300	0.90807300	0.90807300
Ga	-0.90807300	-0.90807300	0.90807300
Ga	-0.90807300	0.90807300	-0.90807300
Ga	0.90807300	-0.90807300	-0.90807300
H	1.82119600	1.82119600	1.82119600
H	-1.82119600	1.82119600	-1.82119600
H	-1.82119600	-1.82119600	1.82119600
H	1.82119600	-1.82119600	-1.82119600

1Ge:

8

E(RB+HF-LYP) = -8310.50829308

Ge	0.87289300	0.87289300	0.87289300
Ge	-0.87289300	-0.87289300	0.87289300
Ge	-0.87289300	0.87289300	-0.87289300
Ge	0.87289300	-0.87289300	-0.87289300
H	1.75663200	1.75663200	1.75663200
H	-1.75663200	1.75663200	-1.75663200
H	-1.75663200	-1.75663200	1.75663200

H 1.75663200 -1.75663200 -1.75663200

1In:

8

E(RB+HF-LYP) = -763.232284688

In 1.04717200 1.04717200 1.04717200

In -1.04717200 -1.04717200 1.04717200

In -1.04717200 1.04717200 -1.04717200

In 1.04717200 -1.04717200 -1.04717200

H 2.06498800 2.06498800 2.06498800

H -2.06498800 2.06498800 -2.06498800

H -2.06498800 -2.06498800 2.06498800

H 2.06498800 -2.06498800 -2.06498800

1Pb:

8

E(RB+HF-LYP) = -774.060473026

Pb 1.11103100 1.11103100 1.11103100

Pb -1.11103100 -1.11103100 1.11103100

Pb -1.11103100 1.11103100 -1.11103100

Pb 1.11103100 -1.11103100 -1.11103100

H 2.15788100 2.15788100 2.15788100

H -2.15788100 2.15788100 -2.15788100

H -2.15788100 -2.15788100 2.15788100

H 2.15788100 -2.15788100 -2.15788100

1Si:

8

E(RB+HF-LYP) = -1160.34422852

Si 0.81881800 0.81881800 0.81881800

Si -0.81881800 -0.81881800 0.81881800

Si -0.81881800 0.81881800 -0.81881800

Si 0.81881800 -0.81881800 -0.81881800

H 1.66878200 1.66878200 1.66878200

H -1.66878200 1.66878200 -1.66878200

H -1.66878200 -1.66878200 1.66878200

H 1.66878200 -1.66878200 -1.66878200

1Sn:

8

E(RB+HF-LYP) = -859.841665923

Sn 1.01791000 1.01791000 1.01791000

Sn -1.01791000 -1.01791000 1.01791000

Sn -1.01791000 1.01791000 -1.01791000

Sn 1.01791000 -1.01791000 -1.01791000

H 2.00803100 2.00803100 2.00803100

H -2.00803100 2.00803100 -2.00803100

H -2.00803100 -2.00803100 2.00803100

H 2.00803100 -2.00803100 -2.00803100

1Tl:

8
 E(RB+HF-LYP) = -692.675261786
 Ti 1.12921300 1.12921300 1.12921300
 Ti -1.12921300 -1.12921300 1.12921300
 Ti -1.12921300 1.12921300 -1.12921300
 Ti 1.12921300 -1.12921300 -1.12921300
 H 2.19311300 2.19311300 2.19311300
 H -2.19311300 2.19311300 -2.19311300
 H -2.19311300 -2.19311300 2.19311300
 H 2.19311300 -2.19311300 -2.19311300

20Al:

8
 E(RB+HF-LYP) = -972.132956259
 Al 0.00000000 1.81266500 0.00000000
 Al 0.00000000 -1.81266500 0.00000000
 Al -1.81266500 0.00000000 0.00000000
 Al 1.81266500 0.00000000 0.00000000
 H 0.00000000 3.40605100 0.00000000
 H 3.40605100 0.00000000 0.00000000
 H -3.40605100 0.00000000 0.00000000
 H 0.00000000 -3.40605100 0.00000000

20B:

8
 E(RB+HF-LYP) = -101.688051651
 B 0.00000000 0.95497500 0.74695800
 B 0.00000000 -0.95497500 -0.74695800
 B 0.00000000 0.95497500 -0.74695800
 B 0.00000000 -0.95497500 0.74695800
 H 0.00000000 1.16965900 1.89874400
 H 0.00000000 -1.16965900 1.89874400
 H 0.00000000 1.16965900 -1.89874400
 H 0.00000000 -1.16965900 -1.89874400

20C:

8
 E(RB+HF-LYP) = -154.739553668
 C -0.78703000 0.66466000 -0.00001100
 C 0.78703000 -0.66466000 0.00001100
 C -0.78703000 -0.66466000 -0.00002000
 C 0.78703000 0.66466000 0.00001400
 H -1.54901100 1.42864000 -0.00003300
 H 1.54901100 1.42864100 0.00006600
 H -1.54901100 -1.42864100 -0.00000200
 H 1.54901100 -1.42864000 0.00000900

20Ge:

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

Ge	0.00000000	-1.11602100	-1.24727000
Ge	0.00000000	1.11602100	-1.24727000
Ge	0.00000000	-1.11602100	1.24727000
H	0.00000000	2.24645200	2.27634000
H	0.00000000	-2.24645200	2.27634000
H	0.00000000	2.24645200	-2.27634000
H	0.00000000	-2.24645200	-2.27634000

20Si:

8

E(RB+HF-LYP) = -1160.35099338

Si	0.00000000	1.06567700	1.18922700
Si	0.00000000	-1.06567700	-1.18922700
Si	0.00000000	1.06567700	-1.18922700
Si	0.00000000	-1.06567700	1.18922700
H	0.00000000	2.15736700	2.18156300
H	0.00000000	-2.15736700	2.18156300
H	0.00000000	2.15736700	-2.18156300
H	0.00000000	-2.15736700	-2.18156300

20Sn:

8

E(RB+HF-LYP) = -859.852057062

Sn	0.00000000	1.29151600	1.42586800
Sn	0.00000000	-1.29151600	-1.42586800
Sn	0.00000000	-1.29151600	1.42586800
Sn	0.00000000	1.29151600	-1.42586800
H	0.00000000	2.55379000	2.56491600
H	0.00000000	2.55379000	-2.56491600
H	0.00000000	-2.55379000	2.56491600
H	0.00000000	-2.55379000	-2.56491600

20Tl:

8

E(RB+HF-LYP) = -692.625793586

Tl	0.00000000	2.05878900	0.00000000
Tl	0.00000000	-2.05878900	0.00000000
Tl	-2.05878900	0.00000000	0.00000000
Tl	2.05878900	0.00000000	0.00000000
H	0.00000000	3.84355800	0.00000000
H	3.84355800	0.00000000	0.00000000
H	-3.84355800	0.00000000	0.00000000
H	0.00000000	-3.84355800	0.00000000

21Al:

8

E(RB+HF-LYP) = -972.182568865

Al	0.00000000	1.82635000	0.00000000
Al	0.09838800	-1.92320100	0.00000000
Al	1.93525900	0.00000000	0.00000000
Al	-1.83326700	-0.05860500	0.00000000

H	-0.16238300	3.40226300	0.00000000
H	-1.13506100	1.10556600	1.12509200
H	-1.13506100	1.10556600	-1.12509200
H	-0.17244500	-3.49536500	0.00000000

21Ga:

8

E(RB+HF-LYP) = -7702.02292378

Ga	-1.87895900	0.03300000	0.00000000
Ga	1.91655400	0.05377900	0.00000000
Ga	0.00000000	1.85755000	0.00000000
Ga	0.03643400	-1.86126400	0.00000000
H	-3.44685800	-0.10702800	0.00000000
H	-1.16648000	-1.10702900	1.14686800
H	-1.16648000	-1.10702900	-1.14686800
H	3.48491900	-0.25395400	0.00000000

21Ge:

8

E(RB+HF-LYP) = -8310.55424394

Ge	-0.21298600	-1.39207600	0.00000000
Ge	0.00000000	1.37034600	0.00000000
Ge	-2.07992700	0.19061500	0.00000000
Ge	2.19801900	-0.10122200	0.00000000
H	0.05831700	-2.93970200	0.00000000
H	1.38230300	-1.07166400	1.09229900
H	1.38230300	-1.07166400	-1.09229900
H	0.21368500	2.91779900	0.00000000

21In:

8

E(RB+HF-LYP) = -763.253678344

In	-2.14173200	0.04637600	0.00000000
In	2.19326500	0.03131100	0.00000000
In	0.00000000	2.11948700	0.00000000
In	0.00000000	-2.13500600	0.00000000
H	-3.87151700	-0.18127900	0.00000000
H	-1.33343800	-1.24774700	1.23697600
H	-1.33343800	-1.24774700	-1.23697600
H	3.92730000	-0.36943500	0.00000000

21Pb:

8

E(RB+HF-LYP) = -774.174448734

Pb	-0.19399600	-1.82956600	0.00000000
Pb	0.00000000	1.70634400	0.00000000
Pb	-2.47745400	0.22650000	0.00000000
Pb	2.62850100	-0.07551700	0.00000000
H	0.49461600	-3.52353600	0.00000000
H	1.44859300	-1.13640600	1.20816400
H	1.44859300	-1.13640600	-1.20816400

H 0.13007300 3.51990900 0.00000000

21Sn:

8

E(RB+HF-LYP) = -859.916281800

Sn -0.19699100 -1.66511100 0.00000000

Sn 0.00000000 1.60448300 0.00000000

Sn -2.37606900 0.21045300 0.00000000

Sn 2.50714000 -0.10304500 0.00000000

H 0.26267800 -3.35712400 0.00000000

H 1.41785900 -1.15876600 1.16035200

H 1.41785900 -1.15876600 -1.16035200

H 0.19762000 3.33568000 0.00000000

21Tl:

8

E(RB+HF-LYP) = -692.723575098

Tl -2.28566800 0.11601200 0.00000000

Tl 2.36458300 -0.04628900 0.00000000

Tl 0.00000000 2.13379900 0.00000000

Tl -0.04529800 -2.16249500 0.00000000

H -4.01540100 -0.29063200 0.00000000

H -1.42240400 -1.25385000 1.26725300

H -1.42240400 -1.25385000 -1.26725300

H 4.13716000 -0.52486000 0.00000000

22Al:

8

E(RB+HF-LYP) = -972.165639588

Al 0.23504800 0.00000000 2.04625900

Al 0.23504800 1.47106500 0.00000000

Al 0.23504800 0.00000000 -2.04625900

Al -0.53451200 -1.33006900 0.00000000

H 0.25540900 0.10098000 3.62508700

H 0.25540900 0.10098000 -3.62508700

H -1.31328700 0.35226000 0.00000000

H -1.41573700 -2.64388900 0.00000000

22Ga:

8

E(RB+HF-LYP) = -7702.00040653

Ga 0.15608800 -0.01808000 1.99240400

Ga 0.15608800 1.50185800 0.00000000

Ga 0.15608800 -0.01808000 -1.99240400

Ga -0.39405100 -1.38466900 0.00000000

H 0.03730300 0.13470400 3.54739500

H 0.03730300 0.13470400 -3.54739500

H -1.44492400 0.06338900 0.00000000

H -0.93033800 -2.84469800 0.00000000

22In:

8
 E(RB+HF-LYP) = -763.223624684
 In 2.24647500 0.00000000 -0.02344800
 In 0.00000000 0.00000000 1.98294500
 In -2.24647500 0.00000000 -0.02344800
 In 0.00000000 0.00000000 -1.84150700
 H 3.98036300 0.00000000 0.21820300
 H -3.98036300 0.00000000 0.21820300
 H 0.00000000 -1.57596200 -2.53626100
 H 0.00000000 1.57596200 -2.53626100

22Tl:

8
 E(RB+HF-LYP) = -692.684202831
 Tl 2.31743600 0.00000000 -0.03098500
 Tl 0.00000000 0.00000000 2.08174500
 Tl -2.31743600 0.00000000 -0.03098500
 Tl 0.00000000 0.00000000 -1.96536900
 H 4.11340100 0.00000000 0.09786800
 H -4.11340100 0.00000000 0.09786800
 H 0.00000000 -1.65149200 -2.30216000
 H 0.00000000 1.65149200 -2.30216000

23Al:

8
 E(RB+HF-LYP) = -972.175190507
 Al -0.37467600 0.05526500 2.04152200
 Al 0.63896800 -1.39030800 0.00000000
 Al -0.37467600 0.05526500 -2.04152200
 Al 0.00000000 1.50667000 0.00000000
 H -0.50909600 -1.53435600 1.29001900
 H -0.50909600 -1.53435600 -1.29001900
 H 1.53213000 -2.69632200 0.00000000
 H 0.93492500 2.78755000 0.00000000

23Ga:

8
 E(RB+HF-LYP) = -7702.01286271
 Ga 0.19375100 -0.14432600 1.97459200
 Ga 0.19375100 1.67750100 0.00000000
 Ga 0.19375100 -0.14432600 -1.97459200
 Ga -0.59663400 -1.50250100 0.00000000
 H 1.25135500 1.19001300 1.30203300
 H 1.25135500 1.19001300 -1.30203300
 H 0.04594900 3.24294100 0.00000000
 H -2.07185100 -2.09974600 0.00000000

23In:

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

In	0.21411600	1.93658100	0.00000000
In	0.21411600	-0.11188500	-2.25593100
In	-0.65728700	-1.79127000	0.00000000
H	1.38478800	1.31312900	1.43933400
H	1.38478800	1.31312900	-1.43933400
H	0.26642700	3.68120300	0.00000000
H	-2.30396500	-2.46293900	0.00000000

23Pb:

8

E(RB+HF-LYP) = -774.196949559

Pb	-0.52326400	-0.14871200	1.92118100
Pb	-0.52326400	2.15109700	0.00000000
Pb	-0.52326400	-0.14871200	-1.92118100
Pb	1.52288800	-1.85689200	0.00000000
H	1.41944700	-0.35226600	1.41072800
H	1.41944700	-0.35226600	-1.41072800
H	-2.32924600	2.56663800	0.00000000
H	3.33641200	-1.59817500	0.00000000

23Si:

8

E(RB+HF-LYP) = -1160.36107393

Si	0.13524900	-0.06068100	2.02812800
Si	0.13524900	1.11971800	0.00000000
Si	0.13524900	-0.06068100	-2.02812800
Si	-0.49010200	-1.13399500	0.00000000
H	1.41766800	0.40043200	1.17078700
H	1.41766800	0.40043200	-1.17078700
H	0.28647300	2.59179000	0.00000000
H	-1.94082600	-1.49372300	0.00000000

23Sn:

8

E(RB+HF-LYP) = -859.919594460

Sn	-0.22865300	-0.09940100	2.48655800
Sn	0.68981800	-1.27979100	0.00000000
Sn	-0.22865300	-0.09940100	-2.48655800
Sn	-0.22865300	1.53269100	0.00000000
H	-1.21122700	-1.21480200	1.36961700
H	-1.21122700	-1.21480200	-1.36961700
H	1.12165700	-2.94970800	0.00000000
H	1.10781700	2.67441000	0.00000000

23Tl:

8

E(RB+HF-LYP) = -692.713838881

Tl	-0.10980900	0.01519500	2.17022500
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

H	-2.52168600	3.42519400	0.00000000
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24Si:

8

E(RB+HF-LYP) = -1160.40074551

Si	1.45806400	-1.56581500	0.00000000
Si	-0.38523500	2.56498700	0.00000000
Si	-0.82705900	-1.72308700	0.00000000
Si	0.00000000	0.24802800	0.00000000
H	0.24192600	3.15056300	1.20770600
H	0.24192600	3.15056300	-1.20770600
H	-2.09075300	-2.50698800	0.00000000
H	-1.83387200	2.86827800	0.00000000

24Sn:

8

E(RB+HF-LYP) = -859.926365461

Sn	1.87321300	-1.69746900	0.00000000
Sn	-0.82820000	3.14369900	0.00000000
Sn	-0.93565500	-2.05816400	0.00000000
Sn	0.00000000	0.44441900	0.00000000
H	-0.21535700	3.93893500	1.39135600
H	-0.21535700	3.93893500	-1.39135600
H	-2.50040400	-2.78710700	0.00000000
H	-2.53680100	3.28497700	0.00000000

24Tl:

8

E(RB+HF-LYP) = -692.690287828

Tl	1.50605600	-2.32871800	0.00000000
Tl	0.06557000	3.93983600	0.00000000
Tl	-1.53412000	-2.57651500	0.00000000
Tl	0.00000000	0.83932700	0.00000000
H	0.96960300	4.04713200	1.50489300
H	0.96960300	4.04713200	-1.50489300
H	-3.32877900	-2.17270200	0.00000000
H	-1.64844200	4.29012600	0.00000000

25Al:

8

E(RB+HF-LYP) = -972.157148870

Al	-0.29379600	-1.24961000	0.00000000
Al	2.28275300	-0.10194300	0.00000000
Al	-2.29189600	0.06208100	0.00000000
Al	0.00000000	1.16143600	0.00000000
H	3.02065000	-0.26897200	1.38423700
H	3.02065000	-0.26897200	-1.38423700
H	-3.77458900	0.59757500	0.00000000
H	1.67150300	1.60483300	0.00000000

25B:

8
 E(RB+HF-LYP) = -101.685883565
 B -0.39988500 -0.79240100 0.00000000
 B 1.45969400 -0.22981700 0.00000000
 B -1.57592900 0.12187100 0.00000000
 B 0.00000000 0.66236300 0.00000000
 H 2.04630100 -0.37426000 1.02354100
 H 2.04630100 -0.37426000 -1.02354100
 H -2.60754300 0.68250900 0.00000000
 H 1.09554800 1.25593500 0.00000000

26Pb:

8
 E(RB+HF-LYP) = -774.204281208
 Pb 0.00000000 1.41175900 0.00000000
 Pb -2.79997800 0.18590000 0.00000000
 Pb 2.69806100 0.13908200 0.00000000
 Pb 0.20184000 -1.71599000 0.00000000
 H -3.65422600 0.83399000 1.42597500
 H -3.65422600 0.83399000 -1.42597500
 H 2.27775700 -1.80165900 0.00000000
 H -3.16301200 -1.56782800 0.00000000

27C:

8
 E(RB+HF-LYP) = -154.802131169
 H -0.86197700 2.83736800 0.00000000
 C -0.45514100 1.85674600 0.00000000
 C 0.00000000 0.74308300 0.00000000
 C 0.57646900 -0.55526700 0.00000000
 C -0.11883400 -1.69404700 0.00000000
 H 1.66124400 -0.59130700 0.00000000
 H -1.20021800 -1.69929600 0.00000000
 H 0.38598400 -2.64985400 0.00000000

28Ge:

8
 E(RB+HF-LYP) = -8310.53179155
 Ge -1.98994500 -2.25055300 0.00000000
 Ge 0.02224200 -1.28433700 0.00000000
 Ge 0.00000000 1.13538600 0.00000000
 Ge 1.92354300 2.28621000 0.00000000
 H -2.53536100 -3.70482400 0.00000000
 H -1.30960300 1.93442200 0.00000000
 H 3.27891100 1.58288300 0.00000000
 H 1.97915300 3.81290200 0.00000000

28Si:

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

Si	-0.06091900	-1.22253500	0.00000000
Si	0.00000000	1.06995400	0.00000000
Si	1.89302300	2.08658100	0.00000000
H	-2.43007700	-3.56924900	0.00000000
H	-1.23815600	1.87543600	0.00000000
H	3.16812500	1.34764000	0.00000000
H	2.02317300	3.55475900	0.00000000

29Al:

8

E(RB+HF-LYP) = -972.169149691

Al	0.00000000	1.25097000	0.00000000
Al	2.52384200	-0.03322600	0.00000000
Al	-0.21274700	-1.32814300	0.00000000
Al	-2.62418800	0.19303300	0.00000000
H	1.64941500	1.66345700	0.00000000
H	0.75650300	-0.13278700	1.02957500
H	0.75650300	-0.13278700	-1.02957500
H	0.90779000	-2.47212900	0.00000000

29Ga:

8

E(RB+HF-LYP) = -7702.01398562

Ga	-0.01272700	1.33369400	-0.01297400
Ga	2.59307700	-0.01308200	0.00000000
Ga	-0.15573500	-1.35785900	0.01320400
Ga	-2.56164700	0.06478600	0.00000000
H	1.63501200	1.77301800	-0.01743400
H	0.77400500	-0.10230700	1.06864800
H	0.77377000	-0.12306100	-1.06665500
H	1.06520400	-2.40138100	0.02320100

29In:

8

E(RB+HF-LYP) = -763.259478149

In	0.00000000	1.55296000	-0.01500400
In	2.85509500	-0.02665700	0.00000000
In	-0.12167600	-1.55095500	0.01499000
In	-2.82700000	0.03638200	0.00000000
H	1.79518300	2.02169800	-0.01931200
H	0.83710000	-0.05706000	1.15551500
H	0.83734800	-0.07936200	-1.15398700
H	1.42655800	-2.46004200	0.02394400

2Al:

8

E(RB+HF-LYP) = -972.149295766

Al	1.10130800	-1.10130800	1.10130800
Al	1.10130800	1.10130800	-1.10130800
Al	-1.10130800	-1.10130800	-1.10130800
Al	-1.10130800	1.10130800	1.10130800

H	0.81712300	0.81712300	0.81712300
H	-0.81712300	-0.81712300	0.81712300
H	0.81712300	-0.81712300	-0.81712300
H	-0.81712300	0.81712300	-0.81712300

2B:

8

E(RB+HF-LYP) = -101.252374030

B	0.81795600	-0.81795600	0.81795600
B	0.81795600	0.81795600	-0.81795600
B	-0.81795600	-0.81795600	-0.81795600
B	-0.81795600	0.81795600	0.81795600
H	0.74051500	0.74051500	0.74051500
H	-0.74051500	-0.74051500	0.74051500
H	0.74051500	-0.74051500	-0.74051500
H	-0.74051500	0.74051500	-0.74051500

2C:

8

E(RB+HF-LYP) = -154.224429611

C	0.61522000	0.61522000	0.61522000
C	-0.61522000	-0.61522000	0.61522000
C	-0.61522000	0.61522000	-0.61522000
C	0.61522000	-0.61522000	-0.61522000
H	0.76341700	-0.76341700	0.76341700
H	0.76341700	0.76341700	-0.76341700
H	-0.76341700	0.76341700	0.76341700
H	-0.76341700	-0.76341700	-0.76341700

2Ga:

8

E(RB+HF-LYP) = -7702.01076676

Ga	1.13227100	-1.13227100	1.13227100
Ga	1.13227100	1.13227100	-1.13227100
Ga	-1.13227100	-1.13227100	-1.13227100
Ga	-1.13227100	1.13227100	1.13227100
H	0.84241300	0.84241300	0.84241300
H	-0.84241300	-0.84241300	0.84241300
H	0.84241300	-0.84241300	-0.84241300
H	-0.84241300	0.84241300	-0.84241300

2Ge:

8

E(RB+HF-LYP) = -8310.52902422

Ge	1.02166300	-1.02166300	1.02166300
Ge	1.02166300	1.02166300	-1.02166300
Ge	-1.02166300	-1.02166300	-1.02166300
Ge	-1.02166300	1.02166300	1.02166300
H	0.82672100	0.82672100	0.82672100
H	-0.82672100	-0.82672100	0.82672100
H	0.82672100	-0.82672100	-0.82672100

H -0.82672100 0.82672100 -0.82672100

2In:

8

E(RB+HF-LYP) = -763.274648770

In 1.25111300 -1.25111300 1.25111300

In 1.25111300 1.25111300 -1.25111300

In -1.25111300 -1.25111300 -1.25111300

In -1.25111300 1.25111300 1.25111300

H 0.91255100 0.91255100 0.91255100

H -0.91255100 -0.91255100 0.91255100

H 0.91255100 -0.91255100 -0.91255100

H -0.91255100 0.91255100 -0.91255100

2Pb:

8

E(RB+HF-LYP) = -774.200788937

Pb 1.20434000 -1.20434000 1.20434000

Pb 1.20434000 1.20434000 -1.20434000

Pb -1.20434000 -1.20434000 -1.20434000

Pb -1.20434000 1.20434000 1.20434000

H 0.92120100 0.92120100 0.92120100

H -0.92120100 -0.92120100 0.92120100

H 0.92120100 -0.92120100 -0.92120100

H -0.92120100 0.92120100 -0.92120100

2Si:

8

E(RB+HF-LYP) = -1160.28532570

Si 0.95536300 -0.95536300 0.95536300

Si 0.95536300 0.95536300 -0.95536300

Si -0.95536300 -0.95536300 -0.95536300

Si -0.95536300 0.95536300 0.95536300

H 0.79485500 0.79485500 0.79485500

H -0.79485500 -0.79485500 0.79485500

H 0.79485500 -0.79485500 -0.79485500

H -0.79485500 0.79485500 -0.79485500

2Sn:

8

E(RB+HF-LYP) = -859.916580679

Sn 1.15305000 1.15305000 -1.15305000

Sn 1.15305000 -1.15305000 1.15305000

Sn -1.15305000 -1.15305000 -1.15305000

Sn -1.15305000 1.15305000 1.15305000

H 0.88610700 0.88610700 0.88610700

H -0.88610700 -0.88610700 0.88610700

H -0.88610700 0.88610700 -0.88610700

H 0.88610700 -0.88610700 -0.88610700

2Tl:

8
 E(RB+HF-LYP) = -692.775226789
 Tl 1.28628300 1.28628300 -1.28628300
 Tl 1.28628300 -1.28628300 1.28628300
 Tl -1.28628300 -1.28628300 -1.28628300
 Tl -1.28628300 1.28628300 1.28628300
 H 0.95036800 0.95036800 0.95036800
 H -0.95036800 -0.95036800 0.95036800
 H -0.95036800 0.95036800 -0.95036800
 H 0.95036800 -0.95036800 -0.95036800

30Ge:
 8
 E(RB+HF-LYP) = -8310.59762962
 Ge 0.45589500 -0.84227300 1.45944900
 Ge 0.45589500 -0.84227300 -1.45944900
 Ge 0.45589500 1.45389900 0.00000000
 Ge -1.55091600 0.16852600 0.00000000
 H 1.50593500 0.48184600 -1.26554200
 H 1.27822500 -1.49625100 0.00000000
 H 1.50593500 0.48184600 1.26554200
 H 1.57333500 2.52044100 0.00000000

31Al:
 8
 E(RB+HF-LYP) = -972.168199820
 Al 0.00000000 1.30965000 0.08843600
 Al 0.00000000 0.00000000 -2.47903900
 Al 0.00000000 -1.30965000 0.08843600
 Al 0.00000000 0.00000000 2.63072600
 H 0.00000000 1.96291600 -1.42283200
 H 1.03171100 0.00000000 -0.71280200
 H -1.03171100 0.00000000 -0.71280200
 H 0.00000000 -1.96291600 -1.42283200

31In:
 8
 E(RB+HF-LYP) = -763.259469595
 In 0.00000000 1.55768100 -0.06103400
 In 0.00000000 0.00000000 2.84394500
 In 0.00000000 -1.55768100 -0.06103400
 In 0.00000000 0.00000000 -2.82241700
 H 0.00000000 2.20252300 1.64791400
 H -1.15733800 0.00000000 0.81532100
 H 1.15733800 0.00000000 0.81532100
 H 0.00000000 -2.20252300 1.64791400

32Ge:
 8
 E(RB+HF-LYP) = -8310.57934692
 Ge -1.84607000 0.08432600 0.57701600

Ge	1.84175200	-0.08603400	0.58971200
Ge	-0.19628300	-1.39030300	-0.60651900
Ge	0.20074700	1.39213000	-0.60119100
H	-2.86226700	0.90393900	-0.28698000
H	-0.86115000	1.42680100	0.93585800
H	0.85484000	-1.43222300	0.93315500
H	2.86391900	-0.90230600	-0.27057400

32Pb:

8

E(RB+HF-LYP) = -774.217752892

Pb	-0.99101300	2.19589400	0.68870700
Pb	0.99101300	-2.19589400	0.68870700
Pb	-1.44980800	-0.72938400	-0.69768900
Pb	1.44980800	0.72938400	-0.69768900
H	0.00000000	3.30017300	-0.43556500
H	0.88097900	1.45515600	1.13120500
H	-0.88097900	-1.45515600	1.13120500
H	0.00000000	-3.30017300	-0.43556500

32Si:

8

E(RB+HF-LYP) = -1160.35847650

Si	-1.69275800	-0.02921700	0.51453200
Si	1.68911300	0.02663900	0.52202700
Si	-0.10986700	-1.32468700	-0.57451700
Si	0.11371700	1.32777000	-0.56733200
H	-2.85946600	0.53330500	-0.22169600
H	-0.93216100	1.30075600	0.95171100
H	0.92352800	-1.30737300	0.94438200
H	2.86523300	-0.53374700	-0.20033500

32Sn:

8

E(RB+HF-LYP) = -859.943319160

Sn	1.26062100	1.78788900	0.69211700
Sn	-1.26062100	-1.78788900	0.69211700
Sn	-1.26062100	0.94615300	-0.70517500
Sn	1.26062100	-0.94615300	-0.70517500
H	2.68266100	1.88235400	-0.35079100
H	1.75453800	-0.06765300	1.00371400
H	-1.75453800	0.06765300	1.00371400
H	-2.68266100	-1.88235400	-0.35079100

33Al:

8

E(RB+HF-LYP) = -972.171756720

Al	0.00000000	-1.25235100	-1.29536300
Al	0.00000000	1.25235100	1.29536300
Al	0.00000000	-1.25235100	1.29536300
Al	0.00000000	1.25235100	-1.29536300

H	1.13565600	0.00000000	-1.78949300
H	-1.13565600	0.00000000	-1.78949300
H	-1.13565600	0.00000000	1.78949300
H	1.13565600	0.00000000	1.78949300

33Ga:

8

E(RB+HF-LYP) = -7701.99523390

Ga	-1.27483500	1.26375600	0.00000000
Ga	1.27483500	-1.26375600	0.00000000
Ga	1.27483500	1.26375600	0.00000000
Ga	-1.27483500	-1.26375600	0.00000000
H	-1.78078800	0.00000000	1.16678800
H	-1.78078800	0.00000000	-1.16678800
H	1.78078800	0.00000000	-1.16678800
H	1.78078800	0.00000000	1.16678800

34Al:

8

E(RB+HF-LYP) = -972.127643150

Al	0.00000000	2.07626800	1.03656600
Al	-2.07626800	0.00000000	-1.03656600
Al	0.00000000	-2.07626800	1.03656600
Al	2.07626800	0.00000000	-1.03656600
H	1.19837900	1.19837900	0.00000000
H	-1.19837900	-1.19837900	0.00000000
H	1.19837900	-1.19837900	0.00000000
H	-1.19837900	1.19837900	0.00000000

34B:

8

E(RB+HF-LYP) = -101.270634815

B	0.00000000	1.59775500	0.75389500
B	-1.59775500	0.00000000	-0.75389500
B	0.00000000	-1.59775500	0.75389500
B	1.59775500	0.00000000	-0.75389500
H	1.03397100	1.03397100	0.00000000
H	-1.03397100	-1.03397100	0.00000000
H	1.03397100	-1.03397100	0.00000000
H	-1.03397100	1.03397100	0.00000000

34Ga:

8

E(RB+HF-LYP) = -7701.99412324

Ga	0.00000000	2.16796300	1.00297800
Ga	-2.16796300	0.00000000	-1.00297800
Ga	0.00000000	-2.16796300	1.00297800
Ga	2.16796300	0.00000000	-1.00297800
H	1.24576400	1.24576400	0.00000000
H	-1.24576400	-1.24576400	0.00000000
H	1.24576400	-1.24576400	0.00000000

H -1.24576400 1.24576400 0.00000000

34In:

8

E(RB+HF-LYP) = -763.258709475

In 0.00000000 2.41125500 1.07325700

In -2.41125500 0.00000000 -1.07325700

In 0.00000000 -2.41125500 1.07325700

In 2.41125500 0.00000000 -1.07325700

H 1.36508100 1.36508100 0.00000000

H -1.36508100 -1.36508100 0.00000000

H 1.36508100 -1.36508100 0.00000000

H -1.36508100 1.36508100 0.00000000

34Tl:

8

E(RB+HF-LYP) = -692.758133506

Tl 0.00000000 2.49746600 1.08161900

Tl -2.49746600 0.00000000 -1.08161900

Tl 0.00000000 -2.49746600 1.08161900

Tl 2.49746600 0.00000000 -1.08161900

H 1.43420600 1.43420600 0.00000000

H -1.43420600 -1.43420600 0.00000000

H 1.43420600 -1.43420600 0.00000000

H -1.43420600 1.43420600 0.00000000

35Al:

8

E(RB+HF-LYP) = -972.153227703

Al 0.00000000 0.00000000 -1.61353200

Al 0.00000000 2.03545900 0.07319700

Al 0.00000000 0.00000000 1.77987000

Al 0.00000000 -2.03545900 0.07319700

H -1.42543800 0.00000000 -2.32407400

H 0.00000000 -3.60813100 0.29131800

H 1.42543800 0.00000000 -2.32407400

H 0.00000000 3.60813100 0.29131800

35B:

8

E(RB+HF-LYP) = -101.680291307

B 0.00000000 0.00000000 -0.79705300

B 0.00000000 1.38944700 0.18114000

B 0.00000000 0.00000000 0.98817800

B 0.00000000 -1.38944700 0.18114000

H -1.00252700 0.00000000 -1.48549600

H 0.00000000 -2.56097800 0.10198200

H 1.00252700 0.00000000 -1.48549600

H 0.00000000 2.56097800 0.10198200

35C:

8
 E(RB+HF-LYP) = -154.674331368
 C 0.00000000 0.00000000 -1.04046500
 C 0.00000000 0.94033700 0.16170800
 C 0.00000000 -0.94033700 0.16170800
 C 0.00000000 0.00000000 1.21762900
 H -0.88816700 0.00000000 -1.67839200
 H 0.00000000 -2.03329900 0.17673300
 H 0.88816700 0.00000000 -1.67839200
 H 0.00000000 2.03329900 0.17673300

35Ga:
 8
 E(RB+HF-LYP) = -7702.00118532
 Ga 0.00000000 0.00000000 -1.59299200
 Ga 1.98652500 0.00000000 0.00000000
 Ga 0.00000000 0.00000000 1.73421900
 Ga -1.98652500 0.00000000 0.00000000
 H 0.00000000 1.41149800 -2.27619700
 H -3.55325500 0.00000000 0.19128500
 H 0.00000000 -1.41149800 -2.27619700
 H 3.55325500 0.00000000 0.19128500

35Ge:
 8
 E(RB+HF-LYP) = -8310.60053427
 Ge 0.00000000 0.00000000 -1.92464500
 Ge 0.00000000 1.46194600 0.05754500
 Ge 0.00000000 0.00000000 1.99035000
 Ge 0.00000000 -1.46194600 0.05754500
 H -1.24490900 0.00000000 -2.84502900
 H 0.00000000 -3.02233800 -0.04770300
 H 1.24490900 0.00000000 -2.84502900
 H 0.00000000 3.02233800 -0.04770300

35In:
 8
 E(RB+HF-LYP) = -763.223769847
 In 0.00000000 0.00000000 -1.83985700
 In 0.00000000 2.24734400 -0.02461800
 In 0.00000000 0.00000000 1.98354800
 In 0.00000000 -2.24734400 -0.02461800
 H -1.57520500 0.00000000 -2.53591800
 H 0.00000000 -3.98054000 0.22176900
 H 1.57520500 0.00000000 -2.53591800
 H 0.00000000 3.98054000 0.22176900

35Pb:
 8
 E(RB+HF-LYP) = -774.174526381
 Pb 0.00000000 0.00000000 2.35069900

Pb	0.00000000	1.82616800	-0.05307200
Pb	0.00000000	0.00000000	-2.33490400
Pb	0.00000000	-1.82616800	-0.05307200
H	1.39972400	0.00000000	3.48807600
H	0.00000000	-3.62705700	0.21628200
H	-1.39972400	0.00000000	3.48807600
H	0.00000000	3.62705700	0.21628200

35Si:

8

E(RB+HF-LYP) = -1160.40887537

Si	0.00000000	0.00000000	-1.79479500
Si	0.00000000	1.33729100	0.10780400
Si	0.00000000	0.00000000	1.95056900
Si	0.00000000	-1.33729100	0.10780400
H	-1.20085800	0.00000000	-2.67119100
H	0.00000000	-2.83567000	0.07152600
H	1.20085800	0.00000000	-2.67119100
H	0.00000000	2.83567000	0.07152600

35Sn:

8

E(RB+HF-LYP) = -859.937757302

Sn	0.00000000	0.00000000	-2.23253600
Sn	0.00000000	1.69631500	0.04821800
Sn	0.00000000	0.00000000	2.27236300
Sn	0.00000000	-1.69631500	0.04821800
H	-1.37341900	0.00000000	-3.28097200
H	0.00000000	-3.43325200	-0.12560900
H	1.37341900	0.00000000	-3.28097200
H	0.00000000	3.43325200	-0.12560900

35Tl:

8

E(RB+HF-LYP) = -692.684202654

Tl	0.00000000	0.00000000	-1.96478500
Tl	0.00000000	2.31814800	-0.03166700
Tl	0.00000000	0.00000000	2.08255600
Tl	0.00000000	-2.31814800	-0.03166700
H	-1.65143100	0.00000000	-2.30041400
H	0.00000000	-4.11417800	0.09566000
H	1.65143100	0.00000000	-2.30041400
H	0.00000000	4.11417800	0.09566000

36Al:

8

E(RB+HF-LYP) = -972.168785473

Al	-0.97625800	-2.61405200	0.00000000
Al	0.97625800	2.61405200	0.00000000
Al	-0.97625800	0.79053800	0.00000000
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

H -0.04810200 2.81834600 1.25127400

37Al:

8

E(RB+HF-LYP) = -972.179716665

Al 0.16523000 1.62121200 0.07311000

Al 1.35255600 -0.64719600 -0.76505500

Al 0.17749200 -0.58171900 1.36527800

Al -1.93935300 -0.56666000 -0.55762600

H 0.38909500 3.16925700 -0.17662900

H -1.43331200 1.26910700 -0.35548800

H 1.77469100 -1.09292800 0.85570500

H 2.44249900 -1.07871300 -1.82778100

37Ga:

8

E(RB+HF-LYP) = -7702.01309274

Ga 0.50661900 1.57876300 0.05777900

Ga 1.33743400 -0.79223100 -0.80562500

Ga 0.08638600 -0.63453800 1.30173700

Ga -2.05737300 -0.21904200 -0.50155900

H 0.91128300 3.04964300 -0.33996300

H -1.17207600 1.52656600 -0.31391600

H 1.71644800 -1.28919700 0.83579000

H 2.47930800 -1.20855700 -1.80423300

38In:

8

E(RB+HF-LYP) = -763.245353074

In 0.66943600 1.67792700 -0.72618700

In 0.04629000 -1.50552800 -1.00740600

In 1.58331700 -0.36594200 1.22775400

In -2.32396000 0.17579200 0.59172500

H 0.42437600 3.18123800 -1.61905400

H -1.02096300 1.74297300 0.34303900

H 1.88360000 -1.56684400 -0.47245100

H -0.06612100 -2.48754300 -2.45994900

39Tl:

8

E(RB+HF-LYP) = -692.751453235

Tl 0.00000000 1.86362100 -1.35617300

Tl 0.15164900 0.34495800 1.93541000

Tl -1.98969000 -1.02168500 -0.17008200

Tl 1.82703500 -1.22739200 -0.43142000

H 1.45386900 0.92468800 0.07496200

H -0.12753300 -0.67116900 -1.33433500

H -1.32375700 1.07385400 0.26530200

H 0.29666200 1.95287900 2.79758000

3Al:

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

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

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

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

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				
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	3Si:			
13	8			
14	E(RB+HF-LYP) =	-1160.38290960		
15	Si	0.00000000	1.19718700	1.05993600
16	Si	-1.19718700	0.00000000	-1.05993600
17	Si	0.00000000	-1.19718700	1.05993600
18	Si	1.19718700	0.00000000	-1.05993600
19	H	1.29438900	1.29438900	0.00000000
20	H	-1.29438900	-1.29438900	0.00000000
21	H	1.29438900	-1.29438900	0.00000000
22	H	-1.29438900	1.29438900	0.00000000
23				
24	3Sn:			
25	8			
26	E(RB+HF-LYP) =	-859.983172356		
27	Sn	0.00000000	1.49130900	1.28190700
28	Sn	-1.49130900	0.00000000	-1.28190700
29	Sn	0.00000000	-1.49130900	1.28190700
30	Sn	1.49130900	0.00000000	-1.28190700
31	H	1.47405400	1.47405400	0.00000000
32	H	-1.47405400	-1.47405400	0.00000000
33	H	1.47405400	-1.47405400	0.00000000
34	H	-1.47405400	1.47405400	0.00000000
35				
36	40Al:			
37	8			
38	E(RB+HF-LYP) =	-972.136858091		
39	Al	0.00000000	0.00000000	1.22102400
40	Al	0.00000000	0.00000000	-1.22102400
41	Al	0.00000000	0.00000000	-3.73625100
42	H	0.00000000	-1.37544500	-4.51871000
43	H	0.00000000	1.37544500	-4.51871000
44	Al	0.00000000	0.00000000	3.73625100
45	H	0.00000000	1.37544500	4.51871000
46	H	0.00000000	-1.37544500	4.51871000
47				
48	40B:			
49	8			
50	E(RB+HF-LYP) =	-101.687637643		
51	B	0.00000000	0.00000000	2.36362500
52	B	0.00000000	0.00000000	-2.36362500
53	B	0.00000000	0.00000000	-0.78043400
54	B	0.00000000	0.00000000	0.78043400

60

H	0.00000000	1.01781800	2.98735500
H	0.00000000	-1.01781800	2.98735500
H	0.00000000	-1.01781800	-2.98735500
H	0.00000000	1.01781800	-2.98735500

40C:

8

E(RB+HF-LYP) = -154.796772661

C	0.00000000	0.00000000	1.94411700
C	0.00000000	0.00000000	-1.94411700
C	0.00000000	0.00000000	-0.63200400
C	0.00000000	0.00000000	0.63200400
H	0.00000000	0.92475900	2.50871300
H	0.00000000	-0.92475900	2.50871300
H	0.00000000	-0.92475900	-2.50871300
H	0.00000000	0.92475900	-2.50871300

40Ga:

8

E(RB+HF-LYP) = -7701.98168355

Ga	0.00000000	0.00000000	1.18472800
Ga	0.00000000	0.00000000	-1.18472800
Ga	0.00000000	0.00000000	-3.59720200
H	0.00000000	-1.37296300	-4.35267000
H	0.00000000	1.37296300	-4.35267000
Ga	0.00000000	0.00000000	3.59720200
H	0.00000000	1.37296300	4.35267000
H	0.00000000	-1.37296300	4.35267000

40Ge:

8

E(RB+HF-LYP) = -8310.49534834

Ge	0.00000000	0.00000000	1.08137900
Ge	0.00000000	0.00000000	-1.08137900
Ge	0.00000000	0.00000000	-3.29931100
H	0.00000000	-1.32009300	-4.05459000
H	0.00000000	1.32009300	-4.05459000
Ge	0.00000000	0.00000000	3.29931100
H	0.00000000	1.32009300	4.05459000
H	0.00000000	-1.32009300	4.05459000

40In:

8

E(RB+HF-LYP) = -763.196597258

In	0.00000000	0.00000000	1.34987500
In	0.00000000	0.00000000	-1.34987500
In	0.00000000	0.00000000	-4.08919000
H	0.00000000	-1.52535300	-4.90372500
H	0.00000000	1.52535300	-4.90372500
In	0.00000000	0.00000000	4.08919000
H	0.00000000	1.52535300	4.90372500

H 0.00000000 -1.52535300 4.90372500

40Pb:

8

E(RB+HF-LYP) = -774.009731566

Pb 0.00000000 0.00000000 1.32837100

Pb 0.00000000 0.00000000 -1.32837100

Pb 0.00000000 0.00000000 -4.04628200

H 0.00000000 -1.58988400 -4.72565000

H 0.00000000 1.58988400 -4.72565000

Pb 0.00000000 0.00000000 4.04628200

H 0.00000000 1.58988400 4.72565000

H 0.00000000 -1.58988400 4.72565000

40Si:

8

E(RB+HF-LYP) = -1160.31356146

Si 0.00000000 0.00000000 1.03802200

Si 0.00000000 0.00000000 -1.03802200

Si 0.00000000 0.00000000 -3.16372100

H 0.00000000 -1.25638800 -3.92662100

H 0.00000000 1.25638800 -3.92662100

Si 0.00000000 0.00000000 3.16372100

H 0.00000000 1.25638800 3.92662100

H 0.00000000 -1.25638800 3.92662100

40Sn:

8

E(RB+HF-LYP) = -859.812928932

Sn 0.00000000 0.00000000 1.25642400

Sn 0.00000000 0.00000000 -1.25642400

Sn 0.00000000 0.00000000 -3.82326400

H 0.00000000 -1.47651100 -4.64749000

H 0.00000000 1.47651100 -4.64749000

Sn 0.00000000 0.00000000 3.82326400

H 0.00000000 1.47651100 4.64749000

H 0.00000000 -1.47651100 4.64749000

40Tl:

8

E(RB+HF-LYP) = -692.641548519

Tl 0.00000000 0.00000000 1.40388600

Tl 0.00000000 0.00000000 -1.40388600

Tl 0.00000000 0.00000000 -4.23532300

H 0.00000000 -1.60328200 -4.88535600

H 0.00000000 1.60328200 -4.88535600

Tl 0.00000000 0.00000000 4.23532300

H 0.00000000 1.60328200 4.88535600

H 0.00000000 -1.60328200 4.88535600

41Pb:

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

41Sn:
 8
 E(RB+HF-LYP) = -859.913148097
 Sn 0.00000000 1.38574700 0.00000000
 Sn 3.05694900 0.54927800 0.00000000
 Sn -0.56416600 -1.76092700 0.00000000
 Sn -2.63658800 -0.20010800 0.00000000
 H 3.15586900 2.32975700 0.00000000
 H 1.50454000 0.70073800 1.15678800
 H 1.50454000 0.70073800 -1.15678800
 H 1.02529500 -2.43071500 0.00000000

42Ge:
 8
 E(RB+HF-LYP) = -8310.54091381
 Ge 0.39264600 -0.19430400 1.86881900
 Ge 0.39264600 1.56330000 0.00000000
 Ge 0.39264600 -0.19430400 -1.86881900
 Ge -1.02554600 -1.16686400 0.00000000
 H -0.60941200 0.13321400 3.03230000
 H -0.60941200 0.13321400 -3.03230000
 H -1.06340100 0.59097600 0.00000000
 H -2.59427300 -1.10792300 0.00000000

42Si:
 8
 E(RB+HF-LYP) = -1160.32525806
 Si 0.40446700 -0.18341400 1.72570800
 Si 0.40446700 1.48629800 0.00000000
 Si 0.40446700 -0.18341400 -1.72570800
 Si -0.90646400 -1.09442700 0.00000000
 H -0.43939000 0.13959400 2.91870800
 H -0.43939000 0.13959400 -2.91870800
 H -1.01743000 0.56331900 0.00000000
 H -2.40091000 -1.19310700 0.00000000

43Ge:
 8
 E(RB+HF-LYP) = -8310.58447627
 Ge 2.18119900 -0.12043600 -0.18796800

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Ge	0.12299200	1.32018300	0.21455100
Ge	-2.15730600	0.00000000	-0.23857500
Ge	-0.14015400	-1.26745100	0.20581300
H	1.72429200	-0.06388200	-1.71484400
H	-1.02585400	1.42889000	-0.97793000
H	-0.46484800	2.31544900	1.24706400
H	-0.44899300	-1.80749000	1.64345000
44C:			
8			
E(RB+HF-LYP) = -154.726103194			
C	-1.08697200	-0.08978400	-0.13872300
C	0.15738500	-0.91669300	0.33674100
C	1.08539500	-0.06049900	-0.18194400
C	0.02994800	0.85440000	0.01302400
H	-1.35599500	-0.35505600	-1.15259000
H	2.15541800	-0.01992100	-0.28547900
H	-1.94861200	-0.01252200	0.52011800
H	0.03465600	1.66295300	0.74336500
44Ge:			
8			
E(RB+HF-LYP) = -8310.60533355			
Ge	-1.74503400	0.13213700	0.29408600
Ge	0.21207900	1.60013300	-0.35262700
Ge	1.68998400	-0.10808800	0.36062300
Ge	-0.08912700	-1.55068700	-0.28823700
H	-2.19706700	0.10003400	1.76500000
H	3.17072400	-0.46839400	0.09681300
H	-2.99740100	0.22782800	-0.60312300
H	-0.14917000	-2.21132300	-1.70175700
44Si:			
8			
E(RB+HF-LYP) = -1160.41062445			
Si	-1.62230700	0.08143800	0.28536700
Si	0.15427700	1.52554800	-0.40641600
Si	1.58811900	0.00000000	0.36741400
Si	0.00000000	-1.43933000	-0.24703600
H	-2.04259400	0.09796900	1.70402500
H	3.06075700	-0.19023100	0.35210700
H	-2.82811500	0.12244700	-0.57855700
H	0.00000000	-2.29963500	-1.46817300
44Sn:			
8			
E(RB+HF-LYP) = -859.940458914			
Sn	2.05795100	0.13412400	-0.35419100
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

H	1.43391300	1.41115200	0.00000000
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48Sn:

8

E(RB+HF-LYP) = -859.908253021

Sn	0.52737400	-2.13323700	0.00000000
Sn	2.38266100	-0.05711300	0.00000000
Sn	0.00000000	1.39702600	0.00000000
Sn	-2.84512600	0.79764200	0.00000000
H	0.79540400	-3.85488400	0.00000000
H	0.30478700	3.12170500	0.00000000
H	-1.20479600	-2.04162100	0.00000000
H	-3.14088500	2.55888500	0.00000000

4Ge:

8

E(RB+HF-LYP) = -8310.60680180

Ge	-1.55522900	-0.20907800	-0.72204700
Ge	0.38853700	1.70845500	0.12913800
Ge	1.31100200	-0.84547300	-0.72845300
Ge	-0.15961900	-0.72776500	1.38274500
H	-1.02824400	1.40514900	-0.98468700
H	0.17550300	0.87810700	1.75503000
H	-0.17904000	-0.74895400	-1.71902100
H	1.52165900	0.82927100	-1.01559900

4Pb:

8

E(RB+HF-LYP) = -774.252771367

Pb	0.95080200	-1.59496400	-0.89985900
Pb	-2.10075700	-0.37954400	0.15950000
Pb	0.31332100	1.81108700	-0.91976500
Pb	0.87128100	0.17074700	1.68780400
H	-1.03803200	-1.68885300	-1.06628900
H	-1.05284500	-0.24533300	1.93329400
H	0.81844200	0.13194600	-2.02185700
H	-1.56860300	1.20156800	-1.11494500

4Sn:

8

E(RB+HF-LYP) = -859.975313181

Sn	-0.59296100	1.66756700	-0.85993000
Sn	2.06410200	-0.03640800	0.15234400
Sn	-0.65549500	-1.64723400	-0.85740500
Sn	-0.87215700	0.01743600	1.60740500
H	1.30139300	1.38915100	-1.00386400
H	1.02764100	-0.03064300	1.81556200
H	-0.75371700	0.01125000	-1.93780500
H	1.25023100	-1.43779400	-0.99464500

5Al:

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

B	0.52149900	-0.58725400	0.88305900
B	0.52149900	0.64196300	0.00000000
B	0.52149900	-0.58725400	-0.88305900
H	-2.04074600	-0.02867100	0.00000000
H	0.58508200	-1.38488800	-1.74468100
H	-1.36227500	1.88907100	0.00000000
H	0.58508200	-1.38488800	1.74468100

6Ga:

8

E(RB+HF-LYP) = -7702.01742096

Ga	-1.82250600	0.15585200	0.00000000
Ga	0.64975700	-0.70920800	1.33174200
Ga	0.64975700	1.36617700	0.00000000
Ga	0.64975700	-0.70920800	-1.33174200
H	-2.69062900	-1.17207700	0.00000000
H	0.72364200	-1.76013600	-2.52231900
H	-2.68634600	1.48034000	0.00000000
H	0.72364200	-1.76013600	2.52231900

6In:

8

E(RB+HF-LYP) = -763.238145315

In	-2.07188200	0.09558100	0.00000000
In	0.72314400	-0.81583700	1.54434200
In	0.72314400	1.61828200	0.00000000
In	0.72314400	-0.81583700	-1.54434200
H	-3.02880600	-1.37929200	0.00000000
H	0.66419400	-2.08923700	-2.77536300
H	-3.07944900	1.53049900	0.00000000
H	0.66419400	-2.08923700	2.77536300

6Tl:

8

E(RB+HF-LYP) = -692.702383246

Tl	-2.14684100	0.07375300	0.00000000
Tl	0.73902500	-0.86455200	1.70597600
Tl	0.73902500	1.71050000	0.00000000
Tl	0.73902500	-0.86455200	-1.70597600
H	-3.21546800	-1.36562400	0.00000000
H	0.35247100	-2.32471900	-2.74845800
H	-3.17844900	1.54803300	0.00000000
H	0.35247100	-2.32471900	2.74845800

7Ga:

8

E(RB+HF-LYP) = -7702.01795942

Ga	-1.73603100	-0.52789000	-0.33748900
Ga	1.35441700	-0.78094600	-0.73046900
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

H 0.00000000 0.00000000 3.29323400

8Ge:

8

E(RB+HF-LYP) = -8310.61039069

Ge 0.00000000 1.74065700 -0.42557900

Ge -1.50745300 -0.87032900 -0.42557900

Ge 1.50745300 -0.87032900 -0.42557900

Ge 0.00000000 0.00000000 1.30452400

H -1.21349900 0.70061400 -1.23739100

H 0.00000000 -1.40122800 -1.23739100

H 1.21349900 0.70061400 -1.23739100

H 0.00000000 0.00000000 2.82304800

8In:

8

E(RB+HF-LYP) = -763.242034450

In 0.00000000 2.20544200 -0.69788700

In -1.90996900 -1.10272100 -0.69788700

In 1.90996900 -1.10272100 -0.69788700

In 0.00000000 0.00000000 2.08042400

H -1.39872700 0.80755500 -1.08002000

H 0.00000000 -1.61511100 -1.08002000

H 1.39872700 0.80755500 -1.08002000

H 0.00000000 0.00000000 3.88871000

8Pb:

8

E(RB+HF-LYP) = -774.227457792

Pb 0.00000000 2.08134400 -0.52997700

Pb -1.80249700 -1.04067200 -0.52997700

Pb 1.80249700 -1.04067200 -0.52997700

Pb 0.00000000 0.00000000 1.59993200

H -1.36625800 0.78880900 -1.39262000

H 0.00000000 -1.57761800 -1.39262000

H 1.36625800 0.78880900 -1.39262000

H 0.00000000 0.00000000 3.35788100

8Si:

8

E(RB+HF-LYP) = -1160.39360685

Si 0.00000000 1.61249200 -0.39625900

Si -1.39645900 -0.80624600 -0.39625900

Si 1.39645900 -0.80624600 -0.39625900

Si 0.00000000 0.00000000 1.25013000

H -1.17665700 0.67934300 -1.19184100

H 0.00000000 -1.35868700 -1.19184100

H 1.17665700 0.67934300 -1.19184100

H 0.00000000 0.00000000 2.71660200

8Sn:

8
 E(RB+HF-LYP) = -859.967357364
 Sn 0.00000000 1.98739200 -0.50280900
 Sn 1.72113200 -0.99369600 -0.50280900
 Sn -1.72113200 -0.99369600 -0.50280900
 Sn 0.00000000 0.00000000 1.52433800
 H 1.31383700 0.75854400 -1.33820900
 H 0.00000000 0.00000000 3.21902800
 H -1.31383700 0.75854400 -1.33820900
 H 0.00000000 -1.51708800 -1.33820900

9Ge:
 8
 E(RB+HF-LYP) = -8310.58187564
 Ge -0.15434100 0.00000000 1.43339000
 Ge 0.51454500 -1.96654200 0.00000000
 Ge -0.15434100 0.00000000 -1.43339000
 Ge -0.15434100 1.90192400 0.00000000
 H -1.30284800 0.05038000 2.48823300
 H -1.30284800 0.05038000 -2.48823300
 H 2.06441000 -1.64825800 0.00000000
 H -1.10740800 3.13603400 0.00000000

9Si:
 8
 E(RB+HF-LYP) = -1160.38446343
 Si -0.14187300 -0.01610500 1.30414500
 Si 0.51807600 -1.85681100 0.00000000
 Si -0.14187300 -0.01610500 -1.30414500
 Si -0.14187300 1.81036200 0.00000000
 H -1.09092400 -0.07050500 2.45571600
 H -1.09092400 -0.07050500 -2.45571600
 H 2.01495300 -1.69664200 0.00000000
 H -1.12752000 2.93887800 0.00000000

9Sn:
 8
 E(RB+HF-LYP) = -859.925047028
 Sn -0.11106800 0.04315300 1.75946900
 Sn -0.11106800 -2.29367100 0.00000000
 Sn -0.11106800 0.04315300 -1.75946900
 Sn 0.36978600 2.15195100 0.00000000
 H -1.62812900 0.65243900 2.40062500
 H -1.62812900 0.65243900 -2.40062500
 H 1.65940700 -2.32424600 0.00000000
 H -0.23228700 3.79002500 0.00000000