Electronic Supporting Information for

Framework for designing main-group single-molecule magnets

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Contents

1 Detailed derivation of the theoretical model

The theoretical crystal-field (CF) model will be derived in detail in this section. The derivation is intended to be self-contained so most of the equations and statements made in the main text will be repeated here to improve readability.

1.1 Model Hamiltonian

The crystal-field model consists of one, two or three electrons occupying two atomic-like p orbitals, chosen as the real np_x and np_y orbitals or, equally, the complex orbitals np_{-1} and np_{+1}. The one-electron states that describe each individual particle in the system are

$$|n\rangle \otimes |lm_l\rangle \otimes |sm_s\rangle \equiv |np_{m_l}\rangle \otimes |sm_s\rangle \equiv |np_{m_l},sm_s\rangle, \tag{S1}$$

where l and s are the orbital and spin angular momenta quantum numbers, respectively, m_l and m_s are the respective angular momentum projections, the principal quantum number n represents radial degrees of freedom that do not depend on angular-momentum degrees of freedom and p is used to denote the one-electron angular-momentum eigenstate with $l = 1$ that we are interested in. The real one-electron states np_x and np_y and the complex states np_{-1} and np_{+1} are related by

$$|np_{\pm1}\rangle = \mp\frac{1}{\sqrt{2}}\left(|np_x\rangle \pm i|np_y\rangle\right), \tag{S2}$$

$$|np_x\rangle = \frac{i}{\sqrt{2}}\left(|np_{-1}\rangle + |np_{+1}\rangle\right) \text{ and} \tag{S3}$$

$$|np_y\rangle = \frac{1}{\sqrt{2}}\left(|np_{-1}\rangle - |np_{+1}\rangle\right). \tag{S4}$$

Since the model is limited to the np_x and np_y orbitals, both of which have the same principal quantum number and orbital quantum number, the possible angular momentum quantum numbers are $l = 1$, $m_l = \pm1$, $s = 1/2$ and $m_s = \pm1/2$. The value of n depends on the element, but is the same for all one-electron states calculated for a given system. The spatial representation of the orbitals np_{m_l} can be further partitioned into a radial function R_{nl} and a spherical harmonic Y_{lm_l}:

$$np_{m_l}(r,\theta,\phi) = R_{nl}(r)Y_{lm_l}(\theta,\phi), \tag{S5}$$

where r represents the spherically symmetric radial degrees of freedom and θ and ϕ represent the angular degrees of freedom.

The many-electron model Hamiltonian is then

$$\begin{aligned}\hat{H} = &\sum_{m_l,m_l'}\sum_{m_s,m_s'}\langle np_{m_l},s,m_s|\hat{h} + \hat{V}_{\mathrm{CF}} + \hat{\xi}\hat{\mathbf{s}}\cdot\hat{\mathbf{l}}|np_{m_l'},sm_s'\rangle\hat{a}^\dagger_{m_l m_s}\hat{a}_{m_l' m_s''} \\ &+ \sum_{\substack{m_l,m_l'\\ m_l'',m_l'''}}\sum_{\substack{m_s,m_s'\\ m_s'',m_s'''}}\left(\langle np_{m_l},sm_s|\otimes\langle np_{m_l'},sm_s'|\right)\hat{g}\left(|np_{m_l''},sm_s''\rangle\otimes|np_{m_l'''},sm_s'''\rangle\right) \\ &\qquad\times\hat{a}^\dagger_{m_l,m_s}\hat{a}^\dagger_{m_l',m_s'}\hat{a}_{m_l''',m_s'''}\hat{a}_{m_l'',m_s''},\end{aligned} \tag{S6}$$

where $\hat{a}^{\dagger}_{m_l,m_s}$ and $\hat{a}_{m_l,m_s}$ are electron creation and annihilation operators, respectively. The free-ion one-electron Hamiltonian $\hat{h}$ is a spherically symmetric operator that includes the kinetic and potential energy terms, and might include many-electron mean-field terms and scalar relativistic corrections. The CF operator $\hat{V}_{\mathrm{CF}}$ accounts for the interactions of the electrons with the rest of the molecule. $\hat{h}_{\mathrm{SOC}} = \hat{\xi}\hat{\mathbf{s}} \cdot \hat{\mathbf{l}}$ is the one-electron spin-orbit coupling (SOC) operator which includes a spherically symmetric radial operator $\hat{\xi}$ and the one-electron spin and orbital angular momentum vector operators $\hat{\mathbf{s}}$ and $\hat{\mathbf{l}}$, respectively. As is common in CF calculations[1–5], two-electron terms of the SOC operator are neglected as the one-electron term is the dominant term of the operator, and the two-electron terms are considerably more difficult to evaluate.[6,7] The operator $\hat{g}$ describes the electron–electron Coulomb repulsion.

Both the $\{np_x, np_y\}$ and $\{np_{-1}, np_{+1}\}$ spatial orbital sets are degenerate eigenstates of $\hat{h}$ with an eigenvalue ϵ. The effects of metal–ligand covalency and other bonding interactions are implicitly included into the matrix elements of $\hat{V}_{\mathrm{CF}}$, which are taken as effective parameters. In the real and complex one-electron bases, the matrix elements of $\hat{V}_{\mathrm{CF}}$ are:

$$V_{\mathrm{CF}} = \begin{array}{c} \\ |np_x\rangle \\ |np_y\rangle \end{array} \begin{array}{c} \begin{array}{cc} |np_x\rangle & |np_y\rangle \end{array} \\ \begin{pmatrix} \Gamma & \eta \\ \eta & \Gamma + \Delta \end{pmatrix} \end{array} \leftrightarrow V_{\mathrm{CF}} = \begin{array}{c} \\ |np_{-1}\rangle \\ |np_{+1}\rangle \end{array} \begin{array}{c} \begin{array}{cc} |np_{-1}\rangle & |np_{+1}\rangle \end{array} \\ \begin{pmatrix} \Phi & \gamma \\ \gamma^* & \Phi \end{pmatrix} \end{array}, \tag{S7}$$

where η, Γ, Δ and Φ are real parameters, and γ is a complex parameter. Note that in the complex orbital basis, both of the diagonal elements are equal. The parameters for the real and complex orbitals are related as

$$\gamma = -\frac{1}{2}\Delta - i\eta \qquad \text{and} \qquad \Phi = \Delta + \frac{1}{2}\Gamma. \tag{S8}$$

In later equations the quantity

$$4|\gamma|^2 = 4\gamma \cdot \gamma^* = \Delta^2 + 4\eta^2, \tag{S9}$$

which describes the square of overall CF streangth will be important.

The one-electron matrix elements of the SOC operator can be evaluated using the partitioning (S5). The spherically symmetric part $\hat{\xi}$ only acts on the radial part. We will introduce this effect as a simple parameter

$$\zeta = \int \mathrm{d}r R_{nl}(r)\hat{\xi}(r)R_{nl}(r) \tag{S10}$$

without defining the radial function R_{nl} further. In practice the ζ is extracted from fits to experimental data or from energy differences between *ab initio* calculated states. Therefore, it parametrically includes effects of two-electron SOC terms in a mean-field manner that are not explicitly included in the Hamiltonian (S6). The one-electron SOC integral ζ is usually a positive quantity.[8] Then, the one-electron matrix element of $\hat{\xi}\hat{\mathbf{s}} \cdot \hat{\mathbf{l}}$ is given by

$$\langle np_{m_l},sm_s|\hat{\xi}\hat{\mathbf{s}} \cdot \hat{\mathbf{l}}|np_{m_l'},sm_s'\rangle = \zeta \sum_{\alpha} \langle lm_l|\hat{l}_\alpha|lm_l'\rangle\langle sm_s|\hat{s}_\alpha|sm_s'\rangle, \tag{S11}$$

where $\alpha \in x, y\, z$, and $\hat{l}_\alpha$ and $\hat{s}_\alpha$ are Cartesian components of $\hat{\mathbf{l}}$ and $\hat{\mathbf{s}}$, respectively. The matrix elements (S11) can be evaluated as

$$\langle np_{m_l},sm_s|\hat{\xi}\hat{\mathbf{s}} \cdot \hat{\mathbf{l}}|np_{m_l'},sm_s'\rangle = m_l m_s \delta_{m_l,m_l'}\delta_{m_s,m_s'}, \tag{S12}$$

where $\delta_{m_l,m_l'}$ and $\delta_{m_s,m_s'}$ are Kronecker deltas. The SOC operator is diagonal in the one-electron basis because the $\hat{\mathbf{l}}$ cannot couple the $m_l = -1$ and $m_l = +1$ states to each other as $\hat{\mathbf{l}}$ is a rank-one tensor operator and $m_l = -1$ and $m_l = +1$ differ by more than one:

$$H_{\mathrm{SOC}} = \begin{array}{c} \\ |np_{-1},s,+1/2\rangle \\ |np_{+1},s,+1/2\rangle \\ |np_{-1},s,-1/2\rangle \\ |np_{+1},s,-1/2\rangle \end{array} \begin{array}{c} \begin{array}{cccc} |np_{-1},s,+1/2\rangle & |np_{+1},s,+1/2\rangle & |np_{-1},s,-1/2\rangle & |np_{+1},s,-1/2\rangle \end{array} \\ \begin{pmatrix} -\zeta/2 & 0 & 0 & 0 \\ 0 & +\zeta/2 & 0 & 0 \\ 0 & 0 & +\zeta/2 & 0 \\ 0 & 0 & 0 & -\zeta/2 \end{pmatrix} \end{array}. \tag{S13}$$

The two-electron integrals can be written in the general form

$$\begin{aligned} &\left(\langle np_{m_l},sm_s| \otimes \langle np_{m_l'},sm_s'|\right)\hat{g}\left(|np_{m_l''},sm_s''\rangle \otimes |np_{m_l'''},sm_s'''\rangle\right) \\ &\quad = \delta_{m_s,m_s''}\delta_{m_s',m_s'''}\left(\langle np_{m_l}| \otimes \langle np_{m_l'}|\right)\frac{1}{|\mathbf{r}_1-\mathbf{r}_2|}\left(|np_{m_l''}\rangle \otimes |np_{m_l'''}\rangle\right) \\ &\quad \equiv \delta_{m_s,m_s''}\delta_{m_s',m_s'''}(np_{m_l},np_{m_l''}|np_{m_l'},np_{m_l'''}) \\ &\quad \equiv \delta_{m_s,m_s''}\delta_{m_s',m_s'''}(m_l,m_l''|m_l',m_l'''), \end{aligned} \tag{S14}$$

where $\mathbf{r}_1$ and $\mathbf{r}_2$ are the coordinates of the two electrons, and the spin-dependent part of the matrix element is reduced to Kronecker deltas as the Coulomb operator does not operate on the spin state. The integrals can be simplified in the atomic orbital basis following a well-established procedure that is explained, for example, in references 1, 2 and 8. For completeness, the procedure will be outlined here as well. The approach is based on expansion of the Coulomb operator as

$$\begin{aligned} \frac{1}{|\mathbf{r}_1-\mathbf{r}_2|} &= \sum_k \frac{(\min[r_1,r_2])^k}{(\max[r_1,r_2])^{k+1}} P_k(\cos\omega_{12}), \\ &= \sum_k \frac{(\min[r_1,r_2])^k}{(\max[r_1,r_2])^{k+1}} \frac{4\pi}{2k+1} \sum_q Y_{kq}(\theta_1,\phi_1)Y_{kq}^*(\theta_2,\phi_2), \end{aligned} \tag{S15}$$

where k is a non-negative integer, q can have integer values between $-k$ and k, $P_k(\cos\omega_{12})$ is an associated Legendre polynomial, ω_{12} is the angle between $\mathbf{r}_1$ and $\mathbf{r}_2$, and in spherical polar coordinates $\mathbf{r}_i = (r_i,\theta_i,\phi_i)$. In the following the indices in $(m_l,m_l''|m_l',m_l''')$ will be further simplified to $(\sigma\tau|\mu\nu)$ to avoid cluttering the notation. The integral $(\sigma\tau|\mu\nu)$ is evaluated as

$$\begin{aligned} (\sigma\tau|\mu\nu) = \sum_k &\iint \mathrm{d}r_1\mathrm{d}r_2 R_{nl}(r_1)R_{nl}(r_2)\frac{(\min[r_1,r_2])^k}{(\max[r_1,r_2])^{k+1}}R_{nl}(r_1)R_{nl}(r_2) \\ &\times \frac{4\pi}{2k+1}\sum_q \int \sin\theta_1 \mathrm{d}\theta_2\mathrm{d}\phi_1 Y_{l\sigma}^*(\theta_1,\phi_1)Y_{kq}(\theta_1,\phi_1)Y_{l\tau}(\theta_1,\phi_1) \\ &\times \int \sin\theta_2\mathrm{d}\theta_2\mathrm{d}\phi_2 Y_{l\mu}^*(\theta_1,\phi_1)Y_{kq}^*(\theta_1,\phi_1)Y_{l\nu}(\theta_1,\phi_1) \end{aligned} \tag{S16}$$

$$= \sum_k R^k(nl,nl,nl,nl)\left(C_{k0,l0}^{l0}\right)^2 \sum_q C_{kq,l\tau}^{l\sigma}C_{kq,l\mu}^{l\nu}, \tag{S17}$$

where the coefficients $C^{l0}_{k0,l0}$ are Clebsch–Gordan (CG) coefficient within the Condon–Shortley phase convention[8],

$$R^k(nl,nl,nl,nl) \equiv \iint \mathrm{d}r_1 \mathrm{d}r_2 R_{nl}(r_1) R_{nl}(r_2) \frac{(\min[r_1,r_2])^k}{(\max[r_1,r_2])^{k+1}} R_{nl}(r_1) R_{nl}(r_2) \equiv F^k(nl,nl), \quad \text{(S18)}$$

and $F^k(nl,nl)$ is Slater–Condon parameter of rank k. Only parameters with even rank k contribute to the expansion (S17).[8] The "triple integral"[9]

$$\int \sin\theta_1 \mathrm{d}\theta_1 \mathrm{d}\phi_1 Y^*_{l\sigma}(\theta_1,\phi_1) Y_{kq}(\theta_1,\phi_1) Y_{l\tau}(\theta_1,\phi_1) = \sqrt{\frac{(2k+1)(2l+1)}{4\pi(2l+1)}} C^{l0}_{k0,l0} C^{l\sigma}_{kq,l\tau} \quad \text{(S19)}$$

of spherical harmonics was used when obtaining equation (S17) from (S16).

Due to the conservation of angular momentum projection in the CG coefficients, only integrals $(\sigma\tau|\mu\nu)$ with $\sigma+\mu=\tau+\nu$ will have non-zero values. Furthermore, due to the equivalence of two orbitals np_{-1} and np_{+1}, and the permutation symmetry $(\sigma\tau|\mu\nu) = (\mu\nu|\sigma\tau)$, we only have three unique two-electron integrals:

$$\begin{aligned} &(+1,+1|+1,+1) = (-1,-1|-1,-1) \equiv U', \\ &(-1,-1|+1,+1) = (+1,+1|-1,-1) \equiv U'' \text{ and} \\ &(-1,+1|+1,-1) = (+1,-1|-1,+1) \equiv K. \end{aligned} \quad \text{(S20)}$$

Following the usual convention, U' and U'' will be referred to as Coulomb integrals and K as an exchange integral. Expansion of the integrals in terms of Slater–Condon parameters with (S16) and explicitly evaluating the CG coefficients gives

$$\begin{aligned} U' &= F^0(nl,nl) + \frac{1}{25}F^2(np,np), \\ U'' &= F^0(nl,nl) + \frac{1}{25}F^2(np,np) \text{ and} \\ K &= \frac{6}{25}F^2(np,np), \end{aligned} \quad \text{(S21)}$$

which shows that two Coulomb integrals are equivalent: $U' = U'' \equiv U$. Thus, we only need to consider two electron-repulsion integrals: the Coulomb integral U and the exchange integral K. Note that the equivalency $U' = U''$ follows from the assumed spherical symmetry. If covalency is explicitly taken into account and the np_{-1} and np_{+1} orbitals are no longer pure p orbitals, the equivalency does not hold, and both parameters need to be included in the model.

After evaluating the one-electron matrix elements and the electron-repulsion integrals, the Hamiltonian (S6) can be simplified to the form

$$\begin{aligned} \hat{H} = {} & (\epsilon+\Phi) \sum_{m_l} \sum_{m_s} \hat{n}_{m_l,m_s} + \sum_{m_s} \left(\gamma \hat{a}^\dagger_{-1,m_s} \hat{a}_{+1,m_s} + \gamma^* \hat{a}^\dagger_{+1,m_s} \hat{a}_{-1,m_s} \right) \\ & + \frac{U}{2} \sum_{m_l,m'_l} \sum_{m_s,m'_s} \hat{n}_{m_l,m_s} \hat{n}_{m'_l,m'_s} - \frac{K}{2} \sum_{m_l} \sum_{m_s,m'_s} \hat{a}^\dagger_{m_l,m_s} \hat{a}^\dagger_{-m_l,m'_s} \hat{a}_{-m_l,m_s} \hat{a}_{m_l,m'_s} \\ & + \zeta \sum_{m_l} \sum_{m_s} m_l m_s \hat{n}_{m_l,m_s}, \end{aligned} \quad \text{(S22)}$$

where $\hat{n}_{m_l,m_s} = \hat{a}^\dagger_{m_l,m_s}\hat{a}_{m_l,m_s}$ is a number operator. The terms $\sum_{m_l}\sum_{m_s}\hat{n}_{m_l,m_s}$ and $1/2\sum_{m_l,m'_l}\sum_{m_s,m'_s}\hat{n}_{m_l,m_s}\hat{n}_{m'_l,m'_s}$ simply count the number of electrons and the number of pairs of electrons in the system, respectively. Since the number of electrons is constant in each system considered, these terms do not contribute to the energy differences between states, and they can be included into the energy origin. Thus, we obtain the final form of the Hamiltonian by energy translation:

$$\hat{H} = \sum_{m_s}\left(\gamma\hat{a}^\dagger_{-1,m_s}\hat{a}_{+1,m_s} + \gamma^*\hat{a}^\dagger_{+1,m_s}\hat{a}_{-1,m_s}\right) + \zeta\sum_{m_l}\sum_{m_s} m_l m_s \hat{n}_{m_l,m_s} - \frac{K}{2}\sum_{m_l}\sum_{m_s,m'_s}\hat{a}^\dagger_{m_l,m_s}\hat{a}^\dagger_{-m_l,m'_s}\hat{a}_{-m_l,m_s}\hat{a}_{m_l,m'_s}. \tag{S23}$$

The model contains one complex parameter γ and two real parameters K and ζ; therefore, a total of four scalar numbers are needed to define the model.

1.2 Magnetic moment operators

The Cartesian components $\hat{\mu}_\alpha$, $\alpha \in x, y, z$ of the magnetic moment operator are

$$\hat{\mu}_\alpha = -\mu_\mathrm{B}\sum_{m_l,m'_l}\sum_{m_s,m'_s}\langle np_{m_l},sm_s|\hat{l}_\alpha + g_e\hat{s}_\alpha|np_{m'_l},sm'_s\rangle\hat{a}^\dagger_{m_l,m_s}\hat{a}_{m'_s,m'_l}, \tag{S24}$$

where μ_B is the Bohr magneton and g_e is the free-electron g factor with a positive sign. The value of g_e will be taken as $g_e \approx 2$ to simplify the following notation. The one-electron matrix elements are then

$$\begin{aligned}
&\langle np_{m_l},sm_s|\hat{l}_x + 2\hat{s}_x|np_{m'_l},sm'_s\rangle = 2\delta_{m_l,m'_l}\delta_{m_s,-m'_s}m_s, \\
&\langle np_{m_l},sm_s|\hat{l}_y + 2\hat{s}_y|np_{m'_l},sm'_s\rangle = -2i\delta_{m_l,m'_l}\delta_{m_s,-m'_s}m_s \text{ and} \\
&\langle np_{m_l},sm_s|\hat{l}_z + 2\hat{s}_z|np_{m'_l},sm'_s\rangle = \delta_{m_l,m'_l}\delta_{m_s,m'_s}\left(m_l + 2m_s\right).
\end{aligned} \tag{S25}$$

1.3 np^1 case

The simplest situation arises when either of the two orbitals is occupied by one electron. The basis states are constructed by creating one electron into a reference "vacuum state" $|np^0\rangle$ with empty orbitals. There are four possible states:

$$\hat{a}^\dagger_{-1,-1/2}|np^0\rangle, \quad \hat{a}^\dagger_{+1,-1/2}|np^0\rangle, \quad \hat{a}^\dagger_{-1,+1/2}|np^0\rangle \quad \text{and} \quad \hat{a}^\dagger_{+1,+1/2}|np^0\rangle, \tag{S26}$$

where the first index refers to the complex orbital and the second to the electron spin. Since the creation operator is a one-electron spin tensor operator, the states are pure spin eigenstates. [10–12] Within the basis (S26), keeping the basis states in the same order, the Hamiltonian (S23) is

$$H^{\text{1-elec}} = \begin{pmatrix} \zeta/2 & \gamma & 0 & 0 \\ \gamma^* & -\zeta/2 & 0 & 0 \\ 0 & 0 & \zeta/2 & \gamma^* \\ 0 & 0 & \gamma & -\zeta/2 \end{pmatrix}. \tag{S27}$$

Since the SOC operator does not mix states with different spins, the Hamiltonian has a block-diagonal structure, and is trivial to diagonalize yielding two eigenvalues each of which is doubly degenerate:

$$E_{\pm}^{\text{1-elec}} = \pm\sqrt{\frac{\zeta^2}{4} + |\gamma|^2} = \pm\sqrt{\frac{\zeta^2}{4} + \frac{\Delta^2}{4} + \eta^2} = \pm\frac{1}{2}\sqrt{\zeta^2 + \Delta^2 + 4\eta^2}, \tag{S28}$$

where we used (S9). The eigenvalue E_- is the ground state energy and corresponds to the energy of a Kramers doublet (KD). If the one-electron system were to display single-molecule magnet (SMM) behavior with an Orbach[13–15] mechanism, the effective barrier height for the reversal of magnetization $U_{\text{eff}}^{\text{1-elec}}$ would correspond to the energy difference between the two KDs; *i. e.*, the difference between the eigenvalues:

$$U_{\text{eff}}^{\text{1-elec}} = E_{+}^{\text{1-elec}} - E_{-}^{\text{1-elec}} = \sqrt{\zeta^2 + \Delta^2 + 4\eta^2}. \tag{S29}$$

It is worth noting that all three one-electron parameters increase the value of $U_{\text{eff}}^{\text{1-elec}}$.

Matrix representations of the magnetic moment operator components (S24) in the basis (S26) are

$$\mu_x^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \qquad \mu_y^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} 0 & 0 & 0 & -i \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ i & 0 & 0 & 0 \end{pmatrix} \text{ and} \tag{S30}$$

$$\mu_z^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

Evaluation of the **g**-tensor for the ground KD (*vide infra*), requires the magnetic moment matrix elements in a basis formed by the two states of the ground KD. The eigenvectors for the two components of the ground KD are

$$w_1 = \begin{pmatrix} c_1 \\ c_2 \\ 0 \\ 0 \end{pmatrix} \qquad \text{and} \qquad w_2 = \begin{pmatrix} 0 \\ 0 \\ c_1^* \\ c_2 \end{pmatrix}, \tag{S31}$$

where

$$c_1 = -e^{i\phi}\sin\frac{\theta}{2}, \qquad c_2 = \cos\frac{\theta}{2} \tag{S32}$$

and

$$\theta = \cos^{-1}\frac{\zeta}{\sqrt{\zeta^2 + 4|\gamma|^2}} = \cos^{-1}\frac{\zeta}{U_{\text{eff}}} \qquad \text{and} \qquad \phi = \tan^{-1}\frac{\text{Im}(\gamma)}{\text{Re}(\gamma)} = \tan^{-1}\frac{2\eta}{\Delta}. \tag{S33}$$

Transformation of the magnetic moment operator components to the eigenbasis, and projection

to the ground KD yields the magnetic moment operator matrices

$$\mu_x^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} 0 & c_2^* c_1 + c_1 c_2 \\ c_1^* c_2 + c_1^* c_2^* & 0 \end{pmatrix}, \tag{S34}$$
$$\mu_y^{\text{1-elec}} = -i\mu_{\text{B}} \begin{pmatrix} 0 & c_2^* c_1 + c_1 c_2 \\ c_1^* c_2 + c_1^* c_2^* & 0 \end{pmatrix} \text{ and}$$
$$\mu_z^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} 2c_1^* c_1 & 0 \\ 0 & -2c_1^* c_1 \end{pmatrix}.$$

By straightforward calculation

$$c_1^* c_1 = \frac{1}{2} - \frac{\zeta}{2U_{\text{eff}}} \qquad \text{and} \qquad c_1^* c_2 + c_1^* c_2^* = \frac{-\Delta + 2i\eta}{U_{\text{eff}}}, \tag{S35}$$

therefore

$$\mu_x^{\text{1-elec}} = \frac{\mu_{\text{B}}}{U_{\text{eff}}} \begin{pmatrix} 0 & -\Delta - 2i\eta \\ -\Delta + 2i\eta & 0 \end{pmatrix}, \tag{S36}$$
$$\mu_y^{\text{1-elec}} = -\frac{i\mu_{\text{B}}}{U_{\text{eff}}} \begin{pmatrix} 0 & -\Delta - 2i\eta \\ -\Delta + 2i\eta & 0 \end{pmatrix} \text{ and}$$
$$\mu_z^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} \left(1 - \dfrac{\zeta}{U_{\text{eff}}}\right) & 0 \\ 0 & -\left(1 - \dfrac{\zeta}{U_{\text{eff}}}\right) \end{pmatrix}.$$

1.4 np^2 case

In the case of two electrons, it is possible to construct six different basis states. In order to minimize the number of non-zero off-diagonal elements in the Hamiltonian matrix, the basis states are constructed using a two-electron spin tensor creation operator [10,11]

$$\hat{Q}^{S,M_S}_{m_l,m_l'} = \sum_{m_s m_s'} C^{SM_S}_{sm_s,sm_s'} \hat{a}^\dagger_{m_l,m_s} \hat{a}^\dagger_{m_l',m_s'} \tag{S37}$$

that creates two-electron states with total spin S and its projection M_S. The six basis states are

$$\hat{Q}^{1,+1}_{-1,+1}|np^0\rangle, \quad \hat{Q}^{1,-1}_{-1,+1}|np^0\rangle, \quad \hat{Q}^{0,0}_{-1,+1}|np^0\rangle, \quad \hat{Q}^{1,0}_{-1,+1}|np^0\rangle, \tag{S38}$$
$$\left(\hat{Q}^{0,0}_{-1,-1} + \hat{Q}^{0,0}_{+1,+1}\right)|np^0\rangle \quad \text{and} \quad \left(\hat{Q}^{0,0}_{-1,-1} - \hat{Q}^{0,0}_{+1,+1}\right)|np^0\rangle.$$

The combinations in the last two basis states in (S38) are taken so that all matrix elements in the Hamiltonian are either purely real or purely imaginary. Using the basis definition (S38), the Hamiltonian takes the form

$$H^{\text{2-elec}} = \begin{pmatrix} -K & 0 & 0 & 0 & 0 & 0 \\ 0 & -K & 0 & 0 & 0 & 0 \\ 0 & 0 & -K & \zeta & 0 & 0 \\ 0 & 0 & \zeta & K & -\Delta & 2i\eta \\ 0 & 0 & 0 & -\Delta & 0 & 0 \\ 0 & 0 & 0 & -2i\eta & 0 & 0 \end{pmatrix}. \tag{S39}$$

While the Hamiltonian (S39) is block-diagonal, the 4×4 block does not yield a simple expression for its eigenvalues. Since we are mostly interested in is the situation when $|\Delta|, |\eta| \ll \zeta$, the CF terms that depend on Δ and η (*i. e.*, the operator $\hat{V}_{\mathrm{CF}}$) can be introduced as a perturbation. The first two eigenvalues corresponding to the 1×1 blocks of the Hamiltonian are $E_1^{2\text{-elec}} = E_2^{2\text{-elec}} = -K$ exactly. The zeroth-order eigenvalues within the 4×4 block are

$$\left(E_3^{2\text{-elec}}\right)^{(0)} = -\sqrt{K^2+\zeta^2}, \quad \left(E_4^{2\text{-elec}}\right)^{(0)} = +\sqrt{K^2+\zeta^2}, \tag{S40}$$
$$\left(E_5^{2\text{-elec}}\right)^{(0)} = 0 \quad \text{and} \quad = \left(E_6^{2\text{-elec}}\right)^{(0)} = 0.$$

Since K is a positive number, at zeroth order the ground state energy is $\left(E_3^{2\text{-elec}}\right)^{(0)}$, which is always lower than $-K$ except if $\zeta = 0$ in which case the ground state energy is equal to $-K$, and the ground manifold is a spin triplet. In the case of a non-vanishing ζ, however, the ground-state is non-degenerate; therefore, it cannot have magnetic anisotropy, and the system cannot be a SMM. A possibility for anisotropy and SMM behavior would only arise if the CF destabilizes the ground state 3 and/or brings the energetically degenerate doublet of states 5 and 6 to below state 3 in energy. The lower-energy doublet of states 1 and 2 is not affected by the perturbation.

In the first-order corrections to all four eigenvalues are zero, and the lowest perturbation correction arises at second order. The corrected energies are

$$\left(E_3^{2\text{-elec}}\right)^{(0)} + \left(E_3^{2\text{-elec}}\right)^{(2)} = -\sqrt{K^2+\zeta^2} - \left(1 - \frac{K}{\sqrt{K^2+\zeta^2}}\right) \cdot \frac{\Delta^2+4\eta^2}{2\sqrt{K^2+\zeta^2}}, \tag{S41}$$
$$\left(E_4^{2\text{-elec}}\right)^{(0)} + \left(E_4^{2\text{-elec}}\right)^{(2)} = +\sqrt{K^2+\zeta^2} + \left(1 + \frac{K}{\sqrt{K^2+\zeta^2}}\right) \cdot \frac{\Delta^2+4\eta^2}{2\sqrt{K^2+\zeta^2}},$$
$$\left(E_5^{2\text{-elec}}\right)^{(0)} + \left(E_5^{2\text{-elec}}\right)^{(2)} = -\frac{4K\eta^2}{K^2+\zeta^2} \text{ and}$$
$$\left(E_6^{2\text{-elec}}\right)^{(0)} + \left(E_6^{2\text{-elec}}\right)^{(2)} = +\frac{K\Delta^2}{K^2+\zeta^2}.$$

Observing the energy expressions (S41) for states 3 and 4 we see that $0 \leq K/\sqrt{K^2+\zeta^2} \leq 1$ and that $(\Delta^2+4\eta^2)/(2\sqrt{K^2+\zeta^2}) \leq 0$. This means that the perturbation further stabilizes state 3 and destabilizes state 4. Thus, the perturbation does not destabilize the ground state.

The energy expression (S41) for state 6 is positive indicating further destabilization of the state. While the state 5 is stabilized, the destabilization of the state 6 means that a doublet consisting of the states 5 and 6 cannot become the ground state. Thus, up to second order in perturbation theory the ground state does not have any degeneracy. Due to Kramers' theorem, the magnetic moment expectation value for the ground singlet is then zero.[5]

1.5 np^3 case

The three electron case is in many ways analogous to the one-electron case as in the three electron case there is one hole in the model orbital space. The basis states can be created by starting from a fully occupied state $|np^4\rangle$ and annihilating one electron. In order to ensure that

the states are spin eigenstates, the states are constructed by a one-electron tensor operator that creates a three-particle state from the four-particle state by annihilating one electron:[12]

$$\hat{q}^{m_s}_{m_l} = (-1)^{l+s-m_l-m_s}\hat{a}_{-m_l,-m_s}. \tag{S42}$$

The basis states are

$$\hat{q}^{+1/2}_{-1}|np^4\rangle, \qquad \hat{q}^{+1/2}_{+1}|np^4\rangle, \qquad \hat{q}^{-1/2}_{+1}|np^4\rangle \quad \text{and} \quad \hat{q}^{-1/2}_{-1}|np^4\rangle, \tag{S43}$$

and in the same order the Hamiltonian is

$$H^{\text{3-elec}} = \begin{pmatrix} K+\zeta/2 & -\gamma & 0 & 0 \\ -\gamma^* & K-\zeta/2 & 0 & 0 \\ 0 & 0 & K+\zeta/2 & -\gamma^* \\ 0 & 0 & -\gamma & K-\zeta/2 \end{pmatrix}. \tag{S44}$$

Since the exchange integral K contributes equally to each diagonal element, it can be included into the energy origin to give

$$H^{\text{3-elec}} \to \begin{pmatrix} \zeta/2 & -\gamma & 0 & 0 \\ -\gamma^* & \zeta/2 & 0 & 0 \\ 0 & 0 & \zeta/2 & -\gamma^* \\ 0 & 0 & -\gamma & \zeta/2 \end{pmatrix}. \tag{S45}$$

We see that the Hamiltonian (S45) is equal to the one-electron Hamiltonian (S27) except with a different phase in the off-diagonal elements. The phases do not, however, affect the eigenvalues. The eigenvalues in the three electron case are also those given in equation (S28) and the effective barrier is the same as in (S29):

$$U^{\text{3-elec}}_{\text{eff}} = U^{\text{1-elec}}_{\text{eff}} \equiv U_{\text{eff}}. \tag{S46}$$

Matrix representations of the magnetic moment operator components (S24) in the basis (S43) are

$$\mu_x^{\text{3-elec}} = \mu_{\text{B}} \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \qquad \mu_y^{\text{3-elec}} = \mu_{\text{B}} \begin{pmatrix} 0 & 0 & 0 & i \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ -i & 0 & 0 & 0 \end{pmatrix} \text{ and} \tag{S47}$$

$$\mu_z^{\text{3-elec}} = \mu_{\text{B}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}.$$

The eigenvectors of (S45) have the same exact structure (S31)–(S33) as in the one-electron case. The differences in the transformation only originate from the differences in the structure of the magnetic moment operators (S47). In the basis of the two components of the ground KD, the magnetic moment operator component matrices are

$$\mu_x^{\text{3-elec}} = -\mu_{\text{B}} \begin{pmatrix} 0 & c_1c_2 + c_1^*c_2 \\ c_1^*c_2^* + c_2^*c_1 & 0 \end{pmatrix}, \tag{S48}$$

$$\mu_y^{\text{1-elec}} = -i\mu_{\text{B}} \begin{pmatrix} 0 & c_1c_2 + c_1^*c_2 \\ c_1^*c_2^* + c_2^*c_1 & 0 \end{pmatrix} \text{ and}$$

$$\mu_z^{\text{1-elec}} = \mu_{\text{B}} \begin{pmatrix} -2c_2^*c_2 & 0 \\ 0 & 2c_2^*c_2 \end{pmatrix}.$$

By a straightforward calculation

$$c_2^* c_2 = \frac{1}{2} + \frac{\zeta}{2U_{\text{eff}}} \qquad \text{and} \qquad c_1^* c_2^* + c_2^* c_1 = \frac{-\Delta + 2i\eta}{U_{\text{eff}}}, \tag{S49}$$

therefore

$$\begin{aligned}
\mu_x^{\text{3-elec}} &= \frac{\mu_{\text{B}}}{U_{\text{eff}}} \begin{pmatrix} 0 & -\Delta - 2i\eta \\ -\Delta + 2i\eta & 0 \end{pmatrix}, \\
\mu_y^{\text{3-elec}} &= -\frac{i\mu_{\text{B}}}{U_{\text{eff}}} \begin{pmatrix} 0 & -\Delta - 2i\eta \\ -\Delta + 2i\eta & 0 \end{pmatrix} \text{ and} \\
\mu_z^{\text{3-elec}} &= \mu_{\text{B}} \begin{pmatrix} -\left(1 + \dfrac{\zeta}{U_{\text{eff}}}\right) & 0 \\ 0 & \left(1 + \dfrac{\zeta}{U_{\text{eff}}}\right) \end{pmatrix},
\end{aligned} \tag{S50}$$

from which we see that $\mu_x^{\text{3-elec}} = \mu_x^{\text{1-elec}}$ and $\mu_y^{\text{3-elec}} = \mu_y^{\text{1-elec}}$ in the KD basis.

1.6 KD g-tensors

The splitting of a KD under an external magnetic field can be described by the Zeeman pseudospin Hamiltonian[5,16,17]

$$\tilde{H} = \mu_{\text{B}} \mathbf{B} \cdot \mathbf{g} \cdot \tilde{\mathbf{S}}, \tag{S51}$$

where $\mathbf{B}$ is the magnetic field, $\mathbf{g}$ is a pseudospin $\mathbf{g}$ tensor and $\tilde{\mathbf{S}}$ is a pseudospin operator acting on a fictitious pseudospin state with $\tilde{S} = 1/2$. The magnitude of the pseudospin is chosen so that its multiplicity $2\tilde{S} + 1 = 2$ is equal to a doublet. The magnitudes and signs of all elements of the pseudospin can be defined rigorously[18], but we will only be interested in the magnitudes of the principal components (eigenvalues), and use a commonly applied approach developed by Abragam and Bleaney[5], Gerloch and McMeeking[19], and Chibotaru and Ungur[16]. The following will follow the notation and presentation of Chibotaru and Ungur.

The $\mathbf{g}$-tensor is related to the dimensionless Abragam–Bleaney tensor[5] $\mathbf{G} = \mathbf{g}\mathbf{g}^T$, which is related to the abstract tensor $\mathbf{A}$:

$$\mathbf{A} = \frac{\mu_{\text{B}}^2}{4} \mathbf{G}, \tag{S52}$$

which has the unit of magnetic moment squared. The elements of the $\mathbf{A}$ tensor can be evaluated as[16]

$$A_{\alpha\beta} = \frac{1}{2} \sum_{i,j} \langle \psi_i | \hat{\mu}_\alpha | \psi_j \rangle \langle \psi_j | \hat{\mu}_\beta | \psi_i \rangle, \tag{S53}$$

where $\alpha, \beta \in x, y, z$, $i, j \in 1, 2$ and $|\psi_i\rangle$ are the two components of the ground KD. In both the one- and three-electron cases the $\mathbf{A}$ tensor is diagonal. The elements are

$$\begin{aligned}
A_{xx}^{\text{1-elec}} = A_{yy}^{\text{1-elec}} = A_{xx}^{\text{3-elec}} = A_{yy}^{\text{3-elec}} &= \frac{\mu_{\text{B}}^2}{U_{\text{eff}}^2} \left(\Delta^2 + 4\eta^2\right), \\
A_{zz}^{\text{1-elec}} &= \mu_{\text{B}}^2 \left(1 - \frac{\zeta}{U_{\text{eff}}}\right)^2 \text{ and} \\
A_{zz}^{\text{3-elec}} &= \mu_{\text{B}}^2 \left(1 + \frac{\zeta}{U_{\text{eff}}}\right)^2.
\end{aligned} \tag{S54}$$

The principal components of the respective **g**-tensors can then be simply evaluated using (S52). Since **A**, and as a consequence **G**, is diagonal, the diagonal elements of **G** are the squares of the principal components of the **g** tensor. The transverse components g_X and g_Y are all equal in both the one- and three-electron cases:

$$g_X = g_Y = \frac{2\sqrt{\Delta^2 + 4\eta^2}}{U_{\text{eff}}}. \tag{S55}$$

The Z components in the two cases are

$$g_Z^{\text{1-elec}} = 2 - \frac{2\zeta}{U_{\text{eff}}} \qquad \text{and} \qquad g_Z^{\text{3-elec}} = 2 + \frac{2\zeta}{U_{\text{eff}}}. \tag{S56}$$

The signs of all principal values were chosen as positive by convention. Since the elements of **g** enter **G** as squares, their sign cannot be obtained when the elements of **g** are extracted from **A** and **G**. The signs do not affect any of the properties we are interested in.

The expression can be further simplified by defining the dimensionless ratio

$$\rho \equiv \frac{\Delta^2 + 4\eta^2}{\zeta^2}, \tag{S57}$$

so that

$$g_Z^{\text{1-elec}} = 2 - \frac{2}{\sqrt{1+\rho}} \qquad \text{and} \qquad g_Z^{\text{3-elec}} = 2 + \frac{2}{\sqrt{1+\rho}}, \tag{S58}$$

and

$$g_X = g_Y = \frac{2}{\sqrt{\frac{1}{\rho} + 1}}. \tag{S59}$$

At the limit of vanishing SOC ($\zeta \to 0$) the ratio ρ tends to infinity, and $g_X, g_Y, g_Z \to 2$ consistent with isotropic magnetism at the absence of SOC. In the high-axiality limit, the CF parameters Δ and η are much smaller than SOC so that $\rho \to 0$. At this limit

$$\lim_{\zeta\to\infty} g_X = \lim_{\zeta\to\infty} g_Y = 0, \qquad \lim_{\zeta\to\infty} g_Z^{\text{1-elec}} = 0 \qquad \text{and} \qquad \lim_{\zeta\to\infty} g_Z^{\text{3-elec}} = 4. \tag{S60}$$

The limits show that in the one-electron case, large SOC leads to a completely non-magnetic ground KD, which results from the perfect cancellation of the orbital and spin momenta. In the three-electron case, large SOC leads to a situation that tends towards perfect axiality[20,21]; *i.e.*, vanishing transverse components g_X and g_Y, and non-zero axial component g_Z.

2 Computational details

2.1 Geometry optimizations

All geometries considered were fully optimized using density function theory (DFT) without any symmetry constraints. Frequency calculations were carried out to ensure that all stationary points correspond to minima on the potential energy surface. The DFT calculations were

carried out using the Amsterdam Density functional (ADF) module[22,23] of the Amsterdam Modeling Suite (AMS) versions 2022.101 and 2023.101.[24] The pure generalized gradient approximation (GGA) PBE for the exchange-correlation (XC) functional[25,26] was used in all optimizations along with the DFT-D3 empirical dispersion correction utilizing the Becke–Johnson (BJ) damping function[27,28]. Scalar relativistic effects were included with the zeroth-order regular approximation (ZORA).[29–31] The standard ADF valence triple-ζ basis set with two sets of polarization functions (TZ2P) designed for ZORA calculations was used throughout.[32] Large frozen cores were used which include the electrons outside the valence s and p shells. The `NumericalQuality` keyword was set to `Good`. Atomic charges and atomic spin densities were calculated using the quantum theory of atoms in molecules (QTAIM)[33,34] as implemented in ADF[35,36].

In order to verify that the use of a pure GGA functional and the inclusion of only scalar relativistic effects for the heavier elements does not introduce any significant error into the geometries, additional calculations were carried out on the geometry **Bi-1b** using the hybrid PBE0 XC functional[25,26,37,38] and two-component ZORA[39] that also includes spin-orbit coupling. The deviations in the Bi–C bond length when using the PBE with two-component ZORA, PBE0 with scalar ZORA and PBE0 with two-component ZORA were less than 0.07 Å in all cases when compared to that calculated with PBE and scalar ZORA. While there is some deviation, this is certainly small enough when considering the possible errors that arise from the lack of any larger substituents on the molecular skeleton. If the calculations were carried out without any treatment of scalar relativistic effects using only a frozen core, the Bi–C bond length in **Bi-1b** would by exaggerated by 0.09 Å compared to scalar ZORA when using PBE and by 0.20 Å when using PBE0.

2.2 Energy-level structure and magnetic property calculations

The electronic structure and magnetic properties were calculated using multireference methods as implemented in the Orca code version 5.0.4.[40–42] First a state-averaged (SA) complete-active space self-consistent field (CASSCF) calculation was carried out.[43–47] In the mono-coordinated structures **1a** the active space contained the np_x and np_y orbitals and the σ and σ^* orbitals of the metal–ligand bond giving a four-orbital active space. In structures **1b** also the six phenyl π-orbitals were included giving a nine-orbital active space. In structures **1c** the active space contained, in addition to the active orbitals of the **1a** structures, also the lone-pair π-orbital at the N atom giving a seven-orbital active space. In **1d**, the active space consisted of the same orbitals as in **1a** as well as the five π-orbitals of the NHC ligand giving a nine-orbital active space. In the larger structures **4**, $[\mathbf{4}]^-$, **5** and $[\mathbf{5}]^-$ the same ten-orbital active space as in the structures **1b** was used. In case of the only selected two-coordinate structures **Sb-2c**, **Sb-3c**, **Bi-2c** and **Bi-3c** the active space consisted of the np_x and np_y and the three combinations of ligand σ-donor orbitals and the np_z orbital giving five-orbital active spaces. Calculations with larger active spaces in case of the two-coordinate systems were attempted, but they invariably led to the rotation of $4d$ or $5d$ orbitals, for Sb and Bi respectively, into the active space. Inclusion of both the ligand orbitals and d orbitals of similar energy into the calculation would have lead to active spaces that are not computationally feasible. In order to keep the electron correlation treatment balanced, all ligand orbitals besides the σ-donating orbitals were then removed from the active spaces of **Sb-2c**, **Sb-3c**, **Bi-2c** and **Bi-3c**. All roots up to an energy cutoff of roughly 50,000 cm^{-1} were solved in the SA-CASSCF calculations. The numbers of roots and

other details are summarized in Table Table S1. All roots were treated using the same set of SA orbitals.

In the SA procedure, only states which arise from the target electron configuration were given non-zero weights for the orbital optimization procedure. In case of np^3 systems, this means that only states which correspond to a leading configuration where three electrons occupy the np_x and np_y orbitals were given non-zero weights. In practice this means the two lowest-energy spin doublets. In case of the np^1 system $[PhSb]^+$ this also means the two lowest-energy doublets. In case of the the np^2 systems PhSb, **4** and **5**, this means the lowest-energy spin triplet and the three lowest-energy spin singlets. Without this constraint, in some cases, the target orbitals rotated out from the active space during the SA-CASSCF iterations.

Electron correlation effects outside the active space were approximated by the second-order N-electron valence state perturbation theory (NEVPT2) in its strongly contracted formulation.[48–50] SOC was introduced with the well-established quasi-degenerate perturbation theory (QDPT) process[51,52] where the spin-orbit coupled Hamiltonian is constructed in a basis of the SA-CASSCF eigenstates using the spin-orbit mean-field (SOMF) approximation[53–55] to the SOC operator. The NEVPT2 correction was included as energy shifts of the diagonal elements of the spin-orbit coupled Hamiltonian. Scalar relativistic effects were treated with the standard second-order Douglas–Kroll–Heß (DKH) transformation[56,57]. DKH-def2-TZVP basis sets[58] were used for C, N and Si atoms, DKH-def2-TZVPP basis sets[58] were used for Ga, Ge, As, Se and Br atoms and SARC-DKH-TZVPP basis sets[59,60] were used for the heavier main-group atoms. In case of the larger structures **4**, $[\mathbf{4}]^-$, **5** and $[\mathbf{5}]^-$, H atoms were treated with the smaller DKH-def2-SVP basis set to reduce computational costs while in case of the other structures, the DKH-def2-TZVP was used for H atoms as well. Auxiliary basis sets used in the integral transformation were generated using the `AutoAux` feature in ORCA.[61] The **g** tensors were calculated with the SINGLE_ANISO module[16,62] as interfaced to ORCA.

2.3 Reduction potential calculations

The Gibbs free energy differences ΔG_r for the reduction processes from **4** to $[\mathbf{4}]^-$ and **5** to $[\mathbf{5}]^-$ were calculated using a compound method. The nuclear vibration, rotation and translation contributions to the internal energy and entropy (U_{nuc} and S_{nuc}, respectively) were evaluated using the standard approach assuming an ideal gas based on the results of the GGA frequency calculations as implemented in ADF. The low-frequency vibrations were corrected using the free rotor interpolation approach.[63] The thermal correction to the electronic internal energy at 298.15 K is less than 10^{-6} kJ mol^{-1} in all systems considered due to the large energy difference between the ground and excited manifolds of states. Thus, the only electronic correction to the free energy taken into account is the contribution from the ground state degeneracy to the entropy following the standard expression[64]:

$$S_{\text{elec}} = R \log Z_{\text{elec}}, \tag{S61}$$

where R is the molar gas constant and the partition function Z_{elec} is 1 in the case of a singlet grounds state (**4** and **5**) and 2 in the case of a doublet ground state ($[\mathbf{4}]^-$ and $[\mathbf{5}]^-$). The ground state electronic energy was first evaluated using the domain-localized pair-natural orbital coupled cluster method with perturbative triple excitations (DLPNO-CCSD(T))[65–69] at scalar-relativistic level using the second-order DKH transformation. The electronic fine structure was then calculated using the results of the multireference calculations. The electronic

Table S1: Details of the SA-CASSCF calculations

			Number of spin states solved			
System	Electrons	Orbitals	Singlets	Doublets	Triplets	Quartets
$[PhSb]^+$	9	10		20		0
PhSb	10	10	9		12	
As-1a	5	4		3		0
As-1b	11	10		13		7
As-1c	7	5		3		0
As-1d	11	9		8		3
At-1a	5	4		4		3
Bi-1a	5	4		4		3
Bi-1b	11	10		14		8
Bi-1c	7	5		3		0
Bi-1d	11	9		8		3
Bi-2c	7	5		3		1
Bi-3c	7	5		7		1
Ga-1a	5	4		7		3
Ge-1a	5	4		3		0
Ge-1b	11	10		18		7
Ge-1c	7	5		2		0
Ge-1d	11	9		9		3
I-1a	5	4		3		1
Pb-1b	11	10		19		8
Pb-1d	11	9		11		3
Po-1a	5	4		6		3
Sb-1a	5	4		3		0
Sb-1b	11	10		13		8
Sb-1c	7	5		3		0
Sb-1d	11	9		8		3
Sb-2c	7	5		3		0
Sb-3c	7	5		3		0
Se-1a	5	4		3		0
Sn-1a	5	4		3		0
Sn-1b	11	10		19		8
Sn-1c	7	5		3		0
Sn-1d	11	9		13		4
Te-1a	5	4		3		1
4	10	10	8		10	
$[\mathbf{4}]^-$	11	10		16		8
5	10	10	8		10	
$[\mathbf{5}]^-$	11	10		16		8

internal energy U_{elec} was calculated by adding a SOC correction to the DLPNO-CCSD(T) ground state energy. The correction was calculated as the energy difference between the lowest NEVPT2 eigenvalue before (E_0(NEVPT2)) and after (E_0(NEVPT2+SOC)) the inclusion of SOC by QDPT:

$$U_{\text{elec}} = E_0(\text{DLPNO-CCSD(T)}) + E_0(\text{NEVPT2+SOC}) - E_0(\text{NEVPT2}). \tag{S62}$$

Solvation effects were implicitly taken into account in the DLPNO-CCSD(T) calculation and are included in the DLPNO-CCSD(T) ground-state energies. The implicit solvation effects were treated using the conductor-like polarizable continuum model (C-PCM) as implemented in ORCA.[70] The default parameters for acetonitrile as a solvent were used. The DLPNO-CCSD(T) calculations were carried out using cc-pVTZ-DK basis sets for all atoms[71,72] and the auxiliary basis sets were generated with the `AutoAux` feature[61] in ORCA. The values of the different energy components and corrections are listed in Tables Table S2 and Table S3. The reduction potential versus the standard hydrogen electrode (SHE) was then calculated from the free energy difference ΔG_r as

$$E^0_{\text{rel,SHE}} = -\frac{\Delta G_r}{F} - E^0_{\text{SHE}}, \tag{S63}$$

where

$$\begin{aligned}\Delta G_r =& U_{\text{elec}}(\text{anion}) - U_{\text{elec}}(\text{neutral}) + U_{\text{nuc}}(\text{anion}) - U_{\text{nuc}}(\text{neutral}) \\ &- T\big(S_{\text{elec}}(\text{anion}) - S_{\text{elec}}(\text{neutral}) + S_{\text{nuc}}(\text{anion}) - S_{\text{nuc}}(\text{neutral})\big),\end{aligned} \tag{S64}$$

F is the Faraday constant and $E^0_{\text{SHE}} = 4.6\,\text{V}$ is the experimentally determined absolute value of the SHE reduction potential in acetonitrile.[73] In the ideal gas approximation the enthalpy correction pV cancels out in the free energy difference and is not explicitly taken into account.

Table S2: Energy components used in the calculations of the reduction potential of **4** in Hartree atomic units

	4	$[\mathbf{4}]^-$
E_0(DLPNO-CCSD(T))	−23680.28252594	−23680.38536387
E_0(NEVPT2)	−23678.70199013	−23678.73739986
E_0(NEVPT2+SOC)	−23678.72208864	−23678.74931486
U_{elec}	−23680.30262445	−23680.39727886
U_{nuc}	1.07106312	1.06795482
S_{elec}	0.00000000	0.00000220
S_{nuc}	0.00046412	0.00046618

Table S3: Energy components used in the calculations of the reduction potential of **5** in Hartree atomic units

	5	$[\mathbf{5}]^-$
E_0(DLPNO-CCSD(T))	−23145.14066008	−23145.24041907
E_0(NEVPT2)	−23143.66470561	−23143.70446831
E_0(NEVPT2+SOC)	−23143.68438805	−23143.71601001
U_{elec}	−23145.16034252	−23145.25196077
U_{nuc}	0.93754860	0.93492996
S_{elec}	0.00000000	0.00000220
S_{nuc}	0.00043527	0.00043412

3 Additional computational data

Table S4: Calculated bond lengths in Ångströms

	a		b		c		d	
Ga-1	2.612		2.308		19.832		2.347	
Ga-2	25.128	18.127	2.365	2.364	12.943	12.044	2.315	2.315
Ga-3	40.501	19.816	12.565	23.670	16.935	33.783	10.338	29.978
In-1	2.754		2.516		18.462		2.569	
In-2	41.939	36.916	2.517	2.517	17.178	16.438	2.621	2.620
In-3	38.394	74.113	2.562	17.506	26.941	48.765	2.600	15.473
Tl-1	2.802		2.602		23.236		2.640	
Tl-2	44.636	37.756	2.712	2.711	13.740	13.694	2.689	2.686
Tl-3	39.401	66.668	7.738	17.889	24.858	50.699	8.486	29.882
Ge-1	2.260		2.059		2.211		1.990	
Ge-2	2.311	2.309	2.091	2.091	2.205	2.180	2.032	2.030
Ge-3	2.260	33.034	2.080	13.483	2.207	21.430	1.993	20.971
Sn-1	2.471		2.287		2.417		2.239	
Sn-2	2.531	2.531	2.320	2.320	20.208	19.172	2.273	2.273
Sn-3	2.457	25.871	2.311	13.296	20.636	43.614	2.304	8.076
Pb-1	2.622		2.448		2.609		2.406	
Pb-2	2.743	2.742	2.493	2.492	20.234	18.976	2.454	2.453
Pb-3	2.621	52.118	2.485	14.079	37.533	76.608	2.503	8.193
As-1	2.098		1.962		2.011		1.923	
As-2	2.129	2.129	1.991	1.989	20.244	2.012	2.020	2.016
As-3	2.098	21.174	13.949	1.971	2.012	36.910	1.944	5.050
Sb-1	2.314		2.187		2.206		2.152	
Sb-2	2.354	2.354	2.211	2.207	2.614	2.511	2.243	2.240
Sb-3	2.314	33.624	2.197	13.685	2.426	3.120	2.178	5.163
Bi-1	2.440		2.322		2.342		2.291	
Bi-2	2.522	2.522	2.352	2.341	2.678	2.653	2.621	2.620
Bi-3	25.169	2.442	2.332	14.672	2.624	3.043	2.435	2.967
Se-1	2.025		1.905		1.873		1.861	
Se-2	3.232	2.032	1.999	1.999	2.169	2.161	2.357	1.908
Se-3	2.032	2.918	1.928	2.867	2.072	2.562	1.881	2.817
Te-1	2.246		2.127		2.069		2.101	
Te-2	2.500	2.462	2.315	2.314	2.330	2.326	2.329	2.324
Te-3	2.255	3.014	2.147	2.988	2.279	2.679	2.107	2.928
Po-1	2.367		2.248		2.187		2.231	
Po-2	2.595	2.595	2.463	2.461	2.434	2.434	2.468	2.466
Po-3	2.376	3.076	2.269	3.040	2.401	2.753	2.411	2.673
Br-1	2.188		1.867		1.846		1.817	
Br-2	3.060	2.065	1.942	2.999	2.104	2.111	16.378	1.856
Br-3	2.082	2.739	1.922	2.760	2.038	2.421	1.888	2.649
I-1	2.582		2.075		2.025		2.038	
I-2	3.080	2.292	2.339	2.337	2.245	2.245	2.306	2.300
I-3	2.293	2.826	2.151	2.822	2.207	2.539	2.189	2.552
At-1	2.644		2.193		2.136		2.164	
At-2	3.084	2.422	2.443	2.443	2.343	2.341	2.421	2.416
At-3	2.419	2.885	2.267	2.878	2.320	2.618	2.346	2.604

Table S5: Calculated QTAIM spin densities for the main group atom

	a	b	c	d
Ga-1	0.9035	1.6924	1.0000	1.5164
Ga-2	1.0000	0.8245	0.0000	−0.0440
Ga-3	1.0000	1.0038	0.9998	1.7365
In-1	0.9081	1.3783	1.0000	1.2076
In-2	1.0000	−0.4053	1.9999	−0.0793
In-3	2.0000	1.0577	1.0000	0.8135
Tl-1	0.9097	1.2123	1.0000	1.0338
Tl-2	1.0000	−0.0506	1.9997	−0.0751
Tl-3	1.0000	0.9958	1.0000	0.5151
Ge-1	0.9168	0.9921	0.9488	0.9461
Ge-2	0.1630	−0.0060	−0.0120	0.0146
Ge-3	0.9172	0.9795	0.9473	0.9474
Sn-1	0.9315	0.9919	0.9518	0.9580
Sn-2	0.2822	−0.0012	1.0000	0.0143
Sn-3	0.9285	0.9776	1.0000	0.8826
Pb-1	0.9482	0.9880	0.9608	0.9697
Pb-2	0.5386	0.0074	1.0000	0.0225
Pb-3	0.9479	0.9818	1.0000	0.8927
As-1	0.9450	0.9755	0.9045	0.9573
As-2	0.0727	0.0082	0.9039	0.0678
As-3	0.9456	0.9709	0.9046	0.9514
Sb-1	0.9567	0.9803	0.9253	0.9714
Sb-2	0.1590	0.0224	0.9220	0.1326
Sb-3	0.9571	0.9767	0.9254	0.9609
Bi-1	0.9713	0.9906	0.9414	0.9847
Bi-2	0.3741	0.0322	0.9292	0.8527
Bi-3	0.9719	0.9859	0.9322	0.8882
Se-1	0.9537	0.7791	0.7357	0.7413
Se-2	0.1631	0.0834	0.6263	0.3597
Se-3	0.6601	0.6251	0.6795	0.5746
Te-1	0.9718	0.8539	0.7928	0.8379
Te-2	0.2989	0.3320	0.7037	0.5752
Te-3	0.6998	0.6735	0.7602	0.6519
Po-1	0.9862	0.8939	0.8183	0.8837
Po-2	0.3170	0.4287	0.7560	0.7112
Po-3	0.7294	0.7054	0.8079	0.6654
Br-1	0.8265	0.3307	0.5544	0.3105
Br-2	−0.0020	0.0325	0.2146	0.2244
Br-3	0.3672	0.2925	0.2627	0.1705
I-1	0.9846	0.4585	0.3853	0.4615
I-2	−0.0036	0.1618	0.3018	0.3424
I-3	0.4698	0.4349	0.3677	0.3598
At-1	0.9991	0.5318	0.4115	0.5418
At-2	0.0065	0.1808	0.3259	0.4065
At-3	0.5181	0.4837	0.3975	0.4447

4 Optimized Cartesian coordinates

Ga-1a

C	6.60080243481170	2.18636250066867	7.87152671815483
C	6.18010493181535	1.25619448433687	6.76925842587585
H	5.08752549896550	1.13972795564431	6.72436728604866
H	6.61074160741467	0.24930343218333	6.89107163745707
H	6.52149914299621	1.64456233907031	5.74698583049095
C	5.96105930133267	3.53630491299146	7.71075888676847
H	4.86341564591063	3.47014458751906	7.68363668775685
H	6.29344817220207	4.03611547082327	6.73579259983800
H	6.23042287605160	4.22076631916312	8.53100093208715
C	8.09549329054303	2.29270783667436	7.96754319787976
H	8.57229046028534	1.31371105639942	8.12786054568027
H	8.41337773897719	2.93476352562049	8.80243720144201
H	8.54642362037319	2.73519547517851	7.00870478677186
Ga	5.70378567971503	1.18364417918448	10.10999782254219

Ga-1b

H	1.11449325900637	-0.15442863445867	2.16504443577540
C	0.57019529761326	-0.07086393584989	1.20345396471977
C	-0.83089167128429	-0.00473077915229	1.18433330736999
H	-1.37183597233904	-0.03359136529698	2.13817457840185
C	-1.57753460792850	0.07864224374369	-0.01080471489892
Ga	-3.88551379454639	0.11840317098828	-0.03327924651184
C	-0.80621367656798	0.12117359230288	-1.19241934256532
H	-1.32724507366496	0.19439253943769	-2.15490478343777
C	0.59505007966711	0.05595338560472	-1.18916471021113
H	1.15909729111309	0.07407174768952	-2.14269675389187
C	1.30232659744736	-0.05046625023566	0.01236957323196
H	2.41716227148398	-0.12542571477331	0.01991369201787

Ga-1c

N	-0.76607574061262	-0.67758953338675	-0.34328854408036
Ga	-11.08454104554357	15.25154527723151	5.41071103776134
Si	0.45207569771217	0.21549007348696	-1.05438875198855
Si	-1.13634277974801	-2.11702678704793	0.42233543650752
H	1.39633511401278	-0.51293476052853	-2.04363858161311
H	-0.03226457082154	1.41160227539749	-1.90940324499606
H	1.47415480854827	0.90047170378543	-0.11369010373412
H	-0.58572338175334	-3.42034848178907	-0.20559406087723
H	-0.68589895706303	-2.27010640324133	1.89738848618775
H	-2.64930914473109	-2.43091336390774	0.52721832683280

Ga-1d

C	0.92899610056405	2.31380656503026	-0.21452588162087
C	-0.31509987734205	2.33958079742248	0.33727758723834
N	1.44947881404663	3.57991253885801	-0.04502490691108
N	-0.48694806928987	3.62786144410170	0.81718542549901
C	0.59726326875359	4.43135161758835	0.59543260790430
H	2.38815620037877	3.86611703815932	-0.36582611671445
H	-1.31853013219254	3.97993170793739	1.29305330208242
H	-1.07364813390451	1.55407495452280	0.42052806586276
H	1.48247931054688	1.50901690629826	-0.70990653836943
Ga	0.78863251843906	6.68236643008144	1.23203333797900

Ga-2a

Ga	7.17604856620273	16.88311338640805	15.13680413226518
C	3.29424368432275	-0.90620482407562	-2.18088182555596
C	2.36584825979942	-0.13781088311389	-1.29001363064164
H	2.51210407863044	0.95548902237119	-1.36527859827633
H	2.46687954763834	-0.40715423488492	-0.22369081720403
H	1.26102140537770	-0.31438108990989	-1.56025801435205
C	3.07958501438211	-2.38352047505116	-2.01382915673365
H	2.01804582808602	-2.69955558111149	-2.32331640680685
H	3.19038337119864	-2.71639469089557	-0.96484817262907

H	3.75711190442580	-2.99155225548051	-2.64165079054128
C	3.12673385627322	-0.49769280399807	-3.61236626000306
H	3.76845442781870	-1.07326026138115	-4.30005356817763
H	3.33397732851367	0.57658344153493	-3.79765309185751
H	2.05204531489527	-0.65517014723967	-3.98610966835543
C	4.26249054871265	-0.11805017408718	9.56409770761748
C	3.14249193525977	-1.09199753027812	9.31127857328953
H	3.42927186103262	-2.12818487062107	9.56334556312211
H	2.81675532891101	-1.09752101253399	8.25740940650138
H	2.21373587839612	-0.86636179039989	9.94111779558864
C	3.84155631321491	1.27587065500503	9.19721908709952
H	2.93879961577338	1.63130854067314	9.79452630440766
H	3.57256727328217	1.37074804232153	8.13133816797058
H	4.64163637115031	2.01348477284385	9.39470099810848
C	4.66229116557048	-0.18121653379492	11.01664802328305
H	5.48886550115591	0.50985870479814	11.24864303150797
H	4.99967688553118	-1.19172046835645	11.30561195531788
H	3.80933473444468	0.09162106125776	11.72803025505507

Ga-2b

H	0.14667534704239	-1.22362583674833	2.31016492881462
C	0.07201556505024	-0.76979043837256	1.30091211521422
C	-1.16063975492413	-0.74839751443499	0.62660890437275
H	-2.03206835982181	-1.18509874918149	1.11961629879843
C	-1.31978679984158	-0.18709856711757	-0.65893939225677
Ga	-3.27691417559618	-0.05480730108675	-1.97823637624082
C	-0.13990875887033	0.35234868786259	-1.21346688307559
H	-0.20081474424902	0.80381210989954	-2.21380258509118
C	1.09907732086037	0.34099485773828	-0.55507156368601
H	2.00358737523047	0.78067813839999	-1.03452847453582
C	1.21996377448080	-0.22492939706674	0.71845740695396
H	2.20532706532728	-0.23928597549609	1.25101175815516
H	-3.95627226463627	-1.60818696311781	1.11006260961972
C	-4.92622306837910	-1.58148221399049	0.60869348735012
C	-6.03986347983063	-2.12330360089594	1.27284399380053
H	-5.92429623706167	-2.56758418292613	2.28275786200024
C	-7.30524683165764	-2.11436871116172	0.67935116833828
H	-8.19669293010041	-2.54528807939325	1.20342960320160
C	-7.42448616284550	-1.54758020788082	-0.59376756401063
H	-8.42614649107361	-1.53137808476145	-1.08154035727643
C	-6.30107773556543	-1.01158247677183	-1.24178325834367
H	-6.42869682910417	-0.57444530393461	-2.24235645764537
C	-5.00879182443406	-1.00245018956182	-0.67609722445734

Ga-2c

N	2.16466828564808	-8.50246861107698	-1.29953502731914
Ga	-2.70822930380597	3.39781304410478	-2.76820566765743
Si	3.08467473023177	-9.87547457169394	-1.18680602985695
Si	1.94628272971856	-7.10175632640084	-0.41235743215451
H	3.25109140129394	-10.63574662704441	-2.50840076990789
H	4.53805150636156	-9.75743403283555	-0.69596809729483
H	2.55132668029682	-10.98978250852833	-0.25510770129170
H	0.89860919121478	-7.17573048498118	0.71291658902519
H	3.15334790930861	-6.49532134510289	0.32641800483412
H	1.43848625601257	-5.91554409952312	-1.23334302276960
N	-6.74527026917704	14.03267231294737	1.18775077510675
Si	-6.37042570723064	14.32028453620088	2.77967391493444
H	-4.95446958884247	13.90258097652889	3.14809896607904
H	-7.22325397686359	13.63644541881629	3.86285727046314
H	-6.41374013237566	15.78552223547456	3.25431019770680
Si	-8.06587086514325	14.13898810591506	0.19291222108694
H	-7.75455922535084	13.84242570546238	-1.26564605153849
H	-8.78584257621254	15.49935621785375	0.09649338337968
H	-9.24849704508469	13.20413005388337	0.48163847717446

Ga-2d

C	0.90902729276694	3.26513367560435	0.64204500741368
C	-0.20381690177200	3.67962175845828	1.31310476497284

N	1.39141475894447	4.38357739628060	-0.01397060148010
N	-0.35136530344228	5.02176825454899	1.02720520107002
C	0.64223153747269	5.50843049142432	0.21751127540775
H	2.26600311613230	4.44350443364916	-0.54171501420541
H	-1.12515496539690	5.60618204778117	1.39108040358663
H	-0.89166971455241	3.14319434174732	1.96703487915279
H	1.39586306642986	2.29289777828342	0.59824657652852
Ga	1.13071505248868	7.48288685947634	-0.88709284597161
C	0.84751881139603	8.51114350917563	1.16774451248271
N	-0.10706503576888	8.55311913256886	2.15101282850010
N	1.73296022247750	9.46616257092018	1.59614176772249
C	0.19106639283126	9.45479539693985	3.15274785714103
C	1.36701415102704	10.04720239550129	2.79700147847295
H	-0.95782379367932	7.96280081061373	2.14170723225075
H	2.61183746155356	9.62085781086016	1.09527659735218
H	1.96938605007554	10.80025165078137	3.30205116994795
H	-0.44815219898406	9.59104968538492	4.02526690965473

Ga-3a

Ga	19.10399150355418	12.50489027502345	6.50487750964537
Cl	-15.04486775593140	-8.39421596397840	0.39135560056231
C	3.74639708361369	-0.00013922166031	5.85438565981536
C	4.21138432480803	-1.36833611790524	6.24689165653207
H	5.27537575966728	-1.56461442149656	5.99617713343679
H	3.60811160720363	-2.17676016444504	5.78505019552569
H	4.12918790693563	-1.54352391637724	7.37865286430522
C	2.27625473247577	0.14938004865346	6.10383424986745
H	2.01891998362332	0.07875228994760	7.22027482074624
H	1.67530502875611	-0.64142224878493	5.61407436970575
H	1.87153892815984	1.12302280986749	5.76467134450812
C	4.52955667500676	1.05693164742990	6.57168854214286
H	4.24892447355067	2.08569035466234	6.27852616063094
H	5.61826863148184	0.95613159171067	6.42237671725352
H	4.37363611709472	1.00924603735282	7.70793417532224

Ga-3b

H	-1.64199130667176	0.15665481895318	-2.15176776566730
C	-1.17168724733728	0.26143551420788	-1.16620313965406
C	-0.43497265986446	1.41046855607550	-0.83476453333273
H	-0.35060779155140	2.17097860605394	-1.63190841696945
C	0.20297026821449	1.65824731812779	0.41735810128406
Ga	-6.82966689190928	-3.17228614195094	-8.80663297956881
C	0.00800850362561	0.57984981982222	1.32197118122668
H	0.44830894780745	0.63857859378070	2.33194646162863
C	-0.71450753488465	-0.59431581328532	1.03313198877756
H	-0.82329507042314	-1.38150054277693	1.79348242065244
C	-1.31492402234559	-0.76275692346147	-0.22237813834754
H	-1.87439322452615	-1.67069072840009	-0.46656488902533
Cl	5.58890802986619	1.03694692285353	10.89939970899570

Ga-3c

N	-2.31337942875794	0.62569194443035	0.84229370348711
Ga	7.86272800735338	1.82337484617938	14.32603056857861
Si	-1.79362332143606	1.88756150327977	-0.10799283254573
Si	-1.92445903267398	-0.98695520413150	0.98322760704021
H	-2.66924541794392	3.13287460061354	0.02444123294616
H	-0.39038291107258	2.44959488104569	0.15403294442218
H	-1.75882627663811	1.67105729342375	-1.62839095728176
H	-2.91606782515981	-1.76493357432996	1.84862617389679
H	-1.88639328976202	-1.82505865116569	-0.30549710913109
H	-0.57915223540719	-1.34507893784054	1.62521536646637
Cl	-8.92461826850173	4.90158129849518	-14.82871669787873

Ga-3d

C	0.01712148348899	3.53063296418389	-0.27963126570059
C	0.92572018324382	3.74095750413574	0.70881757197450
N	0.31325389186118	2.28383703452315	-0.80070286665531

N	1.73392246076163	2.61333960083577	0.71932677322558
C	1.38275141780882	1.66986154918470	-0.21552227000459
H	-0.24675990765326	1.86940120927450	-1.57631014750520
H	2.52512792631879	2.48842294870499	1.35391076426000
H	1.06743512419356	4.57836624948596	1.39133304110290
H	-0.80854825554815	4.13777773533907	-0.64901726645597
Ga	9.57506336417635	-1.69245978488754	5.11787209186298
Cl	-11.03679768865170	19.33920298922002	-0.49573642610429

In-1a

C	6.60180966220944	2.19021665152008	7.86194163177691
C	6.18476404508949	1.25957440651688	6.75853911511012
H	5.09088415184334	1.14849472502132	6.70689000703278
H	6.60826734665880	0.25020322106044	6.88598728029467
H	6.53415668657950	1.64054408639830	5.74045496330532
C	5.96403767291185	3.54150404368106	7.70076543585938
H	4.86587484104319	3.47580805961194	7.66687833961916
H	6.30259505634977	4.04627139541002	6.73442167808594
H	6.22395108751073	4.22327707779424	8.52652376820901
C	8.09710451796610	2.29619534696660	7.95673787876771
H	8.57219865472526	1.31542055065452	8.11411757572621
H	8.41507919743075	2.93737671397050	8.79326970392261
H	8.54342026001210	2.73872949448370	7.00224968699869
In	5.67624722106387	1.13588830236806	10.23216549408544

In-1b

H	1.11315279800753	-0.15494131180899	2.16856201831767
C	0.58178355472968	-0.08062391308479	1.20239700723010
C	-0.81824343501047	-0.02012488149342	1.16766675874169
H	-1.36376680997053	-0.04834586092540	2.11895113815372
C	-1.55788563133297	0.07408662569660	-0.02888925909472
In	-4.07128136098210	0.16989090545221	0.03848005843366
C	-0.78207967180184	0.10464761986065	-1.20683871026097
H	-1.29240386673722	0.17865897641042	-2.17549167951306
C	0.62050924735721	0.04523330902803	-1.19367853347942
H	1.18103128876690	0.07329232699743	-2.14201605391577
C	1.31981005813021	-0.04662482971256	0.01586722173041
H	2.42846382884361	-0.09201896642019	0.03501003365669

In-1c

N	-0.87336221411346	-0.60009481128532	-0.40579273375978
In	-11.18452201390861	14.02680939323461	4.13184333490487
Si	0.40308943033511	0.33094579272151	-0.89835372389198
Si	-1.09343442500464	-1.97488576797348	0.50623795109585
H	-0.00614921042816	1.71555586790665	-1.39078011984051
H	1.51047645001423	0.65219910869398	0.11808957717173
H	1.24188787770468	-0.19320863624870	-2.07858881988439
H	-2.44207264026065	-2.65093498660078	0.27305833160397
H	-0.11064359887447	-3.13994513864615	0.30277780797371
H	-1.06285965546404	-1.81625082180230	2.02915839462652

In-1d

C	0.94009218000131	2.29372628000036	-0.21628387097891
C	-0.31293019868614	2.30797927405288	0.32312238123003
N	1.44590616483718	3.56305321639919	-0.03143011670781
N	-0.49897739879943	3.59193779101550	0.80977085710161
C	0.58067571117024	4.40557095109063	0.60313624503156
H	2.37729094386252	3.87656621318496	-0.33279833770316
H	-1.33580332633328	3.94405174668582	1.27456473567439
H	-1.06090685088861	1.52061398103884	0.39331573412164
H	1.50270908379031	1.49735828720080	-0.70791008136444
In	0.80272369104590	6.88316225933100	1.24471245359510

In-2a

In	20.78641294405005	30.99867267913199	16.23538842663225
C	1.28391578144907	0.26268610923934	-4.59322101716175

C	0.34463206179315	-0.24607922035874	-5.64940972788618
H	0.51224377311293	0.22668879333816	-6.63324641463688
H	-0.71631357637515	-0.09005353268338	-5.38678481613233
H	0.46230204549146	-1.37705248888077	-5.82292960937226
C	0.99994285872088	-0.42774613704264	-3.28989746499654
H	1.14417178128780	-1.56339839850472	-3.36712810331205
H	-0.03805759333452	-0.27834091176808	-2.94475350045820
H	1.66668405556889	-0.09401369269331	-2.47642861337141
C	2.70120175947126	-0.01726502215559	-5.00675220019458
H	3.43861644451311	0.31511706387649	-4.25617456614758
H	2.96857131206963	0.46405753426553	-5.96425172600090
H	2.88735065418195	-1.14012524898662	-5.16115580093140
C	4.75087258935423	-1.99446813482314	12.10198579446419
C	3.85544005906435	-2.96950959234185	12.81392569069785
H	4.17183175622831	-3.15525546908876	13.85573017939718
H	3.80211671153204	-3.94964261935996	12.30795033203750
H	2.77072530298773	-2.59332240029829	12.87901854597524
C	4.23513976666742	-1.77267958724108	10.70592200385346
H	3.16209925241830	-1.37245185746324	10.70630236705910
H	4.21288322144345	-2.70113985609600	10.10995964549890
H	4.83610257921951	-1.03709217742398	10.14437949122670
C	4.76114112442763	-0.68908324389498	12.84796890225124
H	5.40511192451853	0.07080606920845	12.37228007274031
H	5.10184343883920	-0.80047316310339	13.89248164224180
H	3.71497397129882	-0.21850749485118	12.90966146652634

In-2b

H	1.00435546574163	-0.64202768184523	2.27609965030833
C	0.54031291768658	-0.45087446617900	1.29116719356570
C	-0.76867630928571	0.05631449974350	1.22060630886534
H	-1.30615882751366	0.25497707030299	2.15671913531926
C	-1.41721530984510	0.33354585486583	-0.00135740879860
In	-3.63812863798090	1.51184970766275	-0.12880107921438
C	-0.65057360128041	0.05266461717645	-1.15214838143726
H	-1.09875670219562	0.24587894388430	-2.13449991603779
C	0.65793383539484	-0.45444048233073	-1.10001560246141
H	1.22000861207798	-0.64948022594865	-2.03529915150692
C	1.27440818327061	-0.70882534880761	0.12816943954316
H	2.32212342442751	-1.09704844912305	0.17664423843405
H	-5.15829351506632	-0.70133764443284	2.11989950790336
C	-5.58488413738063	-1.07388514879940	1.17970242858475
C	-6.54822856112347	-2.09573732219435	1.23635826547472
H	-6.85810918969417	-2.50634046825247	2.21464926820557
C	-7.13450343392699	-2.59620903173603	0.06844152232342
H	-7.91387149001697	-3.39739611187537	0.10653287274871
C	-6.72150497468263	-2.05291261308467	-1.15110738616730
H	-7.17225349125745	-2.43264562847432	-2.09014730356877
C	-5.75699280311278	-1.03291136446959	-1.18935572412864
H	-5.46111042472878	-0.62807599507385	-2.16493508323669
C	-5.15116102950753	-0.49793271100865	-0.03300279471862

In-2c

N	2.48004552005515	-9.36756966578310	-0.67765877890728
In	-11.59473767880236	-0.32634836931167	3.22446227321118
Si	2.77985244203898	-8.20976655536918	-1.82759129264349
Si	1.44018510589766	-9.53176435658886	0.60947578491445
H	4.09593393479650	-8.43855479821847	-2.57188459907061
H	1.78788759457440	-8.08025418715624	-2.99019602414125
H	2.91560906791459	-6.75182922126469	-1.37120454548554
H	1.83711431022839	-10.67385666300038	1.54094755946705
H	1.31108494072727	-8.34486514593929	1.56868484063428
H	-0.02036002152282	-9.86094386212680	0.29228340719606
N	-5.27971923890722	14.59158408738436	0.43417637050371
Si	-4.71136104614465	15.65015428195252	1.58665803507915
H	-3.26459951923884	15.39090206784944	1.98592853419850
H	-5.44133918122023	15.69405906503180	2.93636874732515
H	-4.68218603758870	17.14179538872568	1.21014152137260
Si	-6.77996807906533	14.22645226060855	-0.17964789815743
H	-6.74632278296239	13.04624102024652	-1.13944754063977

H	-7.48246108612459	15.30885634092765	-1.02022500809995
H	-7.88827824465588	13.84666831203214	0.80642861324313

In-2d

C	1.31967303094210	4.27554677991396	1.38179655475450
C	-0.02030778747449	4.28871766943720	1.63275771492638
N	1.51214122347535	5.13211939543713	0.31269092383635
N	-0.57010005805118	5.15346188904172	0.70352359648466
C	0.35857381957546	5.70649935255727	-0.12172129039919
H	2.42549818733800	5.41844027708818	-0.06472256775343
H	-1.55294203262145	5.45742775579276	0.68138423333102
H	-0.61033326629711	3.79057288651548	2.39981900512390
H	2.13750248659819	3.76340114448911	1.88516081576748
In	0.09227028004675	7.80580763697214	-1.66620529549192
C	0.55221168205536	8.57908012017714	0.79503032113232
N	-0.33506187812414	8.66754809292512	1.82179516069410
N	1.74845832631751	8.64578014870414	1.43844432409732
C	0.27747670360042	8.75981184002434	3.05861279852839
C	1.61821889184579	8.74726389923345	2.81185844837438
H	-1.34615043650253	8.55848964925449	1.66471759741848
H	2.63461317882288	8.51727697223557	0.93172350148435
H	2.47084570953992	8.76794504867012	3.48794727468826
H	-0.27839323903043	8.79353594554925	3.99377323024731

In-3a

In	38.04708497062136	14.49619383344221	13.53490774758743
Cl	-33.10510326147931	-4.46601634872407	5.13224770094963
C	3.82421931843237	-0.65898186883938	4.97737276919505
C	4.54596077788732	-1.38416328337440	6.07559323542701
H	5.61700563583831	-1.12275853197007	6.12953237953682
H	4.48136752439471	-2.48180690120097	5.97709859160327
H	4.11501983994287	-1.13879495204471	7.11194854364882
C	2.37583182382791	-1.05318158535517	4.97072148643726
H	1.85070629267211	-0.79445414232446	5.95953077524610
H	2.23028841877596	-2.13827602656172	4.82956621244750
H	1.79875656339190	-0.54003141275243	4.18202788071128
C	3.94696516403939	0.82348948862167	5.18092321669610
H	3.42924556567860	1.40571568588965	4.39903380143570
H	4.99615217867739	1.16537626488195	5.20238364943256
H	3.48848418729890	1.16272278031193	6.17788300964555

In-3b

H	0.68071376842411	-1.02898833248215	1.54091305098949
C	0.15894917274442	-0.75770363595940	0.60913080797147
C	0.41831074147143	-1.47143380618248	-0.56527941239886
H	1.13552689308184	-2.30153815956925	-0.52075897300247
C	-0.21811345676975	-1.19154475367367	-1.79550925875991
In	0.27952077989425	-2.57510873672840	-3.89332291516708
C	-1.13843725274112	-0.12225184072111	-1.76581599542213
H	-1.66187882513173	0.15078411058796	-2.69085520697223
C	-1.41881752081552	0.60153228528678	-0.59539443114649
H	-2.16815867784022	1.41163304690227	-0.61585858982943
C	-0.76931028716370	0.28575334454895	0.60789986321656
H	-0.99562032503900	0.83345631933685	1.53584611692422
Cl	-3.21053501011501	6.49702015865367	10.66607494359669

In-3c

N	-1.87160626901736	0.69052259169873	0.77488584662788
In	19.65177092217077	7.32836689329969	15.55643541495345
Si	-1.05352651124001	0.44124385850953	-0.64274627529209
Si	-3.36365941196288	1.33693390390449	1.19028340237797
H	-1.07303514769899	1.53123624946929	-1.72880773385141
H	0.45421062515938	0.23785487116104	-0.44422297142890
H	-1.41285323697323	-0.80633061283573	-1.47082386527326
H	-3.74893207631602	2.67746960940520	0.54452981703990
H	-4.59640555348972	0.47054791610349	0.89079147314605
H	-3.48285384495733	1.60686425354421	2.68892694030454
Cl	-16.79652949567457	-4.94499953425982	-14.42598204860416

In-3d

C	0.63611662264245	4.31631039853803	0.57777762854016
C	0.42457816539797	3.33120692415445	-0.34532845530538
N	0.21256680273492	3.79565467892277	1.78764496919467
N	-0.10052128188812	2.26210950494657	0.35457211066707
C	-0.24931937492042	2.50913635826903	1.69198978178389
H	0.21149437034933	4.28407497409980	2.68422291300100
H	-0.36740471644606	1.35290717754957	-0.03314139863013
H	0.63243975154726	3.30520228639811	-1.41040835174506
H	1.01824643086642	5.32424710390828	0.45984390232333
In	-1.13385325588116	0.73778805055589	3.37722165976965
Cl	4.16394648559736	13.34070254265792	-3.87005475959919

Tl-1a

C	6.60533668751262	2.19121799503699	7.86577653726345
C	6.18793546171093	1.26128117899763	6.76217712783055
H	5.09500001190493	1.13706618772862	6.71396220555460
H	6.62411733788590	0.25559947277257	6.87753466808660
H	6.52353729096783	1.65137163625706	5.74277560281321
C	5.96902176510598	3.54231582656912	7.70150807174978
H	4.86967957236538	3.48461993754456	7.68143220828965
H	6.29386131420570	4.03706514912128	6.72476819827417
H	6.24322507338355	4.23346534987800	8.51517717231102
C	8.10128675708215	2.29888160899019	7.95329367517837
H	8.58087935436549	1.32041628120235	8.11330029403641
H	8.42448982963123	2.94764754743451	8.78258821514919
H	8.54350710628102	2.73571830879147	6.99439534759425
Tl	5.61851283899147	1.10283759513330	10.25225323466271

Tl-1b

H	1.13580353836567	-0.15509328399519	2.16769137336621
C	0.59970242938779	-0.08122941262359	1.20852761969861
C	-0.80231221640632	-0.02189940134595	1.19024394144015
H	-1.33457015528527	-0.05123008703605	2.14931375014409
C	-1.55182177419317	0.07233507216500	-0.00170722700690
Tl	-4.15067502380183	0.17698388946502	-0.06901299190349
C	-0.78145787174773	0.10366456372007	-1.18354540201686
H	-1.30179854181029	0.17669273292839	-2.14615368460276
C	0.61876161387755	0.04623747035426	-1.19218891646230
H	1.17243201514174	0.07470880053703	-2.14755580356960
C	1.32606822687709	-0.04646037274872	0.01106535776884
H	2.42895775959477	-0.09157997142028	0.01334198314400

Tl-1c

N	-0.27560309482936	-0.88890000355088	0.10730172932801
Tl	-12.63343263655896	17.86989656981444	6.04830933730681
Si	0.47415223039222	-0.01514199256712	-1.08276867171032
Si	-0.72961788167416	-2.44790433360350	0.43274190701253
H	1.25642681023634	-0.78703885094399	-2.15985488273838
H	-0.43813769252474	0.86892941827073	-1.93403270797228
H	1.51817427130289	0.98190660280061	-0.58935527084304
H	-0.48283798071321	-3.52168124846527	-0.64186142781028
H	-0.09002060474490	-3.07492009406891	1.67284628501616
H	-2.21669342088609	-2.63495606768599	0.73432370241080

Tl-1d

C	0.94185382039881	2.28986442025095	-0.22323628663681
C	-0.31204324480269	2.29653472902740	0.31705285592049
N	1.44605949378024	3.55888225698159	-0.01913415503096
N	-0.49673469435152	3.57260294499127	0.82190166114568
C	0.57897421478187	4.39393216283204	0.62582535029161
H	2.37018849228798	3.88370520947999	-0.31868488512876
H	-1.33714473531925	3.91682050893256	1.28647040175505
H	-1.06146182148466	1.51285876932248	0.37713325673866
H	1.50095165000491	1.50203984727080	-0.72498456099028
Tl	0.81013682470432	6.95677915091091	1.21785636193531

Tl-2a

Tl	29.38764472358845	23.92238633201992	20.49000498993984
C	0.92907843873656	0.63360663156782	-4.80997303352157
C	0.33674654422793	-0.65112514581128	-5.31470176431452
H	-0.50774205101712	-0.48752639695479	-6.00695322150869
H	-0.02751481916790	-1.30020133800448	-4.49949336863771
H	1.10249486070472	-1.27879461286574	-5.89841623172134
C	2.07177386893979	0.33264751320008	-3.88089468194398
H	2.90032525166770	-0.26820297071408	-4.39944520699734
H	1.76504884345197	-0.26654965644196	-3.00666395479470
H	2.55543045367806	1.24695603995535	-3.49584442507736
C	1.42517969610299	1.44525942984014	-5.97224461344820
H	1.89756047122830	2.39301789160810	-5.66090360883366
H	0.62350628514888	1.69662179328490	-6.68900094637934
H	2.22235028397083	0.88359892447832	-6.58247313497407
C	3.66516212601463	-2.45708858462353	12.24481083676372
C	2.49981114899551	-2.10571672682223	13.12821869860795
H	2.65995859664592	-2.39501720133392	14.18209512347019
H	1.55755216715214	-2.57707917530649	12.79733850982596
H	2.29570356585198	-0.97501967451884	13.14231613259168
C	3.37688385540200	-2.01336622894854	10.83708317989472
H	3.22341279783412	-0.87890386542879	10.77048586352795
H	2.45890347227100	-2.46499961963727	10.42157509897784
H	4.20032659224217	-2.24372296929356	10.13860813575890
C	4.89653130145396	-1.75178737187869	12.74401234940476
H	5.78622616405312	-1.95153149361377	12.12217525831191
H	5.15347510641877	-2.02583204913542	13.78269267963046
H	4.76612625440354	-0.61130147462097	12.74641233544664

Tl-2b

H	1.16831011797174	-0.64558793461479	2.21542324066020
C	0.65783755299619	-0.45120073288748	1.25373552991760
C	-0.63621862421255	0.09644410825786	1.23810029279465
H	-1.11523060044850	0.31723053196384	2.20070167988566
C	-1.34922770761905	0.38491004260178	0.05272570860163
Tl	-3.69044498416702	1.75298061540623	0.05629233336596
C	-0.65102347278107	0.05875425988000	-1.13053714523673
H	-1.13851077892032	0.24776830976907	-2.09616458488126
C	0.64534382904619	-0.48662471976955	-1.14178788232468
H	1.14211701252841	-0.70825338681836	-2.10362071637302
C	1.32115542632983	-0.74500808824127	0.05658230522660
H	2.35419377688861	-1.16269552813983	0.06013926296762
H	-5.46356064221760	-0.61296513829433	2.18370703886666
C	-5.78152498571000	-1.02760630137367	1.21843456861798
C	-6.71848469445537	-2.07482968950155	1.22527241164879
H	-7.11845948502093	-2.45744238733804	2.18283640540866
C	-7.16518571360723	-2.63834151999549	0.02424164473065
H	-7.92118190914209	-3.45696019448134	0.02036295950847
C	-6.63855843156832	-2.12900837851699	-1.16864720573016
H	-6.97226175312737	-2.55190650164799	-2.13340388126465
C	-5.69942625584626	-1.08228079455313	-1.14848411758144
H	-5.31796378621570	-0.71424902111282	-2.11020500849987
C	-5.23297389070157	-0.47597755059213	0.03861515969069

Tl-2c

N	2.59631396346193	-8.24028144199451	-1.26910101496260
Tl	-4.07532646778258	3.19898880903748	-4.75673673054224
Si	2.86811157278225	-9.83138326825018	-0.88210922219659
Si	2.63136952175773	-6.76047263841312	-0.48857001186926
H	3.40253245637152	-10.69398022494685	-2.01817176064717
H	3.87335286971442	-10.15777153109298	0.24799331240978
H	1.65878325541177	-10.66772669437211	-0.42767703966312
H	2.93457997321525	-5.59799801077334	-1.40805280976437
H	1.34154240832936	-6.33420403663486	0.21066750406190
H	3.67306838473554	-6.59988334479200	0.63801499805972
N	-7.27258962000867	14.57431664526174	2.25530370821066
Si	-6.07369887030262	13.43120914074124	2.06676207668362
H	-4.87880348285789	13.69027564896466	2.98542813845410

H	-5.40780994778912	13.31433379441997	0.69258647426716
H	-6.40658782721438	11.97506409926511	2.39615427692457
Si	-8.61511506332201	14.88472254661454	1.31340142118587
H	-9.79713133831360	13.91010053610029	1.41434790988918
H	-8.41814864529965	14.99503886749053	-0.20740910813914
H	-9.27806314288920	16.22061110337438	1.65486787763794

Tl-2d

C	1.33349077076459	4.39335997319019	1.44544395432805
C	-0.00352197578724	4.39885674876009	1.70817994582585
N	1.49706661184346	5.16212983156138	0.30655040110133
N	-0.57978299702910	5.17042433733056	0.71482158643340
C	0.32702551680366	5.67090966939470	-0.16879788283822
H	2.40218282788998	5.43484997935445	-0.09629574401309
H	-1.56839217010818	5.45048585096696	0.68593438989271
H	-0.57531319884400	3.95649942713296	2.52132449894644
H	2.16609488993146	3.94406155837694	1.98232595414887
Tl	0.02970079559081	7.83228209528876	-1.74019930825376
C	0.52748476722722	8.65395149142700	0.76802645555816
N	-0.34084882690444	8.63434023157070	1.81658922461511
N	1.73403999551769	8.65977295993905	1.39898101559348
C	0.29159244910271	8.60913236934656	3.04682777662883
C	1.62731976537241	8.62556422433638	2.77815447479323
H	-1.35342050085753	8.53163767009779	1.67292918684407
H	2.61313505145137	8.57648181363315	0.87354940855715
H	2.49049682391552	8.58202593701766	3.43868811511871
H	-0.24836059588038	8.54781383127469	3.98936654671971

Tl-3a

Tl	34.42698347222743	15.41161895048743	-10.30289787281853
Cl	-30.95482839871901	4.21929150884863	-3.62813873396523
C	3.38332594052137	-0.92338478037904	7.63863252079424
C	4.83216680664119	-0.77869838908373	7.26416778166515
H	5.19948818799459	0.25616169587011	7.37642113755751
H	5.03661074551705	-1.08784984909835	6.22436545655345
H	5.51280695333705	-1.42659792854930	7.92397660670690
C	2.96382138701388	-2.35745333954049	7.47773211473953
H	3.57851127503419	-3.06254722948951	8.14500885880758
H	3.09676125419199	-2.72750974528875	6.44615934677282
H	1.90823256320521	-2.52632892756137	7.75334808493239
C	3.19377083963699	-0.50653807393266	9.06994557527104
H	2.14728609395445	-0.60622040858616	9.40748606400525
H	3.49892661507407	0.53835395481784	9.25385516678622
H	3.81812126436949	-1.14726443851471	9.79070889219156

Tl-3b

H	-2.61211608381146	-0.50006799283240	0.41357166011971
C	-1.58803413965569	-0.28123533010015	0.08192434642533
C	-1.27170505867556	-0.33708413871760	-1.28847279588537
H	-2.09078531576391	-0.63731375329482	-1.96613606567513
C	0.00553988156942	-0.01272942145024	-1.83650179443795
Tl	-6.31946704003293	-2.22262572082291	-5.70686150531094
C	0.93857741348467	0.33690316157145	-0.82509656393237
H	1.96750990095078	0.61760502046367	-1.11694447050280
C	0.67874411290386	0.35413720776501	0.55666192103201
H	1.46323328118515	0.65705384810798	1.26729548441547
C	-0.60885283225283	0.05787553407963	1.02606209872431
H	-0.83684724665939	0.05567230176311	2.09478418797885
Cl	1.36635312675786	2.24341928346723	9.81678349704883

Tl-3c

N	-1.98550774309490	0.21386494028578	0.18406947671932
Tl	2.16392749237210	-4.72158085727224	24.19143213581354
Si	-1.84453352023596	1.25821555732401	-1.09621941432209
Si	-1.79229132625674	0.35481780480654	1.83070637390881
H	-2.30738587233857	0.64400637473770	-2.41053411185436
H	-2.63850678768069	2.56903586971982	-1.04713782592414

H	-0.44099928263793	1.76485791331164	-1.45372326475168
H	-2.16794355697734	-0.91802319052364	2.57563145591117
H	-0.38340742209377	0.64586116709169	2.35835799180134
H	-2.62147863055680	1.42331489650992	2.55250729302731
Cl	-3.27529335049937	7.33533952400879	-24.75182011032928

Tl-3d

C	0.26840708238199	3.30383453054043	-0.72141832872145
C	0.47977335945982	3.48660646251640	0.61042909401106
N	-0.59431999799612	2.21833924911453	-0.81317710602008
N	-0.26688648654124	2.51013470109281	1.24594341805534
C	-0.96033926935654	1.69124209595266	0.39897119059933
H	-0.89963546407238	1.81844176416624	-1.70339121692453
H	-0.31849746634436	2.42827119339438	2.27447829609807
H	1.08718522472794	4.21124329332803	1.15040436355117
H	0.67914499005330	3.82116051513324	-1.58391966566570
Tl	-0.93461883873934	-0.97933044032656	-7.65632713760400
Cl	6.90807686642685	20.04939663508794	12.07234709262080

Ge-1a

C	6.57289734016914	2.16406824417765	7.93330420740585
C	6.17303594240492	1.24511105958534	6.78887390671566
H	5.07846762834350	1.13836477684775	6.73053135225552
H	6.60130536565639	0.23952885633506	6.92029607764660
H	6.53147959793479	1.64641878263046	5.80032069080583
C	5.95518348024316	3.53903681139329	7.71882804417570
H	4.85796895480423	3.48010322240034	7.68088039809319
H	6.31653313868290	4.01036799443144	6.75807570975244
H	6.20578119865336	4.22395200962548	8.54365556999012
C	8.08974545334525	2.28612224479613	7.97770473169309
H	8.56180879036028	1.30495175711592	8.12872623659597
H	8.41501430118712	2.92854318331971	8.81123058128927
H	8.49660943552094	2.73125291211897	7.02321643072735
Ge	5.82455977408820	1.26168222068012	9.86529862164735

Ge-1b

H	1.06863259059922	-0.15205156519455	2.17584837590844
C	0.54823725627705	-0.07953924137254	1.20984129198388
C	-0.83919767321851	-0.02379800396863	1.19314166610765
H	-1.37746183136145	-0.05498882616986	2.14841594408096
C	-1.61454073089239	0.07357571306304	-0.01138169407063
Ge	-3.67153256254666	0.16734353172430	-0.02895410328056
C	-0.81430172658872	0.10276946400418	-1.20305621796135
H	-1.33283478380436	0.17425412877755	-2.16702615577426
C	0.57320340135277	0.04766275503338	-1.19694407660262
H	1.11333373022970	0.07798545055686	-2.15430874011382
C	1.30662504822087	-0.04425525775531	0.01268709132594
H	2.39892728173248	-0.08582814869842	0.02175661839637

Ge-1c

N	-1.60055555821405	1.03474429285654	0.46488383272263
Ge	-2.72989639955791	2.76829112067212	1.24422295562853
Si	-0.32907575012240	1.45442670573193	-0.56750752936442
Si	-2.21554901649394	-0.46051358324244	0.95988417170672
H	-0.72236419914140	2.16664050026774	-1.84214915542714
H	0.75301312274570	2.30601124042675	0.05378037899115
H	0.45635718916537	0.21997198473036	-1.09223143795822
H	-3.62221423048375	-0.77807715973969	0.50446710792005
H	-1.39705462887688	-1.66222169889849	0.41076201356374
H	-2.21025052902074	-0.69908340280481	2.45153766221698

Ge-1d

C	0.92150292788450	2.36395054520781	-0.23087475071602
C	-0.31957621165119	2.37964254965457	0.32047731482643
N	1.55180920966457	3.55533591628057	0.12897321158166
N	-0.45026098431813	3.58098974455140	1.01797608369426

C	0.63350941285441	4.45554158990760	0.73325521430860
H	2.32037422334979	3.95468273830223	-0.39600870304051
H	-1.34704261222493	4.00086426710484	1.23062519616757
H	-1.07218233418846	1.59884610320498	0.34735062248948
H	1.43033469511273	1.56785669992535	-0.76381095914902
Ge	0.77231167351673	6.42630984586066	0.97223676983754

Ge-2a

Ge	4.30687100042976	1.57913928723871	4.19785614343244
C	3.58552226725034	0.34342834400383	2.38370293710918
C	2.14309925589404	-0.11951713469996	2.51713111550777
H	1.46336841841833	0.72690472737760	2.70540566264347
H	2.01377241574503	-0.83833665025608	3.34350875161874
H	1.78812444600902	-0.64165378076728	1.57849956821960
C	4.50022986261098	-0.85181271750745	2.15000927986041
H	4.20751286046372	-1.42793723854319	1.21850417478513
H	4.47152056064352	-1.55893880621815	2.99321951410693
H	5.55035385867016	-0.53830576802434	2.03794229930028
C	3.69917221435215	1.29891719263644	1.20513514623499
H	4.72590693933707	1.69601296721521	1.11215396029630
H	3.01849654787793	2.15873524449911	1.31682578396314
H	3.44727248688928	0.78454010510676	0.23453846032044
C	3.56621942118215	0.35714191209782	6.01211919985889
C	3.88483615245155	-1.12497685768877	5.88985847764659
H	4.96010053174391	-1.29325543651062	5.71871437143109
H	3.33965242888472	-1.59770758422363	5.05583948998034
H	3.59392957807730	-1.68968879515126	6.82618464371137
C	2.07153784043460	0.55681526814496	6.22585186284993
H	1.70647632090437	0.02219651293027	7.15628768341320
H	1.48304318348338	0.17379811057553	5.37823254675005
H	1.81929312199087	1.62428462355180	6.32821831407332
C	4.32283938554434	0.93852134173302	7.19707141323528
H	4.14953251010734	2.02603485561906	7.28485066495862
H	5.40939348813922	0.78067108065092	7.09769917124683
H	3.99387890246493	0.46531719620969	8.16546036344564

Ge-2b

H	0.09196707778748	-1.13571146623816	2.34185114145213
C	-0.01733629088972	-0.73347809268090	1.31906217885704
C	-1.27128352703268	-0.76694965309863	0.70200191096240
H	-2.10435198348397	-1.19306074186457	1.26025854069242
C	-1.50252541744950	-0.27006099021590	-0.61762581482707
Ge	-3.24877730048448	-0.19156334843769	-1.76482521180110
C	-0.33312798878190	0.25956456587861	-1.23959858837286
H	-0.43885759936834	0.66045074056672	-2.25806506477260
C	0.91849433435122	0.29686970948267	-0.63275691526623
H	1.78270217306135	0.72357946363795	-1.17520389578082
C	1.10994504007436	-0.20251320916706	0.67411706903189
H	2.10372242792251	-0.17647200794816	1.16290897605689
H	-3.88800760420857	-1.59500320400325	1.25361193954951
C	-4.81778683559087	-1.55916310169297	0.68648462523866
C	-5.97338793832949	-2.06387913966667	1.29013774435024
H	-5.90997786799065	-2.47924169168835	2.31115429713934
C	-7.21390940875590	-2.05793006462574	0.63406605344858
H	-8.12860326971387	-2.45841429084226	1.11206871792443
C	-7.24032760971111	-1.51415682494860	-0.67010544367711
H	-8.19763285346191	-1.48883003293065	-1.22206720455348
C	-6.08518495353426	-1.01414143584536	-1.26322510006543
H	-6.15030640920270	-0.59903631516096	-2.27942904723795
C	-4.80672619520706	-1.00370886851009	-0.63050090834888

Ge-2c

N	-1.96885888139219	1.23371309808178	0.38674342773618
Ge	-2.24195228238191	2.94572329745667	1.74849288708256
Si	-0.59670871964542	1.60315394564342	-0.54339826602902
Si	-2.43267867957895	-0.32068379517812	0.93825162248444
H	-0.63185284191884	2.93901764177244	-1.23295882977632
H	0.77180927730948	1.49751182048874	0.12287424422397

H	-0.43663735875810	0.60459857873673	-1.72553115505802
H	-3.92957941773639	-0.55014868051100	0.96971810749973
H	-1.85806983573657	-1.41836683090679	0.05037685190042
H	-1.94822549861962	-0.70853137302659	2.32882474636243
N	-2.95686396062447	4.42265391455368	0.31303888480053
Si	-1.89579133100443	5.77050870934474	0.40854393817713
H	-0.55828500190675	5.62526978831066	-0.28581454939828
H	-1.59934123729358	6.35193957767519	1.78671779744379
H	-2.57358985317473	6.95218118493672	-0.28997374111490
Si	-4.62750997038728	4.55338147818075	-0.02483168849661
H	-5.27810245804625	3.21756932662009	-0.28825328410440
H	-4.96925669559490	5.38289039270797	-1.28673182479257
H	-5.51212525350911	5.20857792511294	1.04161083105895

Ge-2d

C	0.52281060371277	3.19027295277844	0.23697871240776
C	-0.31666631149220	3.67406821820381	1.18996766847662
N	1.31646185976822	4.25608054253152	-0.15227369792752
N	-0.01530389034854	5.01120024993502	1.35620181555589
C	1.00723771977529	5.41980682018339	0.53059149235208
H	2.06039785172191	4.21515984309664	-0.84417817350318
H	-0.53793626743875	5.62536133593991	2.02974667127407
H	-1.10217347385413	3.19312089401258	1.76663411857855
H	0.62445536359081	2.19727588005672	-0.19188686133016
Ge	2.04273698578890	7.11205431603523	0.09059035452905
C	1.20098953231479	8.35528260486227	1.45720387247694
N	0.19970474319389	8.34107437918681	2.40149674862777
N	1.68156381668652	9.64943899384791	1.55766518046817
C	0.07069969641132	9.55733131088184	3.04208816907554
C	1.00530848523551	10.38985032794578	2.51258555364940
H	-0.42000242466973	7.52158301352962	2.62147961352479
H	2.45790148494089	9.98422541900833	0.99279941221759
H	1.24680897653204	11.42688915530610	2.72795716277787
H	-0.67500475186954	9.71450374265800	3.81675218676878

Ge-3a

Ge	6.20695255759771	2.19949318165322	9.14756958956397
Cl	-14.58307081657566	-12.82832691150663	-11.66602587091529
C	4.93940221935214	1.29971937403775	7.50757466001818
C	5.81795750545566	0.53981322078370	6.52279430054546
H	6.37624308479846	-0.26220423899571	7.02608650874391
H	6.56476562931052	1.20277316074707	6.05851182649584
H	5.20592885338349	0.07877398987074	5.69372656420180
C	4.18066653866897	2.39647594618955	6.77247718868624
H	3.53690681061727	1.97177095164768	5.94824333887458
H	4.87060671998720	3.12394322411663	6.31663938247714
H	3.53366733030167	2.96019199048002	7.45939086890335
C	3.94556270834493	0.33850017523164	8.14306474979396
H	3.29443938268826	0.85983234546180	8.86164900366131
H	4.46458266896656	-0.46797874261430	8.68393774091876
H	3.28737380710278	-0.13774466710317	7.36513114803075

Ge-3b

H	-1.88562054798088	-0.05832099061951	1.61954230399388
C	-1.32554546481444	-0.00740217532114	0.67813293412521
C	-2.00800149807402	0.16829884911652	-0.51963919650992
H	-3.10242522818022	0.22243376751468	-0.48804918138350
C	-1.36563543511177	0.24719801506584	-1.80008509762851
Ge	-2.40363422529117	0.47679115806102	-3.58847113659834
C	0.05967820789005	0.14348428784372	-1.72902708683903
H	0.62490000492904	0.18472992292009	-2.66875470605703
C	0.75665126199021	-0.01634880321687	-0.53555098345679
H	1.85339771872993	-0.08948972977547	-0.55710162066739
C	0.08586797750901	-0.10255709566567	0.70547745891175
H	0.63403297877351	-0.24895589583614	1.63995566060533
Cl	-0.83151575036929	-0.58825131008707	9.76064065150438

Ge-3c

N	-1.63198497249002	-1.15512893136070	0.93735436578973
Ge	-2.11121468195956	-3.18637413883518	1.65362336604799
Si	-2.96812145572889	-0.11914410097083	0.97695827535255
Si	-0.10449238949022	-0.95309344036102	0.23528026948506
H	-4.07867402409294	-0.39707920252133	-0.01753839298639
H	-3.64031185476335	0.02325867113832	2.31860069718384
H	-2.56346676503884	1.34119969789823	0.64743755004261
H	0.31205178048012	-2.02771519583323	-0.73934502858665
H	0.03044034109816	0.35080469883482	-0.58957280469725
H	1.04560693249718	-0.86086481224691	1.22471299484187
Cl	-1.58325291051169	17.55384675425779	-3.71424129247335

Ge-3d

C	0.93075740199819	3.89525716609280	0.13268123089539
C	1.00551470111275	5.12314892320197	0.70718359304793
N	1.80453142801498	3.89177638559174	-0.95564343671875
N	1.92230702788029	5.87205785042898	-0.03149480554398
C	2.61606544730503	5.05580180088397	-0.96189554859673
H	2.19693962774094	3.04343161023003	-1.34528341660727
H	2.41478361289666	6.67164096003733	0.34777511996244
H	0.41316025033284	5.54602630719892	1.51128345029192
H	0.26426732376664	3.06860304729276	0.35327100522526
Ge	4.33948021097782	5.40029719696080	-1.90194081857529
Cl	-12.45951703202616	-3.00870124791931	7.41840362661905

Sn-1a

C	6.58015704745898	2.17189644905276	7.91643697107472
C	6.17874853757416	1.25171961309766	6.77686553697961
H	5.08473451436842	1.14253312449029	6.71588757603514
H	6.60798248904156	0.24579460305924	6.90334860565289
H	6.53645197176837	1.65380272848991	5.78761739477958
C	5.96006655799318	3.54331040325738	7.70910524265650
H	4.86270353422608	3.48564057925209	7.67346556809027
H	6.31898637286608	4.01172570038751	6.74704905702427
H	6.21496738279824	4.23116027224432	8.53022837075377
C	8.09394469340100	2.29149943660326	7.96697568718943
H	8.56818484315443	1.31174337689956	8.12150270815164
H	8.42147228769891	2.93859385459825	8.79569957851845
H	8.49955305301700	2.73164489893456	7.01033907307222
Sn	5.75243711602776	1.18843903509087	10.02642118881544

Sn-1b

H	1.08974529778424	-0.15274857693292	2.17319913735788
C	0.56755159473267	-0.07934012959319	1.20954492093045
C	-0.82290593629461	-0.02013625511310	1.18954765905179
H	-1.35933724612294	-0.04897376756248	2.14546637899854
C	-1.58683561563168	0.07417058129465	-0.01148105317161
Sn	-3.87212261498532	0.16122763574181	-0.02917652831538
C	-0.79777393633559	0.10625158692655	-1.19950726527736
H	-1.31391462442065	0.17979722413932	-2.16415981957298
C	0.59289205922547	0.04794184039819	-1.19638688898271
H	1.13523581189112	0.07688178067155	-2.15124057048427
C	1.31700425063954	-0.04755390028940	0.01261504782351
H	2.40955095951776	-0.09438801968098	0.02159898164214

Sn-1c

N	-1.64805901926779	1.04200764565528	0.41537227165612
Sn	-2.89614570127469	2.93675558792170	1.24849327322134
Si	-0.32639165556400	1.42609072372822	-0.56580617613753
Si	-2.19235880743702	-0.46795747836882	0.94513447653030
H	-0.65141634489785	2.16700983450278	-1.84475075209564
H	0.76725381766018	2.24493515742844	0.08691041792944
H	0.42785428601050	0.17326450546036	-1.06449243792253
H	-3.60410578999405	-0.83570796217237	0.54210942459147
H	-1.34891942074582	-1.63454587728548	0.38433492168829
H	-2.14530136448946	-0.70166213687012	2.44034458053876

Sn-1d

C	0.93371776466912	2.32653629188772	-0.21705553212325
C	-0.31570590277850	2.34065852534896	0.32617231761377
N	1.47517250986948	3.58279127510433	0.00087551950228
N	-0.50145579896206	3.60526120982351	0.86021874976714
C	0.59023222690550	4.45596233505094	0.64644592776379
H	2.36469276924831	3.91481328053234	-0.34634299155412
H	-1.34924351790857	3.95069994152322	1.28895579180884
H	-1.05848746731669	1.55378537755174	0.38421487048423
H	1.46783577466167	1.52479172427144	-0.71338774375701
Sn	0.83402164161174	6.62872003890581	1.13010309049434

Sn-2a

Sn	4.40092754112616	1.77061168921533	4.19754529739640
C	3.58462656811669	0.35936304573805	2.26136643896590
C	2.14360548247155	-0.07701499752220	2.45272090375020
H	1.47439217881973	0.78512219774597	2.60153812662566
H	2.02365367573440	-0.74094575070964	3.32471856633245
H	1.76859755270978	-0.65299252178982	1.55270359542688
C	4.48093161243229	-0.85237308722035	2.07510188781351
H	4.16019476890468	-1.46787987978686	1.17819295290583
H	4.46020762773200	-1.51906935411516	2.95113245786976
H	5.53190876627573	-0.55923782120505	1.92627200619717
C	3.68683170343030	1.25965205652119	1.04388271185329
H	4.71941211591364	1.61942826012087	0.88945458574932
H	3.03802433746433	2.14570515522822	1.13729218769450
H	3.38215482618302	0.71205389199077	0.10265633130249
C	3.57686634582864	0.36455861083610	6.13355978564667
C	3.91906540245617	-1.10257767954383	5.94802919508938
H	5.00077594995342	-1.25247286970235	5.80431135180989
H	3.40752480340727	-1.54035169353552	5.07494871912409
H	3.60326793572168	-1.71220367515832	6.84863678490126
C	2.07854967367161	0.53653661490658	6.31137140478068
H	1.70070964866545	-0.04683914429183	7.20746947526733
H	1.51595231653340	0.18394370580006	5.43313099723631
H	1.80715451420243	1.59383575793536	6.45670490152744
C	4.29911931589495	0.90598840834396	7.35347893930122
H	4.09445085636687	1.98068227888078	7.50389832463099
H	5.39131516616351	0.78591809231901	7.26644074723149
H	3.97173531382026	0.37088670899868	8.29426232356989

Sn-2b

H	0.06673122545360	-1.16081893460751	2.33593772883285
C	0.00880258861293	-0.73876787417292	1.31820290800202
C	-1.22052907654532	-0.71007455810559	0.65168359843694
H	-2.09375658130175	-1.11155622182541	1.16735690821734
C	-1.37583769603339	-0.18351314339262	-0.65951900514556
Sn	-3.28661952444367	-0.01821725346369	-1.96438930442340
C	-0.17340047791525	0.30931265596225	-1.23202120101848
H	-0.21794653460627	0.72938311351415	-2.24697399207015
C	1.05772768085287	0.28755700967747	-0.57807992381586
H	1.95837154569150	0.68723774134313	-1.07905484837756
C	1.17507946820434	-0.24118261475442	0.72102424883810
H	2.14966059244398	-0.26266474075790	1.24679830803127
H	-3.92981198536919	-1.51862246819594	1.15689524516036
C	-4.88634910983295	-1.52603030904665	0.63304682123089
C	-5.99235410213535	-2.07632186796673	1.28953840254960
H	-5.87371024275317	-2.48417440499603	2.30789294181343
C	-7.25409776343544	-2.12102927927127	0.68183185375136
H	-8.13217340200814	-2.55551618727670	1.19887032491944
C	-7.36286187704715	-1.58929982116434	-0.61689081632718
H	-8.34501253513034	-1.61018909541357	-1.12402849821516
C	-6.25282870215263	-1.04475225461888	-1.26061883524603
H	-6.38094077989159	-0.64271605688600	-2.27578114873371
C	-4.95942271065763	-0.98089343458081	-0.67740171641052

Sn-2c

N	1.48303859071434	-9.07292502991561	0.53998756970998
Sn	10.43379314767348	8.65728670979350	-3.18887058302576

Si	2.33955711101467	-8.15501878573896	1.61881178827579
Si	0.63882669227804	-10.48836188170352	0.41852197892376
H	3.39098446727696	-8.86118227142125	2.48698494202363
H	3.14437538295551	-7.04730195622022	0.95806129667729
H	1.53788688249936	-7.38771159327781	2.67748344212112
H	-0.86615678687480	-10.33341333889935	0.19785606674664
H	1.03827103261420	-11.37913523115909	-0.75917446123863
H	0.68932504403032	-11.48373773710056	1.58868437006431
N	-7.68770685409487	13.92514072177044	0.18954478900546
Si	-9.12232561435800	14.22260979263889	-0.59075208833320
H	-9.07139684307985	14.84391371699982	-1.99551016269221
H	-10.12511214225521	15.14620207089885	0.11423300981411
H	-9.95769328397472	12.96884078495761	-0.82229618466689
Si	-6.22394426805168	14.71371260214560	0.22294736022096
H	-5.60589632958347	15.11165275660254	-1.11975758222705
H	-5.13031998263524	13.89408963667500	0.88219670113578
H	-6.14912624614836	16.03629903295463	0.99874774746492

Sn-2d

C	0.60367064081434	3.08163764218906	0.37033973038482
C	-0.26724715952997	3.62443500972191	1.26312742693101
N	1.29795602410748	4.14781589818264	-0.17831131701968
N	-0.08293630566726	4.99052810455467	1.22437623811554
C	0.89138845641036	5.35955680612560	0.33676794539312
H	2.07075623072250	4.06749852004978	-0.83559360517404
H	-0.66032844570094	5.66162176597720	1.79529994244818
H	-1.00091007404410	3.16668785813028	1.92121478529862
H	0.79074632902968	2.05049950745438	0.08406608950196
Sn	1.78806320063264	7.29800266468163	-0.44113016701769
C	1.10229362042633	8.53009938995617	1.34163873257929
N	0.14339515195262	8.43936729851128	2.31392320021606
N	1.67618223092894	9.75497590168394	1.60382784792707
C	0.12703107754667	9.54414760876856	3.13910631194734
C	1.09673149195774	10.38685809134183	2.69220272925053
H	-0.53650944335822	7.64085976674289	2.41407027772092
H	2.48091687624040	10.10096645702953	1.08556811673369
H	1.42162537255060	11.36140950491000	3.04570315531239
H	-0.57283527501979	9.62761220398872	3.96620255945084

Sn-3a

Sn	6.93143006559518	0.18630211076406	8.45530473481161
Cl	-13.50720350399327	-4.93757530604177	-6.55511312508901
C	4.95133455174217	0.56460911198081	7.05111425608535
C	5.22260213975585	0.25058824246173	5.58950942282620
H	5.70785575922345	-0.72329579538531	5.47235055372314
H	5.88158044225649	1.01018943995792	5.13043845832664
H	4.26485890025923	0.27600243437507	4.98781624998607
C	4.42032698966561	1.98141798696901	7.19736772802209
H	3.48284514679727	2.14154629434628	6.58527574699106
H	5.16110315684336	2.72845295988588	6.86934693818761
H	4.22630701059181	2.22699368532887	8.24768515981568
C	3.93446876077284	-0.42089329907977	7.60016590492915
H	3.80511465152500	-0.30460360604659	8.68968276384349
H	4.23065620387043	-1.45822512670647	7.38172220975730
H	2.92870472509472	-0.24647613280971	7.13810399778366

Sn-3b

H	-1.80439001118972	-0.03563269971777	1.69377721433732
C	-1.26663578415020	0.02418933749815	0.73949549772775
C	-1.97023637281913	0.29495996701026	-0.43140013119898
H	-3.05552826633759	0.43594538492613	-0.36438425205357
C	-1.35247892441856	0.39230763843110	-1.71305162839894
Sn	-2.49138384925285	0.82359542245167	-3.67743110430439
C	0.05638946925854	0.19815902909407	-1.69565680956035
H	0.60340585543256	0.26628299098338	-2.64495364170514
C	0.77558953569755	-0.06965949365943	-0.53181974794901
H	1.86381902029800	-0.20953670766338	-0.59020190693679
C	0.12850993916544	-0.16707970171376	0.71762549278926
H	0.68604255794662	-0.36842958866865	1.63566992438207
Cl	-1.08095316963066	-1.25349157897179	9.37940109287079

Sn-3c

N	-2.28190851096558	0.40892034680246	0.44392021093275
Sn	-8.64258308658613	-9.99559021127819	17.09082318875979
Si	-2.99939028661266	1.82475519747350	0.93094352428323
Si	-0.87325231820358	0.00318550513287	-0.33585974417047
H	-4.17838747130484	1.60038986239176	1.86855572304111
H	-2.14250364489213	2.83232870542935	1.70763438028036
H	-3.61536443435645	2.71833552764342	-0.15353989365822
H	-0.58486699212023	-1.49253757770876	-0.29990540455706
H	-0.77644857684502	0.31332901725684	-1.83448667723814
H	0.43487794904010	0.60760170325817	0.18910793355805
Cl	8.36640737284645	11.74899192359870	-16.67392324123146

Sn-3d

C	0.46033338149834	2.93798444432507	0.16479431687144
C	-0.21967554025112	3.84816587390029	0.91820606405841
N	1.54664664929966	3.60597100003140	-0.38923121642827
N	0.48609871797522	5.03585768159456	0.78453806307754
C	1.59779951309585	4.92923266275189	-0.02238799658333
H	2.29839767133377	3.20914651994046	-0.94318277683939
H	0.20815117411607	5.92893003126630	1.17180345325340
H	-1.13137349804710	3.72629254745658	1.51828368508551
H	0.24743378666992	1.89062360067151	-0.00924598040913
Sn	3.18488081167998	6.45912119415674	-0.69288838352022
Cl	-3.23040266737058	2.98801444390519	2.77365077143404

Pb-1a

C	6.58981114821135	2.17729745024418	7.89844374152419
C	6.18437284788629	1.25661702458401	6.76606510491352
H	5.09118782695690	1.14813662947631	6.70379229231571
H	6.61321232752268	0.24919928796215	6.88547192678053
H	6.54320119038180	1.65648896462890	5.77258607112803
C	5.96418719726898	3.54322495553151	7.70442009081235
H	4.86693053232503	3.48427542472996	7.66641210175576
H	6.31822700194778	4.01758076220885	6.74130661812448
H	6.22518481046922	4.23325511144475	8.52229160651668
C	8.09855711399286	2.29338997948542	7.96411106995981
H	8.57470326953819	1.31482138023765	8.12324071703840
H	8.42249240698490	2.94127316108312	8.79278440881757
H	8.51351671861917	2.72922788202414	7.00758560826639
Pb	5.67480600928904	1.15471606181671	10.13243120084051

Pb-1b

H	1.10782706037067	-0.15315388747203	2.17073262715739
C	0.58123571987837	-0.08009046108747	1.20946480856775
C	-0.81194624920054	-0.02186555480052	1.18713241197279
H	-1.34733383622934	-0.05168492755270	2.14410585219623
C	-1.56808998466571	0.07270213443775	-0.01116931898044
Pb	-4.01427275403097	0.17196916371852	-0.03104279854541
C	-0.78699518351218	0.10428844254733	-1.19673873592946
H	-1.30230742551481	0.17717748990146	-2.16237131588761
C	0.60640383324650	0.04709006970100	-1.19603709870771
H	1.15288595031287	0.07599808913909	-2.14850485611197
C	1.32452175046713	-0.04702309555817	0.01272461370979
H	2.41716111887802	-0.09227746297426	0.02172381055865

Pb-1c

N	-1.63339885080533	1.03107156358406	0.41858670794483
Pb	-2.99560531934620	3.07352494416384	1.30272200228993
Si	-0.31976175340509	1.40306438585116	-0.56692117337711
Si	-2.17433649460835	-0.47783439271424	0.93421791121234
H	-0.64538061593698	2.13249538962544	-1.85496373918053
H	0.76924813422874	2.24131488942219	0.07334942582744
H	0.44288467964611	0.15478508412109	-1.05572660592125
H	-3.58487092355452	-0.85012277977952	0.52304828994107
H	-1.33039062908001	-1.64467757338924	0.38174973892648
H	-2.14597822713837	-0.71343151088478	2.43158744233681

Pb-1d

C	0.93857765503990	2.30754650614192	-0.21348366680512
C	-0.31128117645576	2.31946501344270	0.32851788139777
N	1.45582063898387	3.58001693597654	-0.03136264454316
N	-0.51275782437794	3.59946855216250	0.81898288343468
C	0.57460882528009	4.44511116113019	0.61344201421789
H	2.36087683613147	3.90448655651418	-0.34439234717753
H	-1.34710826708276	3.93129955598782	1.28392187439927
H	-1.04935471953253	1.52939033885095	0.40008221662883
H	1.48292098897297	1.50530647739079	-0.69730848299469
Pb	0.84847704304070	6.76192890240240	1.20180027144206

Pb-2a

Pb	4.48720334654973	1.92416856862075	4.19777379109707
C	3.58051443968211	0.35879177173474	2.13622532426027
C	2.14456178853532	-0.04306473101737	2.36976559610234
H	1.49009277741857	0.83190179620558	2.50578931279990
H	2.02933611447688	-0.68530932703319	3.25792293637725
H	1.74187192553369	-0.63461719472027	1.48621465120232
C	4.46350876314268	-0.85839226133507	1.99819409670226
H	4.14624788909691	-1.48913277155866	1.10501444737979
H	4.41928786515090	-1.51035436848851	2.88440558798937
H	5.51981781874076	-0.58573810354324	1.85234783284955
C	3.68987726005555	1.22816099803588	0.90721038931193
H	4.72413142544291	1.56927288815864	0.73310869953080
H	3.05019256282428	2.12245690087882	0.97426569984242
H	3.37093145952676	0.65727544308743	-0.02359141317181
C	3.57716429793238	0.36067202247815	6.25861109759338
C	3.94711821965208	-1.08444827523611	6.02895438626459
H	5.03230955925077	-1.21456648426220	5.89584062396143
H	3.45051842279616	-1.50680326816480	5.14035007125410
H	3.63365467556180	-1.72707508322865	6.91305518690629
C	2.08135386820770	0.51768122084765	6.39162548212209
H	1.69063624106593	-0.07107292782712	7.28435115250526
H	1.54143431704895	0.15246032324870	5.50429287760373
H	1.78939890139607	1.56913770122102	6.53530200423853
C	4.27156085903866	0.89235642785171	7.48875742828219
H	4.05045198435622	1.95927693265083	7.65951393208344
H	5.36599511274131	0.78406320442823	7.42581789262282
H	3.93278410477496	0.33322659696708	8.41970191228866

Pb-2b

H	0.11269588115630	-1.29444109316210	2.27383183958172
C	0.06726165526163	-0.80847509651861	1.28477380381607
C	-1.15119906050173	-0.73818271516698	0.59741005327608
H	-2.03538494037702	-1.17445635841395	1.06696555839299
C	-1.27858893230706	-0.12620334345285	-0.67231779154093
Pb	-3.31640729138088	0.11701677265604	-2.08761662118213
C	-0.07773183190963	0.40917924982222	-1.19268902904375
H	-0.10384356740750	0.90140159528379	-2.17558216699078
C	1.14655248926453	0.34357194168327	-0.52228547238032
H	2.05639113516753	0.77637248736196	-0.97729715174303
C	1.23818420554959	-0.27030955467028	0.73719401526037
H	2.20439384701133	-0.32551954675190	1.27610963165259
H	-3.95816907858256	-1.59354544277154	1.06398978265302
C	-4.93900377937578	-1.57435998142377	0.58420223490038
C	-6.02028727918968	-2.15103185067006	1.26279494288181
H	-5.86589588767511	-2.60600264099449	2.25576019448575
C	-7.30306244519396	-2.16219916895278	0.70205525588149
H	-8.16097658690429	-2.61847896886131	1.23483088510459
C	-7.46662269617478	-1.57445656546495	-0.56246200271679
H	-8.46928049932739	-1.57068415824418	-1.02852559625542
C	-6.37811111371781	-1.00094022336422	-1.22482839255950
H	-6.55264564722261	-0.54961251758684	-2.21227454690648
C	-5.06954857616307	-0.97149282033648	-0.68971942656772

Pb-2c

N	2.78091771122928	-8.19752349485939	0.20312904946975
Pb	-4.79841988125113	4.04776388214279	14.41670485647216
Si	3.09026164567277	-7.57025959037434	-1.30551157618362
Si	2.23336065399750	-9.67365573154581	0.73502368482309
H	2.01232433242838	-7.74279182516814	-2.38569348422182
H	3.31354866650243	-6.06619111548684	-1.29056869477672
H	4.33896970363304	-8.07720833784227	-2.04227369443601
H	1.03326993468239	-10.30012771857399	0.00894470843856
H	3.22778855230239	-10.84064913593814	0.73277357175389
H	1.76985732411242	-9.65058334640451	2.18423022049009
N	-7.73710591290503	14.55386376610724	-1.10938166223827
Si	-6.55385562431886	15.71057498552766	-1.24126432446785
H	-5.54992858755748	15.84937530809891	-0.09397359365186
H	-7.10338410281469	17.13245795317573	-1.37304157376657
H	-5.62974257485225	15.62602137220473	-2.46150491706434
Si	-7.85797856057556	13.07352803953424	-0.35852573358214
H	-7.17178654792476	12.90731679507704	0.99862562545017
H	-7.34367228880517	11.85745154691259	-1.13274972864850
H	-9.29804444355554	12.67159664741235	-0.06724273386002

Pb-2d

C	0.73231234104604	3.07836305193506	0.52738489930582
C	-0.21904429910597	3.62697391014165	1.33159041179513
N	1.30700929725730	4.14087734367519	-0.15314788225057
N	-0.19317000891187	4.98695974047941	1.10479321341299
C	0.75174281033468	5.34635348774674	0.19107913006174
H	2.11713725343499	4.07530530513348	-0.76927265181235
H	-0.83577584997696	5.66750404660196	1.58517241613044
H	-0.90627264877817	3.17644069212175	2.04278719234876
H	1.04648657322891	2.04837074577058	0.38440108192469
Pb	1.42609391916261	7.45368564551601	-0.86978267321148
C	0.98358684813627	8.64859936900332	1.22660376510015
N	0.06232716664677	8.51296674170641	2.22198338803661
N	1.68096407327964	9.76299193813064	1.61661026690557
C	0.18574167497437	9.48436558150472	3.19285305072239
C	1.21296149478210	10.29119489813561	2.81041060655082
H	-0.67154312543929	7.76043972214079	2.24646240308851
H	2.50805509121522	10.08788448697091	1.11615823272927
H	1.64601468376346	11.17337389353372	3.27322140426888
H	-0.46463729505011	9.51192939975207	4.06309174489262

Pb-3a

Pb	8.46259372342395	1.18882049652019	9.40945276437579
Cl	-32.70366632108802	-13.67402489653108	-18.88666286207489
C	6.29473462902062	1.20942850948687	7.93735546434468
C	6.40143268759256	0.13912051469476	6.87063961220659
H	6.53508480025341	-0.85962460919939	7.31063790796912
H	7.25996847644099	0.31158817685209	6.20312833355481
H	5.47295176351943	0.11375132825513	6.22693375674564
C	6.13816550795759	2.57491580250954	7.30064955420675
H	5.20224099687291	2.62347400284492	6.66910805797950
H	6.98903075539196	2.82059788373087	6.64625157949696
H	6.07691029492879	3.37007701773288	8.05757009570445
C	5.11973106904063	0.92142045963812	8.84850268918404
H	5.02697132812222	1.67873009587935	9.64220806428342
H	5.21501342145984	-0.06178642042905	9.33481706420106
H	4.15082186706293	0.91854463801477	8.27017891782206

Pb-3b

H	2.17332659775401	-0.06273687640856	-0.89793770069351
C	1.25157278697213	-0.06724040100643	-0.30112112948189
C	1.32568948768225	-0.06654042332037	1.09145851631897
H	2.32025239324360	-0.10428286871148	1.55445815419185
C	0.18892360054932	0.04676248176984	1.93137297610211
Pb	0.55126797527032	0.20919594979599	4.38469769565876
C	-1.05282757067409	0.08604592104629	1.24240378904980
H	-1.97773828739323	0.16755998392817	1.82600583105039
C	-1.14954634654329	0.03882570365041	-0.15042635538112

H	-2.13659583691139	0.01098118353870	-0.63077120955662
C	0.00311218635206	-0.01978236699436	-0.95211636064172
H	-0.06793183744738	-0.02710242113556	-2.04140684685595
Cl	-10.33735514885420	0.11992413384734	-4.53954735976106

Pb-3c

N	-1.55711701608328	1.23949247408792	-0.13311867749049
Pb	12.86410949156316	-20.69010027876194	26.69632623168204
Si	0.03980804871875	1.59266956643246	-0.42577746733990
Si	-2.35115581222915	0.29419373186406	0.97930004899607
H	0.23506276896059	2.45908271912147	-1.66295968820745
H	0.80547078045397	2.37722622353604	0.64675816254494
H	0.99539685575315	0.42129533461317	-0.68733538125686
H	-3.85397658893768	0.23709435809406	0.73881589910576
H	-1.97136667170414	-1.18962548963918	1.05782019056704
H	-2.27131437674658	0.70942255211084	2.45362991010247
Cl	-20.22833747974875	23.11895880854062	-26.73018922870352

Pb-3d

C	0.52586011849025	2.91574934252514	0.22687397289126
C	-0.21836796342502	3.79825017688182	0.95515159122220
N	1.54669330982443	3.64978213049343	-0.36371953883730
N	0.39933431061303	5.02722636821362	0.76803766438061
C	1.49588964668613	4.97262873513942	-0.04540956694957
H	2.28867299750401	3.31492415592201	-0.97686271663287
H	0.09634031847934	5.90490133794145	1.17540991774264
H	-1.11497455719441	3.62822054986558	1.57022835355601
H	0.39692982936553	1.84934582441593	0.09271613103712
Pb	3.15918271461727	6.64513034123537	-0.88271367487011
Cl	-3.12727072496059	2.85318103736617	2.75462786646000

As-1a

C	6.57295246595529	2.16338495433762	7.94100199022201
C	6.16549731972317	1.23461048545306	6.79838560398743
H	5.07118846982430	1.13404577831282	6.74713955128477
H	6.59095348640062	0.23012021547213	6.93988495507133
H	6.52192873006140	1.62673767075901	5.82098639974091
C	5.95183257732242	3.54429369149932	7.72556195364595
H	4.85676314756713	3.47258539471312	7.67631739567994
H	6.32157828794622	4.01142818692284	6.78447287953501
H	6.19691366361579	4.22037808040441	8.55790885028398
C	8.09700285915431	2.28785448831751	7.98155844910560
H	8.56128635629672	1.30300120207227	8.12567805579559
H	8.41711128146031	2.92542925254849	8.81901188745726
H	8.49115368930937	2.73569208613403	7.04075461249042
As	5.86422806675714	1.30994258851102	9.72227997449371

As-1b

H	1.06325489929955	-0.15155018687964	2.16564815945061
C	0.53967932019117	-0.07843898875269	1.20695822541000
C	-0.85022650481056	-0.02320200872788	1.19685698730940
H	-1.39128288714284	-0.05404732557187	2.14676459471299
C	-1.59387803521935	0.07213694215575	-0.01120308321012
As	-3.55329154266575	0.16160234045802	-0.02807832021621
C	-0.82519434637318	0.10416103743993	-1.20688533614707
H	-1.34667683324598	0.17503659044510	-2.16553458321898
C	0.56458759305997	0.04867689607957	-1.19413077606046
H	1.10768819516675	0.07706562443079	-2.14427321040914
C	1.27709787682508	-0.04299471257567	0.01245180658428
H	2.36733226491515	-0.08531620850140	0.02144553579471

As-1c

N	-1.59279670621965	0.98393871439413	0.41363630480353
As	-2.60064747480828	2.56787445837978	1.13546545751823
Si	-0.30292471561232	1.48390325736720	-0.58830827775140
Si	-2.24361521004271	-0.49001333362255	0.98173445566079

H	-0.74091456670865	2.27331130860615	-1.79322920733997
H	0.74598516604252	2.30292778355650	0.11685753742030
H	0.43535229432386	0.26701159182069	-1.13823726258374
H	-3.68257375186467	-0.70506728318911	0.59500459062552
H	-1.47575453836975	-1.66709003894058	0.38930256584720
H	-2.15970049674035	-0.66660645837221	2.47542383579954

As-1d

C	0.93077146945981	2.35815483008576	-0.20738245778333
C	-0.30811522042049	2.37573482399650	0.34473955800086
N	1.46214023540664	3.63057914949812	-0.03625377412531
N	-0.50729091655948	3.65887397659790	0.83758184118736
C	0.58487080983510	4.46856159187814	0.61630846004413
H	2.37756846029376	3.93374111063406	-0.34081290567370
H	-1.33978424591652	3.98930920385484	1.30697851173573
H	-1.05399209385317	1.59639326751125	0.42776934856201
H	1.47293299093663	1.56020601572358	-0.69727032434781
As	0.82167851081773	6.31246603021983	1.10854174240006

As-2a

As	4.21921166757095	1.44259279747195	4.19801553087429
C	3.57971253998625	0.33329186528309	2.49650902068515
C	2.12458849470137	-0.12316803175913	2.57218783837112
H	1.45389687769455	0.72560883467080	2.77888978609028
H	1.96836608013598	-0.87505736396800	3.36219837188883
H	1.80580634905293	-0.59444238376280	1.60997169517562
C	4.48905626065207	-0.86896689078230	2.23053880458572
H	4.19453047747427	-1.39756028551755	1.28928934013720
H	4.44231391636673	-1.59815854990674	3.05178442885697
H	5.53882448457271	-0.54941608117482	2.13624073068873
C	3.72973293966168	1.32769260118809	1.34355462496777
H	4.75994393387076	1.72162520859099	1.29399629735948
H	3.04735896824787	2.18345298367276	1.46837956678837
H	3.50458556408379	0.83846398470981	0.36608704315716
C	3.55778351190539	0.34604126095191	5.89880268658608
C	3.88860741635067	-1.14321184437037	5.83109393707638
H	4.96098666675402	-1.30087480723240	5.63582942007561
H	3.32379541003663	-1.65524064087274	5.03569159694890
H	3.62903211757939	-1.65265620292897	6.79169929940988
C	2.06022010730613	0.53618318843965	6.15207159007585
H	1.74249086016259	0.02408498531908	7.09478486179816
H	1.45731783551559	0.12530813724328	5.33002686497158
H	1.81253157400036	1.60599823677971	6.23691885219995
C	4.33530542101239	0.97718937824902	7.05537301123066
H	4.15878891848582	2.06612956636561	7.10069054688042
H	5.41875642173925	0.81575665492956	6.93834520395137
H	4.01841118507986	0.53966139841049	8.03185004916845

As-2b

H	-0.57351263000492	-0.23154301545914	2.53914503904627
C	-0.50819350679098	-0.21646204687992	1.44084210076372
C	-1.68418282539186	-0.20827944423868	0.68760453799344
H	-2.65032639893103	-0.18537078340375	1.19491779877548
C	-1.65013770365478	-0.25246187839363	-0.73103568139530
As	-3.24196856939446	-0.21350371439193	-1.92219422933164
C	-0.37114065616712	-0.20487362182347	-1.32902143513624
H	-0.30435645544073	-0.22417556025538	-2.42338502788127
C	0.80255033507379	-0.14022956420536	-0.57569465239462
H	1.77785839677726	-0.08069747180874	-1.08384445055312
C	0.74920357266486	-0.18722759809635	0.82786269723397
H	1.67241762068911	-0.19362302389852	1.42826219701203
H	-3.44191569405753	-2.30878922367475	0.44637021050679
C	-4.45784881753913	-1.96548184190726	0.24204637909108
C	-5.52238442704307	-2.47423805307645	0.98914193152648
H	-5.31781726833035	-3.19166121836382	1.79807901824870
C	-6.84408085632673	-2.10398782784968	0.71759225672894
H	-7.67887050413498	-2.50818883810655	1.31176941270037
C	-7.07896271003226	-1.20921707923720	-0.34050376544122

H	-8.11183640241447	-0.92812098265158	-0.59921414393430
C	-6.00868136960194	-0.64415333513443	-1.03783711408898
H	-6.21097656019325	0.09826531988101	-1.81896221245290
C	-4.66611656975541	-0.98882919702441	-0.76762086701768

As-2c

N	3.53698373900910	-3.85467864712241	0.26257779691183
As	5.44244764100609	-4.13638287911033	-0.31772743439199
Si	2.77222163859837	-5.35180785825839	0.56358885614103
Si	3.04401839863993	-2.23450558765481	0.02299658215783
H	2.69311255805774	-6.27105630921490	-0.62771272713810
H	3.41470658818033	-6.13160739510980	1.67715738868767
H	1.32644299871286	-5.12677834903512	0.99275191788792
H	3.09309015215775	-1.77515632400263	-1.41011065819780
H	1.59578716995640	-2.05934516318636	0.45950037512718
H	3.84833727072543	-1.25490755270190	0.83014778154380
N	-8.89093650160337	10.12286260319328	0.71358709559549
Si	-7.95336330061754	8.94543081830834	0.00926730716782
H	-8.56320481004890	8.20813589411638	-1.18695235245407
H	-7.60958728988822	7.79647297212408	0.94862164344510
H	-6.58391518604684	9.36140702061406	-0.53798882219464
Si	-9.04256912331419	11.76526016598178	0.54080662935564
H	-10.10749983524962	12.26733251386264	-0.44219173930723
H	-7.80878303991979	12.56003002389224	0.09374162148405
H	-9.45090906835546	12.48025405330386	1.82563873817848

As-2d

C	1.41439173768815	4.46103535690858	1.34815933243487
C	0.09854490051675	4.41999015866944	1.69881749066885
N	1.50574349556666	5.28734676654088	0.24143474451425
N	-0.57918450408536	5.21989774886878	0.79473167463066
C	0.27249142896298	5.80239262476988	-0.13407534686977
H	2.35200981779907	5.55456766319996	-0.24383419908868
H	-1.56821066160380	5.43208358645619	0.79986189192871
H	-0.39250089584241	3.88605954754514	2.50252042968431
H	2.27010007924446	3.96960458394902	1.79353123028237
As	-0.01906926661287	7.59366975134624	-1.02013172578606
C	0.41151760856112	8.50346531070775	0.72685467243733
N	-0.41464076199961	8.52980557888644	1.84217101559954
N	1.67335194408252	8.58867275463439	1.29978027150691
C	0.30174240721208	8.60127408466586	3.02447160141169
C	1.61964364209990	8.63922196362184	2.68190556114760
H	-1.41877090144146	8.45086768903323	1.74913621375018
H	2.50776306147181	8.56809437031712	0.72839302570268
H	2.50080719504225	8.70131082772205	3.30796145132374
H	-0.16574032666224	8.62521963215717	4.00071066472081

As-3a

As	5.89175085509012	2.35445207224795	6.42349404857889
Cl	-8.82049062886700	-4.10007238240826	-7.36895097301370
C	4.56227678556631	0.79169325436968	6.85926115355158
C	5.29846900040117	-0.54567611508419	6.96689282841006
H	6.07307885931070	-0.50165975434645	7.74507364568692
H	5.80342465276991	-0.79056806619507	6.02171319039705
H	4.59705444013388	-1.37594445129496	7.21228166169748
C	3.50518370371807	0.70845804557550	5.75856344197997
H	2.77837248441893	-0.10845759340938	5.96332288623244
H	3.96773698919763	0.50482520342289	4.78088016144404
H	2.95599633718559	1.65618232872500	5.67555222309152
C	3.88703777492328	1.11067840677362	8.19248290973071
H	3.33873203150830	2.06134550768243	8.13271116548447
H	4.63099760263357	1.20164420795822	8.99881071087856
H	3.17236411200958	0.30813233598301	8.47868194585001

As-3b

H	-2.31042571362915	0.01899737312957	1.58980322097855
C	-1.70771605651913	0.04658557058302	0.67687702595238

C	-2.34342982106865	0.15493112888885	-0.55806325007102
H	-3.43530697320749	0.20961335081279	-0.59151919065264
C	-1.61923409048273	0.19701275285426	-1.77879016155074
As	-2.51857178370778	0.36157273815205	-3.52458945490799
C	-0.20673357452080	0.11374978217275	-1.65983001894098
H	0.40085480468914	0.13780087259890	-2.56921370820241
C	0.42674170113008	0.00375664747255	-0.42355894098964
H	1.51868609889676	-0.05882335636283	-0.38455701686877
C	-0.31045706883874	-0.02881800638427	0.76865488460061
H	0.18606861354446	-0.11240343545644	1.73620423997196
Cl	3.01167386371395	-0.71236541846120	9.23565237068068

As-3c

N	-0.73608362043666	-0.58971345263405	-0.70975123981637
As	-1.95603096421752	-0.09260029766925	-2.23055531758322
Si	0.87808996504614	-0.15629929374675	-1.05511629516464
Si	-1.61431834422484	-1.30481203652045	0.56795329778894
H	1.44964260742118	-0.85611565721867	-2.25899988766323
H	1.08638861127105	1.31885214759342	-1.26250412606578
H	1.78635543379426	-0.53993164722070	0.10939860446793
H	-2.29661266857404	-2.59175435949549	0.18866396593884
H	-0.67361994909325	-1.66509544717078	1.71372595261720
H	-2.66172114169347	-0.40826116469220	1.16817328656043
Cl	-12.55550992929282	17.45544120877502	6.70228175891989

As-3d

C	0.81430197666060	2.65627852592636	0.00621838578084
C	-0.09217153521780	3.20610419396998	0.86015545240620
N	1.56776830145859	3.72290068493044	-0.47710417450229
N	0.11298589025703	4.56808584595410	0.88418468871726
C	1.13831682291871	4.91744056872890	0.06127204631225
H	2.32183316742094	3.67061408947443	-1.14843023055115
H	-0.52625348297995	5.17459291474690	1.51912484106376
H	-0.87522291552633	2.76579742563778	1.46586372155958
H	0.99176207162950	1.63127202880594	-0.29299747735397
As	1.91441911535815	6.65017793554397	-0.35835869512544
Cl	-1.91944941197945	5.59607578628120	2.75441144169295

Sb-1a

C	6.57828463013409	2.16978345923950	7.92588790049800
C	6.17150380209566	1.24120939956175	6.78483197281416
H	5.07797259153308	1.13517457548468	6.72862761634102
H	6.60207625297213	0.23744644055618	6.91554654934856
H	6.52617458181712	1.64096851795614	5.80873632976039
C	5.95570510626637	3.54813045087851	7.71591805952595
H	4.86003617824581	3.48269298338128	7.67100228540261
H	6.32164118291573	4.00749573705556	6.76914046228544
H	6.20785110095426	4.23082057598366	8.54060725640519
C	8.09989299167630	2.29110640392631	7.97364954561342
H	8.56910044760966	1.30848441923982	8.11834812530103
H	8.42414581158297	2.93379174298115	8.80540616472122
H	8.49076461674326	2.73432137117180	7.02910084228969
Sb	5.79524110684776	1.23807799804134	9.89413944848724

Sb-1b

H	1.08339663270561	-0.15264197486498	2.16490628131478
C	0.55809259845477	-0.07985662658396	1.20755775323981
C	-0.83375141903021	-0.02097596288553	1.19402214428119
H	-1.37209616782093	-0.04924595009070	2.14560845801778
C	-1.57004149318196	0.07310714182294	-0.01131024542862
Sb	-3.75565966508473	0.15934141930807	-0.02823114514399
C	-0.80857459277415	0.10596246273498	-1.20421306539486
H	-1.32669636466683	0.17973333303570	-2.16453477520844
C	0.58333722802788	0.04722419725483	-1.19465205863274
H	1.12862238716434	0.07591344823074	-2.14313091974115
C	1.29097917973018	-0.04520697058314	0.01247467275539
H	2.38148167647603	-0.09022451737895	0.02152289994084

Sb-1c

N	-1.59971724136493	1.01124997404234	0.43578575100447
Sb	-2.73259216991928	2.73987723359302	1.20657864217095
Si	-0.30194296046451	1.44915318186108	-0.58627552613452
Si	-2.21696927327004	-0.49216660521816	0.96346771899254
H	-0.72239858576284	2.20768189670494	-1.81731186914252
H	0.74729486837888	2.28745197562288	0.09503667656249
H	0.41830644613426	0.20718665192752	-1.09042188292022
H	-3.63905987902532	-0.75240847437280	0.54211372059398
H	-1.39690675827560	-1.63429154224777	0.38092933301810
H	-2.17360444643062	-0.67354429191304	2.45774743585473

Sb-1d

C	0.93288595995190	2.33736081294932	-0.20835235306436
C	-0.31043910287497	2.35234941369921	0.33740737559134
N	1.45511888477013	3.61070639358230	-0.03494505896171
N	-0.50993072450192	3.63429137548501	0.82874917009337
C	0.57706721058015	4.44609397375336	0.61168668489532
H	2.37390588722699	3.91372769239404	-0.33091918148603
H	-1.34593789216096	3.96186254202315	1.29505852496301
H	-1.05608140817083	1.57196718420625	0.41418227603400
H	1.47866701629267	1.54164289588227	-0.69805285426059
Sb	0.84552416888684	6.51401771602509	1.14538541619566

Sb-2a

Sb	4.31140084497068	1.63227827249599	4.19734083018940
C	3.58351556967773	0.35246653294118	2.36023571608290
C	2.13359652024625	-0.09649138782940	2.50633351996433
H	1.46146770996943	0.76154834346179	2.66375648032551
H	1.99895534421720	-0.78819048262943	3.35302220188609
H	1.79814545764863	-0.63764276556256	1.58632477926395
C	4.48767231062259	-0.85972525824402	2.15014271988599
H	4.16389579365031	-1.44201787041232	1.25001533543363
H	4.46392086513962	-1.53930166021320	3.01432068411075
H	5.53470011144449	-0.55245244212881	2.00302513386630
C	3.70685583618295	1.28628073151300	1.15971225352727
H	4.74012025646480	1.65512272310038	1.03995647723959
H	3.04699598163499	2.16262559031286	1.26209817083917
H	3.42881380313847	0.75191213081573	0.21681470186407
C	3.56931487480698	0.36118208861239	6.03455231348635
C	3.90514085316566	-1.11915828968900	5.88862012152736
H	4.98395233822269	-1.27265886835230	5.72941257325317
H	3.37154099001775	-1.58192542863419	5.04329882324886
H	3.60576549082047	-1.67939429002056	6.80965129377645
C	2.06737861881194	0.53762052146224	6.24458192113100
H	1.72514495746018	-0.03402008456943	7.14470503442999
H	1.49101134627059	0.17715715087973	5.38026354431186
H	1.80973405695757	1.59797084450831	6.39168461828520
C	4.31620567125850	0.93482406012704	7.23516287392515
H	4.11984766919548	2.01428433641384	7.35456026965479
H	5.40502760111452	0.80079019270977	7.13316494061698
H	3.99183512688954	0.42724330893095	8.17806366787389

Sb-2b

H	-0.45037059724223	-0.19216481499479	2.60807077316922
C	-0.42590572075866	-0.17932345790639	1.50865522753234
C	-1.58814047646215	0.13873832016774	0.80020599846065
H	-2.49675171730547	0.40707663430795	1.34306524900834
C	-1.61712923711534	0.08514175110215	-0.62290886684587
Sb	-3.41696296825459	0.59086944289228	-1.79524841994549
C	-0.39774737654034	-0.18119783682432	-1.27006909528513
H	-0.38242425992097	-0.21894841402296	-2.36522249644196
C	0.79022757827851	-0.41504480020448	-0.56418304535562
H	1.72484469307802	-0.60113414146043	-1.10949608560237
C	0.77130941100329	-0.46894873184198	0.84669314244898
H	1.67713717566722	-0.72775729451582	1.41401224365447
H	-3.37440559407980	-1.90881671504332	0.34393317030938

C	-4.43827914947231	-1.74881205523865	0.15885381255589
C	-5.38360541960144	-2.53579650897535	0.82664955713652
H	-5.04455383270173	-3.28569887552986	1.55597811285952
C	-6.75095645834068	-2.39715829685570	0.56719548415099
H	-7.48964056335962	-3.03091492851762	1.08095154413000
C	-7.16219287050894	-1.43397008543007	-0.36703531796771
H	-8.23202797992316	-1.32882978158145	-0.60946802423434
C	-6.22145065856879	-0.59357141910653	-0.97036838373301
H	-6.57364207737688	0.19218971393393	-1.65100083404183
C	-4.83861190049390	-0.72877770435430	-0.73494374596295

Sb-2c

N	-1.30799049927026	0.58811002728793	0.21627939016597
Sb	-2.41972665859854	2.95208196137439	0.11491363641723
Si	0.34137137607330	0.60147960267214	-0.08940140809925
Si	-2.33234709597324	-0.62732514639325	0.75202766707120
H	0.74298549441959	1.10924871902221	-1.46016006604712
H	1.19687363009606	1.41556459510040	0.86554582225672
H	0.99655349497559	-0.78984896901811	-0.02758680652117
H	-3.57303656369123	-0.84252389138392	-0.09104340180194
H	-1.68134830719042	-2.02059867878888	0.78072604886698
H	-2.87159138992855	-0.48277062295713	2.16484427264660
N	-3.49099859568827	5.22268469110614	0.07190120925712
Si	-2.43517530489925	6.47435067384326	-0.30651169615715
H	-1.81280965090125	6.40090898726725	-1.68593958393423
H	-1.25586603135178	6.65177928628282	0.62801887009902
H	-3.10320956434923	7.85962176854157	-0.29373398619575
Si	-5.09921497758389	5.18516001172458	0.56103034527994
H	-6.01655384118806	4.34231049748461	-0.29907579792305
H	-5.76976928971761	6.56999898183573	0.54123438102419
H	-5.35176622523294	4.70072750499825	1.97463110359470

Sb-2d

C	1.38176430511682	4.33207202002350	1.28695192746368
C	0.07661420611410	4.28690687693898	1.67637830771800
N	1.43209310806328	5.14497169807057	0.16839058138318
N	-0.62899844028451	5.07477197493972	0.78380844221011
C	0.18887343466494	5.65213741084631	-0.17357148765505
H	2.26443179103353	5.41989726654083	-0.33760465438749
H	-1.61843029027073	5.28408853464031	0.82091091195406
H	-0.38918604891510	3.76058484630633	2.49995804115957
H	2.25418857300678	3.85156020020519	1.71150773513890
Sb	-0.15132995737371	7.65373012068698	-1.11934456987838
C	0.40777574968382	8.67938749931382	0.79549344549791
N	-0.36457810407001	8.68494528241468	1.94524256700385
N	1.69167889858709	8.73699364436815	1.31286025326926
C	0.40203879343401	8.71229062728959	3.09712293983729
C	1.70415149436980	8.74552509791391	2.69659357161365
H	-1.37302877966906	8.61464841729927	1.89756137881826
H	2.50065188019786	8.70960430720327	0.70524873613839
H	2.61437718003555	8.77873816944859	3.28201329995088
H	-0.02309779372445	8.71172600554996	4.09287857276394

Sb-3a

Sb	5.57748221438334	3.64359093248402	8.43043890603046
Cl	-8.87966593287326	-19.56785717760636	-11.13546480916403
C	4.47913083305577	1.89789260708158	7.38200017066041
C	5.28143464875813	1.53329060961092	6.13592437807245
H	6.30319531423827	1.22068315525991	6.39704620843108
H	5.35503266140196	2.38624561856764	5.44508386977788
H	4.79650330724347	0.69414233330758	5.58997627448227
C	3.07052944893405	2.32746510600104	6.97888477896603
H	2.53546102521726	1.49573383764574	6.46629059433826
H	3.09990063826250	3.19204853464446	6.30198733423043
H	2.47462244630181	2.61994491282657	7.85591684131010
C	4.40429942959811	0.69335734538393	8.31700614325996
H	3.85161527795390	0.93427981096729	9.23710406225293
H	5.40818048203702	0.36279213269823	8.61605853530892
H	3.88426320548775	-0.15857675887262	7.82251771204282

Sb-3b

H	-2.34523959180431	0.00005117677099	1.70771787178635
C	-1.75894658010430	0.03092182457899	0.78470075982767
C	-2.41656281835080	0.12069718264163	-0.44366379937141
H	-3.50814757075344	0.15661059337197	-0.45791080659680
C	-1.70952447162458	0.16060945669207	-1.66740091727090
Sb	-2.74751190413061	0.29236592026397	-3.59938605483724
C	-0.30104148638824	0.11083113856238	-1.57701240567593
H	0.29366397662115	0.14108769672790	-2.49449669385616
C	0.35858070531141	0.02308982561900	-0.35028949567528
H	1.45083701072734	-0.01102871740075	-0.32674053833621
C	-0.36265090377198	-0.02120465543733	0.84921660093567
H	0.15155766248382	-0.09291956105071	1.80991902093060
Cl	3.98713597178462	-0.57950188134011	8.28241645813971

Sb-3c

N	-1.59722455949818	0.83751062318113	0.09530036783916
Sb	-2.95493672150817	2.80872676684419	0.49310174994254
Si	-0.11670275322259	1.22552256051750	-0.60891427503809
Si	-2.17863262117249	-0.50727520682708	0.92767739950536
H	-0.21503034294522	1.88163619622715	-1.96742493982990
H	0.81327652640469	2.11521516840293	0.19618304575296
H	0.75235258678085	-0.01993926972930	-0.87776587656241
H	-3.52260150886763	-1.01083787798105	0.45068820067662
H	-1.25599762343676	-1.73254829961258	0.78070507556145
H	-2.31800685468437	-0.37036506523241	2.42967088760354
Cl	-4.69991612785014	5.34206440420949	1.01404836454876

Sb-3d

C	0.84704642081498	2.64356622041474	0.01568825074336
C	-0.01463984965096	3.15950194542234	0.93662974357298
N	1.48249257233153	3.74044902303895	-0.55319306075143
N	0.11038885486958	4.53074873447581	0.91176399325092
C	1.03329600154496	4.91668285246011	-0.00252527694866
H	2.19071140220130	3.71573721858178	-1.27538474184517
H	-0.51074907126625	5.11947722373025	1.59264216214701
H	-0.71502795275083	2.69056045613182	1.61754858089004
H	1.06040583814469	1.62434086422197	-0.28018379625560
Sb	1.75607332136355	6.88371656986181	-0.59421872958995
Cl	-1.79170753760256	5.53455889166042	2.90557287478649

Bi-1a

C	6.58342711476565	2.17595812156987	7.90997176566281
C	6.17524692400892	1.24643794047001	6.77558830091510
H	5.08177559622820	1.14297792736866	6.71401217270116
H	6.60252013200186	0.24106723377899	6.90658468728301
H	6.53327598994035	1.64048172606827	5.79713626631762
C	5.95750874724810	3.55000735697081	7.71236311309382
H	4.86136153387343	3.48870036033727	7.67580301808002
H	6.31345926188493	4.01191200598417	6.76113555332999
H	6.21974537218273	4.23538556009910	8.53188267227258
C	8.10041905092593	2.29306434922971	7.97018720493195
H	8.57173030133871	1.31164707598431	8.11677617714292
H	8.42409663619374	2.93837239550666	8.80015515127674
H	8.49928744413039	2.73412124975619	7.02606166723803
Bi	5.75653629667126	1.18937077233365	9.98328480854814

Bi-1b

H	1.09570096509221	-0.15183269717115	2.16483015178086
C	0.56952199489097	-0.07913584512443	1.20828039045473
C	-0.82425449011589	-0.02143779707175	1.19334167058613
H	-1.36169990533721	-0.05125372038241	2.14536490320253
C	-1.55465921100878	0.07225721454253	-0.01107140805311
Bi	-3.87474833842059	0.16539400561058	-0.02979076436067
C	-0.79917255482967	0.10541538457344	-1.20317499680433
H	-1.31656103654062	0.17821819984692	-2.16394147165830

C	0.59465933534001	0.04771970491902	-1.19502981344529
H	1.14068214905954	0.07634120736968	-2.14275131094820
C	1.29948195281630	-0.04644184385560	0.01249947566971
H	2.39013913905373	-0.09211381325684	0.02146317357595

Bi-1c

N	-1.58675685252008	1.00789176301977	0.44759602354196
Bi	-2.80727811148851	2.84179855148826	1.24278404315807
Si	-0.29889427266316	1.43385583693191	-0.58487363595057
Si	-2.20332103397433	-0.49751569914589	0.95681792034316
H	-0.71872065487252	2.17780129621259	-1.82689839736444
H	0.75243918918844	2.28914977258391	0.07434895552231
H	0.42708686732398	0.19158875630250	-1.07825971708388
H	-3.62094097205734	-0.76761636840751	0.52123595693327
H	-1.37538377282494	-1.63765239155001	0.38338725961135
H	-2.18582038611154	-0.68911151743552	2.45151159128876

Bi-1d

C	0.93558537471752	2.32280373830209	-0.20793594930395
C	-0.31035194990747	2.33762759075653	0.33305493377576
N	1.45347491463925	3.59779779338729	-0.03292255727112
N	-0.51120216583229	3.62183170965396	0.81733788985748
C	0.57350227157256	4.43340357116622	0.60535435482752
H	2.36814930264135	3.90485217908549	-0.33796423915346
H	-1.34557449210568	3.94683005230709	1.28872676376340
H	-1.05613269607602	1.55731513573875	0.40937909295006
H	1.48548682247887	1.52679438527734	-0.69263302973878
Bi	0.84784261787192	6.63476384432523	1.17780274029311

Bi-2a

Bi	4.38115528851853	1.74290848341913	4.19743247669477
C	3.58709588401751	0.35387433018783	2.24769967223097
C	2.14124582775758	-0.06996861759027	2.43412805473257
H	1.48136423969277	0.79675073041917	2.58520776922825
H	2.01242147471267	-0.74174582838314	3.29658389073751
H	1.77698116770289	-0.62679259172144	1.52953570060752
C	4.47556430788987	-0.86535692582600	2.06691199931703
H	4.15656441314382	-1.45392503695010	1.16368586037378
H	4.43081501890463	-1.54202305847945	2.93257181252085
H	5.52847650797810	-0.57946398909306	1.93059865278136
C	3.70712507588733	1.26083009810969	1.03446673675605
H	4.73972456213192	1.61527268105316	0.88852998852993
H	3.05895478509964	2.14570377299957	1.11965058949694
H	3.40807351376912	0.70893385110050	0.09991617487089
C	3.56991434203936	0.36457547005405	6.14725416221886
C	3.92556734237814	-1.09993451140317	5.96364311163749
H	5.00635699530379	-1.23873240935155	5.81519211394930
H	3.40997634252351	-1.54809878575382	5.10048566406792
H	3.62308871147317	-1.69238745048759	6.86840512189050
C	2.06948355076133	0.52518657838647	6.32343315029199
H	1.71662438856097	-0.04373836327714	7.22665182270273
H	1.50810507534138	0.14679585471580	5.45693725778917
H	1.79063430338292	1.58031059917699	6.45734632620274
C	4.29174093693115	0.92322402317863	7.36199840289082
H	4.08281328914509	1.99509144047088	7.50570802458179
H	5.38235356535402	0.80327756054377	7.28070200318732
H	3.95973508959881	0.38976009450110	8.29614445971093

Bi-2b

H	-0.43674881854124	-0.19997234356816	2.61767011613325
C	-0.39868150763576	-0.17005857817199	1.51891711433772
C	-1.54403178685362	0.19329309026053	0.79412918187660
H	-2.45248538490621	0.48809796464446	1.32449162892618
C	-1.54884961916490	0.14612057981658	-0.62380157299543
Bi	-3.44405540850216	0.73091279897609	-1.86711654229581
C	-0.34408234144118	-0.17619016709849	-1.26313988115268
H	-0.32244190604125	-0.23360788458325	-2.35708906808660

C	0.83521735599516	-0.43643428553504	-0.54140039749187
H	1.77205883513169	-0.65008188827041	-1.07234709924881
C	0.79457792622920	-0.48313629915372	0.86728223939827
H	1.68802383912704	-0.76308056316462	1.44515523392529
H	-3.39724835850413	-1.87039933411326	0.26937015273859
C	-4.47028636008195	-1.73238947914761	0.11753235878513
C	-5.38189822214961	-2.55870581563301	0.79428924965763
H	-5.01133887057399	-3.30887601560908	1.50781675142342
C	-6.75552376598895	-2.45373200513949	0.55274926829073
H	-7.46650602223231	-3.12728198663054	1.05504169807563
C	-7.21556945737077	-1.47890213896380	-0.34240165893803
H	-8.29293977197831	-1.40421200494727	-0.56346381880158
C	-6.30889162567966	-0.58556372525946	-0.93272351613309
H	-6.69800579198291	0.21967855631080	-1.56904942153350
C	-4.92157293685419	-0.70832847501926	-0.73759201689105

Bi-2c

N	-1.26304528778340	0.49040044860790	0.21441988010150
Bi	-2.39698630112103	2.91566242487684	0.16433189348387
Si	0.37611594536128	0.47186092941680	-0.14507435867207
Si	-2.30068562973493	-0.73473937556422	0.70394040426143
H	0.74444812785651	0.97815657564744	-1.52690007046488
H	1.26614987590341	1.27553937514853	0.78518981570799
H	1.01005652704319	-0.92920864484680	-0.11014473225008
H	-3.51478906805002	-0.95054869204807	-0.17873770164339
H	-1.64099894922673	-2.12433597453180	0.74206850812211
H	-2.88325417878761	-0.59601772092350	2.09880695613672
N	-3.51087534787645	5.32378472071670	0.18949933054906
Si	-2.46723702836973	6.56453364992312	-0.24555030888687
H	-1.88137576899501	6.47286884903069	-1.64183777412443
H	-1.25494701536155	6.74648017859919	0.64636074315312
H	-3.12503080367986	7.95453384644072	-0.23496352665318
Si	-5.13387014992031	5.33917888606185	0.61720242161752
H	-6.06529316664232	4.56970434881079	-0.30132094862117
H	-5.75275131835082	6.74676332598267	0.64264073989806
H	-5.44925046226464	4.79634284865113	1.99776872828469

Bi-2d

C	1.09080606969964	2.29381231473675	0.03263427284065
C	-0.20534168787674	2.22997197661885	0.44880964434633
N	1.39063905558952	3.64389071213557	-0.05758529941856
N	-0.62027329918000	3.54520582367376	0.58807165509688
C	0.34861471533384	4.45118204967554	0.28240924993744
H	2.28545819971235	4.03774368634800	-0.32804551465295
H	-1.53738573571732	3.84826415505266	0.89715221035744
H	-0.84077184730820	1.37648445033584	0.64943080954650
H	1.79694350401108	1.50602023902588	-0.19806066394897
Bi	0.37889490575149	7.04385686219704	0.66870721327800
C	0.69235389032450	9.35425993053344	1.86291445854364
N	-0.17951247386444	10.01916494102005	2.66946039825999
N	1.83091889903199	10.08432011006351	2.01777135045861
C	0.38549110225207	11.11493203583810	3.30281150117683
C	1.68132509231779	11.15690654888768	2.88278924620113
H	-1.13599545802346	9.69917681968115	2.77653247203481
H	2.68526669413695	9.82253053532213	1.53788612204406
H	2.47983452158401	11.84627170379538	3.12694431805548
H	-0.15727614777506	11.76058510505874	3.98176655584268

Bi-3a

Bi	6.75025039548072	2.29503665773388	7.24850691787725
Cl	-15.06461909734248	-2.73584645747292	-4.25326447674106
C	5.00864212082963	0.65026318982426	6.77350634347808
C	5.59139649757773	-0.75153109608492	6.89858325712208
H	5.99895506876298	-0.92554924514839	7.90381867480398
H	6.40798922981994	-0.91610458275418	6.17983976078184
H	4.80940127492119	-1.52164169186906	6.70034991853514
C	4.45921559549312	0.86918987299522	5.36942295419934
H	3.65475565302221	0.13112993019998	5.14226429440979

H	5.24301688528897	0.75452979175833	4.60634580052416
H	4.04109509938951	1.87881942702538	5.25773845141120
C	3.90604243711277	0.85188401599882	7.80425398898990
H	3.47618231892132	1.86288240528000	7.74239336679305
H	4.28190363682189	0.70638411691269	8.82764525255274
H	3.07775788390059	0.12558666560090	7.63936649526240

Bi-3b

H	-2.01811304979990	0.02581698337417	1.98249709154207
C	-1.64261204572246	0.04738160246574	0.95528881241798
C	-2.54408479668447	0.13315181889644	-0.10748595536916
H	-3.61497441142138	0.17103827405603	0.11258888500418
C	-2.11210158833584	0.16663721449453	-1.44928839547389
Bi	-3.62278440406030	0.30132015758511	-3.22062823277089
C	-0.71964535454619	0.10934998960312	-1.66376099818674
H	-0.33237441975522	0.14173781262683	-2.68627843602366
C	0.18616254668795	0.01525934545750	-0.60535500409064
H	1.25901892092074	-0.02939238346516	-0.81400557931431
C	-0.26467596970259	-0.01750474158822	0.71915376502101
H	0.44137125603933	-0.08884314543654	1.54773959764461
Cl	6.07696331638017	-0.64434292806956	7.74660444959933

Bi-3c

N	-1.54522479741457	0.85335488364848	0.18012956517392
Bi	-3.02990704314781	2.98197962255332	0.56504113628194
Si	-0.10408434922131	1.18606388308536	-0.61540121273142
Si	-2.15032074852901	-0.52175975744291	0.93181679570267
H	-0.24667318627066	1.75372535681850	-2.01359731537753
H	0.84697608212925	2.14367252789069	0.08071440893448
H	0.77549102645474	-0.06230528359198	-0.83623633645632
H	-3.51246799795511	-0.97738409033922	0.44904685510359
H	-1.27249666684874	-1.77170739369213	0.72210428879901
H	-2.29220481554468	-0.45574311925640	2.44107345788162
Cl	-4.76250750365210	5.43981337032630	1.02857835668805

Bi-3d

C	0.87708818089641	2.37825337013929	-0.26957413588014
C	-0.32902568391943	2.48230704354002	0.35288176155020
N	1.48018458752971	3.62378766185637	-0.15333251889830
N	-0.41233787185569	3.78354522547515	0.82320926295965
C	0.70561878823628	4.54544799402906	0.53243725090202
H	2.39271991515095	3.87028015756645	-0.51145120344652
H	-1.18888490660351	4.17703749587449	1.33909386541932
H	-1.11272936665041	1.74730941217206	0.49029882997398
H	1.33606719719981	1.53627150062060	-0.77359360528204
Bi	1.10585149761223	6.87120624441290	1.13126609134808
Cl	0.59373766240364	9.54389389431360	2.31310440135377

Se-1a

C	6.58608601094437	2.18061166599691	7.91603734798689
C	6.15511343241818	1.21920283301135	6.80669079220035
H	5.06240053979996	1.12551879829236	6.75321062546815
H	6.59017122533369	0.22036379638998	6.94323360739132
H	6.50882756759780	1.61289842353746	5.83859711608794
C	5.94157291489530	3.55244631458935	7.73724732389700
H	4.84877091783673	3.47571882861532	7.68276933044042
H	6.30633927962262	4.01096052344957	6.80244910512156
H	6.19804694326369	4.22808884770154	8.56381481891324
C	8.10692640586591	2.28432689375879	7.99570799113378
H	8.56702688242567	1.29832985938207	8.13375796914893
H	8.42244547551693	2.93071608305124	8.82535367411904
H	8.49495988608315	2.72348890820348	7.06097378823850
Se	5.89170291979020	1.33683229947823	9.62109906864682

Se-1b

H	1.06994025386452	-0.15088695544398	2.16420658609178
C	0.53369880203606	-0.08007156147426	1.21740570264605
C	-0.85571820181207	-0.02529483103032	1.21097869185504
H	-1.42072253689163	-0.05332236883838	2.14216249622370
C	-1.55405380318222	0.06987882276683	-0.01093121674521
Se	-3.45685661451482	0.16121389817962	-0.02721586779599
C	-0.83040431334054	0.10326701965415	-1.22124834411153
H	-1.37634977509142	0.17511042643344	-2.16137395330630
C	0.55885193027341	0.04824358551485	-1.20480947191042
H	1.11436598522805	0.07788286623791	-2.14261675892281
C	1.24338361056883	-0.04166773705621	0.01215578876589
H	2.33295466286182	-0.08122316494364	0.02130634720980

Se-1c

N	-1.61070852005555	1.04967201315487	0.47102046275288
Se	-2.53526775985301	2.52035009543497	1.17236016241243
Si	-0.28042203479644	1.46823247097848	-0.61176744782170
Si	-2.24181472049753	-0.52057269805472	0.97357823277178
H	-0.80246966487818	2.21332359093721	-1.79651583325187
H	0.71376218398004	2.30934894188519	0.11869179436499
H	0.34913099222128	0.18204361644342	-1.05012695081167
H	-3.65279472383941	-0.67679000897270	0.50873975448718
H	-1.37393282281091	-1.56393541702664	0.34020038197512
H	-2.18307292947028	-0.63148260478008	2.46146944312085

Se-1d

C	0.94411162613202	2.38040826740514	-0.20715648742786
C	-0.31647697500306	2.39823182756824	0.35612068105478
N	1.46358255005743	3.62924615267070	-0.03496895683659
N	-0.50678266159271	3.65851511727309	0.83919562776155
C	0.58283904719357	4.44552471044337	0.61121684922014
H	2.38316472318238	3.94587908540266	-0.33955540045144
H	-1.34047391579270	4.00289742181236	1.31341507266547
H	-1.06194956322025	1.61502795301933	0.43525264115996
H	1.48149803655418	1.57807149854428	-0.70014669416688
Se	0.81126713248914	6.23021796586084	1.08682666702089

Se-2a

Se	3.23315392259163	1.79397251476046	3.79244649488651
C	3.27795310796880	0.57007995080882	2.17055855490221
C	2.16914629891957	0.98032623282033	1.20072649243769
H	2.30353077490857	2.02226700343528	0.87953425684864
H	1.18695003517533	0.90506830359291	1.68654659989074
H	2.16930539784124	0.33067499022430	0.30044994146664
C	3.05697388668244	-0.87165090314451	2.62818068912831
H	3.07049867211553	-1.56720374216084	1.76417704284381
H	2.09089697733309	-0.96986790263844	3.14143325967141
H	3.84139502182688	-1.17728116509436	3.33327333332477
C	4.63873746462872	0.69219364572396	1.48343303723808
H	5.44457266383820	0.41477217946362	2.17622906799081
H	4.81617031037052	1.72797780487438	1.16313094408225
H	4.69448879609668	0.03248712814262	0.59247779543208
C	3.60510526995640	0.01619351719162	6.46570857016990
C	4.95971965833484	-0.56941361587389	6.28319071503253
H	5.68736756466974	0.20212055223421	5.98891726984604
H	4.96475463490770	-1.34725821537848	5.50398848372040
H	5.35008999833943	-1.05046595447370	7.21709558235494
C	2.43288929711956	-0.89840078950134	6.45101539765221
H	2.29968042522798	-1.44112346903257	7.42249221980584
H	2.52803729030952	-1.66777497745611	5.66988166124498
H	1.50096147391987	-0.34382018136995	6.26204214434674
C	3.49690239226441	1.26157282697329	7.27120369703739
H	2.52348373096417	1.75137706310883	7.11802053072341
H	4.27942752900153	1.98423140216415	6.99464884464071
H	3.59976340468766	1.06927380060540	8.37001837328094

Se-2b

H	0.18484923210601	-1.04963738016840	2.23484921606168
C	-0.22597982074650	-0.72452274255387	1.27439190367786
C	-1.28654348344664	0.17437303289673	1.25539850767545
H	-1.71267353534427	0.53697138932781	2.19346447646842
C	-1.82663629566687	0.63662831182045	0.03052743631022
Se	-3.63343035239562	1.49119079683468	0.00567890400364
C	-1.27927296679060	0.12348233060090	-1.17045069492086
H	-1.69968722762588	0.44641103179291	-2.12544779700840
C	-0.21844688755118	-0.77495511952939	-1.14525403267824
H	0.19768405094046	-1.14035712420138	-2.08878274126020
C	0.32926386974724	-1.21234580525645	0.07590405571155
H	1.15863757510980	-1.92072492143665	0.09313693871060
H	-4.98205021181367	-0.19605635282985	2.17881049353587
C	-5.20691145648764	-0.70160821873334	1.23706712912788
C	-5.78126515674601	-1.96772289123980	1.24702721043345
H	-6.01875036489319	-2.44161430059402	2.20410023447402
C	-6.06541381483644	-2.64184756396357	0.04393546710987
H	-6.51041857554380	-3.63776200719842	0.05417956996203
C	-5.75306602323384	-2.00545381807485	-1.17252320792838
H	-5.96879641837242	-2.50882501391782	-2.11963134180498
C	-5.17953007376493	-0.73899408169661	-1.18870870479775
H	-4.93339797120435	-0.26255935449459	-2.14030124503810
C	-4.90944409143967	-0.04692019738446	0.01694822217434

Se-2c

N	-1.39358886977363	1.04849912003792	0.60813704959051
Se	-2.16263991405596	3.01823873961147	1.05453683908996
Si	0.12302810966727	1.10271510523240	-0.17293476336606
Si	-2.63679550283121	-0.12147279413891	0.64816781361937
H	0.11902937250237	1.77358449363463	-1.52333082559896
H	1.15352872618174	1.82549137631548	0.65060678449989
H	0.66580159976857	-0.29115067845451	-0.41538144196362
H	-3.72364181307496	0.07079378287445	-0.37973961348806
H	-2.08608955299010	-1.51107957741623	0.39952792113438
H	-3.32337047204445	-0.16655201182185	1.98517776548169
N	-3.17760257605856	4.89132759821128	0.64740367058242
Si	-2.15038864179881	5.99564766777860	-0.15524811570431
H	-1.68918040880078	5.56584524875922	-1.52618687816869
H	-0.90661480869215	6.27231392001851	0.64258804423853
H	-2.83573112763868	7.33059678930086	-0.36362214268973
Si	-4.87097325921862	4.66729466465781	0.58742745519350
H	-5.36184372962456	3.76827033219446	-0.52023821364807
H	-5.58824470893056	5.98606206847580	0.38196034341733
H	-5.39830242258695	4.08453415472859	1.86884830777992

Se-2d

C	1.26907305694326	3.39394349222149	0.70027456499813
C	-0.01623816433664	3.34203180065202	1.15463027868438
N	1.42542917519771	4.62819040362547	0.10368143643490
N	-0.60029373388151	4.54686604734148	0.82040808582774
C	0.27343236448622	5.35261144756538	0.15525316351395
H	2.26177042801595	4.96541364592786	-0.36227641432043
H	-1.56514741901570	4.81099054225246	0.99252936759266
H	-0.54963327409571	2.55553344357911	1.67350671577310
H	2.06411570321740	2.66052955857024	0.74790028124248
Se	0.00849374057440	7.16206093721970	-0.38808528014541
C	0.45361995319268	8.89255738960752	1.14927674029250
N	-0.30335886342420	9.15798384927409	2.23812893604803
N	1.69442992702725	9.28840320999067	1.51246005050517
C	0.43648217047843	9.74426929589345	3.25340914804998
C	1.71404281500584	9.82804370382207	2.78925966761936
H	-1.30278935858567	8.98586388951774	2.26948077685027
H	2.49368095665704	9.23295319484177	0.88989340489146
H	2.60953891580579	10.22875086943719	3.24755904120452
H	0.00334160673747	10.05758327866031	4.19511003493722

Se-3a

Se	4.47718496466239	1.41311615841381	4.42678276686712

Cl	2.70304596898611	0.06365209119359	2.54402552888423
C	3.63288152395064	0.39619520315567	5.96992856222018
C	3.82968128244903	-1.10049547125049	5.74026713808219
H	4.89864117603960	-1.35375277674558	5.71804354430216
H	3.38530918538373	-1.39151402949501	4.77891203852273
H	3.34691411687492	-1.67604028602305	6.55363039834598
C	2.14539510945875	0.73746125112545	6.02533667699099
H	1.65365947665448	0.16662135921097	6.83639511526664
H	1.67012189126298	0.48505471146115	5.06792054220889
H	1.99958731092283	1.81029925644762	6.21329257482246
C	4.34288172040627	0.84867297139024	7.24492981123813
H	4.22497302354157	1.93022522875532	7.40132401632517
H	5.41770652714011	0.62270855797048	7.20053425504388
H	3.91400172226660	0.32282877438983	8.11944803087925

Se-3b

H	0.76029806896140	-0.13814330788422	2.23648487048907
C	0.29281158231308	-0.06483786709664	1.25125350693347
C	-1.09605909727484	0.01597611131491	1.16532800015969
H	-1.72505293469596	0.00127389971942	2.05831394851743
C	-1.72444646104132	0.11256405998973	-0.08962368917726
Se	-3.64205691542602	0.23980240902675	-0.24355509272726
C	-0.91956255851931	0.11696098878584	-1.24534662417288
H	-1.39364207085700	0.18319367382041	-2.22643716761509
C	0.46928213439707	0.03702171519700	-1.14774965743411
H	1.07116463425888	0.04368759448296	-2.06000451957195
C	1.09132122994475	-0.05212325115305	0.10192898539165
H	2.17835068194053	-0.11348792023502	0.17808015261114
Cl	-4.27025829400126	-0.05027810596809	2.53839728659610

Se-3c

N	-1.44770691132683	0.98740493389027	0.46053394445295
Se	-2.51890387654317	2.67791041122800	0.99564447655895
Si	-0.15400608771373	1.34963283225041	-0.60266122503328
Si	-2.24768860667699	-0.45343744241508	0.92840187113087
H	-0.58710931528298	1.96160144607780	-1.90591138262346
H	0.83842520681431	2.29397203565924	0.01443962106224
H	0.60509906036564	0.08865351195610	-0.95885472546426
H	-3.60370946993417	-0.63060203718311	0.30369169234507
H	-1.43420740306238	-1.66457331888867	0.52119466913292
H	-2.43718306421501	-0.53936760635556	2.41649096288599
Cl	-4.30642953242469	4.49851523378062	0.76030009555202

Se-3d

C	1.08748164404455	2.82831471932810	0.44596873953348
C	-0.25680649061742	2.63232819915871	0.34504804318614
N	1.29227574542688	4.18945962643385	0.54348797722965
N	-0.83953446058508	3.89276376460090	0.39006820044826
C	0.11862883705264	4.84940378621914	0.51185266036542
H	2.16219625871264	4.77525670022335	0.62460250711880
H	-1.82999384333554	4.09861783664809	0.33682474337635
H	-0.84116926594362	1.72650589006354	0.25183583110821
H	1.90284608757077	2.11686560881181	0.45748590852862
Se	-0.08129582858771	6.71632812463450	0.62520011408335
Cl	2.73366131626189	6.73349574387801	0.74196527502170

Te-1a

C	6.58972644608540	2.18369417744236	7.90197416780153
C	6.16219886327032	1.22639054696354	6.79125338002087
H	5.06989716970005	1.12835248531357	6.73306704122934
H	6.59968695467028	0.22726402530230	6.92032261696030
H	6.51550804350447	1.62389716156983	5.82342806656595
C	5.94635641343538	3.55533464512552	7.72693258133602
H	4.85287188881499	3.48501607949562	7.67531117361583
H	6.30948980124022	4.00926332182860	6.78796547034424
H	6.20756901390957	4.23584175379001	8.54824758695932
C	8.10912130115009	2.28816005379684	7.98574135788213

H	8.57490881636885	1.30454910722995	8.12302826010637
H	8.42814244283618	2.93680812142013	8.81233301539462
H	8.49458866124782	2.72638533002057	7.04815505231201
Te	5.82032458516057	1.26854726615881	9.80318278826541

Te-1b

C	4.25457046968020	3.83216184724201	1.82340891843204
C	4.30077456547262	3.31406041107454	3.12970402127424
C	3.44896363692975	2.27531519389308	3.49786448711429
C	2.54669518656549	1.74509507202258	2.57136335724339
H	1.87951448057480	0.93344818036440	2.86343036307079
C	2.49795583213617	2.25506761044580	1.27098397772126
H	1.79436716357931	1.84163978206268	0.54732475372772
C	3.34704688571134	3.29336488469811	0.89428072442636
H	3.31312265879907	3.69322055114462	-0.11889663206851
H	3.48782949734690	1.87727350312884	4.51245791433109
H	5.00529813724549	3.73032960097545	3.84924946317890
Te	5.54452848595885	5.42520936294789	1.25609365154845

Te-1c

N	-1.67346525336559	1.05642257153430	0.40301174223385
Te	-2.76003878921757	2.67946572114434	1.08668662211667
Si	-0.27694453477493	1.44193911535406	-0.59525571625954
Si	-2.20992492431717	-0.52055083712401	0.96946762615390
H	-0.70132874036756	2.25356543562680	-1.77645774933844
H	0.73948947816360	2.20926327187052	0.18976405209362
H	0.31431754111703	0.14158511813777	-1.04684658045937
H	-3.64432447756342	-0.73364897793493	0.60680715761913
H	-1.34923186320687	-1.54591638210779	0.29704050913246
H	-2.05613843646754	-0.63193503650106	2.45343233670771

Te-1d

C	0.93923057995355	2.35479487795739	-0.20977629884812
C	-0.31536912628414	2.37043096977010	0.34899874317990
N	1.45612681490968	3.61102335991250	-0.03490031126915
N	-0.50632975787774	3.63645907514722	0.83568792341346
C	0.57630209091537	4.42134549773270	0.60602522479626
H	2.37533886070751	3.92738022363596	-0.33802444034183
H	-1.34203171868071	3.97361192480597	1.30987354766837
H	-1.06253855537455	1.58935914810401	0.42671145624607
H	1.48102038922147	1.55801805531374	-0.70567318478911
Te	0.83903042250956	6.44159686762041	1.12127733994415

Te-2a

Te	3.76992090614914	0.84087796871367	4.19314717293378
C	3.44441303471769	0.25045602614917	1.82493423055853
C	1.95750574177646	0.13181372295610	1.57397818361077
H	1.43600157124239	1.07074554353907	1.80944334321077
H	1.51119411899622	-0.65858612349690	2.19532555786640
H	1.75324881381922	-0.11670839711073	0.50632035383137
C	4.16647692048657	-1.05271718261649	1.56390221970624
H	4.06622481147638	-1.35498223398412	0.49547849286162
H	3.75781639846809	-1.86464554773810	2.18357641807111
H	5.23835274347933	-0.96907001731547	1.79443700628758
C	4.05859628938519	1.40110905928278	1.05795014042291
H	5.12821903787087	1.51278028011599	1.28945245232621
H	3.56263894972560	2.35391456593650	1.29549043020001
H	3.96674931966504	1.23882020579076	-0.04304478553032
C	3.52860798578331	0.19453629045336	6.59590014943275
C	4.18565296385402	-1.15343875547781	6.77428550012027
H	5.24518421652684	-1.12337479326830	6.48215648937476
H	3.69451000606102	-1.92028529903426	6.15715497332462
H	4.13156892240855	-1.48620530156724	7.83738666362274
C	2.05262761012574	0.16027813166521	6.91426664438647
H	1.88141585605306	-0.10186737110750	7.98499521200002
H	1.53001948828789	-0.58574024389997	6.29769112914548
H	1.57938788494003	1.13454110412811	6.72495427204573

C	4.25308350298186	1.29057467689632	7.34202303598815
H	3.80252118799033	2.27560429103437	7.14928307935404
H	5.31232009054840	1.34337699561959	7.05010774283558
H	4.21605895711257	1.11514134445822	8.44466738983249

Te-2b

H	1.27672826989686	-0.56331715894096	2.21398081288020
C	0.77479417919005	-0.37532381324939	1.25991127915330
C	-0.54471066499766	0.08291735884528	1.24760600824545
H	-1.07260630950171	0.24035166882895	2.19261309251307
C	-1.21136344679468	0.34657070646255	0.04016390123450
Te	-3.48021806175956	0.80341810426124	0.01822117764350
C	-0.51736923168157	0.11514620360902	-1.15833714097026
H	-1.02415990042185	0.29699037873797	-2.11054234251791
C	0.80238986851872	-0.34219892544461	-1.15303633900778
H	1.32609955303005	-0.50391708760638	-2.10021482611963
C	1.45958770736741	-0.59321930585869	0.05786056476481
H	2.48942493037214	-0.95534870646464	0.06451673378284
H	-5.55887354571338	-0.57484173727852	2.16713418546112
C	-5.90831604255303	-1.01085866155252	1.22673387891103
C	-6.90785635124092	-1.98654799131584	1.24612216320333
H	-7.34468762649223	-2.29937463179317	2.19950145076639
C	-7.35478309007899	-2.56557751625592	0.05178883870191
H	-8.13203616765709	-3.33207910533919	0.06439547583727
C	-6.78745877251471	-2.14860100331052	-1.15876586570661
H	-7.12947737634268	-2.58926169320655	-2.10028645635023
C	-5.78976916326429	-1.17101519868435	-1.17130577728379
H	-5.34809842382962	-0.85916132431452	-2.12225820781451
C	-5.33852033353126	-0.57760056012922	0.01851739267200

Te-2c

N	-1.47650111448051	0.79456829694732	-0.05480441299817
Te	-2.54021843440347	2.82934670001334	-0.45006542179953
Si	0.22963460903140	0.88669562609388	-0.11079055490532
Si	-2.48008233654655	-0.39569864637248	0.65041520065059
H	0.72067509583115	1.45604063818735	-1.41358129079722
H	0.85464803281553	1.73048162496304	0.97284170590297
H	0.86099255773909	-0.48294256413607	0.03114888178230
H	-3.72773550890974	-0.62996619603245	-0.15697981445851
H	-1.76985788933089	-1.72960475884708	0.74941148783145
H	-2.94641947404473	-0.08484920095885	2.05213201534164
N	-3.43040240930885	4.94904198652563	-0.09901377963222
Si	-2.28631312572912	6.21506003038858	-0.20198240593063
H	-1.54123589949266	6.19600301611077	-1.50873142235707
H	-1.23128877535003	6.20512266681159	0.87727479124740
H	-2.95338458413666	7.57095812550627	-0.10251598564098
Si	-4.98149371468605	4.94106805993008	0.61939814607677
H	-5.96353895586283	4.11914589644435	-0.16973930030311
H	-5.55572715226090	6.33993746811908	0.70563121800255
H	-5.02537092087419	4.40055123030566	2.02765094198709

Te-2d

C	1.16725207938419	2.79855007776538	0.33548084614639
C	-0.11804535176945	2.74780751857173	0.78844274901426
N	1.40624021431839	4.11966484897202	0.00602537817929
N	-0.60187358273655	4.04064052828117	0.71505448482439
C	0.32050054783696	4.89811724549533	0.22017638762963
H	2.27562807289679	4.48323699701845	-0.37188604852008
H	-1.53833934628619	4.33393155660180	0.97553109184438
H	-0.71145756447470	1.91411786897736	1.14259451619190
H	1.90806952429521	2.01744671139530	0.21867097319601
Te	0.19462380157512	7.21731266402085	0.15577014038901
C	0.59468011425428	9.03946745450993	1.55054457241293
N	-0.22832857217490	9.54576280640863	2.49771460532743
N	1.77239384007296	9.66676476314916	1.77436694014371
C	0.40812023039719	10.48672296248070	3.28542733900728
C	1.68801374245181	10.56543778975665	2.82153009050691
H	-1.20028122317651	9.26587757900834	2.58574021941987

H	2.60004847147898	9.49603198600957	1.21164747080836
H	2.52072198637179	11.17904700513546	3.14191764863807
H	-0.08797698471538	11.01864163644217	4.08765059484026

Te-3a

Te	4.55482569037620	1.55233933629910	4.28645861078761
Cl	2.61533650809797	0.03528363073681	2.54782730920483
C	3.63122021897541	0.39544048273267	5.98717515477934
C	3.84091460814893	-1.09198048970825	5.72611256077505
H	4.91078235815346	-1.34188264101063	5.69970660214316
H	3.39491206901269	-1.37503764569191	4.76293159133437
H	3.36281112265948	-1.68293689386957	6.53197691749636
C	2.14333535815937	0.72495287111210	6.04437552587472
H	1.66282984652570	0.13924415571322	6.85310085691826
H	1.66137375675599	0.47414016453742	5.08975904671244
H	1.98203181716588	1.79272481510536	6.24722991306679
C	4.33914192029870	0.83419788374839	7.26567346707640
H	4.21383645415041	1.91148457625876	7.44452424246007
H	5.41585002710738	0.61715783032592	7.22257766412774
H	3.91278324441241	0.28990492371060	8.13134153724285

Te-3b

H	0.74482832319381	-0.14498097762157	2.24460898035524
C	0.29026781921041	-0.07371424143411	1.25317114137066
C	-1.09932201502304	-0.00918636322427	1.14611824514937
H	-1.73619178091968	-0.02808271230385	2.03457058143154
C	-1.70725495363438	0.08476724079921	-0.11594277917572
Te	-3.84324590552802	0.18166960702099	-0.31544613110522
C	-0.88910555752131	0.11364138380384	-1.25868124164613
H	-1.34576730465775	0.18769511347573	-2.24778259250857
C	0.50018964027501	0.04899849328174	-1.14309791156991
H	1.11620950385535	0.07334708522469	-2.04563673825836
C	1.10301721547795	-0.04589493178500	0.11511223091291
H	2.18974086194113	-0.09571120745764	0.20659416789556
Cl	-4.23121584666949	0.03906151022024	2.64348204714862

Te-3c

N	-1.63375352487827	0.92456528803481	0.14464308844488
Te	-3.00248903680558	2.73266725498222	0.37546562152347
Si	-0.14095049543382	1.27740676502983	-0.61384979402492
Si	-2.20906151820105	-0.49356082926783	0.90959473175856
H	-0.31098130443114	1.82592306876463	-2.00551940939031
H	0.70014586011986	2.27676667149118	0.13318247482566
H	0.70945303545572	0.03068315707783	-0.74502790101864
H	-3.56270852092420	-0.91586771626176	0.40615968318066
H	-1.27542093009676	-1.66053469482088	0.66428187775536
H	-2.33597075811095	-0.37227911129088	2.40581314611319
Cl	-4.23168280669381	4.94303014626084	1.25852648083209

Te-3d

C	1.09227198874580	2.81977484052398	0.47790353729092
C	-0.24917861244751	2.60718910509847	0.35726407355619
N	1.27912548666747	4.18344025887813	0.55140885877785
N	-0.84153952860750	3.86185439722532	0.36072296177103
C	0.10233150267361	4.83070393078446	0.47745564975570
H	2.14561615829619	4.77795519526301	0.64875485914846
H	-1.83342516269771	4.05498068474676	0.28608061583977
H	-0.82334871156950	1.69383463310925	0.27355291555336
H	1.91475816842530	2.11755286533830	0.52045169275527
Te	-0.12325970472816	6.92429996484230	0.53752599962050
Cl	2.78493841524201	6.68775412419001	0.78321883593095

Po-1a

C	6.59425001432057	2.18933109919621	7.88644805089816
C	6.16569113330740	1.23106179329719	6.78195971646501
H	5.07316558061361	1.13471265733144	6.72230954405161

H	6.60060584486892	0.23096292260053	6.91378890784641
H	6.51901658059139	1.62124186086876	5.81060211244738
C	5.94853174185317	3.55807253564854	7.72138792527619
H	4.85457470125974	3.49039080086255	7.67896726476855
H	6.30147437405601	4.01290885212122	6.77786863084392
H	6.21929070645436	4.24038944539726	8.53814316658427
C	8.11016460016557	2.29049190392348	7.98209177957181
H	8.57630190241532	1.30710277048713	8.11996077005671
H	8.42718118326331	2.93977452517254	8.80901387610417
H	8.50317415996147	2.72863915217049	7.04650838583778
Po	5.78696787826334	1.22442375638033	9.89189242804199

Po-1b

H	1.09442228735789	-0.15178644964983	2.16349841469435
C	0.56141874698181	-0.07958881247553	1.21464719473515
C	-0.83208248477333	-0.02190343341123	1.20760539800571
H	-1.38611750281454	-0.04975670827564	2.14565314921885
C	-1.52161542808806	0.07103420841349	-0.01077165671909
Po	-3.76801184451482	0.16084600804611	-0.02904914517104
C	-0.80674766346903	0.10655518983598	-1.21752124243176
H	-1.34107650245145	0.17910431677580	-2.16456659670765
C	0.58666413628395	0.04839289748384	-1.20154108284473
H	1.13936807037290	0.07660927474514	-2.14140884777826
C	1.27172592519086	-0.04591227467305	0.01223742947945
H	2.36114225992383	-0.09046421681509	0.02123698551901

Po-1c

N	-1.63505531284766	1.04712044302091	0.43843281252355
Po	-2.75174705365412	2.76337046193849	1.20676473101003
Si	-0.27945637125604	1.43271332005790	-0.60282873994758
Si	-2.20777900481399	-0.52541884098283	0.95849477055076
H	-0.73615497687559	2.17725125080541	-1.81566028370932
H	0.72694351462086	2.27004613492531	0.12034880913620
H	0.35039259273264	0.13807039603433	-1.01654690359316
H	-3.61846411495151	-0.74803782815350	0.51743856914174
H	-1.31809339505568	-1.55576193935015	0.33353321075184
H	-2.14817587789891	-0.64916339829585	2.44767302413594

Po-1d

C	0.94105687769837	2.33999315540378	-0.20747212401044
C	-0.31470127579217	2.35547683158865	0.34181259597844
N	1.45295477703594	3.60325997435730	-0.03683991865340
N	-0.51005000336286	3.62696501666829	0.82290113513168
C	0.57102555187941	4.41074206758257	0.59796929249427
H	2.37372945378910	3.91431504168467	-0.33865437293939
H	-1.34841075022328	3.96479476959535	1.29067190931189
H	-1.06092099075952	1.57396217970570	0.42193862589137
H	1.49029855618226	1.54251636740694	-0.69366120855879
Po	0.84579780355276	6.55199459600677	1.16153406535435

Po-2a

Po	3.88543142161026	0.89240861102758	4.19751727999317
C	3.54137901209197	0.19906812873276	1.72038102492555
C	2.11605995148581	-0.27597548337666	1.56117023924691
H	1.39576471042442	0.51116789884948	1.82636282960826
H	1.90871965066404	-1.14570453905507	2.20198144086405
H	1.91659545198698	-0.58127447365030	0.50683944339871
C	4.54037821187606	-0.89035993888323	1.40701733790954
H	4.44187384321844	-1.22631112250244	0.34701828337980
H	4.38932974110317	-1.77068000127966	2.04869276007472
H	5.57427348810496	-0.54677982244482	1.55496280770717
C	3.81107987746874	1.46391770684401	0.93921988022265
H	4.83665667860932	1.82995146178939	1.09674667567921
H	3.11916219407920	2.27020422909793	1.22361051157315
H	3.68635015063659	1.28958968603791	-0.15743823006316
C	3.45696573411002	0.24780876191912	6.67434908934695
C	3.75830006885162	-1.22416315209294	6.83337058468200

H	4.80038819678273	-1.45400508225396	6.56881425868132
H	3.10935246264233	-1.83850722454026	6.19189487862974
H	3.59308017190655	-1.54984534563575	7.88749876751106
C	2.01423745445418	0.56825878578824	6.98858399549308
H	1.77348530467150	0.31540063562169	8.04891255320116
H	1.32712189826239	-0.00338626350660	6.34775483772867
H	1.79442012907906	1.63526477162376	6.84012575367792
C	4.41790587681688	1.11358459221279	7.45523505568143
H	4.22173448598039	2.18479959722181	7.29818412579891
H	5.46198447789602	0.91784198537087	7.17014569608680
H	4.32992535518635	0.91805359708437	8.55186911896121

Po-2b

H	1.56078639583788	-0.54444822392519	2.17671471643338
C	1.02769613092991	-0.34985313973841	1.24110820181030
C	-0.32217422668752	0.01649434607792	1.27057381123730
H	-0.83410219371018	0.09737569046487	2.23393671611860
C	-1.03059530795060	0.28219502456391	0.08986584547049
Po	-3.45424859234732	0.70670601336479	0.12698524513817
C	-0.34717447584131	0.14936012413996	-1.12726817605055
H	-0.87956343876216	0.33474649938521	-2.06476195354680
C	1.00256804638995	-0.21606869502859	-1.16702186002806
H	1.51566523544768	-0.30527970108579	-2.12941994537568
C	1.69898639283007	-0.46831962567825	0.01962807975255
H	2.75168929163168	-0.75703041427088	-0.00728849636243
H	-5.69038623317348	-0.80512321907693	2.21340745816435
C	-6.06955204664938	-1.15950565936896	1.25044773526647
C	-7.14309005726622	-2.05624107221094	1.22457253198601
H	-7.59966236129291	-2.38876874168105	2.16183956237317
C	-7.63507004544607	-2.53061907602103	0.00392269497209
H	-8.47053368373166	-3.23326347572563	-0.02004197976224
C	-7.03966895949181	-2.09674715606165	-1.18531073784689
H	-7.41472631769039	-2.46112136100264	-2.14658331605531
C	-5.96787240423027	-1.19847984160138	-1.14938727069230
H	-5.50911384806905	-0.87278308854128	-2.08756316104241
C	-5.47113730072683	-0.70607520697809	0.06596429803977

Po-2c

N	-1.30026831557932	0.74993751279336	0.48220048272901
Po	-2.26090163884354	2.97077315826870	0.74757796977892
Si	0.29647111531693	0.72621830044723	-0.12039428781952
Si	-2.41871788168866	-0.53334679365295	0.60783458750253
H	0.44278892312471	1.23119623953792	-1.53617718292240
H	1.23129142893566	1.56752880721015	0.70786982306877
H	0.87400863067885	-0.67438971746079	-0.13196211525912
H	-3.46355513958618	-0.56623297106938	-0.48181472071226
H	-1.73462995998469	-1.88397565330549	0.55116915303804
H	-3.18570908551580	-0.49699164368966	1.90332231662760
N	-3.35255404377372	5.12492755955947	0.44614207874824
Si	-2.35698203525453	6.35645039992391	-0.18921826961088
H	-1.87827961099104	6.11085437013623	-1.60019391049820
H	-1.11014890070855	6.56475186818243	0.62962810199720
H	-3.06983242379282	7.69256489943557	-0.23183091406123
Si	-5.05060273306192	5.09213904080257	0.61135677494546
H	-5.76774814101332	4.27847033905378	-0.43894379414537
H	-5.65166291105659	6.48045113004295	0.52686208944769
H	-5.48658727720548	4.51963315378403	1.93427181714553

Po-2d

C	1.13158644567377	2.56758646519269	0.17833325905627
C	-0.15378306226752	2.50374712979096	0.62822362199656
N	1.40209879054777	3.90957496477303	-0.01394824833041
N	-0.60313044207599	3.80994359707997	0.68505629381718
C	0.33990130365122	4.69390738237891	0.28320049874220
H	2.28245951491311	4.28474376547396	-0.35231270598979
H	-1.53164475537976	4.09526980971065	0.97946119824360
H	-0.76823212056239	1.65453095185202	0.89972245064297
H	1.85341962003093	1.78478178762494	-0.01812335641206

Po	0.23773407193185	7.15678109706982	0.34200183136822
C	0.63667536334455	9.16843215800266	1.71435164139047
N	-0.20178175898806	9.75085211745702	2.60306326078249
N	1.79464717029483	9.84954043555082	1.87933763938391
C	0.40456725918709	10.78164813028581	3.29650812041896
C	1.68557331486043	10.84348066988510	2.83410503243705
H	-1.16598925797474	9.45648852089129	2.72073500312100
H	2.63174195838598	9.64512274185822	1.34294982897999
H	2.50330031275657	11.50234870454798	3.09793264086418
H	-0.10915372832964	11.37579957057416	4.04180198948722

Po-3a

Po	4.61548252134212	1.56591901096902	4.19523667071259
Cl	2.59859588705371	-0.02105674678727	2.49946706060882
C	3.63145036334961	0.38822916984859	6.00851911872071
C	3.82967185544875	-1.09895288611336	5.75223332518654
H	4.89561467499239	-1.36577190802464	5.74493435881235
H	3.39087763087366	-1.38301057523938	4.78553579749425
H	3.33024889006402	-1.68281359996291	6.55241620340762
C	2.15133246825909	0.74028780423905	6.03367517916340
H	1.64774529548922	0.17057164325655	6.84169073691527
H	1.67952694584242	0.48145229788397	5.07570320076997
H	1.99760262821569	1.81197150438709	6.22117510808117
C	4.33722411346741	0.83695571815920	7.28068185318935
H	4.20624136731637	1.91378316214830	7.45829390531451
H	5.41509193477928	0.62441336575237	7.24063675781855
H	3.91527842350625	0.29305503948342	8.15057172380493

Po-3b

H	0.73432025604419	-0.14530465312153	2.25061865394511
C	0.28958001586974	-0.07302159319800	1.25478720421943
C	-1.09952501004911	-0.00907148422876	1.13160975532719
H	-1.74575290381343	-0.03002562208455	2.01408971115538
C	-1.68868612410628	0.08418244683418	-0.13718481757149
Po	-3.94740119243356	0.18924676920383	-0.32640125084364
C	-0.86407179641292	0.11154520500536	-1.27178360263752
H	-1.30907138532395	0.18399874512526	-2.26644474948286
C	0.52517506162963	0.04724854405157	-1.14082761515187
H	1.15210040279145	0.07011396641339	-2.03597734555088
C	1.11282988887299	-0.04447889279895	0.12427921907670
H	2.19852915031619	-0.09406931108617	0.22721361456488
Cl	-4.26587636338495	0.04124587988438	2.69309122294956

Po-3c

N	-1.56645444728388	0.93362193731273	0.24870382880634
Po	-2.94156719872956	2.86813489565269	0.61256642815744
Si	-0.12308952419759	1.23668881175854	-0.61064931010367
Si	-2.17133327234303	-0.51238222512535	0.92503241230884
H	-0.36275773037341	1.85692915517889	-1.96326923375570
H	0.82362825549718	2.16606474596415	0.10645654417979
H	0.65744787843768	-0.03784855186550	-0.86029130922165
H	-3.54011795901971	-0.87783124014591	0.41007573295699
H	-1.27371328929056	-1.69395933643206	0.61775961864865
H	-2.29639836828601	-0.47083205173997	2.42740249596736
Cl	-4.49906434441110	5.10112385944179	1.01948279205560

Po-3d

C	1.02602354479368	2.45697983784717	0.00140915349836
C	-0.26155409948011	2.47015389847082	0.44882976125995
N	1.40474608477078	3.78253277383011	-0.11008498898356
N	-0.60273944153761	3.80315188561036	0.59029894275235
C	0.41302638977192	4.63664344601137	0.24976794841928
H	2.31557233212065	4.11932751381967	-0.40437370610422
H	-1.49200387301440	4.15733208191483	0.92680474316736
H	-0.94165799056405	1.65773517843902	0.67069725652329
H	1.68193213382089	1.63060657243271	-0.24076441902378
Po	0.59725250825756	7.00427297155765	0.66670433010601
Cl	1.30769241106069	8.84060384006629	2.47505097838495

Br-1a

C	6.64928175894151	2.26696029636211	7.80561024876073
C	6.13104410633283	1.18836139368393	6.86145244803562
H	5.03688961536577	1.12253646560673	6.80193573590507
H	6.59845419287177	0.20409820503562	6.99499110295465
H	6.46526892513549	1.54450156466551	5.85660554432684
C	5.94295381091868	3.58456492814169	7.73902798245268
H	4.85261588123785	3.48756437514299	7.69755287068724
H	6.27352915644502	4.06494592965141	6.80124401400188
H	6.23236200906861	4.25057624422415	8.55987578567357
C	8.13274556210843	2.30026228505242	8.00205728517432
H	8.57121517754364	1.30491887326004	8.13155553796203
H	8.42475419261173	2.95344663553757	8.83225995200247
H	8.55697651879938	2.73933727993465	7.08213254995246
Br	5.81229949401348	1.18742959915886	9.51464150090436

Br-1b

H	1.06749927315799	-0.15002986089198	2.17780284456205
C	0.51920046178149	-0.08172583568246	1.23865731558614
C	-0.85705533638726	-0.02960045549062	1.24009811281676
H	-1.43195074333054	-0.05581577865621	2.16470986471240
C	-1.52697333749384	0.06509431399968	-0.01086677963307
Br	-3.39087425021337	0.16623789771637	-0.02636099755193
C	-0.83109641935960	0.10206593925194	-1.25061378887078
H	-1.38710023353995	0.17514217324895	-2.18418260597043
C	0.54482364071087	0.04877163622999	-1.22643276452180
H	1.11219826591189	0.08010716441539	-2.15613339109964
C	1.22514959758299	-0.04105401309260	0.01197042988331
H	2.31526908117933	-0.07606318104845	0.02137176008699

Br-1c

N	-1.72701483863428	1.09333411554319	0.36901182009121
Br	-2.86683833155732	2.49074340600417	0.76532032297696
Si	-0.27805629397226	1.43878329215478	-0.70535157685454
Si	-2.14224625254963	-0.53544419290832	1.11522006604883
H	-0.50864960037138	2.77949634604149	-1.29531716809588
H	0.87019065655361	1.35809831401769	0.24694721292763
H	-0.30329095829234	0.29024206414722	-1.65602857028612
H	-3.38668655455962	-0.96225607769265	0.41439038293754
H	-0.93649186494878	-1.33455357757891	0.76806503543360
H	-2.33711418792442	-0.26823478327848	2.56512044996350

Br-1d

C	0.96803789265852	2.40176264769137	-0.21107526263606
C	-0.33605220007262	2.42124089121978	0.37012569855171
N	1.48100542626384	3.63350412342423	-0.04503720881098
N	-0.52426742292736	3.66316682877707	0.84833634033073
C	0.58224057686372	4.43839267485726	0.60918421699718
H	2.41222180882772	3.94031286820384	-0.35790802974591
H	-1.37074250866703	3.99848207631268	1.32785524843162
H	-1.07776337867200	1.62356541376986	0.44444136152432
H	1.49846826131233	1.58438027050681	-0.70374926906857
Br	0.80763154441288	6.17921220523709	1.07802690442595

Br-2a

Br	3.50042368888414	0.09109686474101	4.53751232816677
C	3.53838410262872	0.08216149363361	1.47820354660455
C	2.29083150403332	-0.70831375872255	1.28516224144406
H	1.41850338143872	-0.20495823732321	1.72619452119209
H	2.37226864427778	-1.71226092468974	1.72563125110230
H	2.06526588423281	-0.85008758968989	0.20666381869867
C	4.85094519156555	-0.60346813246069	1.31808758750355
H	5.11306112602379	-0.72941606670641	0.24582937174425
H	4.84131934239536	-1.60972204238144	1.76076564903437
H	5.66850158506839	-0.02934929317582	1.77705954995260
C	3.47846709991904	1.55993247843146	1.30142216740641

H	4.34748340246008	2.05967491730178	1.75261580638796
H	2.56546595762711	1.98530413092279	1.74221917461789
H	3.47276857063446	1.83809980213447	0.22592066661535
C	3.38897875584557	0.18358024704529	6.59748896401720
C	3.29403716713602	-1.25029946133114	7.08762741122298
H	4.17731402635688	-1.83148025232150	6.79563022828880
H	2.40066896382957	-1.74896193889785	6.69202582207526
H	3.22971437668761	-1.25071013668117	8.18851871618052
C	2.14233634673723	0.98820253083488	6.92062271524630
H	2.03851949281681	1.06714858115960	8.01560837047533
H	1.24099637868925	0.50415299318195	6.52492057790256
H	2.20397781553506	2.00281159858508	6.50820608057102
C	4.65857852524442	0.87243011494920	7.06534624840405
H	4.73726938707198	1.88625057872010	6.65391478843655
H	5.55134467380973	0.30612545442307	6.77301475491895
H	4.64288361164017	0.94744117021310	8.16542211875847

Br-2b

H	1.80927570743060	1.05203940776793	1.93766704531198
C	1.27371203173038	0.56640783078087	1.12112826738331
C	-0.11104733628632	0.40758469654191	1.21114435579424
H	-0.65907130509097	0.76158541323031	2.08307613266804
C	-0.78308513895012	-0.21324246728225	0.16212306274654
Br	-2.70692985245840	-0.45134143268011	0.27140966693167
C	-0.11102030286207	-0.67706527262979	-0.96553208485184
H	-0.66021102869885	-1.16126333393615	-1.77172955888124
C	1.27323199835040	-0.51090207207093	-1.03985194028403
H	1.80793856404633	-0.87150790177241	-1.91934283360501
C	1.96755698980224	0.10897593358634	0.00007204558292
H	3.04836633079129	0.23521012944091	-0.06287557740547
H	-5.40373749387388	-2.64744094147647	1.86788251985285
C	-6.02963394608234	-2.25220960531212	1.06670139971997
C	-7.36493156177805	-2.66441808907849	0.91711786175186
H	-7.78525407833534	-3.39141830539400	1.61448451995009
C	-8.14659357230068	-2.14721361848365	-0.11819614873323
H	-9.18115502174674	-2.47368765192088	-0.22722591950632
C	-7.61722973086863	-1.21794961806608	-1.01627313418271
H	-8.23347546264659	-0.81922877462083	-1.82427401383405
C	-6.28437680646940	-0.79182676212357	-0.88643152338530
H	-5.85326227323809	-0.06913115168550	-1.58046980061939
C	-5.57034671046474	-1.33480641281503	0.15371565759512

Br-2c

N	-1.54868272531202	0.98138409730108	-0.07862303909501
Br	-2.49164418695685	2.85461190435955	-0.24831096294297
Si	0.19226124201376	1.05339516717566	-0.17390275379656
Si	-2.55352211426876	-0.25924445712230	0.62660913777828
H	0.58881732151233	1.96663979468266	-1.28841510946649
H	0.79568981195897	1.56295195321756	1.10252502912018
H	0.70972855428516	-0.33143619923024	-0.42232827009530
H	-3.92604125815296	-0.17423566337016	0.04142552526512
H	-1.93793340678328	-1.59266122804619	0.32639634117367
H	-2.65672965763294	-0.10948561490286	2.11666502571217
N	-3.35875167977937	4.77011547164618	-0.06008023678217
Si	-2.23033760891827	6.09356379172434	-0.20751826278316
H	-1.18584921946206	5.73652012575751	-1.21417009108642
H	-1.55920121386012	6.40388295248509	1.09918227294476
H	-2.98778261881892	7.31126986791570	-0.64609547883602
Si	-4.93077940063252	4.75737240197731	0.69863887293145
H	-5.73218941626244	3.62025336237844	0.15251900421110
H	-5.60725264677838	6.06308953111478	0.40581495996852
H	-4.82341977615130	4.60297274093594	2.18736803577885

Br-2d

C	0.87084559811247	-3.17344390916118	-1.46848306634552
C	-0.15507492896364	-3.22110680241117	-0.57173293225427
N	0.82835058734802	-1.91252900393132	-2.06404381138606
N	-0.80485666171935	-1.98822522071206	-0.63553614236740

C	-0.17358566461345	-1.23887904768328	-1.52395998796309
H	1.46091510384508	-1.56143169525793	-2.78189997727827
H	-1.61723988788283	-1.70473033533168	-0.08935091588843
H	-0.47668091264832	-4.00233630267959	0.10761192845013
H	1.62671239572850	-3.90457389518414	-1.73185716347487
Br	0.74639858951515	14.93838484974362	0.86155805625084
C	0.95490180951644	15.05015781796116	2.70281778048774
N	-0.01659725177009	15.23449008967312	3.61103801791382
N	2.10809080078629	14.95228106181043	3.38320846349218
C	0.52473789393972	15.25336328087014	4.88458790032795
C	1.86810560204580	15.07540170444772	4.74052318860946
H	-1.00088234046481	15.34794258620824	3.37738610123572
H	3.01672290453110	14.81444852105983	2.94562831941754
H	2.66293013783239	15.02657393797013	5.47478519724959
H	-0.08441363299078	15.39140648811790	5.76961453775102

Br-3a

Br	4.42659854981436	1.36010037680834	4.40656503704609
Cl	2.81847301506517	0.17464226818956	2.53344991376849
C	3.59171137204652	0.34902328640107	6.02333866477471
C	3.81545097069556	-1.12226210388271	5.74561829994149
H	4.88318274012896	-1.36942660428692	5.70919932651598
H	3.34331206977734	-1.42229638194291	4.80254222737325
H	3.35518063467406	-1.69727860449043	6.56512670754049
C	2.12892389593548	0.73927366190447	6.03642022220692
H	1.63931187170617	0.19915282559077	6.86261974142195
H	1.63702979314387	0.45719030160283	5.09792997496646
H	1.99840057388284	1.81509813995013	6.20374039679177
C	4.36470969554281	0.86181648237557	7.22364067315964
H	4.24226582419893	1.94345751325033	7.35687228058957
H	5.43305357198538	0.62459282976489	7.15304059651143
H	3.96438042140254	0.36194900876500	8.12066693739176

Br-3b

H	1.14763890637882	0.27304321479297	2.17670243608412
C	0.51855670062092	0.21780340787627	1.28828712900830
C	-0.83068131733824	0.55691036368251	1.38471855203398
H	-1.26817781004692	0.86919984706757	2.33117666308492
C	-1.61193983312958	0.48141550958258	0.23435426882970
Br	-3.47299275279606	0.94683449726010	0.35519319512762
C	-1.10410097552901	0.06577495699338	-0.99399319489974
H	-1.75069370435831	-0.00125759719479	-1.86700472114997
C	0.24699578519060	-0.27149351759572	-1.06721018950874
H	0.66449694833206	-0.60105716134669	-2.01865448414674
C	1.05723885157757	-0.19377866161142	0.06766455282368
H	2.11177659311500	-0.46087711565769	0.00184428164520
Cl	-4.61596739201684	-1.55090774384906	0.62399151106766

Br-3c

N	-1.72289398382474	0.94045422149094	0.03821705487116
Br	-2.95944918665354	2.54609169304679	0.25782068295590
Si	-0.12276200022335	1.35000237824846	-0.57724518826741
Si	-2.22868879656738	-0.48235963848865	0.94715454377323
H	-0.27620627543260	2.28615796650752	-1.72818118589416
H	0.70760688115892	1.98811976477846	0.49345150312205
H	0.51582183500578	0.06382697584304	-1.00001235535445
H	-3.70074625602176	-0.65234756891417	0.78849621202227
H	-1.47797777138935	-1.64344320621547	0.37597397047700
H	-1.88399404914116	-0.33414326001528	2.39630574081572
Cl	-4.04126833172993	4.53281536738512	1.11905612649526

Br-3d

C	1.02801189227029	2.56528084338915	0.00507362102613
C	-0.23998534825893	2.58405758361359	0.51668127472466
N	1.42929590390586	3.88025586856068	-0.10258157283320
N	-0.57074632489211	3.90988965193881	0.70300463926734
C	0.44671417721800	4.69899497899505	0.31372306805759

H	2.33037530019936	4.20387580405350	-0.45035988431264
H	-1.45238291933268	4.25949976448266	1.07487860091253
H	-0.92233206328473	1.77600506260137	0.75261681864648
H	1.66212561349964	1.73815013309460	-0.29133449491403
Br	0.53353301767864	6.58005375787778	0.45580579325989
Cl	1.20368075099667	8.36327655139280	2.29683213616525

I-1a

C	6.65680690055894	2.26460460420720	7.73349754475050
C	6.15542181867781	1.21659825570475	6.79260791124391
H	5.06154194372581	1.14929553621446	6.75513533142781
H	6.61115961519206	0.23171432270202	6.95117901628806
H	6.47993574923865	1.54683199140923	5.78451630165463
C	5.94230141396090	3.57390321118160	7.72985267958051
H	4.85290365099888	3.47361560101970	7.68745412921630
H	6.25746402222082	4.07586311274840	6.79389532470376
H	6.24168940524686	4.23116952660613	8.55342916585759
C	8.12559965175738	2.29377030251523	7.99232822276661
H	8.56244813059213	1.29871792141712	8.12590835419240
H	8.40528038004956	2.95588788835238	8.81900397775410
H	8.57503750756922	2.72530906708727	7.07644269845068
I	5.75280021160515	1.16222273429218	9.88569190090706

I-1b

H	1.08155068075965	-0.15255207474490	2.17514557507887
C	0.53758710543610	-0.07938857371164	1.23378822698612
C	-0.84199986678178	-0.02168818952520	1.23567049751288
H	-1.40771573731918	-0.04794394652515	2.16576802922121
C	-1.51220043292370	0.07214468193788	-0.01067652673776
I	-3.58542974113783	0.14828259353956	-0.02743857430006
C	-0.81607060340609	0.10996423137059	-1.24573353930628
H	-1.36210217671632	0.18311675053114	-2.18504744802424
C	0.56325781545998	0.05067438186479	-1.22106864409489
H	1.12687337166678	0.07689405867334	-2.15331221017864
C	1.24296482564055	-0.04445585909321	0.01202928283912
H	2.33237475932183	-0.09191805431718	0.02089533100368

I-1c

N	-1.69728073471342	1.11993500939941	0.43420071476045
I	-2.81443582503355	2.70011505280606	1.02925394600109
Si	-0.31530445507403	1.39941336190750	-0.72950302222705
Si	-2.11897869265106	-0.53217240183532	1.09520840750125
H	-0.58098894676793	2.69832277593046	-1.39805862351124
H	0.89922474916739	1.40146433675683	0.14012983668134
H	-0.37260778366887	0.20133678682768	-1.61518214874053
H	-3.27569319480049	-0.99196874531745	0.27222084413893
H	-0.87269320984380	-1.30630290286660	0.83833941858452
H	-2.45858366830169	-0.33810075654965	2.52938550017121

I-1d

C	0.96002835003421	2.37885969747149	-0.21341622635885
C	-0.33220224517570	2.39625687149814	0.36161721861134
N	1.47133320917687	3.61592542694085	-0.04631763022589
N	-0.52297482965089	3.64261596750335	0.84077343017299
C	0.57694985161007	4.42310298054119	0.60381665959885
H	2.40201684796143	3.91585161037082	-0.35928540090045
H	-1.37168542784739	3.96685637368965	1.31897104502426
H	-1.07261141363786	1.59988802415104	0.44041369109607
H	1.49671347060660	1.56556173403094	-0.70236569647977
I	0.83321218692266	6.37910131380252	1.11599290946145

I-2a

I	3.46387613277310	0.15737789630087	3.95068688417057
C	3.54083928900354	0.09088921428725	1.66086242262763
C	2.24030732003277	-0.54453925365455	1.20112068605262
H	1.36953592928745	0.03927686339412	1.52393747203596

H	2.13413593124721	-1.56826614760660	1.58070219212166
H	2.23496672831340	-0.58650803934251	0.09769266737640
C	4.75380189700212	-0.74719624427198	1.29716270429338
H	4.84187809992727	-0.78908078626234	0.19718177501495
H	4.66142025216268	-1.77488083595740	1.66963832007040
H	5.67874700100437	-0.31342856488641	1.69657042339913
C	3.67476954508914	1.53086163211093	1.19564657424603
H	4.58944914908294	1.99665504250185	1.58240932687301
H	2.81568419832516	2.13735890050731	1.50776151643027
H	3.72225832680375	1.54615895243924	0.09251544663225
C	3.35392823814735	0.20425871043979	7.02809512702340
C	3.46509286912365	-1.26534034042725	7.25345446952298
H	4.40823239400312	-1.66919175228030	6.85975816720333
H	2.63171663938588	-1.81427868130466	6.79332725075158
H	3.44318401204384	-1.50047022051209	8.33862903644486
C	2.01295937408627	0.83881441661360	7.17535326847325
H	1.74461549384532	0.94860623472700	8.24749008025409
H	1.22127285840255	0.23434847342710	6.71118894762874
H	1.98553630776321	1.84600674506745	6.73666148345162
C	4.56163111915334	1.04534418630544	7.26673239871958
H	4.46022988521329	2.04359123111204	6.81865001764927
H	5.47182597345295	0.57488128085143	6.86959961221996
H	4.72734380603077	1.19764812858647	8.35424963642323

I-2b

H	1.72156936406590	-0.19471134101983	2.19223135785317
C	1.16002696802680	-0.15253208133719	1.25753733143534
C	-0.23864112215721	-0.20221247063453	1.29057200112023
H	-0.76756339923619	-0.28488545006591	2.24067977433907
C	-0.92694041719266	-0.13536482309684	0.08844421415487
I	-3.26569162160993	-0.15713428998811	0.13376200657896
C	-0.28778303639443	-0.05013645175192	-1.13926845687120
H	-0.85502678969734	-0.01377653516508	-2.06992533450840
C	1.11109946158124	-0.00154010981852	-1.15707378204945
H	1.63414087043081	0.07470779946092	-2.11173747865185
C	1.83131766179930	-0.05303480023115	0.03763116530968
H	2.92090288234715	-0.01947859689589	0.01773756920664
H	-5.44833180404703	-1.43958628364106	2.20466604288412
C	-5.97319811345140	-1.54054020795280	1.25409934736541
C	-7.26015926559475	-2.08914263584623	1.20738934657185
H	-7.73911556251671	-2.41554061506923	2.13197498469150
C	-7.92473300899632	-2.22007210161119	-0.01324595823245
H	-8.92504107799355	-2.65263611844674	-0.04410509761703
C	-7.30908266635028	-1.80410919448778	-1.19496979309373
H	-7.82632766826937	-1.90673884262764	-2.15032194344713
C	-6.02289821241369	-1.25255631845700	-1.16322356288700
H	-5.53651657713313	-0.92911446140668	-2.08412097468448
C	-5.39328686519719	-1.12271406990961	0.06558724053186

I-2c

N	-1.50164171363158	0.85223153768173	-0.02947581043487
I	-2.49913705275187	2.85300065594329	-0.23216362434604
Si	0.24147256413539	0.85158262095594	-0.15698522327303
Si	-2.47825222389038	-0.42538015088230	0.65502249784979
H	0.65946451965270	1.87731547238338	-1.16057795548018
H	0.89734096329248	1.16777347709204	1.15571667244567
H	0.69138030072239	-0.51236318760884	-0.58730173281270
H	-3.89063090164775	-0.26257332426817	0.19387770470927
H	-1.93105049232915	-1.74569346659976	0.20187494564865
H	-2.45679448156279	-0.40034005313804	2.15588561923558
N	-3.39438949530497	4.90327648790334	-0.05048007366189
Si	-2.27141852740392	6.23859995290085	-0.15567865176197
H	-1.19224367719667	5.89467727478848	-1.13108851290824
H	-1.64099847971750	6.54127428816607	1.17256210168811
H	-3.01359660062432	7.45985921595883	-0.60912182974385
Si	-5.01106533706116	4.98237400421373	0.60875918699387
H	-5.76994761226516	3.76571710974935	0.18734608616320
H	-5.68195430164728	6.21950002359247	0.09092736126274
H	-5.00015745076843	5.05012806116764	2.10860123842588

I-2d

C	1.11978435918949	2.67251842086817	0.11891605701249
C	-0.16781818703917	2.59664358081556	0.60176081305969
N	1.42196176837188	4.00824890623159	0.03492450930430
N	-0.58598362564234	3.88996002256043	0.78875716010547
C	0.36517540290533	4.76954253636229	0.39992564001025
H	2.30636322706217	4.38037360358691	-0.30741918985939
H	-1.51013392612382	4.15560255722717	1.12524963903016
H	-0.80295452596104	1.73715805004913	0.79023675244591
H	1.80713948355355	1.89095380022806	-0.18820044018024
I	0.31537425944522	7.05750149985868	0.62770820679186
C	0.64859884334975	9.03173236242282	1.77164191130458
N	-0.19077627534026	9.61728843542533	2.65588471537807
N	1.79710599461002	9.74186565086790	1.85208422449110
C	0.38803404105369	10.72145814807996	3.22889545322059
C	1.66278492364902	10.80128654020083	2.71351871145634
H	-1.14557760503398	9.30854313276981	2.83148402929345
H	2.63266940986451	9.54572943951340	1.30331140946648
H	2.44595265177674	11.53504305681005	2.87450189599668
H	-0.13771021969075	11.37313025612192	3.91921850167223

I-3a

I	4.58696311251532	1.42875305091913	4.27224034919810
Cl	2.79411176748619	0.10354589349196	2.53590556680353
C	3.59824606420722	0.34629689441333	6.03596077110191
C	3.78445111199434	-1.13128788349987	5.76319552445748
H	4.84303035261295	-1.41792795723122	5.76592309867091
H	3.33210122190650	-1.42040922485129	4.80659784370445
H	3.27497699704664	-1.68810829825499	6.56762639419280
C	2.14639337588970	0.77555088948659	6.01376341000631
H	1.62395891605925	0.23538456243446	6.82122766874076
H	1.66792822964739	0.51488316248373	5.06174322392360
H	2.03472560136793	1.85154154825851	6.19409678545391
C	4.35609098685151	0.83733783343724	7.25507930333663
H	4.26139302221229	1.92172086595382	7.39082421947173
H	5.41926954556965	0.57033372597620	7.21525979844185
H	3.91834469463312	0.34741793698241	8.14132704249604

I-3b

H	0.77169076546960	-0.13028366234059	2.24557319713405
C	0.30511328633461	-0.06027714803679	1.26257830988814
C	-1.08744139818339	0.02442039947004	1.17806990774329
H	-1.71435780008839	0.01712589924047	2.07023733751160
C	-1.65671712118728	0.11077583409371	-0.08493961318256
I	-3.79581230977187	0.24555641518936	-0.26207005874595
C	-0.90495024303765	0.11682708240687	-1.25621688124943
H	-1.37837648784798	0.18346199991243	-2.23469378055358
C	0.48499052323534	0.03202837740391	-1.14527317056824
H	1.09142805661434	0.03440956264886	-2.05137594344329
C	1.08945532438206	-0.05601680559732	0.10917288745625
H	2.17459594717776	-0.12213211516645	0.18695122416940
Cl	-4.28746854309714	-0.06428583922452	2.49905658384032

I-3c

N	-1.71307675057234	0.94178962806929	0.06219936464416
I	-3.08945078396617	2.66084561061391	0.21122678952225
Si	-0.10963680568367	1.29476551523432	-0.57162681392393
Si	-2.17159082332850	-0.50199254590663	0.95781498178943
H	-0.23631665951050	2.29613965567441	-1.67042440086091
H	0.77880746299057	1.84098890707200	0.50429148612113
H	0.47245507512765	0.01080402869608	-1.07626638756392
H	-3.65191711541655	-0.66838646650245	0.87643294230752
H	-1.46216907265298	-1.66622435152392	0.33844489314043
H	-1.75953131289018	-0.39037459437114	2.39420226122076
Cl	-4.35099321409732	4.75135461294412	0.90697488360309

I-3d

C	1.02374838006343	2.51154881776296	-0.02543202099894
C	-0.24862564729361	2.51567736130284	0.47874693838386
N	1.42129224448279	3.82863187951346	-0.08819652054841
N	-0.57428869101369	3.83523704017842	0.70151056783203
C	0.43927917209448	4.64777033578793	0.33987651666776
H	2.32569215361428	4.15636147084161	-0.42106192957389
H	-1.45964116969917	4.16852043954239	1.07725650780800
H	-0.93341710094385	1.70070875850510	0.68154620812892
H	1.65707436220939	1.69219908905551	-0.34447050498396
I	0.56904336954462	6.81253350394289	0.63851396125131
Cl	1.22813292694134	8.69015130356690	2.23605027603333

At-1a

C	6.65184889566274	2.25771425997337	7.74194599545738
C	6.15882857882037	1.21972067869409	6.78225029015188
H	5.06536774269586	1.14688954496073	6.74248484771741
H	6.61498414015990	0.23386714039772	6.93363799470045
H	6.48451314458924	1.56056701776948	5.77888001895462
C	5.94297310616133	3.57299418709031	7.72580533326331
H	4.85298532633663	3.47795606558918	7.68051779984765
H	6.26379007546790	4.07184965479102	6.79042561829913
H	6.23818256525735	4.23339540747895	8.54895993483232
C	8.12534316814811	2.29308967195012	7.98803283925061
H	8.56586758203138	1.29989664568147	8.12527175311886
H	8.41027079729616	2.95732896940235	8.81165873088069
H	8.57020000986786	2.72096274983591	7.06857784371726
At	5.73523526889936	1.15327208184297	9.96249355860236

At-1b

H	1.08884942129936	-0.15180948747810	2.17397299077478
C	0.54766796566738	-0.08014447687631	1.23103013409342
C	-0.83493876149099	-0.02324915727243	1.23303046346295
H	-1.39476948420778	-0.05048626084977	2.16651674790129
C	-1.50006131556983	0.07013130469761	-0.01059498429393
At	-3.69117654159126	0.15776744747038	-0.02839536146122
C	-0.80908240245775	0.10806867122789	-1.24300408865757
H	-1.34928984664318	0.18074645616565	-2.18557536621569
C	0.57324793491620	0.04957517343048	-1.21817853061392
H	1.13401825846987	0.07746626374039	-2.15194600144554
C	1.25263145920731	-0.04583582880930	0.01204919688206
H	2.34199331240067	-0.08910010544650	0.02111479957335

At-1c

N	-1.69677351802296	1.11083817653544	0.42241472482480
At	-2.88438883006124	2.77935295647023	1.02956968734925
Si	-0.30646826976100	1.38599514920350	-0.71932920500771
Si	-2.11904181624500	-0.53118851523165	1.08430190423053
H	-0.57353582037712	2.66586034864256	-1.42517968341940
H	0.90256553597741	1.43142579063026	0.15622018857355
H	-0.32373803932872	0.17428167814966	-1.58824993448495
H	-3.24438998404387	-1.02557438082882	0.23753373783856
H	-0.86091395955364	-1.30423678908048	0.88357658603600
H	-2.50841010626263	-0.33602153169389	2.50598242491645

At-1d

C	0.95893478558238	2.36401988722730	-0.20977261139859
C	-0.32924817638846	2.38118786022096	0.35601721385247
N	1.46883828903429	3.60591643909018	-0.04264796849550
N	-0.52303923889070	3.63208642793746	0.83302556618249
C	0.57357623117099	4.41141324570530	0.60029637039398
H	2.39943065646163	3.90253550990471	-0.35432966469745
H	-1.37454699124131	3.95374968866619	1.30490925292114
H	-1.07292826454389	1.58851826864997	0.43077144546014
H	1.49937121910517	1.55438731256048	-0.69901430419491
At	0.84039148970990	6.49020536003743	1.14094469997624

At-2a

At	3.46966395690216	0.12297471503623	3.98210117258899
C	3.49433041280019	0.11346691707880	1.56012334851106
C	3.11979909655095	1.51833499834049	1.13060494438097
H	3.83853699179801	2.26218234972009	1.49596037694262
H	2.11895499622630	1.79871641175998	1.48183578963375
H	3.11478415037363	1.56468129253853	0.02619913257733
C	2.47047196097349	-0.91945165517976	1.13146885251183
H	2.44638586450257	-0.96107184476716	0.02722368652845
H	1.46252684421681	-0.66407390008696	1.48091608522347
H	2.72379557100557	-1.92145037651250	1.49968716612442
C	4.90648069282247	-0.26311317228165	1.15654518336557
H	5.18433310217851	-1.25763303361118	1.52729244883412
H	5.64239608846801	0.46313613300299	1.52331179504734
H	4.97022326392239	-0.28290519843646	0.05335312703793
C	3.40945849091606	0.16896739435841	7.06484454052271
C	4.83878760335814	0.52222899806613	7.31150673804092
H	5.10497627080989	1.49083340503083	6.86728990025340
H	5.52405475763838	-0.24252161526092	6.92138217089196
H	5.03487377907000	0.60207842783564	8.40132936197681
C	2.98906464558374	-1.24144648747163	7.31382017816609
H	2.90995899519931	-1.43510075713656	8.40403153274329
H	3.71469260244954	-1.96258891706148	6.91392151254485
H	2.00369759759802	-1.45817810813707	6.87950126190287
C	2.38776766263207	1.24219387717251	7.24444334496199
H	1.41906117662833	0.96284242511732	6.80840661425863
H	2.71021490135915	2.19354200130725	6.80001484982545
H	2.21266452401633	1.43368371957818	8.32370588460319

At-2b

H	1.69891809789246	-0.23509205732613	2.24263853136115
C	1.18170275441453	-0.16561704801514	1.28414266634898
C	-0.21771745194146	-0.18576469326875	1.25198475976233
H	-0.78836881702033	-0.27076883779490	2.17753948240988
C	-0.85304991938682	-0.08517307580302	0.02187873531360
At	-3.29489163018562	-0.02182861827835	-0.03416171129655
C	-0.15267807134807	0.00365063386793	-1.17311260050180
H	-0.67171767029603	0.06422662294431	-2.13052620203603
C	1.24677069701037	0.02385616055335	-1.12685088342468
H	1.81426426677864	0.10316157660513	-2.05562799822636
C	1.91031496969721	-0.06138781783325	0.09802391040429
H	3.00017898821727	-0.05140258620364	0.12822971454235
H	-5.46676885413177	-1.34421415125467	2.15237949140798
C	-6.01609914590949	-1.49597221007239	1.22246100437246
C	-7.29126668357871	-2.07347384206416	1.24153540475930
H	-7.73300615327402	-2.37062840813585	2.19422926893264
C	-7.99126807752440	-2.27056512375314	0.05005480699556
H	-8.98190779827142	-2.72555036503880	0.06978556471187
C	-7.42223451727388	-1.89330434551109	-1.16725519314256
H	-7.96635265880149	-2.04873215174061	-2.10039960143645
C	-6.14711153101428	-1.31569208731159	-1.20039323247891
H	-5.69998905243542	-1.02587258622441	-2.15212416260946
C	-5.47900174161729	-1.11670498834084	-0.00011175616956

At-2c

N	-1.38183812909178	0.78713114882109	0.22668347368553
At	-2.38517757144937	2.90467358321055	0.21726771498443
Si	0.35248508671984	0.72492654452336	0.04479824999131
Si	-2.39797541967668	-0.60222023555530	0.49587821941283
H	0.78895209672589	1.69363029495647	-1.00978154756907
H	1.03801213403324	1.09016012172144	1.32863053066641
H	0.77157227209912	-0.66408176175708	-0.33771204054556
H	-3.82646531925784	-0.16336913826197	0.53909393495973
H	-2.21157702966925	-1.60647031068040	-0.60437441980066
H	-2.05383868620526	-1.28102786287484	1.79136813170016
N	-3.39865666278493	5.01481440743362	0.20258899815647
Si	-2.37971634996989	6.38287919441813	-0.16618731476996
H	-1.69405233701504	6.18224234826081	-1.48281815466161
H	-1.32525803800266	6.55625008575911	0.88565796158377
H	-3.21561315067830	7.62750297880533	-0.22822718005243

Si	-5.10163396217662	5.13709286449550	0.55153511074553
H	-5.65815505343575	3.76476695781053	0.75852900584915
H	-5.82538296284986	5.80464619361264	-0.58216384903917
H	-5.33930091731488	5.95741258530099	1.78693317470314

At-2d

C	1.09493492979317	2.53648839392047	0.05005154537469
C	-0.18742161872849	2.47210424983410	0.54957366881488
N	1.41532140284961	3.86845725592867	-0.01313741050018
N	-0.57982174557973	3.76828077830888	0.76559002487457
C	0.37970518492681	4.64649736404517	0.38478967950762
H	2.30261602381446	4.22996944503122	-0.35812029474236
H	-1.49350073702699	4.03951681590941	1.12401280790741
H	-0.83027582744139	1.61828302326490	0.73713392961403
H	1.76677558463358	1.74875746727684	-0.27488339057155
At	0.35033663851318	7.04747338636460	0.65446249545916
C	0.68056738137672	9.13630095570722	1.83245828701277
N	-0.17814277800002	9.73825397778533	2.69086981682379
N	1.81639105652156	9.87036158881809	1.91579586613718
C	0.37690871850504	10.86004692360506	3.25105771159231
C	1.65890238669421	10.94466177031396	2.75364387648986
H	-1.13159067708110	9.42358739875151	2.86029550148937
H	2.66307563935990	9.67563643660903	1.38466538224104
H	2.43061665025877	11.69065087074490	2.91316701647036
H	-0.16540821338928	11.51925189778062	3.92097348600506

At-3a

At	4.54397514174289	1.53934075573645	4.17786841125795
Cl	2.67040010852037	0.08544235996368	2.53466683683387
C	3.59226659374591	0.34539053631631	6.05430352409369
C	3.83300754293156	-1.11543164470207	5.74720473187441
H	4.90119653788545	-1.36297221389346	5.72911341586821
H	3.37419766071977	-1.40334165069032	4.79300384084208
H	3.35742945033158	-1.70835066166257	6.54787655815981
C	2.12887305008001	0.72373880931057	6.05167630523174
H	1.63531393642217	0.15580170202569	6.85968824889173
H	1.64761705387072	0.45409141628602	5.10324262608868
H	1.97936428214935	1.79247793436975	6.24663575232207
C	4.35909931530228	0.85775074148181	7.25452386858483
H	4.21609572724456	1.93401119898352	7.41013482759381
H	5.43216713528931	0.64150498983600	7.18409341989193
H	3.97098146376407	0.33557872663860	8.14673863246515

At-3b

H	0.76749688566251	-0.14271086413294	2.24640262171838
C	0.30680875088827	-0.07082999904447	1.26059414011749
C	-1.08664220862495	-0.00270901720753	1.16634023932859
H	-1.71949153794258	-0.02140840959934	2.05532443994638
C	-1.64360970727931	0.08778061025349	-0.10026035247522
At	-3.90033539191263	0.19849638316509	-0.27925474723961
C	-0.88757533852858	0.11345283223920	-1.26640404325291
H	-1.35211454300622	0.18464672897589	-2.24914203162303
C	0.50367666430806	0.04430629217459	-1.14571061063550
H	1.11697943420238	0.06308598857297	-2.04717318650621
C	1.09916069026021	-0.04636533466889	0.11264266033710
H	2.18449221157520	-0.09957129238702	0.19800293033733
Cl	-4.29669590960238	0.02343608165897	2.56570793994721

At-3c

N	-1.67668167838973	0.95598690020405	0.13347775242912
At	-3.12111177742073	2.76810949037084	0.24683273743980
Si	-0.07140839745076	1.27582860608526	-0.50490172901331
Si	-2.15246954445979	-0.53344382906140	0.93111635118247
H	-0.18071560860442	2.20942810885613	-1.66583419161170
H	0.79028217248937	1.90107567018857	0.55065871367737
H	0.54369346332546	-0.02378691507790	-0.92751131939926
H	-3.62954802377415	-0.52121556755113	1.14462752989389
H	-1.75120538070501	-1.68880765885791	0.06479933874668
H	-1.45424612272712	-0.66818226273444	2.25254756965180
Cl	-4.58622037872671	4.88889007142052	0.70427037542485

At-3d

C	1.01913899499137	2.47410428788923	-0.04327448474936
C	-0.25374064924165	2.47679826129222	0.45747869035891
N	1.42020789445619	3.79162798582409	-0.08586446862255
N	-0.57131714139851	3.79579553553793	0.69827267259309
C	0.44412645688547	4.61478400552750	0.35181940741113
H	2.32691434942392	4.11569545197549	-0.41406264985122
H	-1.45709085218487	4.12354546321116	1.07618429787909
H	-0.94286924879341	1.66248335948793	0.64729646734986
H	1.64991732669762	1.65701444821503	-0.37269358451742
At	0.58829291829859	6.93057226004666	0.69974846129525
Cl	1.22470995086530	8.91691894099280	2.25943519085323

Bi-1b calculated using PBE and two-component ZORA

H	1.10339401797814	-0.15267207260683	2.16402658621471
C	0.57451072187769	-0.07989161938365	1.20882382234946
C	-0.82144991504331	-0.02159356979067	1.19167796216599
H	-1.36295429513692	-0.05049288102584	2.14160940946794
C	-1.54874974132312	0.07202883704411	-0.01103790071085
Bi	-3.91121612336376	0.16713693331642	-0.03005432542667
C	-0.79641254992884	0.10510523893086	-1.20150119541444
H	-1.31795194015522	0.17786340867508	-2.16021293643749
C	0.59967586088768	0.04738109618288	-1.19551258799019
H	1.14842108534742	0.07590603124203	-2.14182419919590
C	1.30037560912587	-0.04616599765523	0.01252345271387
H	2.39144726973438	-0.09147540492915	0.02150191226356

Bi-1b calculated using PBE0 and scalar ZORA

H	1.09724693481747	-0.15181274170122	2.15854641085075
C	0.57254102533437	-0.07946833841718	1.20604543465949
C	-0.82031119254218	-0.02182768113373	1.18973059298748
H	-1.35492466557801	-0.05139030623950	2.13889967418537
C	-1.54839245067874	0.07180999913517	-0.01101235257551
Bi	-3.90707074038316	0.16773877186519	-0.03012414432418
C	-0.79533820385675	0.10473685305485	-1.19949342492104
H	-1.30996775840953	0.17744500375085	-2.15733037771145
C	0.59759568818101	0.04716973414483	-1.19276596707379
H	1.14206723639643	0.07556955639287	-2.13646076436949
C	1.29938081338672	-0.04594158044304	0.01252099493571
H	2.38626331333237	-0.09089927040910	0.02146392335667

Bi-1b calculated using PBE0 and two-component ZORA

H	1.10311159912772	-0.15251802295488	2.15827566157662
C	0.57643847432390	-0.07998928908308	1.20682211337179
C	-0.81834221697250	-0.02181780543662	1.18892590277848
H	-1.35675543474341	-0.05056018367676	2.13595232310631
C	-1.54373426962068	0.07174967283784	-0.01098526212442
Bi	-3.93287868967207	0.16852049911010	-0.03025320613983
C	-0.79337104874511	0.10471641267482	-1.19869182965435
H	-1.31187579282495	0.17711753648225	-2.15445212509311
C	0.60155012004254	0.04723060835166	-1.19348990512575
H	1.14800377433193	0.07536196026157	-2.13610199551421
C	1.29985955731831	-0.04577737286221	0.01253498019445
H	2.38708392743433	-0.09090401570469	0.02148334262403

Bi-1b calculated using PBE and no ZORA

H	1.12515654460386	-0.15270283442904	2.16071676767349
C	0.59075524719882	-0.07936938575534	1.21163004455701
C	-0.80519778139313	-0.02318398633568	1.18703173521796
H	-1.35453116924480	-0.05257393320433	2.13178404195505
C	-1.51818695042401	0.06903671196764	-0.00964122020494
Bi	-4.07214150923663	0.17663558673668	-0.03605643677615
C	-0.78134962789916	0.10313717047142	-1.19490168678001
H	-1.31218971951887	0.17453762664173	-2.14793750121325
C	0.61478962636483	0.04722739674652	-1.19770056727158
H	1.16803886062393	0.07579522990183	-2.13834410700629
C	1.30885802503493	-0.04559864018159	0.01246616722937
H	2.39508845389023	-0.08981094255984	0.02097276261936

Bi-1b calculated using PBE0 and no ZORA

H	1.12515654460386	-0.15270283442904	2.16071676767349
C	0.59075524719882	-0.07936938575534	1.21163004455701
C	-0.80519778139313	-0.02318398633568	1.18703173521796
H	-1.35453116924480	-0.05257393320433	2.13178404195505
C	-1.51818695042401	0.06903671196764	-0.00964122020494
Bi	-4.07214150923663	0.17663558673668	-0.03605643677615
C	-0.78134962789916	0.10313717047142	-1.19490168678001
H	-1.31218971951887	0.17453762664173	-2.14793750121325
C	0.61478962636483	0.04722739674652	-1.19770056727158
H	1.16803886062393	0.07579522990183	-2.13834410700629
C	1.30885802503493	-0.04559864018159	0.01246616722937
H	2.39508845389023	-0.08981094255984	0.02097276261936

PhSb

H	3.224354	0.000462	2.155262
C	2.682382	0.000885	1.208406
C	1.287427	0.000566	1.209539
H	0.753207	-0.000004	2.161623
C	0.574730	0.002176	-0.000399
Sb	-1.605663	0.001900	-0.000893
C	1.288220	0.001121	-1.209852
H	0.754640	0.000165	-2.162292
C	2.683179	0.001355	-1.207775
H	3.225773	0.000530	-2.154276
C	3.383124	-0.002049	0.000543
H	4.473434	-0.003485	0.000898

$PhSb^+$

H	3.225934	0.000171	2.161618
C	2.670335	-0.000599	1.224276
C	1.286032	0.000550	1.232760
H	0.746594	0.000563	2.180686
C	0.575897	0.001688	-0.000352
Sb	-1.522844	0.002741	-0.001019
C	1.286816	0.000656	-1.233022
H	0.747990	0.000890	-2.181298
C	2.671115	-0.000529	-1.223649
H	3.227327	0.000566	-2.160628
C	3.359438	-0.002239	0.000533
H	4.450174	-0.000835	0.000881

4

Bi	-1.535700	0.086916	-0.430900
C	0.758226	0.029217	-0.068905
C	1.478084	1.178963	0.294282
C	1.481987	-1.169988	-0.178341
C	-1.175806	-3.658110	-0.208068
C	2.860815	1.134574	0.529236
C	3.558165	-0.068599	0.441846
H	4.631683	-0.107004	0.640214
C	-2.200030	-4.258377	0.525279
H	-3.067405	-4.692382	0.025531
C	0.932369	2.576779	0.559963
C	0.074825	2.663835	1.822929
C	-1.029557	-3.388070	-1.638802
C	-1.948675	4.393135	-2.026883
H	-2.719527	4.873891	-2.626534
C	-0.069002	-3.106951	0.466592
C	-1.108840	3.381906	1.567325
C	-0.012502	3.163507	-0.477853
C	-1.164403	3.696974	0.139477
C	-0.816772	3.852532	-2.655965
C	2.856971	-1.221599	0.092860
C	4.603092	2.858241	-0.060394
H	4.285041	2.804357	-1.110458
H	5.454534	2.175924	0.073416

H	4.955287	3.880034	0.143335
C	-2.130661	4.324867	-0.641845
H	-3.030806	4.745400	-0.190979
C	3.444545	2.491044	0.880484
C	-1.731003	3.105265	3.873081
H	-2.446484	3.284197	4.676483
C	0.942532	-2.550113	-0.532364
C	-0.005910	-3.109656	1.853521
H	0.835202	-2.627457	2.348353
C	-2.115809	-4.273671	1.916203
H	-2.925594	-4.736159	2.481548
C	0.162996	3.245202	-1.848876
H	1.054466	2.805271	-2.299867
C	2.237695	3.445236	0.659731
H	2.365508	3.979302	-0.290730
H	2.150246	4.199733	1.451383
C	-1.475494	-3.211223	-3.993326
H	-2.125836	-3.431054	-4.840643
C	0.161666	-2.664822	-1.836071
C	-0.292443	-2.477611	-4.205311
C	3.424884	-2.624435	-0.006380
C	0.529141	-2.215921	-3.098417
H	1.452181	-1.648077	-3.212244
C	0.333363	2.143988	3.084318
H	1.228316	1.544997	3.239762
C	-2.015210	3.607519	2.604911
H	-2.941888	4.156107	2.429605
C	-1.852412	-3.666205	-2.731249
H	-2.782107	-4.223388	-2.606400
C	4.658804	-2.680432	-0.918751
H	4.427267	-2.275738	-1.913458
H	5.002747	-3.718076	-1.038708
H	5.491159	-2.098155	-0.498594
C	2.246253	-3.428917	-0.619867
C	-0.565225	2.363021	4.139266
C	-1.037440	-3.690520	2.607003
C	-0.630595	3.864454	-4.176378
C	3.951867	2.524984	2.332942
H	4.742893	1.777435	2.486646
H	3.145483	2.317781	3.046184
H	4.368090	3.515225	2.568838
C	-0.594265	2.406615	-4.678021
H	0.222560	1.840469	-4.211707
H	-0.451557	2.377448	-5.768044
H	-1.534650	1.892133	-4.436612
C	-1.767025	4.596491	-4.901802
H	-2.738699	4.115639	-4.724066
H	-1.580801	4.580824	-5.984490
H	-1.837409	5.647480	-4.588909
C	3.803064	-3.148526	1.391212
H	4.577513	-2.516823	1.848648
H	4.192707	-4.174785	1.323509
H	2.933644	-3.157199	2.060546
C	0.697944	4.561712	-4.531231
H	0.694879	5.603891	-4.183448
H	0.847290	4.561155	-5.620689
H	1.557272	4.055028	-4.073336
C	-1.029913	-3.691935	4.139171
C	-0.319185	1.815082	5.549315
C	0.061651	-2.006034	-5.619800
C	0.270106	-3.238067	-6.524235
H	1.092855	-3.861646	-6.148145
H	0.515829	-2.921315	-7.548418
H	-0.632541	-3.861404	-6.568274
C	-0.996214	-5.147020	4.648033
H	-1.862297	-5.718428	4.289402
H	-1.006865	-5.166708	5.747700
H	-0.087434	-5.658400	4.301836
C	0.184560	-2.949571	4.712461
H	1.130386	-3.423226	4.414782

H	0.137588	-2.957993	5.810003
H	0.206480	-1.900636	4.387217
C	-1.089017	-1.148484	-6.183856
H	-2.027764	-1.714303	-6.239482
H	-0.841892	-0.804246	-7.198740
H	-1.261383	-0.266964	-5.553153
C	1.017554	1.068577	5.657356
H	1.057833	0.201704	4.984173
H	1.149032	0.698227	6.683284
H	1.868273	1.724783	5.426321
C	1.344794	-1.164325	-5.646407
H	1.251900	-0.265103	-5.022306
H	1.548031	-0.838304	-6.675691
H	2.215639	-1.738203	-5.300668
C	-2.307024	-2.998511	4.655976
H	-2.369538	-1.968665	4.279359
H	-2.304339	-2.965972	5.755180
H	-3.213317	-3.528024	4.335466
C	-0.298676	2.983190	6.555935
H	0.504285	3.692323	6.311859
H	-0.127355	2.603514	7.573758
H	-1.247544	3.534803	6.556339
C	-1.452860	0.838626	5.921699
H	-2.433625	1.331049	5.896887
H	-1.296833	0.440878	6.935228
H	-1.482395	-0.006787	5.222050
H	2.454354	-3.634640	-1.677350
H	2.100620	-4.394959	-0.120975

$[\mathbf{4}]^-$

Bi	-1.444319	0.110682	-0.855146
C	0.755233	0.012240	-0.182872
C	1.477369	1.154710	0.246138
C	1.503091	-1.192982	-0.192775
C	-0.986783	-3.920075	-0.159654
C	2.834288	1.105872	0.589533
C	3.546818	-0.096362	0.564520
H	4.606393	-0.133868	0.827176
C	-1.922012	-4.627375	0.596540
H	-2.732241	-5.177031	0.113600
C	0.923726	2.554185	0.477860
C	0.053862	2.687932	1.728536
C	-0.892849	-3.655452	-1.593717
C	-1.753010	4.647093	-2.118906
H	-2.459749	5.219668	-2.718132
C	0.041578	-3.209542	0.492705
C	-1.060363	3.509786	1.468600
C	0.019501	3.187060	-0.568488
C	-1.073459	3.836344	0.044500
C	-0.677671	3.996828	-2.743692
C	2.854800	-1.244969	0.171534
C	4.637130	2.797583	0.092984
H	4.398824	2.704714	-0.975440
H	5.469264	2.113732	0.315942
H	4.980810	3.825833	0.286681
C	-1.960682	4.573943	-0.737003
H	-2.815969	5.081927	-0.287485
C	3.404816	2.466727	0.951143
C	-1.729150	3.264723	3.766780
H	-2.442544	3.488495	4.561683
C	0.987535	-2.584296	-0.533083
C	0.096858	-3.152757	1.876999
H	0.853932	-2.526489	2.345255
C	-1.839601	-4.585705	1.988104
H	-2.586953	-5.126433	2.571410
C	0.211651	3.259685	-1.939855
H	1.048121	2.717736	-2.383715
C	2.231604	3.419807	0.604620
H	2.420588	3.886653	-0.371479
H	2.107468	4.226302	1.340258

C	-1.429208	-3.500555	-3.932442
H	-2.083769	-3.773597	-4.761819
C	0.184391	-2.775641	-1.809955
C	-0.365816	-2.605591	-4.158076
C	3.439453	-2.643509	0.077433
C	0.449866	-2.258579	-3.072188
H	1.273477	-1.555425	-3.185816
C	0.253489	2.137701	2.985337
H	1.084654	1.450183	3.129680
C	-1.952472	3.805356	2.500469
H	-2.833024	4.424428	2.318671
C	-1.700344	-4.028444	-2.670202
H	-2.547397	-4.702712	-2.530001
C	4.738192	-2.664333	-0.743286
H	4.578184	-2.210283	-1.730852
H	5.090294	-3.697872	-0.886861
H	5.536702	-2.102870	-0.236327
C	2.317960	-3.418924	-0.657573
C	-0.635390	2.421844	4.034323
C	-0.851550	-3.837642	2.652973
C	-0.492358	3.987143	-4.265036
C	3.804544	2.549060	2.435468
H	4.552846	1.780101	2.676772
H	2.939323	2.400231	3.091501
H	4.238510	3.535216	2.663758
C	-0.741243	2.554110	-4.773930
H	-0.084670	1.832301	-4.271583
H	-0.572776	2.491072	-5.860245
H	-1.771636	2.240947	-4.557216
C	-1.463283	4.934580	-4.982670
H	-2.509012	4.637199	-4.824841
H	-1.269252	4.908370	-6.064828
H	-1.342896	5.972757	-4.640317
C	3.726755	-3.226446	1.473602
H	4.437662	-2.588531	2.018565
H	4.161102	-4.235080	1.389489
H	2.809505	-3.300791	2.069362
C	0.943655	4.417773	-4.624684
H	1.145136	5.437260	-4.265611
H	1.083565	4.398767	-5.716350
H	1.690324	3.748951	-4.178482
C	-0.860688	-3.765116	4.184316
C	-0.469400	1.807104	5.429492
C	-0.205729	-1.951152	-5.534235
C	-0.095722	-3.025989	-6.632106
H	0.790012	-3.656828	-6.469738
H	-0.007071	-2.551518	-7.621564
H	-0.977055	-3.680663	-6.649845
C	-0.693767	-5.180398	4.772603
H	-1.496755	-5.851190	4.439154
H	-0.714042	-5.143385	5.872803
H	0.263859	-5.618677	4.457962
C	0.270404	-2.881961	4.726541
H	1.259564	-3.270617	4.446708
H	0.218473	-2.844409	5.824149
H	0.188448	-1.853665	4.351891
C	-1.444236	-1.066875	-5.792123
H	-2.360056	-1.671879	-5.835768
H	-1.341021	-0.525136	-6.745178
H	-1.563009	-0.336608	-4.979934
C	0.860646	1.054238	5.575478
H	0.932696	0.210984	4.877191
H	0.945505	0.649642	6.594415
H	1.718966	1.717639	5.398875
C	1.042442	-1.060774	-5.608181
H	0.988958	-0.235585	-4.886328
H	1.122982	-0.622961	-6.613723
H	1.959275	-1.634673	-5.411452
C	-2.203150	-3.169639	4.656471
H	-2.354856	-2.172158	4.223154

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H        -2.219744   -3.081014    5.753670
H        -3.049926   -3.798008    4.350465
C        -0.504648    2.912366    6.503548
H         0.309760    3.632992    6.343728
H        -0.386717    2.472096    7.505525
H        -1.452397    3.465882    6.488103
C        -1.623860    0.815142    5.678069
H        -2.597660    1.320441    5.628147
H        -1.526626    0.346282    6.669731
H        -1.620369    0.023441    4.917796
H         2.569987   -3.490212   -1.724283
H         2.186398   -4.441416   -0.277801
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