# What Comes Next: The Fate of Germa, Stanna, and Plumba-*closo*-Dodecaborate Based Electrolytes in Calcium Ion Batteries

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## Computational Details

The modelled anions were fully optimized using M062X functional employing Def2TZVP basis set for C, Si and Ge. In case of Sn and Pb the Def2TZVP basis sets with effective core potential have been generated from the basis set exchange.[1–3] No symmetrical or geometrical constraints were imposed during the optimization. The harmonic frequency calculations were carried out on the same level of theory to depict the nature of the stationary points as local minima. The optimized geometries were used for further calculations and analysis. The zero-point energies of the optimized were considered. The vertical detachment energy (VDE) has been calculated by taking the difference of the energies of the optimized anion and the corresponding one electron less specie,

$$\text{VDE} = E\left[XB_{11}H_{11}{}^{-1}\right] - E\left[XB_{11}H_{11}{}^{-2}\right] \qquad (1)$$

Where, $E\left[XB_{11}H_{11}{}^{-2}\right]$ is the electronic energy of the optimized $\left[XB_{11}H_{11}{}^{-2}\right]$ anion and $E\left[XB_{11}H_{11}{}^{-1}\right]$ is the single energy of same anion with one electron less. Similarly, the VDEs of other considered anions have also been calculated. The cation binding energy has been calculated as follows,

$$\text{Binding energy (BE)} = E_{\text{anion}} + E_{\text{cation}} - E_{\text{ion pair}} \qquad (2)$$

Further, the electrochemical stability window (ESW) has been calculated following the frontier molecular orbital approach.[4,5] The cathodic ($V_{CL}$) and anodic ($V_{AL}$) are calculated by the energies of lowest unoccupied orbital (LUMO) and highest occupied molecular orbital (HOMO), respectively. Then the ESW is calculated by taking the difference between $V_{CL}$ and $V_{AL}$.

$$V_{CL} = \frac{-E_{LUMO}}{e}$$

and,

$$V_{AL} = \frac{-E_{HOMO}}{e}$$

The basin analysis of the electron density and molecular electrostatic potential surfaces of the proposed anions were analysed using Multiwfn software.[6] All the geometry optimizations have been carried out using Gaussian 16 program.[7]

## References


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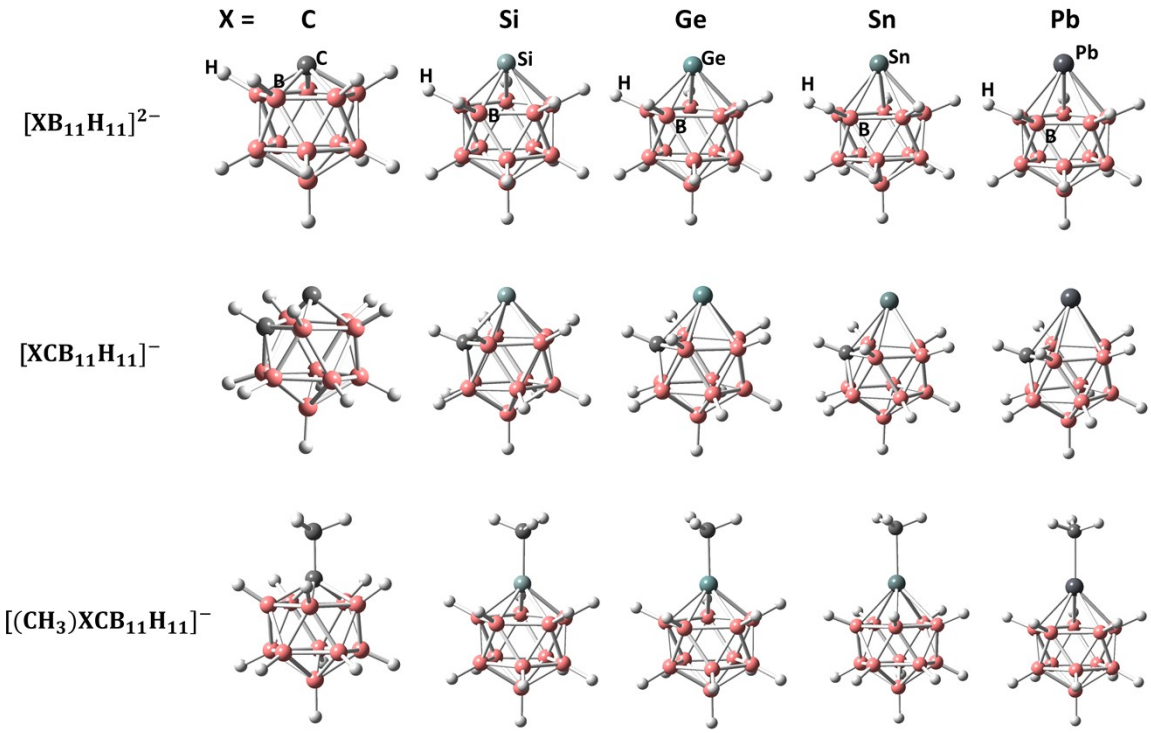



**Figure S1.** Optimized structures of the proposed anions.

**Table S1. Geometrical parameters of $^{XB_{11}H_{11}}{}^{-2}$ anion (where, X=C, Si, Ge, Sn and Pb) (Numbering of the anion cluster has been done as shown in Scheme 2, X is at 1, all the distances are in Å)**

| | C | Si | Ge | Sn | Pb |
|---|---|---|---|---|---|
| P1-1 | 0.848 | 1.450 | 1.554 | 1.789 | 1.886 |
| P1-P2 | 1.521 | 1.498 | 1.493 | 1.487 | 1.485 |
| P2-12 | 0.935 | 0.934 | 0.931 | 0.928 | 0.927 |
| 1-12 | 3.304 | 3.883 | 3.978 | 4.204 | 4.298 |
| 1-H(12) | 4.503 | 5.081 | 5.176 | 5.402 | 5.497 |
| **Top** | | | | | |
| 1-2 | 1.704 | 2.115 | 2.197 | 2.379 | 2.455 |
| 1-3 | 1.704 | 2.115 | 2.197 | 2.380 | 2.456 |
| 1-4 | 1.704 | 2.115 | 2.197 | 2.380 | 2.456 |
| 1-5 | 1.704 | 2.115 | 2.197 | 2.379 | 2.456 |
| 1-6 | 1.704 | 2.115 | 2.197 | 2.380 | 2.455 |
| **UR** | | | | | |
| 2-3 | 1.738 | 1.810 | 1.826 | 1.844 | 1.848 |
| 3-4 | 1.737 | 1.810 | 1.826 | 1.844 | 1.848 |
| 4-5 | 1.737 | 1.810 | 1.826 | 1.844 | 1.848 |
| 5-6 | 1.737 | 1.810 | 1.826 | 1.844 | 1.848 |
| 6-2 | 1.738 | 1.810 | 1.826 | 1.844 | 1.848 |
| 2-H | 1.199 | 1.199 | 1.199 | 1.201 | 1.202 |
| 3-H | 1.199 | 1.199 | 1.199 | 1.201 | 1.202 |
| 4-H | 1.199 | 1.199 | 1.199 | 1.201 | 1.202 |
| 5-H | 1.199 | 1.199 | 1.199 | 1.201 | 1.202 |

| | | | | | |
|---|---|---|---|---|---|
| 6-H | 1.199 | 1.199 | 1.199 | 1.201 | 1.202 |
| **Middle** | | | | | |
| 2-7 | 1.779 | 1.770 | 1.768 | 1.766 | 1.765 |
| 2-8 | 1.779 | 1.770 | 1.768 | 1.766 | 1.765 |
| 3-8 | 1.779 | 1.770 | 1.768 | 1.766 | 1.765 |
| 3-9 | 1.779 | 1.770 | 1.768 | 1.766 | 1.765 |
| 4-9 | 1.780 | 1.769 | 1.768 | 1.766 | 1.765 |
| 4-10 | 1.779 | 1.770 | 1.768 | 1.766 | 1.765 |
| 5-10 | 1.780 | 1.769 | 1.768 | 1.766 | 1.765 |
| 5-11 | 1.780 | 1.770 | 1.768 | 1.766 | 1.765 |
| 5-11 | 1.779 | 1.770 | 1.768 | 1.766 | 1.765 |
| 5-7 | 1.780 | 1.770 | 1.768 | 1.766 | 1.765 |
| **LR** | | | | | |
| 7-8 | 1.772 | 1.773 | 1.774 | 1.776 | 1.777 |
| 8-9 | 1.772 | 1.773 | 1.774 | 1.776 | 1.777 |
| 9-10 | 1.772 | 1.773 | 1.774 | 1.776 | 1.777 |
| 10-11 | 1.772 | 1.773 | 1.774 | 1.776 | 1.777 |
| 11-7 | 1.772 | 1.773 | 1.775 | 1.776 | 1.777 |
| 7-H | 1.199 | 1.198 | 1.198 | 1.198 | 1.199 |
| 8-H | 1.199 | 1.198 | 1.198 | 1.198 | 1.199 |
| 9-H | 1.199 | 1.198 | 1.198 | 1.198 | 1.199 |
| 10-H | 1.199 | 1.198 | 1.198 | 1.198 | 1.199 |
| 11-H | 1.199 | 1.198 | 1.198 | 1.198 | 1.199 |
| **Bottom** | | | | | |
| 7-12 | 1.774 | 1.774 | 1.773 | 1.773 | 1.774 |
| 8-12 | 1.774 | 1.774 | 1.773 | 1.773 | 1.773 |
| 9-12 | 1.774 | 1.774 | 1.773 | 1.773 | 1.774 |
| 10-12 | 1.774 | 1.774 | 1.774 | 1.773 | 1.773 |
| 11-12 | 1.774 | 1.774 | 1.773 | 1.773 | 1.773 |
| 12-H | 1.200 | 1.198 | 1.198 | 1.198 | 1.198 |

**Table S2. Geometrical parameters of $^{XCB_{10}H_{11}}{}^{-1}$ anion (where, X=C, Si, Ge, Sn and Pb) (Numbering of the anion cluster has been done as shown in Scheme 1, all the distances are in Å, 1 = X, 2 = C, and H(12) represents the H atom at 12th position B atom)**

| | **1 = C** | **Si** | **Ge** | **Sn** | **Pb** |
|---|---|---|---|---|---|
| P1-1 | 0.874 | 1.482 | 1.600 | 1.851 | 1.960 |
| P1-P2 | 1.504 | 1.485 | 1.481 | 1.477 | 1.476 |
| P2-12 | 0.936 | 0.934 | 0.933 | 0.932 | 0.931 |
| 1-12 | 3.314 | 3.901 | 4.013 | 4.259 | 4.365 |
| 1-H(12) | 4.502 | 5.089 | 5.201 | 5.447 | 5.553 |
| **Top** | | | | | |
| 1-2 | 1.651 | 2.096 | 2.219 | 2.442 | 2.556 |
| 1-3 | 1.703 | 2.113 | 2.203 | 2.397 | 2.484 |
| 1-4 | 1.709 | 2.103 | 2.182 | 2.358 | 2.427 |
| 1-5 | 1.709 | 2.103 | 2.182 | 2.357 | 2.427 |
| 1-6 | 1.703 | 2.113 | 2.203 | 2.397 | 2.483 |
| **UR** | | | | | |
| 2-3 | 1.664 | 1.704 | 1.709 | 1.709 | 1.704 |

| | | | | | |
|---|---|---|---|---|---|
| 3-4 | 1.740 | 1.793 | 1.811 | 1.820 | 1.824 |
| 4-5 | 1.736 | 1.803 | 1.818 | 1.836 | 1.840 |
| 5-6 | 1.740 | 1.793 | 1.811 | 1.820 | 1.825 |
| 6-2 | 1.664 | 1.704 | 1.709 | 1.709 | 1.704 |
| 2-H | 1.079 | 1.081 | 1.081 | 1.082 | 1.083 |
| 3-H | 1.186 | 1.188 | 1.188 | 1.191 | 1.192 |
| 4-H | 1.187 | 1.191 | 1.191 | 1.193 | 1.194 |
| 5-H | 1.187 | 1.191 | 1.191 | 1.193 | 1.194 |
| 6-H | 1.186 | 1.188 | 1.188 | 1.191 | 1.192 |
| **Middle** | | | | | |
| 2-7 | 1.685 | 1.691 | 1.684 | 1.684 | 1.681 |
| 2-8 | 1.685 | 1.691 | 1.684 | 1.683 | 1.681 |
| 3-8 | 1.790 | 1.764 | 1.765 | 1.763 | 1.764 |
| 3-9 | 1.783 | 1.764 | 1.763 | 1.761 | 1.762 |
| 4-9 | 1.772 | 1.769 | 1.767 | 1.765 | 1.764 |
| 4-10 | 1.775 | 1.769 | 1.767 | 1.764 | 1.763 |
| 5-10 | 1.775 | 1.769 | 1.767 | 1.765 | 1.764 |
| 5-11 | 1.772 | 1.769 | 1.767 | 1.765 | 1.764 |
| 5-11 | 1.783 | 1.764 | 1.764 | 1.761 | 1.762 |
| 5-7 | 1.790 | 1.764 | 1.765 | 1.763 | 1.764 |
| **LR** | | | | | |
| 7-8 | 1.766 | 1.765 | 1.763 | 1.765 | 1.765 |
| 8-9 | 1.759 | 1.765 | 1.766 | 1.768 | 1.768 |
| 9-10 | 1.773 | 1.773 | 1.775 | 1.778 | 1.780 |
| 10-11 | 1.773 | 1.773 | 1.775 | 1.778 | 1.780 |
| 11-7 | 1.759 | 1.765 | 1.766 | 1.768 | 1.768 |
| 7-H | 1.186 | 1.186 | 1.186 | 1.187 | 1.187 |
| 8-H | 1.186 | 1.186 | 1.186 | 1.187 | 1.187 |
| 9-H | 1.188 | 1.188 | 1.188 | 1.189 | 1.189 |
| 10-H | 1.189 | 1.189 | 1.189 | 1.189 | 1.190 |
| 11-H | 1.188 | 1.188 | 1.188 | 1.189 | 1.189 |
| **Bottom** | | | | | |
| 7-12 | 1.763 | 1.767 | 1.767 | 1.768 | 1.769 |
| 8-12 | 1.763 | 1.767 | 1.767 | 1.768 | 1.769 |
| 9-12 | 1.779 | 1.775 | 1.775 | 1.776 | 1.777 |
| 10-12 | 1.767 | 1.770 | 1.768 | 1.769 | 1.768 |
| 11-12 | 1.779 | 1.775 | 1.776 | 1.776 | 1.777 |
| 12-H | 1.189 | 1.188 | 1.188 | 1.188 | 1.188 |

**Table S3. Geometrical parameters of $CH_3XB_{11}H_{11}^{-1}$ (where, X=C, Si, Ge, Sn and Pb) anion (Numbering of the anion cluster has been done as shown in Scheme 1, all the distances are in Å, 1 = X and H(12) represents the H atom at 12th position B atom)**

| | **1 = C** | **Si** | **Ge** | **Sn** | **Pb** |
|---|---|---|---|---|---|
| P1-1 | 0.803 | 1.250 | 1.349 | 1.594 | 1.667 |
| P1-P2 | 1.499 | 1.483 | 1.475 | 1.466 | 1.458 |
| P2-12 | 0.929 | 0.919 | 0.918 | 0.915 | 0.915 |
| 1-12 | 3.231 | 3.652 | 3.742 | 3.975 | 4.040 |

| 1-H(12) | 5.938 | 6.702 | 6.877 | 7.294 | 7.409 |
|---|---|---|---|---|---|
| **Top** | | | | | |
| 1-2 | 1.701 | 2.013 | 2.093 | 2.274 | 2.333 |
| 1-3 | 1.699 | 2.013 | 2.093 | 2.274 | 2.333 |
| 1-4 | 1.703 | 2.013 | 2.093 | 2.274 | 2.334 |
| 1-5 | 1.699 | 2.013 | 2.093 | 2.274 | 2.334 |
| 1-6 | 1.702 | 2.014 | 2.093 | 2.274 | 2.333 |
| 1-C | 1.518 | 1.862 | 1.947 | 2.130 | 2.180 |
| **UR** | | | | | |
| 2-3 | 1.763 | 1.856 | 1.881 | 1.907 | 1.922 |
| 3-4 | 1.762 | 1.855 | 1.881 | 1.906 | 1.920 |
| 4-5 | 1.762 | 1.856 | 1.881 | 1.906 | 1.919 |
| 5-6 | 1.763 | 1.855 | 1.881 | 1.906 | 1.919 |
| 6-2 | 1.761 | 1.855 | 1.881 | 1.907 | 1.922 |
| 2-H | 1.187 | 1.191 | 1.190 | 1.191 | 1.189 |
| 3-H | 1.187 | 1.191 | 1.190 | 1.191 | 1.189 |
| 4-H | 1.187 | 1.191 | 1.190 | 1.191 | 1.189 |
| 5-H | 1.187 | 1.191 | 1.190 | 1.191 | 1.190 |
| 6-H | 1.187 | 1.191 | 1.190 | 1.191 | 1.189 |
| **Middle** | | | | | |
| 2-7 | 1.763 | 1.766 | 1.762 | 1.760 | 1.757 |
| 2-8 | 1.764 | 1.766 | 1.762 | 1.760 | 1.757 |
| 3-8 | 1.765 | 1.765 | 1.763 | 1.760 | 1.756 |
| 3-9 | 1.765 | 1.766 | 1.763 | 1.760 | 1.757 |
| 4-9 | 1.761 | 1.765 | 1.762 | 1.760 | 1.757 |
| 4-10 | 1.761 | 1.765 | 1.762 | 1.760 | 1.757 |
| 5-10 | 1.765 | 1.766 | 1.763 | 1.760 | 1.757 |
| 5-11 | 1.765 | 1.766 | 1.763 | 1.760 | 1.757 |
| 5-11 | 1.763 | 1.765 | 1.763 | 1.760 | 1.756 |
| 5-7 | 1.763 | 1.765 | 1.763 | 1.760 | 1.757 |
| **LR** | | | | | |
| 7-8 | 1.775 | 1.779 | 1.779 | 1.780 | 1.779 |
| 8-9 | 1.774 | 1.779 | 1.779 | 1.780 | 1.779 |
| 9-10 | 1.775 | 1.778 | 1.779 | 1.780 | 1.779 |
| 10-11 | 1.774 | 1.779 | 1.779 | 1.780 | 1.779 |
| 11-7 | 1.775 | 1.779 | 1.779 | 1.780 | 1.779 |
| 7-H | 1.188 | 1.189 | 1.189 | 1.189 | 1.189 |
| 8-H | 1.188 | 1.189 | 1.189 | 1.189 | 1.189 |
| 9-H | 1.188 | 1.189 | 1.189 | 1.189 | 1.189 |
| 10-H | 1.188 | 1.189 | 1.189 | 1.189 | 1.189 |
| 11-H | 1.188 | 1.189 | 1.189 | 1.189 | 1.189 |
| **Bottom** | | | | | |
| 7-12 | 1.773 | 1.770 | 1.770 | 1.769 | 1.768 |
| 8-12 | 1.773 | 1.770 | 1.770 | 1.769 | 1.768 |
| 9-12 | 1.773 | 1.770 | 1.770 | 1.769 | 1.768 |
| 10-12 | 1.773 | 1.770 | 1.770 | 1.769 | 1.769 |
| 11-12 | 1.773 | 1.770 | 1.770 | 1.769 | 1.768 |
| 12-H | 1.189 | 1.188 | 1.188 | 1.189 | 1.189 |

**Table S4. Vertical Detachment Energy (VDE) and Electrochemical Stability Window of the Considered Anions.**

| | X | C | Si | Ge | Sn | Pb |
|---|---|---|---|---|---|---|
| **VDE (eV)** | $XB_{11}H_{11}^{2-}$ | -1.37 | 0.06 | 0.23 | 0.46 | 1.00 |
| | $XCB_{10}H_{11}^{-}$ | 3.60 | 4.67 | 4.81 | 4.79 | 5.98 |
| | $CH_3XB_{11}H_{11}^{-}$ | 5.95 | 5.82 | 5.65 | 5.11 | 4.79 |
| **ESW (V)** | $XB_{11}H_{11}^{2-}$ | 5.83 | 7.03 | 7.36 | 7.02 | 6.50 |
| | $XCB_{10}H_{11}^{-}$ | 7.05 | 7.86 | 8.03 | 7.07 | 6.47 |
| | $CH_3XB_{11}H_{11}^{-}$ | 9.48 | 9.01 | 8.68 | 7.16 | 6.61 |
| **HOMO (eV)** | $XB_{11}H_{11}^{2-}$ | 1.88 | 0.67 | 0.38 | 0.08 | 0.44 |
| | $XCB_{10}H_{11}^{-}$ | -2.99 | -3.88 | -4.13 | -4.08 | -3.69 |
| | $CH_3XB_{11}H_{11}^{-}$ | -5.23 | -5.03 | -4.89 | -4.36 | -4.07 |

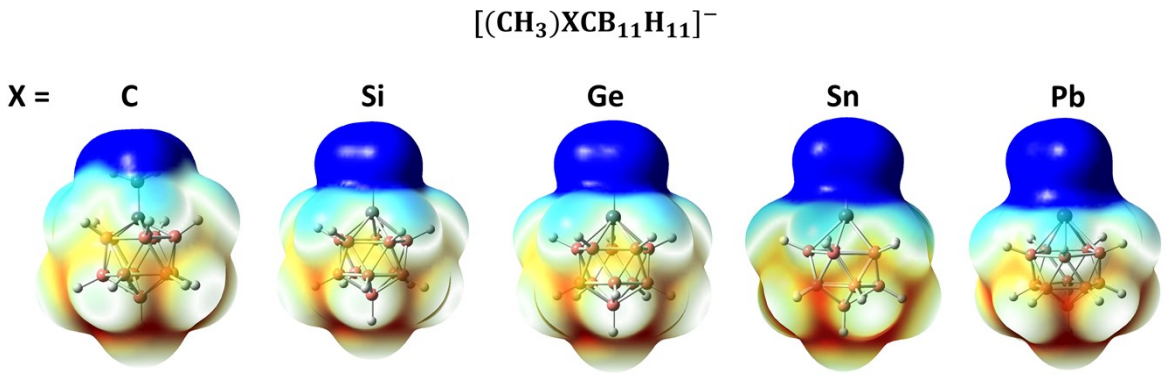



**Figure S2.** MESP surfaces of the -$CH_3$ substituted anion. (surface is plotted at 0.002 a.u. isovalue)

**Table S5. The $Ca^{2+}$ binding energies (BE) and $V_{min}$ of the unique sites of the proposed anions observed from the MESP analysis.**

| $XB_{11}H_{11}^{2-}$ | BE (eV) | | | | |
|---|---|---|---|---|---|
| **Binding sites** | **C** | **Si** | **Ge** | **Sn** | **Pb** |
| **S1** | -18.33 | -18.30 | -18.37 | -18.52 | -18.75 |
| **S2** | -18.34 | -18.21 | -18.27 | -18.40 | -18.63 |
| **S3** | -18.13 | -18.15 | -18.21 | -18.36 | -18.60 |
| **S4** | -19.69 | -18.39 | - | - | - |
| | **$V_{min}$ (kcal/mol)** | | | | |
| **S1** | -178.54 | -176.82 | -177.15 | -177.78 | -178.77 |
| **S2** | -177.50 | -176.46 | -176.88 | -177.88 | -179.14 |
| **S3** | -177.14 | -175.69 | -176.18 | -176.42 | -178.56 |
| **S4** | -194.95 | -174.52 | - | - | - |
| $XCB_{10}H_{11}^{-}$ | **BE (eV)** | | | | |
| **Binding sites** | **C** | **Si** | **Ge** | **Sn** | **Pb** |

| | | | | | |
|---|---|---|---|---|---|
| **S1** | -10.52 | -10.77 | -10.89 | -11.22 | -11.49 |
| **S2** | -11.03 | -11.25 | -11.33 | -11.58 | -11.83 |
| **S3** | -11.00 | -11.26 | -11.36 | -11.66 | -11.93 |
| **S4** | -10.94 | -11.23 | -11.35 | -11.67 | -11.95 |
| **S5** | -10.39 | -10.70 | -11.05 | -11.17 | -11.45 |
| **S6** | -12.01 | -10.81 | -10.73 | -9.85 | - |
| | **$V_{min}$(kcal/mol)** | | | | |
| **S1** | -89.32 | -91.63 | -92.79 | -95.32 | -98.18 |
| **S2** | -95.55 | -96.4 | -96.79 | -98.24 | -100.47 |
| **S3** | -94.67 | -97.04 | -97.91 | -100.15 | -102.78 |
| **S4** | -94.99 | -96.6 | -97.67 | -100.12 | -102.88 |
| **S5** | -88.83 | -90.63 | -91.66 | -94.37 | -97.18 |
| **S6** | -113.92 | -82.84 | -77.85 | -69.1 | - |
| $CH_3XB_{11}H_{11}^-$ | **C** | **Si** | **Ge** | **Sn** | **Pb** |
| **BE (eV)** | -11.31 | -11.63 | -11.69 | -11.93 | -12.01 |
| **V (kcal/mol)** | -98.65 | -100.74 | -101.25 | -102.76 | -102.98 |

**Table S6. Orbital composition analysis of the HOMO of the investigated anions.**

| $XB_{11}H_{11}^{2-}$ | **C** | **Si** | **Ge** | **Sn** | **Pb** |
|---|---|---|---|---|---|
| **Contribution from X** | 75.04% | 74.58% | 67.79% | 17.35% | 19.37% |
| **Contribution from cage** | 24.96% | 25.42% | 32.21% | 82.65 | 80.63% |
| **ODI** | 56.74 | 56.06 | 46.70 | 13.43 | 13.84 |
| $XCB_{10}H_{11}^-$ | | | | | |
| **Contribution from X** | 73.09% | 68.07% | 57.22% | 14.81% | 16.75% |
| **Contribution from cage** | 26.91% | 31.93% | 42.78% | 85.19% | 83.25% |
| **ODI** | 53.92 | 47.34 | 35.02 | 12.71 | 13.02 |
| $CH_3XB_{11}H_{11}^-$ | | | | | |
| **Contribution from X** | 0 | 13.71% | 15.07% | 19.99% | 22.36% |
| **Contribution from cage** | 100% | 86.29% | 84.93% | 80.01% | 77.64% |
| **ODI** | 11.86 | 11.96 | 12.40 | 12.57 | 13.27 |

# Cartesian coordinated of the optimized anions

$XB_{11}H_{11}^{2-}$
C

| | | | |
|---|---|---|---|
| C | 0.00187000 | 0.00125300 | -1.62820200 |
| B | -0.00197400 | -0.00129000 | 1.67566400 |
| B | 1.26139500 | 0.82347700 | 0.74325700 |
| B | -0.53760900 | -1.40926300 | 0.73940100 |
| B | -0.39467000 | 1.45463800 | 0.74181000 |
| B | 0.52723900 | 1.38162000 | -0.77871900 |
| B | -1.50653700 | 0.07456500 | 0.73956800 |
| B | -1.23666000 | -0.80738400 | -0.78221200 |
| B | 1.47706600 | -0.07303100 | -0.77864500 |
| B | 1.17296100 | -0.94640100 | 0.74170900 |
| B | -1.14994500 | 0.92794900 | -0.78089100 |
| H | 2.16639400 | 1.41437000 | 1.26232100 |

| | | | |
|---|---|---|---|
| H | -0.92323200 | -2.42040400 | 1.25561300 |
| H | -0.67778800 | 2.49828300 | 1.25972500 |
| H | 0.90187800 | 2.36339800 | -1.35704700 |
| H | -2.58738100 | 0.12800400 | 1.25582300 |
| H | -2.11525500 | -1.38109300 | -1.36327700 |
| H | 2.52655800 | -0.12483000 | -1.35707300 |
| H | 2.01458600 | -1.62544800 | 1.25952100 |
| H | -1.96695700 | 1.58718100 | -1.36105400 |
| H | -0.00336900 | -0.00230600 | 2.87518200 |
| B | 0.38700100 | -1.42599100 | -0.78084000 |
| H | 0.66201500 | -2.43911800 | -1.36103400 |

**Si**

| | | | |
|---|---|---|---|
| B | 1.92216700 | -0.00011400 | 0.00002600 |
| B | 0.98781300 | -1.50681800 | 0.06851700 |
| B | 0.98791500 | 1.25919000 | 0.83023100 |
| B | 0.98783800 | -0.53082600 | -1.41180000 |
| B | -0.50994500 | -1.28546100 | -0.84752900 |
| B | 0.98802600 | 1.17868400 | -0.94102400 |
| B | -0.50970800 | 1.53818100 | -0.07000900 |
| B | -0.51001600 | -1.20340800 | 0.96067400 |
| B | 0.98786600 | -0.40045900 | 1.45415800 |
| B | -0.50975300 | 0.40887000 | -1.48442900 |
| H | 1.52677400 | -2.57581300 | 0.11715900 |
| H | 1.52697500 | 2.15259700 | 1.41919300 |
| H | 1.52680100 | -0.90752100 | -2.41342400 |
| H | -0.97453100 | -2.20866700 | -1.45625700 |
| H | 1.52709100 | 2.01488900 | -1.60872000 |
| H | -0.97416700 | 2.64291200 | -0.12028200 |
| H | -0.97454100 | -2.06755800 | 1.65072000 |
| H | 1.52689900 | -0.68451200 | 2.48584200 |
| H | -0.97426700 | 0.70236600 | -2.55062300 |
| H | 3.12024300 | -0.00018500 | 0.00002600 |
| B | -0.50987800 | 0.54190900 | 1.44128500 |
| H | -0.97430900 | 0.93120200 | 2.47638700 |
| Si | -1.96032800 | 0.00011100 | -0.00003700 |

**Ge**

| | | | |
|---|---|---|---|
| B | 0.11544800 | -1.23987600 | -0.93523300 |
| H | 0.56181500 | -2.12848500 | -1.60562600 |
| B | 0.11562100 | -1.27246700 | 0.89043900 |
| H | 0.56228500 | -2.18431700 | 1.52865200 |
| B | 0.11521500 | 0.45384800 | 1.48527400 |
| H | 0.56046100 | 0.77933200 | 2.55021600 |
| B | 0.11516300 | 1.55315800 | 0.02776400 |
| H | 0.56051400 | 2.66648100 | 0.04794900 |
| B | -1.37797500 | 1.23655400 | -0.86500500 |
| H | -1.92218700 | 2.11107300 | -1.47729300 |

| | | | |
|---|---|---|---|
| B | -1.37762200 | -0.44078300 | -1.44355700 |
| H | -1.92126400 | -0.75213400 | -2.46498900 |
| B | -1.37750800 | -1.50946800 | -0.02693400 |
| H | -1.92066900 | -2.57736700 | -0.04635600 |
| B | -1.37766200 | -0.49210500 | 1.42694700 |
| H | -1.92123700 | -0.83987800 | 2.43660700 |
| B | -1.37814700 | 1.20471100 | 0.90858200 |
| H | -1.92243700 | 2.05683200 | 1.55159600 |
| B | -2.30885700 | -0.00063500 | -0.00005000 |
| H | -3.50710000 | 0.00004400 | -0.00016100 |
| B | 0.11547100 | 0.50657900 | -1.46832800 |
| H | 0.56094600 | 0.86930400 | -2.52103400 |
| Ge | 1.66916000 | 0.00004800 | 0.00002900 |

**Sn**

| | | | |
|---|---|---|---|
| B | 0.24568000 | -1.56844600 | -0.02846700 |
| H | -0.16832800 | -2.69519600 | -0.04885500 |
| B | 0.24561700 | -0.45758000 | -1.50046700 |
| H | -0.16864900 | -0.78605300 | -2.57834800 |
| B | 0.24550200 | 1.28570600 | -0.89865000 |
| H | -0.16810600 | 2.20928900 | -1.54460300 |
| B | 0.24556200 | 1.25236500 | 0.94499300 |
| H | -0.16837500 | 2.15193600 | 1.62375000 |
| B | 1.73234200 | 0.44071700 | 1.44509000 |
| H | 2.28303400 | 0.75085200 | 2.46320700 |
| B | 1.73223300 | -1.23828300 | 0.86567400 |
| H | 2.28273800 | -2.11054700 | 1.47569500 |
| B | 1.73231600 | -1.20614900 | -0.91025600 |
| H | 2.28281200 | -2.05578200 | -1.55140600 |
| B | 1.73220100 | 0.49305500 | -1.42817700 |
| H | 2.28265400 | 0.84073000 | -2.43423900 |
| B | 1.73221000 | 1.51073700 | 0.02762600 |
| H | 2.28279600 | 2.57491300 | 0.04684800 |
| B | 2.66046000 | -0.00011500 | -0.00017200 |
| H | 3.85839800 | 0.00003700 | -0.00006000 |
| Sn | -1.54358600 | -0.00002000 | 0.00000000 |
| B | 0.24552700 | -0.51185300 | 1.48278600 |
| H | -0.16792900 | -0.87996500 | 2.54808600 |

**Pb**

| | | | |
|---|---|---|---|
| H | -2.67158800 | 1.17110900 | -2.29364200 |
| H | -2.67194000 | -1.81949600 | -1.82248800 |
| H | -2.67159400 | -2.29558500 | 1.16755400 |
| H | -2.67189100 | 0.40098400 | 2.54383200 |
| B | -2.11787200 | 0.68750300 | -1.34642200 |
| B | -2.11819400 | 1.49288500 | 0.23748300 |
| B | -2.11807300 | 0.23529800 | 1.49335000 |
| B | -2.11792200 | -1.34765600 | 0.68534500 |
| B | -2.11808100 | -1.06814800 | -1.06991700 |
| H | -2.67204100 | 2.54312600 | 0.40450800 |

| | | | |
|---|---|---|---|
| H | -0.22629000 | 2.40897700 | -1.22491000 |
| H | -0.22639600 | -0.42063000 | -2.66973700 |
| H | -0.22631300 | -2.66918200 | -0.42505200 |
| H | -0.22614600 | -1.22851100 | 2.40739200 |
| B | -0.63355300 | 1.11085100 | 1.11226300 |
| B | -0.63329400 | 1.40127300 | -0.71229400 |
| B | -0.63329800 | -0.24471400 | -1.55286500 |
| B | -0.63329000 | -1.55261300 | -0.24727500 |
| B | -0.63324100 | -0.71472700 | 1.40027900 |
| H | -0.22672500 | 1.90996400 | 1.91219600 |
| B | -3.04526200 | -0.00015100 | 0.00000800 |
| H | -4.24368500 | -0.00022500 | 0.00002300 |
| Pb | 1.25298800 | 0.00000600 | 0.00000700 |

$XCB_{10}H_{11}^{-}$

C

| | | | |
|---|---|---|---|
| C | 0.00000100 | -0.19794600 | -1.61777200 |
| B | -0.00000100 | 0.17490900 | 1.67524300 |
| B | -1.43632000 | -0.38787200 | 0.78958600 |
| B | 0.88288400 | 1.27309000 | 0.61485800 |
| B | -0.00000700 | -1.42026700 | 0.91482500 |
| B | -0.86796800 | -1.28710300 | -0.62731500 |
| B | 1.43631500 | -0.38788300 | 0.78959000 |
| B | 1.40496700 | 0.35565800 | -0.83077500 |
| B | -1.40496300 | 0.35567200 | -0.83077700 |
| B | -0.88287500 | 1.27309800 | 0.61485700 |
| B | 0.86795800 | -1.28711100 | -0.62731000 |
| H | -2.46694000 | -0.63862700 | 1.32420300 |
| H | 1.47133500 | 2.25977800 | 0.90760700 |
| H | -0.00001600 | -2.42478300 | 1.55014900 |
| H | -1.48544700 | -2.15882400 | -1.14430300 |
| H | 2.46693300 | -0.63864300 | 1.32420900 |
| H | 2.34476000 | 0.72074000 | -1.45454800 |
| H | -2.34474700 | 0.72076500 | -1.45455600 |
| H | -1.47131500 | 2.25979300 | 0.90760600 |
| H | 1.48542800 | -2.15883800 | -1.14430100 |
| H | 0.00000000 | 0.33369000 | 2.85309400 |
| H | 0.00001000 | 2.11804100 | -1.45755300 |
| C | 0.00000600 | 1.24727000 | -0.81981400 |

**Si**

| | | | |
|---|---|---|---|
| B | 1.92827000 | -0.08253400 | -0.00000100 |
| B | 1.04605900 | 1.16799800 | 0.88250200 |
| B | 0.97353900 | -0.50696500 | -1.43541800 |
| B | 0.97353900 | -0.50698800 | 1.43541100 |
| B | -0.48449500 | 0.48596800 | 1.43346700 |
| B | 0.93527100 | -1.54750000 | -0.00001200 |
| B | -0.55231600 | -1.22520800 | -0.90126700 |
| B | 1.04605900 | 1.16801200 | -0.88248400 |
| B | -0.55231600 | -1.22522200 | 0.90124800 |

| | | | |
|---|---|---|---|
| H | 1.51367800 | 2.08568100 | 1.47021200 |
| H | 1.48164900 | -0.82918000 | -2.45976500 |
| H | 1.48165000 | -0.82921700 | 2.45975300 |
| H | -0.96108700 | 0.97169100 | 2.40745100 |
| H | 1.42572100 | -2.63037800 | -0.00002200 |
| H | -1.07373100 | -2.07059500 | -1.55791900 |
| H | -0.74986500 | 2.41525300 | 0.00001900 |
| H | 1.51367800 | 2.08570500 | -1.47017900 |
| H | -1.07373200 | -2.07061900 | 1.55788600 |
| H | 3.11621600 | -0.10146800 | -0.00000100 |
| B | -0.48449500 | 0.48599100 | -1.43345900 |
| H | -0.96108900 | 0.97172700 | -2.40743600 |
| Si | -1.97102000 | 0.03806400 | 0.00000000 |
| C | -0.37739800 | 1.40012500 | 0.00001100 |

**Ge**

| | | | |
|---|---|---|---|
| C | 0.03115900 | -1.41566800 | 0.00024700 |
| H | -0.33261900 | -2.43382900 | 0.00046100 |
| B | -0.08979400 | -0.49403000 | -1.43443500 |
| H | -0.54634800 | -0.98292300 | -2.41669300 |
| B | -0.15803200 | 1.23810600 | -0.90923900 |
| H | -0.65816400 | 2.08944500 | -1.57522200 |
| B | -0.15793700 | 1.23848700 | 0.90882500 |
| H | -0.65798200 | 2.09013800 | 1.57447200 |
| B | -0.08973100 | -0.49350600 | 1.43459200 |
| H | -0.54622700 | -0.98201300 | 2.41707000 |
| B | 1.44484200 | -1.16768900 | 0.88191700 |
| H | 1.92048800 | -2.07742200 | 1.47605500 |
| B | 1.44471900 | -1.16804500 | -0.88151400 |
| H | 1.92042900 | -2.07796000 | -1.47532500 |
| B | 1.36200100 | 0.50702800 | -1.43589900 |
| H | 1.87211000 | 0.83041000 | -2.45910500 |
| B | 1.32451300 | 1.55082700 | -0.00030000 |
| H | 1.81865200 | 2.63223100 | -0.00063800 |
| B | 1.36211400 | 0.50755300 | 1.43569000 |
| H | 1.87223400 | 0.83118700 | 2.45880600 |
| B | 2.31915400 | 0.08917700 | -0.00007700 |
| H | 3.50699100 | 0.11536300 | -0.00009700 |
| Ge | -1.69268000 | -0.01813000 | 0.00002900 |

**Sn**

| | | | |
|---|---|---|---|
| C | -0.41388600 | -1.42905600 | 0.00238300 |
| H | -0.08487200 | -2.46019600 | 0.00430200 |
| B | -0.28250300 | -0.50270800 | 1.43295500 |
| H | 0.15238400 | -1.00400000 | 2.42183400 |
| B | -0.19787500 | 1.24038800 | 0.91604400 |
| H | 0.27664200 | 2.10363400 | 1.58980200 |
| B | -0.19726300 | 1.23737900 | -0.91971400 |

| | | | |
|---|---|---|---|
| H | 0.27681000 | 2.09872300 | -1.59618400 |
| B | -0.28185900 | -0.50759400 | -1.43081700 |
| H | 0.15351300 | -1.01171100 | -2.41806400 |
| B | -1.82252700 | -1.16400400 | -0.88087400 |
| H | -2.31802800 | -2.06539200 | -1.47244000 |
| B | -1.82268900 | -1.16114500 | 0.88401700 |
| H | -2.31834800 | -2.06064700 | 1.47834600 |
| B | -1.71994400 | 0.51506400 | 1.43652200 |
| H | -2.23228300 | 0.84498500 | 2.45696600 |
| B | -1.67029700 | 1.55838000 | -0.00272700 |
| H | -2.15696300 | 2.64356900 | -0.00494000 |
| B | -1.71917800 | 0.51026500 | -1.43824700 |
| H | -2.23085500 | 0.83720000 | -2.46000600 |
| B | -2.68089800 | 0.10685400 | -0.00045600 |
| H | -3.86818900 | 0.14909600 | -0.00084700 |
| Sn | 1.57617300 | -0.01330600 | 0.00006800 |

**Pb**

| | | | |
|---|---|---|---|
| C | -0.83278700 | -1.43776500 | 0.00230400 |
| H | -0.51550300 | -2.47285000 | 0.00416100 |
| B | -0.68352000 | -0.51343600 | 1.42608000 |
| H | -0.25778900 | -1.01940600 | 2.41805500 |
| B | -0.58306500 | 1.23607500 | 0.91827400 |
| H | -0.11212700 | 2.09924600 | 1.59647900 |
| B | -0.58272300 | 1.23314200 | -0.92196800 |
| H | -0.11239500 | 2.09449700 | -1.60287100 |
| B | -0.68311600 | -0.51823900 | -1.42400100 |
| H | -0.25684200 | -1.02692500 | -2.41436800 |
| B | -2.23520000 | -1.15700300 | -0.88087200 |
| H | -2.74500300 | -2.04957700 | -1.47479300 |
| B | -2.23519100 | -1.15417500 | 0.88400200 |
| H | -2.74505300 | -2.04485900 | 1.48074600 |
| B | -2.10967400 | 0.52067800 | 1.43729700 |
| H | -2.61946200 | 0.85789300 | 2.45726200 |
| B | -2.05037700 | 1.56597400 | -0.00262100 |
| H | -2.52865000 | 2.65553000 | -0.00469200 |
| B | -2.10916600 | 0.51594000 | -1.43890000 |
| H | -2.61835700 | 0.85027800 | -2.46013000 |
| B | -3.07632700 | 0.12623300 | -0.00035400 |
| H | -4.26327700 | 0.18578400 | -0.00063900 |
| Pb | 1.28674400 | -0.00950000 | 0.00002800 |

**$CH_3{}^{XCB_{11}H_{11}{}^-}$**

C

| | | | |
|---|---|---|---|
| C | 1.21155400 | -0.00035900 | 0.00001600 |
| B | -2.01975700 | 0.00026800 | -0.00002500 |
| B | -1.09114300 | -1.50933900 | 0.02560900 |
| B | -1.09038200 | 1.20600700 | -0.90825400 |
| B | -1.09040400 | -0.44164700 | 1.44343200 |

| | | | |
|---|---|---|---|
| B | 0.40711500 | -1.19872100 | 0.90102400 |
| B | -1.09046800 | 1.23624100 | 0.86668800 |
| B | 0.40529800 | 1.49979400 | -0.02548000 |
| B | 0.40697700 | -1.22867500 | -0.86001300 |
| B | -1.09023700 | -0.49042800 | -1.42748200 |
| B | 0.41040300 | 0.48756100 | 1.41672500 |
| H | -1.59366500 | -2.58578200 | 0.04400700 |
| H | -1.59210800 | 2.06575000 | -1.55683200 |
| H | -1.59160700 | -0.75641700 | 2.47361700 |
| H | 1.06973300 | -1.98435100 | 1.49456100 |
| H | -1.59227500 | 2.11757400 | 1.48554300 |
| H | 1.06836300 | 2.48384000 | -0.04230900 |
| H | 1.06952600 | -2.03412900 | -1.42640600 |
| H | -1.59153600 | -0.83989100 | -2.44638200 |
| H | 1.07369900 | 0.80650600 | 2.34808900 |
| H | -3.20837100 | 0.00041400 | -0.00009500 |
| B | 0.41061800 | 0.43912200 | -1.43242100 |
| H | 1.07395100 | 0.72647000 | -2.37400100 |
| C | 2.72952200 | 0.00002400 | 0.00011400 |
| H | 3.10950400 | -0.48554800 | 0.89883200 |
| H | 3.10962100 | -0.53481500 | -0.87012900 |
| H | 3.10860500 | 1.02147700 | -0.02828300 |

Si

| | | | |
|---|---|---|---|
| B | 2.24981300 | 0.00005400 | -0.00008200 |
| B | 1.33082800 | 1.05125200 | -1.08815500 |
| B | 1.33109700 | -1.49019400 | 0.26224700 |
| B | 1.33089600 | 1.35984800 | 0.66353000 |
| B | -0.15201600 | 1.55454900 | -0.27365800 |
| B | 1.33089800 | -0.21092200 | 1.49800500 |
| B | -0.15243600 | -1.09683700 | 1.13493300 |
| B | -0.15314100 | 0.22010400 | -1.56261200 |
| B | 1.33074900 | -0.70999200 | -1.33594300 |
| B | -0.15291500 | 0.74071100 | 1.39356100 |
| H | 1.86049400 | 1.79021000 | -1.85390600 |
| H | 1.86121600 | -2.53797900 | 0.44686400 |
| H | 1.86082800 | 2.31581300 | 1.13074600 |
| H | -0.66635300 | 2.61223500 | -0.46005800 |
| H | 1.86028800 | -0.35906200 | 2.55193200 |
| H | -0.66498200 | -1.84300500 | 1.90848500 |
| H | -0.66381000 | 0.36965400 | -2.62778200 |
| H | 1.86013700 | -1.20893500 | -2.27603000 |
| H | -0.66403600 | 1.24468900 | 2.34356400 |
| H | 3.43812300 | 0.00010400 | -0.00014800 |
| B | -0.15233300 | -1.41858500 | -0.69190800 |
| H | -0.66581200 | -2.38377000 | -1.16380500 |
| Si | -1.40240700 | 0.00004100 | 0.00008000 |
| C | -3.26412800 | -0.00003600 | -0.00005000 |
| H | -3.63481600 | -0.71525900 | -0.73335300 |

| | | | |
|---|---|---|---|
| H | -3.63504600 | -0.27758300 | 0.98589100 |
| H | -3.63496100 | 0.99259500 | -0.25280300 |

Ge

| | | | |
|---|---|---|---|
| B | -0.13024200 | -1.45573300 | -0.66441900 |
| B | -0.12900800 | -1.08130600 | 1.17890000 |
| B | -0.12977700 | 0.78741800 | 1.39266100 |
| B | -0.13009800 | 1.56821100 | -0.31825000 |
| B | -0.13051000 | 0.18171000 | -1.59002700 |
| B | -1.60424000 | -1.48297200 | 0.30147600 |
| B | -1.60387800 | -0.17204300 | 1.50382600 |
| B | -1.60448800 | 1.37655300 | 0.62880600 |
| B | -1.60498000 | 1.02246500 | -1.11459400 |
| B | -1.60498800 | -0.74487000 | -1.31690200 |
| B | -2.52245200 | -0.00019500 | 0.00082300 |
| C | 3.16605500 | -0.00035300 | 0.00105100 |
| H | -3.71081600 | -0.00038600 | 0.00125300 |
| H | -2.14210400 | 2.34131600 | 1.06866200 |
| H | -2.14258300 | 1.73935600 | -1.89582600 |
| H | -2.14310000 | -1.26632800 | -2.23982300 |
| H | -2.14130800 | -2.52224500 | 0.51300500 |
| H | -2.14082300 | -0.29314200 | 2.55754700 |
| H | 0.35723200 | 2.63185700 | -0.53498600 |
| H | 0.35672200 | 0.30586000 | -2.66847500 |
| H | 0.35938500 | -2.44257700 | -1.11442200 |
| H | 0.35816800 | -1.81526400 | 1.97871800 |
| H | 0.36056600 | 1.32078700 | 2.33669700 |
| H | 3.52892800 | 0.35041900 | 0.96481800 |
| H | 3.53042400 | -1.01009900 | -0.17574900 |
| H | 3.53218700 | 0.65813100 | -0.78372200 |
| Ge | 1.21919100 | 0.00025800 | -0.00079700 |

Sn

| | | | |
|---|---|---|---|
| Sn | -1.15943300 | 0.00172100 | 0.00069300 |
| B | 0.43452800 | -0.94577000 | 1.31699500 |
| B | 0.43317900 | -1.54448200 | -0.49246700 |
| B | 0.43445500 | -0.00914200 | -1.62112800 |
| B | 0.43588800 | 1.53948200 | -0.51012100 |
| B | 0.43604300 | 0.96076100 | 1.30662200 |
| B | 1.89928000 | -1.43841600 | 0.47542300 |
| B | 1.89928200 | -0.89795300 | -1.22013000 |
| B | 1.90069300 | 0.88166000 | -1.23035700 |
| B | 1.90156100 | 1.44118100 | 0.45919500 |
| B | 1.90079600 | 0.00711100 | 1.51355600 |
| B | 2.81557300 | -0.00192500 | -0.00065400 |
| C | -3.28979200 | -0.00405600 | -0.00157500 |

| | | | |
|---|---|---|---|
| H | 4.00421000 | -0.00256700 | -0.00089900 |
| H | 2.44606400 | 1.49796200 | -2.08896000 |
| H | 2.44739900 | 2.44793300 | 0.77999800 |
| H | 2.44628400 | 0.01300400 | 2.57034800 |
| H | 2.44362900 | -2.44234000 | 0.80748100 |
| H | 2.44353800 | -1.52470400 | -2.07186200 |
| H | -0.00183900 | 2.59095000 | -0.85777400 |
| H | -0.00174400 | 1.61736200 | 2.19841200 |
| H | -0.00570600 | -1.59106300 | 2.21593000 |
| H | -0.00636800 | -2.59903800 | -0.82841900 |
| H | -0.00602500 | -0.01526100 | -2.72761500 |
| H | -3.64957100 | -0.17982200 | -1.01258000 |
| H | -3.64977400 | -0.79338300 | 0.65400200 |
| H | -3.65606900 | 0.95673900 | 0.35206600 |

Pb

| | | | |
|---|---|---|---|
| B | -0.71735100 | -0.13243300 | 1.62817500 |
| B | -0.71622600 | 1.50741500 | 0.62926100 |
| B | -0.71624700 | 1.06523900 | -1.23778100 |
| B | -0.71740000 | -0.84713900 | -1.39653900 |
| B | -0.71810100 | -1.59001900 | 0.37597600 |
| B | -2.17527400 | 0.78851400 | 1.29240000 |
| B | -2.17519300 | 1.47474700 | -0.34908700 |
| B | -2.17558500 | 0.12563600 | -1.50892000 |
| B | -2.17576400 | -1.39435500 | -0.58435900 |
| B | -2.17572300 | -0.98470800 | 1.14691700 |
| B | -3.09031300 | 0.00205100 | -0.00046400 |
| C | 3.12986200 | 0.01051400 | -0.00330700 |
| H | -4.27892700 | 0.00193200 | -0.00034500 |
| H | -2.72048800 | 0.21243400 | -2.56249100 |
| H | -2.72110000 | -2.36937700 | -0.99238100 |
| H | -2.72087400 | -1.67409300 | 1.94824800 |
| H | -2.72013700 | 1.33704800 | 2.19613800 |
| H | -2.71968300 | 2.50382600 | -0.59192400 |
| H | -0.28373900 | -1.42417600 | -2.34191100 |
| H | -0.28573800 | -2.66827500 | 0.63052400 |
| H | -0.28340200 | -0.22298800 | 2.73192300 |
| H | -0.28195000 | 2.52916600 | 1.05607100 |
| H | -0.28167300 | 1.78736100 | -2.07721100 |
| H | 3.46438500 | 0.97647800 | -0.36853800 |
| H | 3.47414700 | -0.15338800 | 1.01305400 |
| H | 3.47518300 | -0.78492200 | -0.65630100 |
| Pb | 0.94964300 | -0.00230300 | 0.00069600 |

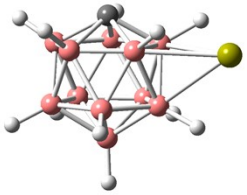
## Cartesian coordinates of the optimized ion pairs of the considered ions

$XB_{11}H_{11}{}^{2-}$

C

S1

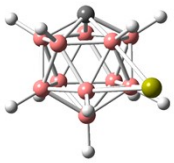
| | | | |
|---|---|---|---|
| C | -0.45964500 | 0.00020600 | -1.54753300 |
| B | -1.08618100 | -0.00019700 | 1.64338200 |
| B | 0.53281300 | -0.00024700 | 1.01521000 |
| B | -2.10490900 | -0.88922200 | 0.50131100 |
| B | -0.45714700 | 1.45791300 | 0.82278600 |
| B | 0.50159200 | 0.86725100 | -0.54903200 |
| B | -2.10477700 | 0.88925900 | 0.50157900 |
| B | -2.07930900 | 0.00022900 | -1.04327300 |
| B | 0.50155100 | -0.86730300 | -0.54924000 |
| B | -0.45734900 | -1.45819100 | 0.82238800 |
| B | -1.08993500 | 1.42907000 | -0.85169600 |
| H | 1.52913300 | -0.00050500 | 1.74205000 |
| H | -3.04709400 | -1.51491900 | 0.85117800 |
| H | -0.17596200 | 2.45997000 | 1.39314400 |
| H | 1.51234400 | 1.46338900 | -0.96885600 |
| H | -3.04687600 | 1.51498900 | 0.85162000 |
| H | -2.96615700 | 0.00039600 | -1.82649000 |
| H | 1.51227900 | -1.46336200 | -0.96911300 |
| H | -0.17637500 | -2.46041100 | 1.39255500 |
| H | -1.26015900 | 2.40313600 | -1.50332300 |
| H | -1.25743700 | -0.00036500 | 2.81607900 |
| B | -1.09010200 | -1.42878300 | -0.85210800 |
| H | -1.26048200 | -2.40264100 | -1.50400400 |
| Ca | 2.80317100 | 0.00001000 | -0.01480900 |



S2

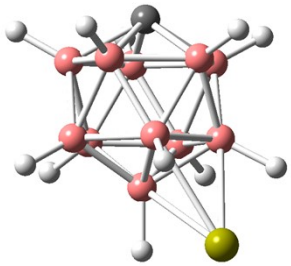
| | | | |
|---|---|---|---|
| C | 0.96572900 | -0.00067500 | -1.56736600 |
| B | 0.54197600 | 0.00075900 | 1.65894900 |
| B | 1.13045100 | 1.45005900 | 0.79796900 |
| B | 1.13213800 | -1.44869700 | 0.79963600 |
| B | -0.50769100 | 0.89000600 | 0.55638500 |
| B | 0.42931000 | 1.43752400 | -0.84412600 |
| B | -0.50689600 | -0.89121000 | 0.55732900 |
| B | 0.43129000 | -1.43884600 | -0.84247000 |
| B | 2.06008200 | 0.87641700 | -0.61130300 |
| B | 2.15180400 | 0.00139100 | 0.93506000 |
| B | -0.52657500 | -0.00152900 | -1.00873200 |
| H | 1.34873800 | 2.46500100 | 1.36872300 |

| | | | |
|---|---|---|---|
| H | 1.35224200 | -2.46270200 | 1.37135200 |
| H | -1.49414200 | 1.51553800 | 0.94530900 |
| H | 0.13912900 | 2.40045200 | -1.47514100 |
| H | -1.49360000 | -1.51671600 | 0.94555100 |
| H | 0.14219800 | -2.40273600 | -1.47249100 |
| H | 2.96264000 | 1.47329700 | -1.09000400 |
| H | 3.13303400 | 0.00231300 | 1.59718500 |
| H | -1.54760700 | -0.00291600 | -1.73360700 |
| H | 0.32803700 | 0.00148900 | 2.82520200 |
| B | 2.06121200 | -0.87544000 | -0.61024800 |
| H | 2.96434300 | -1.47183900 | -1.08845800 |
| Ca | -2.78074500 | 0.00003500 | 0.01341700 |



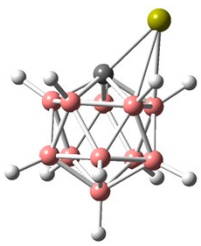
S3

| | | | |
|---|---|---|---|
| C | -2.01676000 | 0.00077800 | -1.00390300 |
| B | 0.50736000 | -0.00089000 | 1.03397200 |
| B | -0.48005100 | -1.45249600 | 0.82528100 |
| B | -0.47872900 | 1.45190800 | 0.82617000 |
| B | 0.52845500 | -0.89308100 | -0.51383200 |
| B | -1.10716200 | -1.41666800 | -0.85659100 |
| B | 0.52889500 | 0.89215300 | -0.51337000 |
| B | -1.10614300 | 1.41740400 | -0.85581500 |
| B | -2.11690300 | -0.87107400 | 0.45144200 |
| B | -1.12267300 | -0.00028500 | 1.64465200 |
| B | -0.48533900 | 0.00036000 | -1.67849200 |
| H | -0.22453300 | -2.45858100 | 1.39983800 |
| H | -0.22270700 | 2.45757000 | 1.40123700 |
| H | 1.51445600 | -1.53136400 | -0.87902400 |
| H | -1.32244600 | -2.40784700 | -1.46982900 |
| H | 1.51470700 | 1.53047600 | -0.87906200 |
| H | -1.32032400 | 2.40917200 | -1.46849800 |
| H | -3.08492600 | -1.48254800 | 0.75320800 |
| H | -1.33258400 | -0.00058100 | 2.81057500 |
| H | -0.23858900 | 0.00061500 | -2.83995900 |
| H | 1.48626700 | -0.00177300 | 1.78071000 |
| B | -2.11611700 | 0.87190700 | 0.45198400 |
| H | -3.08372200 | 1.48395800 | 0.75392400 |
| Ca | 2.78285000 | 0.00000200 | 0.02916500 |



S4

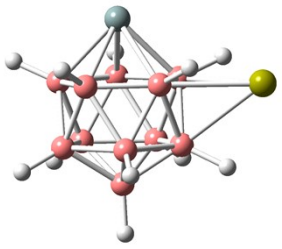
| | | | |
|---|---|---|---|
| C | -0.64605100 | 0.00064700 | -0.73090700 |
| B | 2.23886800 | -0.00060000 | 0.76359300 |
| B | 1.20839400 | 1.44396800 | 0.76463500 |
| B | 1.95824000 | -0.88823100 | -0.74975900 |
| B | 0.74438200 | -0.00064600 | 1.70874600 |
| B | -0.43505700 | 0.86920700 | 0.73088400 |
| B | 1.20783200 | -1.44475500 | 0.76353500 |
| B | 0.28085600 | -1.42932200 | -0.76302900 |
| B | 0.28148600 | 1.43011000 | -0.76195700 |
| B | 1.95860900 | 0.88827500 | -0.74908000 |
| B | -0.43528700 | -0.86922300 | 0.73025000 |
| H | 1.48810800 | 2.46682200 | 1.29226600 |
| H | 2.80327100 | -1.51545600 | -1.29212300 |
| H | 0.68043200 | -0.00108700 | 2.89238100 |
| H | -1.43254700 | 1.43436600 | 1.16282500 |
| H | 1.48703900 | -2.46814000 | 1.29040100 |
| H | -0.15970000 | -2.39279900 | -1.29814700 |
| H | -0.15861600 | 2.39418200 | -1.29635600 |
| H | 2.80390300 | 1.51557300 | -1.29094900 |
| H | -1.43286000 | -1.43455000 | 1.16180200 |
| H | 3.29644800 | -0.00100700 | 1.29651800 |
| B | 0.73944800 | 0.00061800 | -1.68688500 |
| H | 0.63411400 | 0.00108400 | -2.86588500 |
| Ca | -2.74360700 | 0.00000600 | -0.02109700 |



**Si**

S1

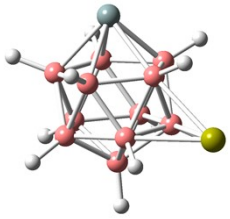
| | | | |
|---|---|---|---|
| B | -0.99941500 | -1.89771200 | 0.00000400 |
| B | -2.04898300 | -0.77758100 | 0.88866700 |
| B | 0.60234200 | -1.20684100 | 0.00022800 |
| B | -2.04878600 | -0.77763600 | -0.88896400 |
| B | -2.12346300 | 0.74957500 | -0.00019100 |
| B | -0.39576300 | -1.05176800 | -1.45007900 |
| B | 0.56384100 | 0.33089000 | -0.90990600 |
| B | -1.08562100 | 0.58983500 | 1.46901300 |
| B | -0.39616600 | -1.05166500 | 1.45019100 |
| B | -1.08530300 | 0.58975200 | -1.46916300 |
| H | -2.97459700 | -1.16602800 | 1.51693800 |
| H | 1.61651000 | -1.90351500 | 0.00041500 |
| H | -2.97428500 | -1.16611000 | -1.51738600 |
| H | -3.11935900 | 1.39494800 | -0.00029700 |
| H | -0.09890300 | -1.61995300 | -2.44861700 |
| H | 1.54890400 | 0.63873200 | -1.58479500 |
| H | -1.30433600 | 1.10807800 | 2.51407000 |
| H | -0.09944200 | -1.61974200 | 2.44883300 |
| H | -1.30367700 | 1.10793000 | -2.51432400 |
| H | -1.14192700 | -3.07405100 | 0.00000900 |
| B | 0.56374400 | 0.33088200 | 0.91024900 |
| H | 1.54886900 | 0.63857900 | 1.58509500 |
| Si | -0.42564000 | 1.99527500 | 0.00000900 |
| Ca | 2.82645400 | -0.07056800 | -0.00001500 |



S2

| | | | |
|---|---|---|---|
| B | 0.09408700 | 1.88492700 | 0.00008500 |
| B | 1.81321000 | 1.47543700 | -0.00093900 |
| B | -0.71924300 | 0.59269800 | 0.89413600 |
| B | 0.83606400 | 1.14253500 | -1.44495000 |
| B | 2.04257100 | -0.02918800 | -0.90469900 |
| B | -0.71993400 | 0.59239600 | -0.89221900 |
| B | -0.51858300 | -0.94087300 | 0.00110600 |
| B | 2.04369400 | -0.02880900 | 0.90310100 |
| B | 0.83771400 | 1.14315200 | 1.44442100 |

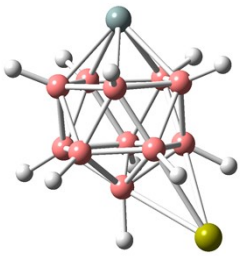
| | | | |
|---|---|---|---|
| B | 0.43881500 | -0.59698900 | -1.47633900 |
| H | 2.63679800 | 2.32648800 | -0.00165400 |
| H | -1.74572600 | 0.82479400 | 1.53360700 |
| H | 0.92567300 | 1.75177700 | -2.45764100 |
| H | 3.02603500 | -0.18911000 | -1.54954400 |
| H | -1.74625200 | 0.82586700 | -1.53153400 |
| H | -1.44224800 | -1.76227400 | 0.00280600 |
| H | 3.02790200 | -0.18852900 | 1.54685300 |
| H | 0.92925000 | 1.75270700 | 2.45674800 |
| H | 0.21264500 | -1.14618700 | -2.50611700 |
| H | -0.34319100 | 2.98820400 | -0.00010400 |
| B | 0.44079800 | -0.59629300 | 1.47676800 |
| H | 0.21570400 | -1.14535300 | 2.50685800 |
| Si | 1.39172500 | -1.83028600 | -0.00009800 |
| Ca | -2.90633500 | -0.18046800 | -0.00006300 |



S3

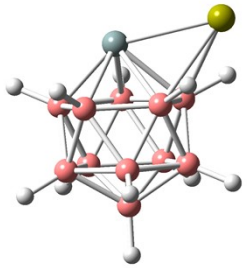
| | | | |
|---|---|---|---|
| B | -0.87165100 | 1.05685800 | -0.00001100 |
| B | 0.13388700 | 0.97803500 | 1.45300400 |
| B | -0.69277900 | -0.48115900 | -0.89515200 |
| B | 0.66591900 | 1.87301700 | 0.00033100 |
| B | 1.80348100 | 0.86200100 | 0.90175600 |
| B | 0.13421800 | 0.97853300 | -1.45276500 |
| B | 0.93917300 | -0.61213400 | -1.46596500 |
| B | 0.93892100 | -0.61263400 | 1.46576800 |
| B | -0.69286400 | -0.48148200 | 0.89462100 |
| B | 1.80366300 | 0.86231800 | -0.90123900 |
| H | -0.21037000 | 1.52104500 | 2.45061000 |
| H | -1.63431400 | -0.95326700 | -1.53297400 |
| H | 0.70556800 | 3.05753400 | 0.00052000 |
| H | 2.64960400 | 1.38326500 | 1.55060100 |
| H | -0.20988900 | 1.52193400 | -2.45021000 |
| H | 1.11688900 | -1.14770900 | -2.51102800 |
| H | 1.11629500 | -1.14863200 | 2.51067400 |
| H | -1.63428100 | -0.95404400 | 1.53229500 |
| H | 2.64987300 | 1.38383300 | -1.54976800 |
| H | -1.93857400 | 1.67163800 | -0.00013000 |
| B | 0.40084800 | -1.53723100 | -0.00033700 |
| H | 0.17971000 | -2.70619100 | -0.00051700 |

| | | | |
|---|---|---|---|
| Si | 2.44959600 | -0.95455200 | -0.00002000 |
| Ca | -2.99494600 | -0.23481400 | 0.00000700 |



S4

| | | | |
|---|---|---|---|
| B | -2.11438000 | -1.22709100 | -0.00000700 |
| B | -2.22956400 | 0.30336900 | -0.89096400 |
| B | -1.11469000 | -0.96171700 | 1.43944200 |
| B | -1.11480700 | -0.96155300 | -1.43950800 |
| B | -0.63301200 | 0.75226700 | -1.48929600 |
| B | -0.42367400 | -1.74717600 | -0.00011200 |
| B | 0.48642400 | -0.52704600 | 0.90465700 |
| B | -1.35627500 | 1.55617100 | 0.00011700 |
| B | -2.22949700 | 0.30326500 | 0.89112600 |
| B | 0.48638800 | -0.52696800 | -0.90488000 |
| H | -3.19084800 | 0.59697000 | -1.51672900 |
| H | -1.25067100 | -1.55695800 | 2.45513100 |
| H | -1.25092300 | -1.55666200 | -2.45525800 |
| H | -0.46730700 | 1.30805400 | -2.52466200 |
| H | -0.06398200 | -2.87949900 | -0.00017400 |
| H | 1.45475800 | -0.89755700 | 1.56695000 |
| H | -1.70979700 | 2.68837000 | 0.00018700 |
| H | -3.19074200 | 0.59680000 | 1.51698300 |
| H | 1.45474900 | -0.89736500 | -1.56718200 |
| H | -3.00006700 | -2.01300700 | -0.00002900 |
| B | -0.63290300 | 0.75209900 | 1.48937200 |
| H | -0.46707300 | 1.30775400 | 2.52479000 |
| Si | 0.67746500 | 1.40399400 | 0.00000900 |
| Ca | 2.82886700 | -0.24654600 | 0.00000700 |



**Ge**

S1

| | | | |
|---|---|---|---|
| B | 1.05187300 | -0.09415900 | 1.48233400 |
| H | 1.35022100 | -0.55570400 | 2.53412800 |
| B | 2.11170900 | -0.09430400 | 0.00007100 |
| H | 3.20174500 | -0.56351100 | 0.00010100 |
| B | 1.05198400 | -0.09418700 | -1.48226600 |
| H | 1.35045300 | -0.55576800 | -2.53401100 |
| B | -0.62939800 | -0.09114300 | -0.92042300 |
| H | -1.56046500 | -0.52770000 | -1.59966300 |
| B | -0.89355000 | 1.41662400 | -0.00008400 |
| H | -2.00009200 | 1.95475000 | -0.00012400 |
| B | 0.11735100 | 1.41804600 | 1.45054700 |
| H | -0.26222200 | 1.93963000 | 2.44653000 |
| B | 1.79303700 | 1.39778400 | 0.88955200 |
| H | 2.64740200 | 1.92777000 | 1.51554700 |
| B | 1.79310000 | 1.39776200 | -0.88946500 |
| H | 2.64750000 | 1.92773300 | -1.51542600 |
| B | 0.11749500 | 1.41800600 | -1.45060100 |
| H | -0.26203900 | 1.93951400 | -2.44663900 |
| B | 0.58515400 | 2.34410700 | -0.00001700 |
| H | 0.54719900 | 3.52839500 | -0.00001800 |
| B | -0.62942500 | -0.09114800 | 0.92032200 |
| H | -1.56047000 | -0.52771200 | 1.59959400 |
| Ge | 0.62330900 | -1.69651300 | 0.00000200 |
| Ca | -2.91958800 | -0.04179500 | 0.00000400 |

S2

| | | | |
|---|---|---|---|
| B | -1.68503300 | 0.76293500 | 0.91273100 |
| H | -2.66951000 | 0.89344400 | 1.56266400 |
| B | -0.28247700 | -0.22586600 | 1.48763500 |
| H | -0.20207500 | -0.80386700 | 2.52329900 |
| B | 0.55316100 | -0.81989100 | -0.00131300 |
| H | 1.22785900 | -1.85416200 | -0.00312800 |
| B | -0.28439100 | -0.22431400 | -1.48819500 |
| H | -0.20500800 | -0.80177500 | -2.52424400 |
| B | -0.20214800 | 1.55539100 | -1.44480000 |
| H | -0.12233400 | 2.17110200 | -2.45459900 |

| | | | |
|---|---|---|---|
| B | -1.05256300 | 2.13978200 | 0.00109800 |
| H | -1.60937900 | 3.18524600 | 0.00192400 |
| B | -0.20064200 | 1.55404700 | 1.44548600 |
| H | -0.11900700 | 2.16877500 | 2.45574500 |
| B | 1.14914100 | 0.60322100 | 0.89278100 |
| H | 2.20165100 | 0.56006000 | 1.53101300 |
| B | 1.14854200 | 0.60381700 | -0.89481600 |
| H | 2.20088300 | 0.55923900 | -1.53314400 |
| B | 0.71286600 | 2.06776800 | 0.00000900 |
| H | 1.43265600 | 3.01150700 | 0.00026400 |
| B | -1.68605000 | 0.76376700 | -0.91098600 |
| H | -2.67122800 | 0.89476300 | -1.55975300 |
| Ge | -1.60846000 | -1.23866500 | 0.00001800 |
| Ca | 3.05771000 | -0.71251600 | 0.00006100 |

S3

| | | | |
|---|---|---|---|
| B | -1.27028900 | 1.19768700 | 0.90977000 |
| H | -2.03312000 | 1.83076900 | 1.56240200 |
| B | -0.58765100 | -0.38521300 | 1.47810300 |
| H | -0.81443900 | -0.89182800 | 2.52816000 |
| B | -0.16344900 | -1.37772700 | -0.00046800 |
| H | -0.07349400 | -2.56406200 | -0.00037600 |
| B | -0.58783100 | -0.38440200 | -1.47843300 |
| H | -0.81525700 | -0.89001300 | -2.52883400 |
| B | 0.40004600 | 1.09616100 | -1.45366300 |
| H | 0.81419500 | 1.59481500 | -2.44811000 |
| B | -0.01755600 | 2.04977100 | 0.00054200 |
| H | 0.09472700 | 3.22985100 | 0.00068500 |
| B | 0.40034100 | 1.09533200 | 1.45412200 |
| H | 0.81472800 | 1.59305900 | 2.44893800 |
| B | 1.04110900 | -0.45601300 | 0.89544600 |
| H | 1.92042400 | -1.03693000 | 1.53326600 |
| B | 1.04108000 | -0.45560200 | -0.89623800 |
| H | 1.92058500 | -1.03577300 | -1.53439600 |
| B | 1.40663400 | 1.04913900 | 0.00010500 |
| H | 2.54061200 | 1.52792000 | -0.00015900 |
| B | -1.27055300 | 1.19821200 | -0.90896300 |
| H | -2.03334000 | 1.83172100 | -1.56121800 |
| Ge | -2.23128400 | -0.57637300 | -0.00004600 |
| Ca | 3.35530200 | -0.49411500 | -0.00002400 |

S4

| | | | |
|---|---|---|---|
| B | -1.38092900 | -1.45561600 | 0.00064000 |
| H | -1.67041500 | -2.60521100 | 0.00086200 |
| B | -0.71681800 | -0.58842700 | 1.50514500 |
| H | -0.52536800 | -1.11905800 | 2.54850800 |
| B | 0.30873400 | 0.77994200 | 0.91394000 |
| H | 1.23274700 | 1.24340300 | 1.58246800 |

| | | | |
|---|---|---|---|
| B | 0.30875800 | 0.77986000 | -0.91470800 |
| H | 1.23301600 | 1.24243500 | -1.58314100 |
| B | -1.32229400 | 1.08235100 | -1.43947800 |
| H | -1.50809400 | 1.66773800 | -2.45315000 |
| B | -2.33472500 | -0.26593500 | -0.89159100 |
| H | -3.27473900 | -0.62775700 | -1.51418700 |
| B | -2.33464500 | -0.26546400 | 0.89223100 |
| H | -3.27462600 | -0.62693400 | 1.51508100 |
| B | -1.32193100 | 1.08291800 | 1.43901400 |
| H | -1.50684900 | 1.66910900 | 2.45239900 |
| B | -0.69188500 | 1.91809600 | -0.00045000 |
| H | -0.42512500 | 3.07640600 | -0.00043700 |
| B | -2.33875900 | 1.26802900 | -0.00006900 |
| H | -3.28200500 | 1.98390400 | -0.00011700 |
| B | -0.71708500 | -0.58891700 | -1.50469900 |
| H | -0.52632500 | -1.12060200 | -2.54766100 |
| Ge | 0.72535600 | -1.22334400 | -0.00007100 |
| Ca | 2.65121600 | 0.78146900 | 0.00008900 |

Sn

S1

| | | | |
|---|---|---|---|
| B | -0.72749800 | -0.25051100 | 0.92881400 |
| H | -1.25994200 | -1.12322900 | 1.61958500 |
| B | 0.64324200 | 0.73729500 | 1.49279300 |
| H | 1.14473000 | 0.56286700 | 2.55657500 |
| B | 1.51107800 | 1.36154600 | 0.00013600 |
| H | 2.66623100 | 1.64475000 | 0.00019600 |
| B | 0.64345500 | 0.73736600 | -1.49266800 |
| H | 1.14516700 | 0.56301800 | -2.55635900 |
| B | -0.99220500 | 1.41797900 | -1.45153200 |
| H | -1.60976300 | 1.62462600 | -2.44379800 |
| B | -1.81137200 | 0.82505800 | -0.00015400 |
| H | -3.02592900 | 0.62775000 | -0.00024700 |
| B | -0.99247100 | 1.41789400 | 1.45142700 |
| H | -1.61016400 | 1.62459300 | 2.44359700 |
| B | 0.38183700 | 2.37758800 | 0.89169700 |
| H | 0.76446200 | 3.30893500 | 1.51599700 |
| B | 0.38196200 | 2.37761900 | -0.89153900 |
| H | 0.76465600 | 3.30897800 | -1.51577900 |
| B | -1.15088600 | 2.44024800 | -0.00003400 |
| H | -1.87285400 | 3.37990800 | -0.00005200 |
| Sn | 1.41448400 | -0.99611100 | 0.00000300 |
| B | -0.72746500 | -0.25048300 | -0.92900300 |
| H | -1.25996500 | -1.12320700 | -1.61970800 |
| Ca | -2.61846100 | -1.52757200 | 0.00000800 |

S2

| | | | |
|---|---|---|---|
| B | -0.00724600 | 0.00156000 | -1.49412400 |

| | | | |
|---|---|---|---|
| H | -0.05341000 | -0.56255900 | -2.54189600 |
| B | -1.11509800 | 1.32527100 | -0.91880400 |
| H | -2.01875300 | 1.73159900 | -1.57687900 |
| B | -1.11502300 | 1.32516100 | 0.91897800 |
| H | -2.01861600 | 1.73142700 | 1.57717600 |
| B | -0.00710400 | 0.00135300 | 1.49407900 |
| H | -0.05317400 | -0.56284200 | 2.54181300 |
| B | 1.58232100 | 0.43613900 | 0.89607100 |
| H | 2.59091000 | 0.13518800 | 1.53708000 |
| B | 1.58228100 | 0.43622400 | -0.89628400 |
| H | 2.59081000 | 0.13510900 | -1.53729700 |
| B | 0.52117800 | 1.70243100 | -1.44588700 |
| H | 0.76148300 | 2.27898700 | -2.45383700 |
| B | -0.15356000 | 2.48615100 | 0.00011300 |
| H | -0.41881500 | 3.64107300 | 0.00021000 |
| B | 0.52128800 | 1.70225000 | 1.44595600 |
| H | 0.76175100 | 2.27866000 | 2.45395200 |
| B | 1.53587300 | 1.96315800 | 0.00000300 |
| H | 2.47305300 | 2.69191400 | 0.00004100 |
| Sn | -1.76455200 | -0.77586300 | 0.00000000 |
| B | 0.65629500 | -0.79348800 | -0.00013100 |
| H | 1.07023400 | -1.95822900 | -0.00034800 |
| Ca | 3.12680500 | -1.28391000 | 0.00000600 |

S3

| | | | |
|---|---|---|---|
| B | -0.22286400 | -0.26094000 | 1.48675800 |
| H | -0.46178700 | -0.74354100 | 2.54795900 |
| B | 0.12591400 | -1.28885700 | 0.00024000 |
| H | 0.15110100 | -2.48070300 | 0.00027100 |
| B | -0.22277900 | -0.26133900 | -1.48661800 |
| H | -0.46146900 | -0.74437800 | -2.54767200 |
| B | -0.78500100 | 1.37914900 | -0.91532700 |
| H | -1.47565500 | 2.08722600 | -1.57570800 |
| B | 0.52539300 | 2.12527500 | -0.00024800 |
| H | 0.73402500 | 3.29274500 | -0.00035400 |
| B | 0.86872800 | 1.14118400 | 1.45555900 |
| H | 1.32592300 | 1.60776400 | 2.44736700 |
| B | 1.38866200 | -0.45657300 | 0.89831400 |
| H | 2.22543300 | -1.09739200 | 1.53787800 |
| B | 1.38867200 | -0.45679400 | -0.89792500 |
| H | 2.22534500 | -1.09793700 | -1.53731400 |
| B | 0.86886100 | 1.14077800 | -1.45575000 |
| H | 1.32614400 | 1.60697900 | -2.44769700 |
| B | 1.86842100 | 1.01632400 | -0.00002200 |
| H | 3.03417300 | 1.40858100 | 0.00006900 |
| Sn | -2.12062800 | -0.39495300 | 0.00000900 |
| B | -0.78509700 | 1.37941500 | 0.91493400 |
| H | -1.47574100 | 2.08769100 | 1.57510700 |
| Ca | 3.68946600 | -0.67337400 | 0.00000400 |

S4

| | | | |
|---|---|---|---|
| B | -0.82569900 | -0.51321500 | -1.51501100 |
| H | -0.60835700 | -1.01182000 | -2.57112800 |
| B | -1.38655200 | -1.44831400 | 0.00013700 |
| H | -1.58547100 | -2.61898700 | 0.00030700 |
| B | -0.82569300 | -0.51300400 | 1.51526600 |
| H | -0.60848900 | -1.01137200 | 2.57151400 |
| B | 0.04687700 | 0.94674300 | 0.93421100 |
| H | 0.86380500 | 1.54913400 | 1.63413700 |
| B | -1.05703200 | 1.97178100 | -0.00024700 |
| H | -0.91849500 | 3.15640600 | -0.00024000 |
| B | -1.61076900 | 1.07725700 | -1.44164000 |
| H | -1.86145200 | 1.65196500 | -2.44808500 |
| B | -2.46353500 | -0.37277200 | -0.89359000 |
| H | -3.36220600 | -0.83422800 | -1.51208800 |
| B | -2.46369400 | -0.37266900 | 0.89367500 |
| H | -3.36235700 | -0.83394200 | 1.51230000 |
| B | -1.61083200 | 1.07748200 | 1.44149000 |
| H | -1.86174900 | 1.65256700 | 2.44766000 |
| B | -2.63404800 | 1.15276200 | -0.00017600 |
| H | -3.64493000 | 1.76963800 | -0.00015700 |
| Sn | 0.90748100 | -1.15076300 | 0.00000200 |
| B | 0.04686900 | 0.94655300 | -0.93420000 |
| H | 0.86411800 | 1.54837800 | -1.63438400 |
| Ca | 2.23160400 | 1.63786900 | 0.00002400 |

Pb

S1

| | | | |
|---|---|---|---|
| H | 2.49882600 | 0.93153700 | -2.44337500 |
| H | 0.98893600 | 3.42155200 | -1.51510900 |
| H | 0.98900200 | 3.42134800 | 1.51543000 |
| H | 2.49894200 | 0.93119300 | 2.44335800 |
| B | 1.84682200 | 0.98581300 | -1.45265200 |
| B | 2.36158000 | 0.11674300 | -0.00011700 |
| B | 1.84695700 | 0.98558900 | 1.45263100 |
| B | 0.96764600 | 2.41306900 | 0.89285700 |
| B | 0.96758100 | 2.41321400 | -0.89263600 |
| H | 3.40246800 | -0.54081800 | -0.00035500 |
| H | 1.09298400 | -1.45240800 | -1.62315600 |
| H | -0.44846400 | 1.06011800 | -2.56224200 |
| H | -1.41491000 | 2.65819900 | 0.00019500 |
| H | -0.44833500 | 1.05964100 | 2.56232900 |
| B | 0.94002100 | -0.44123200 | 0.93005500 |
| B | 0.93996400 | -0.44119500 | -0.93037600 |
| B | 0.07725700 | 1.01348900 | -1.49592200 |
| B | -0.47104400 | 1.93282000 | 0.00012000 |
| B | 0.07738000 | 1.01329700 | 1.49599500 |
| H | 1.09275200 | -1.45250400 | 1.62283100 |

| | | | |
|---|---|---|---|
| B | 2.39748500 | 1.86099100 | 0.00001800 |
| H | 3.43447500 | 2.43495800 | -0.00002000 |
| Pb | -1.42699400 | -0.30065500 | -0.00000100 |
| Ca | 2.17842700 | -2.35410300 | 0.00001800 |

S2

| | | | |
|---|---|---|---|
| H | -2.98654500 | -0.12557100 | 1.53896200 |
| H | -1.48968500 | 2.25940800 | 2.45346800 |
| H | -0.52104400 | 3.77902500 | 0.00009000 |
| H | -1.48958900 | 2.25957200 | -2.45341100 |
| B | -2.02973900 | 0.31439700 | 0.89747700 |
| B | -2.02973200 | 0.31443400 | -0.89757300 |
| B | -1.16509500 | 1.72234300 | -1.44671000 |
| B | -0.61147300 | 2.59695800 | 0.00005000 |
| B | -1.16512800 | 1.72226000 | 1.44674400 |
| H | -2.98650900 | -0.12559200 | -1.53905700 |
| H | -1.17969800 | -1.97999800 | -0.00014100 |
| H | -0.27270100 | -0.43136700 | 2.54661600 |
| H | 1.33740300 | 2.13300500 | 1.58067400 |
| H | 1.33744600 | 2.13309300 | -1.58054800 |
| B | -0.39481500 | 0.11706100 | -1.49544700 |
| B | -0.93589900 | -0.76689500 | -0.00006100 |
| B | -0.39486100 | 0.11696100 | 1.49542600 |
| B | 0.50814100 | 1.59111200 | 0.92062400 |
| B | 0.50816600 | 1.59116600 | -0.92054800 |
| H | -0.27261500 | -0.43121700 | -2.54665900 |
| B | -2.20621100 | 1.83243800 | 0.00000400 |
| H | -3.24011800 | 2.41651800 | 0.00002100 |
| Pb | 1.55613700 | -0.43383800 | 0.00000000 |
| Ca | -3.31281800 | -1.60366500 | 0.00000300 |

S3

| | | | |
|---|---|---|---|
| H | -1.86005000 | 1.60982200 | 2.44796000 |
| H | -1.34759400 | 3.32228700 | 0.00121600 |
| H | -1.85939400 | 1.61280200 | -2.44671400 |
| H | -2.62993600 | -1.13072100 | -1.54125100 |
| B | -1.37787300 | 1.16558600 | 1.45707300 |
| B | -1.82098200 | -0.45549400 | 0.89889600 |
| B | -1.82098700 | -0.45475300 | -0.90026200 |
| B | -1.37754000 | 1.16700800 | -1.45638100 |
| B | -1.08123600 | 2.16608300 | 0.00089400 |
| H | -2.62967500 | -1.13252700 | 1.53916700 |
| H | 0.03180600 | -0.65494200 | 2.55200000 |
| H | 0.91222300 | 2.22863400 | 1.57956200 |
| H | 0.91240600 | 2.23028500 | -1.57748200 |
| H | 0.03285100 | -0.65178000 | -2.55308700 |
| B | -0.52268100 | -1.22720900 | -0.00082000 |
| B | -0.22269100 | -0.18340900 | 1.48829300 |
| B | 0.26168300 | 1.48378900 | 0.91713500 |

| | | | |
|---|---|---|---|
| B | 0.26197900 | 1.48475100 | -0.91574100 |
| B | -0.22246800 | -0.18199000 | -1.48880800 |
| H | -0.49686900 | -2.42013100 | -0.00073600 |
| B | -2.37019700 | 0.99420000 | 0.00012900 |
| H | -3.55329300 | 1.33117400 | -0.00026600 |
| Pb | 1.78110800 | -0.24976300 | -0.00002300 |
| Ca | -4.10492000 | -0.78285600 | -0.00002800 |

S4

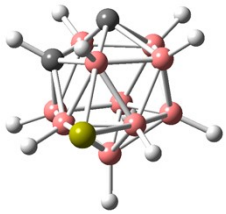
| | | | |
|---|---|---|---|
| H | 2.49965300 | -0.93048400 | 2.44299500 |
| H | 0.99110300 | -3.42111400 | 1.51517100 |
| H | 0.99104200 | -3.42119300 | -1.51504400 |
| H | 2.49951000 | -0.93080000 | -2.44311700 |
| B | 1.84751800 | -0.98486300 | 1.45234100 |
| B | 2.36174100 | -0.11529300 | -0.00007500 |
| B | 1.84743600 | -0.98499000 | -1.45241400 |
| B | 0.96906000 | -2.41285300 | -0.89257300 |
| B | 0.96915000 | -2.41279300 | 0.89266800 |
| H | 3.40178900 | 0.54337500 | -0.00010100 |
| H | 1.09240400 | 1.45268500 | 1.62334900 |
| H | -0.44775900 | -1.06028200 | 2.56227600 |
| H | -1.41328400 | -2.65961300 | 0.00014000 |
| H | -0.44796600 | -1.06037500 | -2.56213700 |
| B | 0.93969000 | 0.44151700 | -0.93077800 |
| B | 0.93981600 | 0.44157200 | 0.93063100 |
| B | 0.07802400 | -1.01368600 | 1.49598000 |
| B | -0.46990700 | -1.93364000 | 0.00008200 |
| B | 0.07790200 | -1.01380500 | -1.49587400 |
| H | 1.09207500 | 1.45258900 | -1.62353500 |
| B | 2.39875100 | -1.85982800 | -0.00002400 |
| H | 3.43595900 | -2.43337800 | 0.00000500 |
| Pb | -1.42691100 | 0.29998600 | 0.00000400 |
| Ca | 2.17581500 | 2.35565400 | -0.00000800 |

$XCB_{10}H_{11}^{-}$

S1

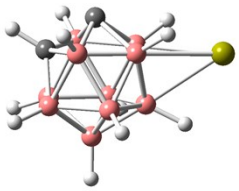
| | | | |
|---|---|---|---|
| C | 1.00946000 | 0.17502700 | -1.59044200 |
| B | 0.53235900 | -0.15226900 | 1.67075900 |
| B | 2.15786300 | -0.05027500 | 0.95389000 |
| B | -0.48651700 | -0.94784300 | 0.47493200 |
| B | 1.09904400 | 1.37773200 | 0.95116800 |
| B | 2.05647500 | 0.97111300 | -0.49790800 |
| B | -0.52677900 | 0.80844700 | 0.62632100 |
| B | -0.50504600 | 0.07631100 | -1.03095600 |
| B | 2.09982700 | -0.77530600 | -0.68376200 |
| B | 1.16496500 | -1.48966300 | 0.68639500 |
| B | 0.41610300 | 1.51160000 | -0.68789300 |

| | | | |
|---|---|---|---|
| H | 3.13270700 | -0.10941200 | 1.61283500 |
| H | -1.42875900 | -1.69061200 | 0.66904400 |
| H | 1.28305900 | 2.33315700 | 1.61794100 |
| H | 2.95022900 | 1.60729500 | -0.92437400 |
| H | -1.51451800 | 1.37914700 | 1.06020000 |
| H | -1.49912900 | 0.00201800 | -1.75036700 |
| H | 2.93901900 | -1.40891800 | -1.20980900 |
| H | 1.36294800 | -2.60001300 | 1.02522600 |
| H | 0.10703500 | 2.49692100 | -1.26017500 |
| H | 0.31004300 | -0.28409900 | 2.82293200 |
| H | 0.31193300 | -2.04946600 | -1.51223500 |
| C | 0.50382900 | -1.22109100 | -0.84504000 |
| Ca | -2.85378900 | -0.00244300 | 0.00734700 |



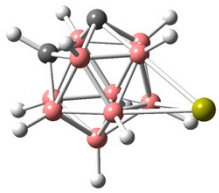
S2

| | | | |
|---|---|---|---|
| C | -0.44885000 | -0.00014900 | -1.58019100 |
| B | -1.09034600 | 0.00015700 | 1.66157400 |
| B | -0.45802700 | -1.45690900 | 0.82696300 |
| B | -2.09692900 | 0.88610800 | 0.51257800 |
| B | 0.53233300 | 0.00054100 | 1.02805800 |
| B | 0.51303800 | -0.86605800 | -0.52704800 |
| B | -0.45882500 | 1.45730200 | 0.82651500 |
| B | -1.08297000 | 1.42702400 | -0.85898700 |
| B | -1.08231800 | -1.42745000 | -0.85852000 |
| B | -2.09648000 | -0.88663700 | 0.51287600 |
| B | 0.51273900 | 0.86666200 | -0.52723300 |
| H | -0.20419600 | -2.46958600 | 1.37766900 |
| H | -3.09353200 | 1.47136200 | 0.73180200 |
| H | 1.51383700 | 0.00102600 | 1.75521300 |
| H | 1.47995000 | -1.46420500 | -0.97608800 |
| H | -0.20551400 | 2.47024500 | 1.37696300 |
| H | -1.35401200 | 2.36065200 | -1.52068200 |
| H | -1.35273400 | -2.36142500 | -1.51998200 |
| H | -3.09280400 | -1.47231000 | 0.73225400 |
| H | 1.47958900 | 1.46485100 | -0.97626400 |
| H | -1.29414700 | 0.00030000 | 2.82300100 |
| H | -2.75521300 | -0.00073300 | -1.63658700 |
| C | -1.94522200 | -0.00043900 | -0.92205200 |
| Ca | 2.86410700 | -0.00001700 | -0.00688600 |



S3

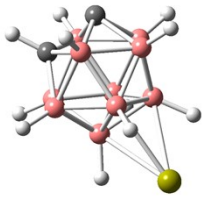
| | | | |
|---|---|---|---|
| C | 0.99535900 | 0.08011400 | -1.60035400 |
| B | 0.51956200 | -0.06812600 | 1.67193400 |
| B | 1.11402200 | 1.42080800 | 0.86317100 |
| B | 1.12647800 | -1.46358200 | 0.75518800 |
| B | -0.52134500 | 0.85452400 | 0.59289100 |
| B | 0.42339200 | 1.46720700 | -0.77959400 |
| B | -0.51057400 | -0.92059400 | 0.50445400 |
| B | 0.45588600 | -1.38964500 | -0.92239500 |
| B | 2.06403000 | 0.91576500 | -0.56910000 |
| B | 2.13122400 | -0.02200200 | 0.96415300 |
| B | -0.53267300 | 0.03773100 | -0.99539100 |
| H | 1.33976900 | 2.40892800 | 1.46483200 |
| H | 1.45246500 | -2.51184400 | 1.17882200 |
| H | -1.49745700 | 1.45635200 | 1.01135100 |
| H | 0.16796400 | 2.44734400 | -1.38410000 |
| H | -1.47432700 | -1.58672000 | 0.83607200 |
| H | 0.29537800 | -2.36278400 | -1.56662900 |
| H | 3.02548400 | 1.44429300 | -0.99118600 |
| H | 3.16023000 | -0.11309000 | 1.52675900 |
| H | -1.50216900 | 0.03193200 | -1.74467100 |
| H | 0.31580800 | -0.13039800 | 2.83276100 |
| H | 2.77459400 | -1.27215900 | -0.99466100 |
| C | 1.94001900 | -0.75448600 | -0.54485600 |
| Ca | -2.85100000 | 0.00369800 | 0.01376800 |



S4

| | | | |
|---|---|---|---|
| C | 0.00000147 | -0.19794590 | -1.61777260 |
| B | -0.00000115 | 0.17490938 | 1.67524348 |
| B | -1.43632023 | -0.38787171 | 0.78958606 |
| B | 0.88288453 | 1.27309037 | 0.61485769 |
| B | -0.00000729 | -1.42026751 | 0.91482481 |

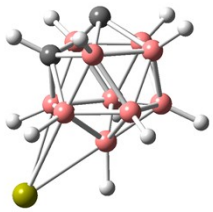
| | | | |
|---|---|---|---|
| B | -0.86796759 | -1.28710286 | -0.62731482 |
| B | 1.43631502 | -0.38788307 | 0.78958995 |
| B | 1.40496754 | 0.35565810 | -0.83077499 |
| B | -1.40496328 | 0.35567236 | -0.83077688 |
| B | -0.88287554 | 1.27309853 | 0.61485741 |
| B | 0.86795830 | -1.28711132 | -0.62731038 |
| H | -2.46693987 | -0.63862752 | 1.32420304 |
| H | 1.47133542 | 2.25977776 | 0.90760695 |
| H | -0.00001650 | -2.42478344 | 1.55014950 |
| H | -1.48544705 | -2.15882373 | -1.14430337 |
| H | 2.46693290 | -0.63864285 | 1.32420865 |
| H | 2.34476031 | 0.72074047 | -1.45454822 |
| H | -2.34474760 | 0.72076493 | -1.45455645 |
| H | -1.47131496 | 2.25979347 | 0.90760643 |
| H | 1.48542844 | -2.15883766 | -1.14430063 |
| H | -0.00000037 | 0.33368964 | 2.85309462 |
| H | 0.00001029 | 2.11804096 | -1.45755337 |
| C | 0.00000642 | 1.24727033 | -0.81981386 |
| Ca | 1.11805300 | -1.42201400 | 2.83704700 |





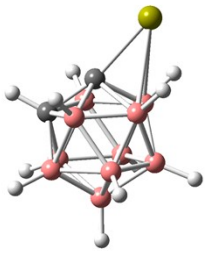
| | | | |
|---|---|---|---|
| C | -2.07437600 | 0.00083700 | -0.96575900 |
| B | 0.52233400 | -0.00094600 | 1.01199800 |
| B | -0.47332900 | 1.45638600 | 0.82255000 |
| B | 0.50562400 | -0.88941600 | -0.51703000 |
| B | -1.08851500 | 0.00023200 | 1.66807900 |
| B | -2.11561200 | 0.87152100 | 0.51053800 |
| B | -0.47531700 | -1.45670800 | 0.82250000 |
| B | -1.16525700 | -1.41732200 | -0.85099900 |
| B | -1.16360000 | 1.41781300 | -0.85101300 |
| B | 0.50639400 | 0.88756100 | -0.51711600 |
| B | -2.11675800 | -0.86978400 | 0.51047200 |
| H | -0.20855800 | 2.46904000 | 1.36881900 |
| H | 1.44799200 | -1.46712200 | -1.02018700 |
| H | -1.26219600 | 0.00032200 | 2.83464300 |
| H | -3.08093700 | 1.48438100 | 0.79135700 |
| H | -0.21179100 | -2.46961300 | 1.36888800 |
| H | -1.32583600 | -2.35746100 | -1.54186100 |
| H | -1.32271100 | 2.35820500 | -1.54188000 |
| H | 1.44888900 | 1.46475600 | -1.02076900 |
| H | -3.08280400 | -1.48145700 | 0.79139600 |
| H | 1.51405400 | -0.00179100 | 1.72773700 |
| H | -0.38752700 | -0.00023700 | -2.56320400 |

| | | | |
|---|---|---|---|
| C | -0.52473100 | -0.00018100 | -1.49124900 |
| Ca | 2.86931200 | 0.00001800 | 0.02486100 |



S6

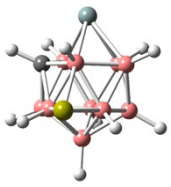
| | | | |
|---|---|---|---|
| C | 0.64282500 | 0.00071200 | -0.70366000 |
| B | -2.25389100 | -0.00056300 | 0.77421100 |
| B | -1.21763400 | -1.44885700 | 0.77324100 |
| B | -1.96574700 | 0.88581800 | -0.73405500 |
| B | -0.76076000 | 0.00019300 | 1.71841500 |
| B | 0.43049100 | -0.86667300 | 0.74561100 |
| B | -1.21879000 | 1.44859100 | 0.77296700 |
| B | -0.28697800 | 1.44010400 | -0.74508800 |
| B | -0.28569900 | -1.43986000 | -0.74477000 |
| B | -1.96501000 | -0.88709700 | -0.73387200 |
| B | 0.43004600 | 0.86799000 | 0.74549000 |
| H | -1.50390900 | -2.47665500 | 1.27401700 |
| H | -2.73890300 | 1.46725100 | -1.40379200 |
| H | -0.71014600 | 0.00025000 | 2.89713300 |
| H | 1.42058100 | -1.44215000 | 1.15042100 |
| H | -1.50631400 | 2.47622100 | 1.27336200 |
| H | 0.11182300 | 2.34799400 | -1.38130600 |
| H | 0.11418700 | -2.34750900 | -1.38067500 |
| H | -2.73767700 | -1.46923800 | -1.40356000 |
| H | 1.42000700 | 1.44387200 | 1.15004700 |
| H | -3.31960600 | -0.00092000 | 1.27715600 |
| H | -0.66797200 | -0.00022800 | -2.58334000 |
| C | -0.74205300 | -0.00019600 | -1.50655600 |
| Ca | 2.80915800 | -0.00001100 | -0.02344600 |



**Si**

S1

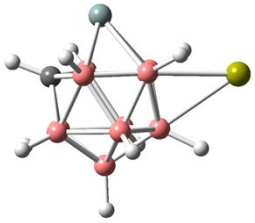
| | | | |
|---|---|---|---|
| B | -0.08545800 | 1.89527000 | 0.08832900 |
| B | -0.84602700 | 1.23589100 | -1.38180600 |
| B | 0.72612100 | 0.54735800 | 0.90071800 |
| B | -1.81383200 | 1.49290100 | 0.07939000 |
| B | -2.02911500 | 0.02339600 | -0.88371500 |
| B | -0.82490900 | 1.08499900 | 1.49762800 |
| B | -0.43551100 | -0.65762200 | 1.43815100 |
| B | 0.71152900 | 0.64605200 | -0.86845800 |
| B | -2.04055100 | -0.05398600 | 0.91375000 |
| H | -0.93040100 | 1.77729100 | -2.42474700 |
| H | 1.75344700 | 0.73256300 | 1.53419900 |
| H | -2.64033900 | 2.33302900 | 0.10325800 |
| H | -2.92833000 | -0.16078500 | -1.62669400 |
| H | -0.90294300 | 1.64063300 | 2.53591000 |
| H | -0.20622300 | -1.28166400 | 2.41848200 |
| H | -0.31349100 | -0.88099000 | -2.32868400 |
| H | 1.69762600 | 0.80355600 | -1.56500600 |
| H | -3.02880900 | -0.25692100 | 1.53125500 |
| H | 0.35893800 | 2.98949100 | 0.11827000 |
| B | 0.48338800 | -0.92583700 | -0.06368400 |
| H | 1.37337000 | -1.74333000 | -0.24767200 |
| Si | -1.44453800 | -1.84030800 | -0.03982700 |
| C | -0.47020300 | -0.43357400 | -1.35623800 |
| Ca | 2.97918700 | -0.20146100 | 0.00224600 |



S2

| | | | |
|---|---|---|---|
| B | -0.95539100 | -1.91629900 | -0.00001800 |
| B | -2.02987600 | -0.82729100 | -0.88728700 |
| B | -0.37249700 | -1.04571400 | 1.45130400 |
| B | -0.37224200 | -1.04573000 | -1.45125300 |
| B | -1.10256800 | 0.57063600 | -1.44132900 |
| B | 0.62377400 | -1.17719300 | 0.00013100 |
| B | 0.56213600 | 0.35683600 | 0.89892300 |
| B | -2.03002300 | -0.82727600 | 0.88707700 |

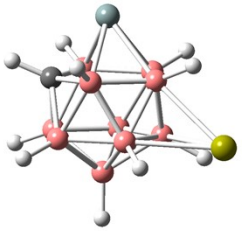
| | | | |
|---|---|---|---|
| B | 0.56221700 | 0.35684000 | -0.89868000 |
| H | -3.00210800 | -1.12971100 | -1.47741500 |
| H | -0.09027300 | -1.59064200 | 2.45987800 |
| H | -0.08987300 | -1.59064000 | -2.45979700 |
| H | -1.45581000 | 1.13165300 | -2.41756900 |
| H | 1.63248600 | -1.86532600 | 0.00027500 |
| H | 1.52241600 | 0.71514400 | 1.56317800 |
| H | -2.94581700 | 1.15304300 | -0.00017700 |
| H | -3.00233800 | -1.12970600 | 1.47706200 |
| H | 1.52248900 | 0.71526800 | -1.56290100 |
| H | -1.09020500 | -3.08768100 | -0.00001300 |
| B | -1.10278000 | 0.57065100 | 1.44126600 |
| H | -1.45621700 | 1.13165900 | 2.41744100 |
| Si | -0.46615700 | 2.01545800 | 0.00001300 |
| C | -2.00614600 | 0.61602400 | -0.00010300 |
| Ca | 2.90522900 | -0.07214500 | -0.00001000 |



S3

| | | | |
|---|---|---|---|
| B | -0.08543300 | 1.88788700 | 0.06002300 |
| B | -1.80383700 | 1.48875400 | 0.05471100 |
| B | 0.71966200 | 0.61472800 | -0.87762600 |
| B | -0.83095400 | 1.09933600 | 1.48321100 |
| B | -2.02502300 | -0.05462800 | 0.88886700 |
| B | 0.72445300 | 0.56135500 | 0.89969000 |
| B | 0.52125300 | -0.93435700 | -0.03507000 |
| B | -0.83861400 | 1.20031000 | -1.39783300 |
| B | -0.43588200 | -0.64164800 | 1.45055600 |
| H | -2.69370100 | 2.25781400 | 0.01394500 |
| H | 1.72261500 | 0.84576500 | -1.53054800 |
| H | -0.94621000 | 1.67035200 | 2.50850300 |
| H | -3.07200500 | -0.23523400 | 1.40349500 |

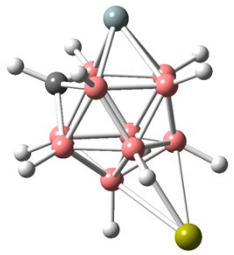
| | | | |
|---|---|---|---|
| H | 1.74292600 | 0.77267400 | 1.54050300 |
| H | 1.42173000 | -1.75920300 | -0.09344700 |
| H | -2.81317700 | -0.06883200 | -1.39698400 |
| H | -1.04507000 | 1.77166200 | -2.40620600 |
| H | -0.24522600 | -1.23564800 | 2.45636900 |
| H | 0.33270800 | 2.99194900 | 0.08057500 |
| B | -0.46661100 | -0.54297700 | -1.46421700 |
| H | -0.39444400 | -1.04459400 | -2.53084500 |
| Si | -1.39735800 | -1.85869500 | -0.02719000 |
| C | -1.90940200 | 0.03474300 | -0.81104000 |
| Ca | 2.98071100 | -0.17736200 | -0.00550000 |



S4

| | | | |
|---|---|---|---|
| B | 0.87969700 | 1.05520700 | 0.07419400 |
| B | -0.66283600 | 1.87151000 | 0.13584600 |
| B | 0.69758600 | -0.40739100 | -0.92517800 |
| B | -0.13787500 | 0.87903200 | 1.51661700 |
| B | -1.79754900 | 0.78427800 | 0.93731200 |
| B | 0.69630200 | -0.53152400 | 0.85117600 |
| B | -0.39891900 | -1.52328800 | -0.10940000 |
| B | -0.13220600 | 1.08319500 | -1.37111200 |
| B | -0.93810800 | -0.71051100 | 1.41531900 |
| H | -0.81362800 | 3.03899600 | 0.14689300 |
| H | 1.61961500 | -0.81488400 | -1.61018700 |
| H | 0.17510200 | 1.36516800 | 2.54600400 |
| H | -2.70343300 | 1.29634700 | 1.49436300 |
| H | 1.62728300 | -1.04541500 | 1.45261300 |
| H | -0.21065300 | -2.68798100 | -0.21153000 |

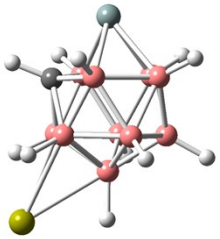
| | | | |
|---|---|---|---|
| H | -2.44887600 | 1.38015500 | -1.30942100 |
| H | 0.08199000 | 1.71462400 | -2.34257300 |
| H | -1.14897500 | -1.30873000 | 2.41342300 |
| H | 1.92951100 | 1.67377300 | 0.09829900 |
| B | -0.95197200 | -0.49381500 | -1.47637800 |
| H | -1.23366000 | -0.84854000 | -2.56646900 |
| Si | -2.46344400 | -0.99349200 | -0.04528000 |
| C | -1.67777400 | 0.85902200 | -0.75779300 |
| Ca | 3.07049900 | -0.25211100 | -0.00863600 |



S5

| | | | |
|---|---|---|---|
| B | -0.88113600 | 1.03231900 | -0.00005200 |
| B | -0.68423800 | -0.49110300 | 0.89021000 |
| B | 0.12477900 | 0.96417800 | -1.45536700 |
| B | 0.12664000 | 0.96761300 | 1.45389500 |
| B | 0.96141600 | -0.60468300 | 1.43831500 |
| B | 0.64577300 | 1.87433200 | -0.00215500 |
| B | 1.79789700 | 0.88233500 | -0.90222400 |
| B | -0.68479300 | -0.49328900 | -0.88691400 |
| B | 1.79897000 | 0.88444500 | 0.89895200 |
| H | -1.58108700 | -1.07588900 | 1.47012800 |
| H | -0.22165600 | 1.47434900 | -2.46310200 |
| H | -0.21855100 | 1.48040300 | 2.46071700 |
| H | 1.12511800 | -1.25929800 | 2.40829700 |
| H | 0.66649500 | 3.05438100 | -0.00349800 |
| H | 2.64477200 | 1.38548300 | -1.55654400 |
| H | 0.28705600 | -2.44157600 | 0.00323800 |

| | | | |
|---|---|---|---|
| H | -1.58150500 | -1.08002900 | -1.46520200 |
| H | 2.64651200 | 1.38921000 | 1.55115400 |
| H | -1.94670400 | 1.62902400 | 0.00023800 |
| B | 0.95991200 | -0.60804500 | -1.43704900 |
| H | 1.12195900 | -1.26505300 | -2.40569100 |
| Si | 2.52369100 | -0.90141300 | 0.00011600 |
| C | 0.43718100 | -1.36984200 | 0.00194500 |
| Ca | -3.08616300 | -0.22463400 | -0.00005400 |



S6

| | | | |
|---|---|---|---|
| B | -2.06893800 | 1.30358800 | -0.00009200 |
| B | -2.25279800 | -0.22123300 | 0.88860100 |
| B | -1.08095700 | 0.98488400 | -1.44203100 |
| B | -1.08065000 | 0.98547600 | 1.44177000 |
| B | -0.67154200 | -0.74139300 | 1.46158900 |
| B | -0.35546400 | 1.73895000 | -0.00041100 |
| B | 0.50283000 | 0.47524600 | -0.90001100 |
| B | -2.25294700 | -0.22157200 | -0.88805700 |
| B | 0.50298300 | 0.47563300 | 0.89949300 |
| H | -3.20049200 | -0.59419600 | 1.47840200 |
| H | -1.19941800 | 1.55813600 | -2.46619300 |
| H | -1.19865100 | 1.55913200 | 2.46575800 |
| H | -0.59737400 | -1.41932800 | 2.42560600 |
| H | 0.04944000 | 2.85094800 | -0.00063300 |
| H | 1.46645800 | 0.77359300 | -1.58879500 |
| H | -1.77032800 | -2.36119300 | 0.00068800 |

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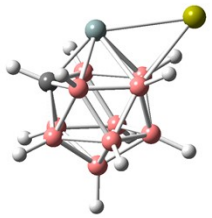
|---|---|---|---|
| H | -3.20068500 | -0.59482000 | -1.47761700 |
| H | 1.46674100 | 0.77421400 | 1.58800500 |
| H | -2.92962400 | 2.10877300 | -0.00025600 |
| B | -0.67189800 | -0.74198400 | -1.46139400 |
| H | -0.59794500 | -1.42001000 | -2.42535600 |
| Si | 0.64362800 | -1.45197100 | 0.00005100 |
| C | -1.36146200 | -1.35874000 | 0.00034400 |
| Ca | 2.90083800 | 0.25284100 | 0.00001700 |



Ge

S1

| | | | |
|---|---|---|---|
| C | -0.24987300 | -0.05353000 | -1.36867200 |
| H | -0.21329600 | -0.51964900 | -2.34415400 |
| B | -1.63492600 | 0.80177500 | -0.89195500 |
| H | -2.54409600 | 0.88663300 | -1.64137900 |
| B | -1.67806000 | 0.73686900 | 0.92084700 |
| H | -2.68007900 | 0.83335500 | 1.54313800 |
| B | -0.28731200 | -0.28853700 | 1.44861500 |
| H | -0.22044100 | -0.93826100 | 2.43729100 |
| B | 0.52447600 | -0.79359000 | -0.07026400 |
| H | 1.16795000 | -1.81610500 | -0.25678400 |
| B | 1.17130900 | 0.66113100 | -0.86854600 |
| H | 2.16956400 | 0.55474100 | -1.55835000 |
| B | -0.16663400 | 1.65112100 | -1.38180600 |
| H | -0.09936200 | 2.20591600 | -2.41912100 |
| B | -1.03564100 | 2.15414700 | 0.07813800 |
| H | -1.60051900 | 3.18867400 | 0.10358800 |
| B | -0.19484700 | 1.49279500 | 1.49926800 |
| H | -0.11810200 | 2.05077600 | 2.53662500 |
| B | 1.15207000 | 0.55400800 | 0.90163100 |
| H | 2.19009300 | 0.45802100 | 1.53808700 |
| B | 0.73712800 | 2.07521900 | 0.09406000 |
| H | 1.46060500 | 3.00853300 | 0.13089200 |
| Ge | -1.67138200 | -1.23907400 | -0.01849200 |
| Ca | 3.12666600 | -0.75828900 | 0.00420000 |

S2

| | | | |
|---|---|---|---|
| C | -1.97697200 | 0.03425500 | -0.00024400 |
| H | -2.99216600 | -0.34018300 | -0.00042100 |
| B | -1.06759300 | -0.07273700 | 1.44220000 |
| H | -1.50793700 | -0.55319500 | 2.42624900 |
| B | 0.62658900 | -0.12040600 | 0.90650900 |

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|---|---|---|---|
| H | 1.52650500 | -0.60071000 | 1.57853000 |
| B | 0.62677800 | -0.12041600 | -0.90597800 |
| H | 1.52661300 | -0.60101100 | -1.57793900 |
| B | -1.06710000 | -0.07274000 | -1.44235900 |
| H | -1.50701000 | -0.55325900 | -2.42657100 |
| B | -1.76230100 | 1.45412300 | -0.88739100 |
| H | -2.66928100 | 1.91117800 | -1.48225800 |
| B | -1.76263400 | 1.45412000 | 0.88693400 |
| H | -2.66979400 | 1.91121600 | 1.48149300 |
| B | -0.09064800 | 1.40592200 | 1.45114400 |
| H | 0.27277400 | 1.90298500 | 2.45860300 |
| B | 0.91500400 | 1.38262900 | 0.00030300 |
| H | 2.01447800 | 1.91407900 | 0.00068800 |
| B | -0.09007500 | 1.40591200 | -1.45101300 |
| H | 0.27365000 | 1.90291000 | -2.45839500 |
| B | -0.52792700 | 2.35866200 | -0.00001700 |
| H | -0.47496200 | 3.53662200 | 0.00001400 |
| Ge | -0.65519400 | -1.72149500 | 0.00000800 |
| Ca | 3.00173500 | -0.04618400 | -0.00002300 |

S3

| | | | |
|---|---|---|---|
| C | -1.53485800 | 0.81012200 | -0.81797900 |
| H | -2.42869300 | 0.97001200 | -1.40606600 |
| B | -1.67220100 | 0.74074200 | 0.88764500 |
| H | -2.72400100 | 0.87539900 | 1.40722900 |
| B | -0.29718500 | -0.26680200 | 1.46184500 |
| H | -0.26514300 | -0.87535500 | 2.47694900 |
| B | 0.55021700 | -0.81429100 | -0.03465500 |
| H | 1.20545000 | -1.84451300 | -0.09644200 |
| B | -0.30854200 | -0.15395700 | -1.46621200 |
| H | -0.36773900 | -0.64292100 | -2.53978500 |
| B | -0.18058800 | 1.62432700 | -1.39512300 |
| H | -0.20992100 | 2.23452700 | -2.40175100 |
| B | -1.02953400 | 2.16413000 | 0.05722200 |
| H | -1.66636800 | 3.15355800 | 0.02617300 |
| B | -0.20525200 | 1.51343500 | 1.48556100 |
| H | -0.15668100 | 2.09477100 | 2.51060800 |
| B | 1.14412200 | 0.56861700 | 0.90273200 |
| H | 2.18084500 | 0.49678500 | 1.54568700 |
| B | 1.15174100 | 0.62434800 | -0.87683900 |
| H | 2.17824000 | 0.57872400 | -1.53326800 |
| B | 0.73257200 | 2.06858400 | 0.06632000 |
| H | 1.44100700 | 3.01311800 | 0.09125800 |
| Ge | -1.62372500 | -1.27393000 | -0.01346900 |
| Ca | 3.12773000 | -0.72473700 | -0.00921000 |

S4

| | | | |
|---|---|---|---|
| C | -1.13070800 | 1.20407700 | -0.76063100 |
| H | -1.82099300 | 1.82685100 | -1.31352700 |

| | | | |
|---|---|---|---|
| B | -1.26233500 | 1.13806500 | 0.93840300 |
| H | -2.08001000 | 1.77766300 | 1.50088100 |
| B | -0.59911700 | -0.46416600 | 1.43305100 |
| H | -0.86544100 | -1.02133300 | 2.44220900 |
| B | -0.17087800 | -1.34988600 | -0.10304100 |
| H | -0.11575500 | -2.52891900 | -0.20588300 |
| B | -0.59718200 | -0.24234600 | -1.47375400 |
| H | -0.91144600 | -0.55403600 | -2.56849300 |
| B | 0.42675100 | 1.21049800 | -1.37075600 |
| H | 0.73059000 | 1.80310600 | -2.34318000 |
| B | 0.00711700 | 2.06342200 | 0.13499300 |
| H | 0.01929800 | 3.24074200 | 0.15155100 |
| B | 0.39426200 | 1.00995300 | 1.51783700 |
| H | 0.77353200 | 1.45327400 | 2.54452400 |
| B | 1.03689500 | -0.50077400 | 0.85482400 |
| H | 1.89646800 | -1.12865800 | 1.45507100 |
| B | 1.04825600 | -0.37905400 | -0.92443900 |
| H | 1.90895200 | -0.90349500 | -1.61080700 |
| B | 1.42590800 | 1.04651800 | 0.07513600 |
| H | 2.54844100 | 1.52002000 | 0.09793500 |
| Ge | -2.25885400 | -0.61234000 | -0.02240000 |
| Ca | 3.42177800 | -0.53879700 | -0.01404800 |

S5

| | | | |
|---|---|---|---|
| C | 0.49466500 | -0.22463700 | -1.37861600 |
| H | 0.71451500 | -0.61143400 | -2.36474200 |
| B | 0.17870800 | -1.33281300 | -0.11674300 |
| H | 0.12910400 | -2.49539700 | -0.33015800 |
| B | 0.60123000 | -0.48037700 | 1.42520700 |
| H | 0.85777400 | -1.07714000 | 2.41460600 |
| B | 1.27905700 | 1.13214800 | 0.95730900 |
| H | 2.07255600 | 1.71610100 | 1.61231800 |
| B | 1.24329100 | 1.21457800 | -0.84871000 |
| H | 1.98361100 | 1.78303600 | -1.57224100 |
| B | -0.43348200 | 1.19757600 | -1.37663900 |
| H | -0.78914600 | 1.68344600 | -2.39074200 |
| B | -1.07370200 | -0.37910800 | -0.91159400 |
| H | -1.90551700 | -0.92653300 | -1.61089800 |
| B | -1.03992600 | -0.50899000 | 0.85994300 |
| H | -1.89438200 | -1.15471500 | 1.44546600 |
| B | -0.38325800 | 0.99918500 | 1.51631500 |
| H | -0.77052200 | 1.43050400 | 2.54623200 |
| B | 0.02067900 | 2.04647700 | 0.11938500 |
| H | -0.06638500 | 3.22186000 | 0.17196100 |
| B | -1.41883400 | 1.04955500 | 0.08542100 |
| H | -2.54144000 | 1.52554600 | 0.10979000 |
| Ge | 2.28400300 | -0.57354000 | -0.01328600 |
| Ca | -3.43575300 | -0.50426600 | 0.00579100 |

S6

| | | | |
|---|---|---|---|
| H | 0.67587200 | -0.82460400 | -2.37339500 |
| B | -0.31497200 | 0.74525600 | -0.86178700 |
| H | -1.21425400 | 1.10007000 | -1.60419500 |
| B | -0.35006100 | 0.64841400 | 0.95400500 |
| H | -1.29863900 | 1.00907700 | 1.63675700 |
| B | 0.75654400 | -0.67528600 | 1.45449000 |
| H | 0.60616800 | -1.31359600 | 2.43890000 |
| B | 1.44693900 | -1.36769500 | -0.10570300 |
| H | 1.77970000 | -2.47791600 | -0.32983400 |
| B | 2.36248200 | -0.07859700 | -0.90115100 |
| H | 3.24075400 | -0.39862600 | -1.61669500 |
| B | 1.28175300 | 1.23564200 | -1.36177100 |
| H | 1.39306700 | 1.80171500 | -2.38945000 |
| B | 0.57063800 | 1.91260500 | 0.12022500 |
| H | 0.21433100 | 3.04158700 | 0.17046800 |
| B | 1.26201900 | 1.03175400 | 1.50826500 |
| H | 1.40361000 | 1.55701400 | 2.55585200 |
| B | 2.35668200 | -0.21580900 | 0.87739200 |
| H | 3.31640500 | -0.57662800 | 1.45887900 |
| B | 2.26963300 | 1.38349200 | 0.10100900 |
| H | 3.16275300 | 2.15188500 | 0.13800300 |
| Ge | -0.68756000 | -1.32854800 | -0.01773600 |
| Ca | -2.71007300 | 0.83525600 | -0.00581600 |

**Sn**

S1

| | | | |
|---|---|---|---|
| C | 0.10074500 | 0.16381800 | -1.37821200 |
| H | 0.04727900 | -0.27693400 | -2.36554000 |
| B | -1.02547800 | 1.33183000 | -0.90103100 |
| H | -1.87055400 | 1.65771700 | -1.66490100 |
| B | -1.10703700 | 1.27979100 | 0.91375100 |
| H | -2.04133300 | 1.65027600 | 1.54527800 |
| B | -0.01784000 | -0.07730200 | 1.44080700 |
| H | -0.09782600 | -0.71180100 | 2.44160400 |
| B | 0.64984900 | -0.75043500 | -0.08218500 |
| H | 1.03198800 | -1.89712500 | -0.28026200 |
| B | 1.64758900 | 0.50119700 | -0.86295500 |
| H | 2.59977800 | 0.16336300 | -1.54544000 |
| B | 0.60457300 | 1.79792400 | -1.37518500 |
| H | 0.82455800 | 2.33079100 | -2.40333000 |
| B | -0.12541300 | 2.48999900 | 0.08303100 |
| H | -0.41012500 | 3.63418600 | 0.11547800 |
| B | 0.50973400 | 1.62640300 | 1.50629500 |
| H | 0.71604500 | 2.14051000 | 2.54920200 |
| B | 1.58596100 | 0.38626300 | 0.90848100 |
| H | 2.56452100 | 0.03641000 | 1.55216700 |
| B | 1.57108100 | 1.96965600 | 0.11246600 |
| H | 2.50429600 | 2.69255200 | 0.16722200 |

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|---|---|---|---|
| Sn | -1.83538900 | -0.76679600 | -0.01331300 |
| Ca | 3.19156400 | -1.34198400 | 0.00530200 |

S2

| | | | |
|---|---|---|---|
| C | -1.32488400 | 1.38881300 | -0.00055400 |
| H | -2.36127800 | 1.70357000 | -0.00094900 |
| B | -0.64453600 | 0.76564400 | 1.43492000 |
| H | -1.28122900 | 0.65084600 | 2.42578700 |
| B | 0.70889400 | -0.26687000 | 0.91241800 |
| H | 1.19601500 | -1.15708200 | 1.59727800 |
| B | 0.70919900 | -0.26709700 | -0.91130400 |
| H | 1.19596300 | -1.15769100 | -1.59601500 |
| B | -0.64364300 | 0.76507000 | -1.43532500 |
| H | -1.27960000 | 0.64968000 | -2.42659300 |
| B | -0.32432600 | 2.41288800 | -0.88936300 |
| H | -0.78890900 | 3.31613600 | -1.48496900 |
| B | -0.32494000 | 2.41326500 | 0.88841400 |
| H | -0.78981100 | 3.31676400 | 1.48341000 |
| B | 1.00520700 | 1.39955200 | 1.45170300 |
| H | 1.59290300 | 1.59534800 | 2.45733900 |
| B | 1.80979700 | 0.79518700 | 0.00068900 |
| H | 3.01602900 | 0.60199100 | 0.00143400 |
| B | 1.00626400 | 1.39887000 | -1.45135800 |
| H | 1.59449000 | 1.59428300 | -2.45676100 |
| B | 1.20505500 | 2.42708100 | 0.00001500 |
| H | 1.93694400 | 3.35197800 | 0.00008800 |
| Sn | -1.45047100 | -1.01870200 | 0.00000600 |
| Ca | 2.69532400 | -1.55407800 | -0.00005400 |

S3

| | | | |
|---|---|---|---|
| C | 0.92657900 | 1.36449000 | -0.82363200 |
| H | 1.72571800 | 1.78839900 | -1.41865400 |
| B | 0.00944700 | 0.10606400 | -1.46523800 |
| H | 0.18699000 | -0.32993300 | -2.55146600 |
| B | -0.63926400 | -0.78380500 | -0.04591700 |
| H | -1.02090400 | -1.94630700 | -0.11320300 |
| B | 0.03968100 | -0.03028900 | 1.46011100 |
| H | 0.15066400 | -0.61619900 | 2.48621900 |
| B | 1.08286700 | 1.31765100 | 0.87826800 |
| H | 2.05542500 | 1.75091400 | 1.39688100 |
| B | 0.07834800 | 2.52130400 | 0.06691000 |
| H | 0.41336300 | 3.64998200 | 0.04394200 |
| B | -0.60034400 | 1.78018900 | -1.38803600 |
| H | -0.75258000 | 2.38587700 | -2.38690600 |
| B | -1.60429100 | 0.45016000 | -0.87544200 |
| H | -2.58550000 | 0.14101500 | -1.53172800 |
| B | -1.57178200 | 0.38356700 | 0.90849600 |
| H | -2.54754900 | 0.03523600 | 1.55834600 |
| B | -0.52918700 | 1.65913200 | 1.49242000 |
| H | -0.73291300 | 2.19975000 | 2.52119600 |

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|---|---|---|---|
| B | -1.59086700 | 1.94576100 | 0.08173500 |
| H | -2.53185800 | 2.65902300 | 0.11919300 |
| Sn | 1.79991400 | -0.79256500 | -0.00999100 |
| Ca | -3.16445300 | -1.35125500 | -0.01245200 |

S4

| | | | |
|---|---|---|---|
| C | -0.62009100 | 1.40473600 | -0.75460100 |
| H | -1.23112200 | 2.10737200 | -1.30675000 |
| B | -0.75890700 | 1.32784600 | 0.93823000 |
| H | -1.50959400 | 2.04541500 | 1.50677100 |
| B | -0.24391800 | -0.32904900 | 1.43205700 |
| H | -0.52995300 | -0.86780900 | 2.44926500 |
| B | 0.10713800 | -1.24003600 | -0.12287700 |
| H | 0.08896700 | -2.42237400 | -0.23506400 |
| B | -0.21838800 | -0.07645700 | -1.47273600 |
| H | -0.54751600 | -0.33984500 | -2.57885300 |
| B | 0.93111600 | 1.27488200 | -1.36263300 |
| H | 1.29846100 | 1.84835000 | -2.32532000 |
| B | 0.58678200 | 2.14819900 | 0.15307400 |
| H | 0.71445400 | 3.31899900 | 0.18216700 |
| B | 0.87292900 | 1.05008600 | 1.52610000 |
| H | 1.29326500 | 1.44811700 | 2.55603500 |
| B | 1.37594300 | -0.50985800 | 0.85030200 |
| H | 2.17695600 | -1.21577300 | 1.44715100 |
| B | 1.40478900 | -0.36931400 | -0.93266600 |
| H | 2.22042000 | -0.95835900 | -1.62336100 |
| B | 1.90752500 | 1.00581100 | 0.08498300 |
| H | 3.06757300 | 1.37638500 | 0.11688300 |
| Sn | -2.15988700 | -0.42251400 | -0.01546500 |
| Ca | 3.74239800 | -0.75268700 | -0.01786200 |

S5

| | | | |
|---|---|---|---|
| C | -0.19193600 | -1.15646600 | 0.00017600 |
| H | -0.18746500 | -2.23946500 | 0.00028500 |
| B | 0.20423500 | -0.31151600 | 1.42718800 |
| H | 0.45084600 | -0.93191800 | 2.40633600 |
| B | 0.77830400 | 1.32223300 | 0.91382300 |
| H | 1.48433300 | 2.00142500 | 1.58300100 |
| B | 0.77823800 | 1.32203700 | -0.91411000 |
| H | 1.48424200 | 2.00107100 | -1.58347600 |
| B | 0.20415600 | -0.31181600 | -1.42707600 |
| H | 0.45063900 | -0.93245700 | -2.40610600 |
| B | -1.43515400 | -0.47530000 | -0.89075400 |
| H | -2.23316000 | -1.18996500 | -1.47385200 |
| B | -1.43514400 | -0.47510400 | 0.89105600 |
| H | -2.23319300 | -1.18959900 | 1.47428700 |
| B | -0.87795400 | 1.09697800 | 1.45684700 |
| H | -1.31252000 | 1.54553300 | 2.46075000 |
| B | -0.51787300 | 2.08662200 | -0.00018500 |
| H | -0.70629900 | 3.25258900 | -0.00029700 |

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|---|---|---|---|
| B | -0.87807100 | 1.09665900 | -1.45696800 |
| H | -1.31271300 | 1.54496400 | -2.46095200 |
| B | -1.88112400 | 0.99816800 | 0.00000200 |
| H | -3.02718400 | 1.41762400 | 0.00003800 |
| Sn | 2.20719300 | -0.36076200 | 0.00000000 |
| Ca | -3.83818000 | -0.60238500 | -0.00001000 |

S6

| | | | |
|---|---|---|---|
| C | 0.14108800 | 1.02687100 | -0.80178500 |
| H | -0.45267800 | 1.66184600 | -1.47885600 |
| B | 0.04733900 | 0.94600900 | 0.91982900 |
| H | -0.73010000 | 1.65303300 | 1.54535500 |
| B | 0.77892900 | -0.59499100 | 1.47544500 |
| H | 0.48620100 | -1.10440100 | 2.50513600 |
| B | 1.26675200 | -1.49625100 | -0.07992600 |
| H | 1.36039000 | -2.67401400 | -0.17643300 |
| B | 0.76728300 | -0.39744200 | -1.49586200 |
| H | 0.41135600 | -0.71145200 | -2.58044700 |
| B | 1.73558500 | 1.08397900 | -1.38474900 |
| H | 1.93100800 | 1.69898500 | -2.37139900 |
| B | 1.26698600 | 1.93871300 | 0.09501000 |
| H | 1.13807500 | 3.11608300 | 0.10211800 |
| B | 1.69672000 | 0.92275300 | 1.48696200 |
| H | 1.96186500 | 1.43217000 | 2.51848200 |
| B | 2.43271900 | -0.56921100 | 0.86743300 |
| H | 3.27821100 | -1.14174700 | 1.45826900 |
| B | 2.42796500 | -0.47253100 | -0.92540400 |
| H | 3.25613500 | -0.97956300 | -1.59469300 |
| B | 2.75131100 | 0.97479300 | 0.06088500 |
| H | 3.80580900 | 1.50187400 | 0.08465300 |
| Sn | -0.97856200 | -1.12492200 | -0.01465100 |
| Ca | -2.21113200 | 1.69764900 | 0.02164700 |

**Pb**

S1

| | | | |
|---|---|---|---|
| C | 0.55347400 | 0.26555700 | -1.38405700 |
| H | 0.44800200 | -0.15715200 | -2.37526200 |
| B | -0.40264500 | 1.56938500 | -0.90540500 |
| H | -1.18897400 | 2.01694900 | -1.67228800 |
| B | -0.50274800 | 1.52938500 | 0.91084500 |
| H | -1.37233100 | 2.03444300 | 1.54375200 |
| B | 0.38467400 | 0.02893900 | 1.43542000 |
| H | 0.22193800 | -0.58808000 | 2.43828400 |
| B | 0.95688300 | -0.71947800 | -0.09171000 |
| H | 1.18084100 | -1.90825600 | -0.29431000 |
| B | 2.12734200 | 0.38273300 | -0.86061700 |
| H | 3.03185700 | -0.07632800 | -1.53873600 |

| | | | |
|---|---|---|---|
| B | 1.27757400 | 1.81415300 | -1.37035500 |
| H | 1.57808000 | 2.31907900 | -2.39262900 |
| B | 0.63992500 | 2.59250400 | 0.08715800 |
| H | 0.51746000 | 3.76547000 | 0.12511300 |
| B | 1.14202200 | 1.64314200 | 1.51140000 |
| H | 1.41435100 | 2.12056900 | 2.55706700 |
| B | 2.03839100 | 0.26837000 | 0.91167500 |
| H | 2.95625400 | -0.21488000 | 1.55929500 |
| B | 2.24838800 | 1.84296000 | 0.12455800 |
| H | 3.27284200 | 2.42891100 | 0.18971900 |
| Pb | -1.62003900 | -0.42767600 | -0.00879300 |
| Ca | 3.39564900 | -1.65125600 | 0.00602700 |

S2

| | | | |
|---|---|---|---|
| C | -0.24900600 | 1.90372100 | 0.00004900 |
| H | -1.06145600 | 2.62002700 | 0.00008600 |
| B | 0.10659100 | 1.04902000 | 1.42867700 |
| H | -0.51557000 | 1.21267600 | 2.42310700 |
| B | 0.91517800 | -0.45437300 | 0.91291900 |
| H | 1.00733500 | -1.46288600 | 1.60308800 |
| B | 0.91516000 | -0.45434200 | -0.91302200 |
| H | 1.00738800 | -1.46283200 | -1.60320700 |
| B | 0.10653900 | 1.04910500 | -1.42864300 |
| H | -0.51566000 | 1.21283900 | -2.42303700 |
| B | 1.08146600 | 2.41989800 | -0.88921000 |
| H | 1.03628300 | 3.43402000 | -1.48660300 |
| B | 1.08150200 | 2.41983900 | 0.88929900 |
| H | 1.03633000 | 3.43392800 | 1.48675000 |
| B | 1.87066300 | 0.94449800 | 1.45186700 |
| H | 2.48859000 | 0.87958700 | 2.45682600 |
| B | 2.35583500 | 0.06389400 | -0.00006100 |
| H | 3.37973900 | -0.60344400 | -0.00014700 |
| B | 1.87059900 | 0.94459800 | -1.45189500 |
| H | 2.48850800 | 0.87973600 | -2.45686800 |
| B | 2.47866700 | 1.79813400 | 0.00000100 |
| H | 3.52925800 | 2.33476800 | -0.00000700 |
| Pb | -1.46848200 | -0.29500300 | 0.00000000 |
| Ca | 2.20589200 | -2.43059300 | 0.00000500 |

S3

| | | | |
|---|---|---|---|
| C | -0.28371700 | 1.62383800 | -0.82593200 |
| H | -1.00062000 | 2.17490900 | -1.42154600 |
| B | -0.45500800 | 1.58774700 | 0.87015200 |
| H | -1.34335100 | 2.17489300 | 1.39109100 |
| B | 0.35881900 | 0.08899800 | 1.45697400 |
| H | 0.16106900 | -0.47073300 | 2.48576000 |
| B | 0.91589300 | -0.75762100 | -0.05161300 |
| H | 1.11892700 | -1.96557700 | -0.12421100 |
| B | 0.41552000 | 0.23561500 | -1.46404600 |

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|---|---|---|---|
| H | 0.17812400 | -0.16010800 | -2.55544500 |
| B | 1.29001700 | 1.78993500 | -1.38275000 |
| H | 1.54689100 | 2.36739100 | -2.37738100 |
| B | 0.73261800 | 2.62383000 | 0.07355400 |
| H | 0.58661300 | 3.79264100 | 0.05865700 |
| B | 1.18638400 | 1.66739700 | 1.49732900 |
| H | 1.47088800 | 2.16489700 | 2.52917700 |
| B | 2.01598500 | 0.24439000 | 0.91213800 |
| H | 2.92356600 | -0.25427500 | 1.56433100 |
| B | 2.06345100 | 0.31295000 | -0.87426100 |
| H | 2.98792600 | -0.14157300 | -1.53007000 |
| B | 2.28732600 | 1.78672500 | 0.09236600 |
| H | 3.33147800 | 2.33823200 | 0.13682800 |
| Pb | -1.59558000 | -0.43471200 | -0.00671500 |
| Ca | 3.32616800 | -1.70085700 | -0.01501000 |

S4

| | | | |
|---|---|---|---|
| C | -0.06952000 | 1.52509200 | -0.75055600 |
| H | -0.63533400 | 2.26640500 | -1.30049400 |
| B | -0.22010500 | 1.44198900 | 0.93603500 |
| H | -0.92606000 | 2.20127300 | 1.51005500 |
| B | 0.20109400 | -0.24304200 | 1.42982900 |
| H | -0.10541000 | -0.76930700 | 2.44884100 |
| B | 0.50311500 | -1.16511800 | -0.13070500 |
| H | 0.42792500 | -2.34563300 | -0.25042500 |
| B | 0.24205700 | 0.02867300 | -1.47021800 |
| H | -0.09690300 | -0.20982000 | -2.58023700 |
| B | 1.47053100 | 1.30926200 | -1.35706800 |
| H | 1.87679400 | 1.86473600 | -2.31520000 |
| B | 1.17363600 | 2.19245300 | 0.16327500 |
| H | 1.37237300 | 3.35347200 | 0.20184800 |
| B | 1.39073900 | 1.07179600 | 1.53085200 |
| H | 1.83272700 | 1.44005400 | 2.56331400 |
| B | 1.80739800 | -0.51213800 | 0.84866700 |
| H | 2.56835000 | -1.26338800 | 1.44426500 |
| B | 1.84613700 | -0.36278300 | -0.93607000 |
| H | 2.62914600 | -0.99221600 | -1.63060100 |
| B | 2.42630500 | 0.97535700 | 0.09204100 |
| H | 3.60599100 | 1.27829400 | 0.12889800 |
| Pb | -1.82143400 | -0.26761500 | -0.01016200 |
| Ca | 4.15102700 | -0.88561100 | -0.02084100 |

S5

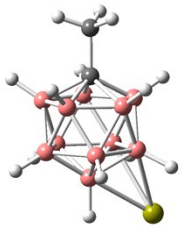
| | | | |
|---|---|---|---|
| C | -0.63267100 | -1.11281600 | 0.00152200 |
| H | -0.59305400 | -2.19527800 | 0.00245200 |
| B | -0.26276700 | -0.25499100 | 1.42094100 |
| H | 0.00471800 | -0.86537200 | 2.40242500 |
| B | 0.25045900 | 1.40223900 | 0.91387600 |
| H | 0.92208300 | 2.11496400 | 1.58555800 |
| B | 0.24995200 | 1.40053600 | -0.91634700 |

| | | | |
|---|---|---|---|
| H | 0.92144900 | 2.11188700 | -1.58962300 |
| B | -0.26333600 | -0.25756800 | -1.41996600 |
| H | 0.00300900 | -0.87006300 | -2.40043700 |
| B | -1.89788500 | -0.47853900 | -0.89063500 |
| H | -2.67374300 | -1.21829900 | -1.47414200 |
| B | -1.89787800 | -0.47686600 | 0.89327100 |
| H | -2.67422300 | -1.21517100 | 1.47784800 |
| B | -1.39463900 | 1.11381300 | 1.45725100 |
| H | -1.84628700 | 1.54846900 | 2.46028100 |
| B | -1.07120100 | 2.11687100 | -0.00158700 |
| H | -1.30453800 | 3.27518600 | -0.00251200 |
| B | -1.39555000 | 1.11105600 | -1.45827800 |
| H | -1.84779100 | 1.54348800 | -2.46201100 |
| B | -2.39457400 | 0.98062000 | 0.00002900 |
| H | -3.55399000 | 1.36222000 | 0.00032700 |
| Pb | 1.86128900 | -0.22578800 | -0.00000100 |
| Ca | -4.29000800 | -0.68432000 | -0.00010000 |

$CH_3XB_{11}H_{11}^-$

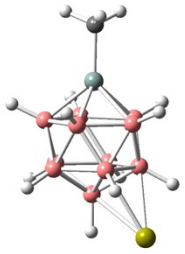
**C**

| | | | |
|---|---|---|---|
| C | 1.84259500 | -0.45578900 | -0.00095500 |
| B | -1.00362900 | 1.01657600 | 0.00141200 |
| B | 0.00372600 | 1.01747100 | -1.45052000 |
| B | 0.00380400 | 1.01174900 | 1.45381500 |
| B | -0.72594400 | -0.49681300 | -0.89083600 |
| B | 0.92878500 | -0.49882600 | -1.43802900 |
| B | -0.72683500 | -0.50021300 | 0.88751300 |
| B | 0.92605800 | -0.50486800 | 1.43584900 |
| B | 1.67131100 | 0.99854900 | -0.88298600 |
| B | 0.47385800 | 1.94716900 | 0.00385800 |
| B | 0.46870200 | -1.44124200 | -0.00236300 |
| H | -0.34336800 | 1.52713000 | -2.45713000 |
| H | -0.34252300 | 1.51802000 | 2.46239200 |
| H | -1.60521000 | -1.05674200 | -1.52058300 |
| H | 1.33227200 | -1.07654000 | -2.38177700 |
| H | -1.60573100 | -1.06317700 | 1.51507300 |
| H | 1.32971600 | -1.08453400 | 2.37818300 |
| H | 2.60531400 | 1.42104700 | -1.46241300 |
| H | 0.46343000 | 3.12611700 | 0.00690100 |
| H | 0.55238300 | -2.61718900 | -0.00607700 |
| H | -2.09588300 | 1.56053300 | 0.00185200 |
| B | 1.67349100 | 0.99289400 | 0.88575800 |
| H | 2.60766400 | 1.41206000 | 1.46785000 |
| C | 3.20248500 | -1.13542400 | -0.00108600 |
| H | 3.23428400 | -1.92226300 | -0.75220300 |
| H | 3.98145100 | -0.40943600 | -0.22424300 |
| H | 3.40564200 | -1.57400700 | 0.97384500 |
| Ca | -3.11282800 | -0.39629900 | -0.00033900 |



**Si**

| | | | |
|---|---|---|---|
| B | 1.32314000 | 0.98263000 | 0.00020700 |
| B | 0.32765600 | 1.07264200 | 1.45664100 |
| B | 0.32732800 | 1.07471900 | -1.45577100 |
| B | 0.91984100 | -0.50184800 | 0.89165600 |
| B | -0.70026800 | -0.37504900 | 1.50256600 |
| B | 0.91960000 | -0.50055600 | -0.89307900 |
| B | -0.70098000 | -0.37285700 | -1.50341400 |
| B | -1.33877400 | 1.25788400 | 0.92754100 |
| B | -0.05980100 | 2.04634700 | 0.00117500 |
| B | -0.30499700 | -1.39435700 | -0.00092800 |
| H | 0.74436100 | 1.55353300 | 2.45212200 |
| H | 0.74435000 | 1.55663200 | -2.45062700 |
| H | 1.76795900 | -1.11714800 | 1.51804800 |
| H | -1.01321700 | -0.88672900 | 2.52159300 |
| H | 1.76791800 | -1.11475500 | -1.52025000 |
| H | -1.01309900 | -0.88353600 | -2.52318300 |
| H | -2.12725400 | 1.87004500 | 1.56104700 |
| H | 0.08173000 | 3.21780000 | 0.00229300 |
| H | -0.32831300 | -2.57768700 | -0.00221200 |
| H | 2.45625100 | 1.43296700 | 0.00014700 |
| B | -1.33848600 | 1.25944200 | -0.92613300 |
| H | -2.12867700 | 1.87131000 | -1.55783400 |
| Si | -2.06742000 | -0.38759400 | -0.00029800 |
| C | -3.76994400 | -1.08593300 | 0.00003000 |
| H | -4.47878100 | -0.31031900 | -0.28774100 |
| H | -3.83360800 | -1.91041300 | -0.70867200 |
| H | -4.01958700 | -1.44685500 | 0.99691800 |
| Ca | 3.30361100 | -0.60289500 | 0.00000200 |



**Ge**

| | | | |
|---|---|---|---|
| B | 0.38122900 | -0.29238900 | 1.52241800 |
| B | 0.95542200 | 1.38617600 | 0.93854200 |
| B | 0.95494000 | 1.38619300 | -0.93883900 |
| B | 0.38142800 | -0.29240600 | -1.52244800 |
| B | 0.02536800 | -1.34249300 | 0.00035200 |
| B | -0.69991700 | 1.11145400 | 1.45631700 |
| B | -0.35505600 | 2.09993000 | -0.00013800 |
| B | -0.70010500 | 1.11137400 | -1.45643400 |
| B | -1.22307200 | -0.48774500 | -0.89237000 |
| B | -1.22321300 | -0.48772300 | 0.89267300 |
| B | -1.68965300 | 0.97819400 | 0.00002400 |
| C | 3.65375600 | -0.93663400 | 0.00011000 |
| H | -2.84117900 | 1.37987200 | 0.00001700 |
| H | -1.14426000 | 1.57544800 | -2.44832200 |
| H | -2.04748100 | -1.13481600 | -1.51904200 |
| H | -2.04775100 | -1.13462500 | 1.51933500 |
| H | -1.14360900 | 1.57602800 | 2.44817400 |
| H | -0.55409200 | 3.26324500 | 0.00011700 |
| H | 0.69038500 | -0.78596900 | -2.55089600 |
| H | 0.07513500 | -2.52464400 | -0.00004200 |
| H | 0.69170800 | -0.78540700 | 2.55071500 |
| H | 1.69619500 | 2.04846800 | 1.57770500 |
| H | 1.69746100 | 2.04727300 | -1.57736800 |
| H | 4.30092100 | -0.19340100 | -0.45994400 |
| H | 3.96855100 | -1.11354300 | 1.02589500 |
| H | 3.69823100 | -1.86426400 | -0.56546300 |
| Ge | 1.84355400 | -0.27420600 | -0.00007300 |
| Ca | -3.59966700 | -0.69060400 | 0.00001600 |

**Sn**

| | | | |
|---|---|---|---|
| Sn | 1.75952900 | -0.19246100 | 0.00007300 |
| B | 0.54945700 | 1.49565400 | -0.94901000 |
| B | 0.05115900 | -0.22530300 | -1.53508700 |
| B | -0.25693200 | -1.29797100 | 0.00002600 |

| | | | |
|---|---|---|---|
| B | 0.05101200 | -0.22521900 | 1.53506500 |
| B | 0.54945700 | 1.49572900 | 0.94897300 |
| B | -1.08676400 | 1.12850100 | -1.45742100 |
| B | -1.53383100 | -0.49345100 | -0.89355200 |
| B | -1.53388000 | -0.49343100 | 0.89343500 |
| B | -1.08688700 | 1.12855700 | 1.45724000 |
| B | -0.78783400 | 2.13318100 | -0.00011900 |
| B | -2.06795200 | 0.94959800 | -0.00013300 |
| C | 3.75577200 | -0.86973600 | -0.00010500 |
| H | -3.23647500 | 1.29829400 | -0.00022100 |
| H | -2.33295700 | -1.17201700 | 1.52157300 |
| H | -1.55790700 | 1.57358400 | 2.44610900 |
| H | -1.04676300 | 3.28518300 | -0.00008200 |
| H | -1.55778700 | 1.57339000 | -2.44635000 |
| H | -2.33292700 | -1.17203600 | -1.52166600 |
| H | 0.33961600 | -0.69707900 | 2.58124800 |
| H | 1.21977100 | 2.22003600 | 1.60105700 |
| H | 1.22040300 | 2.21959600 | -1.60091700 |
| H | 0.33945800 | -0.69728400 | -2.58128100 |
| H | -0.19547100 | -2.48144800 | -0.00002900 |
| H | 3.76493400 | -1.93023700 | -0.23638400 |
| H | 4.31054300 | -0.31200500 | -0.74972600 |
| H | 4.18014400 | -0.69909600 | 0.98555000 |
| Ca | -3.89303500 | -0.80733200 | 0.00005100 |

**Pb**

| | | | |
|---|---|---|---|
| B | -0.31282800 | -0.21122100 | -1.53472600 |
| B | -0.58837200 | -1.27151700 | -0.00017700 |
| B | -0.31314900 | -0.21108600 | 1.53472300 |
| B | 0.14960100 | 1.54110800 | 0.97075600 |
| B | 0.14997400 | 1.54149100 | -0.97051500 |
| B | -1.89007000 | -0.50910400 | -0.89184100 |
| B | -1.89005600 | -0.50891100 | 0.89127000 |
| B | -1.47618800 | 1.11493000 | 1.45960500 |
| B | -1.19007800 | 2.13023400 | 0.00001500 |
| B | -1.47555000 | 1.11504200 | -1.45977700 |
| B | -2.45093000 | 0.92630500 | -0.00046100 |
| C | 3.42630700 | -1.06276600 | -0.00037200 |
| H | -3.62365300 | 1.26005800 | -0.00073100 |
| H | -1.95408200 | 1.56236500 | 2.44439300 |
| H | -1.46944100 | 3.27778800 | -0.00034600 |
| H | -1.95333900 | 1.56253700 | -2.44460500 |
| H | -2.67732400 | -1.19903300 | -1.52374800 |
| H | -2.67735700 | -1.19905900 | 1.52299400 |
| H | 0.79084300 | 2.29053400 | 1.62087300 |
| H | 0.79142700 | 2.29068100 | -1.62065400 |
| H | -0.01372800 | -0.67645100 | -2.58065600 |
| H | -0.49054100 | -2.45288600 | -0.00010500 |
| H | -0.01465800 | -0.67672500 | 2.58063300 |

| | | | |
|---|---|---|---|
| H | 3.43795600 | -1.73517800 | 0.85088600 |
| H | 3.50719200 | -1.59988100 | -0.93941800 |
| H | 4.18250100 | -0.29052200 | 0.08716500 |
| Pb | 1.49772700 | -0.08521800 | 0.00011700 |
| Ca | -4.23845100 | -0.86680700 | 0.00007800 |