Supporting Information

Four-Membered Heterocyclic Molecules Featuring Boron and Heavy Group 14 Elements That Exhibit Both σ-Aromatic and π-Aromatic Properties: A New Synthetic Target

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Computational Details

Geometry optimizations were carried out using density functional theory at the M06-2X[1] level in conjunction with the def2-TZVP basis set.[2] Stationary points were characterized as minima by calculating the Hessian matrix analytically. The calculations were carried out using the program package Gaussian 16, Revision C.01.[3] The NBO analysis[4] was done with the internal module of Gaussian 16 (NBO Version 5.0) at the M06-2X/def2-TZVP level of theory. The quantum theory of atoms in molecules (QTAIM) method[5] was employed for the characterization of the Laplacian of electron density and electron localization function (ELF)[6] using the Multiwfn 3.8 package.[7] For predicting the aromaticity of these four-membered-ring heterocyclic **B_2G14G14′** molecules, Nucleus Independent Chemical Shift (NICS)[8] calculations with the Gauge-Independent Atomic Orbital (GIAO)[9] method, Anisotropy of the Current Induced Density (ACID),[10] and adaptive natural density partitioning (AdNDP)[11] method were conducted at the M06-2X/def2-TZVP level of theory using the Gaussian 16 C.01 program.

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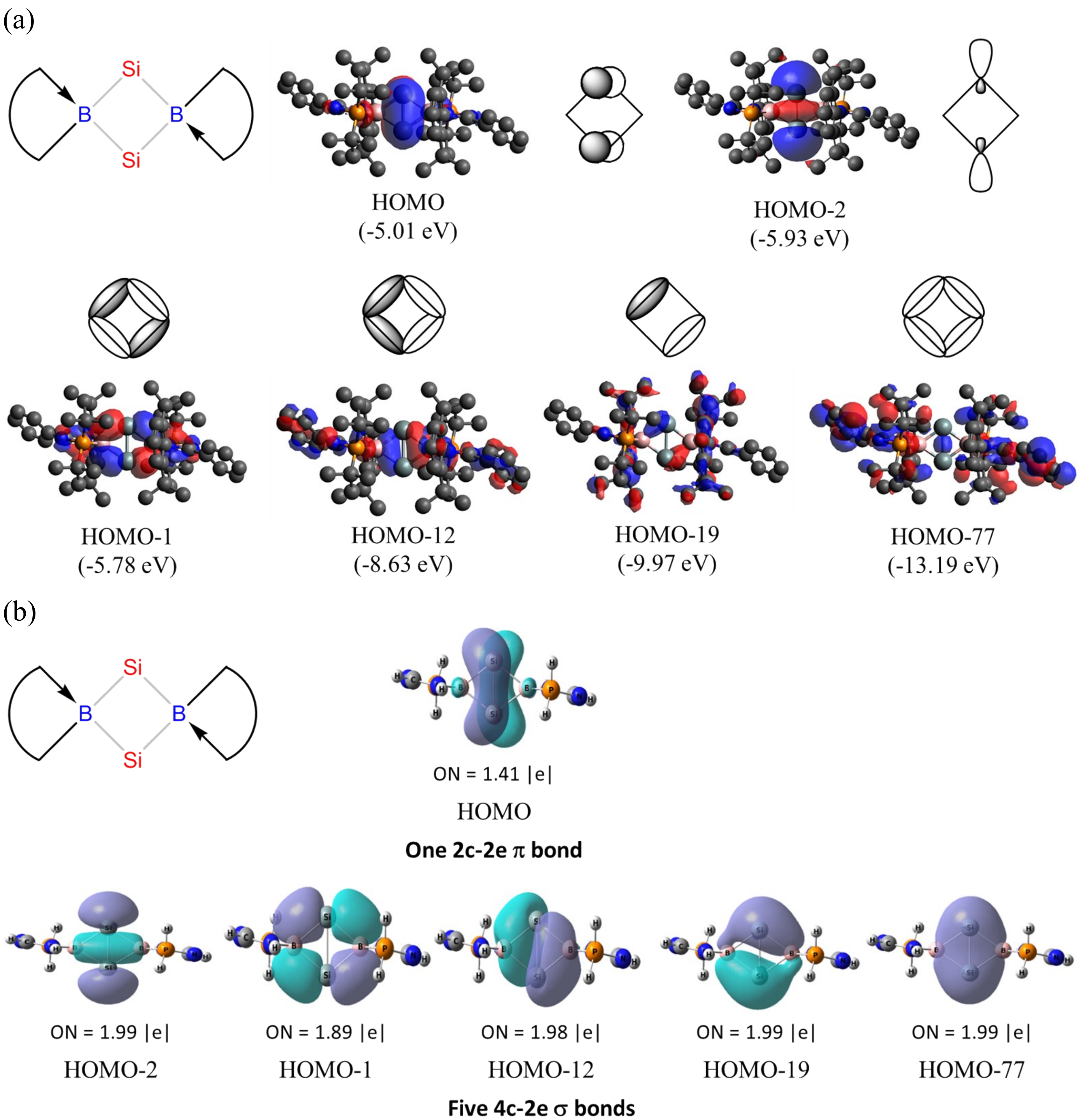


Figure S1. Global minimum structure of the $\mathbf{B_2Si_2}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

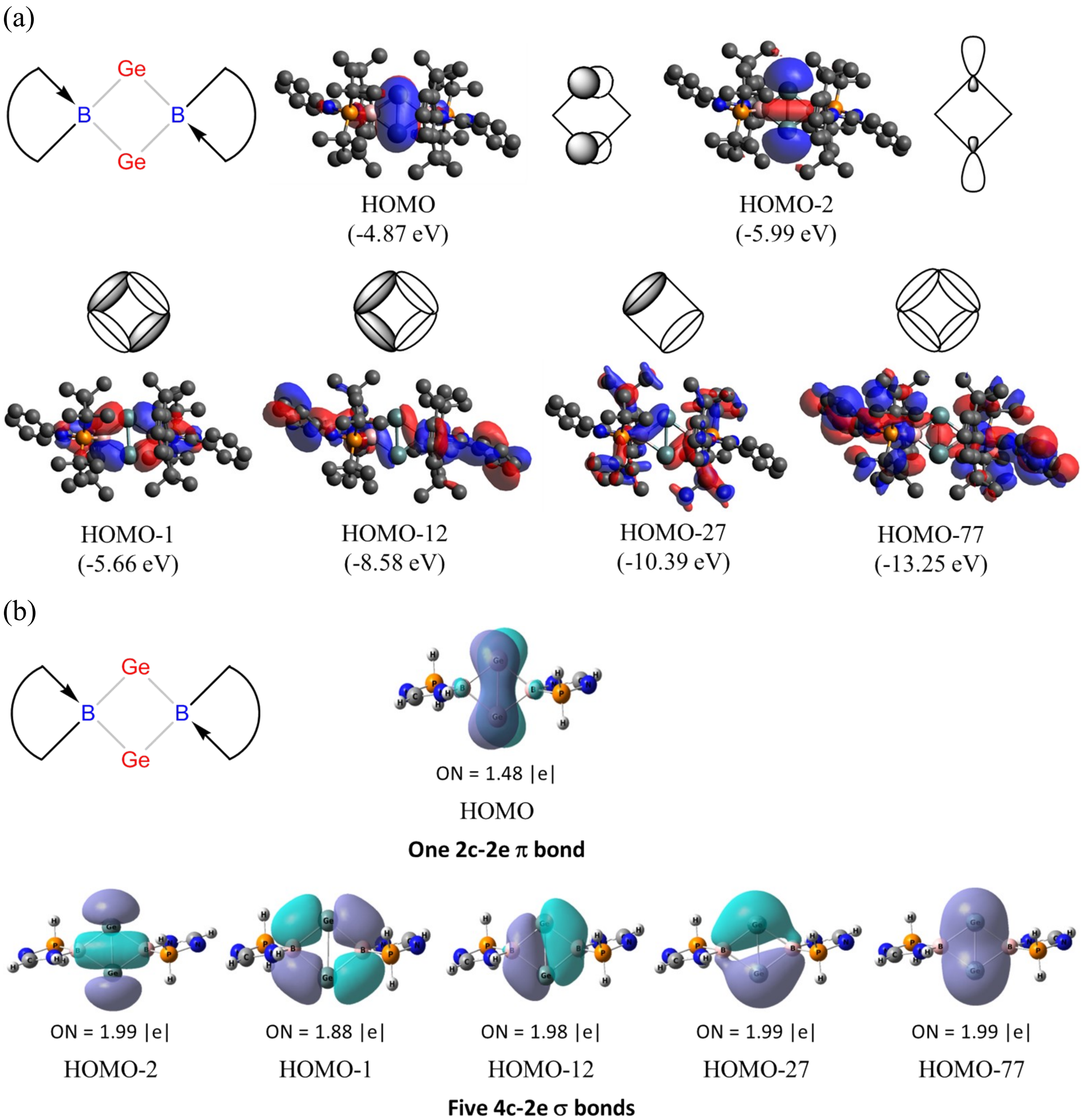


Figure S2. Global minimum structure of the $\mathbf{B_2Ge_2}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

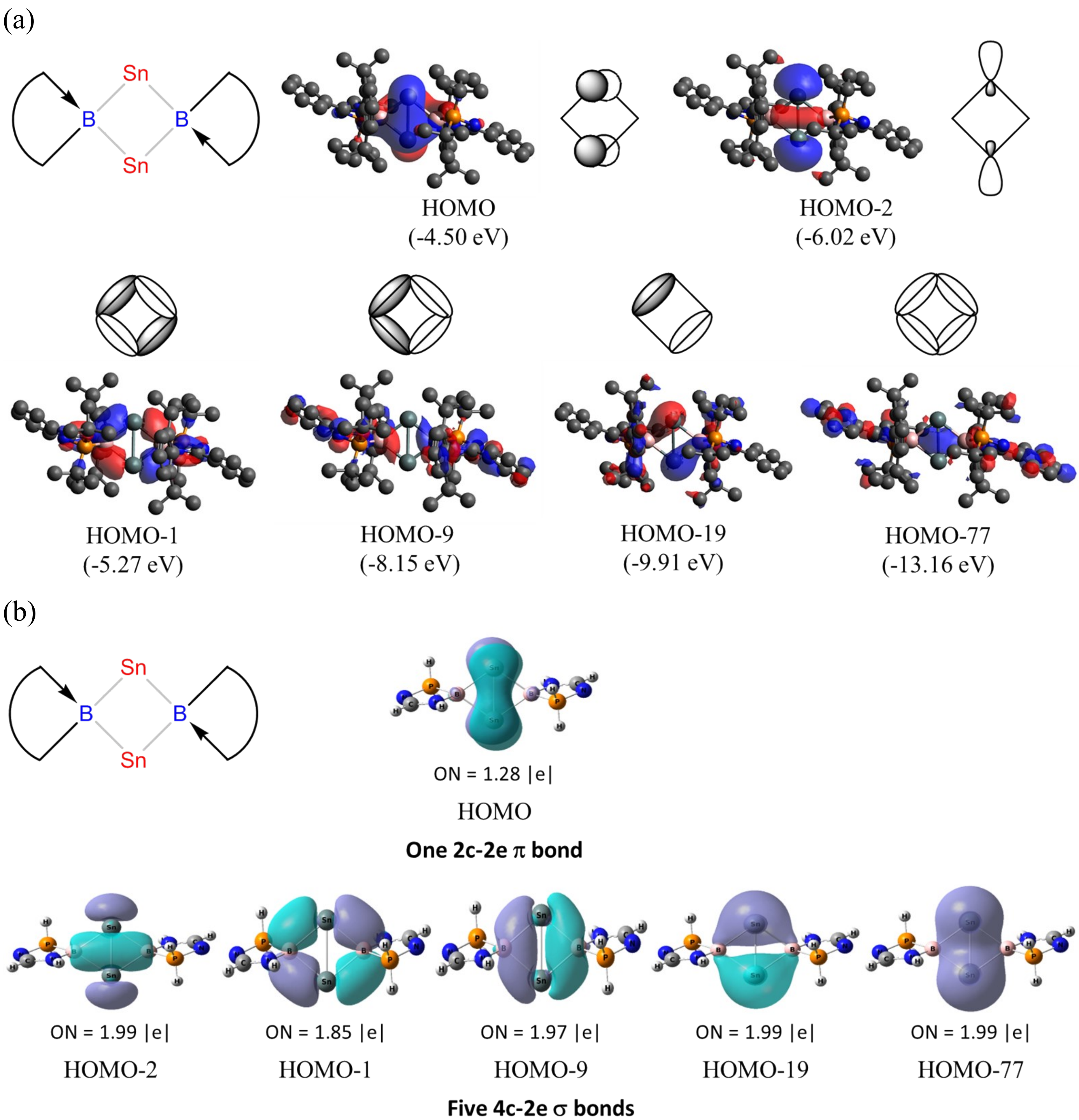


Figure S3. Global minimum structure of the $\mathbf{B_2Sn_2}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

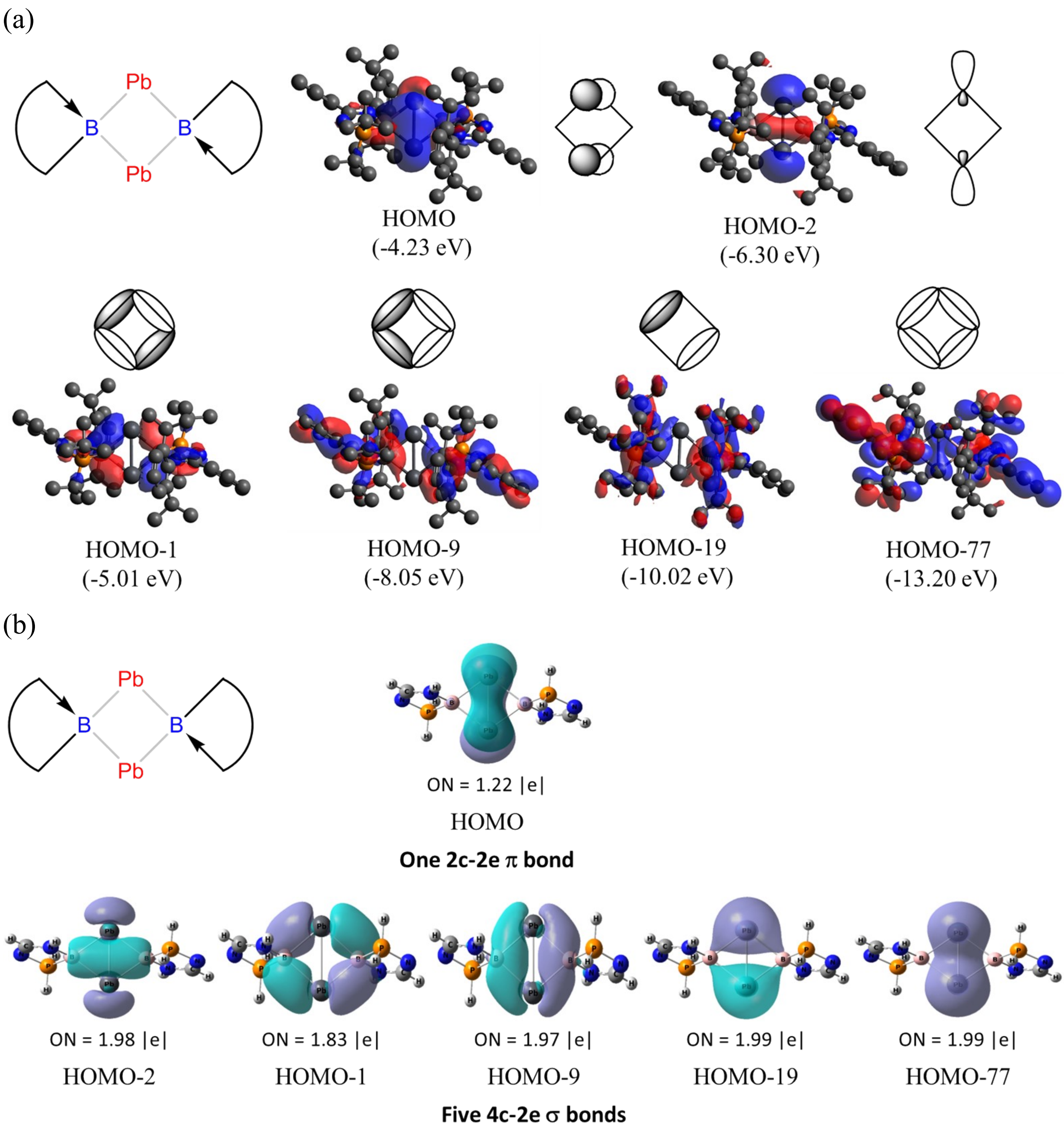


Figure S4. Global minimum structure of the $\mathbf{B_2Pb_2}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

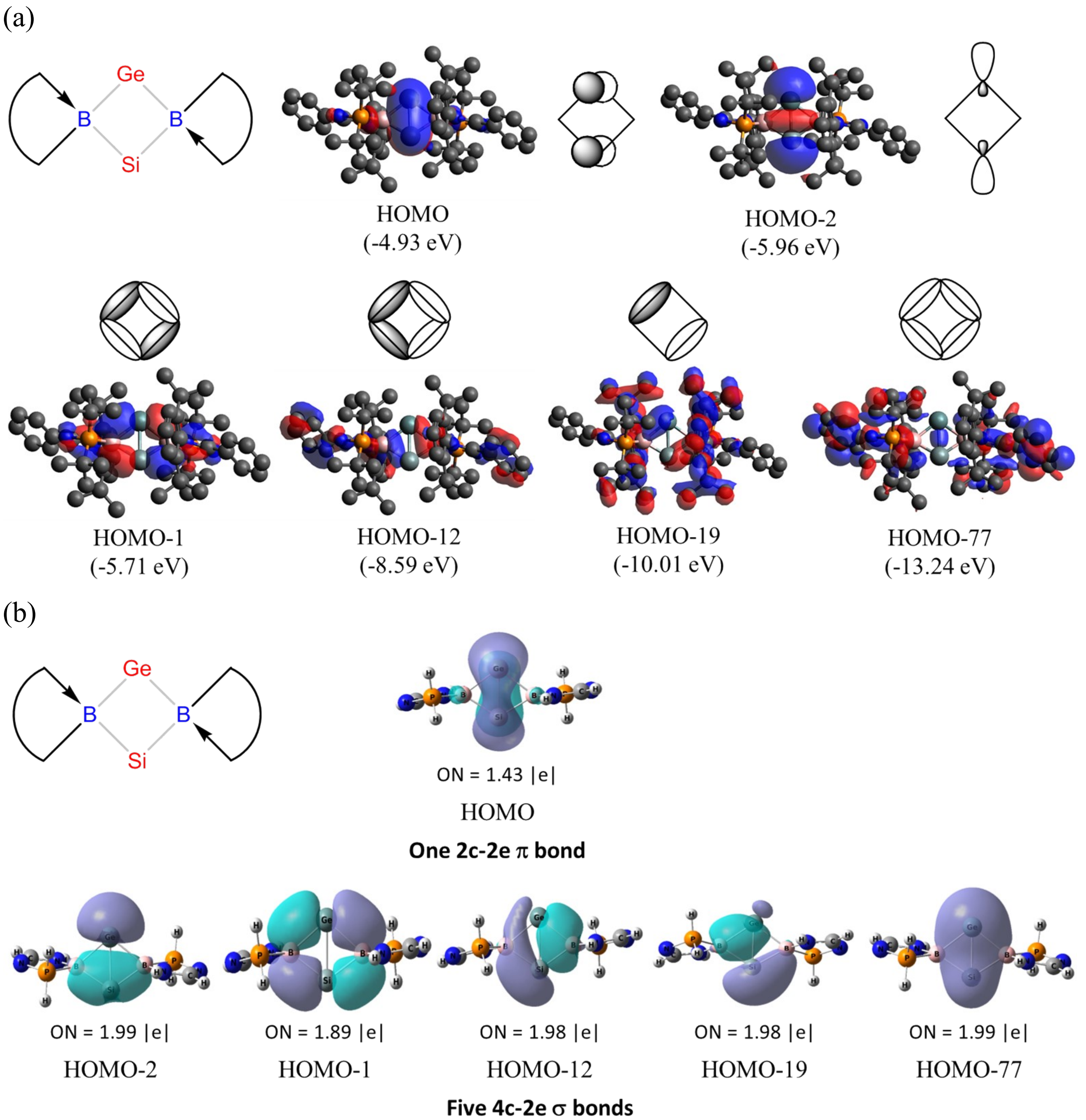


Figure S5. Global minimum structure of the **B_2SiGe** molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

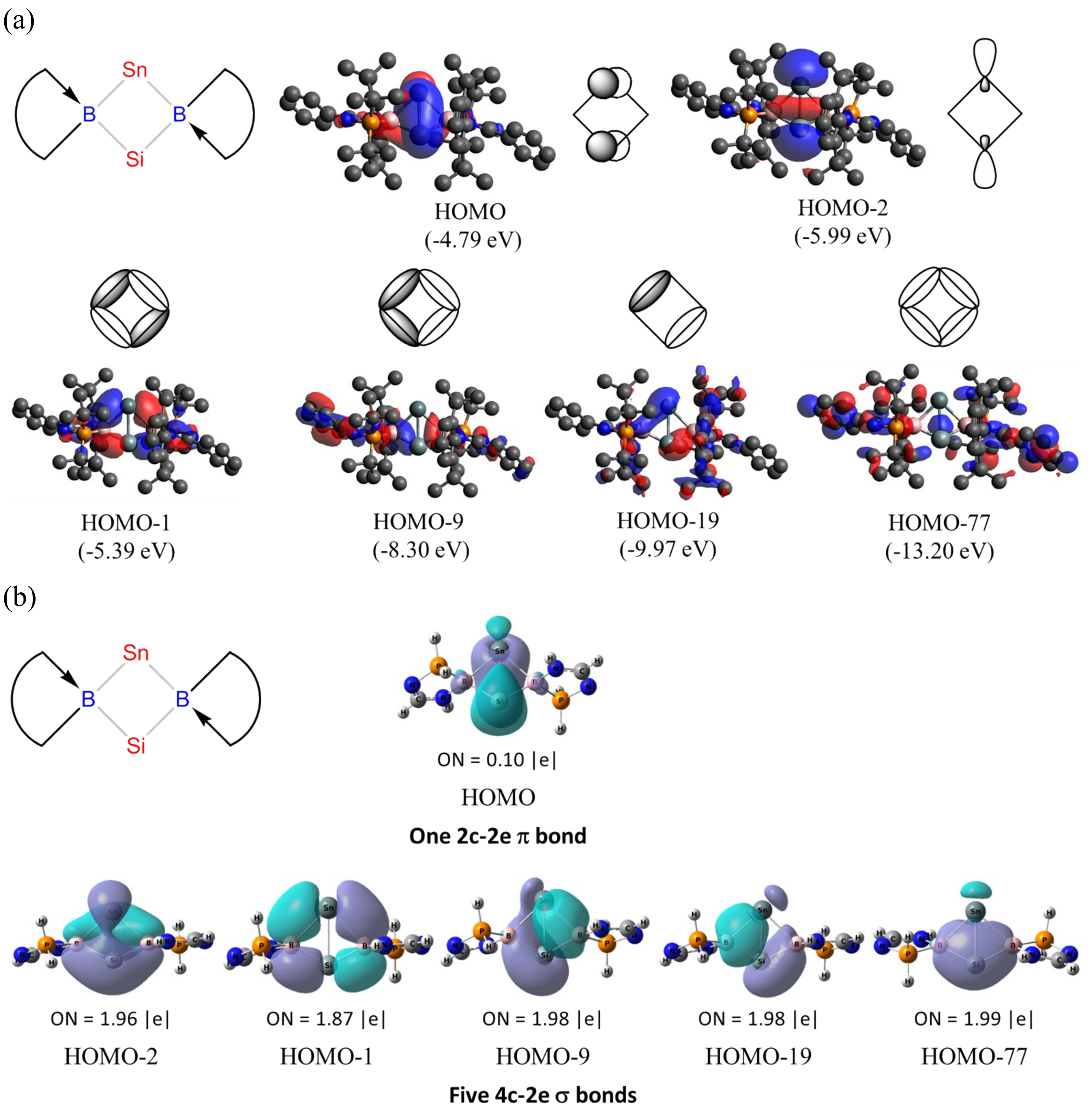


Figure S6. Global minimum structure of the $\mathbf{B_2SiSn}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

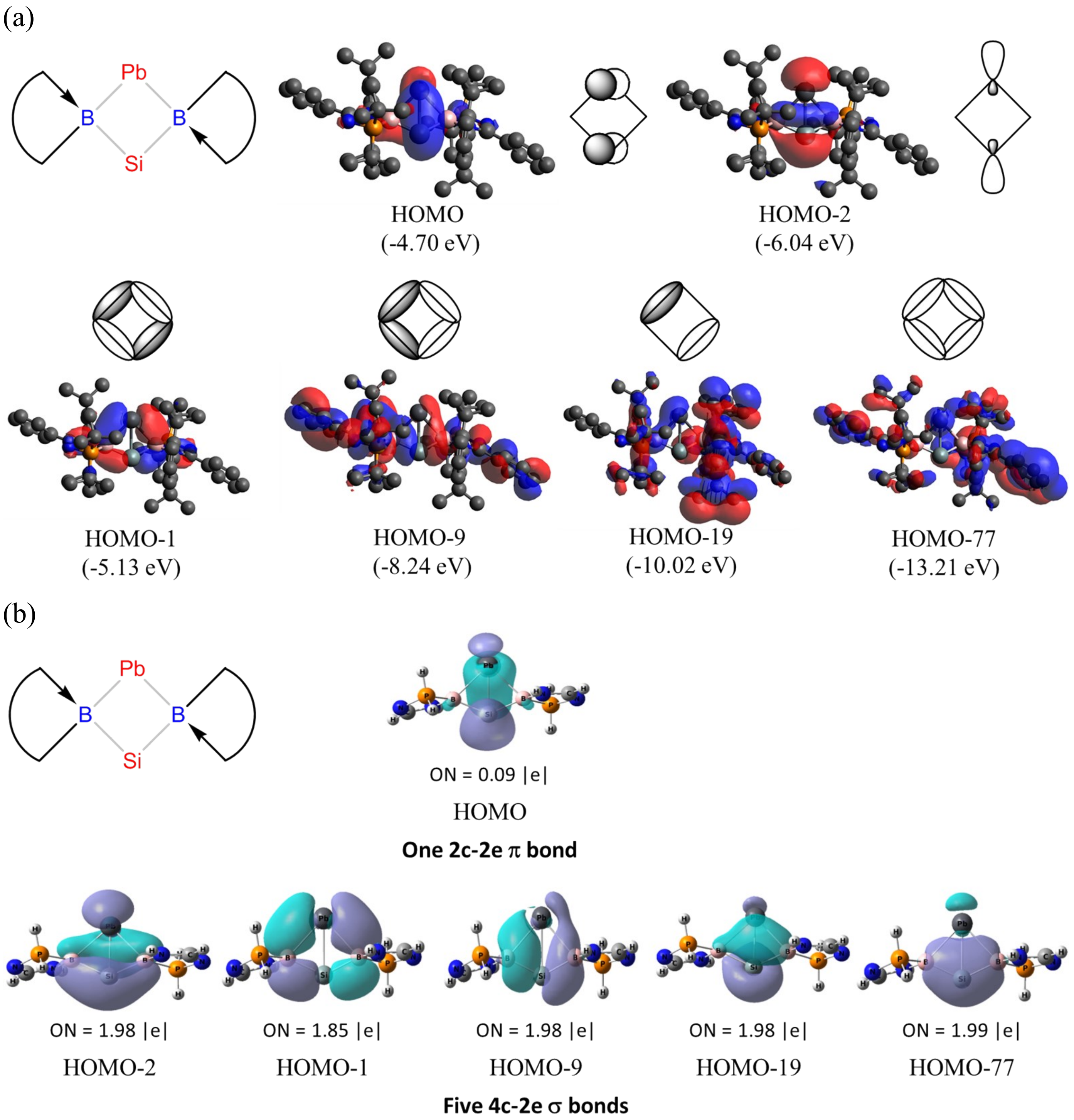


Figure S7. Global minimum structure of the $\mathbf{B_2SiPb}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

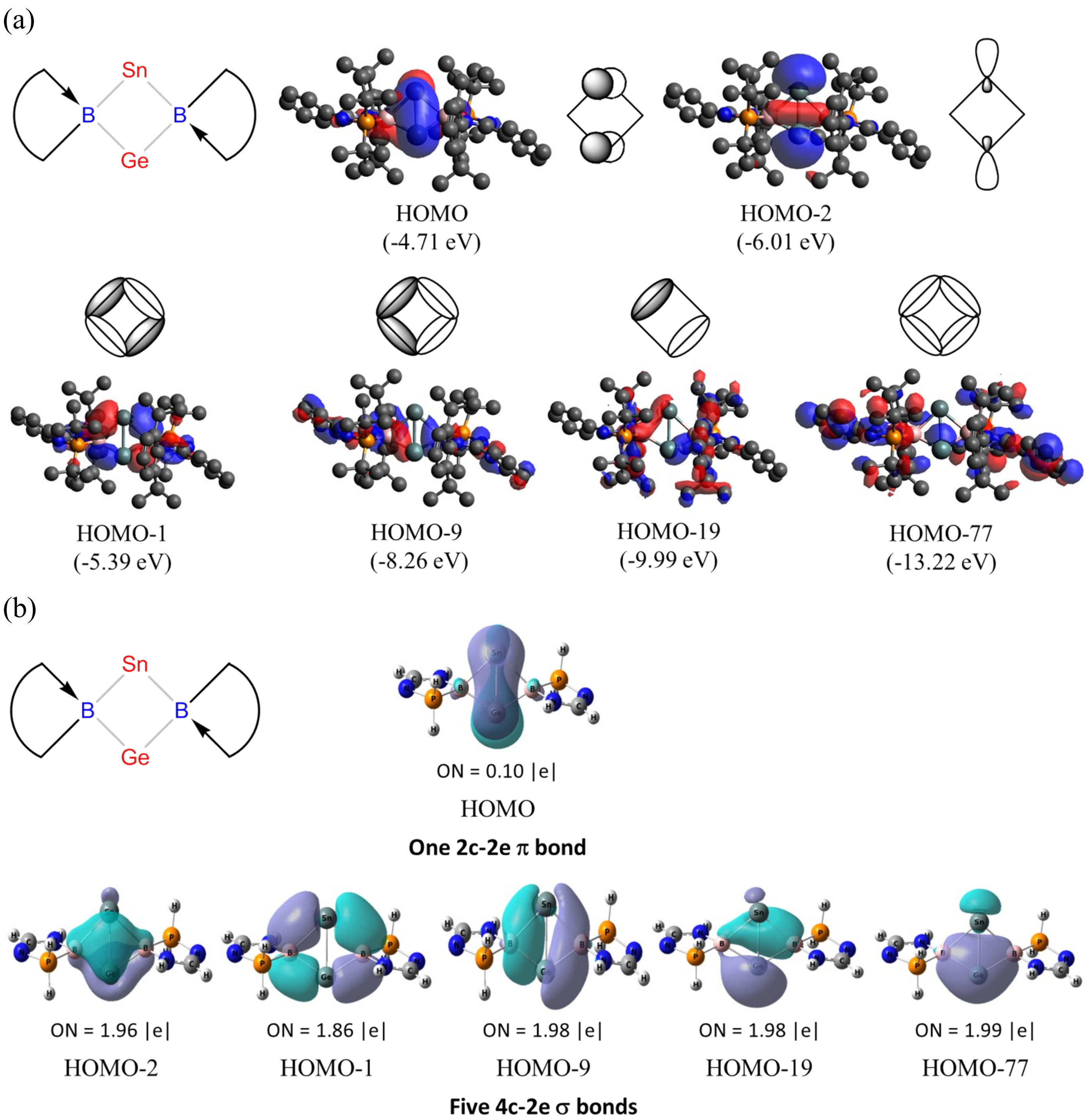


Figure S8. Global minimum structure of the $\mathbf{B_2GeSn}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

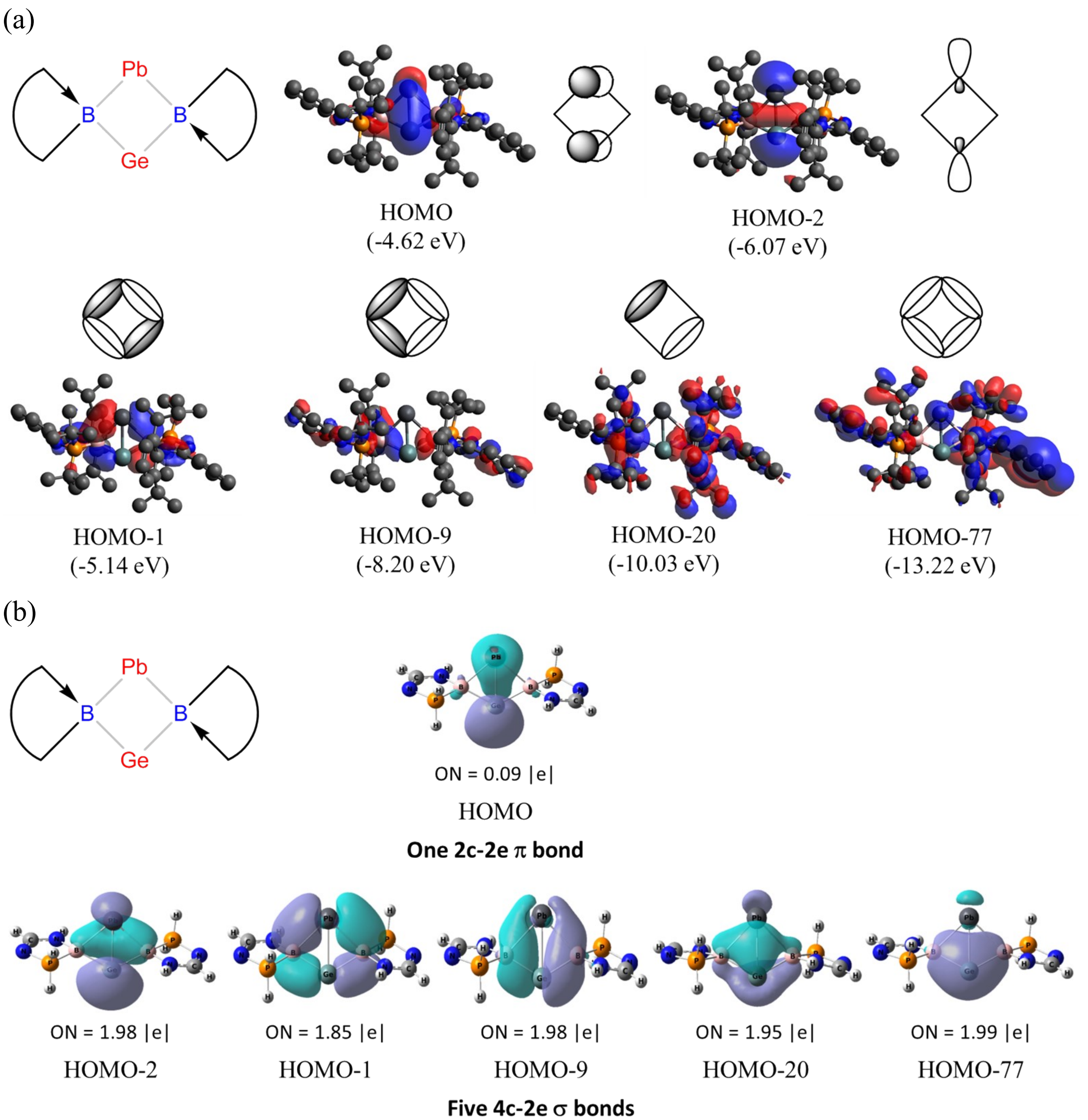


Figure S9. Global minimum structure of the $\mathbf{B_2GePb}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

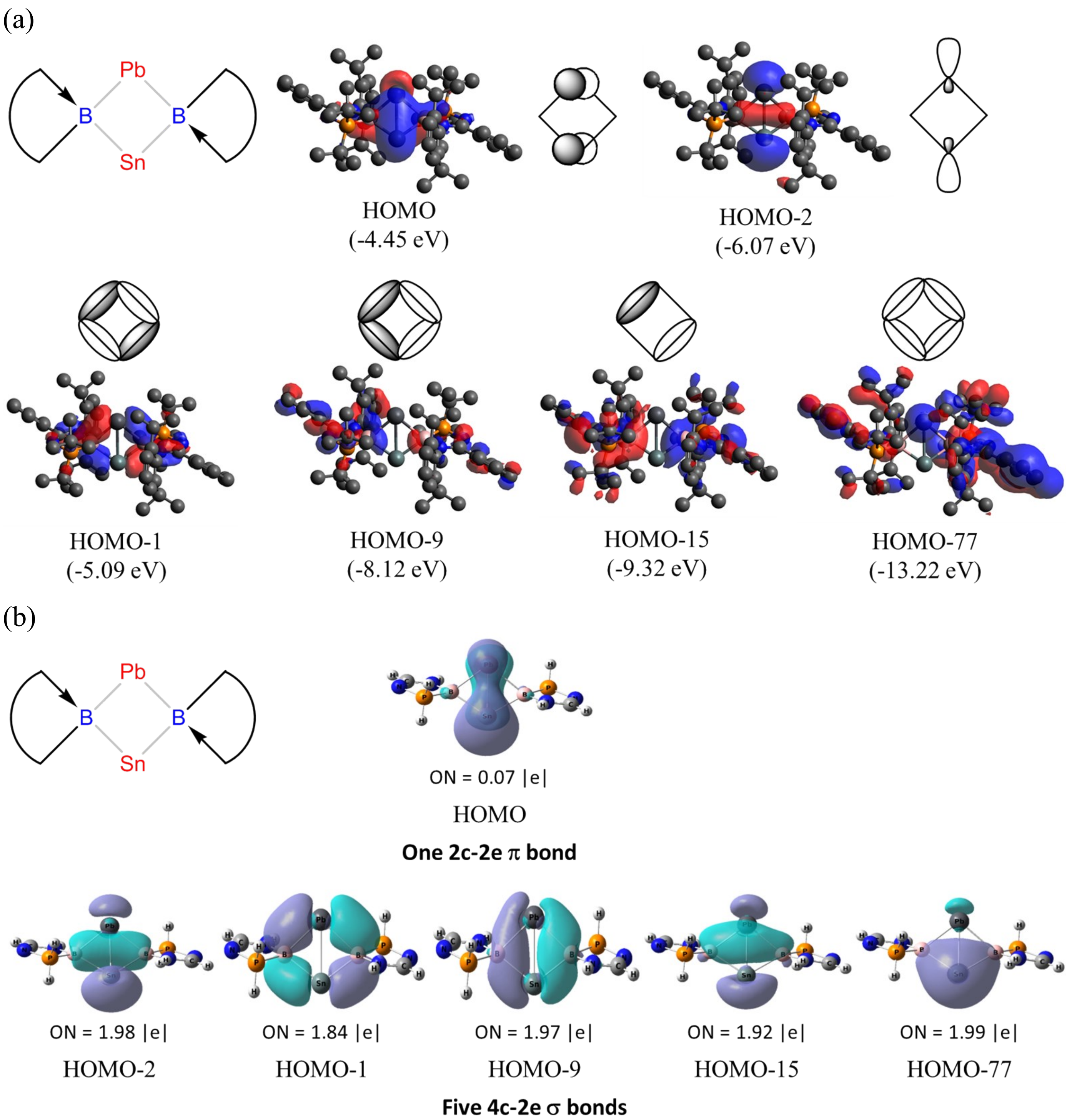


Figure S10. Global minimum structure of the $\mathbf{B_2SnPb}$ molecule. (a) Six significant occupied orbitals. (b) Chemical bonding according to the AdNDP analysis.

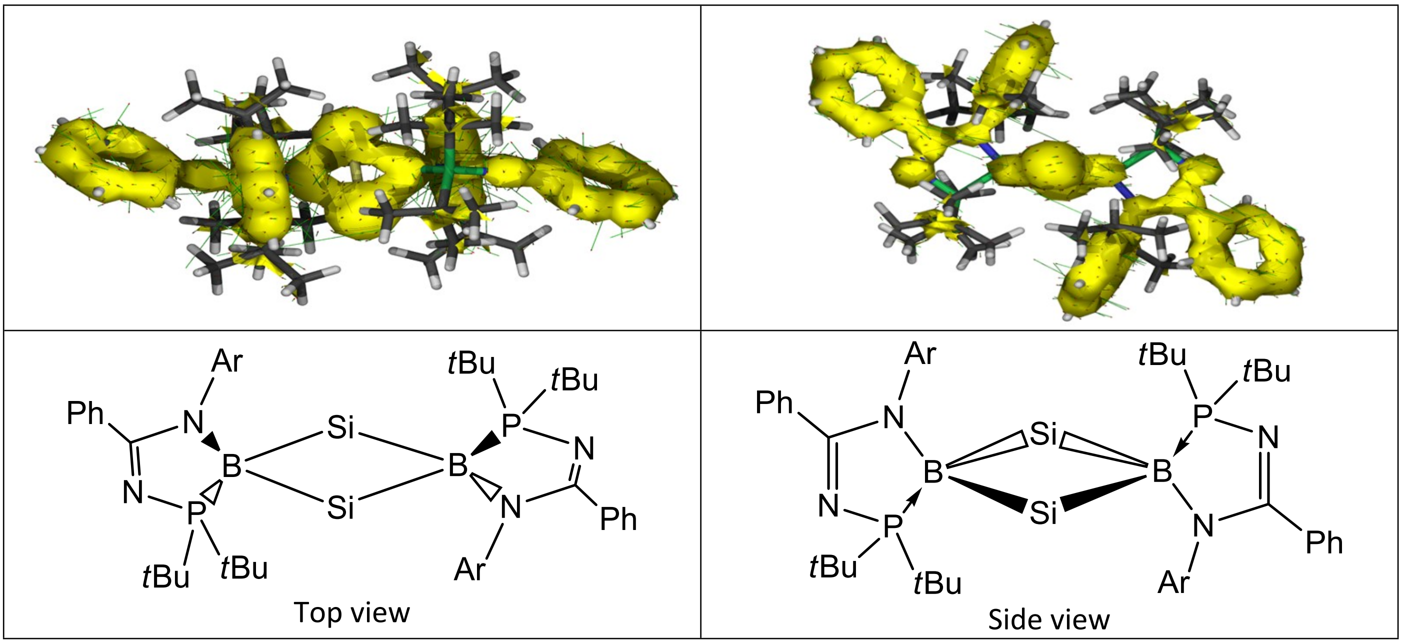


Figure S11. ACID plots for the four-membered $\mathbf{B_2Si_2}$ species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

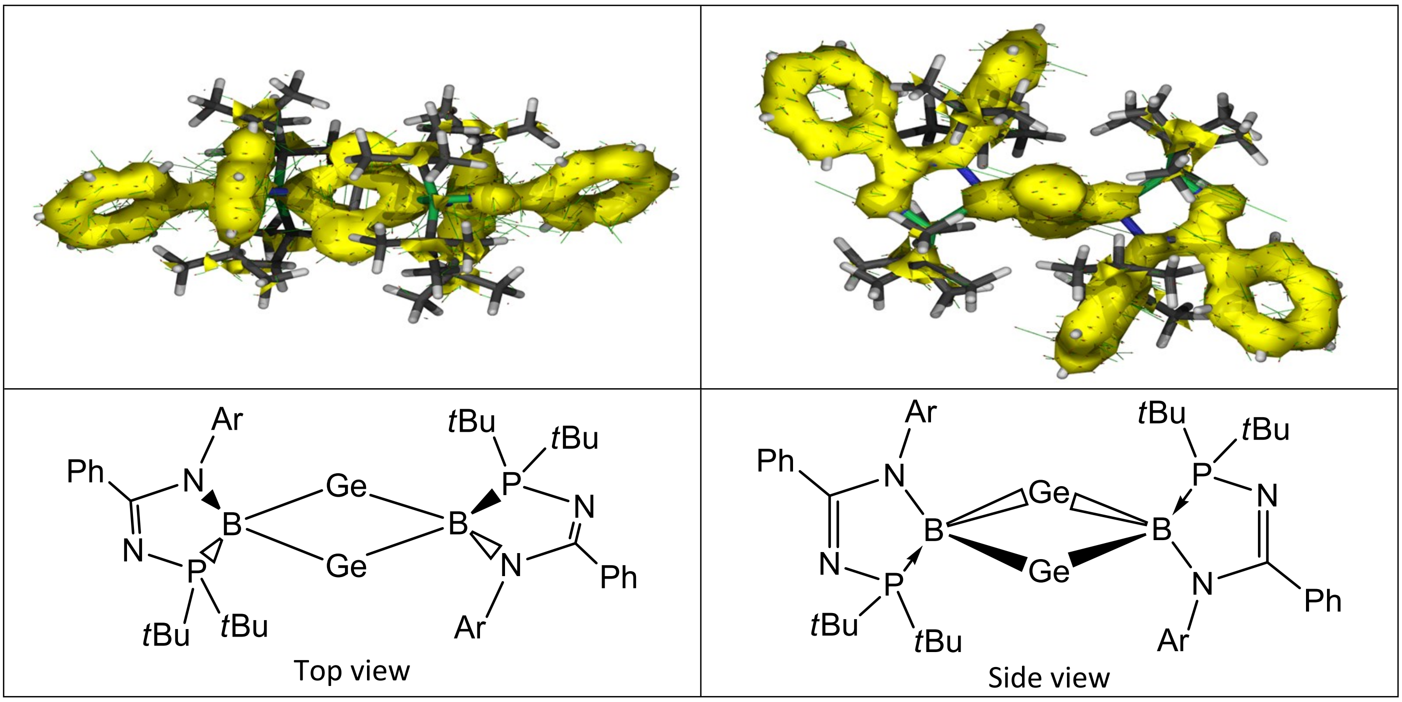


Figure S12. ACID plots for the four-membered $\mathbf{B_2Ge_2}$ species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

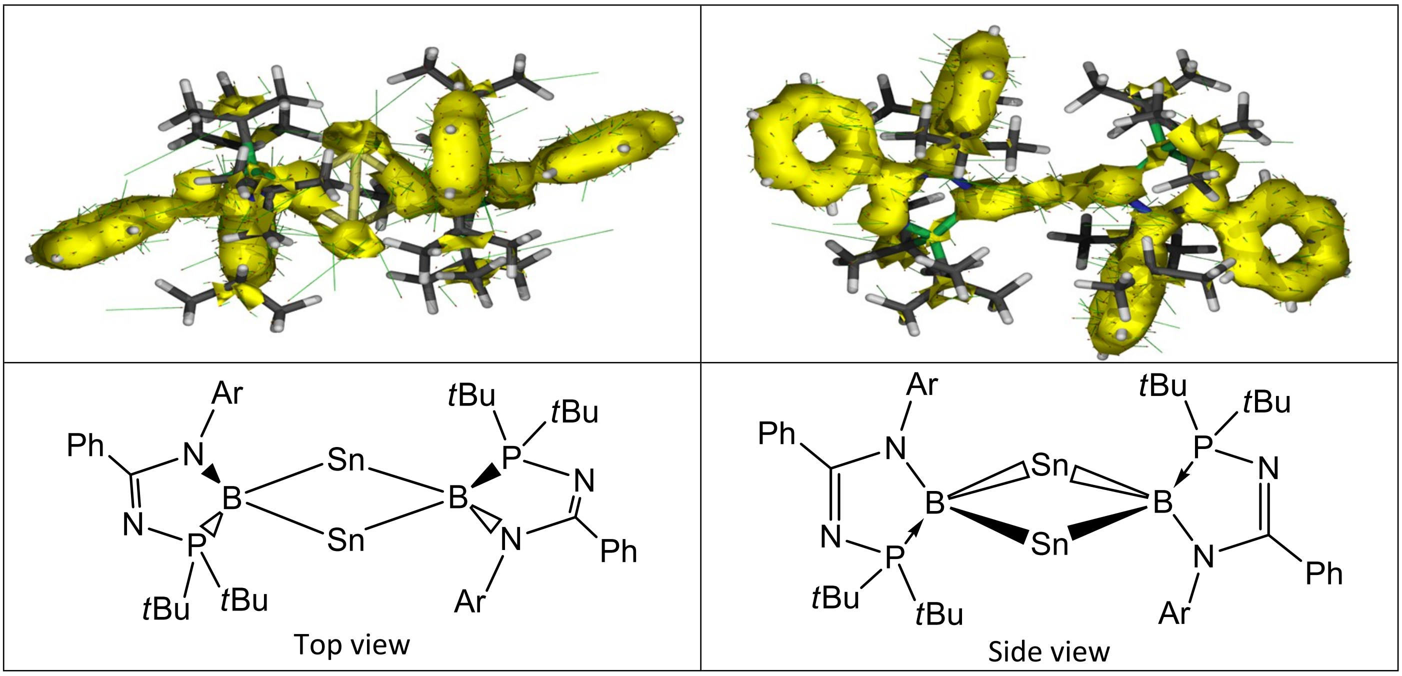


Figure S13. ACID plots for the four-membered B_2Sn_2 species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

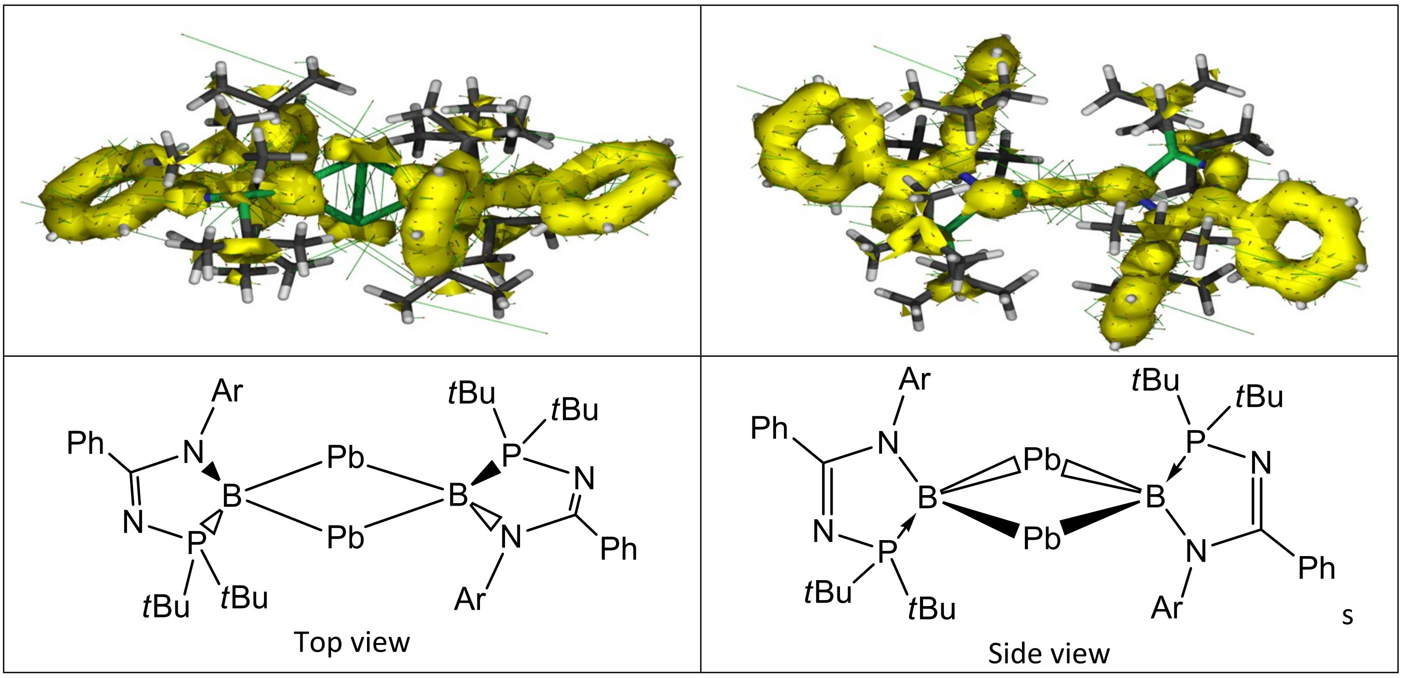


Figure S14. ACID plots for the four-membered B_2Pb_2 species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

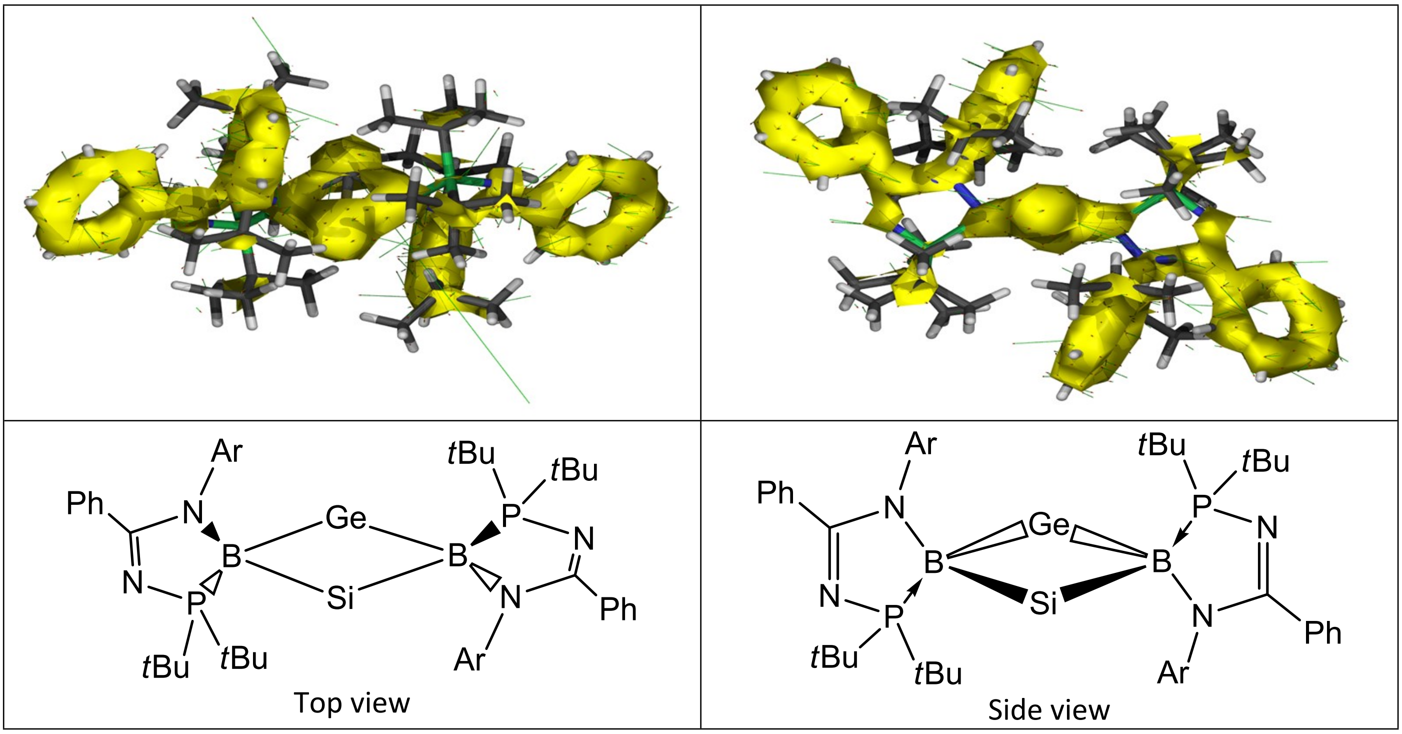


Figure S15. ACID plots for the four-membered **B_2SiGe** species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

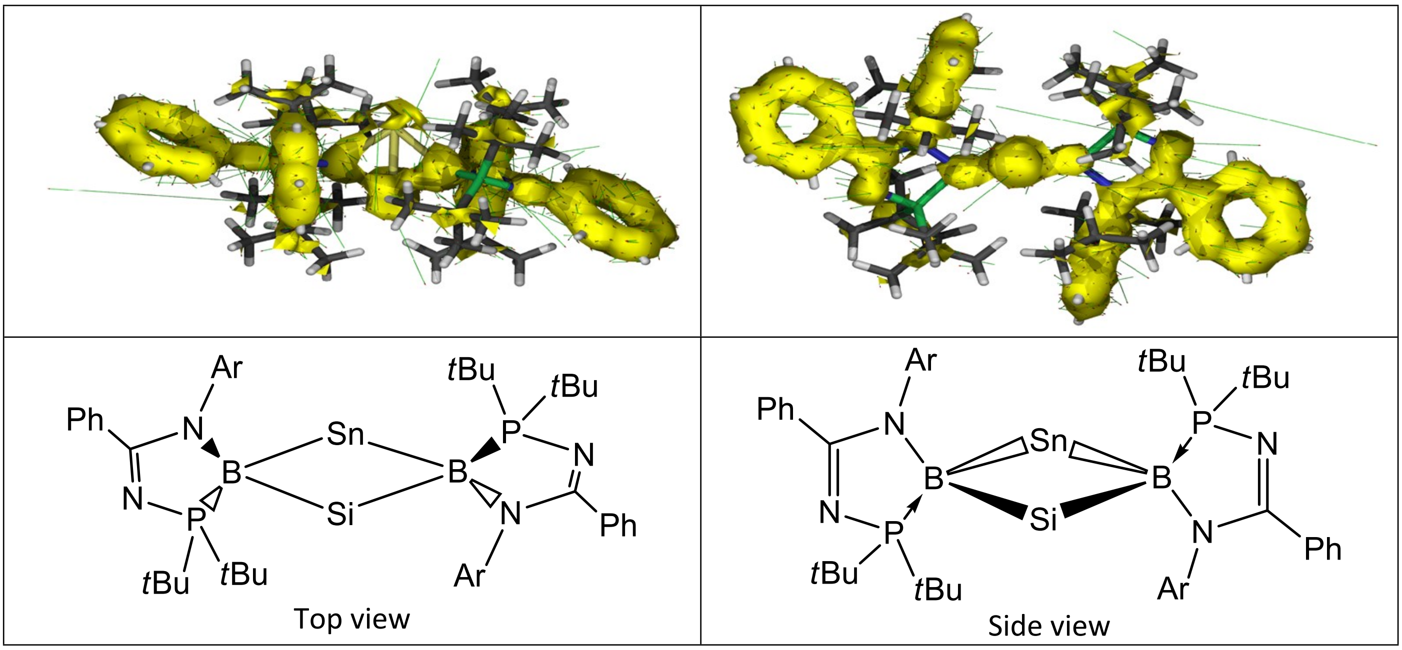


Figure S16. ACID plots for the four-membered **B_2SiSn** species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

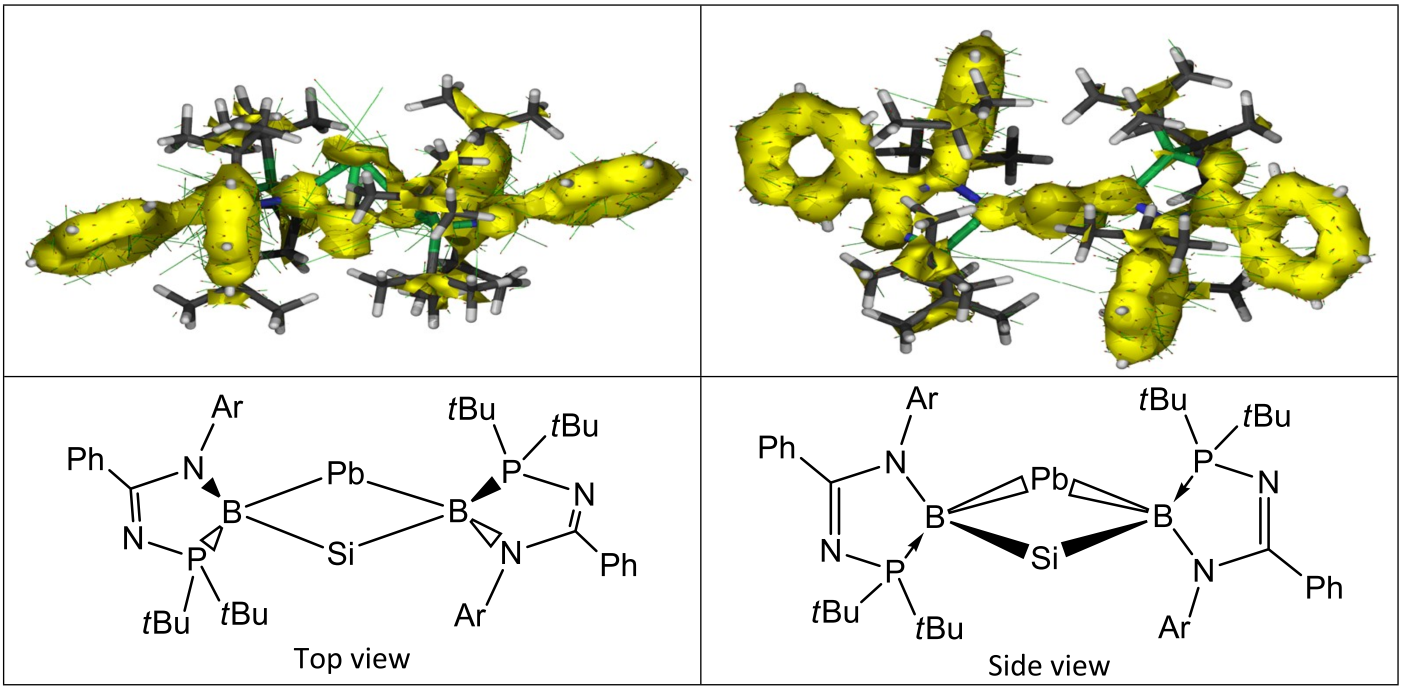


Figure S17. ACID plots for the four-membered $\mathbf{B_2SiPb}$ species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

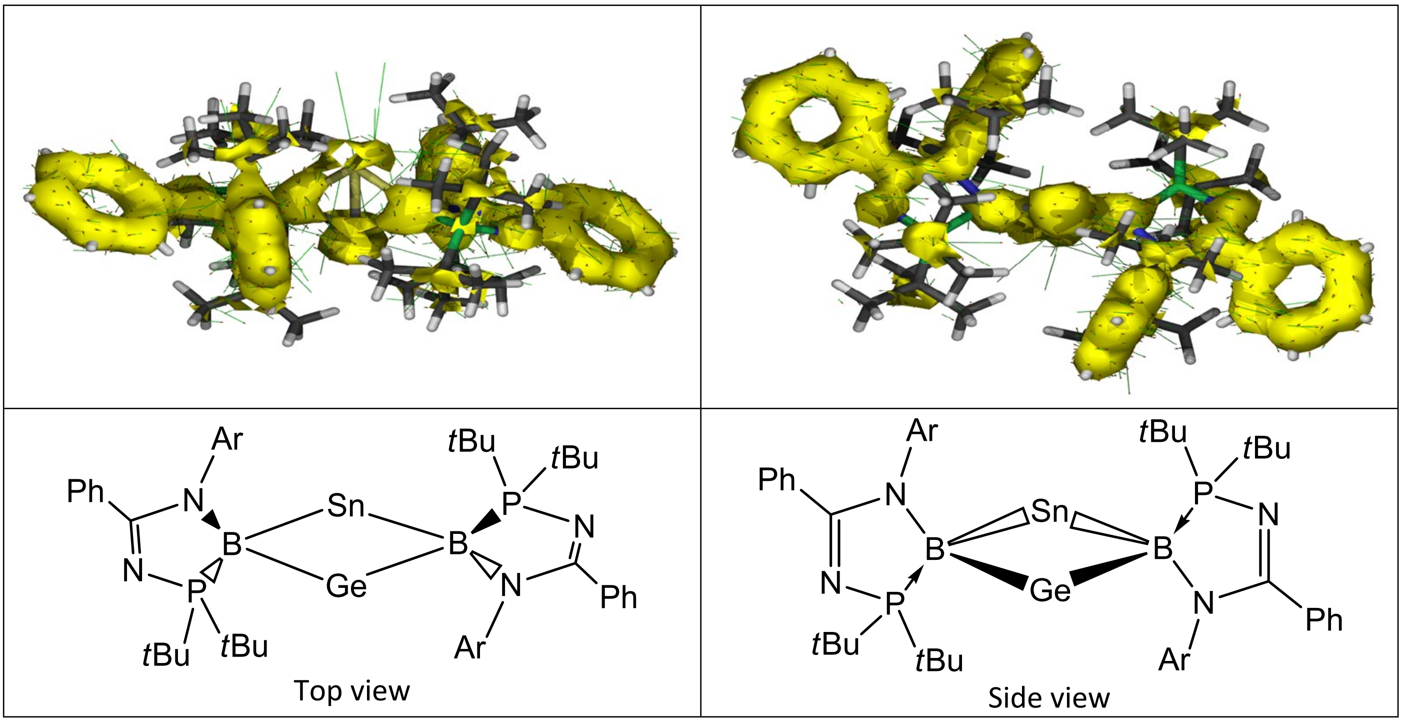


Figure S18. ACID plots for the four-membered $\mathbf{B_2GeSn}$ species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

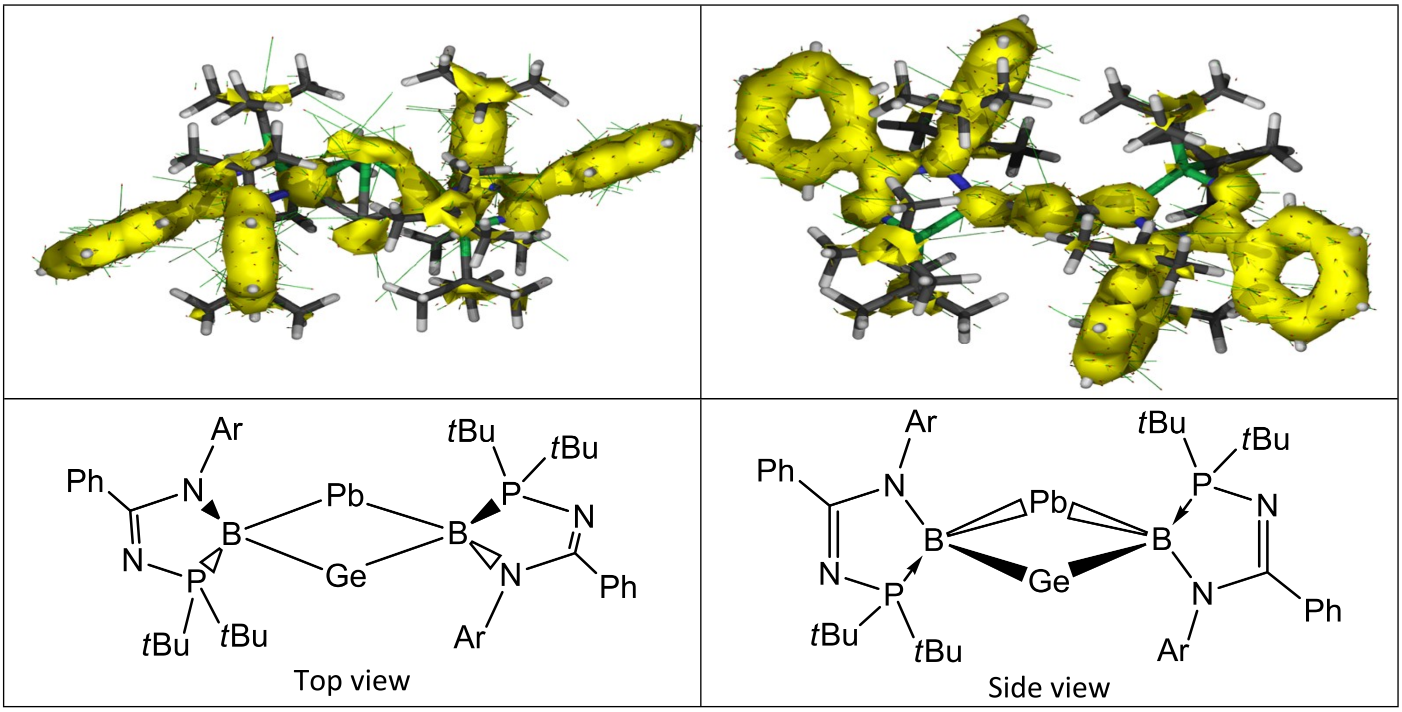


Figure S19. ACID plots for the four-membered $\mathbf{B_2GePb}$ species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

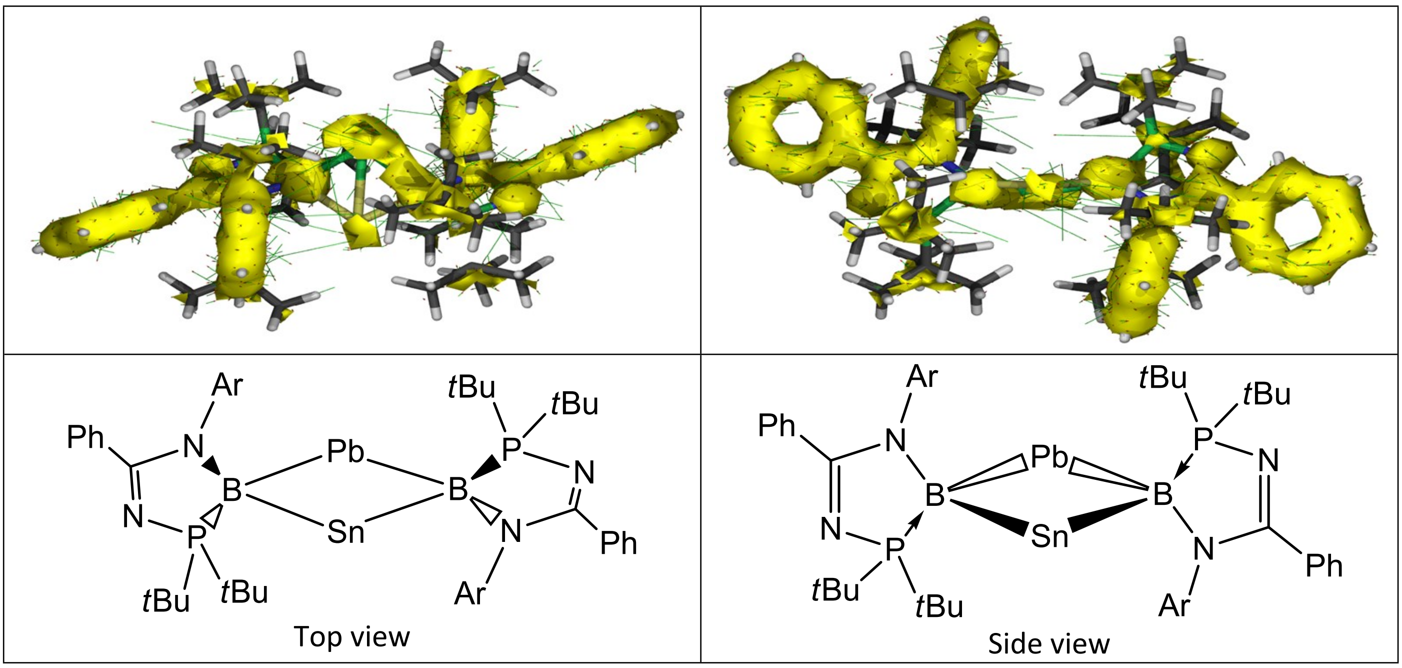


Figure S20. ACID plots for the four-membered $\mathbf{B_2SnPb}$ species. The current density vectors (green arrows with red tips) are plotted onto an iso-surface of contour value 0.05. See the text.

NICS(0)	-38.52 ppm
$NICS(0)_{zz}$	-45.50 ppm
NICS(1)	-22.12 ppm
$NICS(1)_{zz}$	-34.01 ppm

Table S1. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the **B_2Si_2** ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-38.37 ppm
$NICS(0)_{zz}$	-33.32 ppm
NICS(1)	-21.92 ppm
$NICS(1)_{zz}$	-34.65 ppm

Table S2. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the **B_2Ge_2** ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-29.41 ppm
$NICS(0)_{zz}$	-19.80 ppm
NICS(1)	-18.60 ppm
$NICS(1)_{zz}$	-29.06 ppm

Table S3. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the $\mathbf{B_2Sn_2}$ ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-24.53 ppm
$NICS(0)_{zz}$	-15.87 ppm
NICS(1)	-15.42 ppm
$NICS(1)_{zz}$	-25.39 ppm

Table S4. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the $\mathbf{B_2Pb_2}$ ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-38.61 ppm
$NICS(0)_{zz}$	-39.06 ppm
NICS(1)	-21.98 ppm
$NICS(1)_{zz}$	-34.56 ppm

Table S5. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the $\mathbf{B_2SiGe}$ ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-32.96 ppm
$NICS(0)_{zz}$	-28.61 ppm
NICS(1)	-19.87 ppm
$NICS(1)_{zz}$	-30.58 ppm

Table S6. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the $\mathbf{B_2SiSn}$ ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-30.35 ppm
$NICS(0)_{zz}$	-25.01 ppm
NICS(1)	-17.89 ppm
$NICS(1)_{zz}$	-27.66 ppm

Table S7. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the **B_2SiPb** ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-33.57 ppm
$NICS(0)_{zz}$	-25.32 ppm
NICS(1)	-20.15 ppm
$NICS(1)_{zz}$	-31.67 ppm

Table S8. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the **B_2GeSn** ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-30.43 ppm
$NICS(0)_{zz}$	-22.74 ppm
NICS(1)	-18.53 ppm
$NICS(1)_{zz}$	-29.64 ppm

Table S9. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the **B_2GePb** ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

NICS(0)	-25.76 ppm
$NICS(0)_{zz}$	-17.43 ppm
NICS(1)	-17.46 ppm
$NICS(1)_{zz}$	-27.21 ppm

Table S10. Calculated NICS value under the M06-2X/Def2-TZVP of theory. NICS(0) and NICS(1) represents the chemical shift at the **B_2SnPb** ring center and the chemical shift 1Å above the ring center. ZZ represents the chemical shift alone the Z-axis.

Table S11. NBO analysis of $\mathbf{B_2Si_2}$ at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Si_1 (Lone Pair)	1.60	100.00 % Si_1	Si_1:$SP^{0.36}$	2.293	1.012	Si_1: +0.35 Si_2: +0.35 B_1: −0.55 B_2: −0.55
Si_2 (Lone Pair)	1.60	100.00 % Si_2	Si_2: $SP^{0.36}$			
Si_1 (Lone vacancy)	0.76	100.00 % Si_1	Si_1:$P^{99.99}$			
Si_2 (Lone vacancy)	0.76	100.00 % Si_2	Si_2: $P^{99.99}$			
Si_1–B_1 σ	1.59	36.56 % Si_1 + 63.44 % B_1	Si_1: $SP^{6.48}$ B_1: $SP^{3.23}$	2.026	0.968	
Si_1–B_2 σ	1.60	35.81 % Si_1 + 64.19 % B_2	Si_1: $SP^{6.62}$ B_1: $SP^{2.52}$	2.019	0.985	
Si_2–B_1 σ	1.60	35.80 % Si_2 + 64.20 % B_1	Si_1: $SP^{6.62}$ B_1: $SP^{2.52}$	2.026	0.985	
Si_2–B_2 σ	1.59	36.56 % Si_2 + 63.44 % B_2	Si_1: $SP^{6.48}$ B_1: $SP^{3.23}$	2.019	0.968	

Table S12. NBO analysis of $\mathbf{B_2Ge_2}$ at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Ge_1 (Lone Pair)	1.65	100.00 % Ge_1	Ge_1:$SP^{0.31}$	2.436	1.029	Ge_1: +0.25 Ge_2: +0.25 B_1: –0.42 B_2: –0.42
Ge_2 (Lone Pair)	1.65	100.00 % Ge_2	Ge_2: $SP^{0.31}$			
Ge_1 (Lone vacancy)	0.74	100.00 % Ge_1	Ge_1:$P^{99.99}$			
Ge_2 (Lone vacancy)	0.74	100.00 % Ge_2	Ge_2: $P^{99.99}$			
Ge_1–B_1 σ	1.59	38.37 % Ge_1 + 61.63 % B_1	Ge_1: $SP^{7.79}$ B_1: $SP^{2.65}$	2.109	0.972	
Ge_1–B_2 σ	1.59	39.60 % Ge_1 + 60.40 % B_2	Ge_1: $SP^{7.51}$ B_2: $SP^{3.29}$	2.114	0.961	
Ge_2–B_1 σ	1.59	39.60 % Ge_2 + 60.40 % B_1	Ge_1: $SP^{7.51}$ B_1: $SP^{3.29}$	2.114	0.961	
Ge_2–B_2 σ	1.59	38.37 % Ge_2 + 61.63 % B_2	Ge_1: $SP^{7.79}$ B_1: $SP^{2.65}$	2.109	0.972	

Table S13. NBO analysis of $\mathbf{B_2Sn_2}$ at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Sn_1 (Lone Pair)	1.78	100.00 % Sn_1	Sn_1:$SP^{0.23}$	2.834	0.557	Sn_1: +0.69 Sn_2: +0.69 B_1: –0.77 B_2: –0.77
Sn_2 (Lone Pair)	1.78	100.00 % Sn_2	Sn_2: $SP^{0.23}$			
Sn_1 (Lone vacancy)	0.44	100.00 % Sn_1	Sn_1:$P^{99.99}$			
Sn_2 (Lone vacancy)	0.45	100.00 % Sn_2	Sn_2: $P^{99.99}$			
Sn_1–B_1 σ	1.64	28.02 % Sn_1 + 71.98 % B_1	Sn_1: $SP^{10.12}$ B_1: $SP^{2.14}$	2.351	0.806	
Sn_1–B_2 σ	1.67	29.75 % Sn_1 + 70.25 % B_2	Sn_1: $SP^{8.85}$ B_2: $SP^{4.09}$	2.331	0.855	
Sn_2–B_1 σ	1.67	29.80 % Sn_2 + 70.20 % B_1	Sn_1: $SP^{8.86}$ B_1: $SP^{4.07}$	2.330	0.858	
Sn_2–B_2 σ	1.64	28.06 % Sn_2 + 71.94 % B_2	Sn_1: $SP^{10.13}$ B_1: $SP^{2.13}$	2.350	0.809	

Table S14. NBO analysis of $\mathbf{B_2Pb_2}$ at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Pb_1 (Lone Pair)	1.86	100.00 % Pb_1	Pb_1:$SP^{0.12}$	2.996	0.422	Pb_1: +0.75 Pb_2: +0.75 B_1: –0.78 B_2: –0.78
Pb_2 (Lone Pair)	1.86	100.00 % Pb_2	Pb_2: $SP^{0.12}$			
Pb_1 (Lone vacancy)	0.38	100.00 % Pb_1	Pb_1:$P^{99.99}$			
Pb_2 (Lone vacancy)	0.38	100.00 % Pb_2	Pb_2: $P^{99.99}$			
Pb_1–B_1 σ	1.63	25.82 % Pb_1 + 74.18 % B_1	Pb_1: $SP^{15.14}$ B_1: $SP^{2.10}$	2.444	0.722	
Pb_1–B_2 σ	1.66	27.88 % Pb_1 + 72.12 % B_2	Pb_1: $SP^{12.47}$ B_2: $SP^{4.33}$	2.403	0.804	
Pb_2–B_1 σ	1.66	27.87 % Pb_2 + 72.13 % B_1	Pb_1: $SP^{12.47}$ B_1: $SP^{4.31}$	2.404	0.803	
Pb_2–B_2 σ	1.63	25.83 % Pb_2 + 74.17 % B_2	Pb_1: $SP^{15.16}$ B_1: $SP^{2.09}$	2.446	0.722	

Table S15. NBO analysis of $\mathbf{B_2SiGe}$ at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Si (Lone Pair)	0.82	100.00 % Si	Si:$P^{99.99}$	2.359	1.021	Si: +0.36 Ge: +0.25 B_1: −0.49 B_2: −0.49
Ge (Lone Pair)	1.71	100.00 % Ge	Ge: $SP^{0.32}$			
Si (Lone vacancy)	0.61	100.00 % Si	Si:$SP^{9.75}$			
Ge (Lone vacancy)	0.72	100.00 % Ge	Ge: $P^{99.99}$			
Si–B_1 σ	1.87	52.00 % Si_1 + 48.00 % B_1	Si: $SP^{1.17}$ B_1: $SP^{5.73}$	2.008	1.031	
Si–B_2 σ	1.87	51.57 % Si + 48.43 % B_2	Si: $SP^{1.23}$ B_2: $SP^{4.36}$	2.002	1.045	
Ge–B_1 σ	1.62	37.35 % Ge + 62.65 % B_1	Ge: $SP^{7.25}$ B_1: $SP^{1.77}$	2.124	0.913	
Ge–B_2 σ	1.61	38.05 % Ge + 61.95 % B_2	Ge: $SP^{7.11}$ B_1: $SP^{2.19}$	2.129	0.898	

Table S16. NBO analysis of **B_2SiSn** at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Si (Lone Pair)	none	none	none	2.546	0.751	Si: +0.21 Sn: +0.72 B_1: −0.62 B_2: −0.62
Sn (Lone Pair)	1.87	100.00 % Sn	Sn: $SP^{0.18}$			
Si (Lone vacancy)	0.70	100.00 % Si	Si:$SP^{12.83}$			
Sn (Lone vacancy)	none	none	none			
Si–Sn π	1.57	76.12 % Si + 23.88 % Sn	Si: $SP^{7.76}$ Sn: $P^{99.99}$			
Si–B_1 σ	1.87	45.70 % Si_1 + 54.30 % B_1	Si: $SP^{1.42}$ B_1: $SP^{3.23}$	1.986	1.222	
Si–B_2 σ	1.86	45.66 % Si + 54.34 % B_2	Si: $SP^{1.46}$ B_2: $SP^{3.81}$	1.982	1.220	
Sn–B_1 σ	1.55	26.92 % Sn + 73.08 % B_1	Sn: $SP^{11.13}$ B_1: $SP^{2.69}$	2.409	0.623	
Sn–B_2 σ	1.54	27.61 % Sn + 72.39 % B_2	Sn: $SP^{10.18}$ B_2: $SP^{2.99}$	2.397	0.631	

Table S17. NBO analysis of $\mathbf{B_2SiPb}$ at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Si (Lone Pair)	none	none	none			
Pb (Lone Pair)	1.93	100.00 % Pb	Pb: $SP^{0.10}$			
Si (Lone vacancy)	0.72	100.00 % Si	Si:$SP^{15.27}$	2.608	0.702	
Pb (Lone vacancy)	none	none	none			
Si–Pb π	1.59	78.68 % Si + 21.32 % Pb	Si: $SP^{6.18}$ Pb: $P^{99.99}$			Si: +0.17 Pb: +0.75 B_1: −0.60 B_2: −0.60
Si–B_1 σ	1.89	44.78 % Si_1 + 55.22 % B_1	Si: $SP^{1.48}$ B_1: $SP^{2.64}$	1.976	1.262	
Si–B_2 σ	1.88	44.97 % Si + 55.03 % B_2	Si: $SP^{1.49}$ B_2: $SP^{3.17}$	1.973	1.259	
Pb–B_1 σ	1.51	26.04 % Pb + 73.96 % B_1	Pb: $SP^{16.24}$ B_1: $SP^{3.43}$	2.538	0.545	
Pb–B_2 σ	1.51	26.75 % Pb + 73.25 % B_2	Pb: $SP^{14.38}$ B_2: $SP^{3.74}$	2.510	0.560	

Table S18. NBO analysis of $\mathbf{B_2GeSn}$ at the M06-2X/Def2-TZVP level of theory.

<table>
<tr><th>Bond type</th><th>Occupancy</th><th>Polarization</th><th>Hybridization</th><th>Bond Length (Å)</th><th>WBI</th><th>NPA</th></tr>
<tr><td>Ge
(Lone Pair)</td><td>1.57</td><td>100.00 % Ge</td><td>Ge:$SP^{0.43}$</td><td rowspan="4">2.623</td><td rowspan="4">0.779</td><td rowspan="8">Ge: +0.11
Sn: +0.72
B_1: −0.55
B_2: −0.54</td></tr>
<tr><td>Sn
(Lone Pair)</td><td>1.83</td><td>100.00 % Sn</td><td>Sn: $SP^{0.18}$</td></tr>
<tr><td>Ge
(Lone vacancy)</td><td>0.77</td><td>100.00 % Ge</td><td>Ge:$SP^{66.50}$</td></tr>
<tr><td>Sn
(Lone vacancy)</td><td>0.45</td><td>100.00 % Sn</td><td>Sn: $P^{99.99}$</td></tr>
<tr><td>Ge–B_1 σ</td><td>1.74</td><td>42.47 % Ge
+
57.53 % B_1</td><td>Ge: $SP^{5.65}$
B_1: $SP^{2.52}$</td><td>2.079</td><td>1.179</td></tr>
<tr><td>Ge–B_2 σ</td><td>1.72</td><td>40.83 % Ge
+
59.17 % B_2</td><td>Ge: $SP^{6.27}$
B_2: $SP^{1.90}$</td><td>2.077</td><td>1.159</td></tr>
<tr><td>Sn–B_1 σ</td><td>1.53</td><td>27.56 % Sn
+
72.44 % B_1</td><td>Sn: $SP^{11.92}$
B_1: $SP^{3.74}$</td><td>2.401</td><td>0.667</td></tr>
<tr><td>Sn–B_2 σ</td><td>1.54</td><td>28.99 % Sn
+
71.01 % B_2</td><td>Sn: $SP^{11.00}$
B_2: $SP^{5.01}$</td><td>2.384</td><td>0.681</td></tr>
</table>

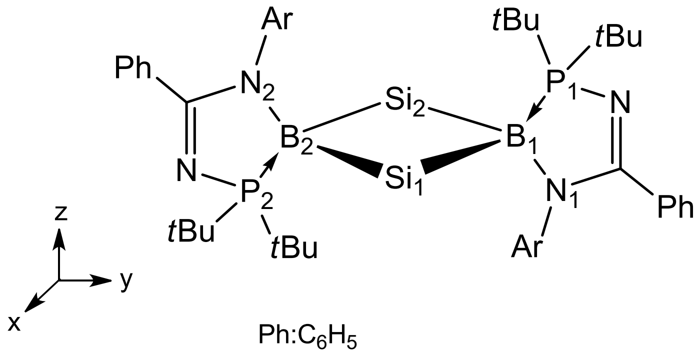
Table S19. NBO analysis of **B_2GePb** at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Ge (Lone Pair)	1.56	100.00 % Ge	Ge:$SP^{0.47}$	2.690	0.699	Ge: +0.07 Pb: +0.77 B_1: −0.52 B_2: −0.54
Pb (Lone Pair)	1.91	100.00 % Pb	Pb: $SP^{0.10}$			
Ge (Lone vacancy)	0.78	100.00 % Ge	Ge:$SP^{54.22}$			
Pb (Lone vacancy)	0.42	100.00 % Pb	Pb: $SP^{17.78}$			
Pb (Lone vacancy)	0.40	100.00 % Pb	Pb: $P^{99.99}$			
Ge–B_1 σ	1.79	42.82 % Ge + 57.18 % B_1	Ge: $SP^{5.16}$ B_1: $SP^{2.25}$	2.068	1.231	
Ge–B_2 σ	1.76	41.31 % Ge + 58.69 % B_2	Ge: $SP^{5.92}$ B_2: $SP^{1.75}$	2.067	1.215	
Pb–B_1 σ	none	none	none	2.529	0.568	
Pb–B_2 σ	1.51	27.27 % Pb + 72.73 % B_2	Pb: $SP^{15.98}$ B_2: $SP^{5.68}$	2.493	0.592	

Table S20. NBO analysis of **B_2SnPb** at the M06-2X/Def2-TZVP level of theory.

Bond type	Occupancy	Polarization	Hybridization	Bond Length (Å)	WBI	NPA
Sn (Lone Pair)	1.74	100.00 % Sn	Sn:$SP^{0.26}$	2.902	0.518	Sn: +0.57 Pb: +0.79 B_1: −0.72 B_2: −0.74
Pb (Lone Pair)	1.89	100.00 % Pb	Pb: $SP^{0.11}$			
Sn (Lone vacancy)	0.52	100.00 % Sn	Sn:$SP^{80.73}$			
Pb (Lone vacancy)	0.35	100.00 % Pb	Pb: $P^{99.99}$			
Sn–B_1 σ	1.73	31.85 % Sn + 68.15 % B_1	Sn: $SP^{8.04}$ B_1: $SP^{2.77}$	2.303	0.984	
Sn–B_2 σ	1.70	29.65 % Sn + 70.35 % B_2	Sn: $SP^{9.66}$ B_2: $SP^{2.20}$	2.317	0.930	
Pb–B_1 σ	1.59	25.52 % Pb + 74.48 % B_1	Pb: $SP^{15.63}$ B_1: $SP^{3.23}$	2.507	0.632	
Pb–B_2 σ	1.61	27.10 % Pb + 72.90 % B_2	Pb: $SP^{13.02}$ B_2: $SP^{4.15}$	2.455	0.696	

Table S21. **B_2Si_2**. All Si_1 lone pair orbital contribution in NBO analysis of second order perturbation theory.

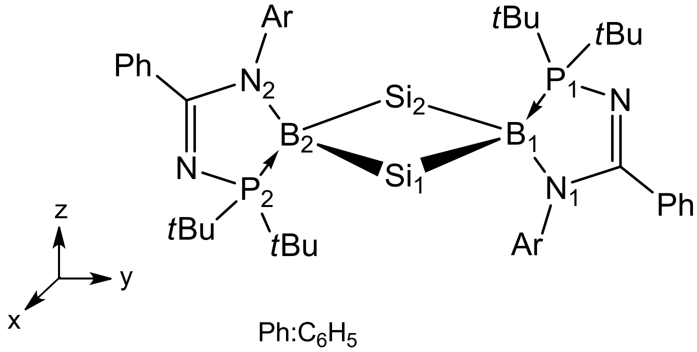


Ph: C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Si_1 (Lone Pair)	BD*Si_1-B_1	8.45
Si_1 (Lone Pair)	BD*Si_1-B_2	9.06
Si_1 (Lone Pair)	BD*B_1-N_1	3.03
Si_1 (Lone Pair)	BD*B_2-P_2	2.68
Si_1 (Lone Pair)	BD*B_1-Si_2	0.85
Si_1 (Lone Pair)	BD*B_2-Si_2	0.58
Si_1 (Lone Pair)	BD*C_{24}- H_{52}	0.76
Si_1 (Lone Pair)	BD*C_{28}- H_{62}	0.58
Si_1 (Lone Pair)	BD*C_{103}- H_{135}	1.22

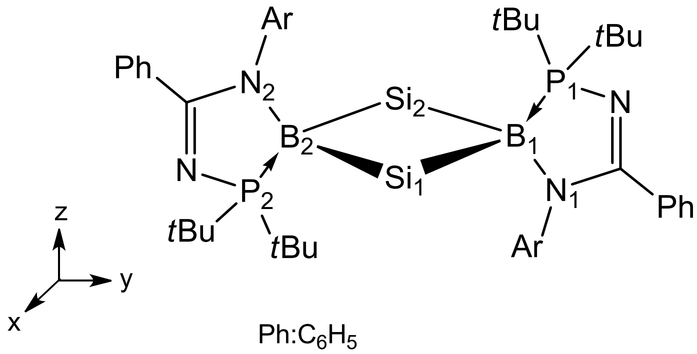
Table S22. **B_2Si_2**. All Si_1 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
BD Si_1- B_2	Si_1 (Lone vacancy)	0.59
BD B_1- P_1	Si_1 (Lone vacancy)	1.03
BD B_1-Si_2	Si_1 (Lone vacancy)	7.06
BD B_2-Si_2	Si_1 (Lone vacancy)	7.62
BD B_2- P_2	Si_1 (Lone vacancy)	0.63
BD B_2- N_2	Si_1 (Lone vacancy)	1.05
BD C_{17}- C_{35}	Si_1 (Lone vacancy)	1.51
BD C_{28}- H_{62}	Si_1 (Lone vacancy)	0.53
BD C_{29}- H_{66}	Si_1 (Lone vacancy)	1.69
BD C_{55}- H_{87}	Si_1 (Lone vacancy)	1.03
BD C_{85}- H_{111}	Si_1 (Lone vacancy)	0.52
BD C_{103}- H_{135}	Si_1 (Lone vacancy)	1.14

Table S23. **B_2Si_2**. All Si_2 lone pair orbital contribution in NBO analysis of second order perturbation theory.

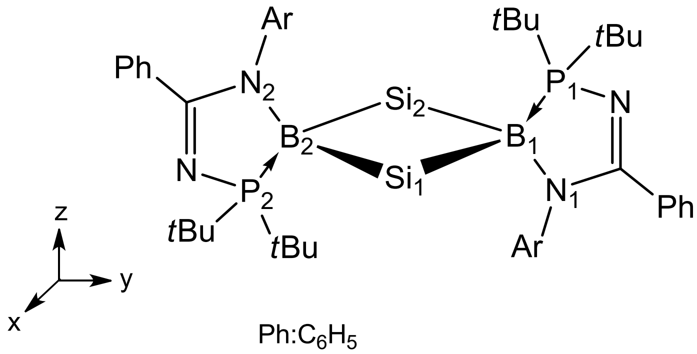


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Si_2 (Lone Pair)	BD*B_1-Si_2	9.05
Si_2 (Lone Pair)	BD*B_2-Si_2	8.45
Si_2 (Lone Pair)	BD*B_2-N_2	3.04
Si_2 (Lone Pair)	BD*B_1-P_1	2.68
Si_2 (Lone Pair)	BD*Si_1- B_1	0.58
Si_2 (Lone Pair)	BD*Si_1- B_2	0.85
Si_2 (Lone Pair)	BD*C_{19}- H_{37}	0.58
Si_2 (Lone Pair)	BD*C_{33}- H_{76}	0.76
Si_2 (Lone Pair)	BD*C_{90}- H_{119}	1.22

Table S24. **B_2Si_2**. All Si_2 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

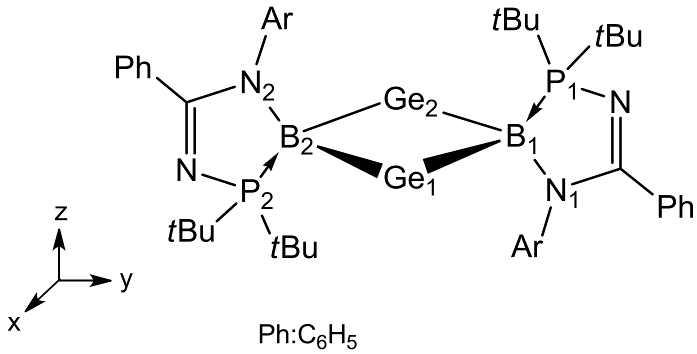


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
BD Si_1- B_1	Si_2 (Lone vacancy)	7.62
BD Si_1- B_2	Si_2 (Lone vacancy)	7.07
BD B_1- P_1	Si_2 (Lone vacancy)	0.63
BD B_1- N_1	Si_2 (Lone vacancy)	1.05
BD B_1-Si_2	Si_2 (Lone vacancy)	0.59
BD B_2- P_2	Si_2 (Lone vacancy)	1.03
BD C_{12}- C_{26}	Si_2 (Lone vacancy)	1.51
BD C_{19}- H_{37}	Si_2 (Lone vacancy)	0.53
BD C_{20}- H_{42}	Si_2 (Lone vacancy)	1.69
BD C_{79}- H_{100}	Si_2 (Lone vacancy)	1.03
BD C_{90}- H_{119}	Si_2 (Lone vacancy)	1.14
BD C_{98}- H_{127}	Si_2 (Lone vacancy)	0.51

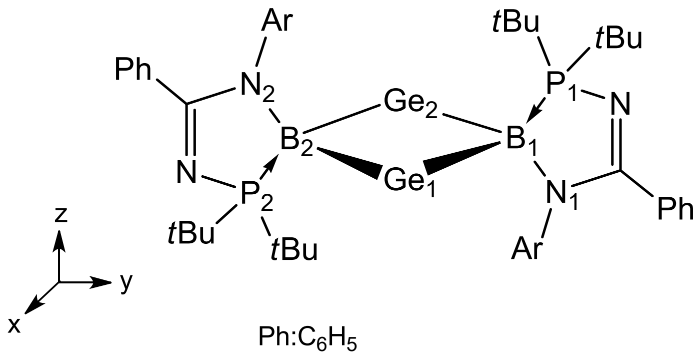
Table S25. **B_2Ge_2**. All Ge_1 lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Ge_1 (Lone Pair)	LV B_2	6.04
Ge_1 (Lone Pair)	BD*Ge_1- B_2	9.17
Ge_1 (Lone Pair)	BD*Ge_1- B_1	9.74
Ge_1 (Lone Pair)	BD*B_1-Ge_2	0.62
Ge_1 (Lone Pair)	BD*B_2- P_2	4.11
Ge_1 (Lone Pair)	BD*C_{24}- H_{52}	0.70
Ge_1 (Lone Pair)	BD*C_{103}- H_{135}	1.09

Table S26. **B_2Ge_2**. All Ge_1 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

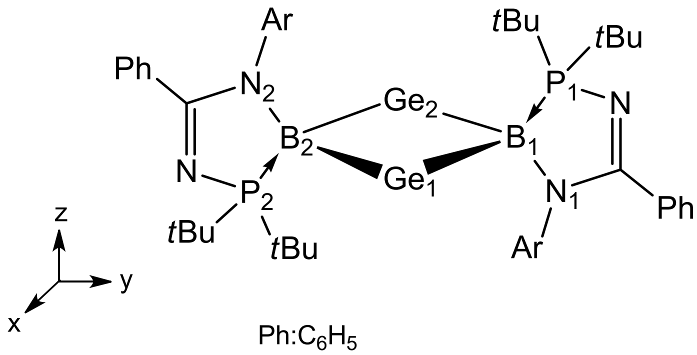


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP N_2	Ge_1 (Lone vacancy)	2.65
LP N_1	Ge_1 (Lone vacancy)	0.58
BD Ge_1- B_1	Ge_1 (Lone vacancy)	1.53
BD B_2-Ge_2	Ge_1 (Lone vacancy)	15.26
BD B_2- P_2	Ge_1 (Lone vacancy)	0.62
BD B_1-Ge_2	Ge_1 (Lone vacancy)	16.50
BD C_{17}- C_{35}	Ge_1 (Lone vacancy)	1.53
BD C_{28}- H_{62}	Ge_1 (Lone vacancy)	0.53
BD C_{29}- H_{66}	Ge_1 (Lone vacancy)	0.99
BD C_{55}- H_{87}	Ge_1 (Lone vacancy)	0.85
BD C_{103}- H_{135}	Ge_1 (Lone vacancy)	0.55

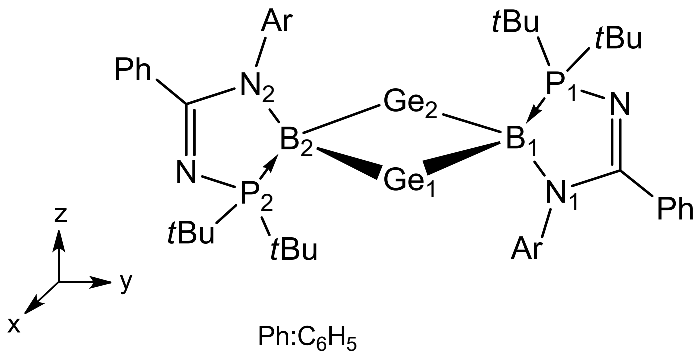
Table S27. **B_2Ge_2**. All Ge_2 lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph: C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Ge_2 (Lone Pair)	LV B_1	6.04
Ge_2 (Lone Pair)	BD*Ge_1- B_1	0.62
Ge_2 (Lone Pair)	BD*B_2-Ge_2	9.74
Ge_2 (Lone Pair)	BD*B_2- P_2	4.11
Ge_2 (Lone Pair)	BD*B_1-Ge_2	9.17
Ge_2 (Lone Pair)	BD*C_{33}- H_{76}	0.70
Ge_2 (Lone Pair)	BD*C_{90}- H_{119}	1.09

Table S28. **B_2Ge_2**. All Ge_2 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

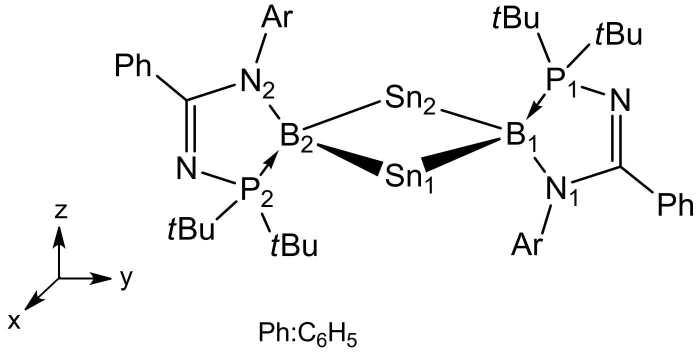


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP N_2	Ge_2 (Lone vacancy)	0.58
LP N_1	Ge_2 (Lone vacancy)	2.65
BD Ge_1- B_2	Ge_2 (Lone vacancy)	16.50
BD Ge_1- B_1	Ge_2 (Lone vacancy)	15.26
BD B_1-Ge_2	Ge_2 (Lone vacancy)	1.53
BD B_1- P_1	Ge_2 (Lone vacancy)	0.62
BD C_{12}- C_{26}	Ge_2 (Lone vacancy)	1.53
BD C_{19}- H_{37}	Ge_2 (Lone vacancy)	0.53
BD C_{20}- H_{42}	Ge_2 (Lone vacancy)	0.99
BD C_{79}- H_{100}	Ge_2 (Lone vacancy)	0.85
BD C_{90}- H_{119}	Ge_2 (Lone vacancy)	0.55

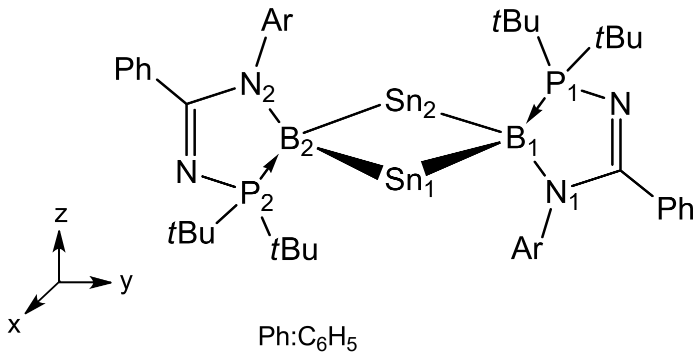
Table S29. **B_2Sn_2**. All Sn_1 lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph: C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Sn_1 (Lone Pair)	LV Sn_1	2.05
Sn_1 (Lone Pair)	LV Sn_2	0.91
Sn_1 (Lone Pair)	BD* Sn_1- B_1	3.82
Sn_1 (Lone Pair)	BD* Sn_1- B_2	4.42
Sn_1 (Lone Pair)	BD* B_1-Sn_2	3.14
Sn_1 (Lone Pair)	BD* B_1- N_1	10.88
Sn_1 (Lone Pair)	BD* B_2-Sn_2	2.38
Sn_1 (Lone Pair)	BD* B_2- P_2	5.17
Sn_1 (Lone Pair)	BD* B_2- N_2	3.44
Sn_1 (Lone Pair)	BD* C_{22}- H_{46}	0.56
Sn_1 (Lone Pair)	BD* C_{24}- H_{52}	0.84
Sn_1 (Lone Pair)	BD* C_{103}- H_{135}	1.61

Table S30. **B_2Sn_2**. All Sn_1 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

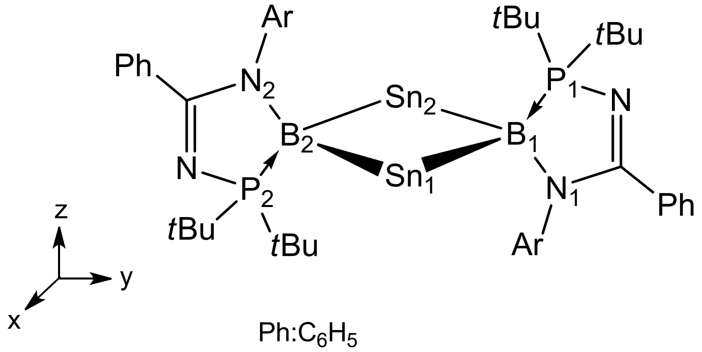


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Sn_1	Sn_1 (Lone vacancy)	2.05
LP Sn_2	Sn_1 (Lone vacancy)	0.89
LP N_1	Sn_1 (Lone vacancy)	0.53
BD B_1-Sn_2	Sn_1 (Lone vacancy)	21.79
BD B_1- P_1	Sn_1 (Lone vacancy)	0.99
BD B_2-Sn_2	Sn_1 (Lone vacancy)	24.68
BD B_2- N_2	Sn_1 (Lone vacancy)	0.92
BD C_{17}- C_{34}	Sn_1 (Lone vacancy)	0.60
BD C_{17}- C_{35}	Sn_1 (Lone vacancy)	1.40
BD C_{20}- H_{42}	Sn_1 (Lone vacancy)	0.97
BD C_{28}- H_{62}	Sn_1 (Lone vacancy)	1.53
BD C_{29}- H_{66}	Sn_1 (Lone vacancy)	0.89
BD C_{55}- H_{87}	Sn_1 (Lone vacancy)	1.20
BD C_{85}- H_{111}	Sn_1 (Lone vacancy)	2.65
BD C_{85}- H_{113}	Sn_1 (Lone vacancy)	0.71

Table S31. **B_2Sn_2**. All Sn_2 lone pair orbital contribution in NBO analysis of second order perturbation theory.

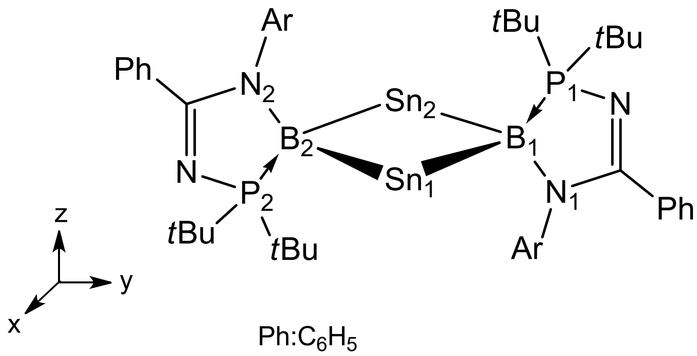


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Sn_2 (Lone Pair)	LV Sn_1	0.89
Sn_2 (Lone Pair)	LV Sn_2	2.04
Sn_2 (Lone Pair)	BD* Sn_1- B_1	2.36
Sn_2 (Lone Pair)	BD* Sn_1- B_2	3.15
Sn_2 (Lone Pair)	BD* B_1-Sn_2	4.49
Sn_2 (Lone Pair)	BD* B_1- P_1	5.26
Sn_2 (Lone Pair)	BD* B_1- N_1	3.46
Sn_2 (Lone Pair)	BD* B_2-Sn_2	3.89
Sn_2 (Lone Pair)	BD* B_2- N_2	11.05
Sn_2 (Lone Pair)	BD* C_{31}- H_{70}	0.57
Sn_2 (Lone Pair)	BD* C_{33}- H_{76}	0.83
Sn_2 (Lone Pair)	BD* C_{90}- H_{119}	1.61

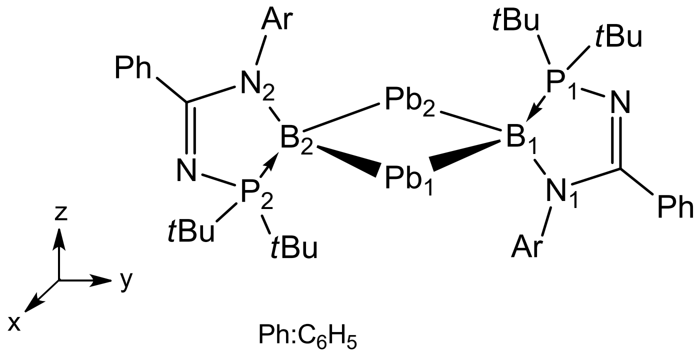
Table S32. **B_2Sn_2**. All Sn_2 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph: C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Sn_1	Sn_2 (Lone vacancy)	0.91
LP Sn_2	Sn_2 (Lone vacancy)	2.04
LP N_2	Sn_2 (Lone vacancy)	0.54
BD Sn_1- B_1	Sn_2 (Lone vacancy)	25.08
BD Sn_1- B_2	Sn_2 (Lone vacancy)	22.25
BD B_1- N_1	Sn_2 (Lone vacancy)	0.91
BD B_2- P_2	Sn_2 (Lone vacancy)	0.99
BD C_{12}- C_{25}	Sn_2 (Lone vacancy)	0.59
BD C_{12}- C_{26}	Sn_2 (Lone vacancy)	1.39
BD C_{19}- H_{37}	Sn_2 (Lone vacancy)	1.52
BD C_{20}- H_{42}	Sn_2 (Lone vacancy)	0.86
BD C_{29}- H_{66}	Sn_2 (Lone vacancy)	0.97
BD C_{79}- H_{100}	Sn_2 (Lone vacancy)	1.18
BD C_{98}- H_{127}	Sn_2 (Lone vacancy)	2.62
BD C_{98}- H_{129}	Sn_2 (Lone vacancy)	0.70

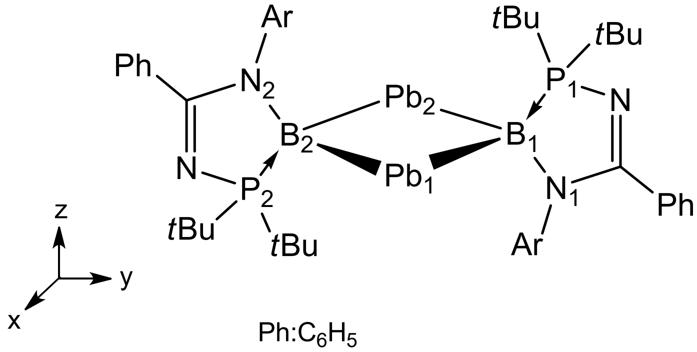
Table S33. $\mathbf{B_2Pb_2}$. All Pb_1 lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Pb_1 (Lone Pair)	LV Pb_1	1.25
Pb_1 (Lone Pair)	LV Pb_2	0.93
Pb_1 (Lone Pair)	BD* Pb_1-B_1	2.25
Pb_1 (Lone Pair)	BD* Pb_1- B_2	3.13
Pb_1 (Lone Pair)	BD* B_1-Pb_2	1.84
Pb_1 (Lone Pair)	BD* B_1- N_1	11.03
Pb_1 (Lone Pair)	BD* B_2-Pb_2	1.47
Pb_1 (Lone Pair)	BD* B_2- P_2	5.77
Pb_1 (Lone Pair)	BD* B_2- N_2	2.83
Pb_1 (Lone Pair)	BD* C_{24}- H_{52}	0.54
Pb_1 (Lone Pair)	BD* C_{103}- H_{135}	1.18

Table S34. **B_2Pb_2**. All Pb_1 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

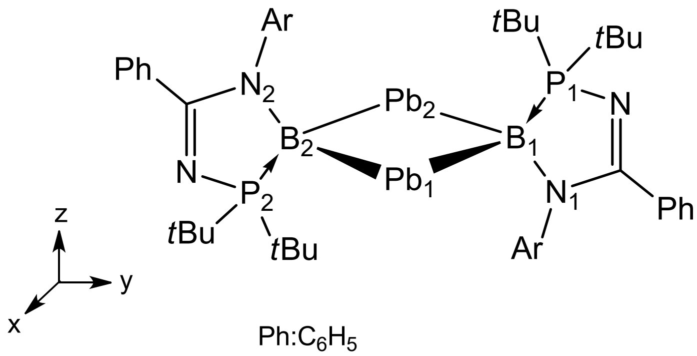


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Pb_1	Pb_1 (Lone vacancy)	1.25
LP Pb_2	Pb_1 (Lone vacancy)	0.94
BD B_1-Pb_2	Pb_1 (Lone vacancy)	18.73
BD B_1- P_1	Pb_1 (Lone vacancy)	0.87
BD B_2-Pb_2	Pb_1 (Lone vacancy)	21.99
BD B_2- N_2	Pb_1 (Lone vacancy)	0.62
BD N_1- C_{17}	Pb_1 (Lone vacancy)	0.58
BD C_{17}- C_{34}	Pb_1 (Lone vacancy)	0.74
BD C_{17}- C_{35}	Pb_1 (Lone vacancy)	1.41
BD C_{20}- H_{42}	Pb_1 (Lone vacancy)	1.36
BD C_{22}- H_{46}	Pb_1 (Lone vacancy)	0.51
BD C_{24}- H_{52}	Pb_1 (Lone vacancy)	0.61
BD C_{28}- H_{62}	Pb_1 (Lone vacancy)	1.76
BD C_{29}- H_{66}	Pb_1 (Lone vacancy)	0.82
BD C_{55}- H_{87}	Pb_1 (Lone vacancy)	1.13
BD C_{85}- H_{111}	Pb_1 (Lone vacancy)	3.00
BD C_{85}- H_{113}	Pb_1 (Lone vacancy)	0.94

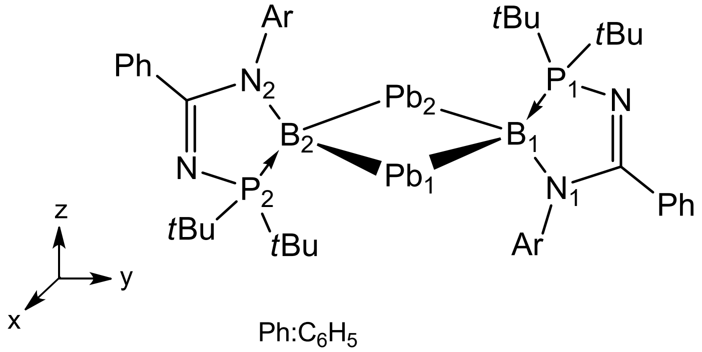
Table S35. **B_2Pb_2**. All Pb_2 lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph: C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Pb_2 (Lone Pair)	LV Pb_1	0.94
Pb_2 (Lone Pair)	LV Pb_2	1.25
Pb_2 (Lone Pair)	BD*Pb_1- B_1	1.48
Pb_2 (Lone Pair)	BD*Pb_1- B_2	1.82
Pb_2 (Lone Pair)	BD* B_1-Pb_2	3.12
Pb_2 (Lone Pair)	BD* B_1- P_1	5.73
Pb_2 (Lone Pair)	BD* B_1- N_1	2.78
Pb_2 (Lone Pair)	BD* B_2-Pb_2	2.22
Pb_2 (Lone Pair)	BD* B_2- N_2	11.09
Pb_2 (Lone Pair)	BD* C_{33}- H_{76}	0.54
Pb_2 (Lone Pair)	BD* C_{90}- H_{119}	1.23

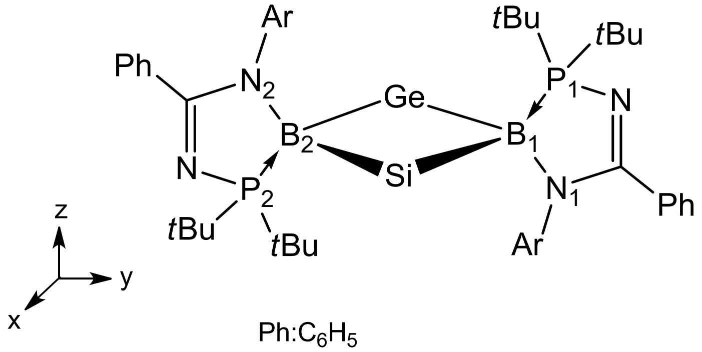
Table S36. **B_2Pb_2**. All Pb_2 lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Pb_1	Pb_2 (Lone vacancy)	0.93
LP Pb_2	Pb_2 (Lone vacancy)	1.25
LP N_2	Pb_2 (Lone vacancy)	0.51
BD Pb_1- B_1	Pb_2 (Lone vacancy)	21.82
BD Pb_1- B_2	Pb_2 (Lone vacancy)	18.78
BD B_1- N_1	Pb_2 (Lone vacancy)	0.62
BD B_2- P_2	Pb_2 (Lone vacancy)	0.87
BD N_1- C_{12}	Pb_2 (Lone vacancy)	0.58
BD C_{12}- C_{25}	Pb_2 (Lone vacancy)	0.74
BD C_{12}- C_{26}	Pb_2 (Lone vacancy)	0.50
BDC_{12}- C_{26}	Pb_2 (Lone vacancy)	1.41
BD C_{19}- H_{37}	Pb_2 (Lone vacancy)	1.77
BD C_{20}- H_{42}	Pb_2 (Lone vacancy)	0.82
BD C_{29}- H_{66}	Pb_2 (Lone vacancy)	1.36
BD C_{31}- H_{70}	Pb_2 (Lone vacancy)	0.51
BD C_{33}- H_{76}	Pb_2 (Lone vacancy)	0.61
BD C_{79}- H_{100}	Pb_2 (Lone vacancy)	1.13
BD C_{98}- H_{127}	Pb_2 (Lone vacancy)	2.97
BD C_{98}- H_{129}	Pb_2 (Lone vacancy)	0.93

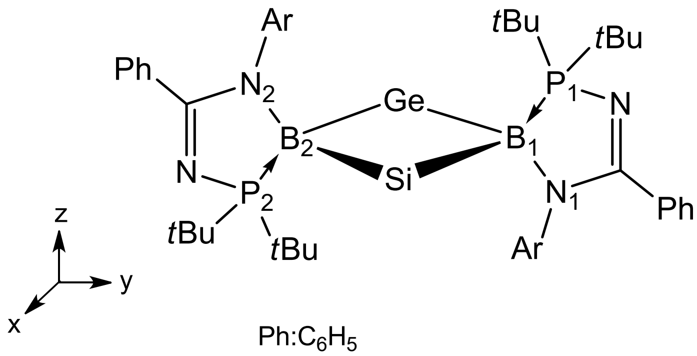
Table S37. **B_2SiGe**. All Si lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Si (Lone Pair)	LV Si	2.64
Si (Lone Pair)	BD* Si- B_2	12.35
Si (Lone Pair)	BD* Si- B_1	2.16
Si (Lone Pair)	BD* B_2- P_2	22.09
Si (Lone Pair)	BD* B_2- N_2	23.53
Si (Lone Pair)	BD* B_1- P_1	15.07
Si (Lone Pair)	BD* B_1- N_1	28.99
Si (Lone Pair)	BD* P_2- N	0.74
Si (Lone Pair)	BD* C_{12}- C_{26}	0.90
Si (Lone Pair)	BD* C_{22}- H_{46}	1.11
Si (Lone Pair)	BD* C_{25}- C_{56}	1.11
Si (Lone Pair)	BD* C_{29}- H_{66}	2.74
Si (Lone Pair)	BD* C_{55}- C_{86}	0.62
Si (Lone Pair)	BD* C_{81}- C_{104}	0.56
Si (Lone Pair)	BD* C_{103}- H_{135}	3.02

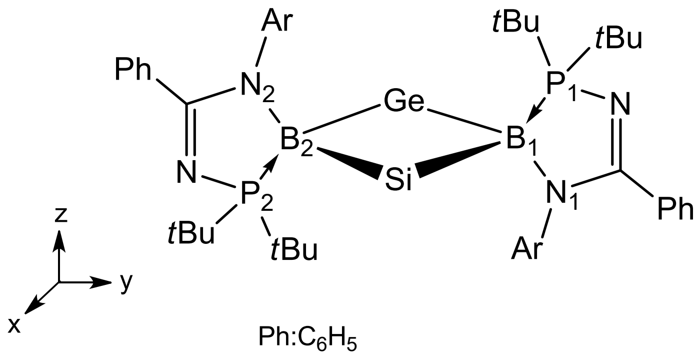
Table S38. **B_2SiGe**. All Si lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph: C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Si	Si (Lone vacancy)	2.64
LP Ge	Si (Lone vacancy)	0.88
BD Si-B_2	Si (Lone vacancy)	15.82
BD Si-B_1	Si (Lone vacancy)	16.40
BD B_2-Ge	Si (Lone vacancy)	113.41
BD B_1-Ge	Si (Lone vacancy)	109.43
BD B_1-N_1	Si (Lone vacancy)	0.56
BD C_{24}-H_{52}	Si (Lone vacancy)	0.67
BD C_{28}-H_{62}	Si (Lone vacancy)	0.69
BD C_{103}-H_{135}	Si (Lone vacancy)	0.88

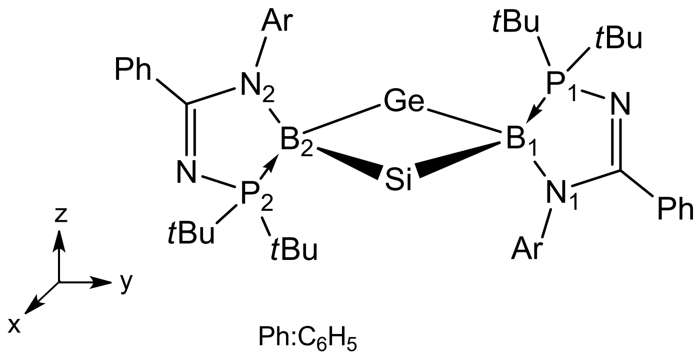
Table S39. **B_2SiGe**. All Ge lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Ge (Lone Pair)	LV Si	0.88
Ge (Lone Pair)	BD* Si- B_2	1.88
Ge (Lone Pair)	BD* Si- B_1	2.26
Ge (Lone Pair)	BD* B_2- P_2	2.54
Ge (Lone Pair)	BD* B_2-Ge	5.80
Ge (Lone Pair)	BD* B_1-Ge	5.31
Ge (Lone Pair)	BD* B_1- N_1	3.05
Ge (Lone Pair)	BD* C_{19}- H_{37}	0.53
Ge (Lone Pair)	BD* C_{33}- H_{76}	0.83
Ge (Lone Pair)	BD* C_{90}- H_{119}	1.01

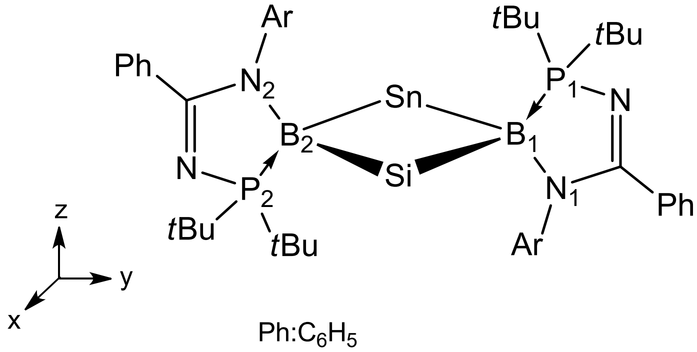
Table S40. **B_2SiGe**. All Ge lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP N_2	Ge (Lone vacancy)	0.56
BD Si- B_2	Ge (Lone vacancy)	1.17
BD Si- B_1	Ge (Lone vacancy)	1.08
BD B_2- N_2	Ge (Lone vacancy)	0.80
BD B_2-Ge	Ge (Lone vacancy)	1.26
BD B_1- P_1	Ge (Lone vacancy)	0.68
BD C_{12}- C_{26}	Ge (Lone vacancy)	1.26
BD C_{20}- H_{42}	Ge (Lone vacancy)	1.19
BD C_{79}- H_{100}	Ge (Lone vacancy)	0.91
BD C_{90}- H_{119}	Ge (Lone vacancy)	1.04

Table S41. **B_2SiSn**. All Si lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

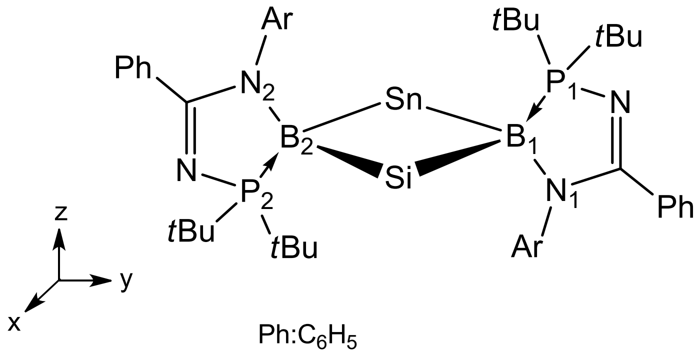


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP N_2	Si (Lone vacancy)	0.79
LP N_2	Si (Lone vacancy)	3.60
LP Sn	Si (Lone vacancy)	3.00
LP N_1	Si (Lone vacancy)	1.11
BD Si- B_2	Si (Lone vacancy)	12.92
BD Si- B_1	Si (Lone vacancy)	11.94
BD B_2-Sn	Si (Lone vacancy)	150.60
BD B_1-Sn	Si (Lone vacancy)	141.24
BD C_{24}- H_{52}	Si (Lone vacancy)	1.10
BD C_{28}- H_{62}	Si (Lone vacancy)	0.66
BD C_{103}- H_{135}	Si (Lone vacancy)	1.63

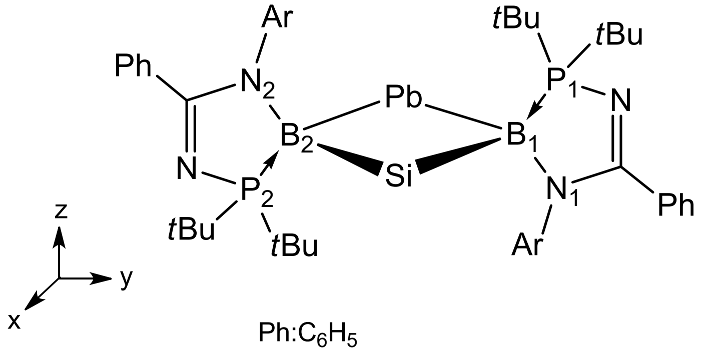
Table S42. **B_2SiSn**. All Sn lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Sn (Lone Pair)	LV Si	3.00
Sn (Lone Pair)	LV B_1	2.56
Sn (Lone Pair)	BD* Si- B_2	0.76
Sn (Lone Pair)	BD* Si- B_1	0.81
Sn (Lone Pair)	BD* Si-Sn	0.59
Sn (Lone Pair)	BD* B_2- P_2	2.12
Sn (Lone Pair)	BD* B_2-Sn	2.32
Sn (Lone Pair)	BD* B_1-Sn	2.18
Sn (Lone Pair)	BD* C_{19}- H_{37}	0.62
Sn (Lone Pair)	BD* C_{33}- H_{76}	0.92
Sn (Lone Pair)	BD* C_{90}- H_{119}	0.81

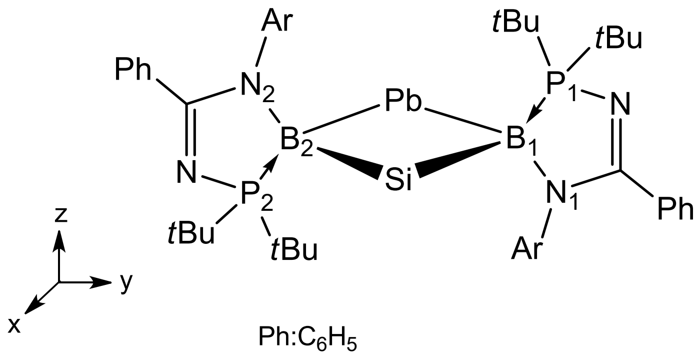
Table S43. **B_2SiPb**. All Si lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP N_2	Si (Lone vacancy)	0.88
LP N_2	Si (Lone vacancy)	3.26
LP Pb	Si (Lone vacancy)	6.54
LP N_1	Si (Lone vacancy)	1.10
BD Si- B_2	Si (Lone vacancy)	11.57
BD Si- B_1	Si (Lone vacancy)	10.17
BD Si-Pb	Si (Lone vacancy)	0.83
BD B_2-Pb	Si (Lone vacancy)	175.74
BD B_1-Pb	Si (Lone vacancy)	164.28
BD C 24- H 52	Si (Lone vacancy)	1.19
BD C_{103}- H_{135}	Si (Lone vacancy)	2.14

Table S44. **B_2SiPb**. All Pb lone pair orbital contribution in NBO analysis of second order perturbation theory.

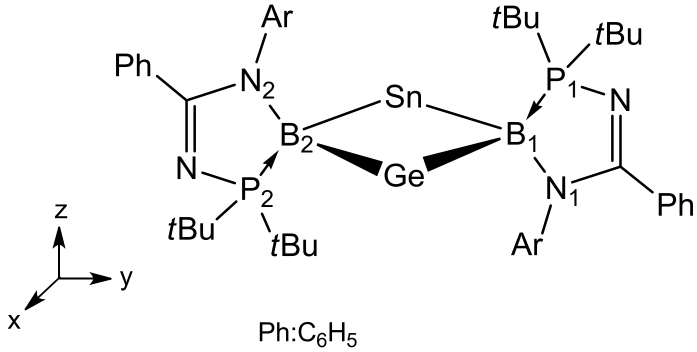


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

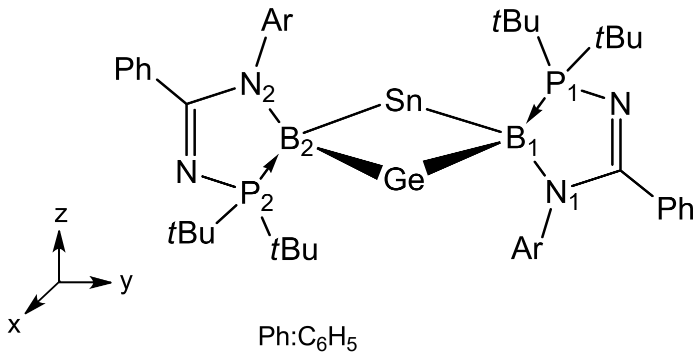
Donor orbital	Acceptor orbital	Energy (kcal/mol)
Pb (Lone Pair)	LV Si	6.54
Pb (Lone Pair)	LV B_1	2.02
Pb (Lone Pair)	BD* B_2- P_2	1.78
Pb (Lone Pair)	BD* B_2-Pb	1.17
Pb (Lone Pair)	BD* B_1-Pb	1.05
Pb (Lone Pair)	BD* C_{33}- H_{76}	0.61

Table S45. **B_2GeSn**. All Ge lone pair orbital contribution in NBO analysis of second order perturbation theory.



Donor orbital	Acceptor orbital	Energy (kcal/mol)
Ge (Lone Pair)	LV Ge	0.86
Ge (Lone Pair)	LV B_2	19.27
Ge (Lone Pair)	LV B_1	5.85
Ge (Lone Pair)	BD* Ge-B_2	6.98
Ge (Lone Pair)	BD* Ge-B_1	7.00
Ge (Lone Pair)	BD* B_2-Sn	2.86
Ge (Lone Pair)	BD* B_1-Sn	1.56
Ge (Lone Pair)	BD* B_1-P_1	9.97
Ge (Lone Pair)	BD* C_{24}- H_{52}	0.77
Ge (Lone Pair)	BD* C_{103}- H_{135}	1.59

Table S46. **B_2GeSn**. All Ge lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

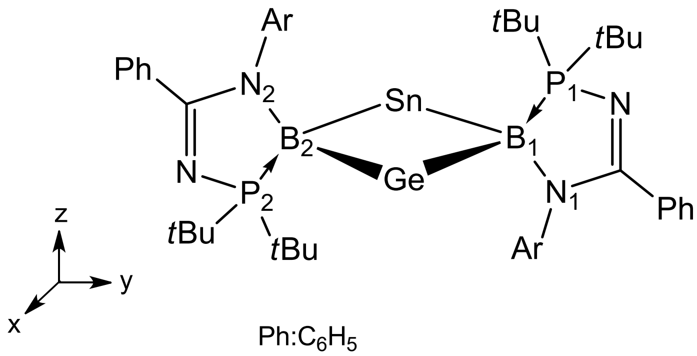


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Ge	Ge (Lone vacancy)	0.86
LP N_2	Ge (Lone vacancy)	0.86
LP N_2	Ge (Lone vacancy)	2.63
BD Ge- B_2	Ge (Lone vacancy)	2.10
BD Ge- B_1	Ge (Lone vacancy)	3.10
BD B_2-Sn	Ge (Lone vacancy)	62.26
BD B_2- P_2	Ge (Lone vacancy)	0.61
BD B_1-Sn	Ge (Lone vacancy)	65.18
BD C_{17}- C_{35}	Ge (Lone vacancy)	1.42
BD C_{28}- H_{62}	Ge (Lone vacancy)	0.61
BD C_{55}- H_{87}	Ge (Lone vacancy)	0.58

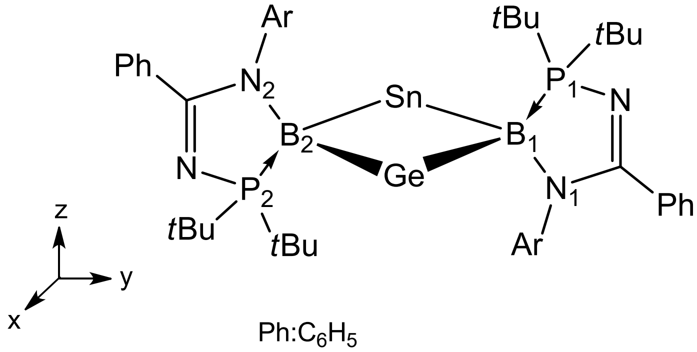
Table S47. **B_2GeSn**. All Sn lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Sn (Lone Pair)	LV B_1	4.94
Sn (Lone Pair)	BD* B_2-Sn	4.28
Sn (Lone Pair)	BD* B_2- P_2	2.94
Sn (Lone Pair)	BD* B $_1$-Sn	4.06
Sn (Lone Pair)	BD* C_{33}- H_{76}	0.83
Sn (Lone Pair)	BD* C_{90}- H_{119}	0.88

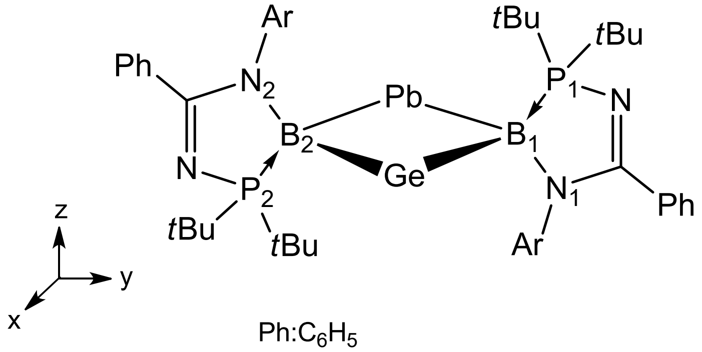
Table S48. **B_2GeSn**. All Sn lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP N_1	Sn (Lone vacancy)	2.52
BD Ge- B_2	Sn (Lone vacancy)	12.81
BD Ge- B_1	Sn (Lone vacancy)	9.88
BD B_2-Sn	Sn (Lone vacancy)	0.63
BD B_1- P_1	Sn (Lone vacancy)	0.64
BD C_{12}- C_{26}	Sn (Lone vacancy)	1.21
BD C_{19}- H_{37}	Sn (Lone vacancy)	0.60
BD C_{20}- H_{42}	Sn (Lone vacancy)	1.92
BD C_{29}- H_{66}	Sn (Lone vacancy)	0.51
BD C_{31}- H_{70}	Sn (Lone vacancy)	0.97
BD C_{79}- H_{100}	Sn (Lone vacancy)	1.41
BD C_{90}- H_{119}	Sn (Lone vacancy)	1.30
BD C_{98}- H_{127}	Sn (Lone vacancy)	1.70

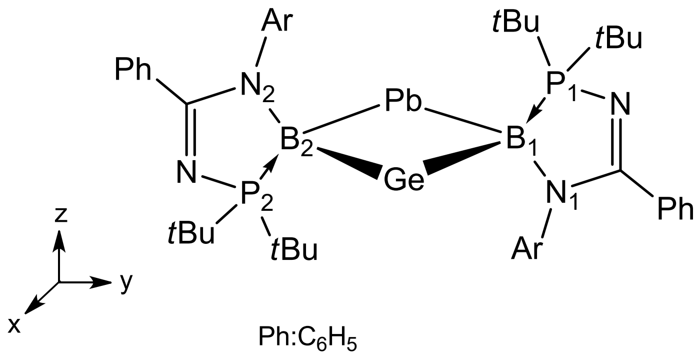
Table S49. **B_2GePb**. All Ge lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Ge (Lone Pair)	LV Ge	0.76
Ge (Lone Pair)	LV B_2	27.00
Ge (Lone Pair)	LV B_1	6.23
Ge (Lone Pair)	LV Pb	0.53
Ge (Lone Pair)	LV Pb	0.94
Ge (Lone Pair)	BD*Ge- B_2	5.89
Ge (Lone Pair)	BD*Ge- B_1	5.56
Ge (Lone Pair)	BD* B_2-Pb	1.88
Ge (Lone Pair)	BD* B_2- P_2	0.62
Ge (Lone Pair)	BD* B_1- P_1	13.04
Ge (Lone Pair)	BD* C_{22}- H_{46}	0.54
Ge (Lone Pair)	BD* C_{24}- H_{52}	0.58
Ge (Lone Pair)	BD* C_{103}- H_{135}	1.59

Table S50. **B_2GePb**. All Ge lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

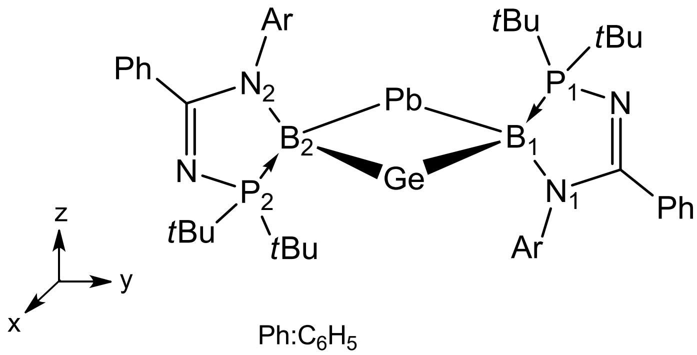


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Ge	Ge (Lone vacancy)	0.76
LP B_1	Ge (Lone vacancy)	160.79
LP Pb	Ge (Lone vacancy)	1.94
LP N_2	Ge (Lone vacancy)	1.14
LP N_2	Ge (Lone vacancy)	2.33
BD Ge- B_2	Ge (Lone vacancy)	2.84
BD Ge- B_1	Ge (Lone vacancy)	3.72
BD B_2-Pb	Ge (Lone vacancy)	95.31
BD B_2- P_2	Ge (Lone vacancy)	0.59
BD C_{17}- C_{35}	Ge (Lone vacancy)	0.85
BD C_{24}- H_{52}	Ge (Lone vacancy)	0.62

Table S51. **B_2GePb**. All Pb lone pair orbital contribution in NBO analysis of second order perturbation theory.

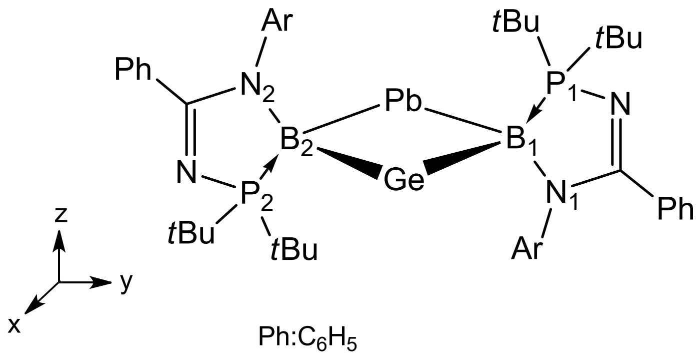


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Pb (Lone Pair)	LV Ge	1.94
Pb (Lone Pair)	LV B_1	3.42
Pb (Lone Pair)	LV Pb	1.27
Pb (Lone Pair)	BD* B_2-Pb	2.47
Pb (Lone Pair)	BD* B_2- P_2	2.47
Pb (Lone Pair)	BD* C_{33}- H_{76}	0.61
Pb (Lone Pair)	BD* C_{90}- H_{119}	0.55

Table S52. **B_2GePb**. All Pb lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

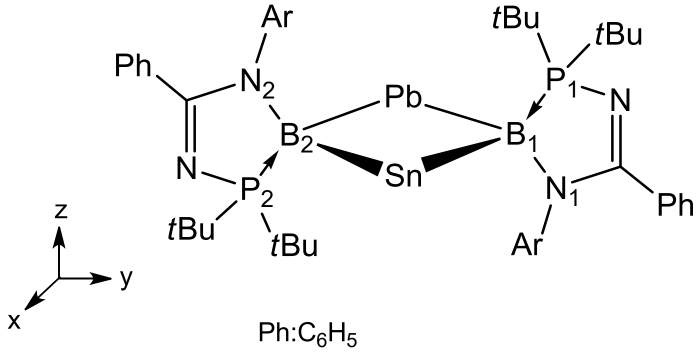


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Ge	Pb (Lone vacancy)	0.53
LP B_1	Pb (Lone vacancy)	206.63
LP Pb	Pb (Lone vacancy)	1.27
LP N_1	Pb (Lone vacancy)	3.13
BD Ge- B_2	Pb (Lone vacancy)	3.84
BD Ge- B_1	Pb (Lone vacancy)	19.32
BD B_1- P_1	Pb (Lone vacancy)	5.13
BD N_1- C_{17}	Pb (Lone vacancy)	0.94
BD N_1- C_{18}	Pb (Lone vacancy)	0.72
BD C_{17}- C_{34}	Pb (Lone vacancy)	0.59
BD C_{19}- H_{37}	Pb (Lone vacancy)	2.02
BD C_{57}- H_{92}	Pb (Lone vacancy)	1.66
BD C_{79}- H_{100}	Pb (Lone vacancy)	1.10
BD C_{90}- H_{119}	Pb (Lone vacancy)	1.20
BD C_{90}- H_{120}	Pb (Lone vacancy)	0.56
LP Ge	Pb (Lone vacancy)	0.94
LP B_1	Pb (Lone vacancy)	9.77
LP N_1	Pb (Lone vacancy)	2.09
BD Ge- B_2	Pb (Lone vacancy)	9.03
BD Ge- B_1	Pb (Lone vacancy)	6.35
BD B_2-Pb	Pb (Lone vacancy)	0.71
BD C_{12}- C_{26}	Pb (Lone vacancy)	1.14
BD C_{19}- H_{37}	Pb (Lone vacancy)	0.62
BD C_{20}- H_{42}	Pb (Lone vacancy)	2.31
BD C_{31}- H_{70}	Pb (Lone vacancy)	1.39
BD C_{79}- H_{100}	Pb (Lone vacancy)	1.53
BD C_{90}- H_{119}	Pb (Lone vacancy)	2.19
BD C_{98}- H_{127}	Pb (Lone vacancy)	2.95
BD C_{98}- H_{129}	Pb (Lone vacancy)	0.75

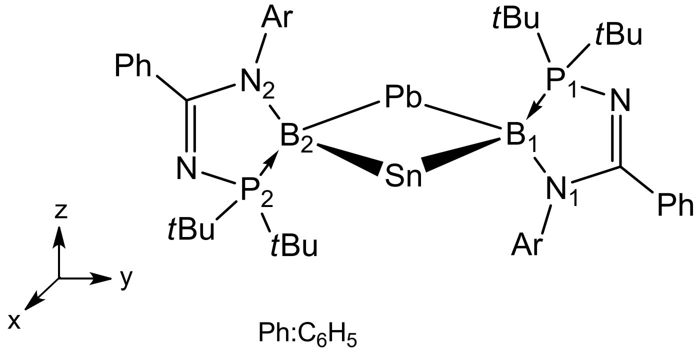
Table S53. **B_2SnPb**. All Sn lone pair orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Sn (Lone Pair)	LV Sn	2.56
Sn (Lone Pair)	LV B_2	20.75
Sn (Lone Pair)	LV B_1	4.73
Sn (Lone Pair)	BD*Sn- B_2	6.13
Sn (Lone Pair)	BD*Sn- B_1	6.15
Sn (Lone Pair)	BD* B_2-Pb	2.41
Sn (Lone Pair)	BD* B_1-Pb	1.21
Sn (Lone Pair)	BD* B_1- P_1	8.88
Sn (Lone Pair)	BD* C_{22}- H_{46}	0.77
Sn (Lone Pair)	BD* C_{24}- H_{52}	0.68
Sn (Lone Pair)	BD* C_{103}- H_{135}	1.94

Table S54. **B_2SnPb**. All Sn lone vacancy orbital contribution in NBO analysis of second order perturbation theory.

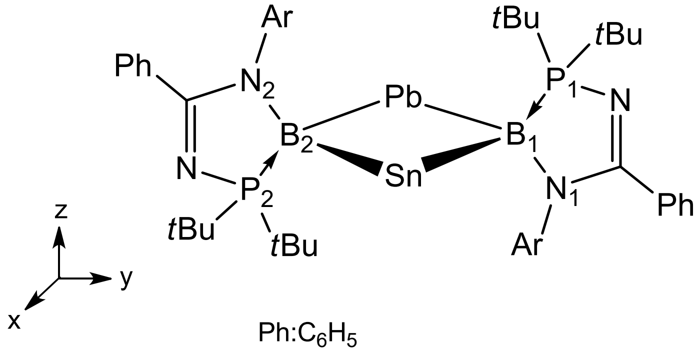


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Sn	Sn (Lone vacancy)	2.56
LP Pb	Sn (Lone vacancy)	2.15
LP N_2	Sn (Lone vacancy)	0.97
LP N_2	Sn (Lone vacancy)	2.47
BD Sn- B_2	Sn (Lone vacancy)	0.71
BD B_2-Pb	Sn (Lone vacancy)	38.47
BD B_2- P_2	Sn (Lone vacancy)	0.88
BD B_1-Pb	Sn (Lone vacancy)	41.50
BD C_{17}- C_{35}	Sn (Lone vacancy)	0.86
BD C_{20}- H_{42}	Sn (Lone vacancy)	0.91
BD C_{24}- H_{52}	Sn (Lone vacancy)	0.85
BD C_{28}- H_{62}	Sn (Lone vacancy)	1.06
BD C_{55}- H_{87}	Sn (Lone vacancy)	0.60
BD C_{85}- H_{111}	Sn (Lone vacancy)	1.84

Table S55. **B_2SnPb**. All Pb lone pair orbital contribution in NBO analysis of second order perturbation theory.

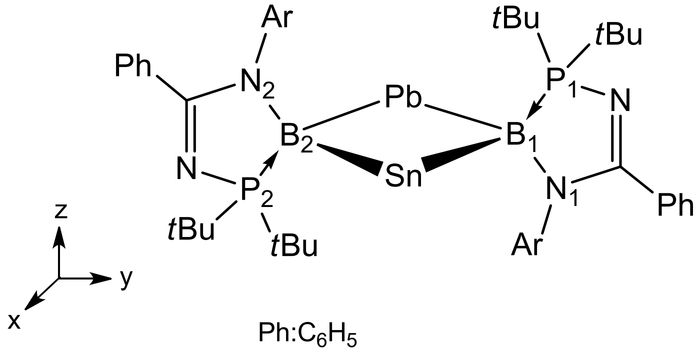


Ph:C_6H_5

Ar: 2,6-diisopropylphenyl

Donor orbital	Acceptor orbital	Energy (kcal/mol)
Pb (Lone Pair)	LV Sn	2.15
Pb (Lone Pair)	LV B_2	1.44
Pb (Lone Pair)	LV B_1	5.83
Pb (Lone Pair)	LV Pb	0.96
Pb (Lone Pair)	BD*Sn- B_2	2.14
Pb (Lone Pair)	BD*Sn- B_1	2.24
Pb (Lone Pair)	BD* B_2-Pb	2.21
Pb (Lone Pair)	BD* B_2- P_2	2.99
Pb (Lone Pair)	BD* B_1-Pb	1.70
Pb (Lone Pair)	BD* C_{33}- H_{76}	0.69
Pb (Lone Pair)	BD* C_{90}- H_{119}	0.95

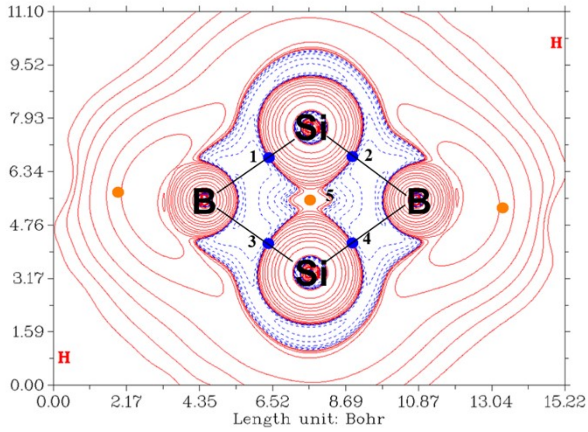
Table S56. **B_2SnPb**. All Pb lone vacancy orbital contribution in NBO analysis of second order perturbation theory.



Ph:C_6H_5
Ar: 2,6-diisopropylphenyl

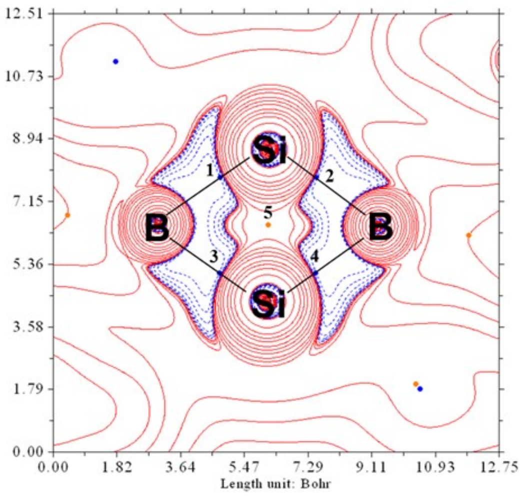
Donor orbital	Acceptor orbital	Energy (kcal/mol)
LP Pb	Pb (Lone vacancy)	0.96
LP N_1	Pb (Lone vacancy)	1.94
BD Sn- B_2	Pb (Lone vacancy)	11.20
BD Sn- B_1	Pb (Lone vacancy)	8.69
BD B_1- P_1	Pb (Lone vacancy)	0.63
BD N_2- C_{12}	Pb (Lone vacancy)	0.57
BD C_{12}- C_{25}	Pb (Lone vacancy)	0.60
BD C_{12}- C_{26}	Pb (Lone vacancy)	0.55
BD C_{12}- C_{26}	Pb (Lone vacancy)	1.37
BD C_{19}- H_{37}	Pb (Lone vacancy)	1.53
BD C_{20}- H_{42}	Pb (Lone vacancy)	1.68
BD C_{29}- H_{66}	Pb (Lone vacancy)	0.95
BD C_{31}- H_{70}	Pb (Lone vacancy)	1.29
BD C_{79}- H_{100}	Pb (Lone vacancy)	1.42
BD C_{90}- H_{119}	Pb (Lone vacancy)	0.87
BD C_{98}- H_{127}	Pb (Lone vacancy)	3.83
BD C_{98}- H_{129}	Pb (Lone vacancy)	1.20

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.095	0.013	–0.060
2	3, –1	0.094	0.004	–0.060
3	3, –1	0.094	0.004	–0.060
4	3, –1	0.095	0.013	–0.060
5	3, +1	0.071	0.008	–0.032

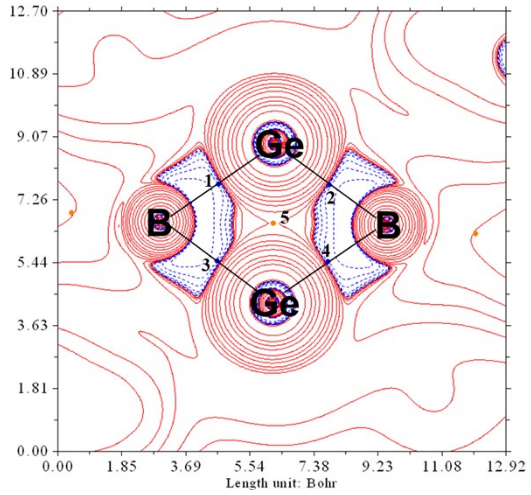
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.091	–0.080	–0.057
2	3, –1	0.092	–0.064	–0.059
3	3, –1	0.092	–0.064	–0.059
4	3, –1	0.091	–0.080	–0.057
5	3, +1	0.049	0.063	–0.017

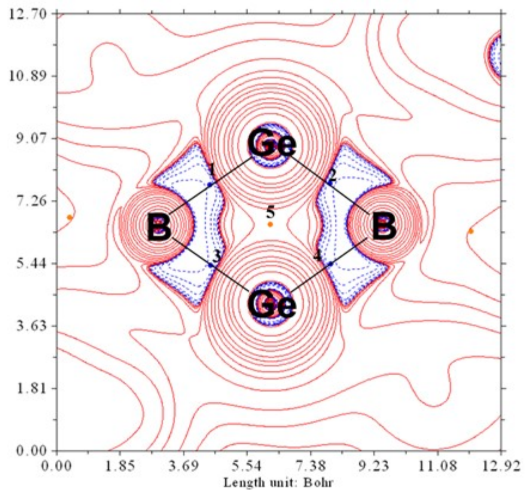
Figure S21: (A) Laplacian distribution of electron energy of the central four-membered ring plane in **B_2Si_2**. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of **B_2Si_2** are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.090	–0.031	–0.044
2	3, –1	0.091	–0.028	–0.044
3	3, –1	0.091	–0.028	–0.044
4	3, –1	0.090	–0.031	–0.044
5	3, +1	0.062	0.041	–0.025

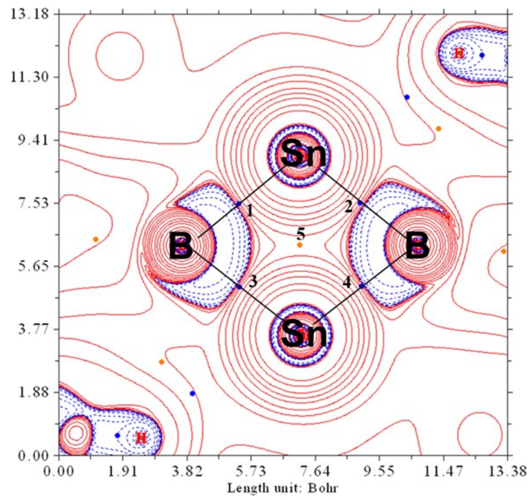
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.085	–0.063	–0.041
2	3, –1	0.086	–0.063	–0.042
3	3, –1	0.086	–0.063	–0.042
4	3, –1	0.085	-0.063	–0.041
5	3, +1	0.044	0.090	–0.012

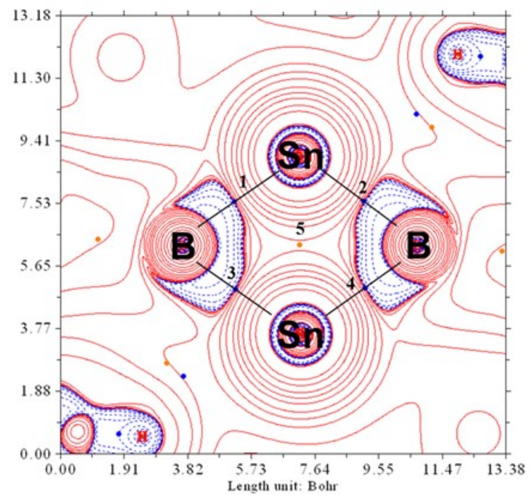
Figure S22: (A) Laplacian distribution of electron energy of the central four-membered ring plane in $\mathbf{B_2Ge_2}$. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of $\mathbf{B_2Ge_2}$ are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.069	0.029	–0.023
2	3, –1	0.072	0.024	–0.025
3	3, –1	0.072	0.024	–0.025
4	3, –1	0.069	0.029	–0.023
5	3, +1	0.040	0.051	–0.008

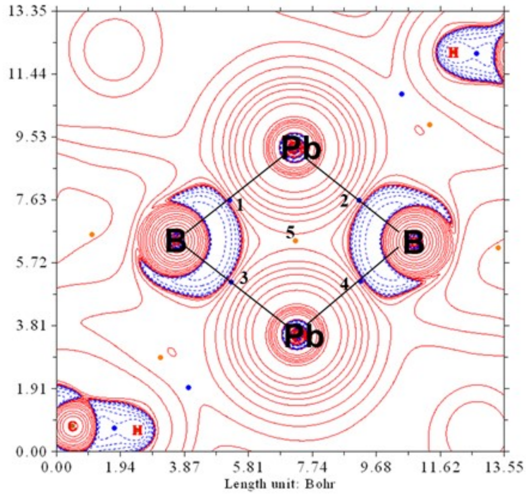
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.067	–0.0007	–0.023
2	3, –1	0.066	0.004	–0.022
3	3, –1	0.066	0.004	–0.022
4	3, –1	0.067	–0.0007	–0.024
5	3, +1	0.029	0.073	–0.003

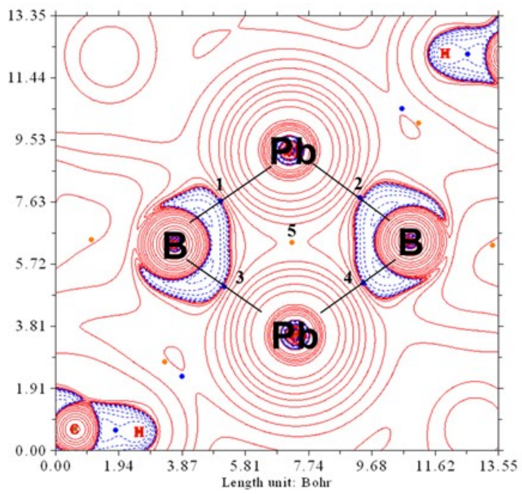
Figure S23: (A) Laplacian distribution of electron energy of the central four-membered ring plane in $\mathbf{B_2Sn_2}$. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of $\mathbf{B_2Sn_2}$ are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.069	0.024	–0.023
2	3, –1	0.065	0.031	–0.019
3	3, –1	0.064	0.031	–0.019
4	3, –1	0.069	0.023	–0.023
5	3, +1	0.035	0.067	–0.005

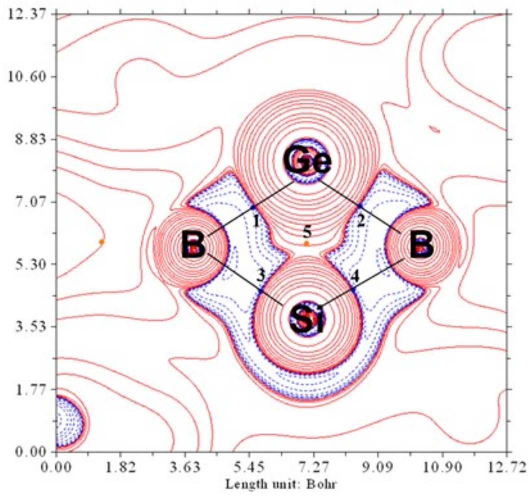
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.062	0.0006	–0.020
2	3, –1	0.059	0.007	–0.018
3	3, –1	0.059	0.007	–0.018
4	3, –1	0.062	0.0006	–0.020
5	3, +1	0.024	0.087	–0.0001

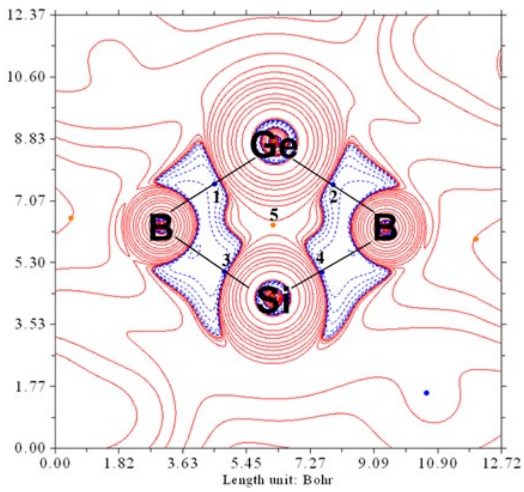
Figure S24: (A) Laplacian distribution of electron energy of the central four-membered ring plane in $\mathbf{B_2Pb_2}$. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of $\mathbf{B_2Pb_2}$ are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.088	–0.019	–0.042
2	3, –1	0.089	–0.016	–0.043
3	3, –1	0.096	0.0001	–0.062
4	3, –1	0.095	–0.010	–0.062
5	3, +1	0.066	0.022	–0.028

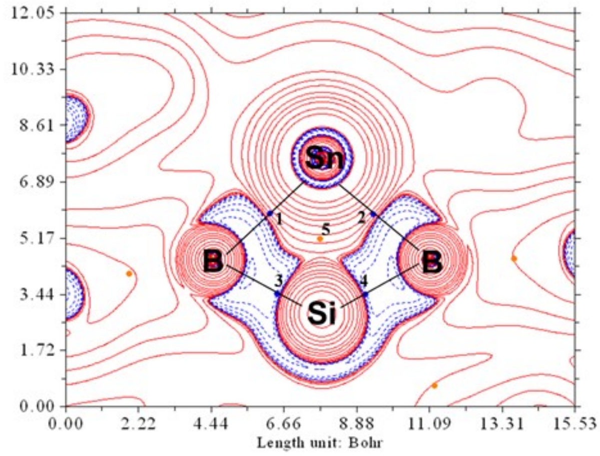
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.084	–0.050	–0.040
2	3, –1	0.082	–0.050	–0.038
3	3, –1	0.094	–0.078	–0.061
4	3, –1	0.095	–0.066	–0.061
5	3, +1	0.046	0.074	–0.015

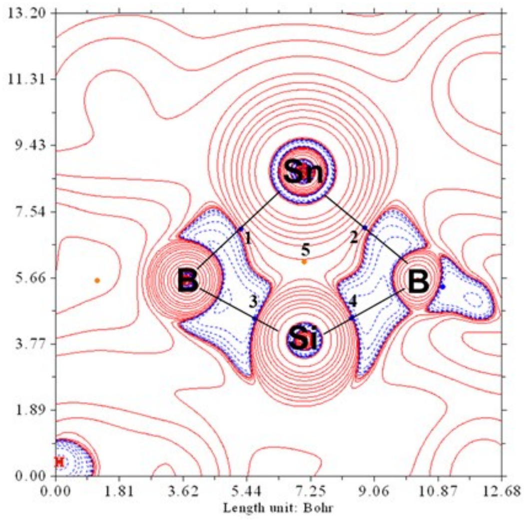
Figure S25: (A) Laplacian distribution of electron energy of the central four-membered ring plane in **B_2SiGe**. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of **B_2SiGe** are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.067	0.038	–0.021
2	3, –1	0.065	0.040	–0.020
3	3, –1	0.098	–0.006	–0.064
4	3, –1	0.097	0.0009	–0.063
5	3, +1	0.053	0.045	–0.017

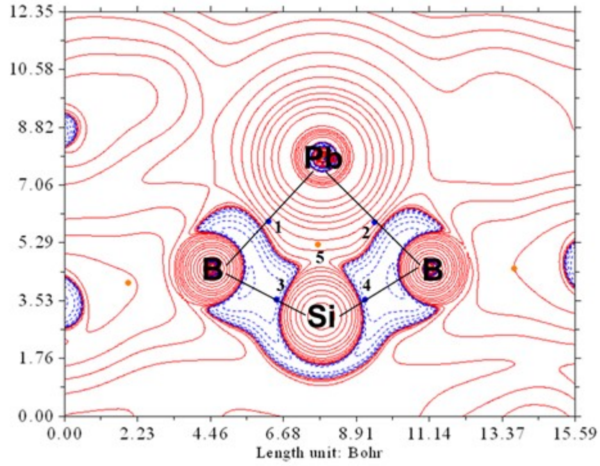
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.060	0.018	–0.018
2	3, –1	0.059	0.017	–0.018
3	3, –1	0.098	–0.050	–0.064
4	3, –1	0.097	–0.039	–0.063
5	3, +1	0.040	0.061	–0.010

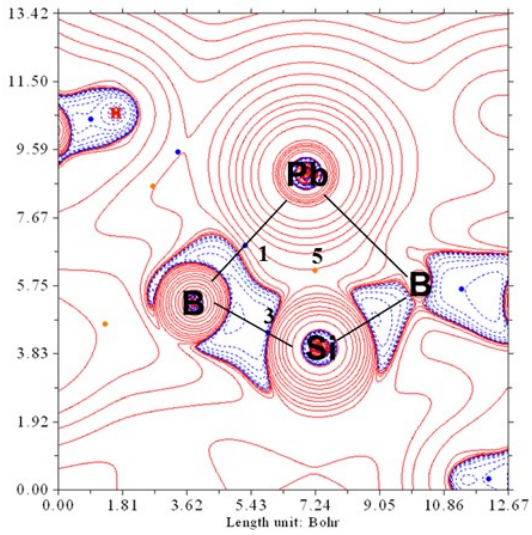
Figure S26: (A) Laplacian distribution of electron energy of the central four-membered ring plane in $\mathbf{B_2SiSn}$. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of $\mathbf{B_2SiSn}$ are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.061	0.044	–0.016
2	3, –1	0.059	0.046	–0.015
3	3, –1	0.099	0.005	–0.064
4	3, –1	0.099	–0.001	–0.066
5	3, +1	0.052	0.045	–0.016

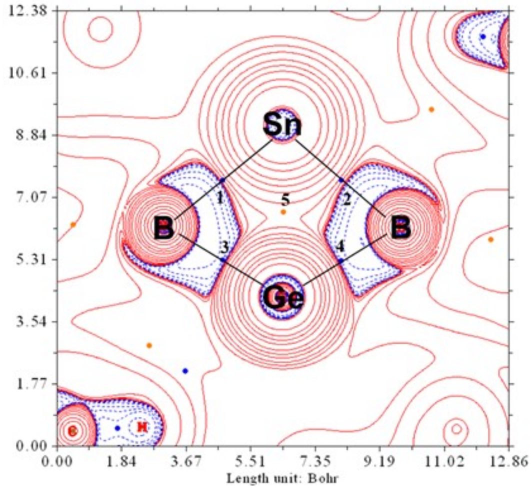
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.051	0.033	–0.012
2	3, –1	0.038	0.061	–0.009
3	3, –1	0.099	–0.035	–0.066
4	3, –1	0.099	–0.027	–0.064
5	3, +1	0.038	0.061	–0.009

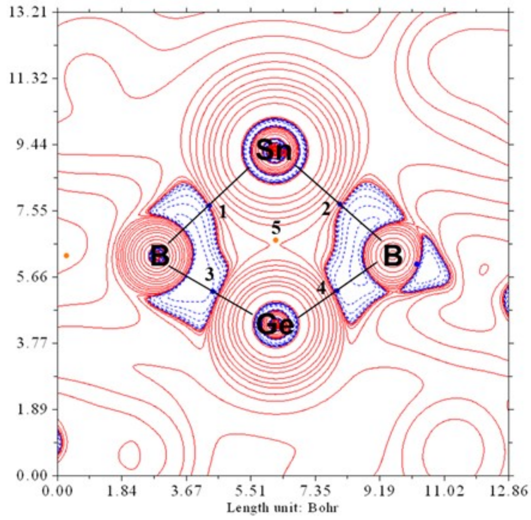
Figure S27: (A) Laplacian distribution of electron energy of the central four-membered ring plane in **B_2SiPb**. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of **B_2SiPb** are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.067	0.031	–0.021
2	3, –1	0.065	0.034	–0.020
3	3, –1	0.093	–0.037	–0.047
4	3, –1	0.094	–0.042	–0.048
5	3, +1	0.050	0.055	–0.014

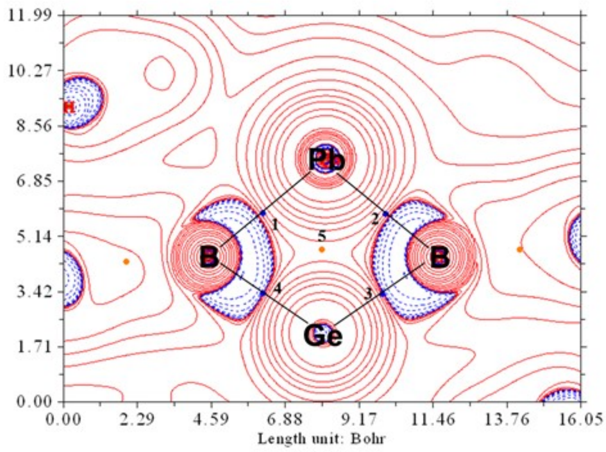
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.060	0.010	–0.019
2	3, –1	0.060	0.007	–0.019
3	3, –1	0.091	–0.074	–0.046
4	3, –1	0.092	–0.071	–0.046
5	3, +1	0.037	0.080	–0.007

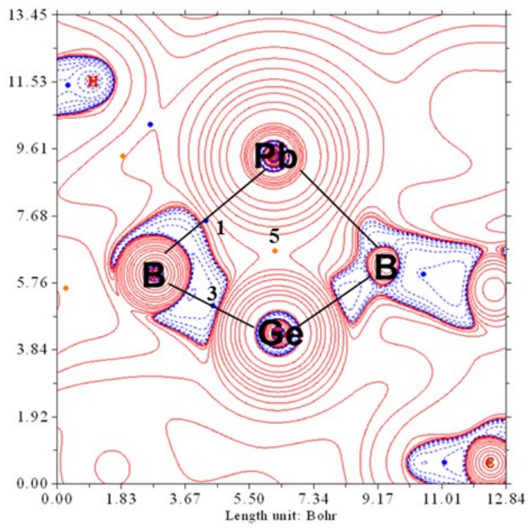
Figure S28: (A) Laplacian distribution of electron energy of the central four-membered ring plane in **B_2GeSn**. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of **B_2GeSn** are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.062	0.036	–0.017
2	3, –1	0.059	0.039	–0.015
3	3, –1	0.096	–0.045	–0.049
4	3, –1	0.095	–0.038	–0.048
5	3, +1	0.048	0.059	–0.013

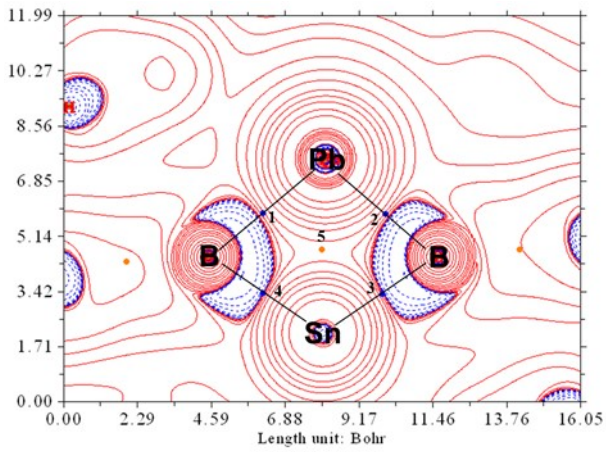
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.051	0.023	–0.013
2	3, –1	0.052	0.023	–0.014
3	3, –1	0.094	–0.078	–0.049
4	3, –1	0.094	–0.072	–0.048
5	3, +1	0.035	0.082	–0.006

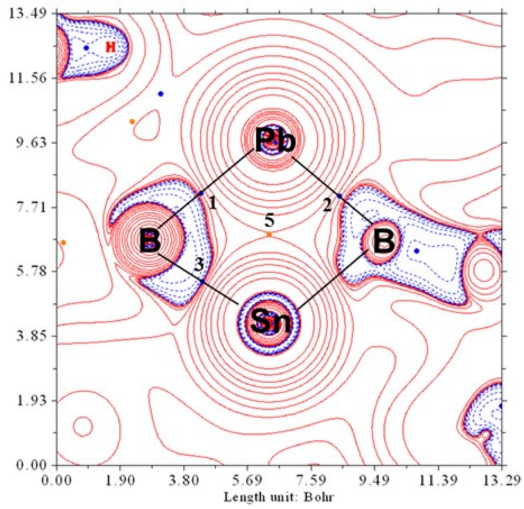
Figure S29: (A) Laplacian distribution of electron energy of the central four-membered ring plane in $\mathbf{B_2GePb}$. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of $\mathbf{B_2GePb}$ are altered.

(A)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.065	0.025	–0.020
2	3, –1	0.060	0.030	–0.016
3	3, –1	0.075	0.025	–0.025
4	3, –1	0.072	0.033	–0.025
5	3, +1	0.038	0.059	–0.007

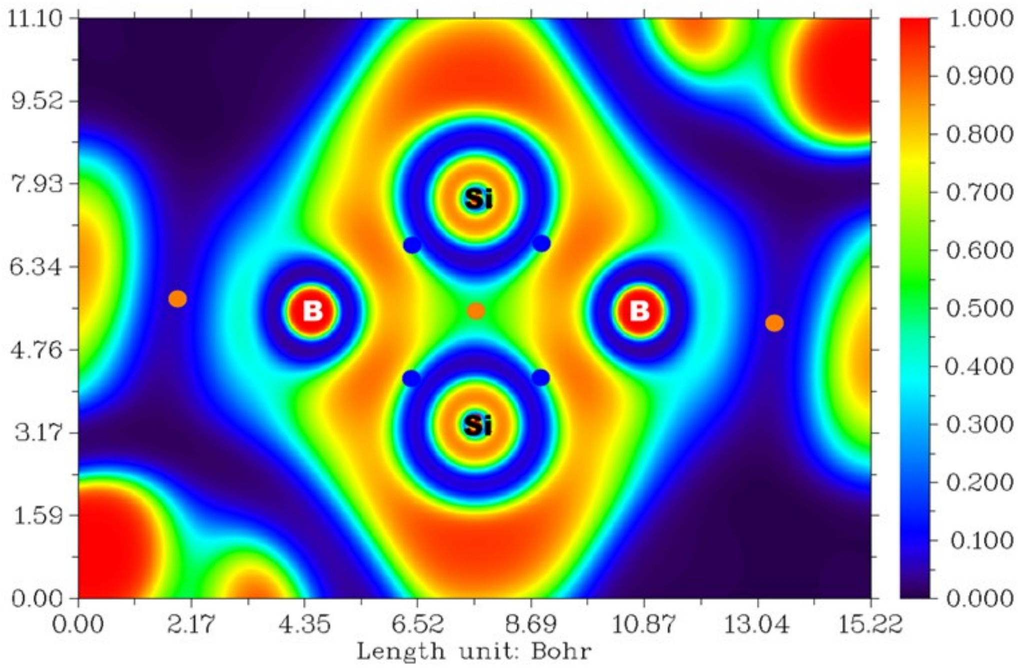
(B)



CP	CP type	Electron density $\rho(r_c)$	Laplacian electron density $\nabla^2\rho(r_c)$	Total energy electron density $H(r_c)$
1	3, –1	0.053	0.013	–0.014
2	3, –1	0.056	0.011	–0.017
3	3, –1	0.071	–0.003	–0.026
4	3, –1	0.070	0.006	–0.025
5	3, +1	0.028	0.073	–0.002

Figure S30: (A) Laplacian distribution of electron energy of the central four-membered ring plane in **B_2SnPb**. Positive and negative area are represented by crimson and blue lines, representing electron depletion and accumulation, respectively. (B) By removing electrons from the σ-bonding HOMO−2, the electron density concentrations within the central four-membered plane of **B_2SnPb** are altered.

(A)



(B)

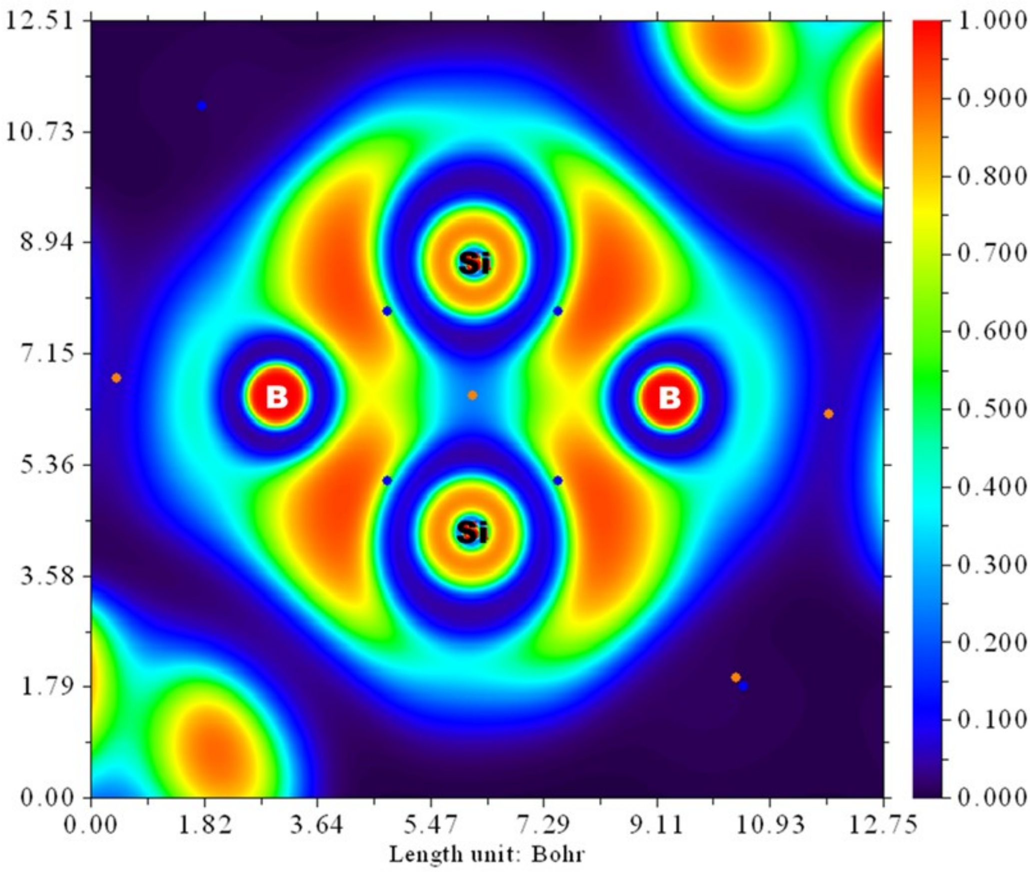
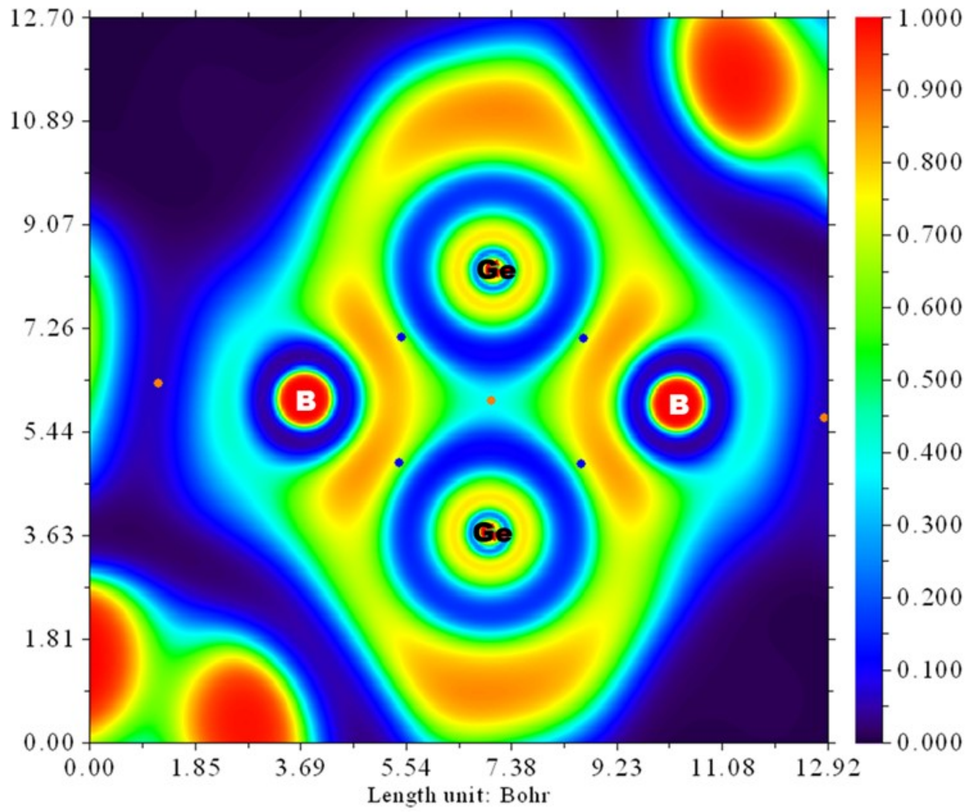


Figure S31. (A) Color-filled map of ELF of $\mathbf{B_2Si_2}$; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

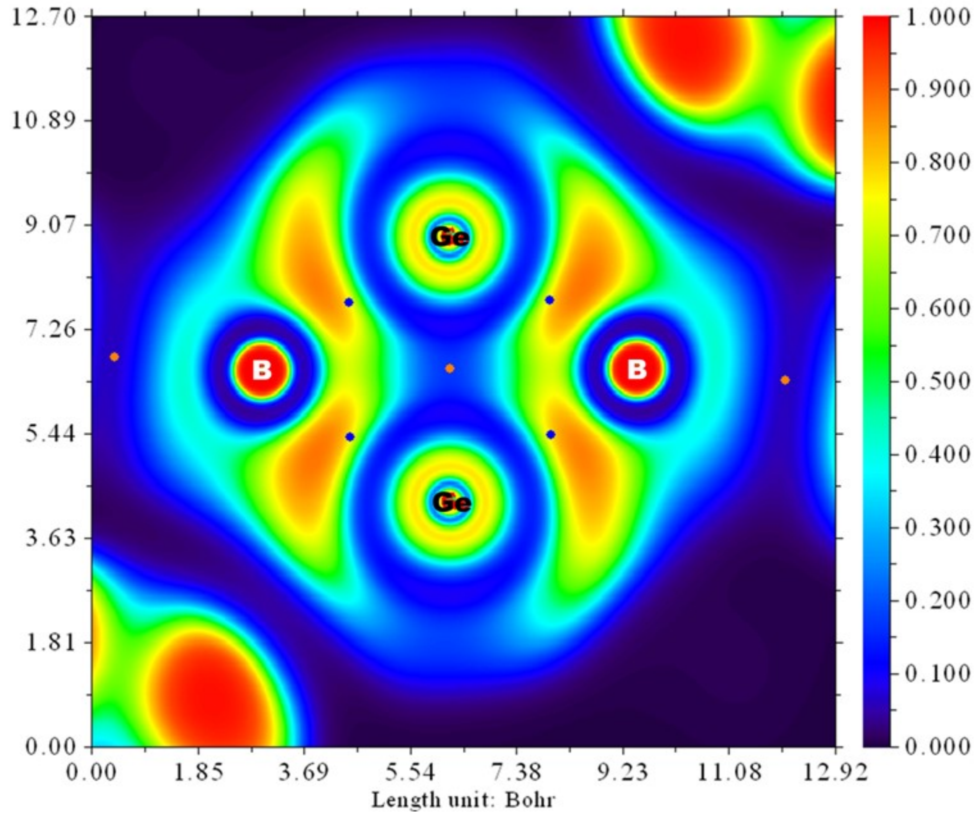
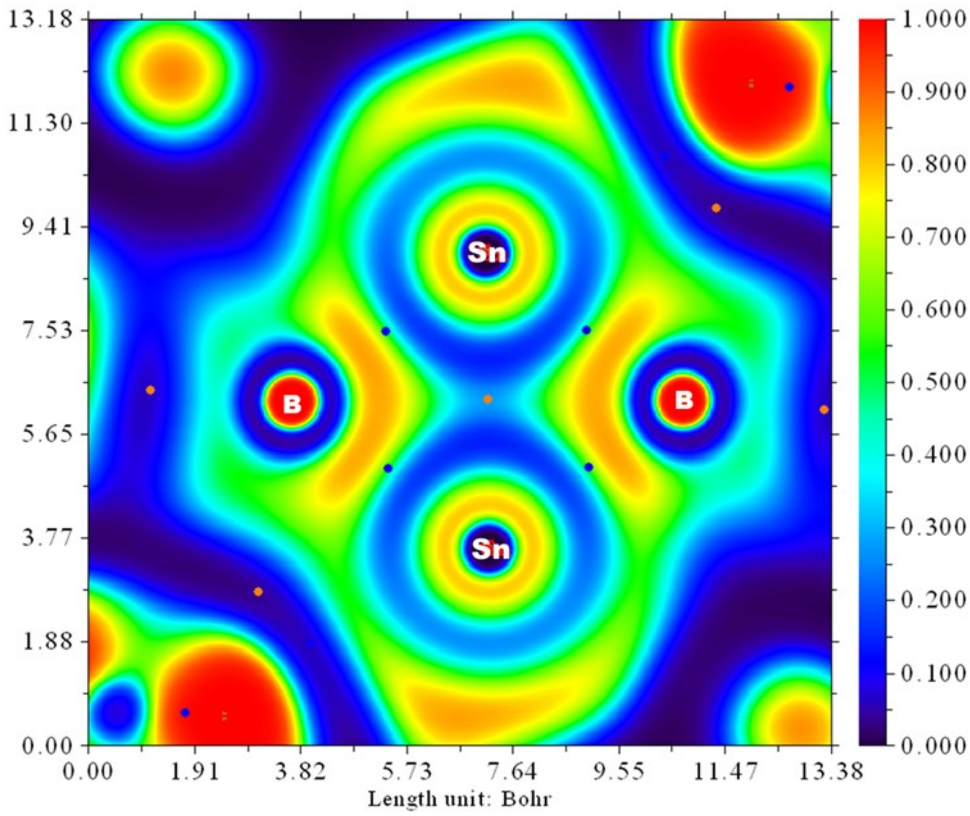


Figure S32. (A) Color-filled map of ELF of **B_2Ge_2**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B). After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

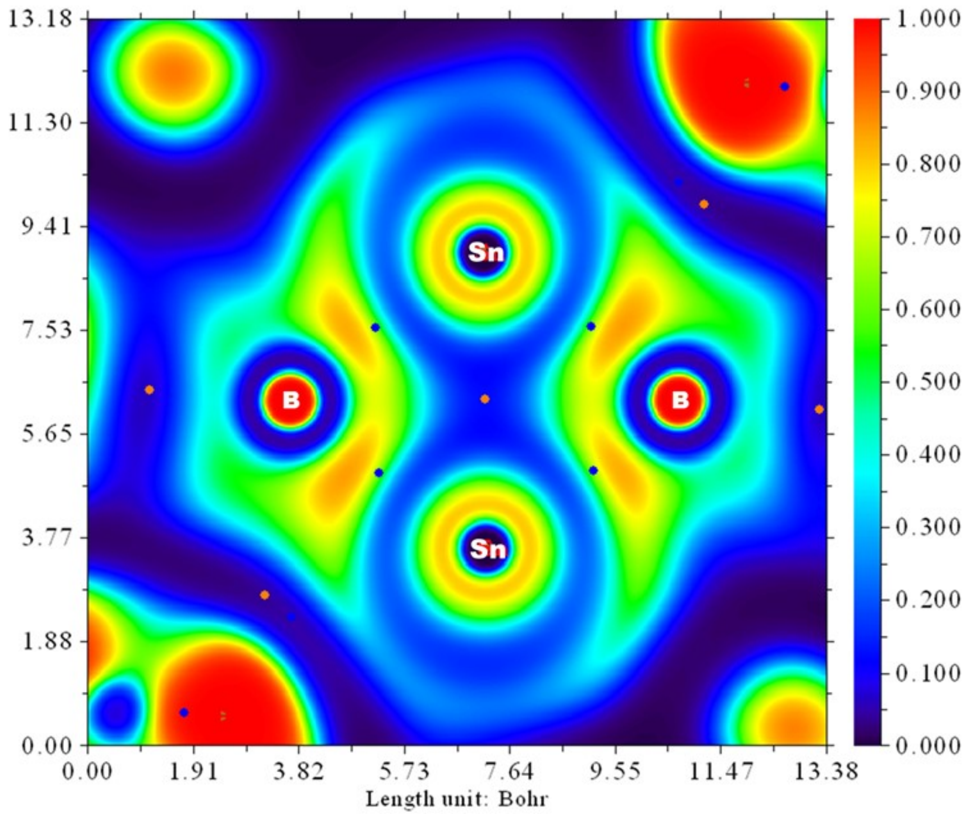
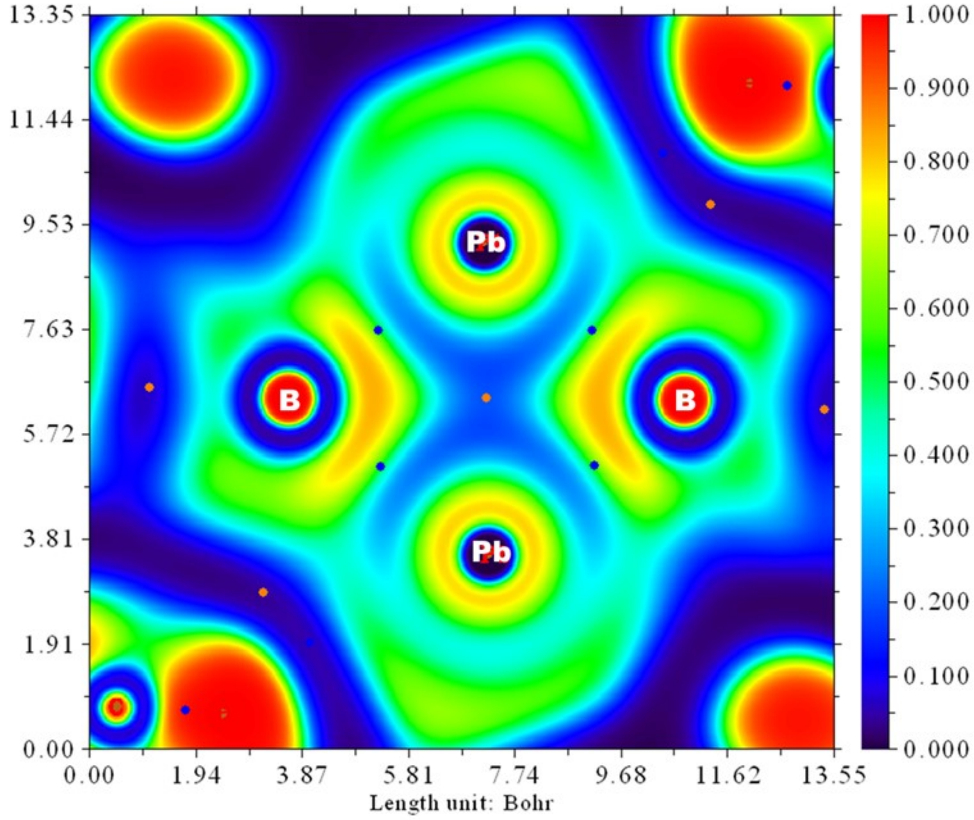


Figure S33. (A) Color-filled map of ELF of **B_2Sn_2**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

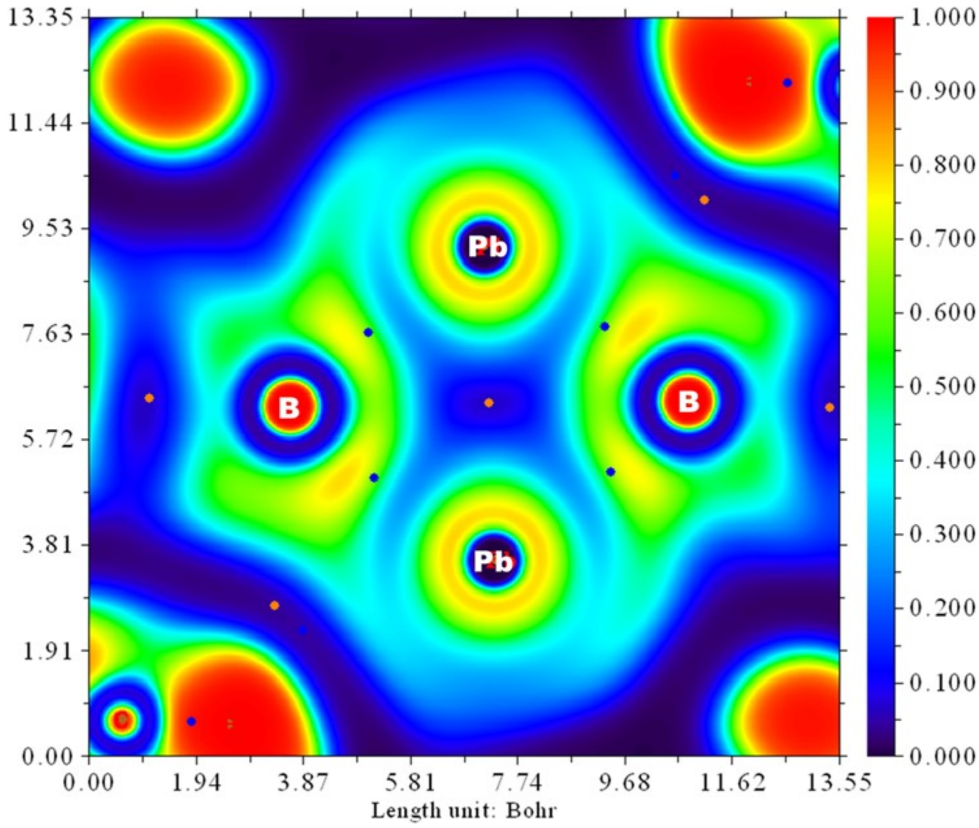
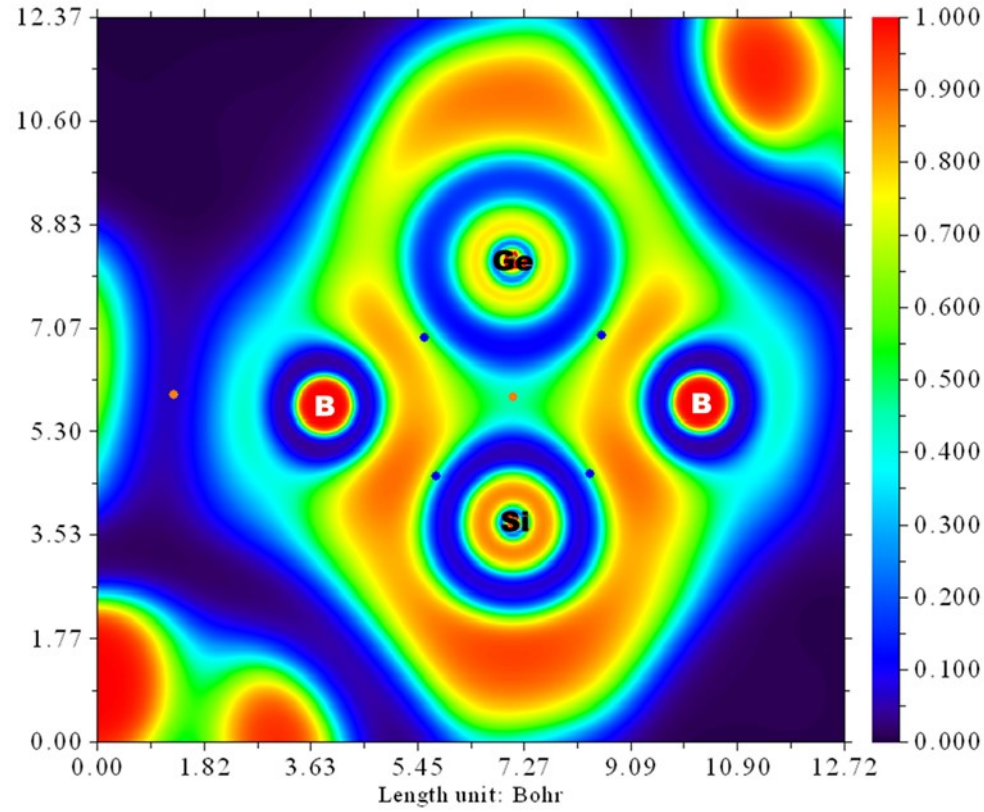


Figure S34. (A) Color-filled map of ELF of $\mathbf{B_2Pb_2}$; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

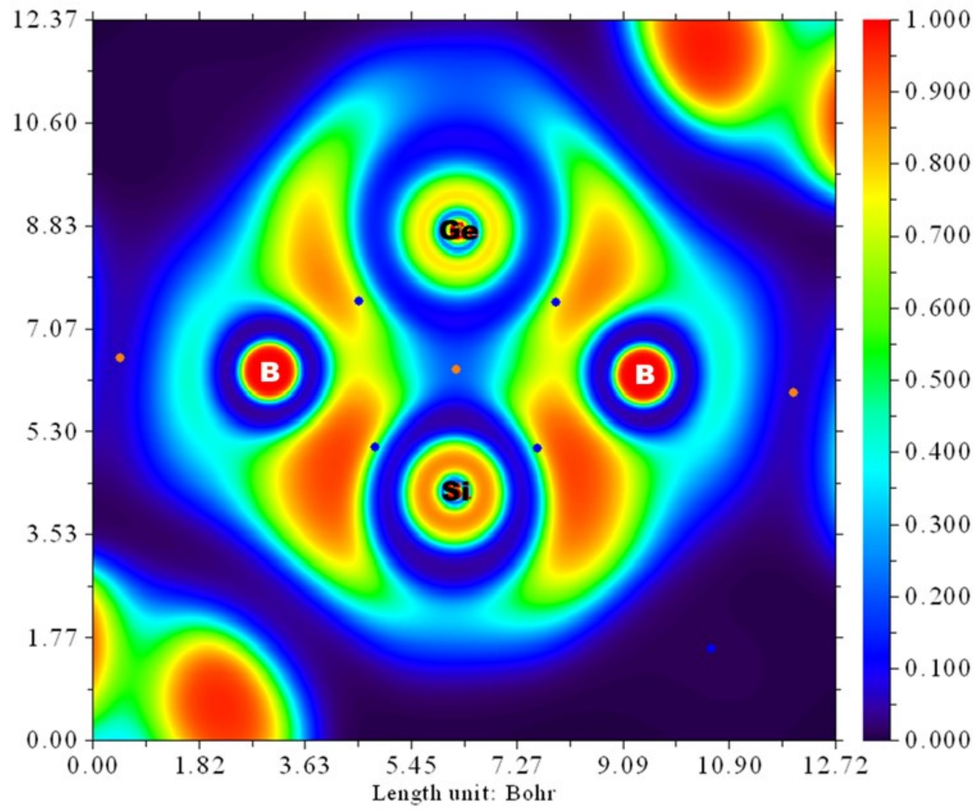
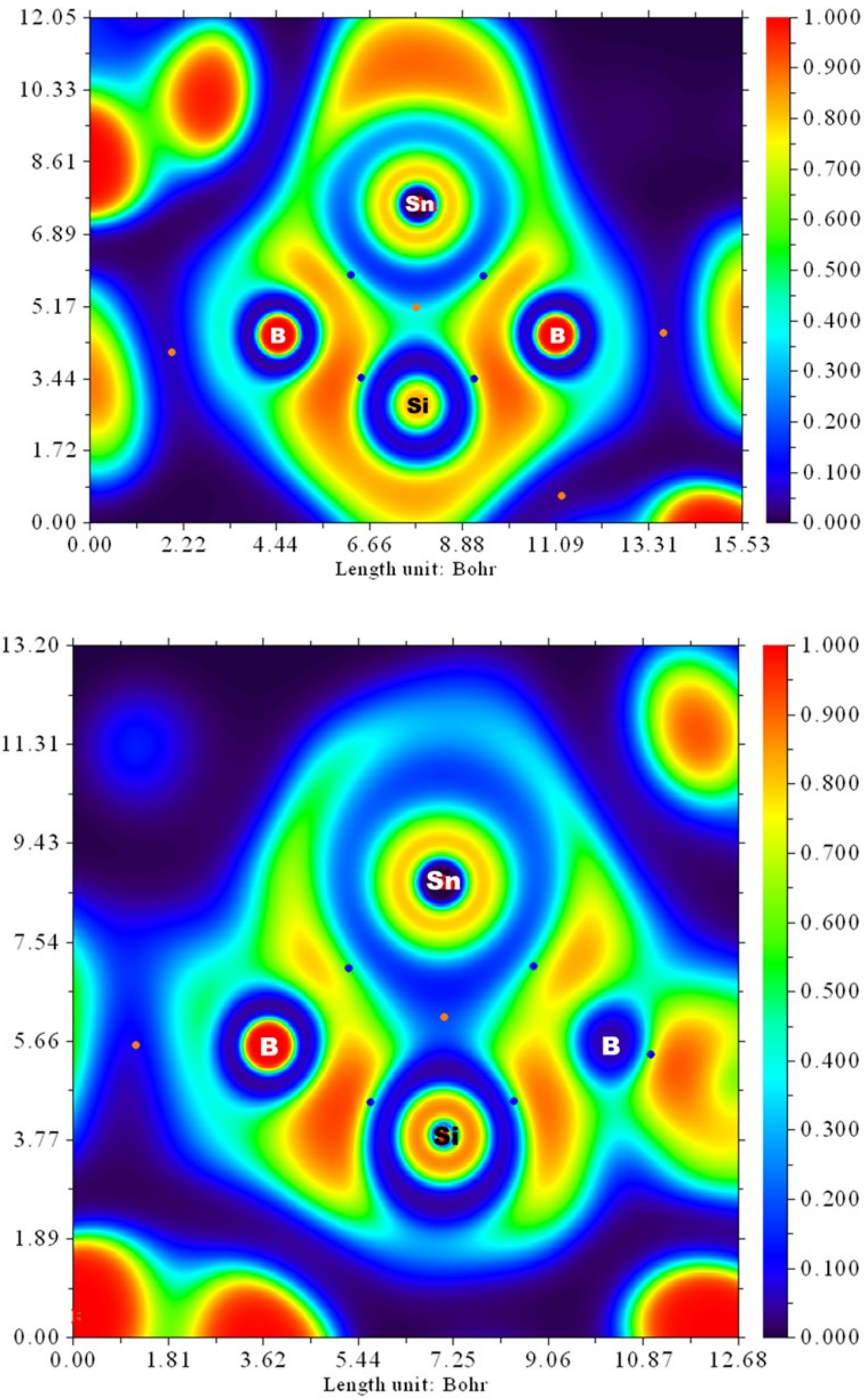


Figure S35. (A) Color-filled map of ELF of **B_2SiGe**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

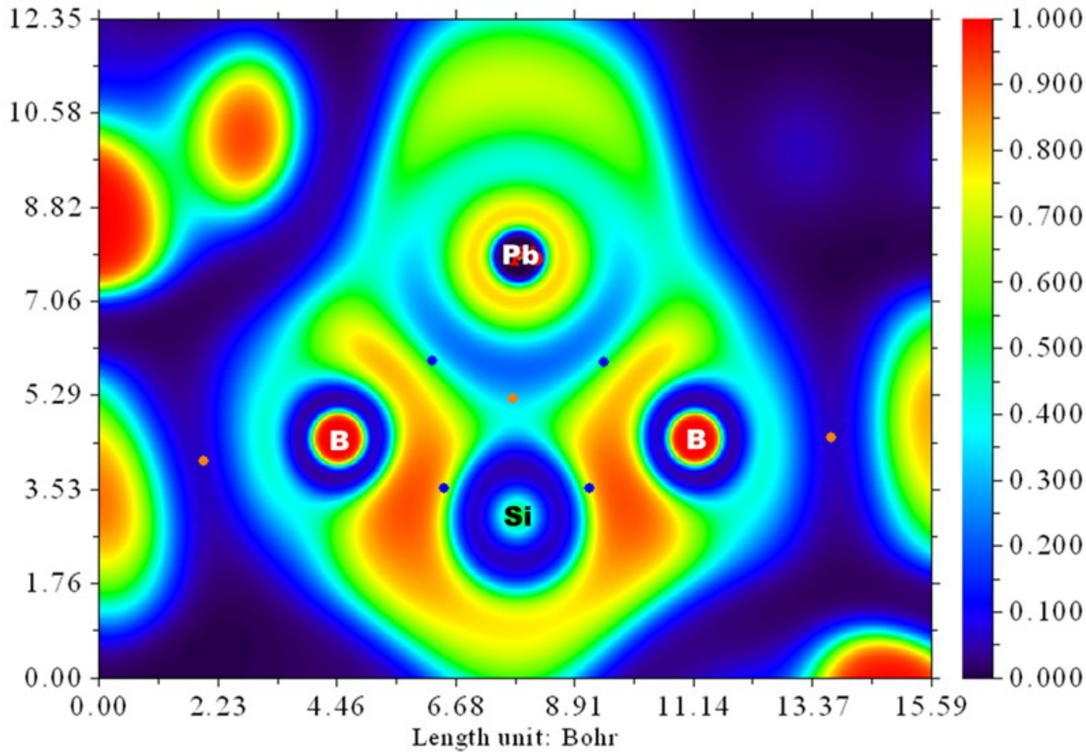
(A)



(B)

Figure S36. (A) Color-filled map of ELF of **B_2SiSn**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

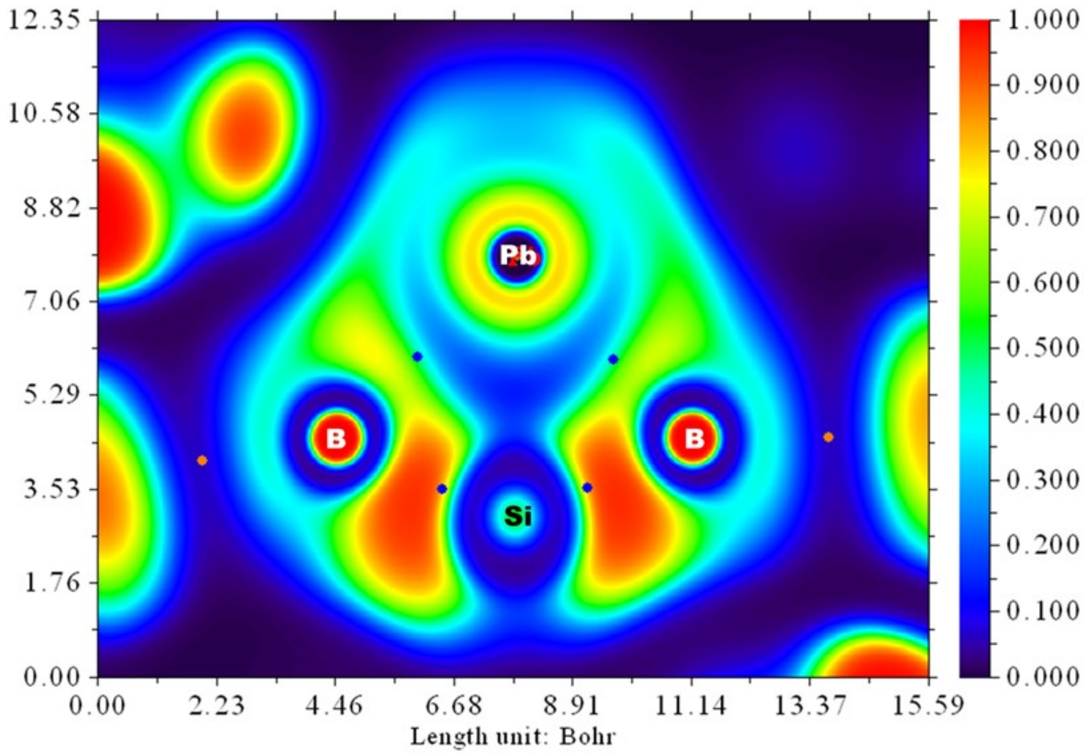
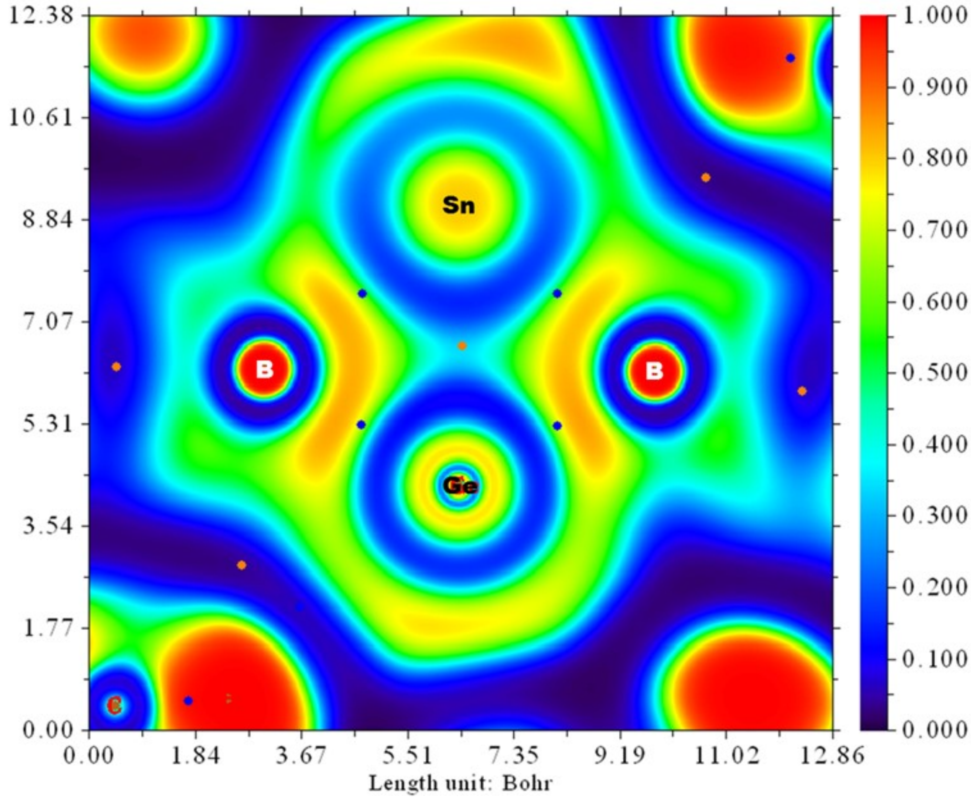


Figure S37. (A) Color-filled map of ELF of **B_2SiPb**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

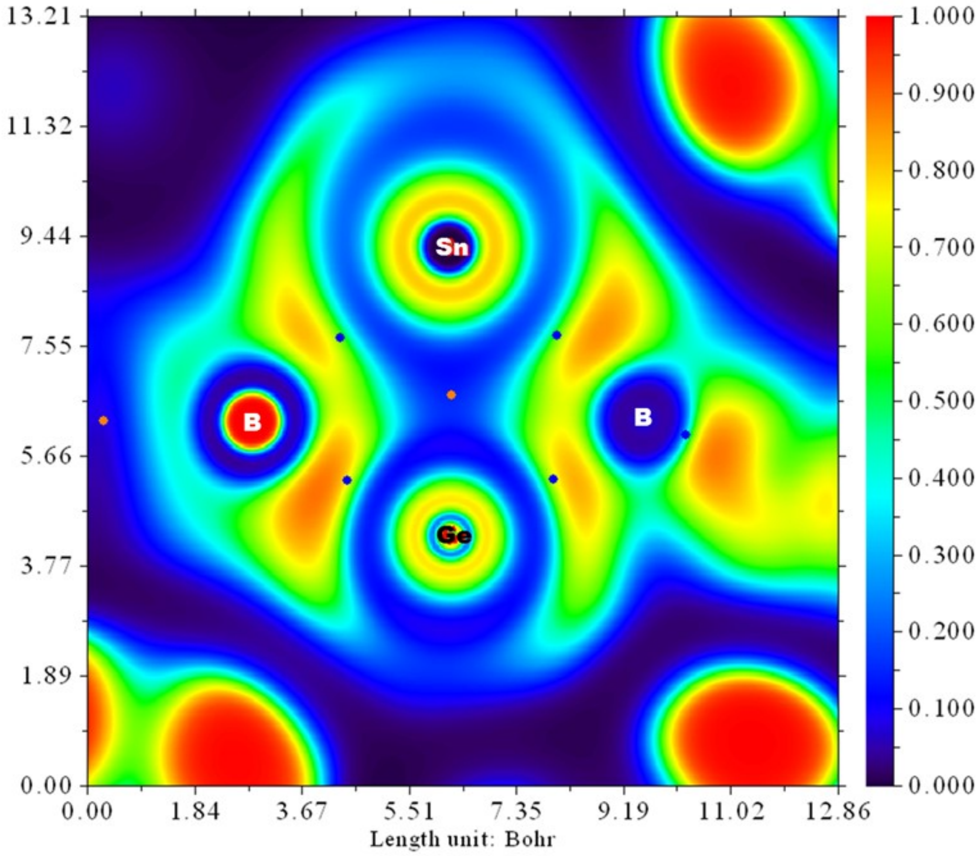
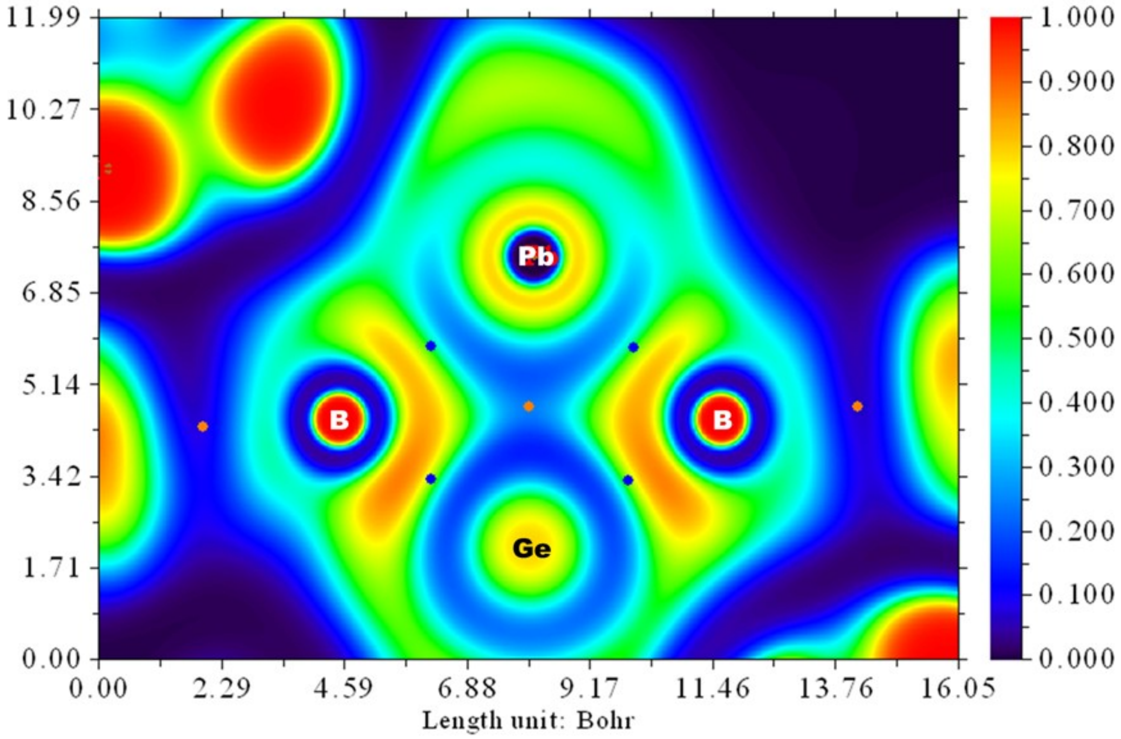


Figure S38. (A) Color-filled map of ELF of **B_2GeSn**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

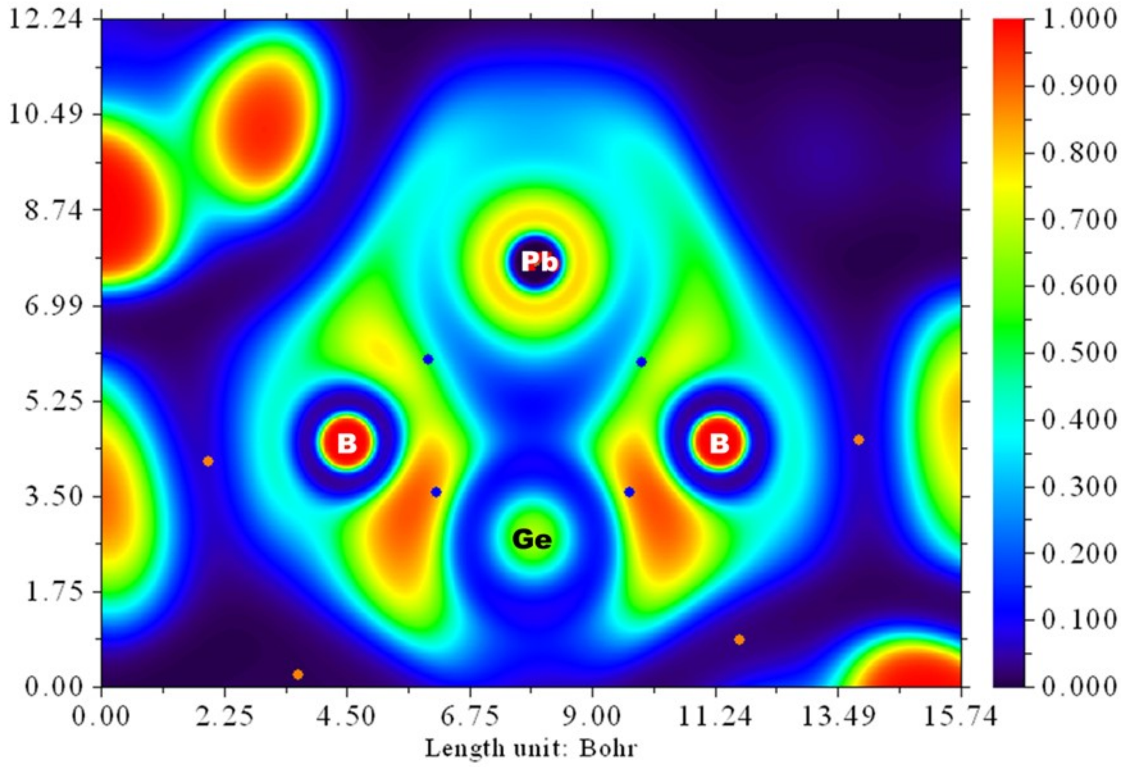
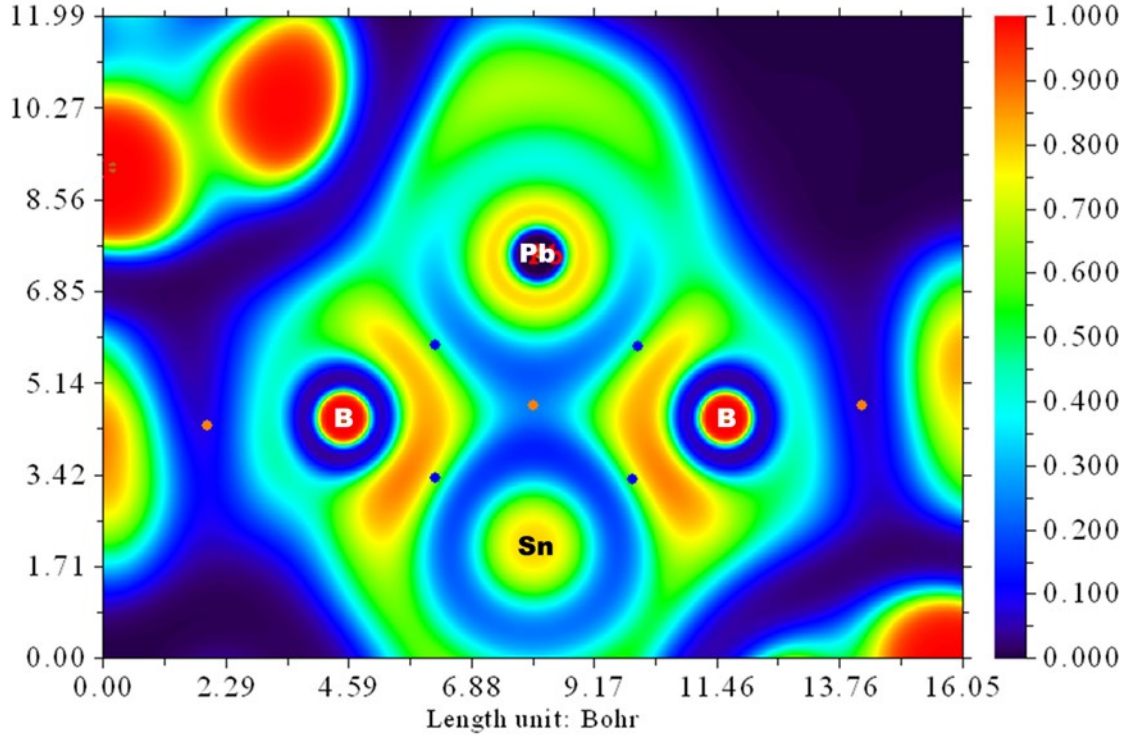


Figure S39. (A) Color-filled map of ELF of **B_2GePb**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

(A)



(B)

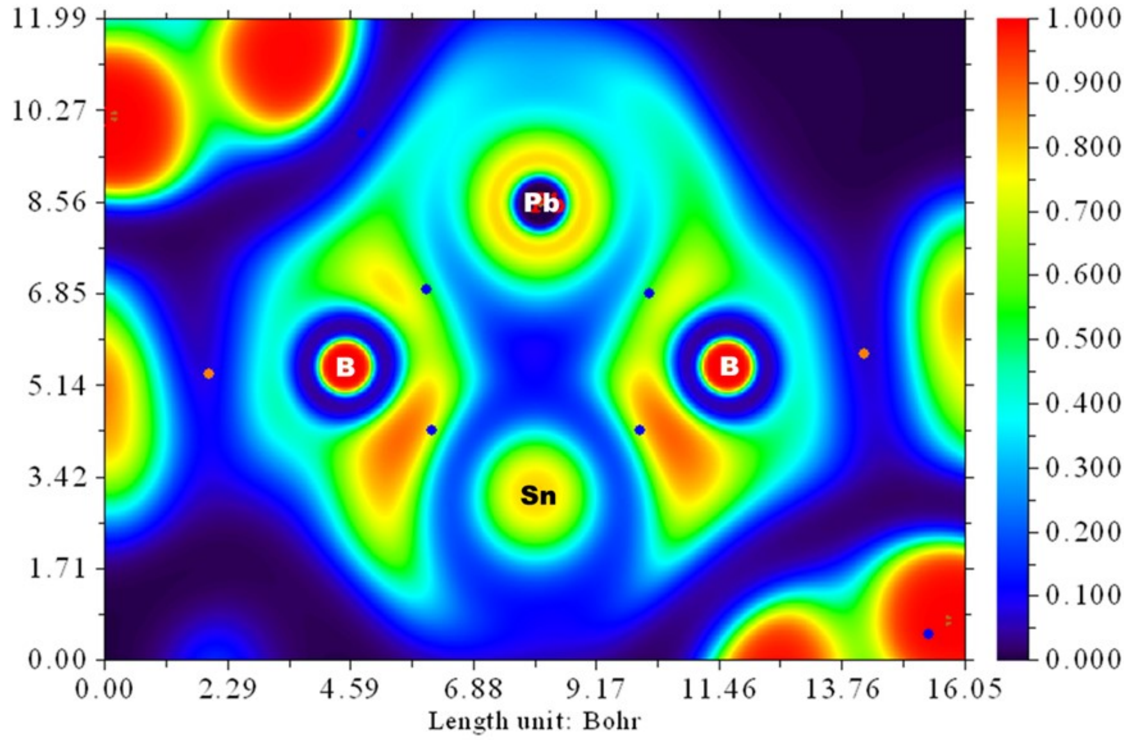


Figure S40. (A) Color-filled map of ELF of **B_2SnPb**; the color reflects the degree of electron localization of the core electrons; red and blue represent strong and weak localization. (B) After removing the σ-electrons from HOMO−2, the distribution of energy density is altered.

Table S57
M06-2X/Def2-TZVP
B2Si2
E= -3636.212786

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-0.16260400	0.11649900	-1.12867300
B	1.51933200	0.66833200	-0.15577900
B	-1.51928400	-0.66833200	0.15626600
P	2.19627400	2.52709100	-0.14733600
N	2.92745600	0.00623200	-0.25322800
Si	0.16272900	-0.11666600	1.12915900
P	-2.19626200	-2.52708300	0.14794100
N	-2.92742100	-0.00617900	0.25340300
C	1.80824200	3.53786100	1.37829200
C	2.02747800	3.51070200	-1.73712000
N	3.83395700	2.13943500	-0.05368900
C	3.04861600	-1.41554600	-0.34428000
C	3.99905500	0.83921900	-0.11409300
C	-1.80784700	-3.53816600	-1.37737500
C	-2.02790500	-3.51045500	1.73792400
N	-3.83390600	-2.13938600	0.05381600
C	-3.04856200	1.41563200	0.34407600
C	-3.99899300	-0.83916200	0.11402200
C	2.31332700	2.71165700	2.57122000
C	0.29430600	3.74101500	1.49922500
C	2.53883200	4.88354800	1.36855600
C	0.65175300	4.17884500	-1.82419600
C	3.15913600	4.53899000	-1.86579400
C	2.18473400	2.49744600	-2.88055600
C	2.93214800	-2.00807000	-1.62219100
C	3.26419600	-2.19303000	0.81072000
C	5.40385800	0.33882100	0.07160200
C	-2.31247200	-2.71215900	-2.57062900
C	-0.29388000	-3.74145800	-1.49775700
C	-2.53855400	-4.88378800	-1.36762700
C	-0.65240900	-4.17901500	1.82531400
C	-3.15989500	-4.53837600	1.86662100
C	-2.18498000	-2.49696500	2.88117600
C	-2.93234600	2.00844200	1.62188800
C	-3.26381800	2.19286900	-0.81115600
C	-5.40373900	-0.33877200	-0.07214700
H	1.80465500	1.73865000	2.63480300
H	2.10324500	3.27046600	3.49688500
H	3.39762900	2.53956100	2.50527200
H	-0.10460700	4.42474200	0.73909900
H	0.06880300	4.17577400	2.48708400
H	-0.25257400	2.79014500	1.41319900
H	2.43997200	5.34368600	2.36459400
H	2.10143900	5.58073700	0.64107100
H	3.61019300	4.76034300	1.15121800

H	-0.16421200	3.48136700	-1.57376100
H	0.58120000	5.05149200	-1.15925600
H	0.48891300	4.53191100	-2.85522000
H	4.13798900	4.05841600	-1.73093400
H	3.07226100	5.36109000	-1.14693600
H	3.11838300	4.97512900	-2.87656100
H	1.34236700	1.79326000	-2.91835800
H	3.12137300	1.92698000	-2.78038000
H	2.22306400	3.04675900	-3.83424800
C	2.74019900	-1.15397400	-2.86846600
C	3.06449100	-3.39420800	-1.72528400
C	3.43649800	-1.59435600	2.20108800
C	3.37977100	-3.58059800	0.65483300
C	6.22036600	1.11450600	0.90928800
C	5.94811300	-0.81599500	-0.50989800
H	-2.10223600	-3.27121800	-3.49610400
H	-1.80364400	-1.73923700	-2.63430900
H	-3.39676300	-2.53986600	-2.50501200
H	0.10460900	-4.42553500	-0.73772400
H	-0.06799700	-4.17584600	-2.48568900
H	0.25309100	-2.79068900	-1.41115200
H	-2.43910900	-5.34426600	-2.36342900
H	-3.61002600	-4.76041700	-1.15099500
H	-2.10169900	-5.58076600	-0.63964400
H	0.16381300	-3.48181700	1.57497100
H	-0.58199100	-5.05176300	1.16049500
H	-0.48988700	-4.53201100	2.85640400
H	-4.13859200	-4.05748700	1.73176900
H	-3.07331600	-5.36050500	1.14775100
H	-3.11926000	-4.97452200	2.87738800
H	-1.34240100	-1.79303200	2.91897300
H	-3.12141500	-1.92622000	2.78077900
H	-2.22362100	-3.04610600	3.83495200
C	-2.74086600	1.15454900	2.86838500
C	-3.06447000	3.39463100	1.72461200
C	-3.43587700	1.59393300	-2.20144700
C	-3.37927600	3.58049400	-0.65561600
C	-6.22002800	-1.11460700	-0.90990800
C	-5.94813900	0.81616600	0.50898300
C	1.89261100	-1.83250900	-3.94428800
C	4.07973600	-0.69207600	-3.45597100
H	2.19747100	-0.25502100	-2.55406500
C	3.28667900	-4.17909800	-0.59575200
H	2.98740400	-3.87106400	-2.70373000
C	2.43543400	-2.17567800	3.20593700
C	4.86140400	-1.81039800	2.73239400
H	3.24808500	-0.51174400	2.12825600
H	3.55810300	-4.20125600	1.53584900
C	7.52758500	0.73085700	1.19092000
H	5.80136600	2.02436000	1.33761000
C	7.26599000	-1.18510900	-0.24348700
H	5.35886300	-1.44361400	-1.17269100
C	-1.89522800	1.83389600	3.94517700

C	-4.08054800	0.69139400	3.45453300
H	-2.19692900	0.25611900	2.55456900
C	-3.28632000	4.17928100	0.59483600
H	-2.98747400	3.87173200	2.70294100
C	-2.43466600	2.17508500	-3.20625600
C	-4.86068300	1.80989400	-2.73306300
H	-3.24746900	0.51133300	-2.12838400
H	-3.55735500	4.20096800	-1.53681500
C	-7.52716100	-0.73098900	-1.19198000
H	-5.80092200	-2.02455100	-1.33793700
C	-7.26593300	1.18525400	0.24213000
H	-5.35906400	1.44390400	1.17181700
H	0.93599800	-2.18675600	-3.53426200
H	2.41323600	-2.68615000	-4.40560900
H	1.67075800	-1.11393100	-4.74691100
H	4.71875500	-1.55375600	-3.70862500
H	4.63598500	-0.04862000	-2.75884300
H	3.90843300	-0.11463600	-4.37730600
H	3.38746600	-5.26143700	-0.69324100
H	2.59354600	-3.25703600	3.34309800
H	1.39899900	-2.01204900	2.88204900
H	2.56538800	-1.69434900	4.18681600
H	5.62837000	-1.40740200	2.05928700
H	5.06032400	-2.88519800	2.86818800
H	4.97442200	-1.32486100	3.71330200
C	8.05617700	-0.42419200	0.61509200
H	8.13744400	1.33899400	1.86052400
H	7.67107400	-2.08452700	-0.70896100
H	-0.93875000	2.18958900	3.53623000
H	-2.41749400	2.68664800	4.40617900
H	-1.67320300	1.11542900	4.74785200
H	-4.72054800	1.55248900	3.70662900
H	-4.63557700	0.04752000	2.75685400
H	-3.90962200	0.11405300	4.37600200
H	-3.38695700	5.26166300	0.69204300
H	-2.59287800	3.25639000	-3.34374800
H	-1.39826800	2.01166700	-2.88213900
H	-2.56438700	1.69347600	-4.18703200
H	-5.62779300	1.40699700	-2.06006700
H	-5.05957100	2.88467700	-2.86904700
H	-4.97349800	1.32422300	-3.71392900
C	-8.05589300	0.42418400	-0.61652400
H	-8.13684200	-1.33924600	-1.86163700
H	-7.67113100	2.08477300	0.70731400
H	9.08180100	-0.72743500	0.83132300
H	-9.08144900	0.72740600	-0.83310300

Table S58
M06-2X/Def2-TZVP
B2Ge2
E= -7211.308379

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ge	1.20967300	-0.00974900	0.05794300
B	-0.01762500	-1.72474100	-0.00718000
B	0.00300700	1.72561200	0.00719100
Ge	-1.22429300	0.01062200	-0.05797300
P	0.08302800	-3.08481300	1.40610100
N	-0.21773100	-2.72942500	-1.16802800
P	-0.09763600	3.08570800	-1.40606600
N	0.20313100	2.73027300	1.16805600
C	-1.22042500	-2.96715300	2.72692600
C	1.76888100	-3.48115400	2.09879900
N	-0.30838300	-4.39431900	0.44791200
C	-0.29716500	-2.27611100	-2.52543800
C	-0.42235800	-4.02485200	-0.80561800
C	1.20579500	2.96804500	-2.72690900
C	-1.78349100	3.48209900	-2.09873200
N	0.29380900	4.39518900	-0.44785900
C	0.28256100	2.27693400	2.52545800
C	0.40778000	4.02570200	0.80566500
C	-2.57149500	-2.98856600	1.99789100
C	-1.08048300	-1.65224900	3.49886500
C	-1.17406900	-4.15479000	3.69042200
C	2.15821600	-2.50663100	3.21266700
C	1.83599200	-4.93202400	2.59094800
C	2.75873800	-3.34766100	0.93345800
C	0.90956700	-2.03867900	-3.20875700
C	-1.54049900	-2.06653800	-3.13780800
C	-0.86028400	-5.08534300	-1.76819300
C	2.55687600	2.98944100	-1.99789800
C	1.06583000	1.65314800	-3.49885800
C	1.15943500	4.15568900	-3.69039700
C	-2.17287400	2.50759900	-3.21260200
C	-1.85057600	4.93297800	-2.59086100
C	-2.77332900	3.34861400	-0.93337500
C	-0.92417500	2.03951300	3.20877500
C	1.52589200	2.06732300	3.13782200
C	0.84572500	5.08617100	1.76825500
H	-2.67209100	-2.15264900	1.30492100
H	-3.36500000	-2.90938000	2.74515900
H	-2.70708700	-3.91986700	1.44582200
H	-0.20356200	-1.63514600	4.14349500
H	-1.96068500	-1.52360700	4.13575000
H	-1.01755700	-0.79302000	2.83044400
H	-2.07784400	-4.13508900	4.30495900
H	-0.32078800	-4.09547900	4.36498600
H	-1.14494200	-5.10736900	3.15838300

H	1.96359000	-1.46662900	2.93675400
H	1.62879400	-2.72450000	4.14057000
H	3.22877600	-2.60684900	3.41070400
H	1.51526000	-5.62316000	1.81150100
H	1.23584600	-5.10844200	3.47899100
H	2.87526800	-5.15567700	2.84538900
H	2.87449100	-2.31127100	0.61907200
H	2.44591800	-3.94828600	0.07585600
H	3.73221200	-3.71717900	1.26460300
C	2.25517200	-2.31348500	-2.55808100
C	0.84590100	-1.60196300	-4.52628400
C	-2.87133400	-2.34565200	-2.45859200
C	-1.54889800	-1.62230200	-4.46016100
C	-1.73616800	-6.04615300	-1.25709700
C	-0.47094600	-5.18239700	-3.10481300
H	3.35036500	2.91024000	-2.74517700
H	2.65747500	2.15352800	-1.30492400
H	2.69248800	3.92074300	-1.44583900
H	0.18888900	1.63605200	-4.14346200
H	1.94601300	1.52451500	-4.13577100
H	1.00292400	0.79391200	-2.83044600
H	2.06319800	4.13598100	-4.30494800
H	1.13032900	5.10826400	-3.15835000
H	0.30614200	4.09639600	-4.36494600
H	-1.97829100	1.46759000	-2.93668800
H	-1.64344900	2.72544800	-4.14050500
H	-3.24343000	2.60786300	-3.41063100
H	-1.52979800	5.62409600	-1.81141300
H	-1.25045200	5.10938800	-3.47892200
H	-2.88985400	5.15666500	-2.84526700
H	-2.88909500	2.31222300	-0.61899700
H	-2.46048400	3.94922600	-0.07577400
H	-3.74680200	3.71815200	-1.26449900
C	-2.26977500	2.31435100	2.55810100
C	-0.86051700	1.60277700	4.52629600
C	2.85673400	2.34643100	2.45861400
C	1.53428400	1.62305900	4.46016700
C	1.72161600	6.04697700	1.25716800
C	0.45639900	5.18320800	3.10488200
C	3.35008200	-1.34093100	-2.99188200
C	2.71359200	-3.75658500	-2.79317800
H	2.12635300	-2.18657500	-1.48685000
C	-0.37407200	-1.39371200	-5.15189400
H	1.76176300	-1.41729400	-5.07288800
C	-3.79499300	-1.12353700	-2.47937400
C	-3.60405400	-3.51756500	-3.12574800
H	-2.67398700	-2.60184000	-1.41472900
H	-2.49845800	-1.46281900	-4.95650800
C	-2.23577400	-7.05549900	-2.06260000
H	-2.02062100	-5.98123200	-0.21633400
C	-0.95401700	-6.21014900	-3.90295900
H	0.20245500	-4.46426300	-3.54418500
C	-3.36470700	1.34180500	2.99187700

C	-2.72816900	3.75745900	2.79322300
H	-2.14095300	2.18745600	1.48686800
C	0.35945400	1.39448700	5.15190000
H	-1.77638200	1.41811900	5.07289900
C	3.78037900	1.12430500	2.47937900
C	3.58946800	3.51832400	3.12579000
H	2.65939400	2.60263900	1.41475400
H	2.48384100	1.46354500	4.95650900
C	2.22123900	7.05630400	2.06268500
H	2.00605900	5.98207100	0.21639900
C	0.93948800	6.21093900	3.90304300
H	-0.21700800	4.46507500	3.54424700
H	3.03495200	-0.30442400	-2.86586500
H	3.64396600	-1.49153600	-4.03289000
H	4.23795900	-1.49890200	-2.37731300
H	2.76544000	-3.97999600	-3.86219000
H	2.04237600	-4.47900200	-2.32658100
H	3.70812800	-3.90490600	-2.36726800
H	-0.40590700	-1.05293300	-6.17915400
H	-4.08558700	-0.87205100	-3.50179000
H	-3.32182500	-0.25309000	-2.02895100
H	-4.70768600	-1.34140600	-1.92158300
H	-3.01013000	-4.42874700	-3.14655500
H	-3.86349000	-3.26091500	-4.15548400
H	-4.53310300	-3.72535100	-2.59155200
C	-1.84492100	-7.14168800	-3.39198200
H	-2.92879300	-7.77740200	-1.65049400
H	-0.63610700	-6.27129900	-4.93554500
H	-3.04960400	0.30529500	2.86580900
H	-3.65857800	1.49237400	4.03289600
H	-4.25258800	1.49982300	2.37732400
H	-2.78002400	3.98084900	3.86223900
H	-2.05693100	4.47987300	2.32664800
H	-3.72269800	3.90581000	2.36730700
H	0.39128400	1.05368900	6.17915300
H	4.07097600	0.87280700	3.50179100
H	3.30720000	0.25386700	2.02895100
H	4.69307200	1.34216800	1.92158500
H	2.99555900	4.42951600	3.14660500
H	3.84889100	3.26165700	4.15552500
H	4.51852500	3.72610200	2.59160400
C	1.83039800	7.14247500	3.39207400
H	2.91426200	7.77820500	1.65058500
H	0.62158700	6.27207400	4.93563400
H	-2.23057800	-7.93088300	-4.02442200
H	2.21606900	7.93165300	4.02452600

Table S59
M06-2X/Def2-TZVP
B2Sn2
E= -3485.744971

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sn	1.38023200	-0.03134300	0.28999400
B	-0.05892700	-1.86075500	-0.04242500
B	0.04489100	1.86329600	0.03781200
Sn	-1.39061600	0.03433200	-0.30384700
P	0.05220800	-3.20351500	1.36966500
N	-0.31224900	-2.85625700	-1.20083800
P	-0.06479400	3.20990600	-1.37056600
N	0.29894700	2.85499000	1.19917900
C	-1.20167900	-3.02195100	2.73895700
C	1.72657900	-3.72329400	2.03970000
N	-0.41231100	-4.50079000	0.42967600
C	-0.37463800	-2.41716100	-2.56620300
C	-0.51437300	-4.14920700	-0.83062400
C	1.18989700	3.03250800	-2.73994200
C	-1.73864400	3.73260400	-2.03999700
N	0.39988400	4.50429400	-0.42647100
C	0.35810800	2.41247800	2.56362000
C	0.50135000	4.14906300	0.83281700
C	-2.58272300	-3.00924100	2.07072300
C	-0.98520200	-1.70714400	3.49366500
C	-1.16162000	-4.20100700	3.71407100
C	2.21497600	-2.82393600	3.17714900
C	1.70051500	-5.18959700	2.49355800
C	2.70643000	-3.63555100	0.86169000
C	0.84079300	-2.14071400	-3.22254000
C	-1.60682300	-2.26195600	-3.22035800
C	-0.90472600	-5.23280800	-1.78485200
C	2.57071500	3.01772400	-2.07129200
C	0.97415400	1.72034900	-3.49956600
C	1.15033100	4.21495500	-3.71101300
C	-2.22672400	2.83772500	-3.18110400
C	-1.71187100	5.20063000	-2.48829200
C	-2.71945900	3.64079000	-0.86313300
C	-0.85905100	2.13738100	3.21731900
C	1.58878100	2.25384200	3.21989600
C	0.89143500	5.22980300	1.79041300
H	-2.68919700	-2.18113400	1.37039300
H	-3.34103800	-2.89874100	2.85011800
H	-2.76818700	-3.94124400	1.53416200
H	-0.07388700	-1.71089400	4.09039900
H	-1.82691000	-1.54863600	4.17433400
H	-0.93255900	-0.85188900	2.81812900
H	-2.03254500	-4.13376000	4.37129600
H	-0.27490100	-4.17773400	4.34609300
H	-1.20408300	-5.15802000	3.19104300

H	2.15921000	-1.76417700	2.91948300
H	1.65128800	-2.99053300	4.09491900
H	3.26146600	-3.06340700	3.38583900
H	1.30841700	-5.83567700	1.70901900
H	1.11710400	-5.34543700	3.39638300
H	2.72837300	-5.49164700	2.71050700
H	2.89056700	-2.60466700	0.56360200
H	2.34034000	-4.19793900	-0.00083600
H	3.65778900	-4.07603200	1.16969000
C	2.18254900	-2.38335200	-2.55293600
C	0.79828600	-1.70452900	-4.54056900
C	-2.95421300	-2.56702400	-2.58435000
C	-1.59177500	-1.82788500	-4.54610600
C	-1.75231900	-6.21998600	-1.27607500
C	-0.48380400	-5.33567300	-3.11151400
H	3.32929800	2.91036500	-2.85086300
H	2.67740100	2.18702800	-1.37409900
H	2.75572300	3.94777100	-1.53121300
H	0.06266500	1.72574200	-4.09603200
H	1.81589100	1.56524700	-4.18096800
H	0.92203000	0.86249100	-2.82727800
H	2.02158400	4.14991100	-4.36801900
H	1.19262100	5.17014700	-3.18464400
H	0.26394900	4.19397600	-4.34356800
H	-2.17278500	1.77705600	-2.92684200
H	-1.66171500	3.00666800	-4.09760300
H	-3.27262100	3.07944100	-3.39029200
H	-1.31960700	5.84359900	-1.70128400
H	-1.12830500	5.35963500	-3.39045500
H	-2.73957800	5.50392000	-2.70422300
H	-2.90366300	2.60888500	-0.56861900
H	-2.35411900	4.20035300	0.00156400
H	-3.67062400	4.08219700	-1.17043300
C	-2.19910200	2.38320100	2.54551000
C	-0.81991600	1.69960900	4.53491900
C	2.93795300	2.55804000	2.58724900
C	1.57035300	1.81766300	4.54493100
C	1.74110400	6.21719700	1.28545300
C	0.46839700	5.32991700	3.11666000
C	3.23443800	-1.33116500	-2.90465600
C	2.72147700	-3.78395800	-2.86287400
H	2.02334000	-2.33184700	-1.47959200
C	-0.40927300	-1.54810300	-5.20346400
H	1.72267800	-1.48944600	-5.06131800
C	-3.93169200	-1.39219600	-2.71994900
C	-3.61611900	-3.79832400	-3.21907000
H	-2.79218900	-2.75882100	-1.52021100
H	-2.53175800	-1.70895700	-5.07058800
C	-2.19612100	-7.25960000	-2.07567500
H	-2.06018600	-6.15058700	-0.24232700
C	-0.91117000	-6.39242800	-3.90318500
H	0.16978300	-4.59830700	-3.54904700
C	-3.25267800	1.33103300	2.89199000

C	-2.73718100	3.78348300	2.85817000
H	-2.03757600	2.33425400	1.47243300
C	0.38604100	1.53966600	5.19981700
H	-1.74576100	1.48584500	5.05364800
C	3.91314700	1.38130000	2.72230500
C	3.60060000	3.78690000	3.22590300
H	2.77839800	2.75236000	1.52321300
H	2.50910100	1.69614100	5.07100800
C	2.18505400	7.25413200	2.08844600
H	2.05048000	6.15008100	0.25196700
C	0.89597600	6.38401500	3.91174800
H	-0.18708200	4.59246600	3.55127100
H	2.85903800	-0.31799200	-2.74803600
H	3.56543900	-1.41477900	-3.94203400
H	4.11281000	-1.46831500	-2.27141300
H	2.81148100	-3.93730500	-3.94159100
H	2.07592500	-4.56515700	-2.45922900
H	3.71118300	-3.90863000	-2.41821200
H	-0.42520200	-1.21059800	-6.23199700
H	-4.25823900	-1.28003600	-3.75594300
H	-3.49189500	-0.45282400	-2.39226500
H	-4.82114400	-1.58261400	-2.11669200
H	-3.01370200	-4.69907700	-3.13688200
H	-3.80327600	-3.61356000	-4.27926700
H	-4.57934500	-3.98477900	-2.74019300
C	-1.77649200	-7.34973700	-3.39608800
H	-2.86872700	-8.00191800	-1.66620200
H	-0.57030500	-6.45650700	-4.92827700
H	-2.87800000	0.31807000	2.73270000
H	-3.58549300	1.41162200	3.92899800
H	-4.12974500	1.47108800	2.25756300
H	-2.82972700	3.93378100	3.93708800
H	-2.08970600	4.56514700	2.45851800
H	-3.72558300	3.91059500	2.41135400
H	0.39934000	1.20082200	6.22794900
H	4.23663500	1.26566100	3.75887100
H	3.47282600	0.44357800	2.39056800
H	4.80453500	1.57195400	2.12201300
H	3.00001800	4.68887400	3.14398800
H	3.78499100	3.59982800	4.28620500
H	4.56525800	3.97252700	2.74959200
C	1.76348200	7.34139700	3.40847800
H	2.85929600	7.99661600	1.68191800
H	0.55351200	6.44593200	4.93647900
H	-2.11957400	-8.16172600	-4.02413000
H	2.10670200	8.15126800	4.03917400

Table S60
M06-2X/Def2-TZVP
B2Pb2
E= -3442.759277

Atomic Number	Coordinates (Angstroms) X	Y	Z
Pb	1.43181600	-0.03446200	0.41243800
B	-0.07540100	-1.90505500	-0.04261500
B	0.05954000	1.90435700	0.04428300
Pb	-1.44952100	0.03334200	-0.40895900
P	0.03071400	-3.24082900	1.36269900
N	-0.33604200	-2.89468700	-1.20113300
P	-0.04787800	3.23966500	-1.36166000
N	0.32169200	2.89472700	1.20174600
C	-1.22037800	-3.05470600	2.73867900
C	1.70180500	-3.77404900	2.04601200
N	-0.43102000	-4.53891500	0.42453600
C	-0.39943500	-2.44484700	-2.56251300
C	-0.52901200	-4.18963700	-0.83938500
C	1.20276100	3.05266800	-2.73787200
C	-1.71940800	3.77127700	-2.04515400
N	0.41474200	4.53838400	-0.42460900
C	0.38531900	2.44663500	2.56362200
C	0.51553500	4.18934300	0.83912600
C	-2.60203400	-3.03621400	2.07290800
C	-0.99833500	-1.73763400	3.48655900
C	-1.18538200	-4.23143300	3.71601800
C	2.18884300	-2.89895000	3.20282200
C	1.67012700	-5.24749100	2.47564900
C	2.69035500	-3.67088500	0.87689500
C	0.81565400	-2.15293400	-3.21372200
C	-1.63186800	-2.29414500	-3.21785200
C	-0.90153500	-5.27490600	-1.79639000
C	2.58459500	3.03547500	-2.07237400
C	0.98087400	1.73468300	-3.48415300
C	1.16695500	4.22829700	-3.71649000
C	-2.20632600	2.89394100	-3.20037700
C	-1.68828700	5.24395700	-2.47745500
C	-2.70771000	3.66989200	-0.87567400
C	-0.82938000	2.15749700	3.21677400
C	1.61824300	2.29582400	3.21768400
C	0.89216900	5.27423600	1.79503300
H	-2.70261000	-2.20630700	1.37351100
H	-3.36071100	-2.92410600	2.85172600
H	-2.79062600	-3.96574400	1.53279300
H	-0.08779400	-1.74068800	4.08451200
H	-1.83978400	-1.56752400	4.16488600
H	-0.94305700	-0.88722800	2.80369200
H	-2.05331300	-4.15907800	4.37674400
H	-0.29639400	-4.21536300	4.34497700
H	-1.23609700	-5.18841000	3.19350600

H	2.14926600	-1.83411500	2.96390900
H	1.61379100	-3.07139600	4.11243400
H	3.23020300	-3.15409800	3.41986100
H	1.28446400	-5.87991800	1.67670700
H	1.07695700	-5.41763900	3.36948500
H	2.69532400	-5.55559600	2.69841400
H	2.87439100	-2.63655800	0.58970500
H	2.33049200	-4.22181300	0.00427600
H	3.64125400	-4.11305700	1.18463200
C	2.15656700	-2.39615000	-2.54252900
C	0.77228900	-1.70389900	-4.52730900
C	-2.97809000	-2.61367300	-2.58533200
C	-1.61768500	-1.84605200	-4.53924100
C	-1.73401800	-6.27797800	-1.29239400
C	-0.47996700	-5.36661200	-3.12449000
H	3.34317200	2.92275400	-2.85119600
H	2.68561600	2.20642100	-1.37199500
H	2.77294000	3.96574800	-1.53341700
H	0.07070600	1.73719600	-4.08268000
H	1.82269900	1.56336000	-4.16172800
H	0.92497100	0.88516000	-2.80025700
H	2.03472100	4.15557600	-4.37740500
H	1.21737500	5.18591900	-3.19508300
H	0.27776100	4.21106000	-4.34514900
H	-2.16575200	1.82943300	-2.95993100
H	-1.63176000	3.06549600	-4.11049300
H	-3.24805000	3.14786200	-3.41733700
H	-1.30312200	5.87802200	-1.67960600
H	-1.09494300	5.41276200	-3.37146000
H	-2.71361100	5.55107600	-2.70104800
H	-2.89130200	2.63605700	-0.58647800
H	-2.34788700	4.22269700	-0.00422500
H	-3.65887200	4.11104600	-1.18410300
C	-2.17107300	2.40030200	2.54672700
C	-0.78474900	1.71120600	4.53132100
C	2.96352100	2.61280200	2.58214500
C	1.60543300	1.85083700	4.54012800
C	1.71874500	6.28026500	1.28682500
C	0.47882200	5.36366200	3.12545200
C	3.20030600	-1.32831600	-2.86974800
C	2.70707200	-3.78701900	-2.87609100
H	1.98964800	-2.36462000	-1.46937400
C	-0.43567000	-1.55036600	-5.19099200
H	1.69626500	-1.47751300	-5.04429800
C	-3.96689700	-1.44713300	-2.71849700
C	-3.63162500	-3.84604700	-3.22694100
H	-2.81564200	-2.81051600	-1.52192700
H	-2.55758100	-1.72945900	-5.06465600
C	-2.16479100	-7.31866400	-2.09780000
H	-2.04115800	-6.21791700	-0.25756800
C	-0.89528400	-6.42342000	-3.92255800
H	0.16393000	-4.61879500	-3.55908300
C	-3.21503600	1.33449700	2.87871700

C	-2.72062300	3.79241600	2.87676200
H	-2.00597300	2.36538400	1.47351400
C	0.42389000	1.55788700	5.19392000
H	-1.70830900	1.48698700	5.04998600
C	3.95412200	1.44817100	2.72085100
C	3.61507100	3.85038600	3.21562300
H	2.79947200	2.80368500	1.51788600
H	2.54589700	1.73442500	5.06462500
C	2.15006900	7.32283400	2.08958100
H	2.02027200	6.22157100	0.25052700
C	0.89424100	6.42250600	3.92085900
H	-0.15951100	4.61313800	3.56362200
H	2.81698100	-0.32174300	-2.68953600
H	3.53175600	-1.38343300	-3.90904300
H	4.08109700	-1.47440900	-2.24142700
H	2.80494100	-3.92016900	-3.95694400
H	2.06365400	-4.57953700	-2.49100500
H	3.69464200	-3.91385400	-2.42727500
H	-0.45218100	-1.20297600	-6.21623100
H	-4.30934300	-1.34897700	-3.75053600
H	-3.53313100	-0.49713300	-2.41290700
H	-4.84660300	-1.63751000	-2.10104600
H	-3.03002300	-4.74606800	-3.13815900
H	-3.80703900	-3.66085500	-4.28928100
H	-4.59989500	-4.03369100	-2.75874400
C	-1.74775200	-7.39507800	-3.42037200
H	-2.82622200	-8.07270200	-1.69132800
H	-0.55512900	-6.47663000	-4.94879500
H	-2.83271500	0.32719000	2.70071500
H	-3.54454300	1.39283700	3.91835300
H	-4.09682900	1.47966500	2.25160300
H	-2.81442500	3.92976400	3.95718600
H	-2.07921000	4.58340300	2.48600900
H	-3.71003000	3.91754600	2.43130500
H	0.44133000	1.21281200	6.21994000
H	4.29889900	1.35700100	3.75288800
H	3.52079500	0.49561600	2.42245800
H	4.83240000	1.63522100	2.10010700
H	3.01036800	4.74867300	3.12224600
H	3.79228500	3.67179700	4.27877100
H	4.58242200	4.03747700	2.74486800
C	1.73971000	7.39805100	3.41393200
H	2.80636100	8.07959900	1.67953700
H	0.55922400	6.47461100	4.94854700
H	-2.08185200	-8.20736600	-4.05306800
H	2.07364700	8.21225800	4.04439900

Table S61
M06-2X/Def2-TZVP
B2SiGe
E= -5423.763376

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-0.16689700	0.14017100	-1.00595600
B	1.54097700	0.67675300	-0.10917200
B	-1.54638700	-0.68571100	0.19786100
P	2.22138500	2.52419600	-0.12785700
N	2.93549100	0.00717400	-0.22025500
Ge	0.18271100	-0.14785900	1.30927500
P	-2.23047800	-2.52792600	0.16977000
N	-2.94739000	-0.01439700	0.26629100
C	1.85365300	3.54164700	1.38491700
C	2.01231300	3.49793000	-1.70518100
N	3.84400100	2.13804000	-0.06447300
C	3.06213600	-1.41540400	-0.33461300
C	4.00712100	0.83705200	-0.11209200
C	-1.77634500	-3.53154400	-1.32729800
C	-2.10826700	-3.50398400	1.75423100
N	-3.84720800	-2.14022800	0.02593900
C	-3.06664000	1.41030100	0.34392700
C	-4.01214800	-0.83986900	0.08861000
C	2.39530700	2.74363800	2.57963500
C	0.34318700	3.73566600	1.54696300
C	2.56134400	4.89748100	1.35026000
C	0.63232900	4.15651100	-1.77052700
C	3.12756500	4.53790900	-1.86603700
C	2.15368900	2.49431000	-2.85720400
C	2.92669100	-1.98339300	-1.61424400
C	3.31066500	-2.20554500	0.79621500
C	5.41271200	0.34269600	0.04654700
C	-2.24269500	-2.71976300	-2.54402100
C	-0.25898800	-3.72346400	-1.39626500
C	-2.48457600	-4.88718100	-1.35191100
C	-0.73900200	-4.17273500	1.89195200
C	-3.23683000	-4.53688900	1.85991100
C	-2.30169700	-2.49602600	2.89557200
C	-2.96157400	2.01034300	1.61189500
C	-3.26170000	2.17309000	-0.81566900
C	-5.40915400	-0.34200500	-0.12354600
H	1.91655700	1.76796400	2.66726500
H	2.18537100	3.30846700	3.49130400
H	3.47392200	2.60033300	2.50194900
H	-0.07578600	4.41189200	0.80392400
H	0.14889900	4.16795400	2.53304900
H	-0.19806300	2.79162100	1.47820400
H	2.47863800	5.35522800	2.33950900
H	2.09711800	5.57745300	0.63690900
H	3.62108300	4.79447100	1.11007800

H	-0.16831800	3.46547300	-1.49217000
H	0.57403600	5.03190500	-1.12345100
H	0.44668500	4.48851600	-2.79556300
H	4.10917400	4.07402000	-1.76856100
H	3.05627600	5.35181800	-1.15015400
H	3.04735700	4.97033800	-2.86676000
H	1.31969100	1.79383200	-2.88725800
H	3.08802500	1.93263000	-2.78096300
H	2.17089300	3.04928500	-3.79839500
C	2.69770500	-1.11904900	-2.84290100
C	3.07120200	-3.35926600	-1.74385200
C	3.50648500	-1.63657900	2.19188900
C	3.43561300	-3.58290100	0.61376300
C	6.22977400	1.09813300	0.89126900
C	5.95304500	-0.78976200	-0.56439200
H	-1.97935700	-3.27469100	-3.44797800
H	-1.75839600	-1.74358800	-2.59015900
H	-3.32381800	-2.57336000	-2.52925700
H	0.11185500	-4.41091700	-0.63818100
H	-0.00006700	-4.14038300	-2.37404000
H	0.27570400	-2.78017400	-1.27923600
H	-2.34123400	-5.33352400	-2.33960100
H	-3.55707200	-4.78663700	-1.17518700
H	-2.06408300	-5.57545400	-0.61966700
H	0.07877200	-3.48663900	1.65429500
H	-0.65376200	-5.04979400	1.24973700
H	-0.60966900	-4.50450200	2.92604900
H	-4.20964000	-4.06762900	1.71349400
H	-3.13560000	-5.35255200	1.14986400
H	-3.20816600	-4.96819000	2.86405400
H	-1.45736100	-1.81281800	2.97744100
H	-3.21836300	-1.91594000	2.76289700
H	-2.38792000	-3.04986500	3.83349500
C	-2.79672300	1.17391100	2.87018600
C	-3.07182100	3.39291200	1.69663700
C	-3.42341800	1.56741000	-2.20045400
C	-3.36074400	3.55760900	-0.67674400
C	-6.19719300	-1.09358300	-0.99857700
C	-5.96845000	0.78970000	0.47156100
C	1.79511400	-1.77457900	-3.88652200
C	4.02032300	-0.68922800	-3.48614300
H	2.19100000	-0.21780700	-2.50987600
C	3.32406100	-4.15785200	-0.63871900
H	2.98054300	-3.81673400	-2.72075700
C	2.55294800	-2.27035500	3.20957800
C	4.94657600	-1.84079600	2.68122100
H	3.29648500	-0.56479000	2.15519000
H	3.63730300	-4.21226300	1.47210400
C	7.53617000	0.71732400	1.14759900
H	5.81664700	1.98693300	1.34684700
C	7.27057000	-1.15479900	-0.32476900
H	5.36298700	-1.40367400	-1.22559900
C	-1.96461900	1.86079100	3.95124800

C	-4.14950400	0.74342200	3.44741600
H	-2.26481800	0.26917500	2.58697600
C	-3.27001900	4.16532600	0.56166700
H	-2.99687100	3.87725200	2.66167300
C	-2.41058900	2.13594400	-3.19946500
C	-4.83727000	1.80237800	-2.74927100
H	-3.25126100	0.49096000	-2.12438900
H	-3.52061000	4.16651800	-1.55855000
C	-7.49453400	-0.71189500	-1.29606800
H	-5.76921100	-1.98120100	-1.44283100
C	-7.27758400	1.15570800	0.19042500
H	-5.39933500	1.40150500	1.15269300
H	0.85535600	-2.10905000	-3.44497700
H	2.27621300	-2.62818000	-4.36887400
H	1.56026900	-1.05004500	-4.66828000
H	4.62622100	-1.55999600	-3.75062700
H	4.60902000	-0.05461800	-2.82183900
H	3.82429500	-0.12283800	-4.39896000
H	3.43245900	-5.22875800	-0.75646600
H	2.76642400	-3.33421100	3.33454400
H	1.51238200	-2.15706100	2.91164300
H	2.68001500	-1.79157800	4.18223200
H	5.68443000	-1.40956900	2.00782200
H	5.16298900	-2.90713800	2.78025700
H	5.07120500	-1.38417200	3.66489400
C	8.06273000	-0.41377300	0.53889700
H	8.14439300	1.30636300	1.82166700
H	7.67210900	-2.03374400	-0.81181900
H	-1.00958700	2.21053000	3.55712200
H	-2.49025800	2.70883000	4.39568500
H	-1.75672500	1.15064200	4.75323600
H	-4.77612200	1.61321500	3.66295900
H	-4.69573800	0.09052500	2.76516500
H	-3.99771400	0.19595300	4.37998700
H	-3.35321700	5.24162700	0.64609600
H	-2.56743600	3.20675700	-3.34821100
H	-1.38575400	1.98059900	-2.86549100
H	-2.53151400	1.64660900	-4.16773000
H	-5.61268900	1.42916000	-2.08302700
H	-5.00956200	2.87014200	-2.90275900
H	-4.94730900	1.30662800	-3.71552100
C	-8.04130600	0.41665700	-0.70016200
H	-8.08046100	-1.29883800	-1.99134500
H	-7.69512900	2.03301400	0.66704800
H	9.08409400	-0.71394900	0.73465800
H	-9.05646100	0.71628300	-0.92676900

Table S62
M06-2X/Def2-TZVP
B2SiSn
E= -3560.983256

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-0.24834900	0.39195300	-0.65669400
B	1.59968700	0.66970700	0.00613900
B	-1.61136100	-0.68556400	0.30551300
P	2.26723000	2.50864000	-0.08150000
N	2.97691100	-0.01604900	-0.14461100
Sn	0.22869700	-0.18272800	1.77796000
P	-2.28545800	-2.52085200	0.22919500
N	-3.02828500	-0.01793100	0.30162700
C	2.02445600	3.56402700	1.43991000
C	1.96028200	3.48546900	-1.64866800
N	3.89124200	2.11895500	-0.11974400
C	3.10742300	-1.43597600	-0.29532800
C	4.05348600	0.81769800	-0.14179000
C	-1.68215100	-3.50447000	-1.22540800
C	-2.32855500	-3.52313000	1.80609600
N	-3.88483100	-2.14319000	-0.04709700
C	-3.16030900	1.40788900	0.35065700
C	-4.06903100	-0.84531200	0.03561000
C	2.67366900	2.80057000	2.60236900
C	0.53728500	3.77989600	1.73513200
C	2.73038500	4.91650800	1.31529600
C	0.59862500	4.18433800	-1.62402300
C	3.08880100	4.49324400	-1.90353900
C	1.99143100	2.47652500	-2.80319300
C	2.90683300	-1.97896600	-1.57870100
C	3.45426800	-2.24733900	0.79436800
C	5.46899300	0.33027400	-0.07227200
C	-2.06385700	-2.69536800	-2.47266800
C	-0.16036600	-3.64380600	-1.16071000
C	-2.34134200	-4.88120000	-1.31977500
C	-0.98361200	-4.18781300	2.10139700
C	-3.44963700	-4.56923600	1.76468800
C	-2.67054900	-2.53293600	2.92856300
C	-3.08878000	2.03326600	1.60832700
C	-3.31022600	2.15133000	-0.82847200
C	-5.45780800	-0.35935700	-0.24138700
H	2.22631900	1.81784400	2.74987500
H	2.52900000	3.37930200	3.51791100
H	3.74439300	2.67297900	2.43787200
H	0.05388100	4.42451000	1.00276500
H	0.44099200	4.25628800	2.71519100
H	-0.01730200	2.84231400	1.75355400
H	2.73134600	5.39488800	2.29830300
H	2.21147600	5.58462000	0.62942500
H	3.76656500	4.80328600	0.99155000

H	-0.20614600	3.50978600	-1.31925300
H	0.59993900	5.04752500	-0.95838400
H	0.37154100	4.54486500	-2.63129300
H	4.06409300	4.00903100	-1.85210600
H	3.07913800	5.32893000	-1.21029000
H	2.95806600	4.89987600	-2.90974100
H	1.15382000	1.78183800	-2.75791600
H	2.92477500	1.90926300	-2.80477500
H	1.93048200	3.02743200	-3.74492900
C	2.57653400	-1.09253700	-2.76695700
C	3.08676200	-3.34486100	-1.75439900
C	3.71943900	-1.71351500	2.19189100
C	3.61024200	-3.61536600	0.56694500
C	6.33494600	1.09880600	0.71056700
C	5.97694000	-0.80403700	-0.70747100
H	-1.68845500	-3.22186200	-3.35406100
H	-1.62320300	-1.69712300	-2.45513900
H	-3.14679200	-2.59628600	-2.56145500
H	0.17300900	-4.27615700	-0.33888900
H	0.19343000	-4.10052400	-2.08948900
H	0.32655900	-2.67282800	-1.05746100
H	-2.09624700	-5.31556400	-2.29264800
H	-3.42798300	-4.81573400	-1.24048100
H	-1.96774800	-5.56229100	-0.55579300
H	-0.15103900	-3.48512600	2.01817000
H	-0.79461300	-5.02967500	1.43499700
H	-0.99574200	-4.57159300	3.12507500
H	-4.40139700	-4.11090400	1.49669300
H	-3.24698500	-5.38152800	1.07237100
H	-3.54388600	-5.00399100	2.76329800
H	-1.85282000	-1.84016000	3.12087900
H	-3.57253900	-1.96285600	2.69388700
H	-2.85896800	-3.09887600	3.84404400
C	-2.98151700	1.22201900	2.88863600
C	-3.16830900	3.41950900	1.66210200
C	-3.41867600	1.52574100	-2.20975100
C	-3.39421400	3.53910800	-0.71987500
C	-6.19647200	-1.10738300	-1.16113600
C	-6.05566000	0.75907400	0.34026000
C	1.64303200	-1.75285100	-3.77981000
C	3.84740900	-0.60415600	-3.47007000
H	2.05569600	-0.22123500	-2.37889000
C	3.43772400	-4.16218900	-0.69048000
H	2.94801800	-3.77964200	-2.73605900
C	2.87984100	-2.44377100	3.24565700
C	5.19827900	-1.84786800	2.57770900
H	3.44863300	-0.65490700	2.20880600
H	3.88773700	-4.25830600	1.39327000
C	7.65729000	0.72759300	0.88737300
H	5.94706000	1.99026600	1.18282500
C	7.30905400	-1.16009100	-0.54736900
H	5.35141700	-1.42531300	-1.32870000
C	-2.20560800	1.93527400	3.99487500

C	-4.35716700	0.79786600	3.41438100
H	-2.44369200	0.30708600	2.64779100
C	-3.32060100	4.17189300	0.50667500
H	-3.11111400	3.92224100	2.61885300
C	-2.35170500	2.06205200	-3.16993700
C	-4.79989200	1.77768100	-2.82929800
H	-3.26821800	0.44787900	-2.11007800
H	-3.51712500	4.13198300	-1.61832000
C	-7.48269700	-0.73472000	-1.51341500
H	-5.73818900	-1.98412800	-1.59661600
C	-7.35430200	1.11574600	0.00398700
H	-5.52257200	1.36928700	1.05111000
H	0.74552000	-2.14227500	-3.29910800
H	2.13064900	-2.56852100	-4.31831900
H	1.33420200	-1.01420500	-4.52190500
H	4.45645800	-1.45024000	-3.79972200
H	4.46048500	0.02218300	-2.82018200
H	3.58407700	-0.01376000	-4.35015400
H	3.57435000	-5.22527200	-0.84412700
H	3.22007000	-3.47439000	3.36553200
H	1.82232200	-2.45984200	2.98863500
H	2.98206600	-1.94698900	4.21189400
H	5.86153200	-1.32305000	1.89418100
H	5.48921400	-2.90065900	2.58833200
H	5.35483900	-1.44961000	3.58207200
C	8.15039800	-0.40740600	0.25830900
H	8.30357000	1.32724500	1.51551700
H	7.68412700	-2.04088800	-1.05198600
H	-1.25286100	2.32664300	3.63398300
H	-2.77648900	2.76441900	4.41856200
H	-1.99773800	1.23486500	4.80534900
H	-4.99427200	1.67006100	3.58339400
H	-4.86903900	0.12864900	2.72214700
H	-4.24483500	0.27028600	4.36400800
H	-3.38324600	5.25118500	0.56646500
H	-2.50173300	3.12642900	-3.36414100
H	-1.34770900	1.92536000	-2.77098800
H	-2.41830500	1.53980200	-4.12643500
H	-5.61425500	1.43681000	-2.19352700
H	-4.93966800	2.84563900	-3.01212500
H	-4.87598600	1.26421000	-3.78968400
C	-8.06861700	0.38036600	-0.92951500
H	-8.02961000	-1.31784000	-2.24277900
H	-7.80221000	1.98315500	0.47084200
H	9.18375700	-0.70067500	0.39214300
H	-9.07526000	0.67286500	-1.19926800

Table S63
M06-2X/Def2-TZVP
B2SiPb
E= -3539.492084

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-0.26763400	0.48537000	-0.53700200
B	1.61604000	0.68652300	0.01678800
B	-1.63166300	-0.66569400	0.31282100
P	2.29862700	2.51504500	-0.07338100
N	2.98022100	-0.01677800	-0.13959500
Pb	0.23428400	-0.12787500	1.94827900
P	-2.27895300	-2.50454900	0.22840800
N	-3.05840300	-0.01856900	0.30990900
C	2.09908400	3.58709400	1.44668400
C	1.98838800	3.49926500	-1.63817100
N	3.91903800	2.10703300	-0.12529400
C	3.09797300	-1.43629900	-0.29886000
C	4.06747100	0.80427100	-0.14428400
C	-1.65742300	-3.47134300	-1.22906200
C	-2.31274500	-3.52021500	1.79887600
N	-3.88374800	-2.15336300	-0.04434200
C	-3.21292200	1.40496700	0.35216100
C	-4.08790300	-0.85761300	0.04157500
C	2.76211000	2.82538000	2.60219000
C	0.62334400	3.83192200	1.77388900
C	2.82511600	4.92653000	1.29640900
C	0.64424800	4.23031600	-1.59723500
C	3.13587000	4.47965400	-1.91450200
C	1.97688800	2.48677800	-2.78947000
C	2.89837200	-1.97225200	-1.58564800
C	3.44235500	-2.25463500	0.78587400
C	5.47716600	0.29994200	-0.07539500
C	-2.04615600	-2.65783700	-2.47125200
C	-0.13429500	-3.58106400	-1.16026100
C	-2.29163200	-4.85849200	-1.33610900
C	-0.95717500	-4.15924500	2.10034200
C	-3.41176900	-4.58886700	1.74421000
C	-2.68456800	-2.54468400	2.92471700
C	-3.16162500	2.03800500	1.60590900
C	-3.36965700	2.13855600	-0.83147400
C	-5.48255300	-0.39140800	-0.23920600
H	2.31093100	1.84633500	2.76231500
H	2.63919900	3.40961500	3.51733400
H	3.82815600	2.68655600	2.41897600
H	0.13630900	4.48052100	1.04767500
H	0.55782200	4.31617500	2.75253700
H	0.05164900	2.90505700	1.80785300
H	2.85562800	5.41299400	2.27499700
H	2.30352000	5.59808000	0.61611500
H	3.85179200	4.79212900	0.95146800

H	-0.17242700	3.57272000	-1.28731900
H	0.67216200	5.09124900	-0.92926300
H	0.41686300	4.59998500	-2.60125000
H	4.10111700	3.97506800	-1.86910300
H	3.15199800	5.32162200	-1.22896900
H	3.00317100	4.88039600	-2.92281400
H	1.13025000	1.80493800	-2.72114900
H	2.90088400	1.90526400	-2.80902200
H	1.90328900	3.03508100	-3.73189600
C	2.56836400	-1.07760800	-2.76776800
C	3.07929900	-3.33692400	-1.76839100
C	3.70341300	-1.72638900	2.18585900
C	3.59873300	-3.62162200	0.55232000
C	6.35370300	1.06084800	0.70329700
C	5.97143500	-0.84309700	-0.70601400
H	-1.66293100	-3.17303400	-3.35600700
H	-1.61610000	-1.65490400	-2.44301100
H	-3.12994800	-2.57014100	-2.56175600
H	0.21176200	-4.20071500	-0.33393000
H	0.23071700	-4.03716200	-2.08467100
H	0.33016400	-2.59816400	-1.06366200
H	-2.03781300	-5.28071700	-2.31209500
H	-3.37932200	-4.81297000	-1.25760300
H	-1.90702500	-5.53930600	-0.57728000
H	-0.13778800	-3.44077000	2.01953000
H	-0.74740700	-4.99525100	1.43277400
H	-0.96418100	-4.54504800	3.12337000
H	-4.36957600	-4.14839000	1.46795900
H	-3.18592800	-5.39443400	1.05130300
H	-3.50763900	-5.02916200	2.74026900
H	-1.88502400	-1.83375000	3.12668800
H	-3.59633400	-1.99194300	2.68640500
H	-2.86649200	-3.11878500	3.83640900
C	-3.04248900	1.23564200	2.89025700
C	-3.27177500	3.42234200	1.65247700
C	-3.44804400	1.50125000	-2.20875100
C	-3.48444200	3.52447500	-0.73155600
C	-6.21035400	-1.15435800	-1.15545800
C	-6.09645200	0.72316200	0.33350200
C	1.65842100	-1.73851600	-3.80119100
C	3.84173500	-0.56872800	-3.45212700
H	2.03054700	-0.21799300	-2.37481200
C	3.42939400	-4.16062500	-0.70879600
H	2.94127200	-3.76650000	-2.75240400
C	2.85090300	-2.45559600	3.23003500
C	5.17833700	-1.86965200	2.58224600
H	3.44101800	-0.66550700	2.20306200
H	3.87530300	-4.26925400	1.37543000
C	7.67123000	0.67365600	0.88163900
H	5.97782800	1.96006900	1.17040000
C	7.29855600	-1.21613800	-0.54336900
H	5.33909900	-1.45783000	-1.32681700
C	-2.26742400	1.96542700	3.98671200

C	-4.41148600	0.80240900	3.42538800
H	-2.50003000	0.32301400	2.65058500
C	-3.43337900	4.16516000	0.49208700
H	-3.23282100	3.93099300	2.60708300
C	-2.36761600	2.04152300	-3.15130800
C	-4.82127000	1.73161300	-2.85330000
H	-3.28754800	0.42617500	-2.09780100
H	-3.61299100	4.10968300	-1.63422800
C	-7.50026200	-0.79993600	-1.51328500
H	-5.74019400	-2.02816100	-1.58394700
C	-7.39811000	1.06234600	-0.00925800
H	-5.57356900	1.34429200	1.04230100
H	0.76026900	-2.14793300	-3.33957500
H	2.16635000	-2.53850400	-4.34415500
H	1.34904200	-0.99430500	-4.53741400
H	4.45922500	-1.40659700	-3.78719400
H	4.44522800	0.05333400	-2.78973000
H	3.58183400	0.03041500	-4.32735400
H	3.56704600	-5.22261200	-0.86893000
H	3.19179700	-3.48517100	3.35676600
H	1.79736900	-2.48377200	2.95592400
H	2.93479900	-1.95737600	4.19729800
H	5.84741500	-1.34265800	1.90613200
H	5.46512500	-2.92348400	2.58776800
H	5.32987900	-1.47830400	3.59005300
C	8.14962100	-0.47107200	0.25895700
H	8.32538600	1.26870300	1.50590900
H	7.66221700	-2.10384200	-1.04418800
H	-1.32810300	2.37797300	3.61307800
H	-2.84911300	2.78503000	4.41403200
H	-2.03726600	1.27275900	4.79818400
H	-5.05630400	1.66954900	3.59021300
H	-4.91879300	0.12366700	2.73911600
H	-4.29097400	0.28257900	4.37835600
H	-3.52034000	5.24304300	0.54568900
H	-2.52451600	3.10297100	-3.35590300
H	-1.37122700	1.91894500	-2.72865100
H	-2.40830500	1.51163700	-4.10506300
H	-5.64142200	1.38809900	-2.22587000
H	-4.97047300	2.79576100	-3.05015400
H	-4.87686800	1.20682200	-3.80896200
C	-8.10115800	0.31230600	-0.93943900
H	-8.03816900	-1.39485700	-2.23966000
H	-7.85746900	1.92762700	0.45032500
H	9.17903600	-0.77711400	0.39425900
H	-9.11041800	0.59106600	-1.21408600

Table S64
M06-2X/Def2-TZVP
B2GeSn
E= -5348.52812

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ge	0.84233400	-0.01244000	0.34771900
B	-0.19984900	-1.77734700	0.00623600
B	-0.13583400	1.80009400	0.06386200
Sn	-1.75593800	0.02932600	-0.01356200
P	-0.04428400	-3.14402100	1.39845100
N	-0.32651400	-2.75783400	-1.17716700
P	-0.20116900	3.13927200	-1.36232900
N	0.18045200	2.81612500	1.20160800
C	-1.42400000	-3.18906100	2.65475900
C	1.62522600	-3.43061900	2.19138500
N	-0.28170200	-4.46144900	0.39962300
C	-0.32306900	-2.30606400	-2.53800100
C	-0.40129600	-4.07797400	-0.84853700
C	1.00535300	2.85928400	-2.74668300
C	-1.87180900	3.71498200	-1.97206700
N	0.35658300	4.42441000	-0.45990700
C	0.33700500	2.37469100	2.55706000
C	0.47974200	4.07925500	0.80050700
C	-2.72638500	-3.34027900	1.85632400
C	-1.46726700	-1.89426500	3.47113200
C	-1.30612300	-4.39230200	3.59336900
C	1.87071800	-2.46845600	3.35642800
C	1.77668300	-4.88844800	2.64561500
C	2.67470200	-3.18910800	1.09841300
C	0.92133200	-2.02081000	-3.13047600
C	-1.51995200	-2.18478200	-3.25776100
C	-0.70166900	-5.15695600	-1.84349700
C	2.39277500	2.79860400	-2.09263600
C	0.70859100	1.52558900	-3.43583800
C	1.00168400	3.99899700	-3.76668300
C	-2.44869800	2.78227100	-3.03729100
C	-1.79548300	5.15300300	-2.50065100
C	-2.79356900	3.72837000	-0.74443000
C	-0.82727400	2.17286300	3.31943100
C	1.61107400	2.12274300	3.08562000
C	1.01672700	5.13282100	1.71849500
H	-2.87875500	-2.51713900	1.15842200
H	-3.56224100	-3.34781300	2.55991100
H	-2.73630800	-4.27627200	1.29625000
H	-0.63606400	-1.81478800	4.16998700
H	-2.39445300	-1.87676700	4.05095600
H	-1.44216100	-1.00822600	2.83627500
H	-2.23856200	-4.48175200	4.15668400
H	-0.50096200	-4.26622200	4.31562800
H	-1.15193400	-5.32121000	3.04169800

H	1.64356400	-1.43247500	3.09076800
H	1.28297700	-2.74067800	4.23359600
H	2.92632800	-2.52095600	3.63772800
H	1.53371400	-5.57763200	1.83675000
H	1.16197100	-5.13255000	3.50689700
H	2.81983100	-5.04591300	2.93175100
H	2.71628400	-2.14259000	0.79990600
H	2.47613200	-3.80442900	0.21747800
H	3.65349500	-3.47261800	1.49273900
C	2.22371500	-2.19721000	-2.36964800
C	0.94503000	-1.63895600	-4.46563900
C	-2.88604300	-2.51327000	-2.67959300
C	-1.44188100	-1.78566300	-4.59255700
C	-1.50620500	-6.20099400	-1.37929900
C	-0.25433000	-5.19992400	-3.16506700
H	3.13130400	2.58545600	-2.86967900
H	2.45030300	2.01141400	-1.33925700
H	2.64676300	3.74947200	-1.62170400
H	-0.22116700	1.54199800	-4.00336000
H	1.51817600	1.30245900	-4.13667500
H	0.65136800	0.70466700	-2.71926600
H	1.85790800	3.86747700	-4.43341100
H	1.09326100	4.97358400	-3.28418700
H	0.10383600	3.98841600	-4.38371500
H	-2.41237500	1.73510800	-2.72884700
H	-1.92534800	2.88304900	-3.98821600
H	-3.49651500	3.04466700	-3.20583500
H	-1.33970000	5.81555700	-1.76539800
H	-1.24249700	5.23388600	-3.43223100
H	-2.81518500	5.49710800	-2.69183700
H	-3.01510700	2.72207900	-0.39275700
H	-2.35578300	4.30373100	0.07453300
H	-3.73555800	4.20599600	-1.02423900
C	-2.20139100	2.50643200	2.76372200
C	-0.69156700	1.71256000	4.62351500
C	2.90383700	2.33671500	2.31477700
C	1.69359200	1.67393200	4.40330200
C	1.91213100	6.04105600	1.14794400
C	0.69395800	5.27505000	3.06875900
C	3.24693200	-1.10351600	-2.67038000
C	2.83663000	-3.57939000	-2.61635200
H	1.99028900	-2.12611900	-1.31172300
C	-0.22711400	-1.52186400	-5.19696600
H	1.89402100	-1.42943600	-4.94310600
C	-3.87188100	-1.35387200	-2.85965100
C	-3.48923600	-3.76442800	-3.33187900
H	-2.76602300	-2.69827000	-1.60907800
H	-2.35400300	-1.69623700	-5.16972800
C	-1.88540800	-7.23644600	-2.21663500
H	-1.83314900	-6.17954200	-0.34934800
C	-0.61696300	-6.25159600	-3.99486600
H	0.37432200	-4.42292800	-3.56930300
C	-3.31474800	1.62314500	3.32417600

C	-2.55700600	3.98200600	2.97576800
H	-2.16406400	2.34264900	1.68842000
C	0.56062700	1.46559700	5.16688300
H	-1.57422300	1.54693500	5.22748400
C	3.76976200	1.07165900	2.28352700
C	3.73853400	3.47316700	2.92108400
H	2.64769100	2.59554300	1.28414800
H	2.66871500	1.48121500	4.83407400
C	2.49313900	7.04194600	1.90783500
H	2.14631500	5.94113300	0.09740300
C	1.26003500	6.29400800	3.82218600
H	0.01031500	4.59707800	3.55355100
H	2.81682400	-0.11135700	-2.52914100
H	3.63552600	-1.17159500	-3.68889600
H	4.09554100	-1.20259700	-1.99066200
H	3.00595600	-3.74604500	-3.68358400
H	2.19594100	-4.38076700	-2.24470200
H	3.79800900	-3.65760600	-2.10427400
H	-0.19086000	-1.22385300	-6.23724400
H	-4.13124000	-1.22553000	-3.91261900
H	-3.46944300	-0.41335700	-2.48765400
H	-4.79438800	-1.56330000	-2.31549400
H	-2.86340600	-4.64596700	-3.21295700
H	-3.63471800	-3.59610100	-4.40145400
H	-4.46621600	-3.97492000	-2.89255700
C	-1.44215500	-7.26503500	-3.53187400
H	-2.52600800	-8.02334800	-1.84033700
H	-0.25541900	-6.26786300	-5.01472400
H	-3.05949700	0.56412800	3.26283600
H	-3.53468100	1.86162900	4.36717500
H	-4.23075100	1.78439400	2.75361200
H	-2.52090500	4.24100600	4.03742900
H	-1.87864500	4.64610500	2.43902700
H	-3.56850700	4.17633000	2.61282600
H	0.64960700	1.11185600	6.18632000
H	4.15045400	0.83760000	3.28018400
H	3.21314800	0.21093200	1.91663200
H	4.63151200	1.22992700	1.63193300
H	3.19242900	4.41149100	2.98599100
H	4.06253000	3.20212000	3.92855700
H	4.63387600	3.63757400	2.31832500
C	2.16816600	7.17282800	3.25143200
H	3.19903300	7.72224200	1.44936900
H	0.99333000	6.38990600	4.86666000
H	-1.73451300	-8.07338900	-4.18956500
H	2.61822800	7.95544000	3.84851000

Table S65
M06-2X/Def2-TZVP
B2GePb
E= -5327.036812

Atomic Number	Coordinates (Angstroms) X	Y	Z
Ge	0.76863400	-0.02684700	0.49007600
B	-0.17650500	-1.80589600	0.02497900
B	-0.11414400	1.80277500	0.10193400
Pb	-1.89166900	0.00341800	0.08697200
P	-0.00170300	-3.19800000	1.38350300
N	-0.33028300	-2.75548800	-1.17779600
P	-0.17037800	3.11074300	-1.35034000
N	0.17553200	2.84803100	1.22025900
C	-1.35440800	-3.28611100	2.67166700
C	1.68320500	-3.51301600	2.14041200
N	-0.26337500	-4.49321100	0.35990100
C	-0.33835900	-2.28044700	-2.53018600
C	-0.40614300	-4.08324400	-0.87705200
C	1.06604100	2.81511300	-2.70416700
C	-1.83225800	3.65906400	-2.01129100
N	0.35317600	4.42317400	-0.46953100
C	0.32056400	2.44278500	2.58790000
C	0.46283600	4.10642800	0.80063200
C	-2.67275000	-3.44431300	1.90235100
C	-1.40175700	-2.01016600	3.51638900
C	-1.19788700	-4.50617000	3.58242800
C	1.94976300	-2.60591100	3.34379400
C	1.84990000	-4.99015000	2.52297900
C	2.71243300	-3.21443400	1.04311100
C	0.90289500	-2.00753800	-3.13579600
C	-1.54206400	-2.13804200	-3.23501600
C	-0.74155700	-5.13851300	-1.88662100
C	2.43634000	2.74763100	-2.01550600
C	0.77567800	1.47752300	-3.38441100
C	1.09546000	3.94418900	-3.73465100
C	-2.37736700	2.69364300	-3.06432100
C	-1.76008300	5.08395600	-2.57529300
C	-2.77841200	3.69842100	-0.80286600
C	-0.84744200	2.25035200	3.34550500
C	1.59181300	2.22517200	3.13551900
C	0.97252100	5.18598500	1.70394800
H	-2.84829200	-2.61802700	1.21357500
H	-3.49327600	-3.46656100	2.62355700
H	-2.68503000	-4.37471300	1.33344100
H	-0.54855700	-1.92386500	4.18724800
H	-2.30850000	-2.02810300	4.12775800
H	-1.41758300	-1.11111600	2.90010600
H	-2.11367500	-4.61806900	4.16883600
H	-0.37469100	-4.38579500	4.28484900
H	-1.04853000	-5.42155300	3.00740000

H	1.73577300	-1.55724600	3.12143700
H	1.36625600	-2.90670900	4.21418700
H	3.00667500	-2.68584200	3.61325100
H	1.58744400	-5.64271700	1.69015700
H	1.25916200	-5.27629900	3.38816900
H	2.90058200	-5.15701400	2.77413600
H	2.73441100	-2.15601600	0.78567700
H	2.50691900	-3.79724000	0.14213000
H	3.70094400	-3.50062900	1.41055800
C	2.20888900	-2.21033300	-2.38711400
C	0.91546400	-1.62022300	-4.46931100
C	-2.90503600	-2.45778500	-2.64392800
C	-1.47540700	-1.72987500	-4.56790500
C	-1.55505100	-6.17762200	-1.42626000
C	-0.31972700	-5.16583500	-3.21713200
H	3.19364200	2.53144600	-2.77360600
H	2.46834100	1.95912500	-1.26177900
H	2.68328300	3.69682400	-1.53737600
H	-0.14282700	1.49040300	-3.96988000
H	1.59613700	1.24115200	-4.06780300
H	0.70207100	0.66735600	-2.65697400
H	1.97125400	3.80584800	-4.37413500
H	1.17274100	4.92345800	-3.25925100
H	0.21684300	3.92751700	-4.37851300
H	-2.31425200	1.65198100	-2.74059000
H	-1.84608500	2.78943300	-4.01147600
H	-3.43022900	2.92374400	-3.24881600
H	-1.31974400	5.76787100	-1.85010400
H	-1.19421900	5.14603200	-3.50036700
H	-2.77941400	5.41577600	-2.79008300
H	-2.99923500	2.70135800	-0.42555500
H	-2.36016900	4.29812900	0.00905700
H	-3.71884500	4.16033700	-1.11293300
C	-2.22054300	2.54524200	2.76773200
C	-0.71867100	1.83823800	4.66617800
C	2.88517500	2.42737800	2.36418200
C	1.66870700	1.82419300	4.46862700
C	1.86468100	6.09392500	1.12717100
C	0.62864500	5.35370200	3.04625200
C	3.26951100	-1.16123000	-2.71634700
C	2.77064100	-3.61699100	-2.61902600
H	1.98833200	-2.10996400	-1.32818900
C	-0.26408100	-1.48183200	-5.18567800
H	1.86111200	-1.42171200	-4.95779700
C	-3.87752200	-1.28248900	-2.79313100
C	-3.53665200	-3.68939400	-3.30652100
H	-2.77309200	-2.66414400	-1.57851700
H	-2.39310400	-1.62472600	-5.13382700
C	-1.96983600	-7.19022800	-2.27493300
H	-1.86015200	-6.17074400	-0.38946900
C	-0.71925600	-6.19429000	-4.05936100
H	0.31758600	-4.39436900	-3.61881900
C	-3.31045000	1.61642800	3.30141300

C	-2.62861600	4.00607800	2.98562800
H	-2.15666500	2.39597800	1.69181000
C	0.53149600	1.62860000	5.22945200
H	-1.60499100	1.68417800	5.26815500
C	3.75119600	1.16210800	2.36005300
C	3.71198100	3.58114300	2.94780300
H	2.63115700	2.66371600	1.32767900
H	2.64235900	1.65939800	4.91414000
C	2.42176200	7.11851600	1.87329500
H	2.11527700	5.97485500	0.08249300
C	1.17126000	6.39555900	3.78549100
H	-0.05395900	4.67834700	3.53622600
H	2.88823300	-0.15107600	-2.56606000
H	3.63205200	-1.24783500	-3.74295100
H	4.12860000	-1.29695700	-2.05643900
H	2.92501900	-3.80242900	-3.68539600
H	2.10583200	-4.39134800	-2.23272900
H	3.73329200	-3.72232500	-2.11430800
H	-0.23607800	-1.17921500	-6.22489400
H	-4.15179800	-1.13722100	-3.84010900
H	-3.45772000	-0.34833100	-2.42325800
H	-4.79413000	-1.48341700	-2.23609500
H	-2.92245100	-4.58157300	-3.20867900
H	-3.69426100	-3.50309000	-4.37141800
H	-4.51051500	-3.89178600	-2.85665800
C	-1.55445000	-7.20117000	-3.59941100
H	-2.61657100	-7.97301100	-1.90024400
H	-0.37839700	-6.19758400	-5.08640900
H	-3.00857200	0.56855400	3.24888600
H	-3.56251000	1.84301200	4.33952600
H	-4.22069800	1.73989500	2.71196500
H	-2.61899900	4.25763200	4.04948900
H	-1.96156300	4.69456100	2.46559500
H	-3.63922200	4.17150500	2.60628700
H	0.61540900	1.31322500	6.26184400
H	4.11416700	0.93736500	3.36565800
H	3.19774000	0.29882000	1.99342400
H	4.62369600	1.31282300	1.72120900
H	3.15644900	4.51585300	2.99448900
H	4.03948400	3.33323900	3.96024000
H	4.60522900	3.74211700	2.34114900
C	2.07631000	7.27390700	3.20905400
H	3.12506300	7.79828600	1.40996400
H	0.88799600	6.51028800	4.82366400
H	-1.87544300	-7.99109900	-4.26631100
H	2.50756000	8.07502800	3.79539600

Table S66
M06-2X/Def2-TZVP
B2SnPb
E= -3464.25345

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sn	1.19628500	-0.08105300	0.63314900
B	-0.08406900	-1.91906500	0.03784900
B	0.04007300	1.85037100	0.14322200
Pb	-1.63030100	-0.01195600	-0.02318900
P	-0.00024700	-3.33861300	1.37250600
N	-0.34818900	-2.83319400	-1.17412700
P	-0.09538900	3.11761300	-1.33620700
N	0.28458300	2.92019300	1.23914800
C	-1.30427700	-3.29867300	2.71404400
C	1.66392300	-3.87479000	2.06349200
N	-0.41962500	-4.58435100	0.34185700
C	-0.35696900	-2.32971000	-2.51793600
C	-0.52248900	-4.15468100	-0.89214500
C	1.13094500	2.84610800	-2.71027200
C	-1.77959900	3.60771200	-2.00561200
N	0.38088000	4.46566400	-0.48359300
C	0.40632900	2.56303900	2.62433400
C	0.49147800	4.18721100	0.79553300
C	-2.66347100	-3.28621600	2.00305500
C	-1.16547900	-2.04303700	3.57717800
C	-1.25337400	-4.54889700	3.59567600
C	2.08908500	-3.05888900	3.28589500
C	1.66266200	-5.37363800	2.39598400
C	2.68248600	-3.66854400	0.93501700
C	0.88492400	-2.06827100	-3.12993900
C	-1.56405800	-2.14052800	-3.21016500
C	-0.89024300	-5.17994500	-1.91749000
C	2.51902900	2.85173500	-2.05648500
C	0.87996100	1.48693100	-3.36425200
C	1.09303000	3.95788700	-3.75987200
C	-2.29827100	2.63411900	-3.06513500
C	-1.75307800	5.03718500	-2.56324700
C	-2.73104800	3.61534700	-0.80093300
C	-0.77649200	2.31624200	3.34465600
C	1.66581900	2.46032600	3.23384300
C	0.89830700	5.32232200	1.67933800
H	-2.78146600	-2.41449600	1.35992700
H	-3.44980900	-3.25934200	2.76127200
H	-2.79700200	-4.18195100	1.39448700
H	-0.27554300	-2.06505600	4.20452500
H	-2.03682800	-1.96938600	4.23419800
H	-1.11383000	-1.13695000	2.97201100
H	-2.14834000	-4.56426700	4.22327200
H	-0.39101200	-4.54495500	4.26040900
H	-1.24175400	-5.46219100	2.99822800

H	2.02350100	-1.98373900	3.10631800
H	1.49285600	-3.30514000	4.16445400
H	3.13027500	-3.29894800	3.51894400
H	1.30019900	-5.96297600	1.55418300
H	1.06771900	-5.61570500	3.27164600
H	2.69317300	-5.67050000	2.60836200
H	2.83199000	-2.61322400	0.71118100
H	2.37257000	-4.18619400	0.02381200
H	3.63937800	-4.09051800	1.25161500
C	2.20081200	-2.33374000	-2.41805400
C	0.89415500	-1.63158000	-4.44815500
C	-2.93446500	-2.45761100	-2.63103800
C	-1.49742700	-1.68529800	-4.52783400
C	-1.74509500	-6.19687000	-1.48435100
C	-0.44159300	-5.20652300	-3.23878100
H	3.26661700	2.66195900	-2.83102300
H	2.60878000	2.07849600	-1.29289700
H	2.73137800	3.81791000	-1.59549800
H	-0.03288600	1.46564400	-3.95839300
H	1.71312800	1.25143500	-4.03263200
H	0.81554200	0.68812300	-2.62299100
H	1.95481800	3.83750400	-4.42155200
H	1.15237100	4.94660400	-3.30164400
H	0.19829900	3.90373200	-4.37862600
H	-2.21381500	1.59226200	-2.74896700
H	-1.77014200	2.74797900	-4.01185000
H	-3.35600500	2.84161600	-3.24970600
H	-1.34390600	5.73344200	-1.83194200
H	-1.18274900	5.12468500	-3.48337200
H	-2.78221200	5.33205400	-2.78496700
H	-2.92529900	2.61105600	-0.42828100
H	-2.33418800	4.22527700	0.01429500
H	-3.68344900	4.05075400	-1.11285600
C	-2.14602800	2.50146900	2.71518600
C	-0.67627400	1.96473900	4.68481400
C	2.98036000	2.72981500	2.51895200
C	1.71082500	2.11289900	4.58349700
C	1.74682700	6.27222300	1.10425600
C	0.49136100	5.50720000	3.00146600
C	3.23829000	-1.23328300	-2.64005000
C	2.78394000	-3.69581800	-2.80958500
H	1.99253500	-2.36003000	-1.35277400
C	-0.28707100	-1.43797000	-5.14742300
H	1.84084200	-1.44254300	-4.93893800
C	-3.89456800	-1.26729300	-2.74087400
C	-3.58688700	-3.65110200	-3.34330000
H	-2.80887700	-2.70411900	-1.57318100
H	-2.41693200	-1.54141400	-5.08186500
C	-2.16956700	-7.18930900	-2.35140300
H	-2.07308900	-6.18872400	-0.45443200
C	-0.84972600	-6.21656300	-4.09873300
H	0.22125700	-4.44621500	-3.61976300
C	-3.15768700	1.44503000	3.16045600

C	-2.70386000	3.90395500	2.97867900
H	-2.02405800	2.40534100	1.63948700
C	0.55935100	1.86402400	5.30560500
H	-1.57635500	1.77671400	5.25639300
C	3.95845900	1.55572500	2.65484900
C	3.67526600	3.98387000	3.06775400
H	2.76658000	2.87666100	1.45660600
H	2.67310700	2.03498900	5.07431000
C	2.20501400	7.35452100	1.83590300
H	2.04488700	6.13830900	0.07387400
C	0.93370400	6.60590400	3.72485700
H	-0.16148600	4.80051400	3.48867200
H	2.84523700	-0.25285700	-2.36644200
H	3.57771600	-1.18939200	-3.67720300
H	4.11445600	-1.42885900	-2.01875100
H	2.92974900	-3.76300800	-3.89102800
H	2.13594600	-4.51803200	-2.50151900
H	3.75333200	-3.83807600	-2.32716300
H	-0.26154700	-1.09699700	-6.17471800
H	-4.15895000	-1.07851100	-3.78315100
H	-3.47301200	-0.35375800	-2.32706900
H	-4.81844000	-1.48672200	-2.20295200
H	-2.98601800	-4.55531500	-3.29607100
H	-3.75278100	-3.41124400	-4.39612900
H	-4.55919200	-3.86124100	-2.89358200
C	-1.72281800	-7.20292500	-3.66592900
H	-2.84758200	-7.95561000	-1.99893000
H	-0.48580100	-6.22154300	-5.11784900
H	-2.75269600	0.43510900	3.06670100
H	-3.46324000	1.58716300	4.19927400
H	-4.05732500	1.51293400	2.54564500
H	-2.76029100	4.10557700	4.05160300
H	-2.08698800	4.67672900	2.51790100
H	-3.71008000	3.98989500	2.56279500
H	0.62145000	1.59380500	6.35208000
H	4.32341400	1.47598500	3.68118000
H	3.50069000	0.60750800	2.38023600
H	4.82504100	1.72210300	2.01208700
H	3.05535400	4.87477500	3.01203200
H	3.94784200	3.82887600	4.11421400
H	4.59540900	4.16959400	2.51029100
C	1.79980600	7.52588300	3.15290100
H	2.87875300	8.06616400	1.37622900
H	0.60403000	6.73240700	4.74785800
H	-2.04957800	-7.97882000	-4.34613000
H	2.15485100	8.37118400	3.72807000
