Electronic Supporting Information (ESI)

Electronic Structure of the Boron Fullerene B_{14} and Its Silicon Derivatives $B_{13}Si^+$, $B_{13}Si^-$ and $B_{12}Si_2$: A Rationalization Using a Cylinder Model

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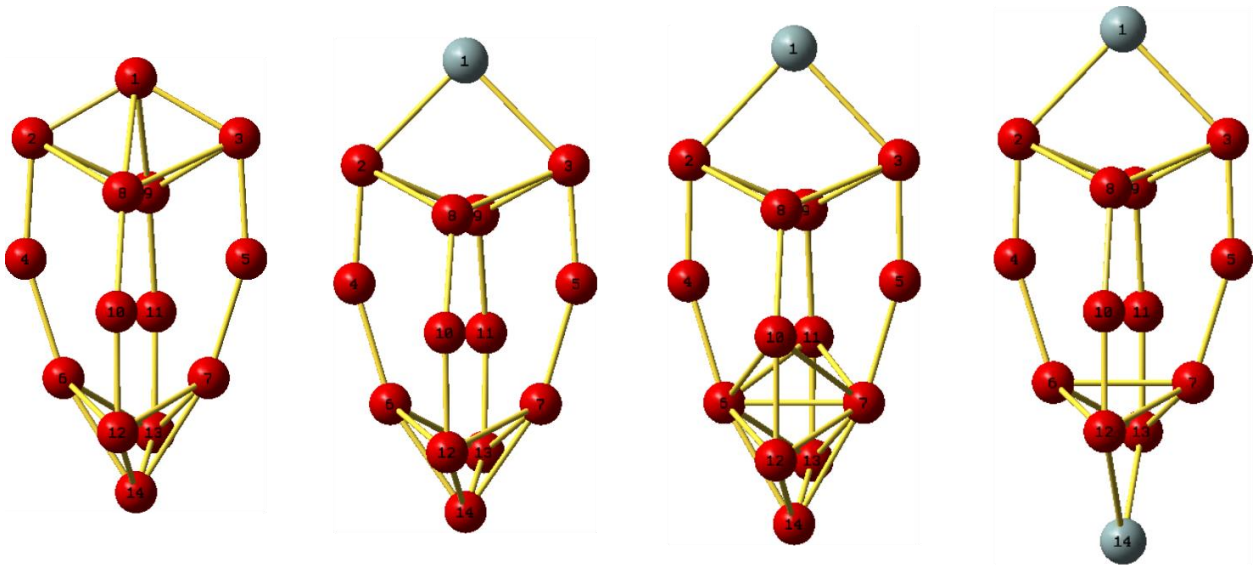
Convergence Criteria:

All density functional theory (DFT) computations were carried out using the Gaussian 09 package. The standard convergence criteria implemented in this program were used:

i) Integral accuracy were reduced to 1.0D-05 until final iterations. Requested convergence on RMS density matrix is = 1.00D-08; requested convergence on MAX density matrix is = 1.00D-06, and requested convergence on energy is =1.00D-06 hartree.

ii) All the geometries were optimized in the framework of DFT using the TPSSh hybrid functional (TPSSh stands for Tao, Perdew, Staroverov and Scuseria exchange functional), which is a time-tested functional for thermochemical calculations, in conjunction with the 6-311+G(d,p) basis set. All geometry optimizations of clusters are carried out in gaseous phase using the Berny's eigenvalue algorithm implemented in G09 package. All the optimized structures are ensured to be energetically minimized from the normal modes of vibration, hang all real vibrational frequencies (for values of harmonic vibrational frequencies, see text). The convergence criteria are: Maximum Force: 0.00045 hartree/bohr, RMS Force: 0.0003 hartree/bohr, Maximum Displacement 0.001800 bohr and RMS Displacement: 0.001200 bohr.



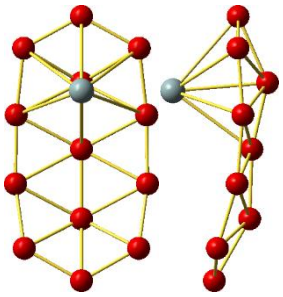
a) **B_{14}.1** (D_{2d}, $^1A_1$)

b) **$B_{13}Si^+$.2** (C_{2v}, $^1A_1$)

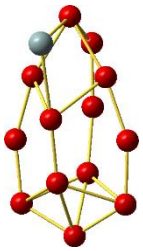
c) **$B_{13}Si^-$.2** (C_{2v}, $^1A_1$)

d) **$B_{12}Si_2$.1** (D_{2d}, $^1A_1$)

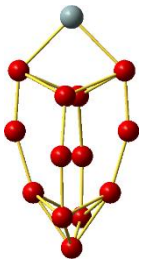
Figure S1. The geometries of **B_{14}.1**, **$B_{13}Si^+$.2**, **$B_{13}Si^-$.2**, and **$B_{12}Si_2$.1** fullerenes



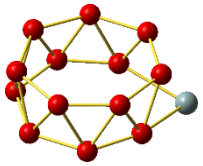
$B_{13}Si^{+}.1$ (C_s, $^1A'$)
[96 – 1349]
ΔE = 0.00



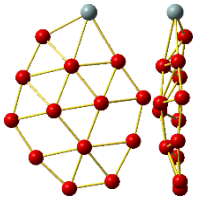
$B_{13}Si^{+}.2$ (C_s, $^1A'$)
[175 – 1360]
ΔE = 0.20



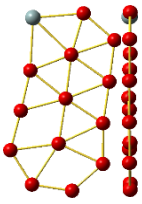
$B_{13}Si^{+}.3$ (C_{2v}, $^1A_1$)
[216 – 1368]
ΔE = 0.31



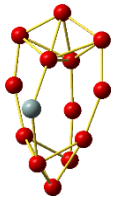
$B_{13}Si^{+}.4$ (C_s, $^1A'$)
[192 – 1288]
ΔE = 0.54



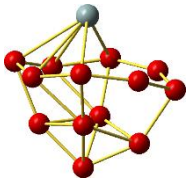
$B_{13}Si^{+}.5$ (C_1, ^1A)
[107 – 1352]
ΔE = 0.57



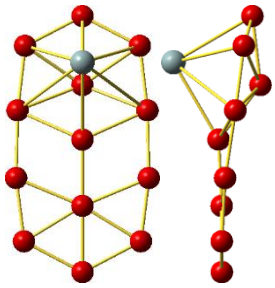
$B_{13}Si^{+}.6$ (C_1, ^1A)
[87 – 1559]
ΔE = 0.57



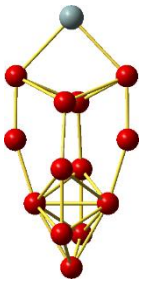
$B_{13}Si^{+}.7$ (C_1, ^1A)
[113 – 1380]
ΔE = 0.58



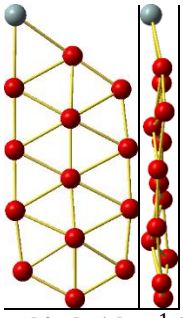
$B_{13}Si^{+}.8$ (C_1, ^1A)
[69 – 1412]
ΔE = 0.62



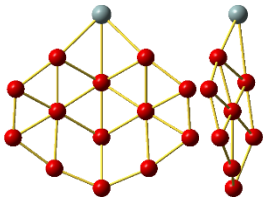
$B_{13}Si^{-}.1$ (C_s, $^1A'$)
[97.29 – 1295]
ΔE = 0.00



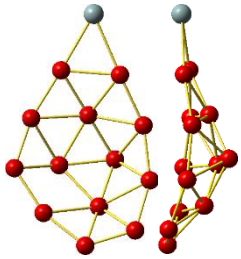
$B_{13}Si^{-}.2$ (C_{2v}, $^1A_1$)
[193 – 1337]
ΔE = 0.13



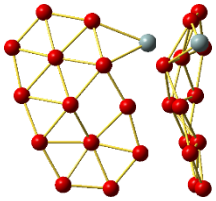
$B_{13}Si^{-}.3$ (C_1, ^1A)
[53 – 1306]
ΔE = 0.24



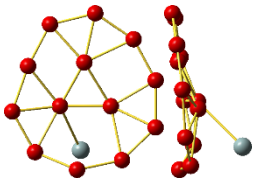
$B_{13}Si^{-}.4$ (C_s, $^1A'$)
[91 – 1343]
ΔE = 0.41



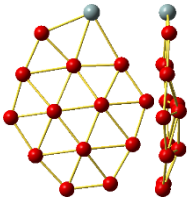
$B_{13}Si^{-}.5$ (C_1, ^1A)
[83 – 1326]
ΔE = 0.46



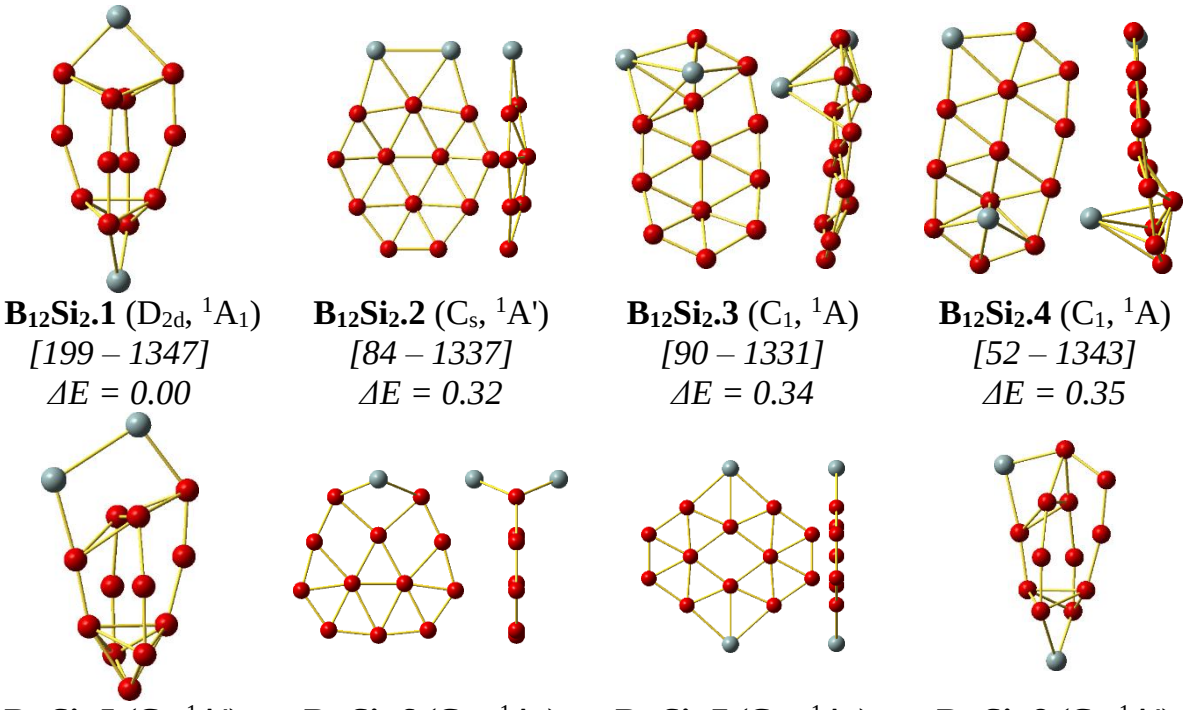
$B_{13}Si^{-}.6$ (C_1, ^1A)
[104 – 1257]
ΔE = 0.56



$B_{13}Si^{-}.7$ (C_1, ^1A)
[69 – 1453]
ΔE = 0.60



$B_{13}Si^{-}.8$ (C_1, ^1A)
[106 – 1286]
ΔE = 0.68



$B_{12}Si_2$.1 (D_{2d}, $^1A_1$)
[199 – 1347]
ΔE = 0.00

$B_{12}Si_2$.2 (C_s, $^1A'$)
[84 – 1337]
ΔE = 0.32

$B_{12}Si_2$.3 (C_1, ^1A)
[90 – 1331]
ΔE = 0.34

$B_{12}Si_2$.4 (C_1, ^1A)
[52 – 1343]
ΔE = 0.35

$B_{12}Si_2$.5 (C_s, $^1A'$)
[133 – 1367]
ΔE = 0.36

$B_{12}Si_2$.6 (C_{2v}, $^1A_1$)
[64 – 1401]
ΔE = 0.38

$B_{12}Si_2$.7 (C_{2v}, $^1A_1$)
[65 – 1310]
ΔE = 0.41

$B_{12}Si_2$.8 (C_s, $^1A'$)
[180 – 1316]
ΔE = 0.45

Figure S2. The geometries of the lower-lying structures of B_{14}, $B_{13}Si^+$, $B_{13}Si^-$, and $B_{12}Si_2$. Some characteristics of these structures include the point group and electronic state giving in parentheses, the lowest and highest frequency giving in brackets (cm^{-1}) and relative energies (eV) (TPSSh/6-311+G(d) + ZPE).

Table S1. A comparison of the computed DFT MOs energies of $B_{13}Si^+$ and the eigenvalue spectrum of the cylinder model with $L^f = 2.92$. DFT MOs of $B_{13}Si^+$ include all 21 valence MOs and 3 LUMOs.

DFT			particle in cylinder model	
	label	E (eV)	label	E (eV)
HOMO – 20	1σ1	-26.32	1σ1	-25.31
HOMO – 19	2σ1	-24.70	2σ1	-23.74
HOMO – 18	3σ1	-20.95	1π1	-21.28
HOMO – 17	1π1	-20.86	1π1	-21.28
HOMO – 16	1π1	-20.73	3σ1	-21.13
HOMO – 15	2π1	-17.80	2π1	-19.72
HOMO – 14	2π1	-17.70	2π1	-19.72
HOMO – 13	4σ1	-17.47	4σ1	-17.48
HOMO – 12	1δ1	-14.74	3π1	-17.10
HOMO – 11	3π1	-14.59	3π1	-17.10
HOMO – 10	1δ1	-14.50	1δ1	-15.99
HOMO – 9	1σ2	-14.49	1δ1	-15.99
HOMO – 8	5σ1	-14.34	2δ1	-14.43
HOMO – 7	3π1	-14.31	2δ1	-14.43
HOMO – 6	4π1	-13.27	1σ2	-14.14
HOMO – 5	2σ2	-13.11	4π1	-13.45
HOMO – 4	4π1	-12.97	4π1	-13.45
HOMO – 3	2δ1	-11.73	5σ1	-12.78
HOMO – 2	2δ1	-11.54	2σ2	-12.57
HOMO – 1	1π2	-11.08	3δ1	-11.82
HOMO	1π2	-10.98	3δ1	-11.82
LUMO	6σ1	-9.14	3σ2	-9.96
LUMO – 1	2π2	-7.22	1ϕ1	-9.51
LUMO – 1′	2π2	-7.14	1ϕ1	-9.51
			5π1	-8.75
			5π1	-8.75
			4δ1	-8.16
			4δ1	-8.16
			2ϕ1	-7.95
			2ϕ1	-7.95
			6σ1	-7.03
			4σ2	-6.31
			1π2	-5.66
			1π2	-5.66
			3ϕ1	-5.34
			3ϕ1	-5.34
			2π2	-4.10
			2π2	-4.10

Table S2. A comparison of computed DFT MOs energies of $B_{13}Si^-$ and the eigenvalue spectrum of the cylinder model with $L^f = 3.11$. DFT MOs of $B_{13}Si^-$ include all 22 valence MOs and 3 LUMOs.

DFT			particle in cylinder model	
	label	E (eV)	label	E (eV)
HOMO – 21	1σ1	-17.90	1σ1	-16.47
HOMO – 20	2σ1	-16.01	2σ1	-15.07
HOMO – 19	3σ1	-12.39	3σ1	-12.74
HOMO – 18	1π1	-12.15	1π1	-12.41
HOMO – 17	1π1	-12.11	1π1	-12.41
HOMO – 16	2π1	-9.01	2π1	-11.01
HOMO – 15	4σ1	-9.01	2π1	-11.01
HOMO – 14	2π1	-9.00	4σ1	-9.47
HOMO – 13	1σ2	-6.00	3π1	-8.68
HOMO – 12	1δ1	-5.94	3π1	-8.68
HOMO – 11	5σ1	-5.88	1δ1	-7.07
HOMO – 10	1δ1	-5.59	1δ1	-7.07
HOMO – 9	3π1	-5.32	2δ1	-5.67
HOMO – 8	3π1	-5.31	2δ1	-5.67
HOMO – 7	2σ2	-4.37	4π1	-5.41
HOMO – 6	4π1	-4.29	4π1	-5.41
HOMO – 5	4π1	-4.14	5σ1	-5.27
HOMO – 4	2δ1	-3.06	1σ2	-5.20
HOMO – 3	2δ1	-3.00	2σ2	-3.80
HOMO – 2	1π2	-2.51	3δ1	-3.34
HOMO – 1	1π2	-2.47	3δ1	-3.34
HOMO	6σ1	-1.56	3σ2	-1.47
LUMO	7σ1	0.93	5π1	-1.21
LUMO – 1	2π2	1.38	5π1	-1.21
LUMO – 1′	2π2	1.77	1ϕ1	-0.53
			1ϕ1	-0.53
			6σ1	-0.14
			4δ1	-0.08
			4δ1	-0.08
			2ϕ1	0.87
			2ϕ1	0.87
			4σ2	1.79
			3ϕ1	3.20
			3ϕ1	3.20
			1π2	3.35
			1π2	3.35
			6π1	3.92
			6π1	3.92
			5δ1	4.12
			5δ1	4.12

			2π2	4.75
			2π2	4.75
			7σ1	5.92

Table S3. A comparison of the computed DFT MOs energies of $B_{12}Si_2$ and the eigenvalue spectrum of the cylinder model with $L^f = 3.11$. DFT MOs of $B_{12}Si_2$ include all 22 valence MOs and 4 LUMOs.

DFT			particle in cylinder model	
	label	E (eV)	label	E (eV)
HOMO – 15	1σ1	-21.85	1σ1	-20.46
HOMO – 14	2σ1	-19.98	2σ1	-19.14
HOMO – 13	3σ1	-16.48	3σ1	-16.93
HOMO – 12'	1π1	-16.29	1π1	-16.44
HOMO – 12	1π1	-16.29	1π1	-16.44
HOMO – 11	4σ1	-13.51	2π1	-15.11
HOMO – 10'	2π1	-13.06	2π1	-15.11
HOMO – 10	2π1	-13.06	4σ1	-13.83
HOMO – 9'	5σ1	-10.53	3π1	-12.90
HOMO – 9	1σ2	-10.06	3π1	-12.90
HOMO – 8	1δ1	-10.05	1δ1	-11.15
HOMO – 7	1δ1	-9.81	1δ1	-11.15
HOMO – 6'	3π1	-9.37	5σ1	-9.86
HOMO – 6	3π1	-9.37	2δ1	-9.82
HOMO – 5	2σ2	-8.74	2δ1	-9.82
HOMO – 4'	4π1	-8.31	4π1	-9.81
HOMO – 4	4π1	-8.31	4π1	-9.81
HOMO – 3	2δ1	-7.34	1σ2	-9.30
HOMO – 2	2δ1	-7.26	2σ2	-7.97
HOMO – 1'	1π2	-6.64	3δ1	-7.61
HOMO – 1	1π2	-6.64	3δ1	-7.61
HOMO	6σ1	-6.48	5π1	-5.83
LUMO	7σ1	-3.93	5π1	-5.83
LUMO – 1	3σ2	-2.52	3σ2	-5.76
LUMO – 1′	2π2	-2.51	6σ1	-4.99
LUMO – 2	2π2	-2.51	1ϕ1	-4.67
			1ϕ1	-4.67
			4δ1	-4.52
			4δ1	-4.52
			2ϕ1	-3.34
			2ϕ1	-3.34
			4σ2	-2.67
			3ϕ1	-1.13
			3ϕ1	-1.13
			6π1	-0.97
			6π1	-0.97

1π2	-0.82
1π2	-0.82
5δ1	-0.54
5δ1	-0.54
2π2	0.51
2π2	0.51
7σ1	0.75

Table S4. The xyz coordination (in Angstrom) of the lowest isomers B_{14}, $B_{13}Si^{+}$, $B_{13}Si^{-}$, and $B_{12}Si_2$ obtained at the TPSSh/6-311+G(d) level of theory.

B_{14}.1	5	0.000000000	1.455856000	0.343122000
	5	0.000000000	1.365426000	1.906562000
	5	0.000000000	-0.956678000	-1.203184000
	5	-0.956678000	0.000000000	1.203184000
	5	-1.455856000	0.000000000	-0.343122000
	5	0.000000000	-1.455856000	0.343122000
	5	1.365426000	0.000000000	-1.906562000
	5	-1.365426000	0.000000000	-1.906562000
	5	0.956678000	0.000000000	1.203184000
	5	1.455856000	0.000000000	-0.343122000
	5	0.000000000	-1.365426000	1.906562000
	5	0.000000000	0.956678000	-1.203184000
	5	0.000000000	0.000000000	2.684682000
	5	0.000000000	0.000000000	-2.684682000
B_{14}.2	5	0.000000000	2.377223000	-0.098126000
	5	0.000000000	0.843781000	0.575930000
	5	0.000000000	-0.843781000	0.575930000
	5	0.000000000	-2.377223000	-0.098126000
	5	-1.459520000	1.736296000	-0.102053000
	5	-1.444731000	0.000000000	0.259670000
	5	-1.459520000	-1.736296000	-0.102053000
	5	-2.777794000	0.767461000	-0.266684000
	5	-2.777794000	-0.767461000	-0.266684000
	5	1.459520000	1.736296000	-0.102053000
	5	1.444731000	0.000000000	0.259670000
	5	1.459520000	-1.736296000	-0.102053000
	5	2.777794000	0.767461000	-0.266684000
	5	2.777794000	-0.767461000	-0.266684000
B_{14}.3	5	0.793458000	0.000000000	0.928134000
	5	-0.793458000	0.000000000	0.928134000
	5	0.000000000	1.388116000	0.275973000
	5	0.000000000	-1.388116000	0.275973000
	5	1.872685000	0.794697000	-0.138245000

	5	-1.872685000	0.794697000	-0.138245000
	5	1.872685000	-0.794697000	-0.138245000
	5	-1.872685000	-0.794697000	-0.138245000
	5	1.391543000	2.314727000	-0.309639000
	5	-1.391543000	2.314727000	-0.309639000
	5	1.391543000	-2.314727000	-0.309639000
	5	-1.391543000	-2.314727000	-0.309639000
	5	0.000000000	2.981747000	-0.308340000
	5	0.000000000	-2.981747000	-0.308340000
B_{14}.4	5	0.000000000	0.000000000	-1.560041000
	5	0.000000000	0.000000000	0.175416000
	5	0.000000000	0.000000000	1.823405000
	5	0.000000000	0.000000000	3.475016000
	5	0.000000000	1.608152000	-0.502752000
	5	0.000000000	-1.608152000	-0.502752000
	5	0.000000000	1.524948000	1.092244000
	5	0.000000000	-1.524948000	1.092244000
	5	0.000000000	1.387129000	2.726561000
	5	0.000000000	-1.387129000	2.726561000
	5	0.000000000	-1.766255000	-2.050755000
	5	0.000000000	1.766255000	-2.050755000
	5	0.000000000	-0.762198000	-3.222194000
	5	0.000000000	0.762198000	-3.222194000
$B_{13}Si^{+}$.1	5	-0.556962000	1.910061000	0.000000000
	5	0.213178000	2.611827000	1.358522000
	5	-0.257152000	1.074233000	-1.567425000
	5	-0.394846000	-0.568663000	1.547807000
	5	-0.979671000	-1.335475000	0.000000000
	5	-0.277276000	-2.160856000	1.372228000
	5	-0.608984000	0.247803000	0.000000000
	5	-0.257152000	1.074233000	1.567425000
	5	0.284827000	3.383373000	0.000000000
	5	0.213178000	2.611827000	-1.358522000
	5	-0.281137000	-2.917809000	0.000000000
	5	-0.394846000	-0.568663000	-1.547807000
	5	-0.277276000	-2.160856000	-1.372228000
	14	1.276470000	-1.143227000	0.000000000
$B_{13}Si^{+}$.2	5	-0.174189000	-2.169867000	1.372619000
	5	-0.193859000	-0.600223000	1.484066000
	5	-0.169636000	-2.957864000	0.000000000
	5	-0.380438000	2.421217000	0.000000000
	5	-0.174189000	-2.169867000	-1.372619000
	5	-0.193859000	-0.600223000	-1.484066000

	5	-0.193859000	0.955683000	-0.964397000
	5	-1.687919000	1.604873000	0.000000000
	5	-0.193859000	0.955683000	0.964397000
	5	1.048185000	0.053583000	0.000000000
	5	-1.596549000	0.044984000	0.000000000
	5	-1.119106000	-1.529051000	0.000000000
	5	0.801654000	-1.540362000	0.000000000
	14	1.509866000	1.975513000	0.000000000
$B_{13}Si^{+}$.3	5	0.000000000	1.536662000	-0.713691000
	5	0.000000000	0.952910000	0.810020000
	5	0.000000000	1.372199000	-2.259605000
	5	0.000000000	-0.952910000	0.810020000
	5	0.000000000	0.000000000	-3.032638000
	5	0.000000000	-1.536662000	-0.713691000
	5	0.000000000	-1.372199000	-2.259605000
	5	1.362323000	0.000000000	1.453511000
	5	-1.362323000	0.000000000	1.453511000
	5	-1.461894000	0.000000000	-0.076786000
	5	1.461894000	0.000000000	-0.076786000
	5	0.990179000	0.000000000	-1.634865000
	5	-0.990179000	0.000000000	-1.634865000
	14	0.000000000	0.000000000	2.812668000
$B_{13}Si^{+}$.4	5	-0.615983000	1.738403000	-0.716888000
	5	-0.127765000	-1.722937000	0.895828000
	5	1.164588000	-0.801029000	1.174574000
	5	-1.916404000	0.803825000	-0.997720000
	5	-0.128665000	1.719427000	0.898089000
	5	-0.615262000	-1.737219000	-0.719120000
	5	-1.914207000	-0.802059000	-0.998670000
	5	-1.680637000	-1.428509000	0.573006000
	5	-1.681412000	1.427440000	0.574064000
	5	-2.436902000	-0.000859000	0.398246000
	5	0.912249000	1.331938000	-0.410640000
	5	1.165345000	0.799536000	1.174213000
	5	0.912915000	-1.330390000	-0.411087000
	14	2.486479000	0.000869000	-0.512105000
$B_{13}Si^{+}$.5	5	-3.292749000	0.346488000	-0.192561000
	5	-3.042491000	-1.175109000	-0.189370000
	5	-2.183059000	1.533156000	-0.080979000
	5	-1.816061000	-0.184262000	0.289000000
	5	-1.595672000	-1.926665000	-0.115195000
	5	2.136644000	1.290410000	-0.371980000
	5	0.680454000	1.989990000	-0.177952000

	5	1.084516000	0.266845000	0.402029000
	5	1.246341000	-1.387998000	-0.118434000
	5	-0.852613000	2.400759000	-0.144474000
	5	-0.515095000	0.895962000	0.524820000
	5	-0.237040000	-0.784742000	0.496994000
	5	-0.047135000	-2.284682000	-0.266756000
	14	3.012129000	-0.350055000	-0.019694000
$B_{13}Si^{+}$.6	5	3.722666000	0.410277000	-0.031288000
	5	2.697626000	1.573908000	0.011894000
	5	3.486235000	-1.099425000	-0.030214000
	5	0.200469000	0.167838000	0.058980000
	5	-3.061322000	0.845406000	-0.036633000
	5	-0.874385000	-1.167992000	0.001812000
	5	0.662209000	-1.522444000	0.022479000
	5	1.139893000	1.576473000	0.022776000
	5	-2.036659000	2.011505000	-0.004435000
	5	2.174537000	-1.916149000	0.012235000
	5	1.923126000	-0.094561000	-0.017858000
	5	-1.479118000	0.379170000	-0.028368000
	5	-0.447144000	1.813072000	0.015169000
	14	-2.895762000	-1.063241000	0.001231000
$B_{13}Si^{+}$.7	5	-2.107642000	0.846158000	-0.000404000
	5	-0.130959000	-1.613431000	0.000786000
	5	1.990995000	-0.104337000	-1.374822000
	5	1.991083000	-0.103241000	1.374628000
	5	0.428263000	-0.259687000	-1.476613000
	5	-1.683944000	-1.775786000	0.000408000
	5	0.428412000	-0.258773000	1.476582000
	5	1.390862000	-1.114038000	0.000641000
	5	2.770998000	-0.032233000	-0.000114000
	5	1.203707000	0.726539000	-0.000823000
	5	-1.145546000	-0.304985000	0.986741000
	5	-2.680715000	-0.584138000	0.000106000
	5	-1.145857000	-0.305824000	-0.987055000
	14	-0.467735000	1.744206000	-0.000021000
$B_{13}Si^{+}$.8	5	1.145337000	1.380589000	0.655187000
	5	-1.756633000	0.008034000	-1.283614000
	5	-1.944592000	0.006423000	0.383237000
	5	1.136312000	-1.392008000	0.648310000
	5	-0.628328000	1.162678000	0.760170000
	5	0.184728000	-2.114232000	-0.380441000
	5	-0.636757000	-1.161688000	0.754859000
	5	-0.994950000	-1.384997000	-1.095804000

	5	0.200361000	2.112937000	-0.372633000
	5	-0.985837000	1.395095000	-1.088893000
	5	0.339384000	-0.004698000	1.716161000
	5	-1.248160000	0.000134000	1.812504000
	5	1.855224000	-0.008884000	0.918131000
	14	1.190683000	0.000220000	-1.223991000
$B_{13}Si^-$.1	5	-0.260968000	1.856848000	0.000000000
	5	-0.392638000	2.718363000	1.417560000
	5	-0.242834000	1.169412000	-1.609712000
	5	-0.242834000	-0.507341000	1.574278000
	5	-0.755294000	-1.209537000	0.000000000
	5	-0.212779000	-2.103700000	1.391541000
	5	0.054038000	0.260110000	0.000000000
	5	-0.242834000	1.169412000	1.609712000
	5	-0.505819000	3.463887000	0.000000000
	5	-0.392638000	2.718363000	-1.417560000
	5	-0.313558000	-2.855063000	0.000000000
	5	-0.242834000	-0.507341000	-1.574278000
	5	-0.212779000	-2.103700000	-1.391541000
	14	1.415633000	-1.453469000	0.000000000
$B_{13}Si^-$.2	5	0.000000000	0.902776000	-1.620678000
	5	0.000000000	-0.902776000	-1.620678000
	5	0.000000000	-1.391371000	-0.063769000
	5	0.000000000	1.391371000	-0.063769000
	5	0.000000000	1.368537000	1.488637000
	5	0.000000000	-1.368537000	1.488637000
	5	-1.362474000	0.000000000	-2.369762000
	5	-1.366583000	0.000000000	-0.782542000
	5	0.000000000	0.000000000	-3.184057000
	5	-0.914781000	0.000000000	0.850276000
	5	1.362474000	0.000000000	-2.369762000
	5	0.914781000	0.000000000	0.850276000
	5	1.366583000	0.000000000	-0.782542000
	14	0.000000000	0.000000000	2.921334000
$B_{13}Si^-$.3	5	2.946550000	-1.714994000	-0.155905000
	5	-0.770044000	0.388265000	0.123760000
	5	3.481586000	1.012606000	0.005811000
	5	-2.392540000	0.854865000	-0.174188000
	5	3.961327000	-0.493544000	-0.010953000
	5	0.798088000	0.067503000	0.012214000
	5	2.377784000	-0.204980000	0.276730000
	5	-1.243797000	1.979394000	-0.216621000
	5	-1.890570000	-0.908236000	-0.128297000

	5	-0.267505000	-1.258518000	-0.081282000
	5	0.332633000	1.781959000	0.009331000
	5	1.931519000	1.488189000	0.091297000
	5	1.326012000	-1.589002000	-0.055082000
	14	-3.782515000	-0.501253000	0.108280000
$B_{13}Si^-$.4	5	-0.128590000	-2.741304000	0.000000000
	5	-0.746200000	-1.157845000	0.000000000
	5	-0.514937000	0.533194000	0.000000000
	5	-0.079303000	-2.128128000	1.459897000
	5	-0.094862000	-0.358563000	1.368437000
	5	0.340183000	1.310002000	1.367667000
	5	0.619782000	0.330673000	2.654145000
	5	-0.079303000	-2.128128000	-1.459897000
	5	-0.094862000	-0.358563000	-1.368437000
	5	0.340183000	1.310002000	-1.367667000
	5	0.283105000	-1.178778000	-2.738103000
	5	0.619782000	0.330673000	-2.654145000
	5	0.283105000	-1.178778000	2.738103000
	14	-0.267172000	2.648409000	0.000000000
$B_{13}Si^-$.5	5	-0.457323000	1.720243000	0.003974000
	5	0.934396000	0.889538000	0.804011000
	5	2.160278000	-0.289407000	0.405636000
	5	1.022250000	2.218343000	-0.204309000
	5	2.350374000	1.352750000	-0.335392000
	5	-0.544846000	0.023630000	0.552962000
	5	0.760840000	-0.765267000	1.130630000
	5	-0.243523000	-1.617373000	0.048777000
	5	1.382966000	-1.807144000	-0.101896000
	5	-1.880153000	0.830968000	-0.040101000
	5	-1.743890000	-0.917797000	-0.189422000
	5	3.323827000	0.112538000	-0.679135000
	5	2.868584000	-1.370006000	-0.644429000
	14	-3.547778000	-0.136077000	-0.268323000
$B_{13}Si^-$.6	5	-1.683744000	-0.116919000	-0.225347000
	5	-2.035360000	-1.732355000	0.029958000
	5	-1.675590000	1.589426000	0.131116000
	5	0.852565000	-0.527159000	0.861226000
	5	1.106699000	1.059768000	0.301482000
	5	2.307461000	-0.141945000	0.004050000
	5	-0.441108000	0.570548000	0.671641000
	5	-0.505839000	-1.314320000	0.346120000
	5	-3.193968000	-0.760928000	-0.386587000
	5	-3.070598000	0.812787000	-0.164757000

	5	2.596269000	1.444051000	-0.255360000
	5	-0.143792000	2.170864000	-0.140969000
	5	1.435280000	2.489955000	-0.398924000
	14	1.589901000	-1.979919000	-0.276303000
$B_{13}Si^{-}$.7	5	-0.320593000	2.424128000	0.435605000
	5	3.069628000	-0.118610000	-0.199791000
	5	1.189888000	1.996789000	0.104880000
	5	2.290845000	-1.455999000	-0.106711000
	5	2.600590000	1.360121000	-0.151763000
	5	-1.637416000	1.569752000	0.543283000
	5	-0.052767000	-0.868067000	-0.101910000
	5	-2.002766000	0.150082000	1.133069000
	5	0.987052000	-2.282750000	0.117596000
	5	-1.688059000	-1.338024000	0.661651000
	5	-0.534838000	-2.382717000	0.494419000
	5	1.437128000	0.135477000	0.112265000
	5	-0.150355000	0.830949000	-0.066473000
	14	-1.852978000	-0.007547000	-1.062900000
$B_{13}Si^{-}$.8	5	-0.158368000	-2.379007000	-0.056492000
	5	-0.284049000	-0.777159000	0.316223000
	5	-0.515232000	0.907066000	0.365025000
	5	-0.737882000	2.450922000	-0.172043000
	5	1.146579000	-1.487689000	-0.174371000
	5	1.100705000	0.214418000	-0.088707000
	5	0.799728000	2.014982000	-0.046168000
	5	2.267189000	1.353910000	0.026908000
	5	-1.694968000	-1.891477000	-0.018062000
	5	-1.865149000	-0.142126000	0.349491000
	5	-2.092796000	1.569935000	-0.059647000
	5	-3.096964000	-1.090934000	-0.166191000
	5	-3.287487000	0.454955000	-0.194934000
	14	3.006676000	-0.427784000	-0.028940000
$B_{12}Si_2$.1	5	0.000000000	1.415713000	0.336911000
	5	0.000000000	1.364381000	1.877905000
	5	0.000000000	-0.913204000	-1.248509000
	5	-0.913204000	0.000000000	1.248509000
	5	-1.415713000	0.000000000	-0.336911000
	5	0.000000000	-1.415713000	0.336911000
	5	1.364381000	0.000000000	-1.877905000
	5	-1.364381000	0.000000000	-1.877905000
	5	0.913204000	0.000000000	1.248509000
	5	1.415713000	0.000000000	-0.336911000
	5	0.000000000	-1.364381000	1.877905000

	5	0.000000000	0.913204000	-1.248509000
	14	0.000000000	0.000000000	-3.286516000
	14	0.000000000	0.000000000	3.286516000
$B_{12}Si_2$.2	5	-0.167777000	0.782837000	2.399439000
	5	-0.076884000	2.246340000	1.745832000
	5	-0.111914000	-0.633638000	-1.724681000
	5	0.399184000	0.691823000	-0.841790000
	5	0.266190000	2.155475000	0.000000000
	5	0.127025000	-0.902774000	0.000000000
	5	0.399184000	0.691823000	0.841790000
	5	-0.076884000	2.246340000	-1.745832000
	5	-0.145430000	3.546434000	0.772164000
	5	-0.111914000	-0.633638000	1.724681000
	5	-0.167777000	0.782837000	-2.399439000
	5	-0.145430000	3.546434000	-0.772164000
	14	-0.033496000	-2.592909000	1.164383000
	14	-0.033496000	-2.592909000	-1.164383000
$B_{12}Si_2$.3	5	2.175254000	-0.235749000	-0.474417000
	5	3.185452000	1.027329000	0.029936000
	5	1.140016000	-1.613834000	-0.026857000
	5	0.134821000	1.816892000	-0.552547000
	5	-0.962887000	0.303721000	-0.833382000
	5	-1.448929000	1.917222000	-0.332462000
	5	0.582966000	0.150546000	-0.198004000
	5	1.714240000	1.482935000	-0.360098000
	5	3.700118000	-0.468565000	0.166936000
	5	2.703381000	-1.675929000	0.219342000
	5	-2.492063000	0.781586000	-0.240236000
	5	-0.453888000	-1.207052000	-0.047974000
	14	-1.116558000	0.365718000	1.380563000
	14	-2.447185000	-1.179684000	-0.434219000
$B_{12}Si_2$.4	5	1.086583000	1.549847000	-0.318137000
	5	3.127468000	-0.350752000	-0.690200000
	5	-0.521539000	1.933046000	-0.123426000
	5	-2.062061000	2.039385000	0.012864000
	5	1.451633000	-0.073472000	-0.971660000
	5	0.582466000	-1.506896000	-0.297342000
	5	-1.027336000	-1.235478000	-0.086109000
	5	2.620416000	1.124035000	-0.499337000
	5	-1.554065000	0.401696000	-0.019344000
	5	-3.094449000	0.888485000	0.076166000
	5	0.097826000	0.167752000	-0.021974000
	5	2.170598000	-1.577459000	-0.482791000

	14	1.902839000	-0.123382000	1.223048000
	14	-2.930532000	-1.076685000	-0.001158000
$B_{12}Si_2$.5	5	0.153692000	-0.662507000	0.932428000
	5	1.495383000	0.260481000	0.000000000
	5	0.153692000	-0.662507000	-0.932428000
	5	0.186521000	2.539148000	-1.374395000
	5	0.153692000	0.955443000	-1.402860000
	5	1.073345000	1.844825000	0.000000000
	5	0.186521000	2.539148000	1.374395000
	5	1.578344000	-1.271488000	0.000000000
	5	-1.105476000	0.337032000	0.000000000
	5	0.153692000	0.955443000	1.402860000
	5	0.192885000	3.336588000	0.000000000
	5	-0.784453000	1.888556000	0.000000000
	14	0.402438000	-2.791469000	0.000000000
	14	-1.630237000	-1.515732000	0.000000000
$B_{12}Si_2$.6	5	0.000000000	2.466578000	1.548693000
	5	0.000000000	-2.466578000	1.548693000
	5	0.000000000	0.839326000	1.325617000
	5	0.000000000	-1.592038000	2.817815000
	5	0.000000000	2.051757000	-0.002670000
	5	0.000000000	0.000000000	-0.213635000
	5	0.000000000	1.374084000	-1.442359000
	5	0.000000000	0.000000000	2.980835000
	5	0.000000000	-2.051757000	-0.002670000
	5	0.000000000	1.592038000	2.817815000
	5	0.000000000	-0.839326000	1.325617000
	5	0.000000000	-1.374084000	-1.442359000
	14	-1.348246000	0.000000000	-2.010963000
	14	1.348246000	0.000000000	-2.010963000
$B_{12}Si_2$.7	5	0.000000000	1.035932000	-0.000066000
	5	0.000000000	-1.035932000	-0.000066000
	5	1.519391000	1.709979000	0.000012000
	5	1.396095000	0.000000000	-0.000018000
	5	1.519391000	-1.709979000	0.000012000
	5	2.852286000	-0.770649000	0.000063000
	5	-1.519391000	1.709979000	0.000012000
	5	-1.396095000	0.000000000	-0.000018000
	5	-1.519391000	-1.709979000	0.000012000
	5	-2.852286000	0.770649000	0.000063000
	5	-2.852286000	-0.770649000	0.000063000
	5	2.852286000	0.770649000	0.000063000
	14	0.000000000	-3.080956000	-0.000024000

	14	0.000000000	3.080956000	-0.000024000
$B_{12}Si_2$.8	5	0.169631000	-0.229961000	1.400513000
	5	0.169631000	1.368139000	0.917833000
	5	0.169631000	1.368139000	-0.917833000
	5	1.038989000	-1.182874000	0.000000000
	5	0.139886000	-1.784904000	-1.366220000
	5	0.139886000	-1.784904000	1.366220000
	5	0.396210000	2.891216000	0.000000000
	5	-1.010334000	0.479480000	0.000000000
	5	-0.763450000	-1.166147000	0.000000000
	5	1.509727000	0.444669000	0.000000000
	5	0.169631000	-0.229961000	-1.400513000
	5	1.666813000	2.009834000	0.000000000
	14	-1.481869000	2.446659000	0.000000000
	14	0.126066000	-3.226203000	0.000000000