Supporting Information

(Si and B)-heterocyclic Carbenes and Theoretical Design of New Molecules

Zeqiong Tian, [a] Congjie Zhang, *[a] Zhipeng Pei, [b] Jinxia Liang *[c] and Yirong Mo *[d]

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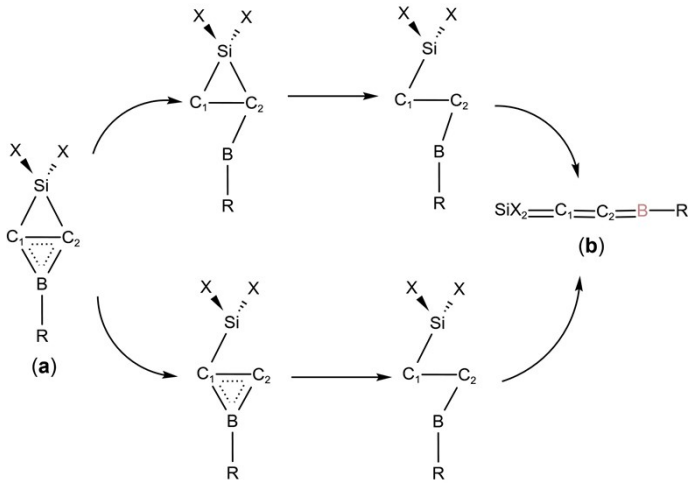
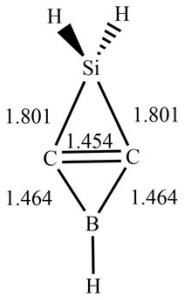
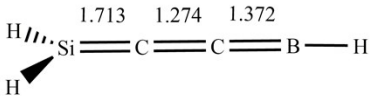


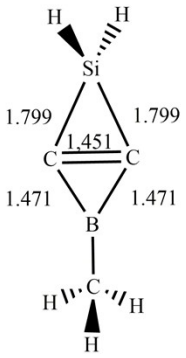
Scheme 1S. The two paths for the isomerization of SiBHCs (**a**) to their linear isomers (**b**).



A1 **0.00** *268.15*



A1-1 **30.25** *147.89i*



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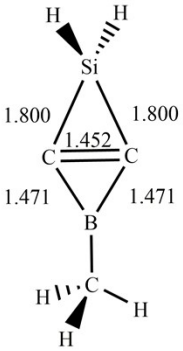
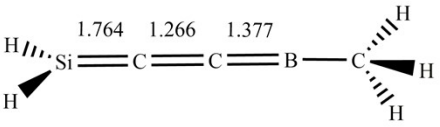
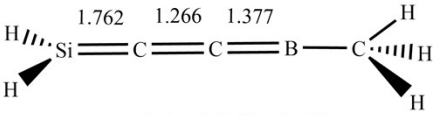


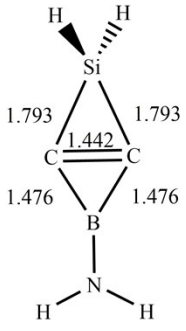
A2-1 **0.03** *48.65i*



A2-2 **26.66** *59.59i*



A2-3 **26.69** *87.83*



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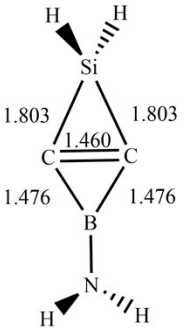
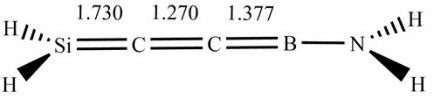
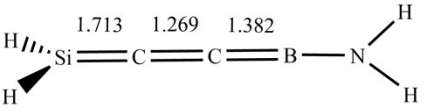


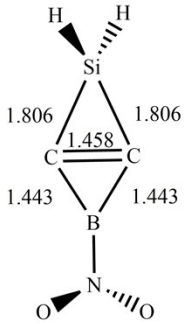
A3-1 **17.63** *597.72i*



A3-2 **41.04** *1246.46i*



A3-3 **23.78** *196.09i*



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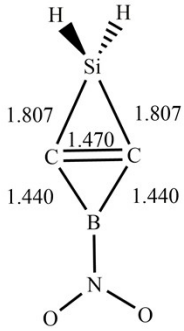
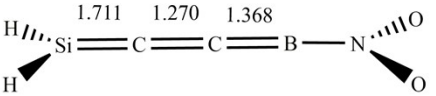
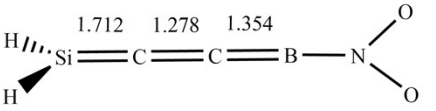


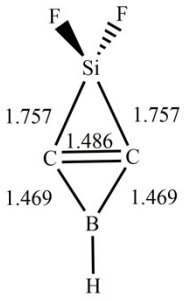
A4-1 **3.43** *87.63i*



A4-2 **32.31** *52.54*



A4-3 **42.07** *396.48i*



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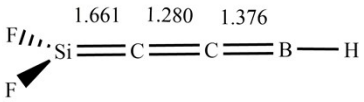
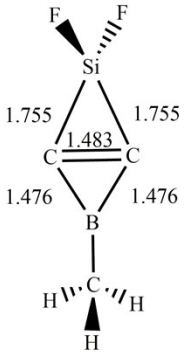
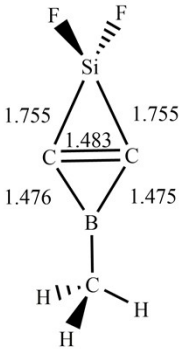


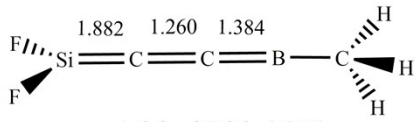
A5-1 **48.96** *253.28i*



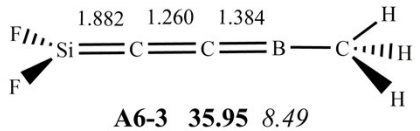
A6 **0.00** *32.94*



A6-1 **0.01** *39.69i*



A6-2 **35.94** *36.71*



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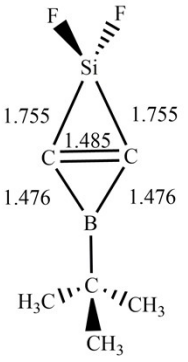

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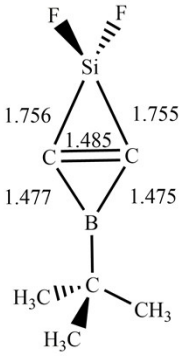

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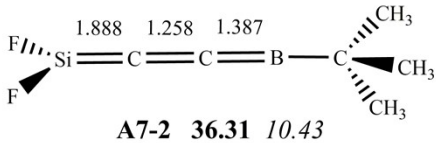
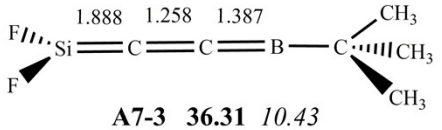
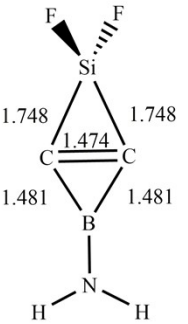


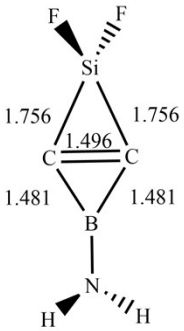
A7-2 **36.31** *10.43*



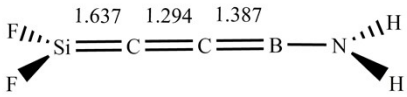
A7-3 **36.31** *10.43*



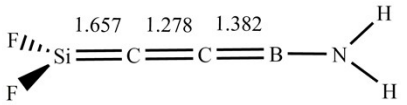
A8 **0.00** *99.13*



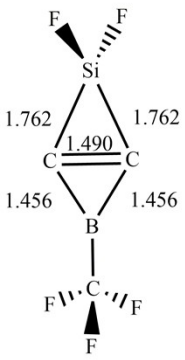
A8-1 **20.12** *646.12i*



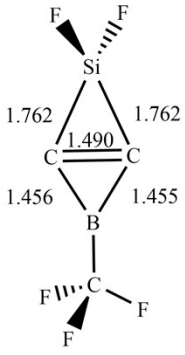
A8-2 **72.67** *277.79i*



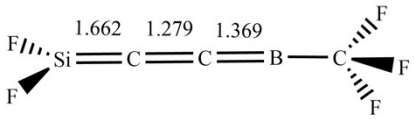
A8-3 **43.92** *268.73i*



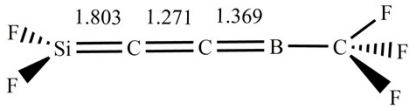
A9 **0.00** *13.37*



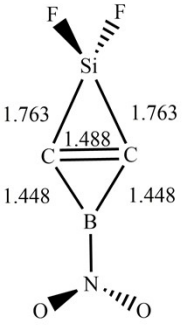
A9-1 **0.03** *7.92i*



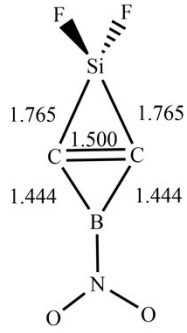
A9-2 **50.70** *206.87i*



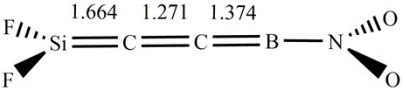
A9-3 **46.02** *6.96*



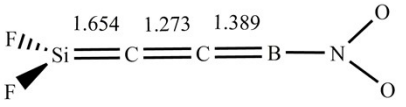
A10 **0.00** *57.11*



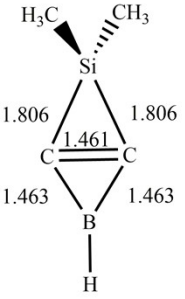
A10-1 **3.65** *62.02i*



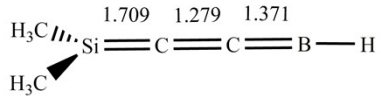
A10-2 **47.52** *157.31i*



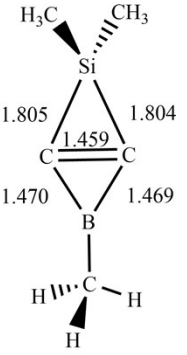
A10-3 **71.18** *172.02i*



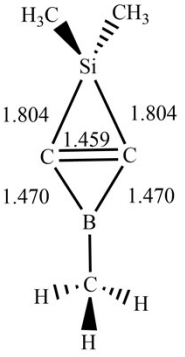
A11 **0.00** *142.03*



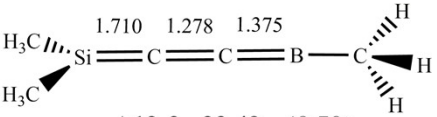
A11-1 **35.39** *45.67*



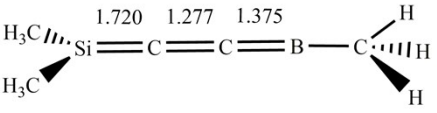
A12 **0.00** *42.73*



A12-1 **0.01** *36.27*



A12-2 **33.49** *48.79i*



A12-3 **33.44** *53.98*

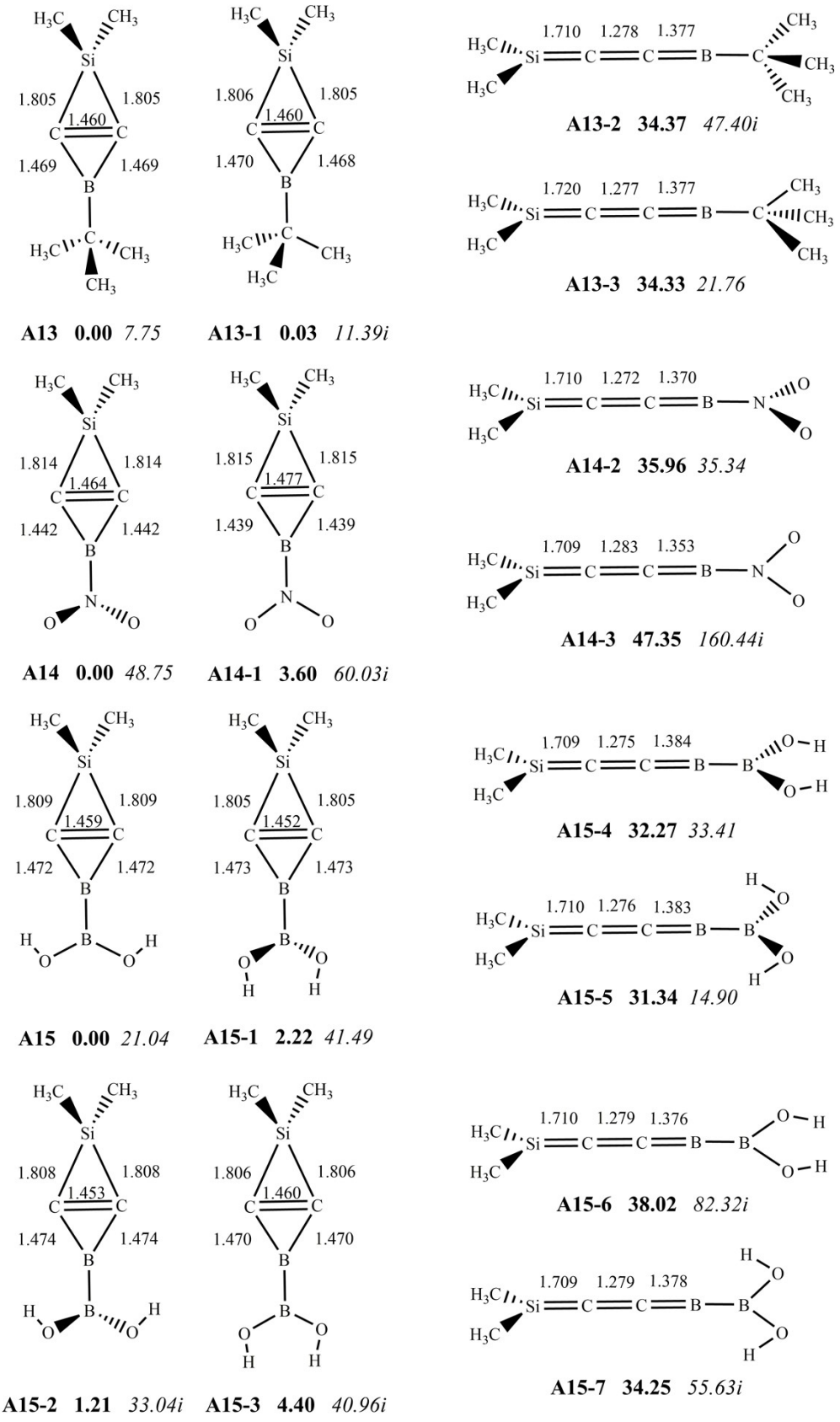


Figure 1S. Optimized geometries of the possible structures of SiBHCs and their linear isomers. Bond lengths (in plain, in Å), relative energies (in bold, in kcal/mol) and the smallest vibrational frequencies (in italic, in cm^{-1}) at M06-2X/6-311G** level.

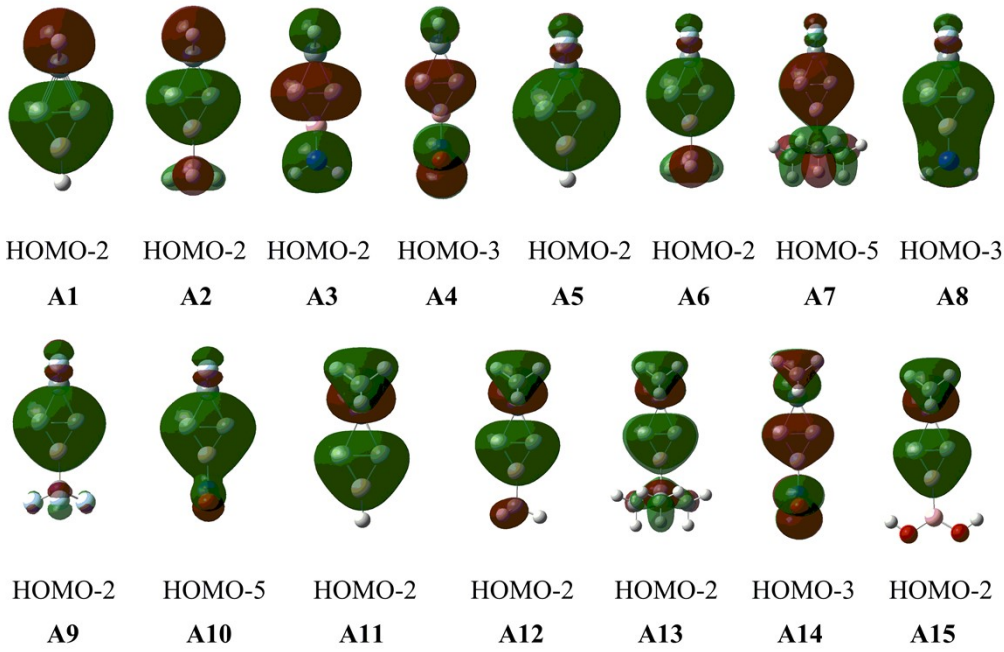


Figure 2S. The π delocalized orbitals covered the three-membered ring CCB of **Ai** (i=1-15).

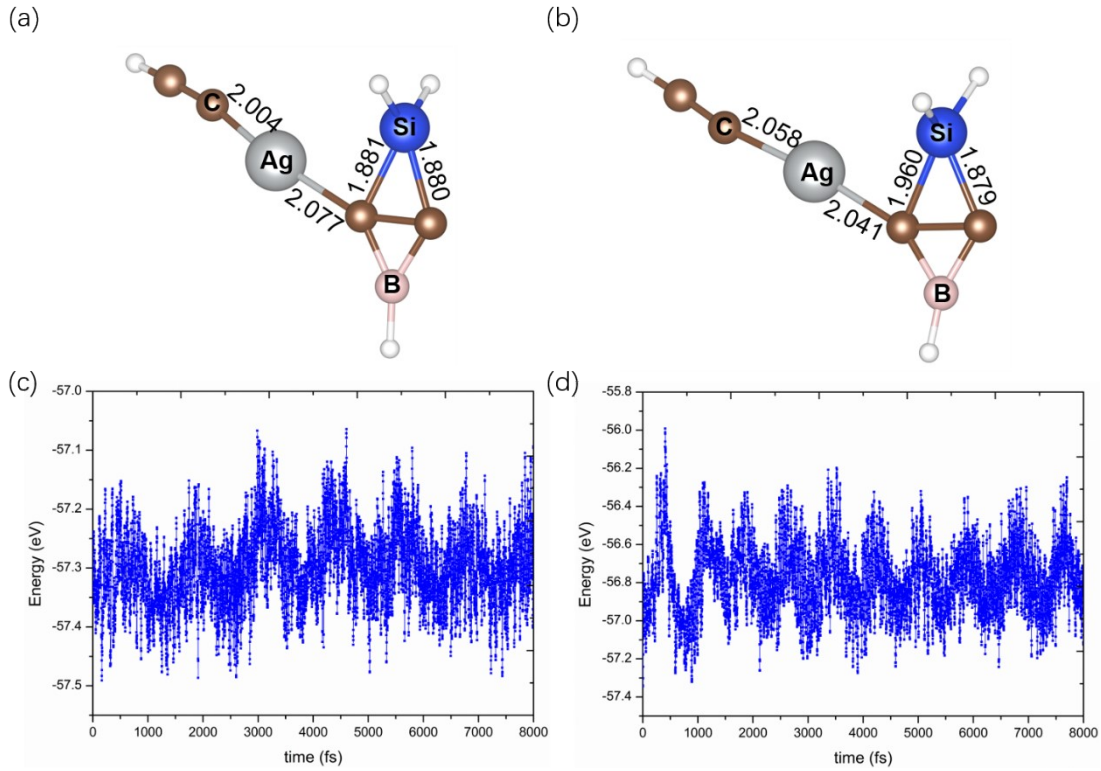


Figure 3S. Selected bond lengths of Ag-C and Si-C in **B1** from ab initio Molecular Dynamics (AIMD) simulations at (a) *T*= 298 K and (b) 673 K for 8000 fs, and the energy evolution of **B1** within 8000 fs from ab initio Molecular Dynamics (AIMD) simulations at (c) *T*= 298 and (d) 673 K.

Table 1S. Symmetry (Symm.), Energy of HOMO ($E_{HOMO,}$ in a.u.) and LUMO ($E_{LUMO,}$ in a.u.), Energy Gaps (E_{gap}, in eV) of **Ai** (i=1-15).

Species	Symm.	E_{HOMO}	E_{LUMO}	E_{gap}
A1	C_{2v}	-0.32146	0.00651	8.92
A2	C_s	-0.31501	0.01316	8.93
A3	C_{2v}	-0.31325	0.02097	9.09
A4	C_{2v}	-0.35298	-0.04246	8.45
A5	C_{2v}	-0.34791	-0.01970	8.93
A6	C_s	-0.34017	-0.01214	8.93
A7	C_s	-0.33467	-0.01376	8.73
A8	C_{2v}	-0.33942	-0.00142	9.20
A9	C_s	-0.36962	-0.04077	8.95
A10	C_{2v}	-0.37529	-0.05218	8.79
A11	C_{2v}	-0.30743	0.01888	8.88
A12	C_s	-0.30198	0.02412	8.87
A13	C_s	-0.30050	0.02114	8.75
A14	C_{2v}	-0.33926	-0.02468	8.56
A15	C_{2v}	-0.30542	-0.00288	8.23

Table 2S. The NICS(0) and NICS(1) values (in ppm) at the centers of the three-membered rings (CCB) of **Ai** (i=1-15). And, electron density (ρ) and Laplacian values ($\nabla^2\rho$) of the inverted C=C bonds in **Ai** (i=1-15) at M06-2X/6-311G** level.

Species	NICS(0)	NICS(1)	ρ	∇^2_ρ
A1	-34.57	-21.59	0.27	-0.39
A2	-30.95	-19.37	0.27	-0.40
A3	-20.50	-17.54	0.27	-0.43
A4	-29.42	-19.90	0.27	-0.39
A5	-37.71	-17.98	0.25	-0.32
A6	-33.68	-15.09	0.25	-0.32
A7	-32.29	-13.89	0.25	-0.32
A8	-21.73	-11.13	0.26	-0.35
A9	-34.33	-15.52	0.25	-0.31
A10	-32.22	-15.64	0.25	-0.31
A11	-36.86	-20.15	0.26	-0.37
A12	-33.42	-17.77	0.26	-0.38
A13	-32.20	-17.27	0.26	-0.37
A14	-31.57	-18.57	0.26	-0.37
A15	-38.44	-19.41	0.26	-0.38

Table 3S. Bonding energies with ZPEs (E_b, in kcal/mol) of the complexes **Bi** (i=1-15) and LAgC≡CH (L= CO, NHC) formed by CO, NHC and AgC≡CH at M06-2X/6-311G** level.

Species	E_b	Species	E_b
B1	-27.58	**B10**	-18.94
B2	-28.77	**B11**	-31.43
B3	-29.75	**B12**	-32.44
B4	-23.24	**B13**	-32.69
B5	-23.13	**B14**	-27.07
B6	-24.49	**B15**	-32.20
B7	-26.20	CO-AgC≡CH	-18.45
B8	-25.79	NHC-AgC≡CH	-45.20
B9	-20.82		

Table 4S. Bond lengths (d1 and d2, in Å) of the transition structures (**TS**) of the Diels-Alder reactions of **Ai** (i=5-13) with butadiene at M06-2X/6-311G** level.

TS	d1	d2	TS	d1	d2
$\mathbf{TS_{A5\text{-}endo}}$	2.323	2.323	$\mathbf{TS_{A5\text{-}exo}}$	2.313	2.313
$\mathbf{TS_{A6\text{-}endo}}$	2.322	2.323	$\mathbf{TS_{A6\text{-}exo}}$	2.316	2.311
$\mathbf{TS_{A7\text{-}endo}}$	2.311	2.329	$\mathbf{TS_{A7\text{-}exo}}$	2.327	2.306
$\mathbf{TS_{A8\text{-}endo}}$	2.330	2.330	$\mathbf{TS_{A8\text{-}exo}}$	2.336	2.336
$\mathbf{TS_{A9\text{-}endo}}$	2.348	2.350	$\mathbf{TS_{A9\text{-}exo}}$	2.338	2.334
$\mathbf{TS_{A10\text{-}endo}}$	2.378	2.378	$\mathbf{TS_{A10\text{-}exo}}$	2.354	2.354
$\mathbf{TS_{A11\text{-}endo}}$	2.300	2.300	$\mathbf{TS_{A11\text{-}exo}}$	2.285	2.285
$\mathbf{TS_{A12\text{-}endo}}$	2.305	2.302	$\mathbf{TS_{A12\text{-}exo}}$	2.274	2.299
$\mathbf{TS_{A13\text{-}endo}}$	2.321	2.283	$\mathbf{TS_{A13\text{-}exo}}$	2.260	2.318

Table 5S. Bond lengths (d, in Å) and WBIs of C_1-C_2 bond of the products of the Diels-Alder reactions of **Ai** (i=5-13) with butadiene at M06-2X/6-311G** level.

Products	d	WBI
$\mathbf{P_{A5}}$	1.794	0.73
$\mathbf{P_{A6}}$	1.789	0.75
$\mathbf{P_{A7}}$	1.789	0.75
$\mathbf{P_{A8}}$	1.777	0.78
$\mathbf{P_{A9}}$	1.826	0.70
$\mathbf{P_{A10}}$	1.828	0.70
$\mathbf{P_{A11}}$	1.705	0.78
$\mathbf{P_{A12}}$	1.703	0.79
$\mathbf{P_{A13}}$	1.708	0.79

Cartesian coordinates, electronic energy (E, in a.u.) and the smallest vibrational frequency (*v,* in cm^{-1}) for all the stable molecules calculated at the M06-2X/6-311G** level.

A1

E= -392.20164

v= 268.15

B	0.000000	0.000000	-1.834183
C	0.000000	0.727179	-0.563128
C	0.000000	-0.727179	-0.563128
H	-1.234889	0.000000	1.878187
H	1.234889	0.000000	1.878187
Si	0.000000	0.000000	1.084306
H	0.000000	0.000000	-3.008200

A2

E= -431.52438

v= 18.74

B	0.016782	-1.158778	0.000000
C	0.004866	0.120829	0.725425
C	0.004866	0.120829	-0.725425
Si	-0.005352	1.767484	0.000000
C	0.004866	-2.706766	0.000000
H	-1.035115	-3.049027	0.000000
H	0.479833	-3.121035	-0.890098
H	0.479833	-3.121035	0.890098
H	1.222472	2.573531	0.000000
H	-1.243608	2.557325	0.000000

A3

E= -447.60660

v= 154.99

B	0.000000	0.000000	-1.200253
C	0.000000	0.720808	0.088124
C	0.000000	-0.720808	0.088124
Si	0.000000	0.000000	1.730105
N	0.000000	0.000000	-2.586387
H	0.000000	0.849638	-3.125067
H	0.000000	-0.849638	-3.125067
H	-1.228149	0.000000	2.538579
H	1.228149	0.000000	2.538579

A4

E= -596.69892

v= 80.24

B	0.000000	0.000000	-0.347487
C	0.729058	0.000000	0.897966
C	-0.729058	0.000000	0.897966
Si	0.000000	0.000000	2.549821
N	0.000000	0.000000	-1.851009
O	0.000000	1.081770	-2.402090
O	0.000000	-1.081770	-2.402090
H	0.000000	1.242071	3.327428
H	0.000000	-1.242071	3.327428

A5

E= -590.81289

v= 169.58

B	0.000000	0.000000	-2.451281
C	0.000000	0.742818	-1.184329
C	0.000000	-0.742818	-1.184329
Si	0.000000	0.000000	0.407710
H	0.000000	0.000000	-3.623659
F	1.265343	0.000000	1.354671
F	-1.265343	0.000000	1.354671

A6

E= -630.13663

v= 32.94

B	0.009120	-1.881477	0.000000
C	0.005095	-0.605530	0.741547
C	0.005095	-0.605530	-0.741547
Si	0.005095	0.984735	0.000000
F	1.267757	1.938727	0.000000
F	-1.258698	1.937292	0.000000
C	-0.016452	-3.425566	0.000000
H	0.450617	-3.845900	-0.891072
H	-1.062125	-3.751516	0.000000
H	0.450617	-3.845900	0.891072

A7

E= -748.04382

v= 17.58

B	0.079321	-0.704928	0.000000
C	-0.139567	0.552027	0.742365
C	-0.139567	0.552027	-0.742365
Si	-0.422601	2.117200	0.000000
F	0.651317	3.279731	0.000000
F	-1.834614	2.832004	0.000000
C	0.410430	-2.223908	0.000000
C	-0.139567	-2.907241	1.259847
H	0.153397	-3.962118	1.273186
H	0.244449	-2.432782	2.165749
H	-1.231130	-2.862172	1.293292
C	-0.139567	-2.907241	-1.259847
H	0.244449	-2.432782	-2.165749
H	0.153397	-3.962118	-1.273186
H	-1.231130	-2.862172	-1.293292
C	1.951446	-2.321128	0.000000
H	2.383902	-1.849723	-0.886326
H	2.383902	-1.849723	0.886326
H	2.246587	-3.375398	0.000000

A8

E= -646.22157

v= 99.13

B	0.000000	0.000000	-1.915022
C	0.000000	0.736942	-0.630561
C	0.000000	-0.736942	-0.630561
Si	0.000000	0.000000	0.954044
F	-1.257991	0.000000	1.918241
F	1.257991	0.000000	1.918241
N	0.000000	0.000000	-3.295826
H	0.000000	-0.848913	-3.836165
H	0.000000	0.848913	-3.836165

A9

E= -927.85215

v= 13.37

B	-0.081265	-0.695945	0.000000
C	0.114823	0.539317	0.744879
C	0.114823	0.539317	-0.744879
Si	0.372880	2.114774	0.000000
F	1.776408	2.833213	0.000000
F	-0.727668	3.243657	0.000000
C	-0.381464	-2.251857	0.000000

F	-1.712064	-2.449429	0.000000
F	0.114823	-2.874153	-1.077690
F	0.114823	-2.874153	1.077690

A10

E= -795.30656

v= 57.11

B	0.000000	0.000000	-1.100869
C	0.743842	0.000000	0.141053
C	-0.743842	0.000000	0.141053
Si	0.000000	0.000000	1.739146
F	0.000000	1.269902	2.669487
F	0.000000	-1.269902	2.669487
N	0.000000	0.000000	-2.601624
O	0.000000	1.082919	-3.148483
O	0.000000	-1.082919	-3.148483

A11

E= -470.84664

v= 142.03

B	0.000000	0.000000	-2.536862
C	0.730491	0.000000	-1.268741
C	-0.730491	0.000000	-1.268741
Si	0.000000	0.000000	0.383414
C	0.000000	1.563265	1.388521
H	0.883694	1.605437	2.029482
H	0.000000	2.437049	0.736552
H	-0.883694	1.605437	2.029482
C	0.000000	-1.563265	1.388521
H	0.883694	-1.605437	2.029482
H	-0.883694	-1.605437	2.029482
H	0.000000	-2.437049	0.736552
H	0.000000	0.000000	-3.711884

A12

E= -510.16862

v= 42.73

B	-0.522571	-1.881224	0.000000
C	-0.886868	-0.458241	0.000000
C	0.519744	-0.844504	0.000000
Si	0.253026	0.940289	0.000000
C	0.519744	1.913616	1.562082
H	-0.162030	2.765944	1.605252
H	0.346531	1.285205	2.435818
H	1.541333	2.297754	1.606187
C	0.519744	1.913616	-1.562082
H	-0.162030	2.765944	-1.605252
H	1.541333	2.297754	-1.606187
H	0.346531	1.285205	-2.435818
C	-0.910128	-3.382976	0.000000
H	-0.483281	-3.880236	-0.875077
H	-0.483281	-3.880236	0.875077
H	-1.988038	-3.544314	0.000000

A13

E= -628.07588

v= 7.75

B	-0.097560	-0.749195	0.000000
C	0.128409	0.505550	0.730067
C	0.128409	0.505550	-0.730067
Si	0.428380	2.129179	0.000000
C	2.147390	2.838426	0.000000
H	2.306207	3.461144	0.883256
H	2.888727	2.039231	0.000000
H	2.306207	3.461144	-0.883256
C	-0.925859	3.403549	0.000000
H	-0.852703	4.042012	0.883269
H	-0.852703	4.042012	-0.883269
H	-1.903029	2.920381	0.000000
C	-0.428887	-2.274835	0.000000
C	-1.966209	-2.392409	0.000000
H	-2.402426	-1.923231	-0.885871
H	-2.254217	-3.449225	0.000000
H	-2.402426	-1.923231	0.885871
C	0.128409	-2.955062	1.258092
H	-0.153280	-4.013607	1.273658
H	1.219661	-2.897540	1.290399
H	-0.258176	-2.482356	2.163951
C	0.128409	-2.955062	-1.258092
H	-0.258176	-2.482356	-2.163951
H	1.219661	-2.897540	-1.290399
H	-0.153280	-4.013607	-1.273658

A14

E= -675.34701

v= 48.75

B	0.000000	0.000000	-1.156083
C	0.732084	0.000000	0.086354
C	-0.732084	0.000000	0.086354
Si	0.000000	0.000000	1.745787
C	0.000000	1.570718	2.728209
H	0.883423	1.617277	3.369023
H	0.000000	2.438572	2.068800
H	-0.883423	1.617277	3.369023
C	0.000000	-1.570718	2.728209
H	0.883423	-1.617277	3.369023
H	-0.883423	-1.617277	3.369023
H	0.000000	-2.438572	2.068800
N	0.000000	0.000000	-2.660308
O	0.000000	1.081055	-3.214181
O	0.000000	-1.081055	-3.214181

A15

E= -646.85375

v= 21.04

B	0.000000	0.000000	-1.078883
C	0.000000	0.729568	0.199116
C	0.000000	-0.729568	0.199116
Si	0.000000	0.000000	1.854291
C	-1.564387	0.000000	2.858034
H	-1.605728	0.883876	3.498470
H	-2.437087	0.000000	2.204829
H	-1.605728	-0.883876	3.498470
C	1.564387	0.000000	2.858034
H	1.605728	0.883876	3.498470
H	1.605728	-0.883876	3.498470
H	2.437087	0.000000	2.204829
B	0.000000	0.000000	-2.776619
O	0.000000	-1.155679	-3.495129
H	0.000000	-1.926339	-2.924922
O	0.000000	1.155679	-3.495129
H	0.000000	1.926339	-2.924922

B1

E= -615.83585

v= 37.19

B	2.570123	1.608064	0.000006
C	2.969550	0.208980	-0.000029
C	1.559690	0.521791	0.000024
H	1.835769	-2.033080	1.251674
H	1.835632	-2.033085	-1.251637
Si	2.000756	-1.292919	0.000003
H	2.804344	2.755076	0.000041
C	-2.679776	-0.138525	0.000071
C	-3.871965	-0.366686	-0.000062
H	-4.919687	-0.559281	0.000152
Ag	-0.644303	0.225054	-0.000007

B2

E= -655.16065

v= 24.61

B	2.522822	0.857235	0.002357
C	1.351160	-0.071998	0.000645
C	2.694502	-0.593282	0.000910
Si	1.504733	-1.925608	-0.000546
C	3.023446	2.314480	0.000089
H	2.594194	2.860141	0.844107
H	4.109236	2.389704	0.046132
H	2.675577	2.821320	-0.904177
H	1.221755	-2.635052	-1.250105
H	1.220587	-2.636965	1.247656
C	-4.134691	0.342744	-0.000193
C	-2.922969	0.267153	-0.000143
H	-5.197697	0.413333	-0.000234
Ag	-0.858994	0.125644	0.000099

B3

E= -671.24444

v= 24.12

B	1.051470	-1.979527	0.000000
C	-0.175934	-2.770543	0.000000
C	-0.327449	-1.344905	0.000000
Si	-1.895517	-2.282795	0.000000
N	2.415048	-1.788872	0.000000
H	3.068955	-2.554314	0.000000
H	2.832264	-0.871608	0.000000
H	-2.673145	-2.353298	1.240699
H	-2.673145	-2.353298	-1.240699
C	0.620640	4.082007	0.000000
C	0.382160	2.891399	0.000000
H	0.823112	5.127854	0.000000
Ag	0.000000	0.856080	0.000000

B4

E= -820.32575

v= 28.70

B	-2.243569	-0.186615	-0.000345
C	-0.819649	-0.498680	-0.000186
C	-1.806729	-1.557902	-0.000403
Si	-0.161837	-2.266782	-0.000180
N	-3.331352	0.845065	-0.000373
O	-3.727392	1.219858	1.082914
O	-3.727075	1.220146	-1.083676
H	0.369068	-2.787178	1.259165
H	0.369449	-2.787059	-1.259413
C	3.263770	0.793223	0.000362
C	4.439744	1.092283	0.000330
H	5.469728	1.364749	0.000417
Ag	1.271653	0.265287	0.000259

B5

E= -814.43986

v= 32.39

B	-1.861272	2.317094	-0.000389
C	-2.577912	1.044720	-0.000404
C	-1.104348	1.038146	-0.000070
Si	-1.923675	-0.575706	-0.000079
H	-1.837985	3.486291	-0.000635
F	-1.936796	-1.490864	1.277759
F	-1.936051	-1.491067	-1.277769
C	4.090810	-0.797606	-0.000356
C	2.950949	-0.382060	-0.000381
H	5.091864	-1.161883	-0.000234
Ag	1.014522	0.331238	0.000240

B6

E= -853.76580

v= 22.26

B	0.947041	1.981749	-0.000108
C	0.921159	0.466612	0.000216
C	2.190224	1.217852	-0.000203
Si	2.405664	-0.520444	0.000082
F	2.872883	-1.324411	-1.271055
F	2.873763	-1.324766	1.270626
C	0.101262	3.265143	0.000042
H	0.703670	4.172444	-0.000669
H	-0.556308	3.273382	0.874277
H	-0.557177	3.272574	-0.873613
C	-3.224449	-0.705662	-0.000088
C	-4.397988	-1.016034	-0.000114
H	-5.427087	-1.291430	-0.000167
Ag	-1.230610	-0.161157	0.000092

B7

E= -971.67555

v= 28.60

B	-0.863169	-1.408879	-0.000081
C	-2.174710	-0.765418	-0.000127
C	-0.982500	0.103579	-0.000089
Si	-2.552112	0.945761	0.000007
F	-3.098050	1.701168	1.270744
F	-3.098294	1.701247	-1.270576
C	0.101831	-2.621759	0.000027
C	-0.690696	-3.937495	0.000084
H	-0.002158	-4.787565	0.000070
H	-1.328007	-4.017676	0.884059
H	-1.328119	-4.017726	-0.883805
C	0.995058	-2.546669	-1.254975
H	1.612175	-1.643320	-1.261527
H	1.668492	-3.408947	-1.264460
H	0.406642	-2.571547	-2.175978
C	0.995114	-2.546607	1.254950
H	1.612202	-1.643237	1.261487
H	0.406759	-2.571500	2.175994
H	1.668587	-3.408855	1.264417
C	4.227802	1.946133	0.000021
C	3.074418	1.567302	-0.000010
H	5.237405	2.286139	0.000024
Ag	1.118737	0.888763	-0.000016

B8

E= -869.85278

v= 23.35

B	-1.416163	-1.534851	0.000000
C	-2.414395	-0.461313	0.000000
C	-1.002206	-0.068929	0.000000
Si	-2.165656	1.266919	0.000000
F	-2.414395	2.176979	1.264625
F	-2.414395	2.176979	-1.264625
N	-1.020503	-2.848788	0.000000
H	-0.050613	-3.125893	0.000000
H	-1.680240	-3.610078	0.000000
C	3.282954	-0.529214	0.000000
C	4.481994	-0.717718	0.000000
H	5.535465	-0.876037	0.000000
Ag	1.236339	-0.234716	0.000000

B9

E= -1151.47519

v= 19.17

B	-1.988305	0.241970	-0.041831
C	-0.529135	0.429597	-0.025025
C	-1.446608	1.586771	-0.020897
Si	0.233412	2.081919	-0.000378
F	0.937894	2.677706	-1.269945
F	0.913039	2.649577	1.295278

C	-3.202099	-0.775337	-0.007925
F	-3.359265	-1.226800	1.246630
F	-4.356876	-0.217402	-0.384423
F	-2.988665	-1.832584	-0.799371
C	3.270861	-1.560599	0.009801
C	4.370738	-2.071803	0.025819
H	5.334822	-2.524516	0.039536
Ag	1.409389	-0.679541	-0.010835

B10

E= -1018.92646

v= 21.31

B	-2.288739	0.080672	0.000153
C	-0.855239	-0.203063	0.000033
C	-1.847474	-1.294330	0.000128
Si	-0.207429	-1.912279	0.000063
F	0.429649	-2.544741	1.285364
F	0.429845	-2.544523	-1.285262
N	-3.387740	1.097320	0.000106
O	-3.784918	1.465214	1.084325
O	-3.785012	1.464809	-1.084220
C	3.167642	1.275232	0.000211
C	4.322155	1.646684	0.000558
H	5.334233	1.979500	0.000848
Ag	1.209130	0.649444	-0.000225

B11

E= -694.48671

v= 31.99

B	1.981118	2.331845	-0.000004
C	2.584634	1.007815	0.000012
C	1.139642	1.114461	-0.000033
Si	1.853917	-0.629094	0.000007
C	1.765748	-1.585816	1.581137
H	2.617682	-2.264989	1.663070
H	1.769871	-0.913737	2.439477
H	0.850240	-2.181443	1.606218
C	1.765835	-1.585832	-1.581118
H	2.617816	-2.264950	-1.663033
H	0.850371	-2.181527	-1.606201
H	1.769918	-0.913764	-2.439466
H	2.048781	3.501422	-0.000006
C	-3.991164	-0.879778	-0.000027
C	-2.880236	-0.389457	-0.000014
H	-4.970106	-1.299672	-0.000043
Ag	-0.972803	0.416562	0.000003

B12

E= -733.81025

v= 30.48

B	-2.303294	-1.497166	0.004765
C	-2.552893	-0.057415	0.002052
C	-1.181757	-0.517050	0.001303
Si	-1.436407	1.343201	-0.000174
C	-1.107743	2.256530	1.576943
H	-1.740336	3.145076	1.641628
H	-1.308541	1.620273	2.439177
H	-0.064142	2.577980	1.613626
C	-1.109724	2.253842	-1.579250
H	-1.742381	3.142295	-1.644580
H	-0.066157	2.575209	-1.617570
H	-1.311478	1.616271	-2.440283
C	-2.744366	-2.977015	0.000589
H	-2.424028	-3.450699	-0.931750
H	-2.251336	-3.522919	0.808581
H	-3.822696	-3.100147	0.096888
C	3.098304	-0.215012	-0.000512
C	4.304505	-0.073974	-0.000739
H	5.363517	0.041620	-0.000735
Ag	1.037357	-0.425178	0.000241

B13

E= -851.71780

v= 11.49

B	-1.957173	0.306130	-0.028742
C	-0.487800	0.564796	-0.019639
C	-1.426158	1.666233	-0.014841
Si	0.260761	2.276446	-0.000815
C	1.031317	2.891057	-1.568040
H	2.088564	2.616468	-1.596499
H	0.535207	2.456764	-2.436186
H	0.961047	3.979410	-1.631279
C	1.012198	2.860412	1.587335
H	2.070036	2.588991	1.622136
H	0.936879	3.946897	1.673292
H	0.507684	2.405523	2.440046
C	-3.069275	-0.779495	-0.008927
C	-2.991454	-1.484229	1.360261
H	-3.185803	-0.790880	2.182984
H	-3.744863	-2.277299	1.405280
H	-2.010252	-1.939621	1.518552
C	-2.788754	-1.810928	-1.115762
H	-3.534652	-2.611024	-1.070774
H	-2.842501	-1.359012	-2.109773
H	-1.799571	-2.261128	-0.998228
C	-4.463572	-0.167977	-0.198706
H	-4.681642	0.569158	0.577910
H	-4.551201	0.329490	-1.167823
H	-5.228020	-0.950317	-0.150021
C	3.053113	-1.842794	0.008545
C	4.073293	-2.501642	0.019146
H	4.965329	-3.084071	0.028234
Ag	1.318969	-0.710486	-0.009127

B14

E= -898.97994

v= 24.40

B	-2.331697	-0.004974	-0.000031
C	-0.887419	-0.186163	-0.000028
C	-1.778830	-1.332411	-0.000074
Si	-0.076963	-1.911778	-0.000023
C	0.662562	-2.488028	1.589909
H	1.728420	-2.248794	1.611551
H	0.176118	-2.007308	2.439109
H	0.550317	-3.570776	1.687416
C	0.662723	-2.487959	-1.589903
H	1.728540	-2.248544	-1.611525
H	0.550667	-3.570732	-1.687358
H	0.176218	-2.007370	-2.439143
N	-3.508705	0.924588	-0.000014
O	-3.938945	1.264486	1.082563
O	-3.938952	1.264550	-1.082563
C	3.122968	1.327732	0.000049
C	4.296667	1.638006	-0.000061
H	5.322384	1.926265	0.000017
Ag	1.140753	0.744373	0.000024

B15

E= -870.49483

v= 24.58

B	-1.412513	0.486258	0.000000
C	-1.135904	1.919181	0.000000
C	0.005693	1.031387	0.000000
Si	0.429421	2.820200	0.000000
C	1.038269	3.576779	1.576866
H	0.769957	4.634792	1.620291
H	0.604304	3.070798	2.439373
H	2.126316	3.503540	1.639052

C	1.038269	3.576779	-1.576866
H	0.769957	4.634792	-1.620291
H	2.126316	3.503540	-1.639052
H	0.604304	3.070798	-2.439373
B	-2.536259	-0.810188	0.000000
O	-2.248104	-2.125191	0.000000
H	-1.325033	-2.411812	0.000000
O	-3.859446	-0.480271	0.000000
H	-4.008541	0.466154	0.000000
C	1.086183	-3.094804	0.000000
C	1.038269	-4.308567	0.000000
H	1.020824	-5.373934	0.000000
Ag	0.882538	-1.028142	0.000000

butadiene

E= -155.94919

v= 160.35

C	0.607451	1.737207	0.000000
C	0.607451	0.405362	0.000000
H	1.527568	2.307609	0.000000
H	-0.322323	2.296905	0.000000
H	1.550318	-0.136359	0.000000
C	-0.607451	-0.405362	0.000000
C	-0.607451	-1.737207	0.000000
H	-1.550318	0.136359	0.000000
H	-1.527568	-2.307609	0.000000
H	0.322323	-2.296905	0.000000

P_{A5}

E= -746.85256

v= 70.45

C	1.221823	1.612420	-0.239592
C	2.241812	0.723733	0.443923
H	1.721574	2.151777	-1.051209
H	0.889232	2.369012	0.477454
H	3.081862	1.265851	0.869135
C	2.244489	-0.602067	0.594382
C	1.227838	-1.625001	0.127820
H	3.086898	-1.032859	1.128384
H	1.728683	-2.327578	-0.546803
H	0.902765	-2.206700	0.995569
B	0.239915	-0.216622	-1.862195
C	0.058681	-0.969523	-0.568541
C	0.058037	0.812309	-0.776066
Si	-1.273811	0.011650	0.109730
H	0.745902	-0.340881	-2.919591
F	-2.772751	-0.058038	-0.428184
F	-1.431605	0.205834	1.687102

P_{A6}

E= -786.17562

v= 63.91

C	-1.006797	-0.588641	-1.625234
C	-1.815272	-1.440444	-0.667119
H	-1.702555	-0.024249	-2.256281
H	-0.455537	-1.254879	-2.295773
H	-2.478942	-2.147257	-1.157536
C	-1.815278	-1.440416	0.667121
C	-1.006854	-0.588556	1.625209
H	-2.478812	-2.147347	1.157555
H	-1.702598	-0.024188	2.256300
H	-0.455568	-1.254799	2.295719
B	-0.622921	1.444483	-0.000052
C	-0.077623	0.352130	-0.894357
C	-0.077632	0.352172	0.894336
Si	1.427761	-0.001429	0.000011
F	2.702385	0.957798	-0.000042
F	2.048228	-1.474222	0.000072
C	-1.650028	2.607310	-0.000003
H	-2.280873	2.611784	-0.891102
H	-1.096594	3.553668	0.000360
H	-2.281190	2.611340	0.890878

P_{A7}

E= -904.08481

v= 29.53

C	0.489447	-1.299998	-1.622776
C	0.331290	-2.465628	-0.667619
H	-0.327880	-1.333284	-2.350514
H	1.413706	-1.447037	-2.190923
H	0.225861	-3.429646	-1.158033
C	0.331276	-2.465625	0.667569
C	0.489515	-1.300020	1.622730
H	0.225621	-3.429618	1.157981
H	-0.327826	-1.333310	2.350451
H	1.413772	-1.447070	2.190884
B	-0.666920	0.411177	-0.000005
C	0.492473	0.025742	0.894561
C	0.492481	0.025745	-0.894583
Si	1.807331	0.838461	-0.000015
F	3.282971	0.223325	0.000088
F	2.041727	2.416513	-0.000067
C	-2.222553	0.531314	0.000008
C	-2.827039	-0.110168	-1.256319
H	-3.912576	0.035797	-1.275301
H	-2.409006	0.331036	-2.165270
H	-2.634048	-1.187003	-1.279528
C	-2.826986	-0.110497	1.256193
H	-2.408995	0.330548	2.165242
H	-3.912535	0.035371	1.275205
H	-2.633893	-1.187320	1.279175
C	-2.536634	2.042933	0.000214
H	-2.130003	2.538371	0.885929
H	-2.130042	2.538612	-0.885384
H	-3.622087	2.188889	0.000255

P_{A8}

E= -802.26351

v= 55.14

C	1.059385	-0.527624	1.613091
C	1.977710	-1.270105	0.666124
H	1.676622	0.063372	2.298259
H	0.542319	-1.266338	2.234130
H	2.722262	-1.887603	1.161107
C	1.977957	-1.269531	-0.666561
C	1.059982	-0.526214	-1.613226
H	2.722832	-1.886428	-1.161806
H	1.677538	0.065692	-2.297320
H	0.543443	-1.264294	-2.235457
B	0.510081	1.515911	0.000551
C	0.072948	0.360438	0.888464
C	0.073035	0.360927	-0.888178
Si	-1.406526	-0.094611	-0.000125
F	-2.769588	0.736983	-0.000148
F	-1.881925	-1.622036	-0.000263
N	1.246103	2.688433	0.000612
H	1.535206	3.149931	-0.845814
H	1.535526	3.149769	0.847016

P_{A9}

E= -1083.89937

v= 22.21

C	0.322005	-1.222084	-1.641339
C	0.223543	-2.381295	-0.667353
H	-0.581433	-1.211994	-2.258750
H	1.165247	-1.404329	-2.313151
H	0.142059	-3.349115	-1.153522
C	0.223523	-2.381256	0.667303

C	0.321940	-1.222016	1.641237
H	0.142219	-3.349072	1.153514
H	-0.581418	-1.211977	2.258763
H	1.165275	-1.404205	2.312949
B	-0.611936	0.571072	-0.000139
C	0.468763	0.092398	-0.912820
C	0.468674	0.092446	0.912683
Si	1.863762	0.759960	-0.000004
F	2.229616	2.307589	-0.000192
F	3.267632	0.005348	0.000242
C	-2.196533	0.592524	-0.000014
F	-2.676615	1.849662	0.001339
F	-2.714762	-0.024008	-1.079548
F	-2.714364	-0.026193	1.078465

P_{A10}
E= -951.35831
v= 62.27

C	-0.094681	-1.156628	-1.636141
C	-0.146412	-2.321818	-0.666290
H	-1.053213	-1.108249	-2.162627
H	0.674255	-1.355562	-2.386575
H	-0.209116	-3.288981	-1.155540
C	-0.146249	-2.321801	0.666505
C	-0.094330	-1.156597	1.636311
H	-0.208749	-3.288964	1.155780
H	-1.052715	-1.108238	2.163072
H	0.674815	-1.355480	2.386541
B	-0.835351	0.740282	0.000120
C	0.173137	0.141520	-0.914175
C	0.173272	0.141561	0.914265
Si	1.629603	0.671208	-0.000088
F	2.152155	2.171075	-0.000200
F	2.940640	-0.230528	-0.000087
N	-2.331613	0.885798	0.000083
O	-2.805399	2.002871	0.000461
O	-2.965257	-0.154843	-0.000568

P_{A11}
E= -626.87690
v= 87.01

C	-1.244634	-0.131754	1.603192
C	-2.266329	0.476458	0.667236
H	-1.748426	-0.882086	2.223140
H	-0.903944	0.648856	2.292627
H	-3.097282	0.971071	1.164033
C	-2.266338	0.476326	-0.667306
C	-1.244634	-0.132005	-1.603178
H	-3.097362	0.970739	-1.164189
H	-1.748424	-0.882470	-2.222959
H	-0.903973	0.648482	-2.292766
B	-0.225225	-1.979092	0.000144
C	-0.085229	-0.753060	0.852435
C	-0.085222	-0.753196	-0.852337
Si	1.268153	0.141831	-0.000008
C	3.022852	-0.494865	0.000019
H	3.562910	-0.145832	0.883323
H	3.031054	-1.585525	0.000048
H	3.562915	-0.145879	-0.883300
C	1.163397	2.010867	-0.000125
H	1.650250	2.435175	0.881107
H	1.650335	2.435114	-0.881336
H	0.116494	2.324273	-0.000176
H	-0.665743	-3.074719	0.000238

P_{A12}
E= -666.19879
v= 29.05

C	1.036838	-0.569464	1.599815
C	1.806323	-1.479506	0.667186
H	1.758067	-0.025201	2.221398
H	0.461026	-1.195052	2.291225
H	2.429778	-2.217735	1.165337
C	1.806359	-1.479456	-0.667226
C	1.036930	-0.569329	-1.599821
H	2.429845	-2.217642	-1.165401
H	1.758206	-0.024986	-2.221280
H	0.461184	-1.194845	-2.291349
B	0.692432	1.510783	0.000065
C	0.143662	0.398061	-0.851421
C	0.143636	0.398013	0.851451
Si	-1.428093	-0.001602	-0.000030
C	-1.938020	-1.803369	-0.000018
H	-2.535551	-2.047981	-0.881452
H	-1.047731	-2.437050	-0.000059
H	-2.535462	-2.047972	0.881480
C	-2.882166	1.171054	-0.000014
H	-3.506209	1.015443	-0.883262
H	-3.505943	1.015737	0.883473
H	-2.536682	2.205827	-0.000237
C	1.698001	2.697224	0.000065
H	2.330071	2.712791	0.890692
H	2.330338	2.712503	-0.890382
H	1.130829	3.635296	-0.000193

P_{A13}
E= -784.10801
v= 22.03

C	-0.561783	-1.282706	1.601494
C	-0.649693	-2.469592	0.667463
H	0.288878	-1.434846	2.275845
H	-1.452779	-1.285376	2.240080
H	-0.733388	-3.432923	1.164625
C	-0.649815	-2.469576	-0.667432
C	-0.561900	-1.282678	-1.601464
H	-0.733754	-3.432881	-1.164602
H	0.288688	-1.434882	-2.275894
H	-1.452968	-1.285256	-2.239939
B	0.778057	0.342456	0.000023
C	-0.420129	0.027302	0.853820
C	-0.420114	0.027318	-0.853777
Si	-1.749310	0.954176	0.000046
C	-1.802023	2.820736	0.000043
H	-2.322116	3.197750	0.883722
H	-0.787302	3.222323	0.000187
H	-2.321864	3.197741	-0.883787
C	-3.442732	0.156724	-0.000035
H	-4.020389	0.445272	0.881285
H	-4.020258	0.445114	-0.881490
H	-3.334989	-0.930981	0.000075
C	2.340744	0.393814	0.000000
C	2.726908	1.887089	-0.000728
H	2.342621	2.400404	0.885449
H	3.818090	1.986659	-0.000977
H	2.342269	2.399611	-0.887205
C	2.913919	-0.275682	-1.256124
H	4.005367	-0.178378	-1.281728
H	2.672887	-1.342914	-1.277287
H	2.508947	0.180005	-2.163826
C	2.914033	-0.274483	1.256694
H	2.509048	0.181984	2.163997
H	2.673098	-1.341714	1.278824
H	4.005472	-0.177058	1.282168

$TS_{A5\text{-}endo}$
E= -746.74748
v= 380.13i

C	1.806569	0.167172	-1.480036

C	1.793685	-0.961404	-0.709686
H	1.694784	0.100653	-2.554604
H	2.214043	1.099262	-1.111255
H	1.568782	-1.906117	-1.194286
C	1.793774	-0.961251	0.709795
C	1.806774	0.167492	1.479901
H	1.568943	-1.905861	1.194633
H	1.695135	0.101230	2.554502
H	2.214163	1.099499	1.110806
B	0.173771	2.232296	-0.000117
C	-0.225856	1.059137	-0.795133
C	-0.225834	1.059233	0.795042
Si	-1.293390	-0.098896	0.000032
H	0.707610	3.280840	-0.000200
F	-2.875887	0.013988	0.000040
F	-1.004060	-1.661623	0.000099

$TS_{A6\text{-}endo}$

E= -786.07106

v= 380.56i

C	-1.267642	1.171051	-1.478607
C	-0.586692	2.072107	-0.709408
H	-1.137881	1.157338	-2.553087
H	-2.151746	0.666315	-1.110364
H	0.155848	2.697529	-1.194487
C	-0.586765	2.072045	0.709548
C	-1.267773	1.170849	1.478565
H	0.155722	2.697414	1.194775
H	-1.138216	1.157067	2.553070
H	-2.151865	0.666217	1.110140
B	-1.215092	-1.448952	-0.000054
C	-0.174588	-0.759998	-0.792781
C	-0.174619	-0.759990	0.792729
Si	1.374414	-0.478547	0.000009
F	2.080996	0.946249	-0.000009
F	2.578164	-1.514607	0.000037
C	-2.606844	-2.130958	-0.000046
H	-3.188345	-1.888185	0.891370
H	-2.464313	-3.216673	-0.000155
H	-3.188441	-1.888027	-0.891359

$TS_{A7\text{-}endo}$

E= -903.97890

v= 380.35i

C	-0.610596	-1.743511	-1.502603
C	-1.650027	-2.073328	-0.678812
H	-0.767377	-1.638181	-2.568625
H	0.417792	-1.870882	-1.194418
H	-2.645357	-2.128188	-1.107764
C	-1.569259	-2.090570	0.737561
C	-0.442735	-1.775639	1.445036
H	-2.508210	-2.159095	1.277683
H	-0.469366	-1.704455	2.524741
H	0.542953	-1.887817	1.009613
B	0.988235	0.411117	-0.000536
C	-0.257715	0.434404	0.795485
C	-0.263332	0.446410	-0.790901
Si	-1.679918	1.121603	0.011559
F	-2.044199	2.667253	0.027188
F	-3.090552	0.386157	0.012804
C	2.540620	0.239524	0.001105
C	3.073338	0.039307	1.425640
H	4.165177	-0.047124	1.417682
H	2.801348	0.879760	2.068529
H	2.667870	-0.869577	1.879275
C	2.958845	-0.946607	-0.883540
H	2.564557	-0.845758	-1.898251
H	4.051123	-0.995899	-0.945839
H	2.614618	-1.901599	-0.473309
C	3.134095	1.531481	-0.595165
H	2.784087	1.692518	-1.617681
H	2.864952	2.408872	-0.000917
H	4.226876	1.459887	-0.612632

$TS_{A8\text{-}endo}$

E= -802.15621

v= 384.60i

C	-1.399530	1.029442	-1.471229
C	-0.836242	2.013375	-0.709668
H	-1.273816	1.028704	-2.546421
H	-2.204890	0.412436	-1.093041
H	-0.185102	2.731271	-1.198072
C	-0.836248	2.013349	0.709723
C	-1.399525	1.029373	1.471243
H	-0.185132	2.731235	1.198174
H	-1.273829	1.028604	2.546438
H	-2.204880	0.412379	1.093026
B	-1.061773	-1.602284	-0.000021
C	-0.106078	-0.782335	-0.784717
C	-0.106085	-0.782339	0.784698
Si	1.406670	-0.354890	-0.000003
F	1.948015	1.141390	-0.000035
F	2.729125	-1.237172	0.000025
N	-2.244659	-2.327734	-0.000020
H	-2.668136	-2.666879	0.847525
H	-2.668136	-2.666891	-0.847561

$TS_{A9\text{-}endo}$

E= -1083.79281

v= 359.68i

C	0.287724	1.730554	-1.489769
C	1.321339	2.153195	-0.705153
H	0.408945	1.654904	-2.562924
H	-0.736106	1.723878	-1.138673
H	2.284468	2.319437	-1.177359
C	1.305175	2.154750	0.716416
C	0.254675	1.733220	1.478747
H	2.257189	2.322152	1.210259
H	0.349658	1.660831	2.554702
H	-0.760819	1.725056	1.103274
B	-0.915610	-0.590731	-0.001203
C	0.299843	-0.516794	-0.803293
C	0.297774	-0.515181	0.802761
Si	1.787333	-1.033911	0.001992
F	3.098040	-0.142439	0.003567
F	2.303031	-2.530447	0.004903
C	-2.485775	-0.376266	-0.000304
F	-3.152275	-1.532105	-0.138723
F	-2.919361	0.200120	1.135772
F	-2.877488	0.431681	-1.006363

$TS_{A10\text{-}endo}$

E= -951.25234

v= 335.82i

C	0.140867	-1.729661	-1.479549
C	-0.885817	-2.193479	-0.712231
H	0.034747	-1.666052	-2.555260
H	1.152121	-1.653378	-1.097384
H	-1.829953	-2.417744	-1.198601
C	-0.885799	-2.193560	0.712171
C	0.140905	-1.729840	1.479510
H	-1.829920	-2.417888	1.198540
H	0.034813	-1.666320	2.555229
H	1.152137	-1.653454	1.097312
B	1.175027	0.706105	0.000017
C	-0.022257	0.543884	0.801578
C	-0.022265	0.543854	-0.801547
Si	-1.535788	0.987569	0.000019

F	-2.122232	2.456229	0.000010
F	-2.794992	0.028683	0.000018
N	2.675337	0.583184	0.000003
O	3.349036	1.587674	0.000031
O	3.106690	-0.559591	-0.000037

$TS_{A11\text{-}endo}$

E= -626.77323

v= 390.23i

C	1.860156	0.237801	-1.481545
C	1.944592	-0.889284	-0.708232
H	1.751100	0.156894	-2.555571
H	2.227954	1.190143	-1.125993
H	1.812300	-1.850645	-1.195685
C	1.944586	-0.889404	0.708088
C	1.860140	0.237548	1.481592
H	1.812290	-1.850849	1.195375
H	1.751071	0.156457	2.555603
H	2.227922	1.189957	1.126204
B	0.230690	2.223721	0.000114
C	-0.173720	1.042819	0.771496
C	-0.173703	1.042890	-0.771389
Si	-1.322026	-0.131750	-0.000011
C	-3.141073	0.275437	-0.000031
H	-3.627629	-0.146356	0.882928
H	-3.292756	1.354604	-0.000129
H	-3.627650	-0.146524	-0.882898
C	-1.036942	-1.977597	-0.000032
H	-0.482664	-2.294978	0.883092
H	-2.005313	-2.482298	-0.000099
H	-0.482551	-2.294942	-0.883091
H	0.786629	3.263160	0.000163

$TS_{A12\text{-}endo}$

E= -666.09569

v= 385.61i

C	-1.500296	-0.930267	1.481152
C	-1.047129	-1.965124	0.707856
H	-1.364498	-0.950268	2.554905
H	-2.273839	-0.262178	1.127195
H	-0.479711	-2.752614	1.194634
C	-1.050892	-1.964455	-0.708976
C	-1.507565	-0.928843	-1.479045
H	-0.486588	-2.751793	-1.199611
H	-1.377010	-0.947855	-2.553467
H	-2.278402	-0.259997	-1.120585
B	-1.022870	1.587190	-0.000298
C	-0.091213	0.745046	0.768703
C	-0.091636	0.745285	-0.769602
Si	1.475573	0.256641	-0.000923
C	2.097903	-1.505357	0.000291
H	3.189931	-1.489163	-0.008674
H	1.770324	-2.044943	0.888716
H	1.755658	-2.052741	-0.877613
C	2.890586	1.472026	-0.001594
H	3.519708	1.329420	0.880595
H	3.517823	1.330568	-0.885308
H	2.515793	2.495450	-0.000568
C	-2.312504	2.453969	0.001585
H	-2.029410	3.511190	0.030421
H	-2.912846	2.311186	-0.899432
H	-2.934127	2.271117	0.880975

$TS_{A13\text{-}endo}$

E= -784.00336

v= 390.02i

C	-0.499004	-1.765796	-1.509476
C	-1.488430	-2.226051	-0.680859
H	-0.684372	-1.654172	-2.570365
H	0.542247	-1.834824	-1.230142
H	-2.475584	-2.385444	-1.104551
C	-1.387371	-2.268717	0.731498
C	-0.293016	-1.847575	1.436681
H	-2.300797	-2.468733	1.283815
H	-0.317429	-1.801223	2.517864
H	0.695393	-1.869195	0.996747
B	0.978863	0.391675	0.003448
C	-0.284945	0.380248	-0.759264
C	-0.271749	0.377699	0.778323
Si	-1.757035	1.093002	0.024724
C	-3.420464	0.243048	0.011665
H	-3.609757	-0.227634	-0.954133
H	-3.504910	-0.517982	0.785748
H	-4.194192	0.995418	0.180606
C	-1.952506	2.948346	0.035746
H	-2.544380	3.276362	-0.822674
H	-2.467964	3.276301	0.941928
H	-0.977954	3.434902	-0.006533
C	2.541503	0.287982	-0.002628
C	3.064079	1.631866	-0.548350
H	2.749195	2.469424	0.080496
H	4.159412	1.621910	-0.570367
H	2.701406	1.813494	-1.563151
C	3.025359	-0.836815	-0.930973
H	4.118765	-0.821701	-0.998761
H	2.737026	-1.824505	-0.556940
H	2.620360	-0.720881	-1.939979
C	3.092195	0.066921	1.412196
H	2.771970	0.865103	2.086088
H	2.744161	-0.880286	1.834056
H	4.187665	0.046322	1.399523

$TS_{A5\text{-}exo}$

E= -746.74404

v= 407.26i

C	-1.449797	-0.603182	-1.473633
C	-2.504337	-0.182481	-0.707806
H	-1.471212	-0.477495	-2.548295
H	-0.746826	-1.338697	-1.102526
H	-3.308147	0.356318	-1.200143
C	-2.504361	-0.181992	0.707876
C	-1.449841	-0.602182	1.474015
H	-3.308149	0.357213	1.199809
H	-1.471263	-0.475708	2.548589
H	-0.746931	-1.338047	1.103482
B	-0.469707	1.969149	-0.000553
C	0.169961	0.901969	-0.794645
C	0.169919	0.902381	0.794123
Si	1.454653	-0.002579	-0.000002
H	-1.219086	2.874253	-0.000785
F	1.408891	-1.596857	0.000387
F	2.998414	0.355239	-0.000045

$TS_{A6\text{-}exo}$

E= -786.06913

v= 407.13i

C	-1.024161	-1.199978	-1.469685
C	-2.156839	-1.064428	-0.711560
H	-1.070229	-1.088138	-2.545199
H	-0.158728	-1.730131	-1.091984
H	-3.071367	-0.755480	-1.208861
C	-2.162623	-1.062100	0.704983
C	-1.036886	-1.199565	1.472728
H	-3.080222	-0.748617	1.193773
H	-1.090814	-1.084056	2.547483
H	-0.168457	-1.730507	1.102850
B	-0.767388	1.505018	0.006890
C	0.158769	0.664930	-0.789261

C	0.160788	0.663070	0.795925
Si	1.637193	0.130829	0.000757
F	3.036742	0.877535	0.000292
F	2.007054	-1.421568	-0.000820
C	-2.058948	2.352423	-0.001347
H	-1.800651	3.402944	-0.171751
H	-2.601007	2.293438	0.943221
H	-2.717065	2.054020	-0.820523

$TS_{A7\text{-}exo}$

E= -903.97660

v= 402.23i

C	-0.764607	1.831631	-1.442761
C	0.253140	2.409815	-0.732366
H	-0.714711	1.782569	-2.522936
H	-1.753406	1.724607	-1.015324
H	1.134492	2.730199	-1.278712
C	0.339209	2.397637	0.681319
C	-0.595030	1.820888	1.499387
H	1.284702	2.704656	1.119696
H	-0.421101	1.749673	2.565239
H	-1.626018	1.719148	1.184072
B	0.740114	-0.550073	-0.005136
C	-0.496732	-0.394171	0.793805
C	-0.509163	-0.364463	-0.788916
Si	-2.008093	-0.829478	0.008892
F	-3.234485	0.191819	0.043367
F	-2.686727	-2.263560	-0.013397
C	2.290509	-0.690022	-0.003171
C	2.958607	0.233454	-1.031534
H	4.020858	-0.018224	-1.122166
H	2.496290	0.133114	-2.017077
H	2.891689	1.280500	-0.726962
C	2.874974	-0.437945	1.391963
H	2.437008	-1.114238	2.129916
H	3.959357	-0.592509	1.385028
H	2.680737	0.585897	1.722293
C	2.552898	-2.157517	-0.410538
H	2.090953	-2.859994	0.288712
H	2.168197	-2.367003	-1.411760
H	3.631766	-2.345512	-0.411680

$TS_{A8\text{-}exo}$

E= -802.15531

v= 393.46i

C	-1.083781	-1.193679	-1.469325
C	-2.203150	-1.003356	-0.709410
H	-1.125473	-1.077158	-2.544637
H	-0.232618	-1.745746	-1.091172
H	-3.102696	-0.645810	-1.200935
C	-2.203149	-1.003357	0.709411
C	-1.083779	-1.193680	1.469324
H	-3.102695	-0.645813	1.200937
H	-1.125471	-1.077162	2.544636
H	-0.232617	-1.745747	1.091169
B	-0.735026	1.560707	0.000000
C	0.154585	0.664669	-0.784908
C	0.154585	0.664668	0.784908
Si	1.618638	0.100197	0.000000
F	3.049972	0.789242	0.000000
F	1.941331	-1.464796	-0.000001
N	-1.838872	2.392262	0.000001
H	-2.262861	2.726853	0.848873
H	-2.262861	2.726855	-0.848872

$TS_{A9\text{-}exo}$

E= -1083.78994

v= 388.37i

C	-0.413499	1.796680	-1.468384
C	0.658431	2.187976	-0.714144
H	-0.326102	1.721655	-2.544585
H	-1.423688	1.849415	-1.080595
H	1.611229	2.326232	-1.214343
C	0.675133	2.182125	0.704591
C	-0.380867	1.791119	1.481087
H	1.639710	2.315252	1.184337
H	-0.269667	1.707953	2.554433
H	-1.399331	1.847852	1.115868
B	0.614145	-0.727093	0.001189
C	-0.572505	-0.433673	-0.799559
C	-0.571749	-0.438599	0.802571
Si	-2.126549	-0.675698	0.001669
F	-2.972659	-2.011377	-0.000784
F	-3.195268	0.502890	0.006002
C	2.196213	-0.807452	-0.000537
F	2.602824	-2.085186	-0.112630
F	2.744034	-0.128574	-1.024121
F	2.745722	-0.315772	1.122847

$TS_{A10\text{-}exo}$

E= -951.24724

v= 363.65i

C	-0.009866	1.779505	-1.474633
C	1.077848	2.089048	-0.710453
H	0.080586	1.696549	-2.550113
H	-1.017985	1.889554	-1.093374
H	2.045785	2.155522	-1.195382
C	1.077979	2.089074	0.710218
C	-0.009580	1.779529	1.474617
H	2.046005	2.155592	1.194962
H	0.081084	1.696619	2.550084
H	-1.017780	1.889484	1.093554
B	0.826328	-0.899405	-0.000008
C	-0.304009	-0.456616	0.802127
C	-0.304039	-0.456579	-0.802078
Si	-1.872064	-0.582131	0.000046
F	-2.846414	0.673827	0.000124
F	-2.811725	-1.851585	-0.000044
N	2.299816	-1.194529	-0.000002
O	3.056418	-0.241843	0.000163
O	2.632844	-2.360494	-0.000141

$TS_{A11\text{-}exo}$

E= -626.76860

v= 427.48i

C	1.561940	0.550037	-1.472981
C	2.622548	0.136906	-0.706591
H	1.579763	0.419275	-2.547054
H	0.875111	1.301860	-1.109545
H	3.422555	-0.408334	-1.198237
C	2.622414	0.137240	0.706749
C	1.561650	0.550711	1.472746
H	3.422327	-0.407771	1.198802
H	1.579290	0.420455	2.546884
H	0.874889	1.302382	1.108853
B	0.553815	-1.922531	0.000291
C	-0.098183	-0.852513	0.769294
C	-0.098191	-0.852792	-0.769085
Si	-1.480857	0.029202	-0.000050
C	-1.580527	1.894544	-0.000284
H	-2.139206	2.222563	0.880257
H	-0.621912	2.410962	-0.001238
H	-2.140765	2.222213	-0.879964
C	-3.189348	-0.711105	0.000095
H	-3.748901	-0.392873	0.883029
H	-3.748943	-0.393136	-0.882906
H	-3.129182	-1.799454	0.000258
H	1.324085	-2.812482	0.000442

$TS_{A12\text{-}exo}$

E= -666.09275

v= 421.19i

C	1.211849	-1.117222	1.481496
C	2.324437	-0.963490	0.693872
H	1.275792	-0.979186	2.552999
H	0.365659	-1.696987	1.139761
H	3.237988	-0.610826	1.163391
C	2.296955	-0.983292	-0.720199
C	1.152351	-1.150108	-1.459128
H	3.192635	-0.648585	-1.235020
H	1.177599	-1.045604	-2.536024
H	0.321638	-1.722952	-1.070367
B	0.776338	1.478398	-0.001357
C	-0.129483	0.609059	0.771525
C	-0.128405	0.595967	-0.764355
Si	-1.677907	0.065343	0.007722
C	-3.179575	1.169906	-0.003921
H	-3.782073	1.010478	0.893658
H	-2.880102	2.217446	-0.040177
H	-3.808756	0.955949	-0.871425
C	-2.194791	-1.730721	0.009716
H	-2.896425	-1.901462	0.830122
H	-2.723443	-1.954890	-0.920494
H	-1.379301	-2.445335	0.112258
C	2.050667	2.358139	-0.015262
H	2.701122	2.095584	-0.852875
H	1.769479	3.408152	-0.146602
H	2.613161	2.282002	0.917015

$TS_{A13\text{-}exo}$

E= -783.99993

v= 418.49i

C	-0.323507	1.885980	-1.507485
C	0.614089	2.414475	-0.657763
H	-0.116849	1.795896	-2.566100
H	-1.369267	1.862226	-1.234801
H	1.590327	2.662282	-1.065153
C	0.484735	2.431685	0.750383
C	-0.583302	1.899159	1.427724
H	1.367461	2.695652	1.324324
H	-0.569027	1.843869	2.508596
H	-1.565571	1.875842	0.977036
B	0.718196	-0.537825	0.010281
C	-0.508474	-0.305017	-0.772838
C	-0.527731	-0.259389	0.759719
Si	-2.100284	-0.713509	-0.019924
C	-2.709954	-2.474118	0.022797
H	-3.248915	-2.717427	-0.896096
H	-1.871645	-3.163492	0.125773
H	-3.393604	-2.627721	0.861244
C	-3.544738	0.473953	-0.056507
H	-4.294514	0.094363	-0.755262
H	-4.012059	0.517065	0.930840
H	-3.295271	1.491405	-0.355357
C	2.258664	-0.789603	0.008874
C	2.412030	-2.280555	0.382209
H	1.896704	-2.929056	-0.332238
H	3.473374	-2.552416	0.377978
H	2.011434	-2.482618	1.379035
C	2.995847	0.056251	1.055609
H	4.035654	-0.278586	1.142586
H	3.009439	1.111379	0.773682
H	2.523666	-0.027692	2.038116
C	2.863499	-0.554414	-1.380558
H	2.372895	-1.178081	-2.131741
H	2.748671	0.487875	-1.688923
H	3.933153	-0.792955	-1.378986

C-1

E= -1199.64585

v= 141.85i

B	0.000000	0.000000	0.000000
B	0.000000	1.698513	0.000000
C	-0.729053	2.978219	0.000000
C	0.729053	2.978219	0.000000
Si	0.000000	4.627440	0.000000
H	0.000000	5.421334	1.234829
H	0.000000	5.421334	-1.234829
B	1.470955	-0.849256	0.000000
C	2.214687	-2.120487	0.000000
C	2.943739	-0.857731	0.000000
Si	4.007480	-2.313720	0.000000
H	4.695013	-2.710667	-1.234829
H	4.695013	-2.710667	1.234829
B	-1.470955	-0.849256	0.000000
C	-2.214687	-2.120487	0.000000
C	-2.943739	-0.857731	0.000000
Si	-4.007480	-2.313720	0.000000
H	-4.695013	-2.710667	1.234829
H	-4.695013	-2.710667	-1.234829

C-2

E= -1199.68543

v= 24.41

B	0.000000	0.000000	0.000000
B	0.000000	1.640638	0.000000
C	0.000000	2.931368	0.718011
C	0.000000	2.931368	-0.718011
Si	0.000000	4.580833	0.000000
H	1.232803	5.377937	0.000000
H	-1.232803	5.377937	0.000000
B	1.420834	-0.820319	0.000000
C	2.538639	-1.465684	0.718011
C	2.538639	-1.465684	-0.718011
Si	3.967118	-2.290417	0.000000
H	4.041028	-3.756607	0.000000
H	5.273831	-1.621330	0.000000
B	-1.420834	-0.820319	0.000000
C	-2.538639	-1.465684	0.718011
C	-2.538639	-1.465684	-0.718011
Si	-3.967118	-2.290417	0.000000
H	-5.273831	-1.621330	0.000000
H	-4.041028	-3.756607	0.000000

D1

E= -7191.08093

v= 4.11

B	4.465837	9.574274	0.000000
B	4.861437	11.166263	0.000000
C	5.170818	12.418118	0.718233
C	5.170818	12.418118	-0.718233
Si	5.569226	14.019275	0.000000
H	6.958125	14.494660	0.000000
H	4.563994	15.089233	0.000000
B	5.645619	8.434004	0.000000
C	6.571371	7.530811	0.715597
C	6.571371	7.530811	-0.715597
Si	7.760494	6.375120	0.000000
H	9.195823	6.700279	0.000000
B	2.888271	9.122718	0.000000
C	1.643076	8.773001	0.715628
C	1.643076	8.773001	-0.715628
Si	0.046516	8.324749	0.000000
H	-0.391671	6.919778	0.000000
Si	7.232702	4.122090	0.000000
C	8.419180	2.963555	0.715628

C	8.419180	2.963555	-0.715628
H	5.796868	3.799086	0.000000
B	9.344641	2.060043	0.000000
B	10.524483	0.919608	0.000000
B	10.126872	-0.672247	0.000000
B	12.100986	1.373004	0.000000
C	9.807560	-1.925569	0.715597
C	9.807560	-1.925569	-0.715597
C	13.339815	1.730999	0.718233
C	13.339815	1.730999	-0.718233
Si	9.401263	-3.533225	0.000000
Si	14.925661	2.186546	0.000000
H	10.400524	-4.613677	0.000000
H	16.031806	1.221417	0.000000
H	15.349656	3.592082	0.000000
Si	7.186186	-4.202659	0.000000
C	6.776104	-5.809446	0.715628
C	6.776104	-5.809446	-0.715628
H	6.188539	-3.120692	0.000000
B	6.456370	-7.062675	0.000000
B	6.058646	-8.654666	0.000000
B	4.481252	-9.106252	0.000000
B	7.239549	-9.793259	0.000000
C	3.236188	-9.456380	0.715597
C	3.236188	-9.456380	-0.715597
C	8.168997	-10.687119	0.718233
C	8.168997	-10.687119	-0.718233
Si	1.640768	-9.908345	0.000000
Si	9.356435	-11.832729	0.000000
H	1.204701	-11.313956	0.000000
H	9.073681	-13.273243	0.000000
H	10.785662	-11.497151	0.000000
Si	-0.046516	-8.324749	0.000000
C	-1.643076	-8.773001	0.715628
C	-1.643076	-8.773001	-0.715628
H	0.391671	-6.919778	0.000000
B	-2.888271	-9.122718	0.000000
B	-4.465837	-9.574274	0.000000
B	-5.645619	-8.434004	0.000000
B	-4.861437	-11.166263	0.000000
C	-6.571371	-7.530811	0.715597
C	-6.571371	-7.530811	-0.715597
C	-5.170818	-12.418118	0.718233
C	-5.170818	-12.418118	-0.718233
Si	-7.760494	-6.375120	0.000000
Si	-5.569226	-14.019275	0.000000
H	-9.195823	-6.700279	0.000000
H	-6.958125	-14.494660	0.000000
H	-4.563994	-15.089233	0.000000
Si	-7.232702	-4.122090	0.000000
C	-8.419180	-2.963555	0.715628
C	-8.419180	-2.963555	-0.715628
H	-5.796868	-3.799086	0.000000
B	-9.344641	-2.060043	0.000000
B	-10.524483	-0.919608	0.000000
B	-10.126872	0.672247	0.000000
B	-12.100986	-1.373004	0.000000
C	-9.807560	1.925569	0.715597
C	-9.807560	1.925569	-0.715597
C	-13.339815	-1.730999	0.718233
C	-13.339815	-1.730999	-0.718233
Si	-9.401263	3.533225	0.000000
Si	-14.925661	-2.186546	0.000000
H	-10.400524	4.613677	0.000000
H	-16.031806	-1.221417	0.000000
H	-15.349656	-3.592082	0.000000
Si	-7.186186	4.202659	0.000000
C	-6.776104	5.809446	0.715628
C	-6.776104	5.809446	-0.715628
H	-6.188539	3.120692	0.000000
B	-6.456370	7.062675	0.000000
B	-6.058646	8.654666	0.000000
B	-4.481252	9.106252	0.000000
B	-7.239549	9.793259	0.000000
C	-3.236188	9.456380	0.715597
C	-3.236188	9.456380	-0.715597
C	-8.168997	10.687119	0.718233
C	-8.168997	10.687119	-0.718233
Si	-1.640768	9.908345	0.000000
Si	-9.356435	11.832729	0.000000
H	-1.204701	11.313956	0.000000
H	-9.073681	13.273243	0.000000
H	-10.785662	11.497151	0.000000

D2

E= -11983.96254

v= 2.10

B	10.566045	9.150068	0.000000
B	12.176413	9.462898	0.000000
C	13.441945	9.709998	0.718231
C	13.441945	9.709998	-0.718231
Si	15.061850	10.023806	0.000000
H	16.078265	8.964674	0.000000
H	15.608005	11.386535	0.000000
B	10.030679	7.599072	0.000000
C	9.603282	6.378205	0.715582
C	9.603282	6.378205	-0.715582
Si	9.059773	4.811955	0.000000
H	9.960407	3.648013	0.000000
B	9.490563	10.389375	0.000000
C	8.647159	11.369819	0.715633
C	8.647159	11.369819	-0.715633
Si	7.565060	12.626574	0.000000
H	6.106845	12.427404	0.000000
Si	6.794951	4.337258	0.000000
C	6.246718	2.771642	0.715678
C	6.246718	2.771642	-0.715678
H	5.892099	5.499526	0.000000
B	5.819115	1.551718	0.000000
B	5.282428	0.001200	0.000000
B	3.671373	-0.310218	0.000000
B	6.357095	-1.238759	0.000000
C	2.401072	-0.551106	0.715641
C	2.401072	-0.551106	-0.715641
C	7.200123	-2.218821	0.715674
C	7.200123	-2.218821	-0.715674
Si	0.772062	-0.861806	0.000000
Si	8.282725	-3.475535	0.000000
H	0.216372	-2.224513	0.000000
H	9.740634	-3.274814	0.000000
Si	-0.772062	0.861806	0.000000
C	-2.401072	0.551106	0.715641
C	-2.401072	0.551106	-0.715641
H	-0.216372	2.224513	0.000000
B	-3.671373	0.310218	0.000000
B	-5.282428	-0.001200	0.000000
B	-6.357095	1.238759	0.000000
B	-5.819115	-1.551718	0.000000
C	-7.200123	2.218821	0.715674
C	-7.200123	2.218821	-0.715674
C	-6.246718	-2.771642	0.715678
C	-6.246718	-2.771642	-0.715678
Si	-8.282725	3.475535	0.000000
Si	-6.794951	-4.337258	0.000000
H	-9.740634	3.274814	0.000000
H	-5.892099	-5.499526	0.000000
Si	-7.561685	5.674400	0.000000
C	-8.645602	6.928998	0.715601

C	-8.645602	6.928998	-0.715601
H	-6.103389	5.872393	0.000000
B	-9.489952	7.908995	0.000000
B	-10.565965	9.147854	0.000000
B	-10.030259	10.698738	0.000000
B	-12.176404	8.835491	0.000000
C	-9.602504	11.919189	0.715613
C	-9.602504	11.919189	-0.715613
C	-13.442083	8.589150	0.718231
C	-13.442083	8.589150	-0.718231
Si	-9.057474	13.485346	0.000000
Si	-15.062351	8.277154	0.000000
H	-9.959450	14.648299	0.000000
H	-16.077690	9.337294	0.000000
H	-15.609816	6.914938	0.000000
Si	-6.792825	13.960444	0.000000
C	-6.245755	15.525888	0.715617
C	-6.245755	15.525888	-0.715617
H	-5.891530	12.796868	0.000000
B	-5.818476	16.746690	0.000000
B	-5.283245	18.297797	0.000000
B	-3.672310	18.609733	0.000000
B	-6.359551	19.535794	0.000000
C	-2.401447	18.849768	0.715593
C	-2.401447	18.849768	-0.715593
C	-7.206848	20.507821	0.718238
C	-7.206848	20.507821	-0.718238
Si	-0.772784	19.161167	0.000000
Si	-8.289438	21.753028	0.000000
H	-0.216686	20.523800	0.000000
H	-7.881565	23.163203	0.000000
H	-9.742542	21.543863	0.000000
Si	0.771647	17.438048	0.000000
C	2.400913	17.747061	0.715612
C	2.400913	17.747061	-0.715612
H	0.215198	16.075487	0.000000
B	3.671729	17.987542	0.000000
B	5.282673	18.299864	0.000000
B	6.358171	17.060655	0.000000
B	5.816371	19.851005	0.000000
C	7.201484	16.080032	0.715601
C	7.201484	16.080032	-0.715601
C	6.234260	21.070904	0.718236
C	6.234260	21.070904	-0.718236
Si	8.285735	14.825491	0.000000
Si	6.771060	22.631160	0.000000
H	9.743881	15.024672	0.000000
H	8.196189	22.983265	0.000000
H	5.863013	23.784789	0.000000
B	10.565965	-9.147854	0.000000
B	12.176404	-8.835491	0.000000
C	13.442083	-8.589150	0.718231
C	13.442083	-8.589150	-0.718231
Si	15.062351	-8.277154	0.000000
H	16.077690	-9.337294	0.000000
H	15.609816	-6.914938	0.000000
B	10.030259	-10.698738	0.000000
C	9.602504	-11.919189	0.715613
C	9.602504	-11.919189	-0.715613
Si	9.057474	-13.485346	0.000000
H	9.959450	-14.648299	0.000000
B	9.489952	-7.908995	0.000000
C	8.645602	-6.928998	0.715601
C	8.645602	-6.928998	-0.715601
Si	7.561685	-5.674400	0.000000
H	6.103389	-5.872393	0.000000
Si	6.792825	-13.960444	0.000000
C	6.245755	-15.525888	0.715617
C	6.245755	-15.525888	-0.715617
H	5.891530	-12.796868	0.000000
B	5.818476	-16.746690	0.000000
B	5.283245	-18.297797	0.000000
B	3.672310	-18.609733	0.000000
B	6.359551	-19.535794	0.000000
C	2.401447	-18.849768	0.715593
C	2.401447	-18.849768	-0.715593
C	7.206848	-20.507821	0.718238
C	7.206848	-20.507821	-0.718238
Si	0.772784	-19.161167	0.000000
Si	8.289438	-21.753028	0.000000
H	0.216686	-20.523800	0.000000
H	7.881565	-23.163203	0.000000
H	9.742542	-21.543863	0.000000
Si	-0.771647	-17.438048	0.000000
C	-2.400913	-17.747061	0.715612
C	-2.400913	-17.747061	-0.715612
H	-0.215198	-16.075487	0.000000
B	-3.671729	-17.987542	0.000000
B	-5.282673	-18.299864	0.000000
B	-6.358171	-17.060655	0.000000
B	-5.816371	-19.851005	0.000000
C	-7.201484	-16.080032	0.715601
C	-7.201484	-16.080032	-0.715601
C	-6.234260	-21.070904	0.718236
C	-6.234260	-21.070904	-0.718236
Si	-8.285735	-14.825491	0.000000
Si	-6.771060	-22.631160	0.000000
H	-9.743881	-15.024672	0.000000
H	-8.196189	-22.983265	0.000000
H	-5.863013	-23.784789	0.000000
Si	-7.565060	-12.626574	0.000000
C	-8.647159	-11.369819	0.715633
C	-8.647159	-11.369819	-0.715633
H	-6.106845	-12.427404	0.000000
B	-9.490563	-10.389375	0.000000
B	-10.566045	-9.150068	0.000000
B	-10.030679	-7.599072	0.000000
B	-12.176413	-9.462898	0.000000
C	-9.603282	-6.378205	0.715582
C	-9.603282	-6.378205	-0.715582
C	-13.441945	-9.709998	0.718231
C	-13.441945	-9.709998	-0.718231
Si	-9.059773	-4.811955	0.000000
Si	-15.061850	-10.023806	0.000000
H	-9.960407	-3.648013	0.000000
H	-16.078265	-8.964674	0.000000
H	-15.608005	-11.386535	0.000000

D3

E= -15578.33056

v= 1.69

B	-6.373423	8.423922	0.000000
B	-6.037823	10.030014	0.000000
C	-5.769112	11.294518	0.715677
C	-5.769112	11.294518	-0.715677
Si	-5.425518	12.917272	0.000000
H	-6.468832	13.955170	0.000000
B	-5.151481	7.328934	0.000000
C	-4.192594	6.461523	0.715641
C	-4.192594	6.461523	-0.715641
Si	-2.962019	5.349881	0.000000
H	-1.539763	5.727736	0.000000
B	-7.932450	7.912102	0.000000
C	-9.161953	7.512979	0.715677
C	-9.161953	7.512979	-0.715677
Si	-10.739257	6.999410	0.000000
H	-11.115711	5.576751	0.000000
Si	-3.406947	3.079055	0.000000
C	-2.177353	1.966045	0.715665

C	-2.177353	1.966045	-0.715665
H	-4.829224	2.701275	0.000000
B	-1.219707	1.097543	0.000000
B	0.000000	0.000000	0.000000
B	-0.340646	-1.605068	0.000000
B	1.560353	0.507526	0.000000
C	-0.613969	-2.868666	0.715665
C	-0.613969	-2.868666	-0.715665
C	2.791322	0.902621	0.715665
C	2.791322	0.902621	-0.715665
Si	-0.963067	-4.490030	0.000000
Si	4.370013	1.410975	0.000000
H	0.075239	-5.532868	0.000000
H	4.753985	2.831593	0.000000
Si	-3.152123	-5.240124	0.000000
C	-3.499546	-6.861654	0.715641
C	-3.499546	-6.861654	-0.715641
H	-4.190484	-4.197342	0.000000
B	-3.771303	-8.125780	0.000000
B	-4.108619	-9.731507	0.000000
B	-5.667336	-10.243915	0.000000
B	-2.885856	-10.825754	0.000000
C	-6.896783	-10.643456	0.715677
C	-6.896783	-10.643456	-0.715677
C	-1.925454	-11.690974	0.715677
C	-1.925454	-11.690974	-0.715677
Si	-8.473927	-11.157273	0.000000
Si	-0.692038	-12.800174	0.000000
H	-8.851116	-12.579758	0.000000
H	0.728248	-12.414864	0.000000
Si	-10.224636	-9.644094	0.000000
C	-11.800100	-10.160415	0.715592
C	-11.800100	-10.160415	-0.715592
H	-9.844948	-8.222302	0.000000
B	-13.030001	-10.561309	0.000000
B	-14.588363	-11.075355	0.000000
B	-15.811071	-9.981214	0.000000
B	-14.922764	-12.681275	0.000000
C	-16.770144	-9.113647	0.715608
C	-16.770144	-9.113647	-0.715608
C	-15.184925	-13.943760	0.718240
C	-15.184925	-13.943760	-0.718240
Si	-18.001965	-8.003448	0.000000
Si	-15.523929	-15.558625	0.000000
H	-19.423905	-8.382754	0.000000
H	-16.894314	-16.084891	0.000000
H	-14.479667	-16.590469	0.000000
Si	-17.558874	-5.732474	0.000000
C	-18.787605	-4.618887	0.715618
C	-18.787605	-4.618887	-0.715618
H	-16.136166	-5.355642	0.000000
B	-19.745397	-3.749657	0.000000
B	-20.964903	-2.651937	0.000000
B	-20.623677	-1.046988	0.000000
B	-22.525190	-3.158527	0.000000
C	-20.349098	0.216886	0.715609
C	-20.349098	0.216886	-0.715609
C	-23.751470	-3.557218	0.718229
C	-23.751470	-3.557218	-0.718229
Si	-20.000906	1.838055	0.000000
Si	-25.321521	-4.064580	0.000000
H	-21.038365	2.881858	0.000000
H	-26.458434	-3.135861	0.000000
H	-25.699457	-5.483105	0.000000
Si	-17.812014	2.588606	0.000000
C	-17.462305	4.209726	0.715632
C	-17.462305	4.209726	-0.715632
H	-16.773694	1.545570	0.000000
B	-17.190173	5.474073	0.000000
B	-16.853833	7.080084	0.000000
B	-15.295383	7.593499	0.000000
B	-18.077907	8.172122	0.000000
C	-14.065290	7.993594	0.715576
C	-14.065290	7.993594	-0.715576
C	-19.041219	9.029240	0.718242
C	-19.041219	9.029240	-0.718242
Si	-12.490577	8.511862	0.000000
Si	-20.272656	10.127533	0.000000
H	-12.111444	9.933757	0.000000
H	-20.046213	11.577991	0.000000
H	-21.687563	9.736143	0.000000
B	10.482042	1.307585	0.000000
B	10.818306	2.913652	0.000000
C	11.087407	4.177995	0.715677
C	11.087407	4.177995	-0.715677
Si	11.431295	5.800765	0.000000
H	10.387464	6.838113	0.000000
B	11.705158	0.213901	0.000000
C	12.665895	-0.651062	0.715677
C	12.665895	-0.651062	-0.715677
Si	13.899445	-1.760000	0.000000
H	15.319948	-1.375412	0.000000
B	8.922783	0.796846	0.000000
C	7.692139	0.400131	0.715641
C	7.692139	0.400131	-0.715641
Si	6.114142	-0.109757	0.000000
H	5.730246	-1.530395	0.000000
Si	13.464349	-4.032748	0.000000
C	14.699227	-5.138979	0.715592
C	14.699227	-5.138979	-0.715592
H	12.043196	-4.414824	0.000000
B	15.661362	-6.003657	0.000000
B	16.885720	-7.096215	0.000000
B	16.549521	-8.702182	0.000000
B	18.443688	-6.582856	0.000000
C	16.277722	-9.966548	0.715608
C	16.277722	-9.966548	-0.715608
C	19.668113	-6.178651	0.718240
C	19.668113	-6.178651	-0.718240
Si	15.932172	-11.588435	0.000000
Si	21.236129	-5.664805	0.000000
H	16.971630	-12.630218	0.000000
H	22.377081	-6.588460	0.000000
H	21.607601	-4.244525	0.000000
Si	13.743905	-12.340194	0.000000
C	13.393876	-13.961100	0.715618
C	13.393876	-13.961100	-0.715618
H	12.706205	-11.296508	0.000000
B	13.119997	-15.225187	0.000000
B	12.779097	-16.830170	0.000000
B	11.218557	-17.337134	0.000000
B	13.997960	-17.928124	0.000000
C	9.986720	-17.731279	0.715609
C	9.986720	-17.731279	-0.715609
C	14.956376	-18.790768	0.718229
C	14.956376	-18.790768	-0.718229
Si	8.408651	-18.240320	0.000000
Si	16.180790	-19.896791	0.000000
H	8.023420	-19.660688	0.000000
H	15.944952	-21.345746	0.000000
H	17.598237	-19.514830	0.000000
Si	6.664208	-16.719960	0.000000
C	5.085423	-17.227663	0.715632
C	5.085423	-17.227663	-0.715632
H	7.048344	-15.299230	0.000000
B	3.854400	-17.624163	0.000000
B	2.295384	-18.135890	0.000000
B	1.071528	-17.042940	0.000000

B	1.961688	-19.741988	0.000000
C	0.109989	-16.177696	0.715576
C	0.109989	-16.177696	-0.715576
C	1.701058	-21.004799	0.718242
C	1.701058	-21.004799	-0.718242
Si	-1.126200	-15.073088	0.000000
Si	1.365627	-22.620401	0.000000
H	-2.547164	-15.455696	0.000000
H	-0.003728	-23.149526	0.000000
H	2.412035	-23.650052	0.000000
B	8.185807	19.482108	0.000000
B	8.527231	21.086651	0.000000
C	8.795094	22.347985	0.718229
C	8.795094	22.347985	-0.718229
Si	9.140731	23.961370	0.000000
H	10.513482	24.481606	0.000000
H	8.101220	24.997935	0.000000
B	9.405120	18.384123	0.000000
C	10.362378	17.514393	0.715609
C	10.362378	17.514393	-0.715609
Si	11.592255	16.402265	0.000000
H	13.014945	16.778830	0.000000
B	6.625400	18.974844	0.000000
C	5.393730	18.579987	0.715618
C	5.393730	18.579987	-0.715618
Si	3.814968	18.072668	0.000000
H	3.429961	16.652151	0.000000
Si	11.147806	14.131354	0.000000
C	12.376882	13.017937	0.715632
C	12.376882	13.017937	-0.715632
H	9.725350	13.753660	0.000000
B	13.335773	12.150090	0.000000
B	14.558449	11.055806	0.000000
B	14.223855	9.449441	0.000000
B	16.116219	11.569866	0.000000
C	13.955301	8.184101	0.715576
C	13.955301	8.184101	-0.715576
C	17.340161	11.975560	0.718242
C	17.340161	11.975560	-0.718242
Si	13.616778	6.561226	0.000000
Si	18.907029	12.492868	0.000000
H	14.658608	5.521940	0.000000
H	19.275529	13.913909	0.000000
Si	-3.239712	13.676842	0.000000
C	-2.899127	15.299394	0.715592
C	-2.899127	15.299394	-0.715592
H	-2.198248	12.637126	0.000000
B	-2.631361	16.564966	0.000000
B	-2.297357	18.171570	0.000000
B	-0.738449	18.683396	0.000000
B	-3.520924	19.264130	0.000000
C	0.492422	19.080195	0.715608
C	0.492422	19.080195	-0.715608
C	-4.483188	20.122411	0.718240
C	-4.483188	20.122411	-0.718240
Si	2.069794	19.591883	0.000000
Si	-5.712200	21.223430	0.000000
H	2.452275	21.012972	0.000000
H	-5.482767	22.673351	0.000000
H	-7.127934	20.834994	0.000000
H	20.049941	11.571534	0.000000

COF-SiBHC-1

E= -2395.85444

B	0.672719	9.116830	0.000136
C	0.900139	7.843963	0.715651
C	0.900125	7.843997	-0.715441
Si	1.187100	6.209934	0.000061
H	2.539992	5.633137	0.000029
Si	-0.561823	4.695770	0.000023
C	-0.274504	3.061744	0.715493
C	-0.274529	3.061803	-0.715595
H	-1.914813	5.272338	0.000073
B	-0.046719	1.789002	-0.000108
B	0.258728	0.176694	-0.000167
B	-0.977688	-0.901969	-0.000133
B	1.810978	-0.356405	-0.000138
C	-1.952085	-1.752040	0.715362
C	-1.952142	-1.751994	-0.715600
C	3.032442	-0.780224	0.715403
C	3.032440	-0.780331	-0.715618
Si	-3.198502	-2.846395	-0.000105
Si	4.599687	-1.323674	-0.000069
H	-2.984181	-4.302170	-0.000158
H	5.761174	-0.419904	-0.000132
Si	-5.403338	-2.145504	0.000000
C	-6.649871	-3.239658	0.715525
C	-6.649946	-3.239637	-0.715433
H	-5.617295	-0.689680	0.000033
B	-7.624571	-4.089409	0.000088
B	-8.860818	-5.167047	0.000155
B	7.864954	-4.555192	0.000157
C	6.643577	-4.131067	0.715650
C	6.643569	-4.131174	-0.715388
Si	5.076374	-3.587607	0.000099
H	3.914733	-4.491182	0.000164
TV	18.277674	0.078327	0.000025
TV	9.228694	15.896327	0.000009