Supplementary Materials

The Effect of Substituents on the Triply Bonded Boron≡Antimony Molecules: A Theoretical Approach

Jia-Syun Lu,[1] Ming-Chung Yang,[1] and Ming-Der Su[1,2]*

[1]Department of Applied Chemistry, National Chiayi University, Chiayi 60004, Taiwan

[2]Department of Medicinal and Applied Chemistry, Kaohsiung Medical University, Kaohsiung 80708, Taiwan

*E-mail: midesu@mail.ncyu.edu.tw

Table of Contents:

Theoretical Methods

Using the Gaussian 09 program package,[1] all geometries are fully optimized using hybrid density functional theory at the M06-2X,[2] B3LYP,[3,4] and B3PW91[4,5] levels, in conjunction with the Def2-TZVP[6] and LANL2DZ+dp[7] basis sets. These DFT calculations are signified as M06-2X/Def2-TZVP, B3PW91/Def2-TZVP and B3LYP/LANL2DZ+dp, respectively. In order to confirm that the reactants and products have no imaginary frequencies and that the transition states possess only one imaginary frequency, frequency calculations were performed for all structures. Thermodynamic corrections to 298 K, heat capacity corrections and entropy corrections (ΔS) are applied to the three levels of DFT. The relative free energy (ΔG) at 298 K is also computed at the same levels of theory.

Next, SiMe(Si*t*Bu$_3$)$_2$–B≡Sb–SiMe(Si*t*Bu$_3$)$_2$, Si*i*PrDis$_2$–B≡Sb–Si*i*PrDis$_2$, and Tbt–B≡Sb–Tbt are the model reactants for this study. Because the Hartree-Fock level of theory cannot accurately describe the entire energy surface, even qualitatively, these stationary points are further computed at the B3LYP/LANL2DZ+dp method. Because of the limitations of the available memory size and CPU time, frequencies are not computed at the B3LYP/LANL2DZ+dp level of theory for the triply bonded R′B≡SbR′ systems that have bulky ligands (R′), so the zero-point energies and the Gibbs free energies that are derived using B3LYP/LANL2DZ+dp cannot be used for these systems.

References:

(1) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J. and Fox, D. J. *Gaussian, Inc*., Wallingford CT, 2013.

(2) Zhao, Y.; Truhlar, D. G. *Acc. Chem. Res*. **2008**, *41*, 157-167.

(3) (a) Becke, A. D. *Phys. Rev. A* **1988**, *38*, 3098-3100. (b) Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648-5652.

(4) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785-789.

(5) Perdew, J. P.; Wang, Y. *Phys. Rev*. **1992**, *B45*, 13244-13249.

(6) Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys*. **2005**, *7*, 3297-3305.

(7) (a) Dunning, T. H., Jr.; Hay, P. J. In *Modern Theoretical Chemistry*, Schaefer, H. F., III, Ed.; Plenum: New York, 1976; p1-28. (b) Hay, P. J.; Wadt, W. R. *J. Chem. Phys*. **1985**, *82*, 270-283. (c) Hay, P. J.; Wadt, W. R. *J. Chem. Phys*. **1985**, *82*, 284-298. (d) Hay, P. J.; Wadt, W. R. *J. Chem. Phys*. **1985**, *82*, 299-310. (e) Check, C. E.; Faust, T. O.; Bailey, J. M.; Wright, B. J.; Gilbert, T. M.; Sunderlin, L. S. *J. Phys. Chem. A* **2001**, *105*, 8111-8116.

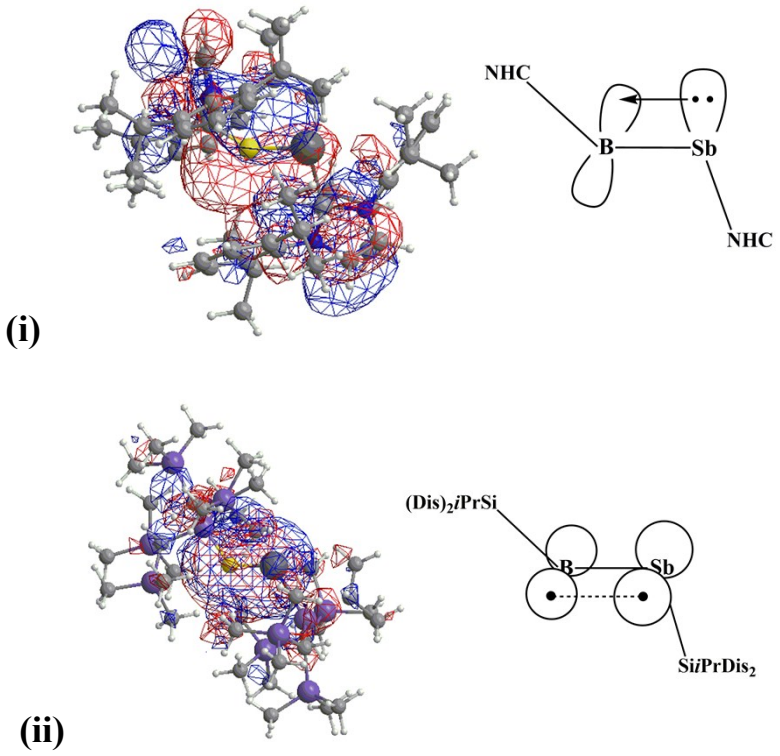

Figure S1: The natural B≡Sb π bonding orbitals ((i) and (ii)) of (Si*i*PrDis$_2$)B≡Sb(Si*i*PrDis$_2$)). For comparison, also see Figure 1.

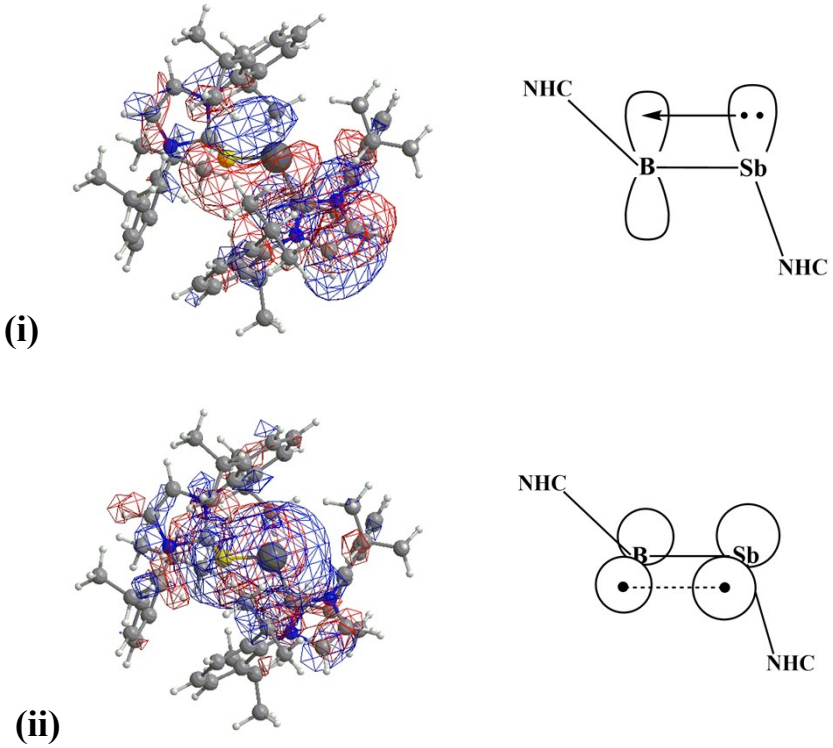

Figure S2: The natural B≡Sb π bonding orbitals ((i) and (ii)) of ((NHC)B≡Sb(NHC)). For comparison, also see Figure 1.

M06-2X/Def2-TZVP

F2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
F	2.032954	-1.130512	-0.000245
F	2.030400	1.131651	-0.000245
B	1.344402	-0.000323	0.001159
Sb	-0.848866	-0.000169	-0.000027

F2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.739213	1.246284	0.000000
Sb	0.000000	-0.701928	0.000000
F	1.372228	0.793944	0.000000
F	-0.961554	2.491269	0.000000

F-B-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	0.517058	-0.307456	-0.000002
B	-1.585916	-0.018508	0.000060
F	0.793375	1.613389	0.000000
F	-2.842304	0.139143	-0.000021

B-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z

B	1.526160	0.747606	1.291248
Sb	-0.210807	-0.356275	0.050535
F	-1.072879	1.338372	-0.156645
F	1.419583	0.265181	-0.847079

B-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.011314	-0.306071	0.240091
B	0.101375	2.058396	0.834664
F	-1.406524	0.344293	-0.903420
F	1.414316	0.246555	-0.920797

(OH)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.344079	-0.002798	-0.001459
Sb	0.866179	-0.001504	0.000105
O	-1.985604	-1.207825	0.001831
H	-2.948174	-1.179107	-0.013901
O	-1.962086	1.215399	-0.002967
H	-2.925055	1.209196	0.024924

(OH)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.366688	-0.446961	0.054321
Sb	0.688001	-0.176992	-0.003397
O	-0.412092	1.589283	-0.099040
H	-0.456433	2.014315	0.761990
O	-2.670747	-0.418625	0.080286

H	-3.135457	-0.118177	-0.710293

HO-B-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.856110	1.641104	-0.117060
H	-0.989894	2.034612	0.747571
O	2.859722	0.169535	-0.092600
H	3.342745	0.335932	0.727409
Sb	-0.515138	-0.326468	0.006501
B	1.578052	-0.041154	-0.025853

B-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.773743	1.365700	1.463821
Sb	0.105433	-0.388652	0.102515
O	-1.506316	0.401884	-0.745530
H	-1.648515	0.265557	-1.685734
O	1.385858	0.954836	-0.551908
H	1.103787	1.873447	-0.482147

B-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-1.507214	0.324625	0.882610
H	-1.896401	-0.359183	1.437491
O	1.505818	0.307909	0.887564
H	1.883707	-0.378152	1.447631
Sb	-0.001529	-0.290281	-0.265536
B	0.020372	2.096282	-0.700839

H2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	2.395082	-1.032533	0.000440
H	2.385077	1.037831	0.000437
B	1.799659	-0.000361	-0.000225
Sb	-0.270166	-0.000068	0.000005

H2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.941762	-0.070761	-0.179320
Sb	0.230160	-0.017026	-0.006899
H	-0.592953	1.503775	0.158036
H	-1.436402	-0.281620	1.090425

H-B-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.029832	2.028230	0.000000
Sb	0.029832	-0.261770	0.000000
H	-1.672375	-0.001250	0.000000
H	0.001757	3.210382	0.000000

B-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z

B	-2.041270	-0.045948	-0.148602
H	-0.381033	1.581674	0.212888
Sb	0.229422	-0.020026	-0.012348
H	-1.113136	-0.330615	1.159868

B-SbH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-2.140214	-0.000461	-0.047003
Sb	0.211079	0.000058	-0.039969
H	-0.034257	1.227006	1.137032
H	-0.029709	-1.227682	1.136397

(CH3)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.048177	1.380774	-0.000069
H	2.700955	1.427005	0.883914
H	2.712219	1.423051	-0.875661
H	1.438773	2.291168	-0.005757
C	2.108963	-1.351498	0.000081
H	2.767827	-1.367487	0.879551
H	2.770522	-1.367357	-0.877348
H	1.538927	-2.285580	-0.001004
B	1.272318	-0.004592	-0.000913
Sb	-0.886934	-0.005363	0.000016

(CH3)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.385140	-0.432391	-0.000227
Sb	0.702615	-0.258624	0.000043

C	-0.132920	1.921642	0.000579
H	0.240911	2.400130	0.901093
H	0.262369	2.397468	-0.892362
H	-1.219982	1.981568	-0.014740
C	-2.914443	-0.325970	0.000042
H	-3.300122	0.173431	-0.891151
H	-3.307823	-1.348676	0.000785
H	-3.298840	0.173827	0.891580

H3C-B-Sb-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.507195	0.106807	-0.009050
Sb	0.486313	-0.387950	0.000299
C	-3.019513	0.323567	0.002224
H	-3.370870	0.838993	0.899789
H	-3.384429	0.844483	-0.886875
H	-3.474312	-0.676993	0.001966
C	1.185028	1.701276	0.000511
H	2.266979	1.654172	-0.112992
H	0.942108	2.184489	0.943515
H	0.761431	2.257200	-0.831825

B-Sb(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.302181	0.406257	1.350297
Sb	-0.291963	-0.419385	-0.015813
C	-0.974741	1.639536	-0.071543
H	-0.899973	2.021119	-1.087414
H	-2.016916	1.661627	0.243784
H	-0.383741	2.259329	0.604562
C	1.853249	0.373142	-0.502506
H	2.729163	-0.217505	-0.233748

H	1.599535	0.119463	-1.546800
H	2.080115	1.437239	-0.481118

B-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.585679	1.023531	-0.371915
H	1.426213	1.474979	-1.349561
H	1.581273	1.815666	0.380992
H	2.551023	0.522348	-0.355727
C	-1.585891	1.023321	-0.372348
H	-1.460067	1.435060	-1.372026
H	-1.546221	1.842955	0.348887
H	-2.553524	0.531578	-0.301520
Sb	0.000131	-0.452092	-0.055321
B	-0.000823	0.630596	1.987180

(SiH3)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.743809	-0.000145	0.000152
Sb	1.297793	-0.000933	-0.000001
Si	-1.787395	-1.725470	-0.000003
H	-2.657133	-1.785489	-1.204256
H	-0.939514	-2.946442	-0.000494
H	-2.656111	-1.785253	1.205109
Si	-1.782657	1.728170	-0.000008
H	-2.652699	1.790711	1.203961
H	-0.931577	2.946929	0.000619
H	-2.650626	1.790034	-1.205477

(SiH3)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.222623	-0.020890	0.008838
Sb	-0.671751	-0.730440	-0.000223
H	-3.039605	1.523319	0.105210
Si	-1.568772	1.698673	0.000089
H	-1.266745	2.410150	-1.263104
H	-1.104037	2.495118	1.155763
Si	3.179273	0.402072	0.000045
H	3.829623	-0.316313	-1.125808
H	3.811965	-0.029876	1.269052
H	3.367988	1.864041	-0.175803

H3Si-B-Sb-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.882708	-0.367006	-0.013552
Sb	1.114259	-0.445274	0.000475
Si	-0.098671	1.910027	0.000304
H	0.387608	2.607373	-1.205145
H	-1.580197	1.997233	-0.009693
H	0.369027	2.597473	1.218811
Si	-2.864874	-0.545089	0.000718
H	-3.452929	0.120421	-1.182167
H	-3.221660	-1.979745	-0.004921
H	-3.425905	0.092121	1.212331

B-Sb(SiH3) (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.460122	0.315704	1.810528
Sb	0.089011	-0.784903	-0.070052
H	2.017753	1.611903	-1.494989

Si	1.815566	1.173776	-0.090431
H	3.085886	0.627263	0.448417
H	1.377575	2.332051	0.728630
Si	-1.938939	0.979360	-0.206200
H	-3.051430	0.658177	0.716933
H	-2.381893	0.671291	-1.592081
H	-1.559645	2.406950	-0.134068

B-Sb(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-1.438492	2.026532	-1.242176
H	-3.083915	0.478806	-0.343557
H	-1.764525	1.850895	1.136230
H	1.494242	1.972131	-1.298068
H	3.095182	0.477769	-0.246280
H	1.697463	1.908556	1.099184
Si	-1.760072	1.096879	-0.142249
Si	1.760614	1.096538	-0.141209
B	-0.002905	0.141618	2.011288
Sb	0.000137	-0.786875	-0.101831

B3PW91/Def2-TZVP

F2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
F	2.031699	-1.135596	-0.000006
F	2.031565	1.135654	-0.000006
B	1.342151	-0.000013	0.000029
Sb	-0.848630	-0.000009	-0.000001

F2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.735271	-1.240084	0.000000
Sb	0.000000	0.700469	0.000000
F	1.396117	-0.794098	0.000000
F	-0.987634	-2.486292	0.000000

F-B-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	0.517924	-0.308227	-0.000002
B	-1.579819	-0.030368	0.000063
F	0.783710	1.624416	0.000000
F	-2.840934	0.139077	-0.000022

B-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.275998	1.184609	1.325741
Sb	0.146331	-0.354638	0.110742
F	1.248247	1.140104	-0.389343
F	-1.368567	0.211395	-0.974720

B-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.006508	-0.318488	-0.227963
B	0.059060	2.027114	-0.905828

F	1.425390	0.311322	0.903721
F	-1.421325	0.367271	0.891309

(OH)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.347743	0.000069	-0.000392
Sb	-0.866534	0.000030	0.000029
O	1.974046	1.216700	-0.000198
H	2.937137	1.199726	0.001833
O	1.973545	-1.216814	-0.000124
H	2.936677	-1.200670	0.001235

(OH)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.360280	-0.421594	0.044283
Sb	0.690410	-0.177337	-0.002983
O	-0.429254	1.600717	-0.102754
H	-0.465248	1.982403	0.780619
O	-2.670019	-0.431640	0.085622
H	-3.150050	-0.182881	-0.712827

HO-B-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.843151	1.659655	-0.117228
H	-0.943981	2.000668	0.776826
O	2.854731	0.161627	-0.099829
H	3.359633	0.306753	0.711352
Sb	-0.516702	-0.327557	0.005236

B	1.568698	-0.034450	-0.003754

B-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.676602	1.319740	1.357900
Sb	-0.131124	-0.420054	0.065043
O	-1.221447	1.202861	-0.362485
H	-1.249332	1.404906	-1.303967
O	1.564810	0.322201	-0.689759
H	1.806761	1.218669	-0.384790

B-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-1.515456	0.284368	0.892198
H	-1.929674	-0.441499	1.375873
O	1.514062	0.276529	0.894556
H	1.917491	-0.449221	1.386977
Sb	-0.000472	-0.278985	-0.273010
B	0.009483	2.126357	-0.626670

H2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	2.394323	-1.038765	-0.000085
H	2.394231	1.038817	-0.000085
B	1.794383	-0.000004	0.000044
Sb	-0.269813	-0.000001	-0.000001

H2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.945095	-0.049914	-0.176775
Sb	0.232840	-0.009954	-0.009448
H	-0.840253	1.331040	0.385712
H	-1.309135	-0.573796	0.979988

H-B-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.029553	2.027787	0.000000
Sb	0.029553	-0.262213	0.000000
H	-1.671653	0.017480	0.000000
H	0.016680	3.216473	0.000000

B-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-2.014002	-0.049155	-0.156102
H	-0.593849	1.480249	0.299762
Sb	0.232677	-0.015035	-0.011144
H	-1.202666	-0.467680	1.049080

B-SbH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	2.125674	0.000220	-0.067035
Sb	-0.213598	-0.000256	-0.037839

H	0.135328	-1.205708	1.138251
H	0.129791	1.217672	1.126722

(CH3)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.045845	1.380930	-0.000023
H	2.699475	1.430053	0.880590
H	2.706082	1.428052	-0.875722
H	1.434768	2.287666	-0.003291
C	2.107944	-1.351029	-0.000059
H	2.761159	-1.372766	0.881798
H	2.773487	-1.367005	-0.872680
H	1.536405	-2.282336	-0.007037
B	1.276651	-0.004719	-0.000743
Sb	-0.886615	-0.005480	0.000011

(CH3)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.264037	-0.355451	-0.000126
Sb	0.740311	-0.196398	0.000004
C	-0.515566	1.747687	-0.000004
H	-0.205606	2.268105	0.902480
H	-0.204715	2.268679	-0.901851
H	-1.609261	1.715870	-0.000551
C	-2.794715	-0.526532	0.000023
H	-3.267924	-0.095237	-0.887689
H	-3.018446	-1.598111	0.001513
H	-3.268054	-0.092688	0.886415

H3C-B-Sb-CH3

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
B	-1.506227	0.117104	-0.006456
Sb	0.483096	-0.388964	0.000226
C	-3.015585	0.329135	0.002279
H	-3.380246	0.820014	0.909215
H	-3.380943	0.869324	-0.876231
H	-3.468626	-0.672658	-0.027604
C	1.199560	1.698966	0.000277
H	2.284943	1.630652	-0.063047
H	0.917229	2.196274	0.925217
H	0.817018	2.239430	-0.862137

B-Sb(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.330707	0.463292	1.283761
Sb	-0.286018	-0.422715	-0.011029
C	-1.036736	1.615923	-0.079073
H	-0.980291	1.999397	-1.096566
H	-2.080842	1.578367	0.235425
H	-0.477834	2.255249	0.607316
C	1.873630	0.398197	-0.477946
H	2.756569	-0.185858	-0.207374
H	1.583173	0.051885	-1.495706
H	2.111254	1.458263	-0.557300

B-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.606565	1.023489	-0.348989
H	1.450980	1.492424	-1.321122
H	1.616287	1.797389	0.423809
H	2.557561	0.492426	-0.342237

C	-1.605660	1.022591	-0.352965
H	-1.447878	1.491273	-1.324772
H	-1.615949	1.796646	0.419566
H	-2.556734	0.491872	-0.347646
Sb	0.000366	-0.443752	-0.065246
B	-0.005674	0.558569	2.006335

(SiH3)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.731694	-0.000183	0.000703
Sb	1.280529	-0.001592	-0.000019
Si	-1.765570	-1.721601	-0.000004
H	-2.630784	-1.783323	-1.210038
H	-0.910570	-2.940290	0.002329
H	-2.635860	-1.781636	1.206465
Si	-1.757586	1.726202	-0.000080
H	-2.622668	1.792577	1.209777
H	-0.897270	2.941175	-0.003043
H	-2.627157	1.789225	-1.206887

(SiH3)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.138257	-0.234630	0.002769
Sb	-0.837605	-0.688205	-0.000145
H	-2.468303	2.157107	0.050525
Si	-0.997096	1.921225	-0.000207
H	-0.468265	2.554769	-1.235920
H	-0.384481	2.566462	1.189658
Si	3.105767	0.106542	-0.000251
H	3.738126	-0.475279	-1.215334
H	3.746455	-0.496597	1.199850
H	3.341638	1.576417	0.011177

H3Si-B-Sb-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.919493	-0.323949	-0.001828
Sb	1.090920	-0.473316	0.000069
Si	0.024206	1.914292	0.000033
H	0.495576	2.619457	-1.217366
H	-1.467164	2.011610	-0.001670
H	0.492612	2.618021	1.219463
Si	-2.903352	-0.477631	0.000159
H	-3.499481	0.163453	-1.202259
H	-3.256702	-1.922645	-0.003568
H	-3.496241	0.155715	1.208317

B-Sb(Si H3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.232297	0.231659	1.943263
Sb	0.041976	-0.769517	-0.086822
H	1.853046	1.721402	-1.470461
Si	1.828706	1.106042	-0.115353
H	3.141830	0.468271	0.172148
H	1.557680	2.164257	0.898465
Si	-1.880266	1.020147	-0.182326
H	-2.861222	0.784419	0.910403
H	-2.543611	0.757894	-1.487633
H	-1.405170	2.424179	-0.143795

B-Sb(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

H	-1.529163	2.001927	-1.284860
H	-3.112334	0.396782	-0.343068
H	-1.819810	1.837352	1.112676
H	1.521843	2.012274	-1.276558
H	3.109848	0.396685	-0.359616
H	1.828800	1.825159	1.117218
Si	-1.799395	1.065105	-0.167101
Si	1.798635	1.064479	-0.169762
B	0.007540	0.331899	1.948077
Sb	-0.000515	-0.783213	-0.078237

B3LYP/LANL2DZ+dp

F2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
F	-2.051187	1.155307	-0.000029
F	-2.051414	-1.155207	-0.000029
B	-1.336048	-0.000023	0.000137
Sb	0.854973	-0.000015	-0.000003

F2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.719459	1.244521	0.000000
Sb	0.000000	-0.711608	0.000000
F	1.403118	0.826354	0.000000
F	-1.003419	2.514692	0.000000

F-B-Sb-F

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.513855	-0.316435	-0.000005
B	1.581077	0.009706	0.000142
F	-0.842805	1.632655	-0.000001
F	2.876271	0.155087	-0.000049

B-SbF2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	2.001279	-0.265150	0.812159
Sb	-0.444617	-0.311279	-0.026219
F	-0.679186	1.618885	0.122013
F	2.086861	0.292333	-0.424640

B-SbF2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	0.000240	-0.345706	-0.203347
B	-0.002403	1.985215	-1.030642
F	1.447717	0.429132	0.862070
F	-1.447745	0.426968	0.862812

(OH)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.352623	-0.000101	-0.000407
Sb	-0.873613	-0.000061	0.000024
O	1.991307	1.227240	-0.000420

H	2.961025	1.192139	0.003855
O	1.992216	-1.226894	0.000247
H	2.961954	-1.191297	-0.001636

(OH)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.358521	-0.418447	0.033444
Sb	0.706114	-0.169559	-0.002518
O	-0.502973	1.590761	-0.101961
H	-0.557573	1.997876	0.777449
O	-2.683567	-0.475712	0.087314
H	-3.169339	-0.178521	-0.699066

HO-B-Sb-OH

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.879714	1.660802	-0.116670
H	-1.026904	2.026686	0.768427
O	2.882455	0.181065	-0.101026
H	3.377853	0.310295	0.726017
Sb	-0.515317	-0.332393	0.005102
B	1.581661	-0.023978	-0.002614

B-Sb(OH)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-0.879714	1.660802	-0.116670
H	-1.026904	2.026686	0.768427
O	2.882455	0.181065	-0.101026
H	3.377853	0.310295	0.726017

Sb	-0.515317	-0.332393	0.005102
B	1.581661	-0.023978	-0.002614

B-Sb(OH)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
O	-1.520723	0.262630	0.901649
H	-1.944274	-0.472579	1.369009
O	1.521637	0.256821	0.901567
H	1.936324	-0.477805	1.376794
Sb	-0.000596	-0.273942	-0.278967
B	0.006207	2.153165	-0.588844

H2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.416410	-1.039942	0.000044
H	-2.416328	1.039986	0.000044
B	-1.813321	-0.000003	-0.000023
Sb	0.272536	-0.000001	0.000001

H2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-2.020042	-0.056488	-0.163383
Sb	0.231218	-0.023928	-0.006670
H	-0.284393	1.626507	0.050796
H	-1.407509	-0.123753	1.106285

H-B-Sb-H

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	0.029509	2.028911	0.000000
Sb	0.029509	-0.261089	0.000000
H	-1.690772	-0.051024	0.000000
H	0.038294	3.222004	0.000000

B-SbH2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-2.042599	-0.023325	-0.156854
H	-0.849334	1.268371	0.534017
Sb	0.239417	-0.006827	-0.012171
H	-1.147917	-0.803559	0.870953

B-SbH2

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-2.174698	-0.000015	-0.035207
Sb	0.212060	0.000006	-0.041602
H	0.029117	1.237670	1.149000
H	0.029296	-1.237917	1.148762

(CH3)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	2.042607	1.385805	0.000176
H	2.711138	1.424459	0.877100
H	2.694190	1.432664	-0.888979

H	1.435362	2.302175	0.009779
C	2.101943	-1.356955	-0.000294
H	2.750462	-1.379276	0.892312
H	2.778082	-1.364115	-0.872320
H	1.532624	-2.296736	-0.016826
B	1.257272	-0.004821	-0.000073
Sb	-0.883441	-0.005258	0.000000

(CH3)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.248719	-0.334786	-0.000038
Sb	0.768221	-0.175463	0.000001
C	-0.697701	1.717162	0.000041
H	-0.394730	2.246361	0.907468
H	-0.392152	2.247367	-0.905947
H	-1.796246	1.684986	-0.001721
C	-2.777159	-0.622179	-0.000001
H	-3.279367	-0.208693	-0.889413
H	-2.944652	-1.709318	0.000426
H	-3.279363	-0.208044	0.889113

H3C-B-Sb-CH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-1.523161	0.117275	-0.010109
Sb	0.487036	-0.392214	0.000332
C	-3.045449	0.333883	0.002584
H	-3.401579	0.849869	0.907305
H	-3.415322	0.863874	-0.888653
H	-3.511428	-0.669240	-0.002789
C	1.216456	1.707989	0.000468
H	2.306513	1.649374	-0.108423
H	0.972754	2.199342	0.948134

H	0.799996	2.272080	-0.840257

B-Sb(CH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.426116	0.387728	1.279992
Sb	-0.305470	-0.422071	-0.014942
C	-1.032421	1.649925	-0.050941
H	-1.015925	2.043929	-1.073464
H	-2.071213	1.631976	0.306375
H	-0.436914	2.286459	0.616169
C	1.931939	0.395577	-0.474409
H	2.815973	-0.235030	-0.310189
H	1.555171	0.130651	-1.499598
H	2.204177	1.455991	-0.525097

B-Sb(CH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.629175	1.095495	0.072543
H	1.584043	1.826280	-0.744932
H	1.538125	1.619761	1.032899
H	2.590611	0.568401	0.031959
C	-1.629411	1.095301	0.072787
H	-1.583191	1.827199	-0.743583
H	-1.539167	1.618193	1.033838
H	-2.590836	0.568397	0.030513
Sb	-0.000002	-0.359783	-0.236399
B	0.000381	-0.564814	2.108736

(SiH3)2B-Sb

Atomic	Coordinates (Angstroms)

Number	X	Y	Z
B	-0.743809	-0.000145	0.000152
Sb	1.297793	-0.000933	-0.000001
Si	-1.787395	-1.725470	-0.000003
H	-2.657133	-1.785489	-1.204256
H	-0.939514	-2.946442	-0.000494
H	-2.656111	-1.785253	1.205109
Si	-1.782657	1.728170	-0.000008
H	-2.652699	1.790711	1.203961
H	-0.931577	2.946929	0.000619
H	-2.650626	1.790034	-1.205477

(SiH3)2B-Sb (TS1)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	1.191619	-0.180144	-0.000060
Sb	-0.772941	-0.719728	-0.000018
H	-2.706780	1.977660	0.206321
Si	-1.236594	1.862028	-0.000388
H	-0.892570	2.488342	-1.299972
H	-0.550626	2.588652	1.096986
Si	3.143350	0.242005	-0.000099
H	3.803836	-0.252962	-1.237408
H	3.818396	-0.371761	1.172543
H	3.295067	1.720448	0.069545

H3Si-B-Sb-SiH3

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-1.068742	-0.510330	0.000056
Si	-0.151613	1.961409	-0.000144
H	-0.682540	2.644779	-1.203253
H	-0.651300	2.629697	1.224658

H	1.327019	2.125924	-0.016351
Si	2.957088	-0.405833	0.000133
H	3.521071	0.254126	1.203954
H	3.368735	-1.833187	0.002690
H	3.524391	0.250947	-1.203844
B	0.964367	-0.364699	-0.002110

B-Sb(SiH3)2 (TS2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.460122	0.315704	1.810528
Sb	0.089011	-0.784903	-0.070052
H	2.017753	1.611903	-1.494989
Si	1.815566	1.173776	-0.090431
H	3.085886	0.627263	0.448417
H	1.377575	2.332051	0.728630
Si	-1.938939	0.979360	-0.206200
H	-3.051430	0.658177	0.716933
H	-2.381893	0.671291	-1.592081
H	-1.559645	2.406950	-0.134068

B-Sb(SiH3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-1.516666	2.291898	-0.768077
H	-3.090132	0.439784	-0.758550
H	-2.307403	1.370120	1.328560
H	1.515787	2.292707	-0.766557
H	3.089629	0.440667	-0.761150
H	2.308706	1.367990	1.328139
Si	-1.923087	1.048100	-0.071802
Si	1.923119	1.047983	-0.072460
B	0.001875	-0.298382	2.141608
Sb	-0.000191	-0.706989	-0.162564

B3LYP/LANL2DZ+dp

(SiMe(SitBu3)2)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-1.895886	0.067905	0.575595
Si	-3.092413	-2.325849	1.123868
Si	-3.504124	1.927380	-0.687686
C	-2.074165	-3.111028	2.849089
C	-2.966658	-3.661740	-0.454064
C	-5.103370	-2.137679	1.734171
C	-3.781528	-4.947605	-0.189382
H	-4.854654	-4.755055	-0.144570
H	-3.497581	-5.445334	0.738138
H	-3.629375	-5.673662	-0.997731
C	-1.506991	-4.054837	-0.669060
H	-0.900097	-3.160785	-0.833506
H	-1.387293	-4.699879	-1.547955
H	-1.121363	-4.614770	0.183525
C	-3.454144	-3.062155	-1.782154
H	-2.881167	-2.169441	-2.049727
H	-4.519442	-2.827258	-1.753583
H	-3.322882	-3.775771	-2.605556
C	-2.382657	-4.607001	3.062080
H	-3.448158	-4.815596	3.151371
H	-1.908847	-4.966449	3.983938
H	-1.984854	-5.223182	2.251449
C	-0.568236	-2.974299	2.635585
H	-0.012529	-3.136148	3.566465
H	-0.329504	-1.983431	2.265172
H	-0.197864	-3.710848	1.926176
C	-2.450809	-2.327114	4.123640
H	-2.303253	-1.254041	4.013204
H	-1.830714	-2.648024	4.969960
H	-3.482418	-2.493083	4.430897

C	-5.576309	-3.335610	2.588270
H	-6.653027	-3.260799	2.787090
H	-5.095088	-3.379244	3.564422
H	-5.410618	-4.291555	2.084307
C	-6.028119	-2.117743	0.505198
H	-5.636978	-1.480128	-0.274682
H	-7.031153	-1.763407	0.769538
H	-6.158377	-3.109534	0.065105
C	-5.262896	-0.849692	2.561412
H	-4.860782	0.012394	2.033758
H	-4.745843	-0.905328	3.522062
H	-6.318135	-0.648754	2.778800
C	-2.408871	2.806467	-2.277936
C	-5.291721	1.223368	-1.602273
C	-4.112854	3.440128	0.689856
C	-2.901178	4.268833	1.127218
H	-3.196755	5.066723	1.819239
H	-2.399012	4.748751	0.285939
H	-2.190349	3.642415	1.658536
C	-4.757290	2.828273	1.949880
H	-5.054729	3.618126	2.650987
H	-4.068949	2.180609	2.488283
H	-5.659134	2.257997	1.726179
C	-5.142498	4.403891	0.059139
H	-5.361082	5.232908	0.744094
H	-6.098301	3.917261	-0.137746
H	-4.792831	4.850837	-0.870682
C	-6.385986	1.007339	-0.542387
H	-6.846034	1.946290	-0.225425
H	-5.999279	0.528361	0.348874
H	-7.201321	0.389492	-0.936484
C	-5.877533	2.215699	-2.632340
H	-6.046318	3.208733	-2.213974
H	-6.847947	1.854807	-2.996673
H	-5.250142	2.326783	-3.516504
C	-4.970144	-0.077130	-2.343799
H	-5.877253	-0.643487	-2.581389
H	-4.324124	-0.688414	-1.726934
H	-4.451232	0.090353	-3.290399
C	-0.976569	3.084660	-1.829513

H	-0.942338	3.909652	-1.117342
H	-0.364608	3.387523	-2.686861
H	-0.503862	2.220320	-1.370048
C	-3.002779	4.160624	-2.723910
H	-2.910757	4.922078	-1.944680
H	-4.052462	4.096497	-3.007868
H	-2.461393	4.544510	-3.597726
C	-2.388653	1.853496	-3.492285
H	-3.300264	1.928368	-4.088626
H	-2.282062	0.809824	-3.197195
H	-1.566836	2.098682	-4.175339
C	-1.756044	0.741933	2.303831
H	-1.486839	1.794434	2.297672
H	-0.993961	0.205775	2.870401
H	-2.690516	0.641623	2.856170
Si	1.949997	-0.079623	0.584024
Si	3.630035	-1.922970	-0.633583
Si	2.993278	2.403621	1.070006
C	3.467717	3.369498	-0.712340
C	4.685364	2.404676	2.370794
C	1.563417	3.534578	2.145085
C	2.345586	3.174776	-1.744299
H	1.493988	3.809583	-1.506334
H	1.997516	2.143349	-1.795373
H	2.673418	3.465515	-2.749423
C	4.765068	2.801517	-1.306207
H	5.625876	2.964857	-0.655451
H	5.002621	3.275931	-2.266079
H	4.661672	1.737201	-1.494838
C	3.666620	4.889363	-0.515449
H	4.434596	5.121914	0.223134
H	2.745603	5.390336	-0.208956
H	3.975817	5.361306	-1.456426
C	5.700460	1.382143	1.884886
H	6.457162	1.156748	2.644674
H	6.242460	1.724625	1.001928
H	5.170871	0.473711	1.645083
C	4.273773	2.028351	3.808735
H	5.156311	1.816002	4.424749
H	3.637761	1.142120	3.841004

H	3.755743	2.846115	4.311800
C	5.405859	3.770361	2.386777
H	6.226875	3.759137	3.114569
H	4.756363	4.600331	2.658041
H	5.855456	4.003512	1.417656
C	0.968568	2.708274	3.298498
H	1.674034	2.536781	4.111572
H	0.636775	1.735427	2.952707
H	0.104471	3.218928	3.740044
C	0.446234	3.934039	1.186342
H	-0.292702	4.542266	1.714569
H	-0.047926	3.051286	0.779069
H	0.803711	4.554080	0.364522
C	2.149644	4.832621	2.738603
H	2.831433	4.636736	3.567759
H	1.351087	5.461269	3.152521
H	2.675679	5.435780	1.997157
C	3.029049	-3.885295	-0.067459
C	3.488419	-1.774793	-2.723224
C	5.658655	-1.839951	-0.026001
C	5.769463	-1.874737	1.517876
H	6.661608	-1.338807	1.860595
H	5.885112	-2.892633	1.901649
H	4.894822	-1.466173	2.022896
C	6.494978	-3.036491	-0.540658
H	7.558348	-2.875912	-0.320663
H	6.416491	-3.189339	-1.615576
H	6.225578	-3.971657	-0.045528
C	6.285843	-0.574320	-0.633250
H	7.263165	-0.358609	-0.187424
H	5.643468	0.284879	-0.486663
H	6.445006	-0.667857	-1.710858
C	3.451054	-4.197349	1.382316
H	4.514576	-4.437990	1.444194
H	2.923517	-5.081117	1.761331
H	3.246762	-3.377677	2.071221
C	1.514412	-3.969666	-0.178147
H	1.036671	-3.112707	0.294434
H	1.143026	-4.884982	0.296055
H	1.191434	-4.009332	-1.220188

C	3.623279	-4.969796	-0.994210
H	4.710983	-4.958917	-1.027211
H	3.268032	-4.881298	-2.021580
H	3.326629	-5.967991	-0.648503
C	3.498010	-0.291856	-3.132343
H	4.468857	0.166589	-2.929052
H	2.735089	0.278839	-2.606919
H	3.314794	-0.177220	-4.207139
C	4.672770	-2.461211	-3.438002
H	5.620250	-1.952409	-3.249145
H	4.525838	-2.443620	-4.525277
H	4.780272	-3.509360	-3.148088
C	2.203038	-2.459795	-3.229910
H	1.362359	-2.311185	-2.557754
H	2.328874	-3.540601	-3.336697
H	1.921158	-2.089731	-4.222495
C	1.964230	-0.780671	2.316398
H	2.938938	-0.637905	2.785508
H	1.787954	-1.853298	2.298428
H	1.217123	-0.326711	2.966237
Sb	-0.023810	-0.250536	-2.471342
B	0.016023	-0.082010	-0.238230

SiMe(SitBu3)2-B-Sb-SiMe(SitBu3)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	-2.713429	-0.277702	-0.612599
Si	-3.555623	2.087735	-1.145294
Si	-3.904550	-1.915132	1.077783
C	-2.249461	2.880059	-2.640283
C	-3.372808	3.218582	0.592302
C	-5.475360	2.192331	-1.938650
C	-4.031465	4.604752	0.449814
H	-5.115675	4.527403	0.330866
H	-3.639523	5.172890	-0.395170
H	-3.858202	5.207973	1.349392
C	-1.885731	3.400510	0.962264

H	-1.371416	2.440710	1.054967
H	-1.783181	3.915604	1.925047
H	-1.350253	4.004484	0.227638
C	-4.058054	2.489871	1.761481
H	-3.620352	1.504288	1.905643
H	-5.131107	2.366510	1.605088
H	-3.933290	3.043430	2.699706
C	-2.265742	4.421747	-2.622677
H	-3.273033	4.829475	-2.729047
H	-1.668422	4.821468	-3.451281
H	-1.831783	4.826622	-1.706049
C	-0.820845	2.394085	-2.372870
H	-0.100179	2.906739	-3.020939
H	-0.731255	1.326136	-2.586453
H	-0.520485	2.571800	-1.340847
C	-2.646593	2.393237	-4.049592
H	-2.778274	1.310048	-4.092204
H	-1.868893	2.652287	-4.778885
H	-3.562840	2.864975	-4.407545
C	-5.769468	3.588612	-2.536570
H	-6.811935	3.651131	-2.872936
H	-5.153641	3.808045	-3.409502
H	-5.619276	4.392983	-1.813905
C	-6.525902	1.946406	-0.844794
H	-6.373748	0.977868	-0.384016
H	-7.540511	1.949699	-1.260945
H	-6.502371	2.712652	-0.066540
C	-5.676696	1.142854	-3.054556
H	-5.401148	0.139740	-2.734215
H	-5.096583	1.366050	-3.950865
H	-6.726915	1.107327	-3.368760
C	-3.245931	-1.531586	3.043464
C	-5.952975	-1.906603	0.905749
C	-3.184552	-3.857861	0.488101
C	-1.651121	-3.791247	0.369807
H	-1.237473	-4.774479	0.116129
H	-1.191294	-3.476859	1.311015
H	-1.328584	-3.100288	-0.409017
C	-3.805062	-4.258176	-0.867193
H	-3.280645	-5.122798	-1.291687

H	-3.767575	-3.462556	-1.607986
H	-4.851262	-4.556586	-0.751823
C	-3.544704	-4.968252	1.501646
H	-3.470437	-5.955797	1.028601
H	-4.554158	-4.878837	1.899961
H	-2.852092	-5.006159	2.343751
C	-6.365167	-1.891388	-0.580601
H	-6.083743	-2.805793	-1.105270
H	-5.904144	-1.060745	-1.108572
H	-7.451681	-1.791616	-0.688390
C	-6.573218	-3.160790	1.559706
H	-6.337005	-4.070344	1.001057
H	-7.667449	-3.085878	1.580438
H	-6.234432	-3.290017	2.593205
C	-6.572900	-0.678670	1.606908
H	-7.570371	-0.455416	1.209966
H	-5.957395	0.213533	1.496293
H	-6.717536	-0.848330	2.677064
C	-1.890697	-0.799425	3.031490
H	-1.119663	-1.400097	2.541140
H	-1.539985	-0.610504	4.053545
H	-1.953609	0.171921	2.537078
C	-3.058720	-2.839289	3.839481
H	-2.200917	-3.408960	3.474586
H	-3.955480	-3.465300	3.813091
H	-2.849624	-2.625312	4.895331
C	-4.265195	-0.687456	3.832807
H	-5.167663	-1.265264	4.053863
H	-4.553949	0.223864	3.312611
H	-3.851015	-0.382115	4.801760
C	-2.709146	-1.136886	-2.265075
H	-2.148163	-2.073155	-2.226216
H	-2.217240	-0.527102	-3.025361
H	-3.719372	-1.359661	-2.615291
Si	3.111676	0.353562	-0.817025
Si	3.799225	1.989270	1.069645
Si	3.685110	-2.102817	-1.091349
C	3.217309	-3.229561	0.581522
C	5.699441	-2.381099	-1.606143
C	2.481795	-2.770942	-2.734396

C	1.815799	-2.870894	1.105250
H	1.034494	-3.228789	0.437059
H	1.677330	-1.800055	1.206891
H	1.626309	-3.327760	2.083561
C	4.253448	-2.963469	1.692770
H	5.218358	-3.423548	1.462003
H	3.926659	-3.390118	2.648345
H	4.419108	-1.896375	1.845898
C	3.209141	-4.745725	0.282337
H	4.152139	-5.102667	-0.132251
H	2.414537	-5.021311	-0.415540
H	3.028826	-5.316450	1.201807
C	6.604825	-1.630532	-0.615739
H	7.658638	-1.701831	-0.909795
H	6.532260	-2.024209	0.399732
H	6.344714	-0.578773	-0.586631
C	5.989803	-1.846883	-3.024283
H	7.057930	-1.933430	-3.258944
H	5.728705	-0.793326	-3.130459
H	5.458766	-2.409441	-3.794081
C	6.099425	-3.871200	-1.553485
H	7.122180	-4.009066	-1.925584
H	5.451311	-4.505264	-2.159856
H	6.091332	-4.255976	-0.530173
C	2.479064	-1.725447	-3.869771
H	3.485373	-1.478918	-4.212653
H	1.979043	-0.800629	-3.569179
H	1.930682	-2.105642	-4.740458
C	1.025327	-2.971247	-2.272936
H	0.369008	-3.163854	-3.130356
H	0.636865	-2.089380	-1.761009
H	0.924742	-3.834161	-1.611528
C	3.011518	-4.107828	-3.291625
H	3.984229	-3.994222	-3.774560
H	2.330010	-4.501935	-4.055409
H	3.104338	-4.874506	-2.520022
C	3.187701	3.926327	0.390984
C	2.791726	1.579125	2.862942
C	5.860391	2.051452	1.407745
C	6.660221	2.175879	0.095268

H	7.738095	2.122158	0.291800
H	6.486809	3.124201	-0.415061
H	6.428821	1.386264	-0.609546
C	6.258716	3.264492	2.281272
H	7.331392	3.235197	2.510071
H	5.735365	3.293929	3.236281
H	6.074862	4.213717	1.772971
C	6.290726	0.766084	2.144882
H	7.382833	0.676065	2.176260
H	5.897690	-0.128995	1.661841
H	5.948030	0.763389	3.183464
C	4.199561	4.499788	-0.621890
H	5.129689	4.804886	-0.136546
H	3.795416	5.399214	-1.102412
H	4.446863	3.794190	-1.415328
C	1.813214	3.814957	-0.295786
H	1.878656	3.264998	-1.237679
H	1.417211	4.808132	-0.539071
H	1.077291	3.318763	0.338692
C	3.081817	4.915607	1.570355
H	4.008453	4.977468	2.144916
H	2.274811	4.658734	2.257604
H	2.863931	5.926283	1.203665
C	2.935081	0.090645	3.219625
H	3.972432	-0.197412	3.400388
H	2.547530	-0.531330	2.421854
H	2.372718	-0.154873	4.128320
C	3.359038	2.388521	4.047096
H	4.365722	2.057977	4.316847
H	2.739439	2.247227	4.941424
H	3.392760	3.460849	3.849363
C	1.292606	1.905940	2.725096
H	0.869471	1.453676	1.832665
H	1.101789	2.979165	2.672139
H	0.726114	1.531346	3.585978
C	3.996793	1.138759	-2.297242
H	5.072338	1.217908	-2.153679
H	3.593934	2.135846	-2.486065
H	3.824009	0.568115	-3.209975
Sb	-0.257996	-0.181023	0.212623

B	1.211619	0.588239	-1.256639

B-Sb(SiMe(SitBu3)2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	2.309662	-0.048144	0.405984
Si	3.221258	2.373442	0.998566
Si	3.882901	-1.844120	-0.861312
C	2.087491	3.002816	2.706354
C	2.878106	3.691370	-0.569000
C	5.217253	2.378711	1.567736
C	3.573057	5.050238	-0.327888
H	4.661201	4.960996	-0.321619
H	3.275728	5.514593	0.613462
H	3.321234	5.758810	-1.126562
C	1.372298	3.938027	-0.729993
H	0.826736	2.995444	-0.819758
H	1.160737	4.526109	-1.631378
H	0.967294	4.507094	0.108481
C	3.385303	3.131964	-1.909060
H	2.901545	2.181782	-2.155129
H	4.469753	3.003310	-1.907042
H	3.160010	3.822354	-2.731582
C	2.221556	4.524407	2.929619
H	3.258499	4.850149	3.017232
H	1.713229	4.821338	3.855258
H	1.754626	5.097289	2.124813
C	0.602023	2.688971	2.486117
H	0.014954	2.929633	3.380557
H	0.435596	1.638154	2.261277
H	0.183124	3.275869	1.672032
C	2.555444	2.270025	3.981452
H	2.557505	1.187083	3.866131
H	1.890736	2.500470	4.823180
H	3.554958	2.573328	4.293887
C	5.579631	3.618326	2.417487
H	6.658971	3.647469	2.613008

H	5.095578	3.616562	3.394206
H	5.319780	4.553198	1.913000
C	6.133622	2.434276	0.331273
H	5.833296	1.719288	-0.423206
H	7.175034	2.222171	0.600310
H	6.128810	3.418525	-0.144115
C	5.522657	1.113723	2.395976
H	5.230354	0.205899	1.869192
H	4.997924	1.110178	3.354547
H	6.593376	1.038713	2.618420
C	2.696804	-2.751368	-2.363991
C	5.566738	-1.047345	-1.818858
C	4.538340	-3.341977	0.484544
C	3.360699	-4.239171	0.903566
H	3.657224	-4.926047	1.705288
H	3.004715	-4.860345	0.078403
H	2.524171	-3.652313	1.272350
C	5.163215	-2.715610	1.747237
H	5.536429	-3.497191	2.420538
H	4.441455	-2.135664	2.317569
H	6.011609	-2.069309	1.516538
C	5.609577	-4.246766	-0.167132
H	5.864786	-5.079753	0.499810
H	6.541200	-3.712044	-0.358893
H	5.275464	-4.685921	-1.107848
C	6.686891	-0.775899	-0.795728
H	7.186148	-1.694534	-0.478210
H	6.312541	-0.291155	0.100770
H	7.466781	-0.135811	-1.224748
C	6.155108	-1.995857	-2.886352
H	6.387033	-2.985135	-2.487571
H	7.090146	-1.585470	-3.288166
H	5.488568	-2.123469	-3.741364
C	5.164452	0.251070	-2.528978
H	6.041366	0.822100	-2.853728
H	4.582007	0.866919	-1.855349
H	4.553620	0.077449	-3.417795
C	1.320365	-3.124764	-1.802857
H	1.386104	-3.854911	-0.995190
H	0.697334	-3.572208	-2.586338

H	0.788442	-2.257485	-1.425529
C	3.332507	-4.050950	-2.901135
H	3.343788	-4.840583	-2.145524
H	4.353171	-3.914533	-3.256580
H	2.751099	-4.438828	-3.746835
C	2.516901	-1.758463	-3.531163
H	3.410680	-1.699347	-4.156627
H	2.293181	-0.748882	-3.177986
H	1.702007	-2.074405	-4.193026
C	2.095024	-0.788218	2.101920
H	1.825104	-1.840855	2.055749
H	1.299722	-0.284650	2.651352
H	3.001845	-0.694277	2.700433
Si	-2.384689	0.117234	0.481999
Si	-3.986748	1.819956	-0.866974
Si	-3.140243	-2.362116	1.039120
C	-3.368055	-3.464014	-0.704349
C	-4.859735	-2.477402	2.235928
C	-1.564303	-3.212262	2.190442
C	-2.202869	-3.189858	-1.673980
H	-1.285513	-3.665664	-1.330370
H	-1.994641	-2.127925	-1.792120
H	-2.410634	-3.600815	-2.668945
C	-4.687978	-3.085729	-1.398379
H	-5.557806	-3.416019	-0.824931
H	-4.766524	-3.557958	-2.384818
H	-4.759740	-2.010756	-1.544414
C	-3.401345	-4.984280	-0.427768
H	-4.190274	-5.267515	0.270401
H	-2.455659	-5.353325	-0.025356
H	-3.582265	-5.538987	-1.356817
C	-5.999426	-1.672818	1.610986
H	-6.855715	-1.586576	2.289936
H	-6.373888	-2.121691	0.689322
H	-5.648547	-0.676728	1.389349
C	-4.580917	-1.899534	3.639423
H	-5.506045	-1.834853	4.225206
H	-4.159947	-0.892531	3.591118
H	-3.900732	-2.530209	4.214862
C	-5.377613	-3.925301	2.376302

H	-6.227299	-3.962622	3.069480
H	-4.629460	-4.617247	2.758988
H	-5.740120	-4.317731	1.421906
C	-1.068949	-2.211238	3.249171
H	-1.865383	-1.838579	3.894088
H	-0.593340	-1.355984	2.773755
H	-0.314280	-2.671138	3.898519
C	-0.386692	-3.559031	1.271913
H	0.463450	-3.900274	1.870418
H	-0.066857	-2.692068	0.691925
H	-0.619496	-4.374819	0.586261
C	-2.010659	-4.502198	2.906251
H	-2.718120	-4.298399	3.712751
H	-1.151884	-4.999772	3.373849
H	-2.463140	-5.223892	2.223028
C	-3.342460	3.788132	-0.379237
C	-3.696289	1.528374	-2.912290
C	-5.984162	1.704012	-0.346799
C	-6.156231	1.754197	1.191101
H	-7.097992	1.284730	1.497899
H	-6.201270	2.780494	1.566662
H	-5.339811	1.274337	1.730575
C	-6.815404	2.878727	-0.918067
H	-7.883029	2.722944	-0.717840
H	-6.706707	2.991617	-1.997518
H	-6.553458	3.832421	-0.453905
C	-6.581299	0.412302	-0.940167
H	-7.569473	0.198404	-0.517513
H	-5.941235	-0.446344	-0.759132
H	-6.712054	0.485433	-2.024214
C	-3.834989	4.178658	1.030065
H	-4.903230	4.408370	1.030323
H	-3.330019	5.086613	1.381230
H	-3.656852	3.398996	1.772048
C	-1.812405	3.849324	-0.413210
H	-1.363334	3.061510	0.186925
H	-1.454006	4.810472	-0.026630
H	-1.421823	3.756351	-1.427994
C	-3.880730	4.825313	-1.389801
H	-4.966976	4.806645	-1.479349

H	-3.466362	4.682772	-2.389619
H	-3.602118	5.839894	-1.079269
C	-3.744716	0.027135	-3.241753
H	-4.723445	-0.402867	-3.017787
H	-2.986480	-0.521845	-2.686878
H	-3.557368	-0.148742	-4.307747
C	-4.788383	2.228578	-3.748521
H	-5.770128	1.771119	-3.601592
H	-4.564109	2.147620	-4.819264
H	-4.872885	3.292910	-3.518063
C	-2.326716	2.087812	-3.346434
H	-1.534914	1.811415	-2.650443
H	-2.334808	3.178020	-3.419647
H	-2.046237	1.717092	-4.339420
C	-2.292351	0.953020	2.142742
H	-3.264661	0.955359	2.640080
H	-1.984728	1.993049	2.043211
H	-1.582695	0.480546	2.820102
B	-0.114312	-0.169656	-2.933333
Sb	-0.052412	0.112189	-0.722308

(SiiPrDis2)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.089711	0.097666	-0.598911
Si	2.022083	0.309746	-0.375938
C	2.817637	0.996211	-2.141049
H	3.246196	1.925985	-1.775093
C	1.844058	1.409370	-3.239729
H	0.969970	1.927439	-2.846240
H	1.511897	0.562454	-3.840455
H	2.338706	2.097837	-3.935564
C	4.032612	0.280841	-2.724215
H	4.625918	0.985981	-3.319556
H	3.764515	-0.526738	-3.405310
H	4.688876	-0.113942	-1.951256
C	2.523998	-1.509522	0.021640

H	1.570355	-1.867669	0.418679
C	2.396224	1.886074	0.821083
H	1.857206	1.719034	1.752488
Si	3.739572	-1.937257	1.390868
Si	2.775177	-2.766397	-1.426981
Si	1.708160	3.589851	0.066253
Si	4.242446	2.286199	1.273695
C	3.218865	-1.308985	3.088774
H	2.922772	-0.265373	3.059478
H	4.038473	-1.420846	3.805013
H	2.373269	-1.890847	3.466316
C	3.749343	-3.843106	1.799760
H	4.259322	-3.989063	2.757097
H	4.298290	-4.398873	1.038120
H	2.725186	-4.211391	1.890322
C	5.544922	-1.579026	1.040708
H	5.902725	-0.686601	1.551927
H	6.167081	-2.408992	1.391817
H	5.740074	-1.457911	-0.025636
C	4.578578	-3.130361	-1.901686
H	5.121032	-2.233928	-2.200729
H	4.593418	-3.823450	-2.749233
H	5.118894	-3.610873	-1.082716
C	2.081489	-4.502745	-0.900107
H	1.314423	-4.384087	-0.136667
H	2.883992	-5.140936	-0.526057
H	1.639408	-4.994583	-1.771607
C	1.861960	-2.511898	-3.047578
H	2.320413	-3.130483	-3.826680
H	0.824183	-2.838102	-2.965405
H	1.884470	-1.488036	-3.400428
C	2.728178	4.394223	-1.305637
H	3.792404	4.162006	-1.253493
H	2.619735	5.482353	-1.253234
H	2.364291	4.082927	-2.288449
C	1.555388	4.869970	1.500050
H	2.321531	5.643394	1.408572
H	1.645677	4.371836	2.468846
H	0.579289	5.361931	1.453430
C	-0.031160	3.510950	-0.593647

H	-0.173047	4.221091	-1.413962
H	-0.750382	3.766286	0.184654
H	-0.247787	2.519066	-0.963136
C	5.536671	1.824951	0.010095
H	5.412099	2.390062	-0.917086
H	5.514084	0.767237	-0.227766
H	6.536600	2.049393	0.395407
C	4.672096	4.156447	1.630650
H	4.094046	4.515311	2.485008
H	4.522330	4.795722	0.761442
H	5.732730	4.210182	1.898457
C	4.702981	1.630925	3.002560
H	5.044922	0.601357	2.982475
H	3.851927	1.728743	3.682226
H	5.526537	2.223962	3.413716
Sb	-0.629140	-0.543654	-2.679677
Si	-1.685541	0.153314	0.711744
C	-1.026267	0.764742	2.580196
H	-1.845334	0.446476	3.218502
C	-0.910184	2.275276	2.787665
H	-1.852505	2.803833	2.638823
H	-0.174859	2.707348	2.122106
H	-0.599480	2.500566	3.814623
C	0.233180	0.074906	3.074190
H	0.834939	0.726340	3.717162
H	0.846691	-0.257788	2.246448
H	0.004227	-0.798930	3.685942
C	-2.992645	1.606269	0.282182
H	-2.476902	2.472360	0.696594
C	-2.628082	-1.585936	0.917339
H	-3.621226	-1.294597	1.261865
Si	-4.612034	1.495530	1.388572
Si	-3.486359	2.222859	-1.422615
Si	-2.050539	-2.755446	2.310635
Si	-2.933774	-2.568292	-0.662601
C	-5.879110	0.241955	0.768969
H	-5.438613	-0.475372	0.077000
H	-6.707718	0.743934	0.261729
H	-6.299860	-0.317285	1.610399
C	-4.353852	1.118238	3.218784

H	-5.309639	1.203176	3.746663
H	-3.662442	1.821655	3.686383
H	-4.002201	0.099216	3.361561
C	-5.482057	3.198871	1.460650
H	-6.022756	3.407408	0.535630
H	-6.209155	3.202652	2.278518
H	-4.748741	3.988347	1.646613
C	-5.203954	1.743177	-2.076587
H	-5.355004	0.664427	-2.069479
H	-5.304350	2.085890	-3.111686
H	-6.001088	2.219540	-1.501841
C	-3.605649	4.182698	-1.275315
H	-4.551427	4.469032	-0.815141
H	-3.561267	4.615245	-2.278525
H	-2.774235	4.560394	-0.678296
C	-2.371054	2.045881	-2.918064
H	-2.577400	1.119260	-3.456450
H	-2.577319	2.854150	-3.628428
H	-1.314994	2.106158	-2.676940
C	-2.532605	-2.157100	4.051147
H	-2.033394	-1.244351	4.364769
H	-2.271643	-2.931273	4.780411
H	-3.614409	-2.006314	4.103441
C	-0.256191	-3.253023	2.269978
H	0.053143	-3.666878	3.234717
H	0.390177	-2.413661	2.045780
H	-0.089092	-4.024342	1.516425
C	-2.959657	-4.461537	2.342311
H	-2.714725	-4.972146	3.279231
H	-2.616653	-5.096318	1.523163
H	-4.041813	-4.319092	2.304697
C	-4.374919	-3.833696	-0.435311
H	-5.092337	-3.456410	0.298093
H	-4.001112	-4.812716	-0.133546
H	-4.893786	-3.965919	-1.389995
C	-3.639212	-1.602800	-2.107589
H	-3.206423	-0.615994	-2.184678
H	-4.721190	-1.491440	-1.998653
H	-3.459593	-2.132461	-3.048268
C	-1.436926	-3.546527	-1.205408

H	-1.352218	-4.484796	-0.649816
H	-0.528487	-2.970158	-1.029992
H	-1.493754	-3.795792	-2.268919

(SiiPrDis2)-B-Sb-(SiiPrDis2)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	0.473708	-0.776943	-0.752151
Si	2.721460	-0.155537	0.418277
C	2.309129	-0.752013	2.220361
H	1.833845	-1.723068	2.043181
C	1.205550	0.068604	2.908631
H	0.334875	0.189547	2.262236
H	1.517638	1.072956	3.184744
H	0.866318	-0.432960	3.821989
C	3.461923	-1.043812	3.171041
H	3.904962	-2.014180	2.933096
H	3.118991	-1.113009	4.209172
H	4.254810	-0.299997	3.125624
C	2.746449	1.720146	0.227548
H	1.673662	1.928938	0.349564
C	4.035549	-1.156936	-0.500976
H	4.111122	-0.693883	-1.489749
Si	3.023027	2.296587	-1.575089
Si	3.495857	2.908587	1.461746
Si	3.449566	-2.943430	-0.927082
Si	5.791046	-1.173635	0.149029
C	2.042719	1.307922	-2.855111
H	2.326251	0.255430	-2.866816
H	2.223036	1.713096	-3.855751
H	0.978532	1.405052	-2.643511
C	2.332513	4.062674	-1.816320
H	2.357537	4.321594	-2.879216
H	2.914757	4.808497	-1.273543
H	1.293858	4.104228	-1.475803
C	4.799507	2.275735	-2.179207
H	5.210813	1.264675	-2.176213

H	4.839974	2.638384	-3.211673
H	5.453013	2.917521	-1.587912
C	4.948339	3.983966	0.881739
H	5.832608	3.377494	0.679293
H	5.211577	4.688764	1.677608
H	4.708308	4.574900	-0.002831
C	2.077315	4.180202	1.866950
H	1.226817	3.644645	2.297260
H	1.761115	4.696514	0.958735
H	2.446756	4.913846	2.588551
C	4.049745	2.366545	3.177925
H	4.968228	1.782757	3.152818
H	4.274677	3.261630	3.769464
H	3.295670	1.816982	3.735360
C	4.846400	-4.117631	-1.497181
H	5.575349	-4.300305	-0.705314
H	5.346740	-3.711840	-2.380180
H	4.410418	-5.082976	-1.774146
C	2.319948	-2.927129	-2.465110
H	2.469632	-3.846214	-3.040417
H	2.561674	-2.079802	-3.110927
H	1.265716	-2.889537	-2.187228
C	2.567138	-3.852432	0.457408
H	3.125198	-3.793429	1.394887
H	2.459418	-4.911210	0.200842
H	1.562044	-3.456284	0.617285
C	6.442306	0.477954	0.757881
H	7.522363	0.419261	0.926643
H	5.983890	0.743356	1.704944
H	6.265374	1.262629	0.024429
C	6.201533	-2.426216	1.488308
H	7.226509	-2.788392	1.358561
H	5.539243	-3.293612	1.478176
H	6.148140	-1.965833	2.478581
C	6.977237	-1.534906	-1.329840
H	6.553843	-1.136095	-2.255533
H	7.153273	-2.606544	-1.436670
H	7.942444	-1.052878	-1.148254
B	-1.236816	0.179280	0.285557
Si	-2.995594	-0.112277	-0.511651

C	-2.742527	-0.360731	-2.534046
H	-3.694158	-0.004257	-2.936921
C	-2.576423	-1.820272	-2.992561
H	-3.497227	-2.395386	-2.863788
H	-1.769484	-2.326714	-2.452568
H	-2.342515	-1.864522	-4.062842
C	-1.594222	0.439065	-3.147866
H	-1.787067	0.609797	-4.213544
H	-0.653590	-0.114003	-3.097437
H	-1.437719	1.406396	-2.682026
C	-3.754621	-1.777441	0.026837
H	-3.455013	-2.431810	-0.790528
C	-4.028665	1.450623	-0.091307
H	-5.087795	1.197176	-0.160542
Si	-5.637167	-1.856168	-0.131749
Si	-3.056532	-2.777762	1.434664
Si	-3.783727	2.934011	-1.265612
Si	-3.720025	2.061248	1.706559
C	-6.608637	-1.023349	1.238726
H	-6.432240	0.052920	1.268642
H	-6.370573	-1.438741	2.219634
H	-7.680863	-1.171602	1.073793
C	-6.253316	-1.131358	-1.777918
H	-7.327070	-1.316979	-1.879963
H	-5.746132	-1.605008	-2.622000
H	-6.095659	-0.053130	-1.826393
C	-6.225771	-3.669574	-0.207787
H	-6.095791	-4.170049	0.754136
H	-7.288848	-3.700172	-0.465081
H	-5.668527	-4.213662	-0.975583
C	-4.115324	-2.967506	2.979044
H	-4.277391	-2.015877	3.485200
H	-3.609637	-3.630656	3.688797
H	-5.086046	-3.415670	2.755539
C	-2.843090	-4.589824	0.766777
H	-3.814234	-5.026857	0.529032
H	-2.355977	-5.199575	1.532841
H	-2.219290	-4.573890	-0.131149
C	-1.324478	-2.367055	2.020824
H	-1.276086	-1.377475	2.470657

H	-1.005089	-3.085923	2.782411
H	-0.611981	-2.429843	1.198461
C	-4.432613	2.577699	-3.013735
H	-3.664610	2.140319	-3.651824
H	-4.747682	3.511732	-3.489706
H	-5.297681	1.911089	-2.976136
C	-2.023615	3.588880	-1.366652
H	-1.766404	3.835549	-2.401363
H	-1.292911	2.866493	-0.994554
H	-1.916310	4.504646	-0.777922
C	-4.870394	4.428764	-0.756639
H	-4.955545	5.122154	-1.598964
H	-4.414132	4.973085	0.072932
H	-5.873821	4.094427	-0.480603
C	-5.205048	3.123265	2.278140
H	-6.128271	2.761609	1.817173
H	-5.060612	4.175600	2.028845
H	-5.310726	3.053421	3.365087
C	-3.685535	0.699686	3.001358
H	-2.796279	0.082693	2.899462
H	-4.582455	0.086044	2.930704
H	-3.662335	1.136648	4.004907
C	-2.149645	3.064737	1.962220
H	-2.239437	4.063886	1.528904
H	-1.278058	2.568824	1.527909
H	-1.959835	3.191925	3.032874

B-Sb(SiiPrDis2)2

Atomic Number	Coordinates (Angstroms) X	Y	Z

Sb	0.125717	-0.088964	-1.148116
Si	-2.436159	-0.205271	-0.516977
C	-3.405634	-0.723911	-2.173198
H	-3.779190	-1.714424	-1.915009
C	-2.524317	-0.940670	-3.406530
H	-1.727525	-1.661381	-3.215123
H	-2.056512	-0.020020	-3.752913

H	-3.120102	-1.337537	-4.236519
C	-4.655588	0.070730	-2.542521
H	-5.328017	-0.552683	-3.144240
H	-4.426053	0.942315	-3.156339
H	-5.215614	0.400525	-1.666719
C	-2.691948	1.591775	0.063280
H	-1.708891	1.801573	0.499248
C	-2.673845	-1.754740	0.682099
H	-2.095125	-1.566489	1.589754
Si	-3.849151	2.008152	1.463441
Si	-2.801851	2.936770	-1.296723
Si	-1.892840	-3.398639	-0.101590
Si	-4.460754	-2.278340	1.213659
C	-3.263017	1.216421	3.078266
H	-2.921479	0.193927	2.933831
H	-4.063478	1.227060	3.823548
H	-2.424523	1.789316	3.486091
C	-3.810119	3.860309	2.003087
H	-4.472458	3.987602	2.865236
H	-4.157927	4.523464	1.209806
H	-2.797802	4.138612	2.307488
C	-5.656807	1.692890	1.107017
H	-5.818191	0.728723	0.630838
H	-6.240103	1.720504	2.032723
H	-6.071969	2.458995	0.447571
C	-4.555938	3.529547	-1.701540
H	-5.249735	2.700714	-1.844072
H	-4.538134	4.115079	-2.626359
H	-4.948829	4.177276	-0.914380
C	-1.860335	4.518792	-0.733467
H	-1.856203	4.634974	0.348336
H	-2.327696	5.399732	-1.183022
H	-0.826242	4.467907	-1.080733
C	-1.977435	2.588897	-2.950352
H	-1.725747	3.534448	-3.442594
H	-1.051550	2.036623	-2.818473
H	-2.634119	2.051258	-3.633071
C	-2.967547	-4.327135	-1.348445
H	-3.984070	-4.511055	-1.002117
H	-2.513547	-5.301900	-1.556032

H	-3.020253	-3.788206	-2.297617
C	-1.465125	-4.587605	1.349716
H	-2.167527	-5.423318	1.386086
H	-1.481137	-4.049062	2.300853
H	-0.461685	-4.999353	1.205050
C	-0.249616	-3.241506	-0.970144
H	-0.357846	-2.719259	-1.918382
H	0.145073	-4.235826	-1.203522
H	0.480171	-2.742502	-0.337399
C	-5.803980	-2.199186	-0.092322
H	-5.544395	-2.769782	-0.986343
H	-6.030907	-1.176527	-0.385980
H	-6.729268	-2.628204	0.306641
C	-4.592219	-4.106889	1.893277
H	-3.890361	-4.243256	2.719298
H	-4.426672	-4.850460	1.114595
H	-5.606518	-4.253465	2.278569
C	-5.094680	-1.431125	2.792097
H	-5.421377	-0.413121	2.617525
H	-4.329890	-1.454038	3.572510
H	-5.966225	-1.975470	3.171189
B	0.580437	0.254240	-3.305304
Si	2.126816	-0.034712	0.538631
C	1.305930	-0.374404	2.391907
H	2.065489	-0.029665	3.091970
C	1.035865	-1.855369	2.697974
H	1.958926	-2.430596	2.801650
H	0.427919	-2.319619	1.921551
H	0.504086	-1.966463	3.649973
C	0.015443	0.394355	2.637512
H	-0.365876	0.197132	3.645623
H	-0.747246	0.095862	1.927254
H	0.130664	1.469592	2.556164
C	3.292640	-1.589823	0.338256
H	2.721344	-2.359590	0.860113
C	3.083636	1.634829	0.466887
H	4.096100	1.414754	0.810547
Si	4.903110	-1.445376	1.390931
Si	3.657374	-2.466446	-1.276638
Si	2.528407	3.035919	1.626798

Si	3.290814	2.337040	-1.288486
C	6.248579	-0.398801	0.587033
H	5.843612	0.281239	-0.164038
H	6.998203	-1.032371	0.104730
H	6.763755	0.201311	1.343427
C	4.652699	-0.766525	3.134942
H	5.595104	-0.818755	3.689681
H	3.912162	-1.349546	3.686975
H	4.350533	0.278161	3.105680
C	5.638932	-3.174983	1.728430
H	6.079973	-3.606737	0.828148
H	6.427163	-3.096292	2.483403
H	4.862310	-3.844717	2.108428
C	5.408810	-2.333818	-1.984583
H	5.712787	-1.297355	-2.133123
H	5.444190	-2.832024	-2.959042
H	6.142494	-2.828432	-1.344425
C	3.471938	-4.377091	-0.871045
H	4.256797	-4.696359	-0.184745
H	3.556625	-4.946389	-1.800636
H	2.493767	-4.556029	-0.418942
C	2.525601	-2.277587	-2.754014
H	2.968950	-1.639818	-3.522656
H	2.345771	-3.249895	-3.224295
H	1.562881	-1.872274	-2.476401
C	2.727268	2.659413	3.474975
H	2.002908	1.939652	3.850647
H	2.578147	3.581885	4.046334
H	3.737809	2.303949	3.687304
C	0.790299	3.653820	1.311804
H	0.267841	3.859390	2.250864
H	0.213793	2.920371	0.748208
H	0.810934	4.585017	0.739189
C	3.650008	4.591564	1.482715
H	3.488848	5.234914	2.353307
H	3.392979	5.171017	0.593751
H	4.703212	4.301063	1.458524
C	4.819999	3.495862	-1.357810
H	5.577284	3.164328	-0.642275
H	4.543259	4.530911	-1.152438

H	5.255974	3.465602	-2.361177
C	3.747283	1.081269	-2.598625
H	2.967696	0.337248	-2.694672
H	4.694306	0.600724	-2.356189
H	3.862246	1.566935	-3.572770
C	1.817794	3.303018	-1.925515
H	1.769238	4.298273	-1.475913
H	0.886539	2.778690	-1.709184
H	1.886238	3.436287	-3.009565

(NHC)2B-Sb

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.564268	-2.244309	1.892144
Sb	0.832518	-2.562027	0.309828
C	-2.202106	-2.230125	1.734386
N	-2.703262	-2.108247	0.305690
C	-3.831487	-1.267489	0.251452
C	-4.018759	-0.683921	1.452097
N	-3.015657	-1.104770	2.373858
H	-4.400679	-1.156713	-0.657619
H	-4.800825	-0.008801	1.758448
C	-3.332316	-1.027305	3.780052
C	-3.959688	-0.789143	6.524816
C	-4.205371	-1.972978	4.397695
C	-2.878252	0.109957	4.516859
C	-3.193831	0.196473	5.888859
C	-4.477049	-1.849778	5.776975
H	-2.852172	1.046777	6.468965
H	-5.126602	-2.573506	6.263144
H	-4.181508	-0.708030	7.585843
C	-2.338313	-2.964956	-0.767418
C	-1.519622	-4.732093	-2.824059
C	-1.561051	-2.460402	-1.864184
C	-2.813775	-4.315234	-0.794599
C	-2.376612	-5.182338	-1.811308
C	-1.149001	-3.386492	-2.860385

H	-2.720462	-6.213641	-1.823623
H	-0.540340	-3.028381	-3.687964
H	-1.178435	-5.416286	-3.596343
C	-3.875097	-4.827549	0.184113
H	-4.163952	-4.006832	0.844786
C	-5.161441	-5.255127	-0.568630
H	-4.985526	-6.128960	-1.208941
H	-5.541749	-4.443566	-1.201080
H	-5.945855	-5.523920	0.151472
C	-3.349147	-5.984346	1.060351
H	-3.004239	-6.827329	0.448012
H	-4.137797	-6.354236	1.726265
H	-2.509768	-5.657110	1.680085
C	-1.245466	-0.985217	-2.207197
H	-0.227614	-1.006381	-2.624113
C	-2.190959	-0.514074	-3.348148
H	-3.234237	-0.501441	-3.006684
H	-2.129012	-1.160483	-4.230893
H	-1.922744	0.506577	-3.650806
C	-1.244846	0.097046	-1.109636
H	-0.733632	-0.229292	-0.204237
H	-2.254982	0.411606	-0.831479
H	-0.712429	0.976415	-1.496850
C	-2.146408	1.272506	3.834744
H	-1.499498	0.851290	3.054933
C	-3.151238	2.237221	3.148134
H	-3.864963	2.635047	3.882869
H	-3.714149	1.754064	2.346941
H	-2.611411	3.087323	2.709627
C	-1.278535	2.107775	4.798590
H	-0.627217	1.481026	5.412345
H	-1.898153	2.721318	5.466772
H	-0.644054	2.792515	4.226188
C	-4.974390	-3.045697	3.618199
H	-4.679609	-3.001397	2.568493
C	-4.691606	-4.475144	4.129212
H	-3.628110	-4.721757	4.051578
H	-5.256314	-5.208005	3.539138
H	-4.991803	-4.596088	5.178129
C	-6.496504	-2.749545	3.655560

H	-7.037592	-3.465517	3.022657
H	-6.712217	-1.738474	3.289841
H	-6.897617	-2.832576	4.673758
C	0.153862	-2.244862	3.438729
N	0.711393	-3.619888	3.793255
C	2.106999	-3.573176	3.673836
C	2.523632	-2.290019	3.491799
N	1.413960	-1.406862	3.501299
H	-0.569277	-1.901867	4.193314
H	2.710276	-4.459572	3.800300
H	3.534543	-1.911779	3.480900
C	1.599090	-0.097005	4.085029
C	2.389136	2.395980	5.152215
C	1.769347	0.051847	5.490960
C	1.805069	1.017548	3.217012
C	2.209254	2.246997	3.772341
C	2.157692	1.309092	6.000489
H	2.395143	3.094077	3.119196
H	2.295607	1.433830	7.070888
H	2.704233	3.352144	5.560825
C	-0.007968	-4.856843	3.906440
C	-1.400503	-7.307601	4.190608
C	0.158949	-5.894837	2.932367
C	-0.805922	-5.099214	5.066482
C	-1.510674	-6.314389	5.170993
C	-0.549316	-7.103044	3.102310
H	-2.125934	-6.506133	6.043988
H	-0.437577	-7.890609	2.362254
H	-1.950213	-8.239637	4.289664
C	1.574461	-1.096542	6.481983
H	1.254808	-1.987228	5.935906
C	2.902113	-1.451604	7.195291
H	3.684477	-1.697811	6.467484
H	2.762948	-2.318445	7.853575
H	3.262886	-0.616559	7.809370
C	0.468581	-0.761388	7.513601
H	0.733946	0.114732	8.118926
H	0.316277	-1.603193	8.200464
H	-0.485183	-0.550419	7.015841
C	1.667300	0.899331	1.701194

H	1.016931	0.047054	1.492533
C	3.036865	0.604938	1.042169
H	3.485238	-0.311324	1.444200
H	3.739681	1.431978	1.210017
H	2.916433	0.468250	-0.040240
C	1.012581	2.133780	1.041725
H	0.041938	2.362098	1.499608
H	0.844292	1.934359	-0.023023
H	1.644764	3.028168	1.108446
C	-0.762841	-4.162441	6.277597
H	-0.637714	-3.132225	5.931821
C	-2.031571	-4.191649	7.156515
H	-1.996398	-3.368458	7.880721
H	-2.111313	-5.126378	7.726430
H	-2.937650	-4.071389	6.556900
C	0.471175	-4.538228	7.141646
H	0.530541	-3.898046	8.030811
H	1.405413	-4.433616	6.578787
H	0.394283	-5.580009	7.480100
C	1.116270	-5.817034	1.736876
H	1.518031	-4.804122	1.666087
C	2.316136	-6.778799	1.916766
H	2.838211	-6.604116	2.866191
H	3.034985	-6.636581	1.099047
H	1.991980	-7.827302	1.901942
C	0.408381	-6.094764	0.393744
H	-0.431855	-5.411387	0.252645
H	0.032907	-7.123925	0.324891
H	1.104871	-5.929090	-0.438186
H	-2.536757	-3.199872	2.169787

NHC-B-Sb-NHC

Atomic Number	Coordinates (Angstroms) X	Y	Z
B	-0.611896	-2.681482	3.511722
Sb	-1.244863	-3.035360	1.609440
C	-2.847500	-1.371494	1.188042

N	-3.384461	-1.447267	-0.171441
C	-4.759504	-1.763680	-0.109017
C	-5.155481	-1.779846	1.191294
N	-4.047988	-1.480450	2.015216
H	-2.275976	-0.451405	1.365499
H	-5.341647	-1.901970	-1.004610
H	-6.135160	-1.938445	1.608905
C	-4.009041	-1.531819	3.446355
C	-3.819477	-1.603428	6.255552
C	-4.206476	-2.768801	4.133754
C	-3.719164	-0.339031	4.164191
C	-3.610106	-0.400859	5.568389
C	-4.127584	-2.769328	5.541715
H	-3.380126	0.501760	6.128582
H	-4.281113	-3.698359	6.083834
H	-3.744536	-1.632318	7.340002
C	-2.564552	-1.505327	-1.353190
C	-0.878154	-1.662940	-3.616752
C	-2.058240	-0.307683	-1.938721
C	-2.260687	-2.779245	-1.933677
C	-1.424928	-2.828824	-3.067717
C	-1.200784	-0.421875	-3.056666
H	-1.192910	-3.788796	-3.520586
H	-0.796738	0.484933	-3.502478
H	-0.223158	-1.718987	-4.482795
C	-2.839823	-4.098684	-1.405687
H	-3.245387	-3.928025	-0.403915
C	-4.006525	-4.580290	-2.305367
H	-3.647757	-4.811266	-3.316825
H	-4.790230	-3.818623	-2.391138
H	-4.456525	-5.490450	-1.887508
C	-1.775225	-5.216552	-1.285364
H	-1.425932	-5.560817	-2.266852
H	-2.202462	-6.081057	-0.761988
H	-0.907564	-4.874343	-0.712374
C	-2.364626	1.135276	-1.498513
H	-2.287565	1.724576	-2.424909
C	-3.780884	1.413840	-0.949876
H	-3.914665	1.054962	0.074155
H	-4.551550	0.944842	-1.573047

H	-3.957943	2.498185	-0.951724
C	-1.273599	1.696573	-0.548819
H	-0.279770	1.626547	-1.006839
H	-1.236584	1.154798	0.402538
H	-1.475340	2.753080	-0.327510
C	-3.564369	1.010875	3.462390
H	-3.796841	0.872662	2.401113
C	-4.579345	2.045486	4.008509
H	-4.378250	2.292023	5.058906
H	-5.604872	1.661254	3.942575
H	-4.521325	2.976008	3.428993
C	-2.115746	1.545573	3.571937
H	-1.385553	0.818901	3.195618
H	-1.852073	1.761138	4.615081
H	-2.002036	2.474212	2.997771
C	-4.519224	-4.086021	3.414881
H	-4.307183	-3.957249	2.347897
C	-3.642316	-5.258944	3.914018
H	-2.582775	-4.995317	3.877913
H	-3.796696	-6.139977	3.276665
H	-3.884366	-5.550814	4.943349
C	-6.019316	-4.447364	3.565766
H	-6.250015	-5.359253	2.999507
H	-6.670072	-3.642152	3.203887
H	-6.267602	-4.631200	4.619373
C	0.583959	-2.745856	4.544172
N	1.107656	-4.154827	4.605701
C	2.495662	-4.155507	4.303880
C	2.881411	-2.913712	3.920465
N	1.773913	-2.035445	3.956007
H	0.346241	-2.363978	5.552081
H	3.079922	-5.057303	4.388167
H	3.853441	-2.566213	3.611655
C	1.769108	-0.658883	3.576171
C	1.665663	2.066214	2.850852
C	1.624737	0.339795	4.581857
C	1.907279	-0.287070	2.201731
C	1.864096	1.082978	1.870993
C	1.548312	1.692820	4.195530
H	1.972662	1.384650	0.832352

H	1.420704	2.461176	4.953811
H	1.616688	3.115247	2.569264
C	0.384874	-5.262214	5.155809
C	-1.114066	-7.404149	6.214746
C	0.029821	-6.361254	4.315159
C	0.044422	-5.273417	6.539016
C	-0.735986	-6.336137	7.038737
C	-0.707673	-7.424858	4.873268
H	-1.023574	-6.343359	8.087252
H	-0.982537	-8.271198	4.249336
H	-1.704079	-8.223036	6.619053
C	1.606266	-0.008942	6.072699
H	1.835142	-1.074426	6.177777
C	2.711759	0.753420	6.844517
H	3.694818	0.586952	6.387096
H	2.753353	0.408054	7.886061
H	2.524344	1.834559	6.858664
C	0.216275	0.254478	6.705509
H	-0.035717	1.322461	6.661736
H	0.207737	-0.052315	7.759693
H	-0.573790	-0.296291	6.181980
C	2.146109	-1.311570	1.087598
H	1.865279	-2.298042	1.469335
C	3.644963	-1.350624	0.693737
H	4.286004	-1.558152	1.558083
H	3.956725	-0.388549	0.265569
H	3.818509	-2.130673	-0.059408
C	1.294219	-1.044617	-0.174967
H	0.240929	-0.907912	0.081775
H	1.355052	-1.899666	-0.860383
H	1.630898	-0.154898	-0.722627
C	0.551165	-4.206908	7.514662
H	1.248603	-3.553394	6.981037
C	-0.607046	-3.337517	8.064566
H	-0.218288	-2.545056	8.717925
H	-1.307903	-3.945819	8.651380
H	-1.172626	-2.867958	7.251570
C	1.355624	-4.844987	8.675702
H	1.797488	-4.061528	9.305627
H	2.167340	-5.475189	8.291751

H	0.718376	-5.468291	9.315785
C	0.469132	-6.445496	2.850319
H	0.811313	-5.452491	2.540131
C	1.660464	-7.428506	2.702339
H	2.497189	-7.147856	3.353072
H	2.020871	-7.438324	1.665141
H	1.357123	-8.450407	2.966764
C	-0.672509	-6.861032	1.893119
H	-1.514260	-6.165483	1.961546
H	-1.039783	-7.874223	2.101889
H	-0.309862	-6.846574	0.857718

B-Sb(NHC)2

Atomic Number	Coordinates (Angstroms) X	Y	Z
Sb	-0.409181	-1.821562	1.755761
B	0.899759	-2.422402	-0.000254
C	-2.677983	-2.196904	1.524423
N	-3.124674	-2.071403	0.123251
C	-4.280066	-1.255708	0.062714
C	-4.527505	-0.745072	1.291970
N	-3.540739	-1.211670	2.197001
H	-4.818446	-1.122457	-0.860749
H	-5.318836	-0.092617	1.622516
C	-3.642106	-1.074423	3.620652
C	-3.861014	-0.778043	6.410916
C	-4.355687	-2.043560	4.377127
C	-3.086141	0.079145	4.250995
C	-3.208056	0.202792	5.650774
C	-4.436148	-1.885391	5.776171
H	-2.801114	1.076601	6.151684
H	-4.974930	-2.619931	6.369435
H	-3.940105	-0.667977	7.489779
C	-2.647407	-2.892841	-0.945820
C	-1.609619	-4.603076	-2.936948
C	-1.828595	-2.342890	-1.982198
C	-3.023328	-4.268403	-0.975412

C	-2.480084	-5.109444	-1.964813
C	-1.314053	-3.235763	-2.953281
H	-2.750216	-6.162224	-1.984324
H	-0.674022	-2.840981	-3.739658
H	-1.186022	-5.262640	-3.690078
C	-4.076900	-4.844172	-0.023519
H	-4.429551	-4.045342	0.636228
C	-5.314849	-5.334339	-0.816843
H	-5.066000	-6.183496	-1.465720
H	-5.719949	-4.534746	-1.449313
H	-6.104121	-5.659493	-0.126181
C	-3.511896	-5.976842	0.863229
H	-3.135905	-6.810226	0.256154
H	-4.291785	-6.369833	1.527432
H	-2.685046	-5.620736	1.485982
C	-1.557526	-0.852007	-2.274129
H	-0.611484	-0.840392	-2.834482
C	-2.653561	-0.310488	-3.231647
H	-3.633323	-0.299993	-2.738175
H	-2.733901	-0.918831	-4.140135
H	-2.415186	0.720467	-3.524342
C	-1.364865	0.139045	-1.112000
H	-0.636013	-0.227963	-0.389510
H	-2.294497	0.355656	-0.577155
H	-0.972142	1.085205	-1.510189
C	-2.457415	1.213062	3.436491
H	-2.095179	0.789661	2.492725
C	-3.527005	2.285013	3.102071
H	-3.917261	2.742958	4.021385
H	-4.371578	1.858018	2.550609
H	-3.086952	3.080567	2.486668
C	-1.258351	1.881526	4.140918
H	-0.535748	1.139275	4.490352
H	-1.572737	2.486643	5.001911
H	-0.739320	2.550693	3.444693
C	-5.106138	-3.201733	3.716616
H	-4.972400	-3.132902	2.632926
C	-4.567994	-4.576791	4.171083
H	-3.500724	-4.680347	3.948438
H	-5.102473	-5.385829	3.657557

H	-4.700622	-4.722195	5.250867
C	-6.628101	-3.088728	3.980211
H	-7.167225	-3.870821	3.430133
H	-7.012501	-2.113812	3.656038
H	-6.861490	-3.205609	5.046111
C	0.567257	-2.299115	3.814499
N	0.988108	-3.682784	4.064043
C	2.398951	-3.744694	4.089911
C	2.906873	-2.492246	3.987377
N	1.840735	-1.566605	3.867476
H	-0.173147	-1.920742	4.532412
H	2.911326	-4.685304	4.212722
H	3.931105	-2.158154	4.016568
C	1.974872	-0.190194	4.268591
C	2.364262	2.469645	5.100496
C	1.879519	0.136525	5.650174
C	2.286161	0.808696	3.301488
C	2.474413	2.134387	3.745329
C	2.071276	1.476033	6.043247
H	2.715623	2.910304	3.023382
H	2.005871	1.740911	7.095252
H	2.515465	3.496928	5.422048
C	0.143916	-4.840890	4.055669
C	-1.399851	-7.197567	4.128004
C	0.181127	-5.742538	2.950036
C	-0.655883	-5.128206	5.201633
C	-1.424550	-6.308223	5.211386
C	-0.599482	-6.917020	3.015919
H	-2.031120	-6.550855	6.078430
H	-0.578476	-7.619125	2.186675
H	-1.994370	-8.107338	4.157059
C	1.621456	-0.920646	6.726188
H	1.486337	-1.893260	6.245146
C	2.843169	-1.059642	7.667549
H	3.751174	-1.291680	7.097752
H	2.677517	-1.868398	8.391088
H	3.023768	-0.134359	8.229290
C	0.333614	-0.615904	7.528999
H	0.420866	0.326728	8.084101
H	0.139101	-1.415172	8.256068

H	-0.537264	-0.536140	6.867344
C	2.471240	0.499900	1.815468
H	2.165580	-0.534912	1.637606
C	3.959358	0.610457	1.406111
H	4.586717	-0.051319	2.016138
H	4.330446	1.636758	1.526098
H	4.081378	0.323052	0.354150
C	1.588047	1.399336	0.918792
H	0.536975	1.339341	1.222108
H	1.653795	1.066913	-0.124681
H	1.901256	2.450845	0.958986
C	-0.591791	-4.250854	6.455712
H	-0.413517	-3.215869	6.149095
C	-1.889325	-4.248879	7.293361
H	-1.827677	-3.472579	8.066648
H	-2.047746	-5.207226	7.804344
H	-2.765013	-4.035946	6.672620
C	0.605960	-4.691393	7.336985
H	0.678135	-4.058068	8.231100
H	1.552856	-4.621621	6.790247
H	0.476924	-5.731031	7.665772
C	1.077429	-5.533842	1.723822
H	1.499505	-4.524815	1.762583
C	2.255507	-6.540170	1.729485
H	2.835141	-6.480909	2.658634
H	2.930593	-6.333033	0.889742
H	1.892135	-7.571108	1.625997
C	0.297517	-5.643069	0.394590
H	-0.538062	-4.939518	0.372700
H	-0.100423	-6.652369	0.227982
H	0.955093	-5.394886	-0.447297
H	-2.813305	-3.214993	1.932018
