

Electronic Supplementary Information for:

" Conformational properties of six-membered heterocycles: Accurate relative energy differences with DFT, the importance of dispersion interactions and silicon substitution effects "

Ragnar Bjornsson and Ingvar Arnason

Contents:	page
Table S1. Alternative version of Table 1 with additional data.	S2
Table S2. Total energies of molecules in Table 1 and S1 with different methods.	S3
Table S3. Total energies of 2-ethoxytetrahydropyran with different methods.	S4
Figure S1 - S4. Graphical diagrams showing the trends in ΔE values of the silacyclohexane families.	S5-S6
Figure S5 . Correlation diagrams of silacyclohexane families.	S7-S8
Table S4. Total energies of 1-trichloromethyl-2,3,4,5,6-pentasilacyclohexane.	S9
Table S5. The convergence of ΔE values with different methods and basis sets.	S10
Table S6. Total energies of molecules in tables 3-7.	S11
Table S7. Cartesian coordinates of all molecules in tables 3-7.	S12-S168

The single-point energy calculations in Table 1 and Table S1 were done using geometries from Tschumper et al. that can be found in the supporting material of references 14 and 15. M06-2X, PBE, PBE0 and B97-1 calculations were done in NWChem and all other calculations (including all dispersion correction calculations) in Orca.

Table S1. Alternative version of Table 1 including data for M06-2X/pc-2, B97-1, PBE, PBE-D, PBE0, TPSS and TPSS-D functionals. Energy differences (kcal/mol) between the axial and equatorial conformers of selected cyclohexanes and heterocycles.

	CCSD(T) ^a	M06-2X/pc-2	PBE ^b	PBE-D ^{b,d}	PBE0 ^{b,d}	B97-1 ^b	TPSS ^c	TPSS-D ^{c,d}
1a	1.75	1.69	2.24	1.48	2.19	2.15	2.07	1.06
1b	0.20	0.14	0.60	0.39	0.52	0.51	0.45	0.18
1c	0.21	0.05	1.02	0.46	0.89	0.97	0.84	0.10
1d	0.56	0.45	1.12	0.86	1.01	1.01	0.87	0.52
2a	2.82	2.60	3.23	2.42	3.18	3.12	3.05	1.96
2b	-2.45	-2.50	-2.13	-2.31	-2.07	-2.15	-2.47	-2.71
2c	-1.27	-1.35	-0.35	-0.92	-0.46	-0.46	-0.69	-1.45
2d	-0.86	-0.91	-0.20	-0.46	-0.26	-0.33	-0.61	-0.96
3a	0.21	0.08	0.58	0.06	0.54	0.53	0.59	-0.10
3b	-0.09	-0.20	-0.06	-0.16	-0.10	-0.11	-0.07	-0.20
3c	-0.15	-0.29	0.21	-0.23	0.17	0.20	0.25	-0.34
3d	0.03	-0.10	0.18	0.01	0.14	0.13	0.16	-0.06
3e	-0.40	-0.63	0.03	-0.36	0.03	-0.01	0.06	-0.47
	MAD	0.19	0.74	0.33	0.66	0.63	0.50	0.38
	MD	-0.19	0.74	0.08	0.65	0.63	0.49	-0.38
	MaxD	0.23	0.92	-0.40	0.81	0.81	0.63	-0.86

^a References 14 and 15.

^b The pc-3 basis set was used.

^c The def2-QZVPP basis set was used.

^d Dispersion correction calculated using Orca version 2.6.71beta.

Table S2. Total energies in hartrees (ZPE exclusive) of all molecules in table1 and table S1.

	CH₃		F		OCH₃		OH		Cl	
M06-2X^b	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>
cyclohexane	-275.1752141	-275.1779309	-335.1271044	-335.1273474	-350.3951581	-350.3953418	-311.0982023	-311.0990037		
2-tetrahydropyran	-311.0850213	-311.0891517	-371.0446072	-371.0406853	-386.2947184	-386.2925663	-346.9990997	-346.9976451		
silacyclohexane	-526.580406	-526.5805644	-586.5951825	-586.5949121	-601.8408436	-601.8404742	-562.5518961	-562.551793	-946.9307549	-946.909514
B3LYP^a										
cyclohexane	-275.1109010	-275.1146706	-335.0698165	-335.070617	-350.323212	-350.3249767	-311.0359305	-311.0376281		
2-tetrahydropyran	-311.0239061	-311.0292967	-370.989331	-370.9856831	-386.2455784	-386.2449959	-346.9577984	-346.9572437		
silacyclohexane	-526.4806192	-526.4817309	-586.4967505	-586.4965492	-601.7318857	-601.7323697	-562.4507302	-562.4509853	-946.7900863	-946.7903143
B3LYP-D^a										
cyclohexane	-275.1399024	-275.1419912	-335.0924205	-335.0927584	-350.3527105	-350.3532257	-311.0600474	-311.0611629		
2-tetrahydropyran	-311.0476017	-311.0511711	-371.0071542	-371.0030968	-386.2694355	-386.2675711	-346.9768901	-346.9757486		
silacyclohexane	-526.5068538	-526.5068028	-586.5192518	-586.5188302	-601.7591034	-601.7586117	-562.4737084	-562.4735961	-946.8139871	-946.8133308
B2PLYP^a										
cyclohexane	-275.105881	-275.1092181	-335.0625881	-335.0631522	-350.3164001	-350.3174189	-311.0305646	-311.0318564		
2-tetrahydropyran	-311.0169283	-311.0219938	-370.9808418	-370.9769816	-386.2373057	-386.2360094	-346.8633657	-346.862397		
silacyclohexane	-526.4776278	-526.4783452	-586.4965289	-586.4962827	-601.7322322	-601.7323232	-562.4506361	-562.4507263	-946.7923128	-946.7919921
B2PLYP-D^a										
cyclohexane	-275.1210722	-275.1235288	-335.0744282	-335.0747501	-350.3318517	-350.3322159	-311.0431973	-311.0441841		
2-tetrahydropyran	-311.0293402	-311.0334518	-370.9901777	-370.9861031	-386.2498023	-386.2478345	-346.9610245	-346.9597387		
silacyclohexane	-526.4913697	-526.4914782	-586.5083153	-586.5079537	-601.7464891	-601.7460690	-562.4626723	-562.46257	-946.8048322	-946.8040483
B97-1^b										
cyclohexane	-275.2169865	-275.2204168	-335.1666017	-335.1674210	-350.4390387	-350.4405810	-311.1373081	-311.1389221		
2-tetrahydropyran	-311.1242413	-311.1292249	-371.0810976	-371.0776763	-386.3559538	-386.3552189	-347.0538739	-347.0533409		
silacyclohexane	-526.6096428	-526.6104919	-586.6171589	-586.6169874	-601.8729005	-601.8732121	-562.5747579	-562.5749707	-946.9221417	-946.9221274
TPSS^a										
cyclohexane	-275.3775146	-275.3792087	-335.3335809	-335.3338626	-350.6300794	-350.6302326	-311.2997922	-311.3006178		
2-tetrahydropyran	-311.2911370	-311.2942649	-371.2545775	-371.2502574	-386.5528472	-386.5505346	-347.2227057	-347.2211779		
silacyclohexane	-526.8000148	-526.7998503	-586.8152255	-586.8149047	-602.0939230	-602.0933867	-562.7683422	-562.768243	-947.1536743	-947.1529198
TPSS-D^a										
cyclohexane	-275.3498942	-275.3531891	-335.3120533	-335.3127755	-350.6019856	-350.6033288	-311.2768237	-311.2782037		
2-tetrahydropyran	-311.2685698	-311.2734322	-371.237603	-371.2336729	-386.5301262	-386.5290344	-347.2045232	-347.2035542		
silacyclohexane	-526.7750295	-526.7759723	-586.7937956	-586.7936847	-602.0680013	-602.0683943	-562.7464582	-562.7467089	-947.1309117	-947.1309994
PBE^b										
cyclohexane	-274.9117881	-274.91535	-334.8450039	-334.8459585	-350.0827112	-350.0843435	-310.8249967	-310.8267811		
2-tetrahydropyran	-310.8117535	-310.8169076	-370.7522067	-370.7488135	-385.9921721	-385.9916139	-346.7342094	-346.7338912		
silacyclohexane	-526.2199106	-526.2208370	-586.2095947	-586.2094977	-601.430112	-601.4304489	-562.1763839	-562.1766638	-946.4392661	-946.4393149
PBE-D^b										
cyclohexane	-274.9325034	-274.9348647	-334.8611496	-334.8617738	-350.1037815	-350.1045213	-310.8422231	-310.8435917		
2-tetrahydropyran	-310.8286789	-310.8325322	-370.7649375	-370.7612519	-386.0092129	-386.0077390	-346.7478463	-346.7471090		
silacyclohexane	-526.2386495	-526.2387456	-586.2256671	-586.2254127	-601.4495533	-601.4491932	-562.1927970	-562.1928144	-946.4563380	-946.4557552
PBE0^b										
cyclohexane	-274.9661588	-274.9696494	-334.8866385	-334.8874678	-350.1319159	-350.1333391	-310.8672563	-310.8688606		
2-tetrahydropyran	-310.8528990	-310.8579724	-370.7809760	-370.7776821	-386.0285994	-386.0278699	-346.7636143	-346.7631999		
silacyclohexane	-526.2955024	-526.2963593	-586.2746611	-586.2745074	-601.502434	-601.5027008	-562.2417496	-562.2419736	-946.5411404	-946.5410065

^a The def2-QZVPP basis set was used.^b The pc-4 basis set was used.

Table S3. Total energies in hartrees (ZPE exclusive) of 2-ethoxytetrahydropyran with different methods.

	<i>axial</i>	<i>equatorial</i>
B3LYP^a	-425.5521818	-425.5518083
B3LYP-D^a	-425.5797129	-425.5778148
B2PLYP^a	-425.5431028	-425.5419047
B2PLYP-D^a	-425.5575238	-425.5555271
M06-2X^b	-425.6304835	-425.6284070

^a The def2-QZVPP basis set was used.

^b The pc-3 basis set was used.

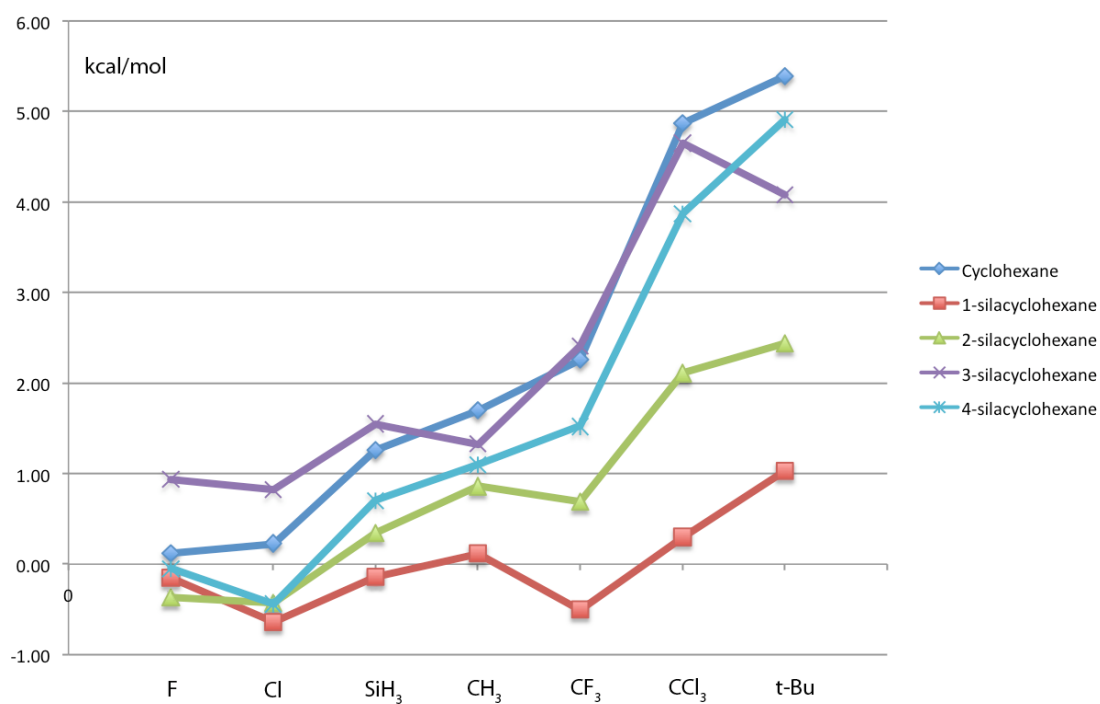


Figure S1. Graphical diagram showing the trends in ΔE values of the monosilacyclohexane families compared to cyclohexane.

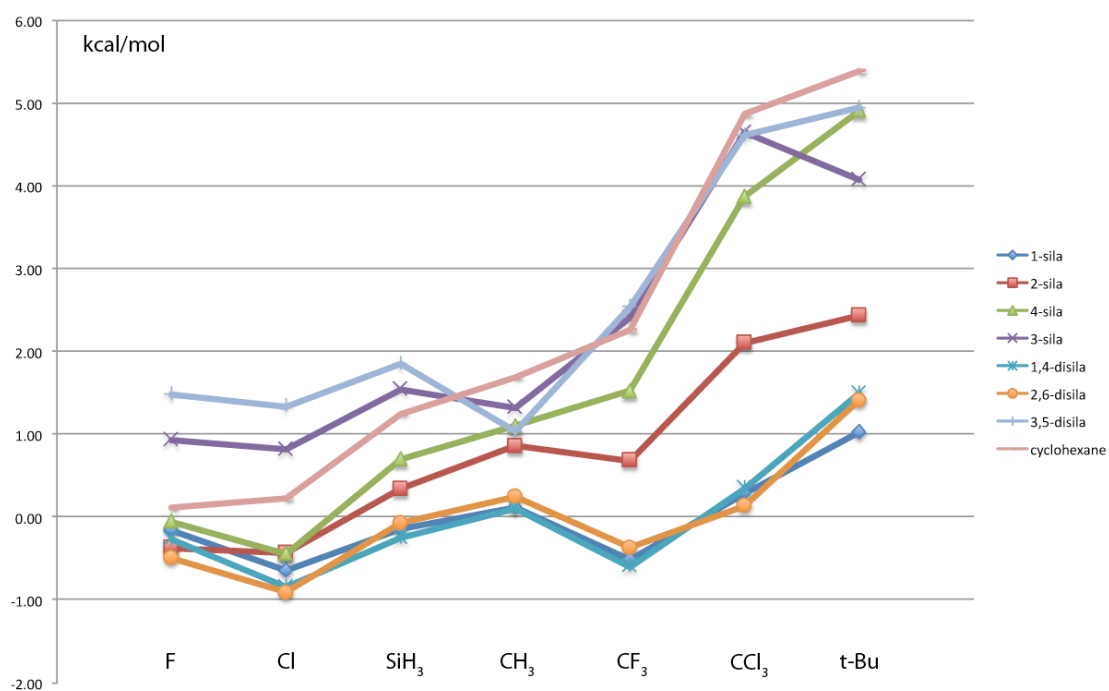


Figure S2. Graphical diagram showing the trends in ΔE values of the disilacyclohexane families compared to the monosilacyclohexane families and cyclohexane.

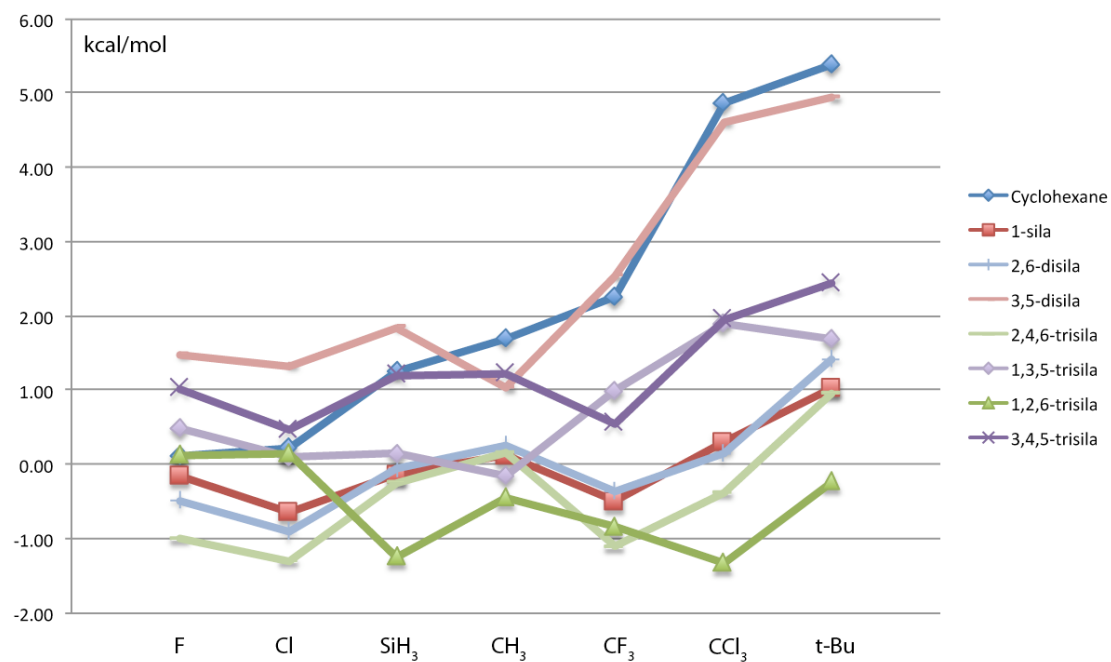


Figure S3. Graphical diagram showing the trends in ΔE values of the trisilacyclohexane families compared to the some of the mono- and disilacyclohexane families and cyclohexane.

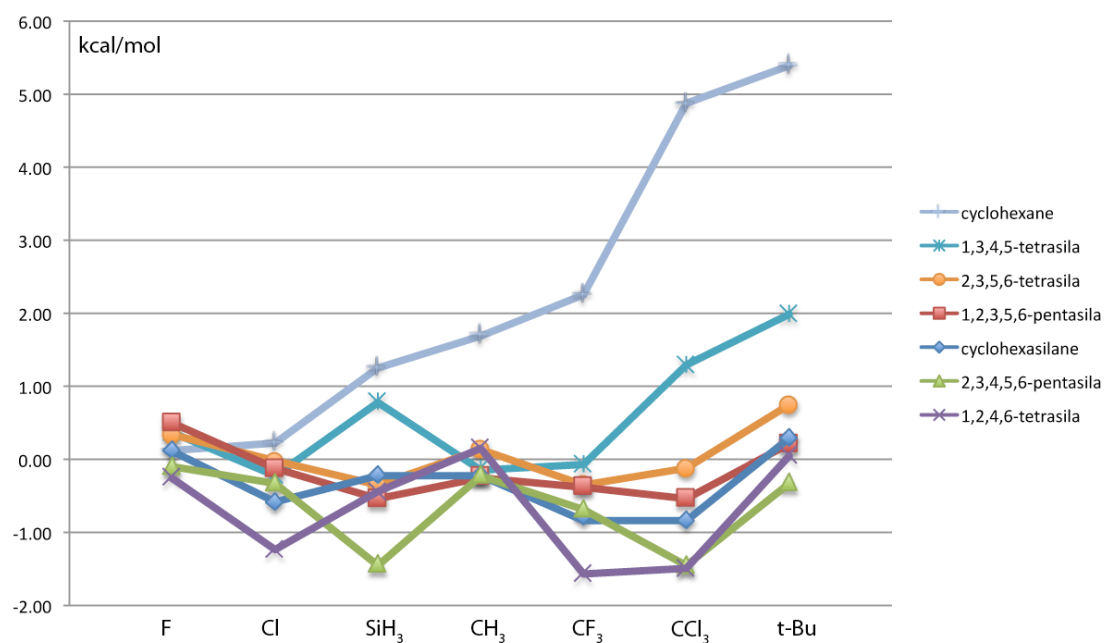
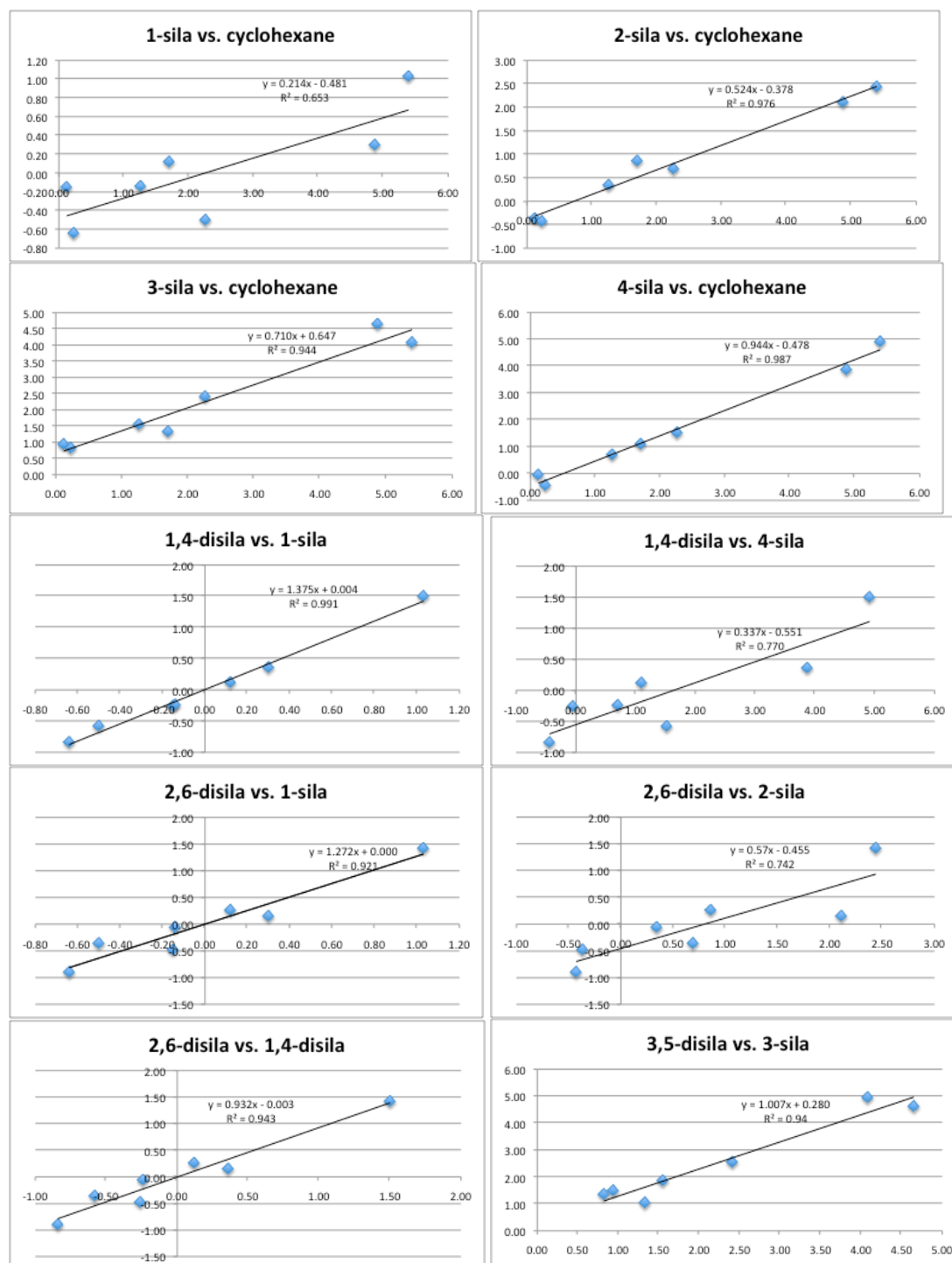


Figure S4. Graphical diagram showing the trends in ΔE values of the tetra-, and pentasilacyclohexane and cyclohexasilane families compared to cyclohexane.

Figure S5. Correlation diagrams for some of the silacyclohexane families (plots of ΔE values of one family vs. ΔE values of another). Both axes in kcal/mol.



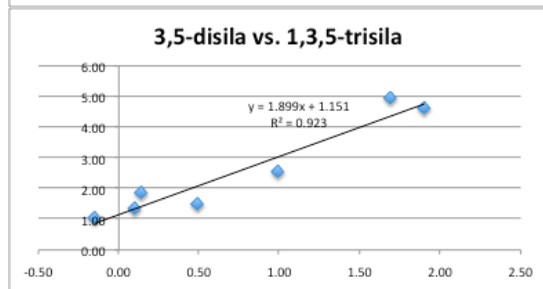
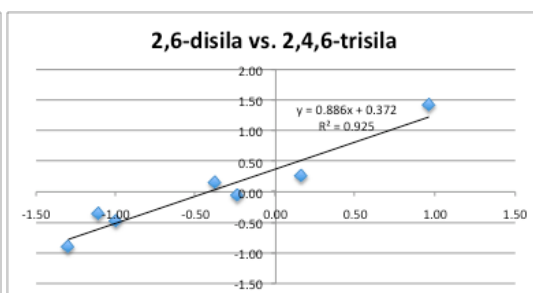
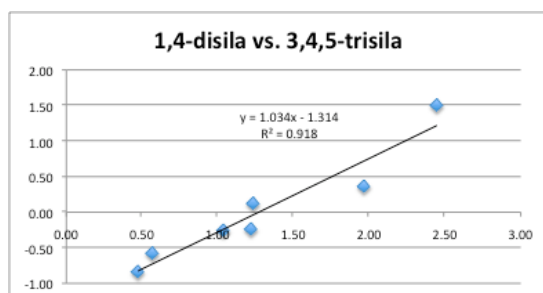


Table S4. Total energies in hartrees (ZPE exclusive) of 1-trichloromethyl-2,3,4,5,6-pentasilacyclohexane with methods from table 8 using a M06-2X/pc-2 geometry (except in the cases of the composite methods G3B3 and CBS-QB3).

	<i>axial</i>	<i>equatorial</i>
G3B3	-2909.775472	-2909.773564
CBS-QB3	-2907.304159	-2907.30203
MP2^a	-2907.125779	-2907.123856
M06-2X^c	-2910.918094	-2910.915776
B3LYP^b	-2910.701232	-2910.702120
B3LYP-D^b	-2910.737288	-2910.736083
B97-1^c	-2910.806466	-2910.806652
B2PLYP^b	-2910.552559	-2910.552253
B2PLYP-D^b	-2910.571445	-2910.570044

^a cc-pVQZ basis set used.

^b Def2-QZVPP basis set used.

^c pc-3 basis set used.

Table S5. The convergence of ΔE values with the M06-2X functional and pc-*n* basis sets and the B2PLYP-D functional and the def2 basis sets for the molecules in Table 1 of paper.

	M06-2X/pc-0	M06-2X/pc-1	M06-2X/pc-2	M06-2X/pc-3	M06-2X/pc-4
<i>Cyclohexanes</i>					
Methyl	-0.86	-1.45	-1.69	-1.70	-1.72
Fluoro	2.25	0.79	-0.14	-0.15	-0.16
Methoxy	2.69	0.98	-0.05	-0.12	-0.11
Hydroxy	2.31	0.47	-0.45	-0.50	-0.50
<i>Tetrahydropyrans</i>					
2-Methyl	-0.52	-2.32	-2.60	-2.59	-2.60
2-Fluoro	6.57	3.81	2.50	2.46	2.45
2-Methoxy	5.93	2.55	1.35	1.31	1.31
2-Hydroxy	5.48	2.09	0.91	0.87	0.87
<i>Silacyclohexanes</i>					
Methyl	0.74	-0.05	-0.08	-0.11	-0.10
Fluoro	-0.74	0.38	0.20	0.16	0.17
Methoxy	0.98	0.63	0.29	0.23	0.24
Hydroxy	0.57	0.37	0.10	0.06	0.06
Chloro	1.80	0.91	0.63	0.63	0.64
	B2PLYP-D / SVP	B2PLYP-D / TZVP	B2PLYP-D / TZVPP	B2PLYP-D / aug-TZVPP	B2PLYP-D / QZVPP
<i>Cyclohexanes</i>					
Methyl	1.49	1.65	1.53	1.54	1.54
Fluoro	-1.10	0.17	0.12	0.17	0.20
Methoxy	-0.72	0.22	0.12	0.21	0.23
Hydroxy	-0.33	0.57	0.49	0.62	0.62
<i>Tetrahydropyrans</i>					
2-Methyl	2.67	2.62	2.56	2.59	2.58
2-Fluoro	-3.50	-2.58	-2.59	-2.59	-2.56
2-Methoxy	-2.05	-1.25	-1.27	-1.24	-1.23
2-Hydroxy	-1.54	-0.87	-0.88	-0.80	-0.81

Table S6. Total energies in hartrees (ZPE exclusive) of molecules in tables 3-7 at the M06-2X/pc-3//M06-2X/pc-2 level.

	F		Cl		CH₃		SiH₃		CF₃		CCl₃		t-Bu	
	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>	<i>ax</i>	<i>eq</i>
cyclohexane	-335.127212	-335.127409	-695.485874	-695.486234	-275.175254	-275.177968	-526.546837	-526.548845	-572.982123	-572.985723	-1654.007522	-1654.015287	-393.102851	-393.111433
1-sila	-586.591266	-586.591034	-946.930793	-946.929774	-526.576964	-526.577154	-777.937134	-777.936914	-824.364610	-824.363815	-1905.410022	-1905.410503	-644.505858	-644.507506
2-sila	-586.500597	-586.500013	-946.866485	-946.865803	-526.558141	-526.559512	-777.938191	-777.938738	-824.367040	-824.368140	-1905.394161	-1905.397523	-644.490913	-644.494800
3-sila	-586.512024	-586.513519	-946.869929	-946.871241	-526.560545	-526.562665	-777.931200	-777.933662	-824.366668	-824.370506	-1905.392602	-1905.400017	-644.489925	-644.496422
4-sila	-586.511795	-586.511712	-946.870652	-946.869949	-526.560580	-526.562329	-777.932023	-777.933145	-824.366690	-824.369113	-1905.391710	-1905.397877	-644.486577	-644.494401
14-disila	-837.978488	-837.978071	-1198.318151	-1198.316807	-777.964416	-777.964602	-1029.324470	-1029.324093	-1075.751581	-1075.750651	-2156.796643	-2156.797211	-895.892307	-895.894705
26-disila	-837.882860	-837.882094	-1198.256542	-1198.255101	-777.951573	-777.951980	-1029.340588	-1029.340500	-1075.761067	-1075.760496	-2156.788152	-2156.788384	-895.885540	-895.887797
35-disila	-837.909113	-837.911490	-1198.266230	-1198.268385	-777.957911	-777.959575	-1029.327648	-1029.330620	-1075.763729	-1075.767792	-2156.790204	-2156.797569	-895.885747	-895.893631
126-trisila	-1089.332384	-1089.332595	-1449.677704	-1449.676367	-1029.329105	-1029.329346	-1280.697768	-1280.697062	-1327.116629	-1327.114658	-2408.161915	-2408.159807	-1147.261707	-1147.261347
246-trisila	-1089.290318	-1089.288722	-1449.664153	-1449.662081	-1029.358732	-1029.358986	-1280.747440	-1280.747050	-1327.167984	-1327.166222	-2408.194086	-2408.193475	-1147.291224	-1147.292755
135-trisila	-1089.395556	-1089.396333	-1449.733881	-1449.734048	-1029.381855	-1029.381615	-1280.740581	-1280.740809	-1327.167279	-1327.168854	-2408.212792	-2408.215821	-1147.309901	-1147.312593
345-trisila	-1089.266930	-1089.268583	-1449.624083	-1449.624989	-1029.316138	-1029.316892	-1280.686174	-1280.688141	-1327.122574	-1327.124518	-2408.150838	-2408.153970	-1147.246554	-1147.250453
2356-tetrasila	-1340.644487	-1340.645021	-1701.017389	-1701.016844	-1280.714097	-1280.714052	-1532.101397	-1532.101621	-1578.521376	-1578.520817	-2659.548797	-2659.548601	-1398.647641	-1398.648831
1246-tetrasila	-1340.740670	-1340.740265	-1701.086250	-1701.084267	-1280.737062	-1280.737300	-1532.105666	-1532.104949	-1578.524983	-1578.522479	-2659.570119	-2659.567737	-1398.669274	-1398.669349
1345-tetrasila	-1340.754370	-1340.754947	-1701.092691	-1701.092577	-1280.740811	-1280.740453	-1532.099705	-1532.099490	-1578.526221	-1578.527472	-2659.572249	-2659.574301	-1398.668053	-1398.671219
23456-pentasila	-1592.012956	-1592.012797	-1952.385846	-1952.384757	-1532.082897	-1532.082378	-1783.470408	-1783.470064	-1829.890440	-1829.888150	-2910.918094	-2910.915776	-1650.016340	-1650.015830
12345-pentasila	-1592.105086	-1592.105880	-1952.449761	-1952.449168	-1532.102488	-1532.102283	-1783.469803	-1783.469431	-1829.887954	-1829.887095	-2910.933559	-2910.932709	-1650.034529	-1650.034864
cyclohexasilane	-1843.474078	-1843.474269	-2203.818754	-2203.817809	-1783.471469	-1783.471119	-2034.838683	-2034.838332	-2081.257030	-2081.255778	-3162.302662	-3162.301331	-1901.403172	-1901.403629

Table S7. Cartesian coordinates (in Å) of all molecules in tables 3-7 at the M06-2X/pc-2 level.

cyclohexane-ccl3-ax

C	0.99446	0.11357	0.00000
C	0.84726	0.97527	-1.26782
C	0.84726	0.97527	1.26782
C	-0.30462	1.98032	-1.25313
C	-0.30462	1.98032	1.25313
C	-0.26516	2.84749	0.00000
H	0.79337	0.34153	-2.15060
H	0.79337	0.34153	2.15060
H	1.78022	1.53927	-1.35100
H	1.78022	1.53927	1.35100
H	-1.26322	1.46529	-1.31033
H	-1.26322	1.46529	1.31033
H	-0.22967	2.60221	-2.14607
H	-0.22967	2.60221	2.14607
H	-1.09562	3.55383	0.00000
H	0.65615	3.43920	0.00000
C	0.15812	-1.17894	0.00000
Cl	-1.60044	-0.90745	0.00000
Cl	0.55994	-2.16648	-1.43469
Cl	0.55994	-2.16648	1.43469
H	2.01149	-0.28500	0.00000

cyclohexane-ccl3-eq

C	-0.37219	-0.44669	0.00000
C	0.13167	-1.16564	-1.25484
C	0.13167	-1.16564	1.25484
C	-0.31787	-2.62568	-1.25382
C	-0.31787	-2.62568	1.25382
C	0.15477	-3.35337	0.00000
H	-0.22818	-0.66369	-2.15063
H	-0.22818	-0.66369	2.15063
H	1.22337	-1.12168	-1.27257
H	1.22337	-1.12168	1.27257
H	-1.40996	-2.66601	-1.30535
H	-1.40996	-2.66601	1.30535

H	0.05799	-3.12147	-2.14896
H	0.05799	-3.12147	2.14896
H	-0.20356	-4.38314	0.00000
H	1.24795	-3.39564	0.00000
C	-0.03016	1.04912	0.00000
H	-1.46687	-0.47298	0.00000
Cl	1.73023	1.32070	0.00000
Cl	-0.72229	1.85139	1.43555
Cl	-0.72229	1.85139	-1.43555

cyclohexane-cf3-ax

C	0.93679	-0.26022	0.00000
C	0.81051	0.59119	-1.27046
C	0.81051	0.59119	1.27046
C	-0.38863	1.53948	-1.25772
C	-0.38863	1.53948	1.25772
C	-0.39183	2.40414	0.00000
H	0.78831	-0.05291	-2.14922
H	0.78831	-0.05291	2.14922
H	1.72310	1.18810	-1.34184
H	1.72310	1.18810	1.34184
H	-1.31816	0.97071	-1.30938
H	-1.31816	0.97071	1.30938
H	-0.35325	2.16733	-2.14854
H	-0.35325	2.16733	2.14854
H	-1.25658	3.06800	0.00000
H	0.49829	3.04165	0.00000
C	-0.01542	-1.43668	0.00000
F	-1.31191	-1.08714	0.00000
F	0.16970	-2.21653	-1.07636
F	0.16970	-2.21653	1.07636
H	1.91882	-0.73828	0.00000

cyclohexane-cf3-eq

C	0.39426	0.10685	0.00000
C	-0.13214	-0.57770	-1.26265
C	-0.13214	-0.57770	1.26265
C	0.22983	-2.06091	-1.25764

C	0.22983	-2.06091	1.25764
C	-0.28756	-2.75383	0.00000
H	0.26920	-0.08814	-2.14942
H	0.26920	-0.08814	2.14942
H	-1.21946	-0.46833	-1.29457
H	-1.21946	-0.46833	1.29457
H	1.31799	-2.16522	-1.30455
H	1.31799	-2.16522	1.30455
H	-0.17152	-2.54074	-2.15030
H	-0.17152	-2.54074	2.15030
H	0.00388	-3.80444	0.00000
H	-1.38129	-2.72697	0.00000
C	0.05350	1.57741	0.00000
H	1.48787	0.06460	0.00000
F	-1.27089	1.79323	0.00000
F	0.54926	2.20580	1.07651
F	0.54926	2.20580	-1.07651

cyclohexane-cl-ax

Cl	-0.76725	1.90221	0.00000
C	0.70348	0.84270	0.00000
H	1.53329	1.54448	0.00000
C	0.72414	-0.00837	1.26213
C	0.72414	-0.00837	-1.26213
C	-0.36385	-1.07860	1.25864
C	-0.36385	-1.07860	-1.25864
C	-0.28203	-1.93979	0.00000
H	0.64287	0.63228	2.13937
H	0.64287	0.63228	-2.13937
H	1.70611	-0.49125	1.30143
H	1.70611	-0.49125	-1.30143
H	-1.34212	-0.59542	1.30569
H	-1.34212	-0.59542	-1.30569
H	-0.26988	-1.69667	2.15170
H	-0.26988	-1.69667	-2.15170
H	-1.07846	-2.68438	0.00000
H	0.66536	-2.48854	0.00000

cyclohexane-cl-eq

H	-1.44480	0.69732	0.00000
C	-0.35467	0.70255	0.00000
Cl	0.10329	2.44517	0.00000
C	0.16633	0.02967	1.25828
C	0.16633	0.02967	-1.25828
C	-0.21082	-1.45254	1.25721
C	-0.21082	-1.45254	-1.25721
C	0.30069	-2.15121	0.00000
H	-0.22996	0.53371	2.13905
H	-0.22996	0.53371	-2.13905
H	1.25385	0.13648	1.28286
H	1.25385	0.13648	-1.28286
H	-1.29964	-1.54846	1.30514
H	-1.29964	-1.54846	-1.30514
H	0.18660	-1.93179	2.15204
H	0.18660	-1.93179	-2.15204
H	-0.00088	-3.19900	0.00000
H	1.39451	-2.13428	0.00000

cyclohexane-f-ax

F	0.80603	1.72470	0.00000
C	-0.46617	1.14463	0.00000
H	-1.17747	1.97252	0.00000
C	-0.60871	0.31407	1.26264
C	-0.60871	0.31407	-1.26264
C	0.34007	-0.88283	1.25665
C	0.34007	-0.88283	-1.25665
C	0.14659	-1.72872	0.00000
H	-0.43027	0.95173	2.12879
H	-0.43027	0.95173	-2.12879
H	-1.64438	-0.03215	1.32027
H	-1.64438	-0.03215	-1.32027
H	1.36976	-0.52032	1.29173
H	1.36976	-0.52032	-1.29173
H	0.18235	-1.48365	2.15255
H	0.18235	-1.48365	-2.15255

H	0.84059	-2.56972	0.00000
H	-0.86385	-2.15042	0.00000
cyclohexane-f-eq			
H	1.41835	1.03335	0.00000
C	0.32348	1.02138	0.00000
F	-0.08760	2.35067	0.00000
C	-0.18477	0.34294	1.25544
C	-0.18477	0.34294	-1.25544
C	0.21233	-1.13316	1.25843
C	0.21233	-1.13316	-1.25843
C	-0.28846	-1.83896	0.00000
H	0.20548	0.85903	2.13266
H	0.20548	0.85903	-2.13266
H	-1.27392	0.43704	1.27514
H	-1.27392	0.43704	-1.27514
H	1.30247	-1.21434	1.30547
H	1.30247	-1.21434	-1.30547
H	-0.17669	-1.62023	2.15240
H	-0.17669	-1.62023	-2.15240
H	0.02907	-2.88210	0.00000
H	-1.38239	-1.83870	0.00000
cyclohexane-ch3-ax			
C	-0.44075	1.14107	0.00000
H	-1.23016	1.89709	0.00000
C	-0.61872	0.27873	-1.25596
C	-0.61872	0.27873	1.25596
C	0.29244	-0.94845	-1.25907
C	0.29244	-0.94845	1.25907
C	0.08318	-1.78712	0.00000
H	-0.44338	0.88421	-2.14772
H	-0.44338	0.88421	2.14772
H	-1.65782	-0.06095	-1.30349
H	-1.65782	-0.06095	1.30349
H	1.33862	-0.63625	-1.31519
H	1.33862	-0.63625	1.31519
H	0.10104	-1.54845	-2.14974

H	0.10104	-1.54845	2.14974
H	0.75292	-2.64815	0.00000
H	-0.93873	-2.17995	0.00000
C	0.89538	1.88163	0.00000
H	0.98487	2.51631	0.88222
H	0.98487	2.51631	-0.88222
H	1.74363	1.19789	0.00000

cyclohexane-ch3-eq

C	0.33735	1.01045	0.00000
C	-0.16661	0.29402	-1.25305
C	-0.16661	0.29402	1.25305
C	0.21279	-1.18462	-1.25790
C	0.21279	-1.18462	1.25790
C	-0.29398	-1.88591	0.00000
H	0.22157	0.79090	-2.14478
H	0.22157	0.79090	2.14478
H	-1.25809	0.38739	-1.29057
H	-1.25809	0.38739	1.29057
H	1.30263	-1.27434	-1.30265
H	1.30263	-1.27434	1.30265
H	-0.18045	-1.67324	-2.15042
H	-0.18045	-1.67324	2.15042
H	0.01005	-2.93349	0.00000
H	-1.38841	-1.87291	0.00000
C	-0.06923	2.47754	0.00000
H	0.30891	2.99361	-0.88298
H	0.30891	2.99361	0.88298
H	-1.15747	2.56894	0.00000
H	1.43237	0.95162	0.00000

cyclohexane-sih3-ax

C	-0.73423	0.75239	0.00000
C	-0.77627	-0.12532	-1.26112
C	-0.77627	-0.12532	1.26112
C	0.32277	-1.18711	-1.26031
C	0.32277	-1.18711	1.26031
C	0.25415	-2.04681	0.00000

H	-0.70808	0.48974	-2.16073
H	-0.70808	0.48974	2.16073
H	-1.74667	-0.63197	-1.30182
H	-1.74667	-0.63197	1.30182
H	1.30319	-0.70507	-1.31303
H	1.30319	-0.70507	1.31303
H	0.23364	-1.81234	-2.14958
H	0.23364	-1.81234	2.14958
H	1.05754	-2.78445	0.00000
H	-0.68814	-2.60393	0.00000
H	-1.62394	1.39132	0.00000
Si	0.68982	1.98958	0.00000
H	2.02781	1.35905	0.00000
H	0.59066	2.84403	-1.20448
H	0.59066	2.84403	1.20448

cyclohexane-sih3-eq

C	0.39727	0.58963	0.00000
C	-0.13169	-0.10853	-1.26118
C	-0.13169	-0.10853	1.26118
C	0.19383	-1.60149	-1.25875
C	0.19383	-1.60149	1.25875
C	-0.34025	-2.27998	0.00000
H	0.27652	0.36349	-2.15706
H	0.27652	0.36349	2.15706
H	-1.21944	0.01651	-1.30846
H	-1.21944	0.01651	1.30846
H	1.27984	-1.72855	-1.30215
H	1.27984	-1.72855	1.30215
H	-0.21742	-2.07713	-2.15037
H	-0.21742	-2.07713	2.15037
H	-0.07923	-3.33899	0.00000
H	-1.43332	-2.22313	0.00000
Si	-0.03147	2.41783	0.00000
H	0.51281	3.08451	1.20384
H	-1.50400	2.57536	0.00000
H	0.51281	3.08451	-1.20384

H	1.49137	0.50983	0.00000
cyclohexane-tbu-ax			
C	-0.18933	2.66705	0.00000
C	-0.30163	1.80248	-1.25028
C	0.76438	0.70495	-1.25636
C	0.80961	-0.18750	0.00000
C	0.76438	0.70495	1.25636
C	-0.30163	1.80248	1.25028
H	0.67652	0.09902	-2.15707
H	-1.30365	1.37361	-1.29496
H	-0.18668	2.41504	-2.14615
H	0.78039	3.17531	0.00000
H	-0.95569	3.44323	0.00000
H	1.80600	-0.64232	0.00000
H	0.67652	0.09902	2.15707
H	1.73605	1.20421	1.32702
H	-1.30365	1.37361	1.29496
H	-0.18668	2.41504	2.14615
H	1.73605	1.20421	-1.32702
C	-0.13324	-1.42866	0.00000
C	-1.63015	-1.11004	0.00000
H	-1.92616	-0.54863	-0.88452
H	-2.19783	-2.04285	0.00000
H	-1.92616	-0.54863	0.88452
C	0.16882	-2.28697	1.23539
H	-0.35847	-3.23928	1.16540
H	1.23687	-2.49874	1.31546
H	-0.15289	-1.80543	2.15760
C	0.16882	-2.28697	-1.23539
H	1.23687	-2.49874	-1.31546
H	-0.35847	-3.23928	-1.16540
H	-0.15289	-1.80543	-2.15760
cyclohexane-tbu-eq			
C	0.17367	-2.86461	0.00000
C	-0.29323	-2.13164	-1.25269
C	0.16606	-0.67422	-1.24857

C	-0.31778	0.07312	0.00000
C	0.16606	-0.67422	1.24857
C	-0.29323	-2.13164	1.25269
H	-0.19082	-0.18269	-2.15293
H	-1.38635	-2.16142	-1.29821
H	0.07298	-2.63532	-2.14846
H	1.26702	-2.91427	0.00000
H	-0.19061	-3.89286	0.00000
H	-0.19082	-0.18269	2.15293
H	1.25982	-0.65089	1.28213
H	-1.38635	-2.16142	1.29821
H	0.07298	-2.63532	2.14846
H	1.25982	-0.65089	-1.28213
H	-1.41542	0.01834	0.00000
C	0.02652	1.58726	0.00000
C	-0.58181	2.25738	-1.23703
H	-0.09804	1.93331	-2.15717
H	-0.46652	3.34011	-1.17123
H	-1.64844	2.03684	-1.31582
C	-0.58181	2.25738	1.23703
H	-1.64844	2.03684	1.31582
H	-0.46652	3.34011	1.17123
H	-0.09804	1.93331	2.15717
C	1.53653	1.83877	0.00000
H	1.73217	2.91244	0.00000
H	2.01546	1.41747	-0.88384
H	2.01546	1.41747	0.88384
1-sila-ccl3-ax			
C	-0.72220	1.41317	-1.50852
C	0.41236	2.42684	-1.28145
C	0.25214	3.24756	0.00000
C	0.41236	2.42684	1.28145
C	-0.72220	1.41317	1.50852
Si	-1.07493	0.36981	0.00000
H	-0.72932	3.73419	0.00000
H	0.46233	3.10159	-2.13739

H	1.37015	1.90372	-1.24447
H	-0.52146	0.78392	-2.37700
H	-1.64780	1.95380	-1.73084
H	0.46233	3.10159	2.13739
H	1.37015	1.90372	1.24447
H	-1.64780	1.95380	1.73084
H	-0.52146	0.78392	2.37700
H	0.99325	4.04789	0.00000
H	-2.43396	-0.20615	0.00000
C	0.04466	-1.19827	0.00000
Cl	1.77063	-0.75284	0.00000
Cl	-0.30208	-2.17109	1.45035
Cl	-0.30208	-2.17109	-1.45035

1-sila-ccl3-eq

C	0.02706	-1.39009	1.49382
C	-0.16914	-2.90360	1.28437
C	0.47692	-3.42958	0.00000
C	-0.16914	-2.90360	-1.28437
C	0.02706	-1.39009	-1.49382
Si	-0.61272	-0.47815	0.00000
H	1.53991	-3.16834	0.00000
H	0.24055	-3.44177	2.14031
H	-1.23816	-3.13648	1.26025
H	-0.46376	-1.05393	2.40717
H	1.09286	-1.17226	1.60501
H	0.24055	-3.44177	-2.14031
H	-1.23816	-3.13648	-1.26025
H	1.09286	-1.17226	-1.60501
H	-0.46376	-1.05393	-2.40717
H	0.42390	-4.51910	0.00000
C	0.01644	1.33711	0.00000
Cl	-0.58442	2.17112	-1.45281
Cl	1.79766	1.37463	0.00000
Cl	-0.58442	2.17112	1.45281
H	-2.08585	-0.36405	0.00000

1-sila-cf3-ax

C	0.68848	0.92726	-1.50272
C	-0.58785	1.75991	-1.28394
C	-0.55981	2.59321	0.00000
C	-0.58785	1.75991	1.28394
C	0.68848	0.92726	1.50272
Si	1.07316	-0.10936	0.00000
H	0.33218	3.22875	0.00000
H	-0.73406	2.42144	-2.13901
H	-1.45656	1.09782	-1.25339
H	0.60449	0.30607	-2.39561
H	1.53637	1.59824	-1.66953
H	-0.73406	2.42144	2.13901
H	-1.45656	1.09782	1.25339
H	1.53637	1.59824	1.66953
H	0.60449	0.30607	2.39561
H	-1.41851	3.26569	0.00000
H	2.42151	-0.70999	0.00000
C	-0.12385	-1.63037	0.00000
F	-1.42731	-1.27003	0.00000
F	0.04678	-2.41900	1.07991
F	0.04678	-2.41900	-1.07991

1-sila-cf3-eq

C	0.05154	-0.86747	1.49141
C	-0.14371	-2.38127	1.28587
C	0.49821	-2.90955	0.00000
C	-0.14371	-2.38127	-1.28587
C	0.05154	-0.86747	-1.49141
Si	-0.59660	0.04391	0.00000
H	1.56285	-2.65534	0.00000
H	0.27027	-2.91816	2.14048
H	-1.21266	-2.61490	1.26665
H	-0.42893	-0.53098	2.41008
H	1.11841	-0.64779	1.59092
H	0.27027	-2.91816	-2.14048
H	-1.21266	-2.61490	-1.26665
H	1.11841	-0.64779	-1.59092

H	-0.42893	-0.53098	-2.41008
H	0.43906	-3.99869	0.00000
C	0.07699	1.85429	0.00000
F	-0.31814	2.55667	-1.08005
F	1.42716	1.88576	0.00000
F	-0.31814	2.55667	1.08005
H	-2.06925	0.16534	0.00000

1-sila-cl-ax

C	0.63751	0.27404	-1.48536
C	-0.44890	1.34441	-1.28512
C	-0.27035	2.15734	0.00000
C	-0.44890	1.34441	1.28512
C	0.63751	0.27404	1.48536
Si	0.71302	-0.84717	0.00000
H	0.72418	2.61586	0.00000
H	-0.45378	2.02123	-2.14084
H	-1.43099	0.86385	-1.26578
H	0.46434	-0.29442	-2.39961
H	1.61448	0.75708	-1.59064
H	-0.45378	2.02123	2.14084
H	-1.43099	0.86385	1.26578
H	1.61448	0.75708	1.59064
H	0.46434	-0.29442	2.39961
H	-0.98940	2.97764	0.00000
Cl	-0.98777	-2.03951	0.00000
H	1.86953	-1.76171	0.00000

1-sila-cl-eq

C	-0.16213	0.22369	1.48216
C	0.17550	1.71325	1.28462
C	-0.41174	2.30384	0.00000
C	0.17550	1.71325	-1.28462
C	-0.16213	0.22369	-1.48216
Si	0.42945	-0.73562	0.00000
H	-0.24614	3.38210	0.00000
H	1.26183	1.84534	1.26701
H	-0.18596	2.28384	2.14150

H	-1.24546	0.09913	1.56345
H	0.27188	-0.15848	2.40643
H	1.26183	1.84534	-1.26701
H	-0.18596	2.28384	-2.14150
H	0.27188	-0.15848	-2.40643
H	-1.24546	0.09913	-1.56345
H	-1.49609	2.15466	0.00000
Cl	-0.33158	-2.65967	0.00000
H	1.90149	-0.85681	0.00000

1-sila-f-ax

C	-0.52670	-0.03640	-1.48353
C	0.40336	1.17442	-1.28457
C	0.11449	1.95598	0.00000
C	0.40336	1.17442	1.28457
C	-0.52670	-0.03640	1.48353
Si	-0.44519	-1.15466	0.00000
H	-0.93391	2.27247	0.00000
H	0.31855	1.84597	-2.14039
H	1.44252	0.83412	-1.26243
H	-0.27503	-0.57529	-2.39831
H	-1.55886	0.30996	-1.59801
H	0.31855	1.84597	2.14039
H	1.44252	0.83412	1.26243
H	-1.55886	0.30996	1.59801
H	-0.27503	-0.57529	2.39831
H	0.71335	2.86786	0.00000
F	0.98459	-1.88655	0.00000
H	-1.46937	-2.21797	0.00000

1-sila-f-eq

C	0.20323	-0.07543	1.48023
C	-0.19064	1.40121	1.28416
C	0.37390	2.01424	0.00000
C	-0.19064	1.40121	-1.28416
C	0.20323	-0.07543	-1.48023
Si	-0.34737	-1.05674	0.00000
H	0.16710	3.08548	0.00000

H	-1.28133	1.49148	1.26444
H	0.14616	1.98620	2.14126
H	1.29127	-0.15407	1.56390
H	-0.21401	-0.46832	2.40808
H	-1.28133	1.49148	-1.26444
H	0.14616	1.98620	-2.14126
H	-0.21401	-0.46832	-2.40808
H	1.29127	-0.15407	-1.56390
H	1.46325	1.90686	0.00000
F	0.30767	-2.51838	0.00000
H	-1.81494	-1.23810	0.00000

1-sila-ch3-ax

C	0.56844	0.01931	-1.48035
C	-0.38935	1.20637	-1.28475
C	-0.12260	1.99479	0.00000
C	-0.38935	1.20637	1.28475
C	0.56844	0.01931	1.48035
Si	0.49064	-1.13420	0.00000
H	0.91789	2.33601	0.00000
H	-0.31966	1.88205	-2.13942
H	-1.42312	0.84684	-1.26581
H	0.33908	-0.51091	-2.40665
H	1.59095	0.39471	-1.58133
H	-0.31966	1.88205	2.13942
H	-1.42312	0.84684	1.26581
H	1.59095	0.39471	1.58133
H	0.33908	-0.51091	2.40665
H	-0.74337	2.89232	0.00000
H	1.62549	-2.08917	0.00000
C	-1.11980	-2.09501	0.00000
H	-1.19448	-2.73199	0.88152
H	-1.19448	-2.73199	-0.88152
H	-1.97847	-1.42267	0.00000

1-sila-ch3-eq

C	-0.17200	-0.01663	1.47935
C	0.18834	1.46509	1.28488

C	-0.38800	2.06533	0.00000
C	0.18834	1.46509	-1.28488
C	-0.17200	-0.01663	-1.47935
Si	0.38928	-1.02609	0.00000
H	-1.47513	1.93358	0.00000
H	-0.16173	2.04737	2.13949
H	1.27698	1.57589	1.26399
H	0.25687	-0.39876	2.40740
H	-1.25833	-0.11536	1.57421
H	-0.16173	2.04737	-2.13949
H	1.27698	1.57589	-1.26399
H	-1.25833	-0.11536	-1.57421
H	0.25687	-0.39876	-2.40740
H	-0.20624	3.14138	0.00000
C	-0.30867	-2.76268	0.00000
H	0.01534	-3.31616	0.88132
H	0.01534	-3.31616	-0.88132
H	-1.39886	-2.73748	0.00000
H	1.87429	-1.08529	0.00000

1-sila-sih3-ax

C	1.48532	0.52034	-0.67596
C	1.28548	1.38181	0.58130
C	0.00013	2.21252	0.55102
C	-1.28528	1.38191	0.58154
C	-1.48542	0.52049	-0.67569
Si	-0.00014	-0.60776	-0.93202
H	0.00007	2.83876	-0.34716
H	2.13951	2.04994	0.70654
H	1.26632	0.74047	1.46819
H	2.41337	-0.04932	-0.61070
H	1.57784	1.17113	-1.55042
H	-2.13923	2.05011	0.70698
H	-1.26599	0.74055	1.46842
H	-1.57803	1.17131	-1.55013
H	-2.41352	-0.04908	-0.61030
H	0.00024	2.89338	1.40358

Si	-0.00010	-2.32485	0.66355
H	-1.19983	-3.18018	0.51965
H	1.19875	-3.18122	0.51851
H	0.00079	-1.77673	2.03983
H	-0.00029	-1.21708	-2.28436

1-sila-sih3-eq

C	0.11930	-0.39462	1.48555
C	-0.13383	-1.89756	1.28514
C	0.48542	-2.45245	0.00000
C	-0.13383	-1.89756	-1.28514
C	0.11930	-0.39462	-1.48555
Si	-0.51534	0.57106	0.00000
H	1.55972	-2.24071	0.00000
H	0.25901	-2.45256	2.13934
H	-1.21155	-2.08595	1.26490
H	-0.34224	-0.04370	2.40950
H	1.19454	-0.21798	1.58488
H	0.25901	-2.45256	-2.13934
H	-1.21155	-2.08595	-1.26490
H	1.19454	-0.21798	-1.58488
H	-0.34224	-0.04370	-2.40950
H	0.38384	-3.53880	0.00000
H	-2.00088	0.53025	0.00000
Si	0.20296	2.79747	0.00000
H	-0.28067	3.51749	1.19903
H	-0.28067	3.51749	-1.19903
H	1.68316	2.84861	0.00000

1-sila-tbu-ax

C	0.36650	2.80643	0.00000
C	0.50970	1.98101	-1.27961
C	-0.63915	0.98220	-1.49391
C	-0.63915	0.98220	1.49391
C	0.50970	1.98101	1.27961
H	-0.46976	0.38922	-2.39506
H	1.46511	1.45041	-1.24102
H	0.57091	2.65460	-2.13670

H	-0.60736	3.30747	0.00000
H	1.12131	3.59453	0.00000
H	-0.46976	0.38922	2.39506
H	-1.56279	1.54165	1.67135
H	1.46511	1.45041	1.24102
H	0.57091	2.65460	2.13670
H	-1.56279	1.54165	-1.67135
C	0.13645	-1.69054	0.00000
C	1.63037	-1.35797	0.00000
H	1.91746	-0.78575	-0.88377
H	2.21961	-2.28039	0.00000
H	1.91746	-0.78575	0.88377
C	-0.19463	-2.51763	1.24638
H	0.37899	-3.44951	1.24101
H	-1.25333	-2.78037	1.28558
H	0.05520	-1.98414	2.16490
C	-0.19463	-2.51763	-1.24638
H	-1.25333	-2.78037	-1.28558
H	0.37899	-3.44951	-1.24101
H	0.05520	-1.98414	-2.16490
Si	-0.93777	-0.12627	0.00000
H	-2.34539	-0.60448	0.00000

1-sila-tbu-eq

C	0.43200	-2.96498	0.00000
C	-0.17787	-2.39860	1.28453
C	0.10216	-0.89939	1.48323
Si	-0.51024	0.07737	0.00000
C	0.10216	-0.89939	-1.48323
C	-0.17787	-2.39860	-1.28453
H	-0.35412	-0.54421	2.40888
H	-1.25885	-2.56787	1.26190
H	0.20201	-2.96199	2.13907
H	1.50993	-2.77189	0.00000
H	0.31127	-4.04958	0.00000
H	-0.35412	-0.54421	-2.40888
H	1.18120	-0.74688	-1.58678

H	-1.25885	-2.56787	-1.26190
H	0.20201	-2.96199	-2.13907
H	1.18120	-0.74688	1.58678
H	-1.99899	0.06316	0.00000
C	0.05525	1.88303	0.00000
C	-0.49172	2.57893	1.24988
H	-0.10547	2.12495	2.16438
H	-0.19730	3.63287	1.25413
H	-1.58188	2.53883	1.28755
C	-0.49172	2.57893	-1.24988
H	-1.58188	2.53883	-1.28755
H	-0.19730	3.63287	-1.25413
H	-0.10547	2.12495	-2.16438
C	1.58385	1.97122	0.00000
H	1.89842	3.01924	0.00000
H	2.01704	1.49880	0.88320
H	2.01704	1.49880	-0.88320

2-sila-ccl3-ax

Si	1.45145	1.32919	-0.53222
C	0.73492	2.62228	0.61537
C	-0.66598	3.05221	0.15668
C	-1.63932	1.88155	0.01695
C	-1.26268	0.89887	-1.09592
C	0.04789	0.09615	-0.93713
H	-0.59381	3.56392	-0.80810
H	1.40537	3.48245	0.65727
H	0.68377	2.21257	1.62567
H	2.64175	0.66005	0.02406
H	1.79520	1.95306	-1.83070
H	-2.62974	2.27471	-0.21700
H	-1.73253	1.36218	0.97138
H	-1.15361	1.47177	-2.02149
H	-2.08603	0.20628	-1.26718
H	-1.07536	3.77930	0.85971
H	0.27716	-0.33441	-1.91445
C	-0.01349	-1.11352	-0.01242

Cl	-0.02986	-0.66080	1.71818
Cl	-1.45428	-2.12997	-0.31742
Cl	1.42183	-2.14172	-0.28822
2-sila-ccl3-eq			
Si	-1.38461	1.32852	0.09221
C	-0.83262	3.05639	-0.37757
C	0.57497	3.35702	0.15285
C	1.61530	2.34343	-0.32145
C	1.38543	0.92282	0.19929
C	0.12261	0.26082	-0.38130
H	0.56208	3.36127	1.24661
H	-1.55181	3.78989	-0.01004
H	-0.83818	3.13617	-1.46844
H	-2.60483	0.93077	-0.63383
H	-1.60621	1.22938	1.55014
H	2.60422	2.66886	0.00293
H	1.63643	2.32988	-1.41549
H	1.31449	0.94961	1.28962
H	2.25336	0.30841	-0.04211
H	0.88118	4.35779	-0.15606
C	0.02468	-1.21825	-0.04245
Cl	1.41757	-2.13151	-0.70857
Cl	-0.01228	-1.48782	1.71913
Cl	-1.45209	-1.92677	-0.74995
H	0.18571	0.29718	-1.47445
2-sila-cf3-ax			
Si	1.46566	0.84466	-0.43628
C	0.70964	2.00313	0.82165
C	-0.69083	2.44651	0.36890
C	-1.64660	1.27774	0.12211
C	-1.24201	0.38203	-1.05307
C	0.08630	-0.38536	-0.88630
H	-0.60968	3.03479	-0.55049
H	1.35491	2.86857	0.97870
H	0.63872	1.48170	1.77890
H	2.67464	0.15026	0.04844

H	1.78000	1.57628	-1.68408
H	-2.64077	1.67415	-0.08815
H	-1.73752	0.68280	1.03312
H	-1.14550	1.00681	-1.94473
H	-2.04052	-0.33064	-1.26197
H	-1.12446	3.10920	1.11938
H	0.33558	-0.86289	-1.83594
C	-0.01612	-1.51928	0.09754
F	-0.06847	-1.09802	1.37778
F	-1.10714	-2.27948	-0.09021
F	1.04144	-2.34022	0.01124

2-sila-cf3-eq

Si	-1.40075	0.72973	0.09483
C	-0.88816	2.48972	-0.28599
C	0.51058	2.78149	0.27799
C	1.58235	1.82506	-0.24666
C	1.39390	0.37152	0.19119
C	0.13062	-0.27728	-0.40167
H	0.48660	2.71770	1.36981
H	-1.61995	3.19475	0.11039
H	-0.88087	2.62537	-1.37121
H	-2.59515	0.30260	-0.65976
H	-1.63130	0.55690	1.54510
H	2.56008	2.16372	0.09735
H	1.60436	1.87246	-1.33988
H	1.34235	0.32988	1.28248
H	2.26760	-0.21153	-0.10388
H	0.79751	3.80606	0.03621
C	0.04575	-1.73207	-0.03871
F	1.09780	-2.43812	-0.48843
F	0.00029	-1.92429	1.28942
F	-1.05032	-2.31324	-0.55408
H	0.19616	-0.25138	-1.49389

2-sila-cl-ax

Si	1.47173	0.35990	-0.38582
C	0.71367	1.48922	0.89628

C	-0.66262	1.97176	0.40649
C	-1.64549	0.82950	0.13978
C	-1.24568	-0.08945	-1.01592
C	0.07088	-0.83899	-0.81145
H	-0.54119	2.55805	-0.50993
H	1.36802	2.33594	1.10654
H	0.59837	0.93534	1.83119
H	2.67362	-0.36675	0.06555
H	1.78739	1.12987	-1.61339
H	-2.62691	1.24927	-0.08370
H	-1.76060	0.23192	1.04700
H	-1.13634	0.50721	-1.92802
H	-2.04262	-0.81128	-1.20293
H	-1.09706	2.64656	1.14576
Cl	-0.08785	-2.00937	0.56131
H	0.29044	-1.45366	-1.68117

2-sila-cl-eq

Si	-1.38591	-0.15856	-0.08952
C	-0.95782	-1.95503	0.23802
C	0.43065	-2.27772	-0.33817
C	1.54111	-1.37769	0.20931
C	1.41424	0.09492	-0.19695
C	0.18448	0.75364	0.42227
H	0.68159	-3.31863	-0.12780
H	-0.95504	-2.12838	1.31779
H	-1.71409	-2.61968	-0.18181
H	-1.59126	0.07109	-1.53560
H	-2.55723	0.32036	0.67132
H	1.55969	-1.45191	1.30119
H	2.50518	-1.74779	-0.14100
H	2.30756	0.64435	0.10469
H	1.35058	0.16919	-1.28590
H	0.40633	-2.18111	-1.42758
Cl	0.08516	2.48683	-0.05638
H	0.28355	0.75755	1.50827

2-sila-f-ax

Si	1.44954	0.16622	0.31652
C	0.87271	-1.33653	-0.63706
C	-0.47912	-1.81595	-0.08082
C	-1.57291	-0.74771	-0.14914
C	-1.33034	0.46038	0.75943
C	-0.09563	1.26979	0.38725
H	-0.35687	-2.13452	0.95932
H	1.61336	-2.13616	-0.60143
H	0.75658	-1.05807	-1.68765
H	2.58017	0.88090	-0.30915
H	1.80449	-0.20579	1.70645
H	-2.52842	-1.19760	0.12283
H	-1.67347	-0.39952	-1.17984
H	-1.21515	0.12620	1.79520
H	-2.19956	1.12107	0.73257
H	-0.80881	-2.69703	-0.63375
F	-0.29394	1.80862	-0.89779
H	0.01285	2.11793	1.06589

2-sila-f-eq

Si	-1.38410	0.24002	-0.11213
C	-0.99162	-1.55478	0.27121
C	0.38374	-1.93382	-0.30034
C	1.51999	-1.04601	0.21300
C	1.42296	0.41477	-0.23748
C	0.22190	1.12749	0.36757
H	0.60759	-2.97357	-0.05605
H	-0.98594	-1.69047	1.35641
H	-1.76795	-2.21399	-0.11921
H	-1.59669	0.42998	-1.56395
H	-2.54984	0.75501	0.63541
H	1.54189	-1.08767	1.30665
H	2.47215	-1.45212	-0.12887
H	2.32857	0.95640	0.04269
H	1.35018	0.45786	-1.32788
H	0.35647	-1.87278	-1.39216
F	0.21611	2.46004	-0.05818

H	0.33320	1.14632	1.45708
2-sila-ch3-ax			
Si	1.41611	0.24058	0.35166
C	0.97172	-1.30452	-0.61639
C	-0.34199	-1.89126	-0.07432
C	-1.51069	-0.90433	-0.12684
C	-1.33776	0.31669	0.78246
C	-0.17229	1.25073	0.40195
H	-0.19851	-2.20919	0.96331
H	1.77364	-2.04235	-0.56923
H	0.84816	-1.04572	-1.67177
H	2.52479	1.00101	-0.27147
H	1.81738	-0.14324	1.72728
H	-2.42516	-1.42391	0.16356
H	-1.66049	-0.57918	-1.16020
H	-1.19868	-0.03632	1.80894
H	-2.26623	0.89547	0.77878
H	-0.60574	-2.78938	-0.63595
H	-0.08538	2.01195	1.18108
C	-0.42215	1.95942	-0.93324
H	-1.39711	2.45242	-0.93558
H	0.33751	2.71593	-1.12775
H	-0.40879	1.26474	-1.77465
2-sila-ch3-eq			
Si	1.35455	0.22727	0.09408
C	1.02860	-1.58592	-0.25879
C	-0.34362	-1.98673	0.30616
C	-1.49199	-1.12428	-0.22362
C	-1.42385	0.34220	0.20845
C	-0.23279	1.11978	-0.37286
H	-0.32507	-1.91197	1.39780
H	1.81621	-2.21945	0.15101
H	1.03466	-1.73903	-1.34178
H	2.52458	0.75368	-0.64712
H	1.59423	0.42241	1.54649
H	-2.43821	-1.54889	0.11526

H	-1.50271	-1.17540	-1.31722
H	-1.38109	0.38858	1.30285
H	-2.35042	0.84826	-0.07887
H	-0.54627	-3.03391	0.07407
C	-0.25214	2.58143	0.07025
H	0.56984	3.14948	-0.36635
H	-1.18609	3.06804	-0.21941
H	-0.16632	2.65653	1.15593
H	-0.31074	1.08023	-1.46555

2-sila-sih3-ax

Si	-1.46442	0.38287	0.39324
C	-0.73077	1.57378	-0.85515
C	0.65528	2.04541	-0.38774
C	1.63149	0.89526	-0.13040
C	1.22741	-0.01299	1.03427
C	-0.07479	-0.81561	0.79379
H	0.55284	2.62744	0.53350
H	-1.39331	2.42510	-1.01638
H	-0.63656	1.06268	-1.81707
H	-2.65592	-0.32113	-0.13592
H	-1.85796	1.12303	1.61701
H	2.61867	1.30917	0.07992
H	1.73623	0.30138	-1.04467
H	1.11126	0.60841	1.92823
H	2.04737	-0.70291	1.24681
H	1.08477	2.72027	-1.13026
Si	0.10758	-2.12780	-0.53527
H	1.43223	-2.78229	-0.42977
H	-0.95233	-3.14679	-0.38289
H	-0.00844	-1.55526	-1.89600
H	-0.33467	-1.36036	1.70622

2-sila-sih3-eq

Si	1.37714	0.21158	-0.06725
C	0.95413	2.01531	0.21809
C	-0.44038	2.32378	-0.34989
C	-1.53940	1.42656	0.22331

C	-1.40591	-0.05016	-0.16038
C	-0.15791	-0.74850	0.42774
H	-0.42601	2.20748	-1.43800
H	1.70547	2.67161	-0.22300
H	0.95967	2.20871	1.29455
H	2.56265	-0.22568	0.70358
H	1.64175	-0.01719	-1.50940
H	-2.50901	1.79039	-0.12090
H	-1.54239	1.51263	1.31450
H	-1.38004	-0.12465	-1.25323
H	-2.30723	-0.58105	0.15685
H	-0.69411	3.36766	-0.15711
H	-0.21284	-0.71236	1.52226
Si	-0.09304	-2.55170	-0.06281
H	1.11131	-3.20819	0.49130
H	-1.29333	-3.26905	0.42439
H	-0.05610	-2.66111	-1.53799

2-sila-tbu-ax

Si	1.44526	0.87289	-0.45780
C	0.74270	2.10891	0.76936
C	-0.65051	2.57400	0.31701
C	-1.63336	1.42439	0.08395
C	-1.21896	0.48042	-1.04968
C	0.06314	-0.36070	-0.83740
H	-2.05322	-0.18012	-1.29005
H	-1.77456	0.86705	1.01229
H	-2.60875	1.84648	-0.16531
H	-0.55715	3.14042	-0.61481
H	-1.06876	3.26278	1.05346
H	0.29267	-0.78889	-1.81914
H	2.68752	0.24104	0.04417
H	1.77200	1.58810	-1.71623
H	0.67287	1.64208	1.75453
H	1.41326	2.96318	0.87532
H	-1.06579	1.09372	-1.94411
C	-0.03841	-1.57897	0.13056

C	0.17658	-1.21730	1.60571
H	-0.55570	-0.49769	1.96662
H	0.08754	-2.11495	2.22010
H	1.17298	-0.80554	1.77699
C	1.05209	-2.58096	-0.26535
H	1.05360	-3.43478	0.41391
H	0.88628	-2.95341	-1.27734
H	2.04139	-2.12277	-0.23056
C	-1.39574	-2.27373	-0.00390
H	-1.61208	-2.51532	-1.04625
H	-1.39605	-3.20465	0.56525
H	-2.20693	-1.65208	0.37679

2-sila-tbu-eq

Si	-1.38704	-0.78660	0.09526
C	-0.88975	-2.55349	-0.29920
C	0.51303	-2.86687	0.23667
C	1.57135	-1.88139	-0.25961
C	1.36337	-0.44792	0.23697
C	0.12512	0.25569	-0.35352
H	2.25938	0.13411	0.01017
H	1.58460	-1.88692	-1.35424
H	2.55497	-2.22502	0.06445
H	0.50124	-2.84438	1.33061
H	0.80204	-3.88072	-0.04682
H	-2.59792	-0.40756	-0.66695
H	-1.69099	-0.65761	1.54260
H	-0.89667	-2.67177	-1.38689
H	-1.62394	-3.25833	0.09369
H	1.28662	-0.47311	1.32872
H	0.19889	0.17215	-1.44733
C	0.05336	1.77301	-0.03152
C	1.13689	2.52507	-0.81218
H	2.13689	2.16679	-0.57027
H	1.10369	3.59026	-0.57699
H	0.98541	2.41276	-1.88712
C	-1.30623	2.33376	-0.45629

H	-1.52898	2.07929	-1.49430
H	-1.31438	3.42086	-0.36409
H	-2.11383	1.94414	0.16617
C	0.24728	2.03636	1.46393
H	0.08818	3.09416	1.67879
H	1.25614	1.78135	1.78791
H	-0.45902	1.46141	2.06471

3-sila-ccl3-ax

C	1.14034	0.92239	-1.04116
Si	1.05520	2.41393	0.11979
C	-0.75819	2.90206	0.19179
C	-1.70076	1.69043	0.13999
C	-1.41459	0.76129	-1.04213
C	-0.08492	-0.01378	-1.05067
H	-0.95548	3.53691	-0.67703
H	1.85784	3.50330	-0.48242
H	1.61798	2.14211	1.45657
H	2.05988	0.35617	-0.89480
H	1.21226	1.34746	-2.04576
H	-2.72990	2.03975	0.04032
H	-1.66255	1.13464	1.07578
H	-1.40128	1.36687	-1.95362
H	-2.23501	0.05684	-1.15945
H	-0.96195	3.51436	1.07079
H	-0.07300	-0.57355	-1.98930
C	0.03055	-1.13975	-0.00536
Cl	0.34665	-0.53974	1.64137
Cl	-1.44481	-2.13633	0.03725
Cl	1.38673	-2.21781	-0.45226

3-sila-ccl3-eq

C	-1.15391	-0.97319	-0.27986
Si	-1.06265	-2.79352	0.18311
C	0.70336	-3.29002	-0.19021
C	1.65966	-2.21376	0.34596
C	1.37531	-0.81128	-0.20081
C	0.04895	-0.22105	0.30250

H	0.82538	-3.37699	-1.27326
H	-2.06264	-3.58351	-0.56575
H	-1.32548	-2.93503	1.63466
H	-2.09218	-0.54365	0.06694
H	-1.14114	-0.88480	-1.36915
H	2.68806	-2.47641	0.09428
H	1.61091	-2.18575	1.43842
H	1.35223	-0.84572	-1.29284
H	2.19600	-0.15448	0.07955
H	0.94429	-4.26531	0.23353
C	-0.03350	1.29689	0.04173
Cl	1.29337	2.15201	0.87550
Cl	0.06520	1.65989	-1.69809
Cl	-1.55970	1.96535	0.67466
H	0.02993	-0.29776	1.39469

3-sila-cf3-ax

C	1.10751	0.46278	-1.04197
Si	1.08451	1.83011	0.26077
C	-0.71678	2.34823	0.36067
C	-1.65140	1.12873	0.35328
C	-1.45158	0.22228	-0.86578
C	-0.09639	-0.49353	-0.97994
H	-0.93617	2.97331	-0.51006
H	1.94277	2.94462	-0.19929
H	1.58989	1.36743	1.56855
H	2.04184	-0.09913	-1.02938
H	1.07050	0.96834	-2.01012
H	-2.68937	1.46536	0.34954
H	-1.52359	0.55296	1.27074
H	-1.56328	0.82671	-1.77003
H	-2.24262	-0.52655	-0.89441
H	-0.89914	2.96681	1.23988
H	-0.12008	-1.09012	-1.89540
C	0.09536	-1.53135	0.10556
F	0.30414	-0.99309	1.31872
F	-0.96693	-2.34079	0.21919

F	1.15392	-2.31425	-0.15053
3-sila-cf3-eq			
C	-1.18898	-0.39040	-0.25265
Si	-1.07185	-2.22608	0.13265
C	0.69482	-2.68044	-0.29507
C	1.65624	-1.63225	0.28708
C	1.36433	-0.20555	-0.18383
C	0.02686	0.34404	0.32869
H	0.79989	-2.70554	-1.38320
H	-2.07237	-3.00360	-0.62816
H	-1.30139	-2.43106	1.58233
H	-2.11501	0.03565	0.13301
H	-1.20070	-0.25811	-1.33783
H	2.68283	-1.88253	0.01627
H	1.61344	-1.65931	1.37995
H	1.36056	-0.17588	-1.27687
H	2.16801	0.45036	0.14983
H	0.94831	-3.67689	0.06788
C	-0.06881	1.82764	0.03983
F	0.93130	2.51541	0.61178
F	-0.02009	2.09056	-1.27459
F	-1.21111	2.35455	0.50200
H	0.01320	0.27173	1.42085
3-sila-cl-ax			
C	1.09065	0.05981	-1.04750
Si	1.05388	1.40116	0.27679
C	-0.76253	1.85523	0.39586
C	-1.63132	0.58870	0.44963
C	-1.42384	-0.34516	-0.74371
C	-0.03221	-0.95916	-0.87155
H	-1.02868	2.44324	-0.48758
H	1.88749	2.54720	-0.14878
H	1.56298	0.90184	1.57058
H	2.05279	-0.44848	-1.09909
H	0.93741	0.55129	-2.01388
H	-2.68618	0.86498	0.48440

H	-1.42716	0.03615	1.36871
H	-1.61052	0.20607	-1.67159
H	-2.15228	-1.15487	-0.70244
H	-0.95633	2.48868	1.26198
Cl	0.31065	-1.99303	0.57814
H	-0.03150	-1.66859	-1.69584

3-sila-cl-eq

C	1.21399	-0.11286	-0.24091
Si	1.05530	1.73257	0.10856
C	-0.71812	2.13268	-0.34318
C	-1.65077	1.07263	0.26335
C	-1.32549	-0.35838	-0.17861
C	0.02107	-0.85384	0.33668
H	-1.00038	3.13051	-0.00630
H	1.26970	1.98193	1.55334
H	2.04828	2.50760	-0.66470
H	1.23453	-0.26305	-1.32342
H	2.14332	-0.51812	0.15828
H	-1.60657	1.12479	1.35543
H	-2.68499	1.28794	-0.00874
H	-2.10194	-1.03296	0.17957
H	-1.32486	-0.42147	-1.27024
H	-0.81799	2.12662	-1.43195
Cl	0.16305	-2.62511	-0.02946
H	0.03393	-0.80596	1.42556

3-sila-f-ax

C	-1.13932	-0.04986	0.66847
Si	-0.97455	1.23139	-0.29283
C	0.66802	1.50260	-0.14657
C	1.49337	0.25194	-0.28233
C	1.25661	-0.70993	0.60566
C	0.03764	-1.22115	0.53294
H	0.83111	1.95740	0.78284
H	-1.71556	2.27212	0.08296
H	-1.28214	0.91953	-1.52984
H	-1.94825	-0.52968	0.59292

H	-1.08203	0.12251	1.65376
H	2.36277	0.47252	-0.19516
H	1.38065	-0.19059	-1.21337
H	1.37037	-0.39627	1.53944
H	1.83376	-1.44458	0.50811
H	0.92924	2.11928	-0.79236
F	0.01884	-1.56192	-0.53121
H	-0.02528	-1.92170	1.03410

3-sila-f-eq

C	-1.26786	0.41113	-0.25476
Si	-0.98783	-1.41343	0.11264
C	0.81367	-1.69744	-0.32142
C	1.67125	-0.56592	0.26867
C	1.24303	0.82723	-0.20004
C	-0.12973	1.23806	0.30731
H	1.15981	-2.66786	0.03557
H	-1.19743	-1.66799	1.55732
H	-1.91672	-2.26476	-0.65987
H	-1.29315	0.55024	-1.33902
H	-2.21883	0.76500	0.14391
H	1.62553	-0.60262	1.36142
H	2.71835	-0.71716	0.00421
H	1.96131	1.57108	0.14514
H	1.23455	0.86853	-1.29296
H	0.91989	-1.70523	-1.40960
F	-0.32958	2.57687	-0.03453
H	-0.13904	1.20223	1.40150

3-sila-ch3-ax

C	-1.26457	0.16045	-0.77175
Si	-0.81501	-1.39733	0.17939
C	1.05250	-1.50523	0.03566
C	1.68546	-0.13006	0.30551
C	1.15402	0.97056	-0.61779
C	-0.32782	1.33794	-0.43768
H	1.30090	-1.82170	-0.98178
H	-1.49104	-2.58376	-0.39287

H	-1.20763	-1.29725	1.60524
H	-2.30508	0.44621	-0.60544
H	-1.17566	-0.08065	-1.83545
H	2.76791	-0.19427	0.18042
H	1.52120	0.15402	1.34800
H	1.31369	0.66041	-1.65541
H	1.74972	1.87406	-0.46945
H	1.46324	-2.26011	0.70707
H	-0.53560	2.13985	-1.15171
C	-0.61014	1.89649	0.95561
H	0.05891	2.72671	1.18511
H	-1.63586	2.25948	1.02200
H	-0.48344	1.14217	1.73253

3-sila-ch3-eq

C	-1.26182	0.36595	-0.26252
Si	-0.98161	-1.44813	0.12219
C	0.81713	-1.74512	-0.31446
C	1.68113	-0.61466	0.26696
C	1.25132	0.78044	-0.19265
C	-0.12579	1.23331	0.30757
H	0.91734	-1.75554	-1.40358
H	-1.90330	-2.33021	-0.62903
H	-1.18465	-1.68578	1.57219
H	-2.22601	0.71006	0.11707
H	-1.29182	0.49465	-1.35005
H	2.72622	-0.77176	-0.00623
H	1.64247	-0.65069	1.36007
H	1.25363	0.81796	-1.28828
H	1.99565	1.50633	0.14189
H	1.16100	-2.71675	0.04194
C	-0.35296	2.70415	-0.02708
H	-1.32327	3.04380	0.33506
H	0.41759	3.33703	0.41462
H	-0.33003	2.85098	-1.10901
H	-0.12905	1.12787	1.39884

3-sila-sih3-ax

C	1.11635	0.10308	-1.02050
Si	1.04853	1.46979	0.27039
C	-0.76644	1.93314	0.37444
C	-1.64262	0.67053	0.41506
C	-1.41460	-0.25814	-0.78154
C	-0.02727	-0.92245	-0.84870
H	-1.02459	2.51996	-0.51199
H	1.89579	2.61546	-0.13021
H	1.52514	0.98009	1.58421
H	2.09109	-0.38931	-1.02274
H	1.01701	0.58564	-1.99900
H	-2.69570	0.95644	0.43850
H	-1.45721	0.12390	1.34438
H	-1.56973	0.32011	-1.69964
H	-2.17976	-1.03704	-0.77654
H	-0.96390	2.56917	1.23806
Si	0.28163	-2.14080	0.55966
H	-0.84728	-3.09509	0.63451
H	1.52903	-2.88614	0.28223
H	0.42398	-1.48505	1.87672
H	-0.03085	-1.56950	-1.73359
3-sila-sih3-eq			
C	-1.21458	-0.08208	0.24643
Si	-1.06771	1.75352	-0.11980
C	0.69972	2.18285	0.33437
C	1.66206	1.14130	-0.25708
C	1.34415	-0.29492	0.17149
C	0.00008	-0.83736	-0.34449
H	0.78987	2.18292	1.42454
H	-2.05583	2.56256	0.62919
H	-1.27586	1.97468	-1.57130
H	-2.15174	-0.48775	-0.13950
H	-1.23854	-0.22388	1.33216
H	2.68727	1.37817	0.03438
H	1.63284	1.19303	-1.34955
H	1.35090	-0.34997	1.26594

H	2.15182	-0.94483	-0.17328
H	0.96401	3.18637	-0.00115
H	-0.01240	-0.72429	-1.43525
Si	-0.15692	-2.67515	0.02472
H	-1.44252	-3.19414	-0.49108
H	0.95295	-3.44446	-0.58227
H	-0.12109	-2.87132	1.49203

3-sila-tbu-ax

C	0.76144	2.46741	-0.30044
C	1.67466	1.23174	-0.29211
C	1.40093	0.30416	0.89515
C	0.06546	-0.46443	0.91589
C	-1.13364	0.51166	0.96515
Si	-1.05060	1.98008	-0.21497
H	2.22121	-0.40612	0.99263
H	1.57883	0.68352	-1.23049
H	2.71691	1.55380	-0.24212
H	0.98648	3.07523	0.58066
H	0.95896	3.09658	-1.16915
H	0.07512	-0.99172	1.87616
H	-2.08118	-0.01919	0.86100
H	-1.15870	0.95897	1.96382
H	-1.57291	1.66984	-1.56416
H	-1.87217	3.08921	0.32425
H	1.43050	0.91555	1.80382
C	-0.09422	-1.60758	-0.13419
C	-0.64024	-1.14323	-1.48789
H	-0.02392	-0.37516	-1.95204
H	-0.67698	-1.99217	-2.17283
H	-1.65260	-0.75081	-1.39821
C	-1.08220	-2.63617	0.43203
H	-1.26108	-3.43163	-0.29292
H	-0.68922	-3.09098	1.34249
H	-2.04451	-2.18210	0.66930
C	1.24014	-2.32248	-0.36077
H	1.68108	-2.64317	0.58503

H	1.08519	-3.21034	-0.97531
H	1.96095	-1.68466	-0.87310
3-sila-tbu-eq			
C	-1.18747	-0.46045	0.26760
Si	-1.05743	-2.28145	-0.16620
C	0.70331	-2.76720	0.24685
C	1.65908	-1.67998	-0.26815
C	1.33218	-0.28180	0.26580
C	0.02454	0.32254	-0.27393
H	2.16693	0.37701	0.02889
H	1.63387	-1.65550	-1.36181
H	2.68464	-1.93207	0.00797
H	0.80251	-2.85135	1.33265
H	0.96078	-3.74160	-0.16973
H	-2.12174	-0.06755	-0.13276
H	-1.24134	-0.35767	1.35584
H	-1.28623	-2.44832	-1.62244
H	-2.06061	-3.09446	0.55852
H	1.27598	-0.32891	1.35827
H	0.03517	0.19766	-1.36527
C	-0.06582	1.85942	-0.03274
C	0.96500	2.58019	-0.90888
H	1.98736	2.28615	-0.67706
H	0.89473	3.65865	-0.76003
H	0.78363	2.37581	-1.96569
C	-1.44887	2.38131	-0.43321
H	-1.72293	2.03925	-1.43369
H	-1.44687	3.47197	-0.44008
H	-2.22236	2.05805	0.26198
C	0.18848	2.21478	1.43368
H	0.02340	3.28155	1.59250
H	1.21294	1.99040	1.73038
H	-0.48647	1.67376	2.09849
4-sila-ccl3-ax			
C	-1.09444	0.82801	-1.28282
C	0.03689	1.84452	-1.50869

Si	0.26425	2.93998	0.00000
C	0.03689	1.84452	1.50869
C	-1.09444	0.82801	1.28282
C	-1.04887	-0.02542	0.00000
H	-0.81090	3.96230	0.00000
H	-0.22097	2.46230	-2.37041
H	0.96857	1.34172	-1.75990
H	-1.18432	0.16988	-2.14544
H	-2.03996	1.37329	-1.22138
H	-0.22097	2.46230	2.37041
H	0.96857	1.34172	1.75990
H	-2.03996	1.37329	1.22138
H	-1.18432	0.16988	2.14544
H	1.57097	3.63249	0.00000
H	-1.97516	-0.60646	0.00000
C	0.01598	-1.13827	0.00000
Cl	1.70065	-0.55512	0.00000
Cl	-0.19230	-2.17857	1.43729
Cl	-0.19230	-2.17857	-1.43729
4-sila-ccl3-eq			
C	-0.23149	-0.87167	1.27197
C	0.34906	-2.28037	1.47714
Si	-0.03995	-3.36876	0.00000
C	0.34906	-2.28037	-1.47714
C	-0.23149	-0.87167	-1.27197
C	0.30843	-0.19705	0.00000
H	-1.48475	-3.69836	0.00000
H	-0.04463	-2.71009	2.39860
H	1.43306	-2.21406	1.60264
H	-0.00550	-0.25705	2.14066
H	-1.32034	-0.92401	1.19778
H	-0.04463	-2.71009	-2.39860
H	1.43306	-2.21406	-1.60264
H	-1.32034	-0.92401	-1.19778
H	-0.00550	-0.25705	-2.14066
H	0.73944	-4.62561	0.00000

C	0.03841	1.31675	0.00000
Cl	0.76843	2.09538	-1.43059
Cl	-1.70939	1.65556	0.00000
Cl	0.76843	2.09538	1.43059
H	1.40078	-0.27313	0.00000

4-sila-cf3-ax

C	-0.98875	0.31011	-1.29275
C	0.19601	1.26986	-1.49511
Si	0.39411	2.38744	0.00000
C	0.19601	1.26986	1.49511
C	-0.98875	0.31011	1.29275
C	-0.97008	-0.52214	0.00000
H	-0.70765	3.38110	0.00000
H	0.02552	1.86349	-2.39400
H	1.11757	0.71179	-1.66104
H	-1.07463	-0.36745	-2.14291
H	-1.91514	0.88918	-1.26844
H	0.02552	1.86349	2.39400
H	1.11757	0.71179	1.66104
H	-1.91514	0.88918	1.26844
H	-1.07463	-0.36745	2.14291
H	1.68397	3.10999	0.00000
H	-1.87542	-1.13411	0.00000
C	0.13983	-1.55185	0.00000
F	1.37342	-1.01874	0.00000
F	0.06976	-2.34829	1.07701
F	0.06976	-2.34829	-1.07701

4-sila-cf3-eq

C	0.19424	-0.27183	1.28476
C	-0.31249	-1.70888	1.47876
Si	0.14872	-2.76811	0.00000
C	-0.31249	-1.70888	-1.47876
C	0.19424	-0.27183	-1.28476
C	-0.34092	0.37564	0.00000
H	1.61164	-3.00421	0.00000
H	0.08758	-2.12337	2.40429

H	-1.40073	-1.70090	1.58539
H	-0.09281	0.34019	2.13978
H	1.28667	-0.26370	1.24428
H	0.08758	-2.12337	-2.40429
H	-1.40073	-1.70090	-1.58539
H	1.28667	-0.26370	-1.24428
H	-0.09281	0.34019	-2.13978
H	-0.54919	-4.07181	0.00000
C	-0.02440	1.85522	0.00000
F	-0.52971	2.47798	-1.07478
F	1.29712	2.08727	0.00000
F	-0.52971	2.47798	1.07478
H	-1.43421	0.31937	0.00000

4-sila-cl-ax

C	-0.90059	-0.19089	-1.28914
C	0.25415	0.80083	-1.48442
Si	0.38856	1.94012	0.00000
C	0.25415	0.80083	1.48442
C	-0.90059	-0.19089	1.28914
C	-0.83917	-1.00557	0.00000
H	-0.76238	2.87661	0.00000
H	0.10361	1.36471	-2.40514
H	1.19005	0.25089	-1.59906
H	-0.95257	-0.88318	-2.13023
H	-1.85290	0.34889	-1.26629
H	0.10361	1.36471	2.40514
H	1.19005	0.25089	1.59906
H	-1.85290	0.34889	1.26629
H	-0.95257	-0.88318	2.13023
H	1.64031	2.72722	0.00000
Cl	0.64927	-2.03798	0.00000
H	-1.65528	-1.72408	0.00000

4-sila-cl-eq

C	0.17721	-0.27031	1.28474
C	-0.29652	1.18037	1.47561
Si	0.19876	2.22801	0.00000

C	-0.29652	1.18037	-1.47561
C	0.17721	-0.27031	-1.28474
C	-0.35542	-0.89632	0.00000
H	-0.46218	3.55090	0.00000
H	-1.38538	1.20064	1.57461
H	0.10712	1.58112	2.40566
H	1.26917	-0.31384	1.25580
H	-0.13959	-0.88476	2.12716
H	-1.38538	1.20064	-1.57461
H	0.10712	1.58112	-2.40566
H	-0.13959	-0.88476	-2.12716
H	1.26917	-0.31384	-1.25580
H	1.66763	2.42274	0.00000
Cl	0.06903	-2.64956	0.00000
H	-1.44573	-0.87038	0.00000

4-sila-f-ax

C	-0.65555	-0.64875	-1.28944
C	0.26253	0.56835	-1.47735
Si	0.12434	1.71484	0.00000
C	0.26253	0.56835	1.47735
C	-0.65555	-0.64875	1.28944
C	-0.40357	-1.41774	0.00000
H	-1.21191	2.36005	0.00000
H	0.02059	1.07850	-2.40968
H	1.29677	0.22850	-1.56065
H	-0.53641	-1.34345	-2.12260
H	-1.70413	-0.33890	-1.28557
H	0.02059	1.07850	2.40968
H	1.29677	0.22850	1.56065
H	-1.70413	-0.33890	1.28557
H	-0.53641	-1.34345	2.12260
H	1.16025	2.77050	0.00000
F	0.92669	-1.84518	0.00000
H	-1.01364	-2.32345	0.00000

4-sila-f-eq

C	0.21569	-0.65334	1.28086
---	---------	----------	---------

C	-0.29523	0.78199	1.47951
Si	0.16694	1.84173	0.00000
C	-0.29523	0.78199	-1.47951
C	0.21569	-0.65334	-1.28086
C	-0.30192	-1.28712	0.00000
H	-0.53339	3.14437	0.00000
H	-1.38408	0.77419	1.58087
H	0.09937	1.19636	2.40711
H	1.30852	-0.66926	1.24712
H	-0.08610	-1.28918	2.11427
H	-1.38408	0.77419	-1.58087
H	0.09937	1.19636	-2.40711
H	-0.08610	-1.28918	-2.11427
H	1.30852	-0.66926	-1.24712
H	1.62918	2.08201	0.00000
F	0.08565	-2.62410	0.00000
H	-1.39748	-1.27928	0.00000

4-sila-ch3-ax

C	-0.69788	-0.61232	-1.28041
C	0.22104	0.60329	-1.49247
Si	0.13021	1.73719	0.00000
C	0.22104	0.60329	1.49247
C	-0.69788	-0.61232	1.28041
C	-0.41691	-1.41501	0.00000
H	-1.18155	2.43031	0.00000
H	-0.06594	1.13585	-2.40016
H	1.25255	0.27734	-1.64195
H	-0.61876	-1.28665	-2.13683
H	-1.73766	-0.27330	-1.25188
H	-0.06594	1.13585	2.40016
H	1.25255	0.27734	1.64195
H	-1.73766	-0.27330	1.25188
H	-0.61876	-1.28665	2.13683
H	1.19972	2.76112	0.00000
H	-1.12116	-2.25144	0.00000
C	0.98978	-2.00868	0.00000

H	1.14787	-2.62916	0.88281
H	1.14787	-2.62916	-0.88281
H	1.75944	-1.23716	0.00000

4-sila-ch3-eq

C	0.20456	-0.60735	1.27792
C	-0.30158	0.82947	1.47899
Si	0.16275	1.88343	0.00000
C	-0.30158	0.82947	-1.47899
C	0.20456	-0.60735	-1.27792
C	-0.30549	-1.28533	0.00000
H	1.62722	2.11905	0.00000
H	0.09095	1.24774	2.40664
H	-1.39101	0.82125	1.57576
H	-0.08227	-1.22102	2.13527
H	1.30010	-0.61345	1.25241
H	0.09095	1.24774	-2.40664
H	-1.39101	0.82125	-1.57576
H	1.30010	-0.61345	-1.25241
H	-0.08227	-1.22102	-2.13527
H	-0.52368	3.19514	0.00000
C	0.09045	-2.75790	0.00000
H	-0.29074	-3.27109	0.88278
H	-0.29074	-3.27109	-0.88278
H	1.17821	-2.85672	0.00000
H	-1.40030	-1.22019	0.00000

4-sila-sih3-ax

C	-0.94205	0.12911	-1.28423
C	0.22406	-0.85183	-1.49548
Si	0.39718	-1.97402	0.00000
C	0.22406	-0.85183	1.49548
C	-0.94205	0.12911	1.28423
C	-0.83760	0.97287	0.00000
H	-0.72001	-2.94982	0.00000
H	0.06209	-1.43889	-2.40051
H	1.15766	-0.30398	-1.64602
H	-1.02462	0.79505	-2.14620

H	-1.87910	-0.43680	-1.24540
H	0.06209	-1.43889	2.40051
H	1.15766	-0.30398	1.64602
H	-1.87910	-0.43680	1.24540
H	-1.02462	0.79505	2.14620
H	1.67435	-2.72157	0.00000
Si	0.64887	2.13612	0.00000
H	0.59624	2.99157	1.20631
H	0.59624	2.99157	-1.20631
H	1.94926	1.43085	0.00000
H	-1.69379	1.65645	0.00000

4-sila-sih3-eq

C	0.17520	0.21873	1.28529
C	-0.29838	-1.23210	1.48218
Si	0.18926	-2.27214	0.00000
C	-0.29838	-1.23210	-1.48218
C	0.17520	0.21873	-1.28529
C	-0.35419	0.87949	0.00000
H	1.65907	-2.47012	0.00000
H	0.10591	-1.64345	2.40820
H	-1.38740	-1.24583	1.58091
H	-0.12197	0.81494	2.15169
H	1.27010	0.24379	1.26160
H	0.10591	-1.64345	-2.40820
H	-1.38740	-1.24583	-1.58091
H	1.27010	0.24379	-1.26160
H	-0.12197	0.81494	-2.15169
H	-0.46512	-3.59974	0.00000
H	-1.44875	0.80223	0.00000
Si	0.06478	2.71388	0.00000
H	-0.48417	3.37456	1.20441
H	-0.48417	3.37456	-1.20441
H	1.53630	2.87879	0.00000

4-sila-tbu-ax

Si	-0.32555	2.53528	0.00000
C	-0.16667	1.42085	-1.49963

C	0.94916	0.38339	-1.27419
C	0.88368	-0.48478	0.00000
C	0.94916	0.38339	1.27419
C	-0.16667	1.42085	1.49963
H	1.03487	-0.26222	-2.14846
H	-1.12053	0.94267	-1.71514
H	0.07470	2.02063	-2.37927
H	0.80889	3.49188	0.00000
H	-1.58708	3.31047	0.00000
H	1.83849	-1.02365	0.00000
H	1.03487	-0.26222	2.14846
H	1.89790	0.92695	1.22228
H	-1.12053	0.94267	1.71514
H	0.07470	2.02063	2.37927
H	1.89790	0.92695	-1.22228
C	-0.15747	-1.64628	0.00000
C	-1.63480	-1.23688	0.00000
H	-1.90660	-0.66410	-0.88300
H	-2.25032	-2.13884	0.00000
H	-1.90660	-0.66410	0.88300
C	0.07910	-2.51908	1.23917
H	-0.52113	-3.42768	1.17631
H	1.12750	-2.81232	1.32210
H	-0.20416	-2.00354	2.15649
C	0.07910	-2.51908	-1.23917
H	1.12750	-2.81232	-1.32210
H	-0.52113	-3.42768	-1.17631
H	-0.20416	-2.00354	-2.15649
4-sila-tbu-eq			
C	-0.25178	-0.34525	-1.26574
C	0.31083	-1.76245	-1.47474
Si	-0.09760	-2.84199	0.00000
C	0.31083	-1.76245	1.47474
C	-0.25178	-0.34525	1.26574
C	0.27826	0.35209	0.00000
H	-0.01888	0.25188	2.14564

H	1.39756	-1.70838	1.58515
H	-0.07572	-2.19036	2.40068
H	-1.54844	-3.15116	0.00000
H	0.65344	-4.11802	0.00000
H	-0.01888	0.25188	-2.14564
H	-1.34354	-0.39577	-1.20767
H	1.39756	-1.70838	-1.58515
H	-0.07572	-2.19036	-2.40068
H	-1.34354	-0.39577	1.20767
H	1.37115	0.23805	0.00000
C	0.01896	1.88705	0.00000
C	0.66459	2.53331	1.23264
H	0.15621	2.26691	2.15719
H	0.62569	3.61967	1.14487
H	1.71315	2.24168	1.32230
C	0.66459	2.53331	-1.23264
H	1.71315	2.24168	-1.32230
H	0.62569	3.61967	-1.14487
H	0.15621	2.26691	-2.15719
C	-1.47740	2.20782	0.00000
H	-1.62706	3.28880	0.00000
H	-1.97306	1.80573	0.88402
H	-1.97306	1.80573	-0.88402

14-disila-ccl3-ax

Si	1.15128	-0.08699	0.00000
C	0.91167	-1.11942	1.54406
C	0.91167	-1.11942	-1.54406
C	-0.29551	-2.08169	1.52681
C	-0.29551	-2.08169	-1.52681
Si	-0.31920	-3.17922	0.00000
H	0.88024	-0.46081	2.41472
H	0.88024	-0.46081	-2.41472
H	1.83695	-1.69720	1.64270
H	1.83695	-1.69720	-1.64270
H	-1.22885	-1.51672	1.55558
H	-1.22885	-1.51672	-1.55558

H	-0.28816	-2.70414	2.42370
H	-0.28816	-2.70414	-2.42370
H	-1.50446	-4.06384	0.00000
H	0.90581	-4.01732	0.00000
H	2.46790	0.58014	0.00000
C	-0.07231	1.40306	0.00000
Cl	-1.76977	0.85527	0.00000
Cl	0.21197	2.39533	-1.45033
Cl	0.21197	2.39533	1.45033

14-disila-ccl3-eq

Si	0.58289	0.22295	0.00000
C	-0.05716	1.08636	-1.52953
C	-0.05716	1.08636	1.52953
C	0.32175	2.58564	-1.52139
C	0.32175	2.58564	1.52139
Si	-0.33100	3.48240	0.00000
H	0.32201	0.59011	-2.42444
H	0.32201	0.59011	2.42444
H	-1.14476	0.97397	-1.54925
H	-1.14476	0.97397	1.54925
H	1.40967	2.69844	-1.54063
H	1.40967	2.69844	1.54063
H	-0.04789	3.07449	-2.42468
H	-0.04789	3.07449	2.42468
H	0.09109	4.89987	0.00000
H	-1.81186	3.41686	0.00000
C	-0.01131	-1.60443	0.00000
Cl	0.60177	-2.43180	-1.45128
Cl	-1.79199	-1.66481	0.00000
Cl	0.60177	-2.43180	1.45128
H	2.05888	0.14445	0.00000

14-disila-cf3-ax

Si	-1.14631	0.43138	0.00000
C	-0.90663	-0.59936	1.54301
C	-0.90663	-0.59936	-1.54301
C	0.38797	-1.44269	1.52495

C	0.38797	-1.44269	-1.52495
Si	0.51060	-2.53849	0.00000
H	-0.94104	0.05111	2.41983
H	-0.94104	0.05111	-2.41983
H	-1.77755	-1.25728	1.62100
H	-1.77755	-1.25728	-1.62100
H	1.26265	-0.78852	1.54185
H	1.26265	-0.78852	-1.54185
H	0.44855	-2.05684	2.42529
H	0.44855	-2.05684	-2.42529
H	1.77154	-3.31040	0.00000
H	-0.63374	-3.48330	0.00000
H	-2.42139	1.17472	0.00000
C	0.21317	1.80957	0.00000
F	1.46897	1.30458	0.00000
F	0.13270	2.61111	-1.08001
F	0.13270	2.61111	1.08001
14-disila-cf3-eq			
Si	0.57114	-0.32184	0.00000
C	-0.06685	0.54181	-1.53029
C	-0.06685	0.54181	1.53029
C	0.30046	2.04345	-1.52336
C	0.30046	2.04345	1.52336
Si	-0.35561	2.93592	0.00000
H	0.31377	0.04703	-2.42568
H	0.31377	0.04703	2.42568
H	-1.15395	0.42145	-1.54903
H	-1.15395	0.42145	1.54903
H	1.38750	2.16399	-1.54509
H	1.38750	2.16399	1.54509
H	-0.07491	2.53065	-2.42515
H	-0.07491	2.53065	2.42515
H	0.05987	4.35510	0.00000
H	-1.83595	2.86225	0.00000
C	-0.09127	-2.13630	0.00000
F	0.30802	-2.83584	-1.08000

F	-1.44105	-2.17428	0.00000
F	0.30802	-2.83584	1.08000
H	2.04536	-0.42814	0.00000
14-disila-cl-ax			
Cl	1.13691	2.12831	0.00000
Si	-0.69006	1.14156	0.00000
H	-1.73853	2.17807	0.00000
C	-0.75758	0.06521	1.52536
C	-0.75758	0.06521	-1.52536
C	0.33124	-1.02906	1.52490
C	0.33124	-1.02906	-1.52490
Si	0.23750	-2.12789	0.00000
H	-0.68521	0.69112	2.41710
H	-0.68521	0.69112	-2.41710
H	-1.75265	-0.39151	1.54919
H	-1.75265	-0.39151	-1.54919
H	1.32053	-0.56450	1.54893
H	1.32053	-0.56450	-1.54893
H	0.25837	-1.64045	2.42619
H	0.25837	-1.64045	-2.42619
H	1.32334	-3.13209	0.00000
H	-1.06805	-2.83328	0.00000
14-disila-cl-eq			
H	1.87484	1.10486	0.00000
Si	0.40127	0.99666	0.00000
Cl	-0.35532	2.92115	0.00000
C	-0.18383	0.08610	-1.52224
C	-0.18383	0.08610	1.52224
C	0.30803	-1.37911	-1.52187
C	0.30803	-1.37911	1.52187
Si	-0.26802	-2.32591	0.00000
H	0.14646	0.61380	-2.41891
H	0.14646	0.61380	2.41891
H	-1.27697	0.11944	-1.52974
H	-1.27697	0.11944	1.52974
H	1.40139	-1.40826	-1.54507

H	1.40139	-1.40826	1.54507
H	-0.02590	-1.89373	-2.42487
H	-0.02590	-1.89373	2.42487
H	0.26768	-3.70465	0.00000
H	-1.74944	-2.38305	0.00000

14-disila-f-ax

F	-1.09208	1.99687	0.00000
Si	0.40704	1.42064	0.00000
H	1.32120	2.57970	0.00000
C	0.60797	0.36329	1.52305
C	0.60797	0.36329	-1.52305
C	-0.34531	-0.85346	1.52164
C	-0.34531	-0.85346	-1.52164
Si	-0.11278	-1.93559	0.00000
H	0.45957	0.97418	2.41652
H	0.45957	0.97418	-2.41652
H	1.64904	0.02591	1.55598
H	1.64904	0.02591	-1.55598
H	-1.38327	-0.51015	1.53531
H	-1.38327	-0.51015	-1.53531
H	-0.20974	-1.44963	2.42593
H	-0.20974	-1.44963	-2.42593
H	-1.06538	-3.06746	0.00000
H	1.27016	-2.47340	0.00000

14-disila-f-eq

H	-1.80985	1.48158	0.00000
Si	-0.33591	1.35663	0.00000
F	0.27186	2.83785	0.00000
C	0.23547	0.43860	-1.51939
C	0.23547	0.43860	1.51939
C	-0.28095	-1.01890	-1.52143
C	-0.28095	-1.01890	1.52143
Si	0.27981	-1.97501	0.00000
H	-0.08395	0.96764	-2.41970
H	-0.08395	0.96764	2.41970
H	1.32949	0.44924	-1.52847

H	1.32949	0.44924	1.52847
H	-1.37484	-1.02978	-1.54180
H	-1.37484	-1.02978	1.54180
H	0.04137	-1.53962	-2.42497
H	0.04137	-1.53962	2.42497
H	-0.27694	-3.34568	0.00000
H	1.76033	-2.05677	0.00000

14-disila-ch3-ax

Si	0.43554	1.41254	0.00000
H	1.45149	2.49263	0.00000
C	0.65824	0.32156	-1.51930
C	0.65824	0.32156	1.51930
C	-0.30770	-0.88355	-1.52711
C	-0.30770	-0.88355	1.52711
Si	-0.09945	-1.96224	0.00000
H	0.53355	0.92215	-2.42380
H	0.53355	0.92215	2.42380
H	1.69307	-0.03310	-1.53239
H	1.69307	-0.03310	1.53239
H	-1.34428	-0.53560	-1.55948
H	-1.34428	-0.53560	1.55948
H	-0.16655	-1.48956	-2.42471
H	-0.16655	-1.48956	2.42471
H	-1.07497	-3.07618	0.00000
H	1.27020	-2.53260	0.00000
C	-1.27869	2.17178	0.00000
H	-1.42909	2.79495	-0.88175
H	-1.42909	2.79495	0.88175
H	-2.05240	1.40312	0.00000

14-disila-ch3-eq

Si	-0.36342	1.29182	0.00000
C	0.19558	0.33171	-1.51959
C	0.19558	0.33171	1.51959
C	-0.31381	-1.12547	-1.52384
C	-0.31381	-1.12547	1.52384
Si	0.24977	-2.07251	0.00000

H	-0.12598	0.85667	-2.42260
H	-0.12598	0.85667	2.42260
H	1.29027	0.34341	-1.53726
H	1.29027	0.34341	1.53726
H	-1.40760	-1.13771	-1.54049
H	-1.40760	-1.13771	1.54049
H	0.00962	-1.65003	-2.42547
H	0.00962	-1.65003	2.42547
H	-0.29198	-3.45050	0.00000
H	1.73190	-2.14751	0.00000
C	0.32786	3.03047	0.00000
H	0.00227	3.58254	0.88150
H	0.00227	3.58254	-0.88150
H	1.41820	3.00946	0.00000
H	-1.84910	1.33764	0.00000
14-disila-sih3-ax			
Si	-0.95402	0.92821	0.00000
C	-0.87030	-0.18132	-1.52543
C	-0.87030	-0.18132	1.52543
C	0.38249	-1.08306	-1.52808
C	0.38249	-1.08306	1.52808
Si	0.47205	-2.17738	0.00000
H	-0.91122	0.43068	-2.42906
H	-0.91122	0.43068	2.42906
H	-1.77346	-0.79877	-1.53459
H	-1.77346	-0.79877	1.53459
H	1.28869	-0.47086	-1.55972
H	1.28869	-0.47086	1.55972
H	0.40738	-1.70618	-2.42463
H	0.40738	-1.70618	2.42463
H	1.71089	-2.98693	0.00000
H	-0.69544	-3.09279	0.00000
Si	0.85573	2.41881	0.00000
H	0.82582	3.28406	-1.20051
H	0.82582	3.28406	1.20051
H	2.14682	1.69193	0.00000

H	-2.21568	1.70757	0.00000
14-disila-sih3-eq			
Si	0.00006	-0.85670	0.49293
C	-1.52649	0.06486	-0.12618
C	1.52644	0.06490	-0.12655
C	-1.52434	1.55136	0.29048
C	1.52435	1.55140	0.29011
Si	-0.00008	2.46002	-0.33329
H	-2.42741	-0.43774	0.23268
H	2.42745	-0.43768	0.23210
H	-1.54713	-0.01670	-1.21719
H	1.54683	-0.01666	-1.21758
H	-1.54240	1.63185	1.38114
H	1.54267	1.63188	1.38077
H	-2.42549	2.05429	-0.06731
H	2.42540	2.05435	-0.06790
H	-0.00005	3.86886	0.12040
H	-0.00026	2.43766	-1.81669
H	0.00025	-0.81932	1.97878
Si	0.00004	-3.08048	-0.23510
H	1.20033	-3.79873	0.24735
H	-1.19929	-3.79929	0.24889
H	-0.00089	-3.12741	-1.71511
14-disila-tbu-ax			
Si	0.40099	2.75407	0.00000
C	0.40205	1.65100	-1.52088
C	-0.79651	0.67764	-1.53021
C	-0.79651	0.67764	1.53021
C	0.40205	1.65100	1.52088
H	-0.77838	0.04888	-2.42410
H	1.34634	1.10135	-1.53178
H	0.40269	2.26650	-2.42316
H	-0.83514	3.57510	0.00000
H	1.57159	3.66083	0.00000
H	-0.77838	0.04888	2.42410
H	-1.72476	1.25381	1.59832

H	1.34634	1.10135	1.53178
H	0.40269	2.26650	2.42316
H	-1.72476	1.25381	-1.59832
C	0.19190	-1.91308	0.00000
C	1.67130	-1.52040	0.00000
H	1.93808	-0.93990	-0.88397
H	2.29469	-2.42005	0.00000
H	1.93808	-0.93990	0.88397
C	-0.09999	-2.75452	1.24717
H	0.51264	-3.66108	1.23837
H	-1.14642	-3.06184	1.29113
H	0.13164	-2.21088	2.16457
C	-0.09999	-2.75452	-1.24717
H	-1.14642	-3.06184	-1.29113
H	0.51264	-3.66108	-1.23837
H	0.13164	-2.21088	-2.16457
Si	-0.97574	-0.41567	0.00000
H	-2.34762	-0.98788	0.00000

14-disila-tbu-eq

Si	-0.26202	-3.02018	0.00000
C	0.33879	-2.09562	1.52303
C	-0.11461	-0.61914	1.52070
Si	0.48983	0.31623	0.00000
C	-0.11461	-0.61914	-1.52070
C	0.33879	-2.09562	-1.52303
H	0.22749	-0.11234	2.42621
H	1.43123	-2.14997	1.53958
H	-0.00468	-2.60681	2.42497
H	-1.74591	-3.03635	0.00000
H	0.22526	-4.41833	0.00000
H	0.22749	-0.11234	-2.42621
H	-1.20802	-0.56921	-1.53822
H	1.43123	-2.14997	-1.53958
H	-0.00468	-2.60681	-2.42497
H	-1.20802	-0.56921	1.53822
H	1.97879	0.29427	0.00000

C	-0.07630	2.12229	0.00000
C	0.46815	2.82346	1.24837
H	0.07520	2.37979	2.16459
H	0.17846	3.87858	1.24243
H	1.55798	2.77922	1.29170
C	0.46815	2.82346	-1.24837
H	1.55798	2.77922	-1.29170
H	0.17846	3.87858	-1.24243
H	0.07520	2.37979	-2.16459
C	-1.60569	2.20402	0.00000
H	-1.92504	3.25052	0.00000
H	-2.03668	1.72949	0.88327
H	-2.03668	1.72949	-0.88327

26-disila-ccl3-ax

Si	-0.76050	1.07861	-1.52319
C	0.54537	2.40232	-1.27831
C	0.36466	3.23206	0.00000
C	0.54537	2.40232	1.27831
Si	-0.76050	1.07861	1.52319
C	-0.89942	-0.06831	0.00000
H	-0.62762	3.69238	0.00000
H	0.50349	3.05301	-2.15528
H	1.53518	1.94059	-1.28442
H	-0.51328	0.31182	-2.75753
H	-2.08405	1.73772	-1.60374
H	0.50349	3.05301	2.15528
H	1.53518	1.94059	1.28442
H	-2.08405	1.73772	1.60374
H	-0.51328	0.31182	2.75753
H	1.08067	4.05581	0.00000
H	-1.92335	-0.45269	0.00000
C	0.00287	-1.28046	0.00000
Cl	1.72602	-0.79245	0.00000
Cl	-0.27355	-2.32141	1.43256
Cl	-0.27355	-2.32141	-1.43256

26-disila-ccl3-eq

Si	-0.17819	-1.09277	1.52678
C	0.43004	-2.85200	1.27831
C	-0.08453	-3.52676	0.00000
C	0.43004	-2.85200	-1.27831
Si	-0.17819	-1.09277	-1.52678
C	0.38873	-0.10395	0.00000
H	-1.17795	-3.52255	0.00000
H	0.12759	-3.42843	2.15543
H	1.52413	-2.85113	1.27898
H	0.37564	-0.52389	2.76985
H	-1.65473	-1.08624	1.58642
H	0.12759	-3.42843	-2.15543
H	1.52413	-2.85113	-1.27898
H	-1.65473	-1.08624	-1.58642
H	0.37564	-0.52389	-2.76985
H	0.21554	-4.57620	0.00000
C	0.05974	1.37229	0.00000
Cl	0.74361	2.19844	-1.43750
Cl	-1.70353	1.64526	0.00000
Cl	0.74361	2.19844	1.43750
H	1.48285	-0.17496	0.00000

26-disila-cf3-ax

Si	-0.71353	0.57969	-1.52767
C	0.70022	1.78624	-1.28372
C	0.58955	2.62400	0.00000
C	0.70022	1.78624	1.28372
Si	-0.71353	0.57969	1.52767
C	-0.85391	-0.54348	0.00000
H	-0.35860	3.16946	0.00000
H	0.73371	2.44332	-2.15554
H	1.64098	1.22973	-1.28032
H	-0.54496	-0.21987	-2.75677
H	-1.99012	1.32538	-1.59209
H	0.73371	2.44332	2.15554
H	1.64098	1.22973	1.28032
H	-1.99012	1.32538	1.59209

H	-0.54496	-0.21987	2.75677
H	1.37430	3.38243	0.00000
H	-1.84241	-1.00800	0.00000
C	0.14461	-1.65960	0.00000
F	1.41340	-1.19597	0.00000
F	0.03562	-2.46127	1.07269
F	0.03562	-2.46127	-1.07269

26-disila-cf3-eq

Si	-0.15046	-0.52482	1.53877
C	0.32952	-2.32077	1.28184
C	-0.23987	-2.94684	0.00000
C	0.32952	-2.32077	-1.28184
Si	-0.15046	-0.52482	-1.53877
C	0.42509	0.42349	0.00000
H	-1.32936	-2.85242	0.00000
H	-0.00732	-2.88400	2.15472
H	1.42083	-2.39817	1.27398
H	0.47751	0.02681	2.75581
H	-1.62073	-0.41112	1.64040
H	-0.00732	-2.88400	-2.15472
H	1.42083	-2.39817	-1.27398
H	-1.62073	-0.41112	-1.64040
H	0.47751	0.02681	-2.75581
H	-0.02893	-4.01763	0.00000
C	0.04941	1.87326	0.00000
F	0.52276	2.52976	-1.07499
F	-1.28201	2.05243	0.00000
F	0.52276	2.52976	1.07499
H	1.51921	0.38656	0.00000

26-disila-cl-ax

Si	-0.68135	0.08804	-1.53986
C	0.71713	1.31054	-1.28640
C	0.58500	2.14327	0.00000
C	0.71713	1.31054	1.28640
Si	-0.68135	0.08804	1.53986
C	-0.76115	-1.00117	0.00000

H	-0.37597	2.66622	0.00000
H	0.75669	1.97097	-2.15511
H	1.66229	0.76115	-1.27368
H	-0.48985	-0.73800	-2.74863
H	-1.96814	0.81834	-1.63228
H	0.75669	1.97097	2.15511
H	1.66229	0.76115	1.27368
H	-1.96814	0.81834	1.63228
H	-0.48985	-0.73800	2.74863
H	1.35081	2.92093	0.00000
Cl	0.70927	-2.05693	0.00000
H	-1.62463	-1.66313	0.00000

26-disila-cl-eq

Si	0.14178	0.02222	1.53645
C	-0.27476	1.83888	1.28644
C	0.31758	2.43760	0.00000
C	-0.27476	1.83888	-1.28644
Si	0.14178	0.02222	-1.53645
C	-0.47165	-0.87851	0.00000
H	0.15154	3.51637	0.00000
H	-1.36217	1.95890	1.27903
H	0.08469	2.39442	2.15536
H	1.60853	-0.14895	1.61030
H	-0.48432	-0.52738	2.75672
H	-1.36217	1.95890	-1.27903
H	0.08469	2.39442	-2.15536
H	-0.48432	-0.52738	-2.75672
H	1.60853	-0.14895	-1.61030
H	1.40237	2.29851	0.00000
Cl	0.04907	-2.59988	0.00000
H	-1.56311	-0.87935	0.00000

26-disila-f-ax

Si	-0.32227	0.49632	-1.54339
C	1.24529	-0.50240	-1.28675
C	2.00735	-0.14270	0.00000
C	1.24529	-0.50240	1.28675

Si	-0.32227	0.49632	1.54339
C	-1.39364	0.24973	0.00000
H	2.24155	0.92597	0.00000
H	1.89291	-0.36418	-2.15486
H	0.97752	-1.56260	-1.26927
H	-1.05078	0.07551	-2.75811
H	0.00539	1.93879	-1.62949
H	1.89291	-0.36418	2.15486
H	0.97752	-1.56260	1.26927
H	0.00539	1.93879	1.62949
H	-1.05078	0.07551	2.75811
H	2.96786	-0.66113	0.00000
F	-1.83293	-1.09736	0.00000
H	-2.28054	0.88609	0.00000

26-disila-f-eq

Si	0.17226	-0.30780	1.54476
C	-0.29963	1.49464	1.28476
C	0.27595	2.11071	0.00000
C	-0.29963	1.49464	-1.28476
Si	0.17226	-0.30780	-1.54476
C	-0.41873	-1.23003	0.00000
H	0.07722	3.18403	0.00000
H	-1.39027	1.57978	1.27417
H	0.03838	2.06179	2.15456
H	1.64390	-0.43358	1.62821
H	-0.43654	-0.85963	2.77363
H	-1.39027	1.57978	-1.27417
H	0.03838	2.06179	-2.15456
H	-0.43654	-0.85963	-2.77363
H	1.64390	-0.43358	-1.62821
H	1.36431	2.00418	0.00000
F	0.00928	-2.56827	0.00000
H	-1.51494	-1.23586	0.00000

26-disila-ch3-ax

Si	-0.51318	0.29187	1.51322
C	0.47952	-1.29034	1.28403

C	0.11982	-2.05591	0.00000
C	0.47952	-1.29034	-1.28403
Si	-0.51318	0.29187	-1.51322
C	-0.26926	1.37765	0.00000
H	-0.95072	-2.28238	0.00000
H	0.32017	-1.92759	2.15639
H	1.54655	-1.04822	1.27710
H	-0.07782	1.00363	2.73897
H	-1.94546	-0.06587	1.65253
H	0.32017	-1.92759	-2.15639
H	1.54655	-1.04822	-1.27710
H	-1.94546	-0.06587	-1.65253
H	-0.07782	1.00363	-2.73897
H	0.63149	-3.02040	0.00000
H	-1.03105	2.16111	0.00000
C	1.13599	2.00994	0.00000
H	1.29735	2.63225	-0.88123
H	1.29735	2.63225	0.88123
H	1.91652	1.24600	0.00000
26-disila-ch3-eq			
Si	0.12717	-0.27609	-1.51311
C	-0.28734	1.54429	-1.28461
C	0.30112	2.15023	0.00000
C	-0.28734	1.54429	1.28461
Si	0.12717	-0.27609	1.51311
C	-0.43452	-1.23160	0.00000
H	1.38698	2.01724	0.00000
H	0.07119	2.09589	-2.15616
H	-1.37533	1.66102	-1.27653
H	-0.49735	-0.81261	-2.74608
H	1.59850	-0.42406	-1.64128
H	0.07119	2.09589	2.15616
H	-1.37533	1.66102	1.27653
H	1.59850	-0.42406	1.64128
H	-0.49735	-0.81261	2.74608
H	0.12930	3.22841	0.00000

C	0.03167	-2.69525	0.00000
H	-0.32390	-3.23372	-0.87998
H	-0.32390	-3.23372	0.87998
H	1.12113	-2.75409	0.00000
H	-1.52994	-1.18778	0.00000

26-disila-sih3-ax

Si	-0.65629	-0.12864	-1.51830
C	0.67997	-1.42781	-1.28164
C	0.51128	-2.25883	0.00000
C	0.67997	-1.42781	1.28164
Si	-0.65629	-0.12864	1.51830
C	-0.71062	0.97496	0.00000
H	-0.47436	-2.73390	0.00000
H	0.67661	-2.08198	-2.15610
H	1.65749	-0.93669	-1.27096
H	-0.39244	0.66432	-2.74178
H	-1.96340	-0.81014	-1.67540
H	0.67661	-2.08198	2.15610
H	1.65749	-0.93669	1.27096
H	-1.96340	-0.81014	1.67540
H	-0.39244	0.66432	2.74178
H	1.23836	-3.07310	0.00000
Si	0.66734	2.23733	0.00000
H	0.60037	3.09578	1.20185
H	0.60037	3.09578	-1.20185
H	1.97744	1.54676	0.00000
H	-1.65485	1.52857	0.00000

26-disila-sih3-eq

Si	-0.08291	0.06303	1.51819
C	0.25492	1.89656	1.28285
C	-0.36210	2.47631	0.00000
C	0.25492	1.89656	-1.28285
Si	-0.08291	0.06303	-1.51819
C	0.47949	-0.88368	0.00000
H	-1.44083	2.29363	0.00000
H	-0.12525	2.43075	2.15629

H	1.33704	2.05808	1.27214
H	0.59470	-0.44293	2.73354
H	-1.54365	-0.13669	1.67922
H	-0.12525	2.43075	-2.15629
H	1.33704	2.05808	-1.27214
H	-1.54365	-0.13669	-1.67922
H	0.59470	-0.44293	-2.73354
H	-0.24030	3.56112	0.00000
H	1.57571	-0.87071	0.00000
Si	-0.07432	-2.66605	0.00000
H	0.42327	-3.37376	1.20026
H	0.42327	-3.37376	-1.20026
H	-1.55127	-2.72401	0.00000

26-disila-tbu-ax

C	-0.43019	2.80664	0.00000
C	-0.61889	1.97659	-1.27744
Si	0.67534	0.62632	-1.49491
C	0.75660	-0.53744	0.00000
Si	0.67534	0.62632	1.49491
C	-0.61889	1.97659	1.27744
H	0.43633	-0.07966	-2.77330
H	-1.62046	1.53841	-1.28151
H	-0.56564	2.62383	-2.15611
H	0.56925	3.25144	0.00000
H	-1.13395	3.64149	0.00000
H	1.78611	-0.91681	0.00000
H	0.43633	-0.07966	2.77330
H	1.99545	1.29682	1.58520
H	-1.62046	1.53841	1.28151
H	-0.56564	2.62383	2.15611
H	1.99545	1.29682	-1.58520
C	-0.18912	-1.77606	0.00000
C	-1.65892	-1.35331	0.00000
H	-1.90482	-0.76210	-0.88407
H	-2.30523	-2.23230	0.00000
H	-1.90482	-0.76210	0.88407

C	0.07574	-2.64648	1.23392
H	-0.51946	-3.55970	1.18401
H	1.12779	-2.93271	1.28435
H	-0.17987	-2.13282	2.15858
C	0.07574	-2.64648	-1.23392
H	1.12779	-2.93271	-1.28435
H	-0.51946	-3.55970	-1.18401
H	-0.17987	-2.13282	-2.15858

26-disila-tbu-eq

Si	0.16698	-0.58428	-1.51375
C	-0.33896	-2.38079	-1.27662
C	0.21590	-3.02609	0.00000
C	-0.33896	-2.38079	1.27662
Si	0.16698	-0.58428	1.51375
C	-0.37119	0.40936	0.00000
H	-0.44002	-0.07260	2.76392
H	-1.43163	-2.44050	1.26943
H	-0.01013	-2.93898	2.15597
H	1.30754	-2.95541	0.00000
H	-0.01871	-4.09253	0.00000
H	-0.44002	-0.07260	-2.76392
H	1.64128	-0.53254	-1.66718
H	-1.43163	-2.44050	-1.26943
H	-0.01013	-2.93898	-2.15597
H	1.64128	-0.53254	1.66718
H	-1.46687	0.30214	0.00000
C	-0.05485	1.93425	0.00000
C	-0.66601	2.59611	1.23916
H	-0.20369	2.23544	2.15801
H	-0.52560	3.67746	1.19882
H	-1.73718	2.39489	1.29999
C	-0.66601	2.59611	-1.23916
H	-1.73718	2.39489	-1.29999
H	-0.52560	3.67746	-1.19882
H	-0.20369	2.23544	-2.15801
C	1.45357	2.19401	0.00000

H	1.64514	3.26815	0.00000
H	1.93395	1.76900	0.88156
H	1.93395	1.76900	-0.88156

35-disila-ccl3-ax

C	-1.23221	0.59364	-1.26913
Si	0.03822	1.96264	-1.58751
C	0.50202	2.85568	0.00000
Si	0.03822	1.96264	1.58751
C	-1.23221	0.59364	1.26913
C	-1.16030	-0.27083	0.00000
H	0.00314	3.82638	0.00000
H	-0.63164	2.90585	-2.51298
H	1.23076	1.44298	-2.28318
H	-1.28855	-0.03654	-2.15695
H	-2.19454	1.11090	-1.21893
H	-0.63164	2.90585	2.51298
H	1.23076	1.44298	2.28318
H	-2.19454	1.11090	1.21893
H	-1.28855	-0.03654	2.15695
H	1.57396	3.05841	0.00000
H	-2.03578	-0.92676	0.00000
C	-0.00110	-1.27959	0.00000
Cl	1.59333	-0.48303	0.00000
Cl	-0.09568	-2.32806	1.43784
Cl	-0.09568	-2.32806	-1.43784

35-disila-ccl3-eq

C	-0.33845	-0.66799	1.26662
Si	0.20725	-2.45382	1.51774
C	-0.27357	-3.43600	0.00000
Si	0.20725	-2.45382	-1.51774
C	-0.33845	-0.66799	-1.26662
C	0.24250	-0.02424	0.00000
H	-1.35775	-3.57455	0.00000
H	-0.40922	-2.98149	2.75348
H	1.68031	-2.47620	1.67021
H	-0.04753	-0.10602	2.15375

H	-1.42999	-0.63495	1.21811
H	-0.40922	-2.98149	-2.75348
H	1.68031	-2.47620	-1.67021
H	-1.42999	-0.63495	-1.21811
H	-0.04753	-0.10602	-2.15375
H	0.18732	-4.42404	0.00000
C	0.05055	1.51112	0.00000
Cl	0.82245	2.24066	-1.43271
Cl	-1.67426	1.94523	0.00000
Cl	0.82245	2.24066	1.43271
H	1.33144	-0.14073	0.00000

35-disila-cf3-ax

C	-1.09726	0.11519	-1.28649
Si	0.24116	1.42660	-1.55645
C	0.37460	2.46115	0.00000
Si	0.24116	1.42660	1.55645
C	-1.09726	0.11519	1.28649
C	-1.05407	-0.72561	0.00000
H	-0.46589	3.16100	0.00000
H	-0.20246	2.25321	-2.70161
H	1.53898	0.81972	-1.90784
H	-1.13581	-0.54150	-2.15709
H	-2.04678	0.65778	-1.28179
H	-0.20246	2.25321	2.70161
H	1.53898	0.81972	1.90784
H	-2.04678	0.65778	1.28179
H	-1.13581	-0.54150	2.15709
H	1.28711	3.05785	0.00000
H	-1.91477	-1.39985	0.00000
C	0.13049	-1.66524	0.00000
F	1.30454	-1.01017	0.00000
F	0.13288	-2.46230	1.07661
F	0.13288	-2.46230	-1.07661

35-disila-cf3-eq

C	-0.29597	-0.06749	1.28123
Si	0.17180	-1.87587	1.52162

C	-0.36375	-2.82429	0.00000
Si	0.17180	-1.87587	-1.52162
C	-0.29597	-0.06749	-1.28123
C	0.28396	0.54907	0.00000
H	-1.45403	-2.90234	0.00000
H	-0.45440	-2.38857	2.75860
H	1.64407	-1.96259	1.65874
H	0.04224	0.49467	2.15308
H	-1.38588	0.01801	1.25653
H	-0.45440	-2.38857	-2.75860
H	1.64407	-1.96259	-1.65874
H	-1.38588	0.01801	-1.25653
H	0.04224	0.49467	-2.15308
H	0.04014	-3.83709	0.00000
C	0.05530	2.04903	0.00000
F	0.59868	2.63716	-1.07548
F	-1.24851	2.36084	0.00000
F	0.59868	2.63716	1.07548
H	1.37318	0.43981	0.00000

35-disila-cl-ax

C	-1.00957	-0.36485	-1.28295
Si	0.27249	1.00026	-1.54105
C	0.29533	2.06438	0.00000
Si	0.27249	1.00026	1.54105
C	-1.00957	-0.36485	1.28295
C	-0.88245	-1.18131	0.00000
H	-0.60988	2.67794	0.00000
H	-0.13936	1.77811	-2.73098
H	1.60949	0.43019	-1.79704
H	-0.99592	-1.03646	-2.14266
H	-1.99752	0.10781	-1.27418
H	-0.13936	1.77811	2.73098
H	1.60949	0.43019	1.79704
H	-1.99752	0.10781	1.27418
H	-0.99592	-1.03646	2.14266
H	1.14857	2.74320	0.00000

Cl	0.70152	-2.06713	0.00000
H	-1.61585	-1.98451	0.00000
35-disila-cl-eq			
C	0.27252	-0.45708	1.27606
Si	-0.15442	1.36646	1.51799
C	0.40995	2.30353	0.00000
Si	-0.15442	1.36646	-1.51799
C	0.27252	-0.45708	-1.27606
C	-0.30259	-1.05148	0.00000
H	0.03214	3.32628	0.00000
H	-1.62367	1.49514	1.65248
H	0.48207	1.85393	2.75986
H	1.35978	-0.57229	1.26403
H	-0.09215	-1.01596	2.13859
H	-1.62367	1.49514	-1.65248
H	0.48207	1.85393	-2.75986
H	-0.09215	-1.01596	-2.13859
H	1.35978	-0.57229	-1.26403
H	1.50181	2.35223	0.00000
Cl	-0.01455	-2.85237	0.00000
H	-1.38914	-0.97091	0.00000
35-disila-f-ax			
C	-0.72914	-0.83685	-1.28150
Si	0.19011	0.79429	-1.53715
C	-0.05452	1.83655	0.00000
Si	0.19011	0.79429	1.53715
C	-0.72914	-0.83685	1.28150
C	-0.35546	-1.56993	0.00000
H	-1.08273	2.20865	0.00000
H	-0.36563	1.45580	-2.73897
H	1.62762	0.54628	-1.76494
H	-0.54411	-1.49136	-2.13507
H	-1.80325	-0.63522	-1.26891
H	-0.36563	1.45580	2.73897
H	1.62762	0.54628	1.76494
H	-1.80325	-0.63522	1.26891

H	-0.54411	-1.49136	2.13507
H	0.60644	2.70375	0.00000
F	1.03218	-1.75950	0.00000
H	-0.78310	-2.57449	0.00000

35-disila-f-eq

C	0.27818	-0.82389	1.27403
Si	-0.15614	0.99335	1.52152
C	0.40196	1.93052	0.00000
Si	-0.15614	0.99335	-1.52152
C	0.27818	-0.82389	-1.27403
C	-0.28893	-1.42239	0.00000
H	0.02001	2.95177	0.00000
H	-1.62515	1.12090	1.66088
H	0.48118	1.48837	2.75980
H	1.36649	-0.93190	1.25750
H	-0.08631	-1.39824	2.12738
H	-1.62515	1.12090	-1.66088
H	0.48118	1.48837	-2.75980
H	-0.08631	-1.39824	-2.12738
H	1.36649	-0.93190	-1.25750
H	1.49367	1.98469	0.00000
F	-0.01346	-2.79465	0.00000
H	-1.38048	-1.34536	0.00000

35-disila-ch3-ax

C	-0.74253	-0.78553	-1.27975
Si	0.17806	0.83944	-1.53080
C	-0.07210	1.89068	0.00000
Si	0.17806	0.83944	1.53080
C	-0.74253	-0.78553	1.27975
C	-0.40485	-1.57444	0.00000
H	-1.10567	2.24816	0.00000
H	-0.34610	1.50466	-2.74546
H	1.62570	0.60452	-1.73744
H	-0.57406	-1.42066	-2.15338
H	-1.81125	-0.54719	-1.28360
H	-0.34610	1.50466	2.74546

H	1.62570	0.60452	1.73744
H	-1.81125	-0.54719	1.28360
H	-0.57406	-1.42066	2.15338
H	0.57793	2.76579	0.00000
H	-1.03445	-2.46890	0.00000
C	1.04531	-2.05130	0.00000
H	1.25380	-2.65574	0.88320
H	1.25380	-2.65574	-0.88320
H	1.74794	-1.21691	0.00000

35-disila-ch3-eq

C	0.29506	-0.78177	1.27566
Si	-0.15751	1.02645	1.52145
C	0.37565	1.97918	0.00000
Si	-0.15751	1.02645	-1.52145
C	0.29506	-0.78177	-1.27566
C	-0.28244	-1.42150	0.00000
H	1.46617	2.05565	0.00000
H	0.47231	1.55024	2.75478
H	-1.62857	1.13329	1.67015
H	-0.04149	-1.34378	2.15071
H	1.38652	-0.87718	1.25692
H	0.47231	1.55024	-2.75478
H	-1.62857	1.13329	-1.67015
H	1.38652	-0.87718	-1.25692
H	-0.04149	-1.34378	-2.15071
H	-0.02678	2.99248	0.00000
C	-0.03032	-2.92757	0.00000
H	-0.46007	-3.39984	0.88382
H	-0.46007	-3.39984	-0.88382
H	1.04347	-3.12622	0.00000
H	-1.36714	-1.26425	0.00000

35-disila-sih3-ax

C	-1.00222	0.30078	-1.28633
Si	0.26247	-1.07495	-1.53344
C	0.26285	-2.15055	0.00000
Si	0.26247	-1.07495	1.53344

C	-1.00222	0.30078	1.28633
C	-0.86294	1.14500	0.00000
H	-0.65693	-2.74213	0.00000
H	-0.10005	-1.84542	-2.74440
H	1.61167	-0.50236	-1.74122
H	-0.98531	0.94885	-2.16635
H	-1.98885	-0.17777	-1.28951
H	-0.10005	-1.84542	2.74440
H	1.61167	-0.50236	1.74122
H	-1.98885	-0.17777	1.28951
H	-0.98531	0.94885	2.16635
H	1.10061	-2.84824	0.00000
Si	0.65981	2.26138	0.00000
H	0.62490	3.11750	1.20624
H	0.62490	3.11750	-1.20624
H	1.92811	1.50479	0.00000
H	-1.68861	1.86659	0.00000

35-disila-sih3-eq

C	-0.29046	0.41708	1.28654
Si	0.15570	-1.39608	1.52653
C	-0.37801	-2.33959	0.00000
Si	0.15570	-1.39608	-1.52653
C	-0.29046	0.41708	-1.28654
C	0.30392	1.03676	0.00000
H	-1.46871	-2.41413	0.00000
H	-0.47475	-1.92833	2.75608
H	1.62714	-1.49606	1.67244
H	0.04527	0.97032	2.16783
H	-1.38090	0.51733	1.26533
H	-0.47475	-1.92833	-2.75608
H	1.62714	-1.49606	-1.67244
H	-1.38090	0.51733	-1.26533
H	0.04527	0.97032	-2.16783
H	0.02087	-3.35453	0.00000
H	1.38824	0.87540	0.00000
Si	0.01559	2.89677	0.00000

H	0.60277	3.52276	1.20583
H	0.60277	3.52276	-1.20583
H	-1.44477	3.14124	0.00000

35-disila-tbu-ax

C	-0.16298	2.69194	0.00000
Si	-0.20333	1.62290	-1.53716
C	0.97529	0.17383	-1.27398
C	0.92026	-0.70073	0.00000
C	0.97529	0.17383	1.27398
Si	-0.20333	1.62290	1.53716
H	0.98315	-0.44945	-2.16876
H	-1.59471	1.22036	-1.83463
H	0.29153	2.36974	-2.71760
H	0.78741	3.23327	0.00000
H	-0.96101	3.43410	0.00000
H	1.86012	-1.26512	0.00000
H	0.98315	-0.44945	2.16876
H	1.95499	0.66788	1.27490
H	-1.59471	1.22036	1.83463
H	0.29153	2.36974	2.71760
H	1.95499	0.66788	-1.27490
C	-0.15656	-1.82204	0.00000
C	-1.59703	-1.31189	0.00000
H	-1.81756	-0.71651	-0.88372
H	-2.28319	-2.16104	0.00000
H	-1.81756	-0.71651	0.88372
C	0.04041	-2.70521	1.23807
H	-0.59426	-3.58943	1.16961
H	1.07623	-3.03988	1.32388
H	-0.22819	-2.18373	2.15600
C	0.04041	-2.70521	-1.23807
H	1.07623	-3.03988	-1.32388
H	-0.59426	-3.58943	-1.16961
H	-0.22819	-2.18373	-2.15600

35-disila-tbu-eq

C	-0.37668	-0.13933	-1.26146
---	----------	----------	----------

Si	0.17988	-1.91688	-1.51645
C	-0.27866	-2.91353	0.00000
Si	0.17988	-1.91688	1.51645
C	-0.37668	-0.13933	1.26146
C	0.20366	0.53212	0.00000
H	-0.09716	0.41020	2.16079
H	1.65300	-1.93181	1.68245
H	-0.43118	-2.46638	2.74839
H	-1.36039	-3.07118	0.00000
H	0.19945	-3.89327	0.00000
H	-0.09716	0.41020	-2.16079
H	-1.47012	-0.12078	-1.21752
H	1.65300	-1.93181	-1.68245
H	-0.43118	-2.46638	-2.74839
H	-1.47012	-0.12078	1.21752
H	1.28922	0.36413	0.00000
C	0.04132	2.08350	0.00000
C	0.72822	2.67874	1.23442
H	0.20543	2.43303	2.15708
H	0.75443	3.76630	1.15821
H	1.75753	2.32365	1.31851
C	0.72822	2.67874	-1.23442
H	1.75753	2.32365	-1.31851
H	0.75443	3.76630	-1.15821
H	0.20543	2.43303	-2.15708
C	-1.42986	2.49804	0.00000
H	-1.51068	3.58622	0.00000
H	-1.94935	2.12834	0.88450
H	-1.94935	2.12834	-0.88450
126-trisila-ccl3-ax			
Si	-0.63519	1.34632	-1.82265
C	0.73365	2.53058	-1.29385
C	0.48119	3.32339	0.00000
C	0.73365	2.53058	1.29385
Si	-0.63519	1.34632	1.82265
Si	-1.15299	-0.02544	0.00000

H	-0.53684	3.72590	0.00000
H	0.86807	3.22761	-2.12434
H	1.67117	1.97645	-1.20842
H	-0.24011	0.57451	-3.02008
H	-1.85161	2.13385	-2.13540
H	0.86807	3.22761	2.12434
H	1.67117	1.97645	1.20842
H	-1.85161	2.13385	2.13540
H	-0.24011	0.57451	3.02008
H	1.14029	4.19308	0.00000
H	-2.50639	-0.61665	0.00000
C	0.04344	-1.53993	0.00000
Cl	1.72970	-0.94187	0.00000
Cl	-0.21358	-2.54034	1.44776
Cl	-0.21358	-2.54034	-1.44776

126-trisila-ccl3-eq

Si	0.02037	-1.37638	1.81804
C	0.26401	-3.17591	1.29594
C	-0.44577	-3.60487	0.00000
C	0.26401	-3.17591	-1.29594
Si	0.02037	-1.37638	-1.81804
Si	0.72317	-0.09005	0.00000
H	-1.47556	-3.23497	0.00000
H	-0.09960	-3.78642	2.12571
H	1.33337	-3.38855	1.21578
H	0.76856	-1.08526	3.05960
H	-1.42077	-1.13225	2.04961
H	-0.09960	-3.78642	-2.12571
H	1.33337	-3.38855	-1.21578
H	-1.42077	-1.13225	-2.04961
H	0.76856	-1.08526	-3.05960
H	-0.52293	-4.69343	0.00000
C	-0.05991	1.66996	0.00000
Cl	0.46306	2.55967	-1.45185
Cl	-1.83594	1.55120	0.00000
Cl	0.46306	2.55967	1.45185

H	2.18368	0.14291	0.00000
---	---------	---------	---------

126-trisila-cf3-ax

Si	-0.62377	0.88169	-1.80683
C	0.87908	1.89953	-1.29577
C	0.73450	2.71634	0.00000
C	0.87908	1.89953	1.29577
Si	-0.62377	0.88169	1.80683
Si	-1.11569	-0.51269	0.00000
H	-0.22051	3.25060	0.00000
H	1.08866	2.57628	-2.12734
H	1.74479	1.23715	-1.21836
H	-0.36555	0.13445	-3.05582
H	-1.77894	1.78588	-2.01413
H	1.08866	2.57628	2.12734
H	1.74479	1.23715	1.21836
H	-1.77894	1.78588	2.01413
H	-0.36555	0.13445	3.05582
H	1.50471	3.48937	0.00000
H	-2.41279	-1.21701	0.00000
C	0.23943	-1.90147	0.00000
F	1.48180	-1.36020	0.00000
F	0.17958	-2.70432	1.07749
F	0.17958	-2.70432	-1.07749

126-trisila-cf3-eq

Si	-0.03693	-0.82246	1.80426
C	0.17492	-2.62855	1.29646
C	-0.53609	-3.05368	0.00000
C	0.17492	-2.62855	-1.29646
Si	-0.03693	-0.82246	-1.80426
Si	0.71499	0.45462	0.00000
H	-1.56375	-2.67856	0.00000
H	-0.20451	-3.22691	2.12797
H	1.24073	-2.86104	1.22362
H	0.68333	-0.54171	3.06396
H	-1.47764	-0.53849	1.99190
H	-0.20451	-3.22691	-2.12797

H	1.24073	-2.86104	-1.22362
H	-1.47764	-0.53849	-1.99190
H	0.68333	-0.54171	-3.06396
H	-0.61848	-4.14183	0.00000
C	-0.09605	2.21452	0.00000
F	0.24743	2.94392	-1.07860
F	-1.44156	2.14335	0.00000
F	0.24743	2.94392	1.07860
H	2.17429	0.68991	0.00000

126-trisila-cl-ax

Si	-0.59912	0.37798	-1.78586
C	0.82587	1.51480	-1.29716
C	0.63415	2.31969	0.00000
C	0.82587	1.51480	1.29716
Si	-0.59912	0.37798	1.78586
Si	-0.84269	-1.10011	0.00000
H	-0.35209	2.79326	0.00000
H	0.97624	2.20476	-2.13051
H	1.74076	0.91985	-1.22914
H	-0.32244	-0.29665	-3.07232
H	-1.83885	1.18149	-1.91534
H	0.97624	2.20476	2.13051
H	1.74076	0.91985	1.22914
H	-1.83885	1.18149	1.91534
H	-0.32244	-0.29665	3.07232
H	1.35580	3.13848	0.00000
Cl	0.83959	-2.33741	0.00000
H	-2.03280	-1.97212	0.00000

126-trisila-cl-eq

Si	0.16588	0.31496	1.78648
C	-0.24954	2.09308	1.29604
C	0.40041	2.60569	0.00000
C	-0.24954	2.09308	-1.29604
Si	0.16588	0.31496	-1.78648
Si	-0.52980	-1.01326	0.00000
H	0.34325	3.69571	0.00000

H	-1.33527	2.20533	1.23081
H	0.06532	2.72352	2.13093
H	1.63535	0.18452	1.91900
H	-0.46566	-0.03135	3.07840
H	-1.33527	2.20533	-1.23081
H	0.06532	2.72352	-2.13093
H	-0.46566	-0.03135	-3.07840
H	1.63535	0.18452	-1.91900
H	1.46710	2.36366	0.00000
Cl	0.31332	-2.90990	0.00000
H	-1.99868	-1.18607	0.00000

126-trisila-f-ax

Si	-0.45554	-0.00231	-1.78061
C	0.59937	1.48893	-1.29756
C	0.19431	2.20959	0.00000
C	0.59937	1.48893	1.29756
Si	-0.45554	-0.00231	1.78061
Si	-0.33429	-1.51142	0.00000
H	-0.88430	2.39264	0.00000
H	0.54778	2.19331	-2.13078
H	1.64543	1.17726	-1.23226
H	-0.01785	-0.55302	-3.08251
H	-1.86831	0.43578	-1.89903
H	0.54778	2.19331	2.13078
H	1.64543	1.17726	1.23226
H	-1.86831	0.43578	1.89903
H	-0.01785	-0.55302	3.08251
H	0.66209	3.19580	0.00000
F	1.10814	-2.23354	0.00000
H	-1.35775	-2.57693	0.00000

126-trisila-f-eq

Si	0.22863	-0.01367	1.78879
C	-0.32974	1.72608	1.29553
C	0.27650	2.28972	0.00000
C	-0.32974	1.72608	-1.29553
Si	0.22863	-0.01367	-1.78879

Si	-0.39425	-1.37896	0.00000
H	0.13071	3.37159	0.00000
H	-1.42102	1.74985	1.22937
H	-0.06820	2.37998	2.13058
H	1.70488	-0.01770	1.91851
H	-0.36128	-0.39294	3.09189
H	-1.42102	1.74985	-1.22937
H	-0.06820	2.37998	-2.13058
H	-0.36128	-0.39294	-3.09189
H	1.70488	-0.01770	-1.91851
H	1.35930	2.13524	0.00000
F	0.29940	-2.82862	0.00000
H	-1.86005	-1.59098	0.00000

126-trisila-ch3-ax

Si	-0.49745	0.03945	-1.76397
C	0.58192	1.52057	-1.29547
C	0.19151	2.25157	0.00000
C	0.58192	1.52057	1.29547
Si	-0.49745	0.03945	1.76397
Si	-0.36612	-1.48440	0.00000
H	-0.88410	2.45207	0.00000
H	0.53698	2.22103	-2.13247
H	1.62514	1.19753	-1.23159
H	-0.04560	-0.51502	-3.06268
H	-1.89331	0.51424	-1.92623
H	0.53698	2.22103	2.13247
H	1.62514	1.19753	1.23159
H	-1.89331	0.51424	1.92623
H	-0.04560	-0.51502	3.06268
H	0.67565	3.23013	0.00000
H	-1.46010	-2.48310	0.00000
C	1.31255	-2.34748	0.00000
H	1.42865	-2.97402	0.88338
H	1.42865	-2.97402	-0.88338
H	2.11788	-1.61237	0.00000

126-trisila-ch3-eq

Si	0.16446	0.02271	1.76232
C	-0.30367	1.79385	1.29523
C	0.32407	2.33460	0.00000
C	-0.30367	1.79385	-1.29523
Si	0.16446	0.02271	-1.76232
Si	-0.47071	-1.37154	0.00000
H	1.39977	2.13498	0.00000
H	-0.00634	2.42902	2.13274
H	-1.39278	1.86963	1.23221
H	-0.44054	-0.33172	3.06793
H	1.64006	-0.04222	1.91576
H	-0.00634	2.42902	-2.13274
H	-1.39278	1.86963	-1.23221
H	1.64006	-0.04222	-1.91576
H	-0.44054	-0.33172	-3.06793
H	0.22387	3.42183	0.00000
C	0.32145	-3.07918	0.00000
H	0.02519	-3.64430	0.88262
H	0.02519	-3.64430	-0.88262
H	1.40715	-2.99064	0.00000
H	-1.95125	-1.48796	0.00000

126-trisila-sih3-ax

Si	-0.60740	-0.45378	-1.77214
C	0.83804	-1.57176	-1.29432
C	0.66218	-2.38291	0.00000
C	0.83804	-1.57176	1.29432
Si	-0.60740	-0.45378	1.77214
Si	-0.91424	1.03296	0.00000
H	-0.31662	-2.87185	0.00000
H	0.99225	-2.25614	-2.13175
H	1.74807	-0.96886	-1.22695
H	-0.31721	0.22584	-3.05574
H	-1.81750	-1.29079	-1.95333
H	0.99225	-2.25614	2.13175
H	1.74807	-0.96886	1.22695
H	-1.81750	-1.29079	1.95333

H	-0.31721	0.22584	3.05574
H	1.39700	-3.19016	0.00000
Si	0.86837	2.54086	0.00000
H	0.85650	3.40165	1.20186
H	0.85650	3.40165	-1.20186
H	2.12949	1.76362	0.00000
H	-2.21566	1.73943	0.00000

126-trisila-sih3-eq

Si	0.09036	0.37352	1.76419
C	-0.20798	2.17824	1.29516
C	0.46987	2.65544	0.00000
C	-0.20798	2.17824	-1.29516
Si	0.09036	0.37352	-1.76419
Si	-0.63841	-0.97196	0.00000
H	1.52104	2.35194	0.00000
H	0.14925	2.78189	2.13281
H	-1.28486	2.35680	1.23218
H	-0.56904	0.06324	3.05292
H	1.55014	0.16759	1.93094
H	0.14925	2.78189	-2.13281
H	-1.28486	2.35680	-1.23218
H	1.55014	0.16759	-1.93094
H	-0.56904	0.06324	-3.05292
H	0.47642	3.74705	0.00000
H	-2.12120	-1.03814	0.00000
Si	0.29622	-3.10883	0.00000
H	-0.11105	-3.86940	1.20043
H	-0.11105	-3.86940	-1.20043
H	1.76900	-2.97829	0.00000

126-trisila-tbu-ax

C	0.47856	2.92909	0.00000
C	0.74380	2.13940	-1.29231
Si	-0.58938	0.89224	-1.78525
Si	-0.95523	-0.57816	0.00000
Si	-0.58938	0.89224	1.78525
C	0.74380	2.13940	1.29231

H	-0.18040	0.20380	-3.03416
H	1.70774	1.62925	-1.21353
H	0.84019	2.83543	-2.12882
H	-0.54817	3.30827	0.00000
H	1.11974	3.81264	0.00000
H	-2.33670	-1.12225	0.00000
H	-0.18040	0.20380	3.03416
H	-1.83688	1.64347	2.06788
H	1.70774	1.62925	1.21353
H	0.84019	2.83543	2.12882
H	-1.83688	1.64347	-2.06788
C	0.27661	-2.03480	0.00000
C	1.71143	-1.50219	0.00000
H	1.91833	-0.89529	-0.88434
H	2.42067	-2.33509	0.00000
H	1.91833	-0.89529	0.88434
C	0.05069	-2.89172	1.24861
H	0.74010	-3.74151	1.24735
H	-0.96518	-3.28840	1.28275
H	0.22303	-2.32485	2.16470
C	0.05069	-2.89172	-1.24861
H	-0.96518	-3.28840	-1.28275
H	0.74010	-3.74151	-1.24735
H	0.22303	-2.32485	-2.16470

126-trisila-tbu-eq

Si	0.10313	-0.86026	-1.77244
C	-0.25196	-2.65539	-1.29558
C	0.41273	-3.14966	0.00000
C	-0.25196	-2.65539	1.29558
Si	0.10313	-0.86026	1.77244
Si	-0.60350	0.48939	0.00000
H	-0.54283	-0.54401	3.06850
H	-1.33388	-2.79904	1.22849
H	0.08225	-3.27434	2.13130
H	1.47187	-2.87500	0.00000
H	0.38960	-4.24121	0.00000

H	-0.54283	-0.54401	-3.06850
H	1.56955	-0.71291	-1.95398
H	-1.33388	-2.79904	-1.22849
H	0.08225	-3.27434	-2.13130
H	1.56955	-0.71291	1.95398
H	-2.09155	0.51760	0.00000
C	0.05274	2.27558	0.00000
C	-0.45727	2.99752	1.25040
H	-0.09787	2.52147	2.16470
H	-0.10390	4.03309	1.25398
H	-1.54758	3.01730	1.28692
C	-0.45727	2.99752	-1.25040
H	-1.54758	3.01730	-1.28692
H	-0.10390	4.03309	-1.25398
H	-0.09787	2.52147	-2.16470
C	1.58324	2.27349	0.00000
H	1.95533	3.30217	0.00000
H	1.98707	1.77442	0.88229
H	1.98707	1.77442	-0.88229

135-trisila-ccl3-ax

Si	1.29022	-0.13470	0.00000
C	0.98027	0.84033	-1.55701
C	0.98027	0.84033	1.55701
Si	-0.42445	2.09142	-1.56782
Si	-0.42445	2.09142	1.56782
C	-0.34473	3.11240	0.00000
H	0.87760	0.14845	-2.39599
H	0.87760	0.14845	2.39599
H	1.89988	1.40565	-1.74419
H	1.89988	1.40565	1.74419
H	-1.73177	1.41040	-1.65297
H	-1.73177	1.41040	1.65297
H	-0.27916	2.95725	-2.75938
H	-0.27916	2.95725	2.75938
H	-1.15403	3.84539	0.00000
H	0.59310	3.67598	0.00000

H	2.64575	-0.72096	0.00000
C	0.16134	-1.69476	0.00000
Cl	-1.55291	-1.22098	0.00000
Cl	0.49954	-2.67192	-1.44926
Cl	0.49954	-2.67192	1.44926

135-trisila-ccl3-eq

Si	0.49815	-0.05841	0.00000
C	-0.17500	-0.86940	-1.52957
C	-0.17500	-0.86940	1.52957
Si	0.14163	-2.72174	-1.56254
Si	0.14163	-2.72174	1.56254
C	-0.55456	-3.48603	0.00000
H	0.24982	-0.40263	-2.41995
H	0.24982	-0.40263	2.41995
H	-1.25647	-0.70583	-1.56022
H	-1.25647	-0.70583	1.56022
H	1.60272	-2.95807	-1.60523
H	1.60272	-2.95807	1.60523
H	-0.46396	-3.32329	-2.76983
H	-0.46396	-3.32329	2.76983
H	-0.36006	-4.56049	0.00000
H	-1.64084	-3.35828	0.00000
C	-0.00582	1.80111	0.00000
Cl	-1.78136	1.95272	0.00000
Cl	0.64863	2.59546	-1.45077
Cl	0.64863	2.59546	1.45077
H	1.97392	-0.03402	0.00000

135-trisila-cf3-ax

Si	-1.20509	0.60608	0.00000
C	-1.01471	-0.40598	-1.55006
C	-1.01471	-0.40598	1.55006
Si	0.42465	-1.61939	-1.56940
Si	0.42465	-1.61939	1.56940
C	0.37686	-2.64149	0.00000
H	-0.95477	0.26281	-2.41161
H	-0.95477	0.26281	2.41161

H	-1.93338	-0.98850	-1.67287
H	-1.93338	-0.98850	1.67287
H	1.70223	-0.88260	-1.64579
H	1.70223	-0.88260	1.64579
H	0.31159	-2.48632	-2.76292
H	0.31159	-2.48632	2.76292
H	1.21135	-3.34587	0.00000
H	-0.54045	-3.23772	0.00000
H	-2.44769	1.40433	0.00000
C	0.19455	1.93959	0.00000
F	1.43070	1.39832	0.00000
F	0.13301	2.74333	-1.08042
F	0.13301	2.74333	1.08042

135-trisila-cf3-eq

Si	0.49617	0.48908	0.00000
C	-0.17499	-0.31866	-1.53371
C	-0.17499	-0.31866	1.53371
Si	0.12860	-2.17331	-1.56464
Si	0.12860	-2.17331	1.56464
C	-0.57292	-2.92899	0.00000
H	0.25600	0.14724	-2.42178
H	0.25600	0.14724	2.42178
H	-1.25488	-0.14521	-1.56736
H	-1.25488	-0.14521	1.56736
H	1.58872	-2.41585	-1.60510
H	1.58872	-2.41585	1.60510
H	-0.47974	-2.77461	-2.77046
H	-0.47974	-2.77461	2.77046
H	-0.38762	-4.00514	0.00000
H	-1.65825	-2.79311	0.00000
C	-0.06666	2.33854	0.00000
F	-1.41300	2.44989	0.00000
F	0.36977	3.01507	-1.08007
F	0.36977	3.01507	1.08007
H	1.97176	0.52985	0.00000

135-trisila-cl-ax

Cl	-1.19625	2.16098	0.00000
Si	0.69581	1.31341	0.00000
H	1.64452	2.44236	0.00000
C	0.86131	0.26814	1.52823
C	0.86131	0.26814	-1.52823
Si	-0.27699	-1.22783	1.56793
Si	-0.27699	-1.22783	-1.56793
C	-0.02186	-2.22208	0.00000
H	0.69676	0.88667	2.41260
H	0.69676	0.88667	-2.41260
H	1.89544	-0.08929	1.57496
H	1.89544	-0.08929	-1.57496
H	-1.68306	-0.77885	1.64587
H	-1.68306	-0.77885	-1.64587
H	0.01825	-2.04756	2.76398
H	0.01825	-2.04756	-2.76398
H	-0.69367	-3.08291	0.00000
H	0.99879	-2.61595	0.00000
135-trisila-cl-eq			
H	-1.84528	1.15727	0.00000
Si	-0.37058	1.14132	0.00000
Cl	0.23184	3.12495	0.00000
C	0.27033	0.29020	1.52143
C	0.27033	0.29020	-1.52143
Si	-0.14522	-1.54240	1.56168
Si	-0.14522	-1.54240	-1.56168
C	0.50431	-2.34874	0.00000
H	-0.12109	0.78177	2.41392
H	-0.12109	0.78177	-2.41392
H	1.35855	0.39974	1.54425
H	1.35855	0.39974	-1.54425
H	-1.61652	-1.70206	1.61044
H	-1.61652	-1.70206	-1.61044
H	0.43056	-2.17241	2.76943
H	0.43056	-2.17241	-2.76943
H	0.24544	-3.40948	0.00000

H	1.59628	-2.28650	0.00000
135-trisila-f-ax			
F	1.13987	2.05279	0.00000
Si	-0.39958	1.60518	0.00000
H	-1.19363	2.84947	0.00000
C	-0.69583	0.58805	1.52461
C	-0.69583	0.58805	-1.52461
Si	0.28640	-1.01351	1.56573
Si	0.28640	-1.01351	-1.56573
C	-0.07050	-1.98032	0.00000
H	-0.47762	1.18443	2.41300
H	-0.47762	1.18443	-2.41300
H	-1.76042	0.33590	1.56473
H	-1.76042	0.33590	-1.56473
H	1.73075	-0.70255	1.63075
H	1.73075	-0.70255	-1.63075
H	-0.07319	-1.80223	2.76522
H	-0.07319	-1.80223	-2.76522
H	0.50960	-2.90539	0.00000
H	-1.12626	-2.26703	0.00000
135-trisila-f-eq			
H	1.76029	1.57858	0.00000
Si	0.28567	1.51142	0.00000
F	-0.24489	3.02302	0.00000
C	-0.32592	0.63929	1.51860
C	-0.32592	0.63929	-1.51860
Si	0.13710	-1.18038	1.56110
Si	0.13710	-1.18038	-1.56110
C	-0.49058	-2.00552	0.00000
H	0.05165	1.13689	2.41415
H	0.05165	1.13689	-2.41415
H	-1.41757	0.71337	1.54384
H	-1.41757	0.71337	-1.54384
H	1.61203	-1.30452	1.61068
H	1.61203	-1.30452	-1.61068
H	-0.42096	-1.82656	2.76882

H	-0.42096	-1.82656	-2.76882
H	-0.20331	-3.05891	0.00000
H	-1.58385	-1.97253	0.00000

135-trisila-ch3-ax

Si	-0.39716	1.56463	0.00000
H	-1.29021	2.74894	0.00000
C	-0.73491	0.52266	-1.52525
C	-0.73491	0.52266	1.52525
Si	0.21020	-1.09402	-1.56297
Si	0.21020	-1.09402	1.56297
C	-0.15981	-2.06018	0.00000
H	-0.50674	1.10430	-2.42152
H	-0.50674	1.10430	2.42152
H	-1.80409	0.29321	-1.56216
H	-1.80409	0.29321	1.56216
H	1.66472	-0.81467	-1.62083
H	1.66472	-0.81467	1.62083
H	-0.14314	-1.88365	-2.76488
H	-0.14314	-1.88365	2.76488
H	0.40445	-2.99485	0.00000
H	-1.22063	-2.32763	0.00000
C	1.38035	2.15045	0.00000
H	1.58779	2.75709	0.88180
H	1.58779	2.75709	-0.88180
H	2.07521	1.31020	0.00000

135-trisila-ch3-eq

Si	0.33831	1.42611	0.00000
C	-0.29786	0.53359	-1.52318
C	-0.29786	0.53359	1.52318
Si	0.14707	-1.28558	-1.56318
Si	0.14707	-1.28558	1.56318
C	-0.48071	-2.10766	0.00000
H	0.08262	1.02472	-2.42176
H	0.08262	1.02472	2.42176
H	-1.38838	0.62549	-1.54874
H	-1.38838	0.62549	1.54874

H	1.62077	-1.42398	-1.62289
H	1.62077	-1.42398	1.62289
H	-0.42027	-1.94226	-2.76340
H	-0.42027	-1.94226	2.76340
H	-0.20105	-3.16309	0.00000
H	-1.57392	-2.06752	0.00000
C	-0.18538	3.22287	0.00000
H	0.19149	3.74004	-0.88244
H	0.19149	3.74004	0.88244
H	-1.27296	3.30397	0.00000
H	1.82014	1.34880	0.00000

135-trisila-sih3-ax

Si	-0.94146	1.11694	0.00000
C	-0.98967	0.02469	-1.53103
C	-0.98967	0.02469	1.53103
Si	0.35162	-1.28430	-1.56543
Si	0.35162	-1.28430	1.56543
C	0.25455	-2.30965	0.00000
H	-0.92112	0.64508	-2.42724
H	-0.92112	0.64508	2.42724
H	-1.96294	-0.47429	-1.56470
H	-1.96294	-0.47429	1.56470
H	1.67370	-0.61861	-1.62784
H	1.67370	-0.61861	1.62784
H	0.21398	-2.14124	-2.76467
H	0.21398	-2.14124	2.76467
H	1.05010	-3.05749	0.00000
H	-0.69422	-2.85431	0.00000
Si	0.97924	2.46354	0.00000
H	0.98205	3.33092	1.19982
H	0.98205	3.33092	-1.19982
H	2.22624	1.66963	0.00000
H	-2.11191	2.02947	0.00000

135-trisila-sih3-eq

Si	0.42008	1.01596	0.00000
C	-0.25283	0.15614	-1.53177

C	-0.25283	0.15614	1.53177
Si	0.12694	-1.68002	-1.56505
Si	0.12694	-1.68002	1.56505
C	-0.53120	-2.47315	0.00000
H	0.15112	0.63229	-2.42772
H	0.15112	0.63229	2.42772
H	-1.33806	0.29180	-1.56104
H	-1.33806	0.29180	1.56104
H	1.59526	-1.86460	-1.62219
H	1.59526	-1.86460	1.62219
H	-0.46394	-2.31721	-2.76405
H	-0.46394	-2.31721	2.76405
H	-0.29273	-3.53871	0.00000
H	-1.62207	-2.39136	0.00000
H	1.89866	0.88690	0.00000
Si	-0.15643	3.28433	0.00000
H	0.36742	3.97219	-1.20107
H	0.36742	3.97219	1.20107
H	-1.63181	3.41679	0.00000

135-trisila-tbu-ax

C	0.32516	2.83575	0.00000
Si	0.47000	1.80333	-1.55558
C	-0.85585	0.47998	-1.54219
C	-0.85585	0.47998	1.54219
Si	0.47000	1.80333	1.55558
H	-0.74919	-0.16412	-2.41823
H	1.81876	1.19386	-1.59966
H	0.32674	2.64975	-2.76278
H	-0.64761	3.33603	0.00000
H	1.08768	3.61693	0.00000
H	-0.74919	-0.16412	2.41823
H	-1.80997	1.00242	1.67077
H	1.81876	1.19386	1.59966
H	0.32674	2.64975	2.76278
H	-1.80997	1.00242	-1.67077
C	0.14169	-2.07198	0.00000

C	1.61261	-1.65212	0.00000
H	1.86672	-1.06305	-0.88215
H	2.25342	-2.53929	0.00000
H	1.86672	-1.06305	0.88215
C	-0.14103	-2.91804	1.24626
H	0.47503	-3.82188	1.22992
H	-1.18605	-3.22969	1.29588
H	0.09621	-2.37857	2.16445
C	-0.14103	-2.91804	-1.24626
H	-1.18605	-3.22969	-1.29588
H	0.47503	-3.82188	-1.22992
H	0.09621	-2.37857	-2.16445
Si	-1.03331	-0.58553	0.00000
H	-2.40263	-1.16536	0.00000

135-trisila-tbu-eq

C	0.48600	-2.99148	0.00000
Si	-0.15496	-2.17915	1.56251
C	0.25821	-0.35201	1.52231
Si	-0.40534	0.52439	0.00000
C	0.25821	-0.35201	-1.52231
Si	-0.15496	-2.17915	-1.56251
H	-0.12845	0.12573	2.42531
H	-1.62578	-2.34355	1.62456
H	0.42580	-2.82364	2.76299
H	1.57841	-2.93383	0.00000
H	0.22304	-4.05118	0.00000
H	-0.12845	0.12573	-2.42531
H	1.34750	-0.24603	-1.54376
H	-1.62578	-2.34355	-1.62456
H	0.42580	-2.82364	-2.76299
H	1.34750	-0.24603	1.54376
H	-1.88763	0.41117	0.00000
C	0.02632	2.36916	0.00000
C	-0.57098	3.02453	1.24852
H	-0.14353	2.61244	2.16403
H	-0.36480	4.09895	1.24369

H	-1.65407	2.89528	1.29206
C	-0.57098	3.02453	-1.24852
H	-1.65407	2.89528	-1.29206
H	-0.36480	4.09895	-1.24369
H	-0.14353	2.61244	-2.16403
C	1.54406	2.56539	0.00000
H	1.78511	3.63252	0.00000
H	2.00859	2.12462	0.88397
H	2.00859	2.12462	-0.88397

246-trisila-ccl3-ax

Si	-0.96603	0.80761	-1.54834
C	0.42404	2.05491	-1.54036
Si	0.47019	3.12224	0.00000
C	0.42404	2.05491	1.54036
Si	-0.96603	0.80761	1.54834
C	-0.95012	-0.31515	0.00000
H	-0.73004	3.98975	0.00000
H	0.29442	2.70378	-2.41039
H	1.37785	1.53973	-1.66287
H	-0.96877	-0.00316	-2.77936
H	-2.25492	1.52665	-1.44511
H	0.29442	2.70378	2.41039
H	1.37785	1.53973	1.66287
H	-2.25492	1.52665	1.44511
H	-0.96877	-0.00316	2.77936
H	1.67005	3.98722	0.00000
H	-1.93546	-0.79478	0.00000
C	0.05573	-1.44598	0.00000
Cl	1.73537	-0.82141	0.00000
Cl	-0.12695	-2.50494	1.43356
Cl	-0.12695	-2.50494	-1.43356

246-trisila-ccl3-eq

Si	-0.33132	-0.82516	1.54102
C	0.47886	-2.51162	1.52517
Si	0.07852	-3.52391	0.00000
C	0.47886	-2.51162	-1.52517

Si	-0.33132	-0.82516	-1.54102
C	0.31931	0.10043	0.00000
H	-1.36747	-3.83862	0.00000
H	0.16385	-3.05966	2.41597
H	1.56212	-2.38257	1.59900
H	-0.01825	-0.08630	2.77705
H	-1.79590	-0.97677	1.42117
H	0.16385	-3.05966	-2.41597
H	1.56212	-2.38257	-1.59900
H	-1.79590	-0.97677	-1.42117
H	-0.01825	-0.08630	-2.77705
H	0.83528	-4.79492	0.00000
C	0.09002	1.59651	0.00000
Cl	0.82456	2.38801	-1.43186
Cl	-1.65774	1.96183	0.00000
Cl	0.82456	2.38801	1.43186
H	1.40571	-0.04404	0.00000

246-trisila-cf3-ax

Si	-0.90157	0.27826	-1.56185
C	0.53064	1.47520	-1.53563
Si	0.57665	2.55087	0.00000
C	0.53064	1.47520	1.53563
Si	-0.90157	0.27826	1.56185
C	-0.87323	-0.80788	0.00000
H	-0.61843	3.42577	0.00000
H	0.47490	2.11465	-2.41946
H	1.46291	0.90980	-1.60389
H	-0.89563	-0.57438	-2.76679
H	-2.17925	1.02019	-1.50101
H	0.47490	2.11465	2.41946
H	1.46291	0.90980	1.60389
H	-2.17925	1.02019	1.50101
H	-0.89563	-0.57438	2.76679
H	1.78119	3.40894	0.00000
H	-1.79862	-1.39085	0.00000
C	0.24888	-1.80086	0.00000

F	1.45604	-1.19290	0.00000
F	0.23582	-2.60848	1.07338
F	0.23582	-2.60848	-1.07338

246-trisila-cf3-eq

Si	-0.23547	-0.23941	1.56777
C	0.42388	-1.98830	1.52401
Si	-0.09272	-2.94931	0.00000
C	0.42388	-1.98830	-1.52401
Si	-0.23547	-0.23941	-1.56777
C	0.38152	0.64275	0.00000
H	-1.56521	-3.09795	0.00000
H	0.08643	-2.51500	2.41928
H	1.51600	-1.95404	1.56954
H	0.22733	0.48645	2.76652
H	-1.71267	-0.25680	1.54444
H	0.08643	-2.51500	-2.41928
H	1.51600	-1.95404	-1.56954
H	-1.71267	-0.25680	-1.54444
H	0.22733	0.48645	-2.76652
H	0.51501	-4.29777	0.00000
C	0.07216	2.11070	0.00000
F	0.57231	2.74786	-1.07339
F	-1.25223	2.34301	0.00000
F	0.57231	2.74786	1.07339
H	1.47349	0.56037	0.00000

246-trisila-cl-ax

Si	-0.78881	-0.25124	-1.58473
C	0.52375	1.07449	-1.53402
Si	0.43573	2.14929	0.00000
C	0.52375	1.07449	1.53402
Si	-0.78881	-0.25124	1.58473
C	-0.66906	-1.27312	0.00000
H	-0.85601	2.87475	0.00000
H	0.43958	1.70291	-2.42306
H	1.50277	0.58999	-1.57216
H	-0.63929	-1.14547	-2.75067

H	-2.13579	0.36432	-1.60848
H	0.43958	1.70291	2.42306
H	1.50277	0.58999	1.57216
H	-2.13579	0.36432	1.60848
H	-0.63929	-1.14547	2.75067
H	1.52689	3.14813	0.00000
Cl	0.94703	-2.09267	0.00000
H	-1.41487	-2.06737	0.00000

246-trisila-cl-eq

Si	0.15729	-0.26958	1.57779
C	-0.37972	1.52395	1.53082
Si	0.20701	2.43556	0.00000
C	-0.37972	1.52395	-1.53082
Si	0.15729	-0.26958	-1.57779
C	-0.46525	-1.09610	0.00000
H	-0.29199	3.82826	0.00000
H	-1.47158	1.56894	1.57302
H	-0.00787	2.03499	2.42173
H	1.63225	-0.35822	1.58134
H	-0.38055	-0.98455	2.75305
H	-1.47158	1.56894	-1.57302
H	-0.00787	2.03499	-2.42173
H	-0.38055	-0.98455	-2.75305
H	1.63225	-0.35822	-1.58134
H	1.68698	2.46981	0.00000
Cl	0.04628	-2.82399	0.00000
H	-1.55700	-1.09525	0.00000

246-trisila-f-ax

Si	-0.53164	-0.62524	-1.58682
C	0.43826	0.97046	-1.53033
Si	0.09418	1.99760	0.00000
C	0.43826	0.97046	1.53033
Si	-0.53164	-0.62524	1.58682
C	-0.15256	-1.59249	0.00000
H	-1.33214	2.39825	0.00000
H	0.23226	1.56102	-2.42517

H	1.50196	0.71745	-1.54946
H	-0.17965	-1.44528	-2.76496
H	-1.98681	-0.35291	-1.59746
H	0.23226	1.56102	2.42517
H	1.50196	0.71745	1.54946
H	-1.98681	-0.35291	1.59746
H	-0.17965	-1.44528	2.76496
H	0.91855	3.22615	0.00000
F	1.23738	-1.87524	0.00000
H	-0.67763	-2.55131	0.00000

246-trisila-f-eq

Si	0.19970	-0.58727	1.58556
C	-0.39445	1.18827	1.52965
Si	0.16918	2.11527	0.00000
C	-0.39445	1.18827	-1.52965
Si	0.19970	-0.58727	-1.58556
C	-0.41019	-1.42997	0.00000
H	-0.36746	3.49395	0.00000
H	-1.48738	1.19782	1.56583
H	-0.04474	1.71298	2.42130
H	1.67760	-0.62726	1.59840
H	-0.31402	-1.31279	2.76613
H	-1.48738	1.19782	-1.56583
H	-0.04474	1.71298	-2.42130
H	-0.31402	-1.31279	-2.76613
H	1.67760	-0.62726	-1.59840
H	1.64762	2.18968	0.00000
F	-0.01676	-2.78187	0.00000
H	-1.50678	-1.41130	0.00000

246-trisila-ch3-ax

Si	-0.56299	-0.60114	-1.55188
C	0.41657	0.99832	-1.53145
Si	0.09444	2.03066	0.00000
C	0.41657	0.99832	1.53145
Si	-0.56299	-0.60114	1.55188
C	-0.17701	-1.58721	0.00000

H	-1.32519	2.45425	0.00000
H	0.17904	1.58338	-2.42234
H	1.48321	0.76302	-1.58365
H	-0.22124	-1.40857	-2.74765
H	-2.00883	-0.28162	-1.59919
H	0.17904	1.58338	2.42234
H	1.48321	0.76302	1.58365
H	-2.00883	-0.28162	1.59919
H	-0.22124	-1.40857	2.74765
H	0.93637	3.24863	0.00000
H	-0.83635	-2.46064	0.00000
C	1.29228	-2.05283	0.00000
H	1.52515	-2.65330	0.88075
H	1.52515	-2.65330	-0.88075
H	1.97918	-1.20405	0.00000

246-trisila-ch3-eq

Si	0.15808	-0.55825	1.55162
C	-0.38979	1.23412	1.52716
Si	0.18773	2.15454	0.00000
C	-0.38979	1.23412	-1.52716
Si	0.15808	-0.55825	-1.55162
C	-0.42070	-1.44162	0.00000
H	1.66791	2.20798	0.00000
H	-0.02635	1.74202	2.42283
H	-1.48247	1.26668	1.56357
H	-0.36331	-1.26274	2.74749
H	1.63899	-0.61832	1.60049
H	-0.02635	1.74202	-2.42283
H	-1.48247	1.26668	-1.56357
H	1.63899	-0.61832	-1.60049
H	-0.36331	-1.26274	-2.74749
H	-0.32206	3.54453	0.00000
C	0.01983	-2.91626	0.00000
H	-0.34509	-3.44760	0.88027
H	-0.34509	-3.44760	-0.88027
H	1.10835	-2.99543	0.00000

H	-1.51577	-1.38481	0.00000
246-trisila-sih3-ax			
Si	-0.80438	-0.19963	1.55035
C	0.50627	1.13766	1.53205
Si	0.43337	2.21590	0.00000
C	0.50627	1.13766	-1.53205
Si	-0.80438	-0.19963	-1.55035
C	-0.64849	-1.24898	0.00000
H	-0.84906	2.95727	0.00000
H	0.39772	1.76265	2.42099
H	1.49339	0.67083	1.58841
H	-0.67210	-1.05436	2.75275
H	-2.14246	0.43519	1.57963
H	0.39772	1.76265	-2.42099
H	1.49339	0.67083	-1.58841
H	-2.14246	0.43519	-1.57963
H	-0.67210	-1.05436	-2.75275
H	1.53617	3.20295	0.00000
Si	0.91601	-2.27288	0.00000
H	0.98808	-3.12921	-1.20313
H	0.98808	-3.12921	1.20313
H	2.10080	-1.38445	0.00000
H	-1.48480	-1.95740	0.00000
246-trisila-sih3-eq			
Si	-0.13758	0.22700	1.55186
C	0.38456	-1.57179	1.52475
Si	-0.20749	-2.48663	0.00000
C	0.38456	-1.57179	-1.52475
Si	-0.13758	0.22700	-1.55186
C	0.44635	1.10605	0.00000
H	-1.68808	-2.51708	0.00000
H	0.01450	-2.07041	2.42313
H	1.47675	-1.61820	1.56027
H	0.39903	0.91325	2.74941
H	-1.61631	0.30516	1.60070
H	0.01450	-2.07041	-2.42313

H	1.47675	-1.61820	-1.56027
H	-1.61631	0.30516	-1.60070
H	0.39903	0.91325	-2.74941
H	0.28265	-3.88329	0.00000
H	1.54282	1.07164	0.00000
Si	-0.04702	2.91066	0.00000
H	0.47497	3.59802	1.20081
H	0.47497	3.59802	-1.20081
H	-1.52150	3.01798	0.00000

246-trisila-tbu-ax

Si	0.58027	2.73108	0.00000
C	0.57075	1.64997	-1.52980
Si	-0.81714	0.38523	-1.52407
C	-0.80107	-0.74280	0.00000
Si	-0.81714	0.38523	1.52407
C	0.57075	1.64997	1.52980
H	-0.81031	-0.38397	-2.78800
H	1.53851	1.15336	-1.62303
H	0.45316	2.28184	-2.41355
H	-0.64331	3.56555	0.00000
H	1.75334	3.63480	0.00000
H	-1.81872	-1.15934	0.00000
H	-0.81031	-0.38397	2.78800
H	-2.09536	1.13344	1.46888
H	1.53851	1.15336	1.62303
H	0.45316	2.28184	2.41355
H	-2.09536	1.13344	-1.46888
C	0.17648	-1.95796	0.00000
C	1.63828	-1.50829	0.00000
H	1.87492	-0.91519	-0.88405
H	2.29829	-2.37709	0.00000
H	1.87492	-0.91519	0.88405
C	-0.06449	-2.83279	1.23562
H	0.54331	-3.73717	1.17925
H	-1.11182	-3.13313	1.30004
H	0.19468	-2.31535	2.15771

C	-0.06449	-2.83279	-1.23562
H	-1.11182	-3.13313	-1.30004
H	0.54331	-3.73717	-1.17925
H	0.19468	-2.31535	-2.15771

246-trisila-tbu-eq

Si	-0.27099	-0.30191	-1.52935
C	0.43135	-2.04139	-1.51507
Si	-0.04927	-3.02756	0.00000
C	0.43135	-2.04139	1.51507
Si	-0.27099	-0.30191	1.52935
C	0.33621	0.63822	0.00000
H	0.12043	0.36848	2.78863
H	1.52216	-1.97571	1.56195
H	0.10505	-2.56066	2.41860
H	-1.51533	-3.23695	0.00000
H	0.60419	-4.35642	0.00000
H	0.12043	0.36848	-2.78863
H	-1.75063	-0.38859	-1.51120
H	1.52216	-1.97571	-1.56195
H	0.10505	-2.56066	-2.41860
H	-1.75063	-0.38859	1.51120
H	1.42553	0.48330	0.00000
C	0.08627	2.17989	0.00000
C	0.72539	2.82725	1.23408
H	0.24330	2.51241	2.15753
H	0.64350	3.91336	1.17068
H	1.78478	2.57221	1.30121
C	0.72539	2.82725	-1.23408
H	1.78478	2.57221	-1.30121
H	0.64350	3.91336	-1.17068
H	0.24330	2.51241	-2.15753
C	-1.41234	2.49065	0.00000
H	-1.57131	3.57003	0.00000
H	-1.90701	2.08048	0.88172
H	-1.90701	2.08048	-0.88172

345-trisila-ccl3-ax

C	-1.39408	0.29359	-1.28266
Si	-0.16995	1.63631	-1.84591
Si	0.59169	2.86329	0.00000
Si	-0.16995	1.63631	1.84591
C	-1.39408	0.29359	1.28266
C	-1.21609	-0.53652	0.00000
H	0.03520	4.23551	0.00000
H	-0.94421	2.49260	-2.77431
H	0.94973	1.04949	-2.60953
H	-1.53345	-0.37660	-2.13168
H	-2.34691	0.81639	-1.16753
H	-0.94421	2.49260	2.77431
H	0.94973	1.04949	2.60953
H	-2.34691	0.81639	1.16753
H	-1.53345	-0.37660	2.13168
H	2.06847	2.95845	0.00000
H	-2.02095	-1.27782	0.00000
C	0.03663	-1.42722	0.00000
Cl	1.55335	-0.48670	0.00000
Cl	0.04385	-2.47535	1.43988
Cl	0.04385	-2.47535	-1.43988

345-trisila-ccl3-eq

C	-0.42059	-0.41221	1.27352
Si	0.26584	-2.10550	1.76816
Si	-0.16159	-3.56676	0.00000
Si	0.26584	-2.10550	-1.76816
C	-0.42059	-0.41221	-1.27352
C	0.19445	0.19102	0.00000
H	-1.59224	-3.95066	0.00000
H	-0.34121	-2.51291	3.05331
H	1.72946	-1.96982	1.95466
H	-0.24197	0.24039	2.12778
H	-1.50415	-0.47796	1.15615
H	-0.34121	-2.51291	-3.05331
H	1.72946	-1.96982	-1.95466
H	-1.50415	-0.47796	-1.15615

H	-0.24197	0.24039	-2.12778
H	0.67264	-4.78663	0.00000
C	0.07565	1.73456	0.00000
Cl	0.88374	2.42914	-1.43064
Cl	-1.62802	2.24199	0.00000
Cl	0.88374	2.42914	1.43064
H	1.27737	0.02757	0.00000

345-trisila-cf3-ax

C	-1.27060	-0.21260	-1.29516
Si	0.01301	1.08279	-1.83546
Si	0.52792	2.44022	0.00000
Si	0.01301	1.08279	1.83546
C	-1.27060	-0.21260	1.29516
C	-1.07774	-1.01860	0.00000
H	-0.35617	3.62927	0.00000
H	-0.62084	1.85610	-2.92718
H	1.21638	0.42362	-2.38125
H	-1.38875	-0.90464	-2.13117
H	-2.22413	0.31324	-1.20867
H	-0.62084	1.85610	2.92718
H	1.21638	0.42362	2.38125
H	-2.22413	0.31324	1.20867
H	-1.38875	-0.90464	2.13117
H	1.93256	2.90173	0.00000
H	-1.81701	-1.82398	0.00000
C	0.24513	-1.74977	0.00000
F	1.29497	-0.90315	0.00000
F	0.38336	-2.53110	1.07736
F	0.38336	-2.53110	-1.07736

345-trisila-cf3-eq

C	-0.34128	0.19616	1.28999
Si	0.26875	-1.53127	1.76318
Si	-0.27649	-2.95822	0.00000
Si	0.26875	-1.53127	-1.76318
C	-0.34128	0.19616	-1.28999
C	0.25469	0.78190	0.00000

H	-1.73252	-3.22971	0.00000
H	-0.31897	-1.91119	3.06540
H	1.74276	-1.47398	1.90474
H	-0.09882	0.84782	2.13130
H	-1.43090	0.18707	1.21024
H	-0.31897	-1.91119	-3.06540
H	1.74276	-1.47398	-1.90474
H	-1.43090	0.18707	-1.21024
H	-0.09882	0.84782	-2.13130
H	0.46198	-4.23827	0.00000
C	0.05978	2.28876	0.00000
F	0.61687	2.86526	-1.07453
F	-1.23678	2.62780	0.00000
F	0.61687	2.86526	1.07453
H	1.34173	0.65252	0.00000

345-trisila-cl-ax

C	-1.09632	-0.73347	-1.29314
Si	0.04931	0.68240	-1.83096
Si	0.38055	2.09793	0.00000
Si	0.04931	0.68240	1.83096
C	-1.09632	-0.73347	1.29314
C	-0.78315	-1.48109	0.00000
H	-0.66625	3.14697	0.00000
H	-0.63304	1.38001	-2.94436
H	1.32647	0.14616	-2.34093
H	-1.11159	-1.45055	-2.11646
H	-2.11288	-0.33847	-1.21136
H	-0.63304	1.38001	2.94436
H	1.32647	0.14616	2.34093
H	-2.11288	-0.33847	1.21136
H	-1.11159	-1.45055	2.11646
H	1.70499	2.75483	0.00000
Cl	0.95784	-2.00235	0.00000
H	-1.32121	-2.42598	0.00000

345-trisila-cl-eq

C	0.28585	-0.72030	1.28722
---	---------	----------	---------

Si	-0.27587	1.03228	1.74745
Si	0.34842	2.44366	0.00000
Si	-0.27587	1.03228	-1.74745
C	0.28585	-0.72030	-1.28722
C	-0.29059	-1.29366	0.00000
H	-0.33373	3.75437	0.00000
H	-1.75370	1.03210	1.85814
H	0.29747	1.37738	3.06560
H	1.37695	-0.75327	1.23729
H	-0.00488	-1.36162	2.12028
H	-1.75370	1.03210	-1.85814
H	0.29747	1.37738	-3.06560
H	-0.00488	-1.36162	-2.12028
H	1.37695	-0.75327	-1.23729
H	1.81506	2.64749	0.00000
Cl	0.00306	-3.09564	0.00000
H	-1.37729	-1.21783	0.00000
345-trisila-f-ax			
C	-0.76216	-1.11846	-1.29138
Si	0.13868	0.47049	-1.80863
Si	0.03833	1.94554	0.00000
Si	0.13868	0.47049	1.80863
C	-0.76216	-1.11846	1.29138
C	-0.27911	-1.76791	0.00000
H	-1.27980	2.62393	0.00000
H	-0.54710	0.99930	-3.00914
H	1.53731	0.16723	-2.17208
H	-0.64763	-1.83038	-2.11117
H	-1.83074	-0.91048	-1.20955
H	-0.54710	0.99930	3.00914
H	1.53731	0.16723	2.17208
H	-1.83074	-0.91048	1.20955
H	-0.64763	-1.83038	2.11117
H	1.10099	2.97328	0.00000
F	1.12345	-1.75261	0.00000
H	-0.55036	-2.82489	0.00000

345-trisila-f-eq

C	0.32001	-1.06948	1.28575
Si	-0.26698	0.66605	1.75966
Si	0.31120	2.08543	0.00000
Si	-0.26698	0.66605	-1.75966
C	0.32001	-1.06948	-1.28575
C	-0.24774	-1.64631	0.00000
H	-0.40893	3.37587	0.00000
H	-1.74271	0.64416	1.89360
H	0.31971	1.03030	3.06648
H	1.41157	-1.08342	1.23114
H	0.03696	-1.73698	2.10220
H	-1.74271	0.64416	-1.89360
H	0.31971	1.03030	-3.06648
H	0.03696	-1.73698	-2.10220
H	1.41157	-1.08342	-1.23114
H	1.77092	2.33582	0.00000
F	0.03192	-3.01880	0.00000
H	-1.33956	-1.57423	0.00000

345-trisila-ch3-ax

C	-0.78732	-1.06817	-1.29033
Si	0.13586	0.50444	-1.80046
Si	0.03070	1.98953	0.00000
Si	0.13586	0.50444	1.80046
C	-0.78732	-1.06817	1.29033
C	-0.35719	-1.79230	0.00000
H	-1.29501	2.65341	0.00000
H	-0.50099	1.04312	-3.02377
H	1.54691	0.19781	-2.12978
H	-0.69371	-1.76441	-2.12877
H	-1.85055	-0.81851	-1.22922
H	-0.50099	1.04312	3.02377
H	1.54691	0.19781	2.12978
H	-1.85055	-0.81851	1.22922
H	-0.69371	-1.76441	2.12877
H	1.08115	3.03074	0.00000

H	-0.88658	-2.74949	0.00000
C	1.13517	-2.11048	0.00000
H	1.41043	-2.68663	0.88389
H	1.41043	-2.68663	-0.88389
H	1.74199	-1.20276	0.00000

345-trisila-ch3-eq

C	0.35602	-1.03129	1.28510
Si	-0.25696	0.69099	1.76233
Si	0.26948	2.12543	0.00000
Si	-0.25696	0.69099	-1.76233
C	0.35602	-1.03129	-1.28510
C	-0.22681	-1.64968	0.00000
H	1.72269	2.41638	0.00000
H	0.32886	1.08966	3.06209
H	-1.73092	0.63844	1.91630
H	0.12063	-1.68444	2.12983
H	1.44835	-1.01897	1.21379
H	0.32886	1.08966	-3.06209
H	-1.73092	0.63844	-1.91630
H	1.44835	-1.01897	-1.21379
H	0.12063	-1.68444	-2.12983
H	-0.47746	3.40165	0.00000
C	0.02221	-3.15835	0.00000
H	-0.40903	-3.62954	0.88337
H	-0.40903	-3.62954	-0.88337
H	1.09556	-3.35951	0.00000
H	-1.31129	-1.49294	0.00000

345-trisila-sih3-ax

C	-1.12367	0.64864	-1.29326
Si	0.06075	-0.73138	-1.82581
Si	0.38668	-2.15668	0.00000
Si	0.06075	-0.73138	1.82581
C	-1.12367	0.64864	1.29326
C	-0.81918	1.43814	0.00000
H	-0.67348	-3.19264	0.00000
H	-0.53486	-1.43250	-2.98566

H	1.34772	-0.14433	-2.26373
H	-1.17744	1.34485	-2.13456
H	-2.12252	0.20677	-1.21080
H	-0.53486	-1.43250	2.98566
H	1.34772	-0.14433	2.26373
H	-2.12252	0.20677	1.21080
H	-1.17744	1.34485	2.13456
H	1.70231	-2.83237	0.00000
Si	0.90038	2.21649	0.00000
H	1.06483	3.05267	1.20869
H	1.06483	3.05267	-1.20869
H	1.95430	1.17811	0.00000
H	-1.49726	2.29886	0.00000

345-trisila-sih3-eq

C	-0.34316	0.68132	1.29525
Si	0.25461	-1.04989	1.77269
Si	-0.27594	-2.47061	0.00000
Si	0.25461	-1.04989	-1.77269
C	-0.34316	0.68132	-1.29525
C	0.26323	1.26999	0.00000
H	-1.73176	-2.74798	0.00000
H	-0.33729	-1.45523	3.06790
H	1.72772	-0.99652	1.93020
H	-0.11103	1.32673	2.14789
H	-1.43417	0.67849	1.21460
H	-0.33729	-1.45523	-3.06790
H	1.72772	-0.99652	-1.93020
H	-1.43417	0.67849	-1.21460
H	-0.11103	1.32673	-2.14789
H	0.45822	-3.75424	0.00000
H	1.34569	1.09755	0.00000
Si	0.00300	3.13630	0.00000
H	0.60076	3.75000	1.20653
H	0.60076	3.75000	-1.20653
H	-1.45320	3.40243	0.00000

345-trisila-tbu-ax

Si	0.67627	2.42181	0.00000
Si	-0.17437	1.25326	-1.84719
C	-1.27413	-0.18094	-1.27650
C	-0.99712	-1.00471	0.00000
C	-1.27413	-0.18094	1.27650
Si	-0.17437	1.25326	1.84719
H	-1.37485	-0.85325	-2.13112
H	0.92861	0.77049	-2.71057
H	-1.01917	2.13732	-2.68415
H	0.23228	3.83423	0.00000
H	2.15686	2.40203	0.00000
H	-1.77730	-1.77527	0.00000
H	-1.37485	-0.85325	2.13112
H	-2.26506	0.26704	1.15559
H	0.92861	0.77049	2.71057
H	-1.01917	2.13732	2.68415
H	-2.26506	0.26704	-1.15559
C	0.31634	-1.83253	0.00000
C	1.60407	-1.00435	0.00000
H	1.70291	-0.38028	-0.88701
H	2.46155	-1.68012	0.00000
H	1.70291	-0.38028	0.88701
C	0.33342	-2.72837	1.24334
H	1.17274	-3.42312	1.19538
H	-0.58518	-3.31354	1.31928
H	0.44330	-2.14309	2.15671
C	0.33342	-2.72837	-1.24334
H	-0.58518	-3.31354	-1.31928
H	1.17274	-3.42312	-1.19538
H	0.44330	-2.14309	-2.15671
345-trisila-tbu-eq			
C	-0.48725	0.12608	-1.26706
Si	0.23090	-1.54614	-1.77307
Si	-0.11941	-3.02203	0.00000
Si	0.23090	-1.54614	1.77307
C	-0.48725	0.12608	1.26706

C	0.12929	0.75894	0.00000
H	-0.34312	0.77301	2.13220
H	1.68747	-1.37750	1.99425
H	-0.38012	-1.99277	3.04585
H	-1.53058	-3.47566	0.00000
H	0.76462	-4.20752	0.00000
H	-0.34312	0.77301	-2.13220
H	-1.56890	0.02731	-1.14323
H	1.68747	-1.37750	-1.99425
H	-0.38012	-1.99277	-3.04585
H	-1.56890	0.02731	1.14323
H	1.20693	0.54612	0.00000
C	0.03973	2.31738	0.00000
C	0.75705	2.88390	1.23158
H	0.22759	2.67371	2.15891
H	0.83699	3.96815	1.14808
H	1.76786	2.47906	1.31510
C	0.75705	2.88390	-1.23158
H	1.76786	2.47906	-1.31510
H	0.83699	3.96815	-1.14808
H	0.22759	2.67371	-2.15891
C	-1.41353	2.78941	0.00000
H	-1.45493	3.87971	0.00000
H	-1.94582	2.43669	0.88416
H	-1.94582	2.43669	-0.88416

1246-tetrasilica-ccl3-ax

Si	-0.77570	1.06900	-1.90002
C	0.63611	2.25364	-1.54850
Si	0.43924	3.29386	0.00000
C	0.63611	2.25364	1.54850
Si	-0.77570	1.06900	1.90002
Si	-1.17418	-0.25093	0.00000
H	-0.91192	3.90413	0.00000
H	0.73670	2.92359	-2.40592
H	1.56765	1.68761	-1.47530
H	-0.50736	0.22305	-3.08228

H	-2.01389	1.84445	-2.14183
H	0.73670	2.92359	2.40592
H	1.56765	1.68761	1.47530
H	-2.01389	1.84445	2.14183
H	-0.50736	0.22305	3.08228
H	1.43697	4.38608	0.00000
H	-2.49655	-0.91071	0.00000
C	0.08879	-1.71345	0.00000
Cl	1.74824	-1.03912	0.00000
Cl	-0.11998	-2.72469	1.44712
Cl	-0.11998	-2.72469	-1.44712

1246-tetrasil-a-ccl3-eq

Si	-0.07497	-1.06661	1.90141
C	-0.40029	-2.88421	1.54652
Si	0.42522	-3.55575	0.00000
C	-0.40029	-2.88421	-1.54652
Si	-0.07497	-1.06661	-1.90141
Si	-0.75080	0.12737	0.00000
H	1.85157	-3.15556	0.00000
H	-0.05772	-3.46656	2.40530
H	-1.47790	-3.05027	1.46624
H	-0.80195	-0.60825	3.10455
H	1.37369	-0.85425	2.10587
H	-0.05772	-3.46656	-2.40530
H	-1.47790	-3.05027	-1.46624
H	1.37369	-0.85425	-2.10587
H	-0.80195	-0.60825	-3.10455
H	0.35760	-5.03355	0.00000
C	0.02174	1.89300	0.00000
Cl	-0.50444	2.78054	-1.45187
Cl	1.79850	1.78098	0.00000
Cl	-0.50444	2.78054	1.45187
H	-2.21275	0.35941	0.00000

1246-tetrasil-a-cf3-ax

Si	-0.79481	0.57621	-1.88747
C	0.72768	1.61900	-1.55076

Si	0.65117	2.67367	0.00000
C	0.72768	1.61900	1.55076
Si	-0.79481	0.57621	1.88747
Si	-1.14000	-0.76717	0.00000
H	-0.61892	3.43755	0.00000
H	0.89122	2.27653	-2.40803
H	1.59827	0.96168	-1.48276
H	-0.64888	-0.24790	-3.10608
H	-1.97893	1.45000	-2.04377
H	0.89122	2.27653	2.40803
H	1.59827	0.96168	1.48276
H	-1.97893	1.45000	2.04377
H	-0.64888	-0.24790	3.10608
H	1.77069	3.64019	0.00000
H	-2.37312	-1.57959	0.00000
C	0.32133	-2.04543	0.00000
F	1.51661	-1.40256	0.00000
F	0.32969	-2.84950	1.07760
F	0.32969	-2.84950	-1.07760

1246-tetrasilica-cf3-eq

Si	-0.01759	-0.52248	1.88103
C	0.35052	-2.33494	1.54970
Si	-0.43732	-3.04477	0.00000
C	0.35052	-2.33494	-1.54970
Si	-0.01759	-0.52248	-1.88103
Si	0.69803	0.67532	0.00000
H	-1.88191	-2.71933	0.00000
H	0.00685	-2.91738	2.40809
H	1.43271	-2.47785	1.48853
H	0.64152	-0.04407	3.11449
H	-1.47789	-0.32702	2.00981
H	0.00685	-2.91738	-2.40809
H	1.43271	-2.47785	-1.48853
H	-1.47789	-0.32702	-2.00981
H	0.64152	-0.04407	-3.11449
H	-0.29131	-4.51674	0.00000

C	-0.11080	2.43665	0.00000
F	0.23332	3.16528	-1.07881
F	-1.45649	2.36670	0.00000
F	0.23332	3.16528	1.07881
H	2.15698	0.92009	0.00000

1246-tetrasil-cl-ax

Si	-0.74116	0.05770	-1.86240
C	0.65381	1.27529	-1.55301
Si	0.48552	2.31609	0.00000
C	0.65381	1.27529	1.55301
Si	-0.74116	0.05770	1.86240
Si	-0.77148	-1.35459	0.00000
H	-0.84475	2.96857	0.00000
H	0.73065	1.94753	-2.41090
H	1.59396	0.71910	-1.50115
H	-0.54675	-0.69803	-3.11869
H	-2.03307	0.77889	-1.93526
H	0.73065	1.94753	2.41090
H	1.59396	0.71910	1.50115
H	-2.03307	0.77889	1.93526
H	-0.54675	-0.69803	3.11869
H	1.51798	3.37576	0.00000
Cl	1.07047	-2.34545	0.00000
H	-1.82623	-2.38706	0.00000

1246-tetrasil-cl-eq

Si	0.15617	0.01897	1.86169
C	-0.38188	1.79441	1.55031
Si	0.31839	2.58808	0.00000
C	-0.38188	1.79441	-1.55031
Si	0.15617	0.01897	-1.86169
Si	-0.52641	-1.22205	0.00000
H	0.00532	4.03416	0.00000
H	-1.47342	1.83600	1.50179
H	-0.08496	2.40053	2.40987
H	1.63245	-0.04401	1.94072
H	-0.40839	-0.51027	3.12222

H	-1.47342	1.83600	-1.50179
H	-0.08496	2.40053	-2.40987
H	-0.40839	-0.51027	-3.12222
H	1.63245	-0.04401	-1.94072
H	1.79094	2.43200	0.00000
Cl	0.30320	-3.12564	0.00000
H	-1.99735	-1.38788	0.00000

1246-tetrasil-f-ax

Si	-0.52117	-0.30090	-1.85268
C	0.54853	1.21571	-1.55192
Si	0.14375	2.19061	0.00000
C	0.54853	1.21571	1.55192
Si	-0.52117	-0.30090	1.85268
Si	-0.26127	-1.71186	0.00000
H	-1.30066	2.51983	0.00000
H	0.45946	1.88503	-2.41092
H	1.59542	0.90345	-1.50389
H	-0.17942	-0.96302	-3.13133
H	-1.94634	0.10369	-1.90263
H	0.45946	1.88503	2.41092
H	1.59542	0.90345	1.50389
H	-1.94634	0.10369	1.90263
H	-0.17942	-0.96302	3.13133
H	0.90476	3.45977	0.00000
F	1.24533	-2.29219	0.00000
H	-1.17998	-2.86987	0.00000

1246-tetrasil-f-eq

Si	0.24030	-0.29659	1.86341
C	-0.43167	1.43383	1.54890
Si	0.20718	2.27894	0.00000
C	-0.43167	1.43383	-1.54890
Si	0.24030	-0.29659	-1.86341
Si	-0.38462	-1.57173	0.00000
H	-0.21499	3.69724	0.00000
H	-1.52317	1.39175	1.49792
H	-0.18437	2.06063	2.40915

H	1.71760	-0.24001	1.94220
H	-0.27284	-0.85076	3.13603
H	-1.52317	1.39175	-1.49792
H	-0.18437	2.06063	-2.40915
H	-0.27284	-0.85076	-3.13603
H	1.71760	-0.24001	-1.94220
H	1.68746	2.23645	0.00000
F	0.28134	-3.03495	0.00000
H	-1.85551	-1.75711	0.00000

1246-tetrasila-ch3-ax

Si	-0.56237	-0.26402	-1.83759
C	0.52259	1.24858	-1.54956
Si	0.12443	2.22806	0.00000
C	0.52259	1.24858	1.54956
Si	-0.56237	-0.26402	1.83759
Si	-0.29159	-1.68789	0.00000
H	-1.31754	2.56821	0.00000
H	0.43550	1.91402	-2.41175
H	1.56874	0.93302	-1.50237
H	-0.20148	-0.92855	-3.11286
H	-1.97513	0.17148	-1.93703
H	0.43550	1.91402	2.41175
H	1.56874	0.93302	1.50237
H	-1.97513	0.17148	1.93703
H	-0.20148	-0.92855	3.11286
H	0.89204	3.49435	0.00000
H	-1.28996	-2.78300	0.00000
C	1.45575	-2.40493	0.00000
H	1.62454	-3.01986	0.88316
H	1.62454	-3.01986	-0.88316
H	2.19774	-1.60584	0.00000

1246-tetrasila-ch3-eq

Si	0.17635	-0.26229	1.83750
C	-0.42231	1.49844	1.54867
Si	0.24347	2.32049	0.00000
C	-0.42231	1.49844	-1.54867

Si	0.17635	-0.26229	-1.83750
Si	-0.44690	-1.57194	0.00000
H	1.72230	2.22908	0.00000
H	-0.14744	2.10947	2.41167
H	-1.51460	1.49731	1.49834
H	-0.35174	-0.79688	3.11509
H	1.65618	-0.25540	1.93698
H	-0.14744	2.10947	-2.41167
H	-1.51460	1.49731	-1.49834
H	1.65618	-0.25540	-1.93698
H	-0.35174	-0.79688	-3.11509
H	-0.12463	3.75478	0.00000
C	0.33240	-3.28644	0.00000
H	0.03162	-3.84929	0.88257
H	0.03162	-3.84929	-0.88257
H	1.41891	-3.20749	0.00000
H	-1.92874	-1.68599	0.00000

1246-tetrasil-sih3-ax

Si	-1.84973	-0.13378	-0.76235
C	-1.55046	-1.32043	0.66527
Si	-0.00167	-2.36855	0.51685
C	1.54821	-1.32225	0.66677
Si	1.85033	-0.13604	-0.76061
Si	0.00122	1.29281	-0.86702
H	-0.00144	-3.04520	-0.80124
H	-2.41235	-1.98645	0.75203
H	-1.49678	-0.75089	1.59727
H	-3.10577	0.62599	-0.56604
H	-1.97245	-0.90435	-2.02087
H	2.40922	-1.98928	0.75448
H	1.49423	-0.75258	1.59868
H	1.97326	-0.90679	-2.01899
H	3.10714	0.62216	-0.56313
H	-0.00279	-3.41147	1.56723
Si	0.00104	2.58684	1.07857
H	1.20394	3.44156	1.16748

H	-1.20158	3.44202	1.16686
H	0.00055	1.67138	2.24402
H	0.00228	2.16119	-2.06714

1246-tetrasila-sih3-eq

Si	-0.08377	-0.07597	1.84219
C	0.36773	-1.87735	1.54907
Si	-0.36720	-2.63865	0.00000
C	0.36773	-1.87735	-1.54907
Si	-0.08377	-0.07597	-1.84219
Si	0.60685	1.19169	0.00000
H	-1.83184	-2.41585	0.00000
H	0.04283	-2.46383	2.41197
H	1.45622	-1.96612	1.49823
H	0.50885	0.42573	3.10292
H	-1.55674	0.04144	1.95458
H	0.04283	-2.46383	-2.41197
H	1.45622	-1.96612	-1.49823
H	-1.55674	0.04144	-1.95458
H	0.50885	0.42573	-3.10292
H	-0.12588	-4.09916	0.00000
H	2.08935	1.28279	0.00000
Si	-0.33138	3.32892	0.00000
H	0.07759	4.08766	1.20093
H	0.07759	4.08766	-1.20093
H	-1.80435	3.20142	0.00000

1246-tetrasila-tbu-ax

Si	-0.39768	2.91153	0.00000
C	-0.64776	1.87572	-1.54242
Si	0.69695	0.59671	-1.86224
Si	0.93783	-0.81524	0.00000
Si	0.69695	0.59671	1.86224
C	-0.64776	1.87572	1.54242
H	0.39175	-0.17287	-3.09303
H	-1.61725	1.37643	-1.46558
H	-0.70357	2.54011	-2.40796
H	0.97884	3.46115	0.00000

H	-1.34316	4.05105	0.00000
H	2.29252	-1.42542	0.00000
H	0.39175	-0.17287	3.09303
H	1.97541	1.31101	2.08773
H	-1.61725	1.37643	1.46558
H	-0.70357	2.54011	2.40796
H	1.97541	1.31101	-2.08773
C	-0.34917	-2.22531	0.00000
C	-1.76371	-1.64135	0.00000
H	-1.94820	-1.02785	-0.88471
H	-2.50338	-2.44727	0.00000
H	-1.94820	-1.02785	0.88471
C	-0.15543	-3.09127	1.24787
H	-0.87323	-3.91717	1.24286
H	0.84630	-3.52217	1.28357
H	-0.31055	-2.52173	2.16518
C	-0.15543	-3.09127	-1.24787
H	0.84630	-3.52217	-1.28357
H	-0.87323	-3.91717	-1.24286
H	-0.31055	-2.52173	-2.16518

1246-tetrasila-tbu-eq

Si	-0.08935	-0.55874	-1.84896
C	0.40532	-2.34996	-1.54861
Si	-0.31645	-3.12368	0.00000
C	0.40532	-2.34996	1.54861
Si	-0.08935	-0.55874	1.84896
Si	0.59166	0.71071	0.00000
H	0.49129	-0.05695	3.11738
H	1.49546	-2.41164	1.49073
H	0.10105	-2.94794	2.41088
H	-1.78547	-2.92926	0.00000
H	-0.04949	-4.58017	0.00000
H	0.49129	-0.05695	-3.11738
H	-1.56502	-0.48787	-1.98047
H	1.49546	-2.41164	-1.49073
H	0.10105	-2.94794	-2.41088

H	-1.56502	-0.48787	1.98047
H	2.08091	0.74191	0.00000
C	-0.05926	2.49987	0.00000
C	0.45158	3.22178	1.25009
H	0.08867	2.75003	2.16512
H	0.10281	4.25888	1.25053
H	1.54190	3.23683	1.28855
C	0.45158	3.22178	-1.25009
H	1.54190	3.23683	-1.28855
H	0.10281	4.25888	-1.25053
H	0.08867	2.75003	-2.16512
C	-1.59004	2.50024	0.00000
H	-1.96064	3.52942	0.00000
H	-1.99529	2.00192	0.88217
H	-1.99529	2.00192	-0.88217

1345-tetrasilica-ccl3-ax

C	-1.41666	0.60425	-1.54525
Si	0.00077	1.79179	-1.93457
Si	0.71854	2.91910	0.00000
Si	0.00077	1.79179	1.93457
C	-1.41666	0.60425	1.54525
Si	-1.39230	-0.42921	0.00000
H	0.15698	4.29089	0.00000
H	-0.48629	2.77367	-2.93042
H	1.11935	1.04730	-2.54608
H	-1.56637	-0.04937	-2.40739
H	-2.32438	1.21213	-1.46288
H	-0.48629	2.77367	2.93042
H	1.11935	1.04730	2.54608
H	-2.32438	1.21213	1.46288
H	-1.56637	-0.04937	2.40739
H	2.19461	3.03630	0.00000
H	-2.50713	-1.39743	0.00000
C	0.15072	-1.58142	0.00000
Cl	1.66812	-0.64434	0.00000
Cl	0.10733	-2.60604	1.45320

Cl	0.10733	-2.60604	-1.45320
----	---------	----------	----------

1345-tetrasila-ccl3-eq

C	-0.21642	-0.61280	1.54751
Si	0.30652	-2.40046	1.84404
Si	-0.39478	-3.65951	0.00000
Si	0.30652	-2.40046	-1.84404
C	-0.21642	-0.61280	-1.54751
Si	0.48043	0.14688	0.00000
H	-1.87477	-3.74572	0.00000
H	-0.25088	-2.89661	3.12063
H	1.78389	-2.45888	1.92784
H	0.08836	-0.01015	2.40606
H	-1.30769	-0.56957	1.49363
H	-0.25088	-2.89661	-3.12063
H	1.78389	-2.45888	-1.92784
H	-1.30769	-0.56957	-1.49363
H	0.08836	-0.01015	-2.40606
H	0.16196	-5.02953	0.00000
C	0.04128	2.02352	0.00000
Cl	0.72122	2.79953	-1.44923
Cl	-1.72851	2.22774	0.00000
Cl	0.72122	2.79953	1.44923
H	1.95656	0.12206	0.00000

1345-tetrasila-cf3-ax

C	-1.27642	0.11980	-1.55942
Si	0.19120	1.26156	-1.90322
Si	0.58559	2.57213	0.00000
Si	0.19120	1.26156	1.90322
C	-1.27642	0.11980	1.55942
Si	-1.24939	-0.89526	0.00000
H	-0.39947	3.68163	0.00000
H	-0.13586	2.12077	-3.06311
H	1.37714	0.45367	-2.24874
H	-1.40046	-0.55354	-2.41094
H	-2.17735	0.73997	-1.52135
H	-0.13586	2.12077	3.06311

H	1.37714	0.45367	2.24874
H	-2.17735	0.73997	1.52135
H	-1.40046	-0.55354	2.41094
H	1.94164	3.16253	0.00000
H	-2.30840	-1.92429	0.00000
C	0.39517	-1.91132	0.00000
F	1.48508	-1.10750	0.00000
F	0.51376	-2.70557	1.08044
F	0.51376	-2.70557	-1.08044

1345-tetrasila-cf3-eq

C	-0.20577	-0.02936	1.55645
Si	0.27190	-1.83126	1.84245
Si	-0.48190	-3.06216	0.00000
Si	0.27190	-1.83126	-1.84245
C	-0.20577	-0.02936	-1.55645
Si	0.48249	0.72211	0.00000
H	-1.96399	-3.08906	0.00000
H	-0.27982	-2.31779	3.12497
H	1.74860	-1.92594	1.90413
H	0.12891	0.56640	2.40917
H	-1.29619	0.04585	1.52037
H	-0.27982	-2.31779	-3.12497
H	1.74860	-1.92594	-1.90413
H	-1.29619	0.04585	-1.52037
H	0.12891	0.56640	-2.40917
H	0.02113	-4.45264	0.00000
C	-0.02568	2.58762	0.00000
F	0.43103	3.25076	-1.08006
F	-1.36771	2.73848	0.00000
F	0.43103	3.25076	1.08006
H	1.95889	0.72099	0.00000

1345-tetrasila-cl-ax

C	-1.03749	-0.42909	-1.54904
Si	0.24889	0.91473	-1.86657
Si	0.27536	2.32658	0.00000
Si	0.24889	0.91473	1.86657

C	-1.03749	-0.42909	1.54904
Si	-0.83094	-1.43828	0.00000
H	-0.97224	3.12958	0.00000
H	-0.09689	1.65121	-3.10278
H	1.57780	0.29630	-2.05321
H	-1.05037	-1.11054	-2.40298
H	-2.02498	0.04130	-1.50520
H	-0.09689	1.65121	3.10278
H	1.57780	0.29630	2.05321
H	-2.02498	0.04130	1.50520
H	-1.05037	-1.11054	2.40298
H	1.42764	3.25385	0.00000
Cl	1.08008	-2.24249	0.00000
H	-1.75323	-2.58874	0.00000

1345-tetrasila-cl-eq

C	0.29026	-0.49783	1.54495
Si	-0.26622	1.28003	1.83827
Si	0.42172	2.55321	0.00000
Si	-0.26622	1.28003	-1.83827
C	0.29026	-0.49783	-1.54495
Si	-0.37744	-1.28851	0.00000
H	-0.15418	3.91528	0.00000
H	-1.74506	1.31385	1.91179
H	0.27176	1.78488	3.12002
H	1.38246	-0.52662	1.50254
H	-0.01064	-1.10653	2.40069
H	-1.74506	1.31385	-1.91179
H	0.27176	1.78488	-3.12002
H	-0.01064	-1.10653	-2.40069
H	1.38246	-0.52662	-1.50254
H	1.90040	2.65995	0.00000
Cl	0.15593	-3.29203	0.00000
H	-1.85194	-1.25201	0.00000

1345-tetrasila-f-ax

C	-0.76813	-0.82424	-1.54445
Si	0.24759	0.73506	-1.85437

Si	-0.03422	2.13492	0.00000
Si	0.24759	0.73506	1.85437
C	-0.76813	-0.82424	1.54445
Si	-0.34526	-1.76691	0.00000
H	-1.42376	2.65472	0.00000
H	-0.18447	1.38452	-3.11202
H	1.67528	0.37435	-1.98818
H	-0.66025	-1.49107	-2.40334
H	-1.82468	-0.54411	-1.49471
H	-0.18447	1.38452	3.11202
H	1.67528	0.37435	1.98818
H	-1.82468	-0.54411	1.49471
H	-0.66025	-1.49107	2.40334
H	0.89638	3.28458	0.00000
F	1.23787	-2.02242	0.00000
H	-0.98208	-3.09822	0.00000

1345-tetrasila-f-eq

C	0.35494	-0.83014	1.54154
Si	-0.27226	0.92143	1.83988
Si	0.35737	2.22314	0.00000
Si	-0.27226	0.92143	-1.83988
C	0.35494	-0.83014	-1.54154
Si	-0.28053	-1.64716	0.00000
H	-0.27710	3.55910	0.00000
H	-1.75116	0.89861	1.91941
H	0.24851	1.44996	3.11930
H	1.44765	-0.80773	1.50030
H	0.08047	-1.45032	2.39860
H	-1.75116	0.89861	-1.91941
H	0.24851	1.44996	-3.11930
H	0.08047	-1.45032	-2.39860
H	1.44765	-0.80773	-1.50030
H	1.83002	2.39601	0.00000
F	0.20180	-3.17490	0.00000
H	-1.75675	-1.66790	0.00000

1345-tetrasila-ch3-ax

C	-0.83511	-0.78450	-1.54474
Si	0.21032	0.74542	-1.86104
Si	0.00390	2.15048	0.00000
Si	0.21032	0.74542	1.86104
C	-0.83511	-0.78450	1.54474
Si	-0.40579	-1.76496	0.00000
H	-1.35683	2.74184	0.00000
H	-0.20287	1.42464	-3.11028
H	1.63007	0.35123	-2.01718
H	-0.75067	-1.44945	-2.40839
H	-1.88471	-0.48313	-1.48515
H	-0.20287	1.42464	3.11028
H	1.63007	0.35123	2.01718
H	-1.88471	-0.48313	1.48515
H	-0.75067	-1.44945	2.40839
H	0.98956	3.25429	0.00000
H	-1.20335	-3.01529	0.00000
C	1.41172	-2.21036	0.00000
H	1.66578	-2.79831	0.88238
H	1.66578	-2.79831	-0.88238
H	2.04271	-1.32089	0.00000

1345-tetrasilica-ch3-eq

C	0.38491	-0.77693	1.54328
Si	-0.26388	0.96072	1.84949
Si	0.31251	2.27287	0.00000
Si	-0.26388	0.96072	-1.84949
C	0.38491	-0.77693	-1.54328
Si	-0.27026	-1.62415	0.00000
H	1.77966	2.49366	0.00000
H	0.27083	1.51667	3.11363
H	-1.74007	0.91460	1.96383
H	0.13832	-1.39831	2.40833
H	1.47673	-0.74198	1.48310
H	0.27083	1.51667	-3.11363
H	-1.74007	0.91460	-1.96383
H	1.47673	-0.74198	-1.48310

H	0.13832	-1.39831	-2.40833
H	-0.35635	3.59283	0.00000
C	0.21577	-3.43136	0.00000
H	-0.17129	-3.94099	0.88236
H	-0.17129	-3.94099	-0.88236
H	1.30153	-3.53456	0.00000
H	-1.75039	-1.51569	0.00000

1345-tetrasila-sih3-ax

C	-1.17652	-0.31997	1.54648
Si	0.19712	0.92001	1.88344
Si	0.42522	2.29488	0.00000
Si	0.19712	0.92001	-1.88344
C	-1.17652	-0.31997	-1.54648
Si	-0.94995	-1.36966	0.00000
H	-0.69282	3.27025	0.00000
H	-0.09440	1.71691	3.09664
H	1.45861	0.18070	2.11963
H	-1.26297	-0.98556	2.40872
H	-2.12847	0.21159	1.46158
H	-0.09440	1.71691	-3.09664
H	1.45861	0.18070	-2.11963
H	-2.12847	0.21159	-1.46158
H	-1.26297	-0.98556	-2.40872
H	1.69676	3.05142	0.00000
Si	1.16120	-2.39594	0.00000
H	1.30715	-3.24697	-1.20218
H	1.30715	-3.24697	1.20218
H	2.25827	-1.40411	0.00000
H	-1.96767	-2.44941	0.00000

1345-tetrasila-sih3-eq

C	-0.32072	0.42278	1.55230
Si	0.25865	-1.34335	1.84968
Si	-0.38127	-2.62482	0.00000
Si	0.25865	-1.34335	-1.84968
C	-0.32072	0.42278	-1.55230
Si	0.36808	1.23604	0.00000

H	-1.85712	-2.77348	0.00000
H	-0.29103	-1.87752	3.11662
H	1.73602	-1.35077	1.95332
H	-0.04318	1.03012	2.41751
H	-1.41271	0.43772	1.49559
H	-0.29103	-1.87752	-3.11662
H	1.73602	-1.35077	-1.95332
H	-1.41271	0.43772	-1.49559
H	-0.04318	1.03012	-2.41751
H	0.22479	-3.97452	0.00000
H	1.84426	1.08024	0.00000
Si	-0.16590	3.51525	0.00000
H	0.37258	4.19032	1.20176
H	0.37258	4.19032	-1.20176
H	-1.63809	3.67685	0.00000

1345-tetrasila-tbu-ax

Si	-0.37116	2.83125	0.00000
Si	-0.17283	1.46576	-1.89281
C	1.12342	0.14763	-1.55062
Si	1.05046	-0.91664	0.00000
C	1.12342	0.14763	1.55062
Si	-0.17283	1.46576	1.89281
H	1.18814	-0.51601	-2.41714
H	-1.47813	0.85383	-2.22475
H	0.23226	2.27441	-3.06622
H	0.77315	3.77617	0.00000
H	-1.61945	3.62621	0.00000
H	2.28104	-1.75147	0.00000
H	1.18814	-0.51601	2.41714
H	2.08611	0.66869	1.50541
H	-1.47813	0.85383	2.22475
H	0.23226	2.27441	3.06622
H	2.08611	0.66869	-1.50541
C	-0.38291	-2.15399	0.00000
C	-1.76158	-1.49072	0.00000
H	-1.91694	-0.87173	-0.88336

H	-2.54093	-2.25911	0.00000
H	-1.91694	-0.87173	0.88336
C	-0.25233	-3.03205	1.24964
H	-1.01967	-3.81159	1.23975
H	0.72060	-3.52444	1.30052
H	-0.38799	-2.45115	2.16392
C	-0.25233	-3.03205	-1.24964
H	0.72060	-3.52444	-1.30052
H	-1.01967	-3.81159	-1.23975
H	-0.38799	-2.45115	-2.16392

1345-tetrasila-tbu-eq

C	-0.35376	-0.08497	-1.53700
Si	0.26891	-1.83153	-1.85043
Si	-0.31270	-3.13965	0.00000
Si	0.26891	-1.83153	1.85043
C	-0.35376	-0.08497	1.53700
Si	0.34168	0.74484	0.00000
H	-0.11318	0.52465	2.41154
H	1.74419	-1.80564	1.97998
H	-0.28643	-2.37685	3.11050
H	-1.78128	-3.35092	0.00000
H	0.34750	-4.46393	0.00000
H	-0.11318	0.52465	-2.41154
H	-1.44458	-0.11085	-1.45793
H	1.74419	-1.80564	-1.97998
H	-0.28643	-2.37685	-3.11050
H	-1.44458	-0.11085	1.45793
H	1.81997	0.58435	0.00000
C	-0.03208	2.60302	0.00000
C	0.58352	3.24614	1.24629
H	0.14048	2.85830	2.16459
H	0.41305	4.32662	1.23201
H	1.66167	3.08185	1.29383
C	0.58352	3.24614	-1.24629
H	1.66167	3.08185	-1.29383
H	0.41305	4.32662	-1.23201

H	0.14048	2.85830	-2.16459
C	-1.54480	2.83696	0.00000
H	-1.76029	3.90951	0.00000
H	-2.01947	2.40655	0.88388
H	-2.01947	2.40655	-0.88388

2356-tetrasil-a-ccl3-ax

Si	-1.14233	0.54365	-1.55013
Si	0.44321	2.27569	-1.58975
C	0.30134	3.26909	0.00000
Si	0.44321	2.27569	1.58975
Si	-1.14233	0.54365	1.55013
C	-1.04711	-0.58081	0.00000
H	-0.68212	3.74720	0.00000
H	0.11647	3.13046	-2.75503
H	1.81814	1.76717	-1.76864
H	-1.12238	-0.25762	-2.78897
H	-2.47321	1.18503	-1.43550
H	0.11647	3.13046	2.75503
H	1.81814	1.76717	1.76864
H	-2.47321	1.18503	1.43550
H	-1.12238	-0.25762	2.78897
H	1.04444	4.06900	0.00000
H	-1.97998	-1.15365	0.00000
C	0.06988	-1.60226	0.00000
Cl	1.66859	-0.80057	0.00000
Cl	-0.00797	-2.67107	1.43448
Cl	-0.00797	-2.67107	-1.43448

2356-tetrasil-a-ccl3-eq

Si	-0.48361	-0.58338	1.53970
Si	0.35610	-2.77420	1.55872
C	-0.18045	-3.67482	0.00000
Si	0.35610	-2.77420	-1.55872
Si	-0.48361	-0.58338	-1.53970
C	0.23990	0.29680	0.00000
H	-1.27010	-3.75452	0.00000
H	-0.11108	-3.46923	2.77852

H	1.83570	-2.70794	1.60092
H	-0.12274	0.12214	2.78375
H	-1.95690	-0.61580	1.41536
H	-0.11108	-3.46923	-2.77852
H	1.83570	-2.70794	-1.60092
H	-1.95690	-0.61580	-1.41536
H	-0.12274	0.12214	-2.78375
H	0.22168	-4.68961	0.00000
C	0.10484	1.80999	0.00000
Cl	0.89267	2.54307	-1.43264
Cl	-1.61170	2.29449	0.00000
Cl	0.89267	2.54307	1.43264
H	1.31480	0.08821	0.00000

2356-tetrasila-cf3-ax

Si	-1.08080	0.01068	-1.56709
Si	0.52154	1.72541	-1.58529
C	0.35759	2.72451	0.00000
Si	0.52154	1.72541	1.58529
Si	-1.08080	0.01068	1.56709
C	-0.91649	-1.06645	0.00000
H	-0.62724	3.19901	0.00000
H	0.27401	2.58276	-2.76686
H	1.88197	1.16025	-1.69844
H	-1.02192	-0.83711	-2.77542
H	-2.42814	0.61865	-1.48238
H	0.27401	2.58276	2.76686
H	1.88197	1.16025	1.69844
H	-2.42814	0.61865	1.48238
H	-1.02192	-0.83711	2.77542
H	1.09870	3.52653	0.00000
H	-1.74995	-1.77364	0.00000
C	0.33650	-1.88996	0.00000
F	1.44267	-1.11753	0.00000
F	0.43363	-2.69043	1.07395
F	0.43363	-2.69043	-1.07395

2356-tetrasila-cf3-eq

Si	-0.37484	0.01292	1.56644
Si	0.29079	-2.23539	1.56182
C	-0.32914	-3.07660	0.00000
Si	0.29079	-2.23539	-1.56182
Si	-0.37484	0.01292	-1.56644
C	0.32587	0.84416	0.00000
H	-1.42149	-3.05669	0.00000
H	-0.21617	-2.90513	2.77957
H	1.77138	-2.28442	1.58776
H	0.11211	0.70899	2.77459
H	-1.85044	0.10464	1.51781
H	-0.21617	-2.90513	-2.77957
H	1.77138	-2.28442	-1.58776
H	-1.85044	0.10464	-1.51781
H	0.11211	0.70899	-2.77459
H	-0.02286	-4.12445	0.00000
C	0.13233	2.33517	0.00000
F	0.68359	2.92664	-1.07348
F	-1.16788	2.67327	0.00000
F	0.68359	2.92664	1.07348
H	1.40700	0.67641	0.00000

2356-tetrasil-cl-ax

Si	-0.89392	-0.56149	-1.59229
Si	0.42200	1.37955	-1.57801
C	0.07126	2.34190	0.00000
Si	0.42200	1.37955	1.57801
Si	-0.89392	-0.56149	1.59229
C	-0.57566	-1.53915	0.00000
H	-0.98196	2.63383	0.00000
H	0.09633	2.19147	-2.77256
H	1.85486	1.02014	-1.63942
H	-0.61354	-1.42504	-2.75843
H	-2.33135	-0.19576	-1.60204
H	0.09633	2.19147	2.77256
H	1.85486	1.02014	1.63942
H	-2.33135	-0.19576	1.60204

H	-0.61354	-1.42504	2.75843
H	0.65945	3.26196	0.00000
Cl	1.16107	-2.04309	0.00000
H	-1.15981	-2.45887	0.00000

2356-tetrasila-cl-eq

Si	0.27069	-0.52464	1.58128
Si	-0.23187	1.76980	1.56764
C	0.45548	2.54825	0.00000
Si	-0.23187	1.76980	-1.56764
Si	0.27069	-0.52464	-1.58128
C	-0.42975	-1.29269	0.00000
H	0.23928	3.61843	0.00000
H	-1.70405	1.93679	1.58702
H	0.31905	2.41728	2.77896
H	1.73664	-0.72315	1.56420
H	-0.29719	-1.20898	2.76124
H	-1.70405	1.93679	-1.58702
H	0.31905	2.41728	-2.77896
H	-0.29719	-1.20898	-2.76124
H	1.73664	-0.72315	-1.56420
H	1.54248	2.43726	0.00000
Cl	-0.09698	-3.06716	0.00000
H	-1.51535	-1.18398	0.00000

2356-tetrasila-f-ax

Si	-0.57648	0.91145	1.59373
Si	0.28281	-1.26978	1.57782
C	-0.27114	-2.13245	0.00000
Si	0.28281	-1.26978	-1.57782
Si	-0.57648	0.91145	-1.59373
C	0.00060	1.77936	0.00000
H	-1.36238	-2.19117	0.00000
H	-0.18849	-2.00386	2.77390
H	1.76022	-1.21380	1.62227
H	-0.13760	1.68275	2.77658
H	-2.05784	0.88360	1.56264
H	-0.18849	-2.00386	-2.77390

H	1.76022	-1.21380	-1.62227
H	-2.05784	0.88360	-1.56264
H	-0.13760	1.68275	-2.77658
H	0.10544	-3.15753	0.00000
F	1.41423	1.77685	0.00000
H	-0.31689	2.82520	0.00000

2356-tetrasila-f-eq

Si	0.27649	-0.84249	1.58687
Si	-0.23089	1.44971	1.56685
C	0.45582	2.22911	0.00000
Si	-0.23089	1.44971	-1.56685
Si	0.27649	-0.84249	-1.58687
C	-0.43479	-1.61100	0.00000
H	0.23662	3.29872	0.00000
H	-1.70325	1.61388	1.58539
H	0.31812	2.09786	2.77833
H	1.74399	-1.03494	1.57782
H	-0.29001	-1.52044	2.77206
H	-1.70325	1.61388	-1.58539
H	0.31812	2.09786	-2.77833
H	-0.29001	-1.52044	-2.77206
H	1.74399	-1.03494	-1.57782
H	1.54302	2.12068	0.00000
F	-0.20297	-2.99877	0.00000
H	-1.52054	-1.46508	0.00000

2356-tetrasila-ch3-ax

Si	0.59570	-0.89041	1.55863
Si	-0.26166	1.29517	1.56811
C	0.28937	2.17858	0.00000
Si	-0.26166	1.29517	-1.56811
Si	0.59570	-0.89041	-1.55863
C	0.03302	-1.79138	0.00000
H	1.38083	2.23565	0.00000
H	0.19258	2.01967	2.77719
H	-1.74322	1.25225	1.60198
H	0.14122	-1.63325	2.75884

H	2.07674	-0.81925	1.59319
H	0.19258	2.01967	-2.77719
H	-1.74322	1.25225	-1.60198
H	2.07674	-0.81925	-1.59319
H	0.14122	-1.63325	-2.75884
H	-0.08850	3.20276	0.00000
H	0.52431	-2.76896	0.00000
C	-1.49473	-1.98361	0.00000
H	-1.82976	-2.53314	-0.88083
H	-1.82976	-2.53314	0.88083
H	-2.01752	-1.02465	0.00000

2356-tetrasila-ch3-eq

Si	0.24441	-0.81193	1.55451
Si	-0.22299	1.48689	1.56614
C	0.46693	2.26883	0.00000
Si	-0.22299	1.48689	-1.56614
Si	0.24441	-0.81193	-1.55451
C	-0.44271	-1.62778	0.00000
H	1.55320	2.14991	0.00000
H	0.33900	2.12729	2.77716
H	-1.69278	1.67906	1.59342
H	-0.31139	-1.47438	2.75913
H	1.71538	-1.01055	1.57476
H	0.33900	2.12729	-2.77716
H	-1.69278	1.67906	-1.59342
H	1.71538	-1.01055	-1.57476
H	-0.31139	-1.47438	-2.75913
H	0.25810	3.34036	0.00000
C	-0.17957	-3.14408	0.00000
H	-0.60576	-3.62562	0.88141
H	-0.60576	-3.62562	-0.88141
H	0.89200	-3.35030	0.00000
H	-1.52164	-1.43878	0.00000

2356-tetrasila-sih3-ax

Si	-0.90565	-0.49637	1.55600
Si	0.42096	1.44139	1.57005

C	0.09209	2.42447	0.00000
Si	0.42096	1.44139	-1.57005
Si	-0.90565	-0.49637	-1.55600
C	-0.59480	-1.51331	0.00000
H	-0.95691	2.73148	0.00000
H	0.10329	2.24194	2.77480
H	1.85541	1.07883	1.63192
H	-0.64329	-1.31510	2.76274
H	-2.32913	-0.08064	1.59105
H	0.10329	2.24194	-2.77480
H	1.85541	1.07883	-1.63192
H	-2.32913	-0.08064	-1.59105
H	-0.64329	-1.31510	-2.76274
H	0.69523	3.33438	0.00000
Si	1.10928	-2.28819	0.00000
H	1.30137	-3.12477	-1.20350
H	1.30137	-3.12477	1.20350
H	2.13481	-1.22245	0.00000
H	-1.31882	-2.33580	0.00000

2356-tetrasila-sih3-eq

Si	0.26983	-0.48478	1.55403
Si	-0.23568	1.80546	1.56727
C	0.43911	2.59808	0.00000
Si	-0.23568	1.80546	-1.56727
Si	0.26983	-0.48478	-1.55403
C	-0.41768	-1.29953	0.00000
H	1.52736	2.49908	0.00000
H	0.31422	2.45647	2.77801
H	-1.70940	1.96374	1.59317
H	-0.26411	-1.15198	2.76437
H	1.74250	-0.66172	1.55548
H	0.31422	2.45647	-2.77801
H	-1.70940	1.96374	-1.59317
H	1.74250	-0.66172	-1.55548
H	-0.26411	-1.15198	-2.76437
H	0.21133	3.66578	0.00000

H	-1.50198	-1.14120	0.00000
Si	-0.10750	-3.14617	0.00000
H	-0.69343	-3.77674	1.20252
H	-0.69343	-3.77674	-1.20252
H	1.35089	-3.38874	0.00000

2356-tetrasila-tbu-ax

C	0.18602	2.91397	0.00000
Si	0.44660	1.91065	-1.56969
Si	-0.99588	0.05536	-1.52645
C	-0.81587	-1.06609	0.00000
Si	-0.99588	0.05536	1.52645
Si	0.44660	1.91065	1.56969
H	-0.91148	-0.69379	-2.80035
H	1.86901	1.50906	-1.66623
H	0.13173	2.72227	-2.76897
H	-0.84481	3.27801	0.00000
H	0.83946	3.78819	0.00000
H	-1.74831	-1.64655	0.00000
H	-0.91148	-0.69379	2.80035
H	-2.36127	0.63349	1.45730
H	1.86901	1.50906	1.66623
H	0.13173	2.72227	2.76897
H	-2.36127	0.63349	-1.45730
C	0.35556	-2.09257	0.00000
C	1.71728	-1.39834	0.00000
H	1.85075	-0.77201	-0.88303
H	2.51637	-2.14116	0.00000
H	1.85075	-0.77201	0.88303
C	0.26336	-2.99351	1.23671
H	1.01573	-3.78166	1.18292
H	-0.71808	-3.46667	1.30149
H	0.43161	-2.43726	2.15757
C	0.26336	-2.99351	-1.23671
H	-0.71808	-3.46667	-1.30149
H	1.01573	-3.78166	-1.18292
H	0.43161	-2.43726	-2.15757

2356-tetrasila-tbu-eq

Si	-0.41566	-0.04791	-1.52392
Si	0.29852	-2.28254	-1.55196
C	-0.28166	-3.16889	0.00000
Si	0.29852	-2.28254	1.55196
Si	-0.41566	-0.04791	1.52392
C	0.27824	0.85225	0.00000
H	-0.00018	0.58067	2.79815
H	1.78064	-2.30618	1.59537
H	-0.19918	-2.95074	2.77643
H	-1.37395	-3.19381	0.00000
H	0.07074	-4.20174	0.00000
H	-0.00018	0.58067	-2.79815
H	-1.89858	-0.02833	-1.48819
H	1.78064	-2.30618	-1.59537
H	-0.19918	-2.95074	-2.77643
H	-1.89858	-0.02833	1.48819
H	1.35097	0.61486	0.00000
C	0.14538	2.40919	0.00000
C	0.83559	2.99837	1.23508
H	0.33230	2.71540	2.15772
H	0.83607	4.08782	1.17826
H	1.87263	2.66328	1.29730
C	0.83559	2.99837	-1.23508
H	1.87263	2.66328	-1.29730
H	0.83607	4.08782	-1.17826
H	0.33230	2.71540	-2.15772
C	-1.32280	2.83717	0.00000
H	-1.39496	3.92568	0.00000
H	-1.84795	2.46811	0.88227
H	-1.84795	2.46811	-0.88227

12356-pentasila-ccl3-ax

Si	-1.05511	0.80907	-1.90824
Si	0.60070	2.44110	-1.60119
C	0.30311	3.38150	0.00000
Si	0.60070	2.44110	1.60119

Si	-1.05511	0.80907	1.90824
Si	-1.27807	-0.53301	0.00000
H	-0.72073	3.76404	0.00000
H	0.54263	3.37349	-2.74994
H	1.94272	1.82210	-1.58012
H	-0.81930	-0.01420	-3.11347
H	-2.35559	1.50676	-2.06000
H	0.54263	3.37349	2.74994
H	1.94272	1.82210	1.58012
H	-2.35559	1.50676	2.06000
H	-0.81930	-0.01420	3.11347
H	0.96180	4.25377	0.00000
H	-2.51257	-1.34589	0.00000
C	0.14910	-1.83265	0.00000
Cl	1.71374	-0.97310	0.00000
Cl	0.05005	-2.86059	1.44784
Cl	0.05005	-2.86059	-1.44784

12356-pentasila-ccl3-eq

Si	-0.28653	-0.82538	1.88302
Si	0.28128	-3.08316	1.59414
C	-0.45756	-3.75417	0.00000
Si	0.28128	-3.08316	-1.59414
Si	-0.28653	-0.82538	-1.88302
Si	0.54141	0.28129	0.00000
H	-1.53480	-3.57200	0.00000
H	-0.19262	-3.86892	2.75486
H	1.75664	-3.19640	1.53365
H	0.27027	-0.27659	3.13753
H	-1.76071	-0.68867	1.89582
H	-0.19262	-3.86892	-2.75486
H	1.75664	-3.19640	-1.53365
H	-1.76071	-0.68867	-1.89582
H	0.27027	-0.27659	-3.13753
H	-0.32169	-4.83865	0.00000
C	0.03534	2.14298	0.00000
Cl	0.68592	2.94354	-1.45038

Cl	-1.73917	2.28617	0.00000
Cl	0.68592	2.94354	1.45038
H	2.02034	0.28963	0.00000

12356-pentasila-cf3-ax

Si	-1.05057	0.31969	-1.90148
Si	0.68419	1.86945	-1.60088
C	0.43450	2.82513	0.00000
Si	0.68419	1.86945	1.60088
Si	-1.05057	0.31969	1.90148
Si	-1.17126	-1.03649	0.00000
H	-0.56583	3.26501	0.00000
H	0.68622	2.79994	-2.75199
H	1.98201	1.16351	-1.56989
H	-0.87701	-0.49548	-3.12275
H	-2.33707	1.05003	-1.99282
H	0.68622	2.79994	2.75199
H	1.98201	1.16351	1.56989
H	-2.33707	1.05003	1.99282
H	-0.87701	-0.49548	3.12275
H	1.14170	3.65871	0.00000
H	-2.27488	-2.01862	0.00000
C	0.45134	-2.09957	0.00000
F	1.54873	-1.30887	0.00000
F	0.55912	-2.89636	1.07823
F	0.55912	-2.89636	-1.07823

12356-pentasila-cf3-eq

Si	-0.26139	-0.25067	1.88582
Si	0.21924	-2.52697	1.59520
C	-0.54798	-3.16331	0.00000
Si	0.21924	-2.52697	-1.59520
Si	-0.26139	-0.25067	-1.88582
Si	0.57650	0.84307	0.00000
H	-1.61628	-2.93448	0.00000
H	-0.28227	-3.29673	2.75469
H	1.68927	-2.69363	1.53138
H	0.31953	0.28706	3.13400

H	-1.72882	-0.05274	1.90134
H	-0.28227	-3.29673	-2.75469
H	1.68927	-2.69363	-1.53138
H	-1.72882	-0.05274	-1.90134
H	0.31953	0.28706	-3.13400
H	-0.46023	-4.25275	0.00000
C	0.00637	2.69685	0.00000
F	0.44430	3.37195	-1.07880
F	-1.33671	2.80430	0.00000
F	0.44430	3.37195	1.07880
H	2.05395	0.88812	0.00000

12356-pentasila-cl-ax

Si	-0.92860	-0.23993	-1.87783
Si	0.53763	1.56758	-1.59769
C	0.14958	2.48240	0.00000
Si	0.53763	1.56758	1.59769
Si	-0.92860	-0.23993	1.87783
Si	-0.66940	-1.60564	0.00000
H	-0.90492	2.76858	0.00000
H	0.41717	2.48380	-2.75385
H	1.92535	1.05720	-1.55288
H	-0.66311	-0.98317	-3.12866
H	-2.32677	0.25452	-1.89860
H	0.41717	2.48380	2.75385
H	1.92535	1.05720	1.55288
H	-2.32677	0.25452	1.89860
H	-0.66311	-0.98317	3.12866
H	0.72657	3.41072	0.00000
Cl	1.30837	-2.26244	0.00000
H	-1.52412	-2.80967	0.00000

12356-pentasila-cl-eq

Si	0.34443	-0.25376	1.86890
Si	-0.24251	2.00132	1.59216
C	0.48705	2.68654	0.00000
Si	-0.24251	2.00132	-1.59216
Si	0.34443	-0.25376	-1.86890

Si	-0.47429	-1.38844	0.00000
H	0.33426	3.76869	0.00000
H	-1.71884	2.10393	1.53444
H	0.22617	2.78527	2.75638
H	1.82055	-0.37796	1.87400
H	-0.19115	-0.80505	3.13238
H	-1.71884	2.10393	-1.53444
H	0.22617	2.78527	-2.75638
H	-0.19115	-0.80505	-3.13238
H	1.82055	-0.37796	-1.87400
H	1.56684	2.52033	0.00000
Cl	0.08621	-3.38732	0.00000
H	-1.95232	-1.35024	0.00000

12356-pentasila-f-ax

Si	-0.65913	-0.60491	-1.86242
Si	0.37022	1.48470	-1.59703
C	-0.20413	2.29726	0.00000
Si	0.37022	1.48470	1.59703
Si	-0.65913	-0.60491	1.86242
Si	-0.08213	-1.90089	0.00000
H	-1.29545	2.35052	0.00000
H	0.05603	2.35187	-2.75462
H	1.83705	1.29246	-1.55053
H	-0.29306	-1.24369	-3.14586
H	-2.13124	-0.42395	-1.82345
H	0.05603	2.35187	2.75462
H	1.83705	1.29246	1.55053
H	-2.13124	-0.42395	1.82345
H	-0.29306	-1.24369	3.14586
H	0.16105	3.32743	0.00000
F	1.51495	-2.10958	0.00000
H	-0.69532	-3.24578	0.00000

12356-pentasila-f-eq

Si	0.38585	-0.57214	1.86726
Si	-0.26479	1.66621	1.59021
C	0.44324	2.37706	0.00000

Si	-0.26479	1.66621	-1.59021
Si	0.38585	-0.57214	-1.86726
Si	-0.42422	-1.72112	0.00000
H	0.25515	3.45361	0.00000
H	-1.74350	1.72951	1.53363
H	0.18210	2.45929	2.75682
H	1.86607	-0.64263	1.87679
H	-0.12702	-1.11770	3.14340
H	-1.74350	1.72951	-1.53363
H	0.18210	2.45929	-2.75682
H	-0.12702	-1.11770	-3.14340
H	1.86607	-0.64263	-1.87679
H	1.52773	2.24533	0.00000
F	-0.00102	-3.27057	0.00000
H	-1.90334	-1.66802	0.00000

12356-pentasila-ch3-ax

Si	-0.72277	-0.57737	-1.84706
Si	0.35248	1.48964	-1.59156
C	-0.19413	2.33165	0.00000
Si	0.35248	1.48964	1.59156
Si	-0.72277	-0.57737	1.84706
Si	-0.14570	-1.89232	0.00000
H	-1.28342	2.41753	0.00000
H	0.08025	2.36402	-2.75508
H	1.81635	1.26008	-1.53629
H	-0.32885	-1.20858	-3.12872
H	-2.18839	-0.35250	-1.87168
H	0.08025	2.36402	2.75508
H	1.81635	1.26008	1.53629
H	-2.18839	-0.35250	1.87168
H	-0.32885	-1.20858	3.12872
H	0.20341	3.34948	0.00000
H	-0.87294	-3.18361	0.00000
C	1.71518	-2.19077	0.00000
H	2.01822	-2.75191	0.88316
H	2.01822	-2.75191	-0.88316

H	2.25332	-1.24246	0.00000
12356-pentasila-ch3-eq			
Si	0.34177	-0.53304	1.84427
Si	-0.25173	1.71978	1.59181
C	0.46493	2.42128	0.00000
Si	-0.25173	1.71978	-1.59181
Si	0.34177	-0.53304	-1.84427
Si	-0.46778	-1.72327	0.00000
H	1.54680	2.26822	0.00000
H	0.21954	2.50563	2.75504
H	-1.72901	1.82233	1.54586
H	-0.16657	-1.06796	3.12933
H	1.82263	-0.63297	1.86443
H	0.21954	2.50563	-2.75504
H	-1.72901	1.82233	-1.54586
H	1.82263	-0.63297	-1.86443
H	-0.16657	-1.06796	-3.12933
H	0.29848	3.50129	0.00000
C	0.02599	-3.53950	0.00000
H	-0.36295	-4.04403	0.88356
H	-0.36295	-4.04403	-0.88356
H	1.11082	-3.63690	0.00000
H	-1.94634	-1.59473	0.00000
12356-pentasila-sih3-ax			
Si	0.96882	0.16591	-1.86265
Si	-0.54926	-1.59915	-1.59175
C	-0.20067	-2.53889	0.00000
Si	-0.54926	-1.59915	1.59175
Si	0.96882	0.16591	1.86265
Si	0.77872	1.56700	0.00000
H	0.84260	-2.86366	0.00000
H	-0.47032	-2.51182	-2.75488
H	-1.92250	-1.04586	-1.54077
H	0.69326	0.90044	-3.11874
H	2.34294	-0.38552	-1.93877
H	-0.47032	-2.51182	2.75488

H	-1.92250	-1.04586	1.54077
H	2.34294	-0.38552	1.93877
H	0.69326	0.90044	3.11874
H	-0.81303	-3.44393	0.00000
Si	-1.36170	2.50643	0.00000
H	-1.57224	3.33925	1.20304
H	-1.57224	3.33925	-1.20304
H	-2.35980	1.41477	0.00000
H	1.80578	2.63582	0.00000

12356-pentasila-sih3-eq

Si	0.28901	-0.19883	1.85073
Si	-0.22787	2.07141	1.59407
C	0.51567	2.73922	0.00000
Si	-0.22787	2.07141	-1.59407
Si	0.28901	-0.19883	-1.85073
Si	-0.54786	-1.35895	0.00000
H	1.59059	2.54316	0.00000
H	0.26793	2.84631	2.75432
H	-1.70103	2.21768	1.54443
H	-0.24612	-0.73333	3.12354
H	1.76331	-0.36192	1.86511
H	0.26793	2.84631	-2.75432
H	-1.70103	2.21768	-1.54443
H	1.76331	-0.36192	-1.86511
H	-0.24612	-0.73333	-3.12354
H	0.39366	3.82520	0.00000
H	-2.02706	-1.24174	0.00000
Si	0.09776	-3.60321	0.00000
H	-0.40762	-4.29832	1.20266
H	-0.40762	-4.29832	-1.20266
H	1.57486	-3.66564	0.00000

12356-pentasila-tbu-ax

C	0.21714	3.02835	0.00000
Si	0.57060	2.08681	-1.58966
Si	-0.95948	0.33197	-1.86777
Si	-0.98705	-1.09009	0.00000

Si	-0.95948	0.33197	1.86777
Si	0.57060	2.08681	1.58966
H	-0.67168	-0.40420	-3.12225
H	1.95269	1.55509	-1.53997
H	0.48614	2.99984	-2.75295
H	-0.82839	3.34618	0.00000
H	0.82405	3.93696	0.00000
H	-2.24482	-1.88134	0.00000
H	-0.67168	-0.40420	3.12225
H	-2.30476	0.94347	2.00376
H	1.95269	1.55509	1.53997
H	0.48614	2.99984	2.75295
H	-2.30476	0.94347	-2.00376
C	0.48027	-2.30568	0.00000
C	1.80521	-1.54140	0.00000
H	1.90973	-0.90756	-0.88288
H	2.64238	-2.24544	0.00000
H	1.90973	-0.90756	0.88288
C	0.39913	-3.18901	1.24854
H	1.21744	-3.91509	1.24223
H	-0.53871	-3.74540	1.28680
H	0.48234	-2.60353	2.16519
C	0.39913	-3.18901	-1.24854
H	-0.53871	-3.74540	-1.28680
H	1.21744	-3.91509	-1.24223
H	0.48234	-2.60353	-2.16519
12356-pentasila-tbu-eq			
Si	-0.32835	-0.29094	-1.84862
Si	0.26137	-2.54436	-1.59253
C	-0.45694	-3.24244	0.00000
Si	0.26137	-2.54436	1.59253
Si	-0.32835	-0.29094	1.84862
Si	0.49106	0.89008	0.00000
H	0.18274	0.23939	3.13483
H	1.73846	-2.64916	1.54633
H	-0.21114	-3.33185	2.75427

H	-1.53845	-3.08675	0.00000
H	-0.29350	-4.32295	0.00000
H	0.18274	0.23939	-3.13483
H	-1.80936	-0.19207	-1.87420
H	1.73846	-2.64916	-1.54633
H	-0.21114	-3.33185	-2.75427
H	-1.80936	-0.19207	1.87420
H	1.97173	0.74870	0.00000
C	0.04497	2.74164	0.00000
C	0.63629	3.39854	1.25026
H	0.22260	2.97076	2.16505
H	0.40812	4.46853	1.25094
H	1.72135	3.28957	1.28705
C	0.63629	3.39854	-1.25026
H	1.72135	3.28957	-1.28705
H	0.40812	4.46853	-1.25094
H	0.22260	2.97076	-2.16505
C	-1.47529	2.91395	0.00000
H	-1.72840	3.97800	0.00000
H	-1.93323	2.46402	0.88263
H	-1.93323	2.46402	-0.88263

23456-pentasila-ccl3-ax

Si	-1.36201	0.25586	-1.57548
Si	0.28622	1.87895	-1.95105
Si	0.54808	3.15330	0.00000
Si	0.28622	1.87895	1.95105
Si	-1.36201	0.25586	1.57548
C	-1.09962	-0.80220	0.00000
H	-0.54846	4.15027	0.00000
H	-0.21922	2.76088	-3.02945
H	1.55594	1.27588	-2.40249
H	-1.55018	-0.62181	-2.74714
H	-2.63548	0.96750	-1.32866
H	-0.21922	2.76088	3.02945
H	1.55594	1.27588	2.40249
H	-2.63548	0.96750	1.32866

H	-1.55018	-0.62181	2.74714
H	1.83444	3.88480	0.00000
H	-1.94946	-1.49457	0.00000
C	0.13790	-1.67519	0.00000
Cl	1.63413	-0.68952	0.00000
Cl	0.19501	-2.73771	1.43836
Cl	0.19501	-2.73771	-1.43836

23456-pentasila-ccl3-eq

Si	-0.59829	-0.33640	1.55489
Si	0.42857	-2.42173	1.85542
Si	-0.08826	-3.74513	0.00000
Si	0.42857	-2.42173	-1.85542
Si	-0.59829	-0.33640	-1.55489
C	0.18319	0.47319	0.00000
H	-1.54541	-4.00826	0.00000
H	-0.02021	-3.03128	3.12641
H	1.89452	-2.21434	1.91829
H	-0.41975	0.51543	2.74439
H	-2.04470	-0.52531	1.31856
H	-0.02021	-3.03128	-3.12641
H	1.89452	-2.21434	-1.91829
H	-2.04470	-0.52531	-1.31856
H	-0.41975	0.51543	-2.74439
H	0.63399	-5.03563	0.00000
C	0.13651	1.99186	0.00000
Cl	0.96581	2.68385	-1.42960
Cl	-1.55534	2.55976	0.00000
Cl	0.96581	2.68385	1.42960
H	1.24435	0.20556	0.00000

23456-pentasila-cf3-ax

Si	-1.23152	-0.29576	-1.59307
Si	0.38715	1.36546	-1.92418
Si	0.44051	2.69873	0.00000
Si	0.38715	1.36546	1.92418
Si	-1.23152	-0.29576	1.59307
C	-0.90167	-1.29314	0.00000

H	-0.80397	3.50393	0.00000
H	-0.01407	2.18224	-3.09231
H	1.70266	0.75400	-2.20241
H	-1.31804	-1.22500	-2.73836
H	-2.55223	0.34231	-1.40401
H	-0.01407	2.18224	3.09231
H	1.70266	0.75400	2.20241
H	-2.55223	0.34231	1.40401
H	-1.31804	-1.22500	2.73836
H	1.59428	3.62462	0.00000
H	-1.62242	-2.11600	0.00000
C	0.45641	-1.92859	0.00000
F	1.44145	-1.00423	0.00000
F	0.66896	-2.70401	1.07512
F	0.66896	-2.70401	-1.07512

23456-pentasila-cf3-eq

Si	-0.45538	0.25997	1.58162
Si	0.40645	-1.90195	1.84677
Si	-0.25627	-3.17025	0.00000
Si	0.40645	-1.90195	-1.84677
Si	-0.45538	0.25997	-1.58162
C	0.28479	1.03244	0.00000
H	-1.73278	-3.27861	0.00000
H	-0.05598	-2.47342	3.13026
H	1.88557	-1.81381	1.87016
H	-0.12574	1.10177	2.74855
H	-1.92458	0.19957	1.42999
H	-0.05598	-2.47342	-3.13026
H	1.88557	-1.81381	-1.87016
H	-1.92458	0.19957	-1.42999
H	-0.12574	1.10177	-2.74855
H	0.32800	-4.52864	0.00000
C	0.15553	2.53228	0.00000
F	0.73073	3.10134	-1.07206
F	-1.13150	2.92070	0.00000
F	0.73073	3.10134	1.07206

H	1.35829	0.82281	0.00000
23456-pentasila-cl-ax			
Si	-0.93058	-0.82486	-1.62259
Si	0.39376	1.08779	-1.88776
Si	0.07184	2.42923	0.00000
Si	0.39376	1.08779	1.88776
Si	-0.93058	-0.82486	1.62259
C	-0.51496	-1.71160	0.00000
H	-1.34065	2.87772	0.00000
H	-0.02584	1.79342	-3.11975
H	1.81615	0.70769	-2.02011
H	-0.73409	-1.77852	-2.73487
H	-2.36188	-0.44562	-1.56521
H	-0.02584	1.79342	3.11975
H	1.81615	0.70769	2.02011
H	-2.36188	-0.44562	1.56521
H	-0.73409	-1.77852	2.73487
H	0.94591	3.62270	0.00000
Cl	1.25362	-2.08829	0.00000
H	-1.02410	-2.67634	0.00000
23456-pentasila-cl-eq			
Si	0.27086	-0.77259	1.60727
Si	-0.37578	1.47073	1.84494
Si	0.43291	2.65429	0.00000
Si	-0.37578	1.47073	-1.84494
Si	0.27086	-0.77259	-1.60727
C	-0.42627	-1.49236	0.00000
H	0.00663	4.07033	0.00000
H	-1.85603	1.54326	1.84794
H	0.12344	2.00346	3.13198
H	1.74467	-0.86577	1.53746
H	-0.21627	-1.58567	2.74002
H	-1.85603	1.54326	-1.84794
H	0.12344	2.00346	-3.13198
H	-0.21627	-1.58567	-2.74002
H	1.74467	-0.86577	-1.53746

H	1.91238	2.59610	0.00000
Cl	-0.06375	-3.26476	0.00000
H	-1.51330	-1.40403	0.00000

23456-pentasila-f-ax

Si	-0.61747	-1.13717	-1.62124
Si	0.36661	0.97152	-1.87823
Si	-0.20515	2.24161	0.00000
Si	0.36661	0.97152	1.87823
Si	-0.61747	-1.13717	1.62124
C	-0.00009	-1.92346	0.00000
H	-1.67448	2.43293	0.00000
H	-0.11554	1.60015	-3.12851
H	1.83558	0.81962	-1.95894
H	-0.29254	-2.03117	-2.75372
H	-2.08946	-1.01462	-1.51973
H	-0.11554	1.60015	3.12851
H	1.83558	0.81962	1.95894
H	-2.08946	-1.01462	1.51973
H	-0.29254	-2.03117	2.75372
H	0.44447	3.57071	0.00000
F	1.41212	-1.87307	0.00000
H	-0.27660	-2.98219	0.00000

23456-pentasila-f-eq

Si	0.30258	-1.07632	1.61284
Si	-0.37759	1.15510	1.85032
Si	0.40740	2.34709	0.00000
Si	-0.37759	1.15510	-1.85032
Si	0.30258	-1.07632	-1.61284
C	-0.40672	-1.79419	0.00000
H	-0.04473	3.75510	0.00000
H	-1.85857	1.20517	1.85938
H	0.11996	1.70078	3.13217
H	1.77871	-1.14384	1.54810
H	-0.17106	-1.90473	2.74115
H	-1.85857	1.20517	-1.85938
H	0.11996	1.70078	-3.13217

H	-0.17106	-1.90473	-2.74115
H	1.77871	-1.14384	-1.54810
H	1.88771	2.31606	0.00000
F	-0.16259	-3.18284	0.00000
H	-1.49349	-1.66019	0.00000

23456-pentasila-ch3-ax

Si	0.62812	-1.12555	-1.58518
Si	-0.33566	0.99427	-1.86719
Si	0.24219	2.27840	0.00000
Si	-0.33566	0.99427	1.86719
Si	0.62812	-1.12555	1.58518
C	0.01602	-1.94143	0.00000
H	1.71295	2.45962	0.00000
H	0.13238	1.61179	-3.12864
H	-1.81122	0.87092	-1.93556
H	0.28170	-1.99152	-2.73775
H	2.10166	-0.97502	-1.54652
H	0.13238	1.61179	3.12864
H	-1.81122	0.87092	1.93556
H	2.10166	-0.97502	1.54652
H	0.28170	-1.99152	2.73775
H	-0.39674	3.61315	0.00000
H	0.46092	-2.94243	0.00000
C	-1.51819	-2.07154	0.00000
H	-1.87619	-2.60724	0.88057
H	-1.87619	-2.60724	-0.88057
H	-2.00015	-1.09188	0.00000

23456-pentasila-ch3-eq

Si	0.28488	-1.04698	1.57746
Si	-0.37257	1.18693	1.84764
Si	0.40709	2.38672	0.00000
Si	-0.37257	1.18693	-1.84764
Si	0.28488	-1.04698	-1.57746
C	-0.40187	-1.81815	0.00000
H	1.88806	2.35801	0.00000
H	0.13253	1.72778	3.12958

H	-1.85362	1.25297	1.86616
H	-0.16326	-1.85355	2.73803
H	1.76581	-1.11187	1.53201
H	0.13253	1.72778	-3.12958
H	-1.85362	1.25297	-1.86616
H	1.76581	-1.11187	-1.53201
H	-0.16326	-1.85355	-2.73803
H	-0.04019	3.79702	0.00000
C	-0.12746	-3.33576	0.00000
H	-0.55003	-3.81927	0.88166
H	-0.55003	-3.81927	-0.88166
H	0.94562	-3.53590	0.00000
H	-1.48237	-1.64148	0.00000

23456-pentasila-sih3-ax

Si	-0.98770	-0.81265	1.57719
Si	0.32608	1.10233	1.91218
Si	0.14070	2.44074	0.00000
Si	0.32608	1.10233	-1.91218
Si	-0.98770	-0.81265	-1.57719
C	-0.49714	-1.71855	0.00000
H	-1.22869	3.00842	0.00000
H	-0.16533	1.83319	3.10260
H	1.73722	0.72559	2.15191
H	-0.85333	-1.73125	2.73104
H	-2.40516	-0.38930	1.49005
H	-0.16533	1.83319	-3.10260
H	1.73722	0.72559	-2.15191
H	-2.40516	-0.38930	-1.49005
H	-0.85333	-1.73125	-2.73104
H	1.10819	3.56045	0.00000
Si	1.32059	-2.16551	0.00000
H	1.66947	-2.94660	-1.20566
H	1.66947	-2.94660	1.20566
H	2.12169	-0.92180	0.00000
H	-1.06220	-2.65783	0.00000

23456-pentasila-sih3-eq

Si	0.34103	-0.72974	1.57198
Si	-0.37529	1.48392	1.85450
Si	0.36145	2.70185	0.00000
Si	-0.37529	1.48392	-1.85450
Si	0.34103	-0.72974	-1.57198
C	-0.37305	-1.48394	0.00000
H	1.84251	2.71866	0.00000
H	0.11840	2.04368	3.13264
H	-1.85763	1.49778	1.87808
H	-0.04856	-1.54764	2.74451
H	1.81926	-0.75665	1.47601
H	0.11840	2.04368	-3.13264
H	-1.85763	1.49778	-1.87808
H	1.81926	-0.75665	-1.47601
H	-0.04856	-1.54764	-2.74451
H	-0.12864	4.09786	0.00000
H	-1.45306	-1.29927	0.00000
Si	-0.12662	-3.34411	0.00000
H	-0.73365	-3.95183	1.20286
H	-0.73365	-3.95183	-1.20286
H	1.32367	-3.63302	0.00000

23456-pentasila-tbu-ax

Si	-0.31417	2.91350	0.00000
Si	-0.34386	1.57057	-1.91841
Si	1.12180	-0.22705	-1.55310
C	0.80193	-1.27358	0.00000
Si	1.12180	-0.22705	1.55310
Si	-0.34386	1.57057	1.91841
H	1.20239	-1.07091	-2.76680
H	-1.72085	1.12869	-2.23399
H	0.15411	2.34971	-3.07623
H	0.98719	3.62346	0.00000
H	-1.39452	3.92515	0.00000
H	1.67513	-1.94316	0.00000
H	1.20239	-1.07091	2.76680
H	2.45446	0.39721	1.37379

H	-1.72085	1.12869	2.23399
H	0.15411	2.34971	3.07623
H	2.45446	0.39721	-1.37379
C	-0.45816	-2.18924	0.00000
C	-1.75432	-1.37862	0.00000
H	-1.83553	-0.74663	-0.88420
H	-2.61369	-2.05092	0.00000
H	-1.83553	-0.74663	0.88420
C	-0.44851	-3.09049	1.23946
H	-1.26867	-3.80793	1.18875
H	0.48675	-3.64846	1.31099
H	-0.56886	-2.51545	2.15747
C	-0.44851	-3.09049	-1.23946
H	0.48675	-3.64846	-1.31099
H	-1.26867	-3.80793	-1.18875
H	-0.56886	-2.51545	-2.15747

23456-pentasila-tbu-eq

Si	-0.52064	0.19921	-1.53246
Si	0.39956	-1.93674	-1.83551
Si	-0.18606	-3.25537	0.00000
Si	0.39956	-1.93674	1.83551
Si	-0.52064	0.19921	1.53246
C	0.22817	1.04682	0.00000
H	-0.29882	0.96646	2.77714
H	1.87670	-1.81166	1.88261
H	-0.05748	-2.51291	3.12047
H	-1.65414	-3.45170	0.00000
H	0.47203	-4.58051	0.00000
H	-0.29882	0.96646	-2.77714
H	-1.98701	0.06052	-1.36826
H	1.87670	-1.81166	-1.88261
H	-0.05748	-2.51291	-3.12047
H	-1.98701	0.06052	1.36826
H	1.28946	0.76669	0.00000
C	0.16257	2.61065	0.00000
C	0.88066	3.17603	1.23126

H	0.37156	2.92366	2.15834
H	0.92805	4.26385	1.16545
H	1.90322	2.79835	1.28924
C	0.88066	3.17603	-1.23126
H	1.90322	2.79835	-1.28924
H	0.92805	4.26385	-1.16545
H	0.37156	2.92366	-2.15834
C	-1.28931	3.09012	0.00000
H	-1.32702	4.18026	0.00000
H	-1.82682	2.73850	0.88285
H	-1.82682	2.73850	-0.88285

cyclohexasilane-ccl3-ax

Si	1.31937	-0.74810	0.00000
Si	1.27206	0.56608	-1.93933
Si	-0.52854	2.06289	-1.96906
Si	-0.49039	3.33017	0.00000
Si	-0.52854	2.06289	1.96906
Si	1.27206	0.56608	1.93933
H	2.51633	1.37078	1.88596
H	-1.81249	1.35279	2.13610
H	-1.81249	1.35279	-2.13610
H	-1.59544	4.31508	0.00000
H	0.79077	4.07668	0.00000
H	-0.34752	2.97916	3.11861
H	1.31770	-0.29126	3.14303
H	-0.34752	2.97916	-3.11861
H	1.31770	-0.29126	-3.14303
H	2.51633	1.37078	-1.88596
H	2.47181	-1.67455	0.00000
C	-0.21941	-1.91317	0.00000
Cl	-1.70863	-0.92786	0.00000
Cl	-0.20833	-2.94246	-1.44985
Cl	-0.20833	-2.94246	1.44985

cyclohexasilane-ccl3-eq

Si	-0.50135	-0.45974	0.00000
Si	0.36158	0.56883	-1.91582

Si	-0.43296	2.77225	-1.90602
Si	0.38007	3.86075	0.00000
Si	-0.43296	2.77225	1.90602
Si	0.36158	0.56883	1.91582
H	1.83759	0.58133	1.81370
H	-1.91272	2.74305	1.84918
H	-1.91272	2.74305	-1.84918
H	-0.01770	5.28597	0.00000
H	1.85904	3.78296	0.00000
H	-0.02246	3.47938	3.13905
H	-0.04351	-0.15743	3.13762
H	-0.02246	3.47938	-3.13905
H	-0.04351	-0.15743	-3.13762
H	1.83759	0.58133	-1.81370
C	-0.05557	-2.33745	0.00000
Cl	-0.72701	-3.12223	-1.44889
Cl	1.71585	-2.52491	0.00000
Cl	-0.72701	-3.12223	1.44889
H	-1.98003	-0.42180	0.00000

cyclohexasilane-cf3-ax

Si	-1.15936	-1.28144	0.00000
Si	-1.23332	0.02256	-1.94188
Si	0.57195	1.51450	-1.95210
Si	0.49007	2.80544	0.00000
Si	0.57195	1.51450	1.95210
Si	-1.23332	0.02256	1.94188
H	-2.49536	0.79605	1.89356
H	1.84375	0.76940	2.04559
H	1.84375	0.76940	-2.04559
H	1.57524	3.81171	0.00000
H	-0.80688	3.52363	0.00000
H	0.45097	2.40148	3.13126
H	-1.25292	-0.84950	3.13581
H	0.45097	2.40148	-3.13126
H	-1.25292	-0.84950	-3.13581
H	-2.49536	0.79605	-1.89356

H	-2.12446	-2.40034	0.00000
C	0.58877	-2.12217	0.00000
F	1.57023	-1.18853	0.00000
F	0.80488	-2.89514	-1.07862
F	0.80488	-2.89514	1.07862

cyclohexasilane-cf3-eq

Si	0.51457	-1.01898	0.00000
Si	-0.31314	0.00665	-1.93131
Si	0.40639	2.23398	-1.90424
Si	-0.46679	3.27894	0.00000
Si	0.40639	2.23398	1.90424
Si	-0.31314	0.00665	1.93131
H	-1.79075	-0.03646	1.86694
H	1.88534	2.25154	1.82727
H	1.88534	2.25154	-1.82727
H	-0.14671	4.72341	0.00000
H	-1.93919	3.12030	0.00000
H	-0.01146	2.93239	3.13943
H	0.14838	-0.71594	3.13534
H	-0.01146	2.93239	-3.13943
H	0.14838	-0.71594	-3.13534
H	-1.79075	-0.03646	-1.86694
C	-0.04753	-2.87586	0.00000
F	0.39223	-3.54932	-1.07869
F	-1.39071	-2.98681	0.00000
F	0.39223	-3.54932	1.07869
H	1.99240	-1.06343	0.00000

cyclohexasilane-cl-ax

Si	0.45215	-1.82194	0.00000
Si	0.92847	-0.58254	1.92599
Si	-0.45728	1.30320	1.92072
Si	0.00963	2.55737	0.00000
Si	-0.45728	1.30320	-1.92072
Si	0.92847	-0.58254	-1.92599
Cl	-1.60256	-2.17163	0.00000
H	2.34647	-0.15690	-1.86156

H	1.11249	-3.14323	0.00000
H	-1.87039	0.86673	-1.90252
H	-1.87039	0.86673	1.90252
H	-0.75797	3.82269	0.00000
H	1.45428	2.88761	0.00000
H	-0.22382	2.11192	-3.13802
H	0.73182	-1.41485	-3.13293
H	-0.22382	2.11192	3.13802
H	0.73182	-1.41485	3.13293
H	2.34647	-0.15690	1.86156

cyclohexasilane-cl-eq

Si	-0.41861	-1.60796	0.00000
Si	0.38630	-0.54003	1.91756
Si	-0.40839	1.66351	1.90126
Si	0.41361	2.75269	0.00000
Si	-0.40839	1.66351	-1.90126
Si	0.38630	-0.54003	-1.91756
H	1.86518	-0.52796	-1.85608
H	-1.88782	1.63515	-1.83280
H	-1.88782	1.63515	1.83280
H	0.02122	4.17935	0.00000
H	1.89226	2.66879	0.00000
H	-0.00845	2.37022	-3.13808
H	-0.04244	-1.26785	-3.13147
H	-0.00845	2.37022	3.13808
H	-0.04244	-1.26785	3.13147
H	1.86518	-0.52796	1.85608
H	-1.89712	-1.58246	0.00000
Cl	0.15772	-3.60337	0.00000

cyclohexasilane-f-ax

Si	-0.11479	-2.02668	0.00000
Si	-0.73394	-0.81718	1.90940
Si	0.46177	1.19517	1.91305
Si	-0.12674	2.40938	0.00000
Si	0.46177	1.19517	-1.91305
Si	-0.73394	-0.81718	-1.90940

F	1.48934	-2.17402	0.00000
H	-2.18158	-0.52104	-1.79157
H	-0.67822	-3.39370	0.00000
H	1.91002	0.89253	-1.87327
H	1.91002	0.89253	1.87327
H	0.52448	3.73842	0.00000
H	-1.59501	2.60778	0.00000
H	0.17441	1.97322	-3.13867
H	-0.50840	-1.59618	-3.14709
H	0.17441	1.97322	3.13867
H	-0.50840	-1.59618	3.14709
H	-2.18158	-0.52104	1.79157

cyclohexasilane-f-eq

Si	0.39803	-1.88230	0.00000
Si	-0.42060	-0.81320	1.91542
Si	0.40157	1.38097	1.89879
Si	-0.40280	2.48636	0.00000
Si	0.40157	1.38097	-1.89879
Si	-0.42060	-0.81320	-1.91542
H	-1.89971	-0.77212	-1.85998
H	1.88083	1.33700	-1.83245
H	1.88083	1.33700	1.83245
H	0.01465	3.90594	0.00000
H	-1.88271	2.42840	0.00000
H	0.00862	2.08920	-3.13696
H	-0.00628	-1.52740	-3.14325
H	0.00862	2.08920	3.13696
H	-0.00628	-1.52740	3.14325
H	-1.89971	-0.77212	1.85998
H	1.87647	-1.80694	0.00000
F	-0.00074	-3.43886	0.00000

cyclohexasilane-ch3-ax

Si	-0.06983	-2.04193	0.00000
Si	-0.74857	-0.84211	-1.89275
Si	0.38879	1.20413	-1.90692
Si	-0.22010	2.41726	0.00000

Si	0.38879	1.20413	1.90692
Si	-0.74857	-0.84211	1.89275
H	-2.20480	-0.57501	1.83363
H	-0.69632	-3.38548	0.00000
H	1.84758	0.94387	1.85770
H	1.84758	0.94387	-1.85770
H	0.40793	3.75788	0.00000
H	-1.69142	2.59287	0.00000
H	0.10192	1.97538	3.13750
H	-0.46492	-1.60031	3.13385
H	0.10192	1.97538	-3.13750
H	-0.46492	-1.60031	-3.13385
H	-2.20480	-0.57501	-1.83363
C	1.80773	-2.20109	0.00000
H	2.15204	-2.73808	-0.88313
H	2.15204	-2.73808	0.88313
H	2.27473	-1.21594	0.00000

cyclohexasilane-ch3-eq

Si	0.44624	-1.89336	0.00000
Si	-0.37633	-0.78302	-1.89024
Si	0.39364	1.42694	-1.90255
Si	-0.41984	2.51961	0.00000
Si	0.39364	1.42694	1.90255
Si	-0.37633	-0.78302	1.89024
H	-1.85814	-0.76727	1.83537
H	1.87435	1.41962	1.85197
H	1.87435	1.41962	-1.85197
H	-0.03118	3.94808	0.00000
H	-1.89942	2.44030	0.00000
H	-0.02516	2.13053	3.13591
H	0.02588	-1.48609	3.13139
H	-0.02516	2.13053	-3.13591
H	0.02588	-1.48609	-3.13139
H	-1.85814	-0.76727	-1.83537
C	-0.01575	-3.71871	0.00000
H	0.38204	-4.21603	0.88373

H	0.38204	-4.21603	-0.88373
H	-1.09865	-3.83636	0.00000
H	1.92285	-1.74349	0.00000

cyclohexasilane-sih3-ax

Si	-0.00006	-1.77214	-0.69853
Si	-1.90283	-0.46304	-1.07428
Si	-1.92421	1.28714	0.47995
Si	0.00011	2.58689	0.18675
Si	1.92449	1.28716	0.47966
Si	1.90286	-0.46326	-1.07430
H	1.86185	0.10765	-2.44060
H	1.93578	0.72041	1.84788
H	-1.93517	0.72016	1.84808
H	0.00019	3.74401	1.10988
H	-0.00001	3.10208	-1.20282
H	3.13709	2.11964	0.31215
H	3.12547	-1.28885	-0.94847
H	-3.13685	2.11963	0.31287
H	-3.12552	-1.28854	-0.94854
H	-1.86176	0.10805	-2.44049
Si	-0.00028	-2.44834	1.53940
H	-1.20474	-3.24737	1.84880
H	1.20337	-3.24862	1.84873
H	0.00035	-1.24420	2.39815
H	-0.00013	-2.95893	-1.58716

cyclohexasilane-sih3-eq

Si	0.00008	-1.53371	0.52433
Si	-1.89454	-0.45433	-0.32473
Si	-1.90554	1.77449	0.38646
Si	-0.00009	2.83641	-0.46142
Si	1.90558	1.77455	0.38604
Si	1.89449	-0.45427	-0.32515
H	1.82094	-0.49072	-1.80485
H	1.85147	1.79952	1.86615
H	-1.85111	1.79947	1.86656
H	-0.00008	4.27667	-0.11983

H	-0.00025	2.70765	-1.93736
H	3.13758	2.47087	-0.04845
H	3.12694	-1.16001	0.09381
H	-3.13766	2.47077	-0.04776
H	-3.12688	-1.16011	0.09450
H	-1.82132	-0.49078	-1.80445
H	0.00025	-1.39952	2.00217
Si	0.00005	-3.79090	-0.07922
H	1.20362	-4.47370	0.44014
H	-1.20331	-4.47377	0.44056
H	-0.00021	-3.88270	-1.55477

cyclohexasilane-tbu-ax

Si	-0.45344	3.08687	0.00000
Si	-0.66733	1.75735	-1.91322
Si	1.04746	0.16123	-1.90940
Si	1.04746	0.16123	1.90940
Si	-0.66733	1.75735	1.91322
H	0.99274	-0.65792	-3.14378
H	-1.99720	1.10537	-1.90870
H	-0.57498	2.59219	-3.13297
H	0.90225	3.68569	0.00000
H	-1.44601	4.18530	0.00000
H	0.99274	-0.65792	3.14378
H	2.32423	0.91559	1.92588
H	-1.99720	1.10537	1.90870
H	-0.57498	2.59219	3.13297
H	2.32423	0.91559	-1.92588
C	-0.37475	-2.46799	0.00000
C	-1.72615	-1.75216	0.00000
H	-1.85300	-1.12357	-0.88326
H	-2.53724	-2.48605	0.00000
H	-1.85300	-1.12357	0.88326
C	-0.26246	-3.34711	1.24919
H	-1.05252	-4.10372	1.24167
H	0.69592	-3.86697	1.29097
H	-0.37074	-2.76462	2.16538

C	-0.26246	-3.34711	-1.24919
H	0.69592	-3.86697	-1.29097
H	-1.05252	-4.10372	-1.24167
H	-0.37074	-2.76462	-2.16538
Si	1.05203	-1.20608	0.00000
H	2.33127	-1.96368	0.00000

cyclohexasilane-tbu-eq

Si	0.38032	-3.34430	0.00000
Si	-0.40884	-2.23561	1.90331
Si	0.39067	-0.03596	1.88333
Si	-0.45330	1.07688	0.00000
Si	0.39067	-0.03596	-1.88333
Si	-0.40884	-2.23561	-1.90331
H	0.02103	0.66148	3.13788
H	-1.88956	-2.20816	1.86130
H	0.00717	-2.94244	3.13592
H	1.86123	-3.29661	0.00000
H	-0.03862	-4.76425	0.00000
H	0.02103	0.66148	-3.13788
H	1.87127	-0.07479	-1.80568
H	-1.88956	-2.20816	-1.86130
H	0.00717	-2.94244	-3.13592
H	1.87127	-0.07479	1.80568
H	-1.93129	0.91088	0.00000
C	-0.04073	2.93768	0.00000
C	-0.64289	3.58717	1.24908
H	-0.22008	3.17253	2.16527
H	-0.43583	4.66137	1.24401
H	-1.72563	3.45752	1.28734
C	-0.64289	3.58717	-1.24908
H	-1.72563	3.45752	-1.28734
H	-0.43583	4.66137	-1.24401
H	-0.22008	3.17253	-2.16527
C	1.47691	3.13345	0.00000
H	1.71408	4.20110	0.00000
H	1.94231	2.69081	0.88269

H	1.94231	2.69081	-0.88269
---	---------	---------	----------