Supporting Information

Probing the Tautomerization of Disilenes, Disilabenzenes with Their Isomeric Silylenes: Significant Substituent, Aromaticity and Base Effects

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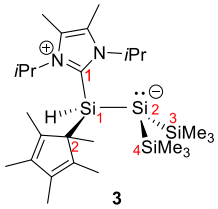
Table S1. Comparison of bond lengths (Å), bond angles (deg), and relative deviations (RD) of compound **3**. Compound **3** was optimized with B3LYP functional, including the Grimme D3 dispersion correction, 6-31+G(d,p) basis set was used to describe all atoms.



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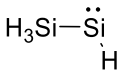
	C1-Si1	C2-Si1	Si1-Si2	Si2-Si3	Si2-Si4	C1-Si1 -Si2	C2-Si1 -Si2	C1-Si1 -C2	Si1-Si2 -Si3	Si1-Si2 -Si4	Si3-Si2 -Si4	RD(%)[a]
exp.	1.945	1.947	2.357	2.361	2.357	110.25	120.54	106.28	94.97	101.61	99.57	0.00
B3LYP-D3	1.973	1.980	2.352	2.395	2.388	109.63	121.79	104.93	93.82	99.49	97.62	1.29

[a] RD = $\Sigma[(|BL_{func.} - BL_{exp.}|)/BL_{exp.}]/n$.

Table S2. Comparison of the relative single point energy between the singlet and triplet states of silylsilyene ($\Delta E_{ST} = \Delta E_T - \Delta E_S$) with different density functionals, 6-311++G(2d,2p) basis set was used to describe all atoms. The structures of silylsilyene in singlet and triplet states were optimized with B3LYP-D3/6-31+G(d,p).



	B3LYP-D3	B3PW91-D3	**M06-2X-D3**	M06-L-D3	M06-D3	PBE0-D3	PBE-D3	TPSS-D3	**CCSD(T)**
ΔE_{ST}	14.1	10.0	**12.3**	11.7	16.8	9.1	10.8	8.9	**12.9**

Table S3. The NICS(1)$_{zz}$ (ppm) and ΔBL (Å) of species **B** and **B'**, relative Gibbs free energies and relative electronic energies (kcal mol^{-1}) of the reactions (Fig. 3b).

Species	**NICS(1)$_{zz}$**	**ΔBL**	**Species**	**NICS(1)$_{zz}$**	**ΔBL**	**ΔG**	**ΔE**
B1(H)	-23.1	0.025	**B'1(H)**	4.9	0.113	16.9	17.7
B2(F)	-21.5	0.031	**B'2(F)**	9.9	0.115	12.0	12.8
B3(Cl)	-21.3	0.029	**B'3(Cl)**	7.9	0.116	12.7	13.6
B4(Me)	-22.5	0.024	**B'4(Me)**	5.2	0.111	18.0	18.3
B5(CF_3)	-22.2	0.029	**B'5(CF_3)**	6.6	0.116	11.4	11.9
B6(CCl_3)	-21.3	0.030	**B'6(CCl_3)**	7.0	0.116	9.8	9.9
B7(SiH_3)	-22.0	0.028	**B'7(SiH_3)**	1.0	0.100	17.0	17.4
B8(SiF_3)	-21.9	0.031	**B'8(SiF_3)**	2.3	0.106	15.4	15.6
B9($SiCl_3$)	-21.4	0.032	**B'9($SiCl_3$)**	1.8	0.107	13.4	13.9
B10(OH)	-20.4	0.033	**B'10(OH)**	8.5	0.112	14.7	15.7
B11(NH_2)	-19.1	0.034	**B'11(NH_2)**	7.0	0.110	16.9	17.9
B12(OMe)	-20.6	0.034	**B'12(OMe)**	8.9	0.113	15.2	15.9
B13($SiMe_3$)	-22.0	0.026	**B'13($SiMe_3$)**	-4.0	0.090	16.9	16.7

Table S4. Energies of species **A** and **A'**. The Gibbs free energies (G) were acquired by employing following formula G = E + G_{ZPE}, where G_{ZPE} is Gibbs free energy correction obtained from B3LYP-D3/6-31+G(d,p) method and electronic energy E was taken from single-point calculations at M06-2X-D3/6-311++G(2d,2p) level. All the calculations were performed by the Gaussian 09 software at 298K.

Species	G_{ZPE}	E	G	Species	G_{ZPE}	E	G
A1(H)	0.006254	-581.276802	-581.270548	**A'1(H)**	0.003875	-581.270845	-581.266970
A2(F)	-0.001354	-680.582738	-680.584092	**A'2(F)**	-0.003281	-680.592283	-680.595564
A3(Cl)	-0.003276	-1040.932056	-1040.935332	**A'3(Cl)**	-0.004665	-1040.943614	-1040.948279
A4(Me)	0.031922	-620.596902	-620.564980	**A'4(Me)**	0.029979	-620.591511	-620.561532
A5(CF3)	0.004750	-918.327933	-918.323183	**A'5(CF3)**	0.003691	-918.327015	-918.323324
A6(CCl3)	-0.002602	-1999.375745	-1999.378347	**A'6(CCl3)**	-0.002715	-1999.383672	-1999.386387
A7(SiH3)	0.018937	-871.962732	-871.943795	**A'7(SiH3)**	0.018354	-871.954443	-871.936089
A8(SiF3)	-0.000844	-1169.921811	-1169.922655	**A'8(SiF3)**	-0.001288	-1169.913631	-1169.914919
A9(SiCl3)	-0.006902	-2250.940588	-2250.947490	**A'9(SiCl3)**	-0.007217	-2250.937172	-2250.944389
A10(OH)	0.009694	-656.551802	-656.542108	**A'10(OH)**	0.008718	-656.565013	-656.556295
A11(NH2)	0.021872	-636.671458	-636.649586	**A'11(NH2)**	0.022785	-636.688852	-636.666067
A12(OMe)	0.034969	-695.841356	-695.806387	**A'12(OMe)**	0.033989	-695.852804	-695.818815
A13(SiMe3)	0.097601	-989.928864	-989.831263	**A'13(SiMe3)**	0.098174	-989.916824	-989.818650

Table S5. Energies of species **B** and **B'**. The Gibbs free energies (G) were acquired by employing following formula G = E + G_{ZPE}, where G_{ZPE} is Gibbs free energy correction obtained from B3LYP-D3/6-31+G(d,p) method and electronic energy E was taken from single-point calculations at M06-2X-D3/6-311++G(2d,2p) level. All the calculations were performed by the Gaussian 09 software at 298K.

Species	G_{ZPE}	E	G	Species	G_{ZPE}	E	G
B1(H)	0.052568	-734.902169	-734.849601	**B'1(H)**	0.051305	-734.873971	-734.822666
B2(F)	0.046056	-834.206635	-834.160579	**B'2(F)**	0.044799	-834.186270	-834.141471
B3(Cl)	0.044008	-1194.556237	-1194.512229	**B'3(Cl)**	0.042547	-1194.534487	-1194.491940
B4(Me)	0.078101	-774.223292	-774.145191	**B'4(Me)**	0.077621	-774.194161	-774.116540
B5(CF3)	0.051454	-1071.950971	-1071.899517	**B'5(CF3)**	0.050680	-1071.931993	-1071.881313
B6(CCl3)	0.044192	-2152.998992	-2152.954800	**B'6(CCl3)**	0.043942	-2152.983164	-2152.939222
B7(SiH3)	0.065396	-1025.586682	-1025.521286	**B'7(SiH3)**	0.064778	-1025.558976	-1025.494198
B8(SiF3)	0.045291	-1323.544357	-1323.499066	**B'8(SiF3)**	0.044874	-1323.519462	-1323.474588
B9(SiCl3)	0.039729	-2404.562874	-2404.523145	**B'9(SiCl3)**	0.038961	-2404.540796	-2404.501835
B10(OH)	0.056901	-810.175193	-810.118292	**B'10(OH)**	0.055354	-810.150218	-810.094864
B11(NH2)	0.068228	-790.289310	-790.221082	**B'11(NH2)**	0.066643	-790.260815	-790.194172
B12(OMe)	0.081944	-849.461911	-849.379967	**B'12(OMe)**	0.080874	-849.436618	-849.355744
B13(SiMe3)	0.145032	-1143.553025	-1143.407993	**B'13(SiMe3)**	0.145237	-1143.526358	-1143.381121

Table S6. Energies of species **C** and **C'**. The Gibbs free energies (G) were acquired by employing following formula G = E + G_{ZPE}, where G_{ZPE} is Gibbs free energy correction obtained from B3LYP-D3/6-31+G(d,p) method and electronic energy E was taken from single-point calculations at M06-2X-D3/6-311++G(2d,2p) level. All the calculations were performed by the Gaussian 09 software at 298K.

Species	G_{ZPE}	E	G	Species	G_{ZPE}	E	G
B1(H)	0.052568	-734.902169	-734.849601	**B'1(H)**	0.051305	-734.873971	-734.822666
C2(F)	0.039160	-933.509570	-933.470410	**C'2(F)**	0.038271	-933.508752	-933.470481
C3(Cl)	0.035234	-1654.209412	-1654.174178	**C'3(Cl)**	0.034052	-1654.197665	-1654.163613
C4(Me)	0.102972	-813.543615	-813.440643	**C'4(Me)**	0.104041	-813.515320	-813.411279
C5(CF3)	0.050940	-1408.998047	-1408.947107	**C'5(CF3)**	0.049118	-1408.986563	-1408.937445
C6(CCl3)	0.036616	-3571.095518	-3571.058902	**C'6(CCl3)**	0.036083	-3571.089679	-3571.053596
C7(SiH3)	0.076973	-1316.271055	-1316.194082	**C'7(SiH3)**	0.077179	-1316.242707	-1316.165528
C8(SiF3)	0.039040	-1912.184729	-1912.145689	**C'8(SiF3)**	0.037159	-1912.161939	-1912.124780
C9(SiCl3)	0.026074	-4074.224012	-4074.197938	**C'9(SiCl3)**	0.025874	-4074.204920	-4074.179046
C10(OH)	0.060818	-885.446352	-885.385534	**C'10(OH)**	0.058467	-885.436131	-885.377664
C11(NH2)	0.083153	-845.674629	-845.591476	**C'11(NH3)**	0.081898	-845.656093	-845.574195
C12(OMe)	0.111089	-964.019080	-963.907991	**C'12(OMe)**	0.110472	-964.007784	-963.897312
C13(SiMe3)	0.237088	-1552.203540	-1551.966452	**C'13(SiMe3)**	0.239182	-1552.176126	-1551.936944

Table S7. Energies of species **D** and **D'**. The Gibbs free energies (G) were acquired by employing following formula G = E + G_{ZPE}, where G_{ZPE} is Gibbs free energy correction obtained from B3LYP-D3/6-31+G(d,p) method and electronic energy E was taken from single-point calculations at M06-2X-D3/6-311++G(2d,2p) level. All the calculations were performed by the Gaussian 09 software at 298K.

Species	G_{ZPE}	E	G	Species	G_{ZPE}	E	G
D1(H)	0.171249	-1039.702103	-1039.530854	**D'1(H)**	0.171660	-1039.713402	-1039.541742
D2(F)	0.157910	-1238.333522	-1238.175612	**D'2(F)**	0.159825	-1238.363586	-1238.203761
D3(Cl)	0.155923	-1959.034773	-1958.878850	**D'3(Cl)**	0.155704	-1959.052517	-1958.896813
D4(Me)	0.224445	-1118.332960	-1118.108515	**D'4(Me)**	0.224112	-1118.356323	-1118.132211
D5(CF3)	0.173472	-1713.833440	-1713.659968	**D'5(CF3)**	0.172799	-1713.847113	-1713.674314
D6(CCl3)	0.160679	-3875.930687	-3875.770008	**D'6(CCl3)**	0.159618	-3875.943845	-3875.784227
D7(SiH3)	0.198406	-1621.071204	-1620.872798	**D'7(SiH3)**	0.198817	-1621.081576	-1620.882759
D8(SiF3)	0.161718	-2217.012214	-2216.850496	**D'8(SiF3)**	0.160765	-2217.016865	-2216.856100
D9(SiCl3)	0.152410	-4379.057211	-4378.904801	**D'9(SiCl3)**	0.149531	-4379.061742	-4378.912211
D10(OH)	0.179497	-1190.259718	-1190.080221	**D'10(OH)**	0.181502	-1190.288685	-1190.107183
D11(NH2)	0.205963	-1150.476390	-1150.270427	**D'11(NH2)**	0.205976	-1150.503361	-1150.297385
D12(OMe)	0.229884	-1268.833691	-1268.603807	**D'12(OMe)**	0.233150	-1268.861608	-1268.628458
D13(SiMe3)	0.360197	-1856.998382	-1856.638185	**D'13(SiMe3)**	0.361305	-1857.010820	-1856.649515

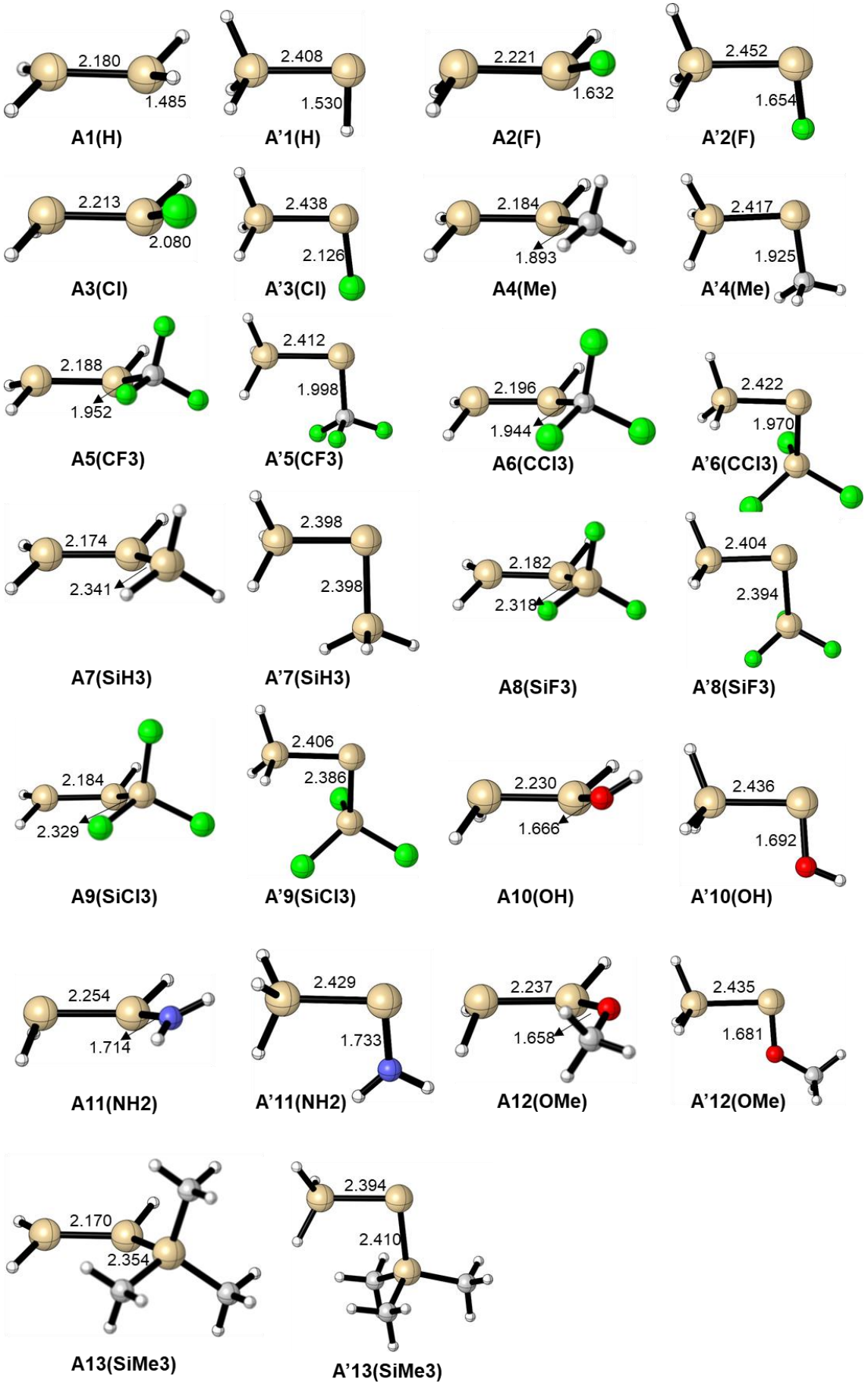


Fig. S1 The selected bond lengths (Å) of optimized disilenes **A** and silylsilylenes **A'**.

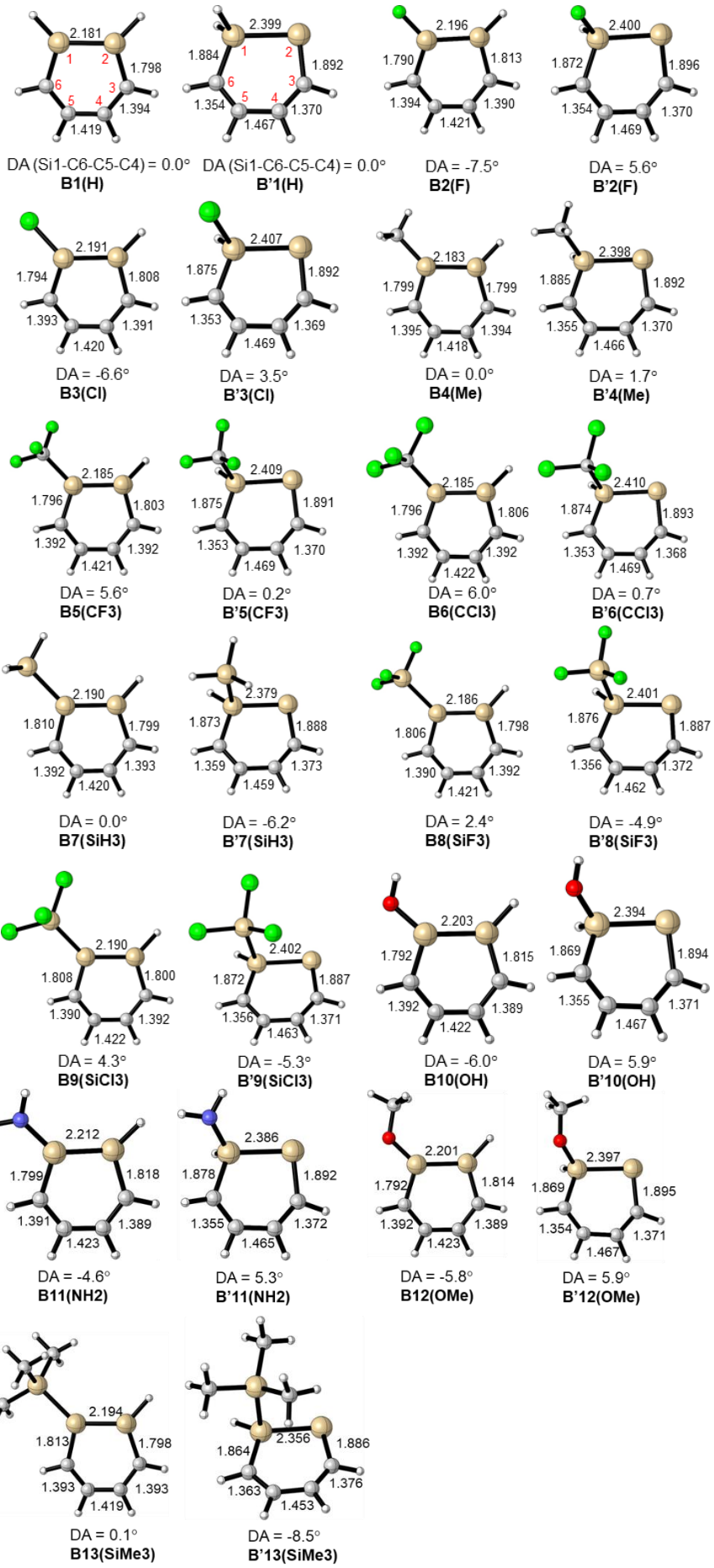


Fig. S2 The selected bond lengths (Å) and dihedral angles of Si1-C6-C5-C4 of optimized disilabenzenes **B** and isomers **B'**.

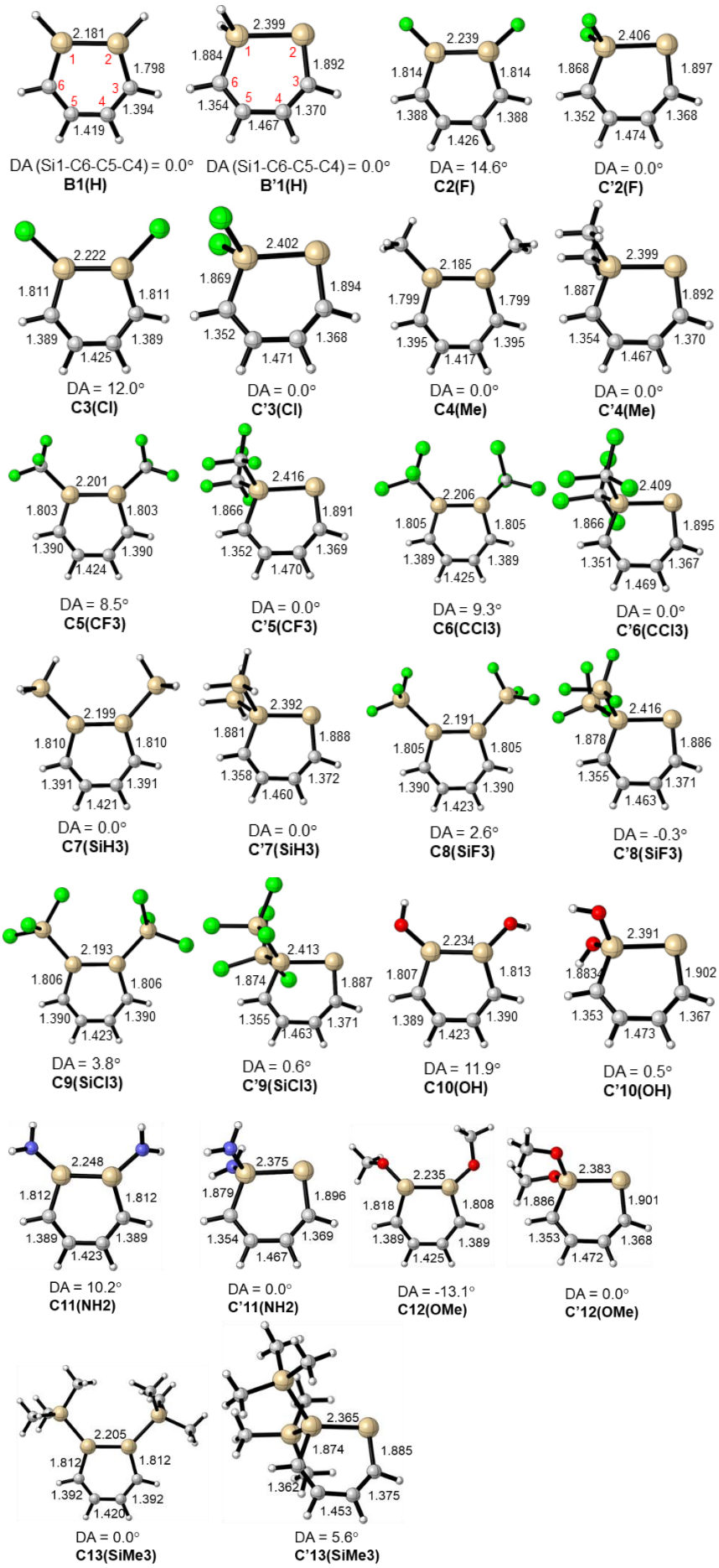


Fig. S3 The selected bond lengths (Å) and dihedral angles of Si1-C6-C5-C4 of optimized disilabenzenes **C** and isomers **C'**.

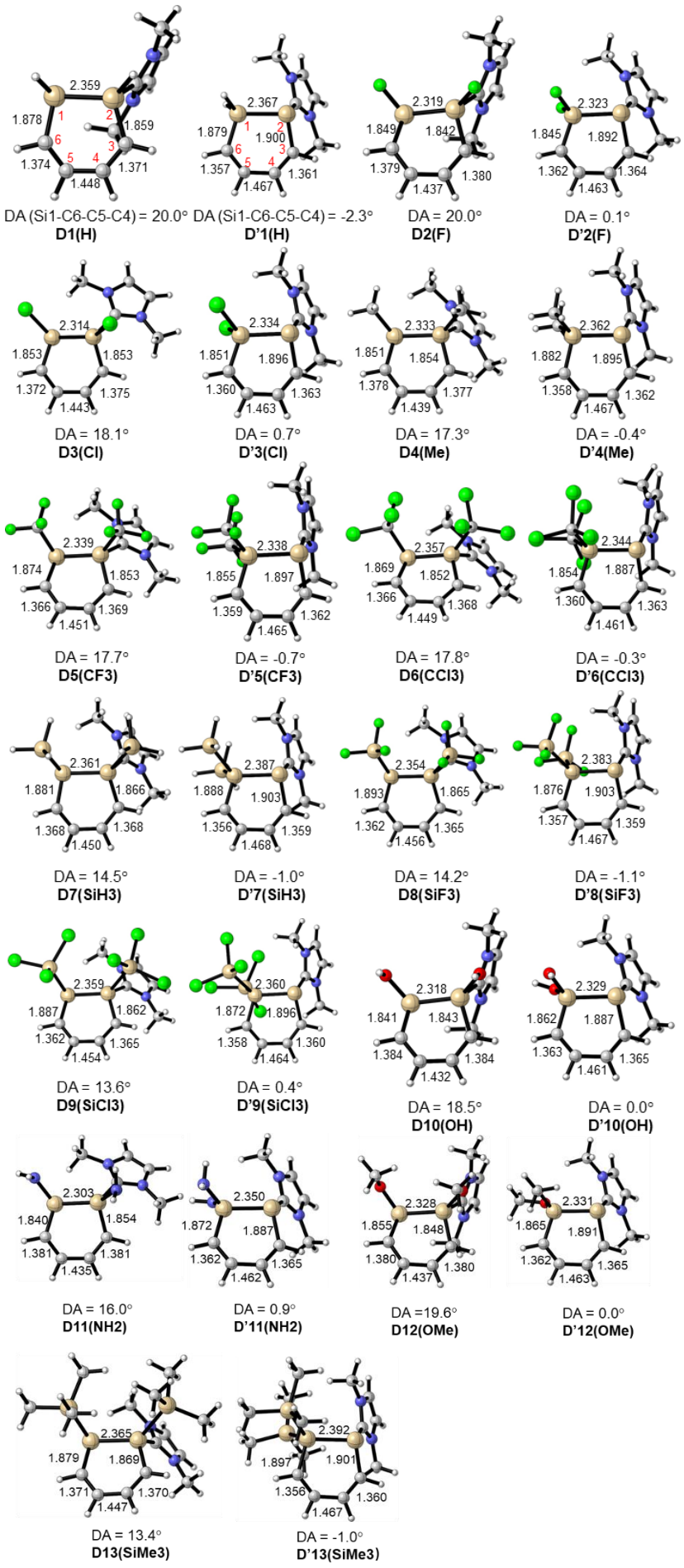


Fig. S4 The selected bond lengths (Å) and dihedral angles of Si1-C6-C5-C4 of optimized **D** and isomers **D'**.

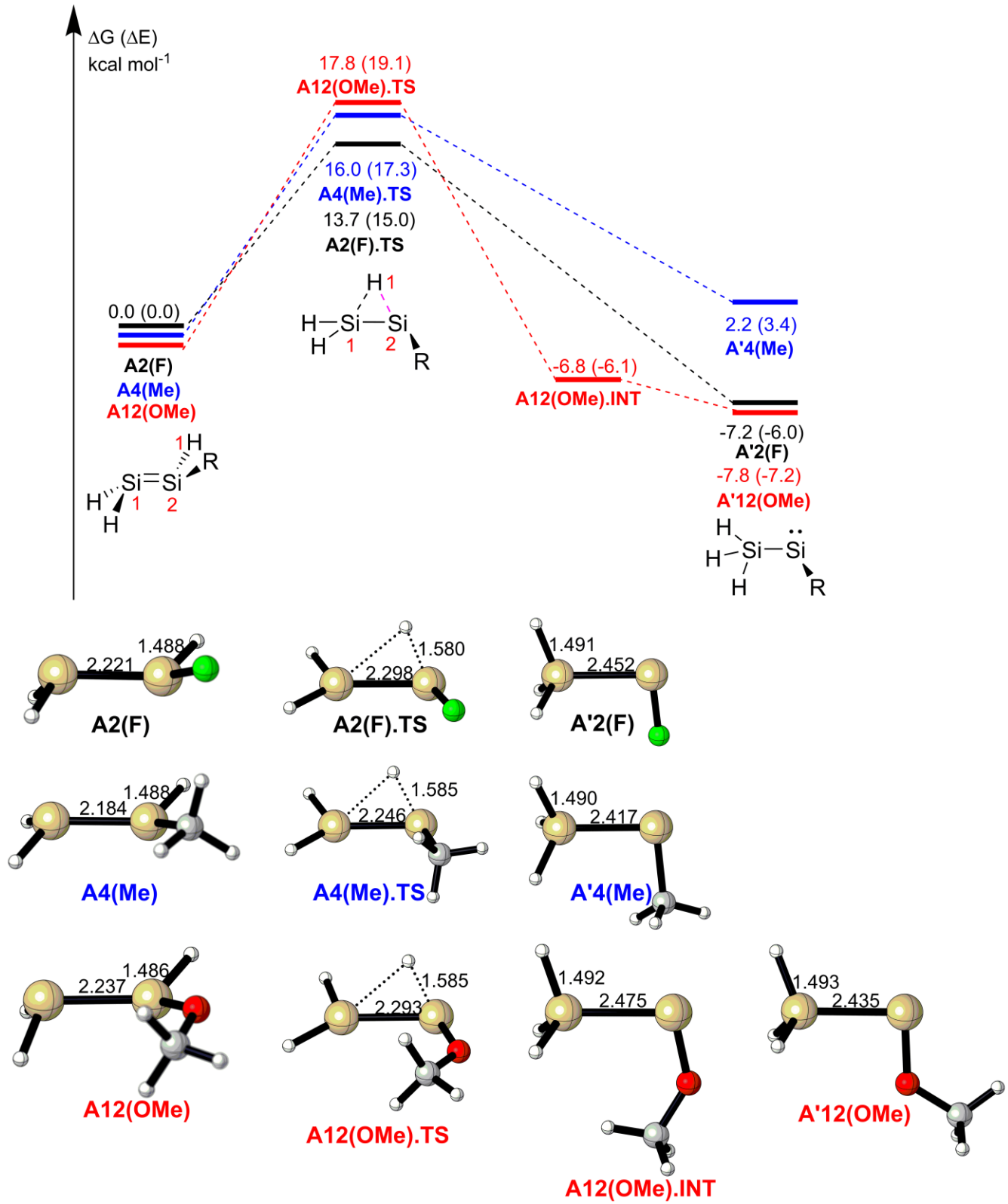


Fig. S5 Energy profile for the isomerization between **A2(F)** to **A'2(F)**, **A4(Me)** to **A'4(Me)** and **A12(OMe)** to **A'12(OMe).** Selected bond lengths (Å) are annotated along the bonds.

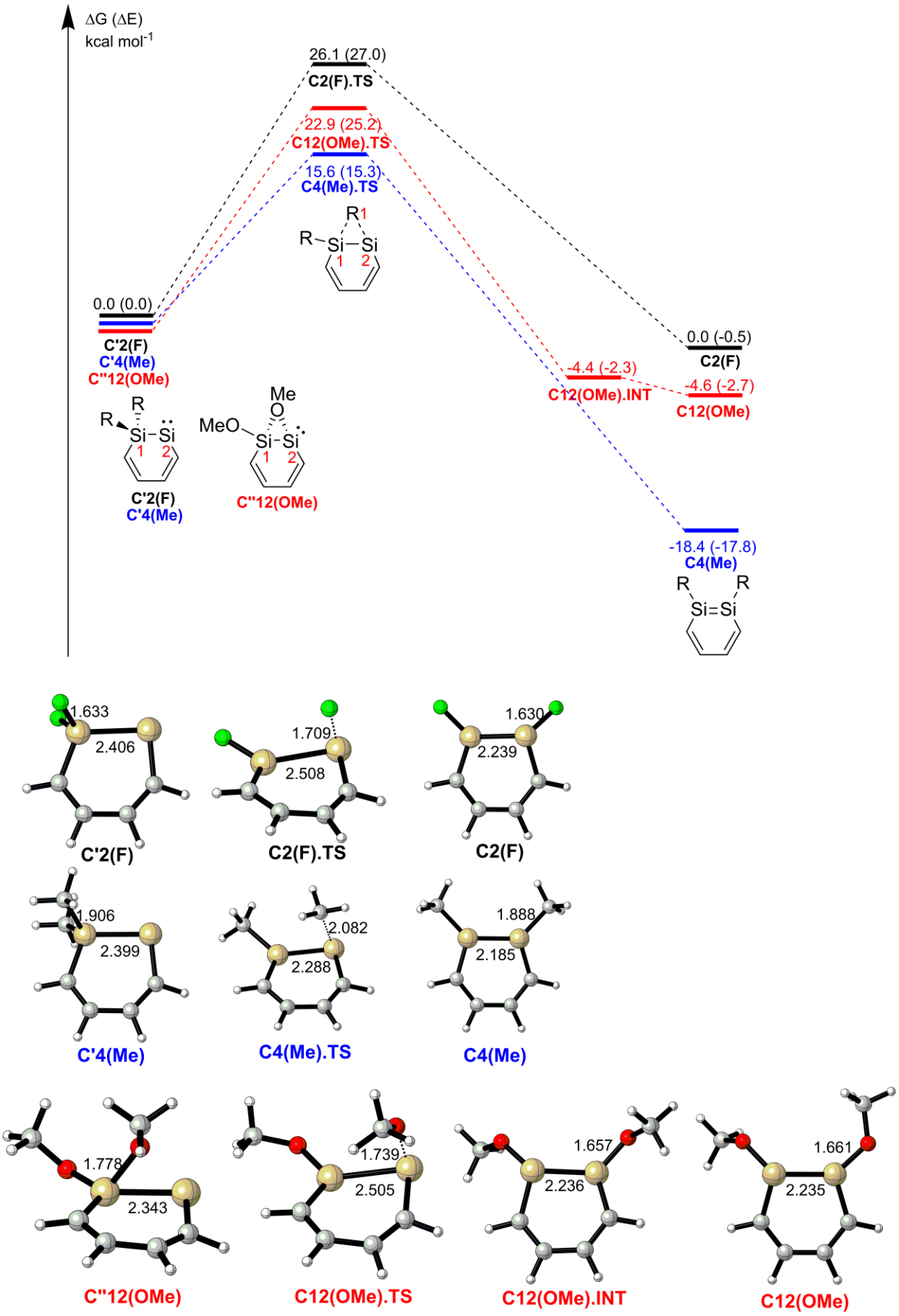


Fig. S6 Energy profile for the isomerization between **C'2(F)** to **C2(F)**, **C'4(Me)** to **C4(Me)** and **C''12(OMe)** to **C12(OMe).** Selected bond lengths (Å) are annotated along the bonds.

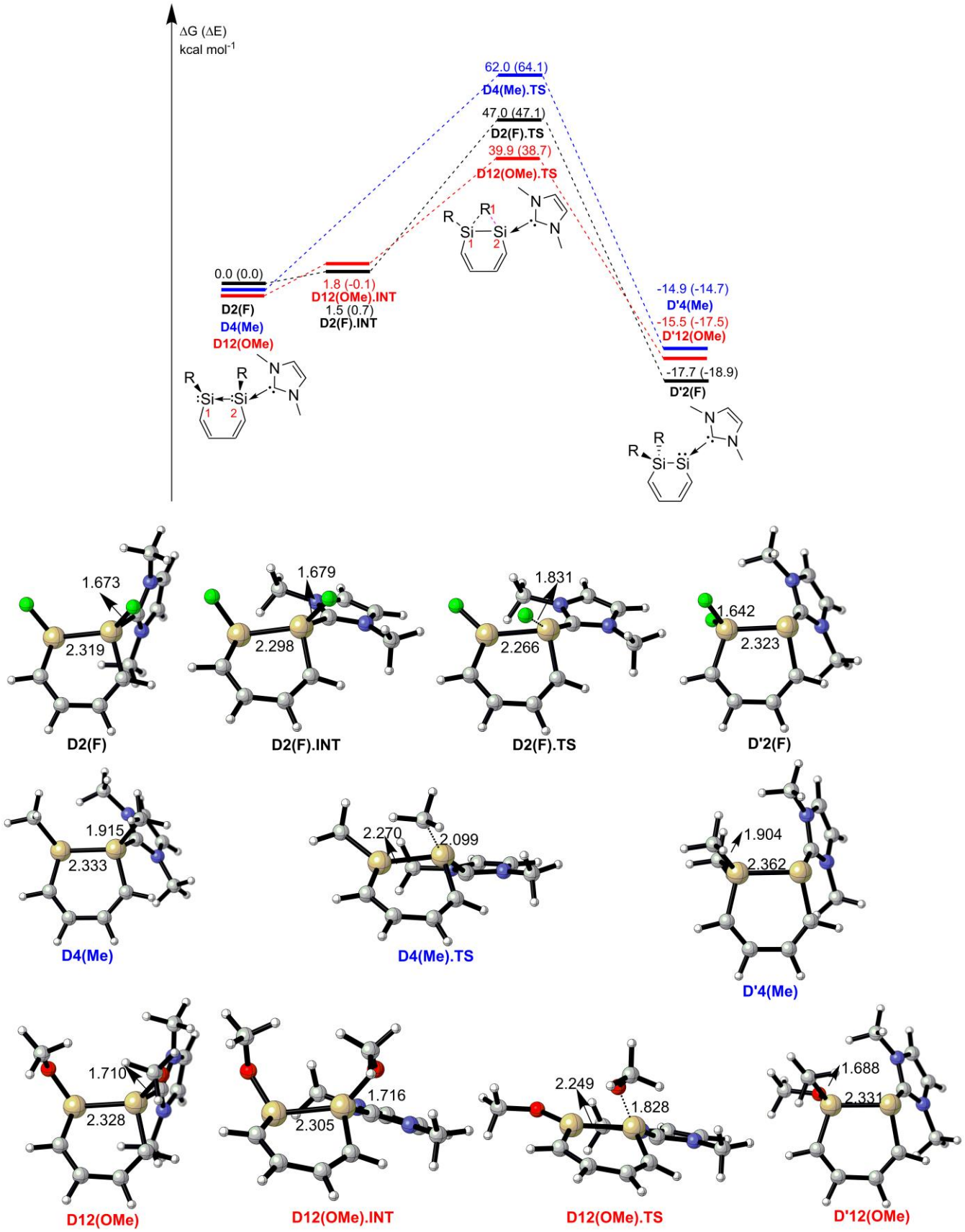


Fig. S7 Energy profile for the isomerization between **D2(F)** to **D'2(F)**, **D4(Me)** to **D'4(Me)** and **D12(OMe)** to **D'12(OMe)**. Selected bond lengths (Å) are annotated along the bonds.

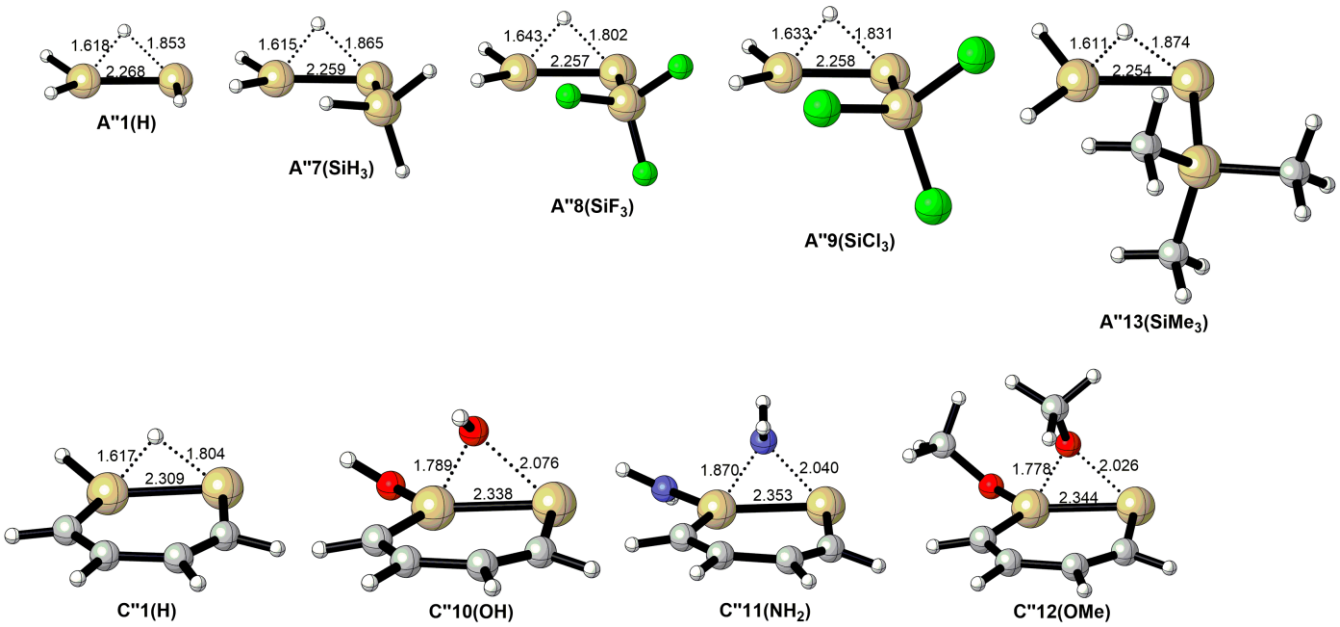


Fig. S8 The selected bond lengths (Å) of optimized species **A''** and **C''** in a monobridged form.

Cartesian coordinates together with the electronic energies for all the complexes optimized at the B3LYP-D3/6-31+G(d,p) level.

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E = -2329.160063 a.u.

Si	-0.37638600	0.59460300	-0.28891100
H	-0.53037300	0.46761900	-1.77176700
Si	-2.22992600	-0.02868000	1.01817400
Si	-3.92626000	1.25518400	-0.06643100
Si	-2.57817700	-2.08022600	-0.16670300
N	1.39885300	-1.35571200	1.13557800
N	1.82647100	-1.29227800	-0.99444500
C	1.09159700	-0.69429100	-0.01442800
C	2.29813900	-2.38480400	0.87371900
C	2.56447800	-2.34882300	-0.46888400
C	2.79905200	-3.37716300	1.87475100
H	3.12081700	-2.90812700	2.80491400
H	3.65827900	-3.91196400	1.46636900
H	2.02881500	-4.11633000	2.11943400
C	3.46002500	-3.25349000	-1.25498000
H	2.99926800	-3.56948700	-2.19273400
H	3.66846300	-4.15600300	-0.67796500
H	4.41796400	-2.77971900	-1.49299100
C	0.93268500	-0.92669000	2.48667900
H	0.22379800	-0.12449700	2.27879400
C	2.09390900	-0.35247500	3.30255200
H	2.78085100	-1.12368500	3.66080600
H	1.68693600	0.15805200	4.18001200
H	2.65230200	0.37229000	2.71134400
C	0.15110300	-2.00872500	3.23083300
H	-0.69814900	-2.35125400	2.63911700
H	-0.25279500	-1.56119500	4.14376800
H	0.77017000	-2.86080900	3.51979800
C	1.80130300	-0.86351400	-2.41787400
H	1.28918900	0.09228100	-2.38830300
C	3.20259500	-0.59891800	-2.97742100
H	3.80239700	-0.02411700	-2.26772800
H	3.09864900	-0.00339300	-3.88937200
H	3.73836500	-1.51202100	-3.24416500
C	0.96199500	-1.81480400	-3.27413500
H	1.40767200	-2.81041600	-3.35082900
H	0.87801300	-1.40568900	-4.28584000
H	-0.04464600	-1.91734600	-2.86350600
C	0.47012600	2.37659800	-0.11640700
C	1.56834100	2.46814600	-1.14587000
C	2.77163000	2.49358200	-0.50412200
C	2.54643100	2.50857000	0.94819100
C	1.20555600	2.46896100	1.19664600
C	-0.60764500	3.46748400	-0.27646900
H	-1.10664500	3.41050300	-1.24766600
H	-0.14352700	4.45831200	-0.19499400
H	-1.37241100	3.38639000	0.49821300
C	1.30390200	2.66985400	-2.61001800
H	0.47395600	2.05339600	-2.97334700
H	2.18429000	2.45011500	-3.22182800
H	1.02171700	3.71270200	-2.81129200
C	4.14543800	2.57266300	-1.10677300
H	4.12040300	2.52689200	-2.19854800
H	4.78776700	1.75611700	-0.75000300
H	4.64917600	3.50715700	-0.82737500
C	3.67570700	2.64698400	1.93015600
H	4.39587100	1.82170200	1.84451600
H	3.32330000	2.67797300	2.96420100
H	4.24009200	3.57067300	1.74820400
C	0.49347300	2.64109100	2.50634000
H	0.09042200	3.65974900	2.59454900
H	1.15697000	2.47936400	3.35997100
H	-0.36344000	1.96433400	2.60276300
C	-3.70019400	1.73304800	-1.90354600
H	-2.81707100	2.36022300	-2.06175300
H	-4.57586600	2.29355600	-2.25725600
H	-3.58951500	0.84350400	-2.53141600
C	-4.26981900	2.87832800	0.88064300
H	-4.47693700	2.66852800	1.93631900
H	-5.14883600	3.38059200	0.45521300
H	-3.43331800	3.58295000	0.83988300
C	-5.58404000	0.30913000	0.01331500
H	-5.59242100	-0.56521200	-0.64502300
H	-6.40001700	0.97304000	-0.30044600
H	-5.80028000	-0.03386700	1.03131300
C	-3.99831500	-3.03020800	0.68272800
H	-3.74016700	-3.25546800	1.72408400
H	-4.19062700	-3.97921700	0.16493300
H	-4.92738500	-2.45233600	0.69127200
C	-3.03289000	-1.98172300	-2.02465200
H	-4.02031200	-1.53259400	-2.17121900
H	-3.05438200	-2.98752900	-2.46572000
H	-2.31359600	-1.37652400	-2.58801800
C	-1.11493100	-3.32380800	-0.13513800
H	-0.23663200	-2.96529900	-0.67892800
H	-1.44446000	-4.25258900	-0.61922200

H	-0.79679400	-3.57776000	0.88072300

A1(H)

E = -581.333136 a.u.

H	0.44278900	1.79659600	-1.22814200
H	0.44278900	1.79659600	1.22814200
H	-0.44278900	-1.79659600	-1.22814200
H	-0.44278900	-1.79659600	1.22814200
Si	0.00000000	1.08985400	0.00000000
Si	0.00000000	-1.08985400	0.00000000

A2(F)

E = -680.635578 a.u

H	-1.09467600	1.73184100	-0.49649500
H	1.82536600	-1.42361200	0.62878400
H	2.37624000	0.93188900	0.41109500
Si	-0.58875300	0.47439000	0.11758300
Si	1.52236500	-0.17162800	-0.12123200
F	-1.79749900	-0.60875500	-0.05469900

A3(Cl)

E = -1040.980296 a.u

H	-0.26942500	2.00816200	-0.54654800
H	2.00589600	-1.61233900	0.63464800
H	3.01256400	0.58160400	0.28498600
Si	-0.03733800	0.70310600	0.12534700
Si	1.90415000	-0.33148900	-0.11670100
Cl	-1.81672900	-0.36353300	-0.02906700

A4(Me)

E = -620.665530 a.u

H	0.71816700	1.92882800	0.39090100
H	-1.83455200	-1.56698600	-0.50534100
H	-2.67032200	0.71738000	-0.16871900
Si	0.46964100	0.54992800	-0.11077000
Si	-1.55875600	-0.23348600	0.09203100
C	2.00886500	-0.53948000	0.05121600
H	2.79734000	-0.17778200	-0.61832100
H	2.40092700	-0.51921100	1.07369800
H	1.78286800	-1.57554000	-0.21717600

A5(CF3)

E = -918.388972 a.u

H	-0.42899900	2.18644200	0.55078600
H	-2.42873400	-1.64825000	-0.55434600
H	-3.69335700	0.39341700	-0.02628900
Si	-0.59021300	0.89892200	-0.16575400
Si	-2.39345800	-0.31374000	0.09065900
C	1.09558700	-0.07068400	0.00552200
F	1.59288500	-0.07665000	1.27361500
F	0.98049600	-1.37344400	-0.37650800
F	2.06539300	0.48342100	-0.78065700

A6(CCl3)

E = -1999.423508 a.u

H	0.77052900	2.34413700	-0.27982400
H	3.08382600	-1.39990200	0.47191600
H	4.11994300	0.80928900	0.21917300
Si	1.01809000	0.99243800	0.27753700
Si	2.92895400	-0.03031100	-0.07577700
C	-0.62816700	-0.00435100	0.00016500
Cl	-1.19903700	0.11523400	-1.71496300
Cl	-0.41093500	-1.74374200	0.43738100
Cl	-1.88790500	0.73455500	1.08717700

A7(SiH3)

E = -872.044191 a.u

H	-0.16406500	2.14644200	0.43932400
H	-2.01469500	-1.76410600	-0.45722200
H	-3.28492700	0.28317000	0.05538900
Si	-0.11941200	0.76626000	-0.11472800
Si	-1.95751700	-0.37938300	0.07147000
H	2.92349000	0.32807300	-0.89407800
H	2.51565700	-0.26217200	1.40594300
H	1.77127200	-1.73486900	-0.36963300
Si	1.95216200	-0.31520100	0.03042000

A8(SiF3)

E = -1169.984716 a.u

H	-1.05395000	-2.28011100	-0.58996400
H	-2.57642600	1.72870000	0.54087500
H	-4.05121000	-0.10427700	-0.18602800
Si	-0.98934000	-1.00165700	0.16191100
Si	-2.65564700	0.38583100	-0.07895300
Si	1.07438700	0.03936700	-0.00720900
F	1.68196500	0.09976200	-1.49802500
F	0.97218500	1.55986600	0.51756600
F	2.19807100	-0.69006000	0.88875000

A9(SiCl3)

E = -2250.993822 a.u

H	1.37726300	-2.51482100	0.29405700
H	3.18182500	1.48335300	-0.38811800
H	4.51762500	-0.53218600	0.07581600
Si	1.40354100	-1.15482000	-0.30372900
Si	3.16512500	0.07781700	0.07761400
Si	-0.61572500	-0.03336200	-0.00596900
Cl	-1.34583600	-0.14026300	1.93422500
Cl	-2.07982300	-0.82203600	-1.24933700
Cl	-0.36362900	1.96869800	-0.49268800

A10(OH)

E = -656.604819 a.u

H	-1.01605600	1.77620000	-0.43249200
H	1.82071000	-1.42290500	0.65397600
H	2.36024900	0.92352000	0.48329600
Si	-0.55743600	0.46396400	0.11704500
Si	1.56189200	-0.18155500	-0.13664900
O	-1.82291200	-0.61246600	-0.00108600
H	-2.64399600	-0.33081700	-0.42163600

A11(NH2)

E = -636.731762 a.u

H	-0.98856200	1.82932200	-0.33400500
H	1.70346500	-1.45925900	0.65759400
H	2.34329000	0.83909500	0.65759500
Si	-0.52805000	0.48262500	0.10815600
Si	1.60638400	-0.19362700	-0.14831500
H	-2.81032700	-0.18717000	-0.38224700
N	-1.91753400	-0.51081100	-0.03498400
H	-1.92181400	-1.49229000	0.20817000

A12(OMe)

E = -695.910601 a.u

H	-0.06855100	2.30321200	0.31358800
H	-1.50153800	-1.76492200	-0.59854300
H	-2.93274400	0.17197900	-0.58330700
Si	-0.05540300	0.88122500	-0.11637500
Si	-1.80140300	-0.49443800	0.13577900
O	1.51527500	0.40906000	0.12343900
C	1.99639300	-0.92985900	-0.03169300
H	1.51961400	-1.43764500	-0.87952300
H	3.07393900	-0.87757200	-0.20365300
H	1.80401600	-1.50338700	0.88243800

A13(SiMe3)

E = -990.046427 a.u

H	1.16321900	-2.33284800	0.29493400
H	2.84514000	1.68693200	-0.36276700
H	4.18641200	-0.33664100	0.04648000
Si	1.02153500	-0.91494600	-0.14259400
Si	2.83032300	0.26563900	0.06320600
Si	-1.11536500	0.06083000	0.00682700
C	-1.82187900	-0.15630000	1.75189500
H	-2.82807500	0.27852300	1.80643100
H	-1.89624900	-1.21477700	2.02353400
H	-1.19346000	0.34052100	2.49813700
C	-0.95170800	1.90204800	-0.40276900
H	-0.54454200	2.05452400	-1.40781700
H	-1.93625700	2.38376300	-0.36026100
H	-0.29572300	2.41279300	0.30997400
C	-2.27055800	-0.77787000	-1.24020500
H	-2.36083600	-1.85213400	-1.04506400
H	-3.27426700	-0.33967500	-1.17445800
H	-1.91139200	-0.64958000	-2.26679100

A'1(H)

E = -581.324086 a.u.

Si	-1.07876100	-0.00328000	0.00000000
H	-1.55047800	0.74221500	1.20563900
H	-1.55047900	0.74223400	-1.20562700
H	-1.74491400	-1.33465100	-0.00001000
Si	1.32703500	-0.10885600	0.00000000
H	1.37003400	1.42011500	0.00000000

A'2(F)

E = -680.643979 a.u.

Si	-1.45410400	0.11089200	0.00000600
H	-1.71455100	0.94690200	1.20808700
H	-1.71502600	0.94478700	-1.20944100
H	-2.42146100	-1.02360300	0.00117100
Si	0.86354800	-0.69077700	0.00000800
F	1.56875800	0.80558900	-0.00000200

A'3(Cl)

E = -1040.988054 a.u.

Si	1.75844100	-0.32538000	-0.00001200
H	1.76750900	-1.19411100	1.21094400
H	1.76687200	-1.19578400	-1.20975000
H	2.99954400	0.49926500	-0.00085800
Si	-0.23267900	1.08108200	-0.00001400
Cl	-1.64085900	-0.51112900	0.00000200

A'4(Me)

E = -620.657114 a.u.

Si	-1.45808200	0.19105600	-0.00631600
H	-1.80702200	0.40823200	1.43412000
H	-1.50500000	1.52664400	-0.67442500
H	-2.53351300	-0.65814500	-0.59168700
Si	0.71981100	-0.85770900	-0.00316600
C	1.73087800	0.77991000	0.00909400
H	1.35379100	1.54587200	0.69957900
H	2.79356200	0.61151000	0.20996300
H	1.64871000	1.21956600	-0.99936800

A'5(CF3)

E = -918.384593 a.u.

Si	2.18765000	-0.32881100	-0.00341300
H	2.39309800	-0.75885300	1.41132700
H	1.88678100	-1.51927000	-0.83923000
H	3.44500000	0.30854700	-0.47838900

Si	0.41822900	1.30880200	0.07827000
C	-1.02603800	-0.07016700	0.02494200
F	-2.24775600	0.40175600	0.39865400
F	-0.83302000	-1.21033000	0.75050400
F	-1.14710700	-0.45023800	-1.29264300

A'6(CCl3)

E = -1999.427716 a.u.

Si	-2.66880900	0.23512600	-0.20395700
H	-2.56697500	0.83306200	1.15236500
H	-2.87049500	1.32409900	-1.20402600
H	-3.86557600	-0.65069800	-0.25383900
Si	-0.74781100	-1.06084600	-0.90803000
C	0.65183500	0.09263700	-0.13833500
Cl	2.30574900	-0.17047600	-0.74946300
Cl	0.36508900	-1.06581000	1.38366400
Cl	0.46002800	1.79498000	0.34834800

A'7(SiH3)

E = -872.032449 a.u.

Si	1.71948400	-0.44206500	-0.00745700
H	1.90795100	-0.73579600	1.44847500
H	1.38344500	-1.72634200	-0.68575800
H	3.02184500	0.04281000	-0.54117500
Si	-0.00000600	1.22975500	0.00000700
H	-1.38363900	-1.72665600	0.68537900
H	-3.02170900	0.04294800	0.54135100
H	-1.90802500	-0.73538200	-1.44850400
Si	-1.71946800	-0.44208900	0.00746600

A'8(SiF3)

E = -1169.973873 a.u.

Si	-2.38596600	0.45379300	0.00699000
H	-1.92335400	1.60525000	0.82433400
H	-2.46508000	0.87630700	-1.42367900
H	-3.74320400	0.04524900	0.45411500
Si	-0.90107500	-1.43526200	-0.07326400
Si	0.99314200	0.02774900	-0.01280600
F	1.25366000	0.44009000	1.53133000
F	0.85165400	1.40291200	-0.85352100
F	2.36648900	-0.64019400	-0.53865900

A'9(SiCl3)

E = -2250.986577 a.u.

Si	2.88058000	-0.18637200	-0.08468100
H	4.18939400	0.50615500	0.04905200
H	2.53485400	-0.84578100	1.19954400
H	3.00359300	-1.22499200	-1.14998100
Si	1.22097900	1.32750300	-0.94682800
Si	-0.57736200	0.02241700	-0.07775200
Cl	-2.39749600	0.37261100	-1.01858400
Cl	-0.38504400	-2.04643100	0.06212800
Cl	-0.69196500	0.80764100	1.86416400

A'10(OH)

E = -656.616966 a.u.

Si	-1.45669900	0.13330900	0.00001000
H	-1.70569600	0.97383200	1.20761900
H	-1.70684700	0.97019200	-1.20990800
H	-2.45511900	-0.97526400	0.00205500
Si	0.82282200	-0.72500500	0.00001200
O	1.53057200	0.81134100	0.00000000
H	2.49736700	0.82426400	-0.00007500

A'11(NH2)

E = -636.747983 a.u.

Si	-1.45041800	0.14505600	0.00002000
H	-2.21791800	-0.30611300	1.19858300
H	-1.45396900	1.64282100	-0.00113900
H	-2.21858200	-0.30732600	-1.19770200
Si	0.79717800	-0.77557900	-0.00000500
H	2.61777200	0.81180500	0.00011900
N	1.60488900	0.75784100	-0.00009300
H	1.18383200	1.68124200	0.00058800

A'12(OMe)

E = -695.921281 a.u

Si	-1.94355400	-0.31918700	-0.00013300
H	-2.00352300	-1.25238400	-1.16305600
H	-2.05857500	-1.12899200	1.24888600
H	-3.13997100	0.57044000	-0.06969600
Si	0.13152500	0.95547700	-0.00072100
O	1.09293700	-0.42343200	-0.00277300
C	2.52448900	-0.40879900	0.00163900
H	2.92197600	0.61525500	0.00706900
H	2.87633300	-0.93971200	0.89143300
H	2.88173500	-0.93242400	-0.89033000

A'13(SiMe3)

E = -990.031414 a.u

Si	-0.99800300	0.04838600	-0.01237500
Si	0.89312000	-1.44191600	-0.12645400
H	2.10309800	1.55318400	0.75086800
H	3.82803000	-0.10871600	0.53077100
H	2.70746400	0.72761400	-1.42507800
Si	2.50381700	0.32477000	0.00348100
C	-1.11742600	0.62243000	1.80191600
H	-0.25068600	1.22647000	2.08926900
H	-2.01638300	1.23981400	1.92463100
H	-1.19832900	-0.21791200	2.50050600

C	-2.59969100	-0.86723500	-0.45999700
H	-3.46812100	-0.20878200	-0.33241300
H	-2.58807300	-1.20782300	-1.50164200
H	-2.74624900	-1.74754200	0.17585100
C	-0.85616600	1.57968600	-1.13144100
H	0.00149500	2.20325600	-0.85972100
H	-0.75449900	1.30388300	-2.18689200
H	-1.76311800	2.18991000	-1.03414800

B1(H)

E = -734.984466 a.u.

C	-0.62702000	1.58355300	0.00000000
C	-1.71274400	0.70931400	0.00000000
C	-1.71274300	-0.70931400	0.00000000
C	-0.62702000	-1.58355300	0.00000000
H	2.18138600	-2.09702000	0.00000000
H	2.18138600	2.09702100	0.00000000
H	-0.86907400	2.64618100	0.00000000
H	-2.70239400	1.16527900	0.00000000
H	-2.70239400	-1.16527900	0.00000000
H	-0.86907400	-2.64618200	0.00000000
Si	1.10204700	1.09071700	0.00000000
Si	1.10204700	-1.09071700	0.00000000

B2(F)

E = -834.284757 a.u.

C	-0.23879700	-1.59589200	-0.08132100
C	1.15189300	-1.67952200	-0.04423400
C	2.10388700	-0.62708400	0.02815200
C	1.87319100	0.74279800	0.08427200
H	0.17886200	3.00697200	0.30136100
H	-0.78693100	-2.53500800	-0.14531800
H	1.57810100	-2.68156600	-0.08670400
H	3.14330200	-0.95120800	0.05865800
H	2.76377800	1.36843900	0.16185200
Si	-1.12045900	-0.05600000	0.15421200
Si	0.29103500	1.60075300	-0.13782800
F	-2.73402500	-0.09733000	-0.04893800

B3(Cl)

E = -1194.630348 a.u.

C	-0.13869100	1.58436500	-0.04473200
C	-1.52801000	1.68856700	-0.04239300
C	-2.49905400	0.65283500	-0.00367700
C	-2.29769700	-0.72303000	0.04502200
H	-0.62349300	-3.01762800	0.24440300
H	0.42460100	2.51554600	-0.08738000
H	-1.93591900	2.69805300	-0.08682400
H	-3.53299100	0.99555300	-0.00082100
H	-3.20061800	-1.33370300	0.08457000
Si	0.73378300	0.03229900	0.17539500
Si	-0.71651500	-1.58623900	-0.10470100
Cl	2.78867000	0.04005400	-0.05111600

B4(Me)

E = -774.317788 a.u.

C	0.15594000	1.57341300	-0.00013400
C	-1.23580900	1.66226700	0.00004300
C	-2.19303900	0.61582500	0.00014100
C	-1.97411100	-0.76038400	0.00010200
H	-0.24144200	-3.02626200	0.00041500
H	0.69025400	2.52476200	-0.00030900
H	-1.65799500	2.66708200	-0.00006000
H	-3.23199300	0.94453100	0.00020500
H	-2.86589600	-1.38720500	0.00016500
Si	1.11765600	0.05312000	-0.00009100
Si	-0.35961100	-1.55414800	-0.00013600
C	3.00197300	0.08167300	0.00018500
H	3.39735600	-0.93834900	-0.00120800
H	3.38379600	0.59780500	-0.88657900
H	3.38356100	0.59526100	0.88852200

B5(CF3)

E = -1072.038780 a.u.

C	0.72227300	-1.57586100	-0.01942600
C	2.10755600	-1.69900900	0.03533900
C	3.09015300	-0.67242300	0.04710600
C	2.91609800	0.70847400	0.00687100
H	1.27412600	3.03299300	-0.18378800
H	0.14860600	-2.50174400	-0.00687000
H	2.50421900	-2.71220000	0.08735000
H	4.11871100	-1.02918900	0.08663400
H	3.83008400	1.30256500	0.01757700
Si	-0.13314200	-0.01114600	-0.23491600
Si	1.33757500	1.57868300	0.05219200
C	-2.05911600	-0.01449300	0.01791200
F	-2.43615400	-0.08108400	1.32447000
F	-2.63505600	-1.08246600	-0.60401600
F	-2.63985700	1.10598700	-0.49485200

B6(CCl3)

E = -2153.073660 a.u.

C	-1.30952900	1.58924700	-0.03452800
C	-2.69564400	1.70108100	0.01564400
C	-3.67218000	0.66756800	0.02072800
C	-3.48709000	-0.71109500	-0.02483100
H	-1.83309900	-3.02181300	-0.23572200
H	-0.74194300	2.51861500	-0.01956800

H	-3.09976600	2.71148800	0.06829300
H	-4.70322000	1.01763700	0.05602800
H	-4.39716800	-1.31170500	-0.02339400
Si	-0.44991900	0.02897300	-0.26248300
Si	-1.90277600	-1.57480300	0.04181300
C	1.46477600	0.01147200	-0.00229100
Cl	2.21737200	1.29517600	-1.04002100
Cl	1.90658400	0.32734400	1.72726700
Cl	2.10609900	-1.61206300	-0.48751500

B7(SiH3)

E = -1025.695845 a.u.

C	-0.27989000	1.57294300	0.00000400
C	-1.66870700	1.66446200	-0.00001500
C	-2.63050900	0.61962100	-0.00000600
C	-2.42168400	-0.75728000	0.00001900
H	-0.69513400	-3.01806600	0.00005400
H	0.25395800	2.52390600	0.00001100
H	-2.08892000	2.67002400	-0.00001000
H	-3.66753500	0.95473200	0.00000900
H	-3.31671400	-1.37902700	0.00004600
Si	0.69669300	0.04856000	0.00002400
Si	-0.80487300	-1.54502500	-0.00002200
Si	3.02988400	0.03796400	-0.00000600
H	3.48543900	-1.37625900	-0.00182800
H	3.56486500	0.72420400	-1.20537400
H	3.56491500	0.72101700	1.20714900

B8(SiF3)

E = -1323.635230 a.u.

C	-1.12455100	1.58508000	-0.02083600
C	-2.51059500	1.68421300	0.02181700
C	-3.47874500	0.64365100	0.04255200
C	-3.28811000	-0.73560300	0.02543800
H	-1.58584900	-3.02537300	-0.07300000
H	-0.57551900	2.52600900	-0.02723700
H	-2.92415400	2.69167000	0.04675700
H	-4.51207300	0.98765800	0.07364000
H	-4.19202200	-1.34380700	0.04552300
Si	-0.19924300	0.03706800	-0.12325100
Si	-1.68839700	-1.55701500	0.01355400
Si	2.10413100	0.01656400	0.01041100
F	2.68795400	-1.39390500	-0.49968700
F	2.68158300	0.23655500	1.49656000
F	2.76054500	1.17370000	-0.89570800

B9(SiCl3)

E = -2404.644797 a.u.

C	-1.69467300	1.57504500	-0.05760800
C	-3.07754100	1.68995700	0.02413800
C	-4.05520000	0.65854700	0.06535700
C	-3.87714200	-0.72196600	0.03443200
H	-2.21006100	-3.02575400	-0.14234300
H	-1.13287600	2.50852800	-0.06999600
H	-3.47941900	2.70147000	0.07104500
H	-5.08407500	1.01202000	0.12584000
H	-4.78587400	-1.32224800	0.07423600
Si	-0.79082300	0.02079600	-0.24351100
Si	-2.28464800	-1.56018300	0.00832700
Si	1.51404100	0.00802300	-0.00222600
Cl	2.30551400	-1.68691900	-0.89486900
Cl	2.13350900	0.01683200	1.97704100
Cl	2.31272200	1.69100300	-0.91352300

B10(OH)

E = -810.254093 a.u.

C	-0.21565600	-1.58908000	-0.07490400
C	1.17321000	-1.67208500	-0.04169000
C	2.12877500	-0.62115200	0.03483700
C	1.89573900	0.74683600	0.09353500
H	0.19114000	2.99419000	0.32700700
H	-0.76249400	-2.52985700	-0.13006700
H	1.59900900	-2.67466100	-0.08153300
H	3.16762600	-0.94700700	0.07035400
H	2.78361600	1.37526800	0.17957700
Si	-1.12211400	-0.05731900	0.13055900
Si	0.30871500	1.59580000	-0.14355300
O	-2.77035400	-0.18882500	-0.05420000
H	-3.32089200	0.56682900	0.17950700

B11(NH2)

E = -790.376232 a.u.

C	-0.22474400	1.57861200	0.06055600
C	1.16243000	1.68650400	0.04333300
C	2.14033800	0.65550600	-0.03129600
C	1.93048900	-0.71546200	-0.09807400
H	0.27043800	-2.97496000	-0.37194200
H	-0.77737800	2.51830100	0.09374500
H	1.56896200	2.69737900	0.08218400
H	3.17238400	1.00292000	-0.06406100
H	2.83002700	-1.32682800	-0.18825900
Si	-1.11658000	0.02816000	-0.13293200
Si	0.35978600	-1.59367700	0.15777100
H	-3.42837300	-0.68749400	-0.23076500
N	-2.82404000	0.08340000	0.01243300
H	-3.32374200	0.87314800	0.39721600

B12(OMe)

E = -849.557135 a.u.

C	0.49139500	-1.65925000	-0.07058300
C	1.87293100	-1.49189700	-0.03586800
C	2.62830400	-0.28831300	0.03334600
C	2.16067800	1.01895600	0.08584300
H	0.08612000	2.93630900	0.31399300
H	0.12129800	-2.68256000	-0.12053400
H	2.47010300	-2.40316300	-0.07039200
H	3.70827300	-0.42694900	0.06721300
H	2.92638100	1.79211500	0.16608700
Si	-0.66866800	-0.30626200	0.12030800
Si	0.44727500	1.57357700	-0.13450000
O	-2.27122500	-0.68352400	-0.05078700
C	-3.34348600	0.25888400	0.01454000
H	-3.28349900	0.97932100	-0.81100800
H	-4.27671200	-0.30248900	-0.07158100
H	-3.34157800	0.80291500	0.96753400

B13(SiMe3)

E = -1143.698606 a.u.

C	-1.16503000	1.54024800	-0.00237200
C	-2.55109400	1.67522000	0.00274300
C	-3.54172700	0.65906500	0.00650700
C	-3.36781600	-0.72342300	0.00509100
H	-1.70852800	-3.02288100	-0.00549100
H	-0.60536100	2.47693900	-0.00757500
H	-2.94186100	2.69286800	0.00306000
H	-4.56952200	1.02205400	0.00965000
H	-4.27824300	-1.32250500	0.00680500
Si	-0.20952200	-0.00099400	-0.00874200
Si	-1.76836800	-1.54520700	0.00346400
Si	2.13880000	0.00959700	0.00112100
C	2.78949700	-0.53115600	1.69531800
H	3.88657800	-0.51566700	1.70150200
H	2.43446700	0.13638000	2.48738800
H	2.46402200	-1.54762400	1.94136900
C	2.69383300	1.78319100	-0.36631000
H	3.78926000	1.84082300	-0.36336000
H	2.33948900	2.11817700	-1.34676800
H	2.31919400	2.48390900	0.38768100
C	2.78400700	-1.17092500	-1.33123200
H	2.44122800	-2.19662800	-1.15624600
H	2.44550400	-0.86855800	-2.32769500
H	3.88103200	-1.17812900	-1.33058400

B'1(H)

E = -734.957826 a.u.

C	-1.50361500	0.92504400	0.00000000
C	-1.86060700	-0.38110700	0.00000000
C	-0.98519000	-1.55774800	0.00000000
C	0.38040000	-1.67042200	0.00000000
H	0.49185400	2.37570600	-1.19411200
H	-2.31503100	1.65399600	0.00000000
H	-2.92262200	-0.62942900	0.00000100
H	-1.54961200	-2.49364700	0.00000100
H	0.72769100	-2.70703000	0.00000000
Si	0.29087500	1.49799200	0.00000000
Si	1.77269200	-0.38869900	0.00000000
H	0.49185400	2.37570700	1.19411100

B'2(F)

E = -834.264585 a.u.

C	-0.25477800	1.66205500	0.04152700
C	1.09323200	1.73895400	-0.06404900
C	2.05849300	0.63195500	-0.08372300
C	1.87848100	-0.72626600	-0.07423600
H	-1.52298500	0.03389800	1.78458600
H	-0.81489300	2.59701100	0.00082600
H	1.55420100	2.72131000	-0.17087500
H	3.09041900	0.98375500	-0.15738600
H	2.81494300	-1.28289700	-0.16667900
Si	-1.12686500	0.03305900	0.34079500
Si	0.33968800	-1.83209900	-0.02283000
F	-2.52819700	0.03258700	-0.51767700

B'3(Cl)

E = -1194.609098 a.u.

C	0.12837500	1.66826400	0.28725000
C	1.42874000	1.73488900	-0.08215600
C	2.35480000	0.62536000	-0.34630000
C	2.17469900	-0.73166700	-0.31432200
H	-1.17138700	0.06090600	2.05374100
H	-0.40883700	2.61007900	0.40199700
H	1.87500700	2.71828400	-0.23270200
H	3.34681300	0.97684100	-0.63987000
H	3.06614200	-1.29104000	-0.61063700
Si	-0.73533300	0.03880700	0.62753100
Si	0.69503200	-1.82900300	0.11876100
Cl	-2.50960100	0.01215300	-0.51102600

B'4(Me)

E = -774.290337 a.u.

C	0.18412800	1.65151500	-0.19348400
C	-1.14677800	1.73091100	0.04674700
C	-2.09872600	0.62823500	0.21370200
C	-1.91930400	-0.73011000	0.20230800
H	1.51434500	-0.01877200	-1.85859000

H	0.72223100	2.59932600	-0.26189300
H	-1.60184700	2.71724200	0.14651600
H	-3.11720800	0.98274900	0.39246000
H	-2.84135200	-1.28756500	0.38852700
Si	1.10657900	0.02313900	-0.41472800
Si	-0.39337900	-1.81509200	-0.06795100
C	2.69416300	0.04436800	0.63298100
H	3.28209300	-0.86309900	0.45943100
H	3.31631100	0.90903700	0.37639300
H	2.45974100	0.09891500	1.70115000

B'5(CF3)

E = -1072.019614 a.u.

C	-0.65521000	1.66484100	-0.44823100
C	-1.89649600	1.74869700	0.08403900
C	-2.80529500	0.65192600	0.44313300
C	-2.66237500	-0.70755400	0.35843000
H	0.60494900	0.01411900	-2.26259900
H	-0.13468700	2.60024300	-0.65300400
H	-2.30935800	2.73801000	0.28238900
H	-3.75281700	1.01604600	0.84699800
H	-3.53981400	-1.25453400	0.71344700
Si	0.15263200	0.02004500	-0.84378600
Si	-1.23574100	-1.83035100	-0.17197100
C	1.83076000	0.00797000	0.15987200
F	1.61954400	-0.09166000	1.50881500
F	2.57490500	1.13787900	-0.02580300
F	2.63076700	-1.04231600	-0.18190900

B'6(CCl3)

E = -2153.057010 a.u.

C	-1.18239400	1.67973900	-0.56679700
C	-2.42341500	1.74404600	-0.03227300
C	-3.31746900	0.63429900	0.32624900
C	-3.15291700	-0.72160500	0.24169000
H	0.09015000	0.06800600	-2.40271900
H	-0.67575800	2.62255100	-0.77158300
H	-2.84931700	2.72728300	0.16942300
H	-4.26971900	0.98490500	0.73115200
H	-4.01965000	-1.28375900	0.59952700
Si	-0.35325200	0.05146700	-0.98239300
Si	-1.69442000	-1.81734600	-0.26472000
C	1.31157000	0.01615100	0.03269300
Cl	0.88872500	-0.08945000	1.80330400
Cl	2.30813700	1.50190500	-0.24561700
Cl	2.27251800	-1.44260000	-0.43272200

B'7(SiH3)

E = -1025.667917 a.u.

C	0.23514900	1.64710000	0.63076600
C	1.37345400	1.72824400	-0.10709100
C	2.15315200	0.62685700	-0.66121700
C	1.99750100	-0.73286100	-0.54685400
H	-0.18108000	2.58395500	1.00248500
H	1.79808800	2.71351400	-0.30176600
H	3.02193100	0.97046800	-1.22780700
H	2.80058900	-1.29695800	-1.02944200
Si	-0.64590400	0.02197000	0.93037500
Si	0.69230200	-1.82911300	0.26619100
Si	-2.36397200	0.03813700	-0.72120100
H	-3.18730700	1.27052000	-0.58587900
H	-1.76456100	0.01750200	-2.08190800
H	-3.25030700	-1.14702800	-0.57082500
H	-1.34685000	0.03807300	2.24640000

B'8(SiF3)

E = -1323.610416 a.u.

C	-0.98063200	1.64720300	-0.73726800
C	-2.03142900	1.76167700	0.11247500
C	-2.78966700	0.68687400	0.75172100
C	-2.69174600	-0.67692100	0.64084100
H	0.28507300	-0.04252900	-2.55035200
H	-0.56305700	2.56795100	-1.14381800
H	-2.39675100	2.76049500	0.35140300
H	-3.58398100	1.06490100	1.39907200
H	-3.45802100	-1.20844500	1.21163500
Si	-0.21418700	-0.01460900	-1.14770600
Si	-1.51562400	-1.83411600	-0.27564600
Si	1.73741900	0.00533600	0.15689000
F	2.59076700	1.36874700	0.01918400
F	1.39295600	-0.15176800	1.72720600
F	2.74639500	-1.20008100	-0.20684300

B'9(SiCl3)

E = -2404.621496 a.u.

C	-1.47558800	1.65211400	-0.86461800
C	-2.52414600	1.76053100	-0.01161600
C	-3.28622900	0.68142000	0.61681500
C	-3.18501200	-0.68107500	0.50038500
H	-0.20824400	-0.02343900	-2.68836400
H	-1.05621900	2.57558100	-1.26282600
H	-2.88698900	2.75795700	0.23680500
H	-4.08468300	1.05550700	1.26133900
H	-3.95310100	-1.21737500	1.06431500
Si	-0.70847000	-0.00285400	-1.28638000
Si	-1.98339500	-1.83152000	-0.39094600
Si	1.25417200	0.00713000	0.01870200

Cl	2.36012800	1.75347300	-0.21080500
Cl	0.75117300	-0.16011600	2.03245100
Cl	2.48533300	-1.59598900	-0.45907700

B'10(OH)

E = -810.229550 a.u.

C	-0.23327300	1.65423500	0.03063800
C	1.11568600	1.73283100	-0.06551500
C	2.07749900	0.62578600	-0.07834300
C	1.89392900	-0.73290700	-0.08172800
H	-1.34890700	-0.01399900	1.81790200
H	-0.79737700	2.58590100	-0.02471400
H	1.57707700	2.71475500	-0.17469700
H	3.11169400	0.97433100	-0.13679700
H	2.82985400	-1.29141900	-0.16828700
Si	-1.11129600	0.03230700	0.33080200
Si	0.34980900	-1.82843200	-0.03530600
O	-2.58227400	0.13931000	-0.47989400
H	-3.17638800	-0.61797500	-0.44152200

B'11(NH2)

E = -790.347630 a.u.

C	-0.16886400	1.67168300	0.03660000
C	1.18003900	1.71157000	-0.08741600
C	2.10762200	0.57759700	-0.10888700
C	1.88437900	-0.77557400	-0.09417300
H	-1.24588400	0.07228100	1.86016700
H	-0.69469900	2.62710000	-0.01121500
H	1.66863300	2.67863600	-0.21185300
H	3.15069100	0.89482300	-0.18769100
H	2.80260200	-1.36205600	-0.18552100
Si	-1.09619600	0.06975500	0.35665400
Si	0.31027100	-1.82157200	-0.01435800
H	-3.03377300	-0.79883900	-0.78307300
N	-2.61871700	0.07637500	-0.49304700
H	-3.33265500	0.76721900	-0.29837800

B'12(OMe)

E = -849.532231 a.u.

C	-0.46532900	-1.71144500	0.03949200
C	-1.80368400	-1.56270700	-0.10592500
C	-2.56837100	-0.31093100	-0.13837000
C	-2.16308800	0.99811700	-0.11376700
H	0.90092200	-0.26805700	1.87399300
H	-0.06283300	-2.72386900	-0.00619400
H	-2.41753700	-2.45349300	-0.24303800
H	-3.64277900	-0.48355900	-0.24048800
H	-2.99032000	1.70419500	-0.22551600
Si	0.66192000	-0.26069700	0.38533100
Si	-0.46084800	1.82283900	0.00373500
O	2.11338000	-0.57751200	-0.39345900
C	3.28137500	0.21027500	-0.18729800
H	4.08190800	-0.21006200	-0.80251600
H	3.12394300	1.25633100	-0.48520300
H	3.59924100	0.18876200	0.86491700

B'13(SiMe3)

E = -1143.670838 a.u.

C	-1.06264500	1.63096100	-0.85605100
C	-2.01435500	1.71680600	0.11628100
C	-2.65231100	0.61732900	0.82039600
C	-2.51539000	-0.74328900	0.66923700
H	0.33683000	0.04620300	-2.66268000
H	-0.75181900	2.56463300	-1.32611900
H	-2.39361100	2.70229900	0.38874000
H	-3.38863500	0.95360200	1.55436100
H	-3.20742200	-1.31327100	1.29603600
Si	-0.24340700	0.01406100	-1.28930800
Si	-1.38481300	-1.83318200	-0.37507100
Si	1.64488000	0.01743800	0.21094500
C	2.63539000	1.60326900	-0.10244700
H	2.03757400	2.49086000	0.13012000
H	3.52921900	1.61841800	0.53449300
H	2.96155100	1.67549700	-1.14541300
C	1.04983000	-0.00503700	2.00756500
H	0.63417600	-0.98061500	2.28032700
H	1.88446100	0.21190600	2.68559300
H	0.27172300	0.74717100	2.17434500
C	2.72532700	-1.49776400	-0.14272900
H	3.06240300	-1.51449000	-1.18483700
H	3.61531100	-1.48474600	0.49907000
H	2.17993400	-2.42756000	0.05052500

C2(F)

E = -933.584862 a.u.

C	1.55672700	1.08605800	0.12422100
C	0.71060900	2.18414500	0.05716000
C	-0.71060900	2.18414500	-0.05716000
C	-1.55672700	1.08605800	-0.12422100
H	2.61941700	1.29986100	0.24867200
H	1.16946000	3.17017800	0.12155200
H	-1.16946000	3.17017800	-0.12155200
H	-2.61941700	1.29986100	-0.24867200
Si	1.08037700	-0.61414000	-0.29287200
Si	-1.08037700	-0.61414000	0.29287200
F	2.20614300	-1.72147700	0.11242600
F	-2.20614300	-1.72147700	-0.11242600

C3(Cl)

E = -1654.276200 a.u.

C	-1.57310000	1.52701000	-0.00802500
C	-0.71225500	2.61671000	-0.00384600
C	0.71225500	2.61671000	0.00384600
C	1.57310000	1.52701000	0.00802500
H	-2.64016500	1.74895300	-0.03817200
H	-1.17136800	3.60440900	-0.02775800
H	1.17136900	3.60440900	0.02775800
H	2.64016500	1.74895300	0.03817200
Si	-1.06788600	-0.18340100	0.30579000
Si	1.06788600	-0.18340100	-0.30579000
Cl	2.49647400	-1.62635700	0.10240800
Cl	-2.49647400	-1.62635700	-0.10240800

C4(Me)

E = -813.650290 a.u.

C	-1.57647200	1.19520400	-0.00005500
C	-0.70862400	2.28695900	-0.00001000
C	0.70855700	2.28697700	0.00006300
C	1.57643500	1.19524500	0.00006200
H	-2.64079000	1.43637300	-0.00008600
H	-1.16777200	3.27547000	0.00000500
H	1.16767700	3.27550100	0.00010700
H	2.64074500	1.43645000	0.00011800
Si	-1.09270800	-0.53761200	-0.00039200
Si	1.09271300	-0.53759000	0.00027800
C	-2.38444900	-1.91387600	0.00031000
H	-1.89628700	-2.89317300	-0.00183900
H	-3.02078600	-1.85242500	0.88905500
H	-3.02401900	-1.85017500	-0.88595500
C	2.38452000	-1.91379400	-0.00021100
H	1.89641600	-2.89312400	0.00180300
H	3.02109100	-1.85229700	-0.88878000
H	3.02385100	-1.85005900	0.88622400

C5(CF3)

E = -1409.091605 a.u.

C	-1.57300000	2.03559500	0.13324100
C	-0.70961100	3.12237100	0.05771100
C	0.70938900	3.12241700	-0.05768000
C	1.57290500	2.03573100	-0.13320900
H	-2.63661100	2.26406100	0.19726500
H	-1.16643100	4.11096600	0.07401800
H	1.16613300	4.11104900	-0.07398300
H	2.63647400	2.26438000	-0.19721600
Si	-1.05306200	0.31887000	0.31967600
Si	1.05315200	0.31894300	-0.31966600
C	-2.44748400	-0.99157000	-0.03472900
C	2.44749400	-0.99154200	0.03480200
F	-2.66800100	-1.20516700	-1.35867000
F	-2.16711100	-2.20287700	0.51418700
F	2.16671300	-2.20290200	-0.51371600
F	3.63123300	-0.57435900	-0.49882200
F	2.66860500	-1.20478300	1.35865700
F	-3.63132600	-0.57411600	0.49824900

C6(CCl3)

E = -3571.162515 a.u.

C	-1.57417300	2.47383600	0.11473600
C	-0.71068000	3.56003000	0.04905100
C	0.71062800	3.55998300	-0.04909100
C	1.57417100	2.47379100	-0.11465200
H	-2.63851900	2.70076000	0.16834200
H	-1.16775000	4.54877700	0.06006100
H	1.16773900	4.54871400	-0.06027700
H	2.63847200	2.70085400	-0.16835600
Si	-1.05290200	0.75862600	0.32839400
Si	1.05276300	0.75860000	-0.32785800
C	-2.41561400	-0.57564000	-0.01016500
C	2.41560100	-0.57567900	0.01022300
Cl	3.90738800	-0.09422900	-0.90813200
Cl	1.83902500	-2.18406500	-0.57880100
Cl	2.82145900	-0.69924500	1.77020700
Cl	-1.83892400	-2.18403300	0.57875000
Cl	-3.90768000	-0.09452600	0.90784900
Cl	-2.82112800	-0.69909100	-1.77033700

C7(SiH3)

E = -1316.407012 a.u.

C	1.58234500	1.68362900	-0.00072100
C	0.71059500	2.76744000	-0.00030600
C	-0.71058200	2.76744500	0.00039300
C	-1.58233900	1.68364000	0.00077000
H	2.64439700	1.93090000	-0.00145500
H	1.16538000	3.75801700	-0.00064600
H	-1.16536000	3.75802500	0.00052500
H	-2.64439000	1.93092000	0.00115500
Si	1.09947000	-0.06067000	-0.00111500
Si	-1.09947700	-0.06066200	0.00116200
Si	2.67114800	-1.78747000	0.00065000
Si	-2.67115200	-1.78746500	-0.00062900
H	-1.94017900	-3.08110800	0.00298900
H	-3.54114500	-1.71843800	1.20318100
H	-3.53531500	-1.72198100	-1.20882300
H	1.94041300	-3.08095200	-0.02725800

H	3.52044200	-1.73685000	1.22004800
H	3.55579500	-1.70371500	-1.19149600

C8(SiF3)

E = -1912.283870 a.u.

C	-1.59120400	2.41200200	0.08306700
C	-0.72804600	3.50084800	0.03728300
C	0.69257800	3.51714000	-0.03603900
C	1.58144900	2.44911200	-0.08320100
H	-2.65480900	2.64137000	0.13550900
H	-1.19205200	4.48616700	0.05604000
H	1.13371000	4.51294400	-0.05279100
H	2.63868000	2.70644600	-0.13401800
Si	-1.07319600	0.68326100	0.12637100
Si	1.10253900	0.70947100	-0.12990100
Si	-2.65190100	-1.00196700	-0.01569100
Si	2.66380700	-0.98999300	0.01542800
F	-2.85844400	-1.56693600	-1.50529100
F	-2.25972700	-2.26121300	0.90062700
F	-4.07876400	-0.45196500	0.48232000
F	1.95583400	-2.40193500	-0.27841500
F	3.85056500	-0.79789000	-1.05169700
F	3.36479500	-1.10143100	1.45709200

C9(SiCl3)

E = -4074.304903 a.u.

C	1.58862500	2.84056700	-0.12012700
C	0.73046100	3.93240900	-0.05382700
C	-0.68856100	3.95368200	0.05182700
C	-1.57982000	2.88854900	0.11763800
H	2.65219300	3.06467800	-0.19466000
H	1.19745100	4.91631300	-0.07992100
H	-1.12566200	4.95120400	0.07881700
H	-2.63530600	3.14780300	0.19243800
Si	1.06124400	1.11432800	-0.18274100
Si	-1.10134000	1.14856500	0.17995700
Si	2.63062900	-0.58751600	0.00510600
Si	-2.65161800	-0.56798300	-0.00520200
Cl	2.84655200	-1.25663900	1.95115600
Cl	4.46124100	0.13581000	-0.64247900
Cl	2.08496200	-2.20215200	-1.16384900
Cl	-1.68392000	-2.34822500	0.40809700
Cl	-4.19585200	-0.29167900	1.34631600
Cl	-3.48579200	-0.70033600	-1.89509000

C10(OH)

E = -885.522502 a.u.

C	-1.54245300	1.14579100	-0.07859100
C	-0.66551700	2.22180500	-0.02696100
C	0.75554700	2.19341900	0.04603900
C	1.58738200	1.08026600	0.08326500
H	-2.60342600	1.38900800	-0.15281400
H	-1.10467000	3.21845100	-0.06296000
H	1.23470900	3.17112100	0.09050700
H	2.65704400	1.29089000	0.15097400
Si	-1.09914400	-0.57671600	0.23928500
Si	1.07520100	-0.62251200	-0.27105400
O	2.17314700	-1.84004800	0.04819000
O	-2.32850400	-1.64493600	-0.13057600
H	2.82621400	-1.69873500	0.74438200
H	-2.24156600	-2.54934800	0.19126800

C11(NH2)

E = -845.766002 a.u.

C	-1.56902500	1.13333600	-0.04140600
C	-0.71334500	2.22704000	-0.02281800
C	0.70937500	2.22827100	0.02289800
C	1.56693600	1.13603800	0.04150500
H	-2.63549700	1.36587100	-0.07301300
H	-1.17293000	3.21506600	-0.05068000
H	1.16726600	3.21707500	0.05087200
H	2.63297400	1.37055300	0.07335300
Si	-1.09554500	-0.59172700	0.24799600
Si	1.09689800	-0.58992300	-0.24833200
N	2.34104000	-1.73927000	0.08096200
N	-2.33820600	-1.74280100	-0.08061700
H	2.33712800	-2.67040100	-0.30826900
H	3.02655000	-1.62559300	0.81523500
H	-2.33210800	-2.67477700	0.30652500
H	-3.02581000	-1.62830900	-0.81280600

C12(OMe)

E = -964.128485 a.u.

C	1.14275000	2.00008800	0.11440200
C	0.00096600	2.78995000	0.13782400
C	-1.35938300	2.37828000	0.03332000
C	-1.85133000	1.08792700	-0.11388400
H	2.09710500	2.52202800	0.19431100
H	0.14857000	3.86571100	0.23249900
H	-2.08964000	3.18482400	0.09581400
H	-2.93931300	0.99940400	-0.15062200
Si	1.14496200	0.19585200	0.23169400
Si	-0.86962600	-0.38055700	-0.54457800
O	-1.62674300	-1.85397200	-0.41291200
O	2.63611400	-0.48792600	-0.02928300
C	2.89015700	-1.89384100	-0.02917100
C	-2.48121000	-2.25529100	0.66253400

H	-2.95686100	-3.19695700	0.37559100
H	-1.89767600	-2.41060300	1.57892900
H	-3.25875600	-1.50727900	0.85929400
H	2.43651500	-2.37190400	-0.90644500
H	3.97346200	-2.03109400	-0.07050100
H	2.50522900	-2.37575200	0.87890700

C13(SiMe3)

E = -1552.412587 a.u.

C	-1.57321300	2.52137500	0.00705900
C	-0.68721400	3.59545400	0.00752500
C	0.73312900	3.57644600	0.00451000
C	1.58898800	2.47829500	-0.00014000
H	-2.63153500	2.78648600	0.00721100
H	-1.12833400	4.59265100	0.00938100
H	1.20101000	4.56137700	0.00506500
H	2.65471600	2.71173000	-0.00364100
Si	-1.11774500	0.76752300	0.00287600
Si	1.08744400	0.73700100	-0.00577600
Si	-2.67941200	-0.98217700	-0.00010800
Si	2.66495500	-1.00167100	-0.00020100
C	2.31369400	-2.18788200	-1.43582800
H	1.31437000	-2.62783000	-1.34874300
H	2.37397900	-1.67511100	-2.40147200
H	3.04352200	-3.00704800	-1.43713800
C	4.39082500	-0.24250200	-0.18786000
H	4.61579500	0.44559700	0.63418700
H	5.15243200	-1.03194100	-0.18486900
H	4.48219900	0.31190800	-1.12797200
C	2.55580400	-1.96538700	1.62865600
H	3.27161600	-2.79690700	1.62739000
H	2.77860900	-1.32362300	2.48749700
H	1.55341500	-2.38314200	1.77343000
C	-3.96633000	-0.71415300	-1.36526200
H	-4.69265500	-1.53659000	-1.36846700
H	-4.51771100	0.22047800	-1.21488400
H	-3.49525700	-0.67077600	-2.35278400
C	-3.55982900	-1.09818300	1.67459800
H	-4.10972400	-0.17797300	1.89982800
H	-4.27723700	-1.92849600	1.66861200
H	-2.84623100	-1.26962100	2.48740100
C	-1.71911800	-2.58524700	-0.32384800
H	-1.22534800	-2.56082200	-1.30109300
H	-0.95196300	-2.75372500	0.44008000
H	-2.39948300	-3.44537500	-0.31056200

C'2(F)

E = -933.581443 a.u.

C	-0.08116700	1.67357600	0.00042400
C	1.26890500	1.75289400	0.00070500
C	2.24749500	0.65045100	0.00031300
C	2.08797900	-0.70824300	-0.00153800
H	-0.64156200	2.60913800	0.00004600
H	1.73211300	2.73988300	0.00100000
H	3.27672300	1.01719300	0.00130300
H	3.03615000	-1.25217900	-0.00211500
Si	-0.95698000	0.02403900	-0.00039900
Si	0.56513600	-1.83893500	-0.00043900
F	-1.94623700	0.00297500	1.29835300
F	-1.94897300	0.00618500	-1.29701200

C'3(Cl)

E = -1654.263601 a.u.

C	0.35821400	1.67068300	0.00012200
C	1.70829100	1.75039500	0.00014400
C	2.68473000	0.65066900	0.00009000
C	2.52043300	-0.70790300	-0.00001600
H	-0.21050300	2.60031500	0.00017600
H	2.16684800	2.73933900	0.00021600
H	3.71459400	1.01476500	0.00015400
H	3.46658600	-1.25576500	-0.00001600
Si	-0.52154000	0.02192300	-0.00001200
Si	1.00012200	-1.83712700	-0.00016400
Cl	-1.74903400	0.00369300	1.70038400
Cl	-1.74906500	0.00402100	-1.70038900

C'4(Me)

E = -813.623433 a.u.

C	0.02611000	1.64719800	0.00032900
C	1.37818600	1.72520800	0.00039600
C	2.34295200	0.61977700	0.00020700
C	2.16091600	-0.73777900	-0.00051700
H	-0.51156000	2.59894500	0.00022700
H	1.84690600	2.71036500	0.00050500
H	3.37790900	0.97225200	0.00053200
H	3.09961100	-1.29851800	-0.00083200
Si	-0.94099200	0.02661300	0.00003100
Si	0.60223700	-1.81047800	0.00023800
C	-2.06131900	0.02551500	-1.54191600
H	-2.67264500	-0.88327800	-1.57278500
H	-2.73613300	0.88979900	-1.52025800
H	-1.47814400	0.07519600	-2.46731100
C	-2.06232500	0.02502300	1.54124500
H	-2.67364700	-0.88380200	1.57111800
H	-1.47976300	0.07415200	2.46704400
H	-2.73707400	0.88933900	1.51952800

C'5(CF3)

E = -1409.077832 a.u.

C	0.90397500	0.00037300	1.66668600
C	2.25254800	0.00046400	1.76769200
C	3.24492200	0.00022500	0.68289600
C	3.10009000	-0.00026000	-0.67859800
H	0.32327900	0.00056800	2.58831200
H	2.69577000	0.00074100	2.76332300
H	4.26931400	0.00044500	1.06136300
H	4.05499400	-0.00042900	-1.21072700
Si	0.05201200	-0.00000600	0.00599100
Si	1.60880400	-0.00056300	-1.84203000
C	-1.14643600	1.54298900	0.00056700
C	-1.14650000	-1.54293900	0.00101600
F	-0.41623500	2.70055100	-0.05056800
F	-1.98224100	1.56232700	-1.07056800
F	-1.92618600	1.62707600	1.11261400
F	-1.98160700	-1.56294400	-1.07067500
F	-1.92700200	-1.62626400	1.11257900
F	-0.41632700	-2.70057700	-0.04885600

C'6(CCl3)

E = -3571.153506 a.u.

C	-0.00350700	1.22679800	1.67242900
C	-0.00733900	2.57474400	1.76822400
C	-0.01002900	3.56382400	0.68183900
C	-0.01036500	3.41006700	-0.67646800
H	-0.00224200	0.64850400	2.59489900
H	-0.00881600	3.01937800	2.76342300
H	-0.01239000	4.58990700	1.05604600
H	-0.01325600	4.36010600	-1.21752600
Si	-0.00073200	0.36015200	0.01960100
Si	-0.00518600	1.90528900	-1.82809400
C	-1.62066400	-0.73040900	0.00621500
C	1.62514400	-0.72143200	0.00630900
Cl	-2.94986900	0.53640700	-0.05503300
Cl	-1.76100900	-1.77063600	-1.45314500
Cl	-1.83642100	-1.73222300	1.48874300
Cl	1.83973200	-1.73064900	1.48419200
Cl	1.77575600	-1.75292300	-1.45844600
Cl	2.94828800	0.55146000	-0.04332300

C'7(SiH3)

E = -1316.378159 a.u.

C	-0.47409400	-0.00078800	1.64300900
C	-1.82810600	-0.00083400	1.74189400
C	-2.80257200	-0.00021700	0.65529300
C	-2.63215400	0.00043800	-0.70622400
H	0.08577200	-0.00133100	2.57947100
H	-2.27532800	-0.00140400	2.73652400
H	-3.83383800	-0.00037600	1.01653900
H	-3.57737200	0.00075000	-1.25661100
Si	0.44263200	0.00004300	-0.00004200
Si	-1.10866700	0.00103900	-1.82099900
Si	1.86681300	1.89280200	0.01249600
Si	1.86639600	-1.89304700	0.01089200
H	1.07219400	-3.15062600	-0.01165200
H	2.75387700	-1.86880300	-1.18244800
H	2.71411800	-1.89615000	1.23494300
H	2.71496100	1.89451400	1.23625300
H	1.07287100	3.15057200	-0.00853200
H	2.75387500	1.86952800	-1.18117400

C'8(SiF3)

E = -1912.260221 a.u.

C	1.21499300	-0.02537000	1.65916600
C	2.56577600	-0.02617200	1.76471900
C	3.55435200	-0.01513800	0.68640600
C	3.40536900	-0.00994800	-0.67683300
H	0.63624900	-0.04555400	2.58174700
H	3.00255100	-0.04087400	2.76308900
H	4.57976500	-0.01595200	1.06161900
H	4.35958300	-0.00976900	-1.21105000
Si	0.34914000	-0.00173700	-0.00734200
Si	1.92161700	0.00600100	-1.84140200
Si	-1.09969600	-1.84138700	-0.00470400
Si	-1.08059000	1.85113000	0.00515000
F	-0.25247600	3.21903800	0.20590000
F	-2.16606400	1.79190800	1.19341000
F	-1.89305500	1.99785400	-1.37500900
F	-1.61104700	-2.21057400	1.47693200
F	-0.37195500	-3.16019000	-0.57854800
F	-2.40403400	-1.59628000	-0.91379700

C'9(SiCl3)

E = -4074.284269 a.u.

C	0.15960600	1.57284300	1.65637800
C	0.35653700	2.90862400	1.76722000
C	0.49555000	3.89023900	0.69104100
C	0.47148800	3.74585900	-0.67195800
H	0.08144200	0.99432100	2.57600200
H	0.42342600	3.33737700	2.76703800
H	0.64271500	4.90421400	1.06870000
H	0.60534200	4.69174900	-1.20439400
Si	0.04214400	0.72176900	-0.00902400
Si	0.25896200	2.27865100	-1.83915600

Si	1.79127900	-0.84810200	-0.00155500
Si	-1.96521800	-0.49682600	-0.00038800
Cl	-3.53873600	0.82261700	0.31366500
Cl	-2.00389400	-1.91764900	1.50792300
Cl	-2.27003700	-1.44640300	-1.81242500
Cl	1.52661600	-2.30617300	-1.44390100
Cl	1.98794100	-1.76822700	1.84504200
Cl	3.56679500	0.15642700	-0.40805100

C'10(OH)

E = -885.511369 a.u.

C	-0.05544200	1.65836400	-0.09977700
C	1.29531600	1.74165100	-0.08218500
C	2.27028100	0.64064800	-0.00798300
C	2.10088700	-0.71582000	0.01540700
H	-0.60045500	2.60275500	-0.18083200
H	1.76072800	2.72685500	-0.13629200
H	3.30076800	1.00437700	0.01785100
H	3.04505000	-1.26597000	0.05182900
Si	-0.96628400	0.01289000	-0.01241300
Si	0.55809400	-1.82883800	0.00125400
O	-1.86213000	0.03688500	1.41566400
O	-2.00802700	-0.14602600	-1.30889700
H	-2.73770600	0.47930000	-1.39872700
H	-1.75872300	0.80002200	1.99548400

C'11(NH2)

E = -845.747538 a.u.

C	-0.02617300	1.66178900	-0.00115400
C	1.32628700	1.71879500	-0.00088400
C	2.27404300	0.59875100	-0.00095700
C	2.07283200	-0.75521800	-0.00151100
H	-0.54987900	2.62128700	-0.00211200
H	1.80954600	2.69672400	-0.00110900
H	3.31418100	0.93538500	-0.00078100
H	3.00412700	-1.32800000	-0.00180500
Si	-0.97010100	0.03693800	-0.00049000
Si	0.50646700	-1.82306600	-0.00182400
H	-2.23148100	0.88082700	-1.92821400
H	-2.20475600	0.87849600	1.94714700
N	-1.84876600	0.03898500	1.50788700
N	-1.85894600	0.04123900	-1.50275000
H	-2.28218600	-0.79362700	1.88394900
H	-2.29662100	-0.79157000	-1.87360900

C'12(OMe)

E = -964.116667 a.u

C	-0.10157800	1.53609400	0.00028900
C	-1.40102700	1.91453900	0.00038400
C	-2.59742900	1.05739100	0.00020100
C	-2.73698800	-0.30310300	-0.00006400
H	0.63155400	2.34511700	0.00042400
H	-1.63623300	2.98003700	0.00061600
H	-3.52142000	1.64176500	0.00028700
H	-3.78115600	-0.62759800	-0.00015700
Si	0.40689900	-0.28009000	-0.00002700
Si	-1.48307300	-1.73172700	-0.00023100
O	1.29559800	-0.56822400	-1.38755400
O	1.29571800	-0.56868400	1.38733300
C	2.33293500	0.24655300	1.92179500
C	2.33268500	0.24727700	-1.92188000
H	2.02584800	1.29816900	1.99933500
H	2.57061200	-0.11929300	2.92486300
H	3.23976500	0.18436600	1.30536900
H	2.02544400	1.29886500	-1.99915500
H	3.23954500	0.18507100	-1.30550800
H	2.57036200	-0.11829700	-2.92505000

C'13(SiMe3)

E = -1552.383324 a.u

C	0.77777000	1.02820200	1.58667100
C	2.01146000	1.59142200	1.71288500
C	2.93478700	1.93594800	0.64524900
C	2.80349200	1.82931000	-0.71935800
H	0.20734400	0.89686500	2.50784700
H	2.36454300	1.85438600	2.71102500
H	3.86367100	2.37894500	1.01319600
H	3.65884500	2.23918400	-1.26469000
Si	0.07338700	0.43516500	-0.04595100
Si	1.48006900	1.08191500	-1.83413000
Si	0.61490900	-1.90442400	0.04004300
Si	-2.28421400	0.65775700	-0.02982800
C	-2.89118500	0.49793800	1.76177500
H	-3.98254500	0.60244800	1.80298800
H	-2.62972600	-0.47489600	2.19173200
H	-2.45623900	1.27597100	2.39869400
C	-2.77637700	2.36275900	-0.69937500
H	-2.46003300	2.48431800	-1.74113800
H	-3.86518400	2.49204000	-0.65819000
H	-2.31764400	3.16688500	-0.11342700
C	-3.11108000	-0.68121200	-1.08908200
H	-2.93283300	-1.68254700	-0.68272100
H	-4.19573100	-0.51894400	-1.11664100
H	-2.74395800	-0.66482500	-2.12099600
C	0.15183400	-2.74262600	-1.59537700
H	0.36683500	-3.81725800	-1.53996200

H	-0.91122700	-2.62297200	-1.82660900
H	0.72631000	-2.32336700	-2.42827900
C	2.46930600	-2.11650800	0.35728600
H	2.79188100	-1.53694900	1.22836700
H	2.70657100	-3.17194000	0.54056500
H	3.05714300	-1.78025400	-0.50328800
C	-0.36151600	-2.70049800	1.45988300
H	-1.44190400	-2.62073200	1.29936800
H	-0.11007800	-3.76583600	1.53935300
H	-0.12509400	-2.22470300	2.41759400

D1(H)

E = -1039.853911 a.u

C	1.37292700	-0.06209900	1.75941200
C	2.56219100	0.56432300	1.49122800
C	3.33581900	0.60813300	0.26744500
C	3.09927400	-0.08289700	-0.89634800
H	1.99362100	-2.29956900	-1.92824800
H	1.04930900	-0.06014400	2.80134000
H	3.04556700	1.06960700	2.33118800
H	4.26584000	1.17238200	0.35049700
H	3.91215000	-0.02208000	-1.62713200
Si	0.42076900	-1.05002100	0.50481800
Si	1.54839600	-0.90605400	-1.56170800
H	-0.22613200	-2.24448900	1.14378100
C	-1.22007900	-0.03473900	0.17523000
N	-1.28874500	1.27437600	-0.17548900
N	-2.50081000	-0.48909700	0.12319100
C	-3.35979500	0.52590400	-0.26122700
C	-2.59389800	1.63526100	-0.44743300
H	-4.42191400	0.37324400	-0.36646600
H	-2.86187500	2.63586900	-0.74635200
C	-0.13299300	2.17054200	-0.31536300
C	-2.92092800	-1.86795600	0.38180000
H	-0.50231400	3.16839700	-0.55420000
H	0.43259900	2.18544300	0.61625600
H	0.51092200	1.80199000	-1.11892000
H	-2.47438500	-2.54097700	-0.35271600
H	-2.61234400	-2.17426900	1.38194900
H	-4.00757900	-1.91614500	0.30311800

D2(F)

E = -1238.478164 a.u

C	1.21898600	-1.08718600	-1.46407400
C	2.54555600	-1.41741300	-1.27549100
C	3.49799800	-0.85751200	-0.35629000
C	3.25437500	0.13658200	0.56745400
H	0.72348000	-1.58802400	-2.30015200
H	2.95446700	-2.18664100	-1.93352200
H	4.51513800	-1.23583600	-0.45986600
H	4.12757400	0.50622600	1.11171500
Si	0.37153200	0.37848100	-0.73847000
Si	1.59385000	0.62891000	1.21586800
C	-1.39486800	-0.19027200	-0.13087000
N	-1.70731300	-1.33290500	0.53468500
N	-2.54438400	0.53562600	-0.16395800
C	-3.56207700	-0.14510300	0.47543100
C	-3.03412200	-1.31950300	0.91674700
H	-4.55934200	0.25614500	0.55800900
H	-3.48326800	-2.13469100	1.46079000
C	-0.76959100	-2.40351300	0.89946700
C	-2.70307700	1.87227400	-0.75336500
H	-1.35233000	-3.27382700	1.20565900
H	-0.13998600	-2.64418500	0.04349000
H	-0.12505800	-2.05855300	1.71184400
H	-3.71316400	2.21897500	-0.53394200
H	-1.97842400	2.55910800	-0.31397000
H	-2.53937700	1.82961900	-1.82895100
F	-0.19684300	1.34757200	-1.97860400
F	1.69659300	2.17454300	1.83706900

D3(Cl)

E = -1959.169869 a.u

C	0.44412500	-2.19042200	0.46435900
C	1.66273900	-2.65269000	0.90231400
C	2.92805900	-1.96666100	1.00546900
C	3.16473500	-0.63921900	0.75045700
H	-0.32448000	-2.95708800	0.37423200
H	1.70570300	-3.70740100	1.17969000
H	3.77105200	-2.60277900	1.27542900
H	4.20439500	-0.31107900	0.80970900
Si	0.17686800	-0.54057900	-0.33623800
Si	1.86486900	0.67856000	0.67390200
C	-1.53155800	0.19131000	0.22999800
N	-1.82616600	1.50049500	0.44598100
N	-2.70499100	-0.47558900	0.39663400
C	-3.71529800	0.40243600	0.73491300
C	-3.16181000	1.64510200	0.76680300
H	-4.72588800	0.07352300	0.91668000
H	-3.59839200	2.60747600	0.97982500
C	-0.88759400	2.62156500	0.34231700
C	-2.89308300	-1.91763600	0.22867500
H	-1.44985300	3.54923400	0.44974400
H	-0.13128000	2.54230200	1.12878800
H	-0.38917800	2.60922000	-0.62778200

H	-3.96290500	-2.11977800	0.17060100
H	-2.41606300	-2.24037100	-0.69825000
H	-2.46238500	-2.45197800	1.07738400
Cl	-0.45114500	-0.92327100	-2.38712800
Cl	2.61886000	2.27267900	-0.56660600

D4(Me)

E = -1118.509443 a.u

C	0.99094400	1.91904500	0.63412700
C	2.06909800	2.32981500	-0.11823800
C	2.97160000	1.56446900	-0.93711500
C	2.98906700	0.19479100	-1.08869800
H	0.56347900	2.68597000	1.28671800
H	2.32570300	3.39019800	-0.05302100
H	3.75898100	2.14917500	-1.41415100
H	3.83673800	-0.19308800	-1.66281900
Si	0.42065600	0.16834600	0.85057700
Si	1.68074400	-1.05137800	-0.68781900
C	-1.40689800	0.01752900	0.10224600
N	-2.02810300	-1.15727700	-0.19473900
N	-2.26426100	0.98511300	-0.32210000
C	-3.39169900	0.42197700	-0.89390900
C	-3.23962100	-0.92721800	-0.81871300
H	-4.19220600	1.02124300	-1.29708600
H	-3.87748500	-1.73060400	-1.15081900
C	-1.43593600	-2.48093200	-0.01831300
C	-2.05115100	2.42861900	-0.19892200
H	-2.20586200	-3.23421500	-0.18898600
H	-0.61333100	-2.59842500	-0.73606300
H	-1.04704800	-2.58688600	0.99497900
H	-2.83997400	2.93987200	-0.75224400
H	-2.09077100	2.72806400	0.85067600
H	-1.07217400	2.68736100	-0.60376300
C	0.01792500	-0.17517800	2.69115600
C	2.51614600	-2.63772700	0.03728700
H	-0.46147900	-1.14838700	2.85176200
H	0.94783900	-0.16144400	3.27032000
H	-0.64670500	0.59810100	3.09958900
H	1.77512400	-3.42290500	0.23038600
H	3.22472200	-3.03791300	-0.69807500
H	3.06454400	-2.44967300	0.96640400

D5(CF3)

E = -1713.991484 a.u

C	0.36329500	2.42729300	0.23786100
C	-0.61723400	3.20590700	0.79223800
C	-1.92726500	2.84605700	1.30220300
C	-2.47198200	1.59554900	1.37082700
H	1.20079700	2.97270800	-0.19556900
H	-0.42249800	4.28005700	0.80890500
H	-2.54103900	3.69760300	1.59559500
H	-3.51313300	1.55450100	1.70072400
Si	0.17923300	0.61070400	-0.07895300
Si	-1.60507600	-0.06273200	1.27443900
C	1.76308700	-0.36804800	0.52019600
N	1.81234100	-1.70659500	0.74075100
N	3.00394300	0.09538400	0.81902600
C	3.81664100	-0.94046500	1.23433100
C	3.06453100	-2.07466400	1.18531600
H	4.84446500	-0.78545400	1.52048900
H	3.31158000	-3.09709100	1.42174900
C	0.69817700	-2.64344600	0.54803200
C	3.45218000	1.48475400	0.68562300
H	1.07594900	-3.65652600	0.68516300
H	-0.08627600	-2.43300400	1.27988800
H	0.29315300	-2.53896600	-0.45768000
H	3.33524700	1.80722900	-0.34991500
H	2.86424400	2.12805400	1.34098200
H	4.50466700	1.53207000	0.96540500
C	0.59230300	0.34688200	-1.99328500
C	-2.79138300	-1.08920600	0.07640100
F	-0.28708000	0.92415800	-2.84138600
F	1.83495200	0.87006300	-2.31420200
F	0.66354500	-0.98143000	-2.34053400
F	-4.02343400	-1.29437800	0.64203700
F	-3.04268400	-0.56345400	-1.16199400
F	-2.28679200	-2.35473600	-0.17608100

D6(CCl3)

E = -3876.064297 a.u

C	-1.09584800	-1.40444300	1.92510300
C	-0.26860500	-1.75060400	2.95810800
C	1.08195500	-1.31891200	3.25583300
C	1.85480800	-0.46059700	2.52688100
H	-2.01314700	-1.98805700	1.84716600
H	-0.64683400	-2.51212500	3.64287700
H	1.52852100	-1.80916200	4.12092200
H	2.88854900	-0.35719200	2.86386400
Si	-0.63296600	-0.30119700	0.51080600
Si	1.34688400	0.76780700	1.21260800
C	-1.97633200	1.12104600	0.37145700
N	-1.81557400	2.31053200	-0.26892700
N	-3.20901800	1.18972200	0.94776000
C	-3.80361600	2.40238700	0.66872800
C	-2.92566600	3.10781700	-0.09484100

H	-4.78678300	2.65612600	1.03083200
H	-2.99525900	4.09445500	-0.52354100
C	-0.60982500	2.75175800	-0.97554400
C	-3.84797700	0.16319800	1.77629000
H	-0.82040300	3.71177800	-1.44681900
H	0.20980500	2.85480600	-0.25787500
H	-0.33233500	2.02495800	-1.73525400
H	-3.96700300	-0.75475300	1.20170300
H	-3.23522200	-0.03143900	2.65669800
H	-4.82749900	0.53478600	2.07775400
C	-1.10786200	-1.35137400	-1.11171600
C	2.79637700	0.51237900	-0.12898800
Cl	-2.93220400	-1.63646300	-1.21217100
Cl	-0.29369900	-2.94956100	-1.03548400
Cl	-0.60395900	-0.49231000	-2.62730200
Cl	3.00599100	-1.18389800	-0.75621700
Cl	4.36532100	1.01162700	0.66509400
Cl	2.55210600	1.59799200	-1.58602700

D7(SiH3)

E = -1621.273951 a.u

C	0.35049500	-2.12623500	-0.78467300
C	1.27876000	-2.90474900	-0.14825500
C	2.29908800	-2.54744500	0.81788500
C	2.60061800	-1.29795100	1.28721900
H	-0.22919700	-2.62825400	-1.56157000
H	1.30054000	-3.95897600	-0.43518300
H	2.92151500	-3.38345000	1.13879500
H	3.47240900	-1.25890600	1.94742800
Si	0.19863600	-0.27833800	-0.57329200
Si	1.65504900	0.32430900	1.18423500
C	-1.58850100	0.12587200	0.14446400
N	-1.96558700	1.34870600	0.60610100
N	-2.65665800	-0.68461200	0.36728000
C	-3.68382500	0.02099200	0.96877000
C	-3.24640000	1.29986300	1.12078800
H	-4.62113900	-0.44173600	1.23282500
H	-3.72745300	2.16559300	1.54683700
C	-1.11243000	2.54117500	0.63448800
C	-2.74664400	-2.10322800	0.00945100
H	-1.71277100	3.38484500	0.97576200
H	-0.27589000	2.36912700	1.31938200
H	-0.73006400	2.75235200	-0.36453100
H	-3.66911100	-2.50361300	0.43140200
H	-2.76423300	-2.21550600	-1.07638000
H	-1.88647900	-2.63966000	0.40904000
Si	-0.06103700	0.68491300	-2.73271800
Si	3.15515500	1.85108600	0.19801400
H	1.21677100	0.62942000	-3.49078000
H	-1.09885900	-0.04073500	-3.52912400
H	-0.49621200	2.11305600	-2.67495600
H	3.84116000	1.45201700	-1.06993800
H	2.40256600	3.10591800	-0.13007600
H	4.23594300	2.25249400	1.14923600

D8(SiF3)

E = -2217.177058 a.u

C	0.64464500	-2.53173900	0.14734700
C	-0.26859100	-3.49810300	-0.16103600
C	-1.59782100	-3.38652400	-0.74348900
C	-2.21409600	-2.25911300	-1.19500100
H	1.52889300	-2.87696400	0.68048000
H	0.00716100	-4.52042000	0.10500000
H	-2.14889800	-4.32622700	-0.77673300
H	-3.23620300	-2.40117200	-1.55466600
Si	0.30759300	-0.70844800	-0.05651200
Si	-1.48942500	-0.55045800	-1.56889100
C	1.84994700	0.21504500	-0.83161100
N	1.81398500	1.47703200	-1.33370700
N	3.14075600	-0.18837900	-0.95366700
C	3.90195400	0.80583300	-1.53644400
C	3.06554900	1.85336200	-1.77451700
H	4.95621200	0.68524000	-1.72694100
H	3.25158900	2.82059600	-2.21284900
C	0.62839400	2.34612200	-1.38456900
C	3.68782800	-1.45973400	-0.46938100
H	0.92886400	3.30627000	-1.80325700
H	-0.13403600	1.89139900	-2.02000000
H	0.23115300	2.50290400	-0.38131300
H	3.57137400	-1.51656000	0.61472200
H	3.17049000	-2.29302300	-0.94466300
H	4.74759900	-1.49315000	-0.72205400
Si	0.68029200	0.25390500	2.06782400
Si	-2.83737100	0.83885200	-0.28546900
F	0.60911800	1.87494600	2.03652700
F	2.21473700	-0.07394700	2.52230100
F	-0.23704400	-0.23901700	3.29293700
F	-2.38572700	2.39463900	-0.50968300
F	-2.78330500	0.69023600	1.33537200
F	-4.41772100	0.79933500	-0.64981300

D9(SiCl3)

E = -4379.203939 a.u

C	-1.06761200	0.84175200	2.39384000
C	-0.25457500	1.46334200	3.29743700

C	1.04475100	2.09093600	3.12161600
C	1.77629800	2.18585100	1.97643500
H	-1.94584300	0.35092000	2.81014600
H	-0.60012900	1.46073900	4.33306300
H	1.48381800	2.46886300	4.04478800
H	2.76712900	2.63169500	2.09596300
Si	-0.62884700	0.56838500	0.60525500
Si	1.28682200	1.87735300	0.18061300
C	-2.06339000	1.25787400	-0.53522600
N	-1.95526800	1.48687100	-1.87054700
N	-3.33784900	1.60242700	-0.21000900
C	-4.01545900	2.04320900	-1.32908400
C	-3.14468400	1.96924700	-2.37284600
H	-5.04353600	2.36502700	-1.28808300
H	-3.26912600	2.21416900	-3.41529800
C	-0.75280300	1.27360200	-2.68708600
C	-3.94626000	1.51918300	1.12300700
H	-1.00750800	1.47960000	-3.72649000
H	0.03915700	1.94822300	-2.35249100
H	-0.41700800	0.24165000	-2.59860800
H	-3.97230100	0.48016600	1.45338600
H	-3.37075000	2.11687400	1.82967400
H	-4.96346300	1.90480000	1.05442600
Si	-1.16399300	-1.72359800	0.22161300
Si	2.84014900	0.22780100	-0.39807200
Cl	-1.63769800	-2.15045000	-1.77520100
Cl	0.26818800	-3.06343500	0.85755900
Cl	-2.92913400	-2.14836400	1.30350700
Cl	3.50543900	-1.08828900	1.08899000
Cl	4.59086100	1.06120900	-1.19930600
Cl	2.03857600	-0.99049300	-1.93065900

D10(OH)

E = -1190.406519 a.u

C	1.24111700	-1.08328200	-1.49156900
C	2.54755100	-1.45589300	-1.22889000
C	3.45432100	-0.94936000	-0.24283800
C	3.20204600	0.06755600	0.66191300
H	0.78922600	-1.54900400	-2.37285300
H	2.97399800	-2.22313200	-1.87880100
H	4.45133100	-1.39047000	-0.26191000
H	4.05608300	0.37081700	1.27553500
Si	0.35753300	0.37390000	-0.78881700
Si	1.55250400	0.70952800	1.16897600
C	-1.39385400	-0.20604700	-0.14737600
N	-1.65694600	-1.36135500	0.51929200
N	-2.55804700	0.49695900	-0.12381900
C	-3.53405800	-0.20939800	0.55226200
C	-2.96581700	-1.37720500	0.95806700
H	-4.53399600	0.17212100	0.68207100
H	-3.37507400	-2.20631700	1.51230100
C	-0.68178100	-2.40797200	0.85464900
C	-2.77159600	1.83869500	-0.68197000
H	-1.23243000	-3.27908900	1.21377900
H	-0.09379900	-2.65933300	-0.02709500
H	-0.00181200	-2.03066300	1.62345400
H	-3.79419500	2.13911400	-0.45098900
H	-2.07091500	2.54133600	-0.22895000
H	-2.60364500	1.82506300	-1.75708900
O	-0.27688100	1.36603900	-2.03476500
O	1.64964400	2.28302600	1.83339000
H	2.21287800	2.89910200	1.35037500
H	0.41711000	1.77814500	-2.56486400

D11(NH2)

E = -1150.635838 a.u

C	0.95049600	1.94417600	-0.26866600
C	2.20407300	2.15628600	-0.80694500
C	3.31061000	1.25292000	-0.93948900
C	3.32389800	-0.08145900	-0.58214100
H	0.33355700	2.84192600	-0.19739300
H	2.41151800	3.17012200	-1.15692100
H	4.22450600	1.69690300	-1.33588400
H	4.28177000	-0.59590500	-0.70312500
Si	0.37600100	0.42236500	0.62034200
Si	1.84620000	-1.12498800	-0.24359200
C	-1.42499700	-0.05775700	0.02005200
N	-1.91962800	-1.27927300	-0.32357100
N	-2.46357700	0.80769600	-0.15457000
C	-3.57630000	0.14345000	-0.63020600
C	-3.23477400	-1.16959700	-0.73582300
H	-4.50327900	0.65185700	-0.84252900
H	-3.80869200	-2.02531600	-1.05327600
C	-1.17990700	-2.54065800	-0.29256300
C	-2.40639300	2.24763700	0.09637900
H	-1.88301300	-3.35542000	-0.47099300
H	-0.39750400	-2.52240300	-1.06054200
H	-0.69130700	-2.67678100	0.67316900
H	-3.42389300	2.61518100	0.23884200
H	-1.81844200	2.42217100	0.99990300
H	-1.94450500	2.75465200	-0.75388400
H	2.66573200	-2.47173300	1.62254400
H	0.57775100	1.48658600	2.75028900
N	-0.14114600	0.98140600	2.23818800

N	2.12648600	-2.56923200	0.76840400
H	-0.56826700	0.30339000	2.86404100
H	2.41807700	-3.41267400	0.28851400

D12(OMe)

E = -1269.012395 a.u

C	0.74665100	1.44750200	1.55048500
C	1.95003700	2.09958900	1.37207400
C	2.95042400	1.90270000	0.35892400
C	2.90059600	0.98764700	-0.67294900
H	0.20623800	1.70202700	2.46733100
H	2.21187400	2.85259700	2.11901300
H	3.84604100	2.51453200	0.47262800
H	3.80484300	0.92656100	-1.28692700
Si	0.20164300	-0.06922600	0.64538400
Si	1.39364900	0.13970800	-1.34390200
C	-1.65235500	0.15449400	0.08720300
N	-2.21528800	1.29174500	-0.39973600
N	-2.59734700	-0.81101800	-0.06827400
C	-3.73466000	-0.28341000	-0.64903800
C	-3.49280200	1.03892600	-0.85906300
H	-4.60571700	-0.88399100	-0.85611000
H	-4.11140100	1.81075800	-1.28770300
C	-1.54368200	2.58870900	-0.55675600
C	-2.43787900	-2.23461400	0.25396300
H	-2.30679200	3.34330700	-0.75502400
H	-0.99143200	2.82875800	0.35074300
H	-0.83221200	2.52636800	-1.38458000
H	-1.62601300	-2.65624400	-0.34172000
H	-2.19402900	-2.34958000	1.30800400
H	-3.37250700	-2.74141600	0.01106000
O	-0.12627300	-1.32742400	1.75529900
O	1.82434300	-1.31221100	-2.12900800
C	2.63105700	-2.30455000	-1.51421700
C	0.94061800	-1.91713400	2.49520800
H	1.45568300	-1.17517200	3.11891000
H	0.51474700	-2.68845600	3.14487500
H	1.68085400	-2.38421600	1.83016000
H	3.59423900	-1.89501600	-1.17773300
H	2.12499700	-2.74405100	-0.63928100
H	2.82236000	-3.10068700	-2.24367300

D13(SiMe3)

E = -1857.273591 a.u

C	-0.64297500	1.06326800	2.09095200
C	0.04332900	2.17513100	2.50159800
C	1.08373800	2.92739600	1.83463800
C	1.72001700	2.60242800	0.66475500
H	-1.29716600	0.61746400	2.84343200
H	-0.18094600	2.53706700	3.50858400
H	1.44074000	3.79329500	2.39399600
H	2.56076100	3.25734700	0.41317900
Si	-0.38846200	0.18251400	0.46190800
Si	1.33645800	1.33770500	-0.67041000
C	-1.99225800	0.52067200	-0.64357400
N	-2.07694300	0.29207600	-1.98304700
N	-3.19883900	1.04706300	-0.29835600
C	-4.01874600	1.15589500	-1.40783500
C	-3.31055800	0.68255800	-2.46788300
H	-5.01858200	1.55484500	-1.34707900
H	-3.57200700	0.59391300	-3.51012800
C	-0.99423500	-0.22453400	-2.82549200
C	-3.61163000	1.43091100	1.05453800
H	-1.39291200	-0.40544800	-3.82446000
H	-0.17963500	0.50717000	-2.85531700
H	-0.61576800	-1.15931400	-2.41421300
H	-4.59874500	1.89061600	0.99157600
H	-3.66049600	0.54806700	1.69446300
H	-2.89232900	2.13315100	1.47501500
Si	-0.76778700	-2.12850800	0.89256400
Si	3.23409500	-0.06661800	-0.62658100
C	4.68217900	0.77738300	-1.53127800
H	4.95030700	1.72396100	-1.04756900
H	5.57198300	0.13458200	-1.52612300
H	4.42281600	0.99744500	-2.57284800
C	3.85943700	-0.52304000	1.11287000
H	3.08799200	-1.04294500	1.68972600
H	4.74682100	-1.16844900	1.06286700
H	4.12578700	0.38343600	1.66786500
C	2.85968300	-1.69440200	-1.55413500
H	2.08651000	-2.28152900	-1.04647600
H	2.51831100	-1.49784100	-2.57737900
H	3.76066300	-2.31799600	-1.61515600
C	0.65304800	-2.83464000	1.92818300
H	0.41392400	-3.84995500	2.26763800
H	1.58130500	-2.87925000	1.35018000
H	0.84094000	-2.21461000	2.81154400
C	-2.38415900	-2.27305100	1.89518400
H	-3.24547500	-1.93348300	1.30698700
H	-2.57104300	-3.31437600	2.18602400
H	-2.33905500	-1.67384200	2.81137600
C	-0.99314700	-3.20746800	-0.66086500
H	-1.18427200	-4.24609300	-0.36314400
H	-1.84948400	-2.87639600	-1.26016400

H	-0.10306500	-3.20715900	-1.29926600

D'1(H)

E = -1039.864801 a.u

C	1.49430000	1.37450500	0.89842500
C	2.72021400	1.50201900	0.32137200
C	3.43843000	0.55759500	-0.54201800
C	3.09609500	-0.69683900	-0.92868000
H	1.17132700	2.25118000	1.46640100
H	3.25408700	2.44289000	0.46966000
H	4.37052500	0.96479400	-0.94013200
H	3.77449000	-1.18152400	-1.63349000
Si	0.46897300	-0.20447500	1.15289800
Si	1.55863500	-1.63256600	-0.38848200
C	-1.18134100	0.09722600	0.21138800
N	-2.13429100	-0.88136100	0.07626900
N	-1.78511000	1.22814100	-0.27189400
C	-3.08291400	0.95629100	-0.68172300
C	-3.29717700	-0.36764900	-0.47130100
H	-3.72652600	1.71856300	-1.09079100
H	-4.16058600	-0.98341000	-0.66622000
C	-1.94951600	-2.26569000	0.49191000
C	-1.17305900	2.55028900	-0.34424200
H	-1.33231400	-2.80761000	-0.22918400
H	-1.45294800	-2.27921700	1.46846500
H	-2.92703700	-2.74474700	0.56941200
H	-0.15341700	2.45959500	-0.71913400
H	-1.76346300	3.17002900	-1.02135000
H	-1.14718000	3.01775200	0.64422000
H	1.97404000	-2.93340200	0.22356100
H	0.77811600	-2.05026400	-1.60464800

D'2(F)

E = -1238.504461 a.u

C	-0.96536200	2.04692900	-0.72411900
C	-2.18767800	2.31905200	-0.18225300
C	-3.12439100	1.41583400	0.48557300
C	-3.03631700	0.07506000	0.70950400
H	-0.45392200	2.92033300	-1.13572600
H	-2.52947000	3.35502300	-0.20604000
H	-4.00824800	1.92578200	0.87370500
H	-3.84218200	-0.38072400	1.28684000
Si	-0.25844700	0.35547500	-1.19399600
Si	-1.60129800	-0.95529300	0.17583700
C	1.42249700	0.16943500	-0.28795100
N	2.10635200	-1.01475600	-0.22267000
N	2.27574200	1.09242900	0.25127300
C	3.46216500	0.48989200	0.64401100
C	3.35048500	-0.83172800	0.35422100
H	4.26717600	1.04855800	1.09368100
H	4.03548600	-1.64957700	0.50998400
C	1.57851700	-2.30242800	-0.66313800
C	1.99770000	2.51655700	0.39970600
H	0.88325500	-2.70232000	0.07888500
H	1.05701300	-2.17168600	-1.61603500
H	2.41102300	-2.99420000	-0.79997200
H	1.02510400	2.65392900	0.87372400
H	2.77645400	2.95875000	1.02264600
H	1.99416800	3.00990900	-0.57603200
F	-2.15448400	-2.30638400	-0.57536500
F	-0.87215700	-1.63935400	1.49036700

D'3(Cl)

E = -1959.185819 a.u

C	-0.36822600	2.42708000	-0.84678100
C	-1.50455600	2.93652800	-0.29326800
C	-2.60671400	2.22516800	0.35528000
C	-2.75853900	0.89597100	0.60104100
H	0.31281500	3.18041700	-1.25144900
H	-1.63121000	4.02003000	-0.29986700
H	-3.40194300	2.88512200	0.70671500
H	-3.64616900	0.58508500	1.15188000
Si	-0.02306200	0.63656600	-1.36716300
Si	-1.49180000	-0.37305500	0.14058700
C	1.60340400	0.12395600	-0.46428300
N	2.08740100	-1.15281900	-0.50935600
N	2.54937500	0.83219700	0.21870500
C	3.59986000	0.00746800	0.59166900
C	3.30285500	-1.23979100	0.14356700
H	4.45052600	0.37631000	1.14180200
H	3.83828900	-2.17086500	0.23667600
C	1.37528900	-2.28796300	-1.08941500
C	2.47305600	2.25108500	0.55597400
H	0.62580800	-2.66313800	-0.38805500
H	0.87807100	-1.96746800	-2.00925000
H	2.09496700	-3.07561200	-1.31787700
H	1.47884300	2.48060300	0.93976000
H	3.22141100	2.46481500	1.32034300
H	2.66959000	2.86751700	-0.32496600
Cl	-0.61065600	-1.14352600	1.93294600
Cl	-2.49751800	-2.06027500	-0.64011100

D'4(Me)

E = -1118.531985 a.u

C	0.93521600	-2.02234300	-0.89407500
C	2.15526500	-2.35993300	-0.39257500

C	3.12602400	-1.50751400	0.30189300
C	3.03656300	-0.19360700	0.63177700
H	0.38786500	-2.85125000	-1.35114300
H	2.47480000	-3.39994000	-0.48412900
H	4.02790300	-2.04265100	0.60789100
H	3.87978200	0.20880100	1.20077300
Si	0.27343800	-0.27806400	-1.22758800
Si	1.59942700	0.96908100	0.27806800
C	-1.41634500	-0.17659600	-0.32434600
N	-2.18251500	0.96382800	-0.34460300
N	-2.20180900	-1.09954100	0.31752300
C	-3.42301200	-0.54450300	0.67368400
C	-3.40555100	0.75087400	0.26810400
H	-4.18322200	-1.11240200	1.18585200
H	-4.14394900	1.53091200	0.36289600
C	-1.76049900	2.21804900	-0.95010600
C	-1.82752000	-2.47931700	0.60616800
H	-1.07065500	2.75529700	-0.29364400
H	-1.24910800	1.99858600	-1.89398900
H	-2.64013300	2.83647800	-1.13756400
H	-0.77856600	-2.51613800	0.90025000
H	-2.45435900	-2.84710300	1.42073200
H	-1.96972400	-3.11163400	-0.27496000
C	2.28526100	2.57670800	-0.47793700
C	0.79631600	1.46879500	1.93919600
H	2.78443200	2.37669400	-1.43172600
H	1.48346200	3.30180700	-0.66560200
H	3.01106700	3.04923300	0.19609400
H	1.53106000	1.95065400	2.59738200
H	0.40025900	0.58991500	2.45888600
H	-0.03107600	2.17480400	1.79415500

D'5(CF3)

E = -1714.004751 a.u

C	0.73100700	2.66452300	-1.03898900
C	-0.17257600	3.50198400	-0.45897900
C	-1.41543300	3.16332600	0.23870000
C	-1.94761200	1.94504600	0.52271900
H	1.60071200	3.16676200	-1.47120600
H	0.03898700	4.57182000	-0.47533100
H	-1.96018900	4.03603900	0.60288600
H	-2.86398500	1.92704100	1.11201500
Si	0.50485100	0.85148100	-1.55016300
Si	-1.14572000	0.34734000	0.02716300
C	1.93591900	-0.11126200	-0.66944800
N	2.13972300	-1.44666600	-0.87022700
N	2.95492700	0.27902100	0.15057200
C	3.77226100	-0.79714300	0.45454700
C	3.25254500	-1.88211400	-0.17704100
H	4.63557900	-0.69884900	1.09278300
H	3.56806100	-2.91290900	-0.18796400
C	1.24911100	-2.31823300	-1.63353500
C	3.13920600	1.61669500	0.71103400
H	0.40392900	-2.62985900	-1.01628500
H	0.87438000	-1.76895400	-2.50155900
H	1.81195700	-3.19250100	-1.96449400
H	2.18357800	1.99380900	1.07365600
H	3.84300400	1.54542800	1.54130700
H	3.53476400	2.30042800	-0.04303500
C	-2.53477900	-0.86681000	-0.62450400
C	-0.58037400	-0.59280200	1.66053200
F	-1.55088100	-0.79699300	2.59115600
F	-2.04051400	-2.11217900	-0.93404200
F	-3.11851200	-0.39980700	-1.76397500
F	-3.54608900	-1.07621600	0.26728300
F	0.41079800	0.11476600	2.29642500
F	-0.03666800	-1.82818200	1.39722100

D'6(CCl3)

E = -3876.076132 a.u

C	1.35056300	2.45794800	-1.56097800
C	0.53568400	3.47633700	-1.16545800
C	-0.74414700	3.38619400	-0.46705100
C	-1.39308900	2.29222300	0.01303500
H	2.27858200	2.77604300	-2.04436800
H	0.86028600	4.49879600	-1.36149400
H	-1.21410100	4.35487400	-0.28859300
H	-2.32093700	2.46447800	0.55679200
Si	0.93059500	0.62742400	-1.74907400
Si	-0.75999100	0.55498900	-0.12762300
C	2.37312800	-0.32081900	-0.88106000
N	2.53082700	-1.67114500	-1.01705400
N	3.46680900	0.08819700	-0.17216400
C	4.27873200	-0.99035500	0.13252700
C	3.68236200	-2.09636400	-0.38550600
H	5.19371900	-0.87797000	0.69172300
H	3.97034900	-3.13487100	-0.35513800
C	1.57147600	-2.55949800	-1.66656400
C	3.78107200	1.45845400	0.22788800
H	1.14064600	-2.04276400	-2.52883300
H	2.09208200	-3.46112300	-1.99389900
H	0.76809200	-2.81908100	-0.97474200
H	2.85575100	2.01426600	0.36091100
H	4.32631100	1.42683500	1.17267500

H	4.39353100	1.94688900	-0.53509900
C	-2.32507000	-0.51259000	-0.69789000
C	-0.26216900	-0.03160800	1.71058700
Cl	-2.02123100	-2.30254300	-0.57253900
Cl	-3.82721000	-0.12388800	0.23560400
Cl	-2.63914900	-0.10689000	-2.43847300
Cl	0.60880800	-1.63287500	1.71253600
Cl	-1.61985000	-0.11965400	2.89578200
Cl	0.92172200	1.22825900	2.30480600

D'7(SiH3)

E = -1621.284202 a.u

C	-0.18673800	2.44573700	-0.95983600
C	-1.25109300	3.07472200	-0.39451400
C	-2.40063400	2.48476400	0.30173500
C	-2.64754700	1.18755300	0.61090700
H	0.55151200	3.11850700	-1.40590500
H	-1.27792200	4.16533100	-0.43037900
H	-3.13208600	3.22349900	0.63586900
H	-3.55283500	0.99424200	1.18898300
Si	-0.00221000	0.60677400	-1.41148000
Si	-1.53780400	-0.27975100	0.18650700
C	1.61566000	0.04433900	-0.50654500
N	2.08406600	-1.23978800	-0.60451100
N	2.57550100	0.70376600	0.21163300
C	3.61361000	-0.15278400	0.54616900
C	3.29831100	-1.37453000	0.04384900
H	4.46939600	0.17718000	1.11302400
H	3.82125900	-2.31600400	0.09419600
C	1.37037100	-2.32602900	-1.26501800
C	2.52177400	2.10369700	0.62410500
H	0.58777900	-2.72347700	-0.61358900
H	0.91088900	-1.94137000	-2.18089200
H	2.07935500	-3.11886200	-1.50928000
H	1.50699100	2.35165300	0.93391800
H	3.20794900	2.24368600	1.46100500
H	2.81314500	2.76102700	-0.19926500
Si	-2.87150600	-2.02884900	-0.66563200
Si	-0.57200100	-1.08170600	2.19674500
H	-1.55311400	-1.49369900	3.24332100
H	0.29573100	-2.26912000	1.92278300
H	0.31428800	-0.04221900	2.79887400
H	-3.51456700	-1.65430000	-1.95575300
H	-2.02970700	-3.23757000	-0.91953600
H	-3.94803100	-2.44170700	0.28171700

D'8(SiF3)

E = -2217.182565 a.u

C	1.21291700	2.74103600	-0.99880600
C	0.53013100	3.66329300	-0.27024300
C	-0.71017000	3.49098400	0.49469100
C	-1.42462400	2.36597400	0.74840800
H	2.12762100	3.12042500	-1.46321100
H	0.93836100	4.67298200	-0.21163600
H	-1.07541400	4.41528900	0.94565700
H	-2.29322700	2.46692100	1.39766700
Si	0.63028400	1.04935500	-1.64699200
Si	-0.94810500	0.67177900	0.09840700
C	1.95855900	-0.20583500	-0.97204600
N	1.90646600	-1.53652500	-1.27710800
N	3.10200200	-0.06054500	-0.24108200
C	3.74385000	-1.27868900	-0.09555000
C	2.98615900	-2.20657100	-0.73643800
H	4.66417700	-1.37861000	0.45690000
H	3.11027100	-3.27227400	-0.84093300
C	0.80562200	-2.18838700	-1.98441500
C	3.57257700	1.17491400	0.38391900
H	-0.00358500	-2.42549100	-1.29125700
H	0.43190400	-1.51415100	-2.75942600
H	1.17732000	-3.10586800	-2.44333000
H	2.73603500	1.68177500	0.86174500
H	4.31449200	0.91337700	1.13909300
H	4.02407000	1.83501400	-0.35981100
Si	-2.84616000	-0.49222700	-0.61049000
Si	-0.11644900	-0.64426000	1.85685700
F	-3.71213300	0.30132400	-1.71633300
F	-3.87874000	-0.88200200	0.56998200
F	-2.42885900	-1.90056900	-1.30008500
F	-0.99121800	-0.83065500	3.20194000
F	0.21236500	-2.14656900	1.32751500
F	1.31687500	-0.06989200	2.36251500

D'9(SiCl3)

E = -4379.208799 a.u

C	-1.78469900	1.28131800	-2.72647200
C	-1.16153200	0.60598300	-3.72936000
C	0.11510200	-0.10952500	-3.67978400
C	0.91046100	-0.38241800	-2.61355500
H	-2.73994800	1.73381300	-3.00609500
H	-1.64949100	0.56722800	-4.70370000
H	0.43932300	-0.49756400	-4.64686800
H	1.80147800	-0.98109200	-2.79828300
Si	-1.05188500	1.87585200	-1.08199800
Si	0.51226600	0.12332700	-0.85519100
C	-2.32637600	1.31727500	0.27133100

N	-2.19382800	1.69284000	1.57757700
N	-3.52677600	0.66919800	0.21431400
C	-4.12577100	0.64737100	1.46284200
C	-3.28129000	1.27793100	2.32022700
H	-5.08094400	0.17671700	1.63127200
H	-3.35030200	1.45085200	3.38202900
C	-1.00756500	2.33319500	2.13840700
C	-4.11545400	0.04572400	-0.97052300
H	-0.59756200	3.02902600	1.40073400
H	-1.29161800	2.87871500	3.03968800
H	-0.25525700	1.58025500	2.38611000
H	-3.33201400	-0.43583400	-1.55307300
H	-4.83252900	-0.70706800	-0.64063800
H	-4.62435500	0.79229500	-1.58493400
Si	2.53943000	0.70613700	0.18326800
Si	-0.14862400	-1.84102200	0.28678200
Cl	3.03896700	2.68913400	-0.18852200
Cl	-0.94371600	-1.39496500	2.17541000
Cl	2.42623000	0.48735500	2.25943700
Cl	4.11276500	-0.47993300	-0.47970500
Cl	-1.70563900	-2.74183500	-0.78709400
Cl	1.32454400	-3.28462700	0.56469800

D'10(OH)

E = -1190.432578 a.u

C	-0.91486100	2.07849500	-0.73717500
C	-2.13720300	2.38582800	-0.21299900
C	-3.09149700	1.50712400	0.45920300
C	-3.02179300	0.16721000	0.69894600
H	-0.37587100	2.93199700	-1.15562700
H	-2.45854000	3.42810700	-0.25414100
H	-3.96799100	2.03683900	0.83914300
H	-3.84136500	-0.25593700	1.28626600
Si	-0.26054000	0.35875700	-1.15568600
Si	-1.61897100	-0.95314700	0.20683600
C	1.43783600	0.16213100	-0.29662800
N	2.11960700	-1.02485900	-0.26353400
N	2.29748600	1.06997500	0.26083500
C	3.48434500	0.45460400	0.63191800
C	3.36644400	-0.85950400	0.31131400
H	4.29337300	0.99982900	1.09083100
H	4.04929500	-1.68307000	0.44482100
O	-2.25432800	-2.34165100	-0.53050600
O	-0.83472200	-1.66400900	1.52399100
H	-2.85866900	-2.17976700	-1.26402000
H	-1.29231800	-2.43915600	1.87719600
C	1.57881900	-2.29906100	-0.72346700
C	2.02290400	2.48880500	0.45319200
H	0.86929400	-2.68914000	0.00952700
H	1.06413200	-2.14753500	-1.67732300
H	2.40311200	-3.00051400	-0.86249700
H	1.03762700	2.61353600	0.90391800
H	2.78580300	2.90330400	1.11404600
H	2.04805000	3.01863500	-0.50306300

D'11(NH2)

E = -1150.661761 a.u

C	0.85602600	-2.09101100	-0.75697800
C	2.07442800	-2.44486500	-0.25445900
C	3.06517800	-1.60276200	0.41335600
C	3.04612000	-0.26314800	0.65768500
H	0.28225100	-2.92047100	-1.17775300
H	2.36148400	-3.49659500	-0.31129100
H	3.92580800	-2.16511400	0.78327200
H	3.88754000	0.12559800	1.23862200
Si	0.25442700	-0.34207500	-1.13005700
Si	1.68619300	0.94555900	0.21756100
C	-1.44874900	-0.13923000	-0.28481800
N	-2.13698300	1.04907100	-0.28057000
N	-2.32396200	-1.04036200	0.26970200
C	-3.52186100	-0.42206700	0.59923800
C	-3.39830300	0.88781400	0.26353300
H	-4.34267300	-0.96218600	1.04331500
H	-4.08751200	1.71061700	0.36629700
C	-1.59846600	2.31045200	-0.77345700
C	-2.05841700	-2.45702800	0.48421200
H	-0.87297400	2.70590900	-0.05696300
H	-1.10411400	2.13241500	-1.73497300
H	-2.42121400	3.01448900	-0.91025000
H	-1.06124200	-2.58198000	0.90794200
H	-2.80611400	-2.85041900	1.17522000
H	-2.11368000	-3.00776000	-0.45919200
N	0.83622800	1.72367200	1.55449100
N	2.51561000	2.33016500	-0.47434000
H	3.25906600	2.13700800	-1.13511000
H	1.96252100	3.11524400	-0.79876200
H	1.38212000	2.35303600	2.13655600
H	0.24808200	1.13470400	2.13317200

D'12(OMe)

E = -1269.037435 a.u

C	-0.04194100	2.50070800	-0.56959300
C	-1.12049300	3.05668200	0.05470700
C	-2.24477200	2.39191000	0.71321500
C	-2.51598200	1.06342400	0.83961500

H	0.68136000	3.22737500	-0.94804100
H	-1.16176100	4.14557500	0.11950800
H	-2.93802200	3.09146200	1.18608700
H	-3.39863900	0.81192100	1.43333700
Si	0.13888100	0.71859700	-1.17527600
Si	-1.46044900	-0.31812800	0.16614100
C	1.73827100	0.01576900	-0.39109200
N	2.08950800	-1.30458900	-0.48156200
N	2.80845700	0.61709600	0.21458500
C	3.79957000	-0.31364600	0.49186500
C	3.34250800	-1.51829500	0.06340100
H	4.72686700	-0.03850800	0.96810400
H	3.79073800	-2.49810600	0.10220100
C	1.22889600	-2.34932200	-1.02536700
C	2.90949200	2.03414900	0.54192300
H	0.43175100	-2.58136200	-0.31507600
H	0.78584900	-1.99872900	-1.96281500
H	1.83399100	-3.23663400	-1.21869400
H	1.98693800	2.36510200	1.02043800
H	3.74965400	2.17375100	1.22410700
H	3.07589500	2.62792500	-0.36135200
O	-2.45785100	-1.41656900	-0.63985400
O	-0.81226400	-1.29475400	1.37429900
C	-3.31298900	-1.02920100	-1.70663700
C	-1.62576800	-2.09467100	2.23097200
H	-2.73906400	-0.65348000	-2.56591800
H	-3.88088000	-1.91025600	-2.02314300
H	-4.01940800	-0.24688800	-1.39468400
H	-2.28825700	-2.75050300	1.65290100
H	-0.96318500	-2.70821400	2.85022700
H	-2.23747400	-1.46901100	2.89593400

D'13(SiMe3)

E = -1857.285896 a.u

C	1.20206400	2.81673500	-0.60486300
C	0.45534500	3.59782900	0.22025200
C	-0.76924200	3.24891000	0.94953400
C	-1.41377700	2.05824000	1.01911500
H	2.08636000	3.31102800	-1.01720800
H	0.79354100	4.62030200	0.39987100
H	-1.17918100	4.07608500	1.53334000
H	-2.28463200	2.02948800	1.67820000
Si	0.72419300	1.16095000	-1.40646300
Si	-0.93831500	0.43856700	0.15406700
C	2.14612900	-0.04775800	-0.92123100
N	2.15240500	-1.35584000	-1.33771700
N	3.35497500	0.11294500	-0.29451200
C	4.08761800	-1.06477500	-0.32809400
C	3.32868900	-1.98762700	-0.97339400
H	5.06792700	-1.14296200	0.11414300
H	3.51759100	-3.02465900	-1.20020200
C	1.06576400	-1.97790800	-2.08069100
C	3.81960800	1.33230700	0.35927200
H	0.22703800	-2.20888800	-1.42141400
H	0.72381400	-1.28094700	-2.85326700
H	1.42996900	-2.89843700	-2.53998000
H	2.99118900	1.79340500	0.89608300
H	4.61191600	1.06821300	1.06189400
H	4.20688600	2.04223900	-0.37645400
Si	-2.89941600	-0.30561400	-0.93602900
Si	-0.29264800	-0.99133100	1.93072900
C	-4.28028800	-0.71284600	0.30896500
H	-5.22279700	-0.91473000	-0.21558600
H	-4.03308700	-1.59884600	0.90464300
H	-4.45387400	0.11805600	1.00204100
C	-3.49691500	1.07908200	-2.08634400
H	-4.39419900	0.77407100	-2.63928200
H	-3.73647600	1.98205200	-1.51404600
H	-2.71820600	1.34343600	-2.81052400
C	-2.59315200	-1.86472800	-1.98686500
H	-1.85553600	-1.67154500	-2.77335900
H	-2.23758100	-2.70433600	-1.37806500
H	-3.52406400	-2.18000900	-2.47441300
C	0.03518800	-2.78875300	1.38604000
H	0.93146900	-2.85231400	0.75929200
H	0.20158100	-3.42454000	2.26467300
H	-0.80695200	-3.21070200	0.82571500
C	1.31213000	-0.33080300	2.71090500
H	2.15965200	-0.46119100	2.03003400
H	1.22131000	0.73702600	2.93920800
H	1.54118800	-0.86163000	3.64344400
C	-1.63359500	-1.01500900	3.27942200
H	-2.57486200	-1.43130200	2.90519600
H	-1.31026400	-1.62028100	4.13580200
H	-1.83819100	-0.00119700	3.64144800

A2(F).TS

E = -680.609685 a.u

H	-0.05771800	-0.78144400	1.32042800
H	2.29229300	1.42599600	-0.11478600
H	2.41971500	-0.95408600	0.08276200
Si	-0.69843500	-0.61521500	-0.11399000
Si	1.45398000	0.18342700	-0.01033300
F	-1.69243700	0.70606300	0.05023600

A4(Me).TS

E = -620.633501 a.u

H	0.21029100	-0.82497200	1.28172500
H	1.97402600	1.66389400	-0.12809400
H	2.62040600	-0.60494900	0.24856900
Si	-0.55145800	-0.77768600	-0.10727400
Si	1.43873500	0.26071400	-0.02875300
C	-1.82238000	0.68441400	0.05145400
H	-1.86869500	1.24047800	-0.89183500
H	-2.81760600	0.26330500	0.22948000
H	-1.60601800	1.39336500	0.85581500

A12(OMe).TS

E = -695.878154 a.u

H	0.60419000	-0.83809500	1.38269500
H	2.03799600	1.93323200	-0.31436100
H	2.96383600	-0.18553500	0.26731400
Si	0.00982600	-1.08022000	-0.06631800
Si	1.67048400	0.50018200	-0.02992900
O	-1.50981900	-0.36226700	-0.09733300
C	-1.86056400	1.00263000	0.07300600
H	-1.38443000	1.63223200	-0.69203700
H	-2.94673400	1.09639700	-0.02148600
H	-1.55726800	1.36464700	1.06595900

A12(OMe).INT

E = -695.920197 a.u

H	-1.66665200	-1.33473000	1.19993100
H	-1.66700200	-1.33375900	-1.20065200
H	-2.99920200	0.26614500	0.00049500
Si	0.12684300	1.24221700	0.00001700
Si	-1.68632300	-0.44215300	0.00000400
O	1.48999100	0.28572400	-0.00002500
C	1.77555800	-1.11191700	0.00001100
H	0.86144900	-1.71802100	0.00077800
H	2.36480600	-1.34757400	-0.89142800
H	2.36605300	-1.34724100	0.89071200

C2(F).TS

E = -933.540714 a.u

C	0.93526000	1.64891500	0.24250800
C	-0.32960300	2.17221400	0.27025000
C	-1.61266700	1.54759300	-0.07250400
C	-1.90026200	0.24466600	-0.32244700
H	1.76268900	2.27991200	0.56301500
H	-0.42865700	3.21037100	0.59363600
H	-2.43398700	2.26621600	-0.09348700
H	-2.95732300	0.08183100	-0.56082200
Si	1.13222300	-0.07244600	-0.31604500
Si	-0.93301600	-1.48602700	-0.47233600
F	2.69088300	-0.48419500	-0.10011800
F	-0.61177100	-1.70469900	1.19213400

C4(Me).TS

E = -813.595214 a.u

C	-0.06229300	1.84304100	0.14889400
C	-1.42403600	1.73972900	0.26811200
C	-2.26428300	0.56885200	0.07623700
C	-1.88711200	-0.71131700	-0.21201400
H	0.38811200	2.80949200	0.37619900
H	-1.97246500	2.63608400	0.56448300
H	-3.32869800	0.77158400	0.20749100
H	-2.73706900	-1.39540100	-0.30272300
Si	0.91564100	0.38890100	-0.36832700
Si	-0.20824800	-1.58463200	-0.64917800
C	2.76625900	0.65908800	-0.11546600
H	3.10737300	1.49683600	-0.73655800
H	2.98585000	0.91391700	0.92786200
H	3.34344300	-0.22801800	-0.39067400
C	0.57938000	-1.61863400	1.27818900
H	1.58063600	-2.05655400	1.25052400
H	0.58390100	-0.74986300	1.94928300
H	-0.10207700	-2.34239900	1.73547000

C12(OMe).TS

E = -964.084392 a.u

C	0.79997100	1.62487900	0.40719600
C	-0.41617400	2.24997400	0.47283400
C	-1.71661400	1.85143500	-0.07822400
C	-2.10714400	0.65761100	-0.59679400
H	1.62731500	2.11087300	0.92417600
H	-0.45864800	3.19517200	1.01904500
H	-2.46184600	2.64633800	-0.00101000
H	-3.15744200	0.65639000	-0.91008800
Si	0.91513900	0.07091500	-0.57464100
Si	-1.25676900	-1.06864700	-1.08355500
O	2.40541200	-0.61157900	-0.43902600
O	-1.11905900	-1.80769200	0.48418800
C	-1.45395300	-1.28645200	1.76238500
C	3.55826900	-0.28980100	0.34322200
H	-0.93640100	-0.33973700	1.97537800
H	-2.53333600	-1.10452000	1.84860500
H	-1.16162100	-2.02519100	2.51669100
H	3.37809700	0.55286700	1.01913200
H	3.82769200	-1.17188800	0.93083000
H	4.38206700	-0.04375500	-0.33302000

C12(OMe).INT

E = -964.128047 a.u

C	1.54597600	1.43807300	0.24747900
C	0.70258400	2.53392800	0.11427100
C	-0.70296700	2.53383800	-0.11417700
C	-1.54613900	1.43784200	-0.24748000
H	2.60128300	1.67101000	0.40420200
H	1.15865600	3.52212300	0.17431300
H	-1.15918600	3.52196500	-0.17407800
H	-2.60151100	1.67060100	-0.40408800
Si	1.00916200	-0.28138600	0.48103600
Si	-1.00921100	-0.28155800	-0.48137200
O	2.18810700	-1.44393500	0.40581300
O	-2.18807300	-1.44426000	-0.40587800
C	-3.26559700	-1.49508700	0.53455800
C	3.26606100	-1.49492800	-0.53412800
H	-2.89329600	-1.78204300	1.52565000
H	-3.77899500	-0.52903100	0.61209400
H	-3.97554200	-2.24955000	0.18568700
H	3.77877600	-0.52858500	-0.61243600
H	3.97639500	-2.24853300	-0.18421100
H	2.89432200	-1.78316500	-1.52504000

D2(F).TS

E = -1238.408771 a.u

C	-0.74345200	-1.86611400	-0.35153100
C	-2.01585400	-2.15548200	-0.82456100
C	-3.14176300	-1.28601800	-0.94975300
C	-3.26543500	0.06926500	-0.64269300
H	-0.00599900	-2.64724800	-0.53445500
H	-2.17627400	-3.15065600	-1.24030000
H	-4.02377600	-1.75771500	-1.38504000
H	-4.20825900	0.55625600	-0.88258300
Si	-0.22132300	-0.42610500	0.67870000
Si	-1.86866800	0.97479000	0.00085900
C	1.52637800	-0.03598500	-0.06714000
N	2.05476700	1.20657000	-0.33418000
N	2.62706100	-0.85824100	0.01965000
C	3.79596900	-0.14435500	-0.19288400
C	3.43904100	1.14638800	-0.41143800
H	4.76619500	-0.61482100	-0.17544700
H	4.03981500	2.01749800	-0.61869000
C	1.27833900	2.42239600	-0.51436000
C	2.56866900	-2.27782700	0.32102900
H	0.54359700	2.28553000	-1.31389600
H	0.75240700	2.68573300	0.40848400
H	1.95526700	3.23407100	-0.78456100
H	2.26280400	-2.85228600	-0.55779300
H	3.55382600	-2.61384600	0.64903400
H	1.84357500	-2.44604900	1.12592400
F	-1.58178900	-0.34245100	1.90158600
F	-2.13681600	2.55912200	0.29810200

D2(F).INT

E = -1238.476936 a.u

C	-0.98872800	-1.84973300	-0.40700500
C	-2.28833400	-2.05765200	-0.82025900
C	-3.41108100	-1.16326100	-0.76920800
C	-3.38586400	0.15018700	-0.35241400
H	-0.34676300	-2.72816400	-0.49219500
H	-2.51783300	-3.04597300	-1.22234400
H	-4.36540000	-1.59961200	-1.06459800
H	-4.34482800	0.67198100	-0.32504500
Si	-0.36934100	-0.41932400	0.59033700
Si	-1.84769900	1.14489000	-0.21383300
C	1.41884500	0.04420700	-0.00557200
N	1.93420300	1.26716400	-0.30849500
N	2.46161700	-0.82412100	-0.12876300
C	3.60187900	-0.15866300	-0.53382700
C	3.27067400	1.15585000	-0.64569900
H	4.53805800	-0.66801900	-0.69756900
H	3.86463900	2.01252800	-0.92049200
C	1.20982600	2.53778200	-0.26871900
C	2.39141200	-2.26744500	0.10332800
H	0.38335100	2.51069200	-0.98720400
H	0.79996000	2.70852100	0.72832700
H	1.90653100	3.33854200	-0.51809300
H	1.99946900	-2.77112300	-0.78332800
H	3.39648900	-2.63290800	0.31836500
H	1.74634500	-2.46459800	0.96024800
F	0.15121100	-1.05116600	2.05643100
F	-2.11831700	2.50241900	0.72022600

D4(Me).TS

E = -1118.409839 a.u

C	-0.60736300	-1.86178100	-0.46419100
C	-1.82991400	-2.19883100	-1.02395300
C	-2.98594100	-1.37085800	-1.16916300
C	-3.18492600	-0.03979300	-0.80123200
H	0.20944600	-2.54617200	-0.69579600
H	-1.90847600	-3.16210600	-1.53074600
H	-3.81198400	-1.85181200	-1.69646400
H	-4.12807000	0.41649100	-1.10157500
Si	-0.22889900	-0.43337500	0.66203000
Si	-1.90082000	0.94678000	-0.01150900
C	1.55996700	-0.03708500	-0.19422400

N	2.06244400	1.22251700	-0.47726500
N	2.69954000	-0.77543300	0.08522000
C	3.83999000	0.01213800	0.02564100
C	3.44332600	1.26188200	-0.32161800
H	4.82493800	-0.38663800	0.21213600
H	4.01670200	2.15971300	-0.49119900
C	1.25073300	2.37358500	-0.80293200
C	2.67848500	-2.17250600	0.45977000
H	0.52051300	2.11183500	-1.57547800
H	0.71239100	2.73075400	0.08509300
H	1.89370200	3.17259900	-1.17762700
H	2.44805700	-2.80960700	-0.39979800
H	3.65293900	-2.45372300	0.86397800
H	1.90880200	-2.33042600	1.22884800
C	-1.74134600	-0.64922300	2.10203100
H	-1.25092000	-0.30081100	3.02246200
H	-2.70220000	-0.09528300	2.04557300
H	-1.99794300	-1.71274300	2.19122800
C	-2.45685800	2.64484900	0.59807100
H	-2.50331800	2.64377800	1.69280200
H	-1.74891500	3.42723300	0.30286400
H	-3.45038400	2.89539400	0.21153000

D12(OMe).TS

E = -1268.955370 a.u

C	-0.09249600	-2.02353900	-0.81271000
C	-1.36091100	-2.48822200	-1.19688100
C	-2.60953300	-1.81635100	-1.17449900
C	-2.93820700	-0.49419500	-0.81255700
H	0.74687200	-2.64777800	-1.11216900
H	-1.40029200	-3.48255200	-1.64366300
H	-3.43931300	-2.41677800	-1.55113500
H	-3.96891200	-0.19004700	-0.98782900
Si	0.16606900	-0.53585700	0.18355900
Si	-1.74033900	0.62303200	-0.10153200
C	1.87839700	0.16641200	-0.13721400
N	2.22089600	1.50621100	-0.13761600
N	3.08863600	-0.49714900	-0.05322500
C	4.13639700	0.40753800	-0.01591600
C	3.59576400	1.65311900	-0.06609000
H	5.16532100	0.08931200	0.03988300
H	4.06726600	2.62299100	-0.06129000
C	1.27149600	2.60065400	-0.25791400
C	3.22660400	-1.93950900	-0.04618700
H	0.71037000	2.51638600	-1.19351800
H	0.55702500	2.58716700	0.57141500
H	1.82151300	3.54294100	-0.24808600
H	3.04405500	-2.35217900	-1.04369500
H	4.23524500	-2.20145200	0.27815400
H	2.49464700	-2.37180400	0.64752700
O	-1.00322100	-0.66356300	1.58233200
O	-2.16013800	2.21867000	0.13826000
C	-1.51701000	-1.87281200	2.17652900
C	-3.49048100	2.72484300	-0.00772700
H	-0.84398900	-2.71168900	1.96876900
H	-1.61553700	-1.73250800	3.25780100
H	-2.49447700	-2.09413400	1.73420500
H	-4.16765200	2.27072400	0.72621100
H	-3.45350600	3.80416300	0.16342400
H	-3.87884100	2.53486700	-1.01623700

D12(OMe).INT

E = -1269.012050 a.u

C	-0.42115500	-1.98128400	-0.81723800
C	-1.61252300	-2.34213800	-1.41380200
C	-2.83186200	-1.59338800	-1.53522500
C	-3.03418500	-0.29426700	-1.11670400
H	0.32455900	-2.77880000	-0.79256200
H	-1.65941800	-3.34774900	-1.83735500
H	-3.66537000	-2.13514800	-1.98357100
H	-4.04557000	0.09866900	-1.25227200
Si	-0.13195700	-0.48609200	0.24235200
Si	-1.69572400	0.90824900	-0.71795000
C	1.64980700	0.20593300	-0.10043000
N	2.03486100	1.48519300	-0.35687600
N	2.79979100	-0.52288100	-0.10551000
C	3.88386000	0.28315000	-0.39084900
C	3.40296600	1.54616200	-0.54812900
H	4.88886600	-0.10315700	-0.44952700
H	3.90932900	2.47276300	-0.76535300
C	1.15382600	2.65298800	-0.40718300
C	2.88419400	-1.96336600	0.13632100
H	0.42547600	2.52915400	-1.21621900
H	0.60689200	2.75585600	0.53129400
H	1.76803400	3.53852900	-0.57377400
H	2.66455700	-2.51118300	-0.78302200
H	3.89471700	-2.19958300	0.47321600
H	2.16753100	-2.23234700	0.91351500
O	0.27928200	-1.01143300	1.82336400
O	-2.26065300	2.21302900	0.22331400
C	-0.69741100	-1.66743600	2.62986600
C	-2.94901700	2.02517100	1.45262900
H	-1.09767600	-2.56199500	2.13377500
H	-0.21822700	-1.96581200	3.56762500

H	-1.53728000	-0.99725900	2.86183400
H	-2.30793700	1.52439300	2.19560700
H	-3.23845500	3.00776300	1.84341300
H	-3.85508700	1.41759300	1.31949600

A''1(H)

E = -581.321433 a.u

H	1.90928700	1.20051300	0.05817100
H	1.87619500	-1.21710000	0.10169100
Si	-1.22885200	-0.09892700	-0.03431700
Si	1.03663200	-0.00013800	-0.06827500
H	0.10198700	-0.02266700	1.25213100
H	-1.19638100	1.42615900	0.02430000

A''7(SiH3)

E = -872.029158 a.u

H	-1.42990200	-1.96087000	0.05204900
H	-3.09904400	-0.20371800	0.05998500
Si	-0.12358000	1.17812700	-0.02990600
Si	-1.64440700	-0.49141100	-0.06486100
H	-1.00975100	0.16886700	1.26475400
Si	1.70420700	-0.39253600	0.00199200
H	2.73048800	0.01127500	1.00404200
H	1.35564600	-1.81915500	0.26150400
H	2.34547700	-0.31492400	-1.34347500

A''8(SiF3)

E = -1169.973396 a.u

H	-1.97822500	-1.93694100	0.03491700
H	-3.77952000	-0.31088700	0.09456600
Si	-1.00215600	1.33974500	0.00714000
Si	-2.31422700	-0.49544400	-0.06608700
H	-1.69854900	0.25048800	1.26236800
Si	0.95115700	-0.02952700	0.00568700
F	0.80944200	-1.60752700	0.34689800
F	2.06636500	0.51482700	1.04251100
F	1.63191000	0.04720000	-1.46121000

A''9(SiCl3)

E = -2250.983535 a.u

H	-2.67516600	1.65664400	0.16329500
H	-4.30791700	-0.11911000	-0.18127600
Si	-1.38132100	-1.47579600	-0.27028000
Si	-2.87150500	0.19326500	0.03066600
H	-2.18254800	-0.25965200	-1.37942200
Si	0.52074800	-0.03469300	-0.02137800
Cl	0.33021800	2.04510100	-0.05379200
Cl	1.93752900	-0.49343100	-1.48031900
Cl	1.34488400	-0.54206600	1.83124500

A''13(SiMe3)

E = -990.027129 a.u

H	-2.15257700	1.83589400	-0.01930900
H	-3.90347300	0.18194600	-0.06795500
Si	-1.00323800	-1.36876000	-0.00149400
Si	-2.43310600	0.37220300	0.06504600
H	-1.84267500	-0.28712800	-1.28132700
Si	0.96307200	0.05286200	-0.00266000
C	0.94212800	1.43000400	-1.31157900
H	0.13697800	2.15023500	-1.13373600
H	1.89411300	1.97526000	-1.28915100
H	0.81403000	1.02147700	-2.31994600
C	2.46065400	-1.06448700	-0.34939600
H	3.39010200	-0.48200100	-0.31998500
H	2.54287100	-1.86538800	0.39441200
H	2.38817700	-1.53421600	-1.33689100
C	1.19774600	0.83635800	1.71405800
H	1.19787600	0.08183500	2.50913100
H	2.15674700	1.36758000	1.76080000
H	0.40046500	1.55497400	1.93298600

C''1(H)

E = -734.957356 a.u

C	1.46912800	-1.00470400	-0.01262900
C	1.88741000	0.29889400	0.03743200
C	1.06250900	1.48408200	0.01929900
C	-0.30486900	1.58387300	-0.04677500
H	2.23435400	-1.77807500	-0.06130900
H	2.96072800	0.49026900	0.06376900
H	1.63011900	2.41601600	0.01745200
H	-0.65429500	2.61617900	-0.14842900
Si	-0.31632600	-1.40865200	-0.08375900
Si	-1.77870000	0.37647600	-0.00539200
H	-0.90135800	-0.63037400	1.20670700
H	-0.62425300	-2.83642700	0.18595500

C''10(OH)

E = -885.509702 a.u

C	0.13678200	1.73705600	-0.04560000
C	-1.22262100	1.77488500	0.06822500
C	-2.16473900	0.66256300	-0.00717900
C	-1.92210900	-0.65586200	-0.27990500
H	0.65856100	2.69090800	-0.12516500
H	-1.70014200	2.75205000	0.15293300
H	-3.20753300	0.97846500	0.05959000
H	-2.83084400	-1.23434300	-0.47472100
Si	1.00955300	0.12511800	-0.24772600
Si	-0.35763900	-1.77142600	-0.27164500
O	2.65936800	0.24350800	-0.37085100

O	0.57012500	-0.72621200	1.26328300
H	3.13361000	0.85715000	0.20359300
H	0.01973200	-0.24612900	1.90227200

C''11(NH2)

E = -845.760512 a.u

C	0.06217500	1.75279500	-0.00360800
C	-1.29706700	1.75316300	0.10727700
C	-2.20573900	0.62054500	-0.03366600
C	-1.91554700	-0.68274900	-0.32500100
H	0.56244800	2.72061100	-0.04253000
H	-1.79962800	2.71413700	0.22608400
H	-3.25884100	0.90867600	-0.01445900
H	-2.79605100	-1.27349100	-0.59620900
Si	0.99828400	0.18406100	-0.23830200
Si	-0.32429700	-1.76103500	-0.30517200
H	3.24474300	1.06714800	0.15797000
H	-0.12765900	-0.33903900	1.96564600
N	2.70855300	0.36513500	-0.33396800
N	0.49079400	-0.77540100	1.28447500
H	1.21068900	-1.32020400	1.75013600
H	3.27011200	-0.19086400	-0.96157400

C''12(OMe)

E = -964.120225 a.u

C	0.10263200	1.70802400	-0.07886300
C	-1.21821700	1.97977300	0.12819000
C	-2.35487800	1.07877100	-0.01942300
C	-2.37724200	-0.21727000	-0.45622000
H	0.79285600	2.55136400	-0.05720800
H	-1.49601000	3.00610900	0.37348200
H	-3.31583500	1.56669800	0.15716200
H	-3.38875900	-0.59392500	-0.64058700
Si	0.64799300	0.02322100	-0.59376900
Si	-1.05251600	-1.58290900	-0.74144200
O	2.28136300	-0.09046400	-0.83489200
O	0.17468200	-1.01765000	0.76788400
C	-0.16969400	-0.69277900	2.12631800
C	3.27375700	0.29026400	0.11923200
H	-0.93545200	0.08655500	2.15749200
H	-0.54538100	-1.60501500	2.59704400
H	0.73176300	-0.34966800	2.64170500
H	3.06834600	1.28226900	0.54366200
H	3.32585800	-0.44318900	0.93330500
H	4.23941900	0.31864900	-0.39244900