Electronic supplementary information

The hierarchy of *ab initio* and DFT methods for describing an intramolecular non-covalent Si···N contact in the silicon compounds using electron diffraction geometries

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Equation S1. Agreement factor being minimized at least-squares procedure of the GED data:

$$R_f = 100\left[\frac{\sum_i^n \omega_i\left[s_i M_{\text{exp.}}(s_i) - k s_i M_{\text{theor.}}(s_i)\right]^2}{\sum_i^n \omega_i\left[s_i M_{\text{exp.}}(s_i)\right]^2}\right]^{1/2}$$

where: ω_i – weight function; k– scale coefficient (index of resolution), $k=s_iM_{exp.}(s_i)/s_iM_{theor.}(s_i)$, $s_iM_{exp.}(s_i)$, $s_iM_{theor.}(s_i)$ – experimental and theoretical molecular scattering intensities, respectively.

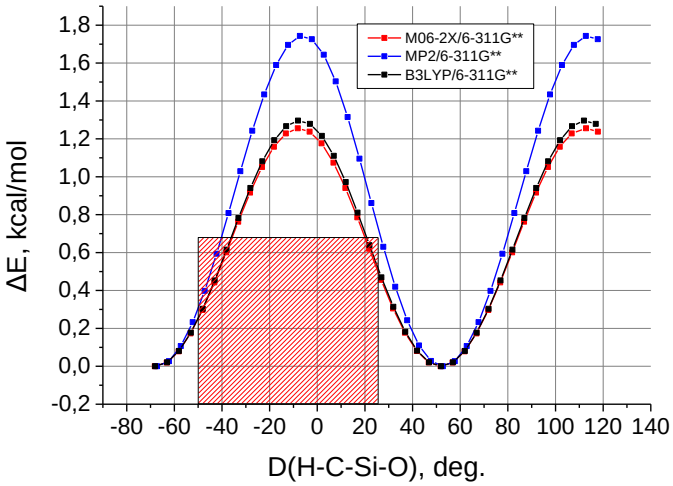


Figure S1. PES of methyl group rotation along with GED data**,** see also main text. The filled rectangle corresponds to the GED value of the angle with error limit.

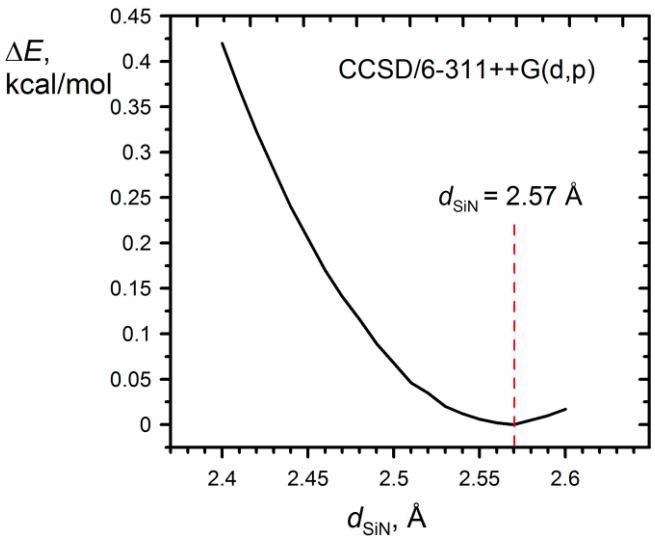


Figure S2. The relative energy of 1-methylsilatrane computed at the CCSD/6-311++G(d,p) level as function of the Si···N distance (the value of the total energy in minimum was set to zero). The PES scan with respect to d_{SiN} was performed with increment of 0.01 Å and using the full MP2/6-311++G(d,p) optimization of the remaining geometric parameters.

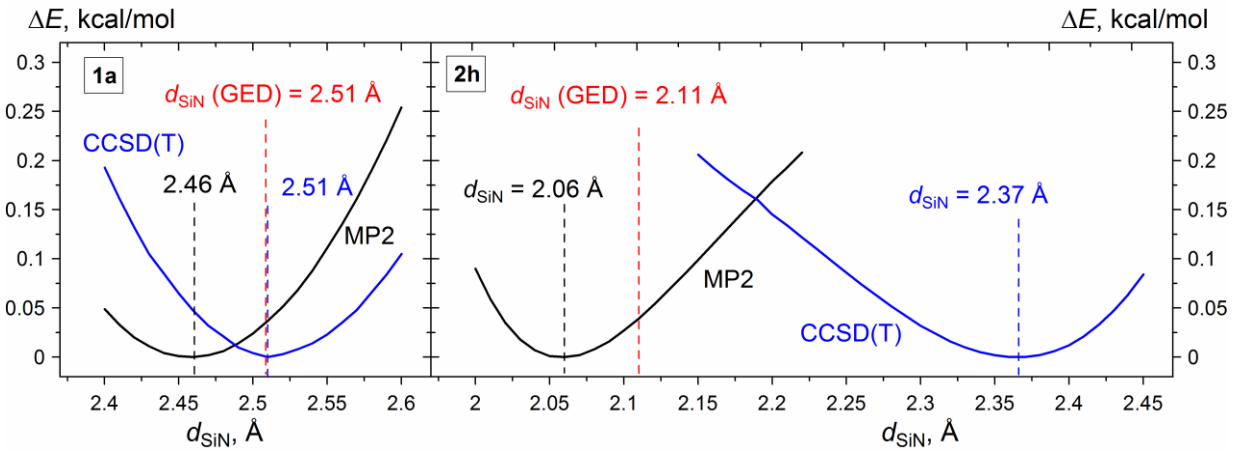


Figure S3. MP2/6-311++G(d,p) and CCSD(T)/6-311++G(d,p) potential functions of deformation of the Si···N contact in molecules **1a** and **2h** (the value of the total energy in minimum was set to zero). The PES scan with respect to d_{SiN} was performed with increment of 0.01 Å and using the full MP2/6-311++G(d,p) optimization of the remaining geometric parameters.

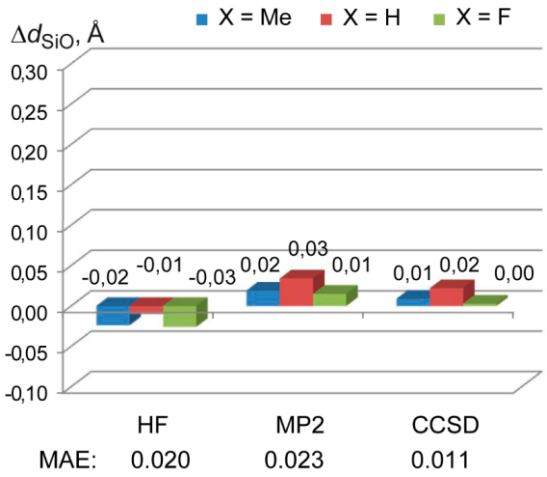


Figure S4. Difference between the ab initio calculated (with the 6-311G(d,p) basis set) and GED experimental values of the Si-O bond lengths (Δd_{SiO}, Å), as well as the corresponding MAE values (in Å) in molecules $XSi(OCH_2CH_2)_3N$.

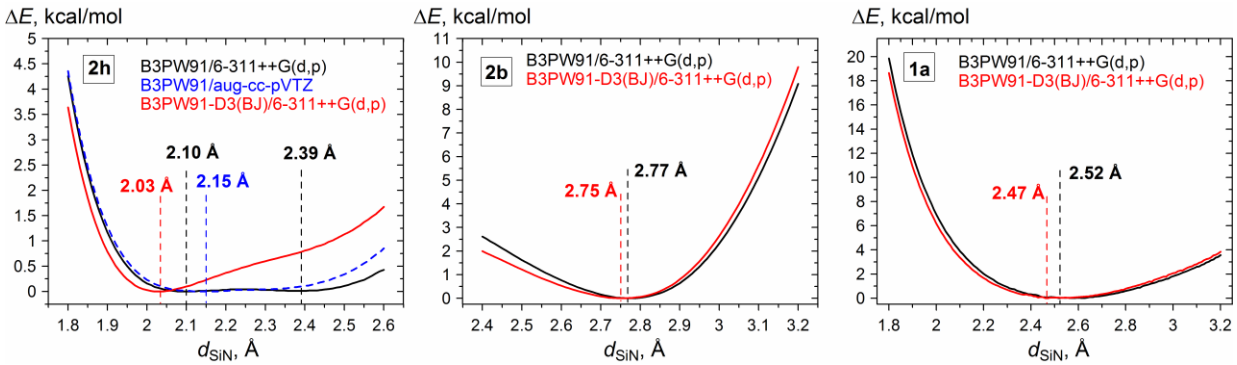


Figure S5. Potential functions of the Si···N contact deformation in the anti-conformer of $(F_3C)F_2SiONMe_2$ (**2h**), $F_3SiCH_2NMe_2$ (**2b**), and 1-methylsilatrane (**1a**) calculated at the B3PW91 and B3PW91-D3(BJ) theory levels.

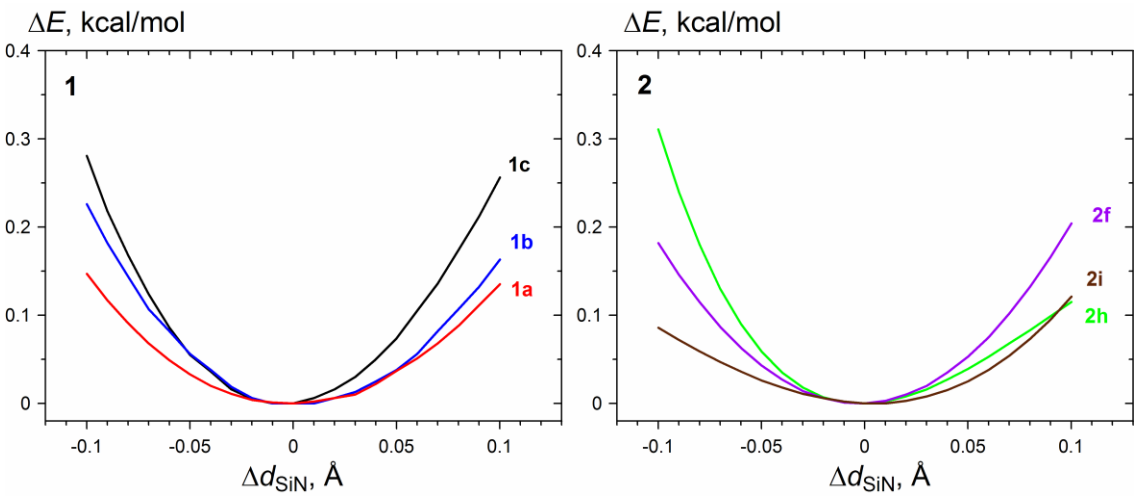


Figure S6. MP2/6-311++G(d,p) potential functions of the Si···N contact deformation in molecules **1** and **2**.

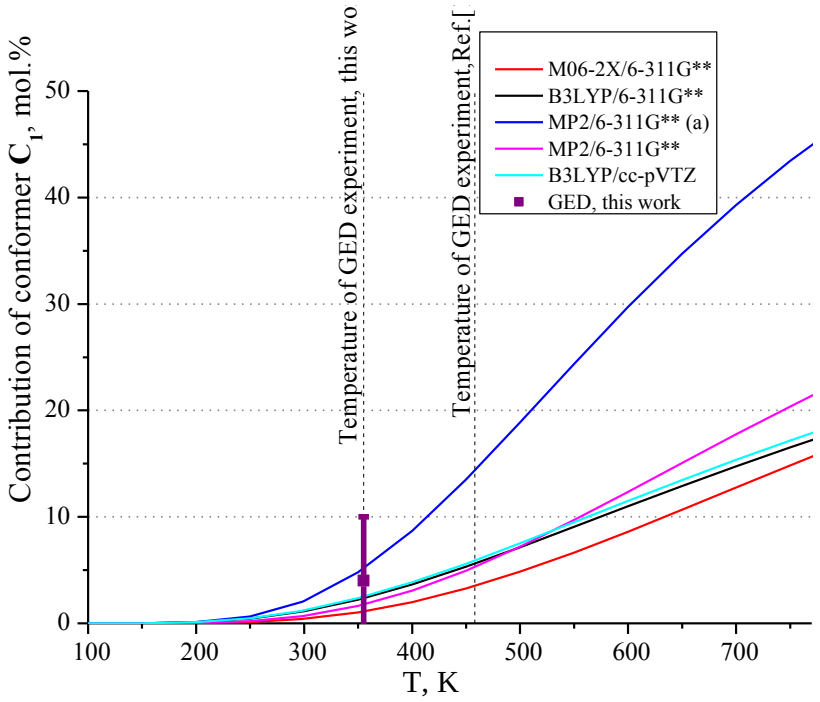


Figure S7. Temperature dependence of conformer C_1 concentration in gas phase as predicted on the base of theoretical calculations at «rigid rotor — harmonic oscillator» approximation. All calculations for conformer C_3 were performed for C_1 equilibrium symmetry which in fact is a qausi-C_3 one (very close to), but, due to difficulties intrinsic to the Gaussian program to keep the symmetry, it was not completely reached. The MP2 results marked by "(a)" correspond to real C_3 symmetry which was easily realized in case of this kind of calculations. Temperature of the GED experiments, from Shen et al (*J. Mol. Struct.* 1980; 64: 257) and this work, along with the GED data of this work, are shown.

Table S1. Starting (QC) and refined (GED) values for internuclear distances (r_a, r_{h1}) and vibrational amplitudes (l) of 1-methylsilatrane based on the B3LYP/6-311G** calculations

Param. #	Atoms	N1	N2	Multiplicity	Starting values			Refined values[b]			Vibrational corrections Δr^a	Gr. #[c]
					r_a	r_{h1}	l	r_a	r_{h1}	l		
69	C H	15	30	3	1.0909	1.093	0.077	1.10845	1.104(2)	0.081(2)	0.0017	1
70	C H	12	23	2	1.0916	1.093	0.077	1.10916	1.104(2)	0.081(2)	0.00121	1
71	C H	10	19	1	1.0916	1.093	0.077	1.10916	1.104(2)	0.081(2)	0.00121	1
72	C H	13	25	3	1.0926	1.094	0.077	1.11019	1.105(2)	0.081(2)	0.00116	1
73	C H	13	24	3	1.0967	1.098	0.078	1.11427	1.109(2)	0.082(2)	0.00104	1
74	C H	10	18	3	1.0988	1.1	0.078	1.11643	1.112(2)	0.083(2)	0.00134	1
75	O C	7	11	2	1.4127	1.415	0.049	1.41939	1.420(3)	0.053(2)	0.00278	1
76	O C	6	9	1	1.4127	1.415	0.049	1.41939	1.420(3)	0.053(2)	0.00278	1
77	N C	2	12	1	1.5063	1.503	0.049	1.46455	1.459(3)	0.053(2)	-0.00373	1
78	N C	2	10	2	1.5063	1.503	0.049	1.46455	1.459(3)	0.053(2)	-0.00373	1
79	C C	13	14	1	1.5371	1.536	0.053	1.53086	1.527(3)	0.058(2)	-0.00123	1
80	C C	11	12	1	1.5371	1.536	0.053	1.53086	1.527(3)	0.058(2)	-0.00123	1
81	C C	9	10	1	1.5371	1.536	0.053	1.53086	1.527(3)	0.058(2)	-0.00124	1
82	Si O	1	6	2	1.6681	1.671	0.047	1.66528	1.667(3)	0.051(2)	0.00305	1
83	Si O	1	7	1	1.668	1.671	0.047	1.66518	1.667(3)	0.051(2)	0.00307	1
84	H H	18	19	1	1.839	1.847	0.124	2.06711	2.067(4)	0.128(2)	0.00836	1
85	H H	22	23	1	1.839	1.847	0.124	2.06711	2.067(4)	0.128(2)	0.00834	1
86	H H	26	27	1	1.839	1.847	0.124	2.06711	2.067(4)	0.128(2)	0.00834	1
87	H H	16	17	2	1.7612	1.769	0.123	1.79526	1.794(4)	0.127(2)	0.00765	1
88	H H	24	25	1	1.7612	1.769	0.123	1.79526	1.794(4)	0.127(2)	0.00765	1
89	H H	28	29	3	1.7589	1.771	0.125	1.78702	1.790(4)	0.129(2)	0.0121	1
90	Si C	1	15	1	1.8582	1.858	0.052	1.84905	1.847(4)	0.057(2)	-5.3E-4	1
91	O H	7	21	3	2.0329	2.04	0.101	2.03214	2.035(4)	0.098(2)	0.00722	2
92	O H	7	20	2	2.0584	2.065	0.101	2.08389	2.086(4)	0.098(2)	0.00657	2
93	O H	6	16	1	2.0584	2.065	0.101	2.08389	2.086(4)	0.098(2)	0.00657	2
94	N H	2	19	3	2.1132	2.116	0.103	2.13047	2.128(4)	0.100(2)	0.00263	2
95	N H	2	18	1	2.175	2.177	0.103	2.08433	2.081(4)	0.100(2)	0.00189	2
96	N H	2	22	2	2.175	2.177	0.103	2.08433	2.081(4)	0.100(2)	0.00191	2
97	C H	13	27	1	2.1481	2.153	0.11	1.6688	1.667(3)	0.106(2)	0.00531	2
98	C H	11	23	1	2.1482	2.153	0.11	1.6689	1.667(3)	0.106(2)	0.00527	2
99	C H	9	19	1	2.1481	2.153	0.11	1.6688	1.667(3)	0.106(2)	0.00531	2
100	C H	14	25	2	2.1678	2.172	0.108	2.1325	2.132(4)	0.105(2)	0.00432	2
101	C H	12	21	1	2.1679	2.172	0.108	2.13261	2.132(4)	0.105(2)	0.00428	2
102	C H	14	24	1	2.1689	2.172	0.108	2.17495	2.173(4)	0.105(2)	0.00343	2
103	C H	12	20	1	2.1688	2.172	0.108	2.17495	2.173(4)	0.105(2)	0.00347	2
104	C H	10	16	1	2.1689	2.172	0.108	2.17495	2.173(4)	0.105(2)	0.00343	2
105	C H	9	18	3	2.1706	2.175	0.11	2.15349	2.152(4)	0.107(2)	0.00429	2
106	H H	19	24	1	2.3948	2.406	0.289	2.43808	2.415(5)	0.286(2)	0.01129	2
107	H H	20	27	1	2.3964	2.406	0.288	2.43954	2.415(5)	0.285(2)	0.00973	2
108	H H	16	23	1	2.3945	2.406	0.289	2.43788	2.415(5)	0.286(2)	0.01156	2
109	H H	17	19	1	2.4209	2.43	0.174	1.85444	1.848(4)	0.171(2)	0.00948	2
110	H H	21	23	1	2.4209	2.43	0.174	1.85444	1.848(4)	0.171(2)	0.00943	2
111	H H	25	27	1	2.4209	2.43	0.174	1.85442	1.848(4)	0.171(2)	0.00949	2
112	O C	8	14	1	2.4249	2.432	0.07	2.4698	2.475(5)	0.067(2)	0.0068	2
113	O C	7	12	1	2.4248	2.432	0.07	2.46969	2.475(5)	0.067(2)	0.00689	2
114	O C	6	10	1	2.4248	2.432	0.07	2.4697	2.475(5)	0.067(2)	0.00683	2
115	H H	19	26	1	2.2851	2.28	0.227	2.68649	2.662(5)	0.224(2)	-0.00554	2
116	H H	18	23	1	2.2844	2.28	0.227	2.68578	2.662(5)	0.224(2)	-0.00487	2
117	H H	22	27	1	2.286	2.28	0.227	2.68742	2.662(5)	0.224(2)	-0.00648	2
118	N C	2	11	2	2.3521	2.352	0.071	2.37565	2.374(5)	0.068(2)	1.3E-4	2
119	N C	2	9	1	2.3522	2.352	0.071	2.37565	2.374(5)	0.068(2)	5E-5	2
120	H H	16	18	1	2.3998	2.407	0.178	2.33642	2.331(5)	0.175(2)	0.00758	2
121	H H	20	22	1	2.3996	2.407	0.178	2.33632	2.331(5)	0.175(2)	0.00772	2
122	H H	24	26	1	2.3997	2.407	0.178	2.33642	2.331(5)	0.175(2)	0.0076	2
123	Si H	1	28	1	2.4554	2.465	0.124	2.45968	2.463(5)	0.121(2)	0.0095	2
124	Si H	1	29	1	2.458	2.465	0.124	2.46227	2.463(5)	0.121(2)	0.00693	2
125	Si H	1	30	1	2.458	2.465	0.124	2.46227	2.463(5)	0.121(2)	0.00688	2
126	C C	10	14	2	2.499	2.498	0.07	2.46638	2.463(5)	0.066(2)	-0.00114	2
127	C C	10	12	1	2.4986	2.498	0.07	2.46589	2.463(5)	0.066(2)	-6.7E-4	2
128	C H	14	19	1	2.5014	2.499	0.143	2.73284	2.723(5)	0.140(2)	-0.00275	2
129	C H	12	27	1	2.5023	2.499	0.143	2.73373	2.723(5)	0.139(2)	-0.0036	2

130	C H	10	23	1	2.501	2.499	0.143	2.73244	2.723(5)	0.140(2)	-0.00232	2
131	H H	25	26	1	2.6151	2.622	0.167	2.62368	2.620(5)	0.164(2)	0.00701	2
132	H H	21	22	1	2.6153	2.622	0.167	2.62379	2.620(5)	0.164(2)	0.00687	2
133	H H	17	18	1	2.6152	2.622	0.167	2.62369	2.620(5)	0.164(2)	0.00696	2
134	Si N	1	2	1	2.4265	2.449	0.182	2.50375	2.514(5)	0.179(2)	0.02276	2
135	C H	12	18	1	2.5795	2.581	0.156	2.50717	2.499(5)	0.153(2)	0.0014	2
136	C H	14	22	1	2.5805	2.581	0.156	2.50817	2.499(5)	0.153(2)	4.1E-4	2
137	C H	10	26	1	2.5799	2.581	0.156	2.50756	2.499(5)	0.153(2)	1E-3	2
138	Si C	1	13	1	2.7311	2.746	0.069	2.72641	2.740(5)	0.066(2)	0.01532	2
139	Si C	1	9	2	2.7311	2.746	0.069	2.72641	2.740(5)	0.066(2)	0.0153	2
140	O H	8	27	1	2.7382	2.754	0.166	2.26574	2.270(5)	0.163(2)	0.01619	2
141	O H	7	23	1	2.7382	2.754	0.166	2.26576	2.270(5)	0.163(2)	0.01615	2
142	O H	6	19	1	2.7381	2.754	0.166	2.26576	2.270(5)	0.163(2)	0.01622	2
143	N O	2	7	1	2.5609	2.571	0.113	2.67749	2.683(5)	0.110(2)	0.00995	2
144	N O	2	6	1	2.5612	2.571	0.113	2.67768	2.683(5)	0.110(2)	0.00973	2
145	N O	2	8	1	2.5611	2.571	0.113	2.67768	2.683(5)	0.110(2)	0.00976	2
146	O O	6	8	1	2.779	2.79	0.095	2.80414	2.812(6)	0.092(2)	0.01069	2
147	O O	7	8	1	2.7797	2.79	0.096	2.80475	2.812(6)	0.092(2)	0.01001	2
148	O O	6	7	1	2.7789	2.79	0.096	2.80404	2.812(6)	0.092(2)	0.01079	2
149	O C	6	15	1	2.8018	2.81	0.102	2.74863	2.754(5)	0.098(2)	0.00869	2
150	O C	7	15	1	2.8026	2.81	0.102	2.74943	2.754(5)	0.099(2)	0.00788	2
151	O C	8	15	1	2.8017	2.81	0.102	2.74853	2.754(5)	0.098(2)	0.00878	2
152	N H	2	24	1	2.7227	2.729	0.156	2.81459	2.813(6)	0.152(2)	0.00622	2
153	N H	2	20	1	2.7227	2.729	0.156	2.8146	2.813(6)	0.153(2)	0.0062	2
154	N H	2	16	1	2.7228	2.729	0.156	2.8147	2.813(6)	0.153(2)	0.00617	2
155	C H	11	27	1	2.8731	2.883	0.208	2.87474	2.870(6)	0.205(2)	0.00958	2
156	C H	13	19	1	2.8719	2.883	0.209	2.87362	2.870(6)	0.206(2)	0.01078	2
157	C H	9	23	1	2.8716	2.883	0.209	2.87332	2.870(6)	0.206(2)	0.01112	2
158	O H	6	28	1	2.9608	2.972	0.247	2.91838	2.910(6)	0.244(2)	0.01164	2
159	O H	7	29	1	2.9652	2.972	0.247	2.92275	2.910(6)	0.244(2)	0.00723	2
160	O H	8	30	1	2.9638	2.972	0.247	2.92124	2.909(6)	0.243(2)	0.00869	2
161	C H	10	24	1	2.9855	3.002	0.218	3.03434	3.036(6)	0.214(2)	0.01658	2
162	C H	14	20	1	2.9865	3.002	0.218	3.03536	3.036(6)	0.215(2)	0.01553	2
163	C H	12	16	1	2.9852	3.002	0.218	3.03407	3.036(6)	0.215(2)	0.01683	2
164	H H	24	27	2	3.0434	3.059	0.126	2.67025	2.679(5)	0.130(3)	0.01519	3
165	H H	16	19	1	3.0434	3.059	0.126	2.67025	2.679(5)	0.130(3)	0.01519	3
166	O H	6	24	1	3.0221	3.06	0.327	3.31754	3.322(7)	0.330(3)	0.03753	3
167	O H	8	20	1	3.0231	3.06	0.329	3.31891	3.322(7)	0.333(3)	0.03661	3
168	O H	7	16	1	3.0215	3.06	0.328	3.31715	3.322(7)	0.331(3)	0.03815	3
169	Si H	1	24	1	3.0401	3.063	0.181	3.16777	3.180(6)	0.184(3)	0.02323	3
170	Si H	1	20	1	3.0402	3.063	0.181	3.16796	3.180(6)	0.185(3)	0.02318	3
171	Si H	1	16	1	3.04	3.063	0.181	3.16771	3.180(6)	0.185(3)	0.02336	3
172	O H	6	29	1	3.0844	3.104	0.252	3.04825	3.046(6)	0.256(3)	0.01988	3
173	O H	8	28	1	3.0816	3.104	0.252	3.04547	3.046(6)	0.256(3)	0.02264	3
174	O H	7	30	1	3.0863	3.104	0.252	3.05016	3.046(6)	0.256(3)	0.01794	3
175	C C	10	13	1	3.1551	3.165	0.11	3.12235	3.128(6)	0.114(3)	0.01	3
176	C C	11	14	1	3.1559	3.165	0.11	3.12314	3.128(6)	0.114(3)	0.00922	3
177	C C	9	12	1	3.155	3.165	0.11	3.12215	3.128(6)	0.114(3)	0.01018	3
178	H H	22	26	1	3.014	3.021	0.229	2.96117	2.949(6)	0.233(3)	0.00651	3
179	H H	18	22	1	3.0132	3.021	0.229	2.96037	2.949(6)	0.233(3)	0.00735	3
180	H H	18	26	1	3.0135	3.021	0.229	2.96065	2.949(6)	0.233(3)	0.007	3
181	C H	12	26	1	3.1272	3.134	0.137	3.09306	3.093(6)	0.141(3)	0.00669	3
182	C H	10	22	1	3.1267	3.134	0.137	3.09256	3.093(6)	0.141(3)	0.00718	3
183	C H	14	18	1	3.1269	3.134	0.137	3.09266	3.093(6)	0.141(3)	0.00705	3
184	Si C	1	14	1	3.194	3.213	0.105	3.15956	3.175(6)	0.109(3)	0.0189	3
185	Si C	1	10	1	3.194	3.213	0.105	3.15966	3.175(6)	0.109(3)	0.01887	3
186	Si C	1	12	1	3.1941	3.213	0.105	3.15975	3.175(6)	0.109(3)	0.01878	3
187	O C	6	13	1	3.257	3.279	0.184	3.37603	3.388(7)	0.187(3)	0.02193	3
188	O C	8	11	1	3.2579	3.279	0.185	3.37697	3.387(7)	0.189(3)	0.02106	3
189	O C	7	9	1	3.2567	3.279	0.184	3.37569	3.388(7)	0.188(3)	0.0223	3
190	O H	7	22	2	3.3437	3.36	0.102	3.35664	3.370(7)	0.106(3)	0.01658	3
191	O H	6	18	1	3.3437	3.36	0.102	3.35664	3.370(7)	0.106(3)	0.01656	3
192	C H	12	19	1	3.3734	3.381	0.104	3.4047	3.409(7)	0.108(3)	0.00745	3
193	C H	14	23	2	3.3736	3.381	0.104	3.4049	3.409(7)	0.108(3)	0.00721	3
194	N H	2	21	1	3.3111	3.321	0.103	3.29564	3.302(7)	0.106(3)	0.0095	3
195	N H	2	25	1	3.3111	3.321	0.103	3.29564	3.302(7)	0.106(3)	0.00949	3
196	N H	2	17	1	3.3111	3.321	0.103	3.29574	3.302(7)	0.106(3)	0.00941	3

197	H H	19	27	1	3.5377	3.549	0.157	3.67428	3.678(7)	0.161(3)	0.01111	3
198	H H	23	27	1	3.5384	3.549	0.157	3.67488	3.678(7)	0.161(3)	0.01044	3
199	H H	19	23	1	3.5373	3.549	0.157	3.67388	3.678(7)	0.161(3)	0.01151	3
200	C H	9	24	1	3.5364	3.562	0.266	3.65867	3.664(7)	0.270(3)	0.02571	3
201	C H	13	20	1	3.5377	3.562	0.268	3.66021	3.664(7)	0.272(3)	0.02446	3
202	C H	11	16	1	3.5359	3.562	0.267	3.65827	3.664(7)	0.271(3)	0.02626	3
203	O C	7	14	1	3.5573	3.576	0.113	3.52897	3.544(7)	0.117(3)	0.0191	3
204	O C	8	10	1	3.557	3.576	0.113	3.52877	3.544(7)	0.117(3)	0.01936	3
205	O C	6	12	1	3.557	3.576	0.113	3.52867	3.544(7)	0.117(3)	0.01937	3
206	O C	6	14	1	3.5853	3.601	0.12	3.65633	3.668(7)	0.124(3)	0.01591	3
207	O C	7	10	1	3.5851	3.601	0.121	3.65604	3.668(7)	0.124(3)	0.01619	3
208	O C	8	12	1	3.5859	3.601	0.121	3.65685	3.668(7)	0.125(3)	0.01539	3
209	O H	7	27	1	3.575	3.606	0.236	3.31906	3.333(7)	0.240(3)	0.03099	3
210	C C	9	14	1	3.606	3.613	0.081	3.58539	3.591(7)	0.085(3)	0.00731	3
211	C C	12	13	1	3.6064	3.613	0.081	3.5858	3.591(7)	0.085(3)	0.00683	3
212	C C	10	11	1	3.6058	3.613	0.081	3.5852	3.591(7)	0.085(3)	0.00751	3
213	O H	8	19	1	3.5746	3.606	0.236	3.31866	3.333(7)	0.240(3)	0.03143	3
214	O H	6	23	1	3.5745	3.606	0.236	3.31858	3.333(7)	0.240(3)	0.03154	3
215	Si H	1	27	1	3.5825	3.614	0.2	3.16463	3.183(6)	0.203(3)	0.03145	3
216	Si H	1	23	1	3.5827	3.614	0.2	3.16481	3.183(6)	0.203(3)	0.03124	3
217	Si H	1	19	1	3.5827	3.614	0.199	3.1648	3.183(6)	0.203(3)	0.03129	3
218	Si H	1	25	1	3.604	3.631	0.102	3.58026	3.604(7)	0.106(3)	0.02713	3
219	Si H	1	17	1	3.604	3.631	0.102	3.58026	3.604(7)	0.106(3)	0.02715	3
220	Si H	1	21	1	3.604	3.631	0.103	3.58017	3.604(7)	0.106(3)	0.02721	3
221	O C	7	13	1	3.706	3.726	0.089	3.68062	3.698(7)	0.092(3)	0.01967	3
222	O C	8	9	1	3.7055	3.726	0.089	3.68012	3.698(7)	0.092(3)	0.02018	3
223	O C	6	11	1	3.7055	3.726	0.089	3.68002	3.698(7)	0.092(3)	0.02021	3
224	O H	6	30	1	3.7161	3.759	0.12	3.68397	3.722(7)	0.124(3)	0.04252	3
225	O H	7	28	1	3.7153	3.759	0.12	3.68307	3.722(7)	0.124(3)	0.04338	3
226	O H	8	29	1	3.7161	3.759	0.12	3.68397	3.722(7)	0.124(3)	0.04254	3
227	H H	19	25	1	3.7924	3.807	0.228	3.90479	3.906(8)	0.232(3)	0.0149	3
228	H H	21	27	1	3.7939	3.807	0.227	3.90623	3.906(8)	0.231(3)	0.01349	3
229	H H	17	23	1	3.792	3.807	0.228	3.90439	3.906(8)	0.232(3)	0.01537	3
230	C C	9	13	1	3.8048	3.822	0.131	3.80296	3.816(8)	0.134(3)	0.01746	3
231	C C	11	13	1	3.8057	3.822	0.131	3.80391	3.816(8)	0.135(3)	0.01655	3
232	C C	9	11	1	3.8045	3.822	0.131	3.80268	3.816(8)	0.135(3)	0.01775	3
233	H H	19	22	1	3.8511	3.862	0.166	4.02805	4.031(8)	0.170(3)	0.01049	3
234	H H	23	26	1	3.8512	3.862	0.166	4.02805	4.031(8)	0.170(3)	0.01042	3
235	H H	18	27	1	3.8512	3.862	0.166	4.02804	4.031(8)	0.170(3)	0.01042	3
236	H H	18	24	1	3.9689	4.001	0.245	4.01846	4.035(8)	0.249(3)	0.03242	3
237	H H	20	26	1	3.9699	4.001	0.245	4.01932	4.035(8)	0.248(3)	0.03148	3
238	H H	16	22	1	3.9687	4.001	0.245	4.01827	4.035(8)	0.249(3)	0.0326	3
239	H H	17	24	1	3.998	4.031	0.311	4.01548	4.023(8)	0.315(3)	0.03256	3
240	H H	20	25	1	3.9998	4.031	0.312	4.01744	4.023(8)	0.316(3)	0.03083	3
241	H H	16	21	1	3.9973	4.031	0.312	4.01486	4.023(8)	0.316(3)	0.03333	3
242	C H	11	18	1	3.9382	3.951	0.157	3.87392	3.880(8)	0.169(10)	0.01319	4
243	C H	9	26	1	3.9386	3.951	0.157	3.87432	3.880(8)	0.169(10)	0.0128	4
244	C H	13	22	1	3.9391	3.951	0.157	3.87494	3.880(8)	0.170(10)	0.01226	4
245	C H	11	26	1	4.081	4.104	0.151	4.05432	4.070(8)	0.164(10)	0.02255	4
246	C H	13	18	1	4.0804	4.104	0.151	4.05374	4.070(8)	0.164(10)	0.02317	4
247	C H	9	22	1	4.0803	4.104	0.151	4.05354	4.070(8)	0.164(10)	0.02328	4
248	C C	9	15	1	4.1086	4.131	0.104	4.09602	4.115(8)	0.117(10)	0.0228	4
249	C C	13	15	1	4.1083	4.131	0.104	4.09582	4.116(8)	0.117(10)	0.02303	4
250	C C	11	15	1	4.1092	4.131	0.104	4.09672	4.116(8)	0.117(10)	0.02214	4
251	C H	12	24	1	4.165	4.181	0.15	4.20585	4.216(8)	0.163(10)	0.01608	4
252	C H	10	20	1	4.1647	4.181	0.151	4.20557	4.216(8)	0.164(10)	0.01641	4
253	C H	14	16	1	4.1648	4.181	0.15	4.20566	4.216(8)	0.163(10)	0.01634	4
254	C H	10	25	1	4.1647	4.184	0.135	4.1415	4.155(8)	0.148(10)	0.01891	4
255	C H	14	21	1	4.1655	4.184	0.135	4.14229	4.155(8)	0.148(10)	0.01809	4
256	C H	12	17	1	4.1644	4.184	0.135	4.1413	4.155(8)	0.148(10)	0.01915	4
257	Si H	1	18	1	4.1071	4.138	0.127	4.05704	4.083(8)	0.140(10)	0.03059	4
258	Si H	1	26	1	4.1071	4.138	0.127	4.05704	4.083(8)	0.140(10)	0.03058	4
259	Si H	1	22	1	4.1072	4.138	0.127	4.05714	4.083(8)	0.140(10)	0.03053	4
260	H H	24	28	1	4.2427	4.25	0.31	4.39482	4.378(9)	0.323(10)	0.00711	4
261	H H	16	29	1	4.2471	4.25	0.31	4.39913	4.378(9)	0.323(10)	0.00275	4
262	H H	20	30	1	4.2483	4.25	0.31	4.40037	4.378(9)	0.323(10)	0.00153	4
263	C H	13	28	1	4.2503	4.273	0.255	4.28829	4.294(9)	0.268(10)	0.02264	4

264	C H	9	29	1	4.2539	4.273	0.255	4.29178	4.294(9)	0.268(10)	0.01908	4
265	C H	11	30	1	4.2555	4.273	0.255	4.29348	4.294(9)	0.268(10)	0.01743	4
266	O H	7	18	1	4.1611	4.189	0.185	4.21199	4.230(8)	0.198(10)	0.02764	4
267	O H	6	26	1	4.1615	4.189	0.185	4.21239	4.230(8)	0.198(10)	0.02726	4
268	O H	8	22	1	4.162	4.189	0.185	4.21292	4.230(8)	0.198(10)	0.02674	4
269	O H	7	24	1	4.2793	4.31	0.177	4.38798	4.410(9)	0.190(10)	0.0305	4
270	O H	6	20	1	4.279	4.31	0.178	4.38774	4.410(9)	0.191(10)	0.03076	4
271	O H	8	16	1	4.279	4.31	0.178	4.3876	4.410(9)	0.191(10)	0.03084	4
272	O H	6	25	1	4.2866	4.322	0.205	4.41933	4.444(9)	0.217(10)	0.03528	4
273	O H	8	21	1	4.2874	4.322	0.206	4.42025	4.444(9)	0.219(10)	0.03448	4
274	O H	7	17	1	4.2862	4.322	0.205	4.41898	4.444(9)	0.218(10)	0.03568	4
275	C H	15	24	1	4.3142	4.342	0.199	4.43037	4.448(9)	0.212(10)	0.02795	4
276	C H	15	16	1	4.3147	4.342	0.199	4.43089	4.448(9)	0.212(10)	0.02745	4
277	C H	15	20	1	4.3152	4.342	0.2	4.43141	4.448(9)	0.212(10)	0.02694	4
278	O H	6	27	1	4.3322	4.36	0.148	4.11293	4.135(8)	0.161(10)	0.02815	4
279	O H	8	23	1	4.3326	4.36	0.148	4.11334	4.135(8)	0.161(10)	0.02779	4
280	O H	7	19	1	4.3321	4.36	0.148	4.11274	4.135(8)	0.161(10)	0.02832	4
281	C H	9	28	1	4.3447	4.378	0.256	4.31241	4.329(9)	0.269(10)	0.03297	4
282	C H	11	29	1	4.3489	4.378	0.256	4.31659	4.329(9)	0.269(10)	0.02874	4
283	C H	13	30	1	4.3474	4.378	0.256	4.31508	4.329(9)	0.269(10)	0.03024	4
284	C H	14	17	1	4.4119	4.429	0.131	4.33731	4.349(9)	0.144(10)	0.01693	4
285	C H	10	21	1	4.4116	4.429	0.131	4.33701	4.349(9)	0.144(10)	0.01724	4
286	C H	12	25	1	4.4125	4.429	0.132	4.33791	4.349(9)	0.144(10)	0.0163	4
287	C H	13	23	2	4.4164	4.434	0.116	4.31334	4.327(9)	0.129(10)	0.01757	4
288	C H	11	19	1	4.4163	4.434	0.116	4.31324	4.327(9)	0.129(10)	0.01769	4
289	H H	16	24	1	4.4646	4.503	0.275	4.63998	4.661(9)	0.287(10)	0.03853	4
290	H H	20	24	1	4.4657	4.503	0.276	4.64118	4.661(9)	0.289(10)	0.03745	4
291	H H	16	20	1	4.4642	4.503	0.275	4.63958	4.661(9)	0.288(10)	0.03899	4
292	C H	13	17	1	4.4991	4.529	0.185	4.41986	4.441(9)	0.198(10)	0.02965	4
293	C H	11	25	1	4.5004	4.529	0.185	4.42108	4.441(9)	0.198(10)	0.02842	4
294	C H	9	21	1	4.4986	4.529	0.185	4.41937	4.441(9)	0.198(10)	0.03015	4
295	O H	8	17	1	4.508	4.543	0.14	4.40054	4.430(9)	0.153(10)	0.03529	4
296	O H	7	25	1	4.5088	4.543	0.14	4.40122	4.430(9)	0.153(10)	0.03455	4
297	O H	6	21	1	4.5078	4.543	0.14	4.40023	4.430(9)	0.153(10)	0.03552	4
298	N C	2	15	1	4.2832	4.307	0.183	4.34558	4.360(9)	0.196(10)	0.02376	4
299	C H	11	24	1	4.5536	4.582	0.175	4.63051	4.651(9)	0.188(10)	0.0284	4
300	C H	13	16	1	4.5529	4.582	0.174	4.62988	4.651(9)	0.187(10)	0.02908	4
301	C H	9	20	1	4.5528	4.582	0.175	4.62973	4.651(9)	0.188(10)	0.02923	4
302	O H	7	26	1	4.5367	4.569	0.134	4.52047	4.548(9)	0.147(10)	0.03208	4
303	O H	8	18	1	4.5365	4.569	0.134	4.52037	4.548(9)	0.147(10)	0.03224	4
304	O H	6	22	1	4.5365	4.569	0.134	4.52037	4.548(9)	0.147(10)	0.03224	4
305	H H	17	26	1	4.5592	4.578	0.214	4.42428	4.431(9)	0.227(10)	0.01881	4
306	H H	18	21	1	4.5587	4.578	0.214	4.42377	4.431(9)	0.227(10)	0.01932	4
307	H H	22	25	1	4.56	4.578	0.214	4.42499	4.431(9)	0.227(10)	0.0181	4
308	H H	22	24	1	4.5859	4.608	0.178	4.55634	4.570(9)	0.191(10)	0.02218	4
309	H H	18	20	1	4.5853	4.608	0.178	4.55574	4.571(9)	0.191(10)	0.02283	4
310	H H	16	26	1	4.5856	4.608	0.178	4.55594	4.570(9)	0.191(10)	0.02255	4
311	C H	15	17	1	4.7408	4.777	0.15	4.72061	4.752(9)	0.163(10)	0.03667	4
312	C H	15	21	2	4.7411	4.777	0.15	4.72091	4.752(9)	0.163(10)	0.03637	4
313	H H	16	28	1	4.7278	4.78	0.295	4.79908	4.832(10)	0.308(10)	0.05264	4
314	H H	24	30	1	4.7296	4.78	0.295	4.80086	4.832(10)	0.308(10)	0.05084	4
315	H H	20	29	1	4.7313	4.78	0.295	4.80256	4.832(10)	0.308(10)	0.04917	4
316	H H	17	28	1	4.7831	4.822	0.318	4.72085	4.737(9)	0.331(10)	0.03908	4
317	H H	21	29	1	4.7875	4.822	0.318	4.72513	4.737(9)	0.331(10)	0.0347	4
318	H H	25	30	1	4.7858	4.822	0.318	4.72342	4.737(9)	0.331(10)	0.0364	4
319	H H	23	24	1	4.7984	4.822	0.199	4.84458	4.859(10)	0.212(10)	0.0236	4
320	H H	19	20	1	4.7988	4.822	0.199	4.845	4.859(10)	0.212(10)	0.02326	4
321	H H	16	27	1	4.7986	4.822	0.199	4.84479	4.859(10)	0.212(10)	0.02341	4
322	H H	25	28	1	4.8194	4.86	0.319	4.89302	4.911(10)	0.332(10)	0.04016	4
323	H H	17	29	1	4.8224	4.86	0.319	4.89602	4.911(10)	0.332(10)	0.03717	4
324	H H	21	30	1	4.8245	4.859	0.319	4.89822	4.911(10)	0.332(10)	0.03498	4
325	C H	9	25	1	4.8826	4.913	0.155	4.89476	4.920(10)	0.168(10)	0.0307	4
326	C H	13	21	1	4.8835	4.913	0.156	4.89571	4.920(10)	0.169(10)	0.02983	4
327	C H	11	17	1	4.8823	4.913	0.155	4.89448	4.920(10)	0.168(10)	0.03104	4
328	C C	14	15	1	4.9182	4.944	0.117	4.87418	4.896(10)	0.130(10)	0.02558	4
329	C C	10	15	1	4.9183	4.944	0.117	4.87417	4.896(10)	0.130(10)	0.02551	4
330	C C	12	15	1	4.9187	4.944	0.117	4.87467	4.896(10)	0.130(10)	0.02505	4

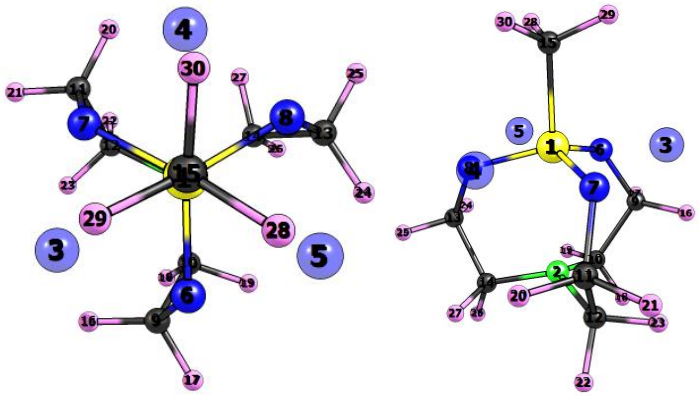
331	N H	2	29	2	4.7681	4.802	0.23	4.83895	4.861(10)	0.243(10)	0.03411	4
332	N H	2	30	1	4.7699	4.802	0.23	4.84066	4.861(10)	0.243(10)	0.03239	4
333	C H	13	29	1	4.9837	5.043	0.128	4.98537	5.041(10)	0.141(10)	0.05959	4
334	C H	9	30	1	4.984	5.043	0.128	4.98576	5.041(10)	0.141(10)	0.05925	4
335	C H	11	28	1	4.9826	5.043	0.128	4.98436	5.041(10)	0.141(10)	0.06064	4
336	H H	21	26	1	5.0283	5.058	0.177	5.00071	5.024(10)	0.190(10)	0.0302	4
337	H H	18	25	1	5.0276	5.058	0.177	5.00002	5.024(10)	0.190(10)	0.0309	4
338	H H	17	22	1	5.0275	5.059	0.177	4.99992	5.024(10)	0.190(10)	0.03107	4
339	H H	24	29	1	5.1546	5.222	0.248	5.30968	5.364(11)	0.261(10)	0.06721	4
340	H H	20	28	1	5.154	5.222	0.249	5.30914	5.364(11)	0.262(10)	0.06775	4
341	H H	16	30	1	5.1556	5.222	0.248	5.3107	5.364(11)	0.261(10)	0.06622	4
342	C H	10	28	1	5.2046	5.235	0.225	5.15531	5.175(10)	0.238(10)	0.03067	4
343	C H	12	29	1	5.209	5.235	0.225	5.15971	5.175(10)	0.238(10)	0.02627	4
344	C H	14	30	1	5.2081	5.235	0.225	5.15881	5.175(10)	0.238(10)	0.02714	4
345	C H	15	27	1	5.2121	5.251	0.226	4.6956	4.722(9)	0.239(10)	0.03884	4
346	C H	15	23	1	5.2127	5.251	0.226	4.69618	4.722(9)	0.239(10)	0.03824	4
347	C H	15	19	1	5.212	5.251	0.226	4.69546	4.722(9)	0.239(10)	0.03892	4
348	C H	14	28	1	5.2805	5.314	0.21	5.27265	5.297(11)	0.223(10)	0.03334	4
349	C H	10	29	1	5.284	5.314	0.21	5.27614	5.297(11)	0.223(10)	0.02982	4
350	C H	12	30	1	5.285	5.314	0.21	5.27714	5.296(11)	0.223(10)	0.0288	4
351	H H	17	27	1	5.3172	5.347	0.141	5.16179	5.187(10)	0.154(10)	0.02953	4
352	H H	19	21	1	5.317	5.347	0.141	5.16159	5.187(10)	0.154(10)	0.02969	4
353	H H	23	25	1	5.3175	5.347	0.141	5.16209	5.187(10)	0.154(10)	0.02922	4
354	H H	27	30	1	5.3177	5.344	0.316	4.76799	4.767(9)	0.358(86)	0.02635	5
355	H H	23	29	1	5.3186	5.344	0.316	4.76885	4.767(9)	0.357(86)	0.02543	5
356	H H	19	28	1	5.3136	5.344	0.316	4.76395	4.767(9)	0.357(86)	0.03038	5
357	H H	17	25	1	5.5443	5.589	0.221	5.49802	5.530(11)	0.263(86)	0.04458	5
358	H H	21	25	1	5.5455	5.589	0.222	5.49935	5.530(11)	0.264(86)	0.04329	5
359	H H	17	21	1	5.5437	5.589	0.221	5.49743	5.530(11)	0.263(86)	0.04517	5
360	H H	21	24	1	5.6275	5.67	0.186	5.70275	5.736(11)	0.228(86)	0.04216	5
361	H H	16	25	1	5.6269	5.67	0.186	5.70213	5.736(11)	0.228(86)	0.04273	5
362	H H	17	20	1	5.6268	5.67	0.187	5.70207	5.736(11)	0.229(86)	0.04289	5
363	C H	14	29	1	5.6223	5.673	0.161	5.58524	5.629(11)	0.202(86)	0.05108	5
364	C H	12	28	1	5.6199	5.673	0.161	5.58284	5.629(11)	0.202(86)	0.05351	5
365	C H	10	30	1	5.6223	5.673	0.161	5.58524	5.629(11)	0.202(86)	0.05111	5
366	H H	27	28	1	5.7048	5.762	0.274	5.19881	5.237(10)	0.315(86)	0.05739	5
367	H H	23	30	1	5.7091	5.762	0.274	5.20308	5.237(10)	0.315(86)	0.05307	5
368	H H	19	29	1	5.7076	5.762	0.273	5.20157	5.237(10)	0.315(86)	0.05456	5
369	H H	17	30	1	5.6897	5.773	0.158	5.67397	5.750(11)	0.200(86)	0.08323	5
370	H H	21	28	2	5.6893	5.773	0.158	5.67347	5.750(11)	0.200(86)	0.08369	5
371	C H	15	18	1	5.8354	5.875	0.135	5.77861	5.813(12)	0.177(86)	0.03935	5
372	C H	15	26	1	5.8353	5.875	0.135	5.77851	5.813(12)	0.177(86)	0.03951	5
373	C H	15	22	1	5.8358	5.875	0.135	5.77901	5.813(12)	0.177(86)	0.03899	5
374	H H	27	29	1	5.909	5.976	0.27	5.45129	5.500(11)	0.312(86)	0.06676	5
375	H H	23	28	1	5.9065	5.976	0.27	5.44878	5.500(11)	0.312(86)	0.06929	5
376	H H	19	30	1	5.9085	5.976	0.27	5.45075	5.500(11)	0.311(86)	0.0673	5
377	H H	18	29	1	6.0981	6.136	0.238	6.06844	6.093(12)	0.280(86)	0.03742	5
378	H H	26	28	1	6.0942	6.136	0.238	6.06456	6.093(12)	0.280(86)	0.04132	5
379	H H	22	30	1	6.099	6.136	0.238	6.06935	6.093(12)	0.280(86)	0.03657	5
380	H H	18	28	1	6.1895	6.239	0.235	6.13275	6.169(12)	0.277(86)	0.04924	5
381	H H	22	29	1	6.1938	6.239	0.235	6.13694	6.169(12)	0.277(86)	0.04498	5
382	H H	26	30	1	6.1928	6.239	0.235	6.13604	6.169(12)	0.277(86)	0.04596	5
383	H H	26	29	2	6.5293	6.597	0.175	6.48259	6.543(13)	0.217(86)	0.06748	5
384	H H	22	28	1	6.5268	6.597	0.175	6.48019	6.543(13)	0.217(86)	0.06995	5

[a] r_{h1} values ($r_{h1}=r_a+\Delta r$) are given for GED results. The vibrational corrections Δr were calculated by the Vibmodule program (Vishnevskiy et al, *J. Phys.: Conf. Ser*., 2015, **633**, 012076) using the so called second approximation, in which harmonic approach with nonlinear relation between Cartesian and internal coordinates were applied on the base of the force field estimated in the quantum chemical calculations at B3LYP/6-311G** level.

[b] Values in parentheses for the GED data are full errors estimated as $\sigma(r_{h1})=[\sigma_{scale}^2+(2.5\sigma_{LS})^2]^{1/2}$, where $\sigma_{scale}=0.002r$ and σ_{LS} is a standard deviation in least-squares refinement for internuclear distances and as $3\sigma_{LS}$ for vibration amplitudes. The place-value is such that the last digit of the uncertainty lines up with the last digit of the nominal value.

[c] All amplitudes were refined being united in 5 groups. The differences between the amplitudes within each group were constrained to the calculated values.

Atomic coordinates of the refined structure of 1-methylsilatrane (for the C_3 conformer) based on the B3LYP/6-311G calculations**



Atom #	Nucleus charge	X	Y	Z
1.	14	0.	0.	0.
2.	7	0.	0.	2.5137
3.	0	2	0.	0.
4.	0	-1.	1.7321	0.
5.	0	-1.	-1.7321	0.
6.	8	1.1479	-1.1479	0.3776
7.	8	0.4202	1.5681	0.3776
8.	8	-1.5681	-0.4202	0.3776
9.	6	1.8096	-1.2564	1.6295
10.	6	0.8872	-1.1117	2.8383
11.	6	0.1833	2.1953	1.6295
12.	6	0.5192	1.3241	2.8383
13.	6	-1.9928	-0.9389	1.6295
14.	6	-1.4063	-0.2125	2.8383
15.	6	0.	0.	-1.8468
16.	1	2.6394	-0.5232	1.6952
17.	1	2.2426	-2.2725	1.6725
18.	1	1.5023	-0.8015	3.7108
19.	1	0.5459	-2.0523	2.3709
20.	1	-0.8666	2.5474	1.6952
21.	1	0.8467	3.0784	1.6725
22.	1	-0.0571	1.7018	3.7108
23.	1	1.5044	1.4989	2.3709
24.	1	-1.7729	-2.0242	1.6952
25.	1	-3.0893	-0.8059	1.6725
26.	1	-1.4452	-0.9003	3.7108
27.	1	-2.0503	0.5534	2.3709
28.	1	-0.1247	-1.0258	-2.236
29.	1	0.9507	0.4049	-2.236
30.	1	-0.826	0.6208	-2.236

Table S2. Starting (QC) and refined (GED) values for internuclear distances (r_a, r_{h1}) and vibrational amplitudes (l) of 1-methylsilatrane based on the MP2/6-311G** calculations

Param. #	Atoms	N1	N2	Multiplicity	Starting values			Refined values[b]			Vibrational corrections Δr^a	Gr. #[c]
					r_a	r_{h1}	l	r_a	r_{h1}	l		
70	C H	15	29	3	1.0913	1.093	0.076	1.10498	1.101(2)	0.077(2)	0.00166	1
71	C H	12	23	1	1.0926	1.094	0.076	1.1063	1.102(2)	0.077(2)	0.00122	1
72	C H	14	27	2	1.0926	1.094	0.076	1.1063	1.102(2)	0.077(2)	0.0012	1
73	C H	13	25	3	1.0931	1.094	0.076	1.10681	1.103(2)	0.077(2)	0.00113	1
74	C H	11	20	3	1.0979	1.099	0.077	1.1117	1.107(2)	0.078(2)	0.00101	1
75	C H	12	22	3	1.0988	1.1	0.077	1.1126	1.109(2)	0.078(2)	0.0014	1
76	O C	7	11	3	1.4069	1.409	0.048	1.40978	1.410(3)	0.049(2)	0.00224	1
77	N C	2	10	3	1.4615	1.459	0.049	1.48107	1.476(3)	0.050(2)	-0.003	1
78	C C	9	10	3	1.5295	1.529	0.051	1.52221	1.519(3)	0.052(2)	-1E-3	1
79	Si O	1	8	3	1.6799	1.682	0.047	1.66791	1.668(3)	0.048(2)	0.00167	1
80	H H	28	29	3	1.7599	1.772	0.124	1.77977	1.783(4)	0.125(2)	0.01174	1
81	H H	20	21	3	1.7675	1.775	0.122	1.87566	1.875(4)	0.123(2)	0.00745	1
82	H H	22	23	3	1.771	1.779	0.123	1.6546	1.653(3)	0.124(2)	0.00789	1
83	Si C	1	15	1	1.8585	1.858	0.052	1.8505	1.848(4)	0.053(2)	-7.7E-4	1
84	O H	7	21	3	2.0352	2.041	0.1	2.04198	2.044(4)	0.097(3)	0.00622	2
85	O H	6	16	3	2.0594	2.065	0.1	2.12385	2.126(4)	0.096(3)	0.00603	2
86	N H	2	19	3	2.0747	2.078	0.102	2.1641	2.163(4)	0.099(3)	0.00352	2
87	N H	2	18	3	2.1347	2.138	0.102	2.23833	2.237(4)	0.098(3)	0.00315	2
88	C H	9	19	3	2.1424	2.148	0.109	2.10446	2.105(4)	0.105(3)	0.00545	2
89	C H	10	16	3	2.1631	2.167	0.106	2.14085	2.140(4)	0.103(3)	0.00371	2
90	C H	14	25	2	2.1658	2.171	0.107	2.00545	2.005(4)	0.103(3)	0.00472	2
91	C H	10	17	1	2.1658	2.171	0.107	2.00545	2.005(4)	0.103(3)	0.00473	2
92	C H	11	22	3	2.1907	2.195	0.108	2.18571	2.185(4)	0.104(3)	0.00397	2
93	H H	16	23	3	2.2686	2.27	0.264	2.63249	2.608(5)	0.260(3)	0.00178	2
94	N C	2	11	2	2.3938	2.395	0.064	2.44219	2.442(5)	0.060(3)	0.00107	2
95	N C	2	13	1	2.3937	2.395	0.064	2.4421	2.442(5)	0.060(3)	0.00111	2
96	O C	8	14	3	2.3889	2.396	0.066	2.39594	2.401(5)	0.063(3)	0.00694	2
97	Si N	1	2	1	2.3935	2.419	0.15	2.48124	2.498(5)	0.146(3)	0.02512	2
98	H H	25	27	3	2.4222	2.433	0.173	2.07443	2.071(4)	0.169(3)	0.01035	2
99	H H	18	23	3	2.4433	2.441	0.224	2.65434	2.634(5)	0.220(3)	-0.0023	2
100	Si H	1	30	3	2.4571	2.465	0.124	2.46028	2.462(5)	0.120(3)	0.00809	2
101	C C	10	14	3	2.4728	2.47	0.069	2.51332	2.509(5)	0.066(3)	-0.00259	2
102	H H	16	18	3	2.4698	2.478	0.175	2.43635	2.432(5)	0.172(3)	0.00802	2
103	C H	10	23	3	2.4885	2.486	0.141	2.60951	2.600(5)	0.137(3)	-0.00233	2
104	H H	25	26	3	2.5959	2.602	0.162	2.43368	2.429(5)	0.159(3)	0.0059	2
105	N O	2	8	3	2.6385	2.649	0.089	2.66202	2.670(5)	0.085(3)	0.01095	2
106	C H	12	18	3	2.6619	2.662	0.153	2.83983	2.832(6)	0.149(3)	3.1E-4	2
107	O H	8	27	3	2.695	2.711	0.162	2.76933	2.776(6)	0.159(3)	0.01578	2
108	Si C	1	11	3	2.7064	2.72	0.067	2.73855	2.750(5)	0.063(3)	0.0134	2
109	O C	8	15	3	2.7403	2.748	0.1	2.75205	2.757(5)	0.096(3)	0.00785	2
110	N H	2	16	3	2.7477	2.755	0.152	2.87568	2.875(6)	0.148(3)	0.00692	2
111	C H	9	23	3	2.778	2.785	0.194	3.04657	3.042(6)	0.189(5)	0.00692	3
112	O O	7	8	2	2.8438	2.851	0.095	2.81695	2.822(6)	0.091(3)	0.00764	2
113	O O	6	8	1	2.8435	2.851	0.095	2.80516	2.810(6)	0.091(3)	0.00796	2
114	O H	8	30	3	2.8865	2.899	0.237	2.92412	2.918(6)	0.233(3)	0.01225	2
115	C H	12	16	3	2.9212	2.932	0.205	3.13943	3.138(6)	0.200(5)	0.01109	3
116	H H	18	22	3	2.9741	2.982	0.227	3.24872	3.241(6)	0.223(5)	0.00761	3
117	O H	6	29	3	3.0042	3.023	0.239	3.03748	3.038(6)	0.235(3)	0.01924	2
118	H H	16	19	3	3.0418	3.057	0.125	2.97445	2.984(6)	0.121(3)	0.01487	2
119	Si H	1	24	3	3.0509	3.072	0.178	3.19484	3.206(6)	0.173(5)	0.02084	3
120	Si C	1	10	3	3.055	3.075	0.103	3.11283	3.129(6)	0.099(5)	0.01966	3
121	C H	10	22	2	3.071	3.078	0.14	3.19933	3.200(6)	0.135(5)	0.00687	3
122	C H	12	26	1	3.0714	3.078	0.14	3.20832	3.209(6)	0.135(5)	0.00645	3
123	C C	11	14	3	3.1089	3.116	0.105	3.23112	3.235(6)	0.100(5)	0.00678	3
124	O H	8	20	3	3.1497	3.18	0.323	3.32916	3.329(7)	0.319(5)	0.03064	3
125	N H	2	21	3	3.3399	3.35	0.099	3.24543	3.253(6)	0.094(5)	0.0101	3
126	O H	7	22	3	3.3435	3.359	0.1	3.35539	3.369(7)	0.095(5)	0.01584	3
127	C H	10	27	3	3.3574	3.364	0.103	3.43859	3.442(7)	0.098(5)	0.00622	3
128	O C	8	11	3	3.3539	3.37	0.176	3.37678	3.385(7)	0.171(5)	0.01647	3
129	Si H	1	19	3	3.4153	3.447	0.192	3.59341	3.615(7)	0.188(5)	0.03128	3
130	O H	6	23	2	3.4482	3.479	0.231	3.66038	3.678(7)	0.226(5)	0.03119	3

131	O H	7	27	1	3.4488	3.479	0.231	3.67403	3.691(7)	0.226(5)	0.0306	3
132	O C	8	10	3	3.4976	3.516	0.113	3.5422	3.557(7)	0.108(5)	0.01858	3
133	H H	19	23	3	3.536	3.547	0.155	3.66165	3.667(7)	0.150(5)	0.01118	3
134	C H	9	24	3	3.5915	3.61	0.256	3.75767	3.759(7)	0.251(5)	0.01823	3
135	Si H	1	21	3	3.5947	3.62	0.1	3.57845	3.601(7)	0.096(5)	0.02523	3
136	C C	10	11	1	3.6192	3.624	0.076	3.63329	3.636(7)	0.071(5)	0.00432	3
137	C C	9	14	2	3.6196	3.623	0.076	3.63369	3.636(7)	0.071(5)	0.0039	3
138	O C	8	12	3	3.6118	3.625	0.107	3.59873	3.609(7)	0.103(5)	0.01309	3
139	O H	8	29	3	3.6756	3.713	0.117	3.69023	3.724(7)	0.112(5)	0.03695	3
140	H H	17	23	3	3.7083	3.719	0.213	3.9916	3.991(8)	0.216(11)	0.01068	4
141	O C	6	11	3	3.7428	3.76	0.086	3.73607	3.751(7)	0.081(5)	0.01709	3
142	H H	16	22	3	3.8267	3.854	0.234	4.03538	4.050(8)	0.229(5)	0.0274	3
143	H H	18	27	3	3.8432	3.854	0.166	4.01793	4.022(8)	0.169(11)	0.0113	4
144	C C	11	13	3	3.8555	3.868	0.123	3.91396	3.922(8)	0.118(5)	0.012	3
145	C H	9	22	3	3.9963	4.017	0.153	4.14686	4.162(8)	0.156(11)	0.0206	4
146	H H	20	25	3	4.0418	4.067	0.298	3.97804	3.981(8)	0.293(5)	0.02488	3
147	C H	11	18	3	4.0583	4.068	0.148	4.18438	4.189(8)	0.151(11)	0.00986	4
148	Si H	1	22	3	4.0377	4.068	0.127	4.1387	4.165(8)	0.130(11)	0.03071	4
149	C C	13	15	3	4.0554	4.076	0.1	4.07833	4.097(8)	0.103(11)	0.0211	4
150	C H	14	21	3	4.1208	4.136	0.131	4.19237	4.203(8)	0.134(11)	0.01507	4
151	C H	14	16	3	4.1553	4.167	0.147	4.26582	4.273(9)	0.150(11)	0.01218	4
152	C H	11	30	2	4.1979	4.219	0.242	4.23754	4.244(8)	0.245(11)	0.02102	4
153	C H	9	29	1	4.1988	4.219	0.242	4.23205	4.238(8)	0.245(11)	0.02012	4
154	H H	24	28	3	4.2351	4.244	0.304	4.36288	4.350(9)	0.307(11)	0.00849	4
155	N C	2	15	1	4.2504	4.276	0.152	4.32565	4.346(9)	0.155(11)	0.02591	4
156	C H	13	30	3	4.2747	4.305	0.242	4.30631	4.323(9)	0.245(11)	0.03041	4
157	O H	8	22	3	4.3024	4.326	0.165	4.37699	4.394(9)	0.168(11)	0.02372	4
158	C H	15	24	3	4.3104	4.336	0.197	4.43371	4.450(9)	0.200(11)	0.02539	4
159	O H	8	23	3	4.3294	4.355	0.14	4.41407	4.435(9)	0.143(11)	0.02541	4
160	O H	6	20	3	4.3483	4.375	0.168	4.44119	4.461(9)	0.171(11)	0.02636	4
161	O H	8	21	3	4.3895	4.42	0.196	4.42872	4.450(9)	0.199(11)	0.03001	4
162	C H	11	19	3	4.416	4.431	0.113	4.52489	4.537(9)	0.116(11)	0.01463	4
163	C H	10	21	3	4.4287	4.442	0.126	4.22202	4.232(8)	0.129(11)	0.01362	4
164	O H	6	22	3	4.5028	4.534	0.137	4.59047	4.617(9)	0.140(11)	0.03129	4
165	H H	16	24	3	4.5198	4.551	0.264	4.73679	4.753(9)	0.267(11)	0.03112	4
166	O H	6	21	3	4.5283	4.562	0.147	4.37544	4.404(9)	0.150(11)	0.03346	4
167	C H	11	25	3	4.5383	4.563	0.178	4.3833	4.400(9)	0.181(11)	0.02451	4
168	C H	11	24	3	4.6069	4.63	0.166	4.74024	4.757(9)	0.169(11)	0.0229	4
169	H H	16	26	3	4.6471	4.666	0.178	4.84745	4.860(10)	0.181(11)	0.01915	4
170	H H	18	21	3	4.7035	4.719	0.201	4.57792	4.584(9)	0.204(11)	0.01518	4
171	C H	15	25	3	4.7079	4.743	0.145	4.74122	4.771(9)	0.148(11)	0.03486	4
172	H H	24	30	3	4.7104	4.757	0.278	4.82079	4.851(10)	0.281(11)	0.04656	4
173	H H	25	30	3	4.7272	4.765	0.3	4.7495	4.768(9)	0.303(11)	0.03741	4
174	N H	2	30	3	4.7368	4.773	0.204	4.81835	4.845(10)	0.207(11)	0.03571	4
175	H H	23	24	3	4.7744	4.794	0.195	5.01341	5.025(10)	0.198(11)	0.01926	4
176	C C	10	15	3	4.773	4.798	0.116	4.82085	4.843(10)	0.119(11)	0.02549	4
177	H H	21	30	3	4.7971	4.834	0.297	4.92032	4.939(10)	0.300(11)	0.03689	4
178	H H	17	22	3	4.9308	4.958	0.179	5.01971	5.040(10)	0.182(11)	0.02715	4
179	C H	13	21	3	4.9345	4.959	0.147	4.97801	4.998(10)	0.150(11)	0.02486	4
180	C H	13	29	3	4.9464	4.999	0.123	4.97911	5.028(10)	0.126(11)	0.05242	4
181	C H	15	19	3	5.0243	5.063	0.221	5.1971	5.226(10)	0.224(11)	0.03822	4
182	C H	14	30	3	5.0466	5.076	0.22	5.11408	5.134(10)	0.223(11)	0.02986	4
183	H H	27	30	2	5.1044	5.136	0.308	5.29502	5.308(11)	0.311(11)	0.03179	4
184	H H	23	29	1	5.1073	5.136	0.308	5.29791	5.308(11)	0.311(11)	0.02888	4
185	C H	12	30	3	5.1533	5.185	0.201	5.19512	5.219(10)	0.204(11)	0.03176	4
186	H H	24	29	3	5.1683	5.227	0.24	5.31116	5.358(11)	0.243(11)	0.05834	4
187	H H	19	21	3	5.3229	5.349	0.138	5.2178	5.240(10)	0.141(11)	0.02643	4
188	C H	10	30	3	5.4829	5.531	0.16	5.54075	5.586(11)	0.128(80)	0.04843	5
189	H H	19	29	2	5.547	5.599	0.261	5.68518	5.728(11)	0.230(80)	0.05209	5
190	H H	27	28	1	5.5436	5.599	0.261	5.68168	5.728(11)	0.230(80)	0.0555	5
191	H H	21	25	3	5.5872	5.626	0.212	5.45576	5.488(11)	0.180(80)	0.03847	5
192	H H	21	24	3	5.6798	5.716	0.178	5.75462	5.787(12)	0.146(80)	0.03605	5
193	H H	25	29	3	5.6687	5.743	0.154	5.69105	5.763(11)	0.123(80)	0.07454	5
194	H H	19	30	3	5.7196	5.783	0.265	5.9177	5.972(12)	0.233(80)	0.06345	5
195	C H	15	22	2	5.767	5.805	0.133	5.83885	5.875(12)	0.101(80)	0.03803	5
196	C H	15	18	1	5.7669	5.805	0.133	5.83866	5.875(12)	0.101(80)	0.03819	5
197	H H	22	30	3	6.061	6.101	0.225	6.12382	6.158(12)	0.194(80)	0.03981	5

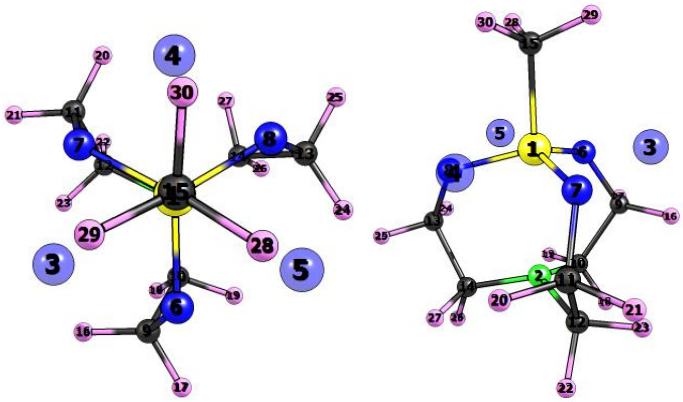
198	H H	26	30	3	6.0857	6.132	0.228	6.15459	6.194(12)	0.197(80)	0.04592	5
199	H H	18	30	3	6.4703	6.533	0.174	6.56658	6.626(13)	0.142(80)	0.06272	5

[a] r_{h1} values ($r_{h1}=r_a+\Delta r$) are given for GED results. The vibrational corrections Δr were calculated by the Vibmodule program (Vishnevskiy et al, *J. Phys.: Conf. Ser*., 2015, **633**, 012076) using the so called second approximation, in which harmonic approach with nonlinear relation between Cartesian and internal coordinates were applied on the base of the force field estimated in the quantum chemical calculations at MP2/6-311G** level.

[b] Values in parentheses for the GED data are full errors estimated as $\sigma(r_{h1})=[\sigma_{scale}^2+(2.5\sigma_{LS})^2]^{½}$, where $\sigma_{scale}=0.002r$ and σ_{LS} is a standard deviation in least-squares refinement for internuclear distances and as $3\sigma_{LS}$ for vibration amplitudes. The place-value is such that the last digit of the uncertainty lines up with the last digit of the nominal value.

[c] All amplitudes were refined being united in 5 groups. The differences between the amplitudes within each group were constrained to the calculated values.

Atomic coordinates of the refined structure of 1-methylsilatrane (for the C_3 conformer) based on the MP2/6-311G calculations**



Atom #	Nucleus charge	X	Y	Z
1.	14	0.	0.	0.
2.	7	0.	0.	2.4978
3.	0	2.	0.	0.
4.	0	-0.9918	1.7367	0.
5.	0	-0.9918	-1.7367	0.
6.	8	0.7745	-1.4282	0.3787
7.	8	0.8561	1.3808	0.3787
8.	8	-1.6243	0.0357	0.3787
9.	6	1.475	-1.7104	1.5698
10.	6	0.6423	-1.3006	2.7728
11.	6	0.7537	2.129	1.5698
12.	6	0.8108	1.2028	2.7728
13.	6	-2.2167	-0.4326	1.5698
14.	6	-1.4479	0.0872	2.7728
15.	6	0.	0.	-1.8483
16.	1	2.4632	-1.2178	1.6522
17.	1	1.4621	-2.8015	1.7268
18.	1	1.2016	-1.4377	3.72
19.	1	-0.08	-2.1183	2.9281
20.	1	-0.164	2.7429	1.6522
21.	1	1.7077	2.659	1.7268
22.	1	0.6526	1.7564	3.72
23.	1	1.8792	0.981	2.9281
24.	1	-2.279	-1.535	1.6522
25.	1	-3.1579	0.1197	1.7268
26.	1	-1.8444	-0.3304	3.72
27.	1	-1.7998	1.12	2.9281
28.	1	-0.4235	-0.9396	-2.2365
29.	1	1.0259	0.0983	-2.2365
30.	1	-0.6059	0.8337	-2.2365

Table S3. Theoretical (QC) and experimental (GED) geometric parameters of 1-methylsilatrane (Å and degrees).

	QC[a]					GED[b]	
Parameter	M06-2X[a]	B3LYP[a]	MP2[a]	CAMB3LYP[c]	B3LYP-D3[c]	MP2[d]	B3LYP[d]
Internuclear distances							
Si ··· N	2.695	2.689	2.419	2.712	2.775	2.498(13)	2.514(17)
Si – O	1.661	1.671	1.682	1.655	1.661	1.668(4)	1.667(4)
O – C	1.409	1.416	1.409	1.406	1.415	1.410(4)	1.420(7)
C – C	1.530	1.536	1.529	1.525	1.532	1.519(5)	1.527(7)
N – C	1.448	1.454	1.458	1.442	1.446	1.476(5[e])[f]	1.459(9[e])[f]
Si – C	1.847	1.858	1.858	1.849	1.856	1.848(7)	1.847(8)
Bond angles							
Si ··· N – C	97.0	97.2	102.1	96.2	95.0	100.7[f]	102.9[f]
N – C – C	109.0	109.8	106.6	110.1	110.6	109.2[f]	105.3[f]
C – C – O	110.1	110.9	109.2	110.9	111.2	110.0(6)	114.2(7)
C – O – Si	124.1	125.5	123.0	125.5	124.8	126.4(5)	125.0(6)
O – Si ··· N	73.7	74.5	78.2	73.9	73.5	76.9(2)	76.9(6)
O – Si – C	106.3	105.5	101.8	106.1	106.5	103.1(2)	103.1(6)
O – Si – O	97.0	97.2	102.1	96.2	95.0	115.5[f]	115.0[f]
Torsion angles							
C-O-Si···N	-33.3	-29.1	-24.3	-30.5	-31.9	-25.1(16)	-19.6(19)
C-C-O-Si	61.8	55.9	49.9	58.0	60.4	47.7(18)	44.2(27)
O-Si···N-C	1.2	-1.3	-5.5	-0.6	0.5	-2.2[f]	-6.4[f]
H-C-Si-O	51.8	51.9	52.8	51.5	50.8	62(36)	34(26)
Flap[g]	47.1	43.5	40.2	45.0	47.1	37.0[f]	41.5[f]
R-factor						4.2%	4.0%

[a] QC calculations with 6-311G(d,p) basis set.

[b] r_{h1} values ($r_{h1}=r_a+\Delta r$) are given for GED results. The vibrational corrections Δr were calculated by the Vibmodule program (Vishnevskiy et al, *J. Phys.: Conf. Ser*., 2015, **633**, 012076) using the so called second approximation, in which harmonic approach with nonlinear relation between Cartesian and internal coordinates were applied on the base of the force field estimated in the specified QC calculations. Values in parentheses are full errors estimated as $\sigma(r_{h1})=[\sigma_{scale}^2+(2.5\sigma_{LS})^2]^{1/2}$, where $\sigma_{scale}=0.002r$ and σ_{LS} is a standard deviation in least-squares refinement for internuclear distances and as $3\sigma_{LS}$ for angles. The place-value is such that the last digit of the uncertainty lines up with the last digit of the nominal value.

[c] QC calculations with cc-pVTZ basis set

[d] Starting model for GED was taken from the corresponding method.

[e] Estimated uncertainty

[f] Dependent parameter.

[g] Flap angle of the OCC fragment relative to the NSi···O plane.

Table S4. GED and DFT values of d_{SiN} and MAE for silatranes $XSi(OCH_2CH_2)_3N$, **1**.

	X = Me		**X = H**		**X = F**		
Method	**d_{SiN}, Å**	**ref.**	**d_{SiN}, Å**	**ref.**	**d_{SiN}, Å**	**ref.**	**MAE, Å**
GED	2.514(17)	-	2.406(27)	[1a]	2.324(14)	[1b]	
B3LYP/6-311G(d,p)	2.689	-	2.549	-	2.433	-	0.14
B3LYP/6-311+G(d,p)	2.711	-	2.563	[2]	2.427	[2]	0.15
B3LYP/6-311++G(d,p)	2.703	[1a]	2.542	[1a]	2.403	[1a]	0.14
B3LYP/def2-TZVPP	2.738	-	2.570	-	2.449	-	0.17
B3LYP/cc-pVTZ	2.719	-	2.567	-	2.424	-	0.16
B3LYP/aug-cc-pVTZ	2.719	-	2.545	-	2.405	-	0.14
B3LYP-D3/6-311G(d,p)	2.728	-	2.591	-	2.468	-	0.18
B3LYP-D3/cc-pVTZ	2.775	-	2.618	-	2.464	-	0.20
B3LYP-D3/aug-cc-pVTZ	2.770	-	2.606	-	2.446	-	0.19
B3LYP-D3(BJ)/6-311G(d,p)	2.657	-	2.521	-	2.405	-	0.11
B3LYP-D3(BJ)/cc-pVTZ	2.696	-	2.536	-	2.394	-	0.13
B3LYP-D3(BJ)/aug-cc-pVTZ	2.688	-	2.526	-	2.380	-	0.12
CAM-B3LYP/6-311G(d,p)	2.677	-	2.549	-	2.409	-	0.13
CAM-B3LYP/cc-pVTZ	2.712	-	2.556	-	2.389	-	0.14
M06-2X/6-311G(d,p)	2.700	[3]	2.535	[3]	2.352	[3]	0.11
M06-2X/ aug-cc-pVTZ	2.755	-	2.562	-	2.340	-	0.14
B3PW91/6-311G(d,p)	2.533	[3]	2.400	[3]	2.321	[3]	0.01
B3PW91/6-311++G(d,p)	2.558	[3]	2.405	[3]	2.304	[3]	0.02
B3PW91/ aug-cc-pVTZ	2.558	-	2.377	-	2.294	-	0.03
B3PW91-D3/6-311G(d,p)	2.585	-	2.437	-	2.347	-	0.04
B3PW91-D3/aug-cc-pVTZ	2.613	-	2.421	-	2.320	-	0.04
B3PW91-D3(BJ)/6-311G(d,p)	2.508	-	2.378	-	2.302	-	0.02
B3PW91-D3(BJ)/aug-cc-pVTZ	2.519	-	2.353	-	2.274	-	0.04
PBE/TZ2P	2.400	[4]	2.301	[4]	2.244	[4]	0.10
PBE0/6-311G(d,p)	2.502	[3]	2.371	[3]	2.293	[3]	0.03
PBE0/6-311++G(d,p)	2.520	[3]	2.376	[3]	2.277	[3]	0.03
PBE0/ aug-cc-pVTZ	2.508	-	2.343	-	2.264	-	0.04
PBE0-D3(BJ)/ aug-cc-pVTZ	2.493	-	2.333	-	2.256	-	0.05
ωB97X/6-311G(d,p)	2.663	[3]	2.511	[3]	2.376	[5]	0.10
ωB97X-D/6-311G(d,p)	2.597	[3]	2.493	[3]	2.372	[5]	0.07
PW6B95/6-311G(d,p)	2.549	-	2.414	-	2.313	-	0.02
PW6B95-D3(BJ)/6-311G(d,p)	2.544	-	2.412	-	2.311	-	0.02

References

[1] a) I. F. Shishkov, L. V. Khristenko, F. M. Rudakov, A. V. Golubinskii, L. V. Vilkov, S. S. Karlov, G. S. Zaitseva, S. Samdal, *Struct. Chem.* **2004**, *15*, 11-16; b) G. Forgacs, M. Kolonits, I. Hargittai, *Struct. Chem*. **1990**, *1*, 245-250.

[2] A. A. Milov, R. M. Minayev, V. I. Minkin, *Russ. J. Org. Chem.*, **2003**, *39*, 340-347.

[3] E. F. Belogolova, V. F. Sidorkin, *J. Phys. Chem. A* **2013**, *117*, 5365-5376.

[4] S. S.Karlov, D. A. Tyurin, M. V. Zabalov, A. V. Churakov, G. S. Zaitseva, *J. Mol. Struct.: THEOCHEM* **2005**, *724*, 31-37.

[5] V. F. Sidorkin, E. F. Belogolova, E. P. Doronina, *Phys. Chem. Chem. Phys.* **2015**, *17*, 26225-26237

Table S5. Different types the GED internuclear Si···N distances (d_{SiN}, Å) in **1** and **2**.

Molecule		Ref.	r_a(Si···N)	r_g(Si···N)	r_{h1}(Si···N)	l	Δr *(vibration correction)*
1a	**$MeSi(OCH_2CH_2)_3N$**	[1a]	2.448(47)[a]	2.453(47)	NA	0.115	NA
		this work	2.491(17)	2.504(17)	2.514(17)	0.179(2)	0.022
1b	**$HSi(OCH_2CH_2)_3N$**	[1c]	2.396(27)	2.406(27)	NA	0.158(57)	NA
1c	**$FSi(OCH_2CH_2)_3N$**	[1b]	2.318(9)	2.324(14)	NA	0.110(3)	NA
2f	*anti-* **$ClH_2SiONMe_2$**	[2a]	2.160(7)	2.164[a] (17)[b]	NA	0.101(15)	NA
2e	*gauche-* **$ClH_2SiONMe_2$**	[2a]	2.468(25)	2.471[a] (29)[b]	NA	0.092(14)	NA
2c	**$F_3SiN(Me)NMe_2$**	[2b]	2.510(6)	2.512[a](6)[c]	NA	0.064	NA
2d	**$F_3SiN(SiMe_3)NMe_2$**	[2b]	2.135(9)	2.140[a] (11)[b]	NA	0.107(5)	NA
2b	**$F_3SiNCH_2NMe_2$**	[2c]	2.731(18)[d]				
2h	*anti-* **$(F_3C)F_2SiONMe_2$**	[2d]	2.127[e]	2.134[a]	2.112	0.121(9)	–0.015
2j	*gauche-* **$(F_3C)F_2SiONMe_2$**	[2d]	2.189[e]	2.196[a]	2.174		
2a	**$H_3SiN(CH_2)_3NMe_2$**	[2e]	2.899[e](35)[f]	2.913[a](36)[b]	2.912(35)	0.205(6)	0.013

Values and uncertainties calculated (estimated) in this work:

[a] – calculated from equation: $r_g = r_a + \frac{l^2}{r_a}$

[b] – uncertainty estimated as a square root of a sum of squares of r_a and l uncertainties

[c] – uncertainty taken equal to that for r_a

[d] – Value and uncertainty estimated on the base of those for r(Si-C), r(N-C) and ∠Si-C-N specified in [2c]

[e] – calculated from equation: $r_a = r_{h1} - \Delta r$

[f] – uncertainty taken equal to that for r_{h1}

References

[1] a) Q. Shen, R. L. Hilderbrandt, *J. Mol. Struct.* **1980**, *64*, 257-262; b) G. Forgacs, M. Kolonits, I. Hargittai, *Struct. Chem.* **1990**, *1*, 245-250; c) I. F. Shishkov, L. V. Khristenko, F. M. Rudakov, A. V. Golubinskii, L. V. Vilkov, S. S. Karlov, G. S. Zaitseva, S. Samdal, *Struct. Chem.* **2004**, *15*, 11-16.

[2] a) N. W. Mitzel, U. Losehand, *J. Am. Chem. Soc.* **1998**, *120*, 7320-7327; b) K. Vojinović, L. J. McLachlan, S. L. Hinchley, D. W. H. Rankin, N. W. Mitzel, *Chem. Eur. J.* **2004**, *10*, 3033-3042; c) N. W. Mitzel, K. Vojinović, T. Foerster, H. E. Robertson, K. B. Borisenko, D. W. H. Rankin, *Chem. Eur. J.* **2005**, *11*, 5114-5125; d) N. W. Mitzel, K. Vojinović, R. Fröhlich, T. Foerster, H. E. Robertson, K. B. Borisenko, D. W. H. Rankin, *J. Am. Chem. Soc.* **2005**, *127*, 13705-13713; e) M. Hagemann, R. J. F. Berger, S. A. Hayes, H.-G. Stammler, N. W. Mitzel, *Chem. Eur. J.* **2008**, *14*, 11027-11038.

GED/MS

The diffraction patterns of 1-methylsilatrane were obtained in a synchronous gas-phase electron diffraction and mass-spectrometric experiment carried out using the *EMR-100*/*APDM-1* unit[1,2]. The samples were loaded in to molybdenum effusion cell filled by crushed pieces of Schott filter with a cylindrical nozzle of 0.6×1.2 mm^2 size (diameter × length) and were kept at 355(5) K in the course of the experiments. Diffraction patterns were recorded on MACO EM/EMS photographic films of 9×12 cm^2.

Accurate wavelengths of the electrons were calibrated using polycrystalline ZnO. The two camera distances resulted in diffraction patterns in the s-range for **1** of 1.3 to 16.4 $Å^{-1}$ and 3.0 to 28.9 $Å^{-1}$ with a step size of 0.1 $Å^{-1}$, where $s=(4\pi/\lambda)\sin(\theta/2)$, λ is electron wavelength and θ is scattering angle, respectively. The optical densities of the diffraction patterns were measured by a computer controlled MD-100 (Carl Zeiss, Jena) microdensitometer[3] with a step size of 0.1 mm. The molecular scattering function, sM(s), was evaluated as $sM(s)=(I(s)/G(s)-1)s$, where I(s) is the total electron scattering intensity, G(s) the experimental background.

Table S6. Conditions of the synchronous GED/MS experiments

	Camera distance	
	Long	Short
Nozzle-to-plate distance, mm	598	338
Number of recorded films	6	5
Primary electron beam current, μA	0.43	1.30
Accelerating voltage [a], kV	81.81	82.54
Temperature of effusion cell, K	360	350
Wavelength of electrons [b], Å	0.041280	0.041082
Exposure time, s	50	65
Residual gas pressure, Torr, in –diffraction chamber –mass spectrometric block	 $3.3\cdot10^{-6}$ $8.0\cdot10^{-7}$	 $1.9\cdot10^{-6}$ $7.4\cdot10^{-7}$
Ionization voltage, V	50	

[a] Approximate value

[b] Accurate wavelengths of electrons were calibrated using diffractions pattern of polycrystalline ZnO

Table S7. Mass-spectra of 1-methylsilatrane

M, Da	Relative intensity, %	
	Our data [a]	NIST[4]
45	28	10
61	21	8
77	19	9
91	13	5
100	23	12
116	38	26
130	15	9
146	100	100
158	17	22
174	56	81
189	22	26

[a] - $U_{ioniz} = 50$.

References

1. Girichev G V., Utkin AN, Revichev YF. UPGRADING THE EMR-100 ELECTRON-DIFFRACTION CAMERA FOR USE WITH GASES. *Instruments Exp Tech New York*. 1984;27(2):457–461.
2. Giricheva NI, Girichev G V., Shlykov SA, Titov VA, Chusova TP. The joint gas electron diffraction and mass spectrometric study of GeI4(g) + Ge(s) system. Molecular structure of germanium diiodide. *J Mol Struct*. 1995;344(1–2):127–134. doi:10.1016/0022-2860(94)08408-A.
3. Girichev EG, Zakharov A V., Girichev G V., Bazanov MI. Automation of a physicochemical experiment: photometry and voltammetry. *Izv Vyss Uchebn Zaved, Tekhnol Tekst Prom*. 2000;(2):142–146.
4. https://webbook.nist.gov/cgi/cbook.cgi?ID=C2288133&Units=SI&Mask=200#Mass-Spec.

Table S8. Observed and Calculated (B3LYP and MP2 methods with 6-311G(d,p) basis set) Frequencies (cm^{-1}) of 1-methylsilatrane molecule. A bold italics in red show data for a benzene solution.

No.	Sym.	Observed[a]	Calculated		Assignment
		cryst/*melt* ***solution***	B3LYP gas phase ***solution (C-PCM)***	MP2 gas phase ***solution (C-PCM)***	
1	A	**84**	90 ***71***	83 ***86***	ν(Si←N) + ρ(NC3)-twist[b] + ring-tors
2	A	-	150 ***160***	171 ***177***	ρ(CH3)-twist
3,4	E	**130**	152 ***151***	155 ***158***	δ(SiO3)-as-bend + ring-tors
5	A	**182**	191 ***193***	219 ***238***	ν(Si←N) + δ(SiO3)-s-def-δ(NC3)-s-def + ring-tors
6,7	E	**242** *170*	198 ***202***	209 ***215***	δ(SiO3)-as-def + ring-def + ring-tors
8,9	E	**264**/*222*	265 ***271***	280 ***280***	δ(SiO3)-as-def + ring-def
10	A	**288**/*280* ***281***	289 ***287***	311 ***312***	ν(Si←N) + ring-tors
11,12	E	**354**/*355* ***355***	358 ***354***	365 ***361***	δ(SiO3)-as-def + ring-tors
13,14	E	**455**/*440*	416 ***424***	437 ***448***	δ(CNC)+ ring-tors' + ring-def
15	A	**471**/*470* ***465***	439 ***453***	465 ***471***	δ(SiO3)-s-def+δ(CNC) +δ(OCC)
16	A	-	552 ***566***	575 ***578***	ring-def"
17,18	E	**580**/*580* ***576***	576 ***590***	596 ***609***	ring-def
19	A	**619**/*606*	598 ***590***	608 ***612***	ν(SiC)-stretch +ν(SiO)-stretch
20,21	E	**718**/*708* ***712***	735 ***730***	747 ***742***	ρ(SiMe)-rock +ν(SiO)-stretch
22	A	**696**	740 ***731***	753 ***738***	ν(SiC)-stretch+ν(NC)-stretch + ν(SiO)
23	A	**769**/*769* ***763***	777 ***768***	791 ***788***	ν(SiC)-stretch-ν(NC)-stretch + ν(SiO)
24,25	E	**818**	855 ***846***	862 ***849***	ρ(SiMe)-rock -ν(SiO)-stretch
26	A	**881**	886 ***895***	925 ***935***	δ(NC3)-s-def+ν(CC)-stretch +ρ(CH2)-rock
27,28	E	-	888 ***887***	905 ***907***	ν(SiO)-stretch + ν(CC)-stretch + ρ(CH2)-rock
29,30	E	**908**/*906* ***902***	926 ***931***	959 ***964***	ν(CC)-stretch +ν(CN) +ρ(CH2)-rock
31	A	**944**/*944* ***934***	998 ***1005***	1039 ***1049***	ν(CC)-stretch +ν(CN)-stretch + ring-def

32,33	E	**1016**/*1008*	1083 ***1075***	1101 ***1095***	ν(CN)-stretch + ρ(CH2)-rock
34	A	**1050**/*1055* ***1055***	1094 ***1094***	1114 ***1117***	ν(CH2)-rock
35,36	E	**1084**/*1085* ***1082***	1125 ***1114***	1162 ***1151***	ν(CO)-stretch + ν(CN)-stretch
37	A	**1113**/*1125*	1152 ***1137***	1186 ***1172***	ν(CO)-stretch
38,39	E	**1171**/*1175*	1207 ***1201***	1223 ***1217***	ρ(CH2)-rock + ν(NC)-stretch
40	A	-	1262 ***1261***	1279 ***1279***	ρ(CH2)-twist
41,42	E	-	1280 ***1277***	1291 ***1288***	ρ(CH2)-twist
43	A	**1237**	1289 ***1289***	1304 ***1307***	ρ(CH2)-twist
44	A	-/*1265*	1311 ***1305***	1321 ***1312***	ρ(SiMe3)-s-def-ν(SiC)-stretch
45,46	E	**1278**/*1280* ***1280***	1329 ***1317***	1333 ***1324***	ρ(CH2)-twist + ρ(CH2)-wag
47,48	E	**1350**	1390 ***1389***	1399 ***1397***	ρ(CH2)-wag
49	A	**1358**/*1358* ***1360***	1392 ***1393***	1402 ***1402***	ρ(CH2)-wag
50	A	-	1405 ***1402***	1420 ***1420***	ρ(CH2)-wag
51,52	E	**1381**	1412 ***1411***	1431 ***1431***	ρ(CH2)-wag
53,54	E	**1407** ***1402***	1465 ***1461***	1476 ***1471***	ρ(SiMe3)-as-def
55,56	E	**1452**/1458 ***1450***	1488 ***1490***	1505 ***1506***	δ(CH2)-sciss
57	A	-	1493 ***1494***	1509 ***1509***	δ(CH2)-sciss
58,59	E	-	1516 ***1514***	1538 ***1539***	δ(CH2)-sciss
60	A	**1487**/1485 ***1480***	1517 ***1519***	1540 ***1541***	δ(CH2)-sciss
61,62	E	-	2963 ***2986***	3045 ***3059***	ν(CH2)-s-stretch
63	A	-	2968 ***2989***	3045 ***3058***	ν(CH2)-s-stretch
64,65	E	**2875**	3000 ***3003***	3054 ***3067***	ν(CH2)-s-stretch
66	A	**2915**	3038 ***3034***	3085 ***3072***	ν(SiMe3)-s-stretch
67	A		3003 ***3007***	3058 ***3079***	ν(CH2)-s-stretch
68,69	E	**2927**	3059 ***3066***	3129 ***3134***	ν(CH2)-as-stretch
70	A	-	3060	3130	ν(CH2)-as-stretch

			3067	***3135***	
71	A	-	3075 ***3084***	3143 ***3153***	ν(CH2)-as-stretch
72,73	E	**2959**	3080 ***3088***	3149 ***3159***	νCH2)-as-stretch
74,75	E	**2975**	3112 ***3106***	3183 ***3175***	ν(SiMe3)-deg-stretch

[a]Raman spectroscopy data for polycrystalline powders (cryst), a liquid state at 155° C (melt) and a solution in C_6H_6 [M. Imbenotte, G. Palavit, P. Legrand, *J. Raman. Spectr*. **1983**, *14*, 135-137].
[b]RelativetoMeSiO$_3$.

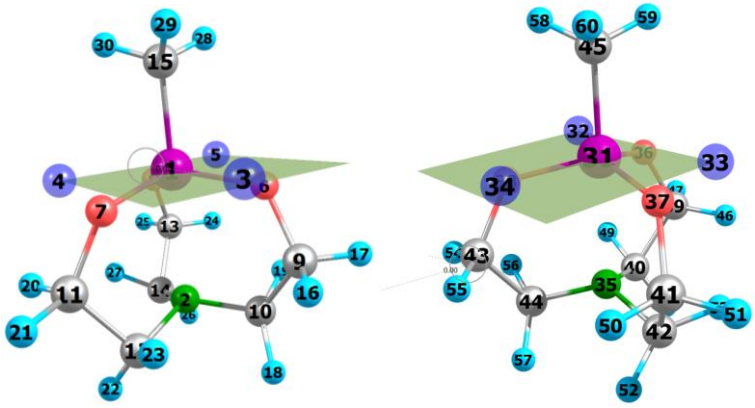


Table S9. Z- matrix for the KCED program input.

N	N1	P1	J1	K1	N2	P2	J2	K2	N3	P3	J3	K3	Code
C_3-conformer													
1		--	--	--	--	--	--	--	--	--	--	--	--
2	1	2.6893	1	0		--	--	--	--	--	--	--	--
3	1	2	2	0	2	90	3	0		--	--	--	--
4	1	2	2	0	2	90	3	0	3	120	31	0	1
5	1	2	2	0	2	90	3	0	3	120	31	0	-1
6	1	1.6711	4	0	2	74.53	5	0	3	45	6	0	0
7	1	1.6711	4	0	2	74.53	5	0	4	45	6	0	0
8	1	1.6711	4	0	2	74.53	5	0	5	45	6	0	0
9	6	1.4155	8	0	1	125.49	9	0	2	-29.12	10	0	0
10	9	1.5359	11	0	6	110.90	12	0	1	55.85	13	0	0
11	7	1.4155	8	0	1	125.49	9	0	2	-29.12	10	0	0
12	11	1.5359	11	0	7	110.90	12	0	1	55.85	13	0	0
13	8	1.4155	8	0	1	125.49	9	0	2	-29.12	10	0	0
14	13	1.5359	11	0	8	110.90	12	0	1	55.85	13	0	0
15	1	1.8577	14	0	3	90	3	0	4	90	3	0	-1
16	9	1.0977	15	0	6	109.86	16	0	10	110.03	17	0	1
17	9	1.0938	15	-18	6	108.10	19	0	10	110.25	20	0	-1
18	10	1.1011	15	21	9	110.09	22	0	2	112.61	23	0	1
19	10	1.0928	15	-24	9	108.84	25	0	2	108.18	26	0	-1
20	11	1.0977	15	0	7	109.86	16	0	12	110.03	17	0	1
21	11	1.0938	15	-18	7	108.10	19	0	12	110.25	20	0	-1
22	12	1.1011	15	21	11	110.09	22	0	2	112.61	23	0	1
23	12	1.0928	15	-24	11	108.84	25	0	2	108.18	26	0	-1
24	13	1.0977	15	0	8	109.86	16	0	14	110.03	17	0	1

25	13	1.0938	15	-18	8	108.10	19	0	14	110.25	20	0	-1
26	14	1.1011	15	21	13	110.09	22	0	2	112.61	23	0	1
27	14	1.0928	15	-24	13	108.84	25	0	2	108.18	26	0	-1
28	15	1.0926	15	-27	1	110.70	28	0	6	51.93	29	0	0
29	15	1.0926	15	-27	1	110.70	28	0	7	51.93	29	0	0
30	15	1.0926	15	-27	1	110.70	28	0	8	51.93	29	0	0
C_1-conformer													
31	1	10	32	0	3	120	31	0	4	120	31	0	1
32	31	2	2	0	1	120	31	0	3	0	0	0	0
33	31	2	2	0	1	120	31	0	32	120	31	0	1
34	31	2	2	0	32	120	-31	0	33	0	0	0	0
35	31	2.6547	1	33	32	90	3	0	33	90	3	0	1
36	31	1.6714	4	34	35	75.36	5	35	32	45	6	0	1
37	31	1.6740	4	36	35	75.52	5	37	36	111.87	38	0	1
38	31	1.6716	4	39	35	75.01	5	40	36	116.15	38	41	-1
39	36	1.4134	8	42	31	124.68	9	-35	35	-28.98	10	0	0
40	39	1.5327	11	44	36	110.56	12	43	31	55.75	13	0	0
41	37	1.4140	8	45	31	126.93	9	46	35	-26.38	10	47	0
42	41	1.5430	11	48	37	111.60	12	49	31	48.86	13	50	0
43	38	1.4132	8	42	31	127.67	9	51	35	26.34	-10	-47	0
44	43	1.5423	11	52	38	111.57	12	49	31	-48.64	-13	-53	0
45	31	1.8585	14	54	32	90	3	0	33	90	3	0	-1
46	39	1.0983	15	55	36	109.97	16	56	40	110.28	17	57	1
47	39	1.0939	15	-18	36	108.27	19	-58	40	110.11	20	59	-1
48	40	1.1009	15	-44	39	110.20	22	60	35	112.59	23	0	1
49	40	1.0913	15	-61	39	108.57	25	0	35	108.05	26	45	-1
50	41	1.0942	15	44	37	108.04	16	-62	42	109.53	17	59	1
51	41	1.0965	15	-63	37	110.01	19	62	42	110.42	20	64	-1
52	42	1.0926	15	-27	41	108.65	22	65	35	107.99	23	66	1
53	42	1.1009	15	-44	41	109.63	25	49	35	111.79	26	67	-1
54	43	1.0942	15	44	38	108.07	16	-62	44	109.47	20	59	1
55	43	1.0968	15	-54	38	109.93	19	62	44	110.59	17	58	-1
56	44	1.1011	15	-44	43	109.60	25	49	35	112.10	26	68	1
57	44	1.0913	15	-61	43	108.57	22	65	35	107.95	23	66	-1
58	45	1.0925	15	-27	31	110.90	28	-57	32	45	6	0	0
59	45	1.0925	15	-27	31	110.90	28	-57	33	45	6	0	0
60	45	1.0925	15	-27	31	110.90	28	-57	34	45	6	0	0

N(i) – atom number; P(i) – parameter value; J(i) – parameter number; K(i) – number of the correction for the parameter specified in the column J(i) was taken as a difference between two analogous parameters adopted from QC calculations; Codes mean: valence angle (1 or -1) and torsion angle (0); atoms 3-5 in C_3-conformer and 32-34 in C_3-conformer are dummies

Table S10. List[a] of independent starting parameters: distances r, valence A and dihedral D angles and differences, dr, dA and dD, between analogous parameters adopted from QC calculations B3LYP/6-311G**

#	Parameter	Value	#	Parameter	Value
1	rSiN	2.4493	35	dA	0.82
2	rXSi	2.	36	dr	0.0029
3	AXSiX	90.	37	dA	0.98
4	rOSi	1.6711	38	A	111.87
5	AOSiN	74.54	39	dr	0.0005
6	AOSiX	45.	40	dA	0.47
7	AOSiO [b]	113.16	41	dA	4.28
8	rCO	1.4155	42	dr	-0.0021
9	ACOSi	125.49	43	dA	-0.33
10	DCOSiN	-29.12	44	dr	-0.0032
11	rCC	1.5359	45	dr	-0.0015
12	ACCO	110.89	46	dA	1.44
13	DCCOSi	55.85	47	dD	2.8
14	rCSi	1.8577	48	dr	0.0071
15	rHC	1.0977	49	dA	0.71
16	AH1C1O	109.86	50	dD	-7.0
17	AH1C1C2	110.03	51	dA	2.18
18	dr	0.0039	52	dr	0.0061
19	AH2C1O	108.1	53	dD	-7.2
20	AH2C1C2	110.25	54	dr	0.0008
21	dr	0.0024	55	dr	0.0006
22	AH3C2C1	110.09	56	dA	-0.3
23	AH3C2N	112.61	57	dA	0.24
24	dr	0.0049	58	dA	0.35
25	AH4C2C1	108.84	59	dA	-0.5
26	AH4C2N	108.18	60	dA	1.98
27	dr	0.0051	61	dr	0.0064
28	A11	110.64	62	dA	1.82
29	D3	51.93	63	dr	0.0012
30	A12	108.22	64	dA	0.17
31	A13	120	65	dA	-1.44
32	rSiSi	10	66	dA	-4.6
33	dr	-0.0346	67	dA	3.61
34	dr	0.0003	68	dA	3.81

[a] Initial values were taken from QC calculations and are specified. All geometric parameters, except the differences, were variables.
[b] parameter #7 was not used

Experimental total intensities and background for 1-methylsilatrane

I(s) long camera s= 1.3 to 16.4 Å^{-1}; step 0.1 Å^{-1}; λ= 0.04128017 Å, sequence in rows

1.03799 0.83911 0.69900 0.64521 0.59580 0.56160 0.53780 0.52190
0.50588 0.48896 0.47150 0.45034 0.43054 0.41036 0.38690 0.36822
0.34863 0.33193 0.31760 0.30429 0.29364 0.28374 0.27602 0.27089
0.26817 0.26761 0.26931 0.27198 0.27541 0.27982 0.28410 0.28959
0.29511 0.30115 0.30789 0.31369 0.32062 0.32705 0.33223 0.33603
0.33786 0.33723 0.33406 0.32768 0.31909 0.30870 0.29716 0.28485
0.27285 0.26154 0.25123 0.24303 0.23672 0.23274 0.23030 0.22948
0.23019 0.23214 0.23458 0.23737 0.23994 0.24236 0.24366 0.24455
0.24467 0.24400 0.24237 0.24076 0.23880 0.23732 0.23583 0.23459
0.23460 0.23465 0.23497 0.23556 0.23638 0.23688 0.23702 0.23688
0.23556 0.23378 0.23174 0.22922 0.22725 0.22508 0.22281 0.22106
0.21930 0.21845 0.21741 0.21636 0.21548 0.21448 0.21335 0.21168
0.21057 0.20956 0.20872 0.20822 0.20786 0.20810 0.20879 0.20939
0.21088 0.21251 0.21409 0.21559 0.21683 0.21834 0.21927 0.21948
0.21901 0.21837 0.21744 0.21624 0.21505 0.21405 0.21258 0.21201
0.21137 0.21104 0.21110 0.21152 0.21204 0.21260 0.21354 0.21380
0.21411 0.21455 0.21409 0.21277 0.21162 0.21015 0.20869 0.20722
0.20595 0.20483 0.20443 0.20406 0.20467 0.20498 0.20589 0.20727
0.20856 0.20956 0.21070 0.21128 0.21218 0.21289 0.21287 0.21391

I(s) short camera s= 3.0 to 28.9 Å^{-1}; step 0.1 Å^{-1}; λ= 0.04108197 Å, sequence in rows

1.99868 1.87638 1.75993 1.65219 1.55887 1.48102 1.41522 1.36147
1.31594 1.27998 1.25075 1.22451 1.20071 1.17739 1.15730 1.14069
1.12479 1.10883 1.09244 1.08219 1.07064 1.05524 1.03843 1.01898
0.99680 0.96883 0.93457 0.89654 0.85425 0.80847 0.76124 0.71623
0.67491 0.63884 0.60807 0.58287 0.56366 0.54978 0.54034 0.53488
0.53195 0.53025 0.52952 0.52886 0.52750 0.52455 0.52011 0.51471
0.50815 0.50022 0.49171 0.48319 0.47523 0.46827 0.46303 0.45804
0.45407 0.45192 0.45035 0.44823 0.44596 0.44291 0.43948 0.43498
0.42910 0.42233 0.41566 0.40884 0.40208 0.39564 0.39011 0.38536
0.38088 0.37652 0.37268 0.36894 0.36533 0.36135 0.35744 0.35365
0.35013 0.34706 0.34435 0.34195 0.34022 0.33977 0.33986 0.34043
0.34138 0.34232 0.34358 0.34400 0.34408 0.34390 0.34294 0.34129
0.33927 0.33672 0.33374 0.33079 0.32737 0.32438 0.32213 0.32045
0.31910 0.31793 0.31751 0.31727 0.31685 0.31624 0.31558 0.31472
0.31334 0.31123 0.30866 0.30567 0.30226 0.29881 0.29563 0.29293
0.29012 0.28802 0.28643 0.28542 0.28513 0.28522 0.28557 0.28625
0.28680 0.28712 0.28721 0.28727 0.28712 0.28686 0.28582 0.28458
0.28286 0.28104 0.27922 0.27772 0.27625 0.27456 0.27312 0.27202
0.27124 0.27035 0.26989 0.26978 0.26994 0.27024 0.27050 0.27143
0.27230 0.27290 0.27321 0.27371 0.27399 0.27390 0.27348 0.27272
0.27192 0.27091 0.27010 0.26911 0.26791 0.26684 0.26561 0.26450
0.26349 0.26261 0.26173 0.26110 0.26085 0.26057 0.26058 0.26058
0.26074 0.26120 0.26131 0.26137 0.26160 0.26158 0.26147 0.26127
0.26094 0.26047 0.26009 0.25981 0.25966 0.25976 0.25958 0.25910
0.25909 0.25922 0.25942 0.25967 0.26001 0.26045 0.26077 0.26126
0.26194 0.26235 0.26264 0.26308 0.26334 0.26316 0.26271 0.26252
0.26220 0.26179 0.26128 0.26074 0.25990 0.25908 0.25862 0.25810
0.25756 0.25737 0.25727 0.25716 0.25714 0.25721 0.25750 0.25787
0.25817 0.25864 0.25918 0.25947 0.25994 0.26023 0.26063 0.26111
0.26165 0.26199 0.26237 0.26309 0.26374 0.26429 0.26459 0.26492

0.26531 0.26577 0.26608 0.26642 0.26663 0.26694 0.26696 0.26711
0.26753 0.26778 0.26768 0.26766 0.26778 0.26787 0.26792 0.26820
0.26851 0.26846 0.26817 0.26816

Background G(s) long camera, sequence in rows

1.09898 0.96108 0.84537 0.76890 0.70255 0.64695 0.60436 0.57435
0.54701 0.52468 0.50301 0.48177 0.46258 0.44416 0.42611 0.41060
0.39530 0.38135 0.37102 0.36124 0.35235 0.34349 0.33528 0.32814
0.32240 0.31838 0.31512 0.31248 0.30997 0.30753 0.30528 0.30326
0.30129 0.29953 0.29769 0.29565 0.29356 0.29159 0.28953 0.28729
0.28525 0.28325 0.28111 0.27920 0.27726 0.27558 0.27367 0.27177
0.26987 0.26797 0.26631 0.26420 0.26228 0.26042 0.25866 0.25684
0.25490 0.25307 0.25119 0.24960 0.24785 0.24614 0.24448 0.24262
0.24105 0.23942 0.23758 0.23602 0.23479 0.23393 0.23323 0.23247
0.23177 0.23113 0.23042 0.22976 0.22920 0.22863 0.22801 0.22740
0.22677 0.22615 0.22549 0.22490 0.22433 0.22378 0.22326 0.22267
0.22206 0.22146 0.22079 0.22015 0.21952 0.21891 0.21842 0.21783
0.21742 0.21705 0.21672 0.21640 0.21607 0.21579 0.21546 0.21517
0.21493 0.21468 0.21444 0.21418 0.21400 0.21381 0.21360 0.21336
0.21313 0.21287 0.21262 0.21242 0.21218 0.21193 0.21162 0.21138
0.21106 0.21073 0.21037 0.21017 0.20996 0.20974 0.20957 0.20946
0.20936 0.20935 0.20932 0.20935 0.20939 0.20945 0.20952 0.20960
0.20965 0.20974 0.20984 0.20993 0.21000 0.21007 0.21017 0.21025
0.21034 0.21045 0.21052 0.21062 0.21076 0.21093 0.21106 0.21126

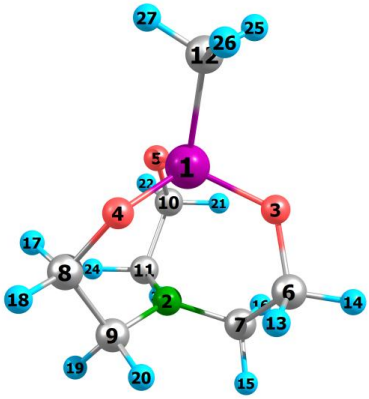
Background G(s) short camera, sequence in rows

2.24435 2.13137 2.02279 1.91628 1.82092 1.73903 1.66129 1.59158
1.52316 1.46136 1.40614 1.35467 1.30356 1.25429 1.20761 1.16420
1.12184 1.08092 1.04025 1.00469 0.96939 0.93670 0.90715 0.88140
0.85782 0.83546 0.81340 0.79293 0.77278 0.75214 0.73218 0.71184
0.69158 0.67297 0.65547 0.63758 0.62266 0.60766 0.59391 0.58313
0.57380 0.56388 0.55448 0.54459 0.53520 0.52572 0.51681 0.50801
0.49935 0.49104 0.48309 0.47638 0.47004 0.46396 0.45840 0.45283
0.44806 0.44420 0.44004 0.43618 0.43217 0.42831 0.42440 0.42054
0.41663 0.41278 0.40892 0.40510 0.40128 0.39744 0.39365 0.38984
0.38613 0.38232 0.37865 0.37527 0.37204 0.36888 0.36588 0.36310
0.36051 0.35801 0.35582 0.35366 0.35159 0.34988 0.34804 0.34629
0.34458 0.34290 0.34130 0.33963 0.33802 0.33636 0.33474 0.33309
0.33151 0.32982 0.32830 0.32659 0.32510 0.32341 0.32193 0.32037
0.31891 0.31737 0.31593 0.31442 0.31296 0.31150 0.31005 0.30862
0.30718 0.30574 0.30433 0.30288 0.30149 0.30005 0.29868 0.29737
0.29604 0.29483 0.29358 0.29245 0.29142 0.29042 0.28944 0.28860
0.28775 0.28692 0.28607 0.28525 0.28441 0.28359 0.28276 0.28196
0.28117 0.28042 0.27958 0.27887 0.27804 0.27734 0.27653 0.27582
0.27513 0.27444 0.27383 0.27328 0.27274 0.27222 0.27167 0.27116
0.27069 0.27021 0.26971 0.26930 0.26881 0.26841 0.26795 0.26753
0.26710 0.26666 0.26626 0.26589 0.26552 0.26520 0.26488 0.26457
0.26427 0.26398 0.26369 0.26346 0.26327 0.26308 0.26293 0.26279
0.26267 0.26257 0.26248 0.26237 0.26226 0.26216 0.26204 0.26193
0.26180 0.26169 0.26156 0.26145 0.26133 0.26122 0.26112 0.26100
0.26087 0.26076 0.26063 0.26049 0.26038 0.26025 0.26014 0.26003
0.25993 0.25984 0.25975 0.25967 0.25960 0.25953 0.25945 0.25939
0.25932 0.25926 0.25919 0.25913 0.25906 0.25901 0.25896 0.25897
0.25908 0.25923 0.25941 0.25957 0.25974 0.25990 0.26009 0.26027

0.26047	0.26065	0.26085	0.26104	0.26123	0.26143	0.26162	0.26183
0.26203	0.26223	0.26245	0.26265	0.26291	0.26315	0.26340	0.26367
0.26395	0.26425	0.26451	0.26480	0.26507	0.26536	0.26560	0.26587
0.26616	0.26645	0.26672	0.26701	0.26729	0.26759	0.26788	0.26822
0.26856	0.26891	0.26929	0.26969				

Cartesian coordinates (Å) for 1-methylsilatrane

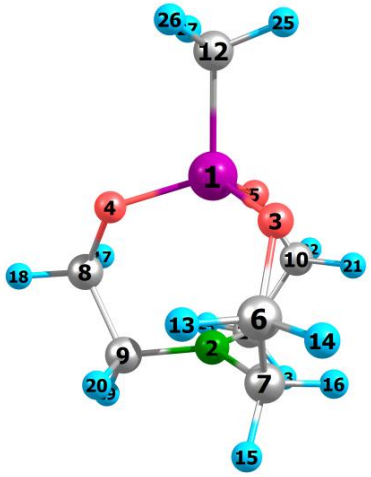
CAM-B3LYP/cc-pVTZ



E(RCAM-B3LYP) = -845.795683497

#	Z	x	y	z
1	14	0.000123	0.000058	0.038621
2	7	0.000230	0.000441	2.750402
3	8	1.564350	-0.286294	0.496576
4	8	-0.533923	1.497963	0.496441
5	8	-1.030039	-1.211283	0.496830
6	6	2.171473	0.192782	1.670736
7	6	1.408020	-0.271543	2.906054
8	6	-1.252244	1.784320	1.670652
9	6	-0.468129	1.355632	2.905899
10	6	-0.918700	-1.976344	1.671158
11	6	-0.939214	-1.082730	2.906253
12	6	0.000099	-0.000217	-1.810358
13	1	2.212956	1.285854	1.646873
14	1	3.197879	-0.175027	1.701056
15	1	1.831651	0.198338	3.802888
16	1	1.537359	-1.347905	3.015219
17	1	-2.219530	1.273540	1.647025
18	1	-1.447074	2.857093	1.700804
19	1	-1.086685	1.487721	3.802840
20	1	0.399351	2.005888	3.014727
21	1	0.007227	-2.558746	1.647475
22	1	-1.750387	-2.681384	1.701593
23	1	-0.744163	-1.684313	3.803255
24	1	-1.936057	-0.656555	3.015215
25	1	0.480475	-0.898770	-2.195221
26	1	0.538040	0.864980	-2.195496
27	1	-1.018201	0.032957	-2.195376

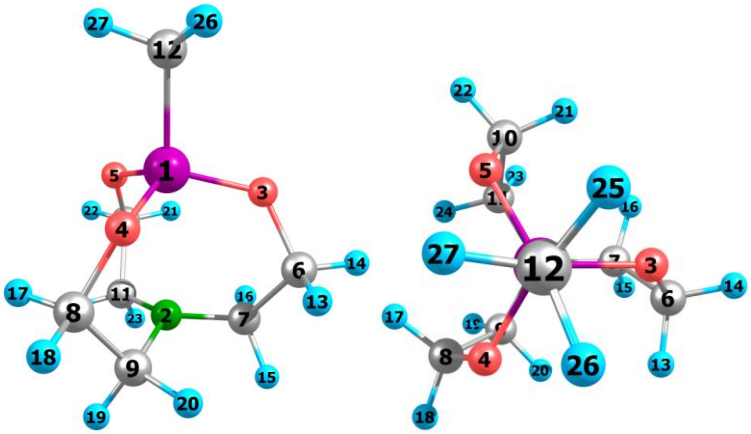
B3LYP-D3/cc-pVTZ



E(RB3LYP) = -846.084482949

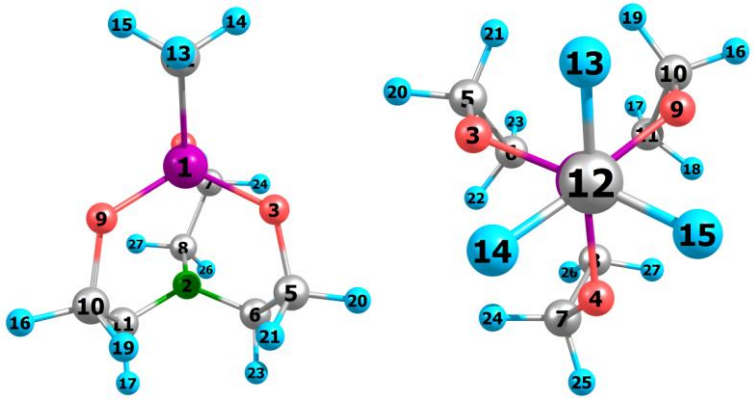
#	Z	x	y	z
1	14	0.000170	0.000073	0.021682
2	7	0.000226	0.000444	2.796541
3	8	1.561451	-0.314931	0.494044
4	8	-0.507472	1.509789	0.493915
5	8	-1.053356	-1.194376	0.494286
6	6	2.167057	0.188826	1.669067
7	6	1.415083	-0.272390	2.921906
8	6	-1.246523	1.782486	1.668921
9	6	-0.470926	1.362178	2.921739
10	6	-0.919985	-1.970517	1.669453
11	6	-0.943472	-1.088442	2.922109
12	6	0.000068	-0.000230	-1.834070
13	1	2.193312	1.283376	1.634523
14	1	3.199322	-0.166350	1.698541
15	1	1.857775	0.200498	3.809998
16	1	1.546383	-1.349210	3.031922
17	1	-2.207474	1.257777	1.634519
18	1	-1.455226	2.854015	1.698219
19	1	-1.101660	1.509267	3.809908
20	1	0.395975	2.014354	3.031459
21	1	0.014751	-2.540620	1.635063
22	1	-1.743755	-2.686844	1.699015
23	1	-0.755285	-1.708068	3.810339
24	1	-1.941690	-0.663755	3.032008
25	1	0.475834	-0.903199	-2.217530
26	1	0.544087	0.863202	-2.217835
27	1	-1.019786	0.039107	-2.217601

B3LYP/6-311G**



E(RB3LYP) = -845.989638011

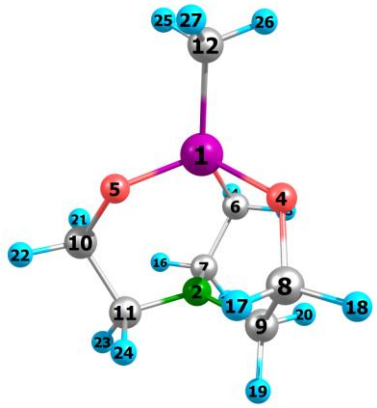
#	Z	x	y	z
1	14	0.000082	0.000049	0.037808
2	7	0.000204	0.000469	2.727088
3	8	1.588322	-0.267583	0.483260
4	8	-0.562305	1.509350	0.483152
5	8	-1.025764	-1.241544	0.483523
6	6	2.198013	0.198667	1.672634
7	6	1.416756	-0.270430	2.909045
8	6	-1.270742	1.804336	1.672605
9	6	-0.473493	1.362692	2.908902
10	6	-0.926644	-2.002335	1.673094
11	6	-0.942665	-1.090843	2.909203
12	6	0.000074	-0.000185	-1.819837
13	1	2.255179	1.294786	1.657487
14	1	3.221507	-0.185940	1.703170
15	1	1.825065	0.201865	3.816066
16	1	1.545968	-1.349885	3.019588
17	1	-2.248477	1.305555	1.657783
18	1	-1.449634	2.882979	1.702949
19	1	-1.086418	1.480317	3.816071
20	1	0.396714	2.014414	3.019020
21	1	-0.005731	-2.599547	1.658190
22	1	-1.771222	-2.696698	1.703750
23	1	-0.738000	-1.680270	3.816482
24	1	-1.942164	-0.663042	3.019299
25	1	0.487859	-0.898389	-2.205926
26	1	0.534023	0.871256	-2.206175
27	1	-1.021624	0.026413	-2.206092



E(RB3LYP) = -845.985283978

#	Z	x	y	z
1	14	-3.195683	0.096184	1.216658
2	7	-0.548451	0.259844	1.328888
3	8	-2.660284	-0.963950	0.036939
4	8	-2.804283	-0.432812	2.753034
5	6	-1.437948	-0.900143	-0.671014
6	6	-0.239849	-0.701752	0.280901
7	6	-1.589465	-1.066262	3.100346
8	6	-0.394422	-0.190371	2.707970
9	8	-2.846513	1.695187	0.876847
10	6	-1.660080	2.219764	0.316161
11	6	-0.406392	1.675924	1.031097
12	6	-5.052519	0.023844	1.188024
13	1	-5.441718	0.383066	0.232729
14	1	-5.400786	-1.000378	1.340291
15	1	-5.473062	0.645230	1.982475
16	1	-1.691577	3.309178	0.413195
17	1	0.486168	1.883516	0.420630
18	1	-0.287098	2.208133	1.976343
19	1	-1.621272	1.993095	-0.756226
20	1	-1.316074	-1.837661	-1.221854
21	1	-1.475217	-0.092742	-1.412001
22	1	-0.010102	-1.657837	0.757224
23	1	0.647584	-0.403918	-0.298568
24	1	-1.522271	-2.045224	2.606888
25	1	-1.589869	-1.239938	4.180346
26	1	0.547283	-0.736527	2.871920
27	1	-0.382957	0.690559	3.351960

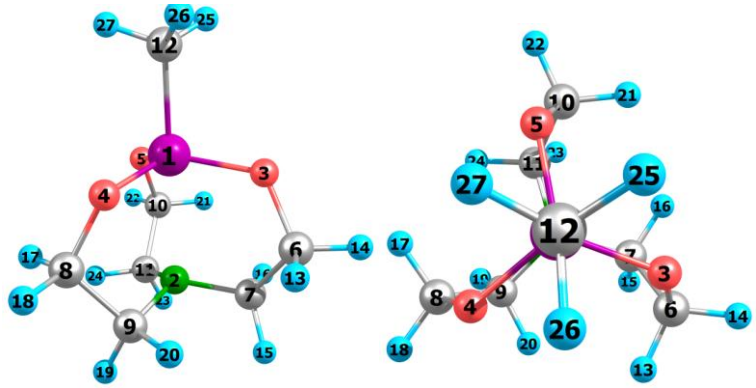
M062X/6-311G**



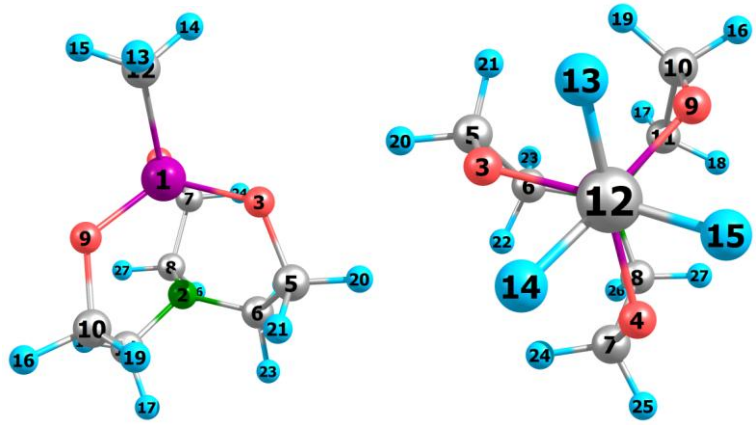
E(RM062X) = -845.732920465

#	Z	x	y	z
1	14	0.000103	0.000098	0.041406
2	7	0.000232	0.000426	2.736510
3	8	1.558779	-0.334612	0.508018
4	8	-0.489223	1.517370	0.507919
5	8	-1.069160	-1.182247	0.508285
6	6	2.167694	0.189482	1.666043
7	6	1.411221	-0.272228	2.913014
8	6	-1.247511	1.782703	1.665972
9	6	-0.469156	1.358710	2.912871
10	6	-0.919680	-1.971408	1.666453
11	6	-0.941376	-1.085175	2.913224
12	6	0.000089	-0.000235	-1.805636
13	1	2.174403	1.285655	1.620058
14	1	3.203529	-0.155236	1.693587
15	1	1.823856	0.206549	3.812355
16	1	1.540824	-1.351983	3.022063
17	1	-2.200125	1.240307	1.620085
18	1	-1.466998	2.852102	1.693430
19	1	-1.089877	1.476878	3.812346
20	1	0.401105	2.010941	3.021496
21	1	0.026308	-2.525272	1.620576
22	1	-1.736106	-2.696132	1.694146
23	1	-0.733128	-1.681716	3.812713
24	1	-1.941292	-0.657555	3.022102
25	1	0.449226	-0.918146	-2.188722
26	1	0.570432	0.847515	-2.189123
27	1	-1.019287	0.069667	-2.189052

MP2/6-311G**

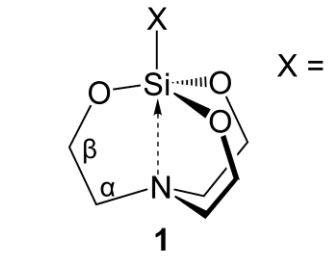


#	Z	x	y	z
1	14	0.000140	0.000047	0.129543
2	7	0.000213	0.000390	2.548151
3	8	1.634580	-0.197533	0.472196
4	8	-0.645912	1.514368	0.472022
5	8	-0.988217	-1.316546	0.472434
6	6	2.222030	0.222082	1.682266
7	6	1.393299	-0.305303	2.853316
8	6	-1.302832	1.813532	1.682146
9	6	-0.431541	1.359742	2.853135
10	6	-0.918638	-2.034813	1.682680
11	6	-0.961092	-1.053139	2.853493
12	6	0.000084	-0.000217	-1.728132
13	1	2.272629	1.319157	1.720658
14	1	3.243940	-0.166369	1.727761
15	1	1.717844	0.117821	3.815665
16	1	1.502854	-1.392798	2.895293
17	1	-2.278220	1.308822	1.720795
18	1	-1.477371	2.892766	1.727469
19	1	-0.960088	1.429424	3.815559
20	1	0.455487	1.998374	2.894844
21	1	0.006155	-2.627161	1.721284
22	1	-1.766005	-2.725576	1.728275
23	1	-0.757003	-1.545536	3.815975
24	1	-1.957671	-0.604259	2.895286
25	1	0.517361	-0.882724	-2.113216
26	1	0.505654	0.888939	-2.113467
27	1	-1.022798	-0.007031	-2.113293



#	Z	x	y	z
1	14	-3.116729	0.104710	1.221961
2	7	-0.689327	0.255095	1.329382
3	8	-2.670460	-0.916611	-0.036610
4	8	-2.801173	-0.505850	2.754598
5	6	-1.427744	-0.870291	-0.699733
6	6	-0.292439	-0.721435	0.319634
7	6	-1.572433	-1.101009	3.099815
8	6	-0.436729	-0.160904	2.707822
9	8	-2.846468	1.735451	0.913583
10	6	-1.677277	2.223095	0.297883
11	6	-0.438742	1.655972	1.005977
12	6	-4.972958	0.031922	1.209168
13	1	-5.369234	0.415397	0.265935
14	1	-5.319061	-0.996272	1.340762
15	1	-5.385134	0.634392	2.023120
16	1	-1.676124	3.315371	0.369635
17	1	0.465462	1.784478	0.392678
18	1	-0.299232	2.197326	1.944901
19	1	-1.666503	1.960522	-0.767326
20	1	-1.300173	-1.800918	-1.262097
21	1	-1.407076	-0.041939	-1.418579
22	1	-0.152063	-1.683748	0.819949
23	1	0.653123	-0.445690	-0.171388
24	1	-1.461078	-2.068634	2.590345
25	1	-1.562348	-1.283832	4.178677
26	1	0.550332	-0.629442	2.839035
27	1	-0.495268	0.726853	3.342076

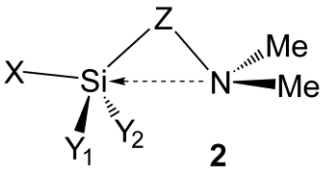
Cartesian coordinates (Å) for molecules 1-2



1

X = Me (**a**), H (**b**), F (**c**)

Z	X	Y_1	Y_2	
$(CH_2)_3$	H	H	H	(**a**)
CH_2	F	F	F	(**b**)
N(Me)	F	F	F	(**c**)
$N(SiMe_3)$	F	F	F	(**d**)
O	H	Cl	H	(**e**)
O	Cl	H	H	(**f**)
O	F	CF_3	F	(**g**)
O	CF_3	F	F	(**h**)
O	F	F	F	(**i**)



2

$H_3Si(CH_2)_3NMe_2$ (**2a**), CCSD/6-311G(d,p)
E(CCSD)=-542.6521219 au

6	1.761924	0.765052	-0.264652
14	1.650837	-1.089868	0.130102
1	0.977359	-1.899985	-0.906254
6	0.575692	1.655296	0.146199
6	-0.740184	1.177747	-0.470423
7	-1.068216	-0.177652	-0.021191
6	-1.687311	-0.168381	1.301027
6	-1.932776	-0.864139	-0.975103
1	3.062465	-1.566396	0.154429
1	1.099509	-1.362768	1.475676
1	2.676889	1.139391	0.214587
1	1.930322	0.866654	-1.347660
1	0.488427	1.678777	1.240161
1	0.754325	2.691301	-0.173261
1	-1.561560	1.885611	-0.250228
1	-0.620249	1.149674	-1.561492
1	-2.142667	-1.876015	-0.611936
1	-2.895343	-0.340094	-1.123509
1	-1.424153	-0.946112	-1.941234
1	-1.826802	-1.198937	1.644565
1	-1.039123	0.339336	2.020322
1	-2.670047	0.339366	1.294139

$H_3Si(CH_2)_3NMe_2$ (**2a**), MP2/6-311G(d,p)
E(MP2)=-542.5603511 au

6	1.751110	0.761379	-0.248382
14	1.578890	-1.097638	0.091948
1	0.904426	-1.869365	-0.971714
6	0.582538	1.667111	0.161291

6	-0.727985	1.194025	-0.459579
7	-1.036259	-0.167010	-0.020477
6	-1.645094	-0.170237	1.304355
6	-1.908132	-0.848106	-0.968820
1	2.981832	-1.602510	0.101924
1	1.035068	-1.403887	1.432277
1	2.667638	1.094455	0.253789
1	1.940529	0.882494	-1.324302
1	0.490778	1.688506	1.253259
1	0.769880	2.700633	-0.155660
1	-1.557671	1.888628	-0.232550
1	-0.606854	1.173534	-1.549661
1	-2.103828	-1.864255	-0.614743
1	-2.874648	-0.328784	-1.094308
1	-1.412547	-0.912907	-1.941018
1	-1.774383	-1.202703	1.640694
1	-0.995740	0.336532	2.020680
1	-2.629746	0.330594	1.304219

$H_3Si(CH_2)_3NMe_2$ (2a), MP2/aug-cc-pVTZ
E(MP2)= -542.7896729 au

6	1.759831	0.745810	-0.205058
14	1.504974	-1.115543	0.075778
1	0.829776	-1.838816	-1.027452
6	0.597058	1.675665	0.141485
6	-0.694468	1.190084	-0.496001
7	-1.013662	-0.152358	-0.019368
6	-1.609863	-0.122547	1.307465
6	-1.892381	-0.852808	-0.941979
1	2.895409	-1.668863	0.083927
1	0.945353	-1.460142	1.405007
1	2.649650	1.028093	0.362800
1	2.029093	0.869981	-1.259425
1	0.476185	1.731565	1.225151
1	0.800187	2.694370	-0.197568
1	-1.527071	1.887327	-0.312372
1	-0.551152	1.130640	-1.578282
1	-2.077944	-1.860896	-0.571514
1	-2.859111	-0.341471	-1.060441
1	-1.412425	-0.927879	-1.916931
1	-1.763853	-1.143355	1.656033
1	-0.946048	0.374614	2.011437
1	-2.577633	0.401152	1.305267

$H_3Si(CH_2)_3NMe_2$ (2a), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -542.5654736 au

6	1.751009	0.781667	-0.261472
14	1.641632	-1.082716	0.092505
1	0.968710	-1.872138	-0.958433
6	0.565482	1.662563	0.172897

6	-0.750993	1.188667	-0.446680
7	-1.062566	-0.180636	-0.020112
6	-1.679801	-0.197266	1.305878
6	-1.933707	-0.853396	-0.982194
1	3.054509	-1.555219	0.097514
1	1.103707	-1.387493	1.435334
1	2.667702	1.145453	0.222373
1	1.915280	0.907288	-1.342349
1	0.483807	1.665530	1.267103
1	0.738700	2.704477	-0.129465
1	-1.577897	1.883956	-0.207809
1	-0.636216	1.181174	-1.538464
1	-2.132803	-1.873476	-0.637838
1	-2.900166	-0.332004	-1.109596
1	-1.432688	-0.910482	-1.953410
1	-1.813507	-1.234418	1.629694
1	-1.031667	0.300321	2.031455
1	-2.664298	0.306104	1.309018

$H_3Si(CH_2)_3NMe_2$ (**2a**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -542.803576 au

6	1.761660	0.768828	-0.233088
14	1.595152	-1.097121	0.094071
1	0.915122	-1.860475	-0.977264
6	0.576729	1.666825	0.145704
6	-0.722650	1.179026	-0.485651
7	-1.048595	-0.169473	-0.017049
6	-1.660176	-0.144922	1.307847
6	-1.922839	-0.864404	-0.955259
1	2.999610	-1.608255	0.102573
1	1.043177	-1.414353	1.432637
1	2.658012	1.099442	0.299907
1	1.988142	0.890912	-1.298570
1	0.471003	1.700859	1.232700
1	0.760293	2.695417	-0.177899
1	-1.549712	1.880546	-0.290564
1	-0.588056	1.130265	-1.569890
1	-2.119023	-1.872709	-0.588967
1	-2.886350	-0.348309	-1.086890
1	-1.431000	-0.940768	-1.924958
1	-1.819457	-1.167730	1.650294
1	-1.002056	0.348831	2.020554
1	-2.628006	0.380223	1.301369

$F_3SiCH_2NMe_2$ (**2b**), CCSD/6-311G(d,p)
E(CCSD)=-761.6636817 au

14	1.114213	-0.051042	-0.010635
6	-0.544978	-0.511347	-0.690445
7	-1.617253	-0.069528	0.212216

9	2.256441	-0.396365	-1.065337
9	1.435961	-0.869666	1.311574
9	1.261729	1.493030	0.344745
1	-0.546608	-1.609336	-0.726229
1	-0.688304	-0.169309	-1.732719
6	-1.979159	1.320127	-0.061427
6	-2.792358	-0.926273	0.076951
1	-2.393514	1.446164	-1.080255
1	-2.730728	1.648012	0.663433
1	-1.102597	1.964852	0.038684
1	-3.193654	-0.926561	-0.954323
1	-2.535897	-1.953459	0.355088
1	-3.576273	-0.572679	0.754454

$F_3SiCH_2NMe_2$ (**2b**), MP2/6-311G(d,p)
E(MP2)=-761.6168225 au

14	1.107974	-0.050521	-0.011023
6	-0.548492	-0.512186	-0.691049
7	-1.611955	-0.069741	0.218333
9	2.256485	-0.380121	-1.070935
9	1.430352	-0.884073	1.307128
9	1.244311	1.495477	0.360903
1	-0.550253	-1.609053	-0.722978
1	-0.700224	-0.172483	-1.732095
6	-1.973890	1.315634	-0.064503
6	-2.787244	-0.921782	0.079704
1	-2.388471	1.431415	-1.083294
1	-2.724428	1.647259	0.657136
1	-1.098502	1.959886	0.029648
1	-3.185123	-0.916812	-0.951661
1	-2.533603	-1.948630	0.354760
1	-3.569916	-0.567651	0.755700

$F_3SiCH_2NMe_2$ (**2b**), MP2/aug-cc-pVTZ
E(MP2)= -762.0029289 au

14	1.113781	-0.054667	-0.008526
6	-0.560890	-0.570495	-0.614595
7	-1.635201	-0.073417	0.243748
9	2.231251	-0.524178	-1.041754
9	1.449598	-0.728089	1.390001
9	1.280101	1.517552	0.176784
1	-0.549340	-1.663661	-0.564066
1	-0.709337	-0.314210	-1.677017
6	-1.944765	1.314086	-0.076203
6	-2.830356	-0.887585	0.072575
1	-2.287718	1.422190	-1.117848
1	-2.733739	1.667038	0.585665
1	-1.069180	1.943119	0.066268
1	-3.193027	-0.869987	-0.967441
1	-2.616761	-1.918357	0.350624

1	-3.619908	-0.510482	0.720996

$F_3SiCH_2NMe_2$ (**2b**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -761.5876054 au

14	1.111880	-0.050017	-0.010669
6	-0.547847	-0.507758	-0.696334
7	-1.617389	-0.068347	0.215468
9	2.260715	-0.382991	-1.069263
9	1.431759	-0.884559	1.307421
9	1.254277	1.495263	0.361287
1	-0.551262	-1.605400	-0.735731
1	-0.695239	-0.160791	-1.736092
6	-1.986793	1.320717	-0.063618
6	-2.792536	-0.929254	0.081917
1	-2.406818	1.439869	-1.080449
1	-2.735229	1.647820	0.664142
1	-1.111693	1.967679	0.029270
1	-3.195984	-0.929932	-0.948047
1	-2.531606	-1.954961	0.359377
1	-3.574486	-0.577271	0.761825

$F_3SiCH_2NMe_2$ (**2b**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -761.9802152 au

14	1.118267	-0.053728	-0.007982
6	-0.559825	-0.564189	-0.621091
7	-1.640948	-0.071434	0.239873
9	2.234453	-0.525205	-1.040445
9	1.450656	-0.731576	1.388178
9	1.292131	1.516181	0.180373
1	-0.550410	-1.658196	-0.577919
1	-0.704149	-0.300813	-1.682222
6	-1.959563	1.319898	-0.075305
6	-2.835328	-0.896113	0.075152
1	-2.308453	1.432846	-1.114570
1	-2.746314	1.666918	0.593609
1	-1.084863	1.951532	0.066449
1	-3.204488	-0.886058	-0.962877
1	-2.613319	-1.924810	0.357372
1	-3.623975	-0.521370	0.727297

$F_3SiN(Me)NMe_2$ (**2c**), CCSD/6-311G(d,p)
E(CCSD) = -816.8835524 au

14	1.115957	-0.100996	-0.000309
7	-0.414844	0.581278	0.000206
7	-1.354123	-0.488502	-0.000100
6	-2.165545	-0.504284	1.215537
6	-2.165964	-0.503218	-1.215471
1	-1.499055	-0.493940	2.081692

1	-2.751775	-1.428505	1.228827
1	-2.860643	0.349340	1.279908
1	-1.499771	-0.492135	-2.081844
1	-2.752212	-1.427419	-1.229357
1	-2.861075	0.350468	-1.278864
9	1.412057	-1.015057	-1.266160
9	1.412509	-1.016046	1.264724
9	2.193548	1.070900	-0.000033
6	-0.854342	1.970812	0.001032
1	-1.443704	2.211631	0.894329
1	0.038220	2.602233	0.000948
1	-1.444427	2.212433	-0.891567

$F_3SiN(Me)NMe_2$ (**2c**), MP2/6-311G(d,p)
E(MP2) = -816.8313659 au

14	1.108591	-0.107958	-0.000151
7	-0.416639	0.591415	-0.000341
7	-1.346082	-0.487864	-0.000335
6	-2.157633	-0.502601	1.212870
6	-2.158859	-0.501431	-1.212725
1	-1.491338	-0.487390	2.076944
1	-2.739699	-1.427411	1.227190
1	-2.854215	0.348263	1.272476
1	-1.493427	-0.485378	-2.077448
1	-2.741014	-1.426185	-1.227387
1	-2.855430	0.349556	-1.270799
9	1.398652	-1.025763	-1.270850
9	1.397567	-1.027431	1.269627
9	2.199120	1.059201	0.001042
6	-0.864080	1.975049	0.000647
1	-1.453346	2.212957	0.892755
1	0.025790	2.607698	0.001225
1	-1.453149	2.214266	-0.891242

$F_3SiN(Me)NMe_2$ (**2c**), MP2/aug-cc-pVTZ
E(MP2)= -817.2604626 au

14	-1.116213	-0.105575	0.000010
7	0.416989	0.583357	-0.000050
7	1.348852	-0.494797	0.000049
6	2.163681	-0.498959	-1.207821
6	2.163743	-0.498679	1.207878
1	1.508197	-0.495372	-2.075612
1	2.759549	-1.410033	-1.215906
1	2.844955	0.359356	-1.261774
1	1.508302	-0.494844	2.075702
1	2.759583	-1.409769	1.216171
1	2.845044	0.359631	1.261576
9	-1.407367	-1.022525	1.265276
9	-1.407184	-1.023074	-1.264898

9	-2.194557	1.066841	-0.000303
6	0.873003	1.959872	-0.000134
1	1.462919	2.191603	-0.888322
1	-0.005748	2.601180	-0.000321
1	1.462696	2.191798	0.888152

$F_3SiN(Me)NMe_2$ (**2c**), SCS-MP2/6-311G(d,p)
E(SCS-MP2) = -816.7975192 au

14	1.111794	-0.109808	-0.000078
7	-0.415327	0.587756	0.000047
7	-1.355461	-0.487722	-0.000219
6	-2.169568	-0.499045	1.216687
6	-2.170092	-0.497948	-1.216785
1	-1.502769	-0.487732	2.081904
1	-2.755840	-1.422733	1.229900
1	-2.863126	0.355343	1.277570
1	-1.503654	-0.485526	-2.082266
1	-2.756152	-1.421759	-1.230768
1	-2.863864	0.356358	-1.276460
9	1.403493	-1.028106	-1.269942
9	1.402965	-1.029558	1.268877
9	2.201653	1.057664	0.000783
6	-0.853086	1.979364	0.000567
1	-1.441681	2.220810	0.893440
1	0.042106	2.606427	0.001147
1	-1.441145	2.221660	-0.892435

$F_3SiN(Me)NMe_2$ (**2c**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -817.2337554 au

14	-1.118699	-0.107292	0.000005
7	0.415136	0.581960	-0.000055
7	1.356767	-0.493374	0.000036
6	2.173263	-0.496958	-1.211935
6	2.173291	-0.496730	1.211990
1	1.516601	-0.495191	-2.079649
1	2.769615	-1.408706	-1.219351
1	2.854127	0.362006	-1.268456
1	1.516648	-0.494763	2.079719
1	2.769621	-1.408491	1.219586
1	2.854176	0.362231	1.268317
9	-1.410742	-1.023885	1.263994
9	-1.410587	-1.024378	-1.263658
9	-2.197685	1.062996	-0.000271
6	0.863801	1.965430	-0.000107
1	1.452982	2.199742	-0.888827
1	-0.019068	2.602214	-0.000274
1	1.452763	2.199892	0.888720

$F_3SiN(SiMe_3)NMe_2$ (2d), CCSD/6-311G(d,p)
E(CCSD)=-1185.5907179 au

14	1.562551	-0.512895	0.001228
7	0.024624	0.171245	-0.102186
7	0.488078	1.547725	0.022944
6	0.239707	2.326851	-1.188713
6	-0.003899	2.195032	1.234679
1	0.636090	1.776849	-2.044879
1	0.778410	3.276157	-1.098387
1	-0.827512	2.536446	-1.349662
1	0.255927	1.576865	2.097209
1	0.490731	3.166927	1.331560
1	-1.094479	2.356165	1.214547
9	2.333914	-0.199090	1.358397
9	2.529992	-0.099630	-1.192455
9	1.458648	-2.105500	-0.057232
14	-1.640163	-0.440234	-0.030184
6	-2.214242	-0.630454	1.749250
1	-3.210355	-1.091044	1.780886
1	-1.531985	-1.277046	2.314751
1	-2.276590	0.330742	2.272137
6	-1.619972	-2.117029	-0.863271
1	-1.278367	-2.040655	-1.902059
1	-0.966753	-2.826891	-0.347152
1	-2.635805	-2.532534	-0.871218
6	-2.817841	0.708679	-0.936897
1	-2.522739	0.852918	-1.982132
1	-3.818253	0.255845	-0.931836
1	-2.904745	1.693462	-0.464249

$F_3SiN(SiMe_3)NMe_2$ (2d), MP2/6-311G(d,p)
E(MP2)=-1185.5016316 au

14	0.598646	-0.721890	-0.022541
7	-0.757674	0.279342	-0.122790
7	0.042937	1.493222	0.021297
6	-0.008980	2.326093	-1.176788
6	-0.273971	2.225225	1.241212
1	0.236837	1.706871	-2.039912
1	0.746083	3.110760	-1.075996
1	-0.992799	2.790731	-1.324599
1	-0.184126	1.547695	2.091350
1	0.450303	3.036588	1.352688
1	-1.286955	2.655965	1.218639
9	1.414539	-0.614072	1.347466
9	1.641343	-0.528577	-1.216381
9	0.141437	-2.256834	-0.103245
14	-2.519578	0.094747	-0.036789
6	-3.114270	0.064350	1.742270
1	-4.190856	-0.137201	1.778179
1	-2.609536	-0.725079	2.308515

1	-2.936916	1.013433	2.256244
6	-2.896639	-1.542807	-0.853785
1	-2.571086	-1.546626	-1.898077
1	-2.402730	-2.374289	-0.346000
1	-3.976959	-1.722531	-0.833651
6	-3.376080	1.491150	-0.949630
1	-3.046500	1.555103	-1.990392
1	-4.455096	1.298470	-0.950952
1	-3.220349	2.465442	-0.477409

$F_3SiN(SiMe_3)NMe_2$ (2d), MP2/aug-cc-pVTZ
E(MP2)= -1186.0292308 au

14	1.569735	-0.503485	0.002772
7	0.010942	0.140215	-0.135228
7	0.505663	1.509498	0.029031
6	0.277968	2.305899	-1.169943
6	-0.021872	2.141926	1.227818
1	0.695266	1.780004	-2.024579
1	0.798054	3.255685	-1.048716
1	-0.784846	2.500264	-1.343586
1	0.196527	1.513578	2.088168
1	0.472578	3.104377	1.353964
1	-1.104255	2.309405	1.163204
9	2.291192	-0.215840	1.394581
9	2.562393	-0.049272	-1.156167
9	1.501307	-2.097962	-0.100699
14	-1.661048	-0.436393	-0.040424
6	-2.253002	-0.540178	1.739398
1	-3.240801	-1.003896	1.778304
1	-1.572569	-1.149784	2.335574
1	-2.326517	0.441731	2.206418
6	-1.637034	-2.144326	-0.800150
1	-1.306009	-2.107731	-1.837924
1	-0.971347	-2.812904	-0.255929
1	-2.642502	-2.568245	-0.776049
6	-2.799214	0.706880	-1.000187
1	-2.479956	0.810301	-2.037104
1	-3.806089	0.283671	-0.996782
1	-2.860475	1.700310	-0.555500

$F_3SiN(SiMe_3)NMe_2$ (2d), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -1185.4685295 au

14	1.560706	-0.520260	0.000954
7	0.018108	0.161624	-0.106982
7	0.513595	1.534286	0.023043
6	0.274389	2.321194	-1.188603
6	0.029268	2.188501	1.237363
1	0.658645	1.764836	-2.045420
1	0.830420	3.259797	-1.096371

1	-0.789514	2.548261	-1.343724
1	0.274334	1.561568	2.097118
1	0.544103	3.149125	1.337475
1	-1.057152	2.370622	1.211898
9	2.332669	-0.217402	1.366490
9	2.536582	-0.112013	-1.194569
9	1.452410	-2.118177	-0.062271
14	-1.656952	-0.427244	-0.030675
6	-2.238374	-0.597121	1.750056
1	-3.239351	-1.046056	1.781273
1	-1.565542	-1.247159	2.321731
1	-2.291912	0.367821	2.265792
6	-1.651755	-2.111576	-0.851378
1	-1.313723	-2.045362	-1.891341
1	-1.000623	-2.820313	-0.331964
1	-2.669593	-2.520952	-0.851705
6	-2.816780	0.732311	-0.949735
1	-2.514057	0.866721	-1.993576
1	-3.822766	0.293113	-0.947785
1	-2.893166	1.720137	-0.482797

$F_3SiN(SiMe_3)NMe_2$ (**2d**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -1186.0069428 au

14	1.573203	-0.505649	0.003261
7	0.018590	0.152308	-0.123684
7	0.495125	1.532613	0.028998
6	0.256270	2.321487	-1.178029
6	-0.036080	2.169425	1.229121
1	0.674273	1.792669	-2.031305
1	0.772298	3.275264	-1.064411
1	-0.807852	2.510683	-1.351178
1	0.195347	1.550473	2.093552
1	0.448921	3.138731	1.344939
1	-1.120955	2.325029	1.171599
9	2.307743	-0.211608	1.384999
9	2.558954	-0.057145	-1.161781
9	1.495186	-2.098112	-0.093150
14	-1.650423	-0.443702	-0.037452
6	-2.246092	-0.566009	1.745029
1	-3.231044	-1.038764	1.779476
1	-1.561767	-1.174626	2.339853
1	-2.329426	0.412194	2.220778
6	-1.623104	-2.151572	-0.810096
1	-1.272552	-2.112759	-1.842634
1	-0.976323	-2.833866	-0.258620
1	-2.634531	-2.565273	-0.809071
6	-2.807720	0.690455	-0.994378
1	-2.495266	0.799062	-2.034000
1	-3.809565	0.252586	-0.987882
1	-2.883078	1.684141	-0.550117

$ClH_2SiONMe_2$, gauche- (**2e**), CCSD/6-311G(d,p)
E(CCSD)=-959.2063619 au

14	0.920388	-0.976681	0.087609
8	-0.544460	-0.544756	0.735399
7	-1.269339	0.193154	-0.284049
17	2.141687	0.654378	-0.201657
1	1.552233	-1.822474	1.104502
1	0.772244	-1.641571	-1.210265
6	-2.500689	-0.562027	-0.503025
6	-1.553080	1.499660	0.307880
1	-3.104846	-0.018910	-1.236591
1	-2.249153	-1.545348	-0.908207
1	-3.067984	-0.686484	0.431364
1	-2.139009	2.076063	-0.415144
1	-2.113494	1.400222	1.249388
1	-0.610470	2.017065	0.496670

$ClH_2SiONMe_2$, gauche- (**2e**), MP2/6-311G(d,p)
E(MP2)=-959.1446701 au

14	0.902225	-0.970077	0.085885
8	-0.555437	-0.556142	0.774653
7	-1.258944	0.186420	-0.271271
17	2.102763	0.667830	-0.224649
1	1.563835	-1.809234	1.089136
1	0.733209	-1.637431	-1.207153
6	-2.488100	-0.561393	-0.505355
6	-1.544990	1.492975	0.311166
1	-3.074365	-0.018835	-1.251294
1	-2.236021	-1.547058	-0.899409
1	-3.069830	-0.675324	0.419917
1	-2.112462	2.068778	-0.424443
1	-2.123478	1.397710	1.240540
1	-0.604378	2.004072	0.516150

$ClH_2SiONMe_2$, gauche- (**2e**), MP2/aug-cc-pVTZ
E(MP2)= -959.4170667 au

14	0.878806	-0.989970	0.078541
8	-0.569199	-0.599660	0.808494
7	-1.211674	0.188700	-0.255065
17	2.051225	0.680709	-0.231288
1	1.581259	-1.846248	1.048703
1	0.680212	-1.645672	-1.222375
6	-2.451231	-0.513734	-0.544846
6	-1.469944	1.490294	0.341358
1	-2.991345	0.059493	-1.297131

1	-2.219151	-1.497322	-0.945708
1	-3.066603	-0.620758	0.354512
1	-1.990585	2.096520	-0.398893
1	-2.082964	1.397183	1.243850
1	-0.522573	1.961357	0.587796

$ClH_2SiONMe_2$, gauche- (**2e**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -959.1368831 au

14	0.911107	-0.969508	0.089499
8	-0.551671	-0.546434	0.761411
7	-1.275714	0.187788	-0.279659
17	2.120889	0.667524	-0.223685
1	1.561836	-1.803767	1.103073
1	0.752927	-1.643893	-1.201067
6	-2.505939	-0.574487	-0.494029
6	-1.567307	1.497210	0.306975
1	-3.108104	-0.038723	-1.234137
1	-2.249542	-1.559803	-0.889582
1	-3.074541	-0.691659	0.439853
1	-2.150382	2.066998	-0.423063
1	-2.132645	1.399442	1.245051
1	-0.627319	2.017242	0.498179

$ClH_2SiONMe_2$, gauche- (**2e**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -959.4141638 au

14	0.895493	-0.985697	0.085782
8	-0.561275	-0.582364	0.786138
7	-1.239970	0.190241	-0.267127
17	2.080024	0.680023	-0.230441
1	1.576818	-1.833877	1.076505
1	0.715626	-1.653003	-1.211572
6	-2.478086	-0.537286	-0.527239
6	-1.511302	1.493337	0.333623
1	-3.044569	0.024392	-1.269962
1	-2.236952	-1.518301	-0.931002
1	-3.072780	-0.653071	0.385249
1	-2.058707	2.087439	-0.398249
1	-2.103232	1.393751	1.249821
1	-0.567202	1.982966	0.558234

$ClH_2SiONMe_2$, anti- (**2f**), CCSD/6-311G(d,p)
E(CCSD)=-959.205623 au

14	0.629206	-0.755772	0.000000
8	-0.625817	0.345575	0.000000
7	0.184776	1.554678	0.000000
17	-0.258000	-2.614170	0.000000
1	1.432518	-0.666817	1.223121
1	1.432518	-0.666817	-1.223121
6	-0.188688	2.286865	-1.208410

6	-0.188688	2.286865	1.208410
1	0.072401	1.687034	-2.083306
1	0.381726	3.220850	-1.231325
1	-1.266427	2.503461	-1.223111
1	0.072401	1.687034	2.083306
1	0.381726	3.220850	1.231325
1	-1.266427	2.503461	1.223111

$ClH_2SiONMe_2$, anti- (**2f**), MP2/6-311G(d,p)
E(MP2)=-959.144603 au

14	0.612904	-0.696439	0.000000
8	-0.711753	0.333682	0.000000
7	0.155212	1.518058	0.000000
17	-0.181154	-2.600692	0.000000
1	1.403127	-0.587269	1.228659
1	1.403127	-0.587269	-1.228659
6	-0.181154	2.262755	-1.208035
6	-0.181154	2.262755	1.208035
1	0.051048	1.649256	-2.079188
1	0.432287	3.166972	-1.230694
1	-1.246298	2.527531	-1.220422
1	0.051048	1.649256	2.079188
1	0.432287	3.166972	1.230694
1	-1.246298	2.527531	1.220422

$ClH_2SiONMe_2$, anti- (**2f**), MP2/aug-cc-pVTZ
E(MP2)= -959.41826 au

14	0.596231	-0.652463	0.000000
8	-0.776105	0.321138	0.000000
7	0.141324	1.478221	0.000000
17	-0.157310	-2.588628	0.000000
1	1.383569	-0.530441	1.236442
1	1.383569	-0.530441	-1.236442
6	-0.157310	2.231171	-1.207982
6	-0.157310	2.231171	1.207982
1	0.047381	1.607868	-2.074272
1	0.491638	3.105554	-1.230209
1	-1.205422	2.542244	-1.219370
1	0.047381	1.607868	2.074272
1	0.491638	3.105554	1.230209
1	-1.205422	2.542244	1.219370

$ClH_2SiONMe_2$, anti- (**2f**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -959.1365312 au

14	0.631705	-0.722186	0.000000
8	-0.667578	0.337165	0.000000
7	0.167034	1.547531	0.000000
17	-0.201428	-2.610614	0.000000

1	1.428785	-0.618937	1.224596
1	1.428785	-0.618937	-1.224596
6	-0.201428	2.283254	-1.210459
6	-0.201428	2.283254	1.210459
1	0.051221	1.678846	-2.083834
1	0.380527	3.209640	-1.233573
1	-1.276065	2.511423	-1.221770
1	0.051221	1.678846	2.083834
1	0.380527	3.209640	1.233573
1	-1.276065	2.511423	1.221770

$ClH_2SiONMe_2$, anti- (**2f**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -959.4148754 au

14	0.612180	-0.680758	0.000000
8	-0.731262	0.325527	0.000000
7	0.153336	1.508910	0.000000
17	-0.176538	-2.601905	0.000000
1	1.406602	-0.558965	1.231022
1	1.406602	-0.558965	-1.231022
6	-0.176538	2.255432	-1.210156
6	-0.176538	2.255432	1.210156
1	0.048930	1.641156	-2.078621
1	0.442548	3.152199	-1.232122
1	-1.235164	2.531221	-1.221481
1	0.048930	1.641156	2.078621
1	0.442548	3.152199	1.232122
1	-1.235164	2.531221	1.221481

$(CF_3)F_2SiONMe_2$, gauche- (**2g**), CCSD/6-311G(d,p)
E(CCSD)=-1034.812434 au

14	0.191123	0.876568	-0.143240
9	-0.060521	1.644965	1.226425
8	-1.185956	0.511402	-0.960438
7	-1.596949	-0.426232	0.091413
6	-2.832156	0.105294	0.668386
1	-3.606963	0.211323	-0.102561
1	-2.625350	1.074912	1.124034
1	-3.164411	-0.591808	1.443275
6	-1.805960	-1.719061	-0.560510
1	-2.589588	-1.644624	-1.326408
1	-0.873349	-2.046447	-1.020757
1	-2.097827	-2.437587	0.210892
9	1.009315	1.876852	-1.072218
6	1.409435	-0.567767	0.171823
9	1.531167	-1.340227	-0.930817
9	2.634394	-0.093948	0.456304
9	1.057183	-1.379277	1.179774

$(CF_3)F_2SiONMe_2$, gauche- (**2g**), MP2/6-311G(d,p)
E(MP2)=-1034.7753796 au

14	0.118286	0.836848	-0.143067
9	-0.143856	1.621588	1.226749
8	-1.233653	0.561304	-1.066595
7	-1.570546	-0.367161	0.038985
6	-2.792802	0.127929	0.668297
1	-3.608517	0.159523	-0.062632
1	-2.609286	1.123061	1.069858
1	-3.041254	-0.551675	1.486567
6	-1.745275	-1.693126	-0.548530
1	-2.580472	-1.682800	-1.257964
1	-0.830921	-1.984308	-1.061463
1	-1.942791	-2.394195	0.265177
9	1.007557	1.843001	-1.017294
6	1.342868	-0.604984	0.165350
9	1.533268	-1.330321	-0.966216
9	2.548236	-0.138459	0.540667
9	0.942743	-1.471888	1.117488

$(CF_3)F_2SiONMe_2$, gauche- (**2g**), MP2/aug-cc-pVTZ
E(MP2) = -1035.3472216 au

14	-0.086051	-0.837710	-0.138063
9	0.181737	-1.606465	1.234604
8	1.250359	-0.550523	-1.087083
7	1.550423	0.379655	0.037718
6	2.783413	-0.081700	0.663966
1	3.597632	-0.073020	-0.063168
1	2.636734	-1.084757	1.050771
1	3.007379	0.594852	1.486819
6	1.687291	1.712219	-0.536552
1	2.517982	1.727324	-1.244831
1	0.767323	1.987431	-1.041538
1	1.873572	2.406856	0.280283
9	-0.963929	-1.861117	-0.999088
6	-1.351194	0.585771	0.158571
9	-1.574777	1.293316	-0.977303
9	-2.541475	0.098298	0.555546
9	-0.964755	1.477982	1.095271

$(CF_3)F_2SiONMe_2$, gauche- (**2g**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -1034.7176377 au

14	0.142316	0.842405	-0.145008
9	-0.106475	1.626630	1.225402
8	-1.220547	0.562689	-1.043308
7	-1.597153	-0.364049	0.053601
6	-2.821316	0.164995	0.662765

1	-3.622438	0.229120	-0.083724
1	-2.615455	1.151691	1.077586
1	-3.108070	-0.514084	1.470557
6	-1.805014	-1.681584	-0.554144
1	-2.624255	-1.639115	-1.282490
1	-0.888450	-1.998984	-1.049851
1	-2.044126	-2.383589	0.249252
9	1.029238	1.834843	-1.034009
6	1.346503	-0.618628	0.166498
9	1.514403	-1.356954	-0.961633
9	2.564569	-0.164127	0.523650
9	0.946462	-1.471567	1.132071

$(CF_3)F_2SiONMe_2$, gauche- (**2g**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -1035.2952203 au

14	-0.100986	-0.840697	-0.140064
9	0.156666	-1.608468	1.232502
8	1.241429	-0.553190	-1.072168
7	1.569745	0.376898	0.046424
6	2.805344	-0.107677	0.662181
1	3.612634	-0.120456	-0.073380
1	2.642506	-1.106081	1.056292
1	3.052415	0.568692	1.479506
6	1.731265	1.707048	-0.540397
1	2.552935	1.701055	-1.260053
1	0.810656	2.000262	-1.035092
1	1.943896	2.402135	0.270552
9	-0.977751	-1.855047	-1.009175
6	-1.355153	0.594964	0.159034
9	-1.568039	1.310944	-0.974468
9	-2.552662	0.111698	0.545683
9	-0.970395	1.479249	1.104406

$(CF_3)F_2SiONMe_2$, anti- (**2h**), CCSD/6-311G(d,p)
E(CCSD)=-1034.810591 au

14	-0.500871	0.231870	0.000000
6	-1.160807	-1.560227	0.000000
9	-1.085808	0.951017	1.288439
9	-0.744649	-2.240167	1.082856
9	-2.505060	-1.593933	0.000000
8	1.128652	0.122469	0.000000
7	1.521354	1.534109	0.000000
6	2.319639	1.715511	1.211130
1	3.181359	1.033369	1.227543
1	1.687629	1.533500	2.082729
1	2.663089	2.754285	1.229545
9	-1.085808	0.951017	-1.288439
9	-0.744649	-2.240167	-1.082856
6	2.319639	1.715511	-1.211130
1	3.181359	1.033369	-1.227543

1	1.687629	1.533500	-2.082729
1	2.663089	2.754285	-1.229545

$(CF_3)F_2SiONMe_2$, anti- (**2h**), CCSD/6-311++G(d,p)
E(CCSD)= -1034.8454047 au

14	0.333229	0.375704	0.000000
6	-1.286713	1.397939	0.000000
9	1.163586	0.799106	1.287096
9	-2.040355	1.132470	1.083678
9	-1.043492	2.721919	0.000000
8	-0.120650	-1.193786	0.000000
7	1.166471	-1.894944	0.000000
6	1.163586	-2.716216	1.210421
1	0.311925	-3.411654	1.219777
1	1.116708	-2.064435	2.085666
1	2.103965	-3.275734	1.231738
9	1.163586	0.799106	-1.287096
9	-2.040355	1.132470	-1.083678
6	1.163586	-2.716216	-1.210421
1	0.311925	-3.411654	-1.219777
1	1.116708	-2.064435	-2.085666
1	2.103965	-3.275734	-1.231738

$(CF_3)F_2SiONMe_2$, anti- (**2h**), MP2/6-311G(d,p)
E(MP2)=-1034.7723229 au

14	-0.257860	0.254312	0.000000
6	-1.151235	-1.437099	0.000000
9	-0.821301	0.961071	1.320991
9	-0.821301	-2.172285	1.086091
9	-2.494842	-1.313611	0.000000
8	1.352405	-0.160290	0.000000
7	1.509385	1.316315	0.000000
6	2.229980	1.676257	1.217514
1	3.215292	1.197345	1.230710
1	1.647230	1.358896	2.080776
1	2.334067	2.763561	1.232123
9	-0.821301	0.961071	-1.320991
9	-0.821301	-2.172285	-1.086091
6	2.229980	1.676257	-1.217514
1	3.215292	1.197345	-1.230710
1	1.647230	1.358896	-2.080776
1	2.334067	2.763561	-1.232123

$(CF_3)F_2SiONMe_2$, anti- (**2h**), MP2/aug-cc-pVTZ
E(MP2)= -1035.3448811 au

14	-0.235457	0.268172	0.000000
6	-1.136898	-1.432609	0.000000
9	-0.813670	0.951023	1.322907

9	-0.813670	-2.173869	1.084961
9	-2.482260	-1.309687	0.000000
8	1.373937	-0.184510	0.000000
7	1.479518	1.305101	0.000000
6	2.188481	1.687285	1.214359
1	3.185463	1.243577	1.217576
1	1.625399	1.349250	2.078003
1	2.259303	2.773479	1.228586
9	-0.813670	0.951023	-1.322907
9	-0.813670	-2.173869	-1.084961
6	2.188481	1.687285	-1.214359
1	3.185463	1.243577	-1.217576
1	1.625399	1.349250	-2.078003
1	2.259303	2.773479	-1.228586

$(CF_3)F_2SiONMe_2$, anti- (**2h**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -1034.7151264 au

14	-0.320883	-0.331269	0.000000
6	1.248797	-1.423197	0.000000
9	-1.154052	-0.730611	1.297188
9	2.015717	-1.189577	1.087165
9	0.945998	-2.739134	0.000000
8	0.213896	1.222077	0.000000
7	-1.117509	1.868728	0.000000
6	-1.154052	2.686200	1.213408
1	-0.330820	3.413197	1.227440
1	-1.085047	2.030921	2.083145
1	-2.116310	3.206094	1.231833
9	-1.154052	-0.730611	-1.297188
9	2.015717	-1.189577	-1.087165
6	-1.154052	2.686200	-1.213408
1	-0.330820	3.413197	-1.227440
1	-1.085047	2.030921	-2.083145
1	-2.116310	3.206094	-1.231833

$(CF_3)F_2SiONMe_2$, anti- (**2h**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -1035.293232 au

14	-0.242687	0.265841	0.000000
6	-1.143157	-1.438366	0.000000
9	-0.818678	0.952818	1.319171
9	-0.818678	-2.180416	1.085917
9	-2.489191	-1.317402	0.000000
8	1.365229	-0.172070	0.000000
7	1.489890	1.317525	0.000000
6	2.208965	1.689980	1.217796
1	3.200176	1.232276	1.221782
1	1.641202	1.359889	2.082298
1	2.295149	2.775797	1.232068
9	-0.818678	0.952818	-1.319171

9	-0.818678	-2.180416	-1.085917
6	2.208965	1.689980	-1.217796
1	3.200176	1.232276	-1.221782
1	1.641202	1.359889	-2.082298
1	2.295149	2.775797	-1.232068

$F_3SiONMe_2$ (**2i**), CCSD/6-311G(d,p)
E(CCSD)= -797.5273531 au

7	-0.552360	1.306859	0.000000
14	0.275516	-0.941021	0.000000
9	1.594569	-1.814337	0.000000
9	-0.560453	-1.337071	1.283755
9	-0.560453	-1.337071	-1.283755
8	0.741076	0.623365	0.000000
6	-0.560453	2.124632	1.210996
6	-0.560453	2.124632	-1.210996
1	-1.502852	2.680345	1.232397
1	-0.514167	1.466910	-2.081329
1	-1.502852	2.680345	-1.232397
1	-0.514167	1.466910	2.081329
1	0.288599	2.822784	-1.227529
1	0.288599	2.822784	1.227529

$F_3SiONMe_2$ (**2i**), MP2/6-311G(d,p)
E(MP2)= -797.4928467 au

7	-0.506709	1.251290	0.000000
14	0.266245	-0.900171	0.000000
9	1.546186	-1.843450	0.000000
9	-0.572705	-1.275560	1.295828
9	-0.572705	-1.275560	-1.295828
8	0.837054	0.640813	0.000000
6	-0.572705	2.060861	1.210227
6	-0.572705	2.060861	-1.210227
1	-1.549963	2.548959	1.230681
1	-0.481875	1.406439	-2.076946
1	-1.549963	2.548959	-1.230681
1	-0.481875	1.406439	2.076946
1	0.226130	2.813436	-1.225555
1	0.226130	2.813436	1.225555

$F_3SiONMe_2$ (**2i**), MP2/aug-cc-pVTZ
E(MP2)= -797.9087611 au

7	-0.430851	1.166015	0.000000
14	0.243607	-0.828842	0.000000
9	1.460325	-1.858423	0.000000
9	-0.583370	-1.196571	1.307900
9	-0.583370	-1.196571	-1.307900
8	0.969170	0.660363	0.000000

6	-0.583370	1.959444	1.210086
6	-0.583370	1.959444	-1.210086
1	-1.599508	2.349919	1.224852
1	-0.430399	1.322408	-2.075627
1	-1.599508	2.349919	-1.224852
1	-0.430399	1.322408	2.075627
1	0.135043	2.782443	-1.218742
1	0.135043	2.782443	1.218742

$F_3SiONMe_2$ (**2i**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -797.4569128 au

7	-0.541411	1.288716	0.000000
14	0.272840	-0.928658	0.000000
9	1.581114	-1.828264	0.000000
9	-0.566230	-1.317872	1.290049
9	-0.566230	-1.317872	-1.290049
8	0.780583	0.630970	0.000000
6	-0.566230	2.106867	1.212506
6	-0.566230	2.106867	-1.212506
1	-1.521720	2.639081	1.234263
1	-0.502996	1.449791	-2.081423
1	-1.521720	2.639081	-1.234263
1	-0.502996	1.449791	2.081423
1	0.265885	2.824183	-1.226592
1	0.265885	2.824183	1.226592

$F_3SiONMe_2$ (**2i**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -797.8775157 au

7	-0.494013	1.228625	0.000000
14	0.262178	-0.885597	0.000000
9	1.523125	-1.849750	0.000000
9	-0.575071	-1.255574	1.294016
9	-0.575071	-1.255574	-1.294016
8	0.872403	0.642734	0.000000
6	-0.575071	2.040181	1.210603
6	-0.575071	2.040181	-1.210603
1	-1.557716	2.510630	1.227279
1	-0.472421	1.394862	-2.078930
1	-1.557716	2.510630	-1.227279
1	-0.472421	1.394862	2.078930
1	0.206331	2.805522	-1.220818
1	0.206331	2.805522	1.220818

1-methylsilatrane (**1a**), CCSD/6-311++G(d,p)
E(CCSD)= -844.0526577 au

14	0.000000	0.000000	1.169338
7	0.000000	0.000000	-1.398809

6	1.242109	-0.717132	-1.648028
6	1.513246	-1.613260	-0.433573
8	1.365830	-0.867698	0.755432
1	1.215328	-1.307385	-2.578720
1	2.052549	0.015674	-1.733424
1	0.816731	-2.464932	-0.431466
1	2.534492	-2.009138	-0.465929
6	-1.242109	-0.717132	-1.648028
6	-2.153747	-0.503880	-0.433573
8	-1.434364	-0.748994	0.755432
1	-1.739893	-0.398813	-2.578720
1	-1.012700	-1.785397	-1.733424
1	-2.543059	0.525157	-0.431466
1	-3.007210	-1.190365	-0.465929
6	0.000000	1.434264	-1.648028
6	0.640501	2.117140	-0.433573
8	0.068534	1.616693	0.755432
1	0.524565	1.706198	-2.578720
1	-1.039849	1.769723	-1.733424
1	1.726329	1.939776	-0.431466
1	0.472719	3.199503	-0.465929
6	0.000000	0.000000	3.025358
1	-0.784603	0.660546	3.411949
1	0.964351	0.349213	3.411949
1	-0.179748	-1.009759	3.411949

1-methylsilatrane (**1a**), MP2/aug-cc-pVTZ
E(MP2)= -844.4016827 au

14	0.000000	0.000000	1.088398
7	0.000000	0.000000	-1.272661
6	0.459081	1.344692	-1.595647
6	-1.394078	-0.274770	-1.595647
6	0.934997	-1.069922	-1.595647
6	0.000000	2.242645	-0.455016
6	-1.942188	-1.121323	-0.455016
6	1.942188	-1.121323	-0.455016
8	0.310410	1.624264	0.771438
8	-1.561859	-0.543309	0.771438
8	1.251449	-1.080955	0.771438
1	0.090939	1.689049	-2.568956
1	-1.508229	-0.765769	-2.568956
1	1.417290	-0.923280	-2.568956
1	1.549015	1.335162	-1.621405
1	-1.930791	0.673905	-1.621405
1	0.381776	-2.009067	-1.621405
1	-1.077911	2.424143	-0.522501
1	-1.560414	-2.145570	-0.522501
1	2.638325	-0.278573	-0.522501
1	0.505349	3.208051	-0.499419
1	-3.030928	-1.166380	-0.499419
1	2.525579	-2.041671	-0.499419

6	0.000000	0.000000	2.951015
1	-0.077052	-1.017266	3.333082
1	0.919505	0.441904	3.333082
1	-0.842452	0.575362	3.333082

1-methylsilatrane (**1a**), MP2/def2-TZVPP
E(MP2)= -844.3676258 au

14	0.000000	0.000000	1.092035
7	0.000000	0.000000	-1.287204
6	-0.455276	1.346083	-1.598948
6	0.000000	2.234033	-0.449497
8	-0.319945	1.611091	0.770047
1	-0.085860	1.701190	-2.566847
1	-1.544201	1.339027	-1.627651
1	1.077929	2.410908	-0.510928
1	-0.499014	3.201602	-0.492660
6	1.393380	-0.278761	-1.598948
6	1.934729	-1.117016	-0.449497
8	1.555218	-0.528465	0.770047
1	1.516203	-0.776238	-2.566847
1	1.931732	0.667804	-1.627651
1	1.548943	-2.138968	-0.510928
1	3.022175	-1.168642	-0.492660
6	-0.938104	-1.067322	-1.598948
6	-1.934729	-1.117016	-0.449497
8	-1.235273	-1.082626	0.770047
1	-1.430343	-0.924952	-2.566847
1	-0.387531	-2.006831	-1.627651
1	-2.626873	-0.271940	-0.510928
1	-2.523162	-2.032959	-0.492660
6	0.000000	0.000000	2.950791
1	0.052551	-1.017466	3.334104
1	-0.907427	0.463222	3.334104
1	0.854876	0.554244	3.334104

1-methylsilatrane (**1a**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -843.9070439 au

14	0.000000	0.000000	1.130881
7	0.000000	0.000000	-1.342692
6	1.240399	-0.716145	-1.630378
6	0.000000	1.432289	-1.630378
6	-1.240399	-0.716145	-1.630378
6	2.176510	-0.483998	-0.438425
6	-0.669101	2.126912	-0.438425
6	-1.507410	-1.642914	-0.438425
8	1.473129	-0.715366	0.764615
8	-0.117040	1.633450	0.764615
8	-1.356090	-0.918084	0.764615
1	1.701851	-0.402060	-2.579903
1	-0.502731	1.674877	-2.579903

1	-1.199120	-1.272817	-2.579903
1	1.012991	-1.785246	-1.693385
1	1.039573	1.769899	-1.693385
1	-2.052564	0.015347	-1.693385
1	2.564774	0.544644	-0.458124
1	-1.754062	1.948837	-0.458124
1	-0.810711	-2.493481	-0.458124
1	3.029109	-1.170423	-0.477845
1	-0.500938	3.208497	-0.477845
1	-2.528171	-2.038074	-0.477845
6	0.000000	0.000000	2.991154
1	-0.967267	0.336246	3.378346
1	0.192435	-1.005801	3.378346
1	0.774831	0.669554	3.378346

1-methylsilatrane (**1a**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -844.3758276 au

14	0.000000	0.000000	1.115577
7	0.000000	0.000000	-1.316887
6	0.441601	1.357453	-1.616792
6	-1.396390	-0.296289	-1.616792
6	0.954788	-1.061165	-1.616792
6	0.000000	2.235481	-0.447633
6	-1.935983	-1.117740	-0.447633
6	1.935983	-1.117740	-0.447633
8	0.343983	1.605503	0.768116
8	-1.562398	-0.504853	0.768116
8	1.218415	-1.100649	0.768116
1	0.050180	1.725968	-2.573008
1	-1.519822	-0.819526	-2.573008
1	1.469642	-0.906441	-2.573008
1	1.531083	1.359324	-1.669161
1	-1.942751	0.646295	-1.669161
1	0.411668	-2.005619	-1.669161
1	-1.081188	2.406589	-0.486828
1	-1.543573	-2.139631	-0.486828
1	2.624761	-0.266958	-0.486828
1	0.496221	3.206483	-0.486981
1	-3.025007	-1.173502	-0.486981
1	2.528786	-2.032982	-0.486981
6	0.000000	0.000000	2.980148
1	-0.092882	-1.016727	3.364012
1	0.926952	0.427925	3.364012
1	-0.834070	0.588801	3.364012

1-methylsilatrane (**1a**), SCS-MP2/def2-TZVPP
E(SCS-MP2)= -844.3404429 au

14	0.000000	0.000000	1.117041
7	0.000000	0.000000	-1.328983
6	-0.439216	1.358281	-1.618447

6	0.000000	2.228103	-0.442846
8	-0.348988	1.594278	0.767243
1	-0.048325	1.735566	-2.570253
1	-1.527658	1.361803	-1.671746
1	1.080548	2.396796	-0.478984
1	-0.491756	3.200244	-0.480618
6	1.395914	-0.298768	-1.618447
6	1.929594	-1.114052	-0.442846
8	1.555179	-0.494906	0.767243
1	1.527207	-0.825932	-2.570253
1	1.943185	0.642089	-1.671746
1	1.535412	-2.134180	-0.478984
1	3.017371	-1.174249	-0.480618
6	-0.956698	-1.059513	-1.618447
6	-1.929594	-1.114052	-0.442846
8	-1.206191	-1.099372	0.767243
1	-1.478882	-0.909634	-2.570253
1	-0.415527	-2.003892	-1.671746
1	-2.615960	-0.262616	-0.478984
1	-2.525615	-2.025995	-0.480618
6	0.000000	0.000000	2.978059
1	0.082482	-1.016160	3.363394
1	-0.921261	0.436648	3.363394
1	0.838779	0.579512	3.363394

1-hydrosilatrane (**1b**), MP2/aug-cc-pVTZ
E(MP2)= -805.1589121 au

14	0.000000	0.000000	1.308244
7	0.000000	0.000000	-0.960083
6	-0.477689	1.337108	-1.307120
6	0.000000	2.262022	-0.195381
8	-0.245056	1.646143	1.045829
1	-0.131245	1.653934	-2.296511
1	-1.567488	1.316397	-1.308445
1	1.068369	2.475512	-0.304903
1	-0.535331	3.211304	-0.233200
6	1.396814	-0.254863	-1.307120
6	1.958969	-1.131011	-0.195381
8	1.548130	-0.610847	1.045829
1	1.497971	-0.713306	-2.296511
1	1.923777	0.699286	-1.308445
1	1.609672	-2.162991	-0.304903
1	3.048736	-1.142042	-0.233200
6	-0.919125	-1.082245	-1.307120
6	-1.958969	-1.131011	-0.195381
8	-1.303074	-1.035296	1.045829
1	-1.366726	-0.940628	-2.296511
1	-0.356289	-2.015683	-1.308445
1	-2.678041	-0.312521	-0.304903
1	-2.513406	-2.069262	-0.233200

1	0.000000	0.000000	2.779471

1-hydrosilatrane (**1b**), MP2/def2-TZVPP
E(MP2)= -805.1274424 au

14	0.000000	0.000000	1.307290
7	0.000000	0.000000	-0.968869
6	-0.475147	1.337828	-1.308573
6	0.000000	2.255996	-0.190807
8	-0.248802	1.635910	1.045389
1	-0.129103	1.662183	-2.294612
1	-1.563984	1.318789	-1.311475
1	1.067649	2.468763	-0.298034
1	-0.532395	3.205749	-0.227662
6	1.396167	-0.257425	-1.308573
6	1.953750	-1.127998	-0.190807
8	1.541141	-0.602486	1.045389
1	1.504044	-0.719285	-2.294612
1	1.924097	0.695055	-1.311475
1	1.604187	-2.158993	-0.298034
1	3.042458	-1.141807	-0.227662
6	-0.921020	-1.080403	-1.308573
6	-1.953750	-1.127998	-0.190807
8	-1.292339	-1.033424	1.045389
1	-1.374941	-0.942898	-2.294612
1	-0.360113	-2.013844	-1.311475
1	-2.671836	-0.309770	-0.298034
1	-2.510063	-2.063942	-0.227662
1	0.000000	0.000000	2.774878

1-hydrosilatrane (**1b**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -804.69634 au

14	0.000000	0.000000	1.355150
7	0.000000	0.000000	-1.023879
6	-0.443051	1.360170	-1.341653
6	0.000000	2.247884	-0.172913
8	-0.337290	1.613933	1.042491
1	-0.050835	1.715147	-2.306693
1	-1.536583	1.361149	-1.387610
1	1.084185	2.425641	-0.219939
1	-0.505394	3.218479	-0.213344
6	1.399468	-0.296392	-1.341653
6	1.946725	-1.123942	-0.172913
8	1.566351	-0.514865	1.042491
1	1.510779	-0.813549	-2.306693
1	1.947081	0.650145	-1.387610
1	1.558575	-2.151752	-0.219939
1	3.039981	-1.171556	-0.213344
6	-0.956417	-1.063779	-1.341653
6	-1.946725	-1.123942	-0.172913

8	-1.229062	-1.099068	1.042491
1	-1.459943	-0.901598	-2.306693
1	-0.410498	-2.011294	-1.387610
1	-2.642759	-0.273889	-0.219939
1	-2.534588	-2.046923	-0.213344
1	0.000000	0.000000	2.820216

1-hydrosilatrane (**1b**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -805.1332429 au

14	0.000000	0.000000	1.324179
7	0.000000	0.000000	-0.981080
6	-0.465762	1.346804	-1.319610
6	0.000000	2.262424	-0.189321
8	-0.262674	1.637300	1.047068
1	-0.102571	1.676365	-2.299471
1	-1.555807	1.333610	-1.340543
1	1.070597	2.474414	-0.281240
1	-0.533823	3.213324	-0.223603
6	1.399247	-0.270041	-1.319610
6	1.959317	-1.131212	-0.189321
8	1.549280	-0.591168	1.047068
1	1.503060	-0.749354	-2.299471
1	1.932844	0.680563	-1.340543
1	1.607607	-2.164371	-0.281240
1	3.049732	-1.144358	-0.223603
6	-0.933486	-1.076763	-1.319610
6	-1.959317	-1.131212	-0.189321
8	-1.286606	-1.046132	1.047068
1	-1.400489	-0.927012	-2.299471
1	-0.377037	-2.014173	-1.340543
1	-2.678204	-0.310043	-0.281240
1	-2.515909	-2.068966	-0.223603
1	0.000000	0.000000	2.794769

1-hydrosilatrane (**1b**), SCS-MP2/def2-TZVPP
E(SCS-MP2)= -805.1006716 au

14	0.000000	0.000000	1.324047
7	0.000000	0.000000	-0.990838
6	-0.463056	1.347668	-1.321329
6	0.000000	2.256167	-0.184610
8	-0.267025	1.627027	1.046449
1	-0.099699	1.685094	-2.297311
1	-1.552090	1.336280	-1.343844
1	1.069954	2.467026	-0.273893
1	-0.530575	3.207687	-0.218091
6	1.398643	-0.272816	-1.321329
6	1.953898	-1.128084	-0.184610
8	1.542560	-0.582263	1.046449
1	1.509184	-0.756205	-2.297311
1	1.933298	0.676010	-1.343844

1	1.601530	-2.160120	-0.273893
1	3.043226	-1.144352	-0.218091
6	-0.935587	-1.074853	-1.321329
6	-1.953898	-1.128084	-0.184610
8	-1.275534	-1.044764	1.046449
1	-1.409484	-0.928889	-2.297311
1	-0.381207	-2.012290	-1.343844
1	-2.671484	-0.306906	-0.273893

1-fluorosilatrane (**1c**), MP2/aug-cc-pVTZ
E(MP2)= -904.3882443 au

14	0.000000	0.000000	1.043757
7	0.000000	0.000000	-1.175756
6	-0.471886	1.340368	-1.529931
6	0.000000	2.259931	-0.411731
8	-0.262310	1.637710	0.822099
1	-0.114653	1.651963	-2.516182
1	-1.561568	1.322600	-1.540138
1	1.070083	2.469529	-0.509218
1	-0.531725	3.210732	-0.448137
6	1.396736	-0.261519	-1.529931
6	1.957158	-1.129966	-0.411731
8	1.549453	-0.591687	0.822099
1	1.487968	-0.726690	-2.516182
1	1.926189	0.691058	-1.540138
1	1.603633	-2.161484	-0.509218
1	3.046438	-1.144879	-0.448137
6	-0.924850	-1.078849	-1.529931
6	-1.957158	-1.129966	-0.411731
8	-1.287143	-1.046022	0.822099
1	-1.373316	-0.925274	-2.516182
1	-0.364621	-2.013657	-1.540138
1	-2.673717	-0.308045	-0.509218
1	-2.514713	-2.065853	-0.448137
9	0.000000	0.000000	2.653139

1-fluorosilatrane (**1c**), MP2/def2-TZVPP
E(MP2)= -904.3533252 au

14	0.000000	0.000000	1.049959
7	0.000000	0.000000	-1.187023
6	-0.468182	1.341095	-1.533024
6	0.000000	2.252386	-0.407190
8	-0.270237	1.626252	0.820486
1	-0.109381	1.661936	-2.514771
1	-1.556908	1.326000	-1.546569
1	1.070024	2.458930	-0.499864
1	-0.526915	3.204673	-0.443164
6	1.395513	-0.265090	-1.533024
6	1.950623	-1.126193	-0.407190
8	1.543494	-0.579094	0.820486

1	1.493969	-0.736241	-2.514771
1	1.926804	0.685322	-1.546569
1	1.594484	-2.156133	-0.499864
1	3.038786	-1.146014	-0.443164
6	-0.927331	-1.076005	-1.533024
6	-1.950623	-1.126193	-0.407190
8	-1.273257	-1.047158	0.820486
1	-1.384588	-0.925694	-2.514771
1	-0.369896	-2.011322	-1.546569
1	-2.664508	-0.302797	-0.499864
1	-2.511871	-2.058659	-0.443164
9	0.000000	0.000000	2.650558

1-fluorosilatrane (**1c**), SCS-MP2/6-311G(d,p)
E(SCS-MP2)= -903.8413953 au

14	0.000000	0.000000	1.075415
7	0.000000	0.000000	-1.228051
6	-0.437576	1.362401	-1.562251
6	0.000000	2.249910	-0.392056
8	-0.353810	1.609324	0.814580
1	-0.034860	1.703653	-2.526575
1	-1.530567	1.366386	-1.615383
1	1.084768	2.424483	-0.427402
1	-0.503971	3.220531	-0.432420
6	1.398662	-0.302249	-1.562251
6	1.948479	-1.124955	-0.392056
8	1.570620	-0.498254	0.814580
1	1.492837	-0.821637	-2.526575
1	1.948609	0.642317	-1.615383
1	1.557280	-2.151678	-0.427402
1	3.041047	-1.173814	-0.432420
6	-0.961086	-1.060152	-1.562251
6	-1.948479	-1.124955	-0.392056
8	-1.216811	-1.111070	0.814580
1	-1.457977	-0.882016	-2.526575
1	-0.418041	-2.008703	-1.615383
1	-2.642048	-0.272805	-0.427402
1	-2.537076	-2.046717	-0.432420
9	0.000000	0.000000	2.685944

1-fluorosilatrane (**1c**), SCS-MP2/aug-cc-pVTZ
E(SCS-MP2)= -904.3505612 au

14	0.000000	0.000000	1.053662
7	0.000000	0.000000	-1.190301
6	0.461504	-1.348999	-1.540489
6	0.000000	-2.263029	-0.407461
8	0.273831	-1.631699	0.822586
1	0.088909	-1.668958	-2.518928
1	1.551270	-1.337917	-1.568122
1	-1.071269	-2.473859	-0.491392

1	0.533395	-3.213661	-0.440145
6	-1.399019	0.274825	-1.540489
6	-1.959840	1.131514	-0.407461
8	-1.550008	0.578705	0.822586
1	-1.489815	0.757482	-2.518928
1	-1.934305	-0.674480	-1.568122
1	-1.606790	2.164675	-0.491392
1	-3.049810	1.144897	-0.440145
6	0.937516	1.074174	-1.540489
6	1.959840	1.131514	-0.407461
8	1.276177	1.052994	0.822586
1	1.400906	0.911477	-2.518928
1	0.383035	2.012397	-1.568122
1	2.678059	0.309183	-0.491392
1	2.516415	2.068764	-0.440145
9	0.000000	0.000000	2.661957

1-fluorosilatrane (**1c**), SCS-MP2/def2-TZVPP
E(SCS-MP2)= -904.3145539 au

14	0.000000	0.000000	1.058478
7	0.000000	0.000000	-1.199961
6	-0.459822	1.349174	-1.542314
6	0.000000	2.256513	-0.403800
8	-0.275597	1.621997	0.821508
1	-0.088432	1.677019	-2.517503
1	-1.548598	1.339608	-1.570306
1	1.070270	2.467236	-0.486937
1	-0.530893	3.207380	-0.435255
6	1.398330	-0.276370	-1.542314
6	1.954197	-1.128256	-0.403800
8	1.542489	-0.572324	0.821508
1	1.496557	-0.761925	-2.517503
1	1.934433	0.671322	-1.570306
1	1.601554	-2.160498	-0.486937
1	3.043119	-1.143923	-0.435255
6	-0.938508	-1.072805	-1.542314
6	-1.954197	-1.128256	-0.403800
8	-1.266892	-1.049673	0.821508
1	-1.408125	-0.915094	-2.517503
1	-0.385835	-2.010929	-1.570306
1	-2.671824	-0.306737	-0.486937