Supplementary material belonging to the publication:

"Unexpected" 29Si NMR Chemical Shifts in Heteroatom-Substituted Silyllithium Compounds: A Quantum Chemical Analysis

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Table of contents for supplementary material pages

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Table 1. Selected bond lengths [pm] and angles [°] for calculated model systems **1**-**3**.[6-31+G(d)][a]

model	method	bond lengths			angles	
		Si-C	Si-Li	Li-O	C-Si-Li	C-Si-C
		194.9		203.1	114.5	100.4
	B3LYP	194.9	265.7	204.0	118.1	100.4
		194.9		204.0	119.6	100.6
		193.6		200.4	116.1	100.2
1	MP2	193.7	260.8	200.4	118.2	100.3
		193.7		201.2	118.3	100.4
		194.4		206.2	115.3	100.9
	HF	194.4	270.9	206.3	117.3	101.0
		194.4		207.1	118.5	101.0
		192.7			114.0	104.5
	B3LYP	192.7	251.8	-	114.1	104.5
		192.7			114.1	104.5
		191.6			114.5	103.9
2	MP2	191.6	254.1	-	114.6	103.9
		191.6			114.6	103.9
		192.4			114.3	104.3
	HF	192.4	258.8	-	114.3	104.3
		192.4			114.3	104.3
		197.1				97.8
	B3LYP	197.1	-	-	-	97.8
		197.1				97.8
		195.4				97.6
3	MP2	195.4	-	-	-	97.6
		195.4				97.6
		196.5				98.4
	HF	196.5	-	-	-	98.4
		196.5				98.4

[a] Standard orientation of models **1**-**3** are in Tables 4 to 12; Optimization of model **2** at the higher B3LYP/6–311++G(d,p) level did not show significant deviation in the structural parameters.

Table 2. Calculated ^{29}Si nuclear shieldings for models $Y_nMe_{3-n}SiX$[a]

model	Y	σ			
		X=H	X=Cl	X=Li	X=Me
Me_3SiX	–	400.5	355.1	400.1	385.9
$(Y)Me_2SiX$	OMe	382.6	370.0	346.6	371.6
	NMe_2	393.3[b]	369.5	362.5	380.2
	SMe	383.3	348.9	366.0[b]	370.1
$(Y)_2MeSiX$	OMe	401.8	405.2[b]	350.8	388.8
	NMe_2	396.7	389.2	352.8	388.1
	SMe	379.5	344.6	351.3	356.4
$(Y)_3SiX$	OMe	–	448.2[b]	394.5[b]	–
	NMe_2	–	410.2	373.5[b]	–
	SMe	–	341.8[c]	335.4[c]	–

[a] GIAO-HF/6-311+G(2d,p)//B3LYP/6-31+G(d) results [b] Values from local minimum structure. [c] Optimization started from a conformationally identical model as the local minimum of the corresponding $(MeO)_3SiX$ system.

Table 3. Calculated ^{29}Si nuclear shieldings for models $Y_nMe_{3-n}SiX$[a]

model	Y	σ			
		X=H	X=Cl	X=Li	X=Me
Me_3SiX	–	343.5	302.2	337.7	326.3
(MeY)Me2SiX	OMe	319.4	322.3	274.6	308.8
	NMe_2	336.6[b]	325.4	295.4	322.0
	SMe	332.8	307.3	310.5[b]	318.4
(MeY)2MeSiX	OMe	343.8	365.7[b]	288.0	331.7
	NMe_2	343.5	350.1	289.2	334.1
	SMe	333.8	315.4	309.7	313.8
(MeY)3SiX	OMe	–	417.7[b]	344.5[b]	–
	NMe_2	–	374.8	322.5[b]	–
	SMe	–	329.2[c]	301.7[c]	–

[a] SGO-BP86/BIII//B3LYP/6-31+G(d) results [b] Values from local minimum structure. [c] Optimization started from a conformationally identical model as the local minimum of the corresponding $(MeO)_3SiX$ system.

Table 4. Standard orientation of **1** [HF/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Li	–0.007776	0.042273	0.122865
2	Si	0.202075	–0.047655	2.822707
3	C	1.577620	1.023234	3.682553
4	C	–1.362783	0.464510	3.855276
5	C	0.580031	–1.802746	3.567802
6	H	2.574265	0.774479	3.314699
7	H	1.429466	2.089631	3.505719
8	H	1.589356	0.877473	4.763878
9	H	1.524862	–2.203515	3.197432
10	H	–0.195483	–2.525363	3.310001
11	H	0.646872	–1.778294	4.656750
12	H	–1.197866	0.353457	4.928249
13	H	–1.639118	1.505437	3.680117
14	H	–2.232118	–0.142814	3.599219
15	O	–1.904391	0.237340	–0.686043
16	C	–2.410785	–0.326640	–1.863803
17	H	–2.811881	0.443685	–2.517320
18	H	–1.599924	–0.835981	–2.362849
19	H	–3.198179	–1.041202	–1.639817
20	C	–2.875348	0.908494	0.081535
21	H	–3.299005	1.733092	–0.485052
22	H	–3.669064	0.225749	0.368719
23	H	–2.390750	1.281505	0.969131
24	O	0.605096	–1.664703	–0.858297
25	C	–0.001023	–2.840627	–0.378348
26	H	0.089509	–3.635765	–1.113265
27	H	0.452918	–3.152100	0.554991
28	H	–1.045178	–2.626247	–0.206592
29	C	1.984346	–1.807200	–1.084538
30	H	2.167937	–2.580079	–1.825621
31	H	2.355855	–0.862259	–1.450137
32	H	2.498141	–2.063007	–0.163552
33	O	1.043868	1.506023	–0.881087
34	C	1.794875	2.445103	–0.147463
35	H	2.745650	2.630606	–0.639145
36	H	1.249515	3.380074	–0.058850
37	H	1.962277	2.033642	0.833964

38	C	0.750932	1.918293	–2.186706
39	H	1.664295	2.130957	–2.735600
40	H	0.221295	1.115904	–2.678351
41	H	0.127511	2.808080	–2.179899

Total Energy of **1** [HF/6-31+G(d)]: E(RHF) = –877.476378165 Hartree
Corrected Zero Point Energy: –877.095789 Hartree

Table 5. Standard orientation of **1** [B3LYP/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Li	–0.041438	0.043312	0.106869
2	Si	0.222944	–0.027053	2.749627
3	C	1.571119	1.085689	3.611166
4	C	–1.335795	0.401148	3.838844
5	C	0.695801	–1.775771	3.469570
6	H	2.580441	0.881887	3.222585
7	H	1.374778	2.158104	3.459732
8	H	1.600944	0.913183	4.699214
9	H	1.661222	–2.127890	3.075897
10	H	–0.055385	–2.539164	3.216606
11	H	0.780618	–1.754348	4.568268
12	H	–1.126664	0.273240	4.913308
13	H	–1.660606	1.442910	3.694657
14	H	–2.193967	–0.243446	3.595770
15	O	–1.926218	0.292312	–0.608083
16	C	–2.415849	0.045853	–1.918996
17	H	–3.339651	–0.549623	–1.883236
18	H	–2.620725	0.989575	–2.445824
19	H	–1.644976	–0.514349	–2.453048
20	C	–2.866638	0.979346	0.221117
21	H	–3.795005	0.397533	0.306386
22	H	–2.402080	1.080472	1.203007
23	H	–3.093496	1.970496	–0.196997
24	O	0.440283	–1.697624	–0.840450
25	C	–0.330861	–2.816860	–0.398120
26	H	–0.224662	–3.652905	–1.104057
27	H	–0.014150	–3.131689	0.603915
28	H	–1.372921	–2.494088	–0.360906
29	C	1.836060	–1.993754	–0.888306
30	H	2.028215	–2.809099	–1.600143
31	H	2.344890	–1.086485	–1.218458
32	H	2.204487	–2.277171	0.106338
33	O	1.139532	1.370739	–0.895111
34	C	1.824328	2.374401	–0.140436
35	H	1.311969	3.342065	–0.236944
36	H	1.807464	2.048987	0.900235
37	H	2.860720	2.472659	–0.493276
38	C	1.061292	1.677667	–2.280269
39	H	0.484536	2.599305	–2.446204
40	H	2.066174	1.802935	–2.708932
41	H	0.561164	0.840343	–2.772044

Total Energy of **1** [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –881.933944578 Hartree
Corrected Zero Point Energy: –881.577469 Hartree

Table 6. Standard orientation of **1** [MP2/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Li	–0.440571	0.055742	–0.052224
2	Si	2.162504	0.053813	0.106026
3	C	3.112294	1.677883	–0.351563
4	C	2.974785	–0.353063	1.816380
5	C	3.083060	–1.221737	–1.024899
6	H	2.887384	2.012316	–1.373783
7	H	2.859339	2.504902	0.326490
8	H	4.200434	1.526118	–0.287444
9	H	2.862544	–1.063614	–2.089845
10	H	2.804476	–2.256830	–0.782868
11	H	4.173627	–1.139556	–0.901066
12	H	4.072521	–0.358372	1.737891
13	H	2.707018	0.386056	2.584443
14	H	2.668013	–1.339501	2.190984
15	O	–1.498157	–0.616829	1.511504
16	C	–2.725752	–1.344672	1.507702
17	H	–2.554757	–2.387661	1.804238
18	H	–3.444955	–0.888498	2.200047
19	H	–3.110595	–1.310247	0.488323
20	C	–0.844641	–0.675452	2.787601
21	H	–0.631408	–1.717844	3.053490
22	H	0.090740	–0.127154	2.684899
23	H	–1.480308	–0.220308	3.557344
24	O	–1.276108	–1.113554	–1.460502
25	C	–0.753788	–2.447770	–1.361983
26	H	–1.298760	–3.113794	–2.042550
27	H	0.315131	–2.455353	–1.599202
28	H	–0.899231	–2.767796	–0.329833
29	C	–1.062048	–0.576216	–2.774177
30	H	–1.582846	–1.190157	–3.519256
31	H	–1.466168	0.435621	–2.768745
32	H	0.010360	–0.544853	–2.999453
33	O	–1.368589	1.771751	–0.509612
34	C	–0.687424	2.975740	–0.128027
35	H	–0.830246	3.169751	0.942555
36	H	0.368920	2.813834	–0.336191
37	H	–1.072298	3.821722	–0.710408
38	C	–2.773992	1.857622	–0.274934
39	H	–2.981556	1.956592	0.798083
40	H	–3.199327	2.715510	–0.810619
41	H	–3.213504	0.933546	–0.652952

Total Energy of **1** [MP2/6-31+G(d)]: EUMP2 = –879.33428849995 Hartree
Corrected Zero Point Energy: Could not be determined, but molecule has same conformation as results from B3LYP and HF calculations.

Table 7. Standard orientation of **2** [HF/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	0.000462	–0.000363	0.346411
2	Li	0.000806	–0.003593	2.904522
3	C	–1.260088	–1.218528	–0.445509
4	C	–0.425430	1.701550	–0.442337
5	C	1.685889	–0.481230	–0.446102
6	H	–1.218809	–1.177300	–1.534424
7	H	–2.282541	–0.988558	–0.150089
8	H	–1.064024	–2.248451	–0.151599

9	H	0.285440	2.471523	–0.146735
10	H	–1.414961	2.046372	–0.146558
11	H	–0.411845	1.646812	–1.531354
12	H	1.629688	–0.463816	–1.534988
13	H	1.997882	–1.482311	–0.152730
14	H	2.479770	0.202886	–0.150642

Total Energy of **2** [HF/6-31+G(d)]: E(RHF) = –415.206817458 Hartree
Corrected Zero Point Energy: –415.088860 Hartree

Table 8. Standard orientation of **2** [B3LYP/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	–0.000007	–0.000474	0.344877
2	Li	–0.004215	–0.003259	2.862381
3	C	–1.263310	–1.223610	–0.443852
4	C	–0.428278	1.706558	–0.440718
5	C	1.692845	–0.481413	–0.440634
6	H	–1.224347	–1.182609	–1.543445
7	H	–2.293164	–0.990288	–0.141163
8	H	–1.062408	–2.261258	–0.144666
9	H	0.303507	2.475384	–0.157665
10	H	–1.416521	2.063068	–0.120115
11	H	–0.438175	1.648063	–1.540195
12	H	1.644097	–0.455838	–1.540304
13	H	2.000343	–1.494355	–0.147329
14	H	2.491873	0.205025	–0.129306

Total Energy of **2** [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –416.770643918 Hartree
Corrected Zero Point Energy: –416.659456 Hartree

Table 9. Standard orientation of **2** [MP2/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	0.000323	0.000300	0.351070
2	Li	0.003301	0.001688	2.891888
3	C	1.581885	–0.731181	–0.446621
4	C	–1.424718	–1.004987	–0.443493
5	C	–0.158586	1.735218	–0.447317
6	H	1.505419	–0.696353	–1.542752
7	H	1.738253	–1.777404	–0.157386
8	H	2.480265	–0.172281	–0.158133
9	H	–2.408492	–0.616014	–0.154356
10	H	–1.390414	–2.061877	–0.152864
11	H	–1.357071	–0.958449	–1.539767
12	H	–0.152842	1.650886	–1.543404
13	H	0.670045	2.393743	–0.160240
14	H	–1.091068	2.234178	–0.157165

Total Energy of **2** [MP2/6-31+G(d)]: E(UMP2) –415.70363835407 Hartree
Corrected Zero Point Energy: –415.589878 Hartree

Table 10. Standard orientation of **3** [HF/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z

1	Si	0.001422	–0.000631	0.515281
2	C	–1.233907	–1.193400	–0.439269
3	C	–0.416120	1.666605	–0.436499
4	C	1.651601	–0.471506	–0.441326
5	H	–1.144948	–1.105094	–1.527838
6	H	–2.270970	–0.977686	–0.175650
7	H	–1.052359	–2.237640	–0.178264
8	H	0.290235	2.456298	–0.173853
9	H	–1.410408	2.031663	–0.172609
10	H	–0.386923	1.546515	–1.525269
11	H	1.530128	–0.435643	–1.529742
12	H	1.983317	–1.478245	–0.180606
13	H	2.465385	0.207016	–0.178869

Total Energy of **3** [HF/6-31+G(d)]: E(RHF) = –407.733331726 Hartree
Corrected Zero Point Energy: –407.619049 Hartree

Table 11. Standard orientation of **3** [B3LYP/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	0.002324	–0.000918	0.533064
2	C	–1.233417	–1.192277	–0.436003
3	C	–0.415612	1.664697	–0.434943
4	C	1.650891	–0.470825	–0.439742
5	H	–1.135329	–1.093920	–1.535123
6	H	–2.280317	–0.973802	–0.172962
7	H	–1.050974	–2.247022	–0.176944
8	H	0.294640	2.464298	–0.172192
9	H	–1.421399	2.031483	–0.176627
10	H	–0.378706	1.529942	–1.533969
11	H	1.516148	–0.425812	–1.538471
12	H	1.984224	–1.489092	–0.184970
13	H	2.473983	0.211501	–0.175634

Total Energy of **3** [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –409.248441736 Hartree
Corrected Zero Point Energy: –409.141115 Hartree

Table 12. Standard orientation of **3** [MP2/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	–0.000597	0.000817	–0.679879
2	C	–1.532347	–0.731936	0.287137
3	C	1.400235	–0.961563	0.284384
4	C	0.132852	1.692392	0.289185
5	H	–1.382938	–0.661600	1.379981
6	H	–1.695592	–1.789292	0.035360
7	H	–2.457771	–0.194379	0.036861
8	H	2.397117	–0.572324	0.033818
9	H	1.398701	–2.031031	0.030950
10	H	1.264436	–0.870726	1.377491
11	H	0.121836	1.526295	1.381827
12	H	–0.702122	2.362455	0.040418
13	H	1.060255	2.225795	0.037361

Total Energy of **3** [MP2/6-31+G(d)]: E(UMP2) = –408.22999184777 Hartree
Corrected Zero Point Energy: – -408.120105 Hartree

Table 13. Standard orientation of **4**·3 THF [B3LYP/TZVP]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	5.64196474886706	3.10977594152814	5.30733089982488
2	C	4.35484254969822	1.32579554820701	3.86247843515848
3	C	4.02186311433392	1.59734569113013	1.24011481708417
4	C	5.06169763249479	3.78324885546995	0.14981947587394
5	C	6.35708968444834	5.58151477276480	1.57252341078541
6	C	6.65090362323161	5.25853397138657	4.16770904449721
7	Si	1.87022056764295	–0.68301125244410	–0.68911571851852
8	C	3.06200248906867	–4.00207779383787	0.46546411228460
9	C	1.42942168612001	–6.08075215972531	0.24537510061757
10	C	2.14073221508473	–8.51883314729119	0.94036091495460
11	C	4.54720745091577	–8.95558262946068	1.90792187681082
12	C	6.21347560045551	–6.93499883464966	2.15826411263421
13	C	5.47408123284833	–4.50944473964300	1.44730152170928
14	N	3.09806457287243	–0.31675645337647	–3.86509755029632
15	C	5.73622268836544	–0.90134442086548	–4.44487720492846
16	C	6.92718837866626	0.76035252772146	–6.49859734706233
17	C	1.36631050054430	–0.47483201896290	–5.99615594616484
18	C	1.05040831873394	–3.10161140816892	–7.19647319071084
19	Li	–2.92694299113344	0.74329441480377	0.33255291154660
20	O	–5.97053852972725	–0.46707202153352	–1.65838204517784
21	C	–6.00545694741867	–2.36171843591853	–3.62807833153502
22	C	–8.67588218304294	–3.44009244812377	–3.58727045022032
23	C	–10.25072223996194	–1.10152086106870	–2.90485488369016
24	C	–8.52799164338040	0.30191418219614	–1.05054584719613
25	O	–3.29463746945033	4.56476829502673	0.00663458559962
26	C	–3.47553560176654	5.58510350470154	–2.52141318975899
27	C	–1.37978426154663	7.55027752179377	–2.71182277012941
28	C	–1.31392297727788	8.61973571094504	–0.01673757648185
29	C	–1.84844504516333	6.28165646185305	1.59642363072632
30	O	–4.00005989383809	–0.30640361230380	3.89143717275141
31	C	–4.36315390095728	–2.98296630501671	4.33553398166950
32	C	–2.99138650775947	–3.56079495663500	6.80275483415444
33	C	–3.30347437237445	–1.07665723911242	8.26725674555563
34	C	–3.08151585072320	0.90147929547056	6.17385588429095
35	H	–0.31267057457698	–3.03061969893785	–8.75262590586341
36	H	2.82847134805834	–3.81340872868304	–7.96583944920369
37	H	–9.21121101000826	–4.28184707639570	–5.38998135730236
38	H	6.07015106075342	0.45466938170686	–8.35190373036052
39	H	–10.59312871199391	0.04397907675073	–4.58858206031101
40	H	0.38524232235353	–4.47198495500501	–5.80186806073283
41	H	1.92610181917009	0.85901757477541	–7.48734358110676
42	H	–5.58218298388303	–1.46116846841634	–5.44310920343361
43	H	8.94107584648761	0.32915415235940	–6.67290907965277
44	H	5.99106894960855	–2.89682215689592	–4.98192945381095
45	H	–0.48228063400794	0.16308721633114	–5.32488337796340
46	H	–8.84749448940717	–4.88694216388356	–2.12327513639541
47	H	–12.07709225563995	–1.56587298350207	–2.07143346680550
48	H	6.73550142547260	2.76333205858899	–6.03312844681982
49	H	–4.52274992192286	–3.72713294638777	–3.21469692063842
50	H	–8.65263708188437	2.35386730285157	–1.21195927410068
51	H	–3.27431854656636	4.02571406770544	–3.85253738342789
52	H	6.82349031004341	–0.65236898308515	–2.71022092386684
53	H	–8.90149748339132	–0.22479928026308	0.91108573760267
54	H	–5.34595524094041	6.44334951988416	–2.76588268832272
55	H	0.82071616927066	–10.07474768051975	0.73264646229603
56	H	–0.46012487026362	–5.78273497569132	–0.50581865425534
57	H	0.40938847405092	6.63041222743601	–3.16793265147817

58	H	5.11737185015585	–10.84486133274074	2.45951206189753
59	H	–1.76975752820961	8.97910978559995	–4.14499817266594
60	H	4.85933369244316	4.06204373109020	–1.87180348322758
61	H	8.09782846423232	–7.25042413264544	2.90400270369426
62	H	–3.60043167611625	–4.00950796614689	2.72122064420609
63	H	6.81369973111351	–2.97452759452969	1.67268848545892
64	H	–6.39446214142161	–3.35628076814094	4.48524752768344
65	H	0.49458482760471	9.47989590633881	0.46419824655752
66	H	–2.79310990847241	10.04025739429020	0.23319867868302
67	H	7.15760654566830	7.23069818332464	0.65171711298535
68	H	–0.99959930556411	–3.94751004470313	6.42996275634065
69	H	–3.79381637781196	–5.18724085540479	7.78119540013616
70	H	–0.10508791402210	5.32620883767008	2.14717593596362
71	H	–2.96766937592962	6.69792578464255	3.27870934091875
72	H	3.61613627201651	–0.34396409546406	4.80082275794027
73	H	–1.11904689470309	1.46772522106248	5.86707426890433
74	H	–4.22385180725744	2.58447490427004	6.51418933190621
75	H	–5.16531895191535	–0.99099669368076	9.15781720534341
76	H	7.66457186348995	6.64712260781820	5.28196686753014
77	H	–1.87934339155771	–0.81538555080023	9.73313138794033
78	H	5.87740077534272	2.81644320910369	7.32367557245343

Total Energy of **4**·3 THF [B3LYP/TZVP]: E(SCF) = –1670.4880514110 Hartree

Table 14. Standard orientation of **5**·3 THF [B3LYP/TZVP]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	H	–3.369322	–0.229269	–4.054623
2	H	–4.783438	0.419387	–3.229079
3	H	0.537682	3.709238	–3.664387
4	H	–1.315185	–0.919646	–3.602877
5	C	–3.697490	0.305781	–3.160010
6	H	–0.861595	–3.329218	–3.405080
7	H	–3.250679	1.302777	–3.180596
8	H	1.177060	1.361835	–3.547341
9	H	–2.515756	–3.035115	–2.875403
10	H	2.958487	3.490279	–3.419446
11	H	3.740962	–3.466199	–2.786037
12	H	2.056690	–2.960971	–2.870657
13	C	–1.468157	–2.836342	–2.637264
14	C	0.912197	3.348433	–2.705754
15	C	–1.162735	–1.329754	–2.594840
16	H	2.906866	–0.733299	–2.592958
17	H	–3.821489	–1.419462	–1.886661
18	H	–0.095182	–1.208385	–2.376259
19	C	0.879010	1.830183	–2.602017
20	C	2.953082	–2.929846	–2.253758
21	H	–0.073038	1.410664	–2.280968
22	H	0.309415	3.792095	–1.910209
23	C	–3.328253	–0.434341	–1.866491
24	C	2.402196	3.645964	–2.490481
25	H	4.465873	–1.362756	–2.021357
26	H	–1.250629	–3.303341	–1.673960
27	C	3.376932	–1.479178	–1.957337
28	H	2.595020	4.663383	–2.149754
29	N	–1.894208	–0.547247	–1.607436
30	H	3.815046	2.220449	–1.579715
31	H	–3.775734	0.105186	–1.030469
32	O	1.866914	1.504810	–1.588955

33	C	2.800529	2.602116	–1.442991
34	H	–2.151595	2.220108	–1.211795
35	C	2.676361	–3.537928	–0.853147
36	H	3.206389	–4.475743	–0.687565
37	H	–3.740281	–3.043621	–0.183649
38	H	1.610204	–3.723904	–0.722376
39	H	–3.060008	4.331422	–0.345991
40	O	2.960581	–1.213224	–0.606050
41	H	2.704442	2.991238	–0.426070
42	C	–2.336525	2.315696	–0.147099
43	Si	–1.137656	–0.369508	0.047611
44	H	–4.897916	–3.080950	1.155876
45	C	–3.833154	–3.055178	0.904002
46	Li	1.505111	0.153388	–0.128438
47	C	3.139890	–2.443894	0.112474
48	C	–2.850392	3.515549	0.338770
49	H	–3.389833	–3.985264	1.268768
50	H	4.200278	–2.559556	0.370414
51	C	–2.064932	1.220702	0.690817
52	H	–1.149033	–3.661160	1.233581
53	H	–3.714511	–0.928833	1.199083
54	H	2.555024	–2.380526	1.028738
55	N	–1.759860	–1.621054	1.208542
56	C	–3.172039	–1.816112	1.526587
57	H	0.120398	–2.454489	1.275785
58	C	–0.877193	–2.681407	1.663613
59	C	–3.107985	3.666966	1.698906
60	H	–3.511856	4.597114	2.082072
61	H	4.236253	0.204018	1.426930
62	O	2.299919	0.857725	1.587957
63	C	–2.335753	1.406588	2.056985
64	H	4.063796	1.959975	1.593097
65	H	–3.323315	–1.861906	2.616110
66	C	3.692823	0.993489	1.946215
67	C	–2.846487	2.602959	2.557440
68	H	–2.152108	0.585763	2.743301
69	C	–0.784363	–2.843157	3.187476
70	H	0.545831	0.549064	2.602166
71	H	–0.064303	–3.626156	3.447932
72	H	–1.742331	–3.126009	3.629925
73	C	1.499475	1.041900	2.776104
74	H	–3.049651	2.700882	3.619088
75	H	–0.465454	–1.908445	3.657185
76	H	1.320414	2.111974	2.935975
77	C	3.768407	0.879983	3.483738
78	H	4.534608	0.174469	3.806732
79	H	2.259104	–0.647368	3.874432
80	C	2.349231	0.441118	3.886802
81	H	4.006269	1.849770	3.926205
82	H	2.061105	0.795319	4.876845

Total Energy of **5**·3 THF [B3LYP/TZVP]: E(SCF) = –1652.0497768721Hartree

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Table 15. Standard orientation of **6**·3 THF [B3LYP/TZVP]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	H	0.137381	5.661974	–1.373385
2	H	1.571057	5.305249	0.626518
3	C	0.516452	4.673938	–1.139942

4	C	1.323929	4.472064	–0.021664
5	H	–0.392468	3.733462	–2.845587
6	H	–3.461210	4.944556	1.536137
7	C	0.218292	3.590734	–1.960716
8	H	–1.107422	4.338836	1.770629
9	H	6.293822	2.149475	–1.230358
10	C	1.816034	3.205747	0.274356
11	C	–3.237230	3.924782	1.847696
12	H	3.877597	2.437028	–1.302986
13	H	–3.966792	3.631781	2.608209
14	H	2.447129	3.057120	1.141993
15	C	–1.805202	3.755941	2.374167
16	H	–1.693586	4.058354	3.415860
17	C	0.721739	2.325220	–1.672376
18	H	–2.853570	3.398824	–0.229579
19	C	5.662781	1.413541	–0.744185
20	C	4.284154	1.581049	–0.782518
21	C	1.523290	2.105527	–0.545722
22	C	–3.258375	2.942919	0.680105
23	H	0.512300	1.492415	–2.330802
24	H	–4.434240	1.035808	–4.231512
25	H	–0.519934	2.030767	1.912659
26	H	–4.248405	2.536851	0.466521
27	H	7.308521	0.187629	–0.079133
28	H	–1.719902	0.826045	–3.549855
29	C	–1.549316	2.262913	2.179497
30	H	–4.438933	1.587930	–1.937111
31	C	6.233427	0.316516	–0.107413
32	O	–2.404088	1.849283	1.077394
33	H	–2.948670	–0.730105	–4.976800
34	C	3.414444	0.654124	–0.171404
35	C	–4.426564	0.146554	–3.597092
36	N	2.009863	0.805932	–0.233237
37	H	–1.828634	1.678953	3.060520
38	C	–4.203433	0.538194	–2.126966
39	C	–2.122017	–0.070246	–3.065308
40	C	–3.201742	–0.723081	–3.916626
41	O	–2.802433	0.309636	–1.846406
42	H	–5.372092	–0.376252	–3.743594
43	C	5.386050	–0.615716	0.484190
44	H	2.753919	–0.791493	–2.287136
45	H	1.385929	0.698208	2.647645
46	H	–1.297115	–0.726208	–2.791091
47	C	4.006690	–0.457022	0.454407
48	H	–4.782544	–0.078941	–1.436276
49	Li	–1.915903	0.222071	–0.029530
50	H	–3.360486	–1.755393	–3.595864
51	H	5.800191	–1.485747	0.983465
52	Si	0.708639	–0.507910	–0.000515
53	H	3.161784	–2.479235	–4.012049
54	C	2.164804	–1.700062	–2.276646
55	H	3.380254	–1.200284	0.922722
56	C	1.293078	–0.365684	2.842556
57	H	1.584337	–0.102360	4.954923
58	C	2.400444	–2.658678	–3.260034
59	C	1.200930	–1.887782	–1.272186
60	C	1.410329	–0.813835	4.154261
61	C	1.089750	–1.245788	1.764551
62	O	–3.070659	–1.213129	0.869211
63	H	–3.532425	–0.438941	2.723981
64	H	–2.055787	–1.432315	2.669724
65	C	–3.086227	–1.344976	2.313973

66	H	–4.424124	–2.333488	–0.227576
67	C	1.678445	–3.848528	–3.273291
68	C	0.469148	–3.087951	–1.329361
69	C	–3.451571	–2.467566	0.256311
70	H	–2.711924	–2.720947	–0.505129
71	C	1.314277	–2.173846	4.442081
72	H	1.868339	–4.599649	–4.031362
73	C	1.011978	–2.611070	2.083821
74	H	–0.313831	–3.273519	–0.599217
75	C	0.705665	–4.058773	–2.299295
76	H	1.405326	–2.528306	5.462335
77	H	0.891639	–3.342703	1.293235
78	C	1.118618	–3.070340	3.396049
79	C	–3.886663	–2.611344	2.597378
80	H	–4.958567	–2.396034	2.610768
81	C	–3.527335	–3.488968	1.391186
82	H	0.131486	–4.979629	–2.295825
83	H	–3.616400	–3.065207	3.550803
84	H	–4.260905	–4.271199	1.193043
85	H	1.065254	–4.135299	3.598797
86	H	–2.555564	–3.962360	1.545580

Total Energy of **6**·3 THF [B3LYP/TZVP]: E(SCF) = –1975.2595826839

Table 16. Standard orientation of **4** [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	–11.526421	6.758750	–1.175812
2	C	–10.177654	6.397603	–1.372064
3	C	–9.548574	6.914565	–2.520798
4	C	–10.218579	7.737567	–3.432540
5	C	–11.556947	8.073264	–3.212468
6	C	–12.209351	7.580499	–2.077904
7	Si	–9.215235	5.194936	–0.200629
8	N	–9.731321	3.516046	–0.529787
9	C	–11.162399	3.185660	–0.529144
10	C	–11.492920	1.766889	–0.043154
11	C	–9.900922	5.587614	1.551938
12	C	–10.147566	6.911788	1.969948
13	C	–10.518101	7.213768	3.284095
14	C	–10.655234	6.190685	4.227670
15	C	–10.416180	4.868334	3.840984
16	C	–10.041611	4.577764	2.525176
17	C	–8.888419	2.628978	–1.328510
18	C	–9.149327	2.633973	–2.845134
19	Li	–6.745320	5.509336	–0.141865
20	H	–8.974981	1.595785	–0.957597
21	H	–7.844022	2.923813	–1.152308
22	H	–11.613623	3.334763	–1.526049
23	H	–11.663855	3.896709	0.136016
24	H	–9.857075	3.543295	2.241392
25	H	–10.523896	4.062362	4.564555
26	H	–10.947384	6.421074	5.249715
27	H	–10.058511	7.726794	1.253063
28	H	–10.707565	8.246792	3.569617
29	H	–12.580847	1.648455	0.039191
30	H	–11.051953	1.577217	0.942924
31	H	–11.132259	0.993061	–0.730809
32	H	–8.448717	1.959274	–3.356082

33	H	–9.027320	3.641433	–3.260614
34	H	–10.164693	2.296980	–3.084341
35	H	–8.503878	6.665385	–2.713029
36	H	–9.697676	8.117167	–4.309506
37	H	–12.085528	8.713746	–3.914912
38	H	–13.250790	7.837877	–1.894811
39	H	–12.056237	6.398795	–0.296189

Total Energy of **4** [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –973.555479420 Hartree
Corrected Zero Point Energy: –973.232975 Hartree

Table 17. Standard orientation of **5** [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	1.808260	4.171905	1.994596
2	C	1.128415	5.150746	2.727100
3	C	0.846260	6.391435	2.147620
4	C	1.252934	6.639323	0.832460
5	C	1.932667	5.653098	0.111176
6	C	2.224790	4.389748	0.665903
7	Si	3.341281	3.122800	–0.259816
8	N	2.818670	3.299829	–1.964143
9	C	3.751835	2.963609	–3.037927
10	C	3.668695	1.526327	–3.582428
11	N	2.923558	1.548284	0.478455
12	C	1.547551	1.053409	0.575731
13	H	1.346039	0.679954	1.594095
14	C	3.946394	0.605709	0.916252
15	C	4.067178	0.448184	2.442292
16	C	1.407021	3.319606	–2.362247
17	C	1.057325	4.337121	–3.460081
18	Li	5.711741	3.792262	0.068314
19	H	3.631883	3.666924	–3.876923
20	H	4.769162	3.127639	–2.653094
21	H	1.067607	2.322318	–2.694081
22	H	0.813304	3.561065	–1.474839
23	H	2.241704	5.864896	–0.910780
24	H	1.037701	7.600180	0.368455
25	H	0.868831	1.902076	0.435896
26	C	1.171109	–0.050298	–0.428790
27	H	3.782326	–0.389648	0.470927
28	H	4.914432	0.949264	0.524249
29	H	0.315488	7.154634	2.712421
30	H	2.019598	3.212570	2.462627
31	H	0.815208	4.943701	3.748794
32	H	–0.029583	4.359751	–3.611824
33	H	1.384578	5.345133	–3.179051
34	H	1.515532	4.088496	–4.424450
35	H	4.423985	1.370432	–4.365043
36	H	3.841384	0.795681	–2.783686
37	H	2.688734	1.313199	–4.025739
38	H	3.131066	0.095715	2.891029
39	H	4.849419	–0.280911	2.696105
40	H	4.320404	1.407232	2.911554
41	H	0.118722	–0.336634	–0.298400
42	H	1.307732	0.293222	–1.459854
43	H	1.775836	–0.954669	–0.291617

Total Energy of **5** [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –955.114535419 Hartree

Corrected Zero Point Energy: –954.743054 Hartree

Table 18. Standard orientation of **6** [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	0.291754	–3.058599	–1.356082
2	C	1.118622	–1.915566	–1.331620
3	C	2.123632	–1.834146	–2.314592
4	C	2.303116	–2.844812	–3.265690
5	C	1.477091	–3.971664	–3.260458
6	C	0.466907	–4.075519	–2.298197
7	Si	0.729413	–0.502716	–0.098800
8	C	1.083093	–1.202566	1.659826
9	C	1.438921	–2.539358	1.922084
10	C	1.607732	–3.011504	3.228763
11	C	1.434478	–2.150906	4.315594
12	C	1.081680	–0.817207	4.083668
13	C	0.899214	–0.361519	2.775946
14	N	2.015510	0.815528	–0.442635
15	C	1.432916	2.073890	–0.730074
16	C	1.621827	3.192695	0.108425
17	C	0.915016	4.376652	–0.103662
18	C	0.000404	4.491723	–1.160182
19	C	–0.167087	3.410515	–2.031334
20	C	0.553879	2.221513	–1.831152
21	C	3.426806	0.762998	–0.316864
22	C	4.059709	–0.263142	0.411471
23	C	5.450808	–0.330968	0.491442
24	C	6.257854	0.618054	–0.141920
25	C	5.641770	1.636463	–0.873949
26	C	4.251408	1.706460	–0.969274
27	Li	–1.042522	1.187833	–0.548624
28	H	3.462166	–1.006308	0.923427
29	H	5.904088	–1.136339	1.064896
30	H	7.340791	0.561976	–0.071830
31	H	6.244919	2.380476	–1.389880
32	H	3.802050	2.493672	–1.567161
33	H	2.307945	3.106741	0.946051
34	H	1.063582	5.213217	0.574962
35	H	–0.552286	5.414348	–1.313147
36	H	–0.827760	3.498476	–2.891560
37	H	0.478988	1.404956	–2.547044
38	H	1.599019	–3.225474	1.093560
39	H	1.882369	–4.051149	3.395795
40	H	1.569700	–2.514334	5.331646
41	H	0.942794	–0.136628	4.921335
42	H	0.608151	0.677713	2.621273
43	H	2.784116	–0.971322	–2.336390
44	H	3.093639	–2.752660	–4.007774
45	H	1.616569	–4.759383	–3.997260
46	H	–0.185667	–4.946224	–2.284019
47	H	–0.512253	–3.157769	–0.626762

Total Energy of **6** [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –1278.43395930 Hartree
Corrected Zero Point Energy: –1278.062874 Hartree

Table 19. Standard orientation of Me_3SiH [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	–1.717422	–0.524898	–0.224118
2	Si	–0.000453	–0.000649	0.379150
3	C	1.314429	–1.222747	–0.223728
4	H	–0.001347	–0.001279	1.874123
5	C	0.403686	1.748382	–0.223277
6	H	–1.763286	–0.556921	–1.320289
7	H	–2.489522	0.175057	0.119597
8	H	–1.984479	–1.521687	0.149055
9	H	1.386110	2.077244	0.138563
10	H	–0.339884	2.474322	0.129307
11	H	0.420697	1.795981	–1.319533
12	H	1.341205	–1.269110	–1.319834
13	H	1.117517	–2.236549	0.147163
14	H	2.315178	–0.932388	0.120489

Total Energy of Me_3SiH [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –409.871446420 Hartree
Corrected Zero Point Energy: –409.752065 Hartree

Table 20. Standard orientation of Me_3SiCl [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	–0.350999	0.000214	–0.000118
2	Cl	1.764065	0.000611	0.000402
3	C	–0.891590	1.750204	–0.429297
4	C	–0.889517	–1.247467	–1.301369
5	C	–0.891018	–0.504047	1.730110
6	H	–1.986906	1.827475	–0.452219
7	H	–0.512249	2.050150	–1.413005
8	H	–0.518529	2.470214	0.308357
9	H	–0.512924	–2.249667	–1.065905
10	H	–0.511578	–0.971220	–2.292592
11	H	–1.984764	–1.303850	–1.361492
12	H	–1.986390	–0.530244	1.806960
13	H	–0.517373	0.201543	2.481226
14	H	–0.511654	–1.499929	1.986819

Total Energy of Me_3SiCl [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = – 869.529324274 Hartree
Corrected Zero Point Energy: –869.416168 Hartree

Table 21. Standard orientation of Me3SiLi (**2**) [B3LYP/6-31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	–0.000007	–0.000474	0.344877
2	Li	–0.004215	–0.003259	2.862381
3	C	–1.263310	–1.223610	–0.443852
4	C	–0.428278	1.706558	–0.440718
5	C	1.692845	–0.481413	–0.440634
6	H	–1.224347	–1.182609	–1.543445
7	H	–2.293164	–0.990288	–0.141163
8	H	–1.062408	–2.261258	–0.144666
9	H	0.303507	2.475384	–0.157665
10	H	–1.416521	2.063068	–0.120115
11	H	–0.438175	1.648063	–1.540195
12	H	1.644097	–0.455838	–1.540304
13	H	2.000343	–1.494355	–0.147329

14	H	2.491873	0.205025	–0.129306

Total Energy of Me_3SiLi (**2**) [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –416.770643918 Hartree
Corrected Zero Point Energy: –416.659456 Hartree

Table 22. Standard orientation of Me_4Si [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	0.000215	–0.000169	0.000842
2	C	1.123432	–1.344569	0.729441
3	C	0.416991	0.247084	–1.833529
4	C	–1.813604	–0.531382	0.168884
5	C	0.272875	1.629082	0.934300
6	H	0.953868	–1.465384	1.807055
7	H	2.184595	–1.100941	0.587742
8	H	0.941631	–2.318058	0.255177
9	H	–0.186992	1.050233	–2.275909
10	H	0.228760	–0.665334	–2.414658
11	H	1.472849	0.513724	–1.970706
12	H	–1.991180	–1.501761	–0.312356
13	H	–2.488882	0.197468	–0.298056
14	H	–2.108523	–0.626559	1.222329
15	H	–0.332231	2.440323	0.508685
16	H	1.323910	1.943390	0.890598
17	H	0.001013	1.533977	1.993731

Total Energy of Me_4Si [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –449.199687169 Hartree
Corrected Zero Point Energy: –449.051860 Hartree

Table 23. Standard orientation of $(MeO)Me_2SiH$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Si	–0.411388	–0.000481	0.349525
2	C	–1.801134	–1.140071	–0.189393
3	O	0.989471	–0.629958	–0.322620
4	C	–0.702905	1.780054	–0.203479
5	C	2.293796	–0.161797	–0.017318
6	H	–0.263788	–0.010803	1.838647
7	H	–2.762443	–0.815825	0.228974
8	H	–1.615639	–2.167598	0.144202
9	H	–1.895123	–1.153518	–1.282072
10	H	–0.819661	1.844989	–1.292622
11	H	0.125955	2.438307	0.085568
12	H	–1.614891	2.183442	0.256343
13	H	3.014491	–0.840669	–0.484084
14	H	2.475154	–0.150913	1.067557
15	H	2.461079	0.849867	–0.413756

Total Energy of $(MeO)Me_2SiH$ [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –485.117828328 Hartree
Corrected Zero Point Energy: –484.992709 Hartree

Table 24. Standard orientation of $(MeO)Me_2SiCl$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Si	–0.220567	–0.385023	0.009483

2	C	–0.225621	–0.931083	1.804784
3	Cl	–0.927695	1.602197	–0.013668
4	O	1.302117	–0.405210	–0.645746
5	C	–1.297130	–1.416395	–1.113612
6	C	2.433542	0.328550	–0.188688
7	H	–1.242282	–0.910154	2.214786
8	H	0.395100	–0.277466	2.428341
9	H	0.158117	–1.955265	1.894997
10	H	–0.946938	–2.455794	–1.130377
11	H	–1.263536	–1.029638	–2.137921
12	H	–2.340462	–1.409456	–0.778064
13	H	3.270671	0.090564	–0.850795
14	H	2.704006	0.047476	0.837849
15	H	2.242379	1.407962	–0.228166

Total Energy of (MeO)Me_2SiCl [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –944.777827535 Hartree
Corrected Zero Point Energy: –944.658755 Hartree

Table 25. Standard orientation of (MeO)Me_2SiLi [B3LYP/6–31+G(d)]

Center	Atom	Coordinates(Angstroms)		
Number	Type	X	Y	Z
1	Si	0.407947	–0.028849	0.343394
2	C	0.731442	1.761745	–0.276015
3	Li	0.148836	–0.309867	2.840615
4	O	–0.994874	–0.576004	–0.493249
5	C	1.758539	–1.083747	–0.499190
6	C	–2.286273	–0.109779	–0.192713
7	H	1.681344	2.141326	0.127342
8	H	–0.054480	2.461990	0.036611
9	H	0.794159	1.793909	–1.373798
10	H	1.736367	–0.944084	–1.589295
11	H	1.620263	–2.152896	–0.295747
12	H	2.757956	–0.800609	–0.140754
13	H	–3.015582	–0.711236	–0.749332
14	H	–2.423885	0.945871	–0.476796
15	H	–2.517168	–0.202065	0.885911

Total Energy of (MeO)Me_2SiLi [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –492.018232106 Hartree
Corrected Zero Point Energy: –491.901494 Hartree

Table 26. Standard orientation of (MeO)Me_2SiMe [B3LYP/6–31+G(d)]

Center	Atom	Coordinates(Angstroms)		
Number	Type	X	Y	Z
1	Si	0.381353	0.003443	0.004784
2	C	0.571401	1.852381	0.358181
3	O	–1.080878	–0.289995	–0.772211
4	C	1.688571	–0.597066	–1.206345
5	C	–2.361702	–0.078346	–0.202970
6	H	0.472574	–0.961451	1.629208
7	H	1.543473	2.063195	0.823708
8	H	–0.202557	2.219623	1.044323
9	H	0.508890	2.442308	–0.564576
10	H	1.593308	–0.082966	–2.170475
11	H	1.582549	–1.672698	–1.391903
12	H	2.701973	–0.415858	–0.826439
13	H	–3.113242	–0.373314	–0.942620
14	H	–2.523839	0.979381	0.051168

15	H	–2.509522	–0.685061	0.701965
16	H	–0.308706	–0.661941	2.339159
17	H	1.439256	–0.793822	2.122278
18	H	0.371442	–2.040205	1.455669

Total Energy of (MeO)Me_2SiMe [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –524.447046721 Hartree
Corrected Zero Point Energy: –524.293493 Hartree

Table 27. Standard orientation of (Me_2N)Me_2SiH [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	H	0.541239	0.000000	–0.226088
2	Si	0.100635	0.000000	1.211144
3	N	1.460562	0.000000	2.319584
4	C	2.259673	1.206965	2.497346
5	H	3.067048	1.300047	1.747292
6	H	1.633263	2.101686	2.433854
7	H	2.731680	1.204375	3.491082
8	C	–0.937595	1.553419	1.484304
9	C	–0.937595	–1.553419	1.484304
10	C	2.259673	–1.206965	2.497346
11	H	3.067048	–1.300047	1.747292
12	H	2.731680	–1.204375	3.491082
13	H	1.633263	–2.101686	2.433854
14	H	–1.250215	–1.647122	2.531655
15	H	–1.843011	–1.503211	0.865641
16	H	–0.407189	–2.470902	1.203959
17	H	–1.250215	1.647122	2.531655
18	H	–0.407189	2.470902	1.203959
19	H	–1.843011	1.503211	0.865641

Total Energy of (Me_2N)Me_2SiH [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –504.539321387 Hartree
Corrected Zero Point Energy: –504.373829 Hartree

Table 28. Standard orientation of (Me_2N)Me_2SiCl [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Cl	0.511575	–0.808219	0.504189
2	Si	0.080540	0.020579	2.421558
3	N	1.532276	0.407210	3.283503
4	C	2.332234	1.576522	2.925576
5	H	3.111614	1.336365	2.183274
6	H	1.701179	2.368326	2.513024
7	H	2.829923	1.977574	3.819952
8	C	–0.923766	1.570493	2.080064
9	C	–0.900849	–1.299630	3.327752
10	C	2.341969	–0.638397	3.905138
11	H	3.116123	–1.026960	3.222540
12	H	2.846729	–0.239807	4.796624
13	H	1.717370	–1.476949	4.224729
14	H	–1.115543	–0.992005	4.358545
15	H	–1.855495	–1.462991	2.813879
16	H	–0.378460	–2.261811	3.354388
17	H	–1.144197	2.108798	3.010080
18	H	–0.411806	2.255684	1.396082
19	H	–1.875352	1.294655	1.610513

Total Energy of $(Me_2N)Me_2SiCl$ [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –964.201459622 Hartree
Corrected Zero Point Energy: –964.041869 Hartree

Table 29. Standard orientation of $(Me_2N)Me_2SiLi$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Li	1.099637	0.000000	0.246381
2	Si	0.120094	0.000000	2.585325
3	N	1.414331	0.000000	3.847360
4	C	2.234838	1.196295	3.943386
5	H	2.961583	1.295949	3.106083
6	H	1.610079	2.094967	3.952699
7	H	2.818048	1.186716	4.876479
8	C	–0.978045	1.511356	3.026016
9	C	–0.978045	–1.511356	3.026016
10	C	2.234838	–1.196295	3.943386
11	H	2.961583	–1.295949	3.106083
12	H	2.818048	–1.186716	4.876479
13	H	1.610079	–2.094967	3.952699
14	H	–1.261550	–1.494254	4.088448
15	H	–1.900656	–1.477906	2.430129
16	H	–0.496458	–2.474511	2.817329
17	H	–1.261550	1.494254	4.088448
18	H	–0.496458	2.474511	2.817329
19	H	–1.900656	1.477906	2.430129

Total Energy of $(Me_2N)Me_2SiLi$ [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –511.439508474 Hartree
Corrected Zero Point Energy: –511.282287 Hartree

Table 30. Standard orientation of $(Me_2N)Me_2SiMe$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	C	0.117911	0.032102	0.024453
2	Si	0.046258	0.083086	1.914773
3	N	1.690499	0.148976	2.534817
4	C	2.659694	1.084059	1.979120
5	H	3.676952	0.670464	2.057117
6	H	2.460941	1.267829	0.918819
7	H	2.661113	2.059871	2.499994
8	C	–1.008362	1.576041	2.436562
9	C	–0.778685	–1.489945	2.566887
10	C	1.986586	–0.174641	3.924014
11	H	3.001249	–0.593175	4.009327
12	H	1.938487	0.707172	4.590185
13	H	1.289083	–0.925518	4.307043
14	H	–0.971763	–1.450194	3.645818
15	H	–1.748945	–1.631316	2.072803
16	H	–0.168835	–2.378922	2.364624
17	H	–1.098611	1.641920	3.528801
18	H	–0.572558	2.520502	2.085148
19	H	–2.025253	1.511166	2.025960
20	H	–0.887317	–0.141980	–0.381568
21	H	0.480941	0.970302	–0.412680
22	H	0.766680	–0.778365	–0.329594

Total Energy of $(Me_2N)Me_2SiMe$ [B3LYP/6-31+G(d)]: E(RB+HF-LYP) = –543.867432669 Hartree
Corrected Zero Point Energy: –-543.673640 Hartree

Table 31. Standard orientation of (MeS)Me_2SiH [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Si	–0.717575	0.101679	0.384120
2	C	–2.085405	–1.133499	–0.013989
3	S	1.118628	–0.771218	–0.365076
4	C	–1.068957	1.794198	–0.378412
5	C	2.378568	0.414488	0.275828
6	H	–0.582190	0.270512	1.861652
7	H	–3.052713	–0.761887	0.347080
8	H	–1.897273	–2.102756	0.461226
9	H	–2.171304	–1.296646	–1.094995
10	H	–1.186329	1.719544	–1.466056
11	H	–0.262771	2.508978	–0.175036
12	H	–1.994470	2.215238	0.036671
13	H	3.358019	–0.008893	0.040050
14	H	2.297844	0.529638	1.360555
15	H	2.293955	1.391133	–0.208166

Total Energy of (MeS)Me_2SiH [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –808.080125569 Hartree
Corrected Zero Point Energy: –807.957779 Hartree

Table 32. Standard orientation of (MeS)Me_2SiCl [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Si	–0.484416	–0.342313	0.122055
2	C	–0.608433	–0.433859	1.995934
3	Cl	–1.182934	1.575881	–0.412017
4	S	1.524223	–0.620319	–0.593186
5	C	–1.543606	–1.618211	–0.755043
6	C	2.446495	0.718793	0.279564
7	H	–1.645772	–0.279584	2.316780
8	H	0.006569	0.331212	2.482361
9	H	–0.277674	–1.417311	2.351201
10	H	–1.222636	–2.634519	–0.496149
11	H	–1.479972	–1.504052	–1.842482
12	H	–2.594276	–1.505515	–0.462506
13	H	3.470803	0.683969	–0.098623
14	H	2.462856	0.555017	1.359831
15	H	2.017502	1.697958	0.053338

Total Energy of (MeS)Me_2SiCl [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1267.73629432 Hartree
Corrected Zero Point Energy: –1267.620146 Hartree

Table 33. Standard orientation of (MeS)Me_2SiLi [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Si	0.736751	0.141603	0.400322
2	C	1.103072	1.691141	–0.675130
3	Li	0.359271	0.316206	2.856063
4	S	–1.123077	–0.770466	–0.424643
5	C	2.019642	–1.161082	–0.188918
6	C	–2.416616	0.416711	0.121083
7	H	2.071578	2.128463	–0.392219

8	H	0.343888	2.472926	–0.545852
9	H	1.143534	1.432287	–1.742141
10	H	1.985183	–1.295231	–1.278929
11	H	1.855696	–2.140694	0.276515
12	H	3.034717	–0.833506	0.074247
13	H	–3.389817	–0.008562	–0.140360
14	H	–2.314611	1.384385	–0.379394
15	H	–2.389836	0.575700	1.207510

Total Energy of (MeS)Me_2SiLi [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –814.987736155 Hartree
Corrected Zero Point Energy: –814.873624 Hartree

Table 34. Standard orientation of (MeS)Me_2SiMe [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Si	–0.663793	–0.058311	–0.000033
2	C	–0.873680	–1.131786	–1.544955
3	S	1.279109	0.920552	0.000120
4	C	–1.905419	1.364175	–0.001486
5	C	2.448581	–0.505814	0.000097
6	C	–0.875105	–1.129649	1.546204
7	H	–1.872498	–1.588454	–1.563085
8	H	–0.141215	–1.947535	–1.580221
9	H	–0.757067	–0.536418	–2.458081
10	H	–1.785468	1.999363	–0.887045
11	H	–1.789434	1.997698	0.885793
12	H	–2.932378	0.976069	–0.004148
13	H	3.456895	–0.084372	–0.000462
14	H	2.328805	–1.123207	–0.894301
15	H	2.329525	–1.122623	0.895001
16	H	–0.146180	–1.948608	1.580537
17	H	–1.875909	–1.581855	1.566783
18	H	–0.753978	–0.534090	2.458613

Total Energy of (MeS)Me_2SiMe [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –847.408992169 Hartree
Corrected Zero Point Energy: –847.257879 Hartree

Table 35. Standard orientation of $(MeO)_2$MeSiH [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	H	0.368744	0.795206	1.857142
2	Si	–0.038649	0.499833	0.461455
3	O	1.313513	0.229235	–0.474313
4	O	–0.976595	–0.868564	0.619446
5	C	–0.948717	1.906021	–0.373893
6	H	–1.178868	1.670152	–1.419867
7	H	–1.889815	2.131154	0.142188
8	H	–0.332687	2.813220	–0.369986
9	C	–1.671046	–1.510545	–0.443280
10	H	–2.175846	–2.389241	–0.030597
11	H	–2.427633	–0.847210	–0.884134
12	H	–0.982197	–1.837371	–1.233519
13	C	2.368838	–0.655770	–0.114940
14	H	3.194709	–0.494626	–0.814489
15	H	2.727395	–0.459231	0.905121
16	H	2.047475	–1.703328	–0.180613

Total Energy of $(MeO)_2MeSiH$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –560.368241937 Hartree
Corrected Zero Point Energy: –560.237022 Hartree

Table 36. Standard orientation of $(MeO)_2MeSiCl$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Cl	–1.772678	–0.730186	–0.762009
2	Si	–0.012202	–0.252985	0.240746
3	O	1.143958	–0.362386	–0.938797
4	O	–0.122159	1.273168	0.858678
5	C	0.261804	–1.404056	1.678306
6	H	1.183391	–1.145026	2.213296
7	H	–0.569383	–1.332728	2.387991
8	H	0.337502	–2.442591	1.338125
9	C	–0.452672	2.458802	0.135683
10	H	–0.358522	3.301161	0.826326
11	H	0.226867	2.610209	–0.712015
12	H	–1.483348	2.409920	–0.234597
13	C	2.536945	–0.136368	–0.732638
14	H	3.027091	–0.194739	–1.708324
15	H	2.723308	0.854562	–0.299050
16	H	2.968594	–0.902341	–0.075195

Total Energy of $(MeO)_2MeSiCl$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1020.02484185 Hartree
Corrected Zero Point Energy: –1019.900135 Hartree

Table 37. Standard orientation of $(MeO)_2MeSiLi$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Li	–0.733551	–0.200353	–2.931475
2	Si	–0.278633	–0.412861	–0.490493
3	O	1.350532	–0.471797	0.036590
4	O	–0.926051	1.086410	0.037507
5	C	–1.004340	–1.769291	0.638176
6	H	–0.716598	–1.623310	1.688106
7	H	–2.100859	–1.790695	0.579246
8	H	–0.632600	–2.755374	0.330664
9	C	–0.963551	1.499546	1.396853
10	H	–1.313676	2.538103	1.431421
11	H	–1.656146	0.880819	1.986094
12	H	0.030045	1.449050	1.864296
13	C	2.362014	0.334680	–0.523026
14	H	3.336611	–0.048638	–0.197373
15	H	2.338291	0.317723	–1.627928
16	H	2.273743	1.382698	–0.199178

Total Energy of $(MeO)_2MeSiLi$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –567.272561807 Hartree
Corrected Zero Point Energy: –567.150003 Hartree

Table 38. Standard orientation of $(MeO)_2MeSiMe$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	C	–0.839427	1.486342	–1.329734
2	Si	0.000000	0.464955	0.000000
3	C	0.839437	1.486331	1.329737

4	O	–1.089542	–0.488492	0.836846
5	O	1.089532	–0.488501	–0.836847
6	C	–1.996043	–1.402986	0.234575
7	C	1.996041	–1.402987	–0.234578
8	H	–1.291275	0.847410	–2.097957
9	H	–1.627698	2.120974	–0.906570
10	H	–0.113567	2.137083	–1.832293
11	H	0.113587	2.137098	1.832279
12	H	1.627732	2.120936	0.906580
13	H	1.291253	0.847393	2.097974
14	H	–1.473564	–2.133876	–0.397475
15	H	–2.514999	–1.938859	1.035650
16	H	–2.744534	–0.879529	–0.376166
17	H	1.473568	–2.133883	0.397471
18	H	2.515001	–1.938856	–1.035653
19	H	2.744528	–0.879525	0.376165

Total Energy of $(MeO)_2MeSiMe$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –599.699256846 Hartree
Corrected Zero Point Energy: –599.539601 Hartree

Table 39. Standard orientation of $(Me_2N)_2MeSiH$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	H	0.241456	0.414451	–0.263038
2	Si	0.151170	0.264934	1.212570
3	N	1.827094	0.142019	1.708170
4	C	2.877119	0.872497	1.011505
5	H	3.793452	0.264512	0.950351
6	H	2.565725	1.108694	–0.011247
7	H	3.142203	1.818987	1.516217
8	N	–0.804726	1.638362	1.729304
9	C	–1.480701	1.706656	3.016571
10	H	–2.443754	2.231708	2.917866
11	H	–1.691164	0.703572	3.400063
12	H	–0.889169	2.245811	3.778526
13	C	–0.749344	–1.304747	1.740169
14	C	2.223772	–0.245424	3.054462
15	H	3.134845	–0.863412	3.025522
16	H	2.436897	0.626173	3.699093
17	H	1.440713	–0.837887	3.538389
18	C	–0.572742	2.955980	1.153225
19	H	–1.523570	3.500137	1.041070
20	H	0.094578	3.580212	1.774260
21	H	–0.123115	2.865951	0.158324
22	H	–0.758817	–1.464651	2.824684
23	H	–1.791607	–1.278352	1.401232
24	H	–0.263793	–2.176777	1.286640

Total Energy of $(Me_2N)_2MeSiH$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –599.211549221 Hartree
Corrected Zero Point Energy: –598.999625 Hartree

Table 40. Standard orientation of $(Me_2N)_2MeSiCl$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Cl	–0.267677	2.032671	–0.809789
2	Si	0.017023	0.260864	0.325151
3	C	0.189152	0.850570	2.101497

4	H	0.392780	0.015114	2.783017
5	H	0.979104	1.600085	2.222818
6	H	–0.753766	1.315103	2.413685
7	N	1.431828	–0.596996	–0.163240
8	C	2.741620	–0.388725	0.444426
9	C	1.523653	–1.186546	–1.497020
10	N	–1.354632	–0.738436	–0.018557
11	C	–1.350670	–2.145635	0.375382
12	C	–2.695944	–0.254069	–0.323582
13	H	2.092190	–0.543162	–2.188092
14	H	2.030530	–2.161855	–1.448351
15	H	0.525606	–1.339999	–1.915935
16	H	3.363137	0.309696	–0.140521
17	H	2.645816	0.007813	1.458248
18	H	3.283811	–1.343715	0.509656
19	H	–3.142896	–0.858985	–1.127040
20	H	–3.363437	–0.318834	0.552547
21	H	–2.669045	0.783690	–0.661085
22	H	–1.769886	–2.769044	–0.429351
23	H	–0.331732	–2.489636	0.572685
24	H	–1.957275	–2.319327	1.280383

Total Energy of $(Me_2N)_2MeSiCl$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1058.87203060 Hartree
Corrected Zero Point Energy: –1058.666209 Hartree

Table 41. Standard orientation of $(Me_2N)_2MeSiLi$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Li	0.345080	–0.396793	0.286899
2	Si	–0.035910	–0.024830	2.754407
3	N	1.477203	0.390285	3.640833
4	C	2.180625	1.587421	3.211228
5	H	2.798616	1.423755	2.300569
6	H	1.465607	2.387233	2.994907
7	H	2.860553	1.940822	4.001829
8	N	–1.062385	1.390958	3.069239
9	C	–2.007709	1.925999	2.113872
10	H	–2.006552	3.030242	2.126281
11	H	–1.746858	1.603272	1.097448
12	H	–3.048883	1.602297	2.307816
13	C	–0.727959	–1.513173	3.757510
14	C	2.406345	–0.671880	3.986046
15	H	3.016444	–1.017583	3.122800
16	H	3.113561	–0.327608	4.756405
17	H	1.874532	–1.538404	4.389397
18	C	–1.335439	1.835792	4.428077
19	H	–1.328330	2.937530	4.489552
20	H	–2.322613	1.495486	4.793981
21	H	–0.565985	1.459010	5.108627
22	H	–0.712687	–1.330274	4.841877
23	H	–1.772523	–1.681530	3.461508
24	H	–0.185191	–2.448054	3.564027

Total Energy of $(Me_2N)_2MeSiLi$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –606.110723692 Hartree
Corrected Zero Point Energy: –605.907958 Hartree

Table 42. Standard orientation of $(Me_2N)_2MeSiMe$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	0.012465	–0.182630	0.251627
2	Si	–0.057691	0.048994	2.130344
3	N	1.504226	0.369505	2.848510
4	C	2.236259	1.581858	2.506369
5	H	3.022905	1.397388	1.752707
6	H	1.552825	2.340019	2.112046
7	H	2.727739	2.003028	3.397933
8	N	–1.044643	1.455325	2.458210
9	C	–2.090090	1.942105	1.571905
10	H	–2.110009	3.043682	1.567845
11	H	–1.918868	1.611225	0.544239
12	H	–3.095672	1.598686	1.876647
13	C	–0.734147	–1.543659	2.901156
14	C	2.361702	–0.650805	3.430495
15	H	3.148815	–0.989357	2.732066
16	H	2.868742	–0.262204	4.328229
17	H	1.780827	–1.526156	3.732581
18	C	–1.202454	1.942745	3.822332
19	H	–1.195865	3.044220	3.843527
20	H	–2.152069	1.610181	4.278934
21	H	–0.377565	1.591476	4.449769
22	H	–0.753365	–1.500703	3.997335
23	H	–1.767610	–1.692475	2.561369
24	H	–0.166477	–2.436330	2.608657
25	H	–0.948232	–0.492486	–0.179269
26	H	0.337541	0.727177	–0.268295
27	H	0.740253	–0.970834	0.017672

Total Energy of $(Me_2N)_2MeSiMe$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –638.539853012 Hartree
Corrected Zero Point Energy: –638.299581 Hartree

Table 43. Standard orientation of $(MeS)_2MeSiH$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	H	–0.335733	0.858699	–1.992011
2	Si	0.026901	0.709011	–0.557513
3	S	–1.716400	0.185200	0.604050
4	S	1.516524	–0.853403	–0.628793
5	C	0.668848	2.319786	0.178379
6	H	0.946137	2.203833	1.232268
7	H	1.553961	2.657913	–0.372600
8	H	–0.096754	3.102222	0.115867
9	C	1.979576	–1.027130	1.149556
10	H	2.616879	–1.911635	1.221756
11	H	2.541389	–0.157402	1.499444
12	H	1.093752	–1.174118	1.773001
13	C	–2.330743	–1.298162	–0.305094
14	H	–3.194217	–1.671492	0.250648
15	H	–2.645491	–1.033700	–1.318067
16	H	–1.564605	–2.076184	–0.346295

Total Energy of $(MeS)_2MeSiH$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1206.29000702 Hartree
Corrected Zero Point Energy: –1206.164488 Hartree

Table 44. Standard orientation of $(MeS)_2MeSiCl$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Cl	–1.363093	–1.672940	–0.769199
2	Si	–0.079600	–0.440497	0.333823
3	S	1.617934	–0.229593	–0.975707
4	S	–1.025971	1.426249	0.810611
5	C	0.312132	–1.271410	1.968443
6	H	1.010905	–0.670928	2.562574
7	H	–0.602565	–1.412728	2.555223
8	H	0.764837	–2.252671	1.788798
9	C	–1.458704	2.085141	–0.857887
10	H	–1.857419	3.089660	–0.698864
11	H	–0.575096	2.141264	–1.497825
12	H	–2.222400	1.462935	–1.329495
13	C	2.718980	0.841825	0.050266
14	H	3.555967	1.122854	–0.593504
15	H	2.199848	1.746640	0.376180
16	H	3.107042	0.300075	0.916390

Total Energy of $(MeS)_2MeSiCl$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1665.94225475 Hartree
Corrected Zero Point Energy: –1665.823279 Hartree

Table 45. Standard orientation of $(MeS)_2MeSiLi$ [B3LYP/6–31+G(d)]

Center Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	Li	0.529438	1.160848	2.882086
2	Si	0.026937	0.806507	0.480266
3	S	1.641503	–0.001378	–0.799337
4	S	–1.542653	–0.735222	0.698823
5	C	–0.658254	2.150954	–0.699824
6	H	–0.917131	1.749384	–1.687601
7	H	–1.561027	2.601584	–0.269352
8	H	0.082796	2.946945	–0.846917
9	C	–2.095048	–1.181040	–1.005978
10	H	–2.707528	–2.083806	–0.929406
11	H	–2.694799	–0.379289	–1.445008
12	H	–1.230025	–1.386158	–1.642976
13	C	2.389750	–1.274043	0.296241
14	H	3.178037	–1.776283	–0.271577
15	H	2.839011	–0.820496	1.187938
16	H	1.644932	–2.015136	0.600502

Total Energy of $(MeS)_2MeSiLi$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1213.20763646 Hartree
Corrected Zero Point Energy: –1213.090307 Hartree

Table 46. Standard orientation of $(MeS)_2MeSiMe$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	C	–0.626889	1.777074	–1.430292
2	Si	0.000081	0.719780	–0.000009
3	S	–1.570568	–0.495214	0.871967
4	S	1.570608	–0.495271	–0.872044
5	C	0.627039	1.776851	1.430446
6	H	0.994609	1.167540	2.263511
7	H	1.448306	2.418868	1.089974
8	H	–0.174660	2.419618	1.814440
9	C	2.168443	–1.463204	0.579555

10	H	2.855074	–2.219680	0.191886
11	H	2.706715	–0.825253	1.285205
12	H	1.336656	–1.959546	1.086100
13	C	–2.168734	–1.463002	–0.579586
14	H	–2.856531	–2.218430	–0.191932
15	H	–2.705792	–0.824724	–1.285847
16	H	–1.337277	–1.960655	–1.085388
17	H	0.175168	2.418616	–1.815560
18	H	–0.996272	1.167828	–2.262600
19	H	–1.446917	2.420338	–1.089162

Total Energy of $(MeS)_2MeSiMe$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1245.62014819 Hartree
Corrected Zero Point Energy: –1245.465911 Hartree

Table 47. Standard orientation of $(MeO)_3SiCl$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Cl	–0.452443	0.784133	0.061739
2	Si	–0.414427	0.502416	2.113645
3	O	1.050177	–0.113973	2.533906
4	C	2.330677	0.415689	2.190955
5	H	3.084547	–0.240475	2.633944
6	H	2.464447	0.436395	1.103129
7	H	2.455993	1.429294	2.590300
8	O	–0.741435	1.968114	2.763587
9	C	–1.090861	2.193581	4.132672
10	H	–1.266933	3.266083	4.248541
11	H	–2.001686	1.644663	4.394821
12	H	–0.276983	1.888889	4.801953
13	O	–1.552234	–0.563334	2.606263
14	C	–1.556037	–1.970967	2.363152
15	H	–0.615845	–2.426808	2.692593
16	H	–2.386369	–2.397007	2.932329
17	H	–1.709581	–2.176545	1.297104

Total Energy of $(MeO)_3SiCl$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1095.27384104 Hartree
Corrected Zero Point Energy: –1095.142793 Hartree

Table 48. Standard orientation of $(MeO)_3SiLi$ [B3LYP/6–31+G(d)]

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	Li	–0.136050	–0.691519	–1.060039
2	Si	0.111429	–0.043959	1.320069
3	O	1.699402	–0.506844	1.676241
4	C	2.371431	–0.176750	2.889720
5	H	3.344121	–0.681852	2.885448
6	H	2.528787	0.905986	2.967785
7	H	1.801432	–0.512490	3.766543
8	O	0.097486	1.596331	1.746582
9	C	–1.085578	2.343734	1.949883
10	H	–0.801678	3.375548	2.187799
11	H	–1.717656	2.362478	1.045696
12	H	–1.680026	1.936347	2.777972
13	O	–0.914861	–0.677955	2.527758
14	C	–1.314907	–2.029242	2.577823
15	H	–0.517740	–2.672334	2.979361
16	H	–1.595387	–2.416392	1.582160

17	H	–2.190204	–2.111087	3.233333

Total Energy of $(MeO)_3SiLi$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –642.527137091 Hartree
Corrected Zero Point Energy: –642.398638 Hartree

Table 49. Standard orientation of $(Me_2N)_3SiCl$ [B3LYP/6–31+G(d)]

Center Number	Atomic Number	Coordinates(Angstroms) X	Y	Z
1	Cl	–0.026437	1.079083	0.585545
2	Si	–0.089679	0.398685	2.604362
3	N	1.534755	0.244810	3.147174
4	C	2.561915	–0.412269	2.347099
5	H	2.988225	–1.275075	2.883810
6	H	2.149395	–0.770811	1.400390
7	H	3.385596	0.280668	2.114158
8	N	–0.910920	1.589173	3.542546
9	C	–2.226921	1.384773	4.133483
10	H	–3.019258	1.890812	3.556369
11	H	–2.463941	0.319021	4.181648
12	H	–2.253565	1.786353	5.158127
13	N	–0.909403	–1.115222	2.569569
14	C	–0.505199	–2.257278	3.379659
15	H	–0.332233	–3.142868	2.747629
16	H	0.419504	–2.037338	3.919211
17	H	–1.280472	–2.521399	4.117938
18	C	2.035987	0.755653	4.415772
19	H	2.456802	–0.057840	5.029274
20	H	2.834761	1.498436	4.257735
21	H	1.230908	1.228809	4.982368
22	C	–2.105705	–1.372454	1.776876
23	H	–1.950120	–2.227679	1.100903
24	H	–2.969628	–1.606035	2.420566
25	H	–2.361749	–0.505619	1.162576
26	C	–0.531686	2.996732	3.467663
27	H	–1.235709	3.574785	2.847475
28	H	–0.515822	3.445910	4.472454
29	H	0.465269	3.107442	3.031264

Total Energy of $(Me_2N)_3SiCl$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1153.54425081 Hartree
Corrected Zero Point Energy: –1153.292632 Hartree

Table 50. Standard orientation of $(Me_2N)_3SiLi$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates(Angstroms) X	Y	Z
1	Li	–0.503827	–0.567864	0.363971
2	Si	–0.209990	–0.033343	2.793223
3	N	1.494733	0.263258	3.228321
4	C	2.422422	0.875448	2.299368
5	H	3.416324	0.397332	2.352592
6	H	2.056935	0.771258	1.269126
7	H	2.572130	1.955689	2.490179
8	N	–1.330593	1.229629	3.366625
9	C	–1.849988	2.258080	2.489496
10	H	–1.316330	3.222626	2.593347
11	H	–1.763661	1.944379	1.440841
12	H	–2.917183	2.455966	2.692522
13	N	–0.607911	–1.381443	3.914372

14	C	0.251928	–2.554520	3.912336
15	H	0.000595	–3.266853	3.097135
16	H	1.298179	–2.262192	3.790775
17	H	0.153940	–3.107889	4.859721
18	C	1.957821	0.374602	4.603788
19	H	2.944299	–0.105313	4.727315
20	H	2.066998	1.427105	4.926269
21	H	1.255358	–0.119539	5.280647
22	C	–2.002063	–1.761091	4.078869
23	H	–2.363499	–2.425461	3.264615
24	H	–2.143409	–2.309308	5.023734
25	H	–2.641247	–0.874807	4.095607
26	C	–1.439689	1.606872	4.768376
27	H	–0.857595	2.517191	5.004883
28	H	–2.489321	1.813819	5.040547
29	H	–1.080687	0.795985	5.408463

Total Energy of $(Me_2N)_3SiLi$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –700.784116348 Hartree
Corrected Zero Point Energy: –700.535238 Hartree

Table 51. Standard orientation of $(MeS)_3SiCl$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Cl	–0.282373	0.476882	–0.012451
2	Si	–0.564281	0.488128	2.062849
3	S	1.164340	–0.346334	3.025559
4	C	2.547505	0.536282	2.178674
5	H	3.462619	0.224517	2.687704
6	H	2.600204	0.251252	1.126203
7	H	2.434429	1.618993	2.269569
8	S	–0.930754	2.550158	2.514437
9	C	–0.990543	2.515383	4.361286
10	H	–1.051472	3.559308	4.678477
11	H	–1.873046	1.979070	4.715631
12	H	–0.085921	2.063668	4.774489
13	S	–2.260901	–0.675239	2.644076
14	C	–1.766126	–2.393139	2.173550
15	H	–0.888403	–2.720816	2.732934
16	H	–2.618008	–3.028501	2.427573
17	H	–1.576261	–2.459465	1.100073

Total Energy of $(MeS)_3SiCl$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –2064.14722839 Hartree
Corrected Zero Point Energy: –2064.025442 Hartree

Table 52. Standard orientation of $(MeS)_3SiLi$ [B3LYP/6–31+G(d)]

Center Number	Atom Type	Coordinates (Angstroms) X	Y	Z
1	Li	–0.497324	–0.500674	–1.000950
2	Si	0.097727	0.000254	1.347933
3	S	2.147949	–0.780400	1.430906
4	C	2.831239	–0.315973	3.082499
5	H	3.759529	–0.877769	3.217683
6	H	3.043029	0.754480	3.126886
7	H	2.123097	–0.585540	3.870348
8	S	0.357371	2.150302	1.785554
9	C	–1.383601	2.751449	1.726533
10	H	–1.353072	3.832888	1.885764

11	H	–1.844913	2.554204	0.752208
12	H	–1.987390	2.290068	2.511486
13	S	–1.017205	–0.683532	3.127840
14	C	–1.489280	–2.386911	2.612256
15	H	–0.605738	–3.016711	2.475552
16	H	–2.078458	–2.377503	1.688435
17	H	–2.102957	–2.808630	3.413200

Total Energy of $(MeS)_3SiLi$ [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1611.41969747 Hartree
Corrected Zero Point Energy: –1611.299620 Hartree

Table 53. Shielding tensor for **4** [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 364.8913	Anisotropy = 85.5672	
	XX = 412.2617	YX = 10.6611	ZX = –35.4557
	XY = 21.9135	YY = 380.4082	ZY = –0.7393
	XZ = –10.3942	YZ = 17.0835	ZZ = 302.0040
Eigenvalues:	295.9115	376.8263	421.9361

Table 54. Shielding tensor for **5** [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 361.2612	Anisotropy = 78.1633	
	XX = 407.7541	YX = 12.4860	ZX = –5.3376
	XY = 29.2672	YY = 333.0137	ZY = –32.8108
	XZ = 11.3974	YZ = –17.2143	ZZ = 343.0159
Eigenvalues:	309.1235	361.2902	413.3701

Table 55. Shielding tensor for **6** [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 362.9025	Anisotropy = 102.8504	
	XX = 415.2963	YX = -15.2893	ZX = 32.3100
	XY = -25.2802	YY = 397.7634	ZY = -9.4826
	XZ = 15.5734	YZ = 6.4560	ZZ = 275.6478
Eigenvalues:	271.6297	385.6084	431.4694

Table 56. Shielding tensor for **4**·3 THF [GIAO–HF/6–311+G(2d,p)//B3LYP/TZVP].

Si	Isotropic = 362.1172	Anisotropy = 131.8445	
	XX = 444.8564	YX = 11.6061	ZX = –9.1695
	XY = –2.6013	YY = 281.0304	ZY = –13.1250
	XZ = –31.7789	YZ = –24.9894	ZZ = 360.4648
Eigenvalues:	276.6948	359.6433	450.0135

Table 57. Shielding tensor for **5**·3 THF [GIAO–HF/6–311+G(2d,p)//B3LYP/TZVP].

Si	Isotropic = 349.7151	Anisotropy = 140.9840	
	XX = 442.1454	YX = 1.7715	ZX = –13.5934
	XY = 16.8298	YY = 288.0587	ZY = –25.4463
	XZ = –6.0456	YZ = –16.1542	ZZ = 318.9412
Eigenvalues:	277.5007	327.9402	443.7044

Table 58. Shielding tensor for **6**·3 THF [GIAO–HF/6–311+G(2d,p)//B3LYP/TZVP].

Si	Isotropic = 366.7565	Anisotropy = 124.1407

	XX = 437.7883	YX = –12.8697	ZX = 44.4906
	XY = –21.5062	YY = 402.9170	ZY = –25.1392
	XZ = 9.1212	YZ = –1.2786	ZZ = 259.5641
Eigenvalues:	254.8557	395.8967	449.5169

Table 59. Shielding tensor for Me_3SiH [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 400.5132	Anisotropy = 20.3420	
	XX = 414.0742	YX = –0.0260	ZX = 0.0363
	XY = 0.0193	YY = 413.9877	ZY = –0.1229
	XZ = 0.1306	YZ = 0.2993	ZZ = 373.4776
Eigenvalues:	373.4772	413.9878	414.0745

Table 60. Shielding tensor for Me_3SiCl [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 355.0845	Anisotropy = 4.0440	
	XX = 357.7803	YX = 0.0166	ZX = 0.0488
	XY = –0.0546	YY = 353.7915	ZY = –0.0529
	XZ = –0.0070	YZ = –0.0594	ZZ = 353.6817
Eigenvalues:	353.6580	353.8150	357.7805

Table 61. Shielding tensor for Me_3SiLi [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 400.1034	Anisotropy = 19.2992	
	XX = 393.6518	YX = –0.0829	ZX = –0.2493
	XY = 0.0670	YY = 393.6900	ZY = 0.0755
	XZ = –0.0240	YZ = 0.0545	ZZ = 412.9683
Eigenvalues:	393.6494	393.6911	412.9695

Table 62. Shielding tensor for Me_4Si [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 385.8591	Anisotropy = 0.2188	
	XX = 385.8553	YX = –0.5095	ZX = 0.1424
	XY = 0.4205	YY = 385.9917	ZY = –0.4635
	XZ = 0.0481	YZ = 0.5116	ZZ = 385.7304
Eigenvalues:	385.6733	385.8991	386.0050

Table 63. Shielding tensor for Si in $(MeO)Me_2SiH$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 382.6067	Anisotropy = 53.6363	
	XX = 414.4888	YX = –0.8612	ZX = –22.7096
	XY = –0.0296	YY = 388.4254	ZY = 7.0292
	XZ = –10.3340	YZ = 8.1828	ZZ = 344.9059
Eigenvalues:	340.0721	389.3837	418.3642

Table 64. Shielding tensor for Si in $(MeO)Me_2SiCl$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 370.0403	Anisotropy = 57.0978	
	XX = 373.7256	YX = 6.5067	ZX = 8.6945
	XY = 19.3338	YY = 338.4250	ZY = 9.6172
	XZ = 19.5045	YZ = 13.3813	ZZ = 397.9704
Eigenvalues:	333.4623	368.5531	408.1055

Table 65. Shielding tensor for Si in (MeO)Me_2SiLi [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 346.5670	Anisotropy = 82.4505	
	XX = 385.0833	YX = 29.3335	ZX = 16.3225
	XY = 41.8436	YY = 271.8343	ZY = –3.0513
	XZ = 7.4265	YZ = –1.9993	ZZ = 382.7834
Eigenvalues:	261.3085	376.8585	401.5339

Table 66. Shielding tensor for Si in (MeO)Me_2SiMe [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 371.5865	Anisotropy = 29.6307	
	XX = 390.2990	YX = 2.0578	ZX = 8.9021
	XY = –1.0759	YY = 359.0284	ZY = 3.2598
	XZ = 1.2723	YZ = 3.5811	ZZ = 365.4322
Eigenvalues:	357.4634	365.9558	391.3403

Table 67. Shielding tensor for Si in (Me_2N)Me_2SiH [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 393.2873	Anisotropy = 58.3882	
	XX = 422.6095	YX = 0.0000	ZX = 30.9572
	XY = 0.0000	YY = 400.3888	ZY = 0.0000
	XZ = 22.8423	YZ = 0.0000	ZZ = 356.8635
Eigenvalues:	347.2603	400.3888	432.2128

Table 68. Shielding tensor for Si in (Me_2N)Me_2SiCl [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 369.5036	Anisotropy = 29.7167	
	XX = 388.2306	YX = 5.7907	ZX = 12.9042
	XY = 0.6046	YY = 376.9418	ZY = –17.6693
	XZ = 0.8625	YZ = –17.7645	ZZ = 343.3384
Eigenvalues:	334.6490	384.5471	389.3147

Table 69. Shielding tensor for Si in (Me_2N)Me_2SiLi [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 362.4871	Anisotropy = 63.9211	
	XX = 399.7999	YX = 0.0000	ZX = 10.1918
	XY = 0.0000	YY = 298.4311	ZY = 0.0000
	XZ = 8.1534	YZ = 0.0000	ZZ = 389.2303
Eigenvalues:	298.4311	383.9290	405.1012

Table 70. Shielding tensor for Si in (Me_2N)Me_2SiMe [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 380.2253	Anisotropy = 36.7478	
	XX = 390.5399	YX = 12.1714	ZX = 12.2522
	XY = 14.8891	YY = 370.5405	ZY = 4.4094
	XZ = 14.1938	YZ = 3.3701	ZZ = 379.5954
Eigenvalues:	363.1589	372.7931	404.7238

Table 71. Shielding tensor for Si in (MeS)Me_2SiH [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 383.3101	Anisotropy = 40.1262	
	XX = 408.0430	YX = 3.1157	ZX = –13.3018
	XY = –5.7056	YY = 383.9161	ZY = –16.8009
	XZ = –6.5889	YZ = –13.6014	ZZ = 357.9710

Eigenvalues:	349.3912	390.4781	410.0609

Table 72. Shielding tensor for Si in (MeS)Me_2SiCl [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 348.9146	Anisotropy = 19.7493	
	XX = 352.4305	YX = 4.8323	ZX = 1.5817
	XY = 8.1490	YY = 340.0805	ZY = –13.7288
	XZ = 8.1103	YZ = –12.3331	ZZ = 354.2328
Eigenvalues:	329.4960	355.1670	362.0808

Table 73. Shielding tensor for Si in (MeS)Me_2SiLi [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 366.0408	Anisotropy = 48.3704	
	XX = 391.1863	YX = –1.0346	ZX = 7.9448
	XY = 38.2293	YY = 310.7230	ZY = –3.5988
	XZ = –4.6092	YZ = 11.0375	ZZ = 396.2133
Eigenvalues:	306.5129	393.3218	398.2878

Table 74. Shielding tensor for Si in (MeS)Me_2SiMe [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 370.1362	Anisotropy = 16.6867	
	XX = 379.9888	YX = 0.8563	ZX = 0.0127
	XY = 1.8376	YY = 349.1594	ZY = 0.0260
	XZ = 0.0243	YZ = 0.0037	ZZ = 381.2603
Eigenvalues:	349.1007	380.0472	381.2606

Table 75. Shielding tensor for Si in $(MeO)_2$MeSiH [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 401.7629	Anisotropy = 47.7187	
	XX = 404.0912	YX = –16.6883	ZX = 1.1826
	XY = –17.3538	YY = 406.4783	ZY = –20.3197
	XZ = 15.8932	YZ = –19.9577	ZZ = 394.7191
Eigenvalues:	378.9437	392.7695	433.5754

Table 76. Shielding tensor for Si in $(MeO)_2$MeSiCl [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 405.2334	Anisotropy = 54.6961	
	XX = 384.8454	YX = –8.4477	ZX = –7.7800
	XY = –3.8849	YY = 409.4060	ZY = –18.8849
	XZ = 8.0113	YZ = –31.6987	ZZ = 421.4487
Eigenvalues:	381.6629	392.3398	441.6974

Table 77. Shielding tensor for Si in $(MeO)_2$MeSiLi [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 350.8385	Anisotropy = 137.4416	
	XX = 345.2640	YX = 2.8161	ZX = 39.0517
	XY = 22.7525	YY = 291.4601	ZY = 23.4214
	XZ = 50.9649	YZ = 23.7711	ZZ = 415.7915
Eigenvalues:	286.6638	323.3856	442.4662

Table 78. Shielding tensor for Si in $(MeO)_2$MeSiMe [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 388.7870	Anisotropy = 53.2009	

	XX = 383.3079	YX = –0.0003	ZX = 17.0912
	XY = 0.0001	YY = 374.6570	ZY = –0.0002
	XZ = 33.8729	YZ = –0.0001	ZZ = 408.3960
Eigenvalues:	367.4497	374.6570	424.2542

Table 79. Shielding tensor for Si in $(Me_2N)_2MeSiH$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 394.3760	Anisotropy = 40.5089	
	XX = 392.9126	YX = 12.9568	ZX = 11.1321
	XY = 13.9590	YY = 410.9973	ZY = 13.2006
	XZ = 5.3816	YZ = 4.2903	ZZ = 379.2181
Eigenvalues:	375.1399	386.6061	421.3820

Table 80. Shielding tensor for Si in $(Me_2N)_2MeSiCl$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 389.1815	Anisotropy = 37.5170	
	XX = 406.8512	YX = 12.9100	ZX = 3.5261
	XY = 2.6228	YY = 405.0131	ZY = –0.3026
	XZ = 7.5388	YZ = 3.0731	ZZ = 355.6802
Eigenvalues:	355.0826	398.2690	414.1928

Table 81. Shielding tensor for Si in $(Me_2N)_2MeSiLi$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 352.7918	Anisotropy = 79.6951	
	XX = 354.7447	YX = –22.6022	ZX = –14.9687
	XY = –36.1742	YY = 303.6889	ZY = 7.8582
	XZ = –11.3277	YZ = 6.8471	ZZ = 399.9419
Eigenvalues:	290.2751	362.1786	405.9219

Table 82. Shielding tensor for Si in $(Me_2N)_2MeSiMe$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 388.0573	Anisotropy = 25.0932	
	XX = 401.1782	YX = –2.4734	ZX = –6.1347
	XY = 0.7197	YY = 380.8016	ZY = 2.1326
	XZ = –11.4496	YZ = 4.1323	ZZ = 382.1921
Eigenvalues:	376.9368	382.4490	404.7861

Table 83. Shielding tensor for Si in $(MeS)_2MeSiH$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 373.4969	Anisotropy = 68.3787	
	XX = 400.8291	YX = 16.9883	ZX = –6.1301
	XY = 11.2393	YY = 401.1179	ZY = –25.7576
	XZ = –2.8048	YZ = –20.2975	ZZ = 318.5438
Eigenvalues:	312.5493	388.8588	419.0827

Table 84. Shielding tensor for Si in $(MeS)_2MeSiCl$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 344.5575	Anisotropy = 49.7179	
	XX = 360.6323	YX = –6.2988	ZX = –5.3868
	XY = –7.3691	YY = 360.5875	ZY = –25.8974
	XZ = 0.7125	YZ = –37.0855	ZZ = 312.4527
Eigenvalues:	296.4736	359.4961	377.7028

Table 85. Shielding tensor for Si in $(MeS)_2MeSiLi$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 351.2563	Anisotropy = 43.8700	
	XX = 363.4211	YX = –21.3454	ZX = 17.3880
	XY = 4.2974	YY = 342.8683	ZY = 31.6023
	XZ = 11.2983	YZ = 35.6400	ZZ = 347.4795
Eigenvalues:	306.9085	366.3575	380.5030

Table 86. Shielding tensor for Si in $(MeS)_2MeSiMe$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 356.4463	Anisotropy = 33.3461	
	XX = 372.7199	YX = –0.0112	ZX = 6.4487
	XY = –0.0056	YY = 378.6770	ZY = –0.0151
	XZ = 10.5951	YZ = 0.0100	ZZ = 317.9420
Eigenvalues:	316.6469	374.0150	378.6771

Table 87. Shielding tensor for Si in $(MeO)_3SiCl$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 448.1875	Anisotropy = 18.6428	
	XX = 447.4452	YX = –10.4129	ZX = 4.0130
	XY = 17.7449	YY = 458.4704	ZY = –5.3961
	XZ = –5.2544	YZ = 15.6789	ZZ = 438.6469
Eigenvalues:	437.1708	446.7757	460.6160

Table 88. Shielding tensor for Si in $(MeO)_3SiLi$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 394.4748	Anisotropy = 138.5827	
	XX = 350.9189	YX = 12.8092	ZX = 21.3528
	XY = 10.4724	YY = 360.6510	ZY = 24.1242
	XZ = 44.1672	YZ = 29.9586	ZZ = 471.8544
Eigenvalues:	341.0263	355.5348	486.8632

Table 89. Shielding tensor for Si in $(Me_2N)_3SiCl$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 410.1845	Anisotropy = 31.2251	
	XX = 430.8496	YX = 4.5602	ZX = 0.9335
	XY = –6.8506	YY = 422.1969	ZY = 11.4066
	XZ = 1.6013	YZ = 12.9222	ZZ = 377.5070
Eigenvalues:	374.3701	425.1822	431.0013

Table 90. Shielding tensor for Si in $(Me_2N)_3SiLi$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 363.2523	Anisotropy = 97.9330	
	XX = 328.3358	YX = 8.2523	ZX = 11.6915
	XY = 5.4705	YY = 341.6274	ZY = 27.8751
	XZ = 11.4229	YZ = 21.1753	ZZ = 419.7936
Eigenvalues:	325.4087	335.8072	428.5409

Table 91. Shielding tensor for Si in $(MeS)_3SiCl$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 341.7796	Anisotropy = 59.0246	
	XX = 362.4364	YX = –0.2603	ZX = 22.1065
	XY = 19.7721	YY = 340.5436	ZY = 24.9483
	XZ = 17.2482	YZ = 28.0187	ZZ = 322.3588

Eigenvalues:	301.4855	342.7239	381.1294

Table 92. Shielding tensor for Si in $(MeS)_3SiLi$ [GIAO–HF/6–311+G(2d,p)//B3LYP/6–31+G(d)].

Si	Isotropic = 335.3773	Anisotropy = 75.4673	
	XX = 317.4748	YX = 36.9313	ZX = 13.2098
	XY = –9.0057	YY = 318.8805	ZY = –18.2612
	XZ = 36.5232	YZ = –33.7704	ZZ = 369.7767
Eigenvalues:	288.3202	332.1230	385.6889

Table 93. Shielding tensor for Si in **4**·3 THF in principal axes [IGLO–BP86/mixed basis//B3LYP/TZVP].

	σ_1	σ_2	σ_3
σ_d	829.4	829.7	827.4
σ_{p0}	444.7	478.1	403.2
σ_{p1}	–1052.4	–994.2	–851.8
σ	221.7	313.5	378.7
prin. axes			
x	–0.0293	0.9689	0.2456
y	0.2357–	0.2321	0.9437
z	0.9714	0.0855	–0.2215

Table 94. Shielding tensor for Si in **5**·3 THF in principal axes [IGLO–BP86/mixed basis//B3LYP/TZVP].

	σ_1	σ_2	σ_3
σ_d	827.0	829.5	826.3
σ_{p0}	415.6	467.7	394.4
σ_{p1}	–1011.6	–1017.6	–849.9
σ	231.0	279.6	370.8
prin. axes			
x	0.0378	0.8736	0.4851
y	0.1412	–0.4852	0.8629
z	0.9893	0.0359	–0.1417

Table 95. Shielding tensor for Si in **6**·3 THF in principal axes [IGLO–BP86/mixed basis//B3LYP/TZVP

	σ_1	σ_2	σ_3
σ_d	829.1	831.3	828.4
σ_{p0}	450.6	504.0	412.1
σ_{p1}	–1067.2	–983.0	–859.1
σ	212.5	352.4	381.4
prin. axes			
x	–0.2158	0.0340	0.9758
y	0.2278	0.9736	0.0164
z	0.9495	–0.2258	0.2179

Table 96. Shielding tensor for Me_3SiH in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	823.6	828.6	828.6
σ_{p0}	399.6	423.1	423.7
σ_{p1}	–905.5	–885.7	–886.3
σ	317.7	366.0	366.1
prin. axes			
x	–0.0012	–0.0022	1.0000

y	–0.0394	–0.9992	–0.0022
z	0.9992	–0.0394	0.0011

Table 97. Shielding tensor for Si in Me_3SiCl in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.0	827.0	827.0
σ_{p0}	389.2	386.3	390.7
σ_{p1}	–934.3	–931.3	–904.3
σ	281.8	282.0	313.5
prin. axes			
x	–0.0011	0.4482	0.8939
y	–0.0012	–0.8939	0.4482
z	1.0000	–0.0006	0.0016

Table 98. Shielding tensor for Si in Me_3SiLi in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	829.1	829.1	827.9
σ_{p0}	438.5	438.5	413.3
σ_{p1}	–932.5	–932.5	–886.1
σ	335.0	335.1	355.1
prin. axes			
x	0.5643	0.8256	0.0012
y	0.8255	–0.5643	0.0096
z	–0.0086	0.0044	1.0000

Table 99. Shielding tensor for Si in Me_3SiMe in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.0	827.0	827.0
σ_{p0}	403.3	404.7	405.7
σ_{p1}	–898.6	–899.7	–900.6
σ	331.8	332.1	332.1
prin. axes			
x	–0.4075	–0.2101	0.8887
y	–0.9114	0.0329	–0.4101
z	0.0569	–0.9771	–0.2049

Table 100. Shielding tensor for Si in $(MeO)Me_2SiH$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	822.0	827.1	828.9
σ_{p0}	389.5	400.8	418.4
σ_{p1}	–943.1	–905.4	–867.6
σ	268.4	322.5	379.6
prin. axes			
x	0.2442	–0.1904	0.9509
y	0.2487	0.9600	0.1284
z	0.9373	–0.2051	–0.2818

Table 101. Shielding tensor for Si in $(MeO)Me_2SiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	825.3	826.8	826.1
σ_{p0}	379.9	378.0	396.5
σ_{p1}	–925.2	–887.1	–889.6
σ	280.0	317.8	332.9
prin. axes			
x	0.1995	–0.9555	0.2172
y	–0.7999	–0.0308	0.5994
z	0.5660	0.2933	0.7704

Table 102. Shielding tensor for Si in (MeO)Me_2SiLi in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.2	826.8	828.8
σ_{p0}	389.0	401.4	434.6
σ_{p1}	–1034.9	–933.5	–911.1
σ	181.2	294.7	352.4
prin. axes			
x	0.2930	–0.9556	–0.0322
y	–0.4540	–0.1687	0.8749
z	0.8414	0.2418	0.4832

Table 103. Shielding tensor for Si in (MeO)Me_2SiMe in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	825.2	825.9	827.4
σ_{p0}	386.3	395.3	406.9
σ_{p1}	–923.9	–920.5	–885.8
σ	287.6	300.7	348.5
prin. axes			
x	–0.0518	–0.9050	0.4222
y	0.3180	–0.4157	–0.8521
z	–0.9467	–0.0901	–0.3094

Table 104. Shielding tensor for Si in (Me_2N)Me_2SiH in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	821.1	826.8	829.9
σ_{p0}	393.8	398.5	426.6
σ_{p1}	–928.9	–877.4	–865.6
σ	286.0	347.8	390.9
prin. axes			
x	–0.8776	–0.4795	0.0004
y	0.0003	0.0003	1.0000
z	0.4795	–0.8776	0.0001

Table 105. Shielding tensor for Si in (Me_2N)Me_2SiCl in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	825.0	825.0	827.5
σ_{p0}	384.4	379.0	385.2
σ_{p1}	–921.2	–883.5	–877.2

σ	288.1	320.5	335.5
prin. axes			
x	–0.5917	–0.0302	0.8056
y	–0.0140	–0.9988	–0.0478
z	–0.8060	0.0396	–0.5905

Table 106. Shielding tensor for Si in $(Me_2N)Me_2SiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.5	825.6	830.7
σ_{p0}	382.1	401.2	439.5
σ_{p1}	–986.3	–910.8	–914.5
σ	223.2	316.0	355.7
prin. axes			
x	0.0000	–1.0000	0.0000
y	–0.1678	0.0000	0.9858
z	–0.9858	0.0000	–0.1678

Table 107. Shielding tensor for Si in $(Me_2N)Me_2SiMe$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	824.6	825.1	828.1
σ_{p0}	399.1	383.3	403.9
σ_{p1}	–920.1	–891.5	–873.4
σ	303.6	316.9	358.7
prin. axes			
x	–0.2223	0.0901	–0.9708
y	–0.0164	0.9952	0.0961
z	0.9749	0.0373	–0.2197

Table 108. Shielding tensor for Si in $(MeS)Me_2SiH$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	823.9	827.5	830.3
σ_{p0}	382.6	407.5	409.8
σ_{p1}	–923.8	–905.2	–873.7
σ	282.7	329.8	366.4
prin. axes			
x	0.2520	0.4093	0.8769
y	–0.0243	–0.9032	0.4286
z	0.9674	–0.1294	–0.2177

Table 109. Shielding tensor for Si in $(MeS)Me_2SiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.2	828.8	825.9
σ_{p0}	367.0	371.7	382.7
σ_{p1}	–939.3	–907.9	–902.9
σ	254.9	292.5	305.7
prin. axes			
x	–0.0548	–0.6639	–0.7458

y	0.9981	–0.0576	–0.0221
z	0.0283	0.7456	–0.6658

Table 110. Shielding tensor for Si in (MeS)Me_2SiLi in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	829.4	828.9	830.0
σ_{p0}	406.6	419.0	437.6
σ_{p1}	–1002.5	–927.1	–915.4
σ	233.5	320.7	352.3
prin. axes			
x	0.2794	–0.9601	0.0081
y	–0.4560	–0.1253	0.8811
z	–0.8450	–0.2499	–0.4728

Table 111. Shielding tensor for Si in (MeS)Me_2SiMe in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.2	826.2	828.7
σ_{p0}	378.1	407.0	390.7
σ_{p1}	–923.5	–912.8	–887.3
σ	281.8	320.4	332.1
prin. axes			
x	0.1970	–0.9804	–0.0001
y	–0.0025	–0.0006	1.0000
z	–0.9804	–0.1970	–0.0026

Table 112. Shielding tensor for Si in $(MeO)_2$MeSiH in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	822.4	827.4	826.5
σ_{p0}	395.3	417.0	404.0
σ_{p1}	–899.4	–896.3	–859.6
σ	318.3	348.0	370.9
prin. axes			
x	0.2496	0.5579	0.7915
y	0.7969	0.3460	–0.4952
z	–0.5501	0.7543	–0.3582

Table 113. Shielding tensor for Si in $(MeO)_2$MeSiCl in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	825.8	825.8	824.9
σ_{p0}	386.2	384.9	394.0
σ_{p1}	–876.6	–867.8	–843.9
σ	335.4	342.9	375.0
prin. axes			
x	0.8727	0.4405	0.2109
y	0.4844	–0.7261	–0.4881
z	0.0619	–0.5281	0.8470

Table 114. Shielding tensor for Si in $(MeO)_2MeSiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	826.9	828.2	826.4
σ_{p0}	388.5	413.2	413.0
σ_{p1}	–992.0	–968.0	–875.1
σ	223.4	273.4	364.2
prin. axes			
x	0.0727	–0.9851	0.1562
y	–0.9143	–0.0032	0.4051
z	0.3986	0.1722	0.9008

Table 115. Shielding tensor for Si in $(MeO)_2MeSiMe$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	825.6	826.0	825.2
σ_{p0}	390.4	397.6	400.9
σ_{p1}	–896.2	–903.3	–867.1
σ	319.8	320.4	359.0
prin. axes			
x	0.0169	0.9998	–0.0082
y	0.8937	–0.0188	–0.4484
z	0.4484	–0.0002	0.8938

Table 116. Shielding tensor for Si in $(Me_2N)_2MeSiH$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	820.3	828.6	824.0
σ_{p0}	372.2	424.6	392.7
σ_{p1}	–867.2	–915.6	–838.7
σ	325.2	337.6	378.1
prin. axes			
x	–0.3101	–0.5371	–0.7845
y	0.9504	–0.1967	–0.2410
z	–0.0249	–0.8203	0.5714

Table 117. Shielding tensor for Si in $(Me_2N)_2MeSiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	822.7	824.2	825.3
σ_{p0}	362.9	379.0	375.5
σ_{p1}	–869.9	–866.8	–838.1
σ	315.7	336.4	362.7
prin. axes			
x	–0.2493	0.8507	–0.4629
y	0.3916	0.5257	0.7552
z	–0.8857	–0.0070	0.4641

Table 118. Shielding tensor for Si in $(Me_2N)_2MeSiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3

σ_d	826.2	829.1	824.0
σ_{p0}	384.9	417.0	389.0
σ_{p1}	–990.2	–936.2	–870.9
σ	221.0	309.9	342.1
prin. axes			
x	–0.0113	–0.9997	0.0203
y	–0.9610	0.0165	0.2760
z	0.2763	0.0164	0.9609

Table 119. Shielding tensor for Si in $(Me_2N)_2MeSiMe$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	823.1	824.4	825.0
σ_{p0}	385.4	388.8	393.6
σ_{p1}	–882.7	–884.3	–861.2
σ	325.8	328.8	357.4
prin. axes			
x	0.5209	0.0365	–0.8528
y	0.0193	–0.9993	–0.0310
z	–0.8534	–0.0004	–0.5213

Table 120. Shielding tensor for Si in $(MeS)_2MeSiH$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	824.4	829.2	829.4
σ_{p0}	350.6	404.9	407.6
σ_{p1}	–942.9	–892.5	–867.3
σ	232.2	341.6	369.6
prin. axes			
x	0.1094	0.2676	0.9573
y	0.7122	–0.6929	0.1123
z	–0.6933	–0.6695	0.2664

Table 121. Shielding tensor for Si in $(MeS)_2MeSiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.5	827.8	827.7
σ_{p0}	343.8	358.8	363.3
σ_{p1}	–942.6	–886.0	–881.6
σ	228.7	300.7	309.4
prin. axes			
x	0.0821	0.3211	0.9435
y	0.8326	0.4982	–0.2420
z	–0.5478	0.8054	–0.2264

Table 122. Shielding tensor for Si in $(MeS)_2MeSiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	830.6	829.9	830.5
σ_{p0}	403.7	408.4	426.5
σ_{p1}	–1005.2	–932.2	–928.6
σ	229.1	306.1	328.3

prin. axes			
x	–0.0020	–0.5718	0.8204
y	0.7980	0.4935	0.3459
z	0.6026	–0.6554	–0.4553

Table 123. Shielding tensor for Si in $(MeS)_2MeSiMe$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.3	828.2	827.7
σ_{p0}	356.0	392.0	379.9
σ_{p1}	–943.1	–901.4	–884.1
σ	240.2	318.9	323.6
prin. axes			
x	0.0514	–0.0001	0.9987
y	0.9987	0.0036	–0.0514
z	–0.0036	1.0000	0.0003

Table 124. Shielding tensor for Si in $(MeO)_3MeSiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	823.9	825.4	825.4
σ_{p0}	400.3	399.7	393.1
σ_{p1}	–833.6	–828.8	–803.4
σ	390.6	396.3	415.0
prin. axes			
x	–0.4625	–0.2130	–0.8606
y	0.4849	0.7519	–0.4467
z	0.7423	–0.6239	–0.2445

Table 125. Shielding tensor for Si in $(MeO)_3MeSiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	827.5	826.8	824.9
σ_{p0}	397.0	395.2	415.2
σ_{p1}	–930.5	–908.3	–823.7
σ	293.9	313.7	416.4
prin. axes			
x	–0.6746	0.6867	0.2709
y	0.7368	0.6489	0.1900
z	0.0453	–0.3278	0.9437

Table 126. Shielding tensor for Si in $(Me_2N)_3MeSiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	818.2	823.3	823.0
σ_{p0}	353.6	377.6	373.7
σ_{p1}	–838.6	–829.3	–814.9
σ	333.2	371.6	381.8
prin. axes			
x	0.0916	–0.0559	0.9942
y	0.5073	–0.8565	–0.0949
z	0.8569	0.5131	–0.0501

Table 127. Shielding tensor for Si in $(Me_2N)_3MeSiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	828.2	825.9	821.9
σ_{p0}	404.9	395.9	384.5
σ_{p1}	–960.6	–928.4	–840.9
σ	272.5	293.3	365.5
prin. axes			
x	0.9998	–0.0204	–0.0087
y	–0.0197	–0.9971	0.0734
z	0.0101	0.0732	0.9973

Table 128. Shielding tensor for Si in $(MeS)_3MeSiCl$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	828.0	828.5	827.6
σ_{p0}	326.8	342.7	344.8
σ_{p1}	–915.4	–891.6	–849.1
σ	239.4	279.6	323.3
prin. axes			
x	0.3806	0.2890	0.8784
y	0.3398	–0.9272	0.1578
z	–0.8601	–0.2384	0.4511

Table 129. Shielding tensor for Si in $(MeS)_3MeSiLi$ in principal axes [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

	σ_1	σ_2	σ_3
σ_d	832.0	830.8	830.0
σ_{p0}	398.5	378.6	407.7
σ_{p1}	–1007.3	–949.9	–919.9
σ	223.1	259.5	317.9
prin. axes			
x	–0.7737	0.1707	–0.6101
y	0.1100	–0.9122	–0.3947
z	–0.6239	–0.3726	0.6870

Table 130. MO contributions to σ in principal axes for Si in **4**·3 THF [IGLO–BP86/mixed basis//B3LYP/TZVP].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(7)	481.9	481.9	481.9	481.9
2	AO O(20)	0.0	0.0	0.0	0.0
3	AO O(30)	0.0	0.0	0.0	0.0
4	AO O(25)	0.0	0.0	0.0	0.0
5	AO N(14)	0.0	0.0	0.0	0.0
6	AO C(24)	0.0	0.0	0.0	0.0
7	AO C(21)	0.0	0.0	0.0	0.0
8	AO C(31)	0.0	0.0	0.0	0.0
9	AO C(34)	0.0	0.0	0.0	0.0
10	AO C(26)	0.0	0.0	0.0	0.0
11	AO C(29)	0.0	0.0	0.0	0.0
12	AO C(23)	0.0	0.0	0.0	0.0

13	AO C(22)	0.0	0.0	0.0	0.0
14	AO C(33)	0.0	0.0	0.0	0.0
15	AO C(32)	0.0	0.0	0.0	0.0
16	AO C(28)	0.0	0.0	0.0	0.0
17	AO C(27)	0.0	0.0	0.0	0.0
18	AO C(17)	0.0	0.0	0.0	0.0
19	AO C(11)	0.0	0.0	0.0	0.0
20	AO C(5)	0.0	0.0	0.0	0.0
21	AO C(10)	0.0	0.0	0.0	0.0
22	AO C(6)	0.0	0.0	0.0	0.0
23	AO C(1)	0.0	0.0	0.0	0.0
24	AO C(12)	0.0	0.0	0.0	0.0
25	AO C(15)	0.0	0.0	0.0	0.0
26	AO C(9)	0.0	0.0	0.0	0.0
27	AO C(2)	0.0	0.0	0.0	0.0
28	AO C(4)	0.0	0.0	0.0	0.0
29	AO C(13)	0.0	0.0	0.0	0.0
30	AO C(18)	0.0	0.0	0.0	0.0
31	AO C(16)	0.0	0.0	0.0	0.0
32	AO C(3)	0.0	–0.1	0.0	0.0
33	AO C(8)	0.0	0.0	–0.1	0.0
34	AO Si(7)	77.6	78.7	71.1	75.8
35	AO Si(7)	76.5	81.9	69.7	76.1
36	AO Si(7)	68.2	66.9	91.4	75.5
37	AO Si(7)	72.3	64.2	88.8	75.1
38	AO Li(19)	0.0	–0.1	0.1	0.0
39	BOND H(50)–C(24)	0.0	–0.1	0.1	0.0
40	BOND H(62)–C(31)	–0.3	0.0	0.1	–0.1
41	BOND H(66)–C(28)	0.0	0.0	0.0	0.0
42	BOND N(14)–C(17)	–3.7	2.0	–3.1	–1.6
43	BOND H(58)–C(11)	0.0	0.0	0.0	0.0
44	BOND C(12)–C(13)	–0.5	–1.5	–1.2	–1.1
45	BOND H(49)–C(21)	–0.1	0.0	0.0	0.0
46	BOND H(77)–C(33)	–0.1	0.0	0.1	0.0
47	BOND H(59)–C(27)	0.1	0.0	0.1	0.0
48	BOND H(37)–C(22)	0.0	0.0	0.0	0.0
49	BOND H(64)–C(31)	0.0	–0.1	0.1	0.0
50	LP O(25)	0.2	0.4	0.1	0.2
51	BOND C(16)–C(15)	–1.5	–0.7	–1.1	–1.1
52	BOND H(67)–C(5)	–0.1	0.1	0.0	0.0
53	BOND H(55)–C(10)	–0.1	0.0	0.1	0.0
54	BOND H(78)–C(1)	0.0	0.1	0.0	0.0
55	BOND C(5)–C(4)	–0.4	–1.7	–0.9	–1.0
56	BOND H(38)–C(16)	0.0	0.0	0.1	0.1
57	BOND H(47)–C(23)	0.0	0.0	0.0	0.0
58	BOND C(22)–C(21)	–0.1	–0.1	0.0	0.0
59	BOND H(69)–C(32)	0.0	0.1	0.1	0.0
60	BOND O(25)–C(29)	0.0	0.0	0.1	0.1
61	BOND H(54)–C(26)	–0.1	0.0	0.0	0.0
62	BOND H(35)–C(18)	0.2	0.1	0.2	0.2
63	BOND C(28)–C(27)	0.1	0.0	0.0	0.0
64	BOND H(76)–C(6)	0.1	0.1	0.1	0.1
65	BOND C(10)–C(11)	–0.1	–0.1	0.0	–0.1
66	BOND H(61)–C(12)	0.0	–0.1	–0.1	–0.1
67	BOND C(6)–C(1)	–0.1	–0.1	–0.1	–0.1
68	BOND H(45)–C(17)	–2.6	0.6	–0.5	–0.9
69	BOND H(53)–C(24)	0.0	0.0	0.1	0.0
70	BOND C(23)–C(24)	–0.1	–0.1	0.1	0.0
71	BOND H(75)–C(33)	0.0	0.0	0.0	0.0
72	BOND H(51)–C(26)	0.0	–0.1	0.0	0.0
73	BOND H(68)–C(32)	–0.1	0.0	0.0	0.0
74	BOND H(71)–C(29)	0.1	0.0	0.0	0.0

75	BOND H(60)–C(4)	–0.2	–0.3	–1.2	–0.5
76	BOND C(12)–C(11)	0.2	0.0	0.7	0.3
77	BOND C(10)–C(9)	0.0	–0.6	–0.1	–0.3
78	BOND H(39)–C(23)	0.0	0.0	0.0	0.0
79	BOND H(74)–C(34)	0.0	0.1	0.0	0.0
80	LP O(20)	–0.2	–0.1	0.2	0.0
81	BOND O(30)–C(34)	0.1	0.0	0.1	0.1
82	BOND O(30)–C(31)	0.0	0.0	0.1	0.1
83	BOND H(44)–C(15)	0.1	0.4	1.0	0.5
84	BOND C(26)–C(27)	0.1	0.0	0.0	0.0
85	BOND C(10)–C(9)	0.1	–0.6	0.2	–0.1
86	BOND H(46)–C(22)	0.0	0.0	0.0	0.0
87	BOND C(8)–C(13)	1.4	–3.6	–2.7	–1.6
88	BOND C(33)–C(32)	0.0	0.1	0.0	0.0
89	BOND C(4)–C(3)	–0.3	–1.4	–6.5	–2.7
90	BOND H(65)–C(28)	0.0	–0.1	0.0	0.0
91	BOND C(8)–C(13)	–0.7	–2.0	–2.5	–1.7
92	BOND H(48)–C(16)	–0.1	0.0	0.0	0.0
93	BOND H(40)–C(18)	0.0	0.2	–0.3	–0.1
94	BOND C(1)–C(2)	–1.0	–0.1	–0.2	–0.4
95	BOND C(2)–C(3)	–1.1	–2.6	–4.1	–2.6
96	BOND H(42)–C(21)	0.1	0.0	0.0	0.0
97	BOND H(43)–C(16)	0.1	0.1	–0.1	0.0
98	BOND H(52)–C(15)	–1.4	–0.6	–0.1	–0.7
99	BOND O(20)–C(24)	0.1	0.0	0.1	0.0
100	BOND C(33)–C(34)	0.0	0.0	0.0	0.0
101	LP O(25)	–0.2	–0.5	–0.1	–0.3
102	BOND H(70)–C(29)	0.0	–0.1	–0.1	–0.1
103	BOND C(28)–C(29)	0.1	0.0	–0.1	0.0
104	BOND H(63)–C(13)	–0.4	–1.3	–0.5	–0.7
105	BOND C(23)–C(22)	0.0	0.0	0.0	0.0
106	BOND O(20)–C(21)	0.0	0.0	0.2	0.1
107	BOND C(18)–C(17)	–0.1	1.1	–0.1	0.3
108	BOND H(73)–C(34)	0.0	–0.1	0.0	0.0
109	BOND H(57)–C(27)	0.0	–0.1	–0.1	–0.1
110	BOND C(31)–C(32)	–0.1	0.0	0.0	0.0
111	BOND C(4)–C(3)	–0.6	1.1	–3.2	–0.9
112	BOND N(14)–Si(7)	–102.6	–35.2	–103.1	–80.3
113	LP O(30)	0.3	0.2	0.1	0.2
114	BOND C(6)–C(5)	0.1	0.1	–0.5	–0.1
115	BOND H(41)–C(17)	–1.7	0.4	0.1	–0.4
116	BOND C(12)–C(11)	0.2	0.5	0.5	0.4
117	BOND H(36)–C(18)	0.1	0.2	0.0	0.1
118	BOND C(6)–C(5)	–0.1	–0.1	0.0	0.0
119	BOND H(56)–C(9)	–0.2	–2.1	0.1	–0.7
120	BOND N(14)–C(15)	–6.4	–1.2	–5.2	–4.3
121	LP O(20)	–0.1	–0.1	0.0	–0.1
122	LP O(30)	–0.6	–0.4	0.0	–0.3
123	BOND O(25)–C(26)	0.1	0.0	0.1	0.1
124	BOND H(72)–C(2)	–0.5	0.1	–0.9	–0.4
125	BOND C(2)–C(1)	0.5	–0.3	–0.4	0.0
126	BOND C(3)–Si(7)	–88.4	–107.1	–132.1	–109.2
127	BOND C(9)–C(8)	–0.9	–2.3	–1.6	–1.6
128	BOND C(8)–Si(7)	–52.4	–96.7	–154.9	–101.3
129	LP N(14)	–10.1	3.4	–8.8	–5.2
130	BOND Si(7)–Li(19)	–278.9	–206.9	7.4	–159.5

Table 131. MO contributions to σ in principal axes for Si in **5**·3 THF [IGLO–BP86/mixed basis//B3LYP/TZVP].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(43)	481.9	481.9	481.9	481.9
2	AO O(40)	0.0	0.0	0.0	0.0
3	AO O(62)	0.0	0.0	0.0	0.0
4	AO O(32)	0.0	0.0	0.0	0.0
5	AO N(29)	0.0	0.0	0.0	0.0
6	AO N(55)	0.0	0.0	0.0	0.0
7	AO C(66)	0.0	0.0	0.0	0.0
8	AO C(47)	0.0	0.0	0.0	0.0
9	AO C(27)	0.0	0.0	0.0	0.0
10	AO C(33)	0.0	0.0	0.0	0.0
11	AO C(73)	0.0	0.0	0.0	0.0
12	AO C(19)	0.0	0.0	0.0	0.0
13	AO C(77)	0.0	0.0	0.0	0.0
14	AO C(24)	0.0	0.0	0.0	0.0
15	AO C(20)	0.0	0.0	0.0	0.0
16	AO C(80)	0.0	0.0	0.0	0.0
17	AO C(35)	0.0	0.0	0.0	0.0
18	AO C(14)	0.0	0.0	0.0	0.0
19	AO C(15)	0.0	0.0	0.0	0.0
20	AO C(58)	0.0	0.0	0.0	0.0
21	AO C(23)	0.0	0.0	0.0	0.0
22	AO C(56)	0.0	0.0	0.0	0.0
23	AO C(59)	0.0	0.0	0.0	0.0
24	AO C(48)	0.0	0.0	0.0	0.0
25	AO C(67)	0.0	0.0	0.0	0.0
26	AO C(42)	0.0	0.0	0.0	0.0
27	AO C(69)	0.0	0.0	0.0	0.0
28	AO C(63)	0.0	0.0	0.0	0.0
29	AO C(13)	0.0	0.0	0.0	0.0
30	AO C(5)	0.0	0.0	0.0	0.0
31	AO C(45)	0.0	0.0	0.0	0.0
32	AO C(51)	0.0	–0.1	0.0	0.0
33	AO Si(43)	70.6	69.8	87.3	75.9
34	AO Si(43)	88.6	85.9	62.6	79.0
35	AO Si(43)	77.2	67.5	84.1	76.3
36	AO Si(43)	64.8	69.5	94.1	76.1
37	AO Li(46)	–0.1	–0.1	0.1	0.0
38	BOND H(11)–C(20)	0.0	0.0	0.0	0.0
39	BOND H(28)–C(24)	0.0	0.0	0.0	0.0
40	LP O(32)	0.2	0.2	0.1	0.2
41	BOND H(72)–C(69)	–0.1	0.2	–0.1	0.0
42	BOND H(7)–C(5)	–0.1	0.1	–0.1	0.0
43	BOND C(59)–C(67)	–0.1	0.0	–0.1	–0.1
44	BOND H(3)–C(14)	0.1	0.0	0.0	0.0
45	BOND H(82)–C(80)	0.0	0.1	0.0	0.0
46	BOND O(40)–C(47)	0.0	0.0	0.1	0.1
47	BOND H(50)–C(47)	0.0	0.0	0.0	0.0
48	BOND H(79)–C(80)	0.0	0.0	0.0	0.0
49	BOND H(81)–C(77)	0.0	0.0	0.0	0.0
50	BOND H(65)–C(56)	–0.5	–0.9	–0.3	–0.6
51	BOND H(4)–C(15)	–0.2	–0.6	–0.1	–0.3
52	BOND H(60)–C(59)	0.1	0.1	0.0	0.1
53	BOND H(68)–C(63)	–0.3	–0.5	–1.4	–0.7
54	BOND H(44)–C(45)	0.4	0.0	0.2	0.2
55	BOND H(31)–C(23)	–0.4	–0.8	–1.1	–0.8
56	BOND H(16)–C(27)	–0.1	–0.1	0.1	0.0
57	BOND H(22)–C(14)	–0.1	0.0	0.0	0.0
58	BOND H(61)–C(66)	0.0	–0.1	0.0	0.0
59	BOND H(70)–C(73)	–0.2	–0.3	–0.1	–0.2
60	BOND H(36)–C(35)	0.1	0.0	0.1	0.1
61	BOND H(30)–C(33)	0.1	0.0	0.0	0.0

62	BOND H(71)–C(69)	0.1	0.2	0.2	0.1
63	BOND H(6)–C(13)	0.2	0.0	0.3	0.2
64	BOND H(34)–C(42)	–0.3	–0.1	–1.2	–0.5
65	BOND C(13)–C(15)	0.2	0.5	0.4	0.4
66	BOND C(69)–C(58)	0.0	–0.2	–0.1	–0.1
67	BOND H(75)–C(69)	–0.2	0.2	–0.2	0.0
68	LP O(40)	0.1	0.3	0.1	0.2
69	BOND C(77)–C(66)	0.0	–0.1	0.0	0.0
70	BOND H(10)–C(24)	0.0	0.0	0.0	0.0
71	BOND H(21)–C(19)	–0.5	–0.1	–0.1	–0.2
72	BOND C(80)–C(73)	–0.1	–0.1	–0.1	–0.1
73	BOND C(20)–C(35)	0.0	0.0	0.1	0.0
74	BOND C(42)–C(51)	0.5	0.8	–3.3	–0.7
75	BOND H(38)–C(35)	–0.1	–0.2	0.0	–0.1
76	BOND H(52)–C(58)	–0.7	1.4	0.7	0.5
77	BOND H(78)–C(77)	0.1	0.0	0.0	0.0
78	BOND C(24)–C(14)	0.0	0.0	0.0	0.0
79	BOND H(57)–C(58)	–2.4	0.3	–0.4	–0.8
80	BOND H(1)–C(5)	0.0	0.1	0.0	0.0
81	BOND H(18)–C(15)	–1.9	–0.1	0.1	–0.6
82	BOND H(8)–C(19)	–0.1	0.1	0.0	0.0
83	BOND C(20)–C(27)	0.0	0.0	0.0	0.0
84	BOND H(64)–C(66)	0.0	0.0	0.1	0.0
85	BOND O(40)–C(27)	0.0	0.1	0.1	0.1
86	BOND O(62)–C(66)	0.1	0.0	0.1	0.1
87	BOND H(39)–C(48)	–0.1	0.1	0.0	0.0
88	BOND O(32)–C(19)	0.0	–0.1	0.2	0.0
89	BOND C(48)–C(59)	0.0	0.4	–0.2	0.0
90	BOND C(42)–C(51)	–0.6	–1.3	–6.3	–2.7
91	LP N(55)	–18.3	2.1	–28.3	–14.8
92	BOND C(5)–C(23)	–0.9	–0.9	–1.0	–0.9
93	BOND N(55)–C(58)	–3.5	2.0	–4.2	–1.9
94	BOND C(67)–C(63)	–0.1	–1.0	–0.8	–0.6
95	BOND H(9)–C(13)	0.3	0.0	0.0	0.1
96	BOND C(77)–C(80)	0.0	0.0	0.0	0.0
97	BOND H(2)–C(5)	0.0	0.2	0.0	0.1
98	BOND H(54)–C(47)	–0.1	–0.1	0.1	0.0
99	BOND C(63)–C(51)	–0.7	–3.8	–3.7	–2.8
100	BOND H(41)–C(33)	–0.1	0.0	0.1	0.0
101	BOND H(76)–C(73)	0.1	0.0	0.0	0.0
102	BOND C(35)–C(47)	0.0	0.0	0.0	0.0
103	BOND C(14)–C(19)	–0.1	0.0	–0.1	–0.1
104	BOND H(25)–C(27)	0.0	0.0	0.0	0.0
105	BOND H(26)–C(13)	0.3	–0.3	–0.3	–0.1
106	BOND H(49)–C(45)	0.0	0.1	0.1	0.1
107	LP O(62)	–0.1	0.0	0.1	0.0
108	BOND O(32)–C(33)	0.1	0.1	0.1	0.1
109	BOND C(33)–C(24)	0.0	0.0	0.0	0.0
110	BOND O(62)–C(73)	–0.1	–0.1	0.2	0.0
111	LP N(29)	–3.5	2.5	–16.5	–5.8
112	BOND H(12)–C(20)	–0.1	–0.1	0.1	0.0
113	BOND H(37)–C(45)	0.0	–0.1	0.0	–0.1
114	BOND C(51)–Si(43)	–54.2	–165.8	–135.1	–118.4
115	BOND C(45)–C(56)	0.1	–0.4	0.6	0.1
116	BOND H(53)–C(56)	–0.8	–0.8	–0.5	–0.7
117	BOND N(29)–C(23)	–5.2	–1.1	–8.5	–4.9
118	BOND N(55)–C(56)	–6.8	–1.7	–6.7	–5.0
119	BOND N(29)–C(15)	–1.5	1.3	–3.9	–1.4
120	BOND H(74)–C(67)	–0.1	0.1	0.0	0.0
121	LP O(40)	–0.4	–0.6	0.1	–0.3
122	BOND H(17)–C(23)	0.4	0.3	0.0	0.2
123	LP O(62)	–0.1	–0.2	–0.1	–0.1

124	LP O(32)	–0.5	–0.3	0.0	–0.3
125	BOND C(48)–C(59)	0.3	0.1	–0.5	0.0
126	BOND C(67)–C(63)	0.3	–0.3	–0.4	–0.1
127	BOND C(48)–C(42)	0.0	–1.5	–1.0	–0.8
128	BOND N(55)–Si(43)	–87.8	–41.8	–98.9	–76.2
129	BOND N(29)–Si(43)	–80.0	–45.7	–129.6	–85.1
130	BOND Si(43)–Li(46)	–282.4	–236.9	11.0	–169.4

Table 132. MO contributions to σ in principal axes for Si in **6**·3 THF [IGLO–BP86/mixed basis//B3LYP/TZVP].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(52)	481.9	481.9	481.9	481.9
2	AO O(41)	0.0	0.0	0.0	0.0
3	AO O(62)	0.0	0.0	0.0	0.0
4	AO O(32)	0.0	0.0	0.0	0.0
5	AO N(36)	0.0	0.0	0.0	0.0
6	AO C(38)	0.0	0.0	0.0	0.0
7	AO C(69)	0.0	0.0	0.0	0.0
8	AO C(22)	0.0	0.0	0.0	0.0
9	AO C(39)	0.0	0.0	0.0	0.0
10	AO C(65)	0.0	0.0	0.0	0.0
11	AO C(29)	0.0	0.0	0.0	0.0
12	AO C(35)	0.0	0.0	0.0	0.0
13	AO C(40)	0.0	0.0	0.0	0.0
14	AO C(11)	0.0	0.0	0.0	0.0
15	AO C(81)	0.0	0.0	0.0	0.0
16	AO C(79)	0.0	0.0	0.0	0.0
17	AO C(21)	0.0	0.0	0.0	0.0
18	AO C(15)	0.0	0.0	0.0	0.0
19	AO C(34)	0.0	0.0	0.0	0.0
20	AO C(7)	0.0	0.0	0.0	0.0
21	AO C(4)	0.0	0.0	0.0	0.0
22	AO C(3)	0.0	0.0	0.0	0.0
23	AO C(78)	0.0	0.0	0.0	0.0
24	AO C(75)	0.0	0.0	0.0	0.0
25	AO C(71)	0.0	0.0	0.0	0.0
26	AO C(17)	0.0	0.0	0.0	0.0
27	AO C(60)	0.0	0.0	0.0	0.0
28	AO C(10)	0.0	0.0	0.0	0.0
29	AO C(67)	0.0	0.0	0.0	0.0
30	AO C(58)	0.0	0.0	0.0	0.0
31	AO C(68)	0.0	0.0	0.0	0.0
32	AO C(19)	0.0	0.0	0.0	0.0
33	AO C(56)	0.0	0.0	0.0	0.0
34	AO C(43)	0.0	0.0	0.0	0.0
35	AO C(73)	0.0	0.0	0.0	0.0
36	AO C(31)	0.0	0.0	0.0	0.0
37	AO C(54)	0.0	0.0	0.0	0.0
38	AO C(20)	0.0	0.0	0.0	0.0
39	AO C(61)	0.0	–0.1	0.0	0.0
40	AO C(59)	0.0	0.0	–0.1	0.0
41	AO C(47)	0.0	0.0	0.0	0.0
42	AO Si(52)	78.0	79.8	72.3	76.7
43	AO Si(52)	77.6	79.2	71.5	76.1
44	AO Si(52)	76.7	62.5	86.0	75.1
45	AO Si(52)	66.3	71.9	88.0	75.4
46	AO Li(49)	–0.1	–0.1	0.1	0.0
47	BOND H(42)–C(35)	0.0	0.0	0.0	0.0
48	BOND H(6)–C(11)	0.0	0.0	0.0	0.0

49	BOND H(84)–C(81)	0.0	0.0	0.0	0.0
50	BOND H(2)–C(4)	0.1	0.0	0.0	0.0
51	BOND C(10)–C(4)	0.0	0.0	0.0	0.0
52	BOND C(56)–C(61)	1.2	0.0	–3.5	–0.8
53	BOND H(72)–C(67)	0.0	0.1	0.1	0.1
54	BOND H(24)–C(35)	0.0	0.0	0.0	0.0
55	BOND C(31)–C(19)	0.1	0.1	0.5	0.2
56	BOND H(83)–C(79)	0.0	0.0	0.1	0.0
57	BOND H(16)–C(15)	0.0	0.1	0.0	0.0
58	BOND O(41)–C(38)	0.2	0.1	0.1	0.1
59	BOND H(66)–C(69)	–0.1	0.1	0.0	0.0
60	BOND H(37)–C(29)	0.1	0.0	0.0	0.0
61	BOND H(1)–C(3)	0.0	0.0	0.0	0.0
62	BOND H(23)–C(17)	0.0	0.2	0.0	0.1
63	BOND C(75)–C(68)	–0.2	–0.9	0.4	–0.2
64	BOND H(76)–C(71)	0.1	0.1	0.1	0.1
65	BOND C(68)–C(59)	0.5	0.2	–2.0	–0.4
66	BOND H(85)–C(78)	–0.1	0.1	0.0	0.0
67	BOND H(27)–C(31)	0.1	0.0	0.0	0.0
68	BOND C(47)–C(43)	–0.2	–0.4	0.4	0.0
69	BOND H(50)–C(40)	0.0	0.0	0.0	0.0
70	BOND H(28)–C(39)	0.1	0.0	0.0	0.0
71	BOND H(86)–C(81)	–0.1	0.0	0.0	0.0
72	BOND H(18)–C(22)	0.0	0.0	0.1	0.0
73	BOND H(64)–C(65)	0.0	–0.1	–0.1	0.0
74	BOND H(13)–C(11)	0.0	0.0	0.0	0.0
75	BOND C(3)–C(7)	0.3	–0.1	0.5	0.2
76	BOND C(31)–C(43)	0.0	0.0	–0.1	0.0
77	BOND H(53)–C(58)	–0.1	0.1	0.0	0.0
78	BOND C(73)–C(78)	–1.1	–0.6	0.2	–0.5
79	BOND H(82)–C(75)	0.0	0.0	0.0	0.0
80	BOND H(9)–C(19)	0.0	0.0	0.0	0.0
81	BOND H(57)–C(60)	–0.1	0.2	0.0	0.0
82	BOND C(20)–C(34)	–0.2	–0.3	0.7	0.1
83	BOND H(30)–C(38)	–0.1	0.0	0.1	0.0
84	BOND H(70)–C(69)	–0.1	–0.1	0.1	0.0
85	BOND H(8)–C(15)	0.0	0.0	0.0	0.0
86	BOND O(62)–C(69)	0.2	0.0	0.1	0.1
87	BOND C(35)–C(40)	0.0	–0.1	0.0	0.0
88	BOND H(5)–C(7)	0.0	0.1	0.0	0.0
89	BOND O(32)–C(22)	0.1	0.1	0.1	0.1
90	BOND C(71)–C(60)	–0.4	0.0	–0.8	–0.4
91	BOND C(58)–C(54)	0.1	–0.6	–1.0	–0.5
92	BOND C(20)–C(34)	–1.0	–0.9	2.1	0.1
93	BOND H(33)–C(40)	0.0	0.0	0.0	0.0
94	BOND C(4)–C(3)	0.0	–0.1	0.0	0.0
95	BOND C(81)–C(79)	0.0	0.0	0.0	0.0
96	LP O(32)	–0.3	–0.4	–0.1	–0.3
97	BOND C(7)–C(17)	0.0	0.1	–0.1	0.0
98	BOND O(62)–C(65)	0.0	0.1	0.2	0.1
99	BOND H(26)–C(22)	0.0	0.0	0.0	0.0
100	BOND C(10)–C(4)	–0.4	0.0	–0.1	–0.2
101	BOND C(40)–C(39)	0.0	–0.2	0.0	–0.1
102	BOND H(45)–C(56)	0.3	–0.6	–0.5	–0.3
103	BOND O(41)–C(39)	–0.1	0.0	0.2	0.0
104	BOND N(36)–C(21)	–1.6	1.2	–1.2	–0.5
105	BOND H(44)–C(54)	–0.3	–0.3	–1.4	–0.7
106	BOND C(69)–C(81)	–0.1	0.0	0.0	0.0
107	BOND C(11)–C(15)	0.0	0.0	0.0	0.0
108	BOND C(68)–C(59)	–1.1	–1.2	–4.9	–2.4
109	BOND C(71)–C(78)	–0.1	–0.1	–0.1	–0.1
110	BOND C(10)–C(21)	0.1	0.2	0.7	0.3

111	BOND C(34)–C(47)	–0.5	–0.7	–0.1	–0.5
112	BOND H(12)–C(20)	0.0	0.0	–0.1	0.0
113	BOND C(67)–C(58)	–0.1	0.0	–0.1	–0.1
114	BOND C(61)–C(73)	–0.5	–3.6	–4.7	–2.9
115	BOND C(20)–C(19)	–0.1	0.1	–0.1	0.0
116	BOND H(46)–C(39)	–0.2	–0.4	0.0	–0.2
117	BOND H(80)–C(79)	0.0	0.0	0.0	0.0
118	BOND C(38)–C(35)	–0.1	–0.1	0.1	0.0
119	BOND C(79)–C(65)	0.0	0.0	–0.1	0.0
120	BOND C(71)–C(60)	0.0	0.0	0.1	0.0
121	BOND C(11)–C(22)	0.0	0.0	0.0	0.0
122	BOND C(75)–C(67)	0.3	–0.1	–0.4	–0.1
123	BOND H(25)–C(29)	–0.1	–0.1	–0.1	–0.1
124	LP O(41)	–0.2	–0.2	0.1	–0.1
125	BOND C(3)–C(7)	0.1	0.0	–0.1	0.0
126	LP O(41)	0.0	–0.2	0.1	0.0
127	BOND H(63)–C(65)	0.1	0.0	0.0	0.0
128	BOND C(15)–C(29)	0.0	–0.1	–0.1	–0.1
129	BOND C(31)–C(19)	0.3	–0.1	0.4	0.2
130	LP O(62)	0.4	0.3	0.1	0.2
131	BOND C(73)–C(78)	0.7	–0.6	–0.6	–0.2
132	BOND C(60)–C(56)	0.2	–1.8	0.0	–0.5
133	BOND O(32)–C(29)	0.0	–0.1	0.2	0.0
134	BOND C(75)–C(67)	0.0	0.6	0.3	0.3
135	BOND C(17)–C(21)	–4.3	0.0	–0.9	–1.7
136	BOND H(51)–C(43)	0.0	0.0	0.0	0.0
137	BOND N(36)–Si(52)	–83.2	–31.5	–100.8	–71.9
138	BOND H(55)–C(47)	0.3	–0.2	0.3	0.1
139	BOND H(74)–C(68)	–0.5	–0.1	0.8	0.1
140	BOND C(59)–Si(52)	–85.1	–77.5	–170.1	–110.9
141	BOND N(36)–C(34)	–0.9	1.6	7.9	2.9
142	BOND H(48)–C(38)	0.0	0.0	0.1	0.0
143	LP O(62)	–0.6	–0.5	–0.1	–0.4
144	LP O(32)	0.1	0.1	0.1	0.1
145	BOND H(77)–C(73)	–0.3	–0.6	–0.3	–0.4
146	BOND H(14)–C(10)	–0.1	0.1	–0.1	0.0
147	BOND C(56)–C(61)	–2.0	–2.6	–8.2	–4.3
148	BOND C(17)–C(21)	–0.9	1.3	1.0	0.5
149	BOND C(61)–Si(52)	–70.2	–123.1	–134.9	–109.4
150	BOND C(58)–C(54)	–0.2	–0.4	–0.2	–0.3
151	BOND C(59)–C(54)	–1.8	–3.0	–4.9	–3.2
152	BOND C(47)–C(43)	0.0	0.2	0.5	0.2
153	BOND N(36)–C(34)	–2.9	–1.9	–2.7	–2.5
154	BOND Si(52)–Li(49)	–311.5	–173.9	8.1	–159.1

Table 133. MO contributions to σ in principal axes for Si in **4** [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(7)	481.9	481.9	481.9	481.9
2	AO N(8)	0.0	0.0	0.0	0.0
3	AO C(17)	0.0	0.0	0.0	0.0
4	AO C(9)	0.0	0.0	0.0	0.0
5	AO C(5)	0.0	0.0	0.0	0.0
6	AO C(4)	0.0	0.0	0.0	0.0
7	AO C(13)	0.0	0.0	0.0	0.0
8	AO C(6)	0.0	0.0	0.0	0.0
9	AO C(3)	0.0	0.0	0.0	0.0
10	AO C(14)	0.0	0.0	0.0	0.0
11	AO C(1)	0.0	0.0	0.0	0.0
12	AO C(12)	0.0	0.0	0.0	0.0

13	AO C(15)	0.0	0.0	0.0	0.0
14	AO C(16)	0.0	0.0	0.0	0.0
15	AO C(2)	0.0	0.0	–0.1	0.0
16	AO C(18)	0.0	0.0	0.0	0.0
17	AO C(11)	0.0	–0.1	0.0	0.0
18	AO C(10)	0.0	0.0	0.0	0.0
19	AO Si(7)	68.3	69.5	86.7	74.8
20	AO Si(7)	83.3	82.3	65.2	76.9
21	AO Si(7)	76.0	70.1	80.5	75.5
22	AO Si(7)	68.8	72.3	84.1	75.1
23	AO Li(19)	–0.1	–0.1	0.1	0.0
24	BOND H(29)–C(10)	0.3	0.2	–0.1	0.1
25	BOND H(37)–C(5)	0.0	0.0	0.1	0.0
26	BOND C(13)–C(12)	–0.6	0.0	–0.1	–0.2
27	BOND H(32)–C(18)	0.3	0.2	0.3	0.2
28	BOND C(6)–C(1)	–0.4	–0.7	–0.9	–0.7
29	BOND H(36)–C(4)	–0.1	0.0	0.2	0.0
30	BOND H(24)–C(16)	0.0	–0.4	–1.0	–0.5
31	BOND H(25)–C(15)	–0.1	0.2	0.0	0.0
32	BOND H(30)–C(10)	–0.1	0.0	0.0	0.0
33	BOND H(33)–C(18)	0.0	0.1	–0.3	–0.1
34	BOND C(4)–C(3)	–0.1	–0.6	0.0	–0.2
35	BOND C(3)–C(2)	–1.7	–2.6	–1.4	–1.9
36	BOND H(26)–C(14)	0.1	0.1	0.1	0.1
37	BOND H(28)–C(13)	0.0	0.1	0.1	0.0
38	BOND H(21)–C(17)	–3.9	0.8	–0.7	–1.2
39	BOND H(38)–C(6)	0.0	–0.1	–0.1	0.0
40	BOND H(22)–C(9)	0.3	0.5	1.1	0.6
41	BOND C(11)–C(12)	–1.1	–2.4	–4.5	–2.7
42	BOND N(8)–C(9)	–5.5	–0.6	–4.1	–3.4
43	BOND H(35)–C(3)	–1.1	–2.7	0.0	–1.2
44	BOND C(14)–C(13)	–0.1	–0.1	–0.1	–0.1
45	BOND C(4)–C(5)	–0.2	–0.2	0.0	–0.1
46	BOND C(15)–C(14)	0.2	0.5	0.1	0.3
47	BOND C(11)–C(16)	0.1	1.7	–3.7	–0.7
48	BOND H(34)–C(18)	0.1	0.2	0.0	0.1
49	BOND C(6)–C(5)	0.2	0.3	0.7	0.4
50	BOND C(13)–C(12)	0.6	–0.4	–0.5	–0.1
51	BOND H(20)–C(17)	–2.5	0.3	0.1	–0.7
52	BOND H(31)–C(10)	0.1	0.0	0.1	0.1
53	BOND C(2)–C(1)	0.0	–2.9	–1.2	–1.4
54	BOND C(10)–C(9)	–0.6	–0.5	–0.9	–0.7
55	BOND C(15)–C(16)	–0.1	–1.4	–0.6	–0.7
56	BOND H(39)–C(1)	–0.4	–0.7	–0.5	–0.5
57	LP N(8)	–9.2	8.7	–9.3	–3.3
58	BOND H(23)–C(9)	–0.4	–0.6	0.1	–0.3
59	BOND N(8)–C(17)	–4.7	1.8	–3.1	–2.0
60	BOND C(18)–C(17)	–0.3	1.6	0.0	0.4
61	BOND C(4)–C(3)	–0.2	–1.0	0.2	–0.3
62	BOND H(27)–C(12)	–0.5	0.2	–1.2	–0.5
63	BOND C(11)–C(16)	0.1	0.6	–6.0	–1.8
64	BOND C(11)–Si(7)	–75.4	–127.7	–136.8	–113.3
65	BOND C(15)–C(14)	0.4	0.5	–0.4	0.2
66	BOND C(6)–C(5)	0.5	–0.1	0.8	0.4
67	BOND C(2)–Si(7)	–66.5	–96.2	–163.4	–108.7
68	BOND C(2)–C(1)	0.9	–3.3	–2.5	–1.6
69	BOND N(8)–Si(7)	–118.3	–43.6	–95.8	–85.9
70	BOND Si(7)–Li(19)	–256.8	–182.4	–4.7	–148.0

Table 134. MO contributions to σ in principal axes for Si in **5** [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(7)	481.9	481.9	481.9	481.9
2	AO N(8)	0.0	0.0	0.0	0.0
3	AO N(11)	0.0	0.0	0.0	0.0
4	AO C(14)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(12)	0.0	0.0	0.0	0.0
7	AO C(16)	0.0	0.0	0.0	0.0
8	AO C(3)	0.0	0.0	0.0	0.0
9	AO C(4)	0.0	0.0	0.0	0.0
10	AO C(2)	0.0	0.0	0.0	0.0
11	AO C(5)	0.0	0.0	0.0	0.0
12	AO C(1)	0.0	0.0	0.0	0.0
13	AO C(15)	0.0	0.0	0.0	0.0
14	AO C(17)	0.0	0.0	0.0	0.0
15	AO C(10)	0.0	0.0	0.0	0.0
16	AO C(6)	0.0	–0.1	0.0	0.0
17	AO C(26)	0.0	0.0	0.0	0.0
18	AO Si(7)	64.4	75.1	84.2	74.5
19	AO Si(7)	78.0	66.7	82.3	75.7
20	AO Si(7)	84.2	84.0	62.4	76.8
21	AO Si(7)	71.9	66.8	88.0	75.6
22	AO Li(18)	–0.1	–0.1	0.1	0.0
23	BOND H(35)–C(10)	0.2	0.1	0.4	0.2
24	BOND H(41)–C(26)	0.5	0.1	0.2	0.3
25	BOND H(30)–C(1)	–0.4	–0.6	–1.2	–0.7
26	BOND N(11)–Si(7)	–76.0	–53.6	–72.3	–67.3
27	BOND H(32)–C(17)	0.1	0.2	0.1	0.1
28	BOND H(31)–C(2)	–0.1	0.1	0.0	0.0
29	BOND H(24)–C(4)	–0.1	0.1	0.0	0.0
30	BOND H(19)–C(9)	–0.4	–0.5	–0.1	–0.3
31	BOND H(40)–C(15)	–0.3	0.3	–0.2	–0.1
32	BOND N(11)–C(14)	–4.3	0.8	–4.3	–2.6
33	BOND H(13)–C(12)	0.0	–0.5	–0.2	–0.2
34	BOND C(4)–C(3)	0.4	0.7	–0.5	0.2
35	BOND H(29)–C(3)	0.1	0.1	0.1	0.1
36	BOND H(33)–C(17)	–0.1	0.1	–0.1	0.0
37	BOND H(25)–C(12)	0.0	–0.9	–0.1	–0.3
38	BOND H(27)–C(14)	–1.5	1.5	0.1	0.0
39	BOND C(6)–C(1)	–0.9	–4.2	–3.3	–2.8
40	BOND C(17)–C(16)	–0.8	–0.1	–0.9	–0.6
41	BOND H(28)–C(14)	–2.8	–0.7	–0.5	–1.3
42	BOND H(34)–C(17)	0.0	0.2	0.0	0.1
43	BOND C(6)–C(5)	–0.4	1.1	–6.1	–1.8
44	BOND C(3)–C(2)	–0.2	0.0	–0.1	–0.1
45	BOND H(39)–C(15)	0.1	0.1	0.4	0.2
46	BOND H(38)–C(15)	–0.1	0.3	–0.1	0.1
47	BOND H(37)–C(10)	0.3	0.0	0.0	0.1
48	BOND H(21)–C(16)	0.8	0.7	–0.1	0.5
49	BOND H(23)–C(5)	–0.2	–0.4	–1.0	–0.5
50	BOND H(36)–C(10)	0.2	–0.3	–0.3	–0.1
51	BOND C(2)–C(1)	0.4	–0.4	–0.4	–0.1
52	BOND C(15)–C(14)	0.3	–0.1	0.2	0.1
53	BOND N(8)–C(9)	–2.6	1.9	–4.5	–1.8
54	BOND H(43)–C(26)	0.1	0.0	0.2	0.1
55	BOND H(42)–C(26)	0.0	–0.2	0.0	–0.1
56	BOND N(8)–C(16)	–4.6	1.1	–9.2	–4.3
57	BOND C(4)–C(5)	0.2	–1.1	–0.8	–0.6
58	BOND H(20)–C(9)	–2.9	–0.4	0.2	–1.0
59	LP N(8)	–1.1	2.8	–24.6	–7.6
60	BOND C(26)–C(12)	0.5	–0.5	1.0	0.3

61	BOND N(11)–C(12)	–5.1	–2.6	–5.2	–4.3
62	BOND C(6)–Si(7)	–45.7	–172.9	–132.0	–116.9
63	BOND C(4)–C(3)	0.1	0.9	–0.1	0.3
64	BOND C(10)–C(9)	–0.1	0.8	0.6	0.4
65	BOND H(22)–C(16)	–0.2	0.0	–1.4	–0.5
66	BOND C(6)–C(5)	0.7	0.4	–2.7	–0.5
67	BOND C(2)–C(1)	–0.2	–0.3	–0.6	–0.4
68	BOND N(11)–Si(7)	–27.8	–6.1	–43.6	–25.8
69	BOND Si(7)–Li(18)	–252.0	–206.2	–2.5	–153.6
70	BOND N(8)–Si(7)	–93.7	–31.8	–131.5	–85.7

Table 135. MO contributions to σ in principal axes for Si in **6** [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(7)	481.9	481.9	481.9	481.9
2	AO N(14)	0.0	0.0	0.0	0.0
3	AO C(15)	0.0	0.0	0.0	0.0
4	AO C(21)	0.0	0.0	0.0	0.0
5	AO C(19)	0.0	0.0	0.0	0.0
6	AO C(17)	0.0	0.0	0.0	0.0
7	AO C(20)	0.0	0.0	0.0	0.0
8	AO C(18)	0.0	0.0	0.0	0.0
9	AO C(16)	0.0	0.0	0.0	0.0
10	AO C(10)	0.0	0.0	0.0	0.0
11	AO C(11)	0.0	0.0	0.0	0.0
12	AO C(25)	0.0	0.0	0.0	0.0
13	AO C(13)	0.0	0.0	0.0	0.0
14	AO C(12)	0.0	0.0	0.0	0.0
15	AO C(23)	0.0	0.0	0.0	0.0
16	AO C(6)	0.0	0.0	0.0	0.0
17	AO C(9)	0.0	0.0	0.0	0.0
18	AO C(1)	0.0	0.0	0.0	0.0
19	AO C(5)	0.0	0.0	0.0	0.0
20	AO C(4)	0.0	0.0	0.0	0.0
21	AO C(26)	0.0	0.0	0.0	0.0
22	AO C(3)	0.0	0.0	0.0	0.0
23	AO C(24)	0.0	0.0	0.0	0.0
24	AO C(8)	0.0	–0.1	–0.1	0.0
25	AO C(22)	0.0	0.0	0.0	0.0
26	AO C(2)	0.0	0.0	–0.1	0.0
27	AO Si(7)	77.3	80.2	72.5	76.7
28	AO Si(7)	75.1	77.5	69.9	74.2
29	AO Si(7)	75.6	63.1	85.3	74.7
30	AO Si(7)	67.0	70.2	88.8	75.3
31	AO Li(27)	–0.1	0.0	0.1	0.0
32	BOND C(18)–C(19)	–0.3	0.0	–0.1	–0.1
33	BOND N(14)–Si(7)	–64.2	–22.5	–108.2	–65.0
34	BOND C(10)–C(9)	0.5	–0.5	–0.8	–0.3
35	BOND C(2)–C(3)	–0.1	–0.7	–4.4	–1.7
36	BOND H(30)–C(24)	0.1	0.1	0.0	0.1
37	BOND H(37)–C(20)	0.1	0.1	0.1	0.1
38	BOND H(41)–C(12)	–0.1	0.1	0.0	0.0
39	BOND C(4)–C(5)	0.5	0.4	–0.1	0.2
40	BOND C(12)–C(11)	–0.2	0.6	–0.5	0.0
41	BOND H(32)–C(26)	0.1	0.0	–0.1	0.0
42	BOND C(6)–C(5)	0.0	–0.1	0.0	–0.1
43	BOND H(45)–C(5)	0.0	0.1	0.1	0.1
44	BOND H(31)–C(25)	0.0	0.0	0.0	0.0
45	BOND H(35)–C(18)	0.0	0.0	0.0	0.0
46	BOND C(20)–C(19)	0.1	0.1	–0.1	0.1

47	BOND C(26)–C(25)	0.0	0.0	0.0	0.0
48	BOND C(11)–C(10)	–0.1	–0.1	–0.1	–0.1
49	BOND C(8)–C(13)	1.8	–1.2	–1.5	–0.3
50	BOND C(4)–C(3)	–1.0	–0.7	–1.1	–0.9
51	BOND C(12)–C(13)	0.5	–1.5	0.4	–0.2
52	BOND H(36)–C(19)	0.0	0.1	0.0	0.0
53	BOND H(34)–C(17)	0.1	0.0	0.0	0.1
54	BOND H(46)–C(6)	0.1	–0.1	0.1	0.0
55	BOND C(24)–C(25)	0.0	0.3	0.4	0.2
56	BOND C(6)–C(1)	–0.7	0.3	0.4	0.0
57	BOND C(16)–C(17)	–0.8	0.0	–0.5	–0.4
58	BOND H(29)–C(23)	0.0	0.0	0.0	0.0
59	BOND N(14)–C(21)	–1.2	–1.6	–3.4	–2.0
60	BOND H(33)–C(16)	0.0	0.1	–0.1	0.0
61	BOND C(18)–C(17)	0.0	–0.1	0.0	0.0
62	BOND H(38)–C(9)	–0.9	–1.0	–0.7	–0.9
63	BOND H(39)–C(10)	0.0	0.0	0.0	0.0
64	BOND C(10)–C(9)	–0.6	–0.8	0.2	–0.4
65	BOND C(8)–C(13)	–2.6	–0.6	–6.4	–3.2
66	BOND C(24)–C(25)	0.3	–0.1	0.5	0.2
67	BOND C(4)–C(5)	0.2	0.2	0.2	0.2
68	BOND C(18)–C(19)	0.1	0.0	0.6	0.2
69	BOND H(40)–C(11)	0.1	0.1	0.1	0.1
70	BOND C(20)–C(15)	–1.3	1.0	1.5	0.4
71	BOND C(21)–C(22)	–0.6	–0.7	–0.2	–0.5
72	BOND C(20)–C(15)	–7.2	–0.5	–1.0	–2.9
73	BOND H(42)–C(13)	0.6	–1.6	–0.1	–0.3
74	BOND H(47)–C(1)	–0.5	0.3	0.5	0.1
75	BOND C(26)–C(21)	0.8	–0.4	0.8	0.4
76	BOND C(15)–C(16)	0.1	0.1	0.9	0.4
77	BOND C(12)–C(11)	0.5	0.5	0.7	0.6
78	BOND C(2)–C(1)	–1.8	–1.3	–4.1	–2.4
79	BOND C(24)–C(23)	0.0	0.0	–0.1	0.0
80	BOND C(8)–Si(7)	–59.4	–145.5	–139.6	–114.8
81	BOND C(8)–C(9)	–1.1	–4.1	–3.8	–3.0
82	BOND H(44)–C(4)	–0.1	0.1	0.0	0.0
83	BOND C(22)–C(23)	–0.2	0.2	0.5	0.2
84	BOND N(14)–C(21)	–0.3	0.6	9.3	3.2
85	BOND C(16)–C(17)	–0.3	0.1	0.1	–0.1
86	BOND N(14)–C(15)	–1.1	0.9	–1.3	–0.5
87	BOND C(26)–C(21)	–1.5	–0.8	1.6	–0.2
88	BOND H(43)–C(3)	–0.3	–0.2	–1.3	–0.6
89	BOND C(2)–C(3)	–0.9	2.0	–4.4	–1.1
90	BOND C(22)–C(23)	0.0	–0.2	0.5	0.1
91	BOND C(6)–C(1)	0.3	0.1	0.0	0.1
92	BOND H(28)–C(22)	–0.1	0.1	0.3	0.1
93	BOND C(2)–Si(7)	–111.4	–66.9	–177.3	–118.5
94	BOND Si(7)–Li(27)	–312.7	–185.3	8.0	–163.3

Table 136. MO contributions to σ in principal axes for Si in Me_3SiH [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO C(1)	0.0	0.0	0.1	0.0
3	AO C(3)	0.0	0.0	0.0	0.0
4	AO C(5)	0.0	0.1	0.0	0.0
5	AO Si(2)	76.0	83.7	67.3	75.7
6	AO Si(2)	82.8	65.3	80.5	76.2
7	AO Si(2)	64.1	79.6	80.8	74.8

8	AO Si(2)	80.1	74.4	74.3	76.3
9	BOND H(7)–C(1)	–0.8	–1.1	0.7	–0.4
10	BOND H(12)–C(3)	–3.0	0.8	1.4	–0.3
11	BOND H(9)–C(5)	–0.8	2.6	–3.0	–0.4
12	BOND H(4)–Si(2)	7.6	–136.0	–135.0	–87.8
13	BOND H(11)–C(5)	–3.0	2.9	–0.7	–0.3
14	BOND H(10)–C(5)	–0.8	1.5	–1.9	–0.4
15	BOND H(8)–C(1)	–0.8	–3.1	2.7	–0.4
16	BOND H(6)–C(1)	–3.0	–0.4	2.6	–0.3
17	BOND H(13)–C(3)	–0.8	–2.1	1.7	–0.4
18	BOND H(14)–C(3)	–0.8	1.0	–1.4	–0.4
19	BOND C(1)–Si(2)	–154.1	–162.0	–27.4	–114.5
20	BOND C(5)–Si(2)	–152.8	–14.7	–176.1	–114.6
21	BOND C(3)–Si(2)	–153.8	–108.2	–82.4	–114.8

Table 137. MO contributions to σ in principal axes for Si in Me_3SiCl [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(2)	0.0	0.0	0.0	0.0
2	AO Si(1)	481.9	481.9	481.9	481.9
3	AO C(3)	0.0	0.1	0.0	0.0
4	AO C(4)	0.1	0.0	0.0	0.0
5	AO C(5)	0.0	0.0	0.0	0.0
6	AO Cl(2)	–0.2	–0.3	0.1	–0.1
7	AO Cl(2)	0.0	0.1	0.1	0.1
8	AO Cl(2)	–0.3	–0.3	0.1	–0.2
9	AO Cl(2)	0.3	0.3	0.1	0.2
10	AO Si(1)	78.2	74.1	80.2	77.5
11	AO Si(1)	82.5	73.0	72.3	75.9
12	AO Si(1)	80.2	75.7	65.1	73.7
13	AO Si(1)	66.4	85.8	80.3	77.5
14	LP Cl(2)	–3.4	–2.7	7.3	0.4
15	BOND H(8)–C(3)	–3.9	3.5	–0.9	–0.5
16	BOND H(9)–C(4)	3.5	–3.9	–0.9	–0.5
17	BOND H(12)–C(5)	0.5	0.0	–2.5	–0.7
18	BOND H(10)–C(4)	1.2	–1.7	–0.9	–0.5
19	BOND H(6)–C(3)	–3.0	3.5	–2.5	–0.7
20	BOND H(7)–C(3)	–2.2	1.7	–0.9	–0.5
21	BOND H(13)–C(5)	–2.0	1.5	–0.9	–0.5
22	BOND H(14)–C(5)	2.0	–2.5	–0.9	–0.5
23	BOND C(4)–Si(1)	–25.5	–226.9	–160.2	–137.5
24	BOND H(11)–C(4)	3.3	–2.7	–2.5	–0.7
25	BOND Cl(2)–Si(1)	–119.8	–119.7	5.3	–78.1
26	LP Cl(2)	–5.3	–0.9	7.3	0.4
27	LP Cl(2)	–0.6	–5.7	7.3	0.3
28	BOND C(3)–Si(1)	–234.7	–16.6	–160.7	–137.3
29	BOND C(5)–Si(1)	–117.1	–135.3	–159.9	–137.4

Table 138. MO contributions to σ in principal axes for Si in Me_3SiLi [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(1)	481.9	481.9	481.9	481.9
2	AO C(4)	0.0	0.0	0.0	0.0
3	AO C(3)	0.1	0.0	0.0	0.0
4	AO C(5)	0.0	0.0	0.0	0.0
5	AO Si(1)	64.6	75.3	81.8	73.9
6	AO Si(1)	83.2	83.2	62.1	76.2

7	AO Si(1)	70.8	67.6	83.2	73.9
8	AO Si(1)	73.8	66.5	81.3	73.9
9	AO Li(2)	–0.1	–0.1	0.2	0.0
10	BOND H(10)–C(4)	0.8	–1.5	–0.9	–0.6
11	BOND C(3)–Si(1)	–21.1	–155.8	–144.1	–107.0
12	BOND H(7)–C(3)	2.6	–3.3	–1.0	–0.6
13	BOND C(5)–Si(1)	–147.4	–31.0	–142.8	–107.0
14	BOND H(12)–C(5)	0.4	2.3	–2.9	–0.1
15	BOND H(14)–C(5)	–3.3	2.6	–0.9	–0.6
16	BOND H(8)–C(3)	1.5	–2.2	–1.0	–0.6
17	BOND H(6)–C(3)	2.5	0.3	–2.9	–0.1
18	BOND H(9)–C(4)	–2.1	1.4	–1.0	–0.5
19	BOND H(13)–C(5)	–1.5	0.9	–1.0	–0.6
20	BOND H(11)–C(4)	1.2	1.5	–2.9	–0.1
21	BOND C(4)–Si(1)	–97.4	–79.0	–144.4	–106.9
22	BOND Si(1)–Li(2)	–175.5	–175.6	10.6	–113.5

Table 139. MO contributions to σ in principal axes for Si in Me_4Si [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(1)	481.9	481.9	481.9	481.9
2	AO C(5)	0.0	0.0	0.1	0.0
3	AO C(2)	0.0	0.0	0.0	0.0
4	AO C(4)	0.0	0.0	0.0	0.0
5	AO C(3)	0.1	0.0	0.0	0.0
6	AO Si(1)	68.3	77.2	81.8	75.8
7	AO Si(1)	83.4	74.5	69.9	75.9
8	AO Si(1)	81.7	77.4	69.3	76.1
9	AO Si(1)	71.0	74.7	82.3	76.0
10	BOND H(6)–C(2)	–3.0	0.9	0.8	–0.4
11	BOND H(15)–C(5)	–1.2	–1.3	1.2	–0.4
12	BOND H(9)–C(3)	2.9	–2.4	–1.8	–0.4
13	BOND H(12)–C(4)	0.1	1.4	–2.7	–0.4
14	BOND C(2)–Si(1)	–160.3	–78.9	–96.8	–112.0
15	BOND H(13)–C(4)	0.2	0.2	–1.7	–0.4
16	BOND H(16)–C(5)	–1.5	–2.3	2.6	–0.4
17	BOND H(11)–C(3)	2.0	–1.8	–1.5	–0.4
18	BOND C(5)–Si(1)	–165.5	–155.1	–16.3	–112.3
19	BOND H(10)–C(3)	3.0	–1.5	–2.9	–0.4
20	BOND H(17)–C(5)	–2.9	–1.2	2.9	–0.4
21	BOND H(8)–C(2)	–1.1	1.6	–1.7	–0.4
22	BOND H(14)–C(4)	–2.4	2.3	–1.2	–0.4
23	BOND H(7)–C(2)	–1.1	–1.0	0.8	–0.4
24	BOND C(3)–Si(1)	–0.9	–164.5	–170.5	–112.0
25	BOND C(4)–Si(1)	–122.5	–49.9	–164.3	–112.2

Table 140. MO contributions to σ in principal axes for Si in $(MeO)Me_2SiH$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(1)	481.9	481.9	481.9	481.9
2	AO O(3)	0.0	0.0	0.1	0.0
3	AO C(5)	0.0	0.0	0.0	0.0
4	AO C(4)	0.0	0.0	0.0	0.0
5	AO C(2)	0.0	0.0	0.0	0.0
6	AO Si(1)	78.7	88.0	69.2	78.6
7	AO Si(1)	87.5	62.9	83.4	78.0
8	AO Si(1)	82.1	80.9	68.9	77.3

9	AO Si(1)	64.0	86.6	79.5	76.7
10	BOND H(6)–Si(1)	–0.7	–193.7	–128.1	–107.5
11	BOND H(10)–C(4)	–3.1	2.4	–0.5	–0.4
12	LP O(3)	–0.6	7.8	13.5	6.9
13	BOND H(8)–C(2)	–0.9	–0.9	0.3	–0.5
14	BOND H(14)–C(5)	–0.2	–3.0	1.4	–0.6
15	BOND H(15)–C(5)	–0.7	–0.5	1.5	0.1
16	BOND H(13)–C(5)	–1.2	–2.9	0.2	–1.3
17	BOND O(3)–Si(1)	–137.1	–146.8	0.1	–94.6
18	BOND H(11)–C(4)	0.1	–0.3	–1.1	–0.4
19	BOND H(12)–C(4)	–1.4	1.5	–2.7	–0.9
20	BOND H(9)–C(2)	–3.3	1.8	0.3	–0.4
21	BOND H(7)–C(2)	–3.1	2.3	–2.6	–1.1
22	BOND C(4)–Si(1)	–170.8	–69.5	–168.9	–136.4
23	BOND C(2)–Si(1)	–207.5	–69.1	–135.4	–137.3
24	LP O(3)	8.5	1.5	14.5	8.2
25	BOND O(3)–C(5)	–3.6	–8.5	4.3	–2.6

Table 141. MO contributions to σ in principal axes for Si in (MeO)Me_2SiCl [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(3)	0.0	0.0	0.0	0.0
2	AO Si(1)	481.9	481.9	481.9	481.9
3	AO O(4)	0.0	0.1	0.0	0.0
4	AO C(6)	0.0	0.0	0.0	0.0
5	AO C(2)	0.0	0.0	0.0	0.0
6	AO C(5)	0.0	0.0	0.1	0.0
7	AO Cl(3)	0.1	–0.2	–0.3	–0.1
8	AO Cl(3)	0.0	0.1	0.1	0.1
9	AO Cl(3)	0.1	–0.4	–0.3	–0.2
10	AO Cl(3)	0.1	0.3	0.3	0.2
11	AO Si(1)	74.6	74.3	87.5	78.8
12	AO Si(1)	69.9	82.4	79.8	77.4
13	AO Si(1)	86.7	87.6	65.5	79.9
14	AO Si(1)	79.1	64.9	90.0	78.0
15	BOND H(13)–C(6)	–1.5	0.1	–2.2	–1.2
16	LP Cl(3)	7.7	–4.6	–7.4	–1.4
17	BOND H(7)–C(2)	–1.6	–2.7	1.2	–1.0
18	LP O(4)	8.7	12.0	3.6	8.1
19	BOND H(10)–C(5)	–2.7	–2.7	3.0	–0.8
20	BOND H(15)–C(6)	–0.4	0.6	–0.2	0.0
21	BOND O(4)–C(6)	–4.7	5.0	–13.8	–4.5
22	BOND H(14)–C(6)	–1.0	0.9	0.1	0.0
23	BOND C(2)–Si(1)	–172.8	–142.5	–129.1	–148.1
24	BOND H(12)–C(5)	–3.5	–2.8	2.4	–1.3
25	BOND H(11)–C(5)	–1.0	–2.1	1.5	–0.5
26	BOND H(9)–C(2)	–2.8	0.6	0.0	–0.7
27	BOND H(8)–C(2)	0.1	1.2	–3.0	–0.5
28	LP Cl(3)	5.9	–2.8	–2.7	0.1
29	BOND C(5)–Si(1)	–211.5	–227.4	–9.7	–149.5
30	BOND Cl(3)–Si(1)	–2.3	–117.6	–154.3	–91.4
31	LP Cl(3)	7.5	0.8	–5.9	0.8
32	BOND O(4)–Si(1)	–136.7	–2.0	–153.2	–97.3
33	LP O(4)	0.1	12.6	–1.7	3.7

Table 142. MO contributions to σ in principal axes for Si in (MeO)Me_2SiLi [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(1)	481.9	481.9	481.9	481.9
2	AO O(4)	0.0	0.0	0.1	0.0
3	AO C(6)	0.0	0.0	0.0	0.0
4	AO C(5)	0.0	0.0	0.0	0.0
5	AO C(2)	0.0	0.0	0.0	0.0
6	AO Si(1)	81.6	74.1	73.2	76.3
7	AO Si(1)	77.9	72.7	78.3	76.3
8	AO Si(1)	67.1	87.7	73.0	75.9
9	AO Si(1)	77.4	82.3	63.6	74.4
10	AO Li(3)	–0.1	0.1	0.0	0.0
11	BOND H(15)–C(6)	–4.5	0.2	1.3	–1.0
12	BOND H(7)–C(2)	2.6	–2.8	–2.7	–1.0
13	BOND C(5)–Si(1)	–91.1	–161.3	–149.7	–134.0
14	BOND H(10)–C(5)	2.1	–2.3	–0.4	–0.2
15	BOND O(4)–C(6)	–6.3	–3.8	4.5	–1.9
16	BOND H(13)–C(6)	–5.0	–1.0	0.2	–1.9
17	BOND H(14)–C(6)	–0.2	–0.7	1.4	0.1
18	LP O(4)	–2.7	6.8	13.6	5.9
19	BOND H(9)–C(2)	2.7	–2.8	–0.6	–0.2
20	BOND H(8)–C(2)	0.1	–0.9	–1.2	–0.7
21	BOND H(11)–C(5)	–0.8	–0.2	–0.9	–0.6
22	BOND H(12)–C(5)	1.6	–2.4	–2.7	–1.2
23	BOND C(2)–Si(1)	–61.8	–186.8	–154.8	–134.5
24	LP O(4)	5.3	4.3	12.2	7.3
25	BOND O(4)–Si(1)	–140.4	–135.0	5.4	–90.0
26	BOND Si(1)–Li(3)	–306.1	–15.4	–143.4	–155.0

Table 143. MO contributions to σ in principal axes for Si in (MeO)Me_2SiMe [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(1)	481.9	481.9	481.9	481.9
2	AO O(3)	0.0	0.0	0.1	0.0
3	AO C(5)	0.0	0.0	0.0	0.0
4	AO C(6)	0.0	0.0	0.0	0.0
5	AO C(2)	0.0	0.0	0.0	0.0
6	AO C(4)	0.0	0.1	0.0	0.0
7	AO Si(1)	85.9	72.0	77.6	78.5
8	AO Si(1)	62.9	88.0	80.0	77.0
9	AO Si(1)	86.6	70.9	75.4	77.6
10	AO Si(1)	81.3	85.4	65.7	77.5
11	BOND H(14)–C(5)	–0.7	–0.8	1.1	–0.1
12	BOND H(9)–C(2)	–0.7	0.1	–1.1	–0.6
13	LP O(3)	3.1	5.8	12.8	7.3
14	BOND H(16)–C(6)	1.9	–2.4	–1.1	–0.5
15	BOND H(12)–C(4)	–4.5	3.2	–2.6	–1.3
16	LP O(3)	1.7	7.2	13.0	7.3
17	BOND H(13)–C(5)	–1.5	–1.9	0.2	–1.1
18	BOND H(15)–C(5)	–0.6	–1.1	1.2	–0.2
19	BOND C(4)–Si(1)	–236.1	–23.8	–139.3	–133.1
20	BOND C(6)–Si(1)	–63.9	–170.2	–156.7	–130.3
21	BOND H(10)–C(4)	–2.7	1.2	–0.2	–0.6
22	BOND H(7)–C(2)	1.5	–2.1	–2.5	–1.0
23	BOND H(17)–C(6)	1.9	–2.3	–2.5	–1.0
24	BOND H(11)–C(4)	–2.3	1.2	–0.3	–0.5
25	BOND H(18)–C(6)	–0.5	–0.1	–1.0	–0.5
26	BOND H(8)–C(2)	2.0	–2.2	–1.2	–0.5
27	BOND O(3)–C(5)	–2.7	–9.6	4.3	–2.7
28	BOND O(3)–Si(1)	–137.2	–135.4	2.3	–90.1

29	BOND C(2)–Si(1)	–69.7	–164.3	–158.6	–130.9

Table 144. MO contributions to σ in principal axes for Si in $(Me_2N)Me_2SiH$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO N(3)	0.0	0.0	0.1	0.0
3	AO C(4)	0.0	0.0	0.0	0.0
4	AO C(10)	0.0	0.0	0.0	0.0
5	AO C(8)	0.0	0.0	0.0	0.0
6	AO C(9)	0.0	0.0	0.0	0.0
7	AO Si(2)	76.5	80.9	74.6	77.3
8	AO Si(2)	69.8	77.9	78.2	75.3
9	AO Si(2)	82.2	71.1	77.4	76.9
10	AO Si(2)	75.1	82.7	70.9	76.2
11	BOND H(1)–Si(2)	6.9	–167.6	–130.7	–97.1
12	BOND H(7)–C(4)	–0.1	–1.2	0.3	–0.3
13	BOND H(19)–C(8)	–2.1	2.1	–2.1	–0.7
14	BOND H(15)–C(9)	–2.1	2.2	–2.1	–0.7
15	BOND H(6)–C(4)	–0.8	–0.5	0.5	–0.3
16	BOND H(13)–C(10)	–0.8	–0.5	0.5	–0.3
17	BOND H(5)–C(4)	–0.1	0.3	0.9	0.3
18	BOND H(11)–C(10)	–0.1	0.3	0.9	0.3
19	BOND H(17)–C(8)	–3.2	1.8	0.0	–0.5
20	BOND H(18)–C(8)	–0.8	–0.7	–0.5	–0.7
21	BOND H(12)–C(10)	–0.1	–1.2	0.3	–0.3
22	BOND H(14)–C(9)	–3.2	1.8	0.0	–0.5
23	BOND H(16)–C(9)	–0.8	–0.7	–0.5	–0.7
24	BOND N(3)–C(4)	–2.3	–6.4	3.7	–1.6
25	BOND N(3)–C(10)	–2.3	–6.5	3.7	–1.7
26	LP N(3)	0.6	–8.5	10.9	1.0
27	BOND C(9)–Si(2)	–179.2	–56.4	–138.2	–124.6
28	BOND C(8)–Si(2)	–177.9	–55.8	–137.8	–123.8
29	BOND N(3)–Si(2)	–130.9	–149.1	–1.8	–93.9

Table 145. MO contributions to σ in principal axes for Si in $(Me_2N)Me_2SiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO Si(2)	481.9	481.9	481.9	481.9
3	AO N(3)	0.0	0.0	0.1	0.0
4	AO C(10)	0.0	0.0	0.0	0.0
5	AO C(4)	0.0	0.0	0.0	0.0
6	AO C(9)	0.0	0.0	0.0	0.0
7	AO C(8)	0.0	0.0	0.0	0.0
8	AO Cl(1)	0.1	–0.2	–0.2	–0.1
9	AO Cl(1)	0.1	0.1	0.1	0.1
10	AO Cl(1)	0.1	–0.4	–0.4	–0.2
11	AO Cl(1)	0.1	0.3	0.3	0.2
12	AO Si(2)	79.9	90.9	63.8	78.2
13	AO Si(2)	71.9	75.5	82.3	76.6
14	AO Si(2)	79.3	64.9	90.1	78.1
15	AO Si(2)	68.0	87.8	74.6	76.8
16	BOND H(13)–C(10)	–0.7	–0.7	0.4	–0.4
17	LP Cl(1)	7.7	–4.3	–2.4	0.3
18	BOND H(5)–C(4)	0.1	0.9	1.0	0.7
19	BOND H(17)–C(8)	–2.5	1.6	–1.7	–0.9

20	BOND H(14)–C(9)	–2.5	1.4	–1.6	–0.9
21	BOND H(6)–C(4)	–0.7	–0.7	0.4	–0.3
22	BOND N(3)–Si(2)	–115.7	–161.6	–8.5	–95.3
23	BOND H(11)–C(10)	0.1	0.9	1.0	0.7
24	BOND N(3)–C(4)	–1.5	–9.7	4.2	–2.3
25	BOND H(7)–C(4)	0.0	–0.4	0.3	0.0
26	BOND H(15)–C(9)	–2.4	2.6	–2.4	–0.7
27	BOND H(19)–C(8)	–2.4	2.7	–2.5	–0.8
28	BOND H(18)–C(8)	–1.2	–0.9	–0.4	–0.8
29	BOND H(16)–C(9)	–1.3	–1.1	–0.2	–0.9
30	BOND N(3)–C(10)	–1.5	–9.8	4.3	–2.3
31	BOND H(12)–C(10)	–0.1	–0.3	0.3	0.0
32	LP Cl(1)	7.4	–5.4	–1.3	0.2
33	LP Cl(1)	6.6	–4.8	–4.2	–0.8
34	BOND C(9)–Si(2)	–191.8	–60.5	–166.0	–139.4
35	BOND C(8)–Si(2)	–191.8	–53.6	–173.1	–139.5
36	BOND Cl(1)–Si(2)	3.3	–137.2	–113.5	–82.4
37	BOND N(3)–Si(2)	–2.2	–39.6	8.8	–11.0

Table 146. MO contributions to σ in principal axes for Si in $(Me_2N)Me_2SiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO N(3)	0.0	0.0	0.1	0.0
3	AO C(10)	0.0	0.0	0.0	0.0
4	AO C(4)	0.0	0.0	0.0	0.0
5	AO C(8)	0.0	0.0	0.0	0.0
6	AO C(9)	0.0	0.0	0.0	0.0
7	AO Si(2)	78.0	75.0	73.5	75.5
8	AO Si(2)	78.2	68.7	79.3	75.4
9	AO Si(2)	68.5	85.3	70.6	74.8
10	AO Si(2)	75.3	79.9	65.8	73.7
11	AO Li(1)	–0.1	0.1	–0.1	0.0
12	BOND N(3)–C(4)	–5.4	–2.7	4.2	–1.3
13	BOND N(3)–C(10)	–5.4	–2.7	4.1	–1.3
14	BOND H(19)–C(8)	2.1	–2.2	–2.2	–0.8
15	BOND H(15)–C(9)	2.1	–2.2	–2.2	–0.8
16	BOND H(7)–C(4)	–4.0	0.2	0.5	–1.1
17	BOND H(13)–C(10)	–0.3	–0.7	0.6	–0.1
18	BOND H(5)–C(4)	–1.7	–0.2	1.0	–0.3
19	BOND H(11)–C(10)	–1.7	–0.2	1.0	–0.3
20	BOND H(6)–C(4)	–0.3	–0.7	0.6	–0.1
21	BOND H(17)–C(8)	1.9	–3.0	0.1	–0.3
22	BOND H(16)–C(9)	–0.4	–0.7	–1.2	–0.8
23	BOND H(12)–C(10)	–4.0	0.2	0.5	–1.1
24	BOND H(18)–C(8)	–0.4	–0.7	–1.1	–0.8
25	BOND H(14)–C(9)	1.9	–2.9	0.1	–0.3
26	LP N(3)	0.6	3.2	10.7	4.8
27	BOND C(9)–Si(2)	–59.7	–164.5	–136.5	–120.2
28	BOND C(8)–Si(2)	–59.0	–163.1	–136.0	–119.4
29	BOND Si(2)–Li(1)	–242.4	2.9	–163.8	–134.4
30	BOND N(3)–Si(2)	–182.3	–134.8	4.2	–104.3

Table 147. MO contributions to σ in principal axes for Si in $(Me_2N)Me_2SiMe$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9

2	AO N(3)	0.0	0.0	0.1	0.0
3	AO C(4)	0.0	0.0	0.0	0.0
4	AO C(10)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(1)	0.0	0.0	0.0	0.0
7	AO C(8)	0.1	0.0	0.0	0.0
8	AO Si(2)	77.4	74.1	80.4	77.3
9	AO Si(2)	65.9	82.2	80.7	76.3
10	AO Si(2)	83.7	74.9	72.2	76.9
11	AO Si(2)	78.0	82.1	70.7	76.9
12	BOND N(3)–Si(2)	–128.3	–134.7	–5.1	–89.3
13	BOND H(15)–C(9)	–1.9	1.3	–1.9	–0.9
14	BOND H(7)–C(4)	–0.1	0.7	0.9	0.5
15	BOND H(20)–C(1)	–2.6	2.0	–2.0	–0.8
16	BOND H(17)–C(8)	3.0	–2.7	–1.7	–0.5
17	BOND H(12)–C(10)	0.1	0.5	0.9	0.5
18	BOND H(5)–C(4)	–0.1	–0.6	0.3	–0.1
19	BOND H(13)–C(10)	–0.8	–0.7	0.4	–0.3
20	BOND H(6)–C(4)	–0.9	–0.4	0.5	–0.3
21	BOND H(18)–C(8)	2.6	–2.4	–1.7	–0.5
22	BOND H(21)–C(1)	–0.9	–0.4	–0.7	–0.7
23	BOND H(22)–C(1)	–3.1	1.9	–0.4	–0.6
24	BOND C(1)–Si(2)	–184.4	–46.6	–134.8	–121.9
25	BOND H(14)–C(9)	–0.6	–0.8	–0.5	–0.6
26	BOND H(19)–C(8)	3.2	–3.0	–2.5	–0.8
27	BOND N(3)–C(10)	–2.2	–6.3	3.2	–1.8
28	BOND H(16)–C(9)	–3.0	1.4	–0.3	–0.6
29	BOND H(11)–C(10)	–0.5	–0.3	0.2	–0.2
30	BOND N(3)–C(4)	–2.5	–6.0	3.2	–1.8
31	BOND C(8)–Si(2)	6.2	–203.7	–169.0	–122.1
32	BOND C(9)–Si(2)	–167.2	–67.6	–129.1	–121.3
33	LP N(3)	0.9	–10.0	12.9	1.3

Table 148. MO contributions to σ in principal axes for Si in (MeS)Me_2SiH [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(3)	0.0	0.0	0.0	0.0
2	AO Si(1)	481.9	481.9	481.9	481.9
3	AO C(5)	0.0	0.0	0.0	0.0
4	AO C(2)	0.0	0.0	0.0	0.0
5	AO C(4)	0.0	0.1	0.0	0.0
6	AO S(3)	–0.2	–0.3	0.0	–0.2
7	AO S(3)	–0.5	–0.4	0.1	–0.3
8	AO S(3)	0.3	0.3	0.0	0.2
9	AO S(3)	0.2	0.1	0.3	0.2
10	AO Si(1)	76.6	82.4	67.3	75.4
11	AO Si(1)	84.0	62.4	83.6	76.6
12	AO Si(1)	77.9	77.5	71.2	75.6
13	AO Si(1)	64.6	80.4	80.6	75.2
14	BOND C(5)–S(3)	–2.1	–2.8	3.7	–0.4
15	BOND H(11)–C(4)	–2.3	2.2	–1.5	–0.6
16	BOND H(8)–C(2)	1.0	–3.1	0.5	–0.5
17	BOND H(13)–C(5)	–0.6	–0.7	0.1	–0.4
18	BOND H(6)–Si(1)	–14.8	–149.3	–130.0	–98.0
19	BOND H(15)–C(5)	–0.6	–0.3	0.7	–0.1
20	BOND H(14)–C(5)	–0.3	–2.0	0.8	–0.5
21	BOND H(10)–C(4)	–3.5	3.1	–0.7	–0.4
22	BOND H(7)–C(2)	1.2	0.3	–2.1	–0.2
23	BOND H(9)–C(2)	–2.1	0.3	0.5	–0.4

24	BOND H(12)–C(4)	–2.1	4.0	–2.5	–0.2
25	LP S(3)	–8.8	–3.1	7.5	–1.5
26	BOND C(2)–Si(1)	–110.6	–150.2	–121.6	–127.5
27	BOND C(4)–Si(1)	–208.1	0.8	–174.5	–127.3
28	BOND S(3)–Si(1)	–146.5	–144.0	–7.9	–99.5
29	LP S(3)	–1.9	–9.7	8.4	–1.1

Table 149. MO contributions to σ in principal axes for Si in (MeS)Me_2SiCl [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(3)	0.0	0.0	0.0	0.0
2	AO S(4)	0.0	0.0	0.0	0.0
3	AO Si(1)	481.9	481.9	481.9	481.9
4	AO C(6)	0.0	0.0	0.0	0.0
5	AO C(5)	0.0	0.0	0.0	0.0
6	AO C(2)	0.0	0.0	0.0	0.0
7	AO Cl(3)	–0.4	–0.2	0.1	–0.2
8	AO S(4)	0.4	0.1	0.4	0.3
9	AO Cl(3)	0.2	0.2	–0.1	0.1
10	AO Cl(3)	–0.1	–0.4	0.1	–0.1
11	AO Cl(3)	0.2	0.3	0.2	0.2
12	AO S(4)	0.0	0.2	–0.1	0.1
13	AO S(4)	–0.3	0.2	–0.1	–0.1
14	AO S(4)	–0.3	0.0	–0.4	–0.3
15	AO Si(1)	85.6	72.7	71.4	76.6
16	AO Si(1)	80.0	80.9	67.0	75.9
17	AO Si(1)	62.2	88.1	84.0	78.1
18	AO Si(1)	83.4	66.9	76.6	75.6
19	LP Cl(3)	0.8	–5.2	7.0	0.9
20	LP S(4)	–7.3	6.4	–2.0	–0.9
21	BOND H(8)–C(2)	–1.1	–2.5	1.6	–0.7
22	BOND H(12)–C(5)	3.9	–2.3	–2.0	–0.1
23	BOND H(13)–C(6)	–1.9	0.0	0.8	–0.4
24	BOND H(14)–C(6)	–0.4	0.7	–0.6	–0.1
25	BOND H(10)–C(5)	1.1	0.2	–3.0	–0.6
26	BOND H(15)–C(6)	–0.5	0.6	–0.5	–0.1
27	BOND H(9)–C(2)	3.1	–2.5	–2.0	–0.5
28	BOND Cl(3)–Si(1)	–126.8	–106.1	–32.2	–88.4
29	LP Cl(3)	–2.7	0.4	2.3	0.0
30	BOND H(7)–C(2)	1.9	–2.5	0.2	–0.1
31	LP Cl(3)	–7.2	0.2	6.6	–0.1
32	BOND H(11)–C(5)	–0.1	0.3	–1.9	–0.6
33	BOND C(5)–Si(1)	–64.3	–159.5	–206.9	–143.6
34	BOND C(2)–Si(1)	–96.1	–226.5	–106.1	–142.9
35	BOND C(6)–S(4)	–4.1	4.5	–2.1	–0.6
36	BOND S(4)–Si(1)	–222.9	–13.7	–128.1	–121.6
37	LP S(4)	–13.0	9.3	–6.3	–3.4

Table 150. MO contributions to σ in principal axes for Si in (MeS)Me_2SiLi [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(4)	0.0	0.0	0.0	0.0
2	AO Si(1)	481.9	481.9	481.9	481.9
3	AO C(6)	0.0	0.0	0.0	0.0
4	AO C(5)	0.0	0.0	0.0	0.0
5	AO C(2)	0.0	0.0	0.0	0.0
6	AO S(4)	–0.5	–0.5	0.2	–0.3

7	AO S(4)	0.0	0.0	0.0	0.0
8	AO S(4)	0.0	0.0	0.1	0.0
9	AO S(4)	0.3	0.3	0.1	0.3
10	AO Si(1)	74.4	73.4	71.7	73.2
11	AO Si(1)	80.2	67.7	78.9	75.6
12	AO Si(1)	63.3	87.3	74.1	74.9
13	AO Si(1)	75.4	78.0	64.1	72.5
14	AO Li(3)	–0.1	0.1	0.0	0.0
15	BOND C(6)–S(4)	–2.3	–1.1	2.7	–0.2
16	BOND H(7)–C(2)	1.9	–0.7	–2.3	–0.4
17	BOND H(11)–C(5)	0.1	–1.5	–1.1	–0.8
18	BOND H(14)–C(6)	–0.1	–0.5	0.5	0.0
19	LP S(4)	–3.7	–6.7	7.1	–1.1
20	BOND H(13)–C(6)	–3.9	0.4	0.1	–1.1
21	BOND H(15)–C(6)	–3.2	0.0	0.7	–0.8
22	BOND H(9)–C(2)	1.4	–2.1	–1.3	–0.7
23	BOND H(12)–C(5)	2.6	–1.4	–2.2	–0.3
24	BOND H(8)–C(2)	–1.0	0.2	–1.4	–0.7
25	BOND H(10)–C(5)	2.1	–3.4	–0.8	–0.7
26	BOND C(5)–Si(1)	–48.5	–174.8	–140.0	–121.1
27	BOND C(2)–Si(1)	–97.7	–123.9	–156.4	–126.0
28	BOND S(4)–Si(1)	–134.2	–124.2	2.7	–85.2
29	BOND Si(1)–Li(3)	–246.7	–22.6	–134.7	–134.7
30	LP S(4)	–8.5	–5.3	7.8	–2.0

Table 151. MO contributions to σ in principal axes for Si in (MeS)Me_2SiMe [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(3)	0.0	0.0	0.0	0.0
2	AO Si(1)	481.9	481.9	481.9	481.9
3	AO C(5)	0.0	0.0	0.0	0.0
4	AO C(4)	0.0	0.0	0.0	0.0
5	AO C(2)	0.0	0.0	0.0	0.0
6	AO C(6)	0.0	0.0	0.0	0.0
7	AO S(3)	0.4	0.4	0.1	0.3
8	AO S(3)	0.0	0.0	0.1	0.1
9	AO S(3)	–0.3	–0.2	0.2	–0.1
10	AO S(3)	–0.3	–0.4	0.0	–0.3
11	AO Si(1)	74.4	74.3	79.5	76.1
12	AO Si(1)	81.2	66.2	82.7	76.7
13	AO Si(1)	68.9	81.1	77.7	75.9
14	AO Si(1)	81.0	77.1	63.9	74.0
15	BOND C(5)–S(3)	–3.0	–2.1	3.5	–0.5
16	BOND H(12)–C(4)	3.3	–2.1	–2.1	–0.3
17	BOND H(7)–C(2)	–0.9	2.1	–2.3	–0.4
18	BOND H(18)–C(6)	0.1	–0.5	–1.2	–0.5
19	BOND H(14)–C(5)	–0.5	–0.6	0.6	–0.2
20	BOND H(11)–C(4)	1.5	–3.0	–0.1	–0.5
21	BOND H(13)–C(5)	–1.7	0.8	0.1	–0.2
22	BOND H(15)–C(5)	–0.5	–0.6	0.6	–0.2
23	BOND H(8)–C(2)	–2.4	1.9	–1.3	–0.6
24	BOND C(2)–Si(1)	–150.2	–57.7	–163.1	–123.6
25	BOND H(17)–C(6)	–0.9	2.1	–2.3	–0.4
26	BOND C(4)–Si(1)	–33.2	–204.2	–131.7	–123.0
27	BOND H(16)–C(6)	–2.3	1.9	–1.4	–0.6
28	BOND H(9)–C(2)	0.2	–0.5	–1.2	–0.5
29	BOND S(3)–Si(1)	–155.5	–122.7	–2.7	–93.6
30	BOND C(6)–Si(1)	–151.5	–57.8	–163.0	–124.1
31	BOND H(10)–C(4)	1.6	–3.0	–0.1	–0.5

32	LP S(3)	–4.8	–6.8	6.8	–1.6
33	LP S(3)	–4.6	–6.8	6.8	–1.5

Table 152. MO contributions to σ in principal axes for Si in $(MeO)_2MeSiH$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO O(4)	0.0	0.0	0.0	0.0
3	AO O(3)	0.0	0.0	0.0	0.0
4	AO C(9)	0.0	0.0	0.0	0.0
5	AO C(13)	0.0	0.0	0.0	0.0
6	AO C(5)	0.0	0.0	0.1	0.0
7	AO Si(2)	72.8	73.2	92.5	79.5
8	AO Si(2)	86.6	85.6	66.1	79.4
9	AO Si(2)	83.4	64.9	88.3	78.9
10	AO Si(2)	77.7	78.3	83.7	79.9
11	BOND H(16)–C(13)	–0.3	0.4	0.3	0.1
12	BOND H(10)–C(9)	–1.3	–0.6	–0.8	–0.9
13	BOND O(3)–Si(2)	–129.6	–35.0	–145.3	–103.3
14	BOND H(12)–C(9)	0.6	–0.1	–0.8	–0.1
15	LP O(3)	–1.8	11.2	12.3	7.3
16	LP O(4)	13.2	13.6	–2.1	8.3
17	BOND H(14)–C(13)	–0.9	–0.6	–1.8	–1.1
18	LP O(3)	7.3	4.0	8.0	6.4
19	BOND O(4)–C(9)	–7.0	1.3	–3.9	–3.2
20	BOND H(15)–C(13)	–0.4	–0.6	–0.9	–0.6
21	BOND H(11)–C(9)	0.4	–0.4	–0.5	–0.2
22	BOND H(7)–C(5)	–4.1	–1.7	1.6	–1.4
23	BOND H(6)–C(5)	–3.2	–1.3	2.6	–0.6
24	BOND H(8)–C(5)	–2.8	–2.8	2.6	–1.0
25	BOND C(5)–Si(2)	–229.0	–214.5	4.2	–146.5
26	BOND H(1)–Si(2)	–25.0	–159.3	–168.8	–117.7
27	BOND O(4)–Si(2)	–107.2	–53.1	–146.9	–102.4
28	BOND O(3)–C(13)	–2.4	2.9	–9.7	–3.1
29	LP O(4)	9.4	0.8	8.2	6.1

Table 153. MO contributions to σ in principal axes for Si in $(MeO)_2MeSiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO Si(2)	481.9	481.9	481.9	481.9
3	AO O(4)	0.0	0.0	0.0	0.0
4	AO O(3)	0.0	0.0	0.0	0.0
5	AO C(13)	0.0	0.0	0.0	0.0
6	AO C(9)	0.0	0.0	0.0	0.0
7	AO C(5)	0.0	0.0	0.1	0.0
8	AO Cl(1)	0.2	0.1	0.2	0.1
9	AO Cl(1)	0.3	–0.1	–0.2	0.0
10	AO Cl(1)	0.0	0.3	0.3	0.2
11	AO Cl(1)	0.0	–0.6	–0.4	–0.3
12	AO Si(2)	84.6	82.7	72.9	80.1
13	AO Si(2)	90.8	77.5	76.4	81.5
14	AO Si(2)	77.3	73.8	94.4	81.8
15	AO Si(2)	68.8	79.5	91.3	79.9
16	BOND H(10)–C(9)	–0.8	–0.1	–2.0	–1.0
17	BOND O(3)–C(13)	–8.3	1.4	–2.1	–3.0
18	LP Cl(1)	8.0	–0.6	–6.2	0.4

19	BOND H(8)–C(5)	–3.6	–3.2	2.7	–1.4
20	BOND H(14)–C(13)	–1.5	–0.7	–0.7	–1.0
21	LP O(4)	–2.8	9.1	–3.6	0.9
22	LP O(3)	8.2	–1.1	9.9	5.7
23	BOND O(4)–C(9)	–3.4	3.6	–15.1	–5.0
24	BOND H(11)–C(9)	–0.6	0.7	–0.1	0.0
25	BOND H(16)–C(13)	0.1	0.0	–0.3	0.0
26	BOND H(12)–C(9)	–0.2	0.4	–0.1	0.0
27	BOND H(15)–C(13)	0.4	0.1	–0.7	–0.1
28	LP Cl(1)	4.1	–5.4	–2.4	–1.2
29	BOND H(6)–C(5)	–1.7	–2.5	2.0	–0.8
30	BOND H(7)–C(5)	–3.0	–1.7	1.6	–1.0
31	BOND C(5)–Si(2)	–218.8	–223.1	3.8	–146.0
32	BOND O(3)–Si(2)	–127.7	–78.1	–131.4	–112.4
33	BOND Cl(1)–Si(2)	–18.2	–147.8	–143.5	–103.2
34	LP Cl(1)	4.3	–4.5	–5.4	–1.9
35	BOND O(4)–Si(2)	–122.0	–20.4	–149.7	–97.4
36	LP O(3)	11.7	15.6	–0.9	8.8
37	LP O(4)	7.6	6.2	2.4	5.4

Table 154. MO contributions to σ in principal axes for Si in $(MeO)_2MeSiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO O(4)	0.0	0.0	0.0	0.0
3	AO O(3)	0.0	0.0	0.0	0.0
4	AO C(13)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(5)	0.0	0.0	0.0	0.0
7	AO Si(2)	70.0	73.2	87.8	77.0
8	AO Si(2)	90.1	87.6	63.7	80.5
9	AO Si(2)	77.9	67.9	86.4	77.4
10	AO Si(2)	67.5	68.5	96.0	77.4
11	AO Li(1)	–0.1	–0.1	0.1	0.0
12	BOND H(11)–C(9)	–0.1	–0.4	–0.3	–0.2
13	BOND H(10)–C(9)	–0.2	–0.8	–1.9	–1.0
14	BOND H(16)–C(13)	0.0	1.2	–0.7	0.2
15	LP O(4)	2.5	12.4	7.0	7.3
16	BOND H(15)–C(13)	–3.8	1.0	–0.5	–1.1
17	BOND H(6)–C(5)	1.4	–0.9	–2.7	–0.8
18	BOND O(3)–Si(2)	–129.7	–17.8	–156.2	–101.2
19	LP O(3)	3.8	16.1	1.6	7.1
20	BOND O(3)–C(13)	–5.0	4.3	–6.2	–2.3
21	BOND H(14)–C(13)	–3.7	–0.2	–0.7	–1.5
22	LP O(4)	13.7	–2.1	3.0	4.9
23	BOND H(8)–C(5)	–1.0	–1.5	–0.6	–1.0
24	BOND H(7)–C(5)	–0.3	–3.0	–1.1	–1.5
25	BOND O(4)–C(9)	2.8	1.0	–11.5	–2.6
26	LP O(3)	1.0	7.0	2.6	3.5
27	BOND O(4)–Si(2)	–47.4	–76.4	–159.2	–94.3
28	BOND C(5)–Si(2)	–120.5	–207.5	–124.2	–150.8
29	BOND H(12)–C(9)	0.0	–0.5	–0.2	–0.2
30	BOND Si(2)–Li(1)	–277.4	–237.6	0.3	–171.6

Table 155. MO contributions to σ in principal axes for Si in $(MeO)_2MeSiMe$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average

1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO O(4)	0.0	0.0	0.0	0.0
3	AO O(5)	0.0	0.0	0.0	0.0
4	AO C(6)	0.0	0.0	0.0	0.0
5	AO C(7)	0.0	0.0	0.0	0.0
6	AO C(1)	0.0	0.0	0.0	0.0
7	AO C(3)	0.0	0.0	0.0	0.0
8	AO Si(2)	76.2	71.7	91.6	79.8
9	AO Si(2)	91.9	84.5	64.2	80.2
10	AO Si(2)	84.6	70.6	82.7	79.3
11	AO Si(2)	65.2	78.0	96.1	79.8
12	BOND H(19)–C(7)	0.2	0.1	–0.7	–0.1
13	BOND O(4)–C(6)	–2.0	2.6	–10.0	–3.2
14	BOND H(10)–C(1)	–2.4	–1.9	0.7	–1.2
15	BOND H(18)–C(7)	–1.0	–0.4	–1.3	–0.9
16	BOND H(13)–C(3)	0.7	–1.7	–0.9	–0.6
17	BOND H(15)–C(6)	–1.0	–0.4	–1.3	–0.9
18	LP O(5)	5.4	12.6	3.9	7.3
19	BOND O(4)–Si(2)	–85.2	–40.2	–166.6	–97.3
20	BOND H(17)–C(7)	0.2	0.2	–0.8	–0.1
21	BOND O(5)–C(7)	–1.5	2.4	–9.9	–3.0
22	BOND H(16)–C(6)	0.2	0.2	–0.7	–0.1
23	BOND H(14)–C(6)	0.2	0.3	–0.8	–0.1
24	BOND H(12)–C(3)	–2.9	–2.8	1.4	–1.4
25	BOND H(8)–C(1)	0.7	–1.7	–0.9	–0.6
26	BOND H(9)–C(1)	–2.8	–2.8	1.4	–1.4
27	BOND H(11)–C(3)	–2.5	–1.8	0.8	–1.1
28	LP O(4)	9.6	2.0	3.8	5.1
29	BOND C(3)–Si(2)	–164.2	–200.5	–58.2	–141.0
30	LP O(4)	5.4	12.6	4.0	7.4
31	BOND C(1)–Si(2)	–165.2	–200.5	–58.8	–141.5
32	BOND O(5)–Si(2)	–81.7	–45.7	–166.9	–98.1
33	LP O(5)	10.0	1.3	4.1	5.1

Table 156. MO contributions to σ in principal axes for Si in $(Me_2N)_2MeSiH$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO N(3)	0.0	0.0	0.0	0.0
3	AO N(8)	0.0	0.0	0.0	0.0
4	AO C(14)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(18)	0.0	0.0	0.0	0.0
7	AO C(4)	0.0	0.0	0.0	0.0
8	AO C(13)	0.0	0.0	0.0	0.0
9	AO Si(2)	85.7	73.0	75.5	78.1
10	AO Si(2)	87.7	79.3	69.1	78.7
11	AO Si(2)	76.5	73.1	82.8	77.5
12	AO Si(2)	70.7	74.1	84.7	76.5
13	BOND H(15)–C(14)	–0.3	0.2	–0.1	0.0
14	BOND H(10)–C(9)	0.1	–0.1	–0.4	–0.2
15	BOND H(19)–C(18)	–0.5	0.0	–0.2	–0.2
16	BOND H(5)–C(4)	–0.3	–0.4	–0.5	–0.4
17	BOND H(23)–C(13)	–1.6	–1.3	0.0	–1.0
18	BOND N(3)–C(4)	–4.6	1.9	–3.3	–2.0
19	BOND N(8)–Si(2)	–119.3	–54.0	–98.8	–90.7
20	BOND H(11)–C(9)	–0.5	–0.6	–0.1	–0.4
21	BOND H(17)–C(14)	–1.3	0.4	0.2	–0.2
22	BOND H(6)–C(4)	0.2	–0.7	–2.4	–0.9

23	BOND H(7)–C(4)	1.1	0.8	–0.2	0.6
24	BOND H(16)–C(14)	–0.1	0.7	0.8	0.5
25	BOND N(8)–C(18)	–5.1	2.6	–3.0	–1.8
26	BOND C(13)–Si(2)	–129.3	–210.1	–61.3	–133.6
27	BOND H(22)–C(13)	–2.3	–1.7	1.6	–0.8
28	BOND H(1)–Si(2)	–10.9	–147.9	–153.9	–104.2
29	BOND H(20)–C(18)	0.6	1.3	–0.1	0.6
30	BOND H(12)–C(9)	0.4	0.1	0.9	0.5
31	BOND H(21)–C(18)	–0.4	0.5	–1.8	–0.6
32	BOND N(3)–C(14)	–8.7	2.2	–2.4	–3.0
33	LP N(3)	–22.1	1.4	0.1	–6.9
34	BOND N(8)–C(9)	–6.4	–0.1	–2.8	–3.1
35	BOND H(24)–C(13)	0.3	–3.0	0.0	–0.9
36	BOND N(3)–Si(2)	–140.8	–37.2	–93.1	–90.4
37	LP N(8)	–25.6	1.3	4.8	–6.5

Table 157. MO contributions to σ in principal axes for Si in $(Me_2N)_2MeSiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO Si(2)	481.9	481.9	481.9	481.9
3	AO N(7)	0.0	0.0	0.0	0.0
4	AO N(10)	0.0	0.0	0.0	0.0
5	AO C(8)	0.0	0.0	0.0	0.0
6	AO C(11)	0.0	0.0	0.0	0.0
7	AO C(9)	0.0	0.0	0.0	0.0
8	AO C(12)	0.0	0.0	0.0	0.0
9	AO C(3)	0.0	0.1	0.0	0.0
10	AO Cl(1)	0.1	–0.4	–0.3	–0.2
11	AO Cl(1)	0.2	0.0	0.0	0.1
12	AO Cl(1)	0.1	–0.2	–0.2	–0.1
13	AO Cl(1)	0.1	0.3	0.3	0.2
14	AO Si(2)	79.5	80.3	77.5	79.1
15	AO Si(2)	84.5	66.5	88.7	79.9
16	AO Si(2)	64.2	81.4	82.8	76.1
17	AO Si(2)	82.5	91.4	65.6	79.8
18	BOND H(20)–C(12)	0.9	0.4	0.3	0.5
19	BOND H(16)–C(8)	0.5	0.5	0.6	0.5
20	LP Cl(1)	6.8	–2.9	–6.3	–0.8
21	BOND N(7)–C(9)	–1.4	–10.1	4.0	–2.5
22	BOND H(24)–C(11)	0.6	0.5	1.0	0.7
23	BOND H(5)–C(3)	–2.6	0.3	–1.2	–1.1
24	BOND N(10)–Si(2)	–36.9	0.5	–4.2	–13.5
25	BOND N(7)–Si(2)	–114.3	–143.8	–12.8	–90.3
26	BOND H(17)–C(8)	–0.8	–0.9	0.0	–0.6
27	BOND N(10)–Si(2)	–117.1	–75.3	–81.3	–91.2
28	BOND H(19)–C(12)	–0.4	–0.7	0.1	–0.3
29	BOND H(18)–C(8)	–1.0	0.3	0.5	–0.1
30	BOND H(22)–C(11)	0.4	0.0	–0.1	0.1
31	BOND H(14)–C(9)	0.4	–0.6	0.3	0.0
32	LP Cl(1)	6.6	–6.5	–0.6	–0.1
33	BOND H(6)–C(3)	–2.2	3.0	–2.9	–0.7
34	BOND H(4)–C(3)	–2.5	2.4	–2.3	–0.8
35	BOND H(13)–C(9)	–0.1	1.2	0.8	0.6
36	BOND N(10)–C(12)	–7.3	–0.1	–4.9	–4.1
37	BOND H(15)–C(9)	–0.6	–0.7	0.3	–0.3
38	BOND H(23)–C(11)	–0.6	–0.3	–0.1	–0.3
39	BOND C(3)–Si(2)	–197.1	–26.8	–196.3	–140.1
40	BOND H(21)–C(12)	–0.6	–0.4	–0.7	–0.6

41	BOND N(7)–C(8)	–2.5	–8.8	2.4	–3.0
42	LP Cl(1)	5.3	–4.8	–3.0	–0.8
43	BOND Cl(1)–Si(2)	2.2	–143.2	–120.5	–87.2
44	BOND N(7)–Si(2)	–6.0	–51.2	–6.6	–21.3
45	BOND N(10)–C(11)	–6.7	2.9	–0.4	–1.4

Table 158. MO contributions to σ in principal axes for Si in $(Me_2N)_2MeSiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO N(3)	0.0	0.0	0.0	0.0
3	AO N(8)	0.0	0.0	0.0	0.0
4	AO C(9)	0.0	0.0	0.0	0.0
5	AO C(14)	0.0	0.0	0.0	0.0
6	AO C(4)	0.0	0.0	0.0	0.0
7	AO C(18)	0.0	0.0	0.0	0.0
8	AO C(13)	0.0	0.0	0.0	0.0
9	AO Si(2)	74.4	75.5	76.1	75.3
10	AO Si(2)	82.1	83.2	65.6	77.0
11	AO Si(2)	77.6	61.9	87.5	75.7
12	AO Si(2)	64.3	76.1	85.2	75.2
13	AO Li(1)	–0.1	–0.1	0.1	0.0
14	BOND H(10)–C(9)	–2.2	0.9	–0.7	–0.7
15	BOND H(5)–C(4)	–0.2	0.1	–0.2	–0.1
16	BOND N(3)–C(14)	–3.7	1.0	–4.6	–2.5
17	LP N(8)	–6.8	–2.7	–11.5	–7.0
18	BOND H(24)–C(13)	1.9	–4.0	–0.8	–1.0
19	BOND H(11)–C(9)	–3.2	–0.4	–0.5	–1.4
20	BOND H(15)–C(14)	–1.6	1.0	–0.2	–0.3
21	BOND H(16)–C(14)	–2.3	–0.4	–0.6	–1.1
22	BOND H(12)–C(9)	0.3	0.5	0.7	0.5
23	BOND H(7)–C(4)	–2.4	–1.3	0.4	–1.1
24	BOND H(6)–C(4)	0.0	–0.1	–0.6	–0.2
25	BOND H(21)–C(18)	–0.5	–0.5	–0.2	–0.4
26	BOND N(8)–C(9)	–3.0	–0.9	–4.4	–2.8
27	BOND H(20)–C(18)	0.2	0.8	0.5	0.5
28	BOND H(23)–C(13)	1.0	–0.9	–2.5	–0.8
29	BOND H(17)–C(14)	–0.4	0.5	–1.0	–0.3
30	BOND H(22)–C(13)	2.3	–0.5	–3.4	–0.6
31	BOND N(8)–C(18)	–3.2	–1.6	–4.2	–3.0
32	BOND H(19)–C(18)	0.1	–0.6	0.1	–0.1
33	BOND N(3)–C(4)	–2.7	0.8	–2.6	–1.5
34	BOND C(13)–Si(2)	–52.1	–176.2	–164.1	–130.8
35	BOND N(3)–Si(2)	–119.0	–51.6	–144.9	–105.2
36	BOND Si(2)–Li(1)	–258.8	–185.2	–10.5	–151.5
37	BOND N(8)–Si(2)	–99.7	–54.6	–100.9	–85.0
38	LP N(3)	–3.4	7.1	2.3	2.0

Table 159. MO contributions to σ in principal axes for Si in $(Me_2N)_2MeSiMe$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO N(3)	0.0	0.0	0.0	0.0
3	AO N(8)	0.0	0.0	0.0	0.0
4	AO C(14)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(4)	0.0	0.0	0.0	0.0

7	AO C(18)	0.0	0.0	0.0	0.0
8	AO C(13)	0.0	0.0	0.0	0.0
9	AO C(1)	0.0	0.0	0.0	0.0
10	AO Si(2)	87.5	75.8	70.6	78.0
11	AO Si(2)	65.8	84.7	79.6	76.7
12	AO Si(2)	77.0	83.3	74.9	78.4
13	AO Si(2)	85.0	64.7	80.3	76.7
14	BOND H(20)–C(18)	0.0	1.0	0.7	0.5
15	BOND H(16)–C(14)	–0.8	0.0	–0.1	–0.3
16	BOND N(8)–C(18)	–5.8	–1.0	1.1	–1.9
17	BOND H(26)–C(1)	–1.0	0.5	–1.6	–0.7
18	BOND H(7)–C(4)	0.0	–0.1	0.4	0.1
19	BOND H(22)–C(13)	–0.6	0.1	–1.6	–0.7
20	BOND H(11)–C(9)	–0.2	–1.2	–0.6	–0.6
21	BOND H(17)–C(14)	–0.2	–1.2	–0.6	–0.6
22	BOND H(15)–C(14)	1.0	0.0	0.3	0.4
23	BOND H(21)–C(18)	–1.0	0.0	0.2	–0.3
24	BOND N(8)–Si(2)	–122.8	–76.1	–48.1	–82.3
25	BOND H(10)–C(9)	–0.9	0.0	0.0	–0.3
26	BOND N(3)–C(14)	–4.6	–2.9	–2.0	–3.1
27	BOND H(6)–C(4)	–1.0	0.0	0.2	–0.2
28	BOND H(25)–C(1)	–1.1	–1.0	–1.0	–1.1
29	BOND H(27)–C(1)	1.7	–1.7	–2.4	–0.8
30	BOND H(24)–C(13)	–0.8	–1.4	–0.9	–1.0
31	BOND H(23)–C(13)	2.1	–2.1	–2.5	–0.8
32	BOND N(8)–C(9)	–4.1	–3.3	–2.1	–3.2
33	BOND H(19)–C(18)	0.0	–0.1	0.4	0.1
34	BOND H(5)–C(4)	0.0	0.9	0.7	0.5
35	BOND N(3)–C(4)	–6.4	–0.6	1.1	–1.9
36	BOND H(12)–C(9)	1.0	0.0	0.3	0.4
37	BOND C(1)–Si(2)	–87.4	–131.5	–160.4	–126.4
38	BOND N(3)–Si(2)	–20.3	–11.6	–2.4	–11.4
39	BOND C(13)–Si(2)	–74.2	–143.3	–160.8	–126.1
40	BOND N(3)–Si(2)	–126.0	–71.8	–46.8	–81.6
41	BOND N(8)–Si(2)	–18.2	–13.2	–1.4	–11.0

Table 160. MO contributions to σ in principal axes for Si in $(MeS)_2MeSiH$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(4)	0.0	0.0	0.0	0.0
2	AO S(3)	0.0	0.0	0.0	0.0
3	AO Si(2)	481.9	481.9	481.9	481.9
4	AO C(9)	0.0	0.0	0.0	0.0
5	AO C(13)	0.0	0.0	0.0	0.0
6	AO C(5)	0.0	0.0	0.0	0.0
7	AO S(4)	–0.5	0.2	–0.5	–0.3
8	AO S(3)	–0.3	–0.4	0.2	–0.2
9	AO S(4)	–0.2	0.1	–0.3	–0.1
10	AO S(3)	0.0	0.2	0.2	0.1
11	AO S(4)	0.3	0.2	0.3	0.3
12	AO S(3)	–0.2	–0.2	–0.2	–0.2
13	AO S(4)	0.2	0.1	0.2	0.2
14	AO S(3)	0.4	0.3	0.1	0.3
15	AO Si(2)	84.4	80.1	62.6	75.7
16	AO Si(2)	65.4	82.8	79.7	76.0
17	AO Si(2)	79.4	68.5	81.9	76.6
18	AO Si(2)	80.3	67.6	75.1	74.4
19	BOND H(15)–C(13)	–0.3	–1.2	0.7	–0.3
20	BOND H(11)–C(9)	–0.1	0.6	–0.5	0.0

21	BOND H(7)–C(5)	2.0	–0.7	–1.7	–0.2
22	BOND H(14)–C(13)	–1.3	–0.2	–0.1	–0.6
23	LP S(3)	–10.5	–2.5	7.1	–2.0
24	BOND C(9)–S(4)	–4.3	4.5	–1.1	–0.3
25	LP S(4)	–6.0	8.4	–7.2	–1.6
26	BOND H(10)–C(9)	–2.0	0.1	0.9	–0.3
27	BOND H(12)–C(9)	–0.5	0.5	–0.6	–0.2
28	BOND H(16)–C(13)	–0.6	–0.5	0.7	–0.1
29	BOND H(8)–C(5)	1.0	–2.9	1.2	–0.2
30	BOND H(6)–C(5)	–2.2	–1.0	1.2	–0.7
31	BOND H(1)–Si(2)	–16.6	–138.2	–152.5	–102.4
32	BOND C(13)–S(3)	–2.8	–1.9	3.5	–0.4
33	BOND C(5)–Si(2)	–120.0	–185.1	–97.8	–134.3
34	LP S(3)	–3.2	–7.1	9.8	–0.2
35	BOND S(4)–Si(2)	–207.3	4.5	–134.9	–112.6
36	LP S(4)	–2.9	8.4	–5.3	0.1
37	BOND S(3)–Si(2)	–181.2	–125.4	–34.8	–113.8

Table 161. MO contributions to σ in principal axes for Si in $(MeS)_2MeSiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO S(4)	0.0	0.0	0.0	0.0
3	AO S(3)	0.0	0.0	0.0	0.0
4	AO Si(2)	481.9	481.9	481.9	481.9
5	AO C(13)	0.0	0.0	0.0	0.0
6	AO C(9)	0.0	0.0	0.0	0.0
7	AO C(5)	0.0	0.0	0.0	0.0
8	AO Cl(1)	0.0	0.3	0.2	0.2
9	AO S(4)	0.3	0.4	0.1	0.3
10	AO S(3)	0.0	–0.2	–0.2	–0.1
11	AO Cl(1)	0.2	–0.1	–0.1	0.0
12	AO Cl(1)	0.3	0.1	0.2	0.2
13	AO Cl(1)	–0.3	–0.2	–0.6	–0.3
14	AO S(4)	0.1	0.0	0.1	0.1
15	AO S(3)	–0.4	0.1	–0.5	–0.3
16	AO S(4)	–0.4	–0.2	0.3	–0.1
17	AO S(3)	0.4	0.1	0.2	0.2
18	AO S(4)	–0.1	–0.4	–0.1	–0.2
19	AO S(3)	0.0	0.3	0.3	0.2
20	AO Si(2)	85.2	81.0	64.8	77.0
21	AO Si(2)	76.2	72.8	85.3	78.1
22	AO Si(2)	83.3	70.7	73.2	75.7
23	AO Si(2)	64.6	81.4	84.9	77.0
24	LP Cl(1)	6.1	–0.3	–0.6	1.7
25	BOND H(12)–C(9)	–0.1	–0.5	0.8	0.1
26	BOND H(16)–C(13)	–0.1	0.7	–0.6	0.0
27	BOND H(7)–C(5)	–0.3	–2.6	2.3	–0.2
28	BOND H(11)–C(9)	–0.6	–0.7	0.8	–0.2
29	BOND C(9)–S(4)	–3.3	–3.6	4.7	–0.7
30	BOND C(13)–S(3)	–0.4	3.7	–4.0	–0.2
31	LP S(3)	–1.5	9.1	–8.4	–0.3
32	BOND H(14)–C(13)	–1.0	–0.3	1.3	0.0
33	BOND H(15)–C(13)	–0.4	0.7	–0.8	–0.2
34	LP S(4)	–7.2	–7.2	10.2	–1.4
35	BOND H(10)–C(9)	–1.8	0.4	–0.2	–0.5
36	BOND H(8)–C(5)	3.0	–1.0	–2.3	–0.1
37	BOND H(6)–C(5)	–1.5	–0.8	0.4	–0.6

38	BOND Cl(1)–Si(2)	–66.4	–81.6	–145.7	–97.9
39	BOND C(5)–Si(2)	–116.3	–199.5	–124.7	–146.8
40	LP Cl(1)	0.1	2.8	–3.2	–0.1
41	BOND S(3)–Si(2)	–157.9	–46.6	–177.6	–127.4
42	LP Cl(1)	5.5	2.8	–6.5	0.6
43	BOND S(4)–Si(2)	–206.2	–163.4	–28.9	–132.8
44	LP S(3)	–5.2	5.3	–8.2	–2.7
45	LP S(4)	–6.8	–4.7	10.3	–0.4

Table 162. MO contributions to σ in principal axes for Si in $(MeS)_2MeSiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(3)	0.0	0.0	0.0	0.0
2	AO S(4)	0.0	0.0	0.0	0.0
3	AO Si(2)	481.9	481.9	481.9	481.9
4	AO C(13)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(5)	0.1	0.0	0.0	0.0
7	AO S(3)	–0.5	–0.6	0.1	–0.3
8	AO S(4)	–0.1	0.3	0.0	0.1
9	AO S(3)	0.1	0.1	0.0	0.0
10	AO S(4)	0.0	0.2	0.0	0.1
11	AO S(3)	–0.1	0.1	0.2	0.0
12	AO S(4)	0.4	0.0	0.3	0.2
13	AO S(3)	0.3	0.3	0.2	0.3
14	AO S(4)	–0.4	–0.1	–0.6	–0.4
15	AO Si(2)	83.6	63.6	72.2	73.1
16	AO Si(2)	67.6	79.3	86.7	77.9
17	AO Si(2)	75.0	79.4	70.1	74.8
18	AO Si(2)	81.2	74.9	65.3	73.8
19	AO Li(1)	0.0	0.0	0.0	0.0
20	BOND H(11)–C(9)	–0.3	0.4	–0.3	–0.1
21	BOND C(13)–S(3)	–3.2	–1.0	3.4	–0.3
22	BOND H(8)–C(5)	1.6	–1.6	–1.0	–0.3
23	BOND H(10)–C(9)	–2.3	–0.1	–0.6	–1.0
24	BOND H(14)–C(13)	–3.0	–0.5	0.1	–1.1
25	BOND C(9)–S(4)	–6.5	2.7	0.7	–1.1
26	BOND H(12)–C(9)	–0.6	0.2	–0.7	–0.4
27	BOND H(16)–C(13)	–0.3	–0.9	0.5	–0.2
28	BOND H(15)–C(13)	–1.5	–0.7	0.6	–0.5
29	BOND C(5)–Si(2)	–33.4	–196.7	–169.8	–133.3
30	BOND H(6)–C(5)	1.6	–4.1	–1.8	–1.4
31	BOND H(7)–C(5)	3.3	–1.7	–2.7	–0.4
32	LP S(4)	–6.7	4.2	–3.9	–2.1
33	LP S(3)	–5.4	–7.7	9.3	–1.2
34	LP S(4)	1.8	2.7	–5.8	–0.4
35	BOND S(3)–Si(2)	–200.4	–113.8	–5.4	–106.5
36	LP S(3)	–12.3	–5.8	6.8	–3.8
37	BOND S(4)–Si(2)	–165.8	–35.0	–106.0	–102.3
38	BOND Si(2)–Li(1)	–126.6	–113.9	–171.4	–137.3

Table 163. MO contributions to σ in principal axes for Si in $(MeS)_2MeSiMe$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(3)	0.0	0.0	0.0	0.0
2	AO S(4)	0.0	0.0	0.0	0.0
3	AO Si(2)	481.9	481.9	481.9	481.9

4	AO C(13)	0.0	0.0	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(1)	0.0	0.0	0.0	0.0
7	AO C(5)	0.0	0.0	0.0	0.0
8	AO S(3)	–0.1	0.3	–0.3	0.0
9	AO S(4)	–0.6	–0.3	–0.3	–0.4
10	AO S(3)	–0.5	–0.3	–0.3	–0.4
11	AO S(4)	0.0	0.3	–0.2	0.1
12	AO S(4)	0.3	0.0	0.2	0.2
13	AO S(3)	0.4	0.1	0.2	0.2
14	AO S(3)	0.1	0.1	0.3	0.2
15	AO S(4)	0.1	0.2	0.4	0.2
16	AO Si(2)	84.1	69.4	72.3	75.3
17	AO Si(2)	65.3	79.7	85.4	76.8
18	AO Si(2)	73.9	73.7	80.9	76.2
19	AO Si(2)	86.7	74.4	64.0	75.0
20	BOND C(9)–S(4)	–3.4	1.2	0.4	–0.6
21	LP S(3)	–7.6	3.3	–1.1	–1.8
22	BOND H(7)–C(5)	3.1	–2.0	–1.9	–0.2
23	BOND H(17)–C(1)	1.4	–0.4	–1.9	–0.3
24	BOND H(12)–C(9)	–0.8	–0.1	0.0	–0.3
25	BOND H(16)–C(13)	–0.8	0.0	0.0	–0.3
26	BOND H(10)–C(9)	–1.8	0.3	0.3	–0.4
27	LP S(4)	–7.9	3.2	–0.7	–1.8
28	BOND H(11)–C(9)	–0.2	0.1	0.0	0.0
29	BOND H(14)–C(13)	–1.8	0.3	0.3	–0.4
30	BOND H(15)–C(13)	–0.2	0.1	0.0	0.0
31	BOND C(5)–Si(2)	–75.6	–171.0	–148.0	–131.5
32	BOND H(8)–C(5)	1.3	–0.4	–1.8	–0.3
33	BOND H(18)–C(1)	–0.6	–2.0	0.3	–0.8
34	BOND H(19)–C(1)	3.1	–2.0	–2.0	–0.3
35	BOND H(6)–C(5)	–0.6	–2.0	0.2	–0.8
36	BOND C(13)–S(3)	–3.4	1.3	0.4	–0.6
37	BOND C(1)–Si(2)	–75.7	–171.7	–145.8	–131.1
38	LP S(3)	–4.4	–1.9	3.5	–0.9
39	BOND S(4)–Si(2)	–185.4	–57.7	–82.9	–108.7
40	LP S(4)	–4.5	–2.0	3.7	–0.9
41	BOND S(3)–Si(2)	–185.7	–57.1	–83.8	–108.9

Table 164. MO contributions to σ in principal axes for Si in $(MeO)_3SiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO Si(2)	481.9	481.9	481.9	481.9
3	AO O(13)	0.0	0.0	0.0	0.0
4	AO O(3)	0.0	0.0	0.0	0.0
5	AO O(8)	0.0	0.0	0.0	0.0
6	AO C(4)	0.0	0.0	0.0	0.0
7	AO C(9)	0.0	0.0	0.0	0.0
8	AO C(14)	0.0	0.0	0.0	0.0
9	AO Cl(1)	0.2	0.2	0.1	0.2
10	AO Cl(1)	0.0	0.0	0.0	0.0
11	AO Cl(1)	0.1	0.2	0.2	0.2
12	AO Cl(1)	0.1	–0.6	–0.6	–0.4
13	AO Si(2)	71.0	83.9	90.4	81.7
14	AO Si(2)	90.1	93.1	66.4	83.2
15	AO Si(2)	93.3	69.7	90.3	84.4
16	AO Si(2)	79.1	82.7	84.7	82.2
17	LP O(3)	7.1	11.0	0.1	6.1

18	BOND H(10)–C(9)	–1.2	–1.1	–0.2	–0.8
19	BOND H(16)–C(14)	–1.2	–0.9	–0.4	–0.8
20	LP Cl(1)	6.9	–5.7	–4.3	–1.0
21	BOND H(5)–C(4)	–0.6	–0.1	–2.2	–1.0
22	BOND O(13)–C(14)	–6.9	–4.7	–4.0	–5.2
23	LP O(8)	2.2	0.1	14.5	5.6
24	BOND H(6)–C(4)	–0.3	1.1	–0.7	0.0
25	BOND H(17)–C(14)	–0.2	–0.8	1.1	0.0
26	BOND H(11)–C(9)	–0.3	0.1	0.4	0.1
27	BOND H(12)–C(9)	–0.2	–0.1	0.2	0.0
28	BOND O(13)–Si(2)	–4.5	–7.5	6.1	–2.0
29	BOND H(7)–C(4)	–0.7	1.1	–0.3	0.1
30	BOND O(8)–Si(2)	–168.2	–124.6	–44.8	–112.5
31	BOND H(15)–C(14)	–0.6	–0.4	1.0	0.0
32	BOND O(3)–C(4)	–4.0	0.0	–12.6	–5.5
33	LP Cl(1)	5.4	–5.2	–2.9	–0.9
34	LP O(8)	5.3	7.4	4.0	5.6
35	LP Cl(1)	3.4	–3.3	–6.5	–2.1
36	BOND O(3)–Si(2)	–119.5	–39.7	–150.7	–103.3
37	LP O(13)	4.3	–4.0	11.3	3.9
38	BOND Cl(1)–Si(2)	–7.7	–149.5	–150.3	–102.5
39	BOND O(8)–C(9)	–11.1	–2.5	3.6	–3.3
40	BOND O(13)–Si(2)	–133.5	–100.3	–58.0	–97.3
41	LP O(3)	0.9	14.6	–3.2	4.1

Table 165. MO contributions to σ in principal axes for Si in $(MeO)_3SiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO O(13)	0.0	0.0	0.0	0.0
3	AO O(8)	0.0	0.0	0.0	0.0
4	AO O(3)	0.0	0.0	0.0	0.0
5	AO C(14)	0.0	0.0	0.0	0.0
6	AO C(9)	0.0	0.0	0.0	0.0
7	AO C(4)	0.0	0.0	0.0	0.0
8	AO Si(2)	78.6	70.0	91.1	79.9
9	AO Si(2)	92.7	92.4	62.4	82.5
10	AO Si(2)	64.9	81.9	93.5	80.1
11	AO Si(2)	76.8	68.8	92.9	79.5
12	AO Li(1)	–0.1	–0.1	0.2	0.0
13	BOND H(16)–C(14)	–4.0	0.7	–0.1	–1.1
14	BOND H(10)–C(9)	–1.7	–0.8	–0.9	–1.1
15	BOND O(3)–C(4)	2.5	–2.5	–12.1	–4.0
16	BOND O(13)–C(14)	–4.8	–1.8	–4.7	–3.8
17	BOND O(8)–C(9)	–7.0	0.1	–5.7	–4.2
18	BOND H(6)–C(4)	–0.7	–0.3	0.5	–0.2
19	BOND H(11)–C(9)	0.0	–1.7	–0.1	–0.6
20	BOND H(12)–C(9)	0.7	0.4	–0.4	0.2
21	LP O(3)	4.2	–9.3	–5.2	–3.4
22	BOND H(17)–C(14)	–2.4	–0.6	–0.7	–1.2
23	BOND H(15)–C(14)	–0.2	1.2	–0.5	0.2
24	BOND H(7)–C(4)	–0.4	–0.4	0.2	–0.2
25	BOND H(5)–C(4)	0.0	–0.5	–1.6	–0.7
26	LP O(13)	–3.2	11.6	3.8	4.1
27	LP O(8)	11.8	7.3	–0.9	6.1
28	BOND O(8)–Si(2)	–119.6	–63.9	–131.0	–104.8
29	BOND O(13)–Si(2)	–121.7	–66.1	–134.7	–107.5
30	LP O(13)	2.2	16.4	–0.6	6.0
31	BOND O(3)–Si(2)	–22.8	–123.0	–126.5	–90.8

32	LP O(8)	7.7	–0.9	3.9	3.6
33	LP O(3)	7.1	–1.9	0.4	1.9
34	BOND Si(2)–Li(1)	–248.9	–245.5	11.1	–161.1

Table 166. MO contributions to σ in principal axes for Si in $(Me_2N)_3SiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO Si(2)	481.9	481.9	481.9	481.9
3	AO N(13)	0.0	0.1	0.0	0.0
4	AO N(8)	0.0	0.0	0.0	0.0
5	AO N(3)	0.0	0.0	0.1	0.0
6	AO C(14)	0.0	0.0	0.0	0.0
7	AO C(9)	0.0	0.0	0.0	0.0
8	AO C(26)	0.0	0.0	0.0	0.0
9	AO C(22)	0.0	0.0	0.0	0.0
10	AO C(18)	0.0	0.0	0.0	0.0
11	AO C(4)	0.0	0.0	0.0	0.0
12	AO Cl(1)	0.2	–0.3	–0.3	–0.1
13	AO Cl(1)	0.1	0.1	0.1	0.1
14	AO Cl(1)	0.1	–0.3	–0.4	–0.2
15	AO Cl(1)	0.1	0.3	0.3	0.2
16	AO Si(2)	78.4	89.7	68.5	78.9
17	AO Si(2)	86.8	71.3	83.9	80.6
18	AO Si(2)	64.4	82.4	82.6	76.5
19	AO Si(2)	83.5	72.9	83.0	79.8
20	BOND H(27)–C(26)	–0.3	1.2	1.3	0.7
21	BOND H(28)–C(26)	1.0	0.1	–0.6	0.2
22	BOND H(20)–C(18)	1.2	–1.4	0.5	0.1
23	LP Cl(1)	6.0	–5.2	–5.2	–1.5
24	BOND N(8)–C(9)	–5.3	–0.4	–4.0	–3.2
25	BOND H(17)–C(14)	–1.0	0.9	1.6	0.5
26	BOND H(7)–C(4)	–0.4	1.4	0.4	0.5
27	BOND H(23)–C(22)	–0.3	0.2	1.2	0.4
28	BOND H(25)–C(22)	–0.2	0.0	–0.9	–0.4
29	BOND H(12)–C(9)	–1.5	0.4	1.2	0.0
30	BOND H(19)–C(18)	–1.0	1.4	0.7	0.4
31	BOND H(16)–C(14)	–1.6	0.2	–0.8	–0.7
32	BOND N(3)–Si(2)	–102.7	–66.4	3.0	–55.4
33	BOND H(11)–C(9)	–1.3	–0.4	–0.7	–0.8
34	BOND N(13)–C(14)	–7.4	4.0	–4.7	–2.7
35	BOND N(8)–C(26)	–2.9	–1.3	–3.9	–2.7
36	BOND H(6)–C(4)	–0.3	–0.9	0.4	–0.3
37	BOND N(13)–C(22)	–6.0	3.1	–7.9	–3.6
38	BOND H(29)–C(26)	–0.2	0.1	–0.4	–0.2
39	LP Cl(1)	4.8	–3.9	–4.9	–1.3
40	BOND H(15)–C(14)	1.0	–0.2	–0.7	0.1
41	BOND H(10)–C(9)	0.8	0.8	–0.5	0.4
42	BOND H(5)–C(4)	1.3	–0.6	0.7	0.5
43	BOND H(24)–C(22)	1.2	0.4	–0.3	0.4
44	BOND H(21)–C(18)	–1.0	–1.8	0.1	–0.9
45	BOND N(3)–C(4)	–5.0	–8.6	4.4	–3.1
46	BOND N(13)–Si(2)	–68.9	–33.5	–87.1	–63.2
47	BOND N(8)–Si(2)	–122.9	–52.6	–74.4	–83.3
48	BOND N(3)–C(18)	–6.9	–7.2	4.2	–3.3
49	BOND Cl(1)–Si(2)	3.6	–130.6	–126.9	–84.6
50	LP Cl(1)	4.7	–4.9	–4.0	–1.4
51	BOND N(13)–Si(2)	–87.9	1.4	–50.3	–45.6
52	BOND N(3)–Si(2)	–48.8	–107.6	–6.6	–54.3

53	BOND N(8)–Si(2)	–14.2	–14.6	–53.0	–27.3

Table 167. MO contributions to σ in principal axes for Si in $(Me_2N)_3SiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Si(2)	481.9	481.9	481.9	481.9
2	AO N(8)	0.0	0.0	0.0	0.0
3	AO N(3)	0.0	0.0	0.0	0.0
4	AO N(13)	0.0	0.1	0.0	0.0
5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(4)	0.0	0.0	0.0	0.0
7	AO C(26)	0.0	0.0	0.0	0.0
8	AO C(18)	0.0	0.0	0.0	0.0
9	AO C(14)	0.0	0.0	0.0	0.0
10	AO C(22)	0.0	0.0	0.0	0.0
11	AO Si(2)	78.0	75.9	76.1	76.7
12	AO Si(2)	82.9	80.0	69.5	77.5
13	AO Si(2)	70.4	69.1	91.4	77.0
14	AO Si(2)	65.9	76.5	84.6	75.7
15	AO Li(1)	–0.1	–0.1	0.2	0.0
16	BOND N(8)–C(9)	2.1	–5.0	–4.2	–2.3
17	BOND H(7)–C(4)	1.4	–0.6	0.7	0.5
18	BOND N(3)–C(4)	2.1	–4.6	–4.1	–2.2
19	BOND N(3)–C(18)	0.4	–5.3	–6.2	–3.7
20	BOND H(28)–C(26)	–0.1	–0.4	–0.5	–0.3
21	BOND H(24)–C(22)	–3.4	0.5	–0.8	–1.2
22	BOND H(12)–C(9)	–0.6	0.0	–0.5	–0.4
23	BOND H(16)–C(14)	–0.5	0.5	–1.1	–0.4
24	BOND H(17)–C(14)	–3.4	0.5	–0.6	–1.2
25	BOND H(6)–C(4)	–0.1	–2.7	–0.3	–1.0
26	BOND H(21)–C(18)	–0.2	–0.2	–0.6	–0.3
27	BOND H(5)–C(4)	–0.6	0.1	–0.6	–0.4
28	BOND N(8)–C(26)	0.7	–5.6	–5.9	–3.6
29	BOND H(27)–C(26)	0.0	0.6	0.2	0.3
30	BOND N(13)–C(14)	–6.8	3.1	–3.6	–2.4
31	BOND H(10)–C(9)	1.6	–0.8	0.7	0.5
32	BOND N(13)–C(22)	–6.8	3.1	–3.9	–2.5
33	BOND H(19)–C(18)	–0.2	–0.5	–0.4	–0.4
34	LP N(3)	4.3	–9.0	–22.1	–8.9
35	BOND H(29)–C(26)	–0.2	–0.2	–0.5	–0.3
36	BOND H(23)–C(22)	–1.1	0.6	–0.1	–0.2
37	BOND H(15)–C(14)	–0.9	0.6	–0.1	–0.2
38	BOND N(3)–Si(2)	–44.7	–111.7	–110.5	–89.0
39	LP N(8)	5.3	–13.1	–21.8	–9.9
40	BOND H(25)–C(22)	–0.6	0.5	–1.2	–0.4
41	BOND H(11)–C(9)	0.1	–3.1	–0.4	–1.1
42	BOND N(13)–Si(2)	–178.5	–2.4	–140.8	–107.3
43	BOND Si(2)–Li(1)	–226.8	–227.5	0.9	–151.1
44	BOND H(20)–C(18)	0.1	0.7	0.1	0.3
45	BOND N(8)–Si(2)	–41.5	–112.8	–109.9	–88.0
46	LP N(13)	–7.8	4.4	0.2	–1.1

Table 168. MO contributions to σ in principal axes for Si in $(MeS)_3SiCl$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO Cl(1)	0.0	0.0	0.0	0.0
2	AO S(3)	0.0	0.0	0.0	0.0

3	AO S(13)	0.0	0.0	0.0	0.0
4	AO S(8)	0.0	0.0	0.0	0.0
5	AO Si(2)	481.9	481.9	481.9	481.9
6	AO C(14)	0.0	0.0	0.0	0.0
7	AO C(4)	0.0	0.0	0.0	0.0
8	AO C(9)	0.0	0.0	0.0	0.0
9	AO Cl(1)	–0.1	–0.3	–0.1	–0.1
10	AO S(3)	0.0	0.0	–0.3	–0.1
11	AO S(13)	0.2	0.3	0.3	0.3
12	AO S(8)	–0.2	0.3	0.1	0.1
13	AO Cl(1)	–0.1	0.2	0.1	0.1
14	AO Cl(1)	0.1	–0.2	–0.4	–0.2
15	AO Cl(1)	0.3	0.2	0.3	0.2
16	AO S(3)	0.1	–0.2	0.3	0.1
17	AO S(13)	0.3	0.0	–0.2	0.0
18	AO S(8)	0.1	–0.1	0.2	0.1
19	AO S(3)	–0.5	–0.1	–0.2	–0.2
20	AO S(13)	–0.2	–0.5	0.0	–0.3
21	AO S(8)	0.4	0.2	0.1	0.2
22	AO S(13)	–0.2	0.0	0.1	0.0
23	AO S(3)	0.3	0.3	0.2	0.3
24	AO S(8)	–0.5	–0.1	–0.6	–0.4
25	AO Si(2)	64.5	87.5	81.1	77.7
26	AO Si(2)	84.0	77.6	71.4	77.7
27	AO Si(2)	76.7	78.5	71.7	75.6
28	AO Si(2)	83.7	67.1	84.1	78.3
29	LP Cl(1)	6.5	0.0	–5.2	0.5
30	BOND H(10)–C(9)	–1.2	0.1	0.6	–0.2
31	BOND H(16)–C(14)	0.2	–1.4	0.4	–0.3
32	LP S(3)	–4.4	–4.7	5.4	–1.2
33	BOND H(7)–C(4)	–0.5	0.0	0.1	–0.2
34	BOND C(14)–S(13)	1.1	–3.2	1.6	–0.2
35	BOND H(17)–C(14)	0.1	–0.3	0.1	0.0
36	LP S(8)	–1.1	10.1	–6.1	0.9
37	LP S(3)	–7.4	6.9	–1.0	–0.5
38	LP Cl(1)	1.9	1.2	–0.1	1.0
39	BOND C(9)–S(8)	–1.7	2.6	–1.2	–0.1
40	BOND H(12)–C(9)	–0.6	0.3	–0.2	–0.2
41	BOND H(11)–C(9)	0.1	0.5	–0.4	0.1
42	BOND H(5)–C(4)	–1.2	0.5	–0.2	–0.3
43	BOND H(15)–C(14)	0.0	–0.2	–0.1	–0.1
44	BOND S(13)–Si(2)	–97.3	–229.7	–79.5	–135.5
45	BOND S(3)–Si(2)	–201.3	–89.9	–113.2	–134.8
46	BOND H(6)–C(4)	0.0	0.2	0.1	0.1
47	LP Cl(1)	7.1	–5.4	2.2	1.3
48	BOND S(8)–Si(2)	–193.6	–57.0	–152.4	–134.3
49	LP S(13)	–5.0	–5.1	7.6	–0.8
50	BOND Cl(1)–Si(2)	–53.7	–133.1	–124.5	–103.8
51	LP S(8)	–3.7	–0.3	0.5	–1.2
52	LP S(13)	6.1	–7.2	–0.7	–0.6
53	BOND C(4)–S(3)	–1.8	1.9	–0.7	–0.2

Table 169. MO contributions to σ in principal axes for Si in $(MeS)_3SiLi$ [IGLO–BP86/BIII//B3LYP/6-31+G(d)].

MO	type	σ_1	σ_2	σ_3	average
1	AO S(13)	0.0	0.0	0.0	0.0
2	AO S(8)	0.0	0.0	0.0	0.0
3	AO S(3)	0.0	0.0	0.0	0.0
4	AO Si(2)	481.9	481.9	481.9	481.9

5	AO C(9)	0.0	0.0	0.0	0.0
6	AO C(14)	0.0	0.0	0.0	0.0
7	AO C(4)	0.0	0.0	0.0	0.0
8	AO S(13)	–0.1	–0.2	–0.2	–0.2
9	AO S(8)	–0.1	–0.3	–0.6	–0.3
10	AO S(3)	–0.2	0.3	0.1	0.1
11	AO S(13)	–0.5	–0.4	0.1	–0.2
12	AO S(8)	–0.2	0.2	0.1	0.1
13	AO S(3)	0.2	–0.1	0.1	0.1
14	AO S(13)	0.3	0.1	0.3	0.2
15	AO S(8)	0.2	–0.2	0.1	0.0
16	AO S(3)	0.3	0.2	0.2	0.2
17	AO S(13)	0.2	0.3	0.1	0.2
18	AO S(8)	0.3	0.3	0.2	0.3
19	AO S(3)	–0.2	–0.3	–0.6	–0.4
20	AO Si(2)	66.0	77.9	81.4	75.1
21	AO Si(2)	81.4	78.2	73.6	77.7
22	AO Si(2)	76.1	70.3	76.4	74.3
23	AO Si(2)	77.9	78.5	69.2	75.2
24	AO Li(1)	0.0	0.0	0.0	0.0
25	BOND H(11)–C(9)	0.2	–1.3	–0.2	–0.4
26	BOND H(17)–C(14)	–1.9	1.1	0.0	–0.3
27	BOND H(6)–C(4)	–0.2	0.5	–0.1	0.1
28	BOND S(13)–Si(2)	–167.5	–160.2	–37.9	–121.9
29	LP S(8)	4.2	–13.0	–8.8	–5.9
30	LP S(3)	–2.6	6.8	–0.8	1.1
31	BOND H(16)–C(14)	–2.1	0.5	0.0	–0.5
32	BOND H(15)–C(14)	–0.2	–0.2	0.2	–0.1
33	BOND H(7)–C(4)	–0.6	–0.1	–0.6	–0.4
34	BOND H(10)–C(9)	–0.4	–1.8	1.0	–0.4
35	BOND H(12)–C(9)	0.6	–0.2	–0.6	–0.1
36	BOND H(5)–C(4)	–2.1	–0.6	–1.5	–1.4
37	BOND C(4)–S(3)	–5.7	1.9	–2.3	–2.0
38	BOND S(3)–Si(2)	–137.7	–71.8	–149.7	–119.7
39	BOND S(8)–Si(2)	–61.0	–149.7	–134.7	–115.1
40	BOND C(14)–S(13)	–1.6	–0.9	2.3	–0.1
41	LP S(8)	8.8	–1.4	–6.0	0.5
42	LP S(13)	–11.7	–5.7	0.3	–5.7
43	LP S(3)	1.2	–0.3	–6.6	–1.9
44	BOND C(9)–S(8)	2.5	–1.2	–2.1	–0.3
45	LP S(13)	–5.1	–7.0	7.4	–1.6
46	BOND Si(2)–Li(1)	–177.4	–122.6	–124.1	–141.4

Table 170. NBO Analysis for bonds to silicon in Me_3SiCl [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Cl	Si	22.47 %	0.47 (17.85 %)	4.54 (81.01 %)	0.06 (1.14 %)	1.97375
	Cl	77.53 %	0.88 (26.14 %)	2.79 (73.03 %)	0.03 (0.83 %)	
Si–C (3x)	Si	26.81 %	0.52 (27.41 %)	2.63 (71.97 %)	0.02 (0.63 %)	1.96908
	C	73.19 %	0.86 (31.79 %)	2.14 (67.95 %)	0.01 (0.26 %)	

Table 171. NBO Analysis for bonds to silicon in Me_3SiLi [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Li	Si	80.37 %	0.8965 (19.08 %)	4.21 (80.40 %)	0.03 (0.52 %)	1.86023
	Li	19.63 %	0.4431 (97.68 %)	0.02 (2.32 %)		
Si–C	Si	27.52 %	0.5246 (27.40 %)	2.63 (72.09 %)	0.02 (0.52 %)	1.97510

(3x)	C	72.48 %	0.8514 (31.84 %)	2.13 (67.94 %)	0.01 (0.21 %)	

Table 172. NBO Analysis for bonds to silicon in (MeO)Me_2SiCl [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Si–C	Si	(25.89 %)	0.51(28.61 %)	2.47 (70.62 %)	0.03 (0.77 %)	(1.96519)
	C	(74.11 %)	0.86 (30.81 %)	2.24 (68.92 %)	0.01 (0.27 %)	
Si–Cl	Si	(21.62 %)	0.47(18.37 %)	4.36 (80.13 %)	0.08 (1.50 %)	(1.97024)
	C	(78.38 %)	0.89(25.37 %)	2.91 (73.80 %)	0.03 (0.83 %)	
Si–O	Si	(13.99 %)	0.37 (23.81 %)	3.14 (74.66 %)	0.06 (1.54 %)	(1.97762)
	O	(86.01 %)	0.93(39.33 %)	1.53 (60.34 %)	0.01 (0.33 %)	
Si–C	Si	(26.28 %)	0.51 (29.26 %)	2.39 (70.03 %)	0.02 (0.71 %)	(1.96546)
	C	(73.72 %)	0.86 (30.91 %)	2.23 (68.81 %)	0.01 (0.29 %)	

Table 173. NBO Analysis for bonds to silicon in (MeO)Me_2SiLi [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Si–C	Si	26.42 %	0.51 (29.06 %)	2.42 (70.26 %)	0.02 (0.68 %)	1.97232
	C	73.58 %	0.86(30.97 %)	2.22 (68.81 %)	0.01 (0.23 %)	
Si–Li	Si	79.70 %	0.89 (20.48 %)	3.85 (78.84 %)	0.03 (0.67 %)	1.83820
	Li	20.30 %	0.45 (97.47 %)	0.03 (2.53 %)	-	
Si–O	Si	14.23 %	0.38(23.50 %)	3.21 (75.36 %)	0.05 (1.15 %)	1.97730
	O	85.77 %	0.93(35.28 %)	1.82 (64.32 %)	0.01 (0.40 %)	
Si–C	Si	26.52 %	0.52(28.70 %)	2.46 (70.66 %)	0.02 (0.63 %)	1.97138
	C	73.48 %	0.86(31.21 %)	2.20 (68.54 %)	0.01 (0.25 %)	

Table 174. NBO Analysis for bonds to silicon in (Me_2N)Me_2SiCl [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Cl–Si	Si	21.68 %	0.47(16.97 %)	4.81 (81.66 %)	0.08 (1.37 %)	1.96744
	Cl	78.32 %	0.89(25.96 %)	2.82 (73.25 %)	0.03 (0.80 %)	
Si–N	Si	17.07 %	0.41 (26.24 %)	2.76 (72.53 %)	0.05 (1.24 %)	1.96309
	N	82.93 %	0.91 (34.90 %)	1.86 (64.86 %)	0.01 (0.24 %)	
Si–C	Si	26.56 %	0.52(28.43 %)	2.49 (70.90 %)	0.02 (0.67 %)	1.96607
	C	73.44 %	0.86(31.76 %)	2.14 (67.96 %)	0.01 (0.27 %)	
Si–C	Si	26.56 %	0.52(28.42 %)	2.49 (70.91 %)	0.02 (0.67 %)	1.96609
	C	73.44 %	0.86(31.76 %)	2.14 (67.96 %)	0.01 (0.27 %)	

Table 175. NBO Analysis for bonds to silicon in (Me_2N)Me_2SiLi [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Li–Si	Si	78.19 %	0.88 (17.51 %)	4.67 (81.84 %)	0.04 (0.64 %)	1.82171
	Li	21.81 %	0.47 (98.21 %)	0.02 (1.79 %)		
Si–N	Si	18.36 %	0.43 (26.46 %)	2.75 (72.67 %)	0.03 (0.87 %)	1.95402
	N	81.64 %	0.90 (27.19 %)	2.67 (72.50 %)	0.01 (0.31 %)	
Si–C	Si	27.29 %	0.52 (28.69 %)	2.47 (70.79 %)	0.02 (0.52 %)	1.97286
	C	72.71 %	0.85 (31.55 %)	2.16 (68.21 %)	0.01 (0.24 %)	
Si–C	Si	27.29 %	0.52 (28.69 %)	2.47 (70.79 %)	0.02 (0.52 %)	1.97286
	C	72.71 %	0.85 (31.55 %)	2.16 (68.21 %)	0.01 (0.24 %)	

Table 176. NBO Analysis for bonds to silicon in (MeS)Me_2SiCl [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–C	Si	27.67 %	0.5260 (29.41 %)	2.38 (69.99 %)	0.02 (0.60 %)	1.96835
	C	72.33 %	0.8505 (31.21 %)	2.20 (68.54 %)	0.01 (0.24 %)	
Si–Cl	Si	23.19 %	0.4815 (19.09 %)	4.17 (79.64 %)	0.07 (1.26 %)	1.97471
	Cl	76.81 %	0.8764 (25.98 %)	2.82 (73.20 %)	0.03 (0.82 %)	
Si–S	Si	30.21 %	0.5497 (22.72 %)	3.36 (76.29 %)	0.04 (1.00 %)	1.95872
	S	69.79 %	0.8354 (20.76 %)	3.76 (78.04 %)	0.06 (1.20 %)	
Si–C	Si	27.71 %	0.5264 (28.83 %)	2.45 (70.59 %)	0.02 (0.58 %)	1.96839
	C	72.29 %	0.8502 (31.50 %)	2.17 (68.24 %)	0.01 (0.25 %)	

Table 177. NBO Analysis for bonds to silicon in (MeS)Me_2SiLi [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–C	Si	28.35 %	0.53 (30.38 %)	2.28 (69.11 %)	0.02 (0.52 %)	1.97649
	C	71.65 %	0.85 (31.39 %)	2.18 (68.40 %)	0.01 (0.22 %)	
Si–Li	Si	85.00 %	0.92 (21.16 %)	3.70 (78.35 %)	0.02 (0.49 %)	1.85402
	Li	15.00 %	0.39 (96.90 %)	0.03 (3.10 %)	-	
Si–S	Si	28.63 %	0.54 (20.88 %)	3.75 (78.36 %)	0.04 (0.76 %)	1.96401
	S	71.37 %	0.84 (19.97 %)	3.96 (79.05 %)	0.05 (0.98 %)	
Si–C	Si	28.20 %	0.53 (28.80 %)	2.45 (70.64 %)	0.02 (0.55 %)	1.97360
	C	71.80 %	0.85 (31.50 %)	2.17 (68.28 %)	0.01 (0.22 %)	

Table 178. NBO Analysis for bonds to silicon in $(MeO)_2$MeSiCl [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–C	Si	25.89 %	0.51 (28.61 %)	2.47 (70.62 %)	0.03 (0.77 %)	1.96519
	C	74.11 %	0.86 (30.81 %)	2.24 (68.92 %)	0.01 (0.27 %)	
Si–Cl	Si	21.62 %	0.47 (18.37 %)	4.36 (80.13 %)	0.08 (1.50 %)	1.97024
	Cl	78.38 %	0.89 (25.37 %)	2.91 (73.80 %)	0.03 (0.83 %)	
Si–O	Si	13.99 %	0.37 (23.81 %)	3.14 (74.66 %)	0.06 (1.54 %)	1.97762
	O	86.01 %	0.93 (39.33 %)	1.53 (60.34 %)	0.01 (0.33 %)	
Si–C	Si	26.28 %	0.51 (29.26 %)	2.39 (70.03 %)	0.02 (0.71 %)	1.96546
	O	73.72 %	0.86 (30.91 %)	2.23 (68.81 %)	0.01 (0.29 %)	

Table 179. NBO Analysis for bonds to silicon in $(MeO)_2$MeSiLi [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Li–Si	Si	83.01 %	0.91 (23.71 %)	3.19 (75.56 %)	0.03 (0.73 %)	1.82773
	Li	16.99 %	0.41 (96.43 %)	0.04 (3.57 %)	-	
Si–O	Si	13.54 %	0.37 (24.40 %)	3.04 (74.24 %)	0.06 (1.35 %)	1.97614
	O	86.46 %	0.93 (35.48 %)	1.81 (64.11 %)	0.01 (0.41 %)	
Si–O	Si	13.25 %	0.36 (23.50 %)	3.19 (75.08 %)	0.06 (1.42 %)	1.97713
	O	86.75 %	0.93 (37.42 %)	1.66 (62.21 %)	0.01 (0.37 %)	
Si–C	Si	25.33 %	0.50 (29.75 %)	2.33 (69.39 %)	0.03 (0.86 %)	1.96598
	C	74.67 %	0.86 (30.64 %)	2.26 (69.10 %)	0.01 (0.26 %)	

Table 180. NBO Analysis for bonds to silicon in $(Me_2N)_2$MeSiCl [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Cl	Si	21.69 %	0.47 (17.83 %)	4.53 (80.76 %)	0.08 (1.42 %)	1.96608
	Cl	78.31 %	0.88 (26.66 %)	2.72 (72.52 %)	0.03 (0.82 %)	

Si–C	Si	25.92 %	0.51 (28.82 %)	2.44 (70.39 %)	0.03 (0.79 %)	1.96063
	C	74.08 %	0.86 (31.69 %)	2.15 (68.03 %)	0.01 (0.28 %)	
Si–N	Si	16.69 %	0.41 (26.71 %)	2.70 (72.01 %)	0.05 (1.29 %)	1.96502
	N	83.31 %	0.91 (37.07 %)	1.69 (62.71 %)	0.01 (0.22 %)	
Si–N	Si	16.99 %	0.41 (26.68 %)	2.70 (72.09 %)	0.05 (1.23 %)	1.96662
	N	83.01 %	0.91 (38.17 %)	1.61 (61.62 %)	0.01 (0.21 %)	

Table 181. NBO Analysis for bonds to silicon in $(Me_2N)_2MeSiLi$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Li	Si	80.49 %	0.90 (18.42 %)	4.40 (80.99 %)	0.03 (0.59 %)	1.81797
	Li	19.51 %	0.44 (97.99 %)	0.02 (2.01 %)	-	
Si–N	Si	17.61 %	0.42 (26.14 %)	2.79 (72.88 %)	0.04 (0.98 %)	1.95522
	N	82.39 %	0.91 (29.00 %)	2.44 (70.71 %)	0.01 (0.29 %)	
Si–N	Si	17.28 %	0.42 (27.05 %)	2.66 (72.04 %)	0.03 (0.91 %)	1.96932
	N	82.72 %	0.91 (37.40 %)	1.67 (62.38 %)	0.01 (0.22 %)	
Si–C	Si	26.40 %	0.51 (29.18 %)	2.41 (70.18 %)	0.02 (0.65 %)	1.96693
	C	73.60 %	0.86 (31.67 %)	2.15 (68.08 %)	0.01 (0.25 %)	

Table 182. NBO Analysis for bonds to silicon in $(MeS)_2MeSiCl$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Cl	Si	24.17 %	0.49 (20.38 %)	3.84 (78.31 %)	0.06 (1.31 %)	1.97609
	Cl	75.83 %	0.87 (26.30 %)	2.77 (72.86 %)	0.03 (0.85 %)	
Si–S	Si	31.40 %	0.56 (24.29 %)	3.07 (74.63 %)	0.04 (1.08 %)	1.95803
	S	68.60 %	0.83 (20.06 %)	3.93 (78.76 %)	0.06 (1.18 %)	
Si–S	Si	31.06 %	0.56 (24.28 %)	3.07 (74.64 %)	0.04 (1.08 %)	1.95967
	S	68.94 %	0.83 (20.49 %)	3.82 (78.34 %)	0.06 (1.17 %)	
Si–C	Si	28.50 %	0.53 (31.07 %)	2.20 (68.38 %)	0.02 (0.54 %)	1.96865
	C	71.50 %	0.85 (31.04 %)	2.21 (68.72 %)	0.01 (0.24 %)	

Table 183. NBO Analysis for bonds to silicon in $(MeS)_2MeSiLi$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Li	Si	89.08 %	0.94 (22.31 %)	3.46 (77.22 %)	0.02 (0.47 %)	1.84130
	Li	10.92 %	0.33 (95.92 %)	0.04 (4.08 %)	-	
Si–S	Si	29.78 %	0.55 (23.03 %)	3.30 (76.10 %)	0.04 (0.87 %)	1.96552
	S	70.22 %	0.84 (20.09 %)	3.93 (78.89 %)	0.05 (1.02 %)	
Si–S	Si	29.52 %	0.54 (23.88 %)	3.15 (75.27 %)	0.04 (0.85 %)	1.96676
	S	70.48 %	0.84 (20.90 %)	3.74 (78.22 %)	0.04 (0.89 %)	
Si–C	Si	29.07 %	0.54 (31.59 %)	2.15 (67.84 %)	0.02 (0.57 %)	1.97313
	C	70.93 %	0.84 (31.13 %)	2.20 (68.64 %)	0.01 (0.22 %)	

Table 184. NBO Analysis for bonds to silicon in $(MeO)_3MeSiCl$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Cl	Si	21.56 %	0.46 (21.37 %)	3.57 (76.40 %)	0.10 (2.22 %)	1.96414
	Cl	78.44 %	0.89 (23.05 %)	3.30 (76.04 %)	0.04 (0.91 %)	
Si–O	Si	13.69 %	0.37 (25.65 %)	2.82 (72.42 %)	0.08 (1.93 %)	1.97434
	O	86.31 %	0.93 (36.32 %)	1.74 (63.32 %)	0.01 (0.37 %)	
Si–O	Si	13.96 %	0.37 (26.71 %)	2.68 (71.58 %)	0.06 (1.71 %)	1.97627
	O	86.04 %	0.93 (37.36 %)	1.67 (62.24 %)	0.01 (0.40 %)	
Si–O	Si	13.87 %	0.37 (26.24 %)	2.74 (72.00 %)	0.07 (1.76 %)	1.97580

	O	86.13 %	0.93 (37.14 %)	1.68 (62.48 %)	0.01 (0.38 %)	

Table 185. NBO Analysis for bonds to silicon in $(MeO)_3MeSiLi$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Li–Si	Si	83.67 %	0.91 (26.35 %)	2.76 (72.66 %)	0.04 (0.99 %)	1.80536
	Li	16.33 %	0.40 (95.70 %)	0.04 (4.30 %)	-	
Si–O	Si	12.96 %	0.36 (25.10 %)	2.92 (73.27 %)	0.06 (1.63 %)	1.97719
	O	87.04 %	0.93 (37.52 %)	1.65 (62.07 %)	0.01 (0.42 %)	
Si–O	Si	13.28 %	0.36 (24.60 %)	3.00 (73.84 %)	0.06 (1.56 %)	1.97557
	O	86.72 %	0.93 (35.37 %)	1.81 (64.17 %)	0.01 (0.46 %)	
Si–O	Si	13.10 %	0.36 (25.76 %)	2.82 (72.64 %)	0.06 (1.60 %)	1.97508
	O	86.90 %	0.93 (34.62 %)	1.88 (64.94 %)	0.01 (0.44 %)	

Table 186. NBO Analysis for bonds to silicon in $(Me_2N)_3MeSiCl$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Cl–Si	Si	21.34 %	0.46 (18.25 %)	4.43 (80.81 %)	0.05 (0.94 %)	1.95993
	Cl	78.66 %	0.89 (26.69 %)	2.71 (72.35 %)	0.04 (0.96 %)	
Si–N	Si	16.43 %	0.41(27.50 %)	2.60 (71.37 %)	0.04 (1.13 %)	1.96623
	N	83.57 %	0.91 (39.59 %)	1.52 (60.10 %)	0.01 (0.31 %)	
Si–N	Si	16.36 %	0.40 (26.99 %)	2.66 (71.81 %)	0.04 (1.20 %)	1.96277
	N	83.64 %	0.91 (37.66 %)	1.65 (62.01 %)	0.01 (0.33 %)	
Si–N	Si	16.40 %	0.40 (27.24 %)	2.63 (71.60 %)	0.04 (1.16 %)	1.96577
	N	83.60 %	0.91 (39.56 %)	1.52 (60.14 %)	0.01 (0.31 %)	

Table 187. NBO Analysis for bonds to silicon in $(Me_2N)_3MeSiLi$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Si–Li	Si	82.38 %	0.91 (21.59 %)	3.60 (77.68 %)	0.03 (0.73 %)	1.82598
	Li	17.62 %	0.42 (98.04 %)	0.02 (1.96 %)	-	
Si–N	Si	16.33 %	0.40 (26.31 %)	2.76 (72.72 %)	0.04 (0.97 %)	1.96679
	N	83.67 %	0.91 (39.05 %)	1.55 (60.68 %)	0.01 (0.27 %)	
Si–N	Si	16.35 %	0.40 (26.25 %)	2.77 (72.78 %)	0.04 (0.97 %)	1.96667
	N	83.65 %	0.91 (39.04 %)	1.55 (60.69 %)	0.01 (0.27 %)	
Si–N	Si	16.31 %	0.40 (26.28 %)	2.77 (72.75 %)	0.04 (0.97 %)	1.96683
	N	83.69 %	0.91 (39.10 %)	1.55 (60.64 %)	0.01 (0.27 %)	

Table 188. NBO Analysis for bonds to silicon in $(MeS)_3MeSiCl$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	s (%)	Hybridization in p (%)	d (%)	overall Occupancy
Si–Cl	Si	75.20 %	0.87 (25.95 %)	2.82 (73.22 %)	0.03 (0.83 %)	1.97693
	Cl	24.80 %	0.50 (21.66 %)	3.56 (77.01 %)	0.06 (1.33 %)	
Si–S	Si	32.13 %	0.57 (26.07 %)	2.79 (72.79 %)	0.04 (1.14 %)	1.95960
	S	67.87 %	0.82 (20.02 %)	3.94 (78.83 %)	0.06 (1.15 %)	
Si–S	Si	32.69 %	0.57 (26.10 %)	2.79 (72.82 %)	0.04 (1.08 %)	1.96033
	S	67.31 %	0.82 (20.07 %)	3.92 (78.74 %)	0.06 (1.19 %)	
Si–S	Si	32.48 %	0.57 (26.15 %)	2.78 (72.76 %)	0.04 (1.09 %)	1.96134
	S	67.52 %	0.82 (20.48 %)	3.83 (78.34 %)	0.06 (1.19 %)	

Table 189. NBO Analysis for bonds to silicon in $(MeS)_3MeSiLi$ [BP86/BIII//B3LYP/6-31+G(d)].

bond	atom	polarization of NBO	Hybridization in s (%)	p (%)	d (%)	overall Occupancy
Si–Li	Si	91.08 %	0.9544(22.92 %)	3.34(76.55 %)	0.02(0.53 %)	1.82917
	Li	8.92 %	0.2986(94.77 %)	0.06(5.23 %)	-	
Si–S	Si	30.14 %	0.5490(27.04 %)	2.66(72.03 %)	0.03(0.93 %)	1.97050
	S	69.86 %	0.8358(19.35 %)	4.12(79.76 %)	0.05(0.88 %)	
Si–S	Si	30.52 %	0.5524(25.45 %)	2.90(73.70 %)	0.03(0.85 %)	1.97213
	S	69.48 %	0.8336(20.05 %)	3.94(78.96 %)	0.05(0.99 %)	
Si–S	Si	30.85 %	0.5554(25.51 %)	2.88(73.55 %)	0.04(0.94 %)	1.96852
	S	69.15 %	0.8316(19.92 %)	3.97(79.04 %)	0.05(1.04 %)	

Table 190. Natural Charges on silicon for selected model systems [BP86/BIII//B3LYP/6-31+G(d)]

model	Y	charge on silicon X=Cl	X=Li
Me_3SiX	–	1.716	0.729
$(Y)Me_2SiX$	OMe	1.924	0.983
	NMe_2	1.839	0.912
	SMe	1.509	0.543
$(Y)_2MeSiX$	OMe	2.096	1.137
	NMe_2	1.978	1.032
	SMe	1.292	0.329
$(Y)_3SiX$	OMe	2.260	1.316
	NMe_2	2.118	1.148
	SMe	1.060	0.133