Supplementary material belonging to the publication:

Understanding Substituent Effects on ^{29}Si Chemical Shifts and Bonding in Disilenes. A Quantum Chemical Analysis

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Standard Orientation of **1** [MP2/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	1.090737	0.000000
2	14	0.000000	–1.090737	0.000000
3	6	–0.487189	2.032785	1.568249
4	6	0.487189	–2.032785	1.568249
5	6	–0.487189	2.032785	–1.568249
6	6	0.487189	–2.032785	–1.568249
7	1	0.090549	2.959879	1.652945
8	1	–0.291447	1.435090	2.463980
9	1	–1.549167	2.300963	1.559908
10	1	–0.090549	–2.959879	1.652945
11	1	0.291447	–1.435090	2.463980
12	1	1.549167	–2.300963	1.559908
13	1	0.090549	2.959879	–1.652945
14	1	–0.291447	1.435090	–2.463980
15	1	–1.549167	2.300963	–1.559908
16	1	–0.090549	–2.959879	–1.652945
17	1	0.291447	–1.435090	–2.463980
18	1	1.549167	–2.300963	–1.559908

Total Energy of **1** [MP2/6–31+G(d)]: E(UMP2) = –736.96092393849 Hartree
Corrected Zero Point Energy: –736.8087219 Hartree

Standard Orientation of **1** [B3LYP/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	1.094140	0.000000
2	14	0.000000	–1.094140	0.000000
3	6	–0.502688	2.043206	1.569639
4	6	0.502688	–2.043206	1.569639
5	6	–0.502688	2.043206	–1.569639
6	6	0.502688	–2.043206	–1.569639
7	1	0.081335	2.968114	1.659261
8	1	–0.320365	1.447377	2.470717
9	1	–1.564010	2.320960	1.551187
10	1	–0.081335	–2.968114	1.659261
11	1	0.320365	–1.447377	2.470717
12	1	1.564010	–2.320960	1.551187
13	1	0.081335	2.968114	–1.659261
14	1	–0.320365	1.447377	–2.470717
15	1	–1.564010	2.320960	–1.551187
16	1	–0.081335	–2.968114	–1.659261
17	1	0.320365	–1.447377	–2.470717
18	1	1.564010	–2.320960	–1.551187

Total Energy of **1** [B3LYP/6–31+G(d)] E(RB+HF–LYP) = –738.632972149 Hartree
Corrected Zero Point Energy: –738.483966 Hartree

Standard Orientation of **1** [HF/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	1.071427	0.000000

2	14	0.000000	–1.071427	0.000000
3	6	–0.267527	2.089618	1.574191
4	6	0.267527	–2.089618	1.574191
5	6	–0.267527	2.089618	–1.574191
6	6	0.267527	–2.089618	–1.574191
7	1	0.465768	2.889006	1.643066
8	1	–0.171892	1.477245	2.465072
9	1	–1.253408	2.546224	1.584446
10	1	–0.465768	–2.889006	1.643066
11	1	0.171892	–1.477245	2.465072
12	1	1.253408	–2.546224	1.584446
13	1	0.465768	2.889006	–1.643066
14	1	–0.171892	1.477245	–2.465072
15	1	–1.253408	2.546224	–1.584446
16	1	–0.465768	–2.889006	–1.643066
17	1	0.171892	–1.477245	–2.465072
18	1	1.253408	–2.546224	–1.584446

Total Energy of **1** [HF/6–31+G(d)] E (RHF) = –736.259041722 Hartree
Corrected Zero Point Energy: –736.100621 Hartree

Standard Orientation of **2** [MP2/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	1.089233	0.000000
2	14	0.000000	–1.089233	0.000000
3	14	–0.376017	2.251785	1.989074
4	14	0.376017	–2.251785	1.989074
5	14	–0.376017	2.251785	–1.989074
6	14	0.376017	–2.251785	–1.989074
7	1	0.589129	3.376262	2.106703
8	1	–0.208475	1.340727	3.148260
9	1	–1.750025	2.819094	2.004182
10	1	–0.589129	–3.376262	2.106703
11	1	0.208475	–1.340727	3.148260
12	1	1.750025	–2.819094	2.004182
13	1	0.589129	3.376262	–2.106703
14	1	–0.208475	1.340727	–3.148260
15	1	–1.750025	2.819094	–2.004182
16	1	–0.589129	–3.376262	–2.106703
17	1	0.208475	–1.340727	–3.148260
18	1	1.750025	–2.819094	–2.004182

Total Energy of **2** [MP2/6–31+G(d)]: E(UMP2) = –1740.9245052382 Hartree
Corrected Zero Point Energy: –1740.8179082 Hartree

Standard Orientation of **2** [B3LYP/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	1.087113	0.000000
2	14	0.000000	–1.087113	0.000000
3	14	–0.135954	2.299439	2.002180
4	14	0.135954	–2.299439	2.002180
5	14	–0.135954	2.299439	–2.002180
6	14	0.135954	–2.299439	–2.002180
7	1	0.965027	3.299572	2.071209
8	1	–0.029473	1.385764	3.168876

9	1	–1.425746	3.039149	2.084517
10	1	–0.965027	–3.299572	2.071209
11	1	0.029473	–1.385764	3.168876
12	1	1.425746	–3.039149	2.084517
13	1	0.965027	3.299572	–2.071209
14	1	–0.029473	1.385764	–3.168876
15	1	–1.425746	3.039149	–2.084517
16	1	–0.965027	–3.299572	–2.071209
17	1	0.029473	–1.385764	–3.168876
18	1	1.425746	–3.039149	–2.084517

Total Energy of **2** [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1744.15328334 Hartree
Corrected Zero Point Energy: –1744.049907 Hartree

Standard Orientation of **2** [HF/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	1.076773	0.000000
2	14	0.000000	–1.076773	0.000000
3	14	0.005366	2.313255	1.999849
4	14	–0.005366	–2.313255	1.999849
5	14	0.005366	2.313255	–1.999849
6	14	–0.005366	–2.313255	–1.999849
7	1	1.204186	3.173468	2.056872
8	1	0.000720	1.412075	3.165249
9	1	–1.185045	3.185065	2.056542
10	1	–1.204186	–3.173468	2.056872
11	1	–0.000720	–1.412075	3.165249
12	1	1.185045	–3.185065	2.056542
13	1	1.204186	3.173468	–2.056872
14	1	0.000720	1.412075	–3.165249
15	1	–1.185045	3.185065	–2.056542
16	1	–1.204186	–3.173468	–2.056872
17	1	–0.000720	–1.412075	–3.165249
18	1	1.185045	–3.185065	–2.056542

Total Energy of **2** [HF/6–31+G(d)]: E(RHF) = –1740.43182464 Hartree
Corrected Zero Point Energy: –1740.321049 Hartree

Standard Orientation of **3** [MP2/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	0.768509	0.000000
2	14	0.774227	–1.267801	0.000000
3	14	–1.046481	1.341370	1.999874
4	6	1.405281	–2.126510	1.554077
5	1	–0.771405	2.758607	2.356495
6	1	–0.521360	0.477095	3.091176
7	1	–2.522516	1.173781	1.925083
8	1	1.053612	–3.164137	1.586149
9	1	1.060231	–1.620564	2.459866
10	1	2.500902	–2.149865	1.566569
11	14	–1.046481	1.341370	–1.999874
12	6	1.405281	–2.126510	–1.554077
13	1	–0.771405	2.758607	–2.356495
14	1	–0.521360	0.477095	–3.091176

15	1	–2.522516	1.173781	–1.925083
16	1	1.053612	–3.164137	–1.586149
17	1	1.060231	–1.620564	–2.459866
18	1	2.500902	–2.149865	–1.566569

Total Energy of **3** [MP2/6–31+G(d)]: E(UMP2) = 1238.9476673373 Hartree
Corrected Zero Point Energy: 1238.8180633 Hartree

Standard Orientation of **3** [B3LYP/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	0.736289	0.000000
2	14	0.737614	–1.320658	0.000000
3	14	–1.005660	1.406223	2.004735
4	6	1.354853	–2.191158	1.562717
5	14	–1.005660	1.406223	–2.004735
6	6	1.354853	–2.191158	–1.562717
7	1	–0.675831	2.825694	2.315210
8	1	–0.496316	0.564884	3.124472
9	1	–2.491788	1.296377	1.977475
10	1	0.965964	–3.216686	1.607802
11	1	1.034172	–1.665873	2.467706
12	1	2.450627	–2.253995	1.569277
13	1	–0.675831	2.825694	–2.315210
14	1	–0.496316	0.564884	–3.124472
15	1	–2.491788	1.296377	–1.977475
16	1	0.965964	–3.216686	–1.607802
17	1	1.034172	–1.665873	–2.467706
18	1	2.450627	–2.253995	–1.569277

Total Energy of **3** [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1241.39739389 Hartree
Corrected Zero Point Energy: –1241.271059 Hartree

Standard Orientation of **3** [HF/6–31+G(d)].

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	0.000000	0.623036	0.000000
2	14	0.253512	–1.512518	0.000000
3	14	–0.347306	1.715443	2.038823
4	6	0.468294	–2.553505	1.558945
5	14	–0.347306	1.715443	–2.038823
6	6	0.468294	–2.553505	–1.558945
7	1	0.608350	2.827298	2.220676
8	1	–0.161658	0.753490	3.145087
9	1	–1.709129	2.280897	2.132806
10	1	–0.268599	–3.352374	1.587869
11	1	0.357551	–1.961087	2.460014
12	1	1.451423	–3.017026	1.577164
13	1	0.608350	2.827298	–2.220676
14	1	–0.161658	0.753490	–3.145087
15	1	–1.709129	2.280897	–2.132806
16	1	–0.268599	–3.352374	–1.587869
17	1	0.357551	–1.961087	–2.460014
18	1	1.451423	–3.017026	–1.577164

Total Energy of **3** [HF/6–31+G(d)]: E(RHF) = –1238.35080131 Hartree
Corrected Zero Point Energy: –1238.216030 Hartree

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

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	–0.071349	2.602523	–0.198428
2	14	–0.021158	0.470704	0.286353
3	6	1.585235	–0.494070	0.117591
4	6	–1.552380	–0.597998	0.062688
5	6	1.426735	3.703943	0.188548
6	6	–1.701615	3.573128	–0.135354
7	6	1.783041	–1.661245	0.886403
8	6	2.983738	–2.372580	0.832304
9	6	4.025207	–1.930039	0.011220
10	6	3.852070	–0.777009	–0.759627
11	6	2.646136	–0.072995	–0.711391
12	6	–1.510259	–1.817954	–0.643817
13	6	–2.657154	–2.598467	–0.806585
14	6	–3.876956	–2.177033	–0.268371
15	6	–3.940147	–0.973787	0.440996
16	6	–2.789987	–0.200023	0.609998
17	1	1.604574	4.416150	–0.627112
18	1	2.335169	3.106527	0.318341
19	1	1.264369	4.283212	1.106359
20	1	–1.857884	4.042169	0.844211
21	1	–2.559339	2.927683	–0.351145
22	1	–1.688176	4.372926	–0.886820
23	1	0.990524	–2.020319	1.540006
24	1	3.106906	–3.269718	1.434504
25	1	4.960953	–2.481915	–0.031366
26	1	4.652295	–0.431229	–1.409935
27	1	2.521588	0.805015	–1.340184
28	1	–0.573217	–2.159045	–1.077120
29	1	–2.599228	–3.533700	–1.358651
30	1	–4.769799	–2.784199	–0.395948
31	1	–4.882756	–0.643272	0.871078
32	1	–2.852866	0.721317	1.185228

Total Energy of **4** [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1122.11655009 Hartree
Corrected Zero Point Energy: –1121.859233 Hartree

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

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	14	–0.223276	2.196942	–0.366448
2	14	0.002178	0.059079	0.064482
3	6	1.668875	–0.796331	0.014583
4	6	–1.422790	–1.158130	0.017669
5	14	1.520383	3.569044	0.385754
6	14	–2.377512	3.097598	–0.185370
7	6	1.890767	–1.961204	0.780441
8	6	3.139493	–2.585811	0.800257
9	6	4.197034	–2.061765	0.050997
10	6	3.997690	–0.911652	–0.718359
11	6	2.749008	–0.287341	–0.736534
12	6	–1.305242	–2.400404	–0.641855
13	6	–2.375509	–3.295665	–0.686831
14	6	–3.587191	–2.972202	–0.067984

15	6	–3.722895	–1.749956	0.596526
16	6	–2.651793	–0.855285	0.639621
17	1	1.820247	4.627914	–0.619379
18	1	2.757171	2.769415	0.594308
19	1	1.181626	4.261201	1.661835
20	1	–2.797023	3.385600	1.216519
21	1	–3.381905	2.179027	–0.786336
22	1	–2.422251	4.387601	–0.929973
23	1	1.082233	–2.385108	1.371855
24	1	3.286151	–3.480308	1.400708
25	1	5.168997	–2.548549	0.063740
26	1	4.813434	–0.503093	–1.309694
27	1	2.608968	0.597279	–1.352078
28	1	–0.371742	–2.668730	–1.130183
29	1	–2.264432	–4.244472	–1.206083
30	1	–4.419897	–3.670339	–0.101393
31	1	–4.660258	–1.495189	1.084714
32	1	–2.770825	0.084936	1.172382

Total Energy of **5** [B3LYP/6–31+G(d)]: E(RB+HF–LYP) = –1624.87960289 Hartree
Corrected Zero Point Energy: –1624.644956 Hartree

Shielding tensor for Si of **1** [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 269.0182	Anisotropy = 158.3546	
	XX = 373.5230	YX = –11.7464	ZX = 0.0000
	XY = 27.2492	YY = 318.1672	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 115.3644
Eigenvalues:	115.3644	317.1023	374.5879

Shielding tensor for Si of **1** [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 201.3853	Anisotropy = 181.1817	
	XX = 317.8345	YX = –3.0409	ZX = 0.0000
	XY = 40.2519	YY = 242.3877	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 43.9338
Eigenvalues:	43.9338	238.0490	322.1732

Shielding tensor for Si of **1** [HF–GIAO/IGLO–III//MP2/6–31+G(d)].

1 Si	Isotropic = 271.3204	Anisotropy = 154.2586	
	XX = 373.2570	YX = –11.9608	ZX = 0.0000
	XY = 25.9165	YY = 320.2026	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 120.5014
Eigenvalues:	120.5014	319.3002	374.1595

Shielding tensor for Si of **1** [BP86–GIAO/IGLO–III//MP2/6–31+G(d)].

1 Si	Isotropic = 203.8753	Anisotropy = 177.6956	
	XX = 318.5003	YX = –3.8230	ZX = 0.0000
	XY = 38.1634	YY = 245.5383	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 47.5873
Eigenvalues:	47.5873	241.6996	322.3390

Shielding tensor for Si of **2** [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 241.6101	Anisotropy = 364.9920	
	XX = 484.0840	YX = 5.0683	ZX = 0.0000
	XY = 18.2958	YY = 325.1602	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –84.4138
Eigenvalues:	–84.4138	324.3061	484.9381

Shielding tensor for Si of **2** [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 189.5830	Anisotropy = 357.0079	
	XX = 426.7432	YX = 7.0089	ZX = 0.0000
	XY = 18.5655	YY = 234.0786	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –92.0730
Eigenvalues:	–92.0730	233.2336	427.5882

Shielding tensor for Si of **2** [HF–GIAO/IGLO–III//MP2/6–31+G(d)].

1 Si	Isotropic = 229.7651	Anisotropy = 391.6680	
	XX = 484.8534	YX = 13.8342	ZX = 0.0000
	XY = 49.9078	YY = 322.2495	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –117.8076
Eigenvalues:	–117.8076	316.2258	490.8770

Shielding tensor for Si of **2** [BP86–GIAO/IGLO–III//MP2/6–31+G(d)].

1 Si	Isotropic = 179.3444	Anisotropy = 383.4129	
	XX = 429.0983	YX = 19.0260	ZX = 0.0000
	XY = 50.7403	YY = 227.1151	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –118.1801
Eigenvalues:	–118.1801	221.2604	434.9530

Shielding tensor for **3** [*Si*(SiH_3)$_2$] [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 413.6964	Anisotropy = 134.7330	
	XX = 496.5916	YX = –20.2296	ZX = 0.0000
	XY = 44.1491	YY = 482.8690	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 261.6286
Eigenvalues:	261.6286	475.9421	503.5184

Shielding tensor for **3** (*Si*Me_2) [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

2 Si	Isotropic = 147.3804	Anisotropy = 305.4893	
	XX = 329.7650	YX = 21.8043	ZX = 0.0000
	XY = 47.4661	YY = 294.6548	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –182.2784
Eigenvalues:	–182.2784	273.3798	351.0400

Shielding tensor for **3** [*Si*(SiH_3)$_2$] [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 341.8096	Anisotropy = 162.6784	
	XX = 434.2839	YX = –3.8902	ZX = 0.0000
	XY = 58.0907	YY = 404.2971	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 186.8478
Eigenvalues:	186.8478	388.3192	450.2619

Shielding tensor for **3** (*Si*Me_2) [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

2 Si	Isotropic = 93.0304	Anisotropy = 312.2698	
	XX = 271.2553	YX = 37.4952	ZX = 0.0000
	XY = 63.3556	YY = 216.3253	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –208.4895
Eigenvalues:	–208.4895	186.3704	301.2102

Shielding tensor for **3** [*Si*(SiH_3)$_2$] [HF–GIAO/IGLO–III//MP2/6–31+G(d)].

1 Si	Isotropic = 420.4221	Anisotropy = 135.7927	
	XX = 506.4030	YX = –23.5944	ZX = 0.0000
	XY = 43.2465	YY = 489.7188	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 265.1444
Eigenvalues:	265.1444	485.1713	510.9505

Shielding tensor for **3** (*Si*Me_2) [HF–GIAO/IGLO–III//MP2/6–31+G(d)].

2 Si	Isotropic = 141.5373	Anisotropy = 312.8748	
	XX = 327.4569	YX = 22.3054	ZX = 0.0000
	XY = 48.0327	YY = 295.5456	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –198.3906
Eigenvalues:	–198.3906	272.8820	350.1205

Shielding tensor for **3** [*Si*(SiH_3)$_2$] [BP86–GIAO/IGLO–III//MP2/6–31+G(d)].

1 Si	Isotropic = 348.8219	Anisotropy = 164.7884	
	XX = 444.5106	YX = –6.7582	ZX = 0.0000
	XY = 58.0351	YY = 412.2926	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = 189.6624
Eigenvalues:	189.6624	398.1224	458.6808

Shielding tensor for **3** (*Si*Me_2) [BP86–GIAO/IGLO–III//MP2/6–31+G(d)].

2 Si	Isotropic = 88.0913	Anisotropy = 320.4014	
	XX = 269.6118	YX = 38.9651	ZX = 0.0000
	XY = 64.6653	YY = 218.0020	ZY = 0.0000
	XZ = 0.0000	YZ = 0.0000	ZZ = –223.3401
Eigenvalues:	–223.3401	185.9217	301.6922

Shielding tensor for **4** (*Si*Me_2) [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 281.9275	Anisotropy = 143.7696	
	XX = 170.7219	YX = –10.4680	ZX = –19.6395
	XY = –0.0744	YY = 298.6330	ZY = –8.4108
	XZ = –0.7966	YZ = 24.2025	ZZ = 376.4277
Eigenvalues:	170.0304	297.9783	377.7739

Shielding tensor for **4** (*Si*Ph_2) [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

2 Si	Isotropic = 280.2758	Anisotropy = 134.1953	
	XX = 163.1084	YX = –23.5677	ZX = –8.6072
	XY = –24.9935	YY = 314.5005	ZY = 4.5665
	XZ = –39.4191	YZ = 17.7476	ZZ = 363.2186
Eigenvalues:	156.9478	314.1404	369.7394

Shielding tensor for **4** (*Si*Me_2) [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 205.7262	Anisotropy = 180.4633	
	XX = 84.7527	YX = –10.8663	ZX = –22.4591
	XY = –1.4746	YY = 207.4844	ZY = –13.1352
	XZ = –6.5925	YZ = 22.5753	ZZ = 324.9416
Eigenvalues:	83.5985	207.5451	326.0351

Shielding tensor for **4** (*Si*Ph_2) [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

2 Si	Isotropic = 213.6784	Anisotropy = 157.6157	
	XX = 88.8885	YX = –24.7610	ZX = –12.4971
	XY = –26.8267	YY = 238.2452	ZY = –3.8032
	XZ = –51.0593	YZ = 8.6333	ZZ = 313.9014
Eigenvalues:	80.4524	241.8272	318.7555

Shielding tensor for **5** [*Si*(SiH_3)$_2$] [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 434.3332	Anisotropy = 119.6322	
	XX = 322.0951	YX = –26.8551	ZX = –15.7819
	XY = –11.7000	YY = 467.1559	ZY = –29.9813
	XZ = 4.6529	YZ = 34.5272	ZZ = 513.7485
Eigenvalues:	319.4366	469.4750	514.0880

Shielding tensor for **5** (*Si*Ph_2) [HF–GIAO/IGLO–III//B3LYP/6–31+G(d)].

2 Si	Isotropic = 176.1833	Anisotropy = 240.9538	
	XX = –114.6167	YX = –62.0464	ZX = –9.4455
	XY = –63.7187	YY = 308.9254	ZY = –6.5733
	XZ = –58.7364	YZ = –3.4471	ZZ = 334.2412
Eigenvalues:	–126.3334	318.0641	336.8192

Shielding tensor for **5** [*Si*(SiH_3)$_2$] [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

1 Si	Isotropic = 349.9269	Anisotropy = 178.7949	
	XX = 226.7228	YX = –24.2040	ZX = –20.6223
	XY = –13.0964	YY = 354.6976	ZY = –26.7817
	XZ = –1.9124	YZ = 35.4491	ZZ = 468.3604
Eigenvalues:	223.6057	357.0516	469.1235

Shielding tensor for **5** (*Si*Ph_2) [BP86–GIAO/IGLO–III//B3LYP/6–31+G(d)].

2 Si	Isotropic = 127.2010	Anisotropy = 247.5568	
	XX = –137.0681	YX = –57.3816	ZX = –10.7130
	XY = –57.2724	YY = 230.2434	ZY = –6.2960
	XZ = –70.0181	YZ = –6.3387	ZZ = 288.4277
Eigenvalues:	–149.6180	238.9822	292.2389

Total Energy of **1** [BP86/IGLO-III//MP2/6–31+G(d)]: E(RB–P86) = –738.763909841 Hartree

Total Energy of **2** [BP86/IGLO-III//MP2/6–31+G(d)]: E(RB–P86) = –1744.36161501 Hartree

Total Energy of **3** [BP86/IGLO-III//MP2/6–31+G(d)]: E(RB–P86) = –1241.56792880 Hartree

GIAO NMR tensors for **1** in principal axes.

	σ_1	σ_2	σ_3
σ_d	888.1	886.8	880.6
σ_{p0}	–71.1	–2.5	–17.6
σ_{p1}	–764.7	–635.8	–533.2
σ	52.3	248.4	329.9
prin. axes			
x	0.0003	–0.2174	0.9761
y	0.0000	0.9761	0.2174
z	1.0000	0.0001	–0.0003

CGO NMR tensors for **1** in principal axes.

	σ_1	σ_2	σ_3
σ_d	1032.0	984.4	1113.6
σ_{p0}	0.0	0.0	0.0
σ_{p1}	–979.0	–744.9	–784.2
σ	53.1	239.5	329.4
prin. axes			
x	0.0000	0.1923	–0.9813
y	0.0000	–0.9813	–0.1923
z	1.0000	0.0000	0.0000

GIAO NMR tensors for **2** in principal axes.

	σ_1	σ_2	σ_3
σ_d	890.0	889.1	880.6
σ_{p0}	–71.8	26.5	86.8
σ_{p1}	–925.1	–682.6	–522.4
σ	–107.0	233.1	445.0
prin. axes			
x	0.0001	–0.1668	0.9860
y	–0.0001	0.9860	0.1668
z	1.0000	0.0001	0.0000

CGO NMR tensors for **2** in principal axes.

	σ_1	σ_2	σ_3
σ_d	1083.0	1057.7	1237.4
σ_{p0}	0.0	0.0	0.0
σ_{p1}	–1173.1	–814.8	–757.9
σ	–90.1	242.9	479.4
prin. axes			
x	0.0000	0.1641	0.9864
y	0.0000	–0.9864	0.1641
z	1.0000	0.0000	0.0000

GIAO NMR tensors for **3** [*Si*$(SiH_3)_2$] in principal axes.

	σ_1	σ_2	σ_3
σ_d	890.7	888.5	882.6

σ_{p0}	9.9	60.7	99.2
σ_{p1}	–706.6	–540.7	–516.2
σ	194.0	408.4	465.6
prin. axes			
x	0.0002	0.4866	–0.8736
y	0.0002	–0.8736	–0.4866
z	1.0000	0.0001	0.0002

GIAO NMR tensors for **3** (*Si*Me_2) in principal axes.

	σ_1	σ_2	σ_3
σ_d	887.8	887.8	880.8
σ_{p0}	–131.4	–28.6	–25.7
σ_{p1}	–969.9	–666.5	–544.4
σ	–213.5	192.7	310.7
prin. axes			
x	0.0001	–0.5284	0.8490
y	0.0000	0.8490	0.5284
z	1.0000	0.0000	0.0000

CGO NMR tensors for **3** [*Si*(SiH_3)$_2$] in principal axes.

	σ_1	σ_2	σ_3
σ_d	1048.8	1049.3	1180.2
σ_{p0}	0.0	0.0	0.0
σ_{p1}	–840.4	–633.0	–689.9
σ	208.4	416.3	490.3
prin. axes			
x	0.0000	0.5289	0.8487
y	0.0000	–0.8487	0.5289
z	1.0000	0.0000	0.0000

CGO NMR tensors for **3** ($SiMe_2$) in principal axes.

	σ_1	σ_2	σ_3
σ_d	1058.4	1005.4	1161.7
σ_{p0}	0.0	0.0	0.0
σ_{p1}	–1270.2	–817.7	–842.6
σ	–211.7	187.7	319.1
prin. axes			
x	0.0000	0.5194	–0.8545
y	0.0000	–0.8545	–0.5194
z	1.0000	0.0000	0.0000

MO contributions to σ in principal axes for **1**.

MO	σ_1	σ_2	σ_3	average
1	241.7	241.0	241.7	241.4
2	241.7	241.0	241.7	241.4
3	0.5	0.4	0.9	0.6
4	0.5	0.5	0.9	0.6
5	0.5	0.4	0.9	0.6
6	0.5	0.5	1.0	0.7
7	49.4	45.2	49.8	48.2
8	49.6	45.2	50.0	48.3
9	29.8	44.9	30.7	35.1
10	66.7	49.3	30.5	48.8

11	26.8	54.8	84.0	55.2
12	26.8	51.0	46.3	41.4
13	35.5	35.3	24.6	31.8
14	74.3	31.0	29.7	45.0
15	7.5	3.8	12.7	8.0
16	15.2	3.6	13.1	10.7
17	3.9	6.3	2.0	4.1
18	3.9	–0.1	9.7	4.5
19	–1.2	5.4	–44.9	–13.5
20	35.9	5.3	38.5	26.6
21	–18.0	0.1	–23.3	–13.7
22	–19.9	–25.4	2.0	–14.5
23	–11.7	–16.5	1.9	–8.8
24	2.8	9.9	–9.7	1.0
25	6.2	–0.4	2.7	2.8
26	–4.8	–4.9	–2.5	–4.1
27	–4.6	–3.2	–3.4	–3.7
28	2.1	–7.3	–27.1	–10.7
29	2.5	–43.6	–264.2	–101.8
30	0.3	–359.7	–231.0	–196.8
31	–718.4	2.4	16.3	–233.2
32	–93.2	–176.5	3.8	–88.6

MO contributions to σ_p in principal axes for **1**.

MO	σ_1	σ_2	σ_3	average
1	–2.5	–0.1	–2.5	–1.7
2	–2.5	–0.1	–2.5	–1.7
3	–6.1	–5.5	–11.5	–7.7
4	–6.1	–5.5	–11.5	–7.7
5	–6.1	–5.5	–11.5	–7.7
6	–6.1	–5.5	–11.4	–7.7
7	0.5	–0.5	1.0	0.3
8	0.7	–0.5	1.2	0.4
9	–25.7	–1.0	–5.1	–10.6
10	11.1	0.1	–2.1	3.0
11	–2.5	2.3	28.6	9.5
12	–2.5	–1.5	–9.1	–4.4
13	–19.8	2.3	–24.0	–13.8
14	19.0	1.3	–22.2	–0.6
15	–0.5	–2.7	0.6	–0.9
16	7.2	–2.5	1.0	1.9
17	–2.4	0.4	–8.9	–3.6
18	–2.5	–6.0	–1.2	–3.2
19	–9.5	–4.6	–54.6	–22.9
20	23.3	–2.9	22.8	14.4
21	–24.4	–5.8	–34.5	–21.6
22	–27.3	–30.9	–7.7	–22.0
23	–19.2	–21.8	–7.9	–16.3
24	–2.3	3.8	–19.9	–6.1
25	–0.2	–7.0	–8.2	–5.1
26	–11.6	–10.0	–12.2	–11.3
27	–11.5	–8.3	–13.1	–10.9
28	–3.0	–13.2	–37.2	–17.8
29	–5.6	–52.2	–278.3	–112.0
30	–8.5	–368.0	–245.6	–207.4
31	–727.2	–4.7	5.4	–242.2
32	–105.0	–188.8	–2.2	–98.6
Sum:	–979.0	–744.9	–784.2	–836.0

Contributions from separate excitations into σ_{p1} (in principal axes) for **1**.

OCC ? VAC	σ_1	σ_2	σ_3	energy denominator, (eV)	|<OZ>| (mHartree/ Zeeman)	|<PSO>| (mZeeman)
29 ? 35	0.00	–1.18	17.65	–7.69	1.5603(+)	1.1521(–)
29 ? 37	0.00	–1.15	–87.17	–9.04	3.0926(+)	2.4940(+)
29 ? 44	0.00	–1.24	–143.93	–9.97	5.5384(–)	2.4135(–)
29 ? 47	0.00	–53.45	–9.74	–10.31	2.4570(+)	2.5687(+)
29 ? 50	0.00	–21.24	–28.01	–10.62	2.6566(–)	1.8472(–)
29 ? 59	0.00	5.19	23.07	–12.41	1.9147(–)	2.0794(+)
29 ? 64	0.00	–0.52	–62.28	–14.38	2.7211(+)	3.2008(+)
29 ? 65	0.00	10.83	–0.09	–15.56	0.6845(–)	2.4480(+)
29 ? 72	0.00	1.23	–11.58	–16.83	1.3796(–)	1.4950(–)
29 ? 78	0.00	–10.64	–1.86	–18.00	1.3516(+)	1.5702(+)
29 ? 82	0.00	7.44	5.56	–19.28	0.7649(–)	5.5771(–)
29 ? 98	0.00	0.16	11.35	–23.45	1.3066(+)	1.9281(–)
29 ? 108	0.00	–0.02	10.48	–26.35	0.6028(+)	4.2235(–)
29 ? 254	0.00	0.13	15.30	–123.61	1.0513(–)	16.8631(+)
Sum:	0.00	–64.46	–261.24			
FullSum:	–5.62	–52.23	–278.25			
30 ? 33	0.00	–327.68	–27.75	–5.62	3.3559(+)	5.5064(+)
30 ? 36	0.00	–32.23	–33.08	–7.53	2.8747(+)	1.9922(+)
30 ? 40	0.00	–5.69	–38.27	–8.89	4.5184(–)	0.8797(–)
30 ? 45	0.00	0.77	–11.44	–9.75	1.4848(–)	0.7527(–)
30 ? 48	0.00	–16.87	–137.28	–9.96	4.6581(–)	3.1803(–)
30 ? 58	0.00	–24.21	5.83	–11.96	2.0140(–)	1.6483(–)
30 ? 62	0.00	7.30	16.59	–13.03	2.5780(+)	1.1092(–)
30 ? 74	0.00	2.32	14.59	–17.00	1.0446(–)	2.5340(+)
30 ? 99	0.00	–3.74	–12.20	–23.41	1.6173(+)	2.2994(+)
30 ? 101	0.00	–11.46	–7.11	–24.08	1.2660(+)	3.4232(+)
30 ? 121	0.00	18.53	–0.78	–30.84	2.4915(+)	2.2040(–)
30 ? 240	0.00	–6.67	–4.09	–109.70	0.6309(+)	17.3793(+)
30 ? 241	0.00	–1.71	–18.52	–112.59	1.4912(+)	16.4150(+)
30 ? 245	0.00	11.17	0.38	–115.98	2.1905(+)	6.0069(–)
30 ? 248	0.00	–0.39	18.21	–116.75	2.3844(–)	8.3981(+)
Sum:	0.00	–390.55	–234.91			
FullSum:	–8.52	–368.04	–245.61			
31 ? 33	–625.95	0.00	0.00	–5.09	3.9112(–)	7.4824(–)
31 ? 36	–63.84	0.00	0.00	–7.00	1.6409(–)	2.5011(–)
31 ? 40	–11.73	0.00	0.00	–8.35	1.2015(–)	0.7492(–)
31 ? 48	–34.52	0.00	0.00	–9.42	1.3372(+)	2.2341(+)
31 ? 61	0.00	–0.02	87.86	–12.30	3.6669(+)	2.7082(–)
31 ? 63	0.00	–0.22	–61.04	–13.24	2.2810(+)	3.3869(+)
31 ? 67	0.00	–0.89	–42.04	–14.83	1.3226(–)	5.1657(–)
31 ? 70	–19.87	0.00	0.00	–15.32	1.0426(–)	2.6830(–)
31 ? 77	0.00	0.30	–12.31	–17.06	0.6687(+)	4.3106(+)
31 ? 80	24.77	0.00	0.00	–17.23	0.7329(–)	5.3500(+)
31 ? 90	–13.04	0.00	0.00	–20.62	0.6674(+)	3.7000(+)
31 ? 91	0.00	–0.02	13.59	–20.75	1.3914(+)	1.8980(–)
31 ? 94	0.00	–0.17	80.05	–21.57	2.2779(+)	7.0201(–)
31 ? 121	19.59	0.00	0.00	–30.30	1.7046(–)	3.1988(+)
31 ? 151	0.00	–0.12	–10.00	–39.33	1.1813(–)	3.3090(–)
31 ? 240	–15.80	0.00	0.00	–109.16	0.7858(+)	20.1635(+)
31 ? 251	0.00	–0.09	–14.55	–121.40	0.7082(+)	24.9475(+)
Sum:	–740.40	–1.24	41.55			
FullSum:	–727.23	–4.74	5.44			
32 ? 34	0.00	–238.04	2.77	–3.77	2.2602(+)	3.7028(+)
32 ? 35	47.49	0.00	0.00	–4.16	1.6261(–)	1.1174(+)

32 ? 37	–54.35	0.00	0.00	–5.52	0.9137(–)	3.0143(–)
32 ? 39	0.00	10.49	–0.07	–5.65	0.2369(+)	2.3306(–)
32 ? 42	10.49	0.00	0.00	–6.26	0.8177(+)	0.7380(–)
32 ? 44	41.88	0.00	0.00	–6.45	0.8462(–)	2.9327(+)
32 ? 47	–70.93	0.00	0.00	–6.79	1.9760(+)	2.2391(+)
32 ? 53	0.00	59.42	–0.74	–7.62	1.5393(+)	2.7455(–)
32 ? 54	–26.40	0.00	0.00	–7.72	1.3624(+)	1.3743(+)
32 ? 71	0.00	–15.05	0.46	–13.09	1.4165(–)	1.3175(–)
32 ? 72	–32.48	0.00	0.00	–13.30	2.0767(+)	1.9112(+)
32 ? 78	–14.90	0.00	0.00	–14.47	2.3103(+)	0.8574(+)
32 ? 82	20.40	0.00	0.00	–15.75	1.0337(+)	2.8568(–)
32 ? 87	–12.52	0.00	0.00	–16.33	0.9912(+)	1.8950(+)
32 ? 100	18.87	0.00	0.00	–20.40	1.0726(–)	3.2963(+)
32 ? 120	–16.46	0.00	0.00	–26.85	0.9375(–)	4.3314(–)
Sum:	–88.91	–183.18	2.41			
FullSum:	–104.97	–188.76	–2.20			

MO contributions to σ in principal axes for **2**.

MO	σ_1	σ_2	σ_3	average
1	1.1	1.2	2.4	1.6
2	1.1	1.2	2.4	1.6
3	1.1	1.2	2.4	1.6
4	1.1	1.2	2.4	1.6
5	241.7	241.0	241.7	241.4
6	241.7	241.0	241.7	241.4
7	1.7	1.8	3.3	2.3
8	1.7	1.8	3.4	2.3
9	1.7	1.8	3.4	2.3
10	1.7	1.8	3.4	2.3
11	48.1	45.6	48.2	47.3
12	48.3	45.6	48.4	47.4
13	1.3	1.8	–3.3	–0.1
14	1.2	–1.1	1.3	0.5
15	–0.3	1.1	2.8	1.2
16	1.5	1.2	3.9	2.2
17	0.3	0.4	0.5	0.4
18	0.3	0.6	1.8	0.9
19	0.3	0.5	0.8	0.5
20	–0.2	–0.2	0.9	0.2
21	0.5	0.3	–0.2	0.2
22	0.0	–0.1	0.7	0.2
23	0.4	0.5	0.0	0.3
24	0.9	0.9	–0.7	0.4
25	26.6	48.5	27.8	34.3
26	78.5	51.7	27.3	52.5
27	46.9	29.0	31.5	35.8
28	26.7	56.3	86.2	56.4
29	26.7	50.9	45.2	40.9
30	65.9	26.6	42.8	45.1
31	5.3	6.6	4.4	5.4
32	27.2	4.5	16.1	15.9
33	3.3	13.5	–0.6	5.4
34	3.2	–5.1	19.0	5.7
35	–15.1	5.4	–53.6	–21.1
36	49.6	8.2	72.0	43.3
37	–33.4	–0.1	–9.4	–14.3
38	2.3	16.0	–4.3	4.6
39	–18.7	–20.4	1.6	–12.5
40	–2.1	–11.2	0.9	–4.1
41	–4.1	–3.1	–0.6	–2.6

42	–4.2	–2.4	–1.2	–2.6
43	–0.1	–0.7	–10.3	–3.7
44	1.6	–5.4	–25.3	–9.7
45	3.9	–39.4	–234.9	–90.1
46	–862.6	5.8	44.3	–270.8
47	0.7	–516.0	–216.5	–243.9
48	–115.2	–67.3	5.7	–59.0

MO contributions to σ_{p1} in principal axes for **2**.

MO	σ_1	σ_2	σ_3	average
1	–3.7	–4.1	–7.8	–5.2
2	–3.7	–4.1	–7.8	–5.2
3	–3.7	–4.1	–7.8	–5.2
4	–3.7	–4.1	–7.8	–5.2
5	–2.5	–0.1	–2.4	–1.7
6	–2.5	–0.1	–2.4	–1.7
7	–3.2	–3.5	–6.8	–4.5
8	–3.2	–3.5	–6.8	–4.5
9	–3.2	–3.5	–6.8	–4.5
10	–3.2	–3.5	–6.8	–4.5
11	–0.7	–0.2	–0.6	–0.5
12	–0.5	–0.1	–0.4	–0.3
13	–3.9	–3.9	–13.8	–7.2
14	–3.9	–6.7	–9.2	–6.6
15	–5.3	–4.3	–7.5	–5.7
16	–3.7	–4.2	–6.5	–4.8
17	–4.6	–4.9	–9.6	–6.4
18	–4.6	–4.7	–8.3	–5.9
19	–4.6	–4.8	–9.3	–6.3
20	–5.1	–5.5	–9.2	–6.6
21	–4.4	–5.0	–10.3	–6.6
22	–4.9	–5.4	–9.4	–6.6
23	–4.5	–4.8	–10.1	–6.4
24	–4.0	–4.4	–10.8	–6.4
25	–28.9	–1.9	–3.5	–11.4
26	23.0	–0.5	–2.2	6.8
27	–8.3	0.8	–21.6	–9.7
28	–2.5	4.1	31.1	10.9
29	–2.5	–1.2	–9.9	–4.6
30	10.6	0.1	–12.2	–0.5
31	–3.4	–2.0	–7.0	–4.1
32	19.1	–1.6	4.7	7.4
33	–1.6	8.1	–9.6	–1.0
34	–1.8	–10.2	10.1	–0.6
35	–21.0	–2.4	–61.2	–28.2
36	37.0	–0.5	57.2	31.2
37	–37.7	–5.7	–18.2	–20.5
38	–1.2	10.5	–12.3	–1.0
39	–24.6	–24.7	–5.9	–18.4
40	–7.9	–15.3	–6.6	–9.9
41	–9.5	–7.1	–7.9	–8.2
42	–9.6	–6.4	–8.5	–8.2
43	–3.6	–6.0	–18.2	–9.3
44	–1.7	–10.7	–33.1	–15.2
45	–2.5	–48.6	–247.1	–99.4
46	–873.0	–0.5	32.6	–280.3
47	–7.1	–524.5	–229.6	–253.8
48	–126.7	–78.8	–0.6	–68.7
Sum:	–1173.1	–814.8	–757.9	–915.3

Contributions from separate excitations into σ_{p1} (in principal axes) for **2**.

OCC ? VAC	σ_1	σ_2	σ_3	energy denominator, (eV)	|<OZ>|, (mHartree /Zeeman)	|<PSO>|, (mZeeman)
45 ? 50	0.00	–0.63	–63.50	–6.09	1.6282(+)	2.2714(+)
45 ? 53	0.00	1.85	–130.43	–6.87	4.6411(–)	1.7986(–)
45 ? 61	0.00	–61.94	0.32	–8.35	2.7652(–)	1.8107(–)
45 ? 65	0.00	–0.04	–16.16	–9.22	2.1111(+)	2.3153(–)
45 ? 69	0.00	5.89	–36.24	–10.29	2.1828(–)	1.8453(–)
45 ? 71	0.00	–28.01	0.07	–10.60	1.9750(+)	1.3850(+)
45 ? 75	0.00	–0.38	19.42	–11.05	1.1949(+)	1.6908(–)
45 ? 82	0.00	0.62	11.79	–12.39	1.2365(–)	1.1441(+)
45 ? 84	0.00	0.01	–39.36	–12.99	1.6145(–)	2.9095(–)
45 ? 90	0.00	20.13	–7.92	–15.24	0.9979(–)	4.1114(–)
45 ? 137	0.00	–0.10	40.45	–25.91	2.1694(–)	4.5032(+)
45 ? 140	0.00	–0.64	–22.68	–27.23	0.9615(–)	6.2214(–)
45 ? 258	0.00	0.18	–10.32	–114.64	1.5409(+)	7.1864(+)
Sum:	0.00	–63.08	–254.57			
FullSum:	–2.52	–48.61	–247.13			
46 ? 49	–871.38	0.00	0.00	–3.94	4.3224(–)	7.2889(–)
46 ? 60	0.00	–0.96	24.55	–7.83	1.0155(+)	1.9415(–)
46 ? 64	0.00	1.21	164.00	–8.45	3.2253(–)	3.9773(+)
46 ? 66	0.00	0.02	–89.30	–9.14	2.6827(–)	2.8044(–)
46 ? 72	–18.44	0.00	0.00	–10.25	0.9992(–)	1.7376(–)
46 ? 77	0.00	–0.19	–20.26	–10.62	2.4894(–)	0.8150(–)
46 ? 79	0.00	0.69	–20.11	–10.78	2.5245(–)	0.8353(–)
46 ? 85	0.00	0.51	–49.85	–12.69	1.2862(+)	4.5735(+)
46 ? 86	23.13	0.00	0.00	–13.01	0.4296(–)	6.4354(+)
46 ? 87	0.00	–0.01	37.30	–14.10	1.2140(+)	3.9933(–)
46 ? 102	0.00	0.41	–10.79	–17.57	0.5417(–)	3.5896(–)
46 ? 107	–21.05	0.00	0.00	–18.34	1.1083(–)	3.1995(–)
46 ? 113	11.11	0.00	0.00	–19.80	0.6335(–)	3.1893(+)
46 ? 118	17.31	0.00	0.00	–20.46	0.6674(–)	4.8772(+)
46 ? 132	0.00	–0.30	22.82	–23.85	0.7748(–)	6.5710(+)
46 ? 147	0.00	0.08	10.37	–28.32	1.6955(+)	1.6028(–)
46 ? 154	0.00	0.20	–11.06	–30.02	1.4263(–)	2.2221(–)
46 ? 261	0.00	0.13	–22.03	–114.73	1.3891(+)	16.8119(+)
Sum:	–859.32	1.79	35.65			
FullSum:	–872.97	–0.53	32.59			
47 ? 49	0.00	–507.99	–1.22	–3.68	3.2151(+)	5.3580(+)
47 ? 51	0.00	2.36	–152.10	–5.48	5.8743(–)	1.3528(–)
47 ? 57	0.00	–0.19	–87.67	–7.15	2.0313(–)	2.8451(–)
47 ? 63	0.00	–39.25	–1.43	–8.06	2.0119(–)	1.5141(–)
47 ? 67	0.00	1.97	13.43	–9.14	0.9931(–)	1.3365(+)
47 ? 70	0.00	0.43	–12.48	–9.63	1.2952(–)	0.9553(–)
47 ? 73	0.00	5.06	8.71	–10.08	2.4789(–)	0.6015(+)
47 ? 81	0.00	0.44	–13.43	–11.61	0.5905(–)	2.5239(–)
47 ? 86	0.00	13.64	3.45	–12.75	0.4907(+)	4.7045(–)
47 ? 89	0.00	0.05	–19.60	–14.48	1.6767(–)	1.5607(–)
47 ? 118	0.00	10.80	3.79	–20.21	0.8454(+)	3.6329(–)
47 ? 133	0.00	0.91	13.01	–24.35	0.9311(+)	3.4162(–)
47 ? 134	0.00	–1.83	–10.30	–24.56	2.3711(–)	1.5533(–)
47 ? 249	0.00	0.64	12.56	–105.06	0.8649(+)	15.7027(–)
Sum:	0.00	–512.96	–243.27			
FullSum:	–7.14	–524.48	–229.64			
48 ? 52	0.00	–118.35	1.27	–4.03	1.2691(+)	3.4980(+)
48 ? 53	14.83	0.00	0.00	–4.63	0.3050(–)	2.0705(+)

48 ? 58	0.00	48.95	1.08	–5.74	1.8788(+)	1.4057(–)
48 ? 59	17.36	0.00	0.00	–5.79	2.3087(–)	0.3999(+)
48 ? 62	0.00	63.73	–1.35	–6.51	1.3669(+)	2.8480(–)
48 ? 65	–73.43	0.00	0.00	–6.99	1.6763(+)	2.8135(+)
48 ? 69	–51.65	0.00	0.00	–8.05	1.7526(+)	2.1806(+)
48 ? 75	–16.13	0.00	0.00	–8.81	0.6303(+)	2.0728(+)
48 ? 82	12.01	0.00	0.00	–10.16	0.8084(+)	1.3858(–)
48 ? 83	0.00	–70.47	1.12	–10.61	1.5602(+)	4.4734(+)
48 ? 84	–96.48	0.00	0.00	–10.75	2.7209(+)	3.5036(+)
48 ? 90	23.83	0.00	0.00	–13.01	0.7527(–)	3.7837(+)
48 ? 94	29.75	0.00	0.00	–14.45	1.3418(–)	2.9431(+)
Sum:	–139.92	–76.14	2.12			
FullSum:	–126.72	–78.80	–0.65			

MO contributions to σ in principal axes for **3** [*Si*(SiH_3)$_2$]

MO	σ_1	σ_2	σ_3	average
1	1.5	0.1	1.5	1.0
2	1.3	2.2	3.2	2.2
3	1.3	2.2	3.2	2.2
4	481.9	481.9	481.9	481.9
5	0.3	0.1	0.4	0.3
6	0.3	0.1	0.5	0.3
7	2.0	0.3	2.0	1.4
8	1.9	3.1	4.5	3.2
9	1.9	3.1	4.5	3.2
10	93.3	90.3	94.1	92.5
11	–0.9	0.2	1.3	0.2
12	1.4	0.2	–1.0	0.2
13	0.6	0.2	0.9	0.6
14	1.2	1.3	0.2	0.9
15	0.7	1.8	3.1	1.8
16	1.3	1.9	–1.5	0.6
17	1.3	1.9	–2.1	0.4
18	–0.8	–1.7	3.0	0.2
19	–0.7	–1.4	3.1	0.3
20	107.0	85.5	71.4	88.0
21	52.3	107.0	130.6	96.6
22	118.3	74.4	63.1	85.2
23	3.8	1.2	3.1	2.7
24	2.3	1.5	3.0	2.3
25	8.5	6.9	15.4	10.3
26	4.1	10.7	17.7	10.8
27	10.9	4.0	–47.1	–10.7
28	–2.4	1.7	–1.4	–0.7
29	–4.5	–0.4	0.8	–1.4
30	0.6	5.7	1.9	2.8
31	43.0	5.3	48.8	32.4
32	–2.9	–0.6	–0.9	–1.5
33	–27.3	–3.2	–25.7	–18.7
34	–16.6	–26.5	–3.9	–15.7
35	2.5	16.6	–36.8	–5.9
36	–4.8	–9.6	–6.4	–6.9
37	0.3	46.9	–25.1	7.3
38	–579.0	2.6	85.3	–163.7
39	4.7	–409.5	–413.9	–272.9
40	–101.9	–91.6	7.4	–62.0

MO contributions to σ_{p1} in principal axes for **3** [*Si*(SiH_3)$_2$]

MO	σ_1	σ_2	σ_3	average

1	–5.0	–0.2	–4.8	–3.3
2	–4.1	–7.2	–10.6	–7.3
3	–4.1	–7.2	–10.6	–7.3
4	0.0	0.0	0.0	0.0
5	–3.9	–1.4	–5.3	–3.5
6	–3.9	–1.4	–5.2	–3.5
7	–4.3	–0.2	–4.2	–2.9
8	–3.6	–6.3	–9.2	–6.4
9	–3.6	–6.3	–9.2	–6.4
10	2.0	–0.8	2.8	1.4
11	–7.3	–0.2	–4.8	–4.1
12	–4.9	–0.3	–7.2	–4.2
13	–5.8	–0.2	–5.2	–3.8
14	–4.4	–8.2	–13.8	–8.8
15	–4.9	–7.7	–10.9	–7.8
16	–4.1	–7.5	–15.2	–8.9
17	–4.1	–7.4	–15.8	–9.1
18	–6.2	–11.1	–10.6	–9.3
19	–6.2	–10.8	–10.6	–9.2
20	2.3	–0.2	0.2	0.8
21	0.0	2.5	26.1	9.5
22	13.9	3.2	–22.4	–1.8
23	–0.4	–0.6	–2.3	–1.1
24	–1.7	–0.4	–2.5	–1.5
25	–2.7	–5.3	–0.2	–2.7
26	–1.7	1.9	5.8	2.0
27	5.8	–1.9	–53.9	–16.7
28	–7.4	–2.3	–8.3	–6.0
29	–8.9	–2.1	–4.3	–5.1
30	–3.0	3.1	–3.8	–1.2
31	31.6	–3.6	35.3	21.1
32	–7.1	–2.2	–6.0	–5.1
33	–31.7	–11.0	–35.5	–26.1
34	–23.8	–33.4	–14.0	–23.7
35	–1.2	9.0	–46.5	–12.9
36	–11.3	–16.3	–15.9	–14.5
37	–4.1	44.0	–31.4	2.8
38	–590.5	–4.4	72.2	–174.2
39	–4.7	–423.9	–432.2	–286.9
40	–115.2	–105.3	0.3	–73.4
Sum:	–840.4	–633.0	–689.9	–721.1

Contributions from separate excitations into σ_{p1} (in principal axes) for **3** [*Si*$(SiH_3)_2$].

OCC ? VAC	σ_1	σ_2	σ_3	energy denominator, (eV)	|<OZ>| (mHartree/ Zeeman)	|<PSO>| (mZeeman)
37 ? 49	0.00	–12.71	–11.28	–9.10	2.8079(+)	0.7187(+)
37 ? 51	0.00	–6.01	–6.23	–9.47	1.1050(+)	0.9813(+)
37 ? 54	0.00	0.02	12.12	–9.85	4.4107(+)	0.2575(–)
37 ? 73	0.00	0.77	–27.66	–13.50	2.1689(–)	1.6261(–)
Sum:	0.00	37.96	–17.17			
FullSum:	–4.10	44.04	–31.44			
38 ? 41	–601.02	0.00	0.00	–4.49	4.0559(–)	6.1075(–)
38 ? 43	0.00	–0.30	42.36	–6.05	0.6632(–)	3.8813(+)
38 ? 46	–14.69	0.00	0.00	–6.98	1.0735(+)	0.8778(+)
38 ? 48	0.00	0.08	69.48	–7.61	2.3031(+)	2.1165(–)
38 ? 49	21.61	0.00	0.00	–7.97	0.6461(+)	2.4486(–)
38 ? 51	–24.74	0.00	0.00	–8.33	0.7092(+)	2.6715(+)
38 ? 52	0.00	–0.41	–63.10	–8.65	1.3948(–)	3.7643(–)

38 ? 56	0.00	0.99	35.90	–9.14	1.2950(+)	3.3301(–)
38 ? 57	0.00	–0.28	29.17	–9.32	1.1716(+)	2.2459(–)
38 ? 62	–16.46	0.00	0.00	–10.04	0.5768(+)	2.6321(+)
38 ? 66	0.00	0.03	–11.03	–10.72	1.6476(–)	0.6621(–)
38 ? 68	–13.33	0.00	0.00	–10.95	1.2446(–)	1.0779(–)
38 ? 71	0.00	0.00	21.90	–11.97	2.2372(+)	1.0770(–)
38 ? 74	0.00	–0.44	–108.57	–12.94	2.2044(+)	5.9459(+)
38 ? 75	0.00	–0.08	54.49	–13.65	1.4998(+)	4.5665(–)
38 ? 77	12.86	0.00	0.00	–14.56	0.5251(+)	3.2774(–)
38 ? 81	28.75	0.00	0.00	–15.18	0.5721(–)	7.0081(+)
38 ? 85	–12.83	0.00	0.00	–16.47	0.5545(+)	3.5023(+)
38 ? 101	0.00	–0.01	–10.00	–19.81	1.0697(–)	1.7062(–)
38 ? 102	0.00	0.00	–18.77	–19.93	1.0393(+)	3.3070(+)
38 ? 108	0.00	–0.21	–9.85	–21.41	1.5742(+)	1.3224(+)
38 ? 109	18.68	0.00	0.00	–21.55	0.5839(+)	6.3333(–)
38 ? 113	10.64	0.00	0.00	–22.53	0.5559(+)	3.9631(–)
38 ? 116	0.00	–0.37	43.99	–23.45	1.1906(+)	8.3137(–)
38 ? 119	0.00	0.18	17.82	–24.57	1.0936(+)	4.1063(–)
38 ? 132	0.00	–0.07	–15.13	–28.16	1.4899(+)	2.6698(+)
Sum:	–590.53	–0.87	78.65			
FullSum:	–590.45	–4.40	72.20			

39 ? 41	0.00	–369.70	–31.89	–4.38	2.5084(+)	6.4485(+)
39 ? 42	0.00	–0.10	–247.50	–5.83	3.7705(–)	3.5166(–)
39 ? 44	0.00	11.02	–69.24	–6.20	3.5278(–)	2.1384(–)
39 ? 49	0.00	–35.65	9.92	–7.86	1.1161(–)	3.2003(+)
39 ? 51	0.00	–67.64	–61.10	–8.23	2.2413(+)	4.5225(+)
39 ? 53	0.00	–2.47	–10.70	–8.58	0.9936(+)	1.0460(+)
39 ? 54	0.00	–0.29	–36.86	–8.61	1.8851(–)	1.5746(–)
39 ? 55	0.00	3.86	9.96	–8.77	1.0798(+)	1.5084(–)
39 ? 62	0.00	–19.93	–6.93	–9.94	0.7390(+)	3.5231(+)
39 ? 63	0.00	7.36	7.06	–10.06	1.6423(+)	0.9355(–)
39 ? 65	0.00	3.47	13.18	–10.61	1.4933(+)	1.2962(–)
39 ? 68	0.00	–15.25	–3.74	–10.85	1.5518(–)	1.5591(+)
39 ? 70	0.00	11.08	27.78	–11.18	1.5040(+)	3.0482(–)
39 ? 73	0.00	5.76	–42.25	–12.26	0.8565(–)	7.3665(–)
39 ? 85	0.00	–7.13	–3.49	–16.36	0.4088(–)	4.0160(–)
39 ? 86	0.00	12.53	0.44	–16.46	0.7038(–)	2.8943(+)
39 ? 95	0.00	3.34	13.06	–18.49	0.5333(–)	5.3212(+)
39 ? 104	0.00	2.53	13.69	–20.45	1.0768(+)	4.2627(–)
39 ? 107	0.00	3.64	–13.96	–21.29	0.9561(+)	3.6992(+)
39 ? 109	0.00	16.94	2.83	–21.45	0.8052(–)	6.4798(–)
39 ? 113	0.00	–4.13	–7.71	–22.42	0.5782(+)	4.8893(+)
39 ? 118	0.00	5.66	10.24	–24.19	1.1150(+)	3.1840(–)
39 ? 120	0.00	–7.79	–5.76	–24.55	1.1479(–)	2.9666(–)
39 ? 121	0.00	1.37	18.39	–24.66	0.9435(+)	5.0057(–)
39 ? 130	0.00	0.19	–10.30	–27.40	0.3603(–)	7.4674(–)
39 ? 133	0.00	–6.01	–5.67	–28.23	0.9439(–)	5.1518(–)
39 ? 255	0.00	0.01	12.72	–116.82	1.1686(–)	11.6950(+)
Sum:	0.00	–447.35	–417.85			
FullSum:	–4.74	–423.89	–432.17			

40 ? 41	10.56	0.00	0.00	–2.48	0.1206(+)	1.9979(–)
40 ? 42	38.02	0.00	0.00	–3.93	0.4080(–)	3.3649(+)
40 ? 43	0.00	–174.89	0.41	–4.05	1.6747(+)	3.8913(+)
40 ? 44	–14.37	0.00	0.00	–4.30	0.5551(+)	1.0224(+)
40 ? 47	65.14	0.00	0.00	–5.43	1.4756(+)	2.2027(–)
40 ? 48	0.00	49.38	–0.09	–5.61	1.1827(+)	2.1564(–)
40 ? 49	–18.99	0.00	0.00	–5.96	0.4659(–)	2.2338(–)
40 ? 50	0.00	18.88	–0.03	–6.13	1.2364(–)	0.8617(+)
40 ? 51	–60.96	0.00	0.00	–6.33	1.0182(–)	3.4821(–)

40 ? 52	0.00	61.40	0.82	–6.64	1.0326(+)	3.8267(–)
40 ? 53	–21.04	0.00	0.00	–6.68	1.3665(–)	0.9454(–)
40 ? 54	–27.38	0.00	0.00	–6.71	1.0977(+)	1.5385(+)
40 ? 55	–41.32	0.00	0.00	–6.87	1.8460(+)	1.4135(+)
40 ? 57	0.00	20.61	1.38	–7.31	1.1217(+)	2.3519(–)
40 ? 59	13.09	0.00	0.00	–7.74	0.7877(+)	1.1815(–)
40 ? 62	–14.97	0.00	0.00	–8.04	0.4929(–)	2.2428(–)
40 ? 68	–17.07	0.00	0.00	–8.95	1.1774(–)	1.1921(–)
40 ? 70	20.18	0.00	0.00	–9.28	0.7662(–)	2.2467(+)
40 ? 73	–76.07	0.00	0.00	–10.36	0.9843(+)	7.3585(+)
40 ? 74	0.00	–16.69	–1.68	–10.94	0.6820(+)	6.0605(+)
40 ? 75	0.00	–45.75	–1.31	–11.64	1.2637(–)	4.7196(–)
40 ? 76	0.00	–20.67	1.33	–12.10	1.6277(+)	3.6482(–)
40 ? 78	12.46	0.00	0.00	–12.63	1.4627(–)	0.9890(+)
40 ? 87	0.00	–13.19	0.55	–14.91	0.7355(+)	3.5745(–)
40 ? 102	0.00	15.33	0.05	–17.93	0.7546(–)	3.3644(+)
40 ? 113	16.39	0.00	0.00	–20.53	0.9874(+)	3.1302(–)
40 ? 130	–17.63	0.00	0.00	–25.50	0.5450(+)	7.5773(+)
Sum:	–133.96	–105.59	1.44			
FullSum:	–115.25	–105.30	0.25			

MO contributions to σ in principal axes for **3** (*Si*Me$_2$).

MO	σ_1	σ_2	σ_3	average
1	481.9	481.9	481.9	481.9
2	0.8	0.5	1.3	0.9
3	0.8	0.5	1.3	0.9
4	1.5	0.1	1.5	1.0
5	0.8	0.7	1.4	1.0
6	0.7	0.8	1.5	1.0
7	97.4	90.8	97.6	95.3
8	1.2	0.7	1.9	1.3
9	1.2	0.7	1.9	1.3
10	2.1	0.3	2.0	1.4
11	89.0	103.6	53.2	81.9
12	52.3	105.4	131.1	96.3
13	111.4	54.3	57.5	74.4
14	0.7	0.5	0.4	0.5
15	0.6	0.5	0.4	0.5
16	0.8	0.5	–0.2	0.3
17	0.8	0.5	–0.3	0.3
18	–0.6	–0.4	1.2	0.1
19	–0.6	–0.3	1.2	0.1
20	–0.1	0.2	1.3	0.5
21	1.4	0.2	–1.2	0.1
22	0.2	0.2	1.3	0.6
23	19.4	7.1	25.5	17.3
24	5.9	3.0	7.5	5.5
25	11.7	2.6	–11.8	0.9
26	2.0	3.6	1.9	2.5
27	0.0	7.6	–21.3	–4.6
28	–35.9	2.8	–24.6	–19.2
29	–27.9	–43.3	2.2	–23.0
30	4.5	–7.6	–38.7	–14.0
31	11.0	1.9	48.6	20.5
32	–6.9	–5.9	–3.5	–5.4
33	–13.4	–0.4	3.7	–3.4
34	–17.5	–1.1	1.7	–5.6
35	1.1	–0.3	1.1	0.6
36	–2.7	–0.7	–1.1	–1.5
37	3.4	–446.5	–467.9	–303.7

38	–897.1	3.9	–20.0	–304.4
39	–1.3	–85.7	–21.6	–36.2
40	–112.4	–95.6	–0.6	–69.6

MO contributions to σ_{p1} in principal axes for **3** (*Si*Me$_2$).

MO	σ_1	σ_2	σ_3	average
1	–0.1	0.0	–0.2	–0.1
2	–2.8	–1.7	–4.3	–2.9
3	–2.8	–1.7	–4.3	–2.9
4	–5.0	–0.2	–4.8	–3.3
5	–8.8	–9.4	–18.2	–12.1
6	–8.8	–9.3	–18.1	–12.1
7	5.9	–0.3	6.1	3.9
8	–2.4	–1.4	–3.8	–2.5
9	–2.4	–1.4	–3.8	–2.5
10	–4.3	–0.1	–4.2	–2.9
11	–15.7	–0.1	–0.2	–5.3
12	0.0	0.8	26.5	9.1
13	7.1	1.1	–45.8	–12.5
14	–2.9	–1.7	–5.3	–3.3
15	–3.0	–1.7	–5.2	–3.3
16	–2.8	–1.7	–5.9	–3.5
17	–2.8	–1.7	–6.0	–3.5
18	–4.2	–2.5	–4.4	–3.7
19	–4.2	–2.5	–4.4	–3.7
20	–6.5	–0.2	–4.9	–3.8
21	–4.9	–0.3	–7.5	–4.2
22	–6.3	–0.2	–4.8	–3.8
23	6.6	–3.7	6.0	3.0
24	–3.4	–6.7	–9.4	–6.5
25	7.2	–1.0	–17.7	–3.8
26	–1.3	1.0	–3.5	–1.3
27	–10.0	–3.8	–33.4	–15.7
28	–47.8	–6.4	–42.4	–32.2
29	–38.9	–52.2	–12.7	–34.6
30	–2.4	–17.1	–53.5	–24.4
31	2.4	–5.4	35.8	10.9
32	–16.8	–14.2	–18.1	–16.4
33	–16.4	–4.2	–2.5	–7.7
34	–21.3	–3.2	–3.1	–9.2
35	–2.0	–4.2	–5.3	–3.9
36	–6.4	–2.7	–5.6	–4.9
37	–8.7	–460.6	–489.5	–319.6
38	–905.1	–2.6	–29.6	–312.4
39	–6.0	–88.9	–28.6	–41.2
40	–122.4	–105.4	–6.1	–78.0
Sum:	–1270.2	–817.7	–842.6	–976.8

Contributions from separate excitations into σ_{p1} (in principal axes) for **3** (*Si*Me$_2$).

OCC ?	VAC	σ_1	σ_2	σ_3	energy denominator, (eV)	|<OZ>| (mHartree/ Zeeman)	|<PSO>| (mZeeman)
37 ?	41	0.00	–380.75	–0.83	–5.62	2.1905(+)	9.0019(+)
37 ?	42	0.00	–3.78	–21.05	–7.07	0.7828(–)	2.2593(–)
37 ?	46	0.00	–4.69	–55.18	–8.12	1.3553(–)	3.2938(–)
37 ?	47	0.00	–2.12	–56.70	–8.57	2.7197(–)	1.7121(–)
37 ?	49	0.00	–30.24	–22.19	–9.10	2.8079(+)	1.6011(+)
37 ?	53	0.00	–1.33	–57.13	–9.82	2.9683(–)	2.0498(–)
37 ?	54	0.00	–0.59	–159.85	–9.85	4.4107(+)	3.3622(+)

37 ? 55	0.00	–37.89	–55.35	–10.01	2.3257(–)	3.8461(–)
37 ? 58	0.00	–54.48	–1.13	–10.77	2.0331(–)	2.7315(–)
37 ? 63	0.00	–0.06	–38.97	–11.30	1.9954(+)	2.0335(+)
37 ? 68	0.00	–14.45	–11.02	–12.09	1.3492(+)	2.1183(+)
37 ? 72	0.00	0.80	30.34	–13.25	1.0163(–)	3.7693(+)
37 ? 73	0.00	0.47	–24.54	–13.50	2.1689(–)	1.4339(–)
37 ? 77	0.00	39.11	–0.23	–15.70	1.2166(+)	4.6697(–)
37 ? 81	0.00	15.01	5.56	–16.31	0.8931(+)	3.5955(–)
37 ? 82	0.00	0.67	–27.55	–16.74	1.3424(+)	3.2471(+)
37 ? 98	0.00	–1.30	–15.77	–20.06	0.8101(–)	4.2765(–)
37 ? 100	0.00	–11.22	–4.84	–20.44	1.0996(–)	6.2539(–)
37 ? 113	0.00	–0.01	19.62	–23.66	1.3198(–)	3.2335(+)
37 ? 114	0.00	–22.95	1.79	–24.00	1.0809(–)	5.0691(–)
37 ? 115	0.00	–21.85	–0.07	–24.30	1.1597(–)	4.2768(–)
37 ? 120	0.00	0.63	–22.17	–25.78	0.8762(+)	6.3576(+)
37 ? 133	0.00	7.16	3.33	–29.47	0.9439(+)	3.1122(–)
37 ? 137	0.00	19.96	–0.41	–31.32	1.7179(+)	4.1863(–)
37 ? 139	0.00	10.08	3.82	–32.21	1.1580(+)	4.4391(–)
37 ? 162	0.00	0.01	15.81	–39.05	1.5868(–)	3.6140(+)
37 ? 176	0.00	12.60	0.01	–42.95	1.4828(–)	3.3700(+)
37 ? 181	0.00	–0.17	10.83	–44.33	1.8061(+)	2.4923(–)
37 ? 183	0.00	–0.18	11.25	–45.57	2.0638(+)	2.3653(–)
37 ? 236	0.00	–14.38	0.05	–101.33	1.7675(–)	7.6709(–)
37 ? 245	0.00	–6.34	–4.36	–109.28	0.4867(–)	24.4459(–)
37 ? 247	0.00	–0.52	–15.72	–112.48	0.7608(–)	23.7590(–)
37 ? 253	0.00	19.86	–0.45	–116.24	1.9309(+)	11.2318(–)
37 ? 257	0.00	0.10	17.68	–121.11	0.7485(–)	26.4836(+)
Sum:	0.00	–482.86	–475.42			
FullSum:	–8.68	–460.57	–489.53			

38 ? 41	–834.90	0.00	0.00	–4.49	4.0559(–)	8.4842(–)
38 ? 42	–10.24	0.00	0.00	–5.93	0.4942(–)	1.1294(–)
38 ? 43	0.00	–1.99	–38.71	–6.05	0.6632(–)	3.5543(–)
38 ? 46	–19.80	0.00	0.00	–6.98	1.0735(+)	1.1832(+)
38 ? 49	–10.42	0.00	0.00	–7.97	0.6461(+)	1.1805(+)
38 ? 50	0.00	–2.39	–18.12	–8.14	0.8457(–)	2.4012(–)
38 ? 57	0.00	0.62	26.00	–9.32	1.1716(+)	1.9997(–)
38 ? 60	0.00	–0.46	13.56	–9.89	1.1241(+)	1.1477(–)
38 ? 64	0.00	0.78	26.67	–10.35	0.6468(–)	4.0784(+)
38 ? 67	0.00	2.01	–43.21	–10.90	1.4653(+)	3.1960(+)
38 ? 68	–19.75	0.00	0.00	–10.95	1.2446(–)	1.5967(–)
38 ? 71	0.00	–0.02	43.71	–11.97	2.2372(+)	2.1622(–)
38 ? 74	0.00	1.27	–68.12	–12.94	2.2044(+)	3.7558(+)
38 ? 75	0.00	–0.15	–18.12	–13.65	1.4998(+)	1.5330(+)
38 ? 77	–17.54	0.00	0.00	–14.56	0.5251(+)	4.4692(+)
38 ? 81	14.10	0.00	0.00	–15.18	0.5721(–)	3.4378(+)
38 ? 90	0.00	1.10	20.58	–17.38	1.0114(–)	3.5976(+)
38 ? 94	0.00	–0.48	20.26	–18.15	0.8245(–)	4.2213(+)
38 ? 97	–11.54	0.00	0.00	–18.82	0.6031(+)	3.3090(+)
38 ? 100	–21.57	0.00	0.00	–19.30	0.6549(+)	5.8407(+)
38 ? 101	0.00	–0.28	–38.23	–19.81	1.0697(–)	6.5570(–)
38 ? 102	0.00	–0.01	19.99	–19.93	1.0393(+)	3.5457(–)
38 ? 108	0.00	–1.93	40.82	–21.41	1.5742(+)	5.5334(–)
38 ? 111	10.00	0.00	0.00	–21.77	1.5296(–)	1.3080(+)
38 ? 114	–12.81	0.00	0.00	–22.86	0.5648(+)	4.7658(+)
38 ? 137	14.18	0.00	0.00	–30.18	1.0906(–)	3.6047(+)
38 ? 142	0.00	–0.22	10.91	–32.79	2.0629(–)	1.6248(+)
38 ? 246	–17.90	0.00	0.00	–108.77	0.7619(–)	23.4812(–)
38 ? 258	0.00	–0.17	–39.44	–120.47	1.5028(+)	29.2527(+)
Sum:	–938.19	–2.32	–41.45			
FullSum:	–905.09	–2.65	–29.56			

39 ? 41	0.00	–88.54	–0.99	–4.38	2.5084(+)	1.4956(–)
39 ? 42	0.00	–0.38	17.77	–5.83	3.7705(–)	0.3354(+)
39 ? 44	0.00	0.04	–11.64	–6.20	3.5278(–)	0.1887(–)
39 ? 46	0.00	–1.23	–12.03	–6.88	1.4653(+)	0.5728(+)
39 ? 54	0.00	–0.15	–14.07	–8.61	1.8851(–)	0.6035(–)
Sum:	0.00	–90.25	–20.96			
FullSum:	–6.01	–88.94	–28.60			

40 ? 41	–11.28	0.00	0.00	–2.48	0.1206(+)	2.1329(+)
40 ? 42	19.17	0.00	0.00	–3.93	0.4080(–)	1.6963(+)
40 ? 43	0.00	–137.78	2.18	–4.05	1.6747(+)	3.1559(+)
40 ? 47	–41.42	0.00	0.00	–5.43	1.4756(+)	1.4008(+)
40 ? 50	0.00	45.48	–0.59	–6.13	1.2364(–)	2.1372(+)
40 ? 53	25.25	0.00	0.00	–6.68	1.3665(–)	1.1345(+)
40 ? 54	44.42	0.00	0.00	–6.71	1.0977(+)	2.4965(–)
40 ? 55	–92.37	0.00	0.00	–6.87	1.8460(+)	3.1596(+)
40 ? 57	0.00	–15.61	–6.94	–7.31	1.1217(+)	1.8161(+)
40 ? 60	0.00	–11.22	0.75	–7.88	0.8536(–)	1.0153(+)
40 ? 62	–13.14	0.00	0.00	–8.04	0.4929(–)	1.9679(–)
40 ? 64	0.00	26.93	–11.07	–8.34	1.0924(–)	3.6644(–)
40 ? 73	–10.64	0.00	0.00	–10.36	0.9843(+)	1.0295(+)
40 ? 74	0.00	9.16	5.26	–10.94	0.6820(+)	3.3534(–)
40 ? 75	0.00	–12.77	–2.00	–11.64	1.2637(–)	1.3401(–)
40 ? 79	21.27	0.00	0.00	–12.84	0.8839(–)	2.8380(+)
40 ? 82	–19.11	0.00	0.00	–13.61	0.8720(–)	2.7399(–)
40 ? 102	0.00	14.26	0.32	–17.93	0.7546(–)	3.2237(+)
40 ? 108	0.00	–14.60	2.52	–19.41	0.6489(–)	5.0615(+)
40 ? 113	14.04	0.00	0.00	–20.53	0.9874(+)	2.6816(–)
Sum:	–63.81	–96.15	–9.56			
FullSum:	–122.35	–105.42	–6.10			

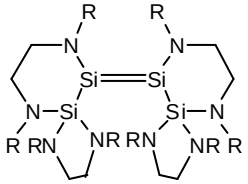
Summary of Natural Population Analysis for **3**.

Atom	No.	Natural Charge	Core	Valence	Rydberg	Total
Si	1	–0.36280	9.99709	4.33974	0.02597	14.36280
Si	2	1.04048	9.99720	2.92998	0.03233	12.95952
Si	3	0.48288	9.99840	3.48337	0.03536	13.51712
C	4	–1.19709	1.99951	5.18559	0.01198	7.19709
Si	5	0.48288	9.99840	3.48337	0.03536	13.51712
C	6	–1.19709	1.99951	5.18559	0.01198	7.19709
H	7	–0.14433	0.00000	1.14356	0.00076	1.14433
H	8	–0.14587	0.00000	1.14520	0.00067	1.14587
H	9	–0.14275	0.00000	1.14182	0.00093	1.14275
H	10	0.26652	0.00000	0.73246	0.00101	0.73348
H	11	0.27428	0.00000	0.72529	0.00043	0.72572
H	12	0.26750	0.00000	0.73110	0.00140	0.73250
H	13	–0.14433	0.00000	1.14356	0.00076	1.14433
H	14	–0.14587	0.00000	1.14520	0.00067	1.14587
H	15	–0.14275	0.00000	1.14182	0.00093	1.14275
H	16	0.26652	0.00000	0.73246	0.00101	0.73348
H	17	0.27428	0.00000	0.72529	0.00043	0.72572
H	18	0.26750	0.00000	0.73110	0.00140	0.73250

Summary of ^{29}Si NMR shifts for various disilene systems ($R^1R^2Si{=}SiR^3R^4$).[a]

R^1	R^2	R^3	R^4	^{29}Si	Lit.
Mes	Mes	Mes	Mes	+63.6	15
Mes	^{t}Bu	Mes	^{t}Bu	+90.3	2,15
^{t}Bu	Mes	Mes	^{t}Bu	+94.3	
Mes	$N(SiMe_3)_2$	Mes	$N(SiMe_3)_2$	+61.3	2,3
$N(SiMe_3)_2$	Mes	Mes	$N(SiMe_3)_2$	+49.4	
Mes	Mes	Mes	Mes	+63.7	
Xyl	Xyl	Xyl	Xyl	+64.1	
Mes	Mes	Xyl	Xyl	+65.2, +62.6	16
Mes	Xyl	Xyl	Mes	+63.87	
Mes	Xyl	Mes	Xyl	+63.86	
Ad	Mes	Ad	Mes	+87.1	9
Ad	Mes	Mes	Ad	+92.6	
Xyl	Xyl	Xyl	Xyl	+64.1	
DMT	DMT	DMT	DMT	+65.2	
Mes	Mes	Xyl	Xyl	+65.2 (Mes) +62.6 (Xyl)	
Mes	Mes	DMT	DMT	+64.2, +64.1	
Mes	Xyl	Mes	Xyl	+63.86, +63.87	4
Mes	Xyl	Xyl	Mes		
Mes	DMT	Mes	DMT	+64.15, +64.37	
Mes	DMT	DMT	Mes		
Mes	Mes	Mes	Xyl	+63.14, +64.42	
Xyl	Xyl	DMT	Xyl	+63.30, +64.63	
Xyl	Xyl	DMT	DMT	+63.24, +65.82	
IS	$SiMe_3$	IS	$SiMe_3$	+97.75	
IS	$SiMe_3$	$SiMe_3$	IS	+97.68	5
IS	^{t}Bu	IS	^{t}Bu	+87.39	
IS	^{t}Bu	^{t}Bu	IS	+96.93	
Mes	TB	TB	Mes	+56.16, +56.74, +57.12, +58.12	6
Mes	TB	Mes	TB	+66.49	
Mes	Mes	IS	IS	+57.86, +59.40	7
^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	+144.5	
^{t}BuMe$_2$Si	^{t}BuMe$_2$Si	^{t}BuMe$_2$Si	^{t}BuMe$_2$Si	+142.1	8
^{i}Pr$_3$Si	^{i}Pr$_3$Si	^{i}Pr$_3$Si	^{i}Pr$_3$Si	+154.5	
Mes	Mes	Mes	Mes	+63.3 (+63.2)	
Mes	Mes	Mes	Mes	+63.3 (+65.0)[c]	
Mes	Mes	Mes	Mes	+63.0 (+59.6)[d]	
IS	IS	IS	IS	+53.4 (+50.8, +53.2)	
Mes	^{t}Bu	Mes	^{t}Bu	+90.3 (+86.1)	17
$(Me_3Si)_2CH$	$(Me_3Si)_2CH$	$(Me_3Si)_2CH$	$(Me_3Si)_2CH$	+90.4 (+86.1, +87.4)	
Me_3Si	IS	Me_3Si	IS	+94.4 (+94.5)	
^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	+144.5 (+143)	
^{i}Pr$_3$Si	^{i}Pr$_3$Si	^{i}Pr$_3$Si	^{i}Pr$_3$Si	+154.5 (+164)	
see below				+119.5[e]	e
$(^t$Bu$_3$Si$)_2$HSi	$(^t$Bu$_3$Si$)_2$HSi	$(^t$Bu$_3$Si$)_2$HSi	$(^t$Bu$_3$Si$)_2$HSi	+141.32	12
^{t}BuMe$_2$Si	^{i}Pr$_2$MeSi	^{t}BuMe$_2$Si	^{i}Pr$_2$MeSi	+141.8	
^{t}BuMe$_2$Si	^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	^{t}BuMe$_2$Si	+141.9	10
^{t}BuMe$_2$Si	^{t}BuMe$_2$Si	^{i}Pr$_2$MeSi	^{i}Pr$_2$MeSi	+131.2, +156.2	
^{t}Bu$_3$Si	Ph	^{t}Bu$_3$Si	Ph	+128	13

[a] ^{29}Si NMR data of various disilenes with selected substituents; solid state ^{29}Si NMR values are given in parentheses. [b] Abbreviation for substituents: Xyl = 2,6-dimethylphenyl, DMT = 4-*tert*-butyl-2,6-dimethylphenyl, IS = 2,4,6-triisopropylphenyl, TB = 2,4,6-tris[bis(trimethylsilyl)-methyl]phenyl [c] $Mes_2SiSiMes_2{\bullet}C_7H_8$ [d] $Mes_2SiSiMes_2{\bullet}$THF, [e] see: Schmedake, T. A.; Haaf, M.; Apeloig, Y.; Müller, T.; Bukalov, S.; West, R. *J. Am. Chem. Soc.* **1999**, *121*, 9479:



R=^{t}Bu