Electronic Supplementary Information for Dalton Transactions

Electronic Supporting Information for

Silaimidazolium and Silaimidazolidinium ions

*Annemarie Schäfer, André Schäfer and Thomas Müller**

Table S1. Calculated absolute electronic energies, E, and free energies G298 of cations and carbene analogues at different levels of theory (in Hartree). Number of imaginary frequencies given in parentheses, Zero point vibrational energies in italics (in kJ mol^{-1}).

cpd	E B3LYP/ 6-31G(d)	G298 B3LYP/ 6-31G(d)	E B3LYP/ 6-311G(2d,p)// B3LYP/6-31G(d)	E B3LYP/ 6-311+G(d,p)
3a	-792.13968 (0), *766.6*	-791.88859	-792.30919	
3c	-1411.49795 (0), *1489.4*	-1410.99567	-1411.82883	-1411.80905 (0), *1475.7*
4	-793.33787 (0), *628.9*	-793.06356	-793.50918	
7a	-1319.13441 (0), *1298.3*	-1318.69579	-1319.39986	
7c	-1938.49634 (0), *2018.9*	-1937.80832	-1938.92271	-1938.89293
7d	-1437.06088 (0), *1522.8*	-1436.53991	-1437.35807	-1437.33988
7f	-2056.42575 (0), *2246.0*	-2055.65048	-2056.88405	-2056.85268
8a	-1320.33434 (0), *1361.0*	-1319.87118	-1320.60226	
8b	-1438.26016 (0), *1587.6*	-1437.71432	-1438.56003	
$SiEt_3^+$	-526.91931 (0), *519.2*	-526.75816	-527.01991	
$Si\mathit{i}Pr_3^+$	-644.85748 (0), *743.6*	-644.61739	-644.98978	

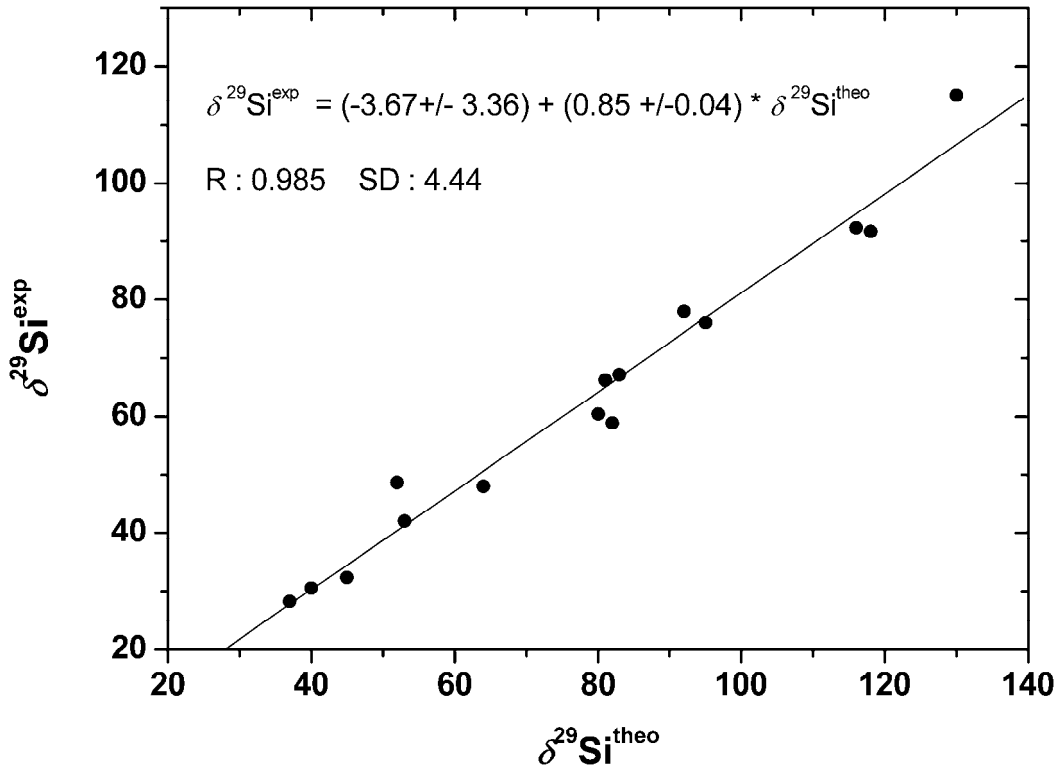

Figure S1. Correlation between calculated ^{29}Si NMR chemical shifts, $\delta^{29}Si^{theo}$ (GIAO/ B3LYP/ 6-311G(2d,p)//B3LYP/6-31G(d) and experimentally determined ^{29}Si NMR chemical shift $\delta^{29}Si^{exp}$ (benzene-d_6, 300K) for silylenes **3**, **4** and silylium ions **7**, **8**.

3a B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.000043	1.184199	-0.000258
2	7	0	-1.236571	-0.111154	-0.000133
3	7	0	1.236545	-0.111109	-0.000182
4	6	0	-0.677992	-1.382130	-0.000319
5	6	0	0.677970	-1.382111	-0.000217
6	1	0	-1.294061	-2.272315	-0.000351
7	1	0	1.294060	-2.272275	0.000032
8	6	0	-2.715730	0.039202	0.000090
9	6	0	2.715727	0.039235	0.000063
10	6	0	-3.304318	-0.617951	1.265837
11	1	0	-2.885561	-0.155590	2.165943
12	1	0	-4.393169	-0.494509	1.288054
13	1	0	-3.089376	-1.690774	1.304598
14	6	0	-3.304687	-0.617353	-1.265776
15	1	0	-3.090187	-1.690247	-1.304999
16	1	0	-4.393497	-0.493504	-1.287693
17	1	0	-2.885975	-0.154819	-2.165817
18	6	0	-3.084890	1.531324	0.000402
19	1	0	-2.694534	2.042408	-0.886118
20	1	0	-4.175253	1.637681	0.000486
21	1	0	-2.694465	2.042118	0.887059
22	6	0	3.304238	-0.617520	1.266012
23	1	0	4.393102	-0.494162	1.288105
24	1	0	2.885571	-0.154769	2.165954
25	1	0	3.089199	-1.690312	1.305164
26	6	0	3.085093	1.531350	-0.000096
27	1	0	4.175473	1.637646	0.000409
28	1	0	2.695178	2.042100	-0.886997
29	1	0	2.694335	2.042561	0.886169
30	6	0	3.304660	-0.617942	-1.265466
31	1	0	4.393524	-0.494567	-1.287233
32	1	0	3.089692	-1.690764	-1.304416
33	1	0	2.886300	-0.155486	-2.165708

3c B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.000018	-0.000002	-1.085896
2	7	0	-1.222703	-0.000088	0.220578
3	7	0	1.222694	0.000026	0.220548
4	6	0	-0.678893	-0.000077	1.501856
5	6	0	0.678904	-0.000018	1.501844
6	1	0	-1.324581	-0.000130	2.371234
7	1	0	1.324614	-0.000004	2.371205
8	6	0	-2.652130	0.000013	0.048663
9	6	0	-3.339702	-1.231820	-0.039022
10	6	0	-4.725939	-1.203271	-0.235241
11	6	0	-5.416807	0.000213	-0.335875
12	6	0	-4.725792	1.203589	-0.235084
13	6	0	-3.339544	1.231933	-0.038881
14	1	0	-5.271347	-2.140039	-0.311611
15	1	0	-6.492732	0.000287	-0.490364
16	1	0	-5.271071	2.140445	-0.311327
17	6	0	2.652121	-0.000020	0.048637
18	6	0	3.339651	1.231823	-0.039100
19	6	0	4.725903	1.203311	-0.235280
20	6	0	5.416813	-0.000147	-0.335831
21	6	0	4.725831	-1.203548	-0.234984
22	6	0	3.339589	-1.231925	-0.038816
23	1	0	5.271277	2.140099	-0.311672
24	1	0	6.492742	-0.000203	-0.490289
25	1	0	5.271154	-2.140385	-0.311152
26	6	0	-2.625503	-2.575999	0.069090
27	1	0	-1.570725	-2.377694	0.278477
28	6	0	-2.625250	2.576019	0.069573
29	1	0	-1.570426	2.377582	0.278600
30	6	0	-2.691217	-3.357616	-1.257454
31	1	0	-2.254080	-2.779889	-2.079129
32	1	0	-2.139695	-4.301952	-1.174086
33	1	0	-3.725690	-3.598357	-1.530403
34	6	0	-3.169154	-3.421954	1.236785
35	1	0	-2.595133	-4.351330	1.332272
36	1	0	-3.099118	-2.880505	2.186735
37	1	0	-4.219829	-3.696670	1.086107
38	6	0	-3.168597	3.421406	1.237835
39	1	0	-3.098166	2.879530	2.187512
40	1	0	-2.594659	4.350809	1.333548
41	1	0	-4.219366	3.696026	1.087632
42	6	0	-2.691276	3.358282	-1.256574
43	1	0	-2.254356	2.780955	-2.078643
44	1	0	-3.725788	3.599243	-1.529183
45	1	0	-2.139691	4.302550	-1.172859
46	6	0	2.625294	-2.576026	0.069583
47	1	0	1.570496	-2.377605	0.278755
48	6	0	3.168774	-3.421602	1.237627
49	1	0	2.594781	-4.350974	1.333319
50	1	0	4.219491	-3.696316	1.087210
51	1	0	3.098561	-2.879864	2.187401
52	6	0	2.691159	-3.358050	-1.256712
53	1	0	2.139513	-4.302298	-1.173157
54	1	0	2.254224	-2.780523	-2.078635
55	1	0	3.725642	-3.599009	-1.529427
56	6	0	2.625464	2.575994	0.069073
57	1	0	1.570695	2.377704	0.278520
58	6	0	3.169199	3.421855	1.236794

59	1	0	3.099281	2.880298	2.186691
60	1	0	4.219847	3.696629	1.086033
61	1	0	2.595135	4.351191	1.332429
62	6	0	2.691130	3.357691	-1.257432
63	1	0	3.725591	3.598349	-1.530495
64	1	0	2.253839	2.780063	-2.079092
65	1	0	2.139716	4.302080	-1.173944

4 B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	0.000001	1.136845	-0.000005
2	7	0	1.252544	-0.094588	0.019323
3	7	0	-1.252547	-0.094599	-0.019387
4	6	0	0.728996	-1.446827	-0.230897
5	6	0	-0.728997	-1.446826	0.230871
6	1	0	1.296463	-2.215341	0.307444
7	1	0	-1.296459	-2.215357	-0.307450
8	6	0	2.719175	0.093038	0.011477
9	6	0	-2.719176	0.093038	-0.011471
10	6	0	3.332260	-0.470688	-1.289632
11	1	0	2.887331	0.014633	-2.165733
12	1	0	4.413490	-0.292982	-1.311406
13	1	0	3.174682	-1.550744	-1.380982
14	6	0	3.348776	-0.616322	1.231939
15	1	0	3.167345	-1.696372	1.217565
16	1	0	4.434889	-0.467255	1.245407
17	1	0	2.933246	-0.213701	2.161871
18	6	0	3.054370	1.591876	0.101106
19	1	0	2.631105	2.043309	1.005269
20	1	0	4.141522	1.725097	0.133682
21	1	0	2.669459	2.143537	-0.763218
22	6	0	-3.348897	-0.616669	-1.231667
23	1	0	-4.434970	-0.467319	-1.245234
24	1	0	-2.933225	-0.214536	-2.161747
25	1	0	-3.167766	-1.696764	-1.216847
26	6	0	-3.054356	1.591856	-0.101532
27	1	0	-4.141509	1.725091	-0.134011
28	1	0	-2.669335	2.143790	0.762568
29	1	0	-2.631190	2.042985	-1.005894
30	6	0	-3.332150	-0.470303	1.289856
31	1	0	-4.413418	-0.292818	1.311566
32	1	0	-3.174344	-1.550292	1.381621
33	1	0	-2.887318	0.015445	2.165769
34	1	0	-0.785443	-1.692470	1.303444
35	1	0	0.785451	-1.692493	-1.303461

7a B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-.392898	.250410	-.281446
2	14	0	1.644093	-1.011705	.211970
3	7	0	-2.034254	-.282330	.011626
4	7	0	-.800232	1.916756	.078368
5	6	0	-2.817250	.814590	.315421
6	6	0	-2.150186	2.000897	.356885
7	1	0	-3.883422	.710156	.455267
8	1	0	-2.620656	2.954789	.538196
9	6	0	-2.706929	-1.622431	-.151542
10	6	0	.067765	3.153878	.076965
11	6	0	-3.772334	-1.519891	-1.259421
12	1	0	-3.319693	-1.215175	-2.208811
13	1	0	-4.244604	-2.496558	-1.403054
14	1	0	-4.564056	-.806808	-1.012071
15	6	0	-3.343132	-2.019829	1.193639
16	1	0	-4.117601	-1.313545	1.507251
17	1	0	-3.811701	-3.004504	1.101622
18	1	0	-2.588028	-2.071550	1.984981
19	6	0	-1.666925	-2.670183	-.555757
20	1	0	-.916813	-2.819892	.226190
21	1	0	-2.163121	-3.632172	-.713529
22	1	0	-1.168607	-2.403721	-1.494370
23	6	0	-.765579	4.412143	-.224457
24	1	0	-.081779	5.254319	-.364902
25	1	0	-1.351231	4.299522	-1.142595
26	1	0	-1.436293	4.682851	.596471
27	6	0	1.124387	2.997348	-1.025445
28	1	0	1.808923	3.850879	-1.010346
29	1	0	1.728856	2.097434	-.885895
30	1	0	.655592	2.952874	-2.013919
31	6	0	.717852	3.284286	1.466565
32	1	0	1.340067	4.183954	1.509349
33	1	0	-.046020	3.362134	2.247071
34	1	0	1.352083	2.422344	1.697815
35	6	0	1.855448	-2.357654	-1.106296
36	1	0	2.872746	-2.742678	-.937331
37	1	0	1.188579	-3.195408	-.872345
38	6	0	1.703468	-1.957184	-2.584674
39	1	0	1.916047	-2.809982	-3.238023
40	1	0	.685556	-1.619414	-2.813985
41	1	0	2.387665	-1.150754	-2.865094
42	6	0	1.287525	-1.707775	1.947375
43	1	0	1.244415	-.863942	2.649281
44	1	0	.294544	-2.171946	1.977531
45	6	0	2.346195	-2.728903	2.418798
46	1	0	3.351973	-2.295965	2.450956
47	1	0	2.112945	-3.078071	3.430332
48	1	0	2.381156	-3.609402	1.768143

49	6	0	3.156147	.136724	.309817
50	1	0	2.890782	1.083303	.794389
51	1	0	3.801447	-.374650	1.040420
52	6	0	3.971353	.393183	-.970885
53	1	0	4.337007	-.541166	-1.408225
54	1	0	3.393737	.913249	-1.742442
55	1	0	4.847358	1.011453	-.747564

7c B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.002712	-0.026897	0.219703
2	14	0	-0.087079	-1.588937	2.063583
3	7	0	1.247490	0.441439	-0.886720
4	7	0	-1.246174	0.471860	-0.880922
5	6	0	0.685604	1.004562	-2.026693
6	6	0	-0.676568	1.023295	-2.022460
7	1	0	1.331075	1.396088	-2.800969
8	1	0	-1.315566	1.435654	-2.791301
9	6	0	1.578682	-1.474811	2.957477
10	1	0	1.437194	-2.037812	3.892724
11	1	0	2.305703	-2.055414	2.374127
12	6	0	2.155736	-0.084397	3.271663
13	1	0	3.082776	-0.173576	3.847818
14	1	0	2.399313	0.460672	2.353188
15	1	0	1.462574	0.528627	3.855469
16	6	0	-0.321624	-3.292103	1.259099
17	1	0	-1.276339	-3.308665	0.720054
18	1	0	0.460749	-3.447839	0.505913
19	6	0	-0.283355	-4.440662	2.291709
20	1	0	-1.073142	-4.342819	3.044682
21	1	0	-0.428730	-5.404992	1.793138
22	1	0	0.677058	-4.486172	2.816346
23	6	0	-1.610967	-1.087713	3.073515
24	1	0	-2.457484	-0.960286	2.385381
25	1	0	-1.860181	-1.976202	3.673017
26	6	0	-1.485381	0.134335	3.999598
27	1	0	-0.724332	-0.019606	4.771511
28	1	0	-1.219698	1.044236	3.448990
29	1	0	-2.434008	0.328024	4.511521
30	6	0	2.689928	0.415673	-0.713230
31	6	0	3.392962	-0.768868	-1.027073
32	6	0	4.782373	-0.758864	-0.852130
33	6	0	5.445687	0.375303	-0.394371
34	6	0	4.730682	1.534630	-0.111208
35	6	0	3.339787	1.589101	-0.265330
36	1	0	5.355142	-1.649800	-1.089010
37	1	0	6.524463	0.359096	-0.269093
38	1	0	5.262209	2.418050	0.228586
39	6	0	-2.689378	0.473741	-0.704794
40	6	0	-3.304311	1.618855	-0.150636
41	6	0	-4.697705	1.596199	-0.008710
42	6	0	-5.447287	0.493569	-0.404087
43	6	0	-4.817321	-0.614428	-0.963076
44	6	0	-3.428013	-0.653550	-1.132043
45	1	0	-5.202700	2.460667	0.410891
46	1	0	-6.527006	0.500853	-0.286172
47	1	0	-5.416869	-1.460602	-1.282023
48	6	0	2.716185	-2.006571	-1.611566
49	1	0	1.635306	-1.911702	-1.457143
50	6	0	2.607723	2.904777	-0.004337
51	1	0	1.529713	2.709077	-0.017335
52	6	0	3.162149	-3.313888	-0.930946
53	1	0	3.038158	-3.270230	0.157446
54	1	0	2.571193	-4.155335	-1.309574
55	1	0	4.213454	-3.543902	-1.133276
56	6	0	2.947360	-2.080166	-3.135945
57	1	0	2.431952	-2.948915	-3.560802
58	1	0	2.574959	-1.183076	-3.642211
59	1	0	4.014266	-2.174697	-3.366875
60	6	0	2.901730	3.922166	-1.127539
61	1	0	2.626270	3.531418	-2.113123
62	1	0	2.340254	4.848131	-0.960735
63	1	0	3.967022	4.176319	-1.158514
64	6	0	2.939576	3.514057	1.371474
65	1	0	2.732745	2.814389	2.188042
66	1	0	3.991195	3.810775	1.444276
67	1	0	2.336799	4.414040	1.535591
68	6	0	-2.779508	-1.851259	-1.822715
69	1	0	-1.713319	-1.854941	-1.566747
70	6	0	-2.878880	-1.713638	-3.357486
71	1	0	-2.389985	-2.561418	-3.850570
72	1	0	-3.926309	-1.694257	-3.678605
73	1	0	-2.403014	-0.794328	-3.714597
74	6	0	-3.363817	-3.202323	-1.370945
75	1	0	-2.765235	-4.023502	-1.780011
76	1	0	-3.378847	-3.299011	-0.279469
77	1	0	-4.388893	-3.345578	-1.728716
78	6	0	-2.534056	2.879502	0.237088
79	1	0	-1.462538	2.650248	0.218273
80	6	0	-2.775963	4.004008	-0.792132
81	1	0	-2.491692	3.695074	-1.803909
82	1	0	-3.832449	4.293097	-0.817848
83	1	0	-2.190782	4.893020	-0.531552
84	6	0	-2.868842	3.366994	1.659418
85	1	0	-3.905904	3.709556	1.740220
86	1	0	-2.721094	2.577591	2.404122
87	1	0	-2.226693	4.213380	1.926793

7d B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.823643	0.045303	-0.442810
2	14	0	1.603318	-0.169674	0.055410
3	7	0	-2.031420	-1.157129	-0.003345
4	7	0	-1.917353	1.366073	-0.039910
5	6	0	-3.193508	-0.514993	0.373760
6	6	0	-3.130421	0.844537	0.359815
7	1	0	-4.087494	-1.077415	0.601056
8	1	0	-3.965972	1.490096	0.581797
9	6	0	-2.075066	-2.660532	-0.140298
10	6	0	-1.740372	2.864968	-0.142443
11	6	0	-3.137013	-3.037232	-1.191539
12	1	0	-2.901117	-2.587188	-2.161645
13	1	0	-3.159862	-4.124484	-1.315340
14	1	0	-4.142246	-2.718745	-0.901255
15	6	0	-2.413952	-3.272523	1.232312
16	1	0	-3.401953	-2.968508	1.590063
17	1	0	-2.414042	-4.364279	1.155735
18	1	0	-1.673876	-2.982306	1.985444
19	6	0	-0.713057	-3.179454	-0.602811
20	1	0	0.065442	-2.985240	0.139722
21	1	0	-0.766225	-4.263504	-0.738724
22	1	0	-0.418814	-2.745360	-1.564221
23	6	0	-3.082211	3.559911	-0.440301
24	1	0	-2.882709	4.610900	-0.669066
25	1	0	-3.583110	3.117219	-1.307362
26	1	0	-3.767856	3.548129	0.412292
27	6	0	-0.781889	3.161391	-1.301972
28	1	0	-0.594646	4.237713	-1.364572
29	1	0	0.185344	2.675315	-1.163152
30	1	0	-1.206486	2.833402	-2.256663
31	6	0	-1.177094	3.378293	1.194955
32	1	0	-1.072072	4.467632	1.164837
33	1	0	-1.848024	3.125053	2.022445
34	1	0	-0.193822	2.948436	1.410487
35	6	0	2.332120	-1.427059	-1.199245
36	1	0	1.963668	-2.407533	-0.871171
37	6	0	1.894162	-1.224811	-2.664087
38	1	0	2.294256	-2.031393	-3.290351
39	1	0	0.804698	-1.225629	-2.787566
40	1	0	2.269009	-0.281617	-3.073803
41	6	0	1.459720	-0.876412	1.844161
42	1	0	0.713696	-1.680677	1.772110
43	6	0	2.762894	-1.531956	2.354173
44	1	0	3.589279	-0.818060	2.427611
45	1	0	2.598006	-1.940515	3.358912
46	1	0	3.086473	-2.360784	1.716912
47	6	0	2.408986	1.573367	-0.033451
48	1	0	1.684627	2.275226	0.401154
49	6	0	2.745971	2.055423	-1.461534
50	1	0	3.571452	1.479092	-1.890537
51	1	0	1.906079	1.989316	-2.160617
52	1	0	3.068239	3.103371	-1.433863
53	6	0	0.917649	0.148067	2.860975
54	1	0	-0.054038	0.560502	2.563145
55	1	0	0.781797	-0.328485	3.839301
56	1	0	1.605131	0.988621	3.005861
57	6	0	3.679509	1.650972	0.848792
58	1	0	4.452751	0.948906	0.519982
59	1	0	4.108136	2.658351	0.779697
60	1	0	3.473109	1.457584	1.904824
61	6	0	3.877868	-1.482301	-1.115677
62	1	0	4.247918	-2.292480	-1.755513
63	1	0	4.339057	-0.555879	-1.471463
64	1	0	4.246395	-1.674139	-0.103636

7f B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.004916	-0.075478	0.008008
2	14	0	0.114626	2.326468	-0.422119
3	7	0	-1.247180	-1.267459	0.194953
4	7	0	1.245779	-1.248060	0.271069
5	6	0	-0.677661	-2.514181	0.446447
6	6	0	0.680966	-2.502608	0.491599
7	1	0	-1.319443	-3.374116	0.581334
8	1	0	1.325389	-3.351077	0.675995
9	6	0	-1.619627	2.820224	-1.062043
10	1	0	-1.852433	2.089792	-1.850900
11	6	0	-2.741401	2.750801	-0.008073
12	1	0	-3.707292	2.977948	-0.475380
13	1	0	-2.832154	1.761786	0.452922
14	1	0	-2.589433	3.486092	0.790189
15	6	0	1.475965	2.353391	-1.772502
16	1	0	2.242664	1.641207	-1.430757
17	6	0	2.175114	3.725262	-1.906816
18	1	0	2.657085	4.038622	-0.975172
19	1	0	2.957185	3.665899	-2.673621
20	1	0	1.481919	4.516444	-2.213653
21	6	0	0.688784	3.099005	1.235719
22	1	0	1.760604	2.853485	1.293205
23	6	0	0.007715	2.543698	2.501439
24	1	0	-1.069565	2.740293	2.502344
25	1	0	0.150765	1.463211	2.620165
26	1	0	0.426095	3.023878	3.394398
27	6	0	-2.691371	-1.134908	0.110327
28	6	0	-3.313048	-1.238877	-1.154569

29	6	0	-4.707950	-1.119664	-1.198563
30	6	0	-5.454379	-0.918102	-0.041657
31	6	0	-4.818246	-0.840724	1.193620
32	6	0	-3.426145	-0.948912	1.303550
33	1	0	-5.218621	-1.198712	-2.153414
34	1	0	-6.535690	-0.832853	-0.101509
35	1	0	-5.413297	-0.700446	2.090745
36	6	0	2.692030	-1.094117	0.266481
37	6	0	3.346175	-0.747013	1.470538
38	6	0	4.740936	-0.621898	1.435420
39	6	0	5.458110	-0.843303	0.264320
40	6	0	4.792402	-1.209707	-0.901220
41	6	0	3.399075	-1.348934	-0.932022
42	1	0	5.274523	-0.359625	2.343337
43	1	0	6.539798	-0.743111	0.262911
44	1	0	5.365782	-1.399155	-1.802891
45	6	0	-2.547041	-1.541654	-2.440791
46	1	0	-1.476126	-1.421920	-2.241559
47	6	0	-2.776133	-0.915179	2.685541
48	1	0	-1.692295	-0.826221	2.552098
49	6	0	-2.904972	-0.582067	-3.591146
50	1	0	-2.768463	0.466737	-3.303295
51	1	0	-2.267692	-0.782289	-4.459631
52	1	0	-3.943568	-0.702820	-3.916986
53	6	0	-2.765523	-3.008670	-2.868218
54	1	0	-2.182340	-3.236688	-3.767629
55	1	0	-2.462247	-3.706467	-2.080121
56	1	0	-3.820689	-3.199479	-3.094123
57	6	0	-3.036304	-2.234122	3.443931
58	1	0	-2.668882	-3.102214	2.885908
59	1	0	-2.534370	-2.220125	4.417977
60	1	0	-4.107775	-2.381649	3.620102
61	6	0	-3.231763	0.290204	3.529569
62	1	0	-3.072068	1.237714	3.003677
63	1	0	-4.293801	0.228867	3.790042
64	1	0	-2.669372	0.323095	4.469276
65	6	0	2.720036	-1.826967	-2.214501
66	1	0	1.648495	-1.608702	-2.136364
67	6	0	2.867236	-3.356050	-2.372946
68	1	0	2.354737	-3.696839	-3.279705
69	1	0	3.922807	-3.638420	-2.455779
70	1	0	2.443448	-3.898495	-1.521465
71	6	0	3.243097	-1.113837	-3.475417
72	1	0	2.634100	-1.393218	-4.342169
73	1	0	3.209714	-0.024679	-3.371306
74	1	0	4.276228	-1.396053	-3.704837
75	6	0	2.612203	-0.591560	2.800542
76	1	0	1.544565	-0.461941	2.590145
77	6	0	2.754341	-1.874839	3.647515
78	1	0	2.371415	-2.753753	3.117797
79	1	0	3.804985	-2.065476	3.893738
80	1	0	2.199542	-1.776797	4.587583
81	6	0	3.071543	0.637410	3.606380
82	1	0	4.101413	0.531544	3.963254
83	1	0	3.017501	1.557086	3.013252
84	1	0	2.436428	0.762961	4.490018
85	6	0	-1.598693	4.217537	-1.728454
86	1	0	-2.586156	4.432955	-2.154567
87	1	0	-1.378642	5.010766	-1.006404
88	1	0	-0.870329	4.291490	-2.541890
89	6	0	0.561372	4.641589	1.211705
90	1	0	1.033234	5.063574	2.107417
91	1	0	1.041366	5.102164	0.343030
92	1	0	-0.488618	4.954138	1.222484
93	6	0	0.954669	1.865582	-3.139040
94	1	0	0.517834	0.859994	-3.090507
95	1	0	0.192491	2.537524	-3.547828
96	1	0	1.774042	1.827995	-3.866449

8a B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	.395956	.282543	.064511
2	14	0	-1.596384	-1.125342	-.192435
3	7	0	2.028167	-.201771	.013682
4	7	0	.639874	1.964681	-.087942
5	6	0	2.881556	1.015622	-.033937
6	6	0	2.035460	2.184459	-.546562
7	1	0	3.736863	.854812	-.695316
8	1	0	2.431785	3.118938	-.148636
9	6	0	2.739613	-1.514116	.140351
10	6	0	-.326325	3.110834	-.101879
11	6	0	3.868554	-1.399904	1.185454
12	1	0	3.478735	-1.073949	2.156044
13	1	0	4.332365	-2.381547	1.321025
14	1	0	4.658498	-.709366	.877258
15	6	0	3.321740	-1.902109	-1.233723
16	1	0	4.029898	-1.153394	-1.603042
17	1	0	3.859504	-2.853007	-1.160716
18	1	0	2.525895	-2.014438	-1.977852
19	6	0	1.761522	-2.596333	.608777
20	1	0	.957227	-2.758278	-.113687
21	1	0	2.289696	-3.548536	.715004
22	1	0	1.328501	-2.347386	1.583892
23	6	0	.380999	4.419866	.297087
24	1	0	-.373004	5.202432	.424587
25	1	0	.915022	4.313174	1.247513
26	1	0	1.081211	4.771633	-.466533
27	6	0	-1.415134	2.827796	.943103
28	1	0	-2.168516	3.621341	.930634
29	1	0	-1.935742	1.888198	.744597

30	1	0	-.984095	2.781612	1.948985
31	6	0	-.931566	3.263308	-1.511051
32	1	0	-1.624892	4.110214	-1.543660
33	1	0	-.151413	3.444395	-2.258313
34	1	0	-1.482860	2.363972	-1.807925
35	6	0	-1.716644	-2.261744	1.322095
36	1	0	-2.724667	-2.698654	1.270208
37	1	0	-1.027350	-3.104151	1.197202
38	6	0	-1.513766	-1.613489	2.703838
39	1	0	-1.660848	-2.348707	3.501924
40	1	0	-.499047	-1.211329	2.819582
41	1	0	-2.216882	-.793815	2.881865
42	6	0	-1.216695	-2.029460	-1.826821
43	1	0	-1.314057	-1.299314	-2.642231
44	1	0	-.180811	-2.384838	-1.863702
45	6	0	-2.174470	-3.215904	-2.073579
46	1	0	-3.224315	-2.902789	-2.090485
47	1	0	-1.961395	-3.681956	-3.041396
48	1	0	-2.068292	-3.989105	-1.305292
49	6	0	-3.179477	-.099147	-.454607
50	1	0	-2.955006	.846014	-.962407
51	1	0	-3.730611	-.689731	-1.202032
52	6	0	-4.098829	.142638	.756460
53	1	0	-4.402285	-.798507	1.225755
54	1	0	-3.626821	.758618	1.528590
55	1	0	-5.012641	.658106	.442431
56	1	0	2.066131	2.242721	-1.643775
57	1	0	3.264694	1.231534	.970639

8b B3LYP/6-31G(d)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	14	0	-0.833706	0.069381	-0.230867
2	14	0	1.629894	-0.205358	0.048564
3	7	0	-2.039493	-1.132802	-0.063322
4	7	0	-1.856816	1.436699	-0.078506
5	6	0	-3.365536	-0.460548	-0.010165
6	6	0	-3.157356	0.972752	0.467266
7	1	0	-4.034593	-0.989899	0.672433
8	1	0	-3.976062	1.595283	0.107136
9	6	0	-2.076832	-2.630881	-0.104689
10	6	0	-1.590998	2.913592	-0.139640
11	6	0	-3.110291	-3.098611	-1.151036
12	1	0	-2.879545	-2.691716	-2.141825
13	1	0	-3.084969	-4.190409	-1.219840
14	1	0	-4.133518	-2.815610	-0.889094
15	6	0	-2.451019	-3.163819	1.293676
16	1	0	-3.433036	-2.810041	1.622853
17	1	0	-2.488126	-4.257930	1.278881
18	1	0	-1.709690	-2.856796	2.039224
19	6	0	-0.709260	-3.188397	-0.502791
20	1	0	0.060144	-2.934979	0.231152
21	1	0	-0.758095	-4.280318	-0.548831
22	1	0	-0.403647	-2.829844	-1.490684
23	6	0	-2.885154	3.687952	-0.459226
24	1	0	-2.626909	4.733618	-0.651732
25	1	0	-3.376485	3.296534	-1.356522
26	1	0	-3.599718	3.682963	0.369272
27	6	0	-0.599415	3.178198	-1.279157
28	1	0	-0.349894	4.242741	-1.326964
29	1	0	0.335981	2.636677	-1.134802
30	1	0	-1.028037	2.884346	-2.243388
31	6	0	-1.030322	3.399948	1.211201
32	1	0	-0.880088	4.484597	1.197188
33	1	0	-1.721891	3.171099	2.029447
34	1	0	-0.067448	2.930190	1.439625
35	6	0	2.252148	-1.468995	-1.255151
36	1	0	1.873439	-2.442604	-0.921642
37	6	0	1.730901	-1.225358	-2.686105
38	1	0	2.077785	-2.022950	-3.354130
39	1	0	0.635318	-1.210734	-2.741656
40	1	0	2.094777	-0.278526	-3.097125
41	6	0	1.533215	-0.920805	1.838863
42	1	0	0.772876	-1.713519	1.792524
43	6	0	2.840426	-1.603132	2.300571
44	1	0	3.678889	-0.902697	2.361698
45	1	0	2.698104	-2.026888	3.302342
46	1	0	3.132511	-2.425068	1.639655
47	6	0	2.495277	1.507826	-0.051794
48	1	0	1.804348	2.234191	0.396020
49	6	0	2.829732	1.982473	-1.483727
50	1	0	3.633409	1.383262	-1.922081
51	1	0	1.981811	1.944665	-2.174433
52	1	0	3.182922	3.020270	-1.456347
53	1	0	-3.147289	1.027011	1.565539
54	1	0	-3.820801	-0.469130	-1.008170
55	6	0	3.797091	-1.576061	-1.262878
56	1	0	4.272683	-0.659122	-1.623619
57	1	0	4.214300	-1.806241	-0.277937
58	1	0	4.100728	-2.383685	-1.939924
59	6	0	3.784107	1.539173	0.806787
60	1	0	4.249082	2.529186	0.724811
61	1	0	3.591088	1.358189	1.867372
62	1	0	4.524111	0.807343	0.466170
63	6	0	1.043929	0.106475	2.880328
64	1	0	0.067991	0.538892	2.623195
65	1	0	0.934093	-0.373423	3.860187
66	1	0	1.747128	0.936783	3.005065