

Supporting Information

Cyclic Disilyl- or Digermylated Germylenes

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1. X-Ray Structures

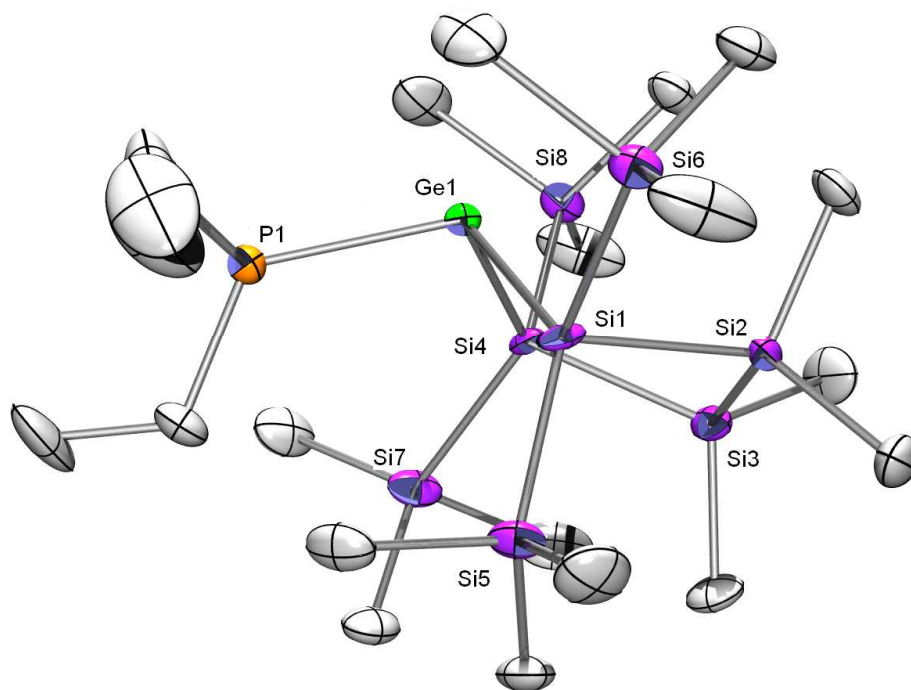


Figure S-1. Crystal structure of **2**. Thermal ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity.

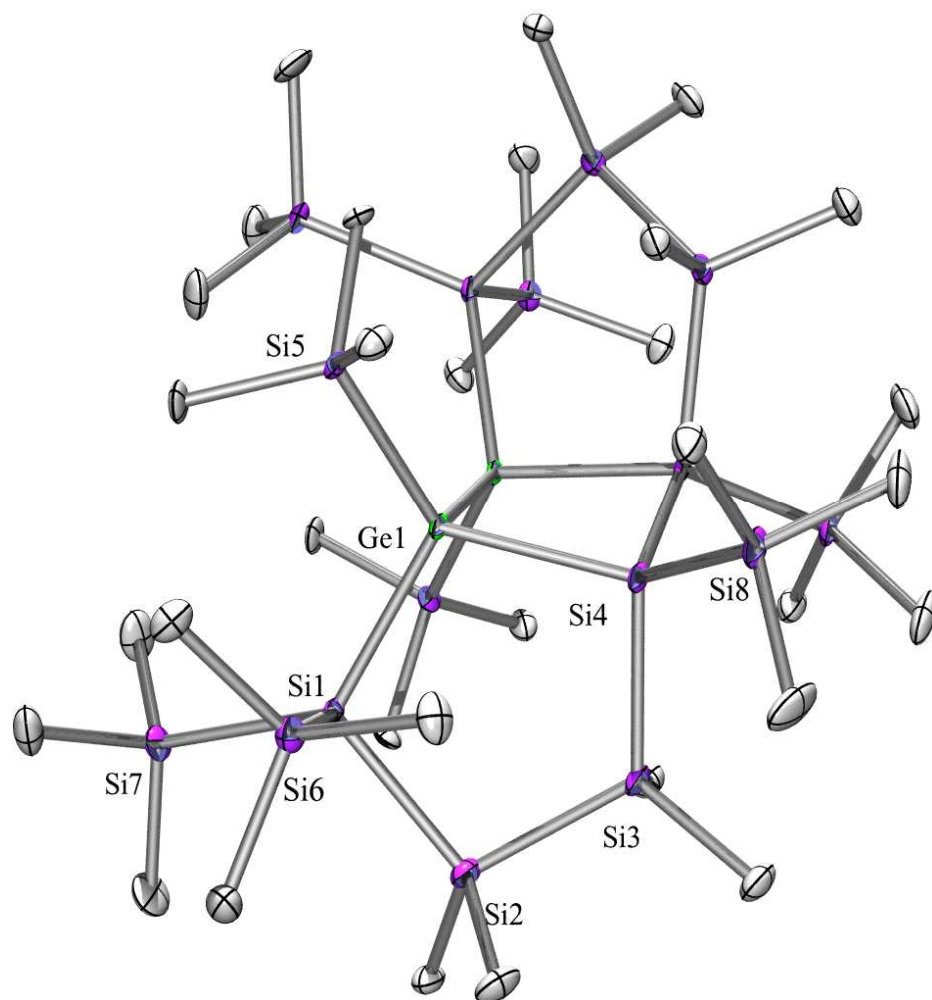


Figure S-2. Crystal structure of **5**. Thermal ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity.

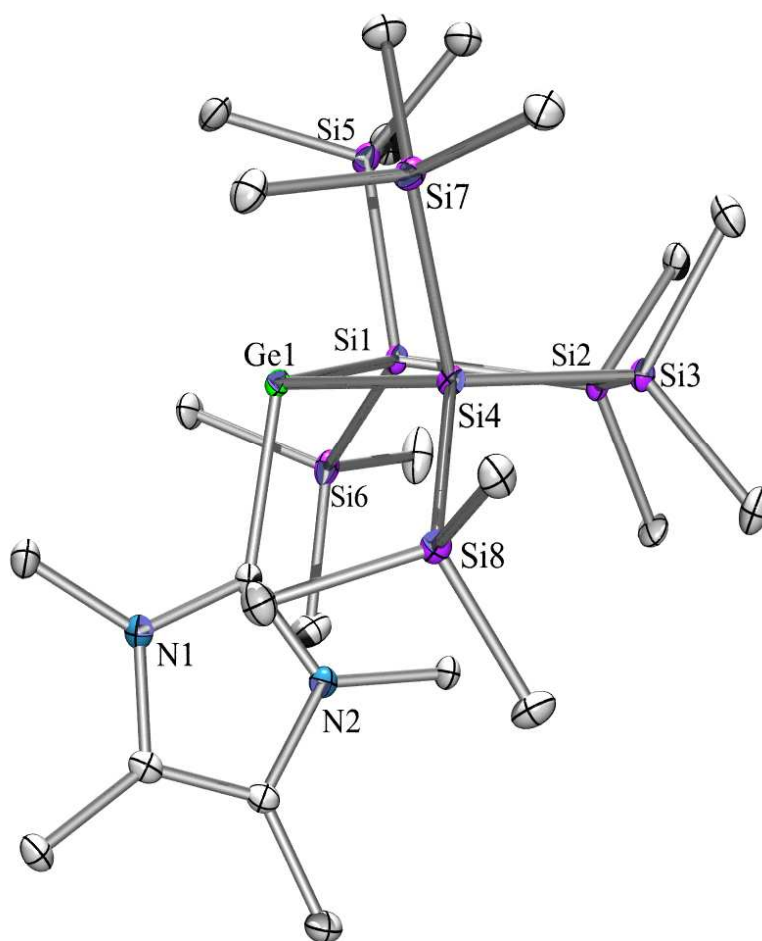


Figure S-3. Crystal structure of **6**. Thermal ellipsoids are represented at the 30% level and hydrogen atoms have been omitted for clarity.

Table S1. Crystallographic data for compounds **2**, **2a**, **5**, **5a**, **6**, and **6a**

	2	2a	5	5a	6	6a
Empirical formula	C ₂₂ H ₆₃ GeSi ₈ P	C ₂₂ H ₆₃ Ge ₃ Si ₆ P	C ₃₂ H ₉₆ Ge ₂ Si ₁₆	C ₃₂ H ₉₆ Ge ₆ Si ₁₂	C ₂₃ H ₆₀ GeSi ₈ N ₂	C ₂₃ H ₆₀ Ge ₃ Si ₈ N ₂
M _w	656.03	745.14	1075.71	1253.71	662.04	751.04
Temperature [K]	100(2)	100(2)	100 (K)	100(2)	100(2)	100(2)
Size [mm]	0.26x0.25x0.16	0.35x0.28x0.22	0.34x0.27x0.18	0.36x0.30x0.24	0.31x0.27x0.16	0.28x0.22x0.18
Crystal system	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic	monoclinic
Space group	P2(1)/n	P2(1)/n	C2/c	C2/c	P2(1)/c	P2(1)/c
a [Å]	13.039(3)	9.7132(2)	27.464(6)	27.672(6)	11.388(2)	11.436(2)
b [Å]	23.653(5)	21.392(4)	12.362(3)	12.496(3)	20.813(4)	20.832(4)
c [Å]	13.088(3)	19.039(4)	20.086(4)	20.276(4)	16.958(3)	17.000(3)
α [°]	90	90	90	90	90	90
β [°]	106.87(3)	102.59(3)	112.87(3)	111.94(3)	107.35(3)	107.05(3)
γ [°]	90	90	90	90	90	90
V [Å ³]	3863(2)	3861(2)	6283(2)	6503(2)	3836(2)	3862(2)
Z	4	4	4	4	4	4
ρ _{calc} [gcm ⁻³]	1.128	1.282	1.137	1.280	1.146	1.288
Absorption coefficient [mm ⁻¹]	1.094	2.559	1.283	2.979	1.064	2.515
F(000)	1416	1560	2304	2592	1424	1568
θ range	1.72<θ<26.36	1.45<θ<25.00	1.61<θ<26.35	1.81<θ<26.76	1.59<θ<26.37	1.59<θ<26.36
Reflections collected/unique	30477/7875	27252/6769	24041/6391	24786/6733	30500/7829	30692/7892
Completeness to θ [%]	99.6	99.5	99.6	97.1	99.9	99.8
Data/restraints/parameters	7875/16/607	6769/0/308	6391/0/242	6733/0/242	7829/0/327	7829/0/327
Goodness of fit on F ²	1.06	1.17	1.24	0.90	1.07	1.05
Final R indices [I>2σ(I)]	R1=0.048, wR2=0.111	R1=0.103, wR2=0.270	R1 = 0.097 wR2 = 0.182	R1=0.053, wR2=0.101	R1 = 0.042, wR2 = 0.091	R1 = 0.027, wR2 = 0.065
R indices (all data)	R1=0.064, wR2=0.117	R1=0.108, wR2=0.272	R1 = 0.126, wR2 = 0.192	R1=0.076, wR2=0.109	R1 = 0.055, wR2 = 0.096	R1 = 0.032, wR2 = 0.066
Largest diff. Peak/hole [e ⁻ /Å ³]	1.27/-0.36	5.07/-1.92	1.55/0.73	0.91/-0.80	0.57/-0.33	0.51/-0.29

2. Computational Details

2.1 General

All quantum chemical calculations were carried out using the Gaussian09 package.¹ The molecular structure optimizations were performed at the density functional M06-2X level of theory² using the def2-tzvp basis set for Ge and the small 6-31G(d) basis set for Si, C, H. Every stationary point was identified by a subsequent frequency calculation either as minimum (Number of imaginary frequencies (NIMAG): 0) or transition state (NIMAG: 1). The SCF energies, $E(\text{SCF})$, for all optimized molecular structures obtained with this method are given in Table S2. Harmonic frequencies were calculated analytically and were used with standard scaling (0.893) to obtain corrections for enthalpy and entropy. The computed Gibbs free energies at $T=298.15\text{K}$ and $p=0.101\text{ MPa}$ (1 atm) in the gas phase, G^{298} , are also given in Table S2. Intrinsic reaction coordinate (IRC) calculations^{3,4} were used to connect transition state structures with the appropriate molecular structures of intermediates. The corresponding computed molecular structures are given in the form of their Cartesian coordinates in Table S3.

Table S2. Absolute SCF energies E(SCF) and free Gibbs enthalpies, G^{298} , for compounds of interest (at M06-2X/(Ge) def2tzvp, (P) 6-311+G(d,p), (C,H,Si) 6-31G(d))

Compound	PG	E(SCF) [H/particle]	G^{298} [H/particle]	(NIMAG), $\nu(\text{IMAG}) [\text{cm}^{-1}]$
3	C ₂	-5031.09931	-5030.57289	
4	C ₁	-5031.10272	-5030.57472	
TS(3/4)	C ₁	-5031.07815	-5030.54826	(1), -63
5	C ₁	-10062.30192	-10061.19193	
9	C ₁	-10062.27270	-10061.16022	
10	C _i	-10062.25064	-10061.14966	
11	C ₂	-10062.26324	-10061.15291	
2	C ₁	-5610.02544	-5609.29990	
2(TS)	C ₁	-5609.99948	-5609.27949	(1), -95
6	C ₁	-5414.42455	-5413.71736	
6(TS)	C ₁	-5414.40721	-5413.69717	(1), -92
8	C ₁	-5031.07907	-5030.54775	
7	C ₁	-5031.10159	-5030.57412	
TS(4/7)	C ₁	-5031.038874	-5030.50679	(1), -59
3a°	C ₂	-8606.24531	-8605.72264	
4a°	C ₁	-8606.24824	-8605.72754	
TS(3a/4a)	C ₁	-8606.22884	-8605.70293	(1), -33
5a°	C ₁	-17212.60049	-17211.50634	
9a°	C ₁	-17212.57566	-17211.47472	
2a	C ₁	-9185.17409	-9184.45350	
2a(TS)	C ₁	-9185.14055	-9184.426716	(1), -106
6a°	C ₁	-8989.57580	-8988.87037	
6a(TS)	C ₁	-8989.54946	-8988.84368	(1), -104
NHC^{Me}	C _{2v}	-383.25575	-383.10469	
PEt₃	C ₁	-578.87647	-578.70900	

Table S3. Calculated molecular structures at M06-2X/def2-tzvp(Ge), 6-311+G(d,p) (P), 6-31G(d) (Si,C,H,N) in the form of their Cartesian coordinates.

Compound **3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-1.141523	0.287544	2.140030
2	14	0	1.141416	-0.287693	2.140063
3	14	0	-1.780882	0.059101	-0.110639
4	14	0	1.780838	-0.059116	-0.110567
5	14	0	-3.616819	1.381222	-0.714036
6	14	0	-2.417861	-2.195876	-0.460254
7	14	0	2.417863	2.195868	-0.460129
8	14	0	3.616838	-1.381134	-0.714039
9	6	0	-3.051905	3.177497	-0.895495
10	1	0	-2.275144	3.268228	-1.663080
11	1	0	-3.887061	3.827438	-1.180989
12	1	0	-2.639286	3.553864	0.047296
13	6	0	-4.340149	0.787924	-2.357262
14	1	0	-5.129455	1.464812	-2.703651
15	1	0	-3.566317	0.744508	-3.131689
16	1	0	-4.775137	-0.212933	-2.260119
17	6	0	-4.946630	1.299832	0.630184
18	1	0	-5.295945	0.274496	0.788937
19	1	0	-4.558341	1.671380	1.584883
20	1	0	-5.812824	1.914650	0.359565
21	6	0	2.486154	2.617566	-2.305482
22	1	0	1.483649	2.633200	-2.749255
23	1	0	2.928654	3.611092	-2.446024
24	1	0	3.083396	1.896102	-2.871749
25	6	0	1.168756	3.373667	0.337973
26	1	0	0.154632	3.188342	-0.038075
27	1	0	1.146905	3.262557	1.426828
28	1	0	1.426760	4.415062	0.111954
29	6	0	4.125808	2.509268	0.292018
30	1	0	4.899058	1.938819	-0.234065
31	1	0	4.383967	3.572385	0.215738
32	1	0	4.157097	2.226279	1.349392
33	6	0	4.340140	-0.787664	-2.357212
34	1	0	4.774989	0.213247	-2.260002
35	1	0	5.129550	-1.464435	-2.703596
36	1	0	3.566335	-0.744319	-3.131671
37	6	0	4.946687	-1.299837	0.630154
38	1	0	5.812937	-1.914506	0.359367
39	1	0	5.295901	-0.274499	0.789097
40	1	0	4.558492	-1.671625	1.584797
41	6	0	3.052016	-3.177425	-0.895654
42	1	0	2.639412	-3.553893	0.047103
43	1	0	2.275271	-3.268150	-1.663254
44	1	0	3.887217	-3.827291	-1.181186
45	6	0	-1.168640	-3.373469	0.337962
46	1	0	-0.154478	-3.187769	-0.037804
47	1	0	-1.147074	-3.262454	1.426834
48	1	0	-1.426272	-4.414916	0.111771
49	6	0	-4.125810	-2.509380	0.291834
50	1	0	-4.899106	-1.939151	-0.234420
51	1	0	-4.383819	-3.572549	0.215750
52	1	0	-4.157210	-2.226182	1.349148
53	6	0	-2.486054	-2.617592	-2.305604
54	1	0	-2.928434	-3.611168	-2.446168
55	1	0	-3.083377	-1.896190	-2.871867
56	1	0	-1.483542	-2.633094	-2.749365
57	6	0	-2.167233	-0.841875	3.280164
58	1	0	-2.097939	-1.894998	2.989336
59	1	0	-1.827870	-0.756668	4.318718
60	1	0	-3.223750	-0.550933	3.247345
61	6	0	-1.419460	2.065580	2.757219
62	1	0	-0.989273	2.200560	3.756072

63	1	0	-0.971472	2.808180	2.091779
64	1	0	-2.492693	2.277923	2.824372
65	6	0	2.167028	0.841796	3.280217
66	1	0	1.827618	0.756616	4.318758
67	1	0	3.223558	0.550898	3.247457
68	1	0	2.097705	1.894906	2.989343
69	6	0	1.419417	-2.065715	2.757258
70	1	0	0.989238	-2.200692	3.756115
71	1	0	0.971438	-2.808339	2.091839
72	1	0	2.492655	-2.278028	2.824404
73	32	0	0.000014	-0.000019	-1.765051

Compound 4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	0.977108	-2.391960	-0.691055
2	14	0	-1.273236	-2.700527	-0.072079
3	14	0	1.644419	-0.244087	-0.009839
4	14	0	-2.092317	-0.520894	0.054746
5	14	0	3.367909	0.528152	-1.395568
6	14	0	2.316049	-0.233699	2.229777
7	14	0	-4.363206	0.008418	-0.000031
8	6	0	2.681425	1.074272	-3.070325
9	1	0	1.958269	1.889577	-2.954764
10	1	0	3.483621	1.422955	-3.730607
11	1	0	2.166189	0.246351	-3.568475
12	6	0	4.330476	1.954241	-0.606185
13	1	0	5.152422	2.263627	-1.262516
14	1	0	3.697200	2.827962	-0.425369
15	1	0	4.767273	1.650935	0.352159
16	6	0	4.582985	-0.904870	-1.642949
17	1	0	4.107101	-1.757106	-2.139646
18	1	0	5.436476	-0.591767	-2.255228
19	1	0	4.970191	-1.255352	-0.679514
20	6	0	-4.999046	-0.026300	-1.778802
21	1	0	-4.833966	-1.007706	-2.235040
22	1	0	-6.073705	0.188074	-1.809518
23	1	0	-4.482689	0.718816	-2.392092
24	6	0	-5.298738	-1.284417	1.014011
25	1	0	-6.374045	-1.072581	1.016861
26	1	0	-5.155783	-2.286948	0.595829
27	1	0	-4.952460	-1.301194	2.052221
28	6	0	-4.646609	1.724883	0.735813
29	1	0	-4.335422	1.755909	1.784886
30	1	0	-4.074052	2.484085	0.191941
31	1	0	-5.706190	2.000582	0.684272
32	6	0	1.109420	-1.271048	3.247954
33	1	0	0.083442	-0.910068	3.110728
34	1	0	1.140957	-2.321846	2.937802
35	1	0	1.349807	-1.227331	4.316301
36	6	0	4.058054	-0.957176	2.401929
37	1	0	4.793189	-0.369410	1.841022
38	1	0	4.372465	-0.973506	3.451727
39	1	0	4.092142	-1.984762	2.023226
40	6	0	2.303655	1.547207	2.868894
41	1	0	2.604362	1.597368	3.921518
42	1	0	2.987390	2.178116	2.290118
43	1	0	1.296778	1.973208	2.783408
44	6	0	2.120411	-3.744864	0.001478
45	1	0	2.091434	-3.769583	1.096218
46	1	0	1.819736	-4.732883	-0.364684
47	1	0	3.158076	-3.572410	-0.305692
48	6	0	1.008375	-2.468752	-2.591619
49	1	0	0.663323	-3.446520	-2.946563
50	1	0	0.344448	-1.703916	-3.010032
51	1	0	2.014606	-2.300487	-2.990099
52	6	0	-2.185306	-3.672406	-1.430527
53	1	0	-1.774179	-4.683368	-1.531835
54	1	0	-3.250865	-3.767290	-1.192576

55	1	0	-2.097537	-3.170088	-2.398904
56	6	0	-1.498688	-3.647462	1.558536
57	1	0	-1.040784	-4.641133	1.493687
58	1	0	-1.046301	-3.114965	2.399490
59	1	0	-2.564012	-3.780960	1.776516
60	32	0	-0.432649	0.937694	-0.134274
61	14	0	-0.623626	3.324651	-0.088193
62	6	0	1.112047	4.052891	-0.228114
63	1	0	1.076881	5.148396	-0.230981
64	1	0	1.731085	3.734782	0.617945
65	1	0	1.605323	3.726332	-1.150076
66	6	0	-1.668083	3.895073	-1.554752
67	1	0	-1.188997	3.622151	-2.500477
68	1	0	-2.661625	3.435352	-1.542248
69	1	0	-1.795867	4.983649	-1.537606
70	6	0	-1.404480	3.901220	1.529962
71	1	0	-0.789658	3.609580	2.387329
72	1	0	-1.500200	4.993573	1.536394
73	1	0	-2.399851	3.469893	1.669282

TS (3/4)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	32	0	0.188396	1.011498	-1.269054
2	14	0	1.207088	-2.091548	1.119595
3	14	0	-1.045391	-1.605007	1.572876
4	14	0	1.798550	-0.340382	-0.345776
5	14	0	-1.693359	-0.071372	-0.095677
6	14	0	4.134466	-0.274117	-0.681371
7	14	0	1.295104	2.585894	0.325147
8	14	0	-2.608891	-1.335411	-1.851600
9	14	0	-3.271102	1.484041	0.671087
10	6	0	4.658061	-2.089319	-0.823606
11	1	0	4.106421	-2.615779	-1.609545
12	1	0	5.726498	-2.156339	-1.060251
13	1	0	4.489041	-2.619196	0.120097
14	6	0	4.609112	0.599765	-2.285278
15	1	0	4.143442	0.090765	-3.135517
16	1	0	4.291140	1.645169	-2.312091
17	1	0	5.695669	0.567789	-2.426899
18	6	0	5.042075	0.442803	0.817044
19	1	0	4.788288	-0.124942	1.719548
20	1	0	6.124576	0.358919	0.664364
21	1	0	4.809630	1.494469	1.006694
22	6	0	-3.061471	-0.207121	-3.302289
23	1	0	-2.223132	0.434863	-3.592954
24	1	0	-3.352942	-0.802654	-4.175323
25	1	0	-3.906952	0.439969	-3.043448
26	6	0	-1.292933	-2.575033	-2.418605
27	1	0	-0.368388	-2.066686	-2.715784
28	1	0	-1.048977	-3.273014	-1.609128
29	1	0	-1.647034	-3.163579	-3.272794
30	6	0	-4.162026	-2.313785	-1.381288
31	1	0	-4.974012	-1.653674	-1.061483
32	1	0	-4.514231	-2.880735	-2.251618
33	1	0	-3.970635	-3.025898	-0.573204
34	6	0	-3.462733	2.880113	-0.592935
35	1	0	-3.832415	2.480058	-1.543284
36	1	0	-4.184362	3.625265	-0.237458
37	1	0	-2.517346	3.391406	-0.797413
38	6	0	-4.971080	0.671083	0.877636
39	1	0	-5.419155	0.448874	-0.096712
40	1	0	-4.906035	-0.266670	1.440782
41	1	0	-5.653734	1.341214	1.413517
42	6	0	-2.778677	2.186803	2.365701
43	1	0	-3.103789	1.509601	3.162552
44	1	0	-1.697887	2.324443	2.473744
45	1	0	-3.260740	3.156707	2.535635
46	6	0	1.704363	2.034341	2.094937

47	1	0	0.850623	1.500549	2.529202
48	1	0	2.567000	1.357350	2.118662
49	1	0	1.929026	2.896072	2.735865
50	6	0	2.823413	3.372824	-0.459975
51	1	0	2.615883	3.659533	-1.495821
52	1	0	3.080290	4.280768	0.099621
53	1	0	3.700726	2.722159	-0.457046
54	6	0	0.010976	3.968968	0.469415
55	1	0	0.387594	4.741163	1.152695
56	1	0	-0.164301	4.426338	-0.509584
57	1	0	-0.948089	3.615014	0.855423
58	6	0	2.289763	-2.031764	2.684257
59	1	0	2.235586	-1.051084	3.168453
60	1	0	1.952312	-2.781562	3.408769
61	1	0	3.339483	-2.242396	2.450792
62	6	0	1.433919	-3.792867	0.298069
63	1	0	1.002844	-4.574277	0.934094
64	1	0	0.940934	-3.841596	-0.677336
65	1	0	2.494820	-4.020349	0.153193
66	6	0	-2.064668	-3.213083	1.553289
67	1	0	-1.711986	-3.896702	2.334108
68	1	0	-3.124011	-3.006021	1.740989
69	1	0	-1.987006	-3.731864	0.592035
70	6	0	-1.196290	-0.892173	3.330941
71	1	0	-0.769040	-1.588419	4.061462
72	1	0	-0.685046	0.069323	3.440420
73	1	0	-2.250626	-0.740965	3.587918

Compound 5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	32	0	-1.113037	-0.363178	-0.628796
2	14	0	-3.230928	-1.209963	0.291850
3	14	0	-3.892401	0.415823	1.894730
4	14	0	-2.312924	2.157070	1.836585
5	14	0	-1.164847	2.063466	-0.234160
6	14	0	-0.966657	-1.396305	-2.808332
7	14	0	-4.963378	-0.995774	-1.311740
8	14	0	-3.380723	-3.442105	1.067715
9	14	0	-1.990818	3.678913	-1.763907
10	6	0	-5.538476	1.275025	1.455261
11	1	0	-6.381899	0.578783	1.440547
12	1	0	-5.501509	1.793487	0.492367
13	1	0	-5.741368	2.027608	2.226868
14	6	0	-4.170238	-0.183377	3.679833
15	1	0	-4.370717	0.691263	4.311068
16	1	0	-3.316831	-0.718445	4.101929
17	1	0	-5.046100	-0.838287	3.734023
18	6	0	-1.073708	2.030343	3.274870
19	1	0	-0.639348	3.018478	3.461581
20	1	0	-0.252876	1.338589	3.061217
21	1	0	-1.572752	1.705899	4.196123
22	6	0	-3.275686	3.763933	2.190861
23	1	0	-3.621123	3.733995	3.232074
24	1	0	-4.154148	3.876164	1.550602
25	1	0	-2.650532	4.656637	2.074757
26	6	0	-1.989861	-0.488442	-4.116940
27	1	0	-2.205854	-1.154842	-4.961152
28	1	0	-1.433420	0.372098	-4.502331
29	1	0	-2.941619	-0.117575	-3.725503
30	6	0	0.805838	-1.513155	-3.465542
31	1	0	1.536284	-1.620986	-2.656046
32	1	0	1.064399	-0.613690	-4.031288
33	1	0	0.912767	-2.376130	-4.135205
34	6	0	-1.632112	-3.154450	-2.574746
35	1	0	-1.680311	-3.682577	-3.535388
36	1	0	-2.637199	-3.145292	-2.144108
37	1	0	-0.988548	-3.731973	-1.904106
38	6	0	-4.969038	-2.142214	-2.825102

39	1	0	-5.877995	-1.912638	-3.396326
40	1	0	-5.016873	-3.197619	-2.541173
41	1	0	-4.115530	-2.005887	-3.492996
42	6	0	-6.587273	-1.411685	-0.394208
43	1	0	-7.282947	-0.566129	-0.418572
44	1	0	-6.421400	-1.671722	0.657513
45	1	0	-7.082406	-2.263751	-0.873006
46	6	0	-5.012346	0.788684	-1.984934
47	1	0	-4.982284	0.789106	-3.080507
48	1	0	-4.158406	1.377474	-1.627780
49	1	0	-5.927664	1.307753	-1.681337
50	6	0	-4.251716	-3.525236	2.745484
51	1	0	-5.258530	-3.095614	2.701986
52	1	0	-3.692784	-2.996999	3.523941
53	1	0	-4.349993	-4.573943	3.051293
54	6	0	-1.695874	-4.277086	1.257908
55	1	0	-1.176678	-3.902378	2.144338
56	1	0	-1.054173	-4.107058	0.386692
57	1	0	-1.826005	-5.359306	1.376296
58	6	0	-4.409112	-4.503669	-0.117858
59	1	0	-4.553483	-5.493292	0.332353
60	1	0	-3.911153	-4.647196	-1.081594
61	1	0	-5.399518	-4.073711	-0.302020
62	6	0	-2.340346	3.063733	-3.517448
63	1	0	-2.718851	3.910150	-4.104136
64	1	0	-3.112018	2.288478	-3.517367
65	1	0	-1.460305	2.667881	-4.027233
66	6	0	-0.728040	5.091171	-1.821185
67	1	0	0.295156	4.733447	-1.978717
68	1	0	-0.747608	5.640359	-0.873736
69	1	0	-0.971248	5.796736	-2.624274
70	6	0	-3.616914	4.443269	-1.162963
71	1	0	-3.467002	5.037451	-0.257593
72	1	0	-4.387127	3.692310	-0.955803
73	1	0	-4.004948	5.109966	-1.942584
74	32	0	1.113083	-0.363138	0.628834
75	14	0	3.230958	-1.209884	-0.291903
76	14	0	1.164804	2.063518	0.234191
77	14	0	0.966721	-1.396359	2.808347
78	14	0	3.892410	0.415967	-1.894705
79	14	0	4.963325	-0.995795	1.311755
80	14	0	3.380837	-3.441987	-1.067816
81	14	0	2.312834	2.157135	-1.836586
82	14	0	1.990750	3.679012	1.763915
83	6	0	1.989870	-0.488497	4.116999
84	6	0	-0.805785	-1.513280	3.465506
85	6	0	1.632243	-3.154468	2.574746
86	6	0	5.538423	1.275227	-1.455114
87	6	0	4.170362	-0.183182	-3.679805
88	6	0	4.968851	-2.142347	2.825033
89	6	0	6.587246	-1.411712	0.394262
90	6	0	5.012261	0.788626	1.985045
91	6	0	4.251955	-3.525088	-2.745526
92	6	0	1.696006	-4.276963	-1.258170
93	6	0	4.409222	-4.503557	0.117757
94	6	0	1.073560	2.030367	-3.274817
95	6	0	3.275510	3.764042	-2.190891
96	6	0	2.340180	3.063890	3.517496
97	6	0	0.728018	5.091310	1.821123
98	6	0	3.616884	4.443320	1.163025
99	1	0	2.205906	-1.154909	4.961190
100	1	0	1.433383	0.372001	4.502415
101	1	0	2.941607	-0.117571	3.725571
102	1	0	-1.536204	-1.621120	2.655987
103	1	0	-1.064395	-0.613832	4.031258
104	1	0	-0.912707	-2.376268	4.135153
105	1	0	1.680397	-3.682609	3.535384
106	1	0	2.637360	-3.145265	2.144184
107	1	0	0.988724	-3.731991	1.904060
108	1	0	6.381866	0.579011	-1.440343
109	1	0	5.501374	1.793673	-0.492213
110	1	0	5.741355	2.027821	-2.226699
111	1	0	4.370820	0.691490	-4.311003

112	1	0	3.317006	-0.718286	-4.101956
113	1	0	5.046266	-0.838039	-3.733974
114	1	0	5.877785	-1.912849	3.396325
115	1	0	5.016648	-3.197737	2.541037
116	1	0	4.115293	-2.006030	3.492876
117	1	0	7.282993	-0.566217	0.418724
118	1	0	6.421374	-1.671624	-0.657491
119	1	0	7.082290	-2.263871	0.872987
120	1	0	4.982048	0.788972	3.080613
121	1	0	4.158376	1.377450	1.627811
122	1	0	5.927616	1.307719	1.681601
123	1	0	5.258760	-3.095452	-2.701936
124	1	0	3.693086	-2.996861	-3.524035
125	1	0	4.350281	-4.573796	-3.051318
126	1	0	1.176913	-3.902207	-2.144638
127	1	0	1.054209	-4.106987	-0.387016
128	1	0	1.826154	-5.359176	-1.376612
129	1	0	4.553520	-5.493196	-0.332446
130	1	0	3.911363	-4.647048	1.081547
131	1	0	5.399664	-4.073621	0.301795
132	1	0	0.639143	3.018485	-3.461495
133	1	0	0.252768	1.338581	-3.061108
134	1	0	1.572547	1.705940	-4.196107
135	1	0	3.620964	3.734092	-3.232099
136	1	0	4.153956	3.876350	-1.550627
137	1	0	2.650299	4.656712	-2.074827
138	1	0	2.718571	3.910347	4.104201
139	1	0	3.111911	2.288696	3.517502
140	1	0	1.460130	2.667981	4.027217
141	1	0	-0.295183	4.733629	1.978722
142	1	0	0.747564	5.640432	0.873635
143	1	0	0.971278	5.796923	2.624154
144	1	0	3.467014	5.037494	0.257644
145	1	0	4.387091	3.692345	0.955906
146	1	0	4.004898	5.110020	1.942655

Compound 9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	32	0	-1.575426	0.094250	-0.905224
2	14	0	-0.248530	1.768122	0.372548
3	32	0	1.443812	-0.000590	0.887755
4	14	0	0.192883	-1.583251	-0.534940
5	14	0	-2.130471	1.108137	-3.046367
6	14	0	1.961099	-0.888746	3.097347
7	14	0	3.759398	0.022242	-0.064234
8	14	0	-3.784800	-0.179493	0.181783
9	14	0	-1.721107	2.296960	2.174589
10	14	0	-0.195865	-3.846333	0.051088
11	14	0	1.561933	-1.890707	-2.438531
12	14	0	0.168441	4.048823	-0.222594
13	14	0	-3.930455	1.762724	1.519440
14	14	0	3.780158	-1.702632	-1.675478
15	14	0	-4.055975	-1.910853	1.765109
16	14	0	-5.471542	-0.801570	-1.364683
17	14	0	5.764461	-0.260104	1.183723
18	14	0	4.237096	2.047551	-1.159885
19	6	0	-0.749057	2.162850	-3.803756
20	1	0	-0.173282	1.642951	-4.572460
21	1	0	-1.205013	3.051154	-4.258688
22	1	0	-0.052051	2.507046	-3.033410
23	6	0	-3.445508	2.389642	-2.586717
24	1	0	-2.952584	3.213980	-2.062763
25	1	0	-3.915917	2.801577	-3.488616
26	1	0	-4.232617	2.006927	-1.935272
27	6	0	-2.779619	-0.067043	-4.380369
28	1	0	-3.727433	-0.534220	-4.101588
29	1	0	-2.941227	0.497313	-5.306897
30	1	0	-2.064692	-0.868328	-4.596310

31	6	0	3.148538	0.318565	3.939307
32	1	0	3.642910	-0.146086	4.800739
33	1	0	3.917420	0.692027	3.259488
34	1	0	2.580578	1.181622	4.305785
35	6	0	2.742596	-2.551278	2.634915
36	1	0	3.336432	-2.965890	3.457691
37	1	0	1.925501	-3.251576	2.428145
38	1	0	3.376104	-2.499733	1.744698
39	6	0	0.712194	-1.360959	4.440993
40	1	0	1.251423	-2.031992	5.122882
41	1	0	0.366605	-0.502893	5.021818
42	1	0	-0.163627	-1.901603	4.072865
43	6	0	0.961795	4.840604	1.323507
44	1	0	1.891831	5.345961	1.043397
45	1	0	0.289034	5.587533	1.755347
46	1	0	1.201941	4.115571	2.109066
47	6	0	1.193407	4.703567	-1.673821
48	1	0	2.259587	4.501051	-1.573876
49	1	0	0.861328	4.358116	-2.655784
50	1	0	1.057091	5.793213	-1.643355
51	6	0	-1.534002	4.837993	-0.538305
52	1	0	-2.369155	4.326142	-0.052740
53	1	0	-1.524146	5.876508	-0.184224
54	1	0	-1.728035	4.862879	-1.615928
55	6	0	-6.134858	0.461034	-2.615010
56	1	0	-6.469185	1.382040	-2.125532
57	1	0	-5.419645	0.735422	-3.393782
58	1	0	-7.006642	0.008260	-3.103444
59	6	0	-7.024068	-1.359638	-0.429072
60	1	0	-7.757040	-1.733756	-1.154105
61	1	0	-6.834136	-2.156395	0.295059
62	1	0	-7.486093	-0.523028	0.107120
63	6	0	-4.789223	-2.295719	-2.319428
64	1	0	-4.849694	-3.206735	-1.716542
65	1	0	-5.364771	-2.462735	-3.237965
66	1	0	-3.739731	-2.157079	-2.601633
67	6	0	-5.679499	-1.703485	2.746534
68	1	0	-6.225388	-2.653868	2.756665
69	1	0	-5.472611	-1.427248	3.785252
70	1	0	-6.347306	-0.945599	2.329271
71	6	0	-2.638600	-1.841889	3.009960
72	1	0	-1.672127	-1.741408	2.500643
73	1	0	-2.768746	-0.970870	3.660148
74	1	0	-2.602137	-2.732632	3.647792
75	6	0	-4.185654	-3.627505	0.969926
76	1	0	-4.153145	-4.399195	1.749367
77	1	0	-5.145789	-3.729055	0.452872
78	1	0	-3.391068	-3.836381	0.250336
79	6	0	-4.816222	3.232217	0.696775
80	1	0	-5.868323	2.969102	0.534581
81	1	0	-4.787863	4.103076	1.362716
82	1	0	-4.394266	3.525453	-0.266170
83	6	0	-4.885382	1.504322	3.149080
84	1	0	-4.833534	2.430666	3.734491
85	1	0	-5.942137	1.280601	2.971603
86	1	0	-4.465761	0.699734	3.759975
87	6	0	-1.803164	4.082152	2.850184
88	1	0	-1.996044	4.850348	2.097650
89	1	0	-2.626826	4.111310	3.575651
90	1	0	-0.886492	4.345081	3.386323
91	6	0	-1.192909	1.294499	3.691445
92	1	0	-1.022203	0.248212	3.440605
93	1	0	-0.244088	1.704972	4.061427
94	1	0	-1.927063	1.346575	4.504542
95	6	0	6.012892	2.190423	-1.807870
96	1	0	6.125590	3.170245	-2.288096
97	1	0	6.768213	2.117431	-1.020120
98	1	0	6.230763	1.425687	-2.561132
99	6	0	3.971313	3.422509	0.112621
100	1	0	4.097072	4.423540	-0.315960
101	1	0	2.966601	3.353732	0.541653
102	1	0	4.684429	3.318235	0.936160
103	6	0	3.126151	2.274895	-2.669377

104	1	0	2.068609	2.248963	-2.387206
105	1	0	3.318556	3.231265	-3.168376
106	1	0	3.300399	1.475695	-3.396708
107	6	0	7.099312	-0.734540	-0.082773
108	1	0	7.054283	-0.144640	-1.001505
109	1	0	8.086798	-0.576786	0.368747
110	1	0	7.032099	-1.791541	-0.358133
111	6	0	6.371089	1.352830	1.983624
112	1	0	7.294133	1.136045	2.535336
113	1	0	6.610234	2.108541	1.228600
114	1	0	5.660600	1.795253	2.687973
115	6	0	5.865969	-1.603075	2.511905
116	1	0	5.195921	-1.427025	3.357241
117	1	0	5.652272	-2.596332	2.104724
118	1	0	6.895488	-1.611389	2.891231
119	6	0	4.885908	-1.280518	-3.169826
120	1	0	5.940964	-1.236675	-2.878009
121	1	0	4.783789	-2.055558	-3.938741
122	1	0	4.616877	-0.321609	-3.623786
123	6	0	4.458343	-3.344858	-0.987223
124	1	0	4.298232	-4.151233	-1.713026
125	1	0	5.536819	-3.267718	-0.814759
126	1	0	3.984805	-3.643864	-0.048525
127	6	0	1.243705	-0.494221	-3.674189
128	1	0	0.270410	-0.651419	-4.153426
129	1	0	1.219012	0.476850	-3.178147
130	1	0	2.007618	-0.461537	-4.460506
131	6	0	1.260844	-3.466894	-3.468775
132	1	0	1.958566	-3.461914	-4.315225
133	1	0	1.395108	-4.406702	-2.929179
134	1	0	0.245404	-3.450975	-3.881161
135	6	0	-1.377895	-4.547374	-1.262142
136	1	0	-1.864729	-5.456912	-0.889768
137	1	0	-2.161003	-3.838713	-1.551202
138	1	0	-0.822174	-4.811971	-2.167152
139	6	0	1.421608	-4.829255	-0.085320
140	1	0	2.035647	-4.561591	-0.946533
141	1	0	2.037758	-4.714213	0.811875
142	1	0	1.163311	-5.892454	-0.173725
143	6	0	-0.821261	-4.303889	1.777704
144	1	0	-0.258225	-3.802116	2.572071
145	1	0	-1.878537	-4.090871	1.928408
146	1	0	-0.674819	-5.384883	1.898301

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-2.625994	0.824982	1.653895
2	14	0	-2.785432	0.864493	3.994438
3	14	0	-0.581142	0.939282	4.732950
4	14	0	0.734648	-0.394171	3.284639
5	14	0	-0.734648	0.394171	-3.284639
6	14	0	0.581142	-0.939282	-4.732950
7	14	0	2.785432	-0.864493	-3.994438
8	14	0	2.625994	-0.824982	-1.653895
9	14	0	0.383191	-2.677068	3.818087
10	14	0	-4.328184	-0.584228	0.853148
11	14	0	-3.007156	3.009794	0.883879
12	14	0	2.900780	0.321460	3.956506
13	14	0	3.007156	-3.009794	-0.883879
14	14	0	4.328184	0.584228	-0.853148
15	14	0	-2.900780	-0.321460	-3.956506
16	14	0	-0.383191	2.677068	-3.818087
17	6	0	-3.359276	-1.914869	-3.046189
18	1	0	-2.720246	-2.734671	-3.390829
19	1	0	-3.230692	-1.828427	-1.964214
20	1	0	-4.401372	-2.191056	-3.247442
21	6	0	-4.278109	0.985041	-3.899719
22	1	0	-4.245980	1.570381	-4.824470
23	1	0	-5.250441	0.479192	-3.857211

24	1	0	-4.226563	1.680023	-3.062584
25	6	0	-2.859303	-0.724605	-5.811196
26	1	0	-3.873757	-1.018995	-6.108745
27	1	0	-2.593028	0.162197	-6.397484
28	1	0	-2.180991	-1.534149	-6.089642
29	6	0	-1.984344	3.523682	-4.366998
30	1	0	-2.783906	3.485375	-3.624977
31	1	0	-1.772698	4.576827	-4.589696
32	1	0	-2.354069	3.060468	-5.289058
33	6	0	0.412728	3.578406	-2.362743
34	1	0	0.472397	4.655129	-2.560681
35	1	0	-0.131161	3.426201	-1.424975
36	1	0	1.431589	3.205808	-2.210426
37	6	0	0.763984	2.849216	-5.313619
38	1	0	1.705499	2.307231	-5.194235
39	1	0	0.272535	2.480863	-6.220154
40	1	0	1.001470	3.908531	-5.469794
41	6	0	0.563585	-0.477097	-6.580709
42	1	0	1.185066	0.402617	-6.769912
43	1	0	0.993040	-1.314912	-7.143570
44	1	0	-0.433467	-0.281912	-6.981524
45	6	0	0.016764	-2.749216	-4.548646
46	1	0	-0.058701	-3.023403	-3.490732
47	1	0	-0.959368	-2.929671	-5.009125
48	1	0	0.738153	-3.425779	-5.022390
49	6	0	3.720265	-2.387473	-4.650578
50	1	0	3.685656	-2.399694	-5.746336
51	1	0	4.773319	-2.360014	-4.349942
52	1	0	3.286881	-3.325797	-4.289716
53	6	0	3.713935	0.652580	-4.674855
54	1	0	3.444604	0.841947	-5.720040
55	1	0	3.506664	1.561177	-4.099101
56	1	0	4.792219	0.469629	-4.639325
57	6	0	1.707991	-4.201311	-1.565132
58	1	0	0.698653	-3.881487	-1.280583
59	1	0	1.744391	-4.271784	-2.656946
60	1	0	1.870590	-5.205679	-1.156565
61	6	0	4.730162	-3.618190	-1.385377
62	1	0	4.941951	-4.573639	-0.890701
63	1	0	4.819090	-3.772221	-2.464053
64	1	0	5.506668	-2.907620	-1.079724
65	6	0	2.933088	-3.080395	1.005726
66	1	0	2.567157	-4.058001	1.340992
67	1	0	3.934263	-2.933722	1.424217
68	1	0	2.272955	-2.311006	1.425755
69	6	0	5.857747	0.519632	-1.972005
70	1	0	6.742609	0.799881	-1.388480
71	1	0	6.030000	-0.485017	-2.375181
72	1	0	5.777902	1.214205	-2.812109
73	6	0	4.853436	-0.100110	0.821185
74	1	0	5.408814	-1.037468	0.694378
75	1	0	5.485670	0.598765	1.381197
76	1	0	3.970772	-0.321558	1.424510
77	6	0	3.758687	2.379649	-0.709538
78	1	0	3.694580	2.835369	-1.704107
79	1	0	2.770949	2.458042	-0.241888
80	1	0	4.468095	2.968918	-0.116829
81	6	0	3.359276	1.914869	3.046189
82	1	0	3.230692	1.828427	1.964214
83	1	0	2.720246	2.734671	3.390829
84	1	0	4.401372	2.191056	3.247442
85	6	0	4.278109	-0.985041	3.899719
86	1	0	5.250441	-0.479192	3.857211
87	1	0	4.245980	-1.570381	4.824470
88	1	0	4.226563	-1.680023	3.062584
89	6	0	2.859303	0.724605	5.811196
90	1	0	2.593028	-0.162197	6.397484
91	1	0	3.873757	1.018995	6.108745
92	1	0	2.180991	1.534149	6.089642
93	6	0	-0.016764	2.749216	4.548646
94	1	0	0.959368	2.929671	5.009125
95	1	0	0.058701	3.023403	3.490732
96	1	0	-0.738153	3.425779	5.022390

97	6	0	-0.563585	0.477097	6.580709
98	1	0	-0.993040	1.314912	7.143570
99	1	0	-1.185066	-0.402617	6.769912
100	1	0	0.433467	0.281912	6.981524
101	6	0	-3.720265	2.387473	4.650578
102	1	0	-4.773319	2.360014	4.349942
103	1	0	-3.685656	2.399694	5.746336
104	1	0	-3.286881	3.325797	4.289716
105	6	0	-3.713935	-0.652580	4.674855
106	1	0	-4.792219	-0.469629	4.639325
107	1	0	-3.506664	-1.561177	4.099101
108	1	0	-3.444604	-0.841947	5.720040
109	6	0	-4.730162	3.618190	1.385377
110	1	0	-4.819090	3.772221	2.464053
111	1	0	-4.941951	4.573639	0.890701
112	1	0	-5.506668	2.907620	1.079724
113	6	0	-1.707991	4.201311	1.565132
114	1	0	-1.744391	4.271784	2.656946
115	1	0	-0.698653	3.881487	1.280583
116	1	0	-1.870590	5.205679	1.156565
117	6	0	-2.933088	3.080395	-1.005726
118	1	0	-3.934263	2.933722	-1.424217
119	1	0	-2.567157	4.058001	-1.340992
120	1	0	-2.272955	2.311006	-1.425755
121	6	0	-4.853436	0.100110	-0.821185
122	1	0	-5.485670	-0.598765	-1.381197
123	1	0	-5.408814	1.037468	-0.694378
124	1	0	-3.970772	0.321558	-1.424510
125	6	0	-5.857747	-0.519632	1.972005
126	1	0	-6.030000	0.485017	2.375181
127	1	0	-6.742609	-0.799881	1.388480
128	1	0	-5.777902	-1.214205	2.812109
129	6	0	-3.758687	-2.379649	0.709538
130	1	0	-2.770949	-2.458042	0.241888
131	1	0	-3.694580	-2.835369	1.704107
132	1	0	-4.468095	-2.968918	0.116829
133	6	0	1.984344	-3.523682	4.366998
134	1	0	1.772698	-4.576827	4.589696
135	1	0	2.783906	-3.485375	3.624977
136	1	0	2.354069	-3.060468	5.289058
137	6	0	-0.412728	-3.578406	2.362743
138	1	0	0.131161	-3.426201	1.424975
139	1	0	-0.472397	-4.655129	2.560681
140	1	0	-1.431589	-3.205808	2.210426
141	6	0	-0.763984	-2.849216	5.313619
142	1	0	-0.272535	-2.480863	6.220154
143	1	0	-1.705499	-2.307231	5.194235
144	1	0	-1.001470	-3.908531	5.469794
145	32	0	-0.321245	0.198206	1.106558
146	32	0	0.321245	-0.198206	-1.106558

Compound 11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-0.405749	-2.263001	2.187345
2	14	0	0.341302	-1.108125	4.090366
3	14	0	-0.341302	1.108125	4.090366
4	14	0	0.405749	2.263001	2.187345
5	14	0	0.135988	2.516982	-1.969039
6	14	0	0.620143	0.984619	-3.694240
7	14	0	-0.620143	-0.984619	-3.694240
8	14	0	-0.135988	-2.516982	-1.969039
9	32	0	-0.000176	1.158173	0.061018
10	32	0	0.000176	-1.158173	0.061018
11	14	0	-2.730579	-2.653398	2.310989
12	14	0	0.922084	-4.208694	2.224370
13	14	0	-0.922084	4.208694	2.224370
14	14	0	2.730579	2.653398	2.310989
15	14	0	-2.002012	3.458259	-2.413718

16	14	0	1.902587	4.096944	-2.317296
17	14	0	-1.902587	-4.096944	-2.317296
18	14	0	2.002012	-3.458259	-2.413718
19	6	0	-3.087919	-4.429799	1.763951
20	1	0	-2.581523	-4.675706	0.826907
21	1	0	-2.733187	-5.130812	2.528800
22	1	0	-4.162776	-4.596394	1.625312
23	6	0	-3.428077	-2.497051	4.063104
24	1	0	-4.498129	-2.736627	4.043394
25	1	0	-2.940661	-3.192403	4.754082
26	1	0	-3.319273	-1.484433	4.462261
27	6	0	-3.639176	-1.412016	1.210672
28	1	0	-3.506783	-0.391903	1.588506
29	1	0	-3.262751	-1.419644	0.182996
30	1	0	-4.713593	-1.630941	1.186500
31	6	0	-1.718348	-5.880719	-1.698707
32	1	0	-2.498914	-6.461936	-2.205900
33	1	0	-0.753626	-6.321331	-1.968706
34	1	0	-1.857144	-6.010544	-0.624462
35	6	0	-2.020912	-4.328419	-4.198774
36	1	0	-2.800919	-5.072541	-4.401388
37	1	0	-2.284188	-3.413634	-4.735806
38	1	0	-1.083353	-4.710531	-4.618499
39	6	0	-3.596140	-3.482322	-1.739544
40	1	0	-3.824596	-2.476283	-2.101558
41	1	0	-4.359103	-4.165104	-2.134025
42	1	0	-3.687299	-3.474871	-0.651479
43	6	0	2.240374	-3.639388	-4.284579
44	1	0	2.231884	-2.676184	-4.802376
45	1	0	3.212093	-4.112813	-4.470712
46	1	0	1.468927	-4.271800	-4.737194
47	6	0	3.411292	-2.368982	-1.750104
48	1	0	3.889475	-1.825345	-2.570759
49	1	0	3.075844	-1.631321	-1.012196
50	1	0	4.173945	-2.995831	-1.273866
51	6	0	2.236841	-5.207300	-1.727742
52	1	0	2.291153	-5.233170	-0.637470
53	1	0	1.438752	-5.885714	-2.045104
54	1	0	3.183505	-5.599632	-2.119610
55	6	0	0.255217	-5.568276	1.101163
56	1	0	-0.676143	-5.986199	1.495843
57	1	0	0.053010	-5.173422	0.100702
58	1	0	0.978901	-6.385760	0.999073
59	6	0	1.021919	-4.921782	3.976284
60	1	0	0.023715	-5.167747	4.356329
61	1	0	1.613213	-5.844881	3.967779
62	1	0	1.490039	-4.230191	4.683813
63	6	0	2.658015	-3.735955	1.638458
64	1	0	3.135921	-3.020108	2.313705
65	1	0	3.302762	-4.620528	1.567371
66	1	0	2.613641	-3.269734	0.648365
67	6	0	-0.341449	-1.911314	5.679628
68	1	0	-0.226629	-2.999877	5.687860
69	1	0	0.210007	-1.509234	6.538363
70	1	0	-1.400896	-1.683644	5.825986
71	6	0	2.236841	-1.167082	4.237388
72	1	0	2.550131	-0.601654	5.123171
73	1	0	2.600942	-2.192439	4.357954
74	1	0	2.729239	-0.731501	3.361835
75	6	0	0.341449	1.911314	5.679628
76	1	0	0.226629	2.999877	5.687860
77	1	0	-0.210007	1.509234	6.538363
78	1	0	1.400896	1.683644	5.825986
79	6	0	-2.236841	1.167082	4.237388
80	1	0	-2.729239	0.731501	3.361835
81	1	0	-2.550131	0.601654	5.123171
82	1	0	-2.600942	2.192439	4.357954
83	6	0	3.639176	1.412016	1.210672
84	1	0	4.713593	1.630941	1.186500
85	1	0	3.506783	0.391903	1.588506
86	1	0	3.262751	1.419644	0.182996
87	6	0	3.087919	4.429799	1.763951
88	1	0	2.581523	4.675706	0.826907

89	1	0	2.733187	5.130812	2.528800
90	1	0	4.162776	4.596394	1.625312
91	6	0	3.428077	2.497051	4.063104
92	1	0	4.498129	2.736627	4.043394
93	1	0	2.940661	3.192403	4.754082
94	1	0	3.319273	1.484433	4.462261
95	6	0	-0.255217	5.568276	1.101163
96	1	0	0.676143	5.986199	1.495843
97	1	0	-0.053010	5.173422	0.100702
98	1	0	-0.978901	6.385760	0.999073
99	6	0	-1.021919	4.921782	3.976284
100	1	0	-1.613213	5.844881	3.967779
101	1	0	-1.490039	4.230191	4.683813
102	1	0	-0.023715	5.167747	4.356329
103	6	0	-2.658015	3.735955	1.638458
104	1	0	-2.613641	3.269734	0.648365
105	1	0	-3.135921	3.020108	2.313705
106	1	0	-3.302762	4.620528	1.567371
107	6	0	3.596140	3.482322	-1.739544
108	1	0	3.824596	2.476283	-2.101558
109	1	0	4.359103	4.165104	-2.134025
110	1	0	3.687299	3.474871	-0.651479
111	6	0	2.020912	4.328419	-4.198774
112	1	0	2.800919	5.072541	-4.401388
113	1	0	2.284188	3.413634	-4.735806
114	1	0	1.083353	4.710531	-4.618499
115	6	0	1.718348	5.880719	-1.698707
116	1	0	1.857144	6.010544	-0.624462
117	1	0	2.498914	6.461936	-2.205900
118	1	0	0.753626	6.321331	-1.968706
119	6	0	-2.236841	5.207300	-1.727742
120	1	0	-2.291153	5.233170	-0.637470
121	1	0	-1.438752	5.885714	-2.045104
122	1	0	-3.183505	5.599632	-2.119610
123	6	0	-2.240374	3.639388	-4.284579
124	1	0	-2.231884	2.676184	-4.802376
125	1	0	-3.212093	4.112813	-4.470712
126	1	0	-1.468927	4.271800	-4.737194
127	6	0	-3.411292	2.368982	-1.750104
128	1	0	-3.889475	1.825345	-2.570759
129	1	0	-3.075844	1.631321	-1.012196
130	1	0	-4.173945	2.995831	-1.273866
131	6	0	2.465816	0.534635	-3.596189
132	1	0	2.678166	-0.347987	-4.212689
133	1	0	3.103390	1.349792	-3.955543
134	1	0	2.752533	0.302877	-2.564598
135	6	0	0.281781	1.654562	-5.458488
136	1	0	1.059774	1.277636	-6.133295
137	1	0	-0.680065	1.295626	-5.839920
138	1	0	0.278705	2.743809	-5.524349
139	6	0	-0.281781	-1.654562	-5.458488
140	1	0	-1.059774	-1.277636	-6.133295
141	1	0	0.680065	-1.295626	-5.839920
142	1	0	-0.278705	-2.743809	-5.524349
143	6	0	-2.465816	-0.534635	-3.596189
144	1	0	-2.678166	0.347987	-4.212689
145	1	0	-3.103390	-1.349792	-3.955543
146	1	0	-2.752533	-0.302877	-2.564598

Compound 7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.378399	-0.298363	-1.783491
2	14	0	1.881358	-2.174775	-0.439954
3	14	0	0.894482	1.030110	-0.550054
4	14	0	0.572742	-0.794987	0.934289
5	14	0	1.467801	3.282863	-0.290313
6	6	0	2.977082	3.401522	0.839742
7	1	0	2.752526	3.001113	1.833725

8	1	0	3.819045	2.833006	0.431901
9	1	0	3.295251	4.444159	0.954780
10	6	0	1.941304	3.889137	-2.019073
11	1	0	1.092868	3.824389	-2.707672
12	1	0	2.273952	4.933072	-1.986430
13	1	0	2.757335	3.288706	-2.436292
14	6	0	0.095817	4.385394	0.390898
15	1	0	0.351602	5.438068	0.223154
16	1	0	-0.864551	4.187414	-0.096204
17	1	0	-0.033084	4.237437	1.466486
18	6	0	4.136462	0.253474	-1.300688
19	1	0	4.243034	0.329314	-0.213695
20	1	0	4.885904	-0.457136	-1.667122
21	1	0	4.366204	1.235149	-1.731614
22	6	0	2.311238	-0.287138	-3.677521
23	1	0	3.052129	-0.979988	-4.091230
24	1	0	1.328639	-0.563757	-4.064585
25	1	0	2.549841	0.717808	-4.043718
26	6	0	1.064438	-3.738181	-1.135425
27	1	0	1.748162	-4.263829	-1.811100
28	1	0	0.814605	-4.417511	-0.312171
29	1	0	0.143546	-3.522447	-1.682173
30	6	0	3.455786	-2.745493	0.463277
31	1	0	4.132986	-3.265223	-0.223767
32	1	0	3.998514	-1.900909	0.898566
33	1	0	3.204734	-3.440092	1.273481
34	32	0	-1.264118	-0.000779	-0.399148
35	14	0	-2.819604	1.263559	0.903085
36	6	0	-3.768329	2.466028	-0.206431
37	1	0	-4.486695	3.044290	0.386822
38	1	0	-3.088643	3.170867	-0.696125
39	1	0	-4.323501	1.938669	-0.988425
40	6	0	-4.065041	0.056092	1.659383
41	1	0	-4.605884	-0.489894	0.878049
42	1	0	-3.565793	-0.682699	2.295146
43	1	0	-4.804781	0.588379	2.268840
44	6	0	-1.954523	2.247544	2.275113
45	1	0	-2.112714	3.320301	2.125981
46	1	0	-2.354747	1.979034	3.257943
47	1	0	-0.873818	2.065106	2.291765
48	14	0	-2.320943	-1.386795	-2.039266
49	6	0	-2.809983	-3.017350	-1.219319
50	1	0	-3.533506	-2.828966	-0.418419
51	1	0	-3.275526	-3.696794	-1.942776
52	1	0	-1.949955	-3.525097	-0.772720
53	6	0	-3.902422	-0.530095	-2.625626
54	1	0	-4.406229	-1.137195	-3.386957
55	1	0	-4.604672	-0.383717	-1.797559
56	1	0	-3.685874	0.450217	-3.062492
57	6	0	-1.220617	-1.674322	-3.545336
58	1	0	-0.239570	-2.076862	-3.275121
59	1	0	-1.695715	-2.373910	-4.242967
60	1	0	-1.060158	-0.726799	-4.070855
61	14	0	0.626472	-1.222804	3.229277
62	6	0	0.217022	-3.062165	3.398334
63	1	0	-0.785504	-3.277166	3.014279
64	1	0	0.929085	-3.676297	2.835916
65	1	0	0.255675	-3.376508	4.447712
66	6	0	2.379016	-0.918948	3.866583
67	1	0	2.669776	0.128050	3.733802
68	1	0	2.451087	-1.160877	4.933273
69	1	0	3.103992	-1.539284	3.329536
70	6	0	-0.593193	-0.232933	4.274021
71	1	0	-1.613789	-0.316368	3.886566
72	1	0	-0.587600	-0.617187	5.300875
73	1	0	-0.330665	0.828179	4.308698

Compound 8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	14	0	2.464600	1.104473	0.354323
2	14	0	1.339444	2.840624	-0.791117
3	14	0	1.009161	-0.746918	0.255685
4	14	0	-0.896558	2.358969	-1.509892
5	14	0	0.968899	-2.172724	2.116846
6	14	0	1.545748	-2.011106	-1.650658
7	6	0	0.866872	-1.276901	3.781032
8	1	0	-0.121677	-0.832729	3.938030
9	1	0	1.035961	-1.998683	4.589142
10	1	0	1.616231	-0.484256	3.876135
11	6	0	-0.513043	-3.342781	2.011695
12	1	0	-0.530713	-4.017386	2.875766
13	1	0	-1.454146	-2.781804	2.001055
14	1	0	-0.482489	-3.955474	1.104493
15	6	0	2.558338	-3.203782	2.100583
16	1	0	3.450256	-2.568764	2.055587
17	1	0	2.627356	-3.821501	3.003495
18	1	0	2.579503	-3.874101	1.234367
19	6	0	1.257809	-0.931733	-3.180092
20	1	0	0.227911	-0.559603	-3.224668
21	1	0	1.927221	-0.063203	-3.165654
22	1	0	1.456211	-1.490079	-4.102260
23	6	0	3.335217	-2.631673	-1.698344
24	1	0	3.618817	-3.131742	-0.766821
25	1	0	3.447642	-3.355813	-2.514096
26	1	0	4.045674	-1.818745	-1.871603
27	6	0	0.430402	-3.542977	-1.720661
28	1	0	0.480005	-4.016243	-2.708584
29	1	0	0.756526	-4.283791	-0.980881
30	1	0	-0.617325	-3.302406	-1.511616
31	6	0	4.064519	0.725687	-0.607997
32	1	0	3.857102	0.506373	-1.660670
33	1	0	4.739554	1.588568	-0.573364
34	1	0	4.590662	-0.134374	-0.179250
35	6	0	3.020825	1.571287	2.112887
36	1	0	3.717227	2.416284	2.064401
37	1	0	2.189219	1.858132	2.760818
38	1	0	3.547791	0.732011	2.581330
39	6	0	1.408904	4.497731	0.151748
40	1	0	2.450183	4.763214	0.366684
41	1	0	0.976063	5.295211	-0.461685
42	1	0	0.868763	4.474315	1.102780
43	6	0	2.288429	3.141091	-2.424262
44	1	0	3.337210	3.380303	-2.215210
45	1	0	2.272052	2.268767	-3.085401
46	1	0	1.847904	3.983118	-2.968621
47	32	0	-1.101232	0.273726	-0.334476
48	14	0	-2.940464	-0.978235	-1.255971
49	6	0	-3.367945	-2.546879	-0.289921
50	1	0	-4.226186	-3.047321	-0.754154
51	1	0	-2.535421	-3.257220	-0.267896
52	1	0	-3.634184	-2.315618	0.747047
53	6	0	-4.440152	0.175751	-1.227658
54	1	0	-4.755953	0.404310	-0.203774
55	1	0	-4.213021	1.122029	-1.731424
56	1	0	-5.288399	-0.288924	-1.744020
57	6	0	-2.601419	-1.435322	-3.059786
58	1	0	-1.756913	-2.124155	-3.163339
59	1	0	-3.484085	-1.917316	-3.496868
60	1	0	-2.381278	-0.538419	-3.649221
61	14	0	-2.021331	1.396427	1.630059
62	6	0	-3.094662	2.891110	1.183169
63	1	0	-3.868466	2.644705	0.449954
64	1	0	-3.587976	3.275163	2.084557
65	1	0	-2.489534	3.705928	0.766026
66	6	0	-3.067066	0.160589	2.606439
67	1	0	-3.439827	0.623890	3.528176
68	1	0	-3.931937	-0.176669	2.025168
69	1	0	-2.482588	-0.723598	2.883425
70	6	0	-0.608556	2.011361	2.718905
71	1	0	0.017988	2.727549	2.175796
72	1	0	-0.995541	2.509962	3.615791

73 1 0 0.032244 1.184377 3.037997

TS (4/7)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-1.139344	-2.483676	-0.024706
2	14	0	-2.824954	-0.972667	0.694830
3	14	0	0.689578	-1.060344	-0.489009
4	14	0	-2.171114	1.319787	0.940036
5	14	0	2.494377	-1.931832	-1.765488
6	14	0	1.075933	-0.090566	2.608866
7	14	0	-2.401674	1.965723	-1.331841
8	6	0	3.093705	-0.657046	-3.020458
9	1	0	3.565379	0.204190	-2.537827
10	1	0	3.833312	-1.117966	-3.685721
11	1	0	2.269224	-0.289388	-3.640484
12	6	0	3.921345	-2.469123	-0.650491
13	1	0	4.687857	-2.946490	-1.272621
14	1	0	4.387614	-1.627021	-0.131280
15	1	0	3.600089	-3.196563	0.101287
16	6	0	1.845878	-3.446686	-2.686712
17	1	0	0.995349	-3.196832	-3.328903
18	1	0	2.635390	-3.867153	-3.320547
19	1	0	1.522723	-4.226341	-1.988452
20	6	0	-1.518924	0.896043	-2.650878
21	1	0	-1.686846	-0.174045	-2.461457
22	1	0	-1.882840	1.118157	-3.661315
23	1	0	-0.436285	1.074297	-2.638312
24	6	0	-4.217070	2.107968	-1.880071
25	1	0	-4.277708	2.686549	-2.809815
26	1	0	-4.679629	1.134243	-2.060560
27	1	0	-4.811358	2.628885	-1.121901
28	6	0	-1.704194	3.730952	-1.490843
29	1	0	-2.397937	4.442453	-1.029687
30	1	0	-0.742253	3.839823	-0.977774
31	1	0	-1.567897	4.022760	-2.539450
32	6	0	-0.373141	-0.854548	3.530400
33	1	0	-1.172525	-0.113457	3.639211
34	1	0	-0.791382	-1.719836	3.008565
35	1	0	-0.055062	-1.177299	4.529264
36	6	0	2.491956	-1.344070	2.492003
37	1	0	3.340555	-0.933612	1.935336
38	1	0	2.843485	-1.608822	3.496753
39	1	0	2.176928	-2.271031	1.996661
40	6	0	1.669343	1.405917	3.601080
41	1	0	1.929760	1.087177	4.618113
42	1	0	2.550828	1.880118	3.159477
43	1	0	0.874250	2.155755	3.671459
44	6	0	-0.565419	-3.902426	1.111400
45	1	0	-0.118906	-3.554618	2.047050
46	1	0	-1.422494	-4.535302	1.367997
47	1	0	0.170561	-4.528903	0.594338
48	6	0	-1.672057	-3.300720	-1.664723
49	1	0	-2.633376	-3.805114	-1.514243
50	1	0	-1.811839	-2.570905	-2.468604
51	1	0	-0.946535	-4.048338	-1.999317
52	6	0	-4.177783	-1.221858	-0.634875
53	1	0	-4.557531	-2.250161	-0.610562
54	1	0	-5.021601	-0.550739	-0.438373
55	1	0	-3.818239	-1.016150	-1.648607
56	6	0	-3.651072	-1.668676	2.268592
57	1	0	-3.944846	-2.715516	2.127672
58	1	0	-3.021894	-1.604830	3.158997
59	1	0	-4.561638	-1.091254	2.465897
60	32	0	0.229228	0.975097	0.514930
61	14	0	2.006584	2.487912	-0.102703
62	6	0	3.668909	1.651875	0.259875
63	1	0	4.496089	2.266153	-0.115460
64	1	0	3.826812	1.497009	1.331998

65	1	0	3.728763	0.673292	-0.230904
66	6	0	1.952726	2.861630	-1.955020
67	1	0	1.989017	1.941971	-2.547381
68	1	0	1.048778	3.408065	-2.239169
69	1	0	2.819570	3.474147	-2.231938
70	6	0	1.889533	4.107442	0.860014
71	1	0	1.999012	3.946632	1.936981
72	1	0	2.676971	4.798509	0.537265
73	1	0	0.923198	4.593633	0.693027

Compound 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	1.182449	-2.537620	0.696642
2	14	0	-0.998500	-2.146450	1.466801
3	14	0	1.956257	-0.423674	0.003011
4	14	0	-1.902777	-0.562544	-0.019269
5	14	0	3.604260	-0.809252	-1.636962
6	14	0	3.158666	0.521956	1.804970
7	14	0	-3.065450	-1.581404	-1.795304
8	14	0	-3.647723	0.484562	1.175929
9	6	0	2.797486	-1.204435	-3.301959
10	1	0	2.166275	-0.377787	-3.644101
11	1	0	3.566003	-1.390584	-4.061723
12	1	0	2.163945	-2.096112	-3.237308
13	6	0	4.672492	0.743596	-1.862983
14	1	0	5.375261	0.615555	-2.694530
15	1	0	4.051494	1.620849	-2.081620
16	1	0	5.257059	0.963054	-0.962674
17	6	0	4.759494	-2.253433	-1.211187
18	1	0	4.206096	-3.196278	-1.144326
19	1	0	5.516114	-2.370298	-1.996430
20	1	0	5.280859	-2.105769	-0.261022
21	6	0	-3.523035	-0.245612	-3.059615
22	1	0	-2.623122	0.280497	-3.398322
23	1	0	-3.999554	-0.697893	-3.937571
24	1	0	-4.215372	0.494252	-2.645195
25	6	0	-1.977155	-2.841036	-2.694804
26	1	0	-1.057708	-2.372117	-3.064600
27	1	0	-1.697589	-3.678568	-2.046972
28	1	0	-2.514758	-3.248368	-3.559548
29	6	0	-4.656912	-2.476064	-1.277547
30	1	0	-5.398653	-1.786162	-0.861232
31	1	0	-5.108629	-2.961674	-2.150716
32	1	0	-4.459610	-3.250334	-0.527912
33	6	0	-4.894862	1.353419	0.038397
34	1	0	-5.433686	0.626710	-0.578989
35	1	0	-5.638088	1.887384	0.643012
36	1	0	-4.427851	2.075718	-0.639143
37	6	0	-4.594021	-0.897577	2.070304
38	1	0	-5.526926	-0.501536	2.489802
39	1	0	-4.847929	-1.723208	1.398769
40	1	0	-4.005605	-1.310101	2.896997
41	6	0	-3.196088	1.727464	2.541030
42	1	0	-2.442503	1.328003	3.228383
43	1	0	-2.835768	2.686936	2.155786
44	1	0	-4.102178	1.931729	3.124849
45	6	0	2.275653	0.472648	3.483353
46	1	0	1.372352	1.090204	3.514843
47	1	0	1.986283	-0.548760	3.751461
48	1	0	2.959161	0.841194	4.258045
49	6	0	4.749694	-0.488962	2.008375
50	1	0	5.423865	-0.336453	1.158786
51	1	0	5.276854	-0.168163	2.915085
52	1	0	4.548696	-1.561432	2.092541
53	6	0	3.759058	2.311040	1.546134
54	1	0	4.534620	2.523437	2.292566
55	1	0	4.208954	2.448676	0.557180
56	1	0	2.976901	3.067251	1.671621

57	6	0	2.287503	-3.386541	1.994143
58	1	0	2.411027	-2.775072	2.894358
59	1	0	1.857676	-4.348595	2.295812
60	1	0	3.282885	-3.579998	1.577362
61	6	0	1.090117	-3.692436	-0.812153
62	1	0	0.555182	-4.617236	-0.565923
63	1	0	0.563184	-3.210579	-1.641164
64	1	0	2.090292	-3.966990	-1.164290
65	6	0	-2.024613	-3.745502	1.578294
66	1	0	-1.570196	-4.458911	2.275088
67	1	0	-3.041502	-3.532761	1.926408
68	1	0	-2.097681	-4.231110	0.598847
69	6	0	-0.894276	-1.359912	3.198589
70	1	0	-0.309340	-1.982976	3.885121
71	1	0	-0.405432	-0.381274	3.136667
72	1	0	-1.886994	-1.214359	3.638525
73	32	0	0.002314	0.405521	-1.301556
74	15	0	-0.101284	2.575040	-0.351109
75	6	0	0.002689	2.733256	1.476808
76	1	0	1.004773	2.382646	1.735992
77	1	0	-0.691685	1.982674	1.869773
78	6	0	-1.685092	3.397051	-0.836533
79	1	0	-2.404498	3.131679	-0.052061
80	1	0	-2.027929	2.896025	-1.749653
81	6	0	1.251150	3.642254	-1.001912
82	1	0	2.175363	3.283206	-0.533997
83	1	0	1.092918	4.671833	-0.659791
84	6	0	-0.266924	4.109798	2.081985
85	1	0	-0.144541	4.070518	3.168626
86	1	0	0.424983	4.865601	1.695233
87	1	0	-1.288184	4.446253	1.876814
88	6	0	-1.641989	4.913395	-1.040529
89	1	0	-2.645569	5.286278	-1.264996
90	1	0	-1.280602	5.439755	-0.153097
91	1	0	-0.993424	5.185394	-1.877898
92	6	0	1.375340	3.577585	-2.525896
93	1	0	1.621356	2.562914	-2.851975
94	1	0	0.441421	3.859980	-3.023380
95	1	0	2.161661	4.254967	-2.870994

2 (TS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	1.064325	-2.654663	-0.813294
2	14	0	-1.184033	-2.751331	-0.117402
3	14	0	2.036709	-0.674713	0.019044
4	14	0	-2.056209	-0.558622	-0.049979
5	14	0	3.614549	0.070677	-1.548468
6	14	0	2.965982	-0.987114	2.146731
7	14	0	-3.181784	0.022193	-2.017975
8	14	0	-3.484987	-0.369580	1.798446
9	6	0	2.792267	0.551260	-3.181642
10	1	0	1.894760	1.152522	-2.996203
11	1	0	3.481831	1.131822	-3.805577
12	1	0	2.484083	-0.332412	-3.748375
13	6	0	4.562644	1.589506	-0.914441
14	1	0	5.415090	1.805527	-1.569327
15	1	0	3.923528	2.480604	-0.906037
16	1	0	4.948179	1.439499	0.100150
17	6	0	4.878018	-1.306112	-1.868934
18	1	0	4.390281	-2.198209	-2.277837
19	1	0	5.635987	-0.978591	-2.590129
20	1	0	5.393014	-1.601711	-0.948872
21	6	0	-3.451585	1.902800	-2.021252
22	1	0	-2.485843	2.422494	-1.980840
23	1	0	-3.966928	2.227340	-2.932760
24	1	0	-4.048550	2.225871	-1.160751
25	6	0	-2.139560	-0.398192	-3.538220
26	1	0	-1.159676	0.086495	-3.457795

27	1	0	-1.972262	-1.475881	-3.637704
28	1	0	-2.625911	-0.045267	-4.455097
29	6	0	-4.876805	-0.816010	-2.147598
30	1	0	-5.543519	-0.475931	-1.346998
31	1	0	-5.357966	-0.583957	-3.104598
32	1	0	-4.786779	-1.905008	-2.069119
33	6	0	-4.432568	1.274685	1.768733
34	1	0	-5.115839	1.307501	0.912221
35	1	0	-5.034201	1.387746	2.678511
36	1	0	-3.764089	2.138625	1.698695
37	6	0	-4.795516	-1.738580	1.719508
38	1	0	-5.518341	-1.630632	2.536694
39	1	0	-5.349254	-1.700015	0.775098
40	1	0	-4.346129	-2.733532	1.800683
41	6	0	-2.522411	-0.526896	3.419370
42	1	0	-2.255084	-1.573174	3.601882
43	1	0	-1.591171	0.049593	3.387825
44	1	0	-3.118834	-0.178550	4.270317
45	6	0	1.777259	-1.989285	3.222609
46	1	0	0.805315	-1.483490	3.269709
47	1	0	1.614892	-2.996605	2.824590
48	1	0	2.161595	-2.086610	4.244500
49	6	0	4.636972	-1.875521	2.040870
50	1	0	5.377900	-1.252365	1.527145
51	1	0	5.026276	-2.101328	3.040273
52	1	0	4.551258	-2.818179	1.489280
53	6	0	3.214956	0.683431	3.003815
54	1	0	3.656984	0.552242	3.998064
55	1	0	3.865301	1.351246	2.427941
56	1	0	2.241890	1.172542	3.124602
57	6	0	2.003345	-4.209272	-0.239380
58	1	0	2.046216	-4.275251	0.852699
59	1	0	1.518457	-5.118914	-0.612426
60	1	0	3.032463	-4.199158	-0.616294
61	6	0	1.075804	-2.638144	-2.713864
62	1	0	0.543462	-3.512175	-3.107422
63	1	0	0.578583	-1.737559	-3.089019
64	1	0	2.096627	-2.658935	-3.111766
65	6	0	-2.192641	-3.839903	-1.311303
66	1	0	-1.745960	-4.836680	-1.403385
67	1	0	-3.215937	-3.963757	-0.938236
68	1	0	-2.249496	-3.402064	-2.313171
69	6	0	-1.261398	-3.593879	1.587096
70	1	0	-0.781387	-4.578704	1.534685
71	1	0	-0.741689	-3.008632	2.351048
72	1	0	-2.294672	-3.746212	1.917640
73	32	0	0.023063	0.537090	-0.024245
74	15	0	0.132981	2.809604	0.101029
75	6	0	1.608296	3.366218	1.051244
76	1	0	1.422396	3.073151	2.088535
77	1	0	2.442008	2.741311	0.709410
78	6	0	1.953931	4.850793	0.951392
79	1	0	1.120755	5.481663	1.280520
80	1	0	2.813936	5.078608	1.587566
81	1	0	2.214225	5.136059	-0.072433
82	6	0	0.284861	3.651176	-1.551352
83	1	0	1.356747	3.623046	-1.791044
84	1	0	-0.194970	2.973010	-2.263988
85	6	0	-0.284385	5.064284	-1.694321
86	1	0	-1.372588	5.060486	-1.578131
87	1	0	0.132286	5.761625	-0.962276
88	1	0	-0.061617	5.454680	-2.691727
89	6	0	-1.317479	3.608753	0.913206
90	1	0	-2.206409	3.233186	0.390054
91	6	0	-1.400204	3.312646	2.409974
92	1	0	-1.356500	2.235339	2.598802
93	1	0	-0.577427	3.788873	2.952820
94	1	0	-2.336995	3.698781	2.821616
95	1	0	-1.269583	4.688677	0.733664

Compound 6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	2.020712	-1.732066	1.461984
2	14	0	-0.260511	-1.988971	1.965646
3	14	0	2.133940	0.089982	-0.035180
4	14	0	-1.427629	-1.193714	0.086503
5	14	0	3.563779	-0.467085	-1.818420
6	14	0	3.128580	1.978270	0.951991
7	14	0	-1.875354	-2.961033	-1.394300
8	14	0	-3.546306	-0.529221	0.847757
9	6	0	2.823413	-1.856036	-2.869124
10	1	0	1.795019	-1.619694	-3.165287
11	1	0	3.415726	-1.995203	-3.781659
12	1	0	2.818420	-2.806838	-2.325649
13	6	0	3.749433	1.055455	-2.932898
14	1	0	4.329923	0.812102	-3.830586
15	1	0	2.765487	1.416344	-3.252794
16	1	0	4.260150	1.875491	-2.416058
17	6	0	5.297283	-1.028476	-1.289152
18	1	0	5.252859	-1.872085	-0.592512
19	1	0	5.864475	-1.354299	-2.169505
20	1	0	5.860140	-0.224754	-0.806402
21	6	0	-2.454946	-2.228111	-3.043198
22	1	0	-1.684462	-1.564986	-3.451915
23	1	0	-2.653057	-3.020302	-3.774747
24	1	0	-3.373301	-1.642583	-2.922337
25	6	0	-0.306497	-3.963733	-1.732064
26	1	0	0.508015	-3.313345	-2.069222
27	1	0	0.030160	-4.492327	-0.833536
28	1	0	-0.484970	-4.710491	-2.514724
29	6	0	-3.204643	-4.173109	-0.789158
30	1	0	-4.183614	-3.690974	-0.690960
31	1	0	-3.311898	-4.997039	-1.504817
32	1	0	-2.941576	-4.605357	0.182981
33	6	0	-4.772040	-0.260240	-0.575964
34	1	0	-4.909335	-1.169898	-1.170176
35	1	0	-5.752562	0.037274	-0.185322
36	1	0	-4.426136	0.532182	-1.250162
37	6	0	-4.248081	-1.883932	1.975400
38	1	0	-5.276045	-1.639957	2.270103
39	1	0	-4.258149	-2.861354	1.484054
40	1	0	-3.652337	-1.978997	2.890377
41	6	0	-3.572930	1.065593	1.878229
42	1	0	-2.841744	1.025697	2.692987
43	1	0	-3.368386	1.946441	1.260209
44	1	0	-4.565970	1.193170	2.325762
45	6	0	2.822618	2.130882	2.828238
46	1	0	1.866675	1.723014	3.171402
47	1	0	3.612096	1.586342	3.357445
48	1	0	2.879315	3.179872	3.144978
49	6	0	5.017038	1.955656	0.784659
50	1	0	5.337004	2.006387	-0.261223
51	1	0	5.449393	2.816103	1.310035
52	1	0	5.440615	1.045521	1.223000
53	6	0	2.545180	3.547441	0.053730
54	1	0	2.947065	4.448761	0.532309
55	1	0	2.911568	3.525850	-0.978885
56	1	0	1.455507	3.640330	0.001545
57	6	0	3.030626	-1.459102	3.054989
58	1	0	2.619058	-0.641545	3.655017
59	1	0	3.021577	-2.366701	3.669607
60	1	0	4.074770	-1.218049	2.824811
61	6	0	2.651549	-3.341769	0.665542
62	1	0	2.535901	-4.175129	1.368902
63	1	0	2.085642	-3.586655	-0.238247
64	1	0	3.710469	-3.274734	0.393758
65	6	0	-0.695850	-3.792372	2.402159
66	1	0	-0.117877	-4.133164	3.269073
67	1	0	-1.759816	-3.892355	2.645253
68	1	0	-0.476670	-4.465589	1.566442
69	6	0	-0.622209	-0.950255	3.528911

70	1	0	-0.074693	-1.369675	4.381326
71	1	0	-0.301415	0.091307	3.415530
72	1	0	-1.687943	-0.949744	3.783603
73	32	0	-0.008321	0.311318	-1.288675
74	6	0	-0.985528	2.029493	-0.644763
75	7	0	-1.852758	2.655159	-1.479252
76	6	0	-1.891769	3.838727	0.374213
77	6	0	-2.428889	3.764984	-0.873595
78	7	0	-1.018877	2.766426	0.488664
79	6	0	-2.132942	4.785975	1.498854
80	1	0	-1.200812	5.248749	1.839400
81	1	0	-2.808855	5.583092	1.183791
82	1	0	-2.589610	4.275130	2.354476
83	6	0	-3.437623	4.634118	-1.544379
84	1	0	-3.763914	5.417767	-0.857965
85	1	0	-3.028832	5.121049	-2.435953
86	1	0	-4.322628	4.063033	-1.843745
87	6	0	-2.154622	2.205814	-2.834618
88	1	0	-1.223015	1.994463	-3.360308
89	1	0	-2.750916	1.290195	-2.809149
90	1	0	-2.708409	2.991235	-3.349077
91	6	0	-0.331478	2.433965	1.720455
92	1	0	0.143594	1.461535	1.582551
93	1	0	0.427447	3.185397	1.953316
94	1	0	-1.054935	2.374651	2.538029

6 (TS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	1.130140	-2.783652	-0.311511
2	14	0	-1.130183	-2.783612	0.311713
3	14	0	2.012645	-0.635451	0.081075
4	14	0	-2.012640	-0.635430	-0.080980
5	14	0	3.730297	-0.416171	-1.515613
6	14	0	2.941356	-0.464532	2.229309
7	14	0	-2.941251	-0.464700	-2.229253
8	14	0	-3.730379	-0.416017	1.515589
9	6	0	3.041429	-0.212532	-3.266135
10	1	0	2.328979	0.617904	-3.322728
11	1	0	3.847640	-0.024778	-3.984534
12	1	0	2.510131	-1.116634	-3.579384
13	6	0	4.969923	0.991181	-1.188955
14	1	0	5.896842	0.776283	-1.734028
15	1	0	4.612796	1.966645	-1.532016
16	1	0	5.225194	1.075198	-0.126368
17	6	0	4.773761	-2.000384	-1.428863
18	1	0	4.187117	-2.901359	-1.632168
19	1	0	5.587613	-1.956956	-2.162644
20	1	0	5.224062	-2.114746	-0.436539
21	6	0	-3.244315	1.364734	-2.631720
22	1	0	-2.326626	1.946008	-2.480100
23	1	0	-3.551233	1.483598	-3.677364
24	1	0	-4.033121	1.795619	-2.004069
25	6	0	-1.732539	-1.135073	-3.519615
26	1	0	-0.759643	-0.641444	-3.411703
27	1	0	-1.580982	-2.214215	-3.408550
28	1	0	-2.102240	-0.948266	-4.534546
29	6	0	-4.594508	-1.380823	-2.385889
30	1	0	-5.344776	-0.959561	-1.706933
31	1	0	-4.987152	-1.301955	-3.406292
32	1	0	-4.486604	-2.444669	-2.147736
33	6	0	-4.970012	0.991255	1.188589
34	1	0	-5.224857	1.075405	0.125911
35	1	0	-5.897141	0.776235	1.733251
36	1	0	-4.613072	1.966696	1.531913
37	6	0	-4.773772	-2.000288	1.429072
38	1	0	-5.587900	-1.956561	2.162530
39	1	0	-5.223704	-2.115079	0.436630
40	1	0	-4.187182	-2.901156	1.632998

41	6	0	-3.041626	-0.212169	3.266127
42	1	0	-2.329136	0.618227	3.322716
43	1	0	-3.847881	-0.024341	3.984460
44	1	0	-2.510399	-1.116284	3.579469
45	6	0	1.732642	-1.134752	3.519746
46	1	0	0.759706	-0.641235	3.411660
47	1	0	1.581197	-2.213931	3.408892
48	1	0	2.102251	-0.947695	4.534664
49	6	0	4.594620	-1.380634	2.385965
50	1	0	5.344768	-0.959615	1.706728
51	1	0	4.987447	-1.301404	3.406269
52	1	0	4.486672	-2.444562	2.148211
53	6	0	3.244536	1.364918	2.631636
54	1	0	3.550829	1.483887	3.677450
55	1	0	4.033820	1.795525	2.004393
56	1	0	2.327077	1.946376	2.479388
57	6	0	2.085950	-4.112226	0.662928
58	1	0	2.061470	-3.910108	1.739198
59	1	0	1.652966	-5.105585	0.497306
60	1	0	3.135906	-4.145945	0.350327
61	6	0	1.210399	-3.252461	-2.155818
62	1	0	0.729192	-4.226160	-2.307608
63	1	0	0.682879	-2.517633	-2.772058
64	1	0	2.239432	-3.325599	-2.521960
65	6	0	-2.086094	-4.112228	-0.662570
66	1	0	-1.653017	-5.105568	-0.497077
67	1	0	-3.135978	-4.146017	-0.349736
68	1	0	-2.061867	-3.910072	-1.738839
69	6	0	-1.210332	-3.252333	2.156052
70	1	0	-0.729091	-4.226013	2.307851
71	1	0	-0.682805	-2.517473	2.772249
72	1	0	-2.239347	-3.325492	2.522244
73	32	0	0.000027	0.615542	-0.000263
74	6	0	-0.000051	2.548750	-0.000125
75	7	0	-1.043232	3.383442	0.278955
76	6	0	0.655168	4.717580	-0.174433
77	6	0	-0.655182	4.717579	0.174465
78	6	0	-2.334123	2.906845	0.714175
79	1	0	-2.959418	3.754903	0.995769
80	1	0	-2.829554	2.345853	-0.084224
81	1	0	-2.201190	2.242474	1.576660
82	6	0	-1.593668	5.847726	0.424640
83	1	0	-1.962431	5.851518	1.456404
84	1	0	-1.086319	6.798552	0.251246
85	1	0	-2.461079	5.805552	-0.243028
86	6	0	1.593706	5.847723	-0.424432
87	1	0	1.962838	5.851368	-1.456063
88	1	0	1.086260	6.798558	-0.251373
89	1	0	2.460881	5.805681	0.243552
90	6	0	2.334038	2.906830	-0.714343
91	1	0	2.959389	3.754889	-0.995810
92	1	0	2.829416	2.345708	0.084006
93	1	0	2.201097	2.242568	-1.576922
94	7	0	1.043161	3.383437	-0.279115

Compound **3a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-1.136815	0.296203	2.179367
2	14	0	1.136788	-0.296281	2.179380
3	14	0	-3.681345	1.454409	-0.687365
4	14	0	-2.556820	-2.236924	-0.460110
5	14	0	2.556799	2.236937	-0.459981
6	14	0	3.681375	-1.454378	-0.687345
7	6	0	-3.067250	3.231202	-0.884570
8	1	0	-2.323509	3.299870	-1.686053
9	1	0	-3.892435	3.910258	-1.128535
10	1	0	-2.599355	3.586297	0.040350
11	6	0	-4.471144	0.880404	-2.305255

12	1	0	-5.253059	1.578692	-2.625522
13	1	0	-3.726181	0.814002	-3.105515
14	1	0	-4.930748	-0.107436	-2.189617
15	6	0	-4.976634	1.404650	0.690332
16	1	0	-5.348976	0.387450	0.849775
17	1	0	-4.556832	1.758465	1.638137
18	1	0	-5.832017	2.044334	0.443133
19	6	0	2.688693	2.616087	-2.307929
20	1	0	1.702114	2.617999	-2.785269
21	1	0	3.138289	3.604232	-2.462540
22	1	0	3.304418	1.876699	-2.829706
23	6	0	1.313893	3.443082	0.299916
24	1	0	0.307702	3.281861	-0.106602
25	1	0	1.258475	3.323395	1.386942
26	1	0	1.601884	4.479963	0.090042
27	6	0	4.248152	2.502625	0.341259
28	1	0	5.012096	1.886155	-0.144974
29	1	0	4.555325	3.551476	0.251445
30	1	0	4.230398	2.242411	1.404799
31	6	0	4.471194	-0.880315	-2.305205
32	1	0	4.930791	0.107524	-2.189528
33	1	0	5.253118	-1.578589	-2.625481
34	1	0	3.726243	-0.813892	-3.105474
35	6	0	4.976642	-1.404649	0.690375
36	1	0	5.832033	-2.044321	0.443171
37	1	0	5.348976	-0.387451	0.849852
38	1	0	4.556827	-1.758492	1.638163
39	6	0	3.067300	-3.231171	-0.884613
40	1	0	2.599394	-3.586298	0.040289
41	1	0	2.323573	-3.299822	-1.686111
42	1	0	3.892496	-3.910211	-1.128586
43	6	0	-1.313958	-3.443120	0.299771
44	1	0	-0.307753	-3.281899	-0.106712
45	1	0	-1.258572	-3.323478	1.386802
46	1	0	-1.601960	-4.479988	0.089847
47	6	0	-4.248198	-2.502612	0.341078
48	1	0	-5.012120	-1.886113	-0.145153
49	1	0	-4.555386	-3.551455	0.251220
50	1	0	-4.230467	-2.242436	1.404627
51	6	0	-2.688678	-2.616008	-2.308074
52	1	0	-3.138293	-3.604138	-2.462731
53	1	0	-3.304373	-1.876588	-2.829841
54	1	0	-1.702088	-2.617927	-2.785390
55	6	0	-2.165982	-0.803574	3.340961
56	1	0	-2.072742	-1.863681	3.083396
57	1	0	-1.844551	-0.680266	4.381350
58	1	0	-3.226247	-0.532800	3.280870
59	6	0	-1.370770	2.095157	2.747752
60	1	0	-0.969717	2.239710	3.757467
61	1	0	-0.866028	2.797769	2.078342
62	1	0	-2.434700	2.356696	2.768561
63	6	0	2.165926	0.803476	3.341017
64	1	0	1.844483	0.680135	4.381398
65	1	0	3.226196	0.532718	3.280932
66	1	0	2.072676	1.863589	3.083479
67	6	0	1.370758	-2.095245	2.747728
68	1	0	0.969680	-2.239830	3.757428
69	1	0	0.866051	-2.797851	2.078287
70	1	0	2.434692	-2.356766	2.768560
71	32	0	0.000018	0.000021	-1.802335
72	32	0	1.829314	-0.045513	-0.110406
73	32	0	-1.829308	0.045509	-0.110441

Compound **4a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	0.969189	-2.423064	-0.696636
2	14	0	-1.284075	-2.685076	-0.078053
3	14	0	3.491833	0.519761	-1.423625

4	14	0	2.346228	-0.196524	2.302372
5	14	0	-4.432158	0.121322	-0.020148
6	6	0	2.809155	1.061160	-3.099990
7	1	0	2.093180	1.883019	-2.987028
8	1	0	3.614249	1.399696	-3.762336
9	1	0	2.287240	0.234335	-3.593153
10	6	0	4.445288	1.948546	-0.631632
11	1	0	5.261172	2.272705	-1.288559
12	1	0	3.799976	2.812318	-0.443931
13	1	0	4.888033	1.644138	0.323572
14	6	0	4.696070	-0.921654	-1.660825
15	1	0	4.215953	-1.767069	-2.165125
16	1	0	5.557990	-0.614936	-2.264686
17	1	0	5.070963	-1.278409	-0.695000
18	6	0	-5.059696	0.059004	-1.799815
19	1	0	-4.906825	-0.934244	-2.234170
20	1	0	-6.131147	0.288325	-1.839451
21	1	0	-4.529692	0.783439	-2.426008
22	6	0	-5.382370	-1.139131	1.018061
23	1	0	-6.455311	-0.914917	1.015070
24	1	0	-5.249041	-2.151248	0.620556
25	1	0	-5.037257	-1.137781	2.056803
26	6	0	-4.684699	1.854469	0.684627
27	1	0	-4.377888	1.894651	1.734686
28	1	0	-4.092888	2.592443	0.132132
29	1	0	-5.738197	2.151176	0.623435
30	6	0	1.095469	-1.192621	3.305642
31	1	0	0.077372	-0.833551	3.113966
32	1	0	1.136811	-2.253354	3.032865
33	1	0	1.292352	-1.112187	4.380859
34	6	0	4.068959	-0.949121	2.521834
35	1	0	4.826758	-0.380023	1.972251
36	1	0	4.360003	-0.962517	3.578527
37	1	0	4.090266	-1.980277	2.152035
38	6	0	2.349156	1.597528	2.899689
39	1	0	2.627167	1.667014	3.957591
40	1	0	3.056079	2.203197	2.321753
41	1	0	1.351429	2.036717	2.781391
42	6	0	2.076148	-3.794220	0.016950
43	1	0	2.037458	-3.804944	1.111578
44	1	0	1.756404	-4.779414	-0.340878
45	1	0	3.119647	-3.647050	-0.283253
46	6	0	1.020283	-2.504535	-2.595343
47	1	0	0.659335	-3.475296	-2.954034
48	1	0	0.378735	-1.725729	-3.022758
49	1	0	2.035505	-2.357806	-2.979527
50	6	0	-2.213907	-3.661350	-1.419740
51	1	0	-1.817357	-4.679566	-1.507129
52	1	0	-3.280071	-3.735899	-1.177919
53	1	0	-2.120057	-3.173671	-2.394984
54	6	0	-1.508380	-3.605078	1.567322
55	1	0	-1.072693	-4.609224	1.508921
56	1	0	-1.031914	-3.070729	2.393898
57	1	0	-2.573243	-3.711173	1.801774
58	32	0	-0.388322	1.013831	-0.187798
59	14	0	-0.551737	3.402394	-0.101106
60	6	0	1.192990	4.113178	-0.224671
61	1	0	1.171825	5.208584	-0.191987
62	1	0	1.812560	3.760151	0.607188
63	1	0	1.677637	3.811054	-1.159713
64	6	0	-1.589988	4.012784	-1.555508
65	1	0	-1.116526	3.755342	-2.508256
66	1	0	-2.587729	3.561932	-1.549033
67	1	0	-1.708273	5.101903	-1.515391
68	6	0	-1.337892	3.955458	1.522715
69	1	0	-0.733697	3.642187	2.379926
70	1	0	-1.426624	5.048152	1.549620
71	1	0	-2.337638	3.528048	1.643874
72	32	0	-2.114685	-0.448470	0.052300
73	32	0	1.711086	-0.238467	-0.007163

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	32	0	0.180980	1.086925	-1.312522
2	14	0	1.231932	-2.080535	1.171244
3	14	0	-1.027768	-1.621903	1.611859
4	14	0	4.257766	-0.192499	-0.590643
5	14	0	1.203133	2.655574	0.333899
6	14	0	-2.612715	-1.386316	-1.885388
7	14	0	-3.391917	1.471681	0.722640
8	6	0	4.829911	-1.992605	-0.711417
9	1	0	4.341379	-2.520560	-1.537162
10	1	0	5.912678	-2.037607	-0.877519
11	1	0	4.607777	-2.535246	0.213853
12	6	0	4.784756	0.714096	-2.158507
13	1	0	4.407232	0.188509	-3.041666
14	1	0	4.407098	1.739472	-2.196947
15	1	0	5.878365	0.748131	-2.228149
16	6	0	5.053457	0.559773	0.952152
17	1	0	4.769735	-0.005343	1.847079
18	1	0	6.145097	0.512529	0.859624
19	1	0	4.774308	1.605278	1.111593
20	6	0	-3.063727	-0.277121	-3.349531
21	1	0	-2.222538	0.360931	-3.640730
22	1	0	-3.350713	-0.881136	-4.218333
23	1	0	-3.909312	0.373447	-3.100207
24	6	0	-1.250336	-2.590207	-2.417036
25	1	0	-0.338138	-2.052296	-2.700585
26	1	0	-0.999193	-3.272064	-1.596046
27	1	0	-1.567136	-3.197549	-3.272797
28	6	0	-4.144099	-2.400042	-1.423575
29	1	0	-4.982533	-1.756049	-1.141462
30	1	0	-4.459782	-3.005549	-2.281868
31	1	0	-3.946648	-3.078600	-0.588397
32	6	0	-3.638654	2.869947	-0.527974
33	1	0	-3.995630	2.462215	-1.480032
34	1	0	-4.386360	3.585711	-0.165970
35	1	0	-2.713081	3.417386	-0.730097
36	6	0	-5.051827	0.583004	0.924545
37	1	0	-5.467396	0.307515	-0.050469
38	1	0	-4.948284	-0.332726	1.517452
39	1	0	-5.778609	1.232295	1.427243
40	6	0	-2.918915	2.170341	2.421129
41	1	0	-3.112989	1.425449	3.199889
42	1	0	-1.862560	2.449546	2.489356
43	1	0	-3.518873	3.058547	2.652349
44	6	0	1.583106	2.085046	2.107156
45	1	0	0.729534	1.534993	2.521531
46	1	0	2.456937	1.421620	2.143012
47	1	0	1.784392	2.942071	2.762264
48	6	0	2.749223	3.470672	-0.390062
49	1	0	2.572331	3.779643	-1.425327
50	1	0	2.996745	4.365104	0.194642
51	1	0	3.623021	2.813927	-0.378351
52	6	0	-0.108345	4.013778	0.468922
53	1	0	0.232557	4.788541	1.167568
54	1	0	-0.277252	4.476981	-0.508612
55	1	0	-1.065414	3.629204	0.830708
56	6	0	2.310047	-1.994586	2.737134
57	1	0	2.239844	-1.011768	3.214999
58	1	0	1.978370	-2.743738	3.465309
59	1	0	3.363490	-2.192906	2.510107
60	6	0	1.492748	-3.777408	0.352173
61	1	0	1.102900	-4.568688	1.002510
62	1	0	0.978289	-3.847900	-0.610790
63	1	0	2.557036	-3.970866	0.183378
64	6	0	-2.021167	-3.244994	1.568923
65	1	0	-1.669030	-3.932685	2.346492
66	1	0	-3.084846	-3.051393	1.746720
67	1	0	-1.927943	-3.751882	0.602758
68	6	0	-1.202127	-0.925073	3.373402

69	1	0	-0.759743	-1.611148	4.104696
70	1	0	-0.718703	0.050155	3.486659
71	1	0	-2.262120	-0.804927	3.623685
72	32	0	1.849455	-0.299170	-0.352476
73	32	0	-1.724330	-0.054578	-0.088412

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	32	0	1.097088	-0.426473	0.639697
2	14	0	3.942614	0.382684	-1.928331
3	14	0	2.381257	2.136985	-1.857473
4	14	0	0.952670	-1.452623	2.818105
5	14	0	5.006079	-1.052014	1.373851
6	14	0	3.419279	-3.569821	-1.084054
7	14	0	2.056442	3.702392	1.833717
8	6	0	5.594354	1.206902	-1.453834
9	1	0	6.420143	0.490271	-1.421303
10	1	0	5.540028	1.714480	-0.485462
11	1	0	5.836041	1.962987	-2.210955
12	6	0	4.217705	-0.235068	-3.706207
13	1	0	4.440774	0.626199	-4.348015
14	1	0	3.351336	-0.754275	-4.122484
15	1	0	5.076435	-0.913241	-3.749251
16	6	0	1.113269	2.028602	-3.271444
17	1	0	0.668323	3.017878	-3.425280
18	1	0	0.301144	1.328262	-3.050516
19	1	0	1.590300	1.725881	-4.211625
20	6	0	3.341887	3.748804	-2.187425
21	1	0	3.687191	3.748945	-3.228850
22	1	0	4.219709	3.846952	-1.543166
23	1	0	2.711184	4.633945	-2.044738
24	6	0	1.978847	-0.519414	4.106463
25	1	0	2.205704	-1.165450	4.963391
26	1	0	1.418610	0.345610	4.476798
27	1	0	2.925033	-0.149036	3.700082
28	6	0	-0.819576	-1.562698	3.475767
29	1	0	-1.542315	-1.740014	2.671649
30	1	0	-1.100552	-0.631696	3.976749
31	1	0	-0.912767	-2.379574	4.202843
32	6	0	1.616591	-3.214281	2.602331
33	1	0	1.671142	-3.731595	3.568508
34	1	0	2.618598	-3.212356	2.163138
35	1	0	0.966296	-3.798556	1.943488
36	6	0	4.971722	-2.213543	2.873363
37	1	0	5.866245	-1.998339	3.472383
38	1	0	5.020573	-3.264713	2.573094
39	1	0	4.100024	-2.082331	3.518773
40	6	0	6.649899	-1.448187	0.486332
41	1	0	7.320964	-0.582777	0.491740
42	1	0	6.498797	-1.741625	-0.558772
43	1	0	7.164061	-2.272588	0.992766
44	6	0	5.025018	0.732193	2.049131
45	1	0	5.040700	0.732092	3.145264
46	1	0	4.139069	1.294028	1.727500
47	1	0	5.910706	1.278725	1.707828
48	6	0	4.285677	-3.638456	-2.763297
49	1	0	5.292492	-3.209163	-2.715323
50	1	0	3.723757	-3.095743	-3.530102
51	1	0	4.381934	-4.681810	-3.087546
52	6	0	1.729684	-4.395339	-1.267068
53	1	0	1.205227	-4.007766	-2.145325
54	1	0	1.097989	-4.226773	-0.388016
55	1	0	1.850367	-5.477428	-1.396701
56	6	0	4.449368	-4.609765	0.116444
57	1	0	4.595430	-5.610307	-0.308540
58	1	0	3.950588	-4.728177	1.083530
59	1	0	5.438753	-4.172417	0.290795
60	6	0	2.343448	3.081677	3.595126
61	1	0	2.713923	3.917959	4.201024

62	1	0	3.100922	2.292329	3.616188
63	1	0	1.438140	2.696220	4.068807
64	6	0	0.814285	5.131468	1.844576
65	1	0	-0.210674	4.790420	2.027255
66	1	0	0.827956	5.640252	0.874295
67	1	0	1.073688	5.867002	2.615209
68	6	0	3.709101	4.410332	1.241932
69	1	0	3.585932	4.978316	0.315683
70	1	0	4.457039	3.629150	1.067082
71	1	0	4.107899	5.090125	2.004607
72	32	0	-1.097131	-0.426539	-0.639466
73	14	0	-0.952891	-1.453148	-2.817681
74	14	0	-3.942808	0.383127	1.928251
75	14	0	-5.005657	-1.052191	-1.374216
76	14	0	-3.419477	-3.569569	1.084500
77	14	0	-2.381291	2.137279	1.857310
78	14	0	-2.056272	3.702245	-1.834074
79	6	0	-1.979229	-0.520250	-4.106133
80	6	0	0.819290	-1.563450	-3.475485
81	6	0	-1.616883	-3.214728	-2.601473
82	6	0	-5.594423	1.207496	1.453590
83	6	0	-4.218085	-0.234368	3.706188
84	6	0	-4.970471	-2.213804	-2.873636
85	6	0	-6.649768	-1.448605	-0.487342
86	6	0	-5.024559	0.731944	-2.049689
87	6	0	-4.286129	-3.638019	2.763620
88	6	0	-1.729908	-4.395060	1.267860
89	6	0	-4.449383	-4.609650	-0.116035
90	6	0	-1.113393	2.028889	3.271359
91	6	0	-3.341805	3.749204	2.187078
92	6	0	-2.343197	3.081346	-3.595428
93	6	0	-0.814057	5.131269	-1.845036
94	6	0	-3.708934	4.410318	-1.242456
95	1	0	-2.206158	-1.166484	-4.962893
96	1	0	-1.419060	0.344709	-4.476719
97	1	0	-2.925391	-0.149820	-3.699730
98	1	0	1.542093	-1.740650	-2.671398
99	1	0	1.100277	-0.632570	-3.976685
100	1	0	0.912367	-2.380480	-4.202402
101	1	0	-1.671531	-3.732248	-3.567534
102	1	0	-2.618865	-3.212658	-2.162211
103	1	0	-0.966568	-3.798892	-1.942553
104	1	0	-6.420320	0.490993	1.421182
105	1	0	-5.540011	1.714917	0.485144
106	1	0	-5.836006	1.963737	2.210588
107	1	0	-4.441123	0.627003	4.347867
108	1	0	-3.351792	-0.753596	4.122595
109	1	0	-5.076878	-0.912457	3.749259
110	1	0	-5.864788	-1.998816	-3.473039
111	1	0	-5.019228	-3.264964	-2.573318
112	1	0	-4.098524	-2.082442	-3.518692
113	1	0	-7.320990	-0.583321	-0.493077
114	1	0	-6.499044	-1.741970	0.557836
115	1	0	-7.163572	-2.273125	-0.993945
116	1	0	-5.039738	0.731722	-3.145830
117	1	0	-4.138836	1.293939	-1.727716
118	1	0	-5.910480	1.278382	-1.708847
119	1	0	-5.292940	-3.208738	2.715444
120	1	0	-3.724330	-3.095218	3.530450
121	1	0	-4.382431	-4.681337	3.087971
122	1	0	-1.205574	-4.007368	2.146138
123	1	0	-1.098093	-4.226608	0.388872
124	1	0	-1.850604	-5.477132	1.397620
125	1	0	-4.595505	-5.610145	0.309037
126	1	0	-3.950459	-4.728164	-1.083035
127	1	0	-5.438742	-4.172322	-0.290580
128	1	0	-0.668352	3.018131	3.425129
129	1	0	-0.301333	1.328437	3.050546
130	1	0	-1.590510	1.726307	4.211542
131	1	0	-3.687154	3.749466	3.228487
132	1	0	-4.219592	3.847366	1.542773
133	1	0	-2.711025	4.634282	2.044339
134	1	0	-2.713609	3.917574	-4.201440

135	1	0	-3.100695	2.292021	-3.616451
136	1	0	-1.437871	2.695811	-4.069013
137	1	0	0.210898	4.790158	-2.027615
138	1	0	-0.827763	5.640169	-0.874816
139	1	0	-1.073387	5.866721	-2.615771
140	1	0	-3.585790	4.978406	-0.316268
141	1	0	-4.456910	3.629184	-1.067551
142	1	0	-4.107669	5.090036	-2.005231
143	32	0	1.218948	2.054237	0.267847
144	32	0	-1.218908	2.054241	-0.267975
145	32	0	3.260610	-1.287305	-0.295946
146	32	0	-3.260687	-1.287150	0.296134

Compound **9a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	32	0	-1.581051	0.050966	-0.944562
2	32	0	1.456215	0.032408	0.934363
3	14	0	-2.109908	0.988650	-3.117170
4	14	0	1.963473	-0.776007	3.169559
5	14	0	-1.776908	2.417832	2.119483
6	14	0	-0.202473	-3.945707	0.205898
7	14	0	1.632144	-2.035008	-2.392370
8	14	0	0.163671	4.132433	-0.386678
9	14	0	-3.979069	1.871883	1.466498
10	14	0	3.839122	-1.810685	-1.619125
11	14	0	-4.113038	-1.887716	1.841976
12	14	0	-5.548607	-0.844584	-1.401070
13	14	0	5.848499	-0.200979	1.251230
14	14	0	4.281737	2.058883	-1.244231
15	6	0	-0.696668	1.967938	-3.917331
16	1	0	-0.143604	1.394152	-4.664325
17	1	0	-1.121618	2.851125	-4.410542
18	1	0	0.016344	2.319462	-3.164580
19	6	0	-3.391067	2.316579	-2.694159
20	1	0	-2.878522	3.125803	-2.163895
21	1	0	-3.831137	2.739976	-3.605940
22	1	0	-4.201971	1.962647	-2.054378
23	6	0	-2.786987	-0.225286	-4.402117
24	1	0	-3.725749	-0.689786	-4.089734
25	1	0	-2.970569	0.307482	-5.343063
26	1	0	-2.070021	-1.028190	-4.605932
27	6	0	3.144767	0.455452	3.985129
28	1	0	3.608006	0.026538	4.881767
29	1	0	3.938326	0.781757	3.308706
30	1	0	2.581819	1.344654	4.291722
31	6	0	2.755611	-2.453493	2.780804
32	1	0	3.339187	-2.831391	3.628583
33	1	0	1.944747	-3.166071	2.589554
34	1	0	3.403643	-2.433667	1.899259
35	6	0	0.676855	-1.194582	4.494268
36	1	0	1.192195	-1.826687	5.229443
37	1	0	0.299751	-0.313533	5.018142
38	1	0	-0.178908	-1.760959	4.116265
39	6	0	0.965583	4.972513	1.126909
40	1	0	1.892588	5.472883	0.827700
41	1	0	0.292373	5.728922	1.542038
42	1	0	1.211808	4.269391	1.930053
43	6	0	1.184931	4.687234	-1.879327
44	1	0	2.247607	4.467785	-1.773005
45	1	0	0.835915	4.280199	-2.831913
46	1	0	1.071244	5.778915	-1.923183
47	6	0	-1.540626	4.912590	-0.710641
48	1	0	-2.366782	4.425676	-0.184896
49	1	0	-1.520224	5.965441	-0.401583
50	1	0	-1.759971	4.891352	-1.783371
51	6	0	-6.156120	0.398359	-2.695037
52	1	0	-6.488904	1.332423	-2.229567
53	1	0	-5.410883	0.647917	-3.454131

54	1	0	-7.019964	-0.046998	-3.204251
55	6	0	-7.114145	-1.346615	-0.458031
56	1	0	-7.856499	-1.724676	-1.171497
57	1	0	-6.933091	-2.131022	0.282528
58	1	0	-7.558280	-0.489872	0.061120
59	6	0	-4.871908	-2.383494	-2.284748
60	1	0	-4.986439	-3.272911	-1.657140
61	1	0	-5.411881	-2.563293	-3.222169
62	1	0	-3.807216	-2.283867	-2.523063
63	6	0	-5.739687	-1.643080	2.804166
64	1	0	-6.235784	-2.611887	2.935577
65	1	0	-5.550025	-1.227512	3.798579
66	1	0	-6.443607	-0.977770	2.296722
67	6	0	-2.695400	-1.798411	3.085778
68	1	0	-1.729931	-1.713352	2.571281
69	1	0	-2.820317	-0.912349	3.716964
70	1	0	-2.661142	-2.675362	3.742774
71	6	0	-4.240468	-3.612678	1.067345
72	1	0	-4.222580	-4.379364	1.852284
73	1	0	-5.193546	-3.711608	0.536775
74	1	0	-3.436319	-3.829825	0.359593
75	6	0	-4.844887	3.306790	0.567744
76	1	0	-5.896314	3.046124	0.398957
77	1	0	-4.817752	4.210917	1.187817
78	1	0	-4.400028	3.542939	-0.401463
79	6	0	-4.953572	1.635875	3.085618
80	1	0	-4.935690	2.571926	3.657261
81	1	0	-6.000495	1.377947	2.895179
82	1	0	-4.519727	0.851498	3.713451
83	6	0	-1.816167	4.221483	2.742525
84	1	0	-2.005339	4.965655	1.964804
85	1	0	-2.624071	4.297404	3.481893
86	1	0	-0.882222	4.482215	3.249702
87	6	0	-1.269675	1.420479	3.646234
88	1	0	-1.113195	0.370528	3.396073
89	1	0	-0.316637	1.816549	4.020021
90	1	0	-2.007526	1.484411	4.455180
91	6	0	6.064417	2.178825	-1.873798
92	1	0	6.184043	3.132644	-2.402519
93	1	0	6.805012	2.149861	-1.068952
94	1	0	6.297367	1.375807	-2.581491
95	6	0	3.987884	3.479293	-0.030898
96	1	0	4.118482	4.463590	-0.495987
97	1	0	2.974515	3.423445	0.380487
98	1	0	4.685465	3.408330	0.809869
99	6	0	3.177826	2.210161	-2.769060
100	1	0	2.119361	2.178922	-2.489568
101	1	0	3.357805	3.147953	-3.307078
102	1	0	3.369326	1.383186	-3.460888
103	6	0	7.185462	-0.716271	0.006767
104	1	0	7.191121	-0.093308	-0.891572
105	1	0	8.170936	-0.630738	0.481531
106	1	0	7.060890	-1.757178	-0.308034
107	6	0	6.420112	1.451134	1.987951
108	1	0	7.357260	1.288746	2.534652
109	1	0	6.620066	2.187204	1.202568
110	1	0	5.700147	1.891195	2.684401
111	6	0	5.917229	-1.496706	2.625800
112	1	0	5.223884	-1.290074	3.445136
113	1	0	5.706110	-2.500689	2.243588
114	1	0	6.935349	-1.500102	3.034930
115	6	0	4.975987	-1.436158	-3.101076
116	1	0	6.019896	-1.344376	-2.781174
117	1	0	4.920750	-2.248179	-3.835873
118	1	0	4.690920	-0.506858	-3.605589
119	6	0	4.492239	-3.411134	-0.822987
120	1	0	4.367003	-4.257560	-1.509176
121	1	0	5.560550	-3.320118	-0.600650
122	1	0	3.972632	-3.656699	0.107250
123	6	0	1.319807	-0.698657	-3.695108
124	1	0	0.326185	-0.846160	-4.134280
125	1	0	1.351207	0.303428	-3.264303
126	1	0	2.059541	-0.749102	-4.503780

127	6	0	1.333821	-3.662713	-3.339111
128	1	0	2.021475	-3.698683	-4.192953
129	1	0	1.483016	-4.571181	-2.751006
130	1	0	0.313261	-3.678058	-3.738506
131	6	0	-1.359004	-4.691448	-1.101209
132	1	0	-1.826612	-5.607255	-0.719732
133	1	0	-2.156178	-4.003426	-1.401809
134	1	0	-0.791601	-4.953130	-1.999913
135	6	0	1.431538	-4.904917	0.139222
136	1	0	2.042868	-4.673560	-0.735175
137	1	0	2.039784	-4.713993	1.029139
138	1	0	1.203539	-5.978316	0.118226
139	6	0	-0.865742	-4.321792	1.935868
140	1	0	-0.301965	-3.802772	2.718775
141	1	0	-1.919583	-4.073167	2.057110
142	1	0	-0.752431	-5.400605	2.103195
143	32	0	-0.256970	1.823461	0.302947
144	32	0	0.207736	-1.652804	-0.466179
145	32	0	-3.832110	-0.164320	0.172920
146	32	0	3.804457	0.026562	-0.046549

Compound **2a**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	1.153929	-2.525293	0.731934
2	14	0	-1.007031	-2.097679	1.527089
3	14	0	3.655479	-0.839300	-1.664171
4	14	0	3.221751	0.590789	1.832920
5	14	0	-3.154013	-1.563435	-1.803931
6	14	0	-3.710148	0.602454	1.204475
7	6	0	2.823748	-1.256022	-3.309956
8	1	0	2.211862	-0.421402	-3.667729
9	1	0	3.576736	-1.485501	-4.073433
10	1	0	2.165742	-2.126542	-3.210992
11	6	0	4.751617	0.686911	-1.925210
12	1	0	5.444145	0.533124	-2.761116
13	1	0	4.145156	1.572478	-2.149782
14	1	0	5.348842	0.906938	-1.033231
15	6	0	4.777913	-2.293991	-1.199009
16	1	0	4.200909	-3.217579	-1.083501
17	1	0	5.522123	-2.463316	-1.986606
18	1	0	5.313376	-2.117466	-0.261608
19	6	0	-3.584280	-0.237827	-3.085621
20	1	0	-2.667674	0.233515	-3.458398
21	1	0	-4.110155	-0.679959	-3.940101
22	1	0	-4.221357	0.546795	-2.664692
23	6	0	-2.086512	-2.858590	-2.675699
24	1	0	-1.161892	-2.409240	-3.056492
25	1	0	-1.815615	-3.681643	-2.005881
26	1	0	-2.628699	-3.282253	-3.529610
27	6	0	-4.750778	-2.417652	-1.245125
28	1	0	-5.476191	-1.705392	-0.837968
29	1	0	-5.223053	-2.924551	-2.095082
30	1	0	-4.548936	-3.170202	-0.474773
31	6	0	-4.947462	1.450423	0.045204
32	1	0	-5.436277	0.715999	-0.603833
33	1	0	-5.728546	1.951584	0.629569
34	1	0	-4.475098	2.197703	-0.601084
35	6	0	-4.652629	-0.756981	2.129516
36	1	0	-5.556079	-0.342024	2.593064
37	1	0	-4.956432	-1.566881	1.459200
38	1	0	-4.039853	-1.194791	2.924640
39	6	0	-3.217193	1.872583	2.526922
40	1	0	-2.468501	1.472410	3.219549
41	1	0	-2.827751	2.804525	2.104024
42	1	0	-4.109121	2.127489	3.112445
43	6	0	2.339568	0.565422	3.510623
44	1	0	1.443031	1.193081	3.538844

45	1	0	2.038457	-0.451821	3.782029
46	1	0	3.026301	0.929244	4.284746
47	6	0	4.794906	-0.444411	2.038334
48	1	0	5.466296	-0.317020	1.182544
49	1	0	5.335553	-0.125332	2.937767
50	1	0	4.571115	-1.511518	2.136535
51	6	0	3.825477	2.368336	1.530835
52	1	0	4.587779	2.614073	2.280431
53	1	0	4.288225	2.469255	0.542993
54	1	0	3.034746	3.121624	1.614580
55	6	0	2.265178	-3.375770	2.020634
56	1	0	2.399931	-2.756840	2.913865
57	1	0	1.832214	-4.332494	2.334412
58	1	0	3.255427	-3.577687	1.596328
59	6	0	1.027921	-3.674793	-0.776486
60	1	0	0.516533	-4.609605	-0.517860
61	1	0	0.464960	-3.195633	-1.583662
62	1	0	2.019673	-3.929620	-1.165547
63	6	0	-2.049313	-3.681219	1.677889
64	1	0	-1.593526	-4.389538	2.379093
65	1	0	-3.059795	-3.453107	2.034273
66	1	0	-2.139503	-4.178347	0.705825
67	6	0	-0.876781	-1.273865	3.238030
68	1	0	-0.306308	-1.893591	3.939772
69	1	0	-0.365047	-0.308706	3.150880
70	1	0	-1.865034	-1.093226	3.675034
71	32	0	-0.006584	0.459843	-1.369967
72	15	0	-0.086575	2.626420	-0.392723
73	6	0	0.028910	2.755372	1.436051
74	1	0	1.024485	2.374207	1.677493
75	1	0	-0.680800	2.017856	1.827123
76	6	0	-1.649212	3.489794	-0.873819
77	1	0	-2.386546	3.211444	-0.110960
78	1	0	-1.985116	3.022438	-1.807150
79	6	0	1.291178	3.670164	-1.026440
80	1	0	2.204280	3.273976	-0.566596
81	1	0	1.163610	4.697822	-0.666108
82	6	0	-0.193251	4.128097	2.068497
83	1	0	-0.043373	4.067924	3.150763
84	1	0	0.505604	4.874732	1.676706
85	1	0	-1.211353	4.490962	1.897399
86	6	0	-1.577380	5.010514	-1.032044
87	1	0	-2.568908	5.406868	-1.268868
88	1	0	-1.228363	5.504199	-0.121502
89	1	0	-0.904313	5.295577	-1.845556
90	6	0	1.410960	3.628761	-2.551762
91	1	0	1.638348	2.615624	-2.895497
92	1	0	0.481073	3.936424	-3.041874
93	1	0	2.208680	4.297101	-2.887748
94	32	0	1.974791	-0.379290	0.003727
95	32	0	-1.940158	-0.500475	-0.013786

2a (TS)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	1.061886	-2.650497	-0.846087
2	14	0	-1.178878	-2.750680	-0.132932
3	14	0	3.685191	0.164911	-1.593138
4	14	0	3.010438	-0.938557	2.207064
5	14	0	-3.234996	0.095001	-2.072456
6	14	0	-3.538859	-0.329602	1.859199
7	6	0	2.840386	0.600487	-3.225408
8	1	0	1.931807	1.184907	-3.039318
9	1	0	3.510963	1.187183	-3.864280
10	1	0	2.547537	-0.298937	-3.775356
11	6	0	4.561626	1.723240	-0.957828
12	1	0	5.399646	1.985370	-1.614630
13	1	0	3.877429	2.579971	-0.941979
14	1	0	4.957406	1.586144	0.054594

15	6	0	4.996672	-1.169120	-1.892409
16	1	0	4.539635	-2.084383	-2.284893
17	1	0	5.743995	-0.828363	-2.618633
18	1	0	5.519955	-1.429628	-0.966271
19	6	0	-3.503273	1.973450	-2.058081
20	1	0	-2.537173	2.488750	-1.984565
21	1	0	-3.995244	2.313244	-2.976995
22	1	0	-4.120558	2.283385	-1.207082
23	6	0	-2.164313	-0.325961	-3.570884
24	1	0	-1.184552	0.154918	-3.467775
25	1	0	-1.999590	-1.405080	-3.661581
26	1	0	-2.627223	0.026281	-4.500056
27	6	0	-4.921601	-0.754793	-2.211825
28	1	0	-5.585146	-0.435176	-1.400149
29	1	0	-5.412495	-0.512665	-3.161416
30	1	0	-4.818006	-1.843720	-2.150999
31	6	0	-4.485128	1.312936	1.832486
32	1	0	-5.162042	1.346573	0.970887
33	1	0	-5.092257	1.426220	2.738668
34	1	0	-3.813697	2.174935	1.766801
35	6	0	-4.837183	-1.707889	1.785184
36	1	0	-5.545365	-1.624143	2.617965
37	1	0	-5.408639	-1.656636	0.851887
38	1	0	-4.374373	-2.698771	1.837185
39	6	0	-2.542868	-0.488150	3.457475
40	1	0	-2.243234	-1.530248	3.612984
41	1	0	-1.628415	0.113920	3.415591
42	1	0	-3.129820	-0.171906	4.327352
43	6	0	1.806249	-1.939365	3.264303
44	1	0	0.829045	-1.441532	3.278148
45	1	0	1.665533	-2.952356	2.872161
46	1	0	2.162774	-2.021402	4.297652
47	6	0	4.685188	-1.818337	2.120538
48	1	0	5.419459	-1.201439	1.590240
49	1	0	5.079649	-2.020935	3.122996
50	1	0	4.602712	-2.772484	1.588699
51	6	0	3.233543	0.743900	3.044272
52	1	0	3.653607	0.629884	4.050208
53	1	0	3.894792	1.403967	2.471942
54	1	0	2.256510	1.231876	3.134168
55	6	0	1.995757	-4.209389	-0.278532
56	1	0	2.032715	-4.277727	0.813816
57	1	0	1.512864	-5.117803	-0.657269
58	1	0	3.026672	-4.196059	-0.649916
59	6	0	1.076718	-2.608352	-2.745262
60	1	0	0.538010	-3.470588	-3.155901
61	1	0	0.590548	-1.696540	-3.108305
62	1	0	2.099899	-2.632026	-3.137513
63	6	0	-2.192850	-3.845462	-1.315076
64	1	0	-1.750993	-4.844994	-1.401284
65	1	0	-3.216412	-3.960444	-0.940166
66	1	0	-2.247816	-3.412401	-2.319226
67	6	0	-1.230926	-3.572856	1.580992
68	1	0	-0.752676	-4.559035	1.538431
69	1	0	-0.697517	-2.972914	2.324230
70	1	0	-2.258684	-3.716652	1.932107
71	32	0	0.029727	0.628015	-0.019188
72	15	0	0.128877	2.891953	0.113614
73	6	0	1.599373	3.456013	1.069188
74	1	0	1.406978	3.168324	2.106797
75	1	0	2.435074	2.829210	0.735527
76	6	0	1.946264	4.939950	0.964012
77	1	0	1.112596	5.572662	1.288326
78	1	0	2.804857	5.170182	1.601319
79	1	0	2.209117	5.220759	-0.060430
80	6	0	0.274636	3.749124	-1.533153
81	1	0	1.345478	3.721337	-1.777673
82	1	0	-0.208513	3.074222	-2.246628
83	6	0	-0.294769	5.163339	-1.666304
84	1	0	-1.383048	5.158294	-1.550986
85	1	0	0.120794	5.855479	-0.928758
86	1	0	-0.071953	5.561706	-2.660628
87	6	0	-1.332415	3.676472	0.923090

88	1	0	-2.215217	3.296513	0.392368
89	6	0	-1.423389	3.371835	2.417408
90	1	0	-1.380436	2.293256	2.598479
91	1	0	-0.602857	3.844004	2.967321
92	1	0	-2.361824	3.756584	2.826821
93	1	0	-1.291417	4.757706	0.749569
94	32	0	2.087837	-0.639001	0.011963
95	32	0	-2.099975	-0.516657	-0.052056

Compound 6a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	0.578753	-2.126500	1.899859
2	14	0	-1.612965	-1.258121	2.059774
3	14	0	2.769997	-2.486981	-1.434317
4	14	0	3.537539	0.422760	0.786627
5	14	0	-3.063240	-1.842476	-1.436998
6	14	0	-3.662894	1.590017	0.088374
7	6	0	1.532935	-3.422984	-2.518135
8	1	0	0.812546	-2.742656	-2.986659
9	1	0	2.066991	-3.951502	-3.317345
10	1	0	0.975596	-4.168326	-1.941019
11	6	0	3.855910	-1.469534	-2.611263
12	1	0	4.291025	-2.119216	-3.380179
13	1	0	3.250130	-0.707678	-3.116018
14	1	0	4.678521	-0.962458	-2.095765
15	6	0	3.844817	-3.789769	-0.575042
16	1	0	3.219778	-4.489217	-0.010464
17	1	0	4.401493	-4.369828	-1.321131
18	1	0	4.566549	-3.348857	0.118633
19	6	0	-3.037865	-1.310718	-3.252785
20	1	0	-2.006829	-1.153576	-3.587580
21	1	0	-3.490172	-2.086807	-3.882143
22	1	0	-3.586131	-0.377633	-3.417230
23	6	0	-2.044779	-3.435309	-1.317132
24	1	0	-0.986881	-3.206751	-1.488596
25	1	0	-2.127610	-3.912722	-0.335451
26	1	0	-2.357632	-4.163356	-2.075292
27	6	0	-4.856419	-2.212793	-0.945908
28	1	0	-5.490538	-1.327946	-1.071968
29	1	0	-5.268530	-3.009834	-1.576416
30	1	0	-4.931672	-2.534795	0.098258
31	6	0	-4.417573	1.877118	-1.625510
32	1	0	-4.979132	0.996351	-1.956063
33	1	0	-5.106356	2.730116	-1.612378
34	1	0	-3.640463	2.074854	-2.371948
35	6	0	-5.050470	1.088989	1.276228
36	1	0	-5.836292	1.852995	1.312462
37	1	0	-5.508106	0.145171	0.960465
38	1	0	-4.668893	0.948191	2.293584
39	6	0	-2.984590	3.269383	0.673520
40	1	0	-2.733414	3.264907	1.740322
41	1	0	-2.092421	3.566376	0.108978
42	1	0	-3.749465	4.040347	0.521949
43	6	0	3.293538	1.449745	2.368367
44	1	0	2.639487	2.307782	2.180640
45	1	0	2.881375	0.869512	3.199748
46	1	0	4.266257	1.844617	2.686174
47	6	0	5.081554	-0.634382	1.092978
48	1	0	5.404119	-1.157130	0.186965
49	1	0	5.913076	-0.003767	1.430638
50	1	0	4.895046	-1.389370	1.865036
51	6	0	3.936719	1.694471	-0.572255
52	1	0	4.983614	2.013917	-0.505318
53	1	0	3.765262	1.296603	-1.578120
54	1	0	3.308858	2.585108	-0.443095
55	6	0	1.469002	-1.859201	3.564446
56	1	0	1.430164	-0.808876	3.871772
57	1	0	0.997425	-2.453644	4.355715

58	1	0	2.522469	-2.153725	3.499220
59	6	0	0.537416	-4.000365	1.577023
60	1	0	-0.127315	-4.503942	2.288564
61	1	0	0.184126	-4.227179	0.566007
62	1	0	1.540345	-4.425751	1.690183
63	6	0	-2.909672	-2.611555	2.402421
64	1	0	-2.667314	-3.161526	3.319156
65	1	0	-3.896407	-2.152373	2.536582
66	1	0	-2.984347	-3.332817	1.584025
67	6	0	-1.702542	-0.136195	3.609777
68	1	0	-1.751317	-0.777297	4.498040
69	1	0	-0.834694	0.517980	3.735756
70	1	0	-2.602642	0.489141	3.603188
71	32	0	0.066330	0.310768	-1.404895
72	6	0	0.530209	2.191332	-0.629422
73	7	0	0.958498	3.219776	-1.400000
74	6	0	0.860127	4.041830	0.638102
75	6	0	1.176142	4.363650	-0.646145
76	7	0	0.477178	2.707182	0.620874
77	6	0	0.859282	4.871227	1.877071
78	1	0	1.567272	4.491553	2.621856
79	1	0	1.145198	5.897177	1.637442
80	1	0	-0.135843	4.897792	2.333863
81	6	0	1.676541	5.632209	-1.247145
82	1	0	1.804961	6.389912	-0.472132
83	1	0	2.645821	5.484801	-1.735359
84	1	0	0.980253	6.028987	-1.993297
85	6	0	1.266687	3.141554	-2.820190
86	1	0	0.900145	2.187222	-3.199807
87	1	0	0.778245	3.963545	-3.348334
88	1	0	2.349356	3.201825	-2.965968
89	6	0	0.033734	1.969652	1.791994
90	1	0	0.473992	0.969666	1.771618
91	1	0	0.366669	2.490369	2.691192
92	1	0	-1.053590	1.882461	1.796392
93	32	0	-2.027067	-0.165001	-0.057094
94	32	0	1.685526	-0.963560	0.086430

6a (TS)

Standard orientation:

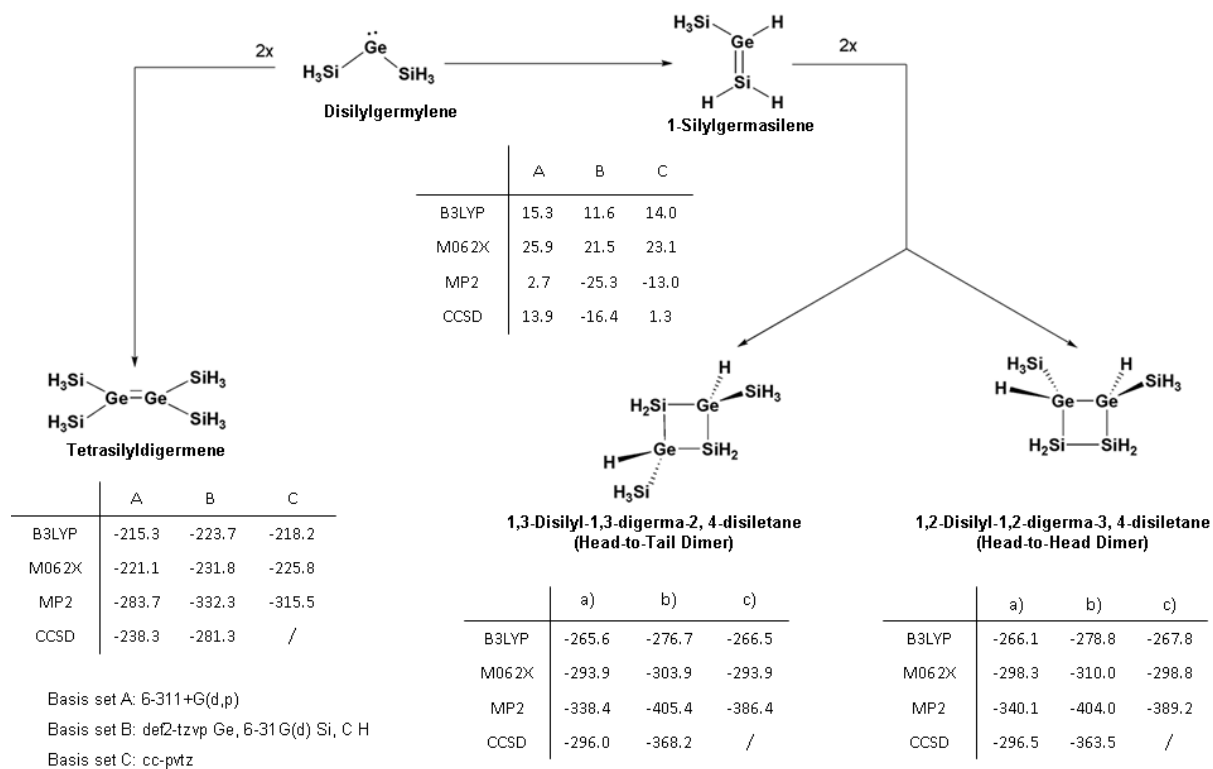
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	14	0	-1.127350	-2.779422	0.322853
2	14	0	1.127305	-2.779452	-0.322769
3	14	0	-3.793299	-0.347836	1.573893
4	14	0	-2.989606	-0.414876	-2.281416
5	14	0	2.989621	-0.414852	2.281414
6	14	0	3.793239	-0.347962	-1.573928
7	6	0	-3.074911	-0.138663	3.310175
8	1	0	-2.376568	0.704429	3.352987
9	1	0	-3.868513	0.032177	4.046679
10	1	0	-2.520998	-1.034811	3.607227
11	6	0	-5.018377	1.067357	1.244033
12	1	0	-5.919282	0.904484	1.848238
13	1	0	-4.620805	2.050232	1.513145
14	1	0	-5.327908	1.100232	0.193272
15	6	0	-4.831176	-1.934055	1.498677
16	1	0	-4.237927	-2.825980	1.723277
17	1	0	-5.655402	-1.887426	2.220567
18	1	0	-5.265679	-2.066529	0.501295
19	6	0	3.300183	1.412465	2.675713
20	1	0	2.381242	1.992635	2.527989
21	1	0	3.617970	1.538402	3.717316
22	1	0	4.082039	1.836964	2.035186
23	6	0	1.758989	-1.083840	3.549874
24	1	0	0.790092	-0.585538	3.427477
25	1	0	1.605827	-2.161582	3.426248
26	1	0	2.110704	-0.906198	4.572836
27	6	0	4.629302	-1.352945	2.431218
28	1	0	5.378601	-0.944869	1.743274

29	1	0	5.033659	-1.279489	3.447514
30	1	0	4.500641	-2.415045	2.195068
31	6	0	5.018341	1.067254	-1.244248
32	1	0	5.327886	1.100240	-0.193494
33	1	0	5.919234	0.904287	-1.848445
34	1	0	4.620792	2.050105	-1.513475
35	6	0	4.831114	-1.934178	-1.498603
36	1	0	5.655301	-1.887634	-2.220543
37	1	0	5.265672	-2.066547	-0.501231
38	1	0	4.237844	-2.826122	-1.723076
39	6	0	3.074748	-0.138952	-3.310182
40	1	0	2.376282	0.704037	-3.353009
41	1	0	3.868287	0.031938	-4.046743
42	1	0	2.520936	-1.035197	-3.607134
43	6	0	-1.758931	-1.083892	-3.549819
44	1	0	-0.790069	-0.585519	-3.427442
45	1	0	-1.605699	-2.161613	-3.426099
46	1	0	-2.110637	-0.906357	-4.572802
47	6	0	-4.629265	-1.353010	-2.431192
48	1	0	-5.378551	-0.944974	-1.743211
49	1	0	-5.033663	-1.279551	-3.447472
50	1	0	-4.500554	-2.415108	-2.195062
51	6	0	-3.300200	1.412422	-2.675777
52	1	0	-3.617962	1.538323	-3.717392
53	1	0	-4.082087	1.836909	-2.035281
54	1	0	-2.381285	1.992630	-2.528045
55	6	0	-2.094388	-4.105689	-0.642154
56	1	0	-2.074118	-3.904726	-1.718828
57	1	0	-1.667915	-5.101888	-0.476489
58	1	0	-3.142850	-4.130062	-0.323513
59	6	0	-1.202311	-3.232445	2.170134
60	1	0	-0.728691	-4.208077	2.332877
61	1	0	-0.669649	-2.493987	2.777854
62	1	0	-2.232473	-3.293281	2.536144
63	6	0	2.094344	-4.105646	0.642338
64	1	0	1.667887	-5.101865	0.476759
65	1	0	3.142809	-4.130031	0.323703
66	1	0	2.074067	-3.904589	1.718995
67	6	0	1.202239	-3.232643	-2.170013
68	1	0	0.728665	-4.208322	-2.332618
69	1	0	0.669516	-2.494282	-2.777799
70	1	0	2.232391	-3.293470	-2.536051
71	32	0	0.000008	0.718048	-0.000036
72	6	0	0.000040	2.642793	-0.000036
73	7	0	1.049031	3.478743	-0.262789
74	6	0	-0.657479	4.813183	0.164227
75	6	0	0.657620	4.813168	-0.164252
76	6	0	2.343734	3.000359	-0.681562
77	1	0	2.973487	3.847139	-0.957596
78	1	0	2.830088	2.437798	0.122394
79	1	0	2.219729	2.333409	-1.544097
80	6	0	1.599933	5.943075	-0.400075
81	1	0	1.985167	5.946457	-1.425923
82	1	0	1.090458	6.894265	-0.234948
83	1	0	2.457038	5.900630	0.280923
84	6	0	-1.599760	5.943108	0.400090
85	1	0	-1.984997	5.946461	1.425937
86	1	0	-1.090257	6.894290	0.235001
87	1	0	-2.456865	5.900715	-0.280912
88	6	0	-2.343647	3.000403	0.681466
89	1	0	-2.973393	3.847189	0.957496
90	1	0	-2.829990	2.437860	-0.122510
91	1	0	-2.219666	2.333438	1.543991
92	7	0	-1.048927	3.478767	0.262727
93	32	0	2.052458	-0.587098	0.074207
94	32	0	-2.052472	-0.587067	-0.074197

2.2 Choice of model chemistry.

The relative energies predicted by the applied method (M06-2X/def2-tzvp (Ge), 6-311+G(d,p) (P), 6-31G(d) (Si, C, N, H)) for a set of small model compounds (disilylsubstituted germylene :Ge(SiH₃)₂, its silagermene isomer, H₂Si=Ge(H)SiH₃, and several dimers) were gauged versus more sophisticated theoretical methods. The results of this comparison are summarized in Figure S-7. The molecular structures obtained with this model chemistry are compared versus experimental data for compounds **2** and **6** and versus computed data obtained using a larger basis set for the same compounds in Table S5. As a short summary of the results depicted in Figure S-7, it can be concluded that the results obtained with the M06-2X functional and the basis set B (def2-tzvp (Ge), 6-31G(d) (Si, C, H)) are always relative close to those obtained from reliable CCSD calculations using the 6-311+G(d,p) basis set (basis set A). The data compiled in Table S4 for compound **6** reveal only minor deviations between the results for both applied basis sets and between the theoretical results and experimental data. For example, bond lengths, extracted from the calculated gas-phase molecular structure (at M06-2X/B) differs only by -1.2 - +1.3 pm from data obtained by X-ray diffraction (XRD) in the solid state. Even the parameter of the donor-acceptor bonds are reliably reproduced by the computations. Important structural parameter of the experimentally not accessible germylenes **3** and **3a** are also given in Table S4. In general, the results of the computations predict for germylenes **3** and **3a** half-chair conformations of almost C₂ molecular symmetry. Acute endocyclic bond angles at the dicoordinated germanium atom (**3**: $\alpha(\text{SiGeSi}) = 94.3^\circ$; **3a**: $\alpha(\text{GeGeGe}) = 94.5^\circ$) and long bonds of the dicoordinated germanium atom to the α -atoms (**3**: $d(\text{Si-Ge(II)}) = 243.2$ pm; **3a**: $d(\text{Ge-Ge(II)}) = 249.2$ pm) are additional characteristics of the cyclic persilylated germylenes **3** and **3a**.

Figure S-7. SCF energies (E^{SCF}) of silagermene, $\text{H}_2\text{Si}=\text{Ge}(\text{H})\text{SiH}_3$, and several dimers relative to germylene, $(\text{H}_3\text{Si})_2\text{Ge}:$, calculated using the indicated methods and basis sets (E^{SCF} in kJ mol^{-1}).



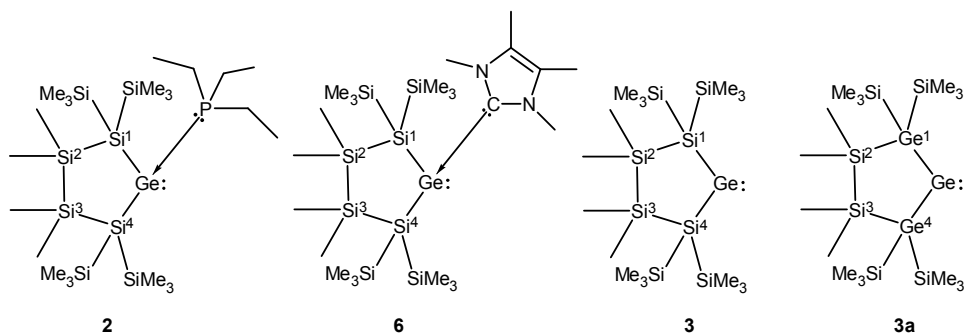


Table S4. Experimental and computed molecular structure parameter for compounds **2**, **3**, **3a** and **6** (bond lengths [pm], angles [°]).

Parameter	Cpd. 2			Cpd. 6			Cpd. 3		Cpd. 3a	
	exp	M06-2X/A ^[a]	M06-2X/B ^[b]	exp	M06-2X/A ^[a]	M06-2X/B ^[b]	M06-2X/B ^[b]	M06-2X/B ^[b]	M06-2X/B ^[b]	
α (Si ¹ GeSi ⁴)	103.9	101.2	101.6	97.4	98.7	99.1	94.3	94.5		
Ω ^[c]	113.6	101.0	101.2	95.0	99.6	99.9	-	-		
Ge-E: ^[d]	236.5	237.2	237.1	207.0	208.3	207.9	-	-		
Ge-Si ¹	246.7	248.9	249.2	247.1	248.1	248.4	243.2	249.2 ^[e]		
Si ¹ -Si ²	243.9	235.3	235.3	235.6	235.0	235.1	235.1	240.5 ^[f]		
Si ² -Si ³	232.9	234.7	234.6	236.2	235.2	235.0	235.4	235.0		
Si ³ -Si ⁴	230.8	235.6	235.6	236.6	236.2	236.1	235.1	240.5 ^[f]		
Si ⁴ -Ge	247.7	248.8	249.2	248.0	248.9	249.2	243.2	249.2 ^[e]		

^[a] Basis set A: 6-311+G(d,p) for all atoms. ^[b] Basis set B: def2-tzvp for Ge, 6-31G(d) for Si, C, and H. ^[c] Angle between the C-Ge vector and the plane spanned by the atoms Si¹GeSi⁴. ^[d] **2** :E = C; **6** E = P. ^[e] Ge-Ge^{1/4}. ^[f] Si^{2/3}-Ge^{1/4}.

2.3 Calculation of inversion barriers in compounds 2, 2a, 6, and 6a

For comparison of the experimentally by VT NMR measurements determined barriers for the inversion of the coordination of the germanium atom with data obtained from calculations, solvent effects were included in the computations. The molecular structures of all relevant intermediates and transition states were reoptimized using the polarized continuum model (PCM) model⁵ and the appropriate parameter for toluene, the solvent used for the NMR measurements. Standard molecular entropies of reaction, ΔS , computed from harmonic frequencies at $p=1$ atm in the gas phase in general are too negative because the translational contributions to entropy are significantly larger in the gas phase than in solution. Following arguments given by Martin et al.⁶ calculating these entropies at the pressure of liquid toluene ($p=23.71$ MPa (234 atm) for $\rho=0.87$ g cm^{-3}) is a straightforward way of modelling the translational degrees of freedom in toluene solution. The Gibbs free energy $G^{\text{T}}(\text{solv})$ for each compound computed in toluene solution at the indicated temperature T and $p=23.71$ MPa is given in Table S5 and is used for the barriers for the inversion process. Bond dissociation energies BDE are calculated using the SCF energies obtained from PCM/M06-2X/B calculations for the donor acceptor complex and its constituent donor- and acceptor-fragment molecules using the solvent parameter of toluene.

Table S5. Calculated SCF energies E(SCF) and Gibbs free energies $G^{\text{T}}(\text{solv})$ in toluene at different temperatures T, which are pertinent for the calculation of the inversion processes found experimentally in compounds **2**, **2a**, **6**, and **6a** (PCM/M06-2X/B at p=23.71 MPa).

Cpd	E(SCF) [H/particle]	T [K]	$G^{\text{T}}(\text{solv})$ [H/particle]
2	-5610.02831	269	-5609.37754
2a	-9185.17667	348	-9184.57681
3	-5031.10093	269	-5030.62828
		293	-5030.63902
3a	-8606.24663	348	-8605.81549
		391	-8605.83864
6	-5414.42985	293	-5413.80875
6a	-8989.58055	391	-8989.01884
2(TS)	-5610.00270	269	-5609.35639
2a(TS)	-9185.14376	348	-9184.54795
6(TS)	-5414.41139	293	-5413.78568
6a(TS)	-8989.55361	391	-8988.98808
NHC^{Me}	-328.25970	293	-383.12396
		391	-383.13874
PEt₃	-578.87786	348	-578.73547
		269	-578.72390

4. References:

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