

SUPPORTING INFORMATION

Theoretical Investigations toward the [3+2]-Dipolar Cycloaddition of Nitrones with Vinyldiazoacetates Catalyzed by $\text{Rh}_2(R\text{-TPCP})_4$: Mechanism and Enantioselectivity

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Table of Contents

1. Computational Details	2
Coordinates of all Stationary Points and Computed Energies	3
Catalyst Configuration	3
2.2. Vinylogous Reactivity vs. Carbenoid Reactivity	9
2.3. C=C-C=N2 <i>s-trans</i> Vinylcarbenoid 2-II and Aryl Nitron 3a	35
2.4. C=C-C=N2 <i>s-trans</i> Vinylcarbenoid 2-II and Styryl Nitron 3b	83
3. Computed Energies	128
4. Functional Effects and Basis Set effects	130
5. Solvent Effects	131

1. Computational Details

All calculations were performed with Gaussian'09 software package. The geometries optimization of all the equilibriums and transition states involving rhodium system were performed by ONIOM methodology, the substrates and dirhodium(II) carboxylates were in the high level layer using DFT/B3LYP method of theory that including the LANL2DZ basis set (aliased as [Rh-LA2] in following) on Rh and 6-31G(d) basis set on smaller atoms. The ligands including adamantly variants and pathalimidos were in the low level layer and performed by semiempirical PM6. Heavy-atom basis set definitions and corresponding pseudopotential parameters were obtained from the EMSL basis set exchange library. At the ONIOM-optimized geometries, vibrational frequencies were calculated to identify whether the optimized geometries is equilibrium or transition state, and to evaluate the zero-point vibration energy (ZPE), as well as to obtain the thermal corrections to the Gibbs free energy (298.15K and 1 atm). The solvent energies for certain important structures were calculated by single point calculations on the optimized structures with ONIOM(B3LYP/6-311+G(d,p)[Rh-LA2]:PM6). All of the relative energies discussed in main text are Gibbs free energies in *n*-pentane with thermal corrections, unless otherwise stated.

2. Coordinates of all Stationary Points and Computed Energies

2.1. Catalysis configuration

Catalyst Rh₂(*R*-TPCP)₄ with *C*₄ symmetry

Sum of electronic and zero-point Energies= -973.821306
 Sum of electronic and thermal Energies= -973.734976
 Sum of electronic and thermal Enthalpies= -973.734032
 Sum of electronic and thermal Free Energies= -973.957564

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.558098	4.309166	3.888069
2	6	0	3.237161	5.198447	3.046165
3	6	0	3.747475	4.753828	1.826572
4	6	0	3.581363	3.411133	1.432597
5	6	0	2.896707	2.528352	2.272906
6	6	0	2.387340	2.979383	3.497161
7	6	0	7.942245	3.898939	-0.029061
8	6	0	8.497987	2.954320	0.838232
9	6	0	7.670360	2.021929	1.473675
10	6	0	6.293330	2.032512	1.242458
11	6	0	5.734324	2.975273	0.364337
12	6	0	6.564079	3.912900	-0.266045
13	6	0	5.073954	1.478419	-2.948541
14	6	0	6.042475	0.710785	-3.601456
15	6	0	6.625616	-0.383857	-2.955476
16	6	0	6.226481	-0.717385	-1.657416
17	6	0	5.257362	0.045044	-0.999711
18	6	0	4.687581	1.157429	-1.637604
19	6	0	4.242162	2.993076	0.152759
20	6	0	3.680038	2.005482	-0.912496
21	6	0	3.668055	3.508334	-1.157631
22	6	0	2.327261	1.288022	-0.857586
23	8	0	1.877922	0.919221	0.273605
24	8	0	1.770414	1.102253	-1.983677
25	45	0	-0.000018	0.000063	0.350491
26	45	0	0.000014	-0.000063	-2.052456
27	6	0	5.694859	-1.491248	2.419550
28	6	0	6.287128	-2.419477	1.554571
29	6	0	5.490742	-3.205355	0.721494
30	6	0	4.088232	-3.071903	0.743215
31	6	0	3.501452	-2.134854	1.599747
32	6	0	4.305512	-1.349310	2.435358
33	6	0	4.378521	-7.642480	0.366829
34	6	0	3.711707	-7.974132	1.549865
35	6	0	2.907044	-7.022319	2.185565
36	6	0	2.767703	-5.743642	1.641041
37	6	0	3.430823	-5.411972	0.449266
38	6	0	4.241573	-6.364706	-0.184047
39	6	0	0.926826	-5.694319	-1.995771
40	6	0	-0.010851	-6.731702	-2.012797
41	6	0	-0.932687	-6.864806	-0.970511
42	6	0	-0.924954	-5.947436	0.086019

43	6	0	0.005221	-4.906478	0.106281
44	6	0	0.947601	-4.784009	-0.928860
45	6	0	3.299965	-4.019753	-0.110686
46	6	0	1.974634	-3.691403	-0.859712
47	6	0	3.287044	-3.818138	-1.617962
48	6	0	1.286893	-2.323141	-0.845214
49	8	0	0.919943	-1.870742	0.287173
50	8	0	1.102563	-1.776687	-1.974138
51	6	0	-5.694872	1.491444	2.419475
52	6	0	-6.287142	2.419731	1.554559
53	6	0	-5.490768	3.205535	0.721402
54	6	0	-4.088265	3.071963	0.742986
55	6	0	-3.501488	2.134862	1.599461
56	6	0	-4.305537	1.349379	2.435142
57	6	0	-4.378446	7.642552	0.366227
58	6	0	-3.711681	7.974245	1.549278
59	6	0	-2.907094	7.022435	2.185078
60	6	0	-2.767781	5.743719	1.640637
61	6	0	-3.430852	5.412007	0.448846
62	6	0	-4.241526	6.364739	-0.184566
63	6	0	-0.926907	5.694149	-1.996357
64	6	0	0.010731	6.731567	-2.013476
65	6	0	0.932502	6.864854	-0.971157
66	6	0	0.924749	5.947630	0.085501
67	6	0	-0.005383	4.906636	0.105854
68	6	0	-0.947705	4.783989	-0.929319
69	6	0	-3.300016	4.019745	-0.111009
70	6	0	-1.974706	3.691359	-0.860060
71	6	0	-3.287145	3.818010	-1.618270
72	6	0	-1.286920	2.323124	-0.845465
73	8	0	-0.919969	1.870842	0.286972
74	8	0	-1.102555	1.776574	-1.974333
75	6	0	-2.557867	-4.310028	3.887841
76	6	0	-3.237721	-5.198914	3.046150
77	6	0	-3.748097	-4.754012	1.826691
78	6	0	-3.581279	-3.411420	1.432626
79	6	0	-2.895846	-2.529056	2.272719
80	6	0	-2.386406	-2.980365	3.496844
81	6	0	-7.942399	-3.898194	-0.028969
82	6	0	-8.497891	-2.953771	0.838695
83	6	0	-7.670034	-2.021759	1.474397
84	6	0	-6.293025	-2.032530	1.243071
85	6	0	-5.734267	-2.975098	0.364583
86	6	0	-6.564253	-3.912342	-0.266063
87	6	0	-5.073823	-1.478227	-2.948430
88	6	0	-6.042345	-0.710567	-3.601312
89	6	0	-6.625620	0.383936	-2.955216
90	6	0	-6.226619	0.717300	-1.657074
91	6	0	-5.257501	-0.045159	-0.999401
92	6	0	-4.687588	-1.157406	-1.637409
93	6	0	-4.242119	-2.993090	0.152899
94	6	0	-3.680026	-2.005497	-0.912358
95	6	0	-3.668145	-3.508341	-1.157556
96	6	0	-2.327252	-1.288049	-0.857545
97	8	0	-1.877963	-0.919082	0.273618
98	8	0	-1.770377	-1.102407	-1.983636
99	1	0	2.165676	4.654057	4.842083

100	1	0	3.373176	6.235312	3.347299
101	1	0	4.289898	5.441538	1.178984
102	1	0	2.731050	1.485322	1.964487
103	1	0	1.852529	2.285272	4.143480
104	1	0	8.582896	4.626809	-0.523488
105	1	0	9.570441	2.943787	1.019310
106	1	0	8.100333	1.286084	2.150533
107	1	0	5.648018	1.309295	1.741966
108	1	0	6.140477	4.653696	-0.941176
109	1	0	4.610596	2.318987	-3.463167
110	1	0	6.341105	0.966680	-4.616280
111	1	0	7.385061	-0.974900	-3.462184
112	1	0	6.671773	-1.572727	-1.150745
113	1	0	4.947049	-0.225094	0.011815
114	1	0	4.318725	3.934063	-1.919900
115	1	0	2.712811	4.039687	-1.141016
116	1	0	6.315169	-0.886603	3.077701
117	1	0	7.369537	-2.532438	1.537284
118	1	0	5.951565	-3.938066	0.060139
119	1	0	2.408369	-1.995209	1.613703
120	1	0	3.837958	-0.624781	3.101310
121	1	0	5.006859	-8.380372	-0.128438
122	1	0	3.818188	-8.969396	1.975683
123	1	0	2.387329	-7.277670	3.107393
124	1	0	2.143253	-5.000709	2.136875
125	1	0	4.766909	-6.113379	-1.102949
126	1	0	1.638334	-5.594968	-2.814231
127	1	0	-0.019001	-7.438161	-2.840875
128	1	0	-1.653904	-7.678939	-0.980419
129	1	0	-1.644717	-6.042410	0.899635
130	1	0	0.000012	-4.177348	0.921818
131	1	0	3.443037	-4.659793	-2.290860
132	1	0	3.736066	-2.914023	-2.037050
133	1	0	-6.315172	0.886849	3.077681
134	1	0	-7.369542	2.532794	1.537382
135	1	0	-5.951593	3.938282	0.060087
136	1	0	-2.408412	1.995118	1.613326
137	1	0	-3.837979	0.624792	3.101028
138	1	0	-5.006725	8.380442	-0.129118
139	1	0	-3.818141	8.969540	1.975031
140	1	0	-2.387419	7.277816	3.106919
141	1	0	-2.143393	5.000787	2.136549
142	1	0	-4.766826	6.113382	-1.103481
143	1	0	-1.638364	5.594653	-2.814843
144	1	0	0.018899	7.437911	-2.841653
145	1	0	1.653684	7.679017	-0.981138
146	1	0	1.644455	6.042751	0.899147
147	1	0	-0.000188	4.177614	0.921489
148	1	0	-3.443179	4.659605	-2.291233
149	1	0	-3.736170	2.913852	-2.037264
150	1	0	-2.165386	-4.655137	4.841752
151	1	0	-3.374294	-6.235686	3.347352
152	1	0	-4.291116	-5.441413	1.179271
153	1	0	-2.729618	-1.486118	1.964243
154	1	0	-1.850983	-2.286559	4.142984
155	1	0	-8.583229	-4.625765	-0.523605
156	1	0	-9.570329	-2.943091	1.019859

157	1	0	-8.099813	-1.286067	2.151545
158	1	0	-5.647532	-1.309614	1.742783
159	1	0	-6.140851	-4.652978	-0.941494
160	1	0	-4.610350	-2.318677	-3.463144
161	1	0	-6.340868	-0.966329	-4.616201
162	1	0	-7.385067	0.974998	-3.461900
163	1	0	-6.672013	1.572536	-1.150312
164	1	0	-4.947296	0.224846	0.012194
165	1	0	-4.318873	-3.934018	-1.919803
166	1	0	-2.712929	-4.039747	-1.141002

Catalyst Rh₂(R-TPCP)₄ with D₂ symmetry

Sum of electronic and zero-point Energies=	-973.658522
Sum of electronic and thermal Energies=	-973.584933
Sum of electronic and thermal Enthalpies=	-973.583988
Sum of electronic and thermal Free Energies=	-973.768310

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.656197	4.516189	-3.355634
2	6	0	0.657547	5.250390	-2.168845
3	6	0	-0.394450	5.119060	-1.261309
4	6	0	-1.461670	4.253321	-1.523758
5	6	0	-1.477810	3.562727	-2.740622
6	6	0	-0.418198	3.673569	-3.642973
7	6	0	-4.882868	7.198935	-0.632162
8	6	0	-5.801367	6.851348	-1.623360
9	6	0	-5.660424	5.636107	-2.294418
10	6	0	-4.620061	4.768097	-1.957251
11	6	0	-3.722501	5.078479	-0.929341
12	6	0	-3.846721	6.323802	-0.300750
13	6	0	-4.852782	2.570483	1.706421
14	6	0	-6.163769	2.152794	1.945076
15	6	0	-6.924213	1.605616	0.910717
16	6	0	-6.363594	1.472043	-0.360048
17	6	0	-5.053270	1.894354	-0.590108
18	6	0	-4.289559	2.472229	0.429273
19	6	0	-2.603403	4.158298	-0.578683
20	6	0	-2.879944	2.860684	0.161885
21	6	0	-2.285248	4.038557	0.894561
22	6	0	-1.961464	1.688089	0.109082
23	8	0	-1.841712	1.061452	-0.992977
24	8	0	-1.781283	1.104483	1.226439
25	45	0	-0.044407	0.031694	-1.181893
26	45	0	0.006574	0.054922	1.356691
27	6	0	-2.891124	-1.042895	5.045881
28	6	0	-2.616811	-2.407956	4.948095
29	6	0	-2.877614	-3.090146	3.758284
30	6	0	-3.394602	-2.415339	2.647097
31	6	0	-3.699579	-1.055508	2.767397
32	6	0	-3.442287	-0.368560	3.955235
33	6	0	-6.865681	-5.175409	1.526509
34	6	0	-7.811399	-4.262843	1.056686
35	6	0	-7.409147	-2.972395	0.709507
36	6	0	-6.066181	-2.607142	0.818285
37	6	0	-5.099509	-3.525594	1.243932
38	6	0	-5.524082	-4.802896	1.628828
39	6	0	-3.658336	-3.967159	-1.997028

40	6	0	-4.336386	-3.908379	-3.216736
41	6	0	-4.936758	-2.718555	-3.630940
42	6	0	-4.851777	-1.586582	-2.819699
43	6	0	-4.170845	-1.656529	-1.603954
44	6	0	-3.576185	-2.844309	-1.166601
45	6	0	-3.668419	-3.133017	1.377411
46	6	0	-2.843255	-2.840548	0.131290
47	6	0	-2.645696	-4.133199	0.886302
48	6	0	-1.649811	-1.928665	0.145229
49	8	0	-1.059429	-1.771202	-0.968124
50	8	0	-1.028433	-1.741781	1.236954
51	6	0	2.816149	1.271382	4.975386
52	6	0	2.549827	2.629456	4.794207
53	6	0	2.850176	3.246465	3.577987
54	6	0	3.400737	2.510877	2.523305
55	6	0	3.694120	1.157747	2.726575
56	6	0	3.397343	0.536554	3.940988
57	6	0	6.971586	5.101323	1.401983
58	6	0	7.901928	4.151360	0.978075
59	6	0	7.470807	2.865839	0.648048
60	6	0	6.115580	2.541295	0.729223
61	6	0	5.165791	3.496177	1.109332
62	6	0	5.616980	4.769868	1.475660
63	6	0	3.968328	3.628109	-2.176565
64	6	0	4.684279	3.375698	-3.349045
65	6	0	5.139003	2.087209	-3.632984
66	6	0	4.879629	1.054054	-2.732384
67	6	0	4.162975	1.319680	-1.565255
68	6	0	3.687490	2.601154	-1.268890
69	6	0	3.720884	3.150802	1.223356
70	6	0	2.906834	2.791387	-0.012902
71	6	0	2.759832	4.152424	0.624247
72	6	0	1.648014	1.971770	0.047689
73	8	0	1.019893	1.813503	-1.044701
74	8	0	1.037802	1.844569	1.154197
75	6	0	0.132143	-3.542631	-4.385720
76	6	0	-0.308090	-4.385901	-3.364907
77	6	0	0.454357	-4.547313	-2.206271
78	6	0	1.668391	-3.868753	-2.051463
79	6	0	2.125251	-3.068085	-3.105212
80	6	0	1.357961	-2.888688	-4.257573
81	6	0	4.358276	-7.368440	-0.750291
82	6	0	5.559185	-7.043370	-1.382227
83	6	0	5.751508	-5.748709	-1.865416
84	6	0	4.756855	-4.783906	-1.694905
85	6	0	3.570519	-5.078096	-1.013794
86	6	0	3.371210	-6.395310	-0.581211
87	6	0	4.229942	-2.994695	2.126246
88	6	0	5.470285	-2.750977	2.720126
89	6	0	6.506080	-2.183962	1.976025
90	6	0	6.292650	-1.855453	0.636812
91	6	0	5.051019	-2.106049	0.051273
92	6	0	4.014148	-2.703529	0.774692
93	6	0	2.501522	-4.053558	-0.834850
94	6	0	2.687594	-2.892146	0.130375
95	6	0	1.824698	-4.067671	0.516859
96	6	0	1.910279	-1.619839	0.063979
97	8	0	1.738060	-1.031993	-1.048530
98	8	0	1.781307	-1.009402	1.170158
99	1	0	1.485781	4.619996	-4.073288
100	1	0	1.483246	5.946359	-1.950701
101	1	0	-0.382772	5.723398	-0.340284
102	1	0	-2.332771	2.918565	-2.999952
103	1	0	-0.438380	3.110018	-4.589761
104	1	0	-4.967607	8.171597	-0.120810
105	1	0	-6.615290	7.543275	-1.892885

106	1	0	-6.361469	5.369048	-3.101969
107	1	0	-4.511059	3.833546	-2.526850
108	1	0	-3.117174	6.637135	0.463078
109	1	0	-4.260782	2.957448	2.550177
110	1	0	-6.589843	2.231583	2.958484
111	1	0	-7.951306	1.255681	1.102263
112	1	0	-6.944936	1.010311	-1.174556
113	1	0	-4.610492	1.745707	-1.587662
114	1	0	-2.906565	4.569319	1.610377
115	1	0	-1.240373	3.970222	1.192110
116	1	0	-2.683225	-0.502537	5.983312
117	1	0	-2.196636	-2.948807	5.811482
118	1	0	-2.667315	-4.170098	3.703740
119	1	0	-4.130402	-0.512247	1.911981
120	1	0	-3.668210	0.706957	4.030611
121	1	0	-7.181405	-6.186832	1.829817
122	1	0	-8.871944	-4.551948	0.982898
123	1	0	-8.153681	-2.236640	0.364310
124	1	0	-5.782066	-1.573887	0.569742
125	1	0	-4.799726	-5.530541	2.028668
126	1	0	-3.177322	-4.915463	-1.715065
127	1	0	-4.385896	-4.801285	-3.861019
128	1	0	-5.463600	-2.669921	-4.597296
129	1	0	-5.312020	-0.638313	-3.140571
130	1	0	-4.094289	-0.758441	-0.973857
131	1	0	-3.004410	-5.064125	0.459556
132	1	0	-1.718673	-4.251581	1.442246
133	1	0	2.576833	0.783244	5.933805
134	1	0	2.104156	3.216932	5.613116
135	1	0	2.645052	4.321852	3.456775
136	1	0	4.148084	0.563718	1.917728
137	1	0	3.615665	-0.534206	4.080543
138	1	0	7.309382	6.108919	1.693979
139	1	0	8.972760	4.406666	0.929080
140	1	0	8.202209	2.100759	0.341376
141	1	0	5.809313	1.510230	0.498862
142	1	0	4.903395	5.526237	1.840510
143	1	0	3.627442	4.655960	-1.992192
144	1	0	4.887550	4.196675	-4.055904
145	1	0	5.700870	1.887226	-4.559462
146	1	0	5.238120	0.033122	-2.940680
147	1	0	3.969602	0.504149	-0.854022
148	1	0	3.169302	5.022735	0.121486
149	1	0	1.829960	4.362212	1.148668
150	1	0	-0.474243	-3.411989	-5.296295
151	1	0	-1.257143	-4.931942	-3.481480
152	1	0	0.091505	-5.225474	-1.417404
153	1	0	3.094149	-2.549460	-3.025127
154	1	0	1.722404	-2.236034	-5.067360
155	1	0	4.185037	-8.397497	-0.395909
156	1	0	6.338129	-7.809912	-1.522683
157	1	0	6.682910	-5.492126	-2.395994
158	1	0	4.922068	-3.783209	-2.119356
159	1	0	2.421470	-6.686407	-0.104380
160	1	0	3.414988	-3.396142	2.748484
161	1	0	5.623566	-2.979699	3.787354
162	1	0	7.477915	-1.971069	2.449486
163	1	0	7.093570	-1.379058	0.048508
164	1	0	4.884291	-1.810182	-0.995574
165	1	0	2.192650	-4.741061	1.286201
166	1	0	0.748387	-3.917982	0.550234

2.2. Vinylogous reactivity vs. carbenoid reactivity

Rh2 complex and C=C-C=N2 *s-cis* vinyl diazoacetate **1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.042582	-3.567988	-4.726435
2	6	0	3.948402	-4.319383	-3.967329
3	6	0	4.419510	-3.824282	-2.751801
4	6	0	3.987517	-2.568743	-2.277729
5	6	0	3.080600	-1.824470	-3.036658
6	6	0	2.610290	-2.326098	-4.257230
7	6	0	8.421079	-2.252288	-0.919602
8	6	0	8.758665	-1.230289	-1.810954
9	6	0	7.748251	-0.486027	-2.430258
10	6	0	6.406611	-0.760949	-2.158745
11	6	0	6.065230	-1.781944	-1.256271
12	6	0	7.078819	-2.530688	-0.642469
13	6	0	5.163846	-0.570137	2.206276
14	6	0	5.999558	0.310814	2.896758
15	6	0	6.453175	1.479722	2.276498
16	6	0	6.053909	1.771735	0.968665
17	6	0	5.217140	0.893861	0.273632
18	6	0	4.783544	-0.292177	0.883907
19	6	0	4.610159	-2.081812	-1.002294
20	6	0	3.920790	-1.263864	0.128038
21	6	0	4.185530	-2.753636	0.295877
22	6	0	2.461642	-0.787471	0.147616
23	8	0	1.924998	-0.425905	-0.939406
24	8	0	1.925555	-0.781768	1.301835
25	45	0	-0.103563	0.157072	-0.928130
26	45	0	-0.012015	0.006731	1.513336
27	6	0	5.186967	2.656734	-3.022037
28	6	0	5.657003	3.623990	-2.125249
29	6	0	4.780947	4.219677	-1.217938
30	6	0	3.419521	3.855988	-1.196718
31	6	0	2.957714	2.878056	-2.083481
32	6	0	3.841526	2.283412	-2.993220
33	6	0	3.031830	8.383092	-0.560979
34	6	0	2.261360	8.674825	-1.690339
35	6	0	1.572535	7.649150	-2.346983
36	6	0	1.652266	6.336305	-1.876991
37	6	0	2.420393	6.043448	-0.739317
38	6	0	3.114189	7.071099	-0.084635
39	6	0	0.019054	5.839485	1.751403
40	6	0	-1.066965	6.714918	1.850740
41	6	0	-2.060551	6.718799	0.867664
42	6	0	-1.972934	5.833716	-0.212602
43	6	0	-0.894146	4.953577	-0.314614
44	6	0	0.116989	4.961861	0.661520
45	6	0	2.527121	4.618380	-0.262748
46	6	0	1.296195	4.047454	0.501517
47	6	0	2.600757	4.332341	1.229218
48	6	0	0.828235	2.590116	0.412546
49	8	0	0.484347	2.164087	-0.730186

50	8	0	0.788893	1.952829	1.510832
51	6	0	-5.523073	-2.070284	-2.981691
52	6	0	-5.944727	-3.132137	-2.172241
53	6	0	-5.017853	-3.833470	-1.401098
54	6	0	-3.653630	-3.481171	-1.429844
55	6	0	-3.239427	-2.409551	-2.227470
56	6	0	-4.173965	-1.709706	-3.001418
57	6	0	-3.307069	-8.046239	-1.348938
58	6	0	-2.591753	-8.221296	-2.537234
59	6	0	-1.909730	-7.139628	-3.105084
60	6	0	-1.941303	-5.886866	-2.488153
61	6	0	-2.654403	-5.711672	-1.292154
62	6	0	-3.341086	-6.795182	-0.725699
63	6	0	-0.139164	-5.881462	0.944548
64	6	0	0.938792	-6.767643	0.857436
65	6	0	1.916039	-6.592662	-0.126496
66	6	0	1.817270	-5.520884	-1.020446
67	6	0	0.745630	-4.630111	-0.935636
68	6	0	-0.246441	-4.811167	0.043218
69	6	0	-2.710239	-4.349040	-0.651787
70	6	0	-1.419642	-3.876427	0.082734
71	6	0	-2.674135	-4.237737	0.863751
72	6	0	-0.946222	-2.419013	0.143382
73	8	0	-0.684479	-1.852564	-0.963513
74	8	0	-0.819945	-1.927505	1.305168
75	6	0	-3.387897	4.210413	-4.121302
76	6	0	-4.200635	4.913579	-3.223504
77	6	0	-4.604683	4.314185	-2.030833
78	6	0	-4.197204	3.001286	-1.719043
79	6	0	-3.381301	2.305527	-2.615485
80	6	0	-2.978922	2.911486	-3.812633
81	6	0	-8.541210	2.706557	-0.170339
82	6	0	-8.962623	1.732309	-1.079487
83	6	0	-8.014508	0.975668	-1.777207
84	6	0	-6.651100	1.190913	-1.566523
85	6	0	-6.225907	2.163355	-0.646780
86	6	0	-7.176970	2.924905	0.046404
87	6	0	-5.263579	0.610902	2.557730
88	6	0	-6.082722	-0.334710	3.180832
89	6	0	-6.496832	-1.474495	2.484400
90	6	0	-6.077357	-1.672619	1.165179
91	6	0	-5.257064	-0.731612	0.537034
92	6	0	-4.858910	0.423828	1.226414
93	6	0	-4.750146	2.404409	-0.458655
94	6	0	-4.014777	1.457902	0.535605
95	6	0	-4.229456	2.927268	0.871591
96	6	0	-2.567410	0.962900	0.410919
97	8	0	-2.108629	0.728310	-0.748644
98	8	0	-1.957866	0.814361	1.514140
99	1	0	2.678045	-3.951694	-5.676706
100	1	0	4.289429	-5.287108	-4.329745
101	1	0	5.136093	-4.401964	-2.169393
102	1	0	2.709803	-0.854028	-2.669795
103	1	0	1.899024	-1.740178	-4.837850
104	1	0	9.204238	-2.834526	-0.437713
105	1	0	9.803177	-1.014068	-2.023683
106	1	0	8.008200	0.308993	-3.126686

107	1	0	5.619148	-0.185600	-2.647045
108	1	0	6.826502	-3.329715	0.051598
109	1	0	4.786952	-1.470979	2.702637
110	1	0	6.295066	0.088337	3.919922
111	1	0	7.110267	2.161176	2.811864
112	1	0	6.393872	2.685919	0.483212
113	1	0	4.902581	1.132885	-0.744713
114	1	0	4.931394	-3.090657	1.013144
115	1	0	3.342241	-3.448038	0.271292
116	1	0	5.867112	2.201617	-3.738585
117	1	0	6.705117	3.916280	-2.141524
118	1	0	5.145012	4.982338	-0.530839
119	1	0	1.903142	2.554015	-2.066965
120	1	0	3.469152	1.524988	-3.681376
121	1	0	3.570341	9.178779	-0.049893
122	1	0	2.197591	9.696332	-2.058461
123	1	0	0.972211	7.873369	-3.227022
124	1	0	1.117567	5.535878	-2.388647
125	1	0	3.719180	6.851342	0.792251
126	1	0	0.789359	5.844575	2.520710
127	1	0	-1.133710	7.398449	2.694966
128	1	0	-2.898298	7.408511	0.940604
129	1	0	-2.745910	5.829251	-0.982130
130	1	0	-0.833856	4.248148	-1.150140
131	1	0	2.652649	5.149177	1.946855
132	1	0	3.197952	3.485923	1.578354
133	1	0	-6.243452	-1.531856	-3.593600
134	1	0	-6.995429	-3.414651	-2.150131
135	1	0	-5.345256	-4.668821	-0.783583
136	1	0	-2.182142	-2.094662	-2.243322
137	1	0	-3.838945	-0.879025	-3.621978
138	1	0	-3.840145	-8.885514	-0.906484
139	1	0	-2.565566	-9.195688	-3.019748
140	1	0	-1.352024	-7.273210	-4.030352
141	1	0	-1.410343	-5.042986	-2.928956
142	1	0	-3.902918	-6.665359	0.196794
143	1	0	-0.899501	-6.028315	1.711205
144	1	0	1.009968	-7.600689	1.554084
145	1	0	2.747565	-7.289570	-0.200706
146	1	0	2.574686	-5.379512	-1.792644
147	1	0	0.674570	-3.784736	-1.629380
148	1	0	-2.685309	-5.129881	1.487905
149	1	0	-3.228759	-3.432504	1.354059
150	1	0	-3.077076	4.675233	-5.054153
151	1	0	-4.522711	5.925569	-3.460323
152	1	0	-5.250601	4.855202	-1.340640
153	1	0	-3.027582	1.290453	-2.374590
154	1	0	-2.339025	2.362136	-4.501655
155	1	0	-9.275997	3.298141	0.372347
156	1	0	-10.024078	1.562571	-1.244893
157	1	0	-8.339749	0.217029	-2.486573
158	1	0	-5.911916	0.605005	-2.114090
159	1	0	-6.858479	3.687280	0.754142
160	1	0	-4.930056	1.488120	3.109345
161	1	0	-6.397151	-0.183297	4.211378
162	1	0	-7.139654	-2.205901	2.968680
163	1	0	-6.389730	-2.561999	0.619171

164	1	0	-4.927728	-0.896591	-0.491265
165	1	0	-4.919296	3.202163	1.667198
166	1	0	-3.368463	3.600604	0.869672
167	6	0	-2.605284	2.479927	5.163567
168	6	0	-1.296270	1.885681	4.733708
169	6	0	-1.137139	0.603286	4.389438
170	6	0	0.104220	-0.052308	3.913099
171	6	0	0.283727	-1.520579	4.221230
172	7	0	1.243553	0.671156	4.051763
173	7	0	2.161935	1.317414	4.111016
174	8	0	1.581535	-1.842189	4.264057
175	6	0	2.039296	-3.251858	4.339457
176	6	0	1.551194	-3.997718	3.098290
177	6	0	1.556434	-3.889701	5.646142
178	6	0	3.562034	-3.099171	4.335173
179	8	0	-0.667395	-2.247571	4.402091
180	1	0	-2.528840	2.939186	6.158022
181	1	0	-3.396982	1.724580	5.193074
182	1	0	-2.916053	3.273370	4.470172
183	1	0	-0.451417	2.574297	4.684639
184	1	0	-1.968700	-0.095964	4.404673
185	1	0	1.969797	-5.010470	3.084374
186	1	0	1.873454	-3.475559	2.191503
187	1	0	0.461524	-4.071640	3.078805
188	1	0	2.009219	-4.881919	5.752190
189	1	0	0.470832	-3.995647	5.657274
190	1	0	1.863355	-3.283466	6.505333
191	1	0	4.035340	-4.086314	4.336237
192	1	0	3.899509	-2.551800	5.221373
193	1	0	3.890772	-2.549797	3.440084

TS 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.045612	-3.576467	-4.687862
2	6	0	4.018981	-4.262389	-3.950362
3	6	0	4.494821	-3.726051	-2.754696
4	6	0	4.001090	-2.493784	-2.277880
5	6	0	3.028122	-1.815303	-3.015538
6	6	0	2.552612	-2.358607	-4.216502
7	6	0	8.442350	-2.014428	-0.999386
8	6	0	8.731132	-0.981495	-1.895296
9	6	0	7.686596	-0.270854	-2.497315
10	6	0	6.359458	-0.590034	-2.203930
11	6	0	6.067182	-1.621933	-1.296731
12	6	0	7.114790	-2.337064	-0.700244
13	6	0	5.193780	-0.429517	2.169561
14	6	0	6.007583	0.481681	2.846930
15	6	0	6.398780	1.671677	2.224255
16	6	0	5.960842	1.953147	0.926375
17	6	0	5.147494	1.044330	0.243641
18	6	0	4.774948	-0.161061	0.856618
19	6	0	4.627015	-1.967952	-1.019022

20	6	0	3.932326	-1.161114	0.115854
21	6	0	4.241511	-2.641081	0.291010
22	6	0	2.461682	-0.718744	0.146879
23	8	0	1.913708	-0.357795	-0.931946
24	8	0	1.937457	-0.736862	1.307497
25	45	0	-0.141195	0.144763	-0.923703
26	45	0	-0.016308	0.003843	1.555362
27	6	0	5.016033	2.748624	-3.105520
28	6	0	5.477794	3.745610	-2.237259
29	6	0	4.605949	4.330331	-1.319214
30	6	0	3.256867	3.925830	-1.257228
31	6	0	2.804147	2.918971	-2.115399
32	6	0	3.683984	2.335554	-3.036709
33	6	0	2.790072	8.447369	-0.623854
34	6	0	1.975418	8.721092	-1.726380
35	6	0	1.285643	7.680307	-2.357847
36	6	0	1.408311	6.370225	-1.889436
37	6	0	2.221136	6.095429	-0.778650
38	6	0	2.915631	7.138197	-0.149126
39	6	0	-0.080829	5.858262	1.788248
40	6	0	-1.181149	6.708759	1.934061
41	6	0	-2.221043	6.680524	1.000575
42	6	0	-2.163191	5.790007	-0.077151
43	6	0	-1.069618	4.935047	-0.225706
44	6	0	-0.014213	4.973328	0.701527
45	6	0	2.371300	4.673821	-0.304506
46	6	0	1.175040	4.081619	0.496434
47	6	0	2.495865	4.388978	1.185025
48	6	0	0.729835	2.615580	0.410635
49	8	0	0.370576	2.184131	-0.720149
50	8	0	0.727599	1.980956	1.514737
51	6	0	-5.416697	-2.217702	-3.023428
52	6	0	-5.810439	-3.320595	-2.255676
53	6	0	-4.874672	-3.996542	-1.473076
54	6	0	-3.528175	-3.579137	-1.447461
55	6	0	-3.143015	-2.468845	-2.205391
56	6	0	-4.086723	-1.793741	-2.990851
57	6	0	-3.034558	-8.135481	-1.375922
58	6	0	-2.297929	-8.278499	-2.555378
59	6	0	-1.646495	-7.170339	-3.108030
60	6	0	-1.729990	-5.923202	-2.484794
61	6	0	-2.464842	-5.779871	-1.297570
62	6	0	-3.120515	-6.890025	-0.746333
63	6	0	-0.003697	-5.898148	1.000716
64	6	0	1.096675	-6.758200	0.932503
65	6	0	2.088353	-6.557335	-0.031801
66	6	0	1.981402	-5.485878	-0.925317
67	6	0	0.887364	-4.621248	-0.859398
68	6	0	-0.118959	-4.828503	0.099767
69	6	0	-2.575632	-4.422643	-0.652594
70	6	0	-1.314976	-3.922548	0.116493
71	6	0	-2.578888	-4.316112	0.864369
72	6	0	-0.876685	-2.453874	0.181938
73	8	0	-0.627265	-1.886965	-0.925366
74	8	0	-0.767443	-1.958729	1.345227
75	6	0	-3.468242	4.363420	-3.900556
76	6	0	-4.394746	4.940578	-3.022912

77	6	0	-4.796812	4.250410	-1.880273
78	6	0	-4.276886	2.969705	-1.597325
79	6	0	-3.351213	2.400325	-2.474911
80	6	0	-2.948723	3.098380	-3.621476
81	6	0	-8.633881	2.401466	-0.157859
82	6	0	-8.992238	1.453058	-1.119768
83	6	0	-7.996973	0.773559	-1.831222
84	6	0	-6.649247	1.040078	-1.582050
85	6	0	-6.287393	1.987148	-0.610027
86	6	0	-7.285540	2.671071	0.097588
87	6	0	-5.339128	0.368169	2.558018
88	6	0	-6.136010	-0.626058	3.132569
89	6	0	-6.493858	-1.756385	2.391172
90	6	0	-6.039997	-1.895737	1.075860
91	6	0	-5.241214	-0.906208	0.496601
92	6	0	-4.899439	0.239572	1.230805
93	6	0	-4.827541	2.282962	-0.381223
94	6	0	-4.078869	1.324844	0.591489
95	6	0	-4.350235	2.770968	0.979967
96	6	0	-2.617098	0.871766	0.460630
97	8	0	-2.172017	0.623457	-0.698051
98	8	0	-1.990033	0.766385	1.560772
99	1	0	2.676007	-3.992480	-5.622373
100	1	0	4.407548	-5.211365	-4.314102
101	1	0	5.262331	-4.253175	-2.189629
102	1	0	2.606355	-0.863281	-2.650260
103	1	0	1.787942	-1.823250	-4.778451
104	1	0	9.252172	-2.570980	-0.531601
105	1	0	9.764200	-0.731082	-2.125413
106	1	0	7.908508	0.532244	-3.197637
107	1	0	5.544807	-0.041733	-2.679022
108	1	0	6.900179	-3.144655	-0.003555
109	1	0	4.868928	-1.349968	2.665286
110	1	0	6.339041	0.264070	3.859848
111	1	0	7.040098	2.376256	2.748587
112	1	0	6.253384	2.882382	0.438052
113	1	0	4.803561	1.273458	-0.768210
114	1	0	5.007334	-2.952773	0.998066
115	1	0	3.416713	-3.358096	0.284025
116	1	0	5.692058	2.301740	-3.831105
117	1	0	6.515570	4.069202	-2.284519
118	1	0	4.963225	5.116287	-0.655467
119	1	0	1.760426	2.558926	-2.069813
120	1	0	3.317320	1.553025	-3.701228
121	1	0	3.329631	9.254814	-0.132875
122	1	0	1.878286	9.740318	-2.093501
123	1	0	0.651155	7.890486	-3.217212
124	1	0	0.873008	5.557640	-2.381495
125	1	0	3.555052	6.932363	0.706218
126	1	0	0.728206	5.892786	2.515528
127	1	0	-1.221961	7.400065	2.773369
128	1	0	-3.070632	7.350942	1.108401
129	1	0	-2.971341	5.762095	-0.809912
130	1	0	-1.032022	4.227075	-1.061547
131	1	0	2.555499	5.207194	1.900021
132	1	0	3.120720	3.554148	1.511229
133	1	0	-6.143305	-1.697070	-3.642920

134	1	0	-6.845873	-3.654305	-2.275102
135	1	0	-5.180690	-4.862830	-0.888136
136	1	0	-2.101532	-2.097894	-2.184602
137	1	0	-3.771534	-0.930819	-3.577373
138	1	0	-3.543867	-8.995300	-0.945351
139	1	0	-2.231441	-9.248345	-3.042944
140	1	0	-1.072252	-7.278778	-4.026436
141	1	0	-1.223284	-5.058280	-2.913860
142	1	0	-3.698702	-6.785375	0.169119
143	1	0	-0.775290	-6.065376	1.751480
144	1	0	1.173887	-7.591480	1.628009
145	1	0	2.937226	-7.234272	-0.091808
146	1	0	2.749342	-5.324946	-1.683347
147	1	0	0.808720	-3.776479	-1.554016
148	1	0	-2.584316	-5.210359	1.485193
149	1	0	-3.166249	-3.526181	1.341103
150	1	0	-3.156852	4.898957	-4.794411
151	1	0	-4.805629	5.924952	-3.237131
152	1	0	-5.528509	4.694618	-1.206734
153	1	0	-2.910018	1.409359	-2.266734
154	1	0	-2.221146	2.644608	-4.293703
155	1	0	-9.405489	2.932725	0.395819
156	1	0	-10.041289	1.243377	-1.315516
157	1	0	-8.273115	0.034884	-2.581414
158	1	0	-5.873142	0.513972	-2.139665
159	1	0	-7.016194	3.412456	0.846490
160	1	0	-5.051976	1.237488	3.145184
161	1	0	-6.476616	-0.519936	4.160289
162	1	0	-7.119679	-2.525750	2.837231
163	1	0	-6.308435	-2.777247	0.494386
164	1	0	-4.883350	-1.025663	-0.528968
165	1	0	-5.065706	2.991327	1.769286
166	1	0	-3.515438	3.474440	1.015615
167	6	0	-2.339151	2.620288	5.015209
168	6	0	-1.328698	1.870592	4.209170
169	6	0	-0.885426	0.635157	4.508126
170	6	0	0.090353	-0.104388	3.699356
171	6	0	0.374851	-1.501163	4.182134
172	7	0	1.605210	0.708734	3.943624
173	7	0	2.412289	1.456184	3.793331
174	8	0	1.674623	-1.807985	4.196495
175	6	0	2.154389	-3.202572	4.354112
176	6	0	1.634263	-4.035554	3.183157
177	6	0	1.725753	-3.759079	5.715908
178	6	0	3.674055	-3.031641	4.287069
179	8	0	-0.559205	-2.222723	4.469923
180	1	0	-1.921026	3.565633	5.387644
181	1	0	-2.702686	2.038232	5.867265
182	1	0	-3.194854	2.889228	4.381399
183	1	0	-0.931939	2.373602	3.329524
184	1	0	-1.278283	0.108500	5.377291
185	1	0	2.060342	-5.044387	3.225584
186	1	0	1.923770	-3.577058	2.231734
187	1	0	0.545172	-4.116986	3.204328
188	1	0	2.205752	-4.731231	5.875523
189	1	0	0.643910	-3.887697	5.768645
190	1	0	2.043839	-3.088190	6.521427

191	1	0	4.162047	-4.011157	4.317614
192	1	0	4.034988	-2.438395	5.133932
193	1	0	3.962322	-2.520023	3.357009

2-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.299674	-0.036903	-3.613292
2	6	0	-6.187128	-0.901629	-2.960221
3	6	0	-5.701246	-1.856431	-2.068205
4	6	0	-4.317213	-1.963562	-1.815084
5	6	0	-3.437245	-1.092729	-2.463570
6	6	0	-3.930675	-0.134452	-3.359952
7	6	0	-5.555783	-6.441786	-1.552212
8	6	0	-4.909139	-6.835781	-2.726836
9	6	0	-3.935376	-6.007443	-3.296072
10	6	0	-3.607572	-4.791573	-2.692901
11	6	0	-4.250039	-4.398093	-1.507380
12	6	0	-5.230322	-5.225854	-0.942765
13	6	0	-2.171192	-5.027353	1.569788
14	6	0	-1.552055	-6.258002	1.803221
15	6	0	-0.734304	-6.829688	0.823060
16	6	0	-0.524095	-6.158712	-0.386047
17	6	0	-1.141874	-4.928549	-0.625759
18	6	0	-1.985560	-4.367108	0.345303
19	6	0	-3.898317	-3.070084	-0.889724
20	6	0	-2.679446	-3.063681	0.077000
21	6	0	-4.088475	-2.852238	0.606010
22	6	0	-1.669130	-1.913380	0.176525
23	8	0	-1.083162	-1.575236	-0.892271
24	8	0	-1.495970	-1.436359	1.341980
25	45	0	0.152724	0.116512	-0.850123
26	45	0	0.012919	0.014606	1.648124
27	6	0	1.116828	-5.092214	-3.965613
28	6	0	1.830101	-6.021713	-3.197854
29	6	0	2.554034	-5.597494	-2.084995
30	6	0	2.580506	-4.233477	-1.722196
31	6	0	1.863889	-3.312504	-2.489569
32	6	0	1.134272	-3.744148	-3.606149
33	6	0	6.852680	-5.574186	-0.548831
34	6	0	7.535067	-4.795057	-1.487304
35	6	0	6.883906	-3.722265	-2.106568
36	6	0	5.556424	-3.428116	-1.788647
37	6	0	4.871959	-4.205763	-0.840349
38	6	0	5.523679	-5.283397	-0.224860
39	6	0	4.826406	-2.533321	2.420207
40	6	0	5.972307	-1.976094	2.994863
41	6	0	6.707812	-1.010074	2.301445
42	6	0	6.288883	-0.598135	1.032154
43	6	0	5.145386	-1.153070	0.452128
44	6	0	4.412929	-2.133885	1.138820
45	6	0	3.432290	-3.887563	-0.533927
46	6	0	3.198766	-2.749060	0.502549

47	6	0	2.850762	-4.190901	0.839912
48	6	0	2.068744	-1.712535	0.432608
49	8	0	1.844964	-1.149127	-0.673434
50	8	0	1.483435	-1.493486	1.543253
51	6	0	-0.490653	5.569805	-3.615981
52	6	0	-1.337573	6.419826	-2.893186
53	6	0	-2.176801	5.897174	-1.910946
54	6	0	-2.187836	4.512140	-1.635701
55	6	0	-1.337443	3.671385	-2.357309
56	6	0	-0.492344	4.201736	-3.342295
57	6	0	-6.615644	5.680069	-0.850497
58	6	0	-7.138448	5.028173	-1.970708
59	6	0	-6.373274	4.061668	-2.633177
60	6	0	-5.091352	3.747301	-2.177824
61	6	0	-4.567002	4.396834	-1.047945
62	6	0	-5.332910	5.368251	-0.388767
63	6	0	-4.862433	2.402132	2.065682
64	6	0	-6.077323	1.817887	2.434841
65	6	0	-6.760065	0.988717	1.539250
66	6	0	-6.216508	0.734643	0.276082
67	6	0	-5.003862	1.318358	-0.100052
68	6	0	-4.329081	2.170143	0.787638
69	6	0	-3.170650	4.060690	-0.592840
70	6	0	-3.050751	2.839041	0.367226
71	6	0	-2.769733	4.248390	0.864127
72	6	0	-1.905703	1.819607	0.357407
73	8	0	-1.549870	1.345714	-0.761056
74	8	0	-1.438936	1.524181	1.503256
75	6	0	5.814443	0.339139	-2.982435
76	6	0	6.650127	1.132970	-2.186687
77	6	0	6.097811	2.034670	-1.278330
78	6	0	4.697895	2.158720	-1.148954
79	6	0	3.869462	1.359491	-1.941768
80	6	0	4.429572	0.454870	-2.854861
81	6	0	6.111192	6.495384	-0.455266
82	6	0	5.506803	7.065202	-1.579432
83	6	0	4.480185	6.380995	-2.239694
84	6	0	4.058223	5.132160	-1.778493
85	6	0	4.660342	4.561668	-0.645747
86	6	0	5.691947	5.245982	0.012357
87	6	0	2.489514	5.209632	2.080256
88	6	0	1.872469	6.447435	2.285962
89	6	0	0.981540	6.955926	1.336421
90	6	0	0.698560	6.216604	0.182903
91	6	0	1.308831	4.978317	-0.027011
92	6	0	2.219347	4.474125	0.916498
93	6	0	4.212686	3.200544	-0.181877
94	6	0	2.899524	3.161658	0.654182
95	6	0	4.240218	2.858733	1.302932
96	6	0	1.856946	2.040426	0.556240
97	8	0	1.380383	1.805296	-0.589930
98	8	0	1.546848	1.472178	1.652585
99	1	0	-5.676612	0.704792	-4.313640
100	1	0	-7.255442	-0.831490	-3.154113
101	1	0	-6.392589	-2.535758	-1.571035
102	1	0	-2.346592	-1.126736	-2.273772
103	1	0	-3.230522	0.538437	-3.855620

104	1	0	-6.315487	-7.082300	-1.108550
105	1	0	-5.162237	-7.782601	-3.198352
106	1	0	-3.432311	-6.310143	-4.212726
107	1	0	-2.855721	-4.141141	-3.140864
108	1	0	-5.741169	-4.926441	-0.030194
109	1	0	-2.787333	-4.567032	2.348169
110	1	0	-1.706570	-6.771226	2.749840
111	1	0	-0.260618	-7.792212	1.001538
112	1	0	0.125378	-6.590949	-1.147947
113	1	0	-0.962674	-4.397749	-1.564292
114	1	0	-4.556804	-3.621243	1.216928
115	1	0	-4.369756	-1.857174	0.966172
116	1	0	0.554440	-5.420871	-4.836390
117	1	0	1.823267	-7.073960	-3.474188
118	1	0	3.113610	-6.322147	-1.494830
119	1	0	1.840142	-2.238890	-2.223731
120	1	0	0.576098	-3.012847	-4.190603
121	1	0	7.355608	-6.410877	-0.067896
122	1	0	8.568925	-5.022271	-1.737173
123	1	0	7.412427	-3.115259	-2.839381
124	1	0	5.046342	-2.595663	-2.275113
125	1	0	4.998695	-5.897070	0.503957
126	1	0	4.258412	-3.286214	2.964286
127	1	0	6.301142	-2.307169	3.977643
128	1	0	7.606787	-0.586273	2.743214
129	1	0	6.857268	0.154091	0.483883
130	1	0	4.821763	-0.825858	-0.540777
131	1	0	3.433880	-4.728209	1.584472
132	1	0	1.797408	-4.476246	0.908091
133	1	0	0.161943	5.975098	-4.385514
134	1	0	-1.343857	7.487411	-3.102826
135	1	0	-2.840580	6.560578	-1.357213
136	1	0	-1.300604	2.582226	-2.160452
137	1	0	0.166823	3.530943	-3.893132
138	1	0	-7.207643	6.432761	-0.333523
139	1	0	-8.136773	5.270887	-2.327151
140	1	0	-6.777489	3.553293	-3.506466
141	1	0	-4.492391	2.998191	-2.696759
142	1	0	-4.933763	5.881194	0.483903
143	1	0	-4.323990	3.030509	2.775138
144	1	0	-6.491982	2.012693	3.421780
145	1	0	-7.711011	0.544723	1.823172
146	1	0	-6.738281	0.083202	-0.424719
147	1	0	-4.581292	1.113036	-1.087033
148	1	0	-3.450337	4.714689	1.574122
149	1	0	-1.739067	4.531982	1.091318
150	1	0	6.243396	-0.359702	-3.696861
151	1	0	7.730739	1.050591	-2.283305
152	1	0	6.751311	2.661952	-0.673254
153	1	0	2.765196	1.407798	-1.858827
154	1	0	3.767435	-0.161550	-3.463888
155	1	0	6.910601	7.024894	0.059182
156	1	0	5.833005	8.037931	-1.940496
157	1	0	4.007629	6.822434	-3.115464
158	1	0	3.259819	4.596711	-2.293166
159	1	0	6.169214	4.808867	0.886232
160	1	0	3.178123	4.819704	2.826759

161	1	0	2.088969	7.015717	3.188257
162	1	0	0.508546	7.922520	1.494003
163	1	0	-0.000507	6.604318	-0.559348
164	1	0	1.073935	4.394040	-0.922696
165	1	0	4.660261	3.559524	2.021730
166	1	0	4.462078	1.831614	1.595773
167	6	0	3.484520	-0.095466	5.065363
168	6	0	2.316231	-0.071480	4.150525
169	6	0	1.009829	-0.046078	4.560374
170	6	0	-0.076728	-0.079970	3.654633
171	6	0	-1.432777	-0.109011	4.264369
172	8	0	-1.943945	-1.335718	4.295056
173	6	0	-3.363308	-1.596888	4.643867
174	6	0	-4.265173	-0.856826	3.654720
175	6	0	-3.620615	-1.189031	6.098315
176	6	0	-3.471561	-3.113147	4.469972
177	8	0	-1.935121	0.929045	4.656095
178	1	0	4.107404	-0.976545	4.847852
179	1	0	3.204571	-0.098834	6.121685
180	1	0	4.126595	0.773863	4.862921
181	1	0	2.524062	-0.093035	3.086412
182	1	0	0.803625	-0.029308	5.632906
183	1	0	-5.310279	-1.134708	3.829908
184	1	0	-3.999554	-1.123791	2.624452
185	1	0	-4.173707	0.227227	3.762081
186	1	0	-4.630295	-1.498820	6.390488
187	1	0	-3.534269	-0.108559	6.225736
188	1	0	-2.907549	-1.684113	6.766611
189	1	0	-4.497184	-3.439404	4.671426
190	1	0	-2.799924	-3.629765	5.163461
191	1	0	-3.199670	-3.404805	3.445045

TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.160902	0.221129	-3.708035
2	6	0	-6.089398	-0.631634	-3.097380
3	6	0	-5.655817	-1.608666	-2.203006
4	6	0	-4.283914	-1.750148	-1.901822
5	6	0	-3.363281	-0.893343	-2.510654
6	6	0	-3.804149	0.087266	-3.410776
7	6	0	-5.694528	-6.186504	-1.605046
8	6	0	-5.057298	-6.608292	-2.775112
9	6	0	-4.055831	-5.815018	-3.346294
10	6	0	-3.691324	-4.606421	-2.749719
11	6	0	-4.324816	-4.184812	-1.568840
12	6	0	-5.332403	-4.977644	-1.002211
13	6	0	-2.349423	-4.846827	1.595884
14	6	0	-1.806335	-6.105226	1.867897
15	6	0	-1.025949	-6.755738	0.906782
16	6	0	-0.776972	-6.135957	-0.322035
17	6	0	-1.318845	-4.878293	-0.599722
18	6	0	-2.125437	-4.235995	0.352433

19	6	0	-3.931084	-2.865621	-0.958658
20	6	0	-2.740210	-2.901736	0.042624
21	6	0	-4.150677	-2.610873	0.527975
22	6	0	-1.672582	-1.805919	0.152490
23	8	0	-1.064167	-1.489984	-0.909172
24	8	0	-1.480693	-1.344752	1.322791
25	45	0	0.226746	0.168665	-0.863426
26	45	0	0.082957	0.048135	1.631619
27	6	0	0.638767	-5.073102	-3.944447
28	6	0	1.385640	-6.035094	-3.252350
29	6	0	2.194300	-5.653192	-2.183661
30	6	0	2.275410	-4.299766	-1.788007
31	6	0	1.522278	-3.347290	-2.478475
32	6	0	0.708416	-3.736169	-3.552249
33	6	0	6.519307	-5.905423	-0.812507
34	6	0	7.190722	-5.193835	-1.810605
35	6	0	6.569750	-4.098878	-2.422028
36	6	0	5.283466	-3.715525	-2.036932
37	6	0	4.610213	-4.425532	-1.029323
38	6	0	5.231493	-5.525376	-0.421586
39	6	0	4.865694	-2.748218	2.211054
40	6	0	6.079883	-2.271094	2.712964
41	6	0	6.839670	-1.363161	1.969096
42	6	0	6.375783	-0.925626	0.724274
43	6	0	5.162830	-1.398636	0.217359
44	6	0	4.406719	-2.323949	0.953665
45	6	0	3.213276	-4.008988	-0.650068
46	6	0	3.118529	-2.855425	0.392688
47	6	0	2.688429	-4.267973	0.756213
48	6	0	2.061865	-1.743942	0.368145
49	8	0	1.874761	-1.136626	-0.724008
50	8	0	1.488593	-1.522335	1.481772
51	6	0	-0.600900	5.666545	-3.632135
52	6	0	-1.404242	6.506552	-2.850402
53	6	0	-2.207669	5.967282	-1.847054
54	6	0	-2.223532	4.575873	-1.610807
55	6	0	-1.418603	3.743958	-2.392401
56	6	0	-0.609263	4.290947	-3.397531
57	6	0	-6.656200	5.637644	-0.707991
58	6	0	-7.187553	4.988589	-1.825794
59	6	0	-6.414026	4.050006	-2.518056
60	6	0	-5.115439	3.760562	-2.094639
61	6	0	-4.582518	4.406441	-0.966609
62	6	0	-5.356777	5.350365	-0.277988
63	6	0	-4.709409	2.332220	2.161072
64	6	0	-5.891944	1.706281	2.564828
65	6	0	-6.602125	0.899684	1.669732
66	6	0	-6.118001	0.710148	0.371655
67	6	0	-4.937138	1.335022	-0.038629
68	6	0	-4.235917	2.164240	0.849666
69	6	0	-3.169101	4.098821	-0.545978
70	6	0	-2.990098	2.874498	0.399558
71	6	0	-2.738355	4.287496	0.902163
72	6	0	-1.818048	1.886424	0.360256
73	8	0	-1.455546	1.436815	-0.763801
74	8	0	-1.339026	1.584916	1.501484
75	6	0	5.979043	0.478325	-2.961528

76	6	0	6.798951	1.229707	-2.110348
77	6	0	6.229158	2.095871	-1.178027
78	6	0	4.827822	2.228804	-1.085157
79	6	0	4.014399	1.469366	-1.931159
80	6	0	4.591746	0.598365	-2.865190
81	6	0	6.218974	6.545814	-0.296290
82	6	0	5.624219	7.140360	-1.412814
83	6	0	4.602261	6.471713	-2.095804
84	6	0	4.175268	5.213807	-1.664795
85	6	0	4.767493	4.618535	-0.539723
86	6	0	5.794611	5.287278	0.141121
87	6	0	2.538503	5.246388	2.089292
88	6	0	1.901771	6.477056	2.277346
89	6	0	1.001549	6.956840	1.321735
90	6	0	0.729160	6.195887	0.179671
91	6	0	1.358747	4.964545	-0.012350
92	6	0	2.278556	4.488937	0.937432
93	6	0	4.317371	3.247320	-0.107645
94	6	0	2.981441	3.185531	0.690801
95	6	0	4.307489	2.889678	1.372215
96	6	0	1.956003	2.051703	0.566941
97	8	0	1.498029	1.817888	-0.588474
98	8	0	1.634355	1.478170	1.656540
99	1	0	-5.496829	0.980523	-4.410329
100	1	0	-7.148766	-0.533992	-3.325562
101	1	0	-6.379318	-2.278919	-1.740087
102	1	0	-2.279493	-0.953676	-2.287650
103	1	0	-3.071800	0.749119	-3.873981
104	1	0	-6.475353	-6.799851	-1.159614
105	1	0	-5.338974	-7.549579	-3.241526
106	1	0	-3.559815	-6.139562	-4.259300
107	1	0	-2.917295	-3.983464	-3.199157
108	1	0	-5.835548	-4.656839	-0.092580
109	1	0	-2.935219	-4.327759	2.361684
110	1	0	-1.991380	-6.578968	2.829435
111	1	0	-0.611594	-7.739460	1.115010
112	1	0	-0.156798	-6.630271	-1.070509
113	1	0	-1.109945	-4.390724	-1.555788
114	1	0	-4.670071	-3.342773	1.142619
115	1	0	-4.400287	-1.595712	0.848748
116	1	0	0.011241	-5.368060	-4.782017
117	1	0	1.338758	-7.079439	-3.553626
118	1	0	2.779402	-6.404358	-1.653967
119	1	0	1.534235	-2.276836	-2.191058
120	1	0	0.126852	-2.978101	-4.077181
121	1	0	6.998933	-6.758465	-0.336589
122	1	0	8.192756	-5.490111	-2.112281
123	1	0	7.089718	-3.544201	-3.200982
124	1	0	4.796114	-2.866097	-2.516451
125	1	0	4.715221	-6.086290	0.354425
126	1	0	4.276880	-3.451727	2.796445
127	1	0	6.438301	-2.614689	3.680817
128	1	0	7.789006	-0.999716	2.355629
129	1	0	6.959767	-0.212743	0.141263
130	1	0	4.799945	-1.046521	-0.752589
131	1	0	3.273523	-4.844063	1.469725
132	1	0	1.623602	-4.478994	0.883137

133	1	0	0.024229	6.085410	-4.417220
134	1	0	-1.404804	7.579606	-3.030316
135	1	0	-2.838883	6.621737	-1.246908
136	1	0	-1.392699	2.651715	-2.223062
137	1	0	0.017268	3.629045	-3.995006
138	1	0	-7.254399	6.369170	-0.168217
139	1	0	-8.198823	5.212123	-2.157499
140	1	0	-6.824682	3.543918	-3.389707
141	1	0	-4.510241	3.033564	-2.637781
142	1	0	-4.951111	5.861422	0.592799
143	1	0	-4.148056	2.942888	2.868322
144	1	0	-6.261093	1.851821	3.577960
145	1	0	-7.528823	0.423911	1.981165
146	1	0	-6.662194	0.078710	-0.330373
147	1	0	-4.561394	1.179516	-1.053358
148	1	0	-3.415701	4.727511	1.631772
149	1	0	-1.711348	4.599845	1.106838
150	1	0	6.422028	-0.192566	-3.693777
151	1	0	7.881091	1.143035	-2.182437
152	1	0	6.870013	2.687353	-0.525490
153	1	0	2.910523	1.527177	-1.871981
154	1	0	3.942831	0.012839	-3.516756
155	1	0	7.015082	7.062945	0.235537
156	1	0	5.954510	8.120031	-1.750427
157	1	0	4.137384	6.932209	-2.965777
158	1	0	3.380533	4.690430	-2.197058
159	1	0	6.264779	4.830155	1.008775
160	1	0	3.236494	4.879485	2.839290
161	1	0	2.111271	7.062637	3.170229
162	1	0	0.513870	7.918270	1.465096
163	1	0	0.023987	6.561936	-0.567821
164	1	0	1.132746	4.362801	-0.898806
165	1	0	4.701070	3.584681	2.111377
166	1	0	4.525359	1.860661	1.664986
167	6	0	3.407362	-0.908643	5.316239
168	6	0	2.084126	-1.039701	4.623754
169	6	0	1.276854	-0.006303	4.337223
170	6	0	0.042647	-0.090901	3.576902
171	6	0	-1.249212	-0.163290	4.299488
172	8	0	-1.732267	-1.389745	4.398058
173	6	0	-3.112929	-1.660005	4.894283
174	6	0	-4.111087	-0.935801	3.989835
175	6	0	-3.217997	-1.235668	6.361561
176	6	0	-3.224865	-3.177194	4.744288
177	8	0	-1.716446	0.888128	4.700074
178	1	0	3.453830	-1.543020	6.210437
179	1	0	3.609518	0.125227	5.613103
180	1	0	4.218824	-1.236943	4.649782
181	1	0	1.794619	-2.038346	4.302265
182	1	0	1.565892	1.017597	4.591769
183	1	0	-5.129684	-1.248275	4.243610
184	1	0	-3.919119	-1.187211	2.940872
185	1	0	-4.042856	0.149293	4.100632
186	1	0	-4.193259	-1.540086	6.757282
187	1	0	-3.119330	-0.153790	6.467668
188	1	0	-2.440962	-1.724077	6.959243
189	1	0	-4.213143	-3.511353	5.076000

190	1	0	-2.465569	-3.683249	5.349077
191	1	0	-3.085762	-3.473969	3.693721

2-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.852067	-1.325744	-3.999462
2	6	0	5.999359	-0.810767	-3.382354
3	6	0	5.881177	0.167199	-2.396619
4	6	0	4.611788	0.649823	-2.009524
5	6	0	3.471756	0.128735	-2.626012
6	6	0	3.595448	-0.855444	-3.617193
7	6	0	7.257353	4.448776	-1.423618
8	6	0	6.757199	5.128635	-2.537407
9	6	0	5.562974	4.705553	-3.131913
10	6	0	4.870827	3.608906	-2.614657
11	6	0	5.367989	2.928830	-1.490226
12	6	0	6.567502	3.350502	-0.900257
13	6	0	3.753028	3.843006	1.820282
14	6	0	3.633613	5.174578	2.225353
15	6	0	3.092358	6.126775	1.355324
16	6	0	2.655931	5.738581	0.084780
17	6	0	2.773863	4.407783	-0.325678
18	6	0	3.342250	3.456683	0.534750
19	6	0	4.615075	1.733288	-0.967960
20	6	0	3.511258	2.032709	0.087844
21	6	0	4.779454	1.292916	0.482107
22	6	0	2.164700	1.302246	0.174235
23	8	0	1.488688	1.209507	-0.889977
24	8	0	1.845126	0.886373	1.333044
25	45	0	-0.227548	-0.003693	-0.873976
26	45	0	-0.055585	0.000941	1.620191
27	6	0	1.055468	5.314039	-3.562718
28	6	0	0.618172	6.406109	-2.802436
29	6	0	-0.315671	6.218112	-1.784862
30	6	0	-0.833623	4.933651	-1.511592
31	6	0	-0.386011	3.847161	-2.267712
32	6	0	0.554714	4.040657	-3.289142
33	6	0	-4.460850	7.661778	-0.637050
34	6	0	-5.272280	7.209479	-1.681358
35	6	0	-4.982461	5.994098	-2.311478
36	6	0	-3.886718	5.232825	-1.899313
37	6	0	-3.074679	5.682780	-0.845783
38	6	0	-3.363174	6.903042	-0.218777
39	6	0	-4.072100	3.995500	2.151335
40	6	0	-5.411442	3.832924	2.517538
41	6	0	-6.289355	3.136065	1.682087
42	6	0	-5.820787	2.592022	0.481561
43	6	0	-4.483429	2.749444	0.110877
44	6	0	-3.603635	3.464725	0.939381
45	6	0	-1.880275	4.861106	-0.436425
46	6	0	-2.177789	3.662099	0.512892
47	6	0	-1.407572	4.874593	1.010909

48	6	0	-1.455091	2.310116	0.450815
49	8	0	-1.423875	1.721426	-0.666715
50	8	0	-0.980508	1.896424	1.557186
51	6	0	-1.594452	-5.393332	-3.481065
52	6	0	-1.041411	-6.469196	-2.774997
53	6	0	-0.016364	-6.247582	-1.856854
54	6	0	0.476510	-4.944380	-1.629837
55	6	0	-0.082757	-3.875278	-2.334207
56	6	0	-1.114851	-4.102568	-3.255311
57	6	0	4.286746	-7.520582	-1.088848
58	6	0	4.960065	-7.055932	-2.222078
59	6	0	4.548461	-5.868672	-2.837914
60	6	0	3.468993	-5.147778	-2.323125
61	6	0	2.795987	-5.609745	-1.180352
62	6	0	3.206147	-6.802089	-0.567678
63	6	0	3.983125	-3.848508	1.754854
64	6	0	5.345105	-3.653184	2.002454
65	6	0	6.141091	-2.983989	1.067969
66	6	0	5.567828	-2.499795	-0.112527
67	6	0	4.207644	-2.692044	-0.365943
68	6	0	3.410263	-3.381477	0.561553
69	6	0	1.616291	-4.831864	-0.658247
70	6	0	1.958233	-3.622969	0.263344
71	6	0	1.279445	-4.861428	0.826187
72	6	0	1.191590	-2.294868	0.283894
73	8	0	0.998406	-1.715399	-0.824265
74	8	0	0.849939	-1.886617	1.439093
75	6	0	-5.736715	1.186614	-3.283165
76	6	0	-6.776107	0.685295	-2.489283
77	6	0	-6.505992	-0.263574	-1.504667
78	6	0	-5.190310	-0.732148	-1.298194
79	6	0	-4.157664	-0.223786	-2.090176
80	6	0	-4.433513	0.732450	-3.077658
81	6	0	-7.740634	-4.475584	-0.352730
82	6	0	-7.329559	-5.236512	-1.450645
83	6	0	-6.170033	-4.880854	-2.148703
84	6	0	-5.423573	-3.769738	-1.751044
85	6	0	-5.831642	-3.008333	-0.643819
86	6	0	-6.996236	-3.362819	0.051366
87	6	0	-3.938374	-4.001572	2.258066
88	6	0	-3.724250	-5.344177	2.583899
89	6	0	-3.085958	-6.195032	1.676640
90	6	0	-2.650078	-5.695939	0.444731
91	6	0	-2.858557	-4.354956	0.114156
92	6	0	-3.517718	-3.503385	1.015402
93	6	0	-5.027857	-1.796137	-0.250482
94	6	0	-3.774971	-2.073736	0.632901
95	6	0	-4.983313	-1.351398	1.205736
96	6	0	-2.445144	-1.316852	0.525200
97	8	0	-1.926918	-1.220080	-0.623624
98	8	0	-1.969838	-0.885057	1.624382
99	1	0	4.942281	-2.085828	-4.771924
100	1	0	6.982837	-1.171027	-3.676891
101	1	0	6.776626	0.573682	-1.927480
102	1	0	2.454123	0.462736	-2.340845
103	1	0	2.694203	-1.252581	-4.084933
104	1	0	8.186575	4.774028	-0.959938

105	1	0	7.294146	5.983494	-2.942012
106	1	0	5.172400	5.231534	-4.001179
107	1	0	3.944475	3.273550	-3.082442
108	1	0	6.965428	2.826967	-0.033574
109	1	0	4.150036	3.093084	2.512068
110	1	0	3.961568	5.470334	3.219325
111	1	0	3.008209	7.165153	1.667131
112	1	0	2.219220	6.472144	-0.593177
113	1	0	2.419173	4.106956	-1.314948
114	1	0	5.507701	1.778754	1.127798
115	1	0	4.720729	0.225499	0.709340
116	1	0	1.779219	5.459628	-4.360981
117	1	0	1.002785	7.402131	-3.011096
118	1	0	-0.659503	7.071741	-1.201955
119	1	0	-0.744510	2.817492	-2.070480
120	1	0	0.893455	3.180592	-3.867056
121	1	0	-4.682587	8.607525	-0.146717
122	1	0	-6.126335	7.800268	-2.004289
123	1	0	-5.611966	5.640034	-3.125852
124	1	0	-3.656931	4.287739	-2.392115
125	1	0	-2.734897	7.263782	0.592565
126	1	0	-3.393939	4.537706	2.807495
127	1	0	-5.771336	4.256195	3.452751
128	1	0	-7.333456	3.019117	1.962583
129	1	0	-6.498957	2.043777	-0.173554
130	1	0	-4.117521	2.313291	-0.823840
131	1	0	-1.863662	5.543851	1.737215
132	1	0	-0.338787	4.769718	1.212784
133	1	0	-2.391133	-5.564819	-4.200943
134	1	0	-1.408680	-7.478664	-2.947581
135	1	0	0.418234	-7.088401	-1.317265
136	1	0	0.260757	-2.835265	-2.171616
137	1	0	-1.541592	-3.256135	-3.793492
138	1	0	4.603367	-8.444346	-0.608697
139	1	0	5.801291	-7.615184	-2.624814
140	1	0	5.070325	-5.505030	-3.721121
141	1	0	3.144393	-4.225031	-2.804826
142	1	0	2.686406	-7.171907	0.313642
143	1	0	3.365939	-4.361315	2.491785
144	1	0	5.785358	-4.028630	2.923818
145	1	0	7.202775	-2.843533	1.255781
146	1	0	6.181329	-1.974151	-0.844792
147	1	0	3.761526	-2.306051	-1.287173
148	1	0	1.822944	-5.512440	1.508109
149	1	0	0.231010	-4.793826	1.128172
150	1	0	-5.946066	1.923269	-4.055167
151	1	0	-7.795302	1.032252	-2.645970
152	1	0	-7.319226	-0.658699	-0.896830
153	1	0	-3.107973	-0.549117	-1.950149
154	1	0	-3.614671	1.119400	-3.684487
155	1	0	-8.642627	-4.748896	0.191095
156	1	0	-7.908701	-6.102684	-1.762200
157	1	0	-5.847770	-5.471317	-3.004468
158	1	0	-4.522125	-3.489157	-2.296643
159	1	0	-7.324564	-2.775046	0.905634
160	1	0	-4.428545	-3.343399	2.972517
161	1	0	-4.056998	-5.726434	3.546591

162	1	0	-2.927632	-7.241142	1.927975
163	1	0	-2.146253	-6.352301	-0.265458
164	1	0	-2.505521	-3.965332	-0.845153
165	1	0	-5.601075	-1.843400	1.954110
166	1	0	-4.903517	-0.283953	1.422258
167	6	0	-2.401222	0.800925	6.489357
168	6	0	-1.211049	0.395850	5.693501
169	6	0	-1.114150	0.496259	4.337172
170	6	0	0.011351	0.040903	3.600182
171	6	0	1.217964	-0.477453	4.292580
172	8	0	2.171865	0.449667	4.360580
173	6	0	3.579876	0.115234	4.698093
174	6	0	4.106710	-0.888454	3.671595
175	6	0	3.660872	-0.407598	6.136113
176	6	0	4.280639	1.468173	4.564543
177	8	0	1.259788	-1.628377	4.689801
178	1	0	-2.813874	-0.067739	7.021306
179	1	0	-3.185144	1.239972	5.866234
180	1	0	-2.110648	1.523294	7.264576
181	1	0	-0.380929	-0.040739	6.247473
182	1	0	5.180729	-1.043482	3.822632
183	1	0	3.947824	-0.507825	2.657017
184	1	0	3.602829	-1.854313	3.758360
185	1	0	4.712450	-0.527911	6.419770
186	1	0	3.157505	-1.370759	6.234154
187	1	0	3.203659	0.306542	6.830108
188	1	0	5.351996	1.353818	4.759357
189	1	0	3.871840	2.187893	5.281385
190	1	0	4.144313	1.874300	3.551239
191	1	0	-1.948627	0.903690	3.769369

TS3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.758756	-3.352685	-2.941005
2	6	0	6.580056	-3.630338	-1.840716
3	6	0	6.475699	-2.863336	-0.681739
4	6	0	5.548705	-1.801159	-0.603191
5	6	0	4.730760	-1.532021	-1.702824
6	6	0	4.837047	-2.307956	-2.865605
7	6	0	9.051140	-0.199064	1.980534
8	6	0	9.438574	0.815859	1.101357
9	6	0	8.562619	1.235308	0.093720
10	6	0	7.304467	0.643647	-0.034573
11	6	0	6.910852	-0.371652	0.852835
12	6	0	7.791439	-0.794155	1.858244
13	6	0	4.722678	0.900318	3.553000
14	6	0	5.055080	2.039237	4.291744
15	6	0	5.344127	3.241514	3.638685
16	6	0	5.287305	3.304037	2.242826
17	6	0	4.954278	2.169033	1.498892
18	6	0	4.684832	0.955787	2.150363
19	6	0	5.559918	-1.014386	0.676547

20	6	0	4.366064	-0.275093	1.349538
21	6	0	4.836024	-1.624286	1.870058
22	6	0	2.953681	-0.161326	0.758165
23	8	0	2.852411	0.180591	-0.455218
24	8	0	2.009335	-0.395905	1.575426
25	45	0	0.947974	0.152316	-1.353444
26	45	0	0.012116	-0.081950	0.961403
27	6	0	5.733663	3.829048	-1.858969
28	6	0	5.633515	4.951279	-1.026905
29	6	0	4.403053	5.302008	-0.473875
30	6	0	3.247832	4.536461	-0.742914
31	6	0	3.356389	3.414143	-1.568631
32	6	0	4.596015	3.065659	-2.123599
33	6	0	1.586118	8.822359	-0.401099
34	6	0	1.151285	8.960400	-1.722319
35	6	0	0.976554	7.823956	-2.519857
36	6	0	1.234786	6.553927	-1.999607
37	6	0	1.666157	6.413651	-0.670950
38	6	0	1.844742	7.553278	0.126029
39	6	0	-1.186116	5.603655	1.147355
40	6	0	-2.420674	6.230167	0.951924
41	6	0	-3.097507	6.087853	-0.263011
42	6	0	-2.539058	5.308560	-1.281909
43	6	0	-1.305967	4.681038	-1.092972
44	6	0	-0.615859	4.834857	0.121153
45	6	0	1.968439	5.037945	-0.136330
46	6	0	0.730445	4.192049	0.289236
47	6	0	1.703271	4.721927	1.329750
48	6	0	0.619670	2.673090	0.098993
49	8	0	0.801457	2.230652	-1.070964
50	8	0	0.319887	2.006026	1.139476
51	6	0	-2.037235	-2.857556	-5.600521
52	6	0	-2.473950	-4.113648	-5.160818
53	6	0	-1.930014	-4.676840	-4.007653
54	6	0	-0.936535	-3.995130	-3.271790
55	6	0	-0.515610	-2.735831	-3.708524
56	6	0	-1.064391	-2.173915	-4.870296
57	6	0	0.273749	-8.408623	-2.841487
58	6	0	1.508977	-8.339954	-3.492157
59	6	0	2.130985	-7.100019	-3.675925
60	6	0	1.521530	-5.932470	-3.211415
61	6	0	0.283207	-6.000823	-2.553648
62	6	0	-0.340721	-7.243359	-2.372603
63	6	0	1.160952	-5.911573	0.719159
64	6	0	2.254340	-6.588648	1.268294
65	6	0	3.557333	-6.193632	0.953372
66	6	0	3.764976	-5.113483	0.088474
67	6	0	2.677390	-4.431885	-0.460298
68	6	0	1.365242	-4.830244	-0.151423
69	6	0	-0.374721	-4.728079	-2.086959
70	6	0	0.211402	-4.106506	-0.782215
71	6	0	-1.176093	-4.726250	-0.792472
72	6	0	0.335102	-2.594444	-0.543261
73	8	0	0.997277	-1.947932	-1.406557
74	8	0	-0.206863	-2.146376	0.514718
75	6	0	-1.601610	4.260875	-5.117742
76	6	0	-2.973311	4.410603	-4.876335

77	6	0	-3.658831	3.452086	-4.132485
78	6	0	-2.985314	2.322675	-3.617178
79	6	0	-1.616885	2.182196	-3.858691
80	6	0	-0.930587	3.149959	-4.605886
81	6	0	-7.222951	0.606776	-4.469871
82	6	0	-6.841304	-0.178646	-5.560971
83	6	0	-5.488610	-0.472644	-5.767031
84	6	0	-4.521465	0.016000	-4.886643
85	6	0	-4.903850	0.800647	-3.785804
86	6	0	-6.258828	1.097470	-3.583547
87	6	0	-5.085587	-1.076465	-0.533363
88	6	0	-5.792942	-2.276472	-0.423470
89	6	0	-5.559269	-3.317079	-1.328626
90	6	0	-4.604396	-3.158266	-2.337480
91	6	0	-3.893500	-1.960435	-2.452621
92	6	0	-4.142493	-0.907235	-1.560467
93	6	0	-3.839273	1.339886	-2.866820
94	6	0	-3.410270	0.397112	-1.703033
95	6	0	-4.169593	1.682820	-1.420655
96	6	0	-1.977821	0.252718	-1.174642
97	8	0	-1.051509	0.100570	-2.022802
98	8	0	-1.867968	0.273256	0.091879
99	1	0	5.840824	-3.947935	-3.847316
100	1	0	7.303084	-4.441528	-1.893463
101	1	0	7.123801	-3.075437	0.167814
102	1	0	3.978604	-0.719707	-1.675443
103	1	0	4.187317	-2.086724	-3.712517
104	1	0	9.730499	-0.528450	2.764112
105	1	0	10.417813	1.278595	1.199113
106	1	0	8.861935	2.024996	-0.592942
107	1	0	6.623132	0.966748	-0.822862
108	1	0	7.498692	-1.584428	2.546018
109	1	0	4.487238	-0.029788	4.067028
110	1	0	5.092011	1.987648	5.377559
111	1	0	5.613203	4.124147	4.213783
112	1	0	5.506603	4.238521	1.726265
113	1	0	4.903753	2.225596	0.407929
114	1	0	5.322729	-1.687705	2.840890
115	1	0	4.204339	-2.499950	1.705357
116	1	0	6.691346	3.557201	-2.296294
117	1	0	6.515638	5.552393	-0.817014
118	1	0	4.328348	6.183155	0.162266
119	1	0	2.482431	2.768247	-1.789279
120	1	0	4.660709	2.185017	-2.763326
121	1	0	1.724267	9.704493	0.220729
122	1	0	0.949176	9.948114	-2.130036
123	1	0	0.637916	7.928452	-3.549090
124	1	0	1.100368	5.667130	-2.619885
125	1	0	2.185550	7.454480	1.154117
126	1	0	-0.666608	5.718896	2.096736
127	1	0	-2.850480	6.836351	1.746908
128	1	0	-4.052300	6.584635	-0.417534
129	1	0	-3.061677	5.190393	-2.232178
130	1	0	-0.874794	4.064303	-1.889261
131	1	0	1.387248	5.504001	2.016737
132	1	0	2.362808	4.014021	1.838232
133	1	0	-2.454063	-2.420143	-6.504526

134	1	0	-3.233959	-4.651889	-5.723013
135	1	0	-2.265528	-5.658948	-3.677211
136	1	0	0.237877	-2.144650	-3.147364
137	1	0	-0.723370	-1.189685	-5.193211
138	1	0	-0.212911	-9.371303	-2.699434
139	1	0	1.985716	-9.247357	-3.855435
140	1	0	3.093019	-7.043566	-4.182173
141	1	0	2.004187	-4.964779	-3.353452
142	1	0	-1.303781	-7.304215	-1.871063
143	1	0	0.150322	-6.236059	0.960658
144	1	0	2.087730	-7.431523	1.935484
145	1	0	4.407011	-6.726259	1.373788
146	1	0	4.779111	-4.801470	-0.166364
147	1	0	2.843187	-3.581902	-1.133592
148	1	0	-1.360641	-5.653978	-0.255128
149	1	0	-2.043506	-4.064284	-0.715854
150	1	0	-1.065464	5.005718	-5.700812
151	1	0	-3.503976	5.272856	-5.274350
152	1	0	-4.727759	3.566873	-3.956175
153	1	0	-1.044945	1.322358	-3.457135
154	1	0	0.138203	3.025344	-4.780495
155	1	0	-8.273703	0.837701	-4.307332
156	1	0	-7.592459	-0.560526	-6.248232
157	1	0	-5.188382	-1.083717	-6.616149
158	1	0	-3.466356	-0.208717	-5.049225
159	1	0	-6.564280	1.707756	-2.736361
160	1	0	-5.256400	-0.274197	0.185851
161	1	0	-6.527163	-2.400315	0.368595
162	1	0	-6.117485	-4.246309	-1.247532
163	1	0	-4.410094	-3.966462	-3.041856
164	1	0	-3.142454	-1.843997	-3.238288
165	1	0	-5.194048	1.630895	-1.053869
166	1	0	-3.644813	2.513588	-0.942451
167	6	0	-1.058244	0.837812	5.011661
168	6	0	-0.636105	0.883129	3.707473
169	6	0	-0.672362	-0.224651	2.834752
170	6	0	-1.214112	-1.527002	3.308877
171	8	0	-0.228698	-2.375743	3.596470
172	6	0	-0.474292	-3.788880	3.975550
173	6	0	-1.340886	-4.481487	2.920835
174	6	0	-1.106562	-3.820272	5.370610
175	6	0	0.938084	-4.374093	3.989065
176	8	0	-2.414988	-1.727853	3.383406
177	1	0	-1.339671	-5.560909	3.109099
178	1	0	-0.926839	-4.294934	1.923867
179	1	0	-2.368417	-4.116968	2.940483
180	1	0	-1.205975	-4.859059	5.705511
181	1	0	-2.098070	-3.362229	5.364727
182	1	0	-0.472703	-3.292103	6.091400
183	1	0	0.905575	-5.424628	4.296318
184	1	0	1.581065	-3.825424	4.683731
185	1	0	1.383858	-4.320051	2.988468
186	1	0	-0.243588	1.817450	3.311487
187	6	0	-5.840444	3.444897	0.943168
188	6	0	-4.795610	3.513525	1.867831
189	6	0	-4.657319	2.547419	2.861817
190	6	0	-5.569885	1.472282	2.932751

191	6	0	-6.614881	1.409255	1.983305
192	6	0	-6.752991	2.386624	1.005371
193	6	0	-5.026310	-2.116651	5.342372
194	6	0	-5.146550	-3.179976	6.239404
195	6	0	-5.064130	-2.956508	7.615336
196	6	0	-4.845691	-1.663106	8.098878
197	6	0	-4.718918	-0.594058	7.214214
198	6	0	-4.831513	-0.828224	5.842734
199	6	0	-5.524352	0.413567	3.916990
200	7	0	-4.714327	0.317926	4.954058
201	8	0	-3.839443	1.202419	5.296239
202	1	0	-5.941053	4.209532	0.177547
203	1	0	-4.076502	4.328829	1.812816
204	1	0	-3.856691	2.600140	3.585537
205	1	0	-7.324001	0.585708	2.026202
206	1	0	-7.570064	2.324670	0.291910
207	1	0	-5.030428	-2.291096	4.272311
208	1	0	-5.289241	-4.186598	5.856884
209	1	0	-5.157588	-3.788088	8.307975
210	1	0	-4.774441	-1.485519	9.168209
211	1	0	-4.540031	0.417034	7.560661
212	1	0	-6.245195	-0.389420	3.833274
213	1	0	-1.479693	-0.083843	5.403523
214	6	0	-0.956943	1.974009	5.962625
215	1	0	-1.951823	2.193428	6.366667
216	1	0	-0.323054	1.688588	6.814863
217	1	0	-0.539122	2.869917	5.495277

TS3'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.542561	2.866161	-3.509021
2	6	0	6.130462	3.696960	-2.546527
3	6	0	5.375823	4.158726	-1.469458
4	6	0	4.016924	3.799407	-1.338217
5	6	0	3.437411	2.969406	-2.300431
6	6	0	4.201122	2.504296	-3.379896
7	6	0	4.000842	8.108247	0.366165
8	6	0	3.256512	8.680555	-0.668982
9	6	0	2.521256	7.860796	-1.532670
10	6	0	2.528914	6.475011	-1.362319
11	6	0	3.270332	5.898842	-0.317554
12	6	0	4.010714	6.720965	0.543124
13	6	0	1.142237	5.079997	2.569909
14	6	0	0.236429	6.008379	3.090927
15	6	0	-0.718670	6.601981	2.259852
16	6	0	-0.773664	6.253588	0.906494
17	6	0	0.127432	5.324306	0.380455
18	6	0	1.102166	4.744225	1.207179
19	6	0	3.286686	4.399350	-0.171159
20	6	0	2.101461	3.782494	0.628602
21	6	0	3.512219	3.764374	1.195003
22	6	0	1.414214	2.445168	0.309396

23	8	0	1.099751	2.225371	-0.895659
24	8	0	1.197720	1.700357	1.313969
25	45	0	0.258949	0.363387	-1.399798
26	45	0	0.034930	-0.055004	1.078795
27	6	0	-0.953715	5.996615	-3.325385
28	6	0	-2.015410	6.583169	-2.624601
29	6	0	-2.866361	5.790573	-1.856778
30	6	0	-2.671634	4.394161	-1.773614
31	6	0	-1.609769	3.816574	-2.473753
32	6	0	-0.756159	4.617886	-3.245680
33	6	0	-7.292882	4.745282	-1.430053
34	6	0	-7.576999	4.190981	-2.681081
35	6	0	-6.594554	3.457984	-3.356474
36	6	0	-5.333742	3.279101	-2.784053
37	6	0	-5.048878	3.829460	-1.523307
38	6	0	-6.032418	4.567685	-0.850656
39	6	0	-5.282023	1.331182	1.272618
40	6	0	-6.392368	0.495829	1.423370
41	6	0	-6.847887	-0.270476	0.345767
42	6	0	-6.181112	-0.207480	-0.881767
43	6	0	-5.069193	0.624361	-1.037627
44	6	0	-4.621832	1.409398	0.035541
45	6	0	-3.672990	3.644905	-0.939485
46	6	0	-3.446509	2.328108	-0.140034
47	6	0	-3.464289	3.671816	0.570067
48	6	0	-2.144469	1.513875	-0.165258
49	8	0	-1.660402	1.234287	-1.298690
50	8	0	-1.693111	1.172189	0.972618
51	6	0	1.731372	-4.558145	-4.630708
52	6	0	2.606063	-5.399042	-3.931287
53	6	0	3.315888	-4.910868	-2.834965
54	6	0	3.169218	-3.569146	-2.424039
55	6	0	2.281846	-2.739382	-3.115968
56	6	0	1.568747	-3.235366	-4.216177
57	6	0	7.633593	-4.349889	-1.772322
58	6	0	8.141421	-3.392518	-2.655187
59	6	0	7.324329	-2.342615	-3.089002
60	6	0	6.004351	-2.248888	-2.642609
61	6	0	5.494973	-3.207235	-1.752355
62	6	0	6.313341	-4.260668	-1.320386
63	6	0	5.870903	-1.609530	1.070619
64	6	0	6.967296	-0.809471	1.404875
65	6	0	7.113662	0.457792	0.833442
66	6	0	6.156265	0.923794	-0.073731
67	6	0	5.057779	0.129976	-0.409497
68	6	0	4.907463	-1.145960	0.160153
69	6	0	4.058331	-3.111393	-1.304984
70	6	0	3.747644	-2.004766	-0.251539
71	6	0	3.700687	-3.475951	0.128939
72	6	0	2.430687	-1.210259	-0.206989
73	8	0	2.141907	-0.557171	-1.252740
74	8	0	1.785491	-1.257707	0.884556
75	6	0	-4.565641	0.073018	-4.832973
76	6	0	-5.416699	-0.987459	-4.496209
77	6	0	-4.974437	-1.990008	-3.635838
78	6	0	-3.670068	-1.956909	-3.091958
79	6	0	-2.832920	-0.888311	-3.422915

80	6	0	-3.280807	0.117639	-4.292552
81	6	0	-4.746993	-6.451427	-3.372454
82	6	0	-3.871781	-6.773116	-4.413623
83	6	0	-2.815637	-5.909996	-4.726619
84	6	0	-2.634299	-4.730113	-4.002170
85	6	0	-3.510355	-4.407710	-2.952928
86	6	0	-4.569869	-5.271811	-2.642635
87	6	0	-2.085215	-5.425951	0.060364
88	6	0	-1.487269	-6.680380	0.210592
89	6	0	-0.358897	-7.016684	-0.543415
90	6	0	0.177027	-6.087340	-1.441029
91	6	0	-0.417635	-4.833161	-1.596640
92	6	0	-1.562971	-4.499255	-0.856273
93	6	0	-3.310195	-3.115472	-2.203391
94	6	0	-2.230027	-3.172888	-1.077047
95	6	0	-3.702791	-3.015517	-0.735609
96	6	0	-1.275657	-2.017319	-0.742638
97	8	0	-0.645032	-1.503496	-1.712603
98	8	0	-1.196414	-1.702523	0.483689
99	1	0	6.129087	2.507060	-4.351392
100	1	0	7.174829	3.985956	-2.643207
101	1	0	5.832973	4.813937	-0.729038
102	1	0	2.379402	2.654089	-2.222207
103	1	0	3.734872	1.852815	-4.119051
104	1	0	4.575121	8.742759	1.038161
105	1	0	3.248544	9.759601	-0.803891
106	1	0	1.941185	8.303507	-2.340342
107	1	0	1.959958	5.835359	-2.038578
108	1	0	4.594470	6.284099	1.350239
109	1	0	1.877377	4.613976	3.222992
110	1	0	0.279723	6.273370	4.144749
111	1	0	-1.414622	7.333489	2.663259
112	1	0	-1.517259	6.709358	0.252228
113	1	0	0.074692	5.049143	-0.676983
114	1	0	3.755229	4.379763	2.058258
115	1	0	4.044476	2.811975	1.244313
116	1	0	-0.291034	6.612504	-3.928513
117	1	0	-2.178127	7.657171	-2.684135
118	1	0	-3.698555	6.249589	-1.324031
119	1	0	-1.404436	2.727820	-2.423089
120	1	0	0.069676	4.148649	-3.781089
121	1	0	-8.054114	5.316806	-0.902965
122	1	0	-8.558270	4.328437	-3.129146
123	1	0	-6.812634	3.025239	-4.331146
124	1	0	-4.565928	2.711470	-3.312426
125	1	0	-5.819694	5.003524	0.122978
126	1	0	-4.925054	1.917181	2.116635
127	1	0	-6.904463	0.442334	2.381380
128	1	0	-7.716894	-0.913630	0.462428
129	1	0	-6.525405	-0.805687	-1.725454
130	1	0	-4.545591	0.663836	-1.997136
131	1	0	-4.286987	3.917146	1.237698
132	1	0	-2.525958	4.076506	0.958167
133	1	0	1.183001	-4.934809	-5.490939
134	1	0	2.737906	-6.430965	-4.249459
135	1	0	4.003792	-5.565310	-2.301987
136	1	0	2.110108	-1.688985	-2.804866

137	1	0	0.881058	-2.573626	-4.743856
138	1	0	8.266371	-5.168422	-1.435618
139	1	0	9.168733	-3.463111	-3.004988
140	1	0	7.717303	-1.595373	-3.776290
141	1	0	5.365590	-1.430773	-2.978009
142	1	0	5.923887	-5.011708	-0.637349
143	1	0	5.775508	-2.602096	1.508660
144	1	0	7.713586	-1.180893	2.103948
145	1	0	7.971840	1.075923	1.085987
146	1	0	6.267545	1.908307	-0.531496
147	1	0	4.309673	0.499812	-1.122900
148	1	0	4.453767	-3.886067	0.799113
149	1	0	2.726821	-3.925104	0.331699
150	1	0	-4.905125	0.852526	-5.510463
151	1	0	-6.421508	-1.030413	-4.910709
152	1	0	-5.640439	-2.816102	-3.387912
153	1	0	-1.808391	-0.785733	-3.000980
154	1	0	-2.608325	0.941314	-4.535299
155	1	0	-5.569585	-7.120157	-3.127453
156	1	0	-4.010633	-7.691272	-4.979442
157	1	0	-2.133004	-6.157881	-5.537238
158	1	0	-1.813043	-4.055038	-4.245152
159	1	0	-5.256524	-5.027526	-1.835069
160	1	0	-2.963805	-5.171751	0.651686
161	1	0	-1.906490	-7.398057	0.912793
162	1	0	0.096186	-7.998308	-0.437336
163	1	0	1.058281	-6.340350	-2.031159
164	1	0	0.004083	-4.107955	-2.300196
165	1	0	-4.234744	-3.826351	-0.242767
166	1	0	-4.052068	-2.051676	-0.352760
167	6	0	-0.736846	1.264794	5.020928
168	6	0	-0.959766	0.754611	3.786576
169	6	0	-0.097164	-0.198760	3.128451
170	6	0	1.073050	-0.677532	3.949426
171	8	0	2.165093	-0.016812	3.569600
172	6	0	3.499937	-0.285069	4.150640
173	6	0	3.883892	-1.742703	3.884715
174	6	0	3.501339	0.062831	5.643885
175	6	0	4.392088	0.673792	3.363425
176	8	0	1.006943	-1.496748	4.850248
177	1	0	4.937403	-1.893629	4.146673
178	1	0	3.753222	-1.966630	2.819948
179	1	0	3.270249	-2.431964	4.466332
180	1	0	4.522084	-0.020399	6.034232
181	1	0	2.855228	-0.611221	6.208720
182	1	0	3.165805	1.094662	5.796423
183	1	0	5.433739	0.570717	3.687067
184	1	0	4.075139	1.710020	3.511595
185	1	0	4.341062	0.446002	2.292201
186	1	0	-1.788046	1.139275	3.196300
187	6	0	-5.561080	-0.691034	6.439542
188	6	0	-4.982082	-0.399385	5.200903
189	6	0	-3.862938	-1.096545	4.754244
190	6	0	-3.305226	-2.119542	5.552564
191	6	0	-3.911980	-2.416584	6.793293
192	6	0	-5.021131	-1.704652	7.236117
193	6	0	0.302242	-4.499300	4.882825

194	6	0	1.209147	-5.500991	4.544423
195	6	0	1.454101	-5.806309	3.202040
196	6	0	0.799519	-5.093180	2.196901
197	6	0	-0.109499	-4.084351	2.518756
198	6	0	-0.361368	-3.812851	3.862630
199	6	0	-2.181451	-2.950991	5.172403
200	7	0	-1.357407	-2.795914	4.159221
201	8	0	-1.467822	-1.815767	3.301368
202	1	0	-6.431719	-0.137190	6.779531
203	1	0	-5.408315	0.377030	4.571360
204	1	0	-3.419453	-0.877199	3.793217
205	1	0	-3.500319	-3.211853	7.410292
206	1	0	-5.468391	-1.943321	8.196769
207	1	0	0.154837	-4.222208	5.920714
208	1	0	1.737259	-6.031366	5.331306
209	1	0	2.160277	-6.590044	2.943963
210	1	0	0.979371	-5.326792	1.149186
211	1	0	-0.619178	-3.509735	1.752621
212	1	0	-2.010251	-3.849126	5.752516
213	1	0	0.094087	0.889877	5.616459
214	6	0	-1.566037	2.336798	5.649428
215	1	0	-1.998006	1.983490	6.596105
216	1	0	-0.948923	3.211981	5.895161
217	1	0	-2.378810	2.661329	4.992835

2.3. C=C-C=N2 *s-trans* vinylcarbenoid **2-II** and aryl nitrene **3a**

s-trans vinyl diazoacetate **2-II** and aryl nitrene **3a** with an approach over *Si*-face

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.758756	-3.352685	-2.941005
2	6	0	6.580056	-3.630338	-1.840716
3	6	0	6.475699	-2.863336	-0.681739
4	6	0	5.548705	-1.801159	-0.603191
5	6	0	4.730760	-1.532021	-1.702824
6	6	0	4.837047	-2.307956	-2.865605
7	6	0	9.051140	-0.199064	1.980534
8	6	0	9.438574	0.815859	1.101357
9	6	0	8.562619	1.235308	0.093720
10	6	0	7.304467	0.643647	-0.034573
11	6	0	6.910852	-0.371652	0.852835
12	6	0	7.791439	-0.794155	1.858244
13	6	0	4.722678	0.900318	3.553000
14	6	0	5.055080	2.039237	4.291744
15	6	0	5.344127	3.241514	3.638685
16	6	0	5.287305	3.304037	2.242826
17	6	0	4.954278	2.169033	1.498892
18	6	0	4.684832	0.955787	2.150363
19	6	0	5.559918	-1.014386	0.676547
20	6	0	4.366064	-0.275093	1.349538
21	6	0	4.836024	-1.624286	1.870058
22	6	0	2.953681	-0.161326	0.758165
23	8	0	2.852411	0.180591	-0.455218
24	8	0	2.009335	-0.395905	1.575426
25	45	0	0.947974	0.152316	-1.353444
26	45	0	0.012116	-0.081950	0.961403
27	6	0	5.733663	3.829048	-1.858969
28	6	0	5.633515	4.951279	-1.026905
29	6	0	4.403053	5.302008	-0.473875
30	6	0	3.247832	4.536461	-0.742914
31	6	0	3.356389	3.414143	-1.568631
32	6	0	4.596015	3.065659	-2.123599
33	6	0	1.586118	8.822359	-0.401099
34	6	0	1.151285	8.960400	-1.722319
35	6	0	0.976554	7.823956	-2.519857
36	6	0	1.234786	6.553927	-1.999607
37	6	0	1.666157	6.413651	-0.670950
38	6	0	1.844742	7.553278	0.126029
39	6	0	-1.186116	5.603655	1.147355
40	6	0	-2.420674	6.230167	0.951924
41	6	0	-3.097507	6.087853	-0.263011
42	6	0	-2.539058	5.308560	-1.281909
43	6	0	-1.305967	4.681038	-1.092972
44	6	0	-0.615859	4.834857	0.121153
45	6	0	1.968439	5.037945	-0.136330
46	6	0	0.730445	4.192049	0.289236
47	6	0	1.703271	4.721927	1.329750
48	6	0	0.619670	2.673090	0.098993
49	8	0	0.801457	2.230652	-1.070964

50	8	0	0.319887	2.006026	1.139476
51	6	0	-2.037235	-2.857556	-5.600521
52	6	0	-2.473950	-4.113648	-5.160818
53	6	0	-1.930014	-4.676840	-4.007653
54	6	0	-0.936535	-3.995130	-3.271790
55	6	0	-0.515610	-2.735831	-3.708524
56	6	0	-1.064391	-2.173915	-4.870296
57	6	0	0.273749	-8.408623	-2.841487
58	6	0	1.508977	-8.339954	-3.492157
59	6	0	2.130985	-7.100019	-3.675925
60	6	0	1.521530	-5.932470	-3.211415
61	6	0	0.283207	-6.000823	-2.553648
62	6	0	-0.340721	-7.243359	-2.372603
63	6	0	1.160952	-5.911573	0.719159
64	6	0	2.254340	-6.588648	1.268294
65	6	0	3.557333	-6.193632	0.953372
66	6	0	3.764976	-5.113483	0.088474
67	6	0	2.677390	-4.431885	-0.460298
68	6	0	1.365242	-4.830244	-0.151423
69	6	0	-0.374721	-4.728079	-2.086959
70	6	0	0.211402	-4.106506	-0.782215
71	6	0	-1.176093	-4.726250	-0.792472
72	6	0	0.335102	-2.594444	-0.543261
73	8	0	0.997277	-1.947932	-1.406557
74	8	0	-0.206863	-2.146376	0.514718
75	6	0	-1.601610	4.260875	-5.117742
76	6	0	-2.973311	4.410603	-4.876335
77	6	0	-3.658831	3.452086	-4.132485
78	6	0	-2.985314	2.322675	-3.617178
79	6	0	-1.616885	2.182196	-3.858691
80	6	0	-0.930587	3.149959	-4.605886
81	6	0	-7.222951	0.606776	-4.469871
82	6	0	-6.841304	-0.178646	-5.560971
83	6	0	-5.488610	-0.472644	-5.767031
84	6	0	-4.521465	0.016000	-4.886643
85	6	0	-4.903850	0.800647	-3.785804
86	6	0	-6.258828	1.097470	-3.583547
87	6	0	-5.085587	-1.076465	-0.533363
88	6	0	-5.792942	-2.276472	-0.423470
89	6	0	-5.559269	-3.317079	-1.328626
90	6	0	-4.604396	-3.158266	-2.337480
91	6	0	-3.893500	-1.960435	-2.452621
92	6	0	-4.142493	-0.907235	-1.560467
93	6	0	-3.839273	1.339886	-2.866820
94	6	0	-3.410270	0.397112	-1.703033
95	6	0	-4.169593	1.682820	-1.420655
96	6	0	-1.977821	0.252718	-1.174642
97	8	0	-1.051509	0.100570	-2.022802
98	8	0	-1.867968	0.273256	0.091879
99	1	0	5.840824	-3.947935	-3.847316
100	1	0	7.303084	-4.441528	-1.893463
101	1	0	7.123801	-3.075437	0.167814
102	1	0	3.978604	-0.719707	-1.675443
103	1	0	4.187317	-2.086724	-3.712517
104	1	0	9.730499	-0.528450	2.764112
105	1	0	10.417813	1.278595	1.199113
106	1	0	8.861935	2.024996	-0.592942

107	1	0	6.623132	0.966748	-0.822862
108	1	0	7.498692	-1.584428	2.546018
109	1	0	4.487238	-0.029788	4.067028
110	1	0	5.092011	1.987648	5.377559
111	1	0	5.613203	4.124147	4.213783
112	1	0	5.506603	4.238521	1.726265
113	1	0	4.903753	2.225596	0.407929
114	1	0	5.322729	-1.687705	2.840890
115	1	0	4.204339	-2.499950	1.705357
116	1	0	6.691346	3.557201	-2.296294
117	1	0	6.515638	5.552393	-0.817014
118	1	0	4.328348	6.183155	0.162266
119	1	0	2.482431	2.768247	-1.789279
120	1	0	4.660709	2.185017	-2.763326
121	1	0	1.724267	9.704493	0.220729
122	1	0	0.949176	9.948114	-2.130036
123	1	0	0.637916	7.928452	-3.549090
124	1	0	1.100368	5.667130	-2.619885
125	1	0	2.185550	7.454480	1.154117
126	1	0	-0.666608	5.718896	2.096736
127	1	0	-2.850480	6.836351	1.746908
128	1	0	-4.052300	6.584635	-0.417534
129	1	0	-3.061677	5.190393	-2.232178
130	1	0	-0.874794	4.064303	-1.889261
131	1	0	1.387248	5.504001	2.016737
132	1	0	2.362808	4.014021	1.838232
133	1	0	-2.454063	-2.420143	-6.504526
134	1	0	-3.233959	-4.651889	-5.723013
135	1	0	-2.265528	-5.658948	-3.677211
136	1	0	0.237877	-2.144650	-3.147364
137	1	0	-0.723370	-1.189685	-5.193211
138	1	0	-0.212911	-9.371303	-2.699434
139	1	0	1.985716	-9.247357	-3.855435
140	1	0	3.093019	-7.043566	-4.182173
141	1	0	2.004187	-4.964779	-3.353452
142	1	0	-1.303781	-7.304215	-1.871063
143	1	0	0.150322	-6.236059	0.960658
144	1	0	2.087730	-7.431523	1.935484
145	1	0	4.407011	-6.726259	1.373788
146	1	0	4.779111	-4.801470	-0.166364
147	1	0	2.843187	-3.581902	-1.133592
148	1	0	-1.360641	-5.653978	-0.255128
149	1	0	-2.043506	-4.064284	-0.715854
150	1	0	-1.065464	5.005718	-5.700812
151	1	0	-3.503976	5.272856	-5.274350
152	1	0	-4.727759	3.566873	-3.956175
153	1	0	-1.044945	1.322358	-3.457135
154	1	0	0.138203	3.025344	-4.780495
155	1	0	-8.273703	0.837701	-4.307332
156	1	0	-7.592459	-0.560526	-6.248232
157	1	0	-5.188382	-1.083717	-6.616149
158	1	0	-3.466356	-0.208717	-5.049225
159	1	0	-6.564280	1.707756	-2.736361
160	1	0	-5.256400	-0.274197	0.185851
161	1	0	-6.527163	-2.400315	0.368595
162	1	0	-6.117485	-4.246309	-1.247532
163	1	0	-4.410094	-3.966462	-3.041856

164	1	0	-3.142454	-1.843997	-3.238288
165	1	0	-5.194048	1.630895	-1.053869
166	1	0	-3.644813	2.513588	-0.942451
167	6	0	-1.058244	0.837812	5.011661
168	6	0	-0.636105	0.883129	3.707473
169	6	0	-0.672362	-0.224651	2.834752
170	6	0	-1.214112	-1.527002	3.308877
171	8	0	-0.228698	-2.375743	3.596470
172	6	0	-0.474292	-3.788880	3.975550
173	6	0	-1.340886	-4.481487	2.920835
174	6	0	-1.106562	-3.820272	5.370610
175	6	0	0.938084	-4.374093	3.989065
176	8	0	-2.414988	-1.727853	3.383406
177	1	0	-1.339671	-5.560909	3.109099
178	1	0	-0.926839	-4.294934	1.923867
179	1	0	-2.368417	-4.116968	2.940483
180	1	0	-1.205975	-4.859059	5.705511
181	1	0	-2.098070	-3.362229	5.364727
182	1	0	-0.472703	-3.292103	6.091400
183	1	0	0.905575	-5.424628	4.296318
184	1	0	1.581065	-3.825424	4.683731
185	1	0	1.383858	-4.320051	2.988468
186	1	0	-0.243588	1.817450	3.311487
187	6	0	-5.840444	3.444897	0.943168
188	6	0	-4.795610	3.513525	1.867831
189	6	0	-4.657319	2.547419	2.861817
190	6	0	-5.569885	1.472282	2.932751
191	6	0	-6.614881	1.409255	1.983305
192	6	0	-6.752991	2.386624	1.005371
193	6	0	-5.026310	-2.116651	5.342372
194	6	0	-5.146550	-3.179976	6.239404
195	6	0	-5.064130	-2.956508	7.615336
196	6	0	-4.845691	-1.663106	8.098878
197	6	0	-4.718918	-0.594058	7.214214
198	6	0	-4.831513	-0.828224	5.842734
199	6	0	-5.524352	0.413567	3.916990
200	7	0	-4.714327	0.317926	4.954058
201	8	0	-3.839443	1.202419	5.296239
202	1	0	-5.941053	4.209532	0.177547
203	1	0	-4.076502	4.328829	1.812816
204	1	0	-3.856691	2.600140	3.585537
205	1	0	-7.324001	0.585708	2.026202
206	1	0	-7.570064	2.324670	0.291910
207	1	0	-5.030428	-2.291096	4.272311
208	1	0	-5.289241	-4.186598	5.856884
209	1	0	-5.157588	-3.788088	8.307975
210	1	0	-4.774441	-1.485519	9.168209
211	1	0	-4.540031	0.417034	7.560661
212	1	0	-6.245195	-0.389420	3.833274
213	1	0	-1.479693	-0.083843	5.403523
214	6	0	-0.956943	1.974009	5.962625
215	1	0	-1.951823	2.193428	6.366667
216	1	0	-0.323054	1.688588	6.814863
217	1	0	-0.539122	2.869917	5.495277

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.457937	-3.286218	-3.298293
2	6	0	6.405347	-3.448186	-2.279213
3	6	0	6.377101	-2.615110	-1.162398
4	6	0	5.401301	-1.600906	-1.044856
5	6	0	4.457400	-1.448122	-2.062797
6	6	0	4.487956	-2.290075	-3.183539
7	6	0	9.062575	0.291167	1.076120
8	6	0	9.310121	1.273583	0.113476
9	6	0	8.317191	1.602205	-0.816447
10	6	0	7.081972	0.952175	-0.784483
11	6	0	6.829320	-0.030847	0.186671
12	6	0	7.826517	-0.362055	1.114396
13	6	0	4.875226	1.297318	3.024446
14	6	0	5.227040	2.488137	3.666037
15	6	0	5.384500	3.665150	2.927575
16	6	0	5.177167	3.649368	1.544668
17	6	0	4.825065	2.461871	0.897993
18	6	0	4.686255	1.274720	1.633081
19	6	0	5.499479	-0.738459	0.181716
20	6	0	4.345664	-0.009820	0.931941
21	6	0	4.924364	-1.307851	1.472494
22	6	0	2.878513	0.015027	0.475582
23	8	0	2.650982	0.281629	-0.740201
24	8	0	2.028385	-0.208625	1.391671
25	45	0	0.675734	0.082619	-1.469178
26	45	0	-0.027422	-0.037473	0.942434
27	6	0	5.233071	3.818003	-2.627255
28	6	0	5.161749	5.001201	-1.881124
29	6	0	3.970400	5.358238	-1.251798
30	6	0	2.825503	4.538687	-1.356673
31	6	0	2.907299	3.353662	-2.093405
32	6	0	4.107393	2.999527	-2.726631
33	6	0	1.086266	8.794705	-1.240271
34	6	0	0.518112	8.809057	-2.517299
35	6	0	0.290265	7.604113	-3.191361
36	6	0	0.628663	6.388898	-2.592181
37	6	0	1.195085	6.373052	-1.307699
38	6	0	1.425749	7.581073	-0.634336
39	6	0	-1.451343	5.734096	0.705696
40	6	0	-2.710330	6.317098	0.531344
41	6	0	-3.498612	5.973431	-0.570740
42	6	0	-3.025015	5.039150	-1.498377
43	6	0	-1.766909	4.457261	-1.331846
44	6	0	-0.966296	4.808841	-0.231525
45	6	0	1.582325	5.054486	-0.689533
46	6	0	0.406194	4.215273	-0.102296
47	6	0	1.436481	4.855386	0.813175
48	6	0	0.339464	2.681487	-0.163520
49	8	0	0.423224	2.163825	-1.314500
50	8	0	0.173992	2.084037	0.944223
51	6	0	-2.516748	-3.290600	-5.234915
52	6	0	-2.845735	-4.539508	-4.692864

53	6	0	-2.176343	-5.007702	-3.563584
54	6	0	-1.162682	-4.236590	-2.953844
55	6	0	-0.852612	-2.983134	-3.489211
56	6	0	-1.526790	-2.517401	-4.627419
57	6	0	0.268629	-8.566847	-2.398949
58	6	0	1.437648	-8.491093	-3.161522
59	6	0	1.989627	-7.242091	-3.467271
60	6	0	1.376185	-6.072527	-3.013236
61	6	0	0.204336	-6.147647	-2.243886
62	6	0	-0.349382	-7.399512	-1.940021
63	6	0	1.385881	-5.875090	0.866288
64	6	0	2.555488	-6.481185	1.335055
65	6	0	3.805211	-6.021873	0.910218
66	6	0	3.882311	-4.949984	0.014276
67	6	0	2.717904	-4.340103	-0.455732
68	6	0	1.458733	-4.800867	-0.034079
69	6	0	-0.461537	-4.874554	-1.788490
70	6	0	0.219308	-4.156298	-0.582639
71	6	0	-1.135572	-4.826412	-0.424304
72	6	0	0.296074	-2.628099	-0.437824
73	8	0	0.848645	-2.008798	-1.394009
74	8	0	-0.168927	-2.140992	0.637581
75	6	0	-2.425909	3.708864	-5.286210
76	6	0	-3.780584	3.800076	-4.941386
77	6	0	-4.340776	2.872195	-4.065559
78	6	0	-3.556656	1.832232	-3.518937
79	6	0	-2.205875	1.750342	-3.863999
80	6	0	-1.645757	2.687255	-4.744064
81	6	0	-7.739930	-0.175391	-3.850706
82	6	0	-7.404496	-1.027599	-4.906223
83	6	0	-6.058523	-1.262961	-5.209077
84	6	0	-5.052364	-0.649838	-4.460235
85	6	0	-5.387437	0.201572	-3.394153
86	6	0	-6.736194	0.439955	-3.095788
87	6	0	-5.166681	-1.396986	0.020798
88	6	0	-5.788794	-2.617752	0.294919
89	6	0	-5.587604	-3.715351	-0.548657
90	6	0	-4.749557	-3.591577	-1.660961
91	6	0	-4.124453	-2.373099	-1.940192
92	6	0	-4.343358	-1.264477	-1.109565
93	6	0	-4.283141	0.872054	-2.619560
94	6	0	-3.704622	0.058604	-1.423898
95	6	0	-4.513201	1.322491	-1.182832
96	6	0	-2.225621	0.035227	-1.009684
97	8	0	-1.370113	-0.129905	-1.928088
98	8	0	-2.011710	0.157584	0.235727
99	1	0	5.479890	-3.933159	-4.171943
100	1	0	7.166070	-4.221315	-2.362617
101	1	0	7.122388	-2.737966	-0.377460
102	1	0	3.661787	-0.678698	-2.002179
103	1	0	3.739738	-2.158956	-3.965562
104	1	0	9.832984	0.032427	1.799558
105	1	0	10.271262	1.781406	0.086185
106	1	0	8.507187	2.366588	-1.567627
107	1	0	6.308746	1.204699	-1.511761
108	1	0	7.642816	-1.126577	1.865971
109	1	0	4.743483	0.386577	3.605471

110	1	0	5.383626	2.496734	4.742083
111	1	0	5.668793	4.588566	3.425947
112	1	0	5.293293	4.563058	0.961814
113	1	0	4.657519	2.456054	-0.182887
114	1	0	5.506570	-1.297746	2.391083
115	1	0	4.318922	-2.215280	1.417407
116	1	0	6.158962	3.541560	-3.125796
117	1	0	6.035066	5.644392	-1.797930
118	1	0	3.917653	6.286258	-0.684023
119	1	0	2.045311	2.659330	-2.180710
120	1	0	4.150445	2.069820	-3.295170
121	1	0	1.265984	9.730283	-0.714795
122	1	0	0.253811	9.753784	-2.986505
123	1	0	-0.152461	7.612195	-4.185766
124	1	0	0.451888	5.448317	-3.115366
125	1	0	1.870458	7.578112	0.358094
126	1	0	-0.843024	6.010135	1.565254
127	1	0	-3.071490	7.047693	1.252339
128	1	0	-4.472200	6.436346	-0.711441
129	1	0	-3.632537	4.766006	-2.362613
130	1	0	-1.398604	3.723667	-2.059435
131	1	0	1.148237	5.683661	1.456748
132	1	0	2.152693	4.207558	1.325158
133	1	0	-3.029455	-2.928463	-6.122699
134	1	0	-3.619742	-5.146474	-5.157261
135	1	0	-2.428543	-5.985118	-3.154544
136	1	0	-0.091089	-2.320068	-3.025756
137	1	0	-1.269138	-1.536676	-5.029046
138	1	0	-0.163515	-9.536656	-2.161555
139	1	0	1.917311	-9.399983	-3.516926
140	1	0	2.900295	-7.180088	-4.060376
141	1	0	1.804823	-5.097610	-3.249083
142	1	0	-1.260873	-7.466017	-1.350553
143	1	0	0.417108	-6.249353	1.192901
144	1	0	2.489842	-7.319377	2.025191
145	1	0	4.714060	-6.499067	1.268617
146	1	0	4.853589	-4.589097	-0.328008
147	1	0	2.782078	-3.498790	-1.157483
148	1	0	-1.229319	-5.726649	0.179227
149	1	0	-2.018600	-4.192685	-0.299907
150	1	0	-1.987357	4.429746	-5.971922
151	1	0	-4.395943	4.592431	-5.361912
152	1	0	-5.397282	2.940283	-3.809166
153	1	0	-1.547856	0.963371	-3.442717
154	1	0	-0.588292	2.609679	-4.997791
155	1	0	-8.785308	0.010646	-3.613409
156	1	0	-8.186151	-1.506611	-5.490953
157	1	0	-5.793977	-1.925793	-6.030867
158	1	0	-4.002605	-0.828894	-4.698722
159	1	0	-7.006352	1.102076	-2.276412
160	1	0	-5.306866	-0.549506	0.691447
161	1	0	-6.429899	-2.714439	1.167536
162	1	0	-6.079516	-4.661791	-0.338980
163	1	0	-4.579798	-4.443662	-2.318427
164	1	0	-3.463160	-2.283781	-2.806264
165	1	0	-5.499141	1.248988	-0.728700
166	1	0	-3.996488	2.216190	-0.824571

167	6	0	-0.503256	1.095095	5.090993
168	6	0	-0.428805	1.069945	3.687328
169	6	0	-0.503026	-0.077575	2.924585
170	6	0	-0.836593	-1.387389	3.543170
171	8	0	0.257228	-2.144016	3.664710
172	6	0	0.218748	-3.553749	4.110671
173	6	0	-0.779561	-4.361071	3.276244
174	6	0	-0.103865	-3.590073	5.608484
175	6	0	1.650674	-4.018142	3.841703
176	8	0	-1.975611	-1.698710	3.864051
177	1	0	-0.631934	-5.428445	3.476703
178	1	0	-0.604157	-4.172851	2.211615
179	1	0	-1.810660	-4.093311	3.508462
180	1	0	-0.048582	-4.622311	5.972879
181	1	0	-1.107597	-3.206722	5.804383
182	1	0	0.621000	-2.992569	6.172376
183	1	0	1.775711	-5.059046	4.159293
184	1	0	2.370634	-3.396702	4.382337
185	1	0	1.875621	-3.954488	2.770395
186	1	0	-0.211298	2.007523	3.178041
187	6	0	-5.411819	3.167165	1.453843
188	6	0	-4.234965	3.456567	2.150118
189	6	0	-3.824396	2.660548	3.214001
190	6	0	-4.595232	1.539548	3.591496
191	6	0	-5.777466	1.251935	2.871705
192	6	0	-6.184501	2.059902	1.817820
193	6	0	-3.557737	-1.533575	6.546450
194	6	0	-3.536861	-2.368210	7.665493
195	6	0	-3.259355	-1.849547	8.931821
196	6	0	-2.989636	-0.486443	9.082721
197	6	0	-3.005423	0.359893	7.975796
198	6	0	-3.304838	-0.171073	6.718605
199	6	0	-4.305792	0.660202	4.699383
200	7	0	-3.351001	0.751227	5.598011
201	8	0	-2.454263	1.713192	5.613349
202	1	0	-5.721884	3.801808	0.627922
203	1	0	-3.626737	4.309446	1.854840
204	1	0	-2.919193	2.886325	3.757848
205	1	0	-6.376842	0.390055	3.154185
206	1	0	-7.100856	1.829669	1.282462
207	1	0	-3.702155	-1.939160	5.552089
208	1	0	-3.722038	-3.430897	7.539175
209	1	0	-3.242418	-2.506333	9.796694
210	1	0	-2.769492	-0.078699	10.065021
211	1	0	-2.802637	1.420363	8.068164
212	1	0	-4.994935	-0.156676	4.875540
213	1	0	-0.641513	0.152782	5.614575
214	6	0	0.107045	2.211679	5.874936
215	1	0	-0.282412	2.256586	6.893446
216	1	0	1.192273	2.039180	5.926077
217	1	0	-0.049306	3.175332	5.380592

4a-I

Standard orientation:

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

S-42

1	6	0	4.938672	-2.787781	-4.710321
2	6	0	5.685824	-3.575305	-3.825241
3	6	0	5.749370	-3.237335	-2.474043
4	6	0	5.065180	-2.103551	-1.987831
5	6	0	4.317481	-1.324534	-2.874267
6	6	0	4.254615	-1.669435	-4.230936
7	6	0	8.886628	-1.882887	0.663267
8	6	0	9.424552	-0.773502	0.005460
9	6	0	8.608085	0.008314	-0.819591
10	6	0	7.260536	-0.316654	-0.984659
11	6	0	6.714779	-1.425767	-0.317260
12	6	0	7.536653	-2.211238	0.502844
13	6	0	4.889045	-0.645241	2.832964
14	6	0	5.483418	0.166062	3.803043
15	6	0	6.012176	1.412008	3.450081
16	6	0	5.928477	1.851921	2.125145
17	6	0	5.337452	1.043322	1.150666
18	6	0	4.832860	-0.219334	1.496679
19	6	0	5.263371	-1.774201	-0.537547
20	6	0	4.245678	-1.110742	0.438044
21	6	0	4.523971	-2.606019	0.500465
22	6	0	2.802547	-0.680027	0.123320
23	8	0	2.489396	-0.402171	-1.069588
24	8	0	2.048829	-0.646468	1.147500
25	45	0	0.487071	0.097265	-1.522793
26	45	0	0.055987	-0.031624	0.953659
27	6	0	6.107589	2.976870	-1.888252
28	6	0	6.196082	3.934589	-0.870953
29	6	0	5.034609	4.465516	-0.308910
30	6	0	3.769887	4.043708	-0.761979
31	6	0	3.684469	3.057452	-1.751293
32	6	0	4.853549	2.532026	-2.314815
33	6	0	3.011838	8.534585	-0.613020
34	6	0	2.601638	8.729938	-1.935038
35	6	0	2.173584	7.639040	-2.699725
36	6	0	2.153967	6.357098	-2.145836
37	6	0	2.559340	6.161129	-0.816502
38	6	0	2.992784	7.253944	-0.052144
39	6	0	-0.405693	6.065084	0.422542
40	6	0	-1.471625	6.858710	-0.012791
41	6	0	-2.161990	6.530691	-1.183087
42	6	0	-1.785265	5.400046	-1.916568
43	6	0	-0.721283	4.605303	-1.486822
44	6	0	-0.014015	4.938135	-0.317730
45	6	0	2.569419	4.769956	-0.236157
46	6	0	1.184726	4.126491	0.073364
47	6	0	2.109106	4.568707	1.198053
48	6	0	0.905518	2.616579	-0.046915
49	8	0	0.934339	2.136230	-1.218509
50	8	0	0.629763	2.018839	1.037436
51	6	0	-4.730838	-2.863182	-3.818222
52	6	0	-5.078199	-3.882020	-2.923748
53	6	0	-4.107289	-4.442838	-2.092746
54	6	0	-2.777036	-3.987025	-2.150028
55	6	0	-2.440224	-2.941221	-3.017840
56	6	0	-3.416946	-2.387768	-3.853485

57	6	0	-1.904149	-8.457260	-2.117400
58	6	0	-1.109377	-8.537644	-3.264650
59	6	0	-0.515997	-7.381375	-3.783103
60	6	0	-0.715354	-6.148368	-3.158032
61	6	0	-1.508679	-6.067774	-2.003201
62	6	0	-2.106102	-7.226239	-1.485994
63	6	0	0.995061	-5.935119	0.135831
64	6	0	2.193669	-6.644887	0.018088
65	6	0	3.161088	-6.243471	-0.907485
66	6	0	2.930770	-5.119755	-1.708487
67	6	0	1.740057	-4.401225	-1.588009
68	6	0	0.756242	-4.812412	-0.672466
69	6	0	-1.749286	-4.729937	-1.353310
70	6	0	-0.548248	-4.075316	-0.613575
71	6	0	-1.731937	-4.634755	0.163288
72	6	0	-0.327333	-2.553404	-0.539773
73	8	0	0.006135	-1.967546	-1.611895
74	8	0	-0.467994	-2.049315	0.615674
75	6	0	-2.490513	2.963369	-5.900111
76	6	0	-3.425494	3.808587	-5.289412
77	6	0	-3.992225	3.453883	-4.065707
78	6	0	-3.628129	2.246861	-3.434993
79	6	0	-2.687033	1.411203	-4.042643
80	6	0	-2.121566	1.771859	-5.273006
81	6	0	-8.123245	2.248809	-2.564381
82	6	0	-8.446883	1.031882	-3.171423
83	6	0	-7.439169	0.099450	-3.441293
84	6	0	-6.113499	0.381317	-3.104700
85	6	0	-5.787970	1.598876	-2.488009
86	6	0	-6.797804	2.535128	-2.223294
87	6	0	-5.560529	0.766604	0.818105
88	6	0	-6.481119	-0.089569	1.430295
89	6	0	-6.539121	-1.437634	1.065683
90	6	0	-5.668963	-1.928365	0.085506
91	6	0	-4.753717	-1.076097	-0.535707
92	6	0	-4.701200	0.282940	-0.181562
93	6	0	-4.347527	1.904570	-2.164251
94	6	0	-3.756648	1.198549	-0.905528
95	6	0	-4.022155	2.699013	-0.910321
96	6	0	-2.290958	0.751388	-0.713518
97	8	0	-1.575427	0.595658	-1.736338
98	8	0	-1.951428	0.592251	0.504366
99	1	0	4.890878	-3.048631	-5.764842
100	1	0	6.220876	-4.447775	-4.193494
101	1	0	6.339252	-3.844419	-1.788847
102	1	0	3.744541	-0.452929	-2.512463
103	1	0	3.659095	-1.058932	-4.908951
104	1	0	9.518646	-2.494596	1.303806
105	1	0	10.473824	-0.518528	0.133021
106	1	0	9.024424	0.871392	-1.335373
107	1	0	6.624836	0.286518	-1.634183
108	1	0	7.127723	-3.077892	1.018400
109	1	0	4.442694	-1.603556	3.118201
110	1	0	5.532413	-0.172593	4.835124
111	1	0	6.482932	2.037924	4.203719
112	1	0	6.324031	2.826948	1.844441
113	1	0	5.268119	1.394958	0.118810

114	1	0	5.052333	-3.022967	1.354959
115	1	0	3.753020	-3.301185	0.156001
116	1	0	7.012941	2.581826	-2.343881
117	1	0	7.170907	4.272210	-0.525909
118	1	0	5.103426	5.222691	0.469799
119	1	0	2.702201	2.675800	-2.081326
120	1	0	4.777044	1.772653	-3.093395
121	1	0	3.349697	9.380552	-0.018179
122	1	0	2.616978	9.726682	-2.369555
123	1	0	1.855100	7.787814	-3.730098
124	1	0	1.820886	5.504796	-2.739803
125	1	0	3.320662	7.107272	0.974314
126	1	0	0.134638	6.336124	1.328520
127	1	0	-1.752380	7.743244	0.554709
128	1	0	-2.980394	7.157175	-1.529446
129	1	0	-2.314895	5.138329	-2.834784
130	1	0	-0.428379	3.713826	-2.064322
131	1	0	1.842821	5.422677	1.816804
132	1	0	2.583834	3.791833	1.803150
133	1	0	-5.481073	-2.446272	-4.486888
134	1	0	-6.102530	-4.246213	-2.886252
135	1	0	-4.370622	-5.251838	-1.414135
136	1	0	-1.412403	-2.542007	-3.036799
137	1	0	-3.143899	-1.584927	-4.539008
138	1	0	-2.368175	-9.354715	-1.713927
139	1	0	-0.952331	-9.496159	-3.753674
140	1	0	0.104257	-7.440987	-4.675853
141	1	0	-0.251605	-5.246052	-3.558839
142	1	0	-2.728965	-7.169233	-0.596572
143	1	0	0.241227	-6.263493	0.849767
144	1	0	2.367819	-7.517897	0.643206
145	1	0	4.087880	-6.803131	-1.007686
146	1	0	3.681798	-4.798186	-2.432509
147	1	0	1.570491	-3.504182	-2.201802
148	1	0	-1.608135	-5.529952	0.769514
149	1	0	-2.391595	-3.923985	0.667306
150	1	0	-2.050542	3.237530	-6.856222
151	1	0	-3.712813	4.739637	-5.772803
152	1	0	-4.729700	4.104872	-3.600019
153	1	0	-2.350793	0.488616	-3.542367
154	1	0	-1.380240	1.117881	-5.731488
155	1	0	-8.904280	2.977775	-2.358028
156	1	0	-9.478469	0.811086	-3.435649
157	1	0	-7.687680	-0.848070	-3.915817
158	1	0	-5.324722	-0.342025	-3.316367
159	1	0	-6.553385	3.487327	-1.758172
160	1	0	-5.535139	1.818747	1.096509
161	1	0	-7.168425	0.301860	2.177632
162	1	0	-7.266496	-2.099113	1.529239
163	1	0	-5.706354	-2.978308	-0.206832
164	1	0	-4.079985	-1.467943	-1.304215
165	1	0	-4.819741	3.113692	-0.297688
166	1	0	-3.167805	3.381145	-0.941927
167	6	0	-0.667671	0.786132	5.280876
168	6	0	-0.444910	0.902966	3.818103
169	6	0	-0.262550	-0.159227	2.995658
170	6	0	-0.267123	-1.553814	3.507110

171	8	0	0.972238	-1.902076	3.913086
172	6	0	1.351955	-3.300015	4.179869
173	6	0	1.145037	-4.134908	2.914238
174	6	0	0.564732	-3.847877	5.377077
175	6	0	2.840730	-3.179637	4.519946
176	8	0	-1.250794	-2.274418	3.526724
177	1	0	1.525448	-5.150691	3.073291
178	1	0	1.688864	-3.688710	2.074600
179	1	0	0.089304	-4.188964	2.642016
180	1	0	0.945045	-4.840656	5.644820
181	1	0	-0.498357	-3.924441	5.144518
182	1	0	0.691731	-3.193008	6.247413
183	1	0	3.270920	-4.172328	4.691581
184	1	0	2.982657	-2.577971	5.424303
185	1	0	3.383142	-2.693321	3.696149
186	1	0	-0.370078	1.908981	3.409022
187	6	0	-3.106768	5.357909	3.171303
188	6	0	-2.976140	4.513578	2.067111
189	6	0	-2.971699	3.133638	2.241746
190	6	0	-3.080312	2.579252	3.532134
191	6	0	-3.203916	3.440474	4.646147
192	6	0	-3.227996	4.816544	4.457127
193	6	0	-4.556077	-1.413183	4.155450
194	6	0	-5.054344	-2.684476	4.421063
195	6	0	-4.589358	-3.414621	5.516982
196	6	0	-3.617400	-2.861705	6.351582
197	6	0	-3.094827	-1.597929	6.089198
198	6	0	-3.554361	-0.884055	4.978113
199	6	0	-3.190751	1.135163	3.631540
200	7	0	-3.032296	0.425038	4.732056
201	8	0	-2.197838	0.937267	5.684547
202	1	0	-3.112008	6.435256	3.033338
203	1	0	-2.864823	4.930646	1.068220
204	1	0	-2.832103	2.462409	1.400235
205	1	0	-3.292875	3.027431	5.642528
206	1	0	-3.338808	5.472713	5.315095
207	1	0	-4.955756	-0.852096	3.315219
208	1	0	-5.820721	-3.096116	3.771572
209	1	0	-4.990614	-4.401652	5.724309
210	1	0	-3.257568	-3.415143	7.213388
211	1	0	-2.346097	-1.163548	6.737005
212	1	0	-3.558893	0.589030	2.766326
213	1	0	-0.426434	-0.214408	5.644422
214	6	0	-0.026268	1.861440	6.137232
215	1	0	-0.349187	1.783541	7.180615
216	1	0	1.061361	1.741593	6.100479
217	1	0	-0.277820	2.857963	5.761480

TS4a-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.918510	-2.820677	-4.703318
2	6	0	5.676469	-3.579101	-3.802233
3	6	0	5.752512	-3.200085	-2.462544

4	6	0	5.068899	-2.054635	-2.004645
5	6	0	4.310245	-1.304328	-2.906611
6	6	0	4.235774	-1.689941	-4.251620
7	6	0	8.921917	-1.665096	0.575318
8	6	0	9.417998	-0.553330	-0.110811
9	6	0	8.567192	0.190273	-0.936438
10	6	0	7.226761	-0.174839	-1.073850
11	6	0	6.723224	-1.286223	-0.377808
12	6	0	7.579345	-2.033713	0.442700
13	6	0	4.906280	-0.470510	2.775295
14	6	0	5.482812	0.382527	3.719921
15	6	0	5.969373	1.635189	3.331743
16	6	0	5.862103	2.038880	1.997047
17	6	0	5.288720	1.188522	1.047796
18	6	0	4.825563	-0.079586	1.429510
19	6	0	5.279277	-1.678988	-0.567438
20	6	0	4.255000	-1.014701	0.400044
21	6	0	4.574446	-2.499747	0.502717
22	6	0	2.800454	-0.629845	0.084353
23	8	0	2.475330	-0.377804	-1.110304
24	8	0	2.048335	-0.600671	1.111030
25	45	0	0.458383	0.059094	-1.555737
26	45	0	0.037107	-0.032660	0.914427
27	6	0	5.983315	3.093624	-2.025845
28	6	0	6.053033	4.069039	-1.024012
29	6	0	4.881686	4.577913	-0.461985
30	6	0	3.625590	4.116047	-0.899539
31	6	0	3.559841	3.115276	-1.875673
32	6	0	4.738572	2.611540	-2.438903
33	6	0	2.727038	8.583895	-0.806201
34	6	0	2.293719	8.747179	-2.125254
35	6	0	1.890349	7.632606	-2.868773
36	6	0	1.918564	6.358662	-2.296836
37	6	0	2.347410	6.194832	-0.970669
38	6	0	2.755921	7.311521	-0.227347
39	6	0	-0.616536	5.998647	0.342393
40	6	0	-1.718103	6.749675	-0.079473
41	6	0	-2.399983	6.403964	-1.249671
42	6	0	-1.979931	5.297417	-1.996059
43	6	0	-0.880372	4.544888	-1.579880
44	6	0	-0.181725	4.897375	-0.411647
45	6	0	2.409376	4.813651	-0.370843
46	6	0	1.050646	4.130887	-0.032615
47	6	0	1.975965	4.618080	1.072662
48	6	0	0.815902	2.614450	-0.131453
49	8	0	0.850194	2.112915	-1.292644
50	8	0	0.564232	2.023238	0.965541
51	6	0	-4.617141	-2.996418	-3.921532
52	6	0	-4.974457	-4.010853	-3.025714
53	6	0	-4.019804	-4.546620	-2.160269
54	6	0	-2.695448	-4.070346	-2.183554
55	6	0	-2.349446	-3.031061	-3.055140
56	6	0	-3.310026	-2.501996	-3.925024
57	6	0	-1.766157	-8.530469	-2.033410
58	6	0	-0.943239	-8.621921	-3.159845
59	6	0	-0.354892	-7.467532	-3.687990
60	6	0	-0.587040	-6.225309	-3.093083

61	6	0	-1.408284	-6.133599	-1.958846
62	6	0	-2.000980	-7.290228	-1.432212
63	6	0	1.026975	-5.929199	0.269836
64	6	0	2.234431	-6.630829	0.204775
65	6	0	3.221657	-6.249510	-0.708292
66	6	0	3.001882	-5.154375	-1.550831
67	6	0	1.801839	-4.444381	-1.483834
68	6	0	0.799257	-4.835252	-0.579732
69	6	0	-1.683838	-4.786643	-1.342471
70	6	0	-0.512001	-4.107530	-0.576354
71	6	0	-1.716333	-4.661788	0.171523
72	6	0	-0.301233	-2.585543	-0.524579
73	8	0	0.030986	-2.011707	-1.602823
74	8	0	-0.445665	-2.063303	0.624594
75	6	0	-2.701644	2.922982	-5.894378
76	6	0	-3.664691	3.716400	-5.258425
77	6	0	-4.195012	3.320786	-4.030863
78	6	0	-3.765023	2.124698	-3.421442
79	6	0	-2.797659	1.340087	-4.055338
80	6	0	-2.269087	1.741402	-5.289293
81	6	0	-8.248083	1.875737	-2.412694
82	6	0	-8.518410	0.687782	-3.097920
83	6	0	-7.466300	-0.159101	-3.463638
84	6	0	-6.149591	0.179120	-3.144585
85	6	0	-5.877064	1.367087	-2.448663
86	6	0	-6.931566	2.218100	-2.088702
87	6	0	-5.422243	0.493245	0.956756
88	6	0	-6.274714	-0.402395	1.609444
89	6	0	-6.389585	-1.720607	1.158466
90	6	0	-5.643356	-2.143318	0.053020
91	6	0	-4.793479	-1.252094	-0.606269
92	6	0	-4.686766	0.076600	-0.164052
93	6	0	-4.446978	1.733711	-2.144141
94	6	0	-3.802510	1.036599	-0.908682
95	6	0	-4.129866	2.524189	-0.884804
96	6	0	-2.322311	0.646987	-0.747108
97	8	0	-1.611889	0.492040	-1.774626
98	8	0	-1.955848	0.523097	0.469475
99	1	0	4.861466	-3.113483	-5.749126
100	1	0	6.210675	-4.460902	-4.149373
101	1	0	6.352384	-3.783284	-1.765326
102	1	0	3.739283	-0.424589	-2.564873
103	1	0	3.632905	-1.101759	-4.942684
104	1	0	9.581096	-2.247395	1.216104
105	1	0	10.461785	-0.267140	-0.004937
106	1	0	8.951327	1.054759	-1.474529
107	1	0	6.564743	0.398456	-1.724001
108	1	0	7.203413	-2.902276	0.979623
109	1	0	4.495366	-1.435944	3.086835
110	1	0	5.552548	0.070644	4.759424
111	1	0	6.427052	2.293833	4.065642
112	1	0	6.226283	3.018056	1.688881
113	1	0	5.202332	1.511662	0.007924
114	1	0	5.124036	-2.876299	1.362764
115	1	0	3.819333	-3.225688	0.188725
116	1	0	6.895939	2.714580	-2.480772
117	1	0	7.020988	4.437863	-0.691238

118	1	0	4.935646	5.349076	0.304300
119	1	0	2.586147	2.706799	-2.196191
120	1	0	4.677241	1.840430	-3.207087
121	1	0	3.044956	9.448767	-0.227531
122	1	0	2.271486	9.737796	-2.573617
123	1	0	1.553402	7.756645	-3.896591
124	1	0	1.604284	5.488389	-2.874392
125	1	0	3.100628	7.190455	0.796976
126	1	0	-0.086947	6.281212	1.251287
127	1	0	-2.035969	7.613233	0.501122
128	1	0	-3.247556	6.997306	-1.584543
129	1	0	-2.504895	5.021052	-2.912576
130	1	0	-0.554926	3.672210	-2.165947
131	1	0	1.688857	5.472541	1.682436
132	1	0	2.485520	3.868440	1.682449
133	1	0	-5.354615	-2.597658	-4.615089
134	1	0	-5.994233	-4.389878	-3.012502
135	1	0	-4.291484	-5.350490	-1.478434
136	1	0	-1.327949	-2.616523	-3.051672
137	1	0	-3.029558	-1.702834	-4.611522
138	1	0	-2.226932	-9.426540	-1.622779
139	1	0	-0.760958	-9.587714	-3.625461
140	1	0	0.286500	-7.535738	-4.565041
141	1	0	-0.128333	-5.324458	-3.502328
142	1	0	-2.646364	-7.224955	-0.559299
143	1	0	0.257790	-6.242235	0.974511
144	1	0	2.399919	-7.482629	0.861088
145	1	0	4.155368	-6.803751	-0.767406
146	1	0	3.767562	-4.850093	-2.266814
147	1	0	1.638330	-3.572390	-2.132740
148	1	0	-1.605700	-5.543412	0.800145
149	1	0	-2.401404	-3.949078	0.638364
150	1	0	-2.290615	3.228760	-6.853815
151	1	0	-4.003126	4.638679	-5.725620
152	1	0	-4.955272	3.930129	-3.545103
153	1	0	-2.416674	0.425269	-3.574550
154	1	0	-1.508414	1.126904	-5.769721
155	1	0	-9.063998	2.538082	-2.130223
156	1	0	-9.543238	0.422768	-3.347616
157	1	0	-7.673484	-1.083887	-3.998867
158	1	0	-5.327081	-0.476773	-3.432655
159	1	0	-6.730096	3.147025	-1.559921
160	1	0	-5.339836	1.518360	1.313452
161	1	0	-6.860286	-0.066794	2.463102
162	1	0	-7.059757	-2.413777	1.660838
163	1	0	-5.723631	-3.170314	-0.302957
164	1	0	-4.212912	-1.590826	-1.468488
165	1	0	-4.930295	2.892519	-0.245983
166	1	0	-3.308171	3.244412	-0.921434
167	6	0	-0.405710	0.945389	5.238136
168	6	0	-0.542226	1.000280	3.729979
169	6	0	-0.280277	-0.107280	2.922495
170	6	0	-0.240449	-1.477569	3.498039
171	8	0	1.008241	-1.789031	3.877951
172	6	0	1.417075	-3.173142	4.208927
173	6	0	1.179517	-4.071514	2.994341
174	6	0	0.666762	-3.658955	5.454302

175	6	0	2.912132	-3.015341	4.497776
176	8	0	-1.228243	-2.184750	3.569270
177	1	0	1.575334	-5.073614	3.194448
178	1	0	1.692550	-3.666411	2.115262
179	1	0	0.116274	-4.151176	2.759875
180	1	0	1.061048	-4.634950	5.759954
181	1	0	-0.402468	-3.752798	5.259402
182	1	0	0.814499	-2.960759	6.286241
183	1	0	3.359658	-3.993502	4.703210
184	1	0	3.071651	-2.370766	5.368815
185	1	0	3.424534	-2.562722	3.636630
186	1	0	-0.353784	1.968669	3.270906
187	6	0	-3.418283	5.293362	3.081606
188	6	0	-3.154581	4.427596	2.018630
189	6	0	-2.870394	3.085146	2.259780
190	6	0	-2.847725	2.590713	3.574319
191	6	0	-3.112412	3.467791	4.642353
192	6	0	-3.400074	4.806874	4.391919
193	6	0	-4.272047	-1.220272	4.620074
194	6	0	-4.791369	-2.462447	4.970346
195	6	0	-4.311344	-3.144955	6.090869
196	6	0	-3.300900	-2.569475	6.862556
197	6	0	-2.756322	-1.334359	6.515749
198	6	0	-3.230230	-0.667178	5.379448
199	6	0	-2.627918	1.137892	3.784289
200	7	0	-2.724089	0.611659	5.041489
201	8	0	-1.756344	1.144493	5.878257
202	1	0	-3.636748	6.340170	2.890984
203	1	0	-3.158268	4.800605	0.996161
204	1	0	-2.649120	2.409250	1.439339
205	1	0	-3.100672	3.097667	5.659919
206	1	0	-3.612512	5.472492	5.223537
207	1	0	-4.677021	-0.689206	3.762818
208	1	0	-5.586141	-2.891129	4.366865
209	1	0	-4.729459	-4.108578	6.365215
210	1	0	-2.928535	-3.082889	7.744462
211	1	0	-1.980506	-0.879913	7.118569
212	1	0	-2.982820	0.486495	2.988933
213	1	0	-0.065725	-0.042955	5.560197
214	6	0	0.471827	2.037390	5.826384
215	1	0	0.452083	2.001114	6.920248
216	1	0	1.505394	1.899090	5.493053
217	1	0	0.127850	3.024407	5.501543

5a-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.287044	4.394467	-4.687435
2	6	0	-4.268023	4.932261	-3.844669
3	6	0	-4.711061	4.208111	-2.738823
4	6	0	-4.176943	2.932969	-2.457981
5	6	0	-3.197037	2.402585	-3.300435
6	6	0	-2.754325	3.134443	-4.410522

7	6	0	-8.580950	2.248986	-1.287287
8	6	0	-8.863408	1.263255	-2.237097
9	6	0	-7.815170	0.583721	-2.867662
10	6	0	-6.489619	0.887058	-2.550036
11	6	0	-6.204797	1.871708	-1.590388
12	6	0	-7.255567	2.555693	-0.963371
13	6	0	-5.483129	0.239886	1.514830
14	6	0	-6.274062	-0.801790	2.008447
15	6	0	-6.440627	-1.972482	1.262665
16	6	0	-5.806529	-2.101014	0.022596
17	6	0	-5.015383	-1.063207	-0.476233
18	6	0	-4.857528	0.119228	0.263752
19	6	0	-4.768130	2.207658	-1.284600
20	6	0	-4.039342	1.248085	-0.296963
21	6	0	-4.375157	2.675896	0.108827
22	6	0	-2.558671	0.848293	-0.364652
23	8	0	-2.045721	0.625889	-1.495634
24	8	0	-1.987560	0.753091	0.770987
25	45	0	0.018013	0.214725	-1.608265
26	45	0	-0.005168	0.025392	0.890317
27	6	0	-5.014310	-2.225022	-4.132125
28	6	0	-5.433970	-3.365606	-3.436297
29	6	0	-4.543855	-4.041489	-2.602575
30	6	0	-3.218260	-3.584865	-2.449831
31	6	0	-2.806232	-2.442125	-3.141942
32	6	0	-3.704223	-1.767371	-3.980054
33	6	0	-2.578314	-8.144566	-2.338013
34	6	0	-1.781218	-8.248449	-3.481613
35	6	0	-1.155447	-7.109245	-3.999718
36	6	0	-1.324543	-5.870359	-3.377459
37	6	0	-2.119572	-5.766131	-2.225237
38	6	0	-2.750108	-6.907347	-1.709577
39	6	0	0.159170	-5.732405	0.450801
40	6	0	1.269891	-6.579785	0.511229
41	6	0	2.284661	-6.479743	-0.444708
42	6	0	2.192604	-5.519024	-1.457644
43	6	0	1.087544	-4.668086	-1.522471
44	6	0	0.055766	-4.781740	-0.575446
45	6	0	-2.318331	-4.417740	-1.584471
46	6	0	-1.151211	-3.897596	-0.694522
47	6	0	-2.473439	-4.317880	-0.073140
48	6	0	-0.738316	-2.424332	-0.594078
49	8	0	-0.404071	-1.845181	-1.666060
50	8	0	-0.739062	-1.933370	0.581660
51	6	0	5.096377	2.876451	-3.642467
52	6	0	5.515458	3.905295	-2.789763
53	6	0	4.619110	4.468149	-1.881938
54	6	0	3.286344	4.011682	-1.813717
55	6	0	2.876965	2.975162	-2.658123
56	6	0	3.781605	2.412967	-3.569190
57	6	0	2.734571	8.521646	-1.189851
58	6	0	1.917169	8.781356	-2.293736
59	6	0	1.245353	7.729079	-2.925557
60	6	0	1.388722	6.421436	-2.456238
61	6	0	2.204665	6.160601	-1.344367
62	6	0	2.880797	7.214985	-0.714141
63	6	0	-0.095837	5.966444	1.120959

64	6	0	-1.215651	6.796233	1.234698
65	6	0	-2.270528	6.683793	0.324977
66	6	0	-2.205749	5.731738	-0.698436
67	6	0	-1.094098	4.895261	-0.812135
68	6	0	-0.026458	5.011818	0.095135
69	6	0	2.376604	4.741394	-0.868840
70	6	0	1.178830	4.134015	-0.076746
71	6	0	2.488278	4.460984	0.622368
72	6	0	0.757584	2.661436	-0.173146
73	8	0	0.435451	2.246985	-1.324034
74	8	0	0.732832	2.011796	0.920327
75	6	0	3.224825	-3.777650	-5.053429
76	6	0	4.277319	-4.342655	-4.321789
77	6	0	4.727614	-3.723911	-3.156953
78	6	0	4.134032	-2.525610	-2.703962
79	6	0	3.084120	-1.968847	-3.437365
80	6	0	2.631918	-2.596322	-4.606567
81	6	0	8.552545	-1.896926	-1.407762
82	6	0	8.831660	-0.898683	-2.345131
83	6	0	7.780753	-0.233579	-2.986807
84	6	0	6.456554	-0.564168	-2.692586
85	6	0	6.174194	-1.562591	-1.745518
86	6	0	7.228078	-2.231206	-1.107703
87	6	0	5.299435	-0.252306	1.642128
88	6	0	6.100940	0.698722	2.279584
89	6	0	6.458527	1.876394	1.615353
90	6	0	5.999408	2.106785	0.314860
91	6	0	5.195645	1.160717	-0.327087
92	6	0	4.855093	-0.031701	0.328547
93	6	0	4.737339	-1.921717	-1.467838
94	6	0	4.025930	-1.070015	-0.374750
95	6	0	4.341868	-2.537961	-0.132135
96	6	0	2.557582	-0.630204	-0.400678
97	8	0	2.075280	-0.211470	-1.489147
98	8	0	1.959340	-0.705285	0.723004
99	1	0	-2.943239	4.956887	-5.552594
100	1	0	-4.688548	5.913025	-4.057222
101	1	0	-5.485294	4.621493	-2.093904
102	1	0	-2.744805	1.417453	-3.091897
103	1	0	-1.984295	2.711601	-5.055281
104	1	0	-9.394186	2.780793	-0.797215
105	1	0	-9.895002	1.025123	-2.486382
106	1	0	-8.032291	-0.183821	-3.608309
107	1	0	-5.672054	0.360043	-3.043947
108	1	0	-7.044672	3.326630	-0.225628
109	1	0	-5.355580	1.147135	2.103031
110	1	0	-6.766026	-0.696881	2.973453
111	1	0	-7.063717	-2.778701	1.643427
112	1	0	-5.933055	-3.010137	-0.565532
113	1	0	-4.523998	-1.170110	-1.447337
114	1	0	-5.133327	2.857331	0.868073
115	1	0	-3.561920	3.399153	0.207847
116	1	0	-5.704888	-1.702498	-4.790384
117	1	0	-6.453394	-3.728317	-3.551911
118	1	0	-4.867491	-4.939036	-2.076883
119	1	0	-1.780313	-2.044208	-3.030477
120	1	0	-3.368559	-0.877475	-4.513018

121	1	0	-3.067345	-9.028794	-1.933906
122	1	0	-1.647502	-9.212102	-3.967936
123	1	0	-0.534340	-7.187197	-4.890352
124	1	0	-0.839360	-4.981469	-3.781264
125	1	0	-3.374160	-6.834795	-0.821658
126	1	0	-0.621934	-5.812682	1.205327
127	1	0	1.339812	-7.319304	1.306762
128	1	0	3.141831	-7.147645	-0.403693
129	1	0	2.982721	-5.432617	-2.204692
130	1	0	1.023756	-3.906849	-2.306719
131	1	0	-2.519816	-5.217371	0.538541
132	1	0	-3.126818	-3.545870	0.338447
133	1	0	5.791907	2.443283	-4.357646
134	1	0	6.539484	4.269644	-2.840443
135	1	0	4.945185	5.276817	-1.229312
136	1	0	1.847777	2.569645	-2.614338
137	1	0	3.446587	1.605227	-4.220292
138	1	0	3.260502	9.338027	-0.698850
139	1	0	1.804189	9.798596	-2.661796
140	1	0	0.608770	7.928348	-3.785952
141	1	0	0.866877	5.599694	-2.947872
142	1	0	3.522753	7.019977	0.141923
143	1	0	0.728414	6.075914	1.824033
144	1	0	-1.258709	7.538925	2.028828
145	1	0	-3.135637	7.337739	0.407322
146	1	0	-3.021403	5.643452	-1.417928
147	1	0	-1.049094	4.143222	-1.609612
148	1	0	2.533155	5.281063	1.336476
149	1	0	3.120022	3.633448	0.957195
150	1	0	2.874182	-4.257515	-5.964202
151	1	0	4.746699	-5.261822	-4.666430
152	1	0	5.553492	-4.160471	-2.596107
153	1	0	2.583074	-1.040459	-3.105624
154	1	0	1.807954	-2.151405	-5.164051
155	1	0	9.367458	-2.416593	-0.907426
156	1	0	9.862331	-0.639079	-2.575780
157	1	0	7.995333	0.543492	-3.718049
158	1	0	5.637235	-0.049800	-3.196392
159	1	0	7.020789	-3.010013	-0.376757
160	1	0	5.010740	-1.159289	2.170821
161	1	0	6.444553	0.521350	3.296828
162	1	0	7.089639	2.611031	2.109863
163	1	0	6.267622	3.025033	-0.206572
164	1	0	4.833846	1.350030	-1.340581
165	1	0	5.100238	-2.810535	0.599528
166	1	0	3.521861	-3.260142	-0.117054
167	6	0	-1.922096	-1.174888	4.252912
168	6	0	-0.553814	-1.365925	3.519858
169	6	0	-0.099110	-0.132771	2.856339
170	6	0	0.310532	1.031103	3.682133
171	8	0	-0.612745	1.976861	3.755528
172	6	0	-0.372539	3.278007	4.451954
173	6	0	0.889310	3.944963	3.901010
174	6	0	-0.291716	3.016620	5.957133
175	6	0	-1.620900	4.078282	4.082211
176	8	0	1.426765	1.018403	4.178643
177	1	0	0.928434	4.978627	4.261183

178	1	0	0.858048	3.953391	2.805768
179	1	0	1.793307	3.423752	4.217250
180	1	0	-0.200664	3.972240	6.485407
181	1	0	0.573859	2.399764	6.207004
182	1	0	-1.194118	2.512838	6.317149
183	1	0	-1.594996	5.054098	4.577552
184	1	0	-2.528096	3.552324	4.394394
185	1	0	-1.666831	4.241046	2.998900
186	1	0	-0.661974	-2.165322	2.785145
187	6	0	2.332963	-5.605215	3.674327
188	6	0	2.546459	-4.454922	2.909654
189	6	0	1.905782	-3.261304	3.240190
190	6	0	1.043860	-3.204857	4.346010
191	6	0	0.830538	-4.358649	5.106615
192	6	0	1.472988	-5.552843	4.771180
193	6	0	0.856862	-0.679488	7.429041
194	6	0	0.962042	0.172191	8.527047
195	6	0	-0.179652	0.670294	9.159040
196	6	0	-1.435884	0.294833	8.679446
197	6	0	-1.559447	-0.553941	7.579759
198	6	0	-0.409964	-1.035507	6.932239
199	6	0	0.389208	-1.880216	4.710874
200	7	0	-0.509217	-1.964748	5.866308
201	8	0	-1.816005	-2.109516	5.351804
202	1	0	2.832361	-6.534142	3.413398
203	1	0	3.205008	-4.489375	2.045218
204	1	0	2.071920	-2.377807	2.626279
205	1	0	0.166514	-4.310541	5.962742
206	1	0	1.299691	-6.441593	5.371927
207	1	0	1.756400	-1.082100	6.974972
208	1	0	1.949466	0.438275	8.894430
209	1	0	-0.090889	1.328286	10.018245
210	1	0	-2.336199	0.659205	9.167479
211	1	0	-2.535593	-0.860964	7.225101
212	1	0	1.160752	-1.137318	4.916717
213	1	0	-2.002301	-0.158222	4.657568
214	6	0	-3.140286	-1.533872	3.426340
215	1	0	-4.048629	-1.449030	4.031406
216	1	0	-3.228430	-0.854128	2.571348
217	1	0	-3.063078	-2.558292	3.050551

7a-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.323782	-4.084324	-2.295405
2	6	0	6.105452	-4.190280	-1.138613
3	6	0	6.146195	-3.137797	-0.223797
4	6	0	5.404166	-1.963253	-0.456597
5	6	0	4.612296	-1.867371	-1.605717
6	6	0	4.576141	-2.926329	-2.521582
7	6	0	9.260218	-0.054034	1.121308
8	6	0	9.555856	0.749615	0.016226
9	6	0	8.557060	1.042712	-0.918609

10	6	0	7.266478	0.535552	-0.750221
11	6	0	6.967267	-0.265895	0.362280
12	6	0	7.969944	-0.563258	1.296313
13	6	0	5.395163	1.999982	2.436595
14	6	0	5.808311	3.325560	2.602856
15	6	0	5.703212	4.233867	1.545661
16	6	0	5.171891	3.815936	0.320507
17	6	0	4.753325	2.495104	0.149825
18	6	0	4.874611	1.574980	1.205198
19	6	0	5.582195	-0.836804	0.517033
20	6	0	4.468768	0.147268	0.983503
21	6	0	4.973535	-0.952916	1.905111
22	6	0	3.010088	0.075300	0.521578
23	8	0	2.787895	0.231865	-0.720379
24	8	0	2.145386	-0.089510	1.435770
25	45	0	0.809325	0.121853	-1.401355
26	45	0	0.115895	-0.001573	0.914889
27	6	0	4.058396	4.662018	-3.926313
28	6	0	4.240362	5.644152	-2.944994
29	6	0	3.293061	5.805168	-1.933849
30	6	0	2.151362	4.980679	-1.891007
31	6	0	1.976884	3.996594	-2.868566
32	6	0	2.930076	3.840177	-3.882735
33	6	0	0.043684	8.933710	-0.788630
34	6	0	-0.809536	8.976986	-1.894838
35	6	0	-1.033175	7.818163	-2.646550
36	6	0	-0.407969	6.620413	-2.293630
37	6	0	0.441973	6.573163	-1.176971
38	6	0	0.670661	7.736544	-0.429049
39	6	0	-1.371948	5.129995	1.655308
40	6	0	-2.668305	5.536344	1.984565
41	6	0	-3.690529	5.465061	1.033298
42	6	0	-3.414064	4.975186	-0.247140
43	6	0	-2.120729	4.565392	-0.581783
44	6	0	-1.089115	4.652996	0.365884
45	6	0	1.135071	5.280735	-0.829838
46	6	0	0.308913	4.247098	-0.009415
47	6	0	1.488752	4.977469	0.617961
48	6	0	0.402194	2.720838	-0.121043
49	8	0	0.636827	2.206112	-1.257366
50	8	0	0.207989	2.093672	0.967185
51	6	0	-0.494988	-3.938218	-5.760559
52	6	0	-1.193718	-4.990957	-5.156940
53	6	0	-0.963147	-5.304887	-3.817698
54	6	0	-0.031187	-4.564557	-3.063335
55	6	0	0.658859	-3.509725	-3.667687
56	6	0	0.425463	-3.199952	-5.013604
57	6	0	1.075503	-8.736257	-1.413542
58	6	0	2.390010	-8.747415	-1.888279
59	6	0	2.998044	-7.549713	-2.280516
60	6	0	2.296107	-6.345440	-2.197183
61	6	0	0.978514	-6.331266	-1.711625
62	6	0	0.368364	-7.532957	-1.325988
63	6	0	0.918565	-5.255341	1.807699
64	6	0	1.800663	-5.790571	2.750157
65	6	0	3.180261	-5.747686	2.525346
66	6	0	3.675789	-5.154646	1.359776

67	6	0	2.798592	-4.615043	0.415178
68	6	0	1.413002	-4.676341	0.628892
69	6	0	0.224697	-5.027169	-1.659791
70	6	0	0.469769	-4.133489	-0.407896
71	6	0	-0.869595	-4.825333	-0.623350
72	6	0	0.477345	-2.601106	-0.379385
73	8	0	0.915500	-1.974819	-1.392083
74	8	0	0.048070	-2.083863	0.700690
75	6	0	-2.631642	4.434666	-4.359248
76	6	0	-3.932025	4.445299	-3.840120
77	6	0	-4.427960	3.323969	-3.175020
78	6	0	-3.626177	2.175930	-3.018771
79	6	0	-2.324165	2.173282	-3.529338
80	6	0	-1.831926	3.300958	-4.198574
81	6	0	-7.656325	0.098502	-3.866008
82	6	0	-7.276597	-0.546616	-5.046567
83	6	0	-5.919465	-0.698700	-5.350932
84	6	0	-4.944669	-0.209374	-4.478482
85	6	0	-5.324723	0.431507	-3.288808
86	6	0	-6.685071	0.588838	-2.987820
87	6	0	-4.959729	-2.001327	-0.693732
88	6	0	-5.369217	-3.330267	-0.840221
89	6	0	-4.803070	-4.136372	-1.832172
90	6	0	-3.812071	-3.614726	-2.670953
91	6	0	-3.392970	-2.290797	-2.524758
92	6	0	-3.978105	-1.472202	-1.544322
93	6	0	-4.264247	0.982762	-2.372236
94	6	0	-3.553061	-0.036788	-1.435300
95	6	0	-4.507834	1.004303	-0.871149
96	6	0	-2.081894	0.041525	-1.017497
97	8	0	-1.208688	0.002953	-1.940708
98	8	0	-1.866194	0.093992	0.232024
99	1	0	5.302296	-4.899924	-3.015165
100	1	0	6.687470	-5.091971	-0.956732
101	1	0	6.766080	-3.215448	0.668552
102	1	0	4.001520	-0.969710	-1.791429
103	1	0	3.960120	-2.840086	-3.416070
104	1	0	10.036283	-0.285460	1.848578
105	1	0	10.560191	1.145695	-0.117255
106	1	0	8.784926	1.667603	-1.780428
107	1	0	6.487971	0.761848	-1.478546
108	1	0	7.748746	-1.191689	2.156443
109	1	0	5.484223	1.298102	3.265202
110	1	0	6.219063	3.646949	3.558296
111	1	0	6.036120	5.261498	1.673453
112	1	0	5.085637	4.519618	-0.508391
113	1	0	4.322850	2.171089	-0.803456
114	1	0	5.555065	-0.693784	2.788786
115	1	0	4.308641	-1.791589	2.127412
116	1	0	4.793664	4.540776	-4.718818
117	1	0	5.117729	6.287354	-2.976097
118	1	0	3.425862	6.580809	-1.180775
119	1	0	1.106893	3.324734	-2.829411
120	1	0	2.787489	3.069192	-4.638323
121	1	0	0.221635	9.834103	-0.203476
122	1	0	-1.298113	9.908765	-2.171276
123	1	0	-1.696225	7.849366	-3.509163

124	1	0	-0.578539	5.718708	-2.882702
125	1	0	1.335886	7.713543	0.431478
126	1	0	-0.583496	5.177367	2.404745
127	1	0	-2.880622	5.909922	2.984673
128	1	0	-4.697436	5.788133	1.288890
129	1	0	-4.206860	4.914009	-0.992132
130	1	0	-1.914444	4.180192	-1.582808
131	1	0	1.311474	5.717034	1.397154
132	1	0	2.405041	4.420001	0.828160
133	1	0	-0.669554	-3.697625	-6.806905
134	1	0	-1.911443	-5.569185	-5.735636
135	1	0	-1.493690	-6.135000	-3.352904
136	1	0	1.365255	-2.902134	-3.083195
137	1	0	0.965519	-2.374815	-5.475115
138	1	0	0.598940	-9.666545	-1.109796
139	1	0	2.939021	-9.684239	-1.953250
140	1	0	4.021015	-7.556018	-2.652082
141	1	0	2.768135	-5.413012	-2.507878
142	1	0	-0.655629	-7.534912	-0.958252
143	1	0	-0.158734	-5.276309	1.999413
144	1	0	1.411272	-6.237704	3.663313
145	1	0	3.865192	-6.170382	3.257156
146	1	0	4.749683	-5.111200	1.181914
147	1	0	3.193516	-4.147806	-0.489189
148	1	0	-1.166951	-5.641785	0.032397
149	1	0	-1.741721	-4.221911	-0.890022
150	1	0	-2.249110	5.304619	-4.888958
151	1	0	-4.558854	5.326821	-3.962095
152	1	0	-5.446042	3.326215	-2.786925
153	1	0	-1.672487	1.294700	-3.398053
154	1	0	-0.817784	3.287305	-4.596556
155	1	0	-8.711405	0.220225	-3.627767
156	1	0	-8.033929	-0.929075	-5.727362
157	1	0	-5.621038	-1.199409	-6.270318
158	1	0	-3.887594	-0.323436	-4.717268
159	1	0	-6.989640	1.092149	-2.072321
160	1	0	-5.402727	-1.378712	0.084443
161	1	0	-6.132965	-3.736700	-0.179546
162	1	0	-5.132390	-5.166159	-1.952114
163	1	0	-3.363592	-4.239327	-3.443846
164	1	0	-2.604874	-1.887720	-3.166070
165	1	0	-5.466766	0.691154	-0.459177
166	1	0	-4.096332	1.824660	-0.278037
167	6	0	-2.813035	1.232253	4.341863
168	6	0	-2.233994	-0.154712	4.149776
169	6	0	-0.796540	-0.447426	3.905588
170	6	0	0.198590	0.269086	4.822023
171	8	0	0.318855	1.557725	4.469032
172	6	0	1.340468	2.446048	5.069557
173	6	0	2.732486	1.866771	4.800605
174	6	0	1.059229	2.632686	6.563979
175	6	0	1.134003	3.751319	4.298166
176	8	0	0.783610	-0.289220	5.724854
177	1	0	3.494834	2.596092	5.096253
178	1	0	2.853336	1.658033	3.730379
179	1	0	2.894407	0.943348	5.358655
180	1	0	1.752122	3.375601	6.974859

181	1	0	1.184931	1.695530	7.108415
182	1	0	0.038622	2.999398	6.719594
183	1	0	1.870267	4.495991	4.617990
184	1	0	0.131036	4.151825	4.477894
185	1	0	1.248338	3.575349	3.222683
186	1	0	-0.526320	-0.134412	2.860590
187	6	0	-3.052345	-5.331234	4.163900
188	6	0	-2.353768	-4.586339	3.212863
189	6	0	-2.430957	-3.193162	3.209653
190	6	0	-3.200669	-2.524900	4.177774
191	6	0	-3.911118	-3.283412	5.125661
192	6	0	-3.836141	-4.674060	5.116570
193	6	0	-6.735788	0.325926	4.314930
194	6	0	-7.984600	0.225296	3.709866
195	6	0	-8.219159	-0.723874	2.710742
196	6	0	-7.177698	-1.561760	2.313878
197	6	0	-5.912379	-1.459525	2.895338
198	6	0	-5.686222	-0.517955	3.911036
199	6	0	-3.247802	-1.050727	4.238793
200	7	0	-4.447747	-0.409768	4.597937
201	8	0	-4.120668	0.955641	4.910209
202	1	0	-2.990192	-6.415853	4.163003
203	1	0	-1.734462	-5.085119	2.465877
204	1	0	-1.907092	-2.632958	2.440373
205	1	0	-4.508891	-2.769983	5.871842
206	1	0	-4.384992	-5.246319	5.859256
207	1	0	-6.553957	1.057873	5.092830
208	1	0	-8.783312	0.889683	4.029032
209	1	0	-9.198653	-0.806601	2.248723
210	1	0	-7.340025	-2.299300	1.531948
211	1	0	-5.112743	-2.107774	2.557704
212	1	0	-0.594237	-1.516788	3.976231
213	1	0	-2.281888	1.796375	5.116402
214	6	0	-2.911015	2.072254	3.065604
215	1	0	-3.461606	2.998165	3.266838
216	1	0	-1.910532	2.339858	2.705567
217	1	0	-3.422679	1.519805	2.271764

s-trans vinyl diazoacetate 2-**II** and aryl nitron 3**a** with an approach over *Re*-face
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.903755	-3.746240	-5.067957
2	6	0	3.273118	-3.853500	-4.794520
3	6	0	3.909108	-2.881071	-4.023828
4	6	0	3.186004	-1.780458	-3.517737
5	6	0	1.817180	-1.684515	-3.784859
6	6	0	1.181861	-2.666010	-4.558236
7	6	0	7.230653	0.097072	-4.588812
8	6	0	6.781482	1.004505	-5.552546
9	6	0	5.426054	1.347653	-5.607568
10	6	0	4.522063	0.787102	-4.702514
11	6	0	4.973212	-0.119756	-3.730701
12	6	0	6.330805	-0.466416	-3.678872
13	6	0	5.290114	1.866771	-1.108796

14	6	0	5.798707	3.167113	-1.182054
15	6	0	5.039963	4.187894	-1.761821
16	6	0	3.764488	3.905397	-2.262660
17	6	0	3.251034	2.609116	-2.191670
18	6	0	4.015960	1.577027	-1.621613
19	6	0	3.980176	-0.741261	-2.781833
20	6	0	3.477803	0.176591	-1.624948
21	6	0	4.391447	-1.004968	-1.340390
22	6	0	2.050065	0.132850	-1.058296
23	8	0	1.113816	0.353885	-1.877808
24	8	0	1.953585	-0.086459	0.191191
25	45	0	-0.871820	0.085601	-1.235158
26	45	0	0.026613	-0.026183	1.104640
27	6	0	0.964640	4.678670	-4.959440
28	6	0	1.295659	5.827292	-4.229049
29	6	0	0.858316	5.966555	-2.912965
30	6	0	0.077329	4.959695	-2.305438
31	6	0	-0.248331	3.816608	-3.038831
32	6	0	0.197745	3.678555	-4.360586
33	6	0	-1.733865	8.774928	-0.394441
34	6	0	-2.980670	8.682365	-1.018943
35	6	0	-3.380926	7.472567	-1.597456
36	6	0	-2.539234	6.359457	-1.551605
37	6	0	-1.289101	6.448884	-0.917424
38	6	0	-0.887293	7.662825	-0.343365
39	6	0	-1.362332	5.046597	2.507595
40	6	0	-2.362275	5.399880	3.418107
41	6	0	-3.709912	5.263024	3.070922
42	6	0	-4.054918	4.758480	1.813118
43	6	0	-3.059863	4.400119	0.899851
44	6	0	-1.706908	4.557479	1.237393
45	6	0	-0.387051	5.242414	-0.905310
46	6	0	-0.638005	4.215328	0.237621
47	6	0	0.629183	5.053946	0.213731
48	6	0	-0.528456	2.689705	0.094016
49	8	0	-1.081233	2.160801	-0.909860
50	8	0	0.089519	2.095961	1.036411
51	6	0	-5.531815	-3.191171	-2.710637
52	6	0	-5.498582	-4.481282	-2.165927
53	6	0	-4.327828	-4.962305	-1.583772
54	6	0	-3.160665	-4.166288	-1.533444
55	6	0	-3.207435	-2.876038	-2.067756
56	6	0	-4.387746	-2.395818	-2.655450
57	6	0	-1.692829	-8.531693	-1.739035
58	6	0	-1.116541	-8.483332	-3.011598
59	6	0	-0.809077	-7.246809	-3.590080
60	6	0	-1.076799	-6.062364	-2.900369
61	6	0	-1.653399	-6.109972	-1.621067
62	6	0	-1.962241	-7.349364	-1.042789
63	6	0	0.921919	-5.918878	0.490326
64	6	0	2.132507	-6.599873	0.334042
65	6	0	3.022152	-6.229447	-0.678354
66	6	0	2.695175	-5.173141	-1.534836
67	6	0	1.486658	-4.489817	-1.383466
68	6	0	0.589081	-4.858629	-0.368180
69	6	0	-1.959181	-4.818481	-0.906557
70	6	0	-0.721503	-4.136626	-0.238830

71	6	0	-1.831424	-4.737522	0.608462
72	6	0	-0.507858	-2.617994	-0.194126
73	8	0	-0.615586	-1.999578	-1.293542
74	8	0	-0.219792	-2.125270	0.941450
75	6	0	-5.539001	3.904857	-2.067058
76	6	0	-6.412578	3.917757	-0.972110
77	6	0	-6.362495	2.893845	-0.028001
78	6	0	-5.435499	1.837049	-0.160357
79	6	0	-4.565907	1.831436	-1.253884
80	6	0	-4.620456	2.863248	-2.201820
81	6	0	-9.009810	-0.384592	1.852174
82	6	0	-9.379839	-1.097710	0.708720
83	6	0	-8.486760	-1.204774	-0.363443
84	6	0	-7.229249	-0.602323	-0.293054
85	6	0	-6.852850	0.109311	0.858486
86	6	0	-7.750821	0.219583	1.929073
87	6	0	-4.556397	-1.769764	3.297225
88	6	0	-4.878755	-3.046087	3.765703
89	6	0	-5.277998	-4.044065	2.870433
90	6	0	-5.339171	-3.765279	1.501822
91	6	0	-5.015088	-2.491154	1.026868
92	6	0	-4.638757	-1.482031	1.924919
93	6	0	-5.501618	0.772587	0.898837
94	6	0	-4.325648	-0.098936	1.429667
95	6	0	-4.834317	1.087628	2.232025
96	6	0	-2.901709	-0.059433	0.864376
97	8	0	-2.766490	-0.205027	-0.385529
98	8	0	-1.977429	0.087880	1.725942
99	1	0	1.407283	-4.501106	-5.673413
100	1	0	3.841689	-4.692975	-5.189364
101	1	0	4.976622	-2.962248	-3.824338
102	1	0	1.207376	-0.851832	-3.383188
103	1	0	0.112826	-2.577086	-4.754420
104	1	0	8.283809	-0.173596	-4.546125
105	1	0	7.483169	1.442248	-6.258995
106	1	0	5.073403	2.053364	-6.357778
107	1	0	3.465113	1.052584	-4.743699
108	1	0	6.687246	-1.175980	-2.935890
109	1	0	5.896779	1.075647	-0.672172
110	1	0	6.792321	3.381369	-0.792478
111	1	0	5.442291	5.195908	-1.830443
112	1	0	3.167823	4.695386	-2.722337
113	1	0	2.251550	2.390275	-2.588339
114	1	0	5.416791	-0.832950	-1.020250
115	1	0	3.970521	-1.870540	-0.823414
116	1	0	1.302437	4.569604	-5.987568
117	1	0	1.888550	6.613423	-4.692063
118	1	0	1.106648	6.866692	-2.352129
119	1	0	-0.847167	3.000225	-2.591898
120	1	0	-0.061022	2.777862	-4.917585
121	1	0	-1.419353	9.714768	0.055019
122	1	0	-3.638574	9.547724	-1.055721
123	1	0	-4.351421	7.397492	-2.084885
124	1	0	-2.849534	5.417554	-2.006625
125	1	0	0.081496	7.744885	0.143678
126	1	0	-0.316003	5.147259	2.787403
127	1	0	-2.090074	5.784070	4.398892

128	1	0	-4.487003	5.547510	3.776736
129	1	0	-5.103405	4.645562	1.536232
130	1	0	-3.335692	3.997919	-0.079093
131	1	0	0.776308	5.828490	0.963324
132	1	0	1.579384	4.563006	-0.022429
133	1	0	-6.441794	-2.815700	-3.172109
134	1	0	-6.386264	-5.109215	-2.201585
135	1	0	-4.311367	-5.970321	-1.170194
136	1	0	-2.335178	-2.185973	-2.031624
137	1	0	-4.398202	-1.384777	-3.064320
138	1	0	-1.933479	-9.491981	-1.287417
139	1	0	-0.907280	-9.404050	-3.551246
140	1	0	-0.359336	-7.206652	-4.580441
141	1	0	-0.835875	-5.097299	-3.347823
142	1	0	-2.413394	-7.394759	-0.054074
143	1	0	0.230978	-6.224125	1.275249
144	1	0	2.377209	-7.425964	0.998417
145	1	0	3.960519	-6.764013	-0.804231
146	1	0	3.380507	-4.882021	-2.331369
147	1	0	1.233452	-3.667016	-2.060919
148	1	0	-1.638888	-5.630474	1.200310
149	1	0	-2.502655	-4.065294	1.152430
150	1	0	-5.580182	4.700005	-2.807609
151	1	0	-7.133972	4.724785	-0.861961
152	1	0	-7.053213	2.899552	0.814832
153	1	0	-3.809847	1.032658	-1.388250
154	1	0	-3.931818	2.843599	-3.046775
155	1	0	-9.701799	-0.299150	2.687750
156	1	0	-10.358520	-1.568494	0.651633
157	1	0	-8.772295	-1.759055	-1.255608
158	1	0	-6.535104	-0.681325	-1.131016
159	1	0	-7.471420	0.772061	2.823915
160	1	0	-4.226865	-1.001285	3.995758
161	1	0	-4.816414	-3.262294	4.830387
162	1	0	-5.538810	-5.033588	3.238195
163	1	0	-5.641034	-4.539130	0.796592
164	1	0	-5.053979	-2.282050	-0.045361
165	1	0	-5.358703	0.914000	3.169978
166	1	0	-4.210929	1.982118	2.307923
167	6	0	2.313492	2.243428	5.571695
168	6	0	1.738094	1.067764	4.880583
169	6	0	1.203725	1.077802	3.618935
170	6	0	0.736941	-0.089110	2.969445
171	6	0	0.714681	-1.378702	3.715621
172	8	0	1.663852	-2.208748	3.297672
173	6	0	1.781624	-3.599650	3.813897
174	6	0	0.451926	-4.340424	3.648408
175	6	0	2.247086	-3.540952	5.272281
176	6	0	2.856478	-4.195146	2.906579
177	8	0	-0.119545	-1.570506	4.584205
178	1	0	3.409594	2.105817	5.615199
179	1	0	1.960683	2.299725	6.609248
180	1	0	2.099500	3.180935	5.051810
181	1	0	1.774734	0.124082	5.422570
182	1	0	0.614766	-5.408434	3.830538
183	1	0	0.081850	-4.209872	2.625286
184	1	0	-0.305762	-3.972595	4.340718

185	1	0	2.423129	-4.557773	5.640655
186	1	0	1.490592	-3.071837	5.905745
187	1	0	3.186442	-2.983421	5.353341
188	1	0	3.059374	-5.230576	3.199740
189	1	0	3.787352	-3.625448	2.970625
190	1	0	2.516951	-4.194030	1.863177
191	1	0	1.143960	2.015798	3.071710
192	6	0	7.023552	-3.565639	4.111836
193	6	0	6.750707	-2.610318	5.094051
194	6	0	6.297877	-1.338091	4.748997
195	6	0	6.104736	-1.001733	3.390142
196	6	0	6.382589	-1.979181	2.407521
197	6	0	6.836861	-3.244004	2.763477
198	6	0	5.333147	3.773036	3.548571
199	6	0	4.927005	4.971296	2.967079
200	6	0	4.076554	4.962667	1.857225
201	6	0	3.632097	3.749006	1.331046
202	6	0	4.040663	2.538134	1.894649
203	6	0	4.900521	2.566118	2.994483
204	7	0	5.345103	1.341973	3.647030
205	8	0	5.443896	1.401677	4.932557
206	1	0	7.379654	-4.552935	4.392609
207	1	0	6.897460	-2.855130	6.142625
208	1	0	6.096350	-0.590689	5.503277
209	1	0	6.234259	-1.734870	1.358522
210	1	0	7.044019	-3.980010	1.991715
211	1	0	5.974123	3.747884	4.421249
212	1	0	5.272835	5.912884	3.382970
213	1	0	3.756813	5.898499	1.408804
214	1	0	2.949496	3.734100	0.479906
215	1	0	3.664292	1.601335	1.492738
216	1	0	5.559896	0.435559	1.845524
217	6	0	5.651894	0.287647	2.914091

TS3a-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.854226	-4.433535	-4.816320
2	6	0	2.074245	-5.015185	-4.449078
3	6	0	2.978419	-4.302330	-3.662681
4	6	0	2.679432	-2.991451	-3.235781
5	6	0	1.452747	-2.422273	-3.590784
6	6	0	0.546738	-3.143713	-4.380711
7	6	0	7.163877	-2.725092	-4.151675
8	6	0	7.100949	-1.771637	-5.171826
9	6	0	5.957566	-0.977268	-5.312643
10	6	0	4.881198	-1.133628	-4.436727
11	6	0	4.946082	-2.086154	-3.407571
12	6	0	6.090023	-2.885176	-3.270390
13	6	0	5.832972	-0.174655	-0.847855
14	6	0	6.767016	0.859129	-0.968996
15	6	0	6.437452	2.028641	-1.659765
16	6	0	5.162062	2.168301	-2.219061
17	6	0	4.225076	1.140878	-2.099016

18	6	0	4.559946	-0.046731	-1.424860
19	6	0	3.762171	-2.266559	-2.491255
20	6	0	3.571077	-1.173278	-1.396384
21	6	0	4.003411	-2.581663	-1.021327
22	6	0	2.191225	-0.692137	-0.907644
23	8	0	1.448271	-0.170791	-1.785777
24	8	0	1.959623	-0.833876	0.333313
25	45	0	-0.555065	0.298007	-1.295029
26	45	0	0.097971	-0.078116	1.113489
27	6	0	2.921048	3.871349	-4.937539
28	6	0	3.593268	4.854088	-4.199352
29	6	0	3.171008	5.166557	-2.908399
30	6	0	2.063730	4.504867	-2.334313
31	6	0	1.399468	3.524877	-3.075043
32	6	0	1.830866	3.209878	-4.371167
33	6	0	1.604791	8.754614	-0.540277
34	6	0	0.431239	9.084155	-1.223803
35	6	0	-0.338278	8.073917	-1.811899
36	6	0	0.062890	6.739942	-1.717273
37	6	0	1.238208	6.406378	-1.024169
38	6	0	2.010497	7.419907	-0.440057
39	6	0	0.566118	5.185577	2.417116
40	6	0	-0.275192	5.888301	3.284319
41	6	0	-1.568647	6.235465	2.881902
42	6	0	-2.023279	5.865319	1.612273
43	6	0	-1.187723	5.160374	0.741927
44	6	0	0.118396	4.830378	1.134465
45	6	0	1.664982	4.963411	-0.960266
46	6	0	1.032624	4.113184	0.180917
47	6	0	2.511694	4.460474	0.202258
48	6	0	0.604097	2.640893	0.053914
49	8	0	-0.041630	2.320136	-0.983266
50	8	0	0.915223	1.891984	1.032358
51	6	0	-5.933376	-0.897154	-3.138706
52	6	0	-6.446386	-2.099947	-2.636202
53	6	0	-5.606592	-2.994332	-1.976394
54	6	0	-4.231964	-2.710780	-1.803873
55	6	0	-3.732845	-1.502413	-2.296766
56	6	0	-4.581495	-0.604720	-2.962945
57	6	0	-4.597175	-7.306481	-1.945350
58	6	0	-3.955326	-7.513939	-3.169584
59	6	0	-3.142334	-6.510303	-3.708181
60	6	0	-2.971594	-5.303267	-3.027016
61	6	0	-3.614489	-5.094378	-1.796263
62	6	0	-4.429409	-6.100426	-1.257930
63	6	0	-1.377603	-5.909054	0.522425
64	6	0	-0.543189	-7.028389	0.454923
65	6	0	0.501267	-7.072298	-0.472955
66	6	0	0.708974	-5.989055	-1.333085
67	6	0	-0.123478	-4.869505	-1.271382
68	6	0	-1.176681	-4.821779	-0.343630
69	6	0	-3.437926	-3.772697	-1.093317
70	6	0	-2.088136	-3.628750	-0.316569
71	6	0	-3.410575	-3.714491	0.427748
72	6	0	-1.284049	-2.321175	-0.244655
73	8	0	-1.061479	-1.743770	-1.350473
74	8	0	-0.902271	-1.954364	0.907786

75	6	0	-3.450953	5.516433	-2.401902
76	6	0	-4.324702	5.870679	-1.365930
77	6	0	-4.705568	4.921069	-0.419682
78	6	0	-4.217977	3.597727	-0.490346
79	6	0	-3.341889	3.252919	-1.522761
80	6	0	-2.963017	4.211173	-2.473779
81	6	0	-8.472671	2.893268	1.283599
82	6	0	-9.010813	2.347360	0.115160
83	6	0	-8.157830	1.897769	-0.899226
84	6	0	-6.773387	1.993063	-0.746560
85	6	0	-6.230203	2.535401	0.430331
86	6	0	-7.086541	2.989578	1.442860
87	6	0	-4.938457	-0.023450	2.993140
88	6	0	-5.740688	-1.081123	3.429170
89	6	0	-6.432924	-1.867813	2.502389
90	6	0	-6.307076	-1.603062	1.135369
91	6	0	-5.503374	-0.548341	0.693025
92	6	0	-4.829657	0.258379	1.621429
93	6	0	-4.734244	2.653457	0.558996
94	6	0	-3.997809	1.419979	1.159105
95	6	0	-4.082392	2.724539	1.934528
96	6	0	-2.623457	0.924986	0.689678
97	8	0	-2.477388	0.712879	-0.550738
98	8	0	-1.766393	0.747491	1.610498
99	1	0	0.150603	-4.985746	-5.435027
100	1	0	2.318729	-6.020965	-4.783887
101	1	0	3.930813	-4.753778	-3.390062
102	1	0	1.161800	-1.410028	-3.244151
103	1	0	-0.406445	-2.684814	-4.646490
104	1	0	8.049958	-3.347136	-4.043244
105	1	0	7.937165	-1.648404	-5.856228
106	1	0	5.904791	-0.235434	-6.107741
107	1	0	3.987708	-0.517449	-4.545839
108	1	0	6.143548	-3.634484	-2.484439
109	1	0	6.108182	-1.090291	-0.329228
110	1	0	7.758141	0.745205	-0.534287
111	1	0	7.171587	2.823115	-1.771337
112	1	0	4.895929	3.077674	-2.762060
113	1	0	3.223597	1.251986	-2.537162
114	1	0	5.012055	-2.763606	-0.659879
115	1	0	3.283509	-3.216369	-0.498938
116	1	0	3.246449	3.628548	-5.946441
117	1	0	4.439833	5.378345	-4.637396
118	1	0	3.687962	5.939964	-2.342107
119	1	0	0.537328	2.971992	-2.652609
120	1	0	1.303613	2.438866	-4.933495
121	1	0	2.205662	9.537975	-0.082946
122	1	0	0.116082	10.122321	-1.298750
123	1	0	-1.253245	8.327189	-2.344590
124	1	0	-0.535222	5.952373	-2.179099
125	1	0	2.925305	7.173086	0.093199
126	1	0	1.567196	4.908866	2.739639
127	1	0	0.078651	6.167286	4.274110
128	1	0	-2.219085	6.790257	3.553974
129	1	0	-3.031916	6.127868	1.292468
130	1	0	-1.551623	4.865838	-0.246690
131	1	0	2.890968	5.151426	0.951540

132	1	0	3.239237	3.670433	0.002866
133	1	0	-6.584420	-0.200394	-3.660561
134	1	0	-7.500160	-2.336950	-2.764590
135	1	0	-6.016544	-3.929337	-1.595807
136	1	0	-2.668343	-1.197690	-2.164894
137	1	0	-4.165338	0.332370	-3.335354
138	1	0	-5.230191	-8.084972	-1.524674
139	1	0	-4.086862	-8.452544	-3.702552
140	1	0	-2.640721	-6.669853	-4.660738
141	1	0	-2.336432	-4.519941	-3.442709
142	1	0	-4.934137	-5.944827	-0.307062
143	1	0	-2.192217	-5.887132	1.245426
144	1	0	-0.713962	-7.870086	1.122438
145	1	0	1.144733	-7.946379	-0.530612
146	1	0	1.518717	-6.015777	-2.062461
147	1	0	0.040113	-4.025608	-1.950556
148	1	0	-3.641704	-4.595337	1.023758
149	1	0	-3.798699	-2.816329	0.919410
150	1	0	-3.158640	6.253757	-3.145544
151	1	0	-4.710310	6.885989	-1.303563
152	1	0	-5.397141	5.196352	0.376059
153	1	0	-2.913637	2.232912	-1.603893
154	1	0	-2.276816	3.923450	-3.270709
155	1	0	-9.132697	3.243838	2.074489
156	1	0	-10.088737	2.271380	-0.006013
157	1	0	-8.573679	1.472083	-1.810536
158	1	0	-6.108314	1.646871	-1.539579
159	1	0	-6.676765	3.415141	2.356628
160	1	0	-4.384671	0.574288	3.716674
161	1	0	-5.824610	-1.291991	4.493252
162	1	0	-7.065734	-2.683045	2.844421
163	1	0	-6.834883	-2.216418	0.405869
164	1	0	-5.398470	-0.353420	-0.377761
165	1	0	-4.690940	2.773516	2.835424
166	1	0	-3.178062	3.326372	2.055801
167	6	0	2.107551	1.793738	5.842255
168	6	0	1.852199	0.543924	5.059068
169	6	0	1.445274	0.609669	3.696578
170	6	0	0.642322	-0.317180	3.083186
171	6	0	0.008816	-1.408518	3.876543
172	8	0	0.416942	-2.625981	3.501958
173	6	0	-0.251058	-3.849632	4.004090
174	6	0	-1.744829	-3.810352	3.669358
175	6	0	-0.001751	-4.000490	5.509858
176	6	0	0.454080	-4.950326	3.213338
177	8	0	-0.815358	-1.165876	4.745661
178	1	0	2.698712	1.597090	6.740453
179	1	0	1.131996	2.190943	6.157302
180	1	0	2.602720	2.557908	5.236701
181	1	0	1.487820	-0.299660	5.637250
182	1	0	-2.188750	-4.787619	3.890391
183	1	0	-1.876833	-3.590443	2.605265
184	1	0	-2.264845	-3.047008	4.249561
185	1	0	-0.389915	-4.968602	5.847661
186	1	0	-0.500844	-3.208465	6.070468
187	1	0	1.071511	-3.972416	5.724360
188	1	0	0.037130	-5.929480	3.472695

189	1	0	1.526731	-4.959871	3.424235
190	1	0	0.315793	-4.788821	2.137324
191	1	0	1.748126	1.486432	3.127302
192	6	0	4.227872	-5.410852	4.660620
193	6	0	3.955263	-4.382106	5.567852
194	6	0	3.949738	-3.053456	5.153908
195	6	0	4.242350	-2.736353	3.809247
196	6	0	4.514523	-3.785116	2.902499
197	6	0	4.500411	-5.109591	3.322735
198	6	0	5.334604	1.901207	4.126122
199	6	0	5.812881	3.085006	3.569457
200	6	0	5.610385	3.355915	2.213052
201	6	0	4.918533	2.443709	1.415143
202	6	0	4.432429	1.251723	1.954000
203	6	0	4.663594	0.991189	3.305076
204	7	0	4.225587	-0.251994	3.908208
205	8	0	3.697722	-0.158174	5.118315
206	1	0	4.225858	-6.444532	4.994652
207	1	0	3.744800	-4.617813	6.606949
208	1	0	3.747012	-2.253947	5.852459
209	1	0	4.735948	-3.547968	1.865220
210	1	0	4.704871	-5.905176	2.612708
211	1	0	5.478847	1.668054	5.174255
212	1	0	6.347594	3.793186	4.194968
213	1	0	5.983367	4.279858	1.781873
214	1	0	4.732907	2.660881	0.363524
215	1	0	3.847227	0.566428	1.346243
216	1	0	4.848859	-1.295737	2.307747
217	6	0	4.413241	-1.396500	3.295616

4a-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.089390	1.719848	-2.783651
2	6	0	-7.052619	0.976200	-2.089936
3	6	0	-6.675808	-0.161564	-1.379221
4	6	0	-5.327387	-0.582453	-1.347477
5	6	0	-4.369090	0.177559	-2.024003
6	6	0	-4.753568	1.320279	-2.741372
7	6	0	-7.794165	-4.463546	-1.157740
8	6	0	-7.423060	-4.989166	-2.398607
9	6	0	-6.282418	-4.503036	-3.047382
10	6	0	-5.515057	-3.495528	-2.458998
11	6	0	-5.884537	-2.969517	-1.210763
12	6	0	-7.029104	-3.455569	-0.562816
13	6	0	-4.021669	-4.692513	0.901541
14	6	0	-3.767745	-6.063055	0.792306
15	6	0	-2.922191	-6.544511	-0.211108
16	6	0	-2.327343	-5.648513	-1.106015
17	6	0	-2.578130	-4.279142	-1.002346
18	6	0	-3.431239	-3.790675	0.002129
19	6	0	-5.059879	-1.861567	-0.605682
20	6	0	-3.726158	-2.320713	0.065071
21	6	0	-4.879827	-1.798883	0.904786

22	6	0	-2.427070	-1.499769	0.024760
23	8	0	-2.012688	-1.190815	-1.134135
24	8	0	-1.883308	-1.238708	1.139053
25	45	0	-0.547737	0.293776	-1.292699
26	45	0	-0.080288	-0.079569	1.161514
27	6	0	-1.316718	-4.725639	-4.751390
28	6	0	-0.538407	-5.799147	-4.299411
29	6	0	0.532845	-5.569358	-3.437934
30	6	0	0.848680	-4.259237	-3.017325
31	6	0	0.064452	-3.194132	-3.466068
32	6	0	-1.014669	-3.430574	-4.329455
33	6	0	4.993610	-6.240733	-3.343023
34	6	0	5.509655	-5.434382	-4.361380
35	6	0	4.907072	-4.204327	-4.648172
36	6	0	3.793817	-3.780507	-3.919476
37	6	0	3.278556	-4.586816	-2.891854
38	6	0	3.879969	-5.821037	-2.608618
39	6	0	4.587911	-3.318231	0.052324
40	6	0	5.928817	-2.943928	0.180663
41	6	0	6.435384	-1.875982	-0.565351
42	6	0	5.590836	-1.175236	-1.433671
43	6	0	4.251176	-1.545495	-1.566026
44	6	0	3.742249	-2.631741	-0.834177
45	6	0	2.058763	-4.124000	-2.137988
46	6	0	2.316476	-3.054971	-1.035390
47	6	0	1.899524	-4.469743	-0.663293
48	6	0	1.358050	-1.894160	-0.698130
49	8	0	0.940939	-1.193594	-1.659233
50	8	0	1.120456	-1.745948	0.540373
51	6	0	-0.882575	6.082444	-3.284950
52	6	0	-1.406258	6.947375	-2.315473
53	6	0	-2.072482	6.429659	-1.206335
54	6	0	-2.229503	5.035215	-1.045738
55	6	0	-1.700557	4.178971	-2.014277
56	6	0	-1.030074	4.704008	-3.128126
57	6	0	-6.104760	6.678946	0.958553
58	6	0	-6.960356	6.293517	-0.076964
59	6	0	-6.529042	5.356429	-1.022764
60	6	0	-5.248674	4.807168	-0.933943
61	6	0	-4.389358	5.188109	0.110272
62	6	0	-4.821749	6.130417	1.053624
63	6	0	-4.190342	2.766925	3.038627
64	6	0	-5.343501	2.296981	3.672680
65	6	0	-6.401020	1.779941	2.916995
66	6	0	-6.295374	1.721621	1.524086
67	6	0	-5.143833	2.189151	0.884576
68	6	0	-4.091527	2.729010	1.638080
69	6	0	-3.003170	4.600321	0.167053
70	6	0	-2.864743	3.265175	0.955915
71	6	0	-2.244340	4.547373	1.487496
72	6	0	-1.938625	2.103120	0.566925
73	8	0	-1.960007	1.715342	-0.639419
74	8	0	-1.254369	1.621450	1.522434
75	6	0	4.280197	0.392333	-5.002297
76	6	0	5.388333	1.020101	-4.419282
77	6	0	5.223946	1.810881	-3.283370
78	6	0	3.946709	1.988953	-2.708255

79	6	0	2.846072	1.358435	-3.294134
80	6	0	3.016326	0.563559	-4.436603
81	6	0	5.992679	6.050682	-1.904983
82	6	0	5.166592	6.829433	-2.720031
83	6	0	3.926172	6.330135	-3.133124
84	6	0	3.512209	5.057993	-2.733123
85	6	0	4.338195	4.277103	-1.908519
86	6	0	5.582617	4.776626	-1.499311
87	6	0	3.161276	4.608181	1.450760
88	6	0	2.808343	5.842043	2.005719
89	6	0	1.785761	6.603803	1.433048
90	6	0	1.106651	6.121574	0.308938
91	6	0	1.452135	4.888317	-0.247672
92	6	0	2.493476	4.130477	0.312809
93	6	0	3.884400	2.896382	-1.512659
94	6	0	2.883488	2.826809	-0.322155
95	6	0	4.304714	2.314470	-0.167866
96	6	0	1.716036	1.828798	-0.230698
97	8	0	0.943538	1.781321	-1.229007
98	8	0	1.625480	1.175116	0.853631
99	1	0	-6.382601	2.600424	-3.349795
100	1	0	-8.095560	1.284105	-2.110647
101	1	0	-7.433123	-0.740261	-0.851783
102	1	0	-3.285524	-0.078464	-2.000814
103	1	0	-3.987963	1.896773	-3.262282
104	1	0	-8.681486	-4.838402	-0.652018
105	1	0	-8.018795	-5.773407	-2.859338
106	1	0	-5.990963	-4.910619	-4.013560
107	1	0	-4.624906	-3.114998	-2.961485
108	1	0	-7.326211	-3.048702	0.401147
109	1	0	-4.687269	-4.326886	1.682172
110	1	0	-4.238312	-6.755960	1.486299
111	1	0	-2.732974	-7.611129	-0.300920
112	1	0	-1.669930	-6.015541	-1.895223
113	1	0	-2.111802	-3.578749	-1.706612
114	1	0	-5.425826	-2.475868	1.558368
115	1	0	-4.779768	-0.816206	1.376720
116	1	0	-2.151615	-4.902519	-5.425522
117	1	0	-0.767922	-6.811355	-4.625106
118	1	0	1.139578	-6.406397	-3.096223
119	1	0	0.261226	-2.153410	-3.138842
120	1	0	-1.619899	-2.587450	-4.664355
121	1	0	5.457459	-7.199693	-3.121357
122	1	0	6.375556	-5.762598	-4.931714
123	1	0	5.305117	-3.575619	-5.442746
124	1	0	3.319931	-2.823886	-4.144415
125	1	0	3.480229	-6.457229	-1.822546
126	1	0	4.211492	-4.169299	0.617587
127	1	0	6.584401	-3.504542	0.844076
128	1	0	7.485162	-1.604552	-0.488848
129	1	0	5.977676	-0.343256	-2.025211
130	1	0	3.592146	-0.995081	-2.249050
131	1	0	2.604957	-5.136442	-0.174301
132	1	0	0.889589	-4.627589	-0.276322
133	1	0	-0.367380	6.484252	-4.153764
134	1	0	-1.298144	8.023440	-2.431983
135	1	0	-2.488897	7.106383	-0.460763

136	1	0	-1.781701	3.076537	-1.919199
137	1	0	-0.622274	4.019128	-3.871794
138	1	0	-6.436716	7.406927	1.695926
139	1	0	-7.958358	6.719182	-0.147794
140	1	0	-7.192950	5.053442	-1.830200
141	1	0	-4.910168	4.079436	-1.673518
142	1	0	-4.163210	6.435471	1.864241
143	1	0	-3.360652	3.148866	3.631870
144	1	0	-5.415581	2.331633	4.757645
145	1	0	-7.300871	1.422974	3.411673
146	1	0	-7.110490	1.313071	0.927963
147	1	0	-5.062755	2.133294	-0.204179
148	1	0	-2.654234	5.011092	2.382435
149	1	0	-1.157189	4.654229	1.469843
150	1	0	4.404847	-0.220433	-5.891944
151	1	0	6.375627	0.896619	-4.858786
152	1	0	6.085636	2.311682	-2.844901
153	1	0	1.825144	1.455581	-2.868105
154	1	0	2.144901	0.077550	-4.877495
155	1	0	6.958170	6.436076	-1.584721
156	1	0	5.485879	7.820815	-3.033100
157	1	0	3.280372	6.934522	-3.768072
158	1	0	2.546672	4.666163	-3.056628
159	1	0	6.231751	4.176067	-0.867974
160	1	0	3.953852	4.017852	1.903415
161	1	0	3.332474	6.211055	2.883930
162	1	0	1.517287	7.567321	1.859821
163	1	0	0.303330	6.707633	-0.140209
164	1	0	0.907870	4.505277	-1.117652
165	1	0	5.002529	2.853255	0.468655
166	1	0	4.468994	1.238733	-0.095488
167	6	0	2.034464	0.126600	5.047839
168	6	0	1.500136	0.273684	3.666177
169	6	0	0.415606	-0.354806	3.160400
170	6	0	-0.444057	-1.176858	4.054733
171	8	0	-0.668579	-2.410160	3.580320
172	6	0	-1.686365	-3.294390	4.185706
173	6	0	-3.059002	-2.614855	4.132145
174	6	0	-1.281255	-3.675089	5.615417
175	6	0	-1.652960	-4.513753	3.264959
176	8	0	-0.905015	-0.730851	5.099067
177	1	0	-3.831271	-3.333756	4.429011
178	1	0	-3.261547	-2.276445	3.110743
179	1	0	-3.103608	-1.754840	4.802112
180	1	0	-1.970841	-4.436911	5.997929
181	1	0	-1.311772	-2.807970	6.276203
182	1	0	-0.270107	-4.096550	5.627518
183	1	0	-2.415208	-5.239913	3.567387
184	1	0	-0.675201	-5.002524	3.298386
185	1	0	-1.851841	-4.210852	2.230412
186	1	0	2.020719	0.994424	3.034803
187	6	0	2.434827	-5.252165	4.689258
188	6	0	2.173447	-4.912389	3.358967
189	6	0	2.483059	-3.640882	2.889788
190	6	0	3.073308	-2.693295	3.753119
191	6	0	3.306689	-3.033621	5.105575
192	6	0	2.994219	-4.308938	5.559936

193	6	0	5.936570	0.037302	2.290202
194	6	0	6.870638	0.927637	1.766024
195	6	0	6.897906	2.256014	2.196061
196	6	0	5.974822	2.696423	3.148047
197	6	0	5.020999	1.824592	3.667318
198	6	0	5.000199	0.496171	3.226319
199	6	0	3.575707	-1.479420	3.150495
200	7	0	4.061199	-0.423113	3.779388
201	8	0	3.574028	-0.078891	5.012780
202	1	0	2.197052	-6.248127	5.052081
203	1	0	1.722861	-5.637139	2.688178
204	1	0	2.243735	-3.346927	1.870070
205	1	0	3.758139	-2.310660	5.774653
206	1	0	3.191860	-4.573454	6.594323
207	1	0	5.955217	-1.007481	1.989427
208	1	0	7.591774	0.571117	1.036870
209	1	0	7.640813	2.941341	1.799924
210	1	0	5.995214	3.726288	3.491371
211	1	0	4.307537	2.159135	4.408281
212	1	0	3.725736	-1.470507	2.072892
213	1	0	1.655339	-0.769152	5.542002
214	6	0	1.860255	1.336944	5.951073
215	1	0	0.797839	1.405967	6.202040
216	1	0	2.437505	1.229306	6.875971
217	1	0	2.157502	2.261757	5.445260

TS4a-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-6.134304	0.919682	-3.042584
2	6	0	-6.969559	0.062887	-2.314169
3	6	0	-6.422784	-0.996946	-1.593008
4	6	0	-5.028526	-1.219218	-1.586185
5	6	0	-4.200375	-0.356917	-2.309109
6	6	0	-4.755258	0.707225	-3.034377
7	6	0	-6.593233	-5.608473	-1.335829
8	6	0	-6.235000	-5.946767	-2.643503
9	6	0	-5.332572	-5.141457	-3.347640
10	6	0	-4.789453	-4.004202	-2.747033
11	6	0	-5.141759	-3.666913	-1.429254
12	6	0	-6.050788	-4.471400	-0.728430
13	6	0	-2.591610	-4.636140	1.261934
14	6	0	-2.090510	-5.936939	1.351874
15	6	0	-1.611951	-6.584196	0.208147
16	6	0	-1.623787	-5.918133	-1.021302
17	6	0	-2.122028	-4.615567	-1.114109
18	6	0	-2.626194	-3.972054	0.025961
19	6	0	-4.561479	-2.420995	-0.813524
20	6	0	-3.203801	-2.589419	-0.070539
21	6	0	-4.475479	-2.277883	0.701353
22	6	0	-2.074783	-1.547591	-0.095257
23	8	0	-1.684664	-1.163047	-1.236997
24	8	0	-1.620679	-1.201670	1.038833
25	45	0	-0.309262	0.427544	-1.375863

26	45	0	0.029493	0.135374	1.100479
27	6	0	-1.345393	-4.239202	-4.861269
28	6	0	-0.569687	-5.360596	-4.539781
29	6	0	0.484903	-5.242994	-3.637460
30	6	0	0.792966	-4.001174	-3.034391
31	6	0	0.003154	-2.892803	-3.349495
32	6	0	-1.056236	-3.014025	-4.262259
33	6	0	4.756814	-6.421908	-3.124417
34	6	0	5.344061	-5.722677	-4.182509
35	6	0	4.838417	-4.472364	-4.555952
36	6	0	3.751250	-3.922169	-3.874024
37	6	0	3.163567	-4.620925	-2.806718
38	6	0	3.668335	-5.875507	-2.437176
39	6	0	4.501135	-3.585463	0.211063
40	6	0	5.887516	-3.462956	0.345918
41	6	0	6.592885	-2.549833	-0.443108
42	6	0	5.902942	-1.740657	-1.352886
43	6	0	4.519027	-1.860614	-1.493858
44	6	0	3.812025	-2.803520	-0.729355
45	6	0	1.974826	-4.014138	-2.103491
46	6	0	2.344239	-2.999839	-0.972093
47	6	0	1.708941	-4.340104	-0.639356
48	6	0	1.553769	-1.720088	-0.662374
49	8	0	1.227268	-0.999748	-1.643454
50	8	0	1.312054	-1.503097	0.568999
51	6	0	-1.542362	6.111802	-3.630524
52	6	0	-2.112578	6.923860	-2.641789
53	6	0	-2.687766	6.346060	-1.511060
54	6	0	-2.707173	4.943681	-1.353484
55	6	0	-2.134627	4.139670	-2.341723
56	6	0	-1.552189	4.725074	-3.474105
57	6	0	-6.798563	6.045654	0.557741
58	6	0	-7.577616	5.492781	-0.462241
59	6	0	-7.002683	4.591697	-1.365624
60	6	0	-5.655472	4.244210	-1.249748
61	6	0	-4.872585	4.793036	-0.220282
62	6	0	-5.448986	5.699624	0.679983
63	6	0	-4.386937	2.513499	2.744555
64	6	0	-5.478180	1.894094	3.359855
65	6	0	-6.409210	1.185371	2.593479
66	6	0	-6.237048	1.085632	1.209457
67	6	0	-5.148403	1.704008	0.588172
68	6	0	-4.227576	2.437309	1.351295
69	6	0	-3.413702	4.425652	-0.133927
70	6	0	-3.080191	3.142791	0.683434
71	6	0	-2.676080	4.516648	1.194932
72	6	0	-1.977521	2.128862	0.349463
73	8	0	-1.839798	1.773393	-0.856561
74	8	0	-1.321436	1.711746	1.356976
75	6	0	5.128986	0.439089	-4.312007
76	6	0	6.116332	1.067299	-3.542671
77	6	0	5.752007	1.929926	-2.509391
78	6	0	4.392392	2.183099	-2.234660
79	6	0	3.410345	1.541740	-2.995825
80	6	0	3.781626	0.674208	-4.031660
81	6	0	6.197201	6.355263	-1.595828
82	6	0	5.474555	7.036845	-2.579239

83	6	0	4.302239	6.474810	-3.096763
84	6	0	3.852829	5.236283	-2.633594
85	6	0	4.574735	4.553617	-1.641997
86	6	0	5.751463	5.115641	-1.126814
87	6	0	2.792534	5.287306	1.220081
88	6	0	2.257340	6.547624	1.503615
89	6	0	1.218695	7.062771	0.722933
90	6	0	0.706566	6.307768	-0.337875
91	6	0	1.233941	5.047159	-0.623744
92	6	0	2.290772	4.534603	0.147616
93	6	0	4.096013	3.203620	-1.175587
94	6	0	2.877930	3.199800	-0.207611
95	6	0	4.263360	2.814202	0.286409
96	6	0	1.783312	2.121634	-0.208904
97	8	0	1.120008	1.977428	-1.275177
98	8	0	1.628908	1.502571	0.891311
99	1	0	-6.559716	1.743316	-3.611128
100	1	0	-8.045707	0.222649	-2.315497
101	1	0	-7.076456	-1.669006	-1.038167
102	1	0	-3.097949	-0.477351	-2.311256
103	1	0	-4.092977	1.371984	-3.589797
104	1	0	-7.296638	-6.230860	-0.786299
105	1	0	-6.656633	-6.832079	-3.113715
106	1	0	-5.053566	-5.400761	-4.367324
107	1	0	-4.092320	-3.371658	-3.298711
108	1	0	-6.337306	-4.215127	0.289364
109	1	0	-2.947646	-4.123485	2.163057
110	1	0	-2.082514	-6.449427	2.310791
111	1	0	-1.235187	-7.602060	0.273216
112	1	0	-1.245803	-6.412016	-1.916873
113	1	0	-2.118637	-4.096012	-2.076654
114	1	0	-4.908076	-3.032823	1.353812
115	1	0	-4.598939	-1.281292	1.135231
116	1	0	-2.163758	-4.325579	-5.571824
117	1	0	-0.787845	-6.322031	-4.999616
118	1	0	1.086142	-6.121163	-3.402344
119	1	0	0.164422	-1.892399	-2.886791
120	1	0	-1.654893	-2.131460	-4.492023
121	1	0	5.146451	-7.395325	-2.833336
122	1	0	6.190845	-6.148976	-4.715477
123	1	0	5.292112	-3.926993	-5.381552
124	1	0	3.352374	-2.950193	-4.166357
125	1	0	3.214983	-6.428108	-1.617247
126	1	0	3.961939	-4.309391	0.819332
127	1	0	6.419489	-4.092089	1.057247
128	1	0	7.674684	-2.476446	-0.357274
129	1	0	6.443482	-1.018766	-1.966556
130	1	0	3.982394	-1.228329	-2.209139
131	1	0	2.287919	-5.104680	-0.126651
132	1	0	0.669436	-4.360373	-0.298310
133	1	0	-1.095804	6.560842	-4.514458
134	1	0	-2.111164	8.005387	-2.759293
135	1	0	-3.137914	6.979083	-0.747301
136	1	0	-2.115110	3.038822	-2.239397
137	1	0	-1.103851	4.084478	-4.233119
138	1	0	-7.241919	6.747483	1.261319
139	1	0	-8.627233	5.761580	-0.554413

140	1	0	-7.606471	4.160022	-2.161585
141	1	0	-5.205785	3.546352	-1.957547
142	1	0	-4.850212	6.135598	1.477124
143	1	0	-3.650353	3.043837	3.348258
144	1	0	-5.602459	1.966757	4.438287
145	1	0	-7.264322	0.714711	3.072127
146	1	0	-6.953659	0.529614	0.605690
147	1	0	-5.016058	1.617110	-0.493352
148	1	0	-3.165370	4.927382	2.076174
149	1	0	-1.618783	4.791862	1.188690
150	1	0	5.411428	-0.226057	-5.124666
151	1	0	7.167624	0.892098	-3.760155
152	1	0	6.521075	2.428671	-1.922199
153	1	0	2.334360	1.693540	-2.785979
154	1	0	3.004046	0.183413	-4.617737
155	1	0	7.109636	6.789883	-1.193049
156	1	0	5.821744	8.001712	-2.941572
157	1	0	3.736993	7.003681	-3.862317
158	1	0	2.939430	4.796452	-3.035651
159	1	0	6.320096	4.590105	-0.363821
160	1	0	3.600963	4.893983	1.832825
161	1	0	2.654064	7.128818	2.333261
162	1	0	0.808730	8.046490	0.939180
163	1	0	-0.109053	6.700476	-0.947099
164	1	0	0.819009	4.448171	-1.442390
165	1	0	4.792413	3.469769	0.975443
166	1	0	4.456128	1.769513	0.536120
167	6	0	1.989274	0.386551	5.050347
168	6	0	1.650702	0.247806	3.592325
169	6	0	0.386936	-0.023271	3.104679
170	6	0	-0.748103	-0.221671	4.043274
171	8	0	-1.227991	-1.464098	4.087375
172	6	0	-2.464474	-1.777386	4.845486
173	6	0	-3.632181	-0.982254	4.255672
174	6	0	-2.249402	-1.504627	6.339082
175	6	0	-2.644480	-3.274830	4.596864
176	8	0	-1.172216	0.742644	4.664794
177	1	0	-4.573711	-1.330836	4.694635
178	1	0	-3.674461	-1.132980	3.171371
179	1	0	-3.530332	0.087558	4.449616
180	1	0	-3.115321	-1.870473	6.902476
181	1	0	-2.127933	-0.438706	6.535655
182	1	0	-1.362229	-2.038603	6.698372
183	1	0	-3.539220	-3.633580	5.116412
184	1	0	-1.777711	-3.834051	4.961501
185	1	0	-2.757829	-3.474588	3.520424
186	1	0	2.307750	0.783328	2.905632
187	6	0	1.052527	-5.002064	5.013072
188	6	0	0.882839	-4.632964	3.676144
189	6	0	1.462698	-3.462876	3.194356
190	6	0	2.229308	-2.647591	4.048894
191	6	0	2.387637	-3.018609	5.398230
192	6	0	1.803249	-4.190918	5.870250
193	6	0	5.474233	-0.534563	2.305676
194	6	0	6.478867	0.193585	1.673236
195	6	0	6.927613	1.402965	2.208662
196	6	0	6.359935	1.879302	3.391059

197	6	0	5.340122	1.173565	4.027000
198	6	0	4.881118	-0.029584	3.472948
199	6	0	2.911592	-1.493495	3.447460
200	7	0	3.856035	-0.774483	4.117811
201	8	0	3.363505	-0.199133	5.284413
202	1	0	0.602839	-5.917604	5.387366
203	1	0	0.293318	-5.253298	3.005529
204	1	0	1.323784	-3.162162	2.158935
205	1	0	2.979768	-2.398814	6.061363
206	1	0	1.940557	-4.477079	6.909082
207	1	0	5.169578	-1.493954	1.893447
208	1	0	6.918643	-0.199955	0.760223
209	1	0	7.718982	1.958984	1.715907
210	1	0	6.708355	2.810602	3.827594
211	1	0	4.904912	1.539237	4.946570
212	1	0	3.044063	-1.532394	2.369650
213	1	0	1.323930	-0.227180	5.664444
214	6	0	2.010551	1.817016	5.570732
215	1	0	0.982576	2.190365	5.592540
216	1	0	2.421755	1.852999	6.585359
217	1	0	2.604251	2.467339	4.920597

5a-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.576838	-3.836104	-4.615512
2	6	0	-3.144823	-5.123005	-4.271268
3	6	0	-1.918495	-5.299704	-3.631440
4	6	0	-1.100683	-4.190443	-3.331479
5	6	0	-1.540775	-2.907375	-3.669799
6	6	0	-2.775928	-2.734713	-4.309159
7	6	0	2.002550	-7.355512	-4.522899
8	6	0	2.538296	-6.695969	-5.632852
9	6	0	2.333187	-5.320970	-5.791583
10	6	0	1.596012	-4.606627	-4.844550
11	6	0	1.062836	-5.266948	-3.726490
12	6	0	1.265031	-6.645592	-3.570397
13	6	0	3.339860	-4.573574	-1.356531
14	6	0	4.714372	-4.588355	-1.612477
15	6	0	5.290692	-3.603233	-2.419990
16	6	0	4.488848	-2.592217	-2.960858
17	6	0	3.115420	-2.573540	-2.710853
18	6	0	2.529126	-3.575628	-1.918714
19	6	0	0.241037	-4.489739	-2.730354
20	6	0	1.039244	-3.589194	-1.738195
21	6	0	0.329191	-4.842769	-1.252975
22	6	0	0.542359	-2.234079	-1.218194
23	8	0	0.296956	-1.347610	-2.084981
24	8	0	0.462856	-2.121420	0.047788
25	45	0	-0.531220	0.476701	-1.458145
26	45	0	0.003280	-0.226348	0.884288
27	6	0	3.877157	0.283770	-5.867137
28	6	0	5.149628	0.279544	-5.281763
29	6	0	5.320427	0.749860	-3.980488

30	6	0	4.218667	1.234290	-3.244483
31	6	0	2.951730	1.234624	-3.832754
32	6	0	2.784313	0.757921	-5.139786
33	6	0	7.484751	4.174239	-1.730333
34	6	0	6.949293	5.307066	-2.349277
35	6	0	5.626682	5.290199	-2.806305
36	6	0	4.842292	4.146553	-2.644657
37	6	0	5.376278	3.009841	-2.015364
38	6	0	6.703035	3.026578	-1.563636
39	6	0	4.359728	2.644028	1.599816
40	6	0	4.481185	3.702560	2.504088
41	6	0	3.954593	4.959838	2.190385
42	6	0	3.294330	5.152284	0.972824
43	6	0	3.167481	4.096968	0.065202
44	6	0	3.713553	2.840834	0.368373
45	6	0	4.520074	1.778132	-1.877992
46	6	0	3.609349	1.711328	-0.617835
47	6	0	4.794766	0.770774	-0.770465
48	6	0	2.198958	1.109825	-0.559274
49	8	0	1.392157	1.363704	-1.494677
50	8	0	1.968055	0.419353	0.488429
51	6	0	-5.532868	3.529712	-2.487707
52	6	0	-6.608100	3.098415	-1.700462
53	6	0	-6.525331	1.892190	-1.007871
54	6	0	-5.367066	1.086553	-1.089478
55	6	0	-4.294002	1.531914	-1.865745
56	6	0	-4.381272	2.746523	-2.562323
57	6	0	-8.864961	-1.855247	-0.498560
58	6	0	-8.816109	-2.464299	-1.755760
59	6	0	-7.664493	-2.346739	-2.541915
60	6	0	-6.565355	-1.623108	-2.074349
61	6	0	-6.612143	-1.013748	-0.810351
62	6	0	-7.767311	-1.130412	-0.024271
63	6	0	-5.140651	-3.190851	1.257925
64	6	0	-5.351468	-4.572127	1.225211
65	6	0	-4.866213	-5.332121	0.157157
66	6	0	-4.166562	-4.704166	-0.878424
67	6	0	-3.953309	-3.324134	-0.851301
68	6	0	-4.441678	-2.556401	0.218438
69	6	0	-5.425658	-0.213195	-0.336427
70	6	0	-4.240248	-1.068365	0.216791
71	6	0	-5.068452	-0.192028	1.142874
72	6	0	-2.760883	-0.716671	0.022340
73	8	0	-2.389967	-0.449698	-1.158352
74	8	0	-2.037367	-0.745994	1.068227
75	6	0	1.594492	5.968646	-2.957871
76	6	0	1.485508	6.882554	-1.901873
77	6	0	0.646152	6.605923	-0.824369
78	6	0	-0.099881	5.407971	-0.782094
79	6	0	0.019189	4.497039	-1.834897
80	6	0	0.863658	4.780674	-2.917842
81	6	0	-3.011821	8.333473	1.384441
82	6	0	-3.947544	8.387084	0.347787
83	6	0	-3.925252	7.416605	-0.660236
84	6	0	-2.972670	6.396153	-0.631954
85	6	0	-2.035933	6.336595	0.413273
86	6	0	-2.056312	7.312846	1.418908

87	6	0	-2.869669	3.840392	3.145153
88	6	0	-4.125916	3.813399	3.756647
89	6	0	-5.286750	3.779197	2.977217
90	6	0	-5.186739	3.757285	1.582797
91	6	0	-3.933143	3.780611	0.965283
92	6	0	-2.768359	3.839045	1.744524
93	6	0	-1.002861	5.241292	0.407631
94	6	0	-1.419700	3.904126	1.087128
95	6	0	-0.350741	4.788919	1.708335
96	6	0	-1.024709	2.519638	0.563102
97	8	0	-1.307884	2.246971	-0.638737
98	8	0	-0.462970	1.756657	1.413210
99	1	0	-4.530912	-3.697234	-5.118926
100	1	0	-3.763828	-5.985669	-4.509363
101	1	0	-1.580500	-6.302990	-3.375794
102	1	0	-0.937131	-2.011813	-3.430706
103	1	0	-3.106248	-1.727418	-4.564111
104	1	0	2.158511	-8.425296	-4.398710
105	1	0	3.112558	-7.249825	-6.372101
106	1	0	2.748654	-4.804893	-6.655441
107	1	0	1.434045	-3.535241	-4.967027
108	1	0	0.847542	-7.166874	-2.712009
109	1	0	2.899258	-5.347832	-0.730340
110	1	0	5.334413	-5.375033	-1.186347
111	1	0	6.357292	-3.625226	-2.631684
112	1	0	4.931798	-1.817278	-3.588908
113	1	0	2.489001	-1.779057	-3.133666
114	1	0	0.911931	-5.700921	-0.922950
115	1	0	-0.559510	-4.726628	-0.629185
116	1	0	3.743127	-0.079843	-6.883397
117	1	0	6.005829	-0.085029	-5.845623
118	1	0	6.312704	0.757825	-3.531251
119	1	0	2.068286	1.589689	-3.273601
120	1	0	1.789209	0.758108	-5.584000
121	1	0	8.513480	4.183475	-1.375336
122	1	0	7.558289	6.199211	-2.476225
123	1	0	5.207159	6.170486	-3.289924
124	1	0	3.813211	4.131259	-3.006845
125	1	0	7.128914	2.149198	-1.081404
126	1	0	4.763953	1.663761	1.851720
127	1	0	4.993016	3.548305	3.451932
128	1	0	4.060418	5.785719	2.890198
129	1	0	2.878553	6.128135	0.722022
130	1	0	2.645015	4.252544	-0.882655
131	1	0	5.657710	0.881885	-0.115860
132	1	0	4.606227	-0.287233	-0.965846
133	1	0	-5.597643	4.466707	-3.035308
134	1	0	-7.510185	3.703017	-1.634430
135	1	0	-7.370036	1.562017	-0.403736
136	1	0	-3.344924	0.959384	-1.944337
137	1	0	-3.531057	3.072777	-3.161915
138	1	0	-9.759640	-1.944486	0.114374
139	1	0	-9.670588	-3.028334	-2.122477
140	1	0	-7.623780	-2.820680	-3.520904
141	1	0	-5.666210	-1.531312	-2.684400
142	1	0	-7.813810	-0.657050	0.954049
143	1	0	-5.528831	-2.605247	2.090757

144	1	0	-5.901896	-5.053927	2.030633
145	1	0	-5.036670	-6.405646	0.128185
146	1	0	-3.788787	-5.289755	-1.717079
147	1	0	-3.408902	-2.837585	-1.667333
148	1	0	-5.720702	-0.652488	1.882868
149	1	0	-4.612249	0.711304	1.558672
150	1	0	2.241865	6.187087	-3.804070
151	1	0	2.052066	7.811215	-1.926160
152	1	0	0.552057	7.325958	-0.011933
153	1	0	-0.529051	3.534382	-1.833450
154	1	0	0.945133	4.057956	-3.730179
155	1	0	-3.025979	9.087010	2.169547
156	1	0	-4.691204	9.180368	0.323917
157	1	0	-4.652026	7.456659	-1.469576
158	1	0	-2.950815	5.643388	-1.420683
159	1	0	-1.332010	7.279350	2.230091
160	1	0	-1.969175	3.850352	3.756898
161	1	0	-4.198832	3.816665	4.842384
162	1	0	-6.263819	3.767464	3.454604
163	1	0	-6.086558	3.721246	0.968792
164	1	0	-3.859925	3.749897	-0.124841
165	1	0	-0.560155	5.307244	2.642186
166	1	0	0.690453	4.458157	1.683997
167	6	0	1.592830	0.397245	4.747832
168	6	0	1.738528	-0.310618	3.360518
169	6	0	0.445771	-0.689918	2.749544
170	6	0	-0.603779	-1.288628	3.612516
171	8	0	-0.578867	-2.613872	3.639867
172	6	0	-1.605580	-3.416990	4.371864
173	6	0	-2.963009	-3.183522	3.712053
174	6	0	-1.595894	-3.046214	5.857712
175	6	0	-1.111868	-4.847758	4.156265
176	8	0	-1.369628	-0.525677	4.175800
177	1	0	-3.708456	-3.843694	4.168482
178	1	0	-2.912923	-3.411601	2.640375
179	1	0	-3.289729	-2.148476	3.828732
180	1	0	-2.237130	-3.748817	6.401814
181	1	0	-1.970916	-2.034009	6.017252
182	1	0	-0.584170	-3.117450	6.267574
183	1	0	-1.799682	-5.551161	4.636941
184	1	0	-0.115608	-4.983772	4.588538
185	1	0	-1.066838	-5.082228	3.087776
186	1	0	2.319136	0.291742	2.661681
187	6	0	6.326893	-1.826084	1.663906
188	6	0	5.142675	-2.197139	1.022024
189	6	0	3.926652	-2.140065	1.701892
190	6	0	3.879695	-1.705365	3.034345
191	6	0	5.069649	-1.340551	3.675359
192	6	0	6.286156	-1.400786	2.992136
193	6	0	2.182201	-2.751246	7.293059
194	6	0	2.230142	-3.919294	8.051229
195	6	0	2.722907	-5.108302	7.508274
196	6	0	3.171262	-5.113675	6.187162
197	6	0	3.125558	-3.955536	5.409952
198	6	0	2.625555	-2.761424	5.958302
199	6	0	2.531667	-1.633889	3.733142
200	7	0	2.644537	-1.564972	5.207632

201	8	0	1.604796	-0.679261	5.674479
202	1	0	7.274209	-1.877868	1.134762
203	1	0	5.162397	-2.540740	-0.010957
204	1	0	3.008392	-2.421213	1.189665
205	1	0	5.039748	-1.035192	4.715714
206	1	0	7.202995	-1.122756	3.504644
207	1	0	1.803244	-1.831594	7.720454
208	1	0	1.878756	-3.894723	9.079397
209	1	0	2.759932	-6.013952	8.106291
210	1	0	3.562952	-6.026838	5.747043
211	1	0	3.497852	-3.980240	4.391971
212	1	0	1.935684	-2.511092	3.446584
213	1	0	0.606192	0.849827	4.867631
214	6	0	2.691414	1.430228	4.987037
215	1	0	2.593273	2.251417	4.266601
216	1	0	2.596209	1.840102	5.997166
217	1	0	3.686370	0.992256	4.876386

7a-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.904316	-4.564317	2.607934
2	6	0	-5.659472	-4.987116	1.506964
3	6	0	-5.830905	-4.141464	0.411522
4	6	0	-5.250689	-2.856134	0.401339
5	6	0	-4.491954	-2.442075	1.500048
6	6	0	-4.321464	-3.295826	2.598121
7	6	0	-9.246140	-2.042863	-1.736854
8	6	0	-9.782650	-1.157405	-0.797601
9	6	0	-8.943013	-0.540405	0.136206
10	6	0	-7.571821	-0.806080	0.131497
11	6	0	-7.031045	-1.689901	-0.815540
12	6	0	-7.874008	-2.311584	-1.747628
13	6	0	-5.690821	0.370897	-3.316266
14	6	0	-6.343086	1.508563	-3.801740
15	6	0	-6.589606	2.593518	-2.955593
16	6	0	-6.171344	2.543689	-1.621328
17	6	0	-5.517558	1.411589	-1.131009
18	6	0	-5.285097	0.312281	-1.974733
19	6	0	-5.555400	-1.991850	-0.787228
20	6	0	-4.622426	-0.914442	-1.417523
21	6	0	-4.818122	-2.263952	-2.090071
22	6	0	-3.227143	-0.563047	-0.894616
23	8	0	-3.143365	-0.173832	0.311574
24	8	0	-2.273750	-0.649757	-1.727487
25	45	0	-1.248138	0.158338	1.101717
26	45	0	-0.354722	-0.003850	-1.140807
27	6	0	-6.028136	3.979269	2.233617
28	6	0	-6.107414	4.929501	1.207971
29	6	0	-4.975138	5.240840	0.455618
30	6	0	-3.745327	4.605747	0.722432
31	6	0	-3.672122	3.654866	1.743975
32	6	0	-4.812873	3.343306	2.494838

33	6	0	-2.038395	8.842887	-0.128416
34	6	0	-1.587845	9.072838	1.174375
35	6	0	-1.450170	7.999881	2.062095
36	6	0	-1.760051	6.702486	1.649349
37	6	0	-2.204592	6.468300	0.337510
38	6	0	-2.348244	7.545276	-0.548038
39	6	0	0.491342	5.110435	-1.988840
40	6	0	1.742314	5.723620	-2.096504
41	6	0	2.471876	6.039345	-0.945573
42	6	0	1.951251	5.726313	0.313590
43	6	0	0.703138	5.106838	0.427754
44	6	0	-0.040798	4.811030	-0.723800
45	6	0	-2.562174	5.065369	-0.078253
46	6	0	-1.400332	4.178718	-0.611884
47	6	0	-2.502212	4.661238	-1.544223
48	6	0	-1.248000	2.670878	-0.383913
49	8	0	-1.448527	2.216877	0.786071
50	8	0	-0.888404	2.003761	-1.402447
51	6	0	1.465119	-2.990789	5.690085
52	6	0	2.174518	-4.079947	5.168409
53	6	0	1.842893	-4.592947	3.915143
54	6	0	0.794088	-4.022738	3.163946
55	6	0	0.091219	-2.935159	3.688142
56	6	0	0.429216	-2.421808	4.947355
57	6	0	0.116026	-8.483960	2.016423
58	6	0	-1.089723	-8.614931	2.710746
59	6	0	-1.785160	-7.471106	3.118605
60	6	0	-1.278420	-6.201804	2.832891
61	6	0	-0.070186	-6.068217	2.128563
62	6	0	0.627711	-7.215174	1.726128
63	6	0	-0.418620	-5.283195	-1.580525
64	6	0	-1.238700	-6.054568	-2.408076
65	6	0	-2.554171	-6.338500	-2.026803
66	6	0	-3.052037	-5.834340	-0.821613
67	6	0	-2.237802	-5.059189	0.009341
68	6	0	-0.910549	-4.795628	-0.358643
69	6	0	0.471670	-4.689094	1.857745
70	6	0	-0.011704	-4.001423	0.548103
71	6	0	1.433890	-4.452366	0.701558
72	6	0	-0.295803	-2.506453	0.375223
73	8	0	-0.965093	-1.911154	1.274489
74	8	0	0.147262	-1.990998	-0.699310
75	6	0	0.539208	5.093540	4.297911
76	6	0	1.873245	5.422988	4.026857
77	6	0	2.718182	4.483791	3.437580
78	6	0	2.242121	3.197310	3.106715
79	6	0	0.909895	2.875085	3.379051
80	6	0	0.063996	3.822324	3.972339
81	6	0	6.601270	2.290555	4.325203
82	6	0	6.315027	1.509662	5.448703
83	6	0	5.035849	0.966510	5.611253
84	6	0	4.045828	1.201887	4.654604
85	6	0	4.334065	1.980781	3.522801
86	6	0	5.614820	2.528416	3.363189
87	6	0	5.000861	-0.258836	0.857830
88	6	0	5.793887	-1.401685	0.998056
89	6	0	5.411411	-2.418545	1.877596

90	6	0	4.226772	-2.293971	2.611351
91	6	0	3.428503	-1.156235	2.473049
92	6	0	3.818796	-0.125735	1.601905
93	6	0	3.245982	2.249324	2.516632
94	6	0	2.970464	1.109229	1.490638
95	6	0	3.598108	2.420417	1.045645
96	6	0	1.586483	0.740583	0.948874
97	8	0	0.682194	0.482274	1.803049
98	8	0	1.470550	0.680959	-0.312912
99	1	0	-4.774999	-5.221113	3.465195
100	1	0	-6.117417	-5.974487	1.509144
101	1	0	-6.427920	-4.469212	-0.438933
102	1	0	-4.005956	-1.451402	1.513668
103	1	0	-3.726321	-2.960375	3.446798
104	1	0	-9.897457	-2.525728	-2.462991
105	1	0	-10.850197	-0.948629	-0.792012
106	1	0	-9.358465	0.148850	0.869239
107	1	0	-6.917148	-0.328263	0.860047
108	1	0	-7.465128	-3.004763	-2.479669
109	1	0	-5.500746	-0.468781	-3.982766
110	1	0	-6.662189	1.545574	-4.841685
111	1	0	-7.105396	3.473804	-3.332731
112	1	0	-6.354934	3.389329	-0.957491
113	1	0	-5.178040	1.378686	-0.091646
114	1	0	-5.360855	-2.324981	-3.031825
115	1	0	-3.988346	-2.975779	-2.087318
116	1	0	-6.909923	3.739520	2.823776
117	1	0	-7.051748	5.430202	1.002789
118	1	0	-5.034576	5.988534	-0.334405
119	1	0	-2.726194	3.129944	1.951094
120	1	0	-4.745876	2.597882	3.286026
121	1	0	-2.148629	9.675448	-0.820921
122	1	0	-1.345538	10.082665	1.498090
123	1	0	-1.101340	8.176256	3.077949
124	1	0	-1.659263	5.868072	2.344249
125	1	0	-2.700091	7.376972	-1.563938
126	1	0	-0.066107	4.851943	-2.888271
127	1	0	2.147848	5.955400	-3.079729
128	1	0	3.438960	6.529914	-1.030031
129	1	0	2.514490	5.968184	1.214645
130	1	0	0.308360	4.855995	1.415183
131	1	0	-2.270535	5.396982	-2.312788
132	1	0	-3.230574	3.939975	-1.920538
133	1	0	1.720579	-2.592644	6.669551
134	1	0	2.981007	-4.529570	5.744674
135	1	0	2.386730	-5.448738	3.516108
136	1	0	-0.719793	-2.459964	3.112353
137	1	0	-0.123577	-1.571009	5.343460
138	1	0	0.659969	-9.371553	1.698120
139	1	0	-1.486797	-9.602760	2.933815
140	1	0	-2.723509	-7.570414	3.661040
141	1	0	-1.817222	-5.311090	3.156647
142	1	0	1.567483	-7.124066	1.184877
143	1	0	0.598652	-5.048534	-1.892783
144	1	0	-0.850557	-6.432291	-3.352602
145	1	0	-3.187715	-6.947902	-2.667344
146	1	0	-4.078285	-6.044815	-0.522564

147	1	0	-2.636711	-4.660868	0.944609
148	1	0	1.800210	-5.287608	0.106121
149	1	0	2.216027	-3.699510	0.819971
150	1	0	-0.119513	5.823687	4.762728
151	1	0	2.251533	6.411254	4.281543
152	1	0	3.759406	4.738896	3.241631
153	1	0	0.499059	1.883322	3.120385
154	1	0	-0.972825	3.556764	4.176519
155	1	0	7.595281	2.715010	4.196868
156	1	0	7.084614	1.324098	6.194797
157	1	0	4.810491	0.358018	6.485302
158	1	0	3.048524	0.781084	4.781274
159	1	0	5.845814	3.138623	2.492638
160	1	0	5.307941	0.527122	0.168803
161	1	0	6.714837	-1.494674	0.420133
162	1	0	6.034540	-3.302953	1.992795
163	1	0	3.922752	-3.084062	3.298689
164	1	0	2.497616	-1.066623	3.039690
165	1	0	4.638365	2.441001	0.723567
166	1	0	3.001584	3.110372	0.441969
167	6	0	4.482638	-2.838923	-3.127511
168	6	0	4.029308	-1.404990	-2.952728
169	6	0	2.626321	-1.030500	-2.584692
170	6	0	1.588552	-1.358535	-3.651608
171	8	0	0.560653	-0.453376	-3.627797
172	6	0	-0.382133	-0.370134	-4.800807
173	6	0	-1.263151	-1.619760	-4.853953
174	6	0	0.438832	-0.170650	-6.081487
175	6	0	-1.208536	0.883171	-4.515733
176	8	0	1.658818	-2.284635	-4.427326
177	1	0	-2.003036	-1.498607	-5.653879
178	1	0	-1.802218	-1.745740	-3.910329
179	1	0	-0.671389	-2.513079	-5.056636
180	1	0	-0.249133	0.037331	-6.908228
181	1	0	1.026232	-1.053216	-6.334857
182	1	0	1.109511	0.689344	-5.977023
183	1	0	-1.872141	1.072643	-5.366637
184	1	0	-0.564221	1.756655	-4.377667
185	1	0	-1.828463	0.761227	-3.624993
186	1	0	2.320075	-1.569960	-1.676817
187	6	0	5.288053	3.676065	-3.555364
188	6	0	4.557301	3.106063	-2.511305
189	6	0	4.501582	1.719389	-2.364254
190	6	0	5.163798	0.876755	-3.274553
191	6	0	5.908355	1.462987	-4.314450
192	6	0	5.967587	2.848011	-4.452235
193	6	0	7.731625	-0.397907	-1.862847
194	6	0	8.966088	-0.420715	-1.209569
195	6	0	9.903142	-1.415396	-1.483847
196	6	0	9.594068	-2.394289	-2.433184
197	6	0	8.375718	-2.374673	-3.105060
198	6	0	7.428513	-1.374124	-2.824203
199	6	0	5.082709	-0.597570	-3.190377
200	7	0	6.223463	-1.358691	-3.586623
201	8	0	5.741799	-2.698398	-3.827536
202	1	0	5.331992	4.755845	-3.666330
203	1	0	4.026124	3.741557	-1.805421

204	1	0	3.945852	1.294773	-1.532423
205	1	0	6.429807	0.817438	-5.013264
206	1	0	6.543683	3.281600	-5.265149
207	1	0	7.016178	0.378870	-1.623694
208	1	0	9.183798	0.344857	-0.468899
209	1	0	10.858603	-1.430478	-0.967230
210	1	0	10.311050	-3.179583	-2.659028
211	1	0	8.137158	-3.131608	-3.842537
212	1	0	2.546467	0.025812	-2.342325
213	1	0	3.826311	-3.379372	-3.815764
214	6	0	4.634481	-3.618101	-1.815406
215	1	0	3.656434	-3.751675	-1.335552
216	1	0	5.058961	-4.608249	-2.008402
217	1	0	5.288783	-3.083220	-1.117665

2.4. C=C-C=N2 *s-trans* vinylcarbenoid **2-II** and styryl nitrene **3b**

s-trans vinyl diazoacetate **2-II** and styryl nitrene **3b** with an approach over *Si*-face

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.994950	-2.441779	-3.585643
2	6	0	6.842758	-2.858171	-2.551165
3	6	0	6.708086	-2.311037	-1.276453
4	6	0	5.722239	-1.334950	-1.013673
5	6	0	4.879592	-0.925519	-2.049281
6	6	0	5.016891	-1.480282	-3.329325
7	6	0	9.147910	0.011028	1.813658
8	6	0	9.472230	1.173608	1.109192
9	6	0	8.568191	1.697880	0.178351
10	6	0	7.345093	1.063493	-0.047164
11	6	0	7.014422	-0.101067	0.665475
12	6	0	7.923316	-0.627679	1.593526
13	6	0	4.760808	0.548269	3.554508
14	6	0	5.038532	1.555395	4.482836
15	6	0	5.282906	2.862726	4.050424
16	6	0	5.236080	3.162135	2.685325
17	6	0	4.957984	2.159408	1.752534
18	6	0	4.733719	0.842642	2.181621
19	6	0	5.700938	-0.783002	0.383192
20	6	0	4.474364	-0.245385	1.177522
21	6	0	5.029823	-1.633802	1.453825
22	6	0	3.045210	-0.117388	0.629662
23	8	0	2.896396	0.379415	-0.523431
24	8	0	2.133489	-0.504593	1.425892
25	45	0	0.963473	0.407768	-1.366941
26	45	0	0.109733	-0.181599	0.916633
27	6	0	5.680024	4.199299	-1.391635
28	6	0	5.573142	5.187036	-0.404350
29	6	0	4.344318	5.433384	0.205693
30	6	0	3.197749	4.695486	-0.160067
31	6	0	3.313713	3.704271	-1.138644
32	6	0	4.551496	3.461415	-1.751087
33	6	0	1.476588	8.866405	0.781281
34	6	0	1.037322	9.179956	-0.508082
35	6	0	0.878222	8.162704	-1.455711
36	6	0	1.156362	6.836838	-1.116648
37	6	0	1.591982	6.519878	0.179874
38	6	0	1.755099	7.540470	1.127267
39	6	0	-1.242236	5.433813	1.857480
40	6	0	-2.476431	6.079998	1.737553
41	6	0	-3.140130	6.106829	0.507599
42	6	0	-2.574629	5.467273	-0.600918
43	6	0	-1.343435	4.818755	-0.487144
44	6	0	-0.661106	4.813248	0.741177
45	6	0	1.916437	5.087850	0.518260
46	6	0	0.693094	4.171418	0.825485
47	6	0	1.661283	4.569242	1.927145
48	6	0	0.610109	2.691565	0.426881

49	8	0	0.769500	2.425071	-0.798288
50	8	0	0.356849	1.876265	1.369580
51	6	0	-2.072020	-2.266045	-5.866457
52	6	0	-2.441708	-3.578462	-5.546535
53	6	0	-1.816728	-4.241948	-4.491592
54	6	0	-0.807332	-3.605063	-3.738755
55	6	0	-0.451583	-2.290695	-4.055234
56	6	0	-1.082765	-1.627638	-5.117030
57	6	0	0.666980	-7.946211	-3.921549
58	6	0	1.871724	-7.725312	-4.595175
59	6	0	2.420730	-6.438857	-4.636122
60	6	0	1.768973	-5.376340	-4.006232
61	6	0	0.561675	-5.598144	-3.325294
62	6	0	0.010535	-6.886899	-3.287421
63	6	0	1.629067	-5.851380	-0.164151
64	6	0	2.796243	-6.505170	0.242208
65	6	0	4.047903	-5.953345	-0.044095
66	6	0	4.128948	-4.740466	-0.736788
67	6	0	2.966831	-4.080430	-1.140120
68	6	0	1.705910	-4.634307	-0.858853
69	6	0	-0.145539	-4.435931	-2.677474
70	6	0	0.470241	-3.929309	-1.337556
71	6	0	-0.871485	-4.643339	-1.355792
72	6	0	0.498189	-2.451317	-0.919709
73	8	0	1.082598	-1.658174	-1.714164
74	8	0	-0.033419	-2.176255	0.200779
75	6	0	-1.854134	4.873592	-4.514916
76	6	0	-3.218070	4.948951	-4.204706
77	6	0	-3.845562	3.885852	-3.557987
78	6	0	-3.121116	2.723628	-3.213058
79	6	0	-1.760372	2.657890	-3.521096
80	6	0	-1.132182	3.731035	-4.168676
81	6	0	-7.357026	1.005551	-4.087315
82	6	0	-7.012447	0.391303	-5.294551
83	6	0	-5.665221	0.174384	-5.604957
84	6	0	-4.666334	0.569836	-4.713094
85	6	0	-5.011237	1.182666	-3.497028
86	6	0	-6.361261	1.402090	-3.189273
87	6	0	-5.024032	-1.123598	-0.580769
88	6	0	-5.691874	-2.350118	-0.627492
89	6	0	-5.436697	-3.251025	-1.666471
90	6	0	-4.499989	-2.926021	-2.652445
91	6	0	-3.828198	-1.701255	-2.610589
92	6	0	-4.099023	-0.786516	-1.581969
93	6	0	-3.915775	1.627077	-2.562885
94	6	0	-3.411351	0.549144	-1.556868
95	6	0	-4.190353	1.760575	-1.071727
96	6	0	-1.958149	0.381215	-1.096486
97	8	0	-1.053842	0.384480	-1.980607
98	8	0	-1.809215	0.224621	0.157108
99	1	0	6.100258	-2.865609	-4.581528
100	1	0	7.609792	-3.605027	-2.744773
101	1	0	7.377172	-2.628411	-0.477472
102	1	0	4.084800	-0.174403	-1.878655
103	1	0	4.347021	-1.153346	-4.124652
104	1	0	9.849171	-0.399922	2.537112
105	1	0	10.424129	1.669828	1.283073

106	1	0	8.818134	2.602880	-0.372289
107	1	0	6.641974	1.469140	-0.776291
108	1	0	7.679780	-1.532738	2.145672
109	1	0	4.557787	-0.464759	3.897118
110	1	0	5.067113	1.319506	5.544236
111	1	0	5.509376	3.643159	4.772775
112	1	0	5.420811	4.179203	2.340063
113	1	0	4.916896	2.400763	0.686850
114	1	0	5.531970	-1.835152	2.397626
115	1	0	4.449181	-2.504359	1.140510
116	1	0	6.635778	4.011814	-1.875198
117	1	0	6.448531	5.766073	-0.118103
118	1	0	4.263531	6.212633	0.962594
119	1	0	2.447815	3.080083	-1.439602
120	1	0	4.622051	2.683008	-2.511509
121	1	0	1.602817	9.655697	1.519504
122	1	0	0.819800	10.211539	-0.774857
123	1	0	0.536417	8.403903	-2.460667
124	1	0	1.034459	6.042788	-1.854116
125	1	0	2.099418	7.305181	2.131719
126	1	0	-0.730488	5.420922	2.817668
127	1	0	-2.915267	6.570479	2.603924
128	1	0	-4.089307	6.628279	0.409511
129	1	0	-3.091029	5.475263	-1.562022
130	1	0	-0.906385	4.310646	-1.354041
131	1	0	1.336226	5.244761	2.715369
132	1	0	2.332811	3.807882	2.332860
133	1	0	-2.553384	-1.749395	-6.693343
134	1	0	-3.212895	-4.081936	-6.125508
135	1	0	-2.100439	-5.266097	-4.253716
136	1	0	0.313629	-1.740329	-3.471497
137	1	0	-0.793567	-0.601872	-5.347553
138	1	0	0.236847	-8.945107	-3.890665
139	1	0	2.381259	-8.550580	-5.087077
140	1	0	3.358868	-6.263891	-5.159924
141	1	0	2.194967	-4.372712	-4.036363
142	1	0	-0.928821	-7.065278	-2.769278
143	1	0	0.659694	-6.299527	0.047861
144	1	0	2.727689	-7.451951	0.773534
145	1	0	4.955593	-6.467136	0.263380
146	1	0	5.102594	-4.307389	-0.972449
147	1	0	3.034327	-3.126670	-1.678734
148	1	0	-0.963146	-5.638272	-0.925313
149	1	0	-1.773827	-4.058857	-1.155846
150	1	0	-1.363336	5.700277	-5.022718
151	1	0	-3.788204	5.835422	-4.473911
152	1	0	-4.908466	3.944601	-3.325795
153	1	0	-1.149950	1.773928	-3.250670
154	1	0	-0.068639	3.663181	-4.397612
155	1	0	-8.403534	1.175383	-3.843490
156	1	0	-7.788247	0.082354	-5.990941
157	1	0	-5.394022	-0.303547	-6.544320
158	1	0	-3.615931	0.405440	-4.956148
159	1	0	-6.637176	1.877943	-2.249000
160	1	0	-5.213296	-0.429692	0.239001
161	1	0	-6.412038	-2.603007	0.146384
162	1	0	-5.963979	-4.200662	-1.707379

163	1	0	-4.289561	-3.625502	-3.460913
164	1	0	-3.090979	-1.455370	-3.379211
165	1	0	-5.198531	1.633935	-0.675037
166	1	0	-3.667228	2.536481	-0.508215
167	6	0	-1.051701	0.175849	5.029709
168	6	0	-0.662070	0.407211	3.735339
169	6	0	-0.511286	-0.609392	2.767091
170	6	0	-0.810652	-2.025056	3.119983
171	8	0	0.308632	-2.736657	3.229554
172	6	0	0.307125	-4.201230	3.466083
173	6	0	-0.564159	-4.913266	2.428007
174	6	0	-0.157446	-4.463623	4.902074
175	6	0	1.780666	-4.563742	3.278465
176	8	0	-1.958659	-2.416612	3.252121
177	1	0	-0.375630	-5.991307	2.484529
178	1	0	-0.303711	-4.562217	1.423211
179	1	0	-1.625010	-4.726400	2.595054
180	1	0	-0.072736	-5.533030	5.126071
181	1	0	-1.198919	-4.164911	5.040358
182	1	0	0.470165	-3.917287	5.614477
183	1	0	1.930783	-5.631335	3.470547
184	1	0	2.413623	-3.991185	3.962685
185	1	0	2.098602	-4.349905	2.250928
186	1	0	-0.444483	1.426383	3.421633
187	6	0	-6.819411	3.806726	0.462951
188	6	0	-5.767582	3.736641	1.383584
189	6	0	-5.546711	2.574046	2.113528
190	6	0	-6.375303	1.445192	1.941974
191	6	0	-7.424998	1.531695	1.005541
192	6	0	-7.647327	2.697860	0.276645
193	6	0	-4.369321	-4.007646	5.117706
194	6	0	-4.279877	-5.258474	5.730181
195	6	0	-4.090653	-5.357893	7.110369
196	6	0	-3.975908	-4.197887	7.881845
197	6	0	-4.060122	-2.943004	7.282589
198	6	0	-4.277865	-2.857212	5.905769
199	6	0	-5.197756	-1.311795	4.308454
200	7	0	-4.379331	-1.533079	5.326572
201	8	0	-3.671757	-0.610338	5.884031
202	1	0	-6.986923	4.716927	-0.106039
203	1	0	-5.108673	4.590770	1.525150
204	1	0	-4.716215	2.534362	2.812091
205	1	0	-8.071855	0.669921	0.855809
206	1	0	-8.467545	2.741480	-0.434911
207	1	0	-4.457370	-3.927666	4.039842
208	1	0	-4.340880	-6.155815	5.121035
209	1	0	-4.019479	-6.334474	7.580778
210	1	0	-3.819721	-4.269915	8.954486
211	1	0	-3.963816	-2.026634	7.852258
212	1	0	-5.798584	-2.150630	3.982273
213	1	0	-1.304730	-0.831190	5.346864
214	6	0	-1.190503	1.237826	6.058003
215	1	0	-2.229498	1.253095	6.410179
216	1	0	-0.571186	0.997423	6.933670
217	1	0	-0.909549	2.224818	5.679919
218	6	0	-5.302175	-0.038043	3.679136
219	1	0	-4.629503	0.729741	4.045813

220	6	0	-6.189148	0.200728	2.678355
221	1	0	-6.850804	-0.613654	2.380689

TS3b-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.972509	-1.943857	-3.820545
2	6	0	6.942402	-2.103183	-2.822425
3	6	0	6.807540	-1.435859	-1.606345
4	6	0	5.698831	-0.594910	-1.367119
5	6	0	4.734825	-0.442110	-2.365801
6	6	0	4.873271	-1.116956	-3.586669
7	6	0	9.049947	1.578551	0.988394
8	6	0	9.125739	2.694053	0.149951
9	6	0	8.081015	2.967387	-0.740258
10	6	0	6.965056	2.129998	-0.791969
11	6	0	6.883971	1.012529	0.055340
12	6	0	7.933612	0.737277	0.942580
13	6	0	4.784640	1.641367	3.040712
14	6	0	4.960381	2.781108	3.830235
15	6	0	4.936578	4.051668	3.246470
16	6	0	4.724417	4.178681	1.870145
17	6	0	4.548072	3.042587	1.075820
18	6	0	4.591991	1.765520	1.655079
19	6	0	5.682608	0.108360	-0.039939
20	6	0	4.442612	0.541162	0.796159
21	6	0	5.233157	-0.703988	1.167765
22	6	0	2.976234	0.381435	0.364007
23	8	0	2.670881	0.694896	-0.822156
24	8	0	2.198037	-0.031695	1.278510
25	45	0	0.702331	0.308152	-1.496476
26	45	0	0.120247	-0.114779	0.909662
27	6	0	4.718768	4.775677	-2.293566
28	6	0	4.503389	5.843356	-1.413049
29	6	0	3.284155	5.964153	-0.748151
30	6	0	2.256606	5.018154	-0.951667
31	6	0	2.482588	3.947922	-1.822069
32	6	0	3.709658	3.831943	-2.490394
33	6	0	-0.076765	8.950589	-0.413502
34	6	0	-0.625149	9.019237	-1.697360
35	6	0	-0.663423	7.873587	-2.499946
36	6	0	-0.156278	6.663466	-2.021775
37	6	0	0.389367	6.591829	-0.730166
38	6	0	0.431113	7.741369	0.071494
39	6	0	-2.154758	5.324665	1.197420
40	6	0	-3.476963	5.755940	1.052255
41	6	0	-4.176935	5.494193	-0.129005
42	6	0	-3.558469	4.776332	-1.158615
43	6	0	-2.239259	4.341480	-1.019048
44	6	0	-1.522132	4.631604	0.154295
45	6	0	0.960379	5.285211	-0.242302
46	6	0	-0.078894	4.231018	0.247532
47	6	0	0.850070	4.921336	1.232186

48	6	0	0.075732	2.716884	0.042210
49	8	0	0.210537	2.323199	-1.151896
50	8	0	0.021437	2.003895	1.092340
51	6	0	-2.181257	-3.299704	-5.384368
52	6	0	-2.305247	-4.607731	-4.899342
53	6	0	-1.504826	-5.038727	-3.842454
54	6	0	-0.563384	-4.169045	-3.251539
55	6	0	-0.454510	-2.860427	-3.731057
56	6	0	-1.260681	-2.431917	-4.795140
57	6	0	1.566553	-8.228546	-3.118951
58	6	0	2.669464	-7.908944	-3.916071
59	6	0	3.003594	-6.568193	-4.137118
60	6	0	2.238903	-5.549758	-3.564006
61	6	0	1.133834	-5.869828	-2.759707
62	6	0	0.797985	-7.213480	-2.540895
63	6	0	2.467788	-5.620347	0.250964
64	6	0	3.752053	-6.041787	0.608064
65	6	0	4.872015	-5.318384	0.188755
66	6	0	4.702813	-4.168243	-0.589528
67	6	0	3.422480	-3.740557	-0.945706
68	6	0	2.293067	-4.465820	-0.528329
69	6	0	0.300174	-4.759338	-2.174184
70	6	0	0.927569	-4.013077	-0.956609
71	6	0	-0.281585	-4.916276	-0.776501
72	6	0	0.750825	-2.508196	-0.700220
73	8	0	1.141622	-1.739457	-1.626926
74	8	0	0.267800	-2.182080	0.427607
75	6	0	-3.065168	3.687332	-4.985818
76	6	0	-4.395532	3.585792	-4.559077
77	6	0	-4.779335	2.545084	-3.715371
78	6	0	-3.839774	1.581927	-3.286398
79	6	0	-2.514267	1.692379	-3.712284
80	6	0	-2.131398	2.743228	-4.557602
81	6	0	-7.742493	-0.936994	-3.536722
82	6	0	-7.367403	-1.665574	-4.668941
83	6	0	-6.024273	-1.700046	-5.060413
84	6	0	-5.059984	-1.009103	-4.324044
85	6	0	-5.434447	-0.280859	-3.182706
86	6	0	-6.781006	-0.244732	-2.793982
87	6	0	-4.842458	-2.070609	0.039799
88	6	0	-5.280620	-3.383278	0.233234
89	6	0	-4.946599	-4.379757	-0.689720
90	6	0	-4.160673	-4.060753	-1.801295
91	6	0	-3.718508	-2.749853	-1.999402
92	6	0	-4.070540	-1.744173	-1.087061
93	6	0	-4.381502	0.480696	-2.420177
94	6	0	-3.632219	-0.325367	-1.316803
95	6	0	-4.586012	0.797654	-0.945762
96	6	0	-2.147501	-0.171946	-0.959661
97	8	0	-1.316785	-0.121500	-1.912690
98	8	0	-1.896792	-0.138246	0.285913
99	1	0	6.077289	-2.461768	-4.770944
100	1	0	7.803510	-2.744105	-2.999145
101	1	0	7.570087	-1.552517	-0.837269
102	1	0	3.843059	0.194566	-2.208788
103	1	0	4.108211	-0.991163	-4.352862
104	1	0	9.861298	1.362380	1.680435

105	1	0	9.993760	3.347969	0.188241
106	1	0	8.137440	3.835027	-1.395021
107	1	0	6.152248	2.339766	-1.489085
108	1	0	7.883746	-0.129574	1.597730
109	1	0	4.791975	0.655507	3.501659
110	1	0	5.121271	2.677901	4.900746
111	1	0	5.084301	4.937215	3.859655
112	1	0	4.700010	5.165231	1.407532
113	1	0	4.377357	3.148423	0.000864
114	1	0	5.825209	-0.714633	2.080118
115	1	0	4.780375	-1.683466	0.998324
116	1	0	5.665348	4.685562	-2.821120
117	1	0	5.285775	6.582134	-1.253339
118	1	0	3.115838	6.804776	-0.076245
119	1	0	1.715939	3.164279	-1.990012
120	1	0	3.867402	2.989957	-3.165192
121	1	0	-0.044144	9.840306	0.211911
122	1	0	-1.020996	9.960159	-2.072254
123	1	0	-1.089800	7.923973	-3.500253
124	1	0	-0.184139	5.769617	-2.645969
125	1	0	0.859067	7.697002	1.070299
126	1	0	-1.615466	5.536990	2.118394
127	1	0	-3.956887	6.305541	1.859360
128	1	0	-5.195838	5.853559	-0.251873
129	1	0	-4.102264	4.556569	-2.078728
130	1	0	-1.758484	3.771648	-1.822657
131	1	0	0.446709	5.633303	1.948890
132	1	0	1.653607	4.337001	1.687495
133	1	0	-2.798355	-2.964494	-6.214554
134	1	0	-3.022643	-5.289027	-5.351585
135	1	0	-1.596936	-6.060585	-3.477310
136	1	0	0.247480	-2.131575	-3.276726
137	1	0	-1.162304	-1.406976	-5.154245
138	1	0	1.303360	-9.270247	-2.947758
139	1	0	3.266436	-8.699745	-4.364228
140	1	0	3.862161	-6.316330	-4.757192
141	1	0	2.497631	-4.503778	-3.733756
142	1	0	-0.061458	-7.469428	-1.925626
143	1	0	1.602952	-6.201763	0.567041
144	1	0	3.878249	-6.942540	1.204806
145	1	0	5.871150	-5.651878	0.458593
146	1	0	5.572301	-3.603680	-0.930709
147	1	0	3.294609	-2.837145	-1.556250
148	1	0	-0.182146	-5.856024	-0.237308
149	1	0	-1.247702	-4.453212	-0.555937
150	1	0	-2.764162	4.496569	-5.646618
151	1	0	-5.129756	4.316475	-4.891119
152	1	0	-5.816473	2.464581	-3.391798
153	1	0	-1.741724	0.970430	-3.381913
154	1	0	-1.091477	2.816121	-4.875858
155	1	0	-8.785888	-0.908403	-3.230262
156	1	0	-8.116261	-2.204522	-5.244239
157	1	0	-5.729184	-2.266699	-5.941446
158	1	0	-4.013332	-1.031966	-4.630804
159	1	0	-7.080233	0.318933	-1.911397
160	1	0	-5.090741	-1.298709	0.768451
161	1	0	-5.882756	-3.629865	1.103984

162	1	0	-5.295838	-5.398627	-0.543026
163	1	0	-3.890296	-4.832141	-2.521618
164	1	0	-3.098221	-2.507298	-2.866159
165	1	0	-5.529323	0.564623	-0.450900
166	1	0	-4.178485	1.729313	-0.546850
167	6	0	-0.340122	0.629288	5.118951
168	6	0	-0.426319	0.699496	3.732244
169	6	0	-0.237372	-0.388363	2.885243
170	6	0	-0.179679	-1.772477	3.428435
171	8	0	1.065516	-2.248000	3.396884
172	6	0	1.403784	-3.649448	3.732714
173	6	0	0.524628	-4.626181	2.946916
174	6	0	1.275917	-3.834345	5.248490
175	6	0	2.861150	-3.748649	3.280016
176	8	0	-1.179780	-2.361109	3.813229
177	1	0	0.943500	-5.634805	3.039448
178	1	0	0.516981	-4.343630	1.888512
179	1	0	-0.503030	-4.630605	3.310137
180	1	0	1.601280	-4.843563	5.525817
181	1	0	0.241809	-3.702688	5.574962
182	1	0	1.911069	-3.116201	5.778614
183	1	0	3.259834	-4.742539	3.510607
184	1	0	3.477135	-2.996284	3.780909
185	1	0	2.934081	-3.590958	2.197287
186	1	0	-0.526466	1.682715	3.275909
187	6	0	-7.469767	2.447334	0.524495
188	6	0	-6.313885	2.876001	1.187276
189	6	0	-5.665731	2.036895	2.086335
190	6	0	-6.161509	0.742052	2.347360
191	6	0	-7.323499	0.324767	1.666759
192	6	0	-7.971514	1.166658	0.766479
193	6	0	-2.624669	-3.036156	6.531573
194	6	0	-2.280865	-3.965360	7.514581
195	6	0	-1.976962	-3.545836	8.811645
196	6	0	-2.005984	-2.184646	9.127003
197	6	0	-2.345842	-1.244937	8.156015
198	6	0	-2.668656	-1.680379	6.867936
199	6	0	-4.007562	-0.910198	5.018087
200	7	0	-3.051291	-0.675097	5.900032
201	8	0	-2.465914	0.485535	6.003039
202	1	0	-7.971744	3.107435	-0.177233
203	1	0	-5.910786	3.867785	0.995473
204	1	0	-4.763974	2.383299	2.582532
205	1	0	-7.717741	-0.671481	1.854339
206	1	0	-8.867854	0.824813	0.256333
207	1	0	-2.792732	-3.350602	5.508359
208	1	0	-2.234476	-5.019504	7.256763
209	1	0	-1.707602	-4.275132	9.570212
210	1	0	-1.765894	-1.852211	10.132864
211	1	0	-2.377161	-0.184346	8.375026
212	1	0	-4.473474	-1.886257	5.070901
213	1	0	-0.166497	-0.335883	5.586117
214	6	0	-0.106270	1.838077	5.959703
215	1	0	-0.508135	1.709807	6.966147
216	1	0	0.980190	1.996460	6.042703
217	1	0	-0.537798	2.733148	5.502340
218	6	0	-4.468492	0.070048	4.095773

219	1	0	-3.944251	1.018947	4.093819
220	6	0	-5.538347	-0.172901	3.292579
221	1	0	-6.012513	-1.152227	3.365167

TS4b-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	6.026176	-0.952333	-4.006693
2	6	0	7.056247	-0.755632	-3.077907
3	6	0	6.818880	-0.018002	-1.919490
4	6	0	5.545749	0.539546	-1.670454
5	6	0	4.522884	0.337480	-2.599450
6	6	0	4.765077	-0.408000	-3.761731
7	6	0	8.343326	3.730218	0.209060
8	6	0	8.092112	4.724574	-0.740246
9	6	0	6.972758	4.623233	-1.574144
10	6	0	6.107714	3.533358	-1.459424
11	6	0	6.354548	2.536890	-0.500498
12	6	0	7.479176	2.637217	0.330054
13	6	0	4.297262	2.933983	2.582016
14	6	0	4.214228	4.159889	3.248134
15	6	0	3.859821	5.317923	2.548828
16	6	0	3.575357	5.243202	1.181721
17	6	0	3.656288	4.020234	0.510515
18	6	0	4.033906	2.860773	1.204626
19	6	0	5.421960	1.356606	-0.415919
20	6	0	4.160451	1.552458	0.475326
21	6	0	5.263543	0.592840	0.893059
22	6	0	2.762207	0.992165	0.172041
23	8	0	2.327857	1.110182	-1.009580
24	8	0	2.159119	0.487705	1.170774
25	45	0	0.492434	0.200590	-1.506482
26	45	0	0.139404	-0.112057	0.957320
27	6	0	3.182813	5.418441	-3.008250
28	6	0	2.755181	6.486082	-2.208882
29	6	0	1.586899	6.370571	-1.457353
30	6	0	0.823628	5.183653	-1.491085
31	6	0	1.261326	4.118492	-2.283144
32	6	0	2.436091	4.239936	-3.038841
33	6	0	-2.396353	8.447743	-1.055265
34	6	0	-3.040111	8.244051	-2.279141
35	6	0	-2.844886	7.047280	-2.977516
36	6	0	-2.009970	6.057092	-2.455246
37	6	0	-1.367351	6.258202	-1.223328
38	6	0	-1.560536	7.459346	-0.526320
39	6	0	-3.338242	4.583661	1.082767
40	6	0	-4.735749	4.623623	1.073508
41	6	0	-5.448817	4.064212	0.009219
42	6	0	-4.759584	3.456408	-1.045760
43	6	0	-3.364060	3.413529	-1.042266
44	6	0	-2.643956	3.987195	0.019241
45	6	0	-0.446554	5.191751	-0.689728
46	6	0	-1.143750	3.970847	-0.017444

47	6	0	-0.347114	4.963824	0.812644
48	6	0	-0.632082	2.526388	-0.116972
49	8	0	-0.465597	2.063802	-1.282152
50	8	0	-0.459236	1.923721	0.988553
51	6	0	-1.639697	-4.425239	-4.785252
52	6	0	-1.436780	-5.654548	-4.145766
53	6	0	-0.503075	-5.759544	-3.115594
54	6	0	0.247938	-4.636388	-2.709254
55	6	0	0.026855	-3.407436	-3.338469
56	6	0	-0.912109	-3.307042	-4.374370
57	6	0	3.304110	-8.039602	-2.365931
58	6	0	4.233188	-7.571256	-3.299446
59	6	0	4.210521	-6.227884	-3.690434
60	6	0	3.263113	-5.354985	-3.151064
61	6	0	2.332639	-5.823303	-2.210099
62	6	0	2.354129	-7.170237	-1.821041
63	6	0	3.754401	-4.857613	0.670989
64	6	0	5.124825	-4.923629	0.939835
65	6	0	6.010883	-4.055877	0.295156
66	6	0	5.520812	-3.115238	-0.617211
67	6	0	4.153224	-3.043564	-0.888538
68	6	0	3.260039	-3.920654	-0.249737
69	6	0	1.295569	-4.877517	-1.661434
70	6	0	1.800143	-3.861820	-0.591227
71	6	0	0.868246	-4.999309	-0.206215
72	6	0	1.271028	-2.425768	-0.466286
73	8	0	1.408963	-1.687535	-1.486429
74	8	0	0.778462	-2.109061	0.660741
75	6	0	-3.933021	2.442508	-4.969225
76	6	0	-5.202419	2.060832	-4.515595
77	6	0	-5.331087	1.014603	-3.604684
78	6	0	-4.192005	0.326327	-3.129585
79	6	0	-2.930098	0.715924	-3.582716
80	6	0	-2.804912	1.770708	-4.498787
81	6	0	-7.435614	-3.020397	-3.111776
82	6	0	-6.918747	-3.713770	-4.209507
83	6	0	-5.610377	-3.461980	-4.637831
84	6	0	-4.821570	-2.522577	-3.971179
85	6	0	-5.336597	-1.830158	-2.862452
86	6	0	-6.649446	-2.079438	-2.439099
87	6	0	-4.296277	-3.151701	0.564864
88	6	0	-4.456556	-4.498650	0.898859
89	6	0	-4.010503	-5.495682	0.025186
90	6	0	-3.389341	-5.138993	-1.175790
91	6	0	-3.228346	-3.792635	-1.514613
92	6	0	-3.699926	-2.790537	-0.654205
93	6	0	-4.472902	-0.803263	-2.177597
94	6	0	-3.569279	-1.340903	-1.026467
95	6	0	-4.736087	-0.415151	-0.728537
96	6	0	-2.138095	-0.859763	-0.748366
97	8	0	-1.376315	-0.731418	-1.748183
98	8	0	-1.850711	-0.663005	0.474662
99	1	0	6.210091	-1.525571	-4.912307
100	1	0	8.042841	-1.174713	-3.263931
101	1	0	7.625215	0.141682	-1.204635
102	1	0	3.506704	0.743342	-2.431545
103	1	0	3.953707	-0.560881	-4.473354

104	1	0	9.213709	3.805176	0.857806
105	1	0	8.764196	5.574618	-0.831584
106	1	0	6.774903	5.395643	-2.315052
107	1	0	5.237760	3.451256	-2.112866
108	1	0	7.683563	1.867253	1.070743
109	1	0	4.557319	2.033078	3.134888
110	1	0	4.429199	4.212219	4.313030
111	1	0	3.806422	6.272923	3.065815
112	1	0	3.292748	6.139721	0.630143
113	1	0	3.425858	3.966692	-0.557126
114	1	0	5.889846	0.831567	1.749954
115	1	0	5.073128	-0.481786	0.846389
116	1	0	4.089369	5.509717	-3.601776
117	1	0	3.332278	7.407816	-2.179322
118	1	0	1.251323	7.208822	-0.848100
119	1	0	0.709929	3.157061	-2.319011
120	1	0	2.762319	3.397399	-3.649394
121	1	0	-2.544690	9.378303	-0.511289
122	1	0	-3.690627	9.013436	-2.688385
123	1	0	-3.344733	6.885981	-3.930955
124	1	0	-1.855449	5.124189	-2.998529
125	1	0	-1.060412	7.626787	0.424821
126	1	0	-2.790139	5.023874	1.913451
127	1	0	-5.267131	5.100101	1.894034
128	1	0	-6.535601	4.099843	0.000353
129	1	0	-5.308892	3.016408	-1.879318
130	1	0	-2.825470	2.929840	-1.865212
131	1	0	-0.861181	5.623256	1.508287
132	1	0	0.611527	4.644458	1.230005
133	1	0	-2.358883	-4.344399	-5.596685
134	1	0	-2.002036	-6.529559	-4.459063
135	1	0	-0.339362	-6.720345	-2.629652
136	1	0	0.567835	-2.491829	-3.025285
137	1	0	-1.069067	-2.341004	-4.854930
138	1	0	3.318682	-9.084087	-2.061578
139	1	0	4.971904	-8.248672	-3.721314
140	1	0	4.933201	-5.860227	-4.416735
141	1	0	3.243831	-4.307340	-3.453473
142	1	0	1.632194	-7.542449	-1.097764
143	1	0	3.071451	-5.540729	1.174155
144	1	0	5.501208	-5.659633	1.647086
145	1	0	7.077648	-4.114602	0.497173
146	1	0	6.206303	-2.436550	-1.127217
147	1	0	3.771056	-2.301903	-1.600902
148	1	0	1.236901	-5.813564	0.414792
149	1	0	-0.162171	-4.756015	0.064271
150	1	0	-3.830112	3.256408	-5.682924
151	1	0	-6.087473	2.578778	-4.878781
152	1	0	-6.321291	0.715320	-3.262496
153	1	0	-2.003787	0.221678	-3.223554
154	1	0	-1.810251	2.062534	-4.836907
155	1	0	-8.453271	-3.212249	-2.777881
156	1	0	-7.531018	-4.446110	-4.730602
157	1	0	-5.206057	-3.998614	-5.494233
158	1	0	-3.803799	-2.320541	-4.308837
159	1	0	-7.060666	-1.542253	-1.587116
160	1	0	-4.620414	-2.373551	1.259779

161	1	0	-4.928629	-4.773057	1.839290
162	1	0	-4.142445	-6.544435	0.280829
163	1	0	-3.025345	-5.909699	-1.855537
164	1	0	-2.731629	-3.519908	-2.449957
165	1	0	-5.612089	-0.799052	-0.210381
166	1	0	-4.534020	0.613450	-0.418166
167	6	0	-0.648955	0.961950	5.135714
168	6	0	-0.932254	0.572607	3.700678
169	6	0	-0.093210	-0.267335	2.968630
170	6	0	0.711259	-1.324574	3.629520
171	8	0	1.946908	-0.903127	3.916477
172	6	0	3.038346	-1.836439	4.291917
173	6	0	3.218106	-2.877397	3.187415
174	6	0	2.733189	-2.468877	5.653086
175	6	0	4.248230	-0.903258	4.369444
176	8	0	0.247522	-2.436027	3.828161
177	1	0	4.109335	-3.481662	3.393515
178	1	0	3.354453	-2.386002	2.217919
179	1	0	2.353938	-3.539707	3.115438
180	1	0	3.595041	-3.062598	5.979270
181	1	0	1.857646	-3.117709	5.599480
182	1	0	2.550896	-1.694293	6.405966
183	1	0	5.147368	-1.475616	4.621221
184	1	0	4.098382	-0.134749	5.134858
185	1	0	4.400297	-0.408111	3.405072
186	1	0	-1.459090	1.330167	3.120777
187	6	0	-8.229991	1.656810	1.967831
188	6	0	-7.180486	2.402749	2.511962
189	6	0	-5.960231	1.795285	2.796439
190	6	0	-5.763609	0.424808	2.541670
191	6	0	-6.825286	-0.309376	1.979351
192	6	0	-8.047588	0.297972	1.701395
193	6	0	-2.019137	-3.132380	5.954152
194	6	0	-1.546109	-4.200225	6.710203
195	6	0	-0.728168	-3.980634	7.821711
196	6	0	-0.388516	-2.673272	8.172079
197	6	0	-0.843005	-1.592319	7.418066
198	6	0	-1.646828	-1.822398	6.293029
199	6	0	-2.503960	-0.710174	4.224666
200	7	0	-2.166663	-0.729757	5.559204
201	8	0	-1.809872	0.536654	5.986372
202	1	0	-9.180115	2.133850	1.745181
203	1	0	-7.309497	3.464248	2.704104
204	1	0	-5.140115	2.392526	3.186208
205	1	0	-6.691975	-1.370380	1.778757
206	1	0	-8.857285	-0.288264	1.276219
207	1	0	-2.674630	-3.318975	5.110497
208	1	0	-1.829773	-5.210984	6.431851
209	1	0	-0.370895	-4.818275	8.413048
210	1	0	0.234032	-2.485813	9.042494
211	1	0	-0.597439	-0.577064	7.702718
212	1	0	-2.355149	-1.651945	3.703708
213	1	0	0.226286	0.427551	5.518169
214	6	0	-0.511064	2.457987	5.358773
215	1	0	-0.395480	2.679651	6.424395
216	1	0	0.369379	2.830948	4.826310
217	1	0	-1.392531	2.988047	4.983497

218	6	0	-4.509222	-0.262587	2.862856
219	6	0	-3.657052	0.098454	3.844535
220	1	0	-3.856341	0.964807	4.468182
221	1	0	-4.294052	-1.166836	2.283045

5b-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.956683	1.711204	-4.020203
2	6	0	-6.978304	1.511190	-3.082982
3	6	0	-6.775702	0.653786	-2.002690
4	6	0	-5.545504	-0.018831	-1.843195
5	6	0	-4.530387	0.185038	-2.780530
6	6	0	-4.737694	1.049986	-3.863625
7	6	0	-8.455010	-3.286350	-0.287739
8	6	0	-8.250623	-4.174725	-1.347031
9	6	0	-7.136703	-4.019608	-2.179857
10	6	0	-6.230258	-2.981867	-1.954419
11	6	0	-6.429637	-2.093197	-0.884956
12	6	0	-7.549190	-2.246317	-0.055669
13	6	0	-4.323277	-2.880326	2.126642
14	6	0	-4.267303	-4.170408	2.661302
15	6	0	-3.982235	-5.262227	1.835158
16	6	0	-3.740997	-5.057687	0.472993
17	6	0	-3.793470	-3.769753	-0.067057
18	6	0	-4.100728	-2.675340	0.755252
19	6	0	-5.454021	-0.963737	-0.679839
20	6	0	-4.194133	-1.293080	0.172364
21	6	0	-5.265705	-0.352353	0.702205
22	6	0	-2.782064	-0.739553	-0.064483
23	8	0	-2.344798	-0.699266	-1.248013
24	8	0	-2.164540	-0.402296	0.997166
25	45	0	-0.442528	0.144872	-1.596876
26	45	0	-0.117851	0.114602	0.885238
27	6	0	-3.425306	-4.678106	-3.810131
28	6	0	-3.079848	-5.862073	-3.146087
29	6	0	-1.922733	-5.914774	-2.371011
30	6	0	-1.089233	-4.782419	-2.244123
31	6	0	-1.442652	-3.602794	-2.904523
32	6	0	-2.606938	-3.554917	-3.684435
33	6	0	1.979472	-8.249330	-2.098494
34	6	0	2.606577	-7.964794	-3.314774
35	6	0	2.439249	-6.707916	-3.906713
36	6	0	1.649212	-5.738378	-3.285456
37	6	0	1.024254	-6.020634	-2.060048
38	6	0	1.188397	-7.281995	-1.470784
39	6	0	2.972166	-4.632801	0.653847
40	6	0	4.359463	-4.789428	0.724849
41	6	0	5.172766	-4.330766	-0.315813
42	6	0	4.595842	-3.696817	-1.421139
43	6	0	3.210429	-3.535164	-1.496972
44	6	0	2.389332	-4.019640	-0.466226
45	6	0	0.153817	-4.970329	-1.421623

46	6	0	0.897969	-3.890361	-0.581587
47	6	0	0.005716	-4.919537	0.093685
48	6	0	0.490722	-2.413326	-0.522543
49	8	0	0.371036	-1.799050	-1.618831
50	8	0	0.340684	-1.936584	0.649425
51	6	0	1.902481	5.154019	-4.197833
52	6	0	1.751750	6.278406	-3.376796
53	6	0	0.817031	6.266929	-2.342047
54	6	0	0.011013	5.131683	-2.116543
55	6	0	0.175197	4.007191	-2.931089
56	6	0	1.118422	4.022279	-3.967536
57	6	0	-2.915918	8.559245	-1.295895
58	6	0	-3.859724	8.264176	-2.283992
59	6	0	-3.888783	6.989636	-2.860665
60	6	0	-2.978458	6.012457	-2.451808
61	6	0	-2.033899	6.306320	-1.456080
62	6	0	-2.003039	7.584815	-0.881033
63	6	0	-3.536428	5.003652	1.194212
64	6	0	-4.909054	5.071535	1.450433
65	6	0	-5.803802	4.303604	0.699870
66	6	0	-5.320095	3.461916	-0.307521
67	6	0	-3.950000	3.386585	-0.565127
68	6	0	-3.047432	4.161967	0.182893
69	6	0	-1.035253	5.253912	-1.047715
70	6	0	-1.583594	4.107127	-0.143499
71	6	0	-0.622532	5.145881	0.412193
72	6	0	-1.098809	2.653428	-0.218820
73	8	0	-1.232423	2.070881	-1.334126
74	8	0	-0.643284	2.161863	0.863435
75	6	0	4.011833	-2.133325	-5.117865
76	6	0	5.279971	-1.925453	-4.560376
77	6	0	5.446344	-0.998800	-3.532940
78	6	0	4.347335	-0.257867	-3.045001
79	6	0	3.084900	-0.475052	-3.602009
80	6	0	2.921375	-1.410054	-4.634098
81	6	0	7.888698	2.712932	-2.476433
82	6	0	7.524971	3.564454	-3.523358
83	6	0	6.232160	3.500226	-4.055139
84	6	0	5.306325	2.589134	-3.542784
85	6	0	5.668605	1.736550	-2.486892
86	6	0	6.965426	1.799501	-1.958153
87	6	0	4.592534	2.913566	0.846596
88	6	0	4.832178	4.222522	1.272809
89	6	0	4.414452	5.303739	0.490353
90	6	0	3.744657	5.070905	-0.714849
91	6	0	3.499904	3.764099	-1.145449
92	6	0	3.936484	2.678059	-0.372089
93	6	0	4.661360	0.742665	-1.969000
94	6	0	3.713435	1.271388	-0.850452
95	6	0	4.767268	0.218769	-0.543623
96	6	0	2.237112	0.893274	-0.694978
97	8	0	1.496539	0.947188	-1.718474
98	8	0	1.888495	0.577046	0.488659
99	1	0	-6.114305	2.378040	-4.864934
100	1	0	-7.932111	2.021237	-3.201883
101	1	0	-7.576167	0.489517	-1.282377
102	1	0	-3.550482	-0.313717	-2.674241

103	1	0	-3.934048	1.204610	-4.583382
104	1	0	-9.321615	-3.402786	0.360239
105	1	0	-8.955395	-4.983866	-1.524849
106	1	0	-6.975818	-4.708869	-3.006860
107	1	0	-5.365665	-2.856769	-2.608088
108	1	0	-7.718036	-1.558423	0.770017
109	1	0	-4.536195	-2.031937	2.774961
110	1	0	-4.452158	-4.325123	3.722309
111	1	0	-3.950898	-6.267212	2.250118
112	1	0	-3.515914	-5.903188	-0.177303
113	1	0	-3.598524	-3.616326	-1.132162
114	1	0	-5.891467	-0.664629	1.535778
115	1	0	-5.041548	0.714255	0.774462
116	1	0	-4.323247	-4.637725	-4.422479
117	1	0	-3.712090	-6.742585	-3.240821
118	1	0	-1.649316	-6.842440	-1.869118
119	1	0	-0.829813	-2.684132	-2.817175
120	1	0	-2.867635	-2.625454	-4.191441
121	1	0	2.106674	-9.226493	-1.636555
122	1	0	3.222888	-8.717972	-3.800517
123	1	0	2.925589	-6.484055	-4.854541
124	1	0	1.514197	-4.760355	-3.748037
125	1	0	0.702550	-7.512879	-0.525317
126	1	0	2.346161	-4.991024	1.469152
127	1	0	4.804562	-5.277832	1.589808
128	1	0	6.250309	-4.470196	-0.269157
129	1	0	5.225075	-3.327165	-2.231878
130	1	0	2.763318	-3.029575	-2.358234
131	1	0	0.449923	-5.691695	0.718781
132	1	0	-0.949174	-4.594363	0.514070
133	1	0	2.626058	5.164162	-5.009588
134	1	0	2.359482	7.163898	-3.551298
135	1	0	0.697154	7.146537	-1.711111
136	1	0	-0.417450	3.087058	-2.767324
137	1	0	1.234577	3.136861	-4.592705
138	1	0	-2.889612	9.550602	-0.847963
139	1	0	-4.569368	9.023356	-2.604835
140	1	0	-4.622486	6.757277	-3.630582
141	1	0	-2.999166	5.018465	-2.899778
142	1	0	-1.268250	7.823154	-0.115251
143	1	0	-2.848008	5.617772	1.773810
144	1	0	-5.280600	5.732894	2.230595
145	1	0	-6.872294	4.365085	0.892710
146	1	0	-6.012956	2.865656	-0.903538
147	1	0	-3.574122	2.723447	-1.353985
148	1	0	-0.973569	5.871730	1.143586
149	1	0	0.397284	4.833789	0.652040
150	1	0	3.880676	-2.852173	-5.923095
151	1	0	6.135963	-2.483366	-4.934265
152	1	0	6.436468	-0.833722	-3.108439
153	1	0	2.190430	0.068223	-3.239038
154	1	0	1.928141	-1.566685	-5.054923
155	1	0	8.893275	2.760419	-2.060939
156	1	0	8.244001	4.275258	-3.923901
157	1	0	5.946718	4.161458	-4.871114
158	1	0	4.300730	2.534239	-3.960235
159	1	0	7.256281	1.140822	-1.141484

160	1	0	4.911043	2.072929	1.462336
161	1	0	5.345132	4.399758	2.215474
162	1	0	4.608404	6.322041	0.818864
163	1	0	3.409226	5.909044	-1.325203
164	1	0	2.967883	3.587958	-2.083497
165	1	0	5.620889	0.472645	0.086150
166	1	0	4.449315	-0.805643	-0.335715
167	6	0	-0.138665	-1.986531	4.375068
168	6	0	0.798832	-1.137596	3.461246
169	6	0	0.116483	0.005138	2.835497
170	6	0	-0.403030	1.101619	3.688994
171	8	0	-1.702132	0.994224	3.932875
172	6	0	-2.465818	2.043322	4.671326
173	6	0	-2.323285	3.380224	3.944020
174	6	0	-1.969898	2.096733	6.118649
175	6	0	-3.899273	1.518326	4.587889
176	8	0	0.368988	1.972522	4.057222
177	1	0	-3.025785	4.101684	4.375192
178	1	0	-2.562856	3.258847	2.880761
179	1	0	-1.310833	3.777193	4.026501
180	1	0	-2.591964	2.797202	6.687014
181	1	0	-0.932393	2.431727	6.171362
182	1	0	-2.043525	1.113316	6.594233
183	1	0	-4.575986	2.204777	5.107078
184	1	0	-3.979604	0.531154	5.053141
185	1	0	-4.216564	1.438412	3.542952
186	1	0	1.207141	-1.793325	2.689296
187	6	0	8.051021	-0.893990	1.714497
188	6	0	7.076205	-1.895245	1.668286
189	6	0	5.828156	-1.691639	2.251041
190	6	0	5.526866	-0.480839	2.902404
191	6	0	6.514506	0.520215	2.930754
192	6	0	7.764136	0.316498	2.347599
193	6	0	1.841760	0.395132	7.247641
194	6	0	1.446349	1.052812	8.410728
195	6	0	0.420771	0.541212	9.208897
196	6	0	-0.199318	-0.650835	8.830304
197	6	0	0.182203	-1.320078	7.667567
198	6	0	1.196566	-0.790617	6.853000
199	6	0	1.975097	-0.737089	4.471111
200	7	0	1.652125	-1.489063	5.703905
201	8	0	0.801976	-2.550516	5.316791
202	1	0	9.022286	-1.055146	1.255182
203	1	0	7.284835	-2.835317	1.164120
204	1	0	5.069865	-2.467865	2.175432
205	1	0	6.298038	1.464097	3.426262
206	1	0	8.512489	1.103608	2.386802
207	1	0	2.664253	0.791224	6.661379
208	1	0	1.954576	1.969857	8.696430
209	1	0	0.120359	1.055602	10.116811
210	1	0	-0.987907	-1.074200	9.447130
211	1	0	-0.286783	-2.255780	7.389383
212	1	0	1.950295	0.332200	4.681841
213	1	0	-0.837491	-1.336447	4.915430
214	6	0	-0.871002	-3.116781	3.679028
215	1	0	-1.413544	-3.721186	4.412741
216	1	0	-1.592098	-2.714002	2.958783

217	1	0	-0.169431	-3.759494	3.139405
218	6	0	4.223170	-0.216327	3.527996
219	6	0	3.304596	-1.122684	3.896085
220	1	0	3.477919	-2.190960	3.777391
221	1	0	4.000459	0.836874	3.704950

7a-I

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.339909	5.116637	-4.131198
2	6	0	3.379056	6.140768	-3.177109
3	6	0	2.415618	6.194166	-2.169856
4	6	0	1.401820	5.218035	-2.102615
5	6	0	1.370577	4.192917	-3.052808
6	6	0	2.338686	4.145316	-4.063823
7	6	0	-1.196668	8.884058	-1.134213
8	6	0	-2.075743	8.768070	-2.214756
9	6	0	-2.169658	7.556444	-2.908279
10	6	0	-1.389172	6.464309	-2.523124
11	6	0	-0.512317	6.576806	-1.432593
12	6	0	-0.414261	7.793249	-0.742593
13	6	0	-2.147977	5.091477	1.360651
14	6	0	-3.493486	5.345726	1.642833
15	6	0	-4.481995	5.017932	0.710225
16	6	0	-4.120871	4.426534	-0.504724
17	6	0	-2.777877	4.171841	-0.793772
18	6	0	-1.782089	4.514567	0.134617
19	6	0	0.349507	5.400551	-1.050358
20	6	0	-0.336054	4.284989	-0.205380
21	6	0	0.727503	5.187666	0.406541
22	6	0	-0.025455	2.784549	-0.263504
23	8	0	0.367397	2.285910	-1.363089
24	8	0	-0.207483	2.158772	0.827261
25	45	0	0.869916	0.248222	-1.422698
26	45	0	0.076345	0.080669	0.861800
27	6	0	-3.212082	3.884929	-4.528672
28	6	0	-4.500476	3.668092	-4.025538
29	6	0	-4.805180	2.471160	-3.376602
30	6	0	-3.821085	1.475527	-3.222731
31	6	0	-2.530505	1.701929	-3.713017
32	6	0	-2.230885	2.904010	-4.365845
33	6	0	-7.354615	-1.226843	-4.315361
34	6	0	-6.798185	-1.846568	-5.438238
35	6	0	-5.413586	-1.815102	-5.636319
36	6	0	-4.586576	-1.167566	-4.715430
37	6	0	-5.143714	-0.551247	-3.584496
38	6	0	-6.532044	-0.578640	-3.389162
39	6	0	-4.519172	-2.922286	-1.192096
40	6	0	-4.643007	-4.296661	-1.419145
41	6	0	-3.756919	-4.951205	-2.279559
42	6	0	-2.734153	-4.229149	-2.904415
43	6	0	-2.602745	-2.857834	-2.678538
44	6	0	-3.506194	-2.192814	-1.831835

45	6	0	-4.248867	0.174331	-2.613950
46	6	0	-3.389326	-0.706662	-1.659540
47	6	0	-4.558298	0.108905	-1.127298
48	6	0	-1.985953	-0.334107	-1.170627
49	8	0	-1.077042	-0.214700	-2.050119
50	8	0	-1.849343	-0.223859	0.087066
51	6	0	6.141440	-3.120114	-1.928284
52	6	0	6.851167	-3.049509	-0.723442
53	6	0	6.644106	-1.979764	0.147729
54	6	0	5.721491	-0.966260	-0.177305
55	6	0	5.000535	-1.049875	-1.373053
56	6	0	5.214365	-2.124493	-2.245244
57	6	0	9.070755	1.665638	1.515627
58	6	0	9.286599	2.465214	0.389352
59	6	0	8.312205	2.534634	-0.612227
60	6	0	7.125085	1.808878	-0.489064
61	6	0	6.904364	1.011885	0.644786
62	6	0	7.883808	0.938260	1.645514
63	6	0	4.836514	3.038621	2.516226
64	6	0	5.007615	4.421912	2.630601
65	6	0	4.820917	5.248768	1.519352
66	6	0	4.448746	4.689597	0.291749
67	6	0	4.269025	3.310319	0.173260
68	6	0	4.476398	2.474066	1.283776
69	6	0	5.636016	0.206244	0.752898
70	6	0	4.339559	0.988883	1.116130
71	6	0	4.978041	0.032512	2.112291
72	6	0	2.942475	0.641128	0.590951
73	8	0	2.768484	0.691517	-0.667247
74	8	0	2.067438	0.380195	1.471804
75	6	0	0.785828	-4.221794	-5.635169
76	6	0	0.276303	-5.371911	-5.020033
77	6	0	0.448906	-5.565688	-3.649557
78	6	0	1.132323	-4.606630	-2.875807
79	6	0	1.633884	-3.456797	-3.492739
80	6	0	1.459313	-3.267621	-4.869470
81	6	0	2.944385	-8.347984	-0.809808
82	6	0	4.252822	-8.123583	-1.246729
83	6	0	4.616612	-6.863268	-1.733919
84	6	0	3.677057	-5.831585	-1.783509
85	6	0	2.363796	-6.052788	-1.337545
86	6	0	1.999828	-7.317698	-0.855369
87	6	0	1.767481	-4.789265	2.105448
88	6	0	2.655631	-5.081579	3.144415
89	6	0	4.020415	-4.812514	3.000262
90	6	0	4.493993	-4.236780	1.817072
91	6	0	3.611099	-3.939311	0.775408
92	6	0	2.244717	-4.228462	0.910408
93	6	0	1.356297	-4.935546	-1.429774
94	6	0	1.302237	-3.947401	-0.226816
95	6	0	0.158339	-4.915903	-0.493504
96	6	0	0.986984	-2.448965	-0.289863
97	8	0	1.331377	-1.794343	-1.321479
98	8	0	0.404848	-1.983028	0.740335
99	1	0	4.086853	5.078974	-4.921087
100	1	0	4.157080	6.900079	-3.226672
101	1	0	2.434721	7.001945	-1.439458

102	1	0	0.605125	3.405777	-2.992827
103	1	0	2.308162	3.341825	-4.798006
104	1	0	-1.119976	9.826018	-0.594274
105	1	0	-2.685225	9.617206	-2.516073
106	1	0	-2.853131	7.463706	-3.750235
107	1	0	-1.460191	5.520740	-3.064992
108	1	0	0.269782	7.893688	0.097304
109	1	0	-1.385489	5.338714	2.097316
110	1	0	-3.770598	5.801342	2.591858
111	1	0	-5.528145	5.220199	0.929792
112	1	0	-4.886776	4.165093	-1.234160
113	1	0	-2.504944	3.709757	-1.744833
114	1	0	0.444447	5.916116	1.164793
115	1	0	1.708243	4.765288	0.639792
116	1	0	-2.978608	4.812464	-5.047506
117	1	0	-5.267212	4.431127	-4.147482
118	1	0	-5.812513	2.295876	-3.000822
119	1	0	-1.741398	0.946347	-3.577061
120	1	0	-1.224844	3.069410	-4.750184
121	1	0	-8.431792	-1.247905	-4.160416
122	1	0	-7.440049	-2.351680	-6.156765
123	1	0	-4.977900	-2.296365	-6.510232
124	1	0	-3.507970	-1.141587	-4.869223
125	1	0	-6.972945	-0.094905	-2.520023
126	1	0	-5.215439	-2.420969	-0.520750
127	1	0	-5.434138	-4.856583	-0.922125
128	1	0	-3.864909	-6.017327	-2.466171
129	1	0	-2.036896	-4.733779	-3.574643
130	1	0	-1.793584	-2.294729	-3.155498
131	1	0	-5.453759	-0.398076	-0.769624
132	1	0	-4.343457	0.976372	-0.498448
133	1	0	6.314867	-3.946152	-2.614967
134	1	0	7.570275	-3.826328	-0.469824
135	1	0	7.208661	-1.916806	1.077120
136	1	0	4.252446	-0.283473	-1.629315
137	1	0	4.653058	-2.178124	-3.177517
138	1	0	9.828779	1.607500	2.294584
139	1	0	10.210308	3.031376	0.291038
140	1	0	8.478441	3.155438	-1.490979
141	1	0	6.366412	1.860415	-1.269819
142	1	0	7.725681	0.314051	2.522393
143	1	0	4.989174	2.401728	3.386529
144	1	0	5.294861	4.853096	3.587868
145	1	0	4.967347	6.323130	1.607123
146	1	0	4.300983	5.328795	-0.579659
147	1	0	3.960468	2.873643	-0.782419
148	1	0	5.454301	0.422976	3.010348
149	1	0	4.463210	-0.905619	2.336971
150	1	0	0.657007	-4.073615	-6.705088
151	1	0	-0.247730	-6.118693	-5.613434
152	1	0	0.068267	-6.468773	-3.174175
153	1	0	2.142178	-2.684825	-2.896267
154	1	0	1.850631	-2.367472	-5.340839
155	1	0	2.657858	-9.327226	-0.430572
156	1	0	4.986488	-8.925723	-1.208073
157	1	0	5.634639	-6.685950	-2.075452
158	1	0	3.959192	-4.851055	-2.168088

159	1	0	0.983816	-7.502735	-0.512324
160	1	0	0.702974	-4.986107	2.230199
161	1	0	2.280628	-5.516542	4.069510
162	1	0	4.710191	-5.047553	3.807823
163	1	0	5.554828	-4.019746	1.700461
164	1	0	3.987426	-3.485819	-0.143611
165	1	0	-0.021854	-5.737129	0.200287
166	1	0	-0.790632	-4.524928	-0.868159
167	6	0	-2.859063	1.370887	4.487981
168	6	0	-2.449498	-0.033417	4.101885
169	6	0	-1.061824	-0.438037	3.762156
170	6	0	-0.007418	0.100593	4.733248
171	8	0	0.415467	1.310670	4.339717
172	6	0	1.506172	2.030480	5.035841
173	6	0	2.775184	1.172005	5.028321
174	6	0	1.055952	2.399448	6.453276
175	6	0	1.686775	3.274665	4.165033
176	8	0	0.352968	-0.506458	5.719071
177	1	0	3.613221	1.762644	5.414259
178	1	0	3.004751	0.863883	4.001604
179	1	0	2.657207	0.282423	5.648669
180	1	0	1.826469	3.013162	6.933145
181	1	0	0.892570	1.506218	7.058929
182	1	0	0.129635	2.983964	6.422279
183	1	0	2.489444	3.902827	4.565851
184	1	0	0.765286	3.864130	4.129734
185	1	0	1.948221	2.985583	3.140641
186	1	0	-0.787643	-0.058154	2.741826
187	6	0	-3.253344	-7.097473	2.022457
188	6	0	-3.571053	-6.651103	3.309395
189	6	0	-3.519897	-5.294490	3.616039
190	6	0	-3.153569	-4.348885	2.638618
191	6	0	-2.821638	-4.815855	1.353813
192	6	0	-2.876502	-6.173937	1.045762
193	6	0	-6.844978	0.806499	4.969826
194	6	0	-8.204419	0.793052	4.673963
195	6	0	-8.737071	-0.146986	3.787569
196	6	0	-7.879953	-1.068770	3.186350
197	6	0	-6.511424	-1.060353	3.455598
198	6	0	-5.982214	-0.125682	4.362812
199	6	0	-3.550158	-0.829261	4.182845
200	7	0	-4.623397	-0.119588	4.732428
201	8	0	-4.147031	1.170550	5.129546
202	1	0	-3.293532	-8.157331	1.787606
203	1	0	-3.852197	-7.365418	4.078285
204	1	0	-3.746601	-4.966420	4.626296
205	1	0	-2.535286	-4.095121	0.588206
206	1	0	-2.630187	-6.507860	0.041114
207	1	0	-6.436453	1.533494	5.660379
208	1	0	-8.854378	1.523653	5.148358
209	1	0	-9.800338	-0.157134	3.567187
210	1	0	-8.271175	-1.799029	2.482904
211	1	0	-5.862014	-1.767654	2.955323
212	1	0	-0.971478	-1.525738	3.733801
213	1	0	-2.214427	1.793039	5.268060
214	6	0	-2.966330	2.347288	3.314548
215	1	0	-3.351289	3.314099	3.657226

216	1	0	-1.984171	2.507588	2.854225
217	1	0	-3.641957	1.954866	2.547254
218	6	0	-3.106021	-2.906150	2.896821
219	6	0	-3.679261	-2.261965	3.935879
220	1	0	-4.290760	-2.806568	4.652324
221	1	0	-2.595645	-2.314788	2.137214

s-trans vinyl diazoacetate **2-II** and styryl nitrene **3b** with an approach over *Re*-face

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.891936	2.166427	5.476168
2	6	0	4.140622	1.547287	5.338764
3	6	0	4.261072	0.377901	4.589068
4	6	0	3.132186	-0.194293	3.965675
5	6	0	1.890030	0.433299	4.098568
6	6	0	1.774399	1.609342	4.852801
7	6	0	5.508411	-3.889491	5.296152
8	6	0	4.565413	-4.422845	6.179434
9	6	0	3.230437	-4.010142	6.105064
10	6	0	2.838122	-3.068737	5.150961
11	6	0	3.783068	-2.537324	4.259248
12	6	0	5.121489	-2.947837	4.337604
13	6	0	3.277731	-4.419389	1.568845
14	6	0	3.034866	-5.794640	1.640008
15	6	0	1.816920	-6.269745	2.134788
16	6	0	0.835110	-5.362934	2.549434
17	6	0	1.071630	-3.988872	2.479971
18	6	0	2.302078	-3.507214	2.000218
19	6	0	3.350962	-1.498352	3.256005
20	6	0	2.567399	-2.031207	2.016597
21	6	0	3.981918	-1.494101	1.871004
22	6	0	1.432229	-1.255956	1.327944
23	8	0	0.432275	-0.976943	2.049836
24	8	0	1.597401	-1.002792	0.093949
25	45	0	-1.045244	0.295003	1.264484
26	45	0	0.018965	-0.042503	-0.989861
27	6	0	-2.294246	-4.648012	4.797653
28	6	0	-2.511638	-5.789089	4.014640
29	6	0	-2.804534	-5.658200	2.658209
30	6	0	-2.891102	-4.381455	2.062425
31	6	0	-2.671509	-3.247945	2.848237
32	6	0	-2.371483	-3.384436	4.210674
33	6	0	-6.179644	-6.665486	-0.270763
34	6	0	-7.261840	-5.948308	0.246520
35	6	0	-7.044106	-4.716005	0.873063
36	6	0	-5.750496	-4.201956	0.981729
37	6	0	-4.662705	-4.917975	0.455360
38	6	0	-4.881806	-6.154689	-0.166931
39	6	0	-3.609301	-3.626272	-2.852297
40	6	0	-4.536700	-3.395726	-3.872315
41	6	0	-5.652853	-2.586427	-3.638454
42	6	0	-5.832141	-1.997337	-2.382862
43	6	0	-4.907031	-2.221945	-1.359959

44	6	0	-3.797668	-3.051176	-1.585185
45	6	0	-3.273457	-4.356770	0.610120
46	6	0	-2.827470	-3.329376	-0.471332
47	6	0	-2.185623	-4.705363	-0.397755
48	6	0	-1.963440	-2.085377	-0.209740
49	8	0	-2.259795	-1.369915	0.787122
50	8	0	-1.041655	-1.878141	-1.062729
51	6	0	-3.429498	5.478928	2.643508
52	6	0	-2.680362	6.573752	2.193762
53	6	0	-1.381504	6.385107	1.726513
54	6	0	-0.798023	5.097665	1.699101
55	6	0	-1.557698	4.010355	2.138429
56	6	0	-2.864935	4.204357	2.610295
57	6	0	2.679661	8.049895	2.314747
58	6	0	3.049362	7.660764	3.605400
59	6	0	2.636397	6.420043	4.103704
60	6	0	1.855639	5.571102	3.316330
61	6	0	1.484877	5.960646	2.019338
62	6	0	1.899106	7.203939	1.520801
63	6	0	3.757070	4.570304	0.100045
64	6	0	5.127533	4.512120	0.366368
65	6	0	5.616333	3.649843	1.352176
66	6	0	4.725839	2.847428	2.072240
67	6	0	3.354958	2.902466	1.809927
68	6	0	2.858565	3.763470	0.818067
69	6	0	0.618982	5.040493	1.197650
70	6	0	1.379683	3.831321	0.562753
71	6	0	0.819870	4.944473	-0.308431
72	6	0	0.777766	2.425667	0.428818
73	8	0	0.254588	1.935502	1.472247
74	8	0	0.881443	1.875667	-0.711536
75	6	0	-7.042508	-0.600602	1.451145
76	6	0	-7.685302	-0.136195	0.296430
77	6	0	-7.024509	0.736146	-0.566452
78	6	0	-5.705920	1.160067	-0.291678
79	6	0	-5.069552	0.690229	0.860079
80	6	0	-5.738828	-0.186361	1.726146
81	6	0	-7.440259	4.944686	-2.383860
82	6	0	-7.491879	5.726157	-1.226450
83	6	0	-6.766402	5.340067	-0.093654
84	6	0	-5.992373	4.178364	-0.117476
85	6	0	-5.933933	3.395099	-1.282433
86	6	0	-6.665229	3.780879	-2.414251
87	6	0	-2.805209	3.910291	-3.402766
88	6	0	-2.386350	5.186618	-3.787976
89	6	0	-2.280370	6.208641	-2.838903
90	6	0	-2.580486	5.945894	-1.498822
91	6	0	-2.996751	4.670511	-1.106917
92	6	0	-3.127630	3.650608	-2.060862
93	6	0	-5.113955	2.132141	-1.273581
94	6	0	-3.611941	2.288574	-1.653518
95	6	0	-4.571413	1.553549	-2.574764
96	6	0	-2.473746	1.508498	-0.985602
97	8	0	-2.411218	1.546566	0.277693
98	8	0	-1.675440	0.916306	-1.779202
99	1	0	2.795505	3.076191	6.064238
100	1	0	5.015835	1.976748	5.821828

101	1	0	5.231514	-0.107450	4.496542
102	1	0	0.983460	0.033658	3.602349
103	1	0	0.798387	2.087768	4.942298
104	1	0	6.547792	-4.206221	5.354485
105	1	0	4.868151	-5.155747	6.923839
106	1	0	2.494216	-4.422781	6.792734
107	1	0	1.798539	-2.744437	5.091913
108	1	0	5.862211	-2.533145	3.657983
109	1	0	4.235313	-4.059654	1.197153
110	1	0	3.801993	-6.496076	1.317321
111	1	0	1.635613	-7.339765	2.204937
112	1	0	-0.118362	-5.725259	2.938524
113	1	0	0.300024	-3.279054	2.805088
114	1	0	4.798785	-2.172286	1.634791
115	1	0	4.120347	-0.538970	1.358604
116	1	0	-2.068723	-4.748001	5.856941
117	1	0	-2.458662	-6.776921	4.467535
118	1	0	-2.984507	-6.546779	2.054652
119	1	0	-2.714849	-2.232117	2.411432
120	1	0	-2.197615	-2.489918	4.808982
121	1	0	-6.345699	-7.624735	-0.756953
122	1	0	-8.270623	-6.346201	0.163051
123	1	0	-7.885003	-4.155217	1.277372
124	1	0	-5.580246	-3.243283	1.474370
125	1	0	-4.045791	-6.720604	-0.570968
126	1	0	-2.738795	-4.250177	-3.042570
127	1	0	-4.390887	-3.850363	-4.849631
128	1	0	-6.379084	-2.415893	-4.429855
129	1	0	-6.697942	-1.362328	-2.193354
130	1	0	-5.048538	-1.752419	-0.382257
131	1	0	-2.373721	-5.429323	-1.187506
132	1	0	-1.157376	-4.785636	-0.041340
133	1	0	-4.440864	5.623759	3.015038
134	1	0	-3.111749	7.572237	2.213469
135	1	0	-0.806119	7.245552	1.386177
136	1	0	-1.171774	2.966527	2.113466
137	1	0	-3.436720	3.338407	2.946004
138	1	0	2.999442	9.014223	1.925186
139	1	0	3.656842	8.319935	4.221104
140	1	0	2.924826	6.113945	5.107570
141	1	0	1.536225	4.601258	3.700495
142	1	0	1.613253	7.514196	0.518228
143	1	0	3.386221	5.257134	-0.660422
144	1	0	5.813609	5.146828	-0.190625
145	1	0	6.682078	3.608919	1.563211
146	1	0	5.096880	2.179809	2.850167
147	1	0	2.662438	2.278070	2.384921
148	1	0	1.498488	5.620235	-0.826139
149	1	0	-0.050866	4.734535	-0.937682
150	1	0	-7.558657	-1.276198	2.129026
151	1	0	-8.702845	-0.452383	0.076529
152	1	0	-7.533141	1.107064	-1.455882
153	1	0	-4.027931	0.979131	1.106422
154	1	0	-5.224767	-0.544350	2.618537
155	1	0	-8.003305	5.241843	-3.266409
156	1	0	-8.093495	6.631848	-1.205418
157	1	0	-6.804872	5.946438	0.809440

158	1	0	-5.430905	3.874494	0.767235
159	1	0	-6.630822	3.179160	-3.320073
160	1	0	-2.868721	3.113191	-4.142256
161	1	0	-2.140619	5.383022	-4.829670
162	1	0	-1.964300	7.203803	-3.142501
163	1	0	-2.492788	6.734145	-0.751495
164	1	0	-3.218858	4.467081	-0.055903
165	1	0	-4.839074	1.995945	-3.532451
166	1	0	-4.486299	0.468173	-2.669946
167	6	0	0.296611	-2.692374	-5.778468
168	6	0	0.851514	-1.636631	-4.892913
169	6	0	0.463803	-1.450400	-3.584729
170	6	0	0.812914	-0.325414	-2.816144
171	6	0	1.640571	0.760428	-3.419515
172	8	0	2.804956	0.910128	-2.795440
173	6	0	3.732233	2.024538	-3.127604
174	6	0	3.008280	3.369939	-3.028895
175	6	0	4.319084	1.781861	-4.521587
176	6	0	4.796565	1.895920	-2.039065
177	8	0	1.215368	1.417083	-4.356777
178	1	0	1.102383	-3.178850	-6.335552
179	1	0	-0.372058	-2.220374	-6.514691
180	1	0	-0.272804	-3.441109	-5.221240
181	1	0	1.511525	-0.910275	-5.357411
182	1	0	3.752264	4.174080	-3.055801
183	1	0	2.462534	3.426622	-2.080872
184	1	0	2.300502	3.510550	-3.845816
185	1	0	5.072158	2.547441	-4.739185
186	1	0	3.541359	1.831942	-5.286736
187	1	0	4.807624	0.803655	-4.566724
188	1	0	5.575568	2.651588	-2.185377
189	1	0	5.260773	0.906393	-2.062295
190	1	0	4.348972	2.051539	-1.049573
191	1	0	-0.205611	-2.176579	-3.128455
192	6	0	9.844229	0.724269	-4.354537
193	6	0	8.812967	0.365945	-5.230012
194	6	0	7.758265	-0.426125	-4.789531
195	6	0	7.704825	-0.880094	-3.454695
196	6	0	8.755275	-0.514415	-2.589431
197	6	0	9.811136	0.279159	-3.031694
198	6	0	2.075378	-5.362351	-3.816122
199	6	0	1.209611	-6.296830	-3.253726
200	6	0	0.795120	-6.161243	-1.924979
201	6	0	1.244064	-5.082603	-1.161843
202	6	0	2.120264	-4.142610	-1.707721
203	6	0	2.537229	-4.303853	-3.029838
204	7	0	3.452219	-3.364484	-3.647801
205	8	0	3.191573	-3.022384	-4.865074
206	1	0	10.666431	1.342364	-4.703744
207	1	0	8.835082	0.704222	-6.262349
208	1	0	6.973256	-0.702257	-5.486951
209	1	0	8.733188	-0.857123	-1.557661
210	1	0	10.607666	0.549759	-2.344201
211	1	0	2.407295	-5.437071	-4.844740
212	1	0	0.860045	-7.132747	-3.852365
213	1	0	0.118065	-6.889961	-1.489296
214	1	0	0.908063	-4.957197	-0.133656

215	1	0	2.425229	-3.277124	-1.125918
216	1	0	4.651913	-3.346555	-1.987687
217	6	0	5.493738	-2.093275	-3.585422
218	6	0	6.623177	-1.709565	-2.934741
219	6	0	4.524931	-2.951955	-2.987997
220	1	0	5.285347	-1.788477	-4.605592
221	1	0	6.757693	-2.048806	-1.907301

TS3b-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.217346	1.803963	5.428858
2	6	0	4.409917	1.089685	5.258437
3	6	0	4.420849	-0.079172	4.498282
4	6	0	3.236286	-0.555982	3.898591
5	6	0	2.051523	0.168560	4.060666
6	6	0	2.046039	1.343345	4.825664
7	6	0	5.311356	-4.433379	5.204154
8	6	0	4.342325	-4.880127	6.107028
9	6	0	3.046436	-4.354810	6.053743
10	6	0	2.718972	-3.387569	5.101099
11	6	0	3.689517	-2.943117	4.189436
12	6	0	4.989124	-3.466327	4.246914
13	6	0	2.958965	-4.790403	1.545285
14	6	0	2.593627	-6.136218	1.650071
15	6	0	1.346480	-6.488601	2.173861
16	6	0	0.457215	-5.487859	2.581807
17	6	0	0.816261	-4.142886	2.478830
18	6	0	2.078164	-3.784648	1.972771
19	6	0	3.330192	-1.874416	3.188159
20	6	0	2.479216	-2.340059	1.966260
21	6	0	3.933593	-1.934141	1.792100
22	6	0	1.407394	-1.463327	1.293372
23	8	0	0.445365	-1.107815	2.032182
24	8	0	1.580303	-1.214868	0.060097
25	45	0	-0.934192	0.302718	1.295633
26	45	0	0.080267	-0.071667	-0.983033
27	6	0	-2.622298	-4.579721	4.716414
28	6	0	-2.953754	-5.674301	3.907328
29	6	0	-3.243933	-5.480874	2.557831
30	6	0	-3.214720	-4.186465	1.995505
31	6	0	-2.880847	-3.099853	2.806936
32	6	0	-2.583313	-3.299740	4.162078
33	6	0	-6.747863	-6.061742	-0.346045
34	6	0	-7.743815	-5.253569	0.208879
35	6	0	-7.392550	-4.068393	0.865062
36	6	0	-6.051832	-3.692062	0.965979
37	6	0	-5.050169	-4.499403	0.401993
38	6	0	-5.403292	-5.688800	-0.250204
39	6	0	-3.880763	-3.237217	-2.898325
40	6	0	-4.787772	-2.896188	-3.905527
41	6	0	-5.828996	-2.001012	-3.640722
42	6	0	-5.952120	-1.437031	-2.367050

43	6	0	-5.046485	-1.771834	-1.356804
44	6	0	-4.014630	-2.687377	-1.613003
45	6	0	-3.609017	-4.087264	0.549398
46	6	0	-3.069700	-3.086421	-0.514351
47	6	0	-2.573529	-4.522616	-0.479650
48	6	0	-2.081054	-1.942271	-0.231744
49	8	0	-2.298524	-1.229770	0.787853
50	8	0	-1.150362	-1.804220	-1.087005
51	6	0	-2.954313	5.563430	2.828480
52	6	0	-2.133473	6.621060	2.416329
53	6	0	-0.854233	6.361923	1.929477
54	6	0	-0.361387	5.039260	1.844112
55	6	0	-1.192703	3.990565	2.245820
56	6	0	-2.480084	4.255422	2.737854
57	6	0	3.309739	7.754280	2.459595
58	6	0	3.670036	7.317904	3.737718
59	6	0	3.183133	6.097718	4.219769
60	6	0	2.338210	5.316404	3.428694
61	6	0	1.976611	5.753337	2.144208
62	6	0	2.465004	6.976052	1.662080
63	6	0	4.125549	4.283195	0.139842
64	6	0	5.495665	4.150802	0.380492
65	6	0	5.956348	3.251099	1.346165
66	6	0	5.038242	2.484887	2.071049
67	6	0	3.667645	2.615370	1.835477
68	6	0	3.198875	3.516429	0.866095
69	6	0	1.042181	4.906000	1.319098
70	6	0	1.721205	3.669690	0.643741
71	6	0	1.209793	4.832048	-0.192254
72	6	0	1.038327	2.301921	0.493165
73	8	0	0.495329	1.828128	1.534696
74	8	0	1.100484	1.765795	-0.655426
75	6	0	-6.991378	-0.043491	1.534372
76	6	0	-7.600579	0.502879	0.397464
77	6	0	-6.870312	1.326740	-0.457013
78	6	0	-5.514471	1.619080	-0.191763
79	6	0	-4.912031	1.067014	0.941596
80	6	0	-5.651146	0.239908	1.799473
81	6	0	-6.914413	5.588901	-2.192948
82	6	0	-6.895830	6.342131	-1.016021
83	6	0	-6.206484	5.864531	0.104424
84	6	0	-5.538522	4.639863	0.048868
85	6	0	-5.550366	3.884261	-1.135718
86	6	0	-6.245496	4.362206	-2.255095
87	6	0	-2.389878	4.155964	-3.276550
88	6	0	-1.866721	5.398964	-3.642573
89	6	0	-1.684604	6.397028	-2.679553
90	6	0	-2.012845	6.142195	-1.344565
91	6	0	-2.533119	4.899587	-0.971845
92	6	0	-2.741115	3.906237	-1.939919
93	6	0	-4.845723	2.553405	-1.160957
94	6	0	-3.339384	2.583631	-1.554843
95	6	0	-4.369296	1.956916	-2.479881
96	6	0	-2.266445	1.690034	-0.919502
97	8	0	-2.196502	1.686281	0.344835
98	8	0	-1.525485	1.058529	-1.736349
99	1	0	3.206037	2.712877	6.025929

100	1	0	5.326643	1.444552	5.724524
101	1	0	5.347446	-0.638518	4.379914
102	1	0	1.105972	-0.151054	3.577919
103	1	0	1.113265	1.897370	4.938612
104	1	0	6.320761	-4.837307	5.246412
105	1	0	4.594614	-5.632714	6.850516
106	1	0	2.290212	-4.699453	6.756981
107	1	0	1.710160	-2.975056	5.058669
108	1	0	5.750353	-3.118951	3.552564
109	1	0	3.939388	-4.527147	1.153675
110	1	0	3.288980	-6.910885	1.332763
111	1	0	1.070934	-7.535961	2.272277
112	1	0	-0.519526	-5.753622	2.991094
113	1	0	0.117071	-3.358317	2.797997
114	1	0	4.682152	-2.683924	1.548195
115	1	0	4.146132	-0.997176	1.271733
116	1	0	-2.399188	-4.727994	5.770470
117	1	0	-2.991979	-6.673954	4.334767
118	1	0	-3.512391	-6.332157	1.933931
119	1	0	-2.829827	-2.073288	2.395577
120	1	0	-2.319587	-2.441561	4.780468
121	1	0	-7.017799	-6.984505	-0.855538
122	1	0	-8.788981	-5.544128	0.131589
123	1	0	-8.165933	-3.436646	1.298442
124	1	0	-5.777588	-2.770142	1.481668
125	1	0	-4.635198	-6.324544	-0.683993
126	1	0	-3.067315	-3.926843	-3.112272
127	1	0	-4.684992	-3.331293	-4.896909
128	1	0	-6.540340	-1.744225	-4.422162
129	1	0	-6.758659	-0.735238	-2.153404
130	1	0	-5.142862	-1.320951	-0.364905
131	1	0	-2.843273	-5.204307	-1.283080
132	1	0	-1.556862	-4.716793	-0.136829
133	1	0	-3.950515	5.762685	3.215242
134	1	0	-2.493992	7.645366	2.480060
135	1	0	-0.223573	7.194124	1.618207
136	1	0	-0.882978	2.922607	2.173790
137	1	0	-3.108310	3.417432	3.042660
138	1	0	3.686895	8.702665	2.082608
139	1	0	4.327369	7.924359	4.356238
140	1	0	3.463848	5.754901	5.213848
141	1	0	1.960767	4.362444	3.799875
142	1	0	2.186894	7.322811	0.669341
143	1	0	3.777469	4.995286	-0.607906
144	1	0	6.203681	4.756686	-0.180820
145	1	0	7.021813	3.153059	1.537879
146	1	0	5.387454	1.786505	2.831741
147	1	0	2.953699	2.018484	2.413333
148	1	0	1.915458	5.480318	-0.708767
149	1	0	0.316369	4.686224	-0.808100
150	1	0	-7.561291	-0.680781	2.206123
151	1	0	-8.645739	0.288403	0.184949
152	1	0	-7.351863	1.762116	-1.332141
153	1	0	-3.844096	1.249971	1.178617
154	1	0	-5.162663	-0.183348	2.677532
155	1	0	-7.449414	5.957083	-3.066042
156	1	0	-7.414750	7.296647	-0.970247

157	1	0	-6.190090	6.448718	1.022654
158	1	0	-5.005132	4.265179	0.924031
159	1	0	-6.264871	3.783220	-3.176083
160	1	0	-2.512266	3.375222	-4.026263
161	1	0	-1.599453	5.588003	-4.680224
162	1	0	-1.287850	7.367248	-2.968413
163	1	0	-1.865985	6.910644	-0.586161
164	1	0	-2.776716	4.701186	0.075466
165	1	0	-4.605454	2.441578	-3.425210
166	1	0	-4.381762	0.870421	-2.598045
167	6	0	-0.021253	-2.573798	-5.838002
168	6	0	0.806235	-1.727078	-4.929637
169	6	0	0.432713	-1.491763	-3.593710
170	6	0	0.834107	-0.394226	-2.857187
171	6	0	1.664326	0.672088	-3.489700
172	8	0	2.849627	0.818614	-2.889306
173	6	0	3.746162	1.953060	-3.219183
174	6	0	3.010334	3.285633	-3.051036
175	6	0	4.292220	1.775182	-4.640336
176	6	0	4.850548	1.807995	-2.173191
177	8	0	1.248512	1.331688	-4.430378
178	1	0	0.569860	-2.978943	-6.662816
179	1	0	-0.806501	-1.933676	-6.267925
180	1	0	-0.511426	-3.388984	-5.298233
181	1	0	1.456980	-1.004239	-5.410001
182	1	0	3.738848	4.102756	-3.103285
183	1	0	2.516321	3.312261	-2.074388
184	1	0	2.256893	3.430289	-3.825557
185	1	0	5.024321	2.562969	-4.851764
186	1	0	3.488810	1.838083	-5.376635
187	1	0	4.800132	0.810754	-4.739962
188	1	0	5.602325	2.593657	-2.305266
189	1	0	5.344195	0.836043	-2.256716
190	1	0	4.429812	1.900416	-1.164445
191	1	0	-0.272723	-2.182417	-3.135285
192	6	0	9.418276	0.142339	-4.727449
193	6	0	8.338654	-0.147502	-5.569623
194	6	0	7.233316	-0.835945	-5.082735
195	6	0	7.180141	-1.250089	-3.734878
196	6	0	8.280532	-0.958168	-2.903863
197	6	0	9.385758	-0.266356	-3.392584
198	6	0	1.355476	-5.424892	-3.858122
199	6	0	0.538710	-6.385382	-3.266922
200	6	0	0.253456	-6.320153	-1.899869
201	6	0	0.776074	-5.281819	-1.127124
202	6	0	1.596998	-4.310779	-1.701526
203	6	0	1.891122	-4.407616	-3.063105
204	7	0	2.774189	-3.459932	-3.703220
205	8	0	2.457585	-3.083794	-4.918638
206	1	0	10.279883	0.679929	-5.112808
207	1	0	8.363226	0.162299	-6.610485
208	1	0	6.410656	-1.065743	-5.752806
209	1	0	8.256700	-1.273888	-1.863736
210	1	0	10.220856	-0.047088	-2.733571
211	1	0	1.595338	-5.452484	-4.914119
212	1	0	0.130099	-7.188153	-3.873205
213	1	0	-0.382732	-7.070654	-1.440360

214	1	0	0.538380	-5.211234	-0.066955
215	1	0	1.947410	-3.468780	-1.110462
216	1	0	4.076688	-3.478793	-2.134349
217	6	0	4.858007	-2.245519	-3.764573
218	6	0	6.051251	-1.976558	-3.170096
219	6	0	3.888918	-3.063763	-3.117610
220	1	0	4.614873	-1.901192	-4.763122
221	1	0	6.202803	-2.343304	-2.154659

4b-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.577155	-4.194582	-5.165596
2	6	0	0.389827	-5.157246	-4.847836
3	6	0	1.418574	-4.845212	-3.961268
4	6	0	1.503227	-3.561497	-3.378055
5	6	0	0.530773	-2.609718	-3.692650
6	6	0	-0.504170	-2.928986	-4.583856
7	6	0	5.913823	-4.792142	-3.894965
8	6	0	6.277969	-3.804715	-4.814649
9	6	0	5.478513	-2.666191	-4.966744
10	6	0	4.319967	-2.513962	-4.202273
11	6	0	3.956358	-3.502666	-3.273713
12	6	0	4.755573	-4.644710	-3.125177
13	6	0	5.088278	-2.409515	-0.197000
14	6	0	6.363940	-1.860599	-0.033594
15	6	0	6.697586	-0.656791	-0.660540
16	6	0	5.743596	0.005257	-1.441856
17	6	0	4.469273	-0.539430	-1.609263
18	6	0	4.136949	-1.762376	-1.002003
19	6	0	2.686484	-3.330016	-2.481029
20	6	0	2.788886	-2.369641	-1.258064
21	6	0	2.596758	-3.864117	-1.056452
22	6	0	1.665410	-1.409120	-0.813974
23	8	0	1.152474	-0.692219	-1.715737
24	8	0	1.402208	-1.418509	0.427262
25	45	0	-0.603766	0.444083	-1.285332
26	45	0	-0.086029	-0.031264	1.145166
27	6	0	4.095602	1.539332	-4.891231
28	6	0	5.085600	2.311288	-4.269913
29	6	0	4.796842	2.998958	-3.092578
30	6	0	3.511106	2.928197	-2.512655
31	6	0	2.529311	2.153942	-3.136527
32	6	0	2.824403	1.464011	-4.321290
33	6	0	4.880557	7.211925	-1.445922
34	6	0	3.938090	7.896280	-2.218348
35	6	0	2.793586	7.230221	-2.671157
36	6	0	2.591028	5.885696	-2.353379
37	6	0	3.534092	5.198496	-1.572088
38	6	0	4.682279	5.865797	-1.122680
39	6	0	2.340171	5.104041	1.816173
40	6	0	1.799770	6.222106	2.458587

41	6	0	0.669665	6.856609	1.934607
42	6	0	0.072369	6.361915	0.770268
43	6	0	0.606093	5.244125	0.125338
44	6	0	1.753067	4.616743	0.638247
45	6	0	3.309223	3.741389	-1.265196
46	6	0	2.338702	3.439213	-0.085845
47	6	0	3.823801	3.149321	0.041920
48	6	0	1.344082	2.265993	-0.075643
49	8	0	0.571340	2.182051	-1.072024
50	8	0	1.378687	1.513972	0.945909
51	6	0	-6.267552	0.996368	-2.772770
52	6	0	-7.093405	0.042607	-2.164156
53	6	0	-6.531210	-1.067114	-1.536379
54	6	0	-5.130448	-1.249518	-1.504818
55	6	0	-4.312377	-0.281072	-2.093657
56	6	0	-4.882978	0.832762	-2.727899
57	6	0	-6.892137	-5.493877	-1.698747
58	6	0	-6.420757	-5.842651	-2.967564
59	6	0	-5.371569	-5.117732	-3.543775
60	6	0	-4.795259	-4.048120	-2.855378
61	6	0	-5.265433	-3.699092	-1.579285
62	6	0	-6.318241	-4.424771	-1.003822
63	6	0	-3.159592	-5.256553	0.399074
64	6	0	-2.667123	-6.545761	0.175706
65	6	0	-1.728407	-6.775894	-0.834089
66	6	0	-1.280503	-5.709023	-1.620536
67	6	0	-1.768490	-4.419616	-1.401224
68	6	0	-2.714703	-4.183276	-0.389294
69	6	0	-4.651238	-2.521767	-0.864701
70	6	0	-3.262748	-2.798612	-0.204547
71	6	0	-4.496644	-2.561045	0.649362
72	6	0	-2.129637	-1.760445	-0.147125
73	8	0	-1.754773	-1.304629	-1.270996
74	8	0	-1.663339	-1.484078	0.997350
75	6	0	-1.858030	6.203996	-2.821315
76	6	0	-2.538968	6.891721	-1.808581
77	6	0	-3.127072	6.185952	-0.760755
78	6	0	-3.047621	4.776726	-0.705768
79	6	0	-2.360582	4.098569	-1.715411
80	6	0	-1.770057	4.812720	-2.767850
81	6	0	-7.171485	5.607287	1.305016
82	6	0	-7.936760	5.167335	0.221626
83	6	0	-7.343438	4.387462	-0.777601
84	6	0	-5.991618	4.048898	-0.694388
85	6	0	-5.222057	4.484578	0.397306
86	6	0	-5.817285	5.269488	1.394552
87	6	0	-4.666918	1.904432	3.142656
88	6	0	-5.733240	1.201221	3.709309
89	6	0	-6.678338	0.575409	2.889617
90	6	0	-6.545504	0.643864	1.499487
91	6	0	-5.480504	1.345138	0.927209
92	6	0	-4.544150	1.992390	1.746257
93	6	0	-3.759115	4.128187	0.448568
94	6	0	-3.415297	2.775445	1.138517
95	6	0	-3.022162	4.095669	1.781999
96	6	0	-2.305466	1.817542	0.681236
97	8	0	-2.267444	1.509926	-0.547530

98	8	0	-1.541771	1.402261	1.607220
99	1	0	-1.379310	-4.434655	-5.859633
100	1	0	0.339454	-6.146450	-5.297508
101	1	0	2.172230	-5.595081	-3.726161
102	1	0	0.536593	-1.596403	-3.237957
103	1	0	-1.257172	-2.173376	-4.811872
104	1	0	6.531502	-5.680226	-3.777993
105	1	0	7.178854	-3.921276	-5.412723
106	1	0	5.758494	-1.896579	-5.684007
107	1	0	3.693546	-1.628268	-4.321927
108	1	0	4.475927	-5.420584	-2.416732
109	1	0	4.851318	-3.363310	0.270039
110	1	0	7.105865	-2.387052	0.563926
111	1	0	7.699559	-0.247111	-0.559104
112	1	0	5.994486	0.943904	-1.939568
113	1	0	3.724742	-0.021497	-2.227188
114	1	0	3.403147	-4.467076	-0.647395
115	1	0	1.623861	-4.217061	-0.704441
116	1	0	4.316359	1.006626	-5.813112
117	1	0	6.077199	2.380091	-4.711636
118	1	0	5.564826	3.612291	-2.623778
119	1	0	1.508363	2.049301	-2.709846
120	1	0	2.044245	0.862968	-4.790749
121	1	0	5.771634	7.727367	-1.094320
122	1	0	4.092647	8.943612	-2.467266
123	1	0	2.057445	7.760874	-3.272735
124	1	0	1.700462	5.364260	-2.707541
125	1	0	5.420630	5.339985	-0.523339
126	1	0	3.215528	4.611018	2.232337
127	1	0	2.261183	6.600154	3.367673
128	1	0	0.254568	7.730752	2.430704
129	1	0	-0.814016	6.847046	0.358935
130	1	0	0.127898	4.848740	-0.777227
131	1	0	4.430640	3.749975	0.715703
132	1	0	4.156884	2.110830	0.047301
133	1	0	-6.704031	1.856119	-3.274994
134	1	0	-8.173805	0.165798	-2.186463
135	1	0	-7.181487	-1.809292	-1.075045
136	1	0	-3.200580	-0.344639	-2.062006
137	1	0	-4.223881	1.574709	-3.180828
138	1	0	-7.709010	-6.054507	-1.249291
139	1	0	-6.868017	-6.674472	-3.506283
140	1	0	-5.002380	-5.387251	-4.531500
141	1	0	-3.976513	-3.481681	-3.301013
142	1	0	-6.693076	-4.156440	-0.018663
143	1	0	-3.899181	-5.088597	1.180859
144	1	0	-3.024895	-7.372788	0.785006
145	1	0	-1.355172	-7.780574	-1.014182
146	1	0	-0.554856	-5.879676	-2.416661
147	1	0	-1.418489	-3.584801	-2.022005
148	1	0	-4.919966	-3.377260	1.230785
149	1	0	-4.574122	-1.620557	1.204020
150	1	0	-1.403661	6.751920	-3.642898
151	1	0	-2.613714	7.976309	-1.843767
152	1	0	-3.665448	6.724283	0.018758
153	1	0	-2.249386	2.994151	-1.702388
154	1	0	-1.236882	4.264780	-3.545047

155	1	0	-7.629375	6.213488	2.083951
156	1	0	-8.989976	5.429042	0.154931
157	1	0	-7.936572	4.042714	-1.622482
158	1	0	-5.527065	3.444354	-1.475294
159	1	0	-5.229701	5.615509	2.242433
160	1	0	-3.921678	2.372384	3.784541
161	1	0	-5.825153	1.139567	4.791580
162	1	0	-7.512072	0.036317	3.332458
163	1	0	-7.271928	0.152573	0.853287
164	1	0	-5.375955	1.388428	-0.160141
165	1	0	-3.516161	4.414566	2.697561
166	1	0	-1.967220	4.378936	1.802822
167	6	0	1.719591	1.415679	6.011804
168	6	0	1.973387	0.268159	5.048825
169	6	0	1.394167	0.431829	3.687892
170	6	0	0.424531	-0.330382	3.140549
171	6	0	-0.306511	-1.306782	3.992545
172	8	0	-0.381341	-2.533058	3.451942
173	6	0	-1.295029	-3.556145	4.001573
174	6	0	-2.732531	-3.023622	3.993404
175	6	0	-0.838359	-3.982016	5.402541
176	6	0	-1.142851	-4.704290	3.005453
177	8	0	-0.803933	-0.987450	5.066584
178	1	0	2.340772	1.327404	6.909962
179	1	0	0.666317	1.369700	6.304912
180	1	0	1.900411	2.387727	5.540690
181	1	0	1.679703	-0.675511	5.508246
182	1	0	-3.422935	-3.839019	4.238097
183	1	0	-2.974800	-2.640950	2.996583
184	1	0	-2.865088	-2.221057	4.720392
185	1	0	-1.453253	-4.822276	5.746262
186	1	0	-0.934204	-3.160263	6.113146
187	1	0	0.204642	-4.317898	5.378212
188	1	0	-1.825083	-5.522532	3.260534
189	1	0	-0.121264	-5.094019	3.005694
190	1	0	-1.377712	-4.355004	1.993492
191	1	0	1.803831	1.254754	3.101463
192	6	0	2.571682	-7.412421	3.955104
193	6	0	2.905958	-6.459343	4.925224
194	6	0	3.065227	-5.125511	4.570422
195	6	0	2.890465	-4.712185	3.231042
196	6	0	2.557779	-5.687070	2.267567
197	6	0	2.398098	-7.022878	2.625297
198	6	0	4.675450	2.404957	3.848242
199	6	0	5.476266	3.459391	3.416141
200	6	0	6.409936	3.271823	2.394423
201	6	0	6.546685	2.012647	1.805716
202	6	0	5.764876	0.944086	2.237025
203	6	0	4.813606	1.148867	3.246037
204	7	0	4.028086	0.053032	3.703667
205	8	0	3.530699	0.165868	4.975330
206	1	0	2.447491	-8.453652	4.238180
207	1	0	3.042563	-6.762048	5.959189
208	1	0	3.332054	-4.401252	5.333633
209	1	0	2.411592	-5.380279	1.235273
210	1	0	2.133728	-7.757141	1.870241
211	1	0	3.960370	2.544228	4.646980

212	1	0	5.368952	4.432785	3.885008
213	1	0	7.034351	4.097350	2.067312
214	1	0	7.278784	1.849168	1.020612
215	1	0	5.916195	-0.042703	1.805925
216	1	0	3.867649	-0.944241	1.920294
217	6	0	3.361310	-2.263620	3.579444
218	6	0	3.067145	-3.340162	2.794162
219	6	0	3.723644	-1.025476	2.994888
220	1	0	3.404499	-2.331284	4.660939
221	1	0	2.944263	-3.158214	1.726053

TS4b-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.596627	2.486581	-3.156386
2	6	0	-6.647562	1.760703	-2.581009
3	6	0	-6.385344	0.568762	-1.908993
4	6	0	-5.065991	0.074869	-1.797779
5	6	0	-4.022088	0.811446	-2.363415
6	6	0	-4.290875	2.010114	-3.041217
7	6	0	-7.699309	-3.716678	-1.925976
8	6	0	-7.262375	-4.202412	-3.161623
9	6	0	-6.065617	-3.729648	-3.711640
10	6	0	-5.307813	-2.775061	-3.030017
11	6	0	-5.743422	-2.289803	-1.786428
12	6	0	-6.944072	-2.761994	-1.237752
13	6	0	-4.042396	-4.093282	0.658646
14	6	0	-3.861876	-5.478440	0.600714
15	6	0	-3.111204	-6.047813	-0.431997
16	6	0	-2.532284	-5.224483	-1.403689
17	6	0	-2.706735	-3.840265	-1.348753
18	6	0	-3.471834	-3.265386	-0.320525
19	6	0	-4.924647	-1.239692	-1.081718
20	6	0	-3.685004	-1.779129	-0.301753
21	6	0	-4.877861	-1.200707	0.440023
22	6	0	-2.336964	-1.048016	-0.234078
23	8	0	-1.835235	-0.706373	-1.346449
24	8	0	-1.839816	-0.886133	0.922730
25	45	0	-0.231951	0.650947	-1.362545
26	45	0	0.035584	0.109342	1.078716
27	6	0	-1.737083	-3.696455	-5.182380
28	6	0	-1.150958	-4.928510	-4.864495
29	6	0	-0.096149	-4.984771	-3.956058
30	6	0	0.396976	-3.809461	-3.345540
31	6	0	-0.198086	-2.586097	-3.662413
32	6	0	-1.259484	-2.533718	-4.578452
33	6	0	4.080435	-6.599935	-3.622875
34	6	0	4.767844	-5.874331	-4.599844
35	6	0	4.414909	-4.544704	-4.856385
36	6	0	3.379608	-3.941790	-4.139030
37	6	0	2.691782	-4.668103	-3.153406
38	6	0	3.043499	-6.001298	-2.900351

39	6	0	4.069985	-3.956004	-0.041535
40	6	0	5.456601	-3.945958	0.137182
41	6	0	6.248380	-3.025222	-0.555487
42	6	0	5.645909	-2.100106	-1.414954
43	6	0	4.261791	-2.108059	-1.600738
44	6	0	3.466714	-3.051587	-0.929696
45	6	0	1.559633	-4.003615	-2.412454
46	6	0	1.993066	-3.109187	-1.209279
47	6	0	1.242219	-4.411163	-0.978873
48	6	0	1.308402	-1.791471	-0.816202
49	8	0	1.092576	-0.959343	-1.737566
50	8	0	1.042772	-1.660532	0.422867
51	6	0	-0.208423	6.679995	-2.955340
52	6	0	-0.709866	7.481114	-1.921403
53	6	0	-1.453038	6.906222	-0.891785
54	6	0	-1.713034	5.518865	-0.882222
55	6	0	-1.207450	4.725249	-1.914476
56	6	0	-0.455863	5.306710	-2.944862
57	6	0	-5.665097	7.120854	1.020459
58	6	0	-6.445839	6.888180	-0.114922
59	6	0	-5.969666	6.044708	-1.125105
60	6	0	-4.719309	5.436366	-1.000793
61	6	0	-3.935606	5.663220	0.143269
62	6	0	-4.412524	6.512535	1.151150
63	6	0	-3.956922	2.904726	2.856900
64	6	0	-5.157233	2.422127	3.384447
65	6	0	-6.213813	2.082134	2.532660
66	6	0	-6.059433	2.210466	1.149164
67	6	0	-4.859684	2.690393	0.615274
68	6	0	-3.809531	3.058548	1.468220
69	6	0	-2.577425	5.018135	0.239716
70	6	0	-2.529099	3.614921	0.911370
71	6	0	-1.912535	4.824568	1.596311
72	6	0	-1.612402	2.459075	0.490575
73	8	0	-1.556460	2.160648	-0.738192
74	8	0	-1.016729	1.879071	1.453865
75	6	0	5.030174	0.186550	-4.496519
76	6	0	6.127528	0.587786	-3.724363
77	6	0	5.931398	1.368878	-2.586156
78	6	0	4.633069	1.767592	-2.205035
79	6	0	3.540711	1.355646	-2.973953
80	6	0	3.742665	0.568116	-4.115554
81	6	0	7.104610	5.490559	-1.095017
82	6	0	6.498423	6.388705	-1.978024
83	6	0	5.253545	6.081111	-2.538086
84	6	0	4.615909	4.880759	-2.217120
85	6	0	5.221034	3.980685	-1.325823
86	6	0	6.470387	4.287894	-0.768470
87	6	0	3.646769	4.558763	1.747537
88	6	0	3.355894	5.836713	2.234393
89	6	0	2.450663	6.658410	1.556638
90	6	0	1.826289	6.193728	0.394121
91	6	0	2.109973	4.917233	-0.095689
92	6	0	3.033510	4.096711	0.573052
93	6	0	4.534941	2.676309	-1.014449
94	6	0	3.363012	2.745804	0.007941
95	6	0	4.672845	2.066552	0.373476

96	6	0	2.096469	1.882095	-0.073287
97	8	0	1.408035	1.962514	-1.129843
98	8	0	1.846196	1.186610	0.963090
99	1	0	-5.799521	3.412645	-3.688888
100	1	0	-7.669038	2.125892	-2.663082
101	1	0	-7.209634	0.005223	-1.473105
102	1	0	-2.960396	0.491002	-2.281120
103	1	0	-3.459941	2.569040	-3.473366
104	1	0	-8.630457	-4.081233	-1.496995
105	1	0	-7.850774	-4.945348	-3.695035
106	1	0	-5.723036	-4.106203	-4.673742
107	1	0	-4.375102	-2.404608	-3.457624
108	1	0	-7.292426	-2.386498	-0.278243
109	1	0	-4.636907	-3.658840	1.461255
110	1	0	-4.316738	-6.113547	1.358134
111	1	0	-2.987596	-7.126445	-0.488931
112	1	0	-1.950497	-5.660603	-2.216703
113	1	0	-2.253566	-3.196956	-2.111303
114	1	0	-5.515706	-1.853309	1.032239
115	1	0	-4.773560	-0.226627	0.929037
116	1	0	-2.557202	-3.648983	-5.894976
117	1	0	-1.516588	-5.840630	-5.331535
118	1	0	0.362267	-5.945698	-3.724093
119	1	0	0.129981	-1.633149	-3.195114
120	1	0	-1.710885	-1.567694	-4.808533
121	1	0	4.351721	-7.634621	-3.422621
122	1	0	5.574530	-6.341524	-5.160228
123	1	0	4.947611	-3.977977	-5.617977
124	1	0	3.100782	-2.906786	-4.339811
125	1	0	2.512018	-6.574349	-2.143935
126	1	0	3.463326	-4.683963	0.494244
127	1	0	5.920602	-4.665424	0.809775
128	1	0	7.329185	-3.034686	-0.432855
129	1	0	6.254895	-1.372955	-1.953957
130	1	0	3.794477	-1.384360	-2.277040
131	1	0	1.748964	-5.256389	-0.517798
132	1	0	0.200512	-4.364096	-0.651709
133	1	0	0.368955	7.127378	-3.760928
134	1	0	-0.523540	8.553037	-1.925229
135	1	0	-1.848723	7.532690	-0.092974
136	1	0	-1.375775	3.632209	-1.930303
137	1	0	-0.064466	4.672824	-3.740285
138	1	0	-6.031631	7.776539	1.807895
139	1	0	-7.420222	7.360774	-0.213946
140	1	0	-6.574778	5.862132	-2.011162
141	1	0	-4.345604	4.783782	-1.791434
142	1	0	-3.812254	6.699613	2.039512
143	1	0	-3.126482	3.146143	3.521354
144	1	0	-5.268298	2.312895	4.461302
145	1	0	-7.151927	1.719643	2.945756
146	1	0	-6.873652	1.939715	0.477853
147	1	0	-4.741629	2.777873	-0.467912
148	1	0	-2.371080	5.218607	2.501679
149	1	0	-0.824685	4.897768	1.661920
150	1	0	5.181966	-0.416397	-5.388720
151	1	0	7.133891	0.298035	-4.019093
152	1	0	6.787756	1.690703	-1.995468

153	1	0	2.505080	1.626987	-2.692259
154	1	0	2.879791	0.255428	-4.704200
155	1	0	8.073116	5.727076	-0.659233
156	1	0	6.992354	7.324496	-2.229377
157	1	0	4.779014	6.778899	-3.225866
158	1	0	3.646447	4.638741	-2.653574
159	1	0	6.949181	3.593383	-0.082395
160	1	0	4.351340	3.924535	2.281922
161	1	0	3.838721	6.192022	3.142263
162	1	0	2.231329	7.655359	1.931679
163	1	0	1.113492	6.827058	-0.135919
164	1	0	1.607412	4.548695	-0.996011
165	1	0	5.328668	2.518237	1.115920
166	1	0	4.687100	0.979563	0.472567
167	6	0	1.906903	-0.223776	5.075124
168	6	0	1.621014	-0.209111	3.592872
169	6	0	0.340088	-0.273836	3.051235
170	6	0	-0.836393	-0.475469	3.935198
171	8	0	-1.385526	-1.684906	3.857384
172	6	0	-2.676107	-1.992342	4.528621
173	6	0	-3.761757	-1.058472	3.987205
174	6	0	-2.508878	-1.888052	6.048647
175	6	0	-2.935624	-3.437664	4.106276
176	8	0	-1.218209	0.460906	4.622643
177	1	0	-4.741146	-1.387641	4.351271
178	1	0	-3.762257	-1.089663	2.892585
179	1	0	-3.598650	-0.025896	4.301915
180	1	0	-3.423208	-2.241597	6.538612
181	1	0	-2.321185	-0.858779	6.358033
182	1	0	-1.680207	-2.520823	6.386141
183	1	0	-3.894580	-3.777886	4.510607
184	1	0	-2.147765	-4.102049	4.472448
185	1	0	-2.966270	-3.515496	3.013713
186	1	0	2.332315	0.366193	2.995941
187	6	0	5.350578	-1.166635	2.353592
188	6	0	6.475294	-0.500187	1.874540
189	6	0	7.065330	0.526847	2.615485
190	6	0	6.517652	0.878152	3.849933
191	6	0	5.383365	0.231278	4.338118
192	6	0	4.783271	-0.784506	3.580278
193	6	0	2.625969	-1.945247	3.277562
194	7	0	3.657410	-1.488764	4.077314
195	8	0	3.157489	-1.033122	5.296791
196	1	0	4.932334	-1.990351	1.779393
197	1	0	6.896066	-0.799880	0.917992
198	1	0	7.948816	1.034541	2.241371
199	1	0	6.973657	1.664038	4.445122
200	1	0	4.965993	0.494673	5.300383
201	1	0	2.802405	-1.886548	2.207404
202	1	0	1.131174	-0.774661	5.614264
203	6	0	2.096580	1.150602	5.700786
204	1	0	1.130298	1.664053	5.715292
205	1	0	2.459909	1.058179	6.729945
206	1	0	2.804791	1.755630	5.125907
207	6	0	1.871981	-3.094675	3.761176
208	1	0	1.968966	-3.318512	4.819320
209	6	0	1.137903	-3.861171	2.925356

210	1	0	1.045948	-3.528683	1.891059
211	6	0	0.431398	-5.096700	3.257854
212	6	0	-0.411586	-5.671355	2.287371
213	6	0	0.557794	-5.750102	4.500596
214	6	0	-1.114490	-6.845395	2.550331
215	1	0	-0.528274	-5.175511	1.325460
216	6	0	-0.142238	-6.923734	4.761552
217	1	0	1.216395	-5.343269	5.262227
218	6	0	-0.982854	-7.476261	3.788577
219	1	0	-1.767987	-7.262197	1.788420
220	1	0	-0.030229	-7.414190	5.724477
221	1	0	-1.527424	-8.392883	3.996332

5b-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-5.926399	3.389992	-2.369606
2	6	0	-6.943651	2.992028	-1.492832
3	6	0	-6.808180	1.817692	-0.754949
4	6	0	-5.653611	1.013335	-0.880807
5	6	0	-4.639046	1.423192	-1.749570
6	6	0	-4.779037	2.605950	-2.490285
7	6	0	-9.046485	-1.986232	0.007848
8	6	0	-9.053870	-2.625880	-1.234961
9	6	0	-7.953358	-2.498568	-2.089809
10	6	0	-6.849216	-1.735090	-1.704793
11	6	0	-6.838858	-1.095679	-0.454788
12	6	0	-7.943337	-1.221460	0.399605
13	6	0	-5.104187	-3.146027	1.700987
14	6	0	-5.285888	-4.531296	1.748412
15	6	0	-4.937353	-5.324073	0.651196
16	6	0	-4.400325	-4.726226	-0.493727
17	6	0	-4.217762	-3.342632	-0.547669
18	6	0	-4.576725	-2.541983	0.548854
19	6	0	-5.649945	-0.252523	-0.070909
20	6	0	-4.419006	-1.051157	0.462485
21	6	0	-5.226956	-0.155355	1.387929
22	6	0	-2.958190	-0.678048	0.186199
23	8	0	-2.638389	-0.455410	-1.017998
24	8	0	-2.195686	-0.650284	1.204220
25	45	0	-0.776842	0.428384	-1.421395
26	45	0	-0.162787	-0.167038	0.929782
27	6	0	-3.961325	-3.951130	-4.331325
28	6	0	-3.543261	-5.231815	-3.948694
29	6	0	-2.308031	-5.405512	-3.325610
30	6	0	-1.467484	-4.299718	-3.079679
31	6	0	-1.893282	-3.022871	-3.456951
32	6	0	-3.137123	-2.853051	-4.080184
33	6	0	1.575966	-7.578945	-4.147298
34	6	0	2.096373	-6.986217	-5.301324
35	6	0	1.900172	-5.619995	-5.531218
36	6	0	1.187426	-4.847956	-4.611178

37	6	0	0.670100	-5.440864	-3.448667
38	6	0	0.862946	-6.810919	-3.221563
39	6	0	2.984180	-4.652086	-1.028893
40	6	0	4.361891	-4.709194	-1.260367
41	6	0	4.960291	-3.828423	-2.166169
42	6	0	4.178605	-2.875879	-2.828958
43	6	0	2.802596	-2.812952	-2.601027
44	6	0	2.194114	-3.714082	-1.710642
45	6	0	-0.124347	-4.601175	-2.481964
46	6	0	0.703592	-3.679348	-1.536706
47	6	0	-0.035584	-4.890028	-0.990083
48	6	0	0.252923	-2.286651	-1.076889
49	8	0	0.006401	-1.438549	-1.981949
50	8	0	0.210537	-2.110274	0.182109
51	6	0	1.352262	5.747104	-3.353755
52	6	0	1.310425	6.731873	-2.358423
53	6	0	0.527801	6.540971	-1.221295
54	6	0	-0.228072	5.359665	-1.056694
55	6	0	-0.176182	4.378356	-2.050105
56	6	0	0.611351	4.575732	-3.193594
57	6	0	-2.910130	8.513302	1.046226
58	6	0	-3.939918	8.495653	0.101453
59	6	0	-4.034017	7.434061	-0.805432
60	6	0	-3.103524	6.393543	-0.768008
61	6	0	-2.072349	6.406417	0.185426
62	6	0	-1.976248	7.473272	1.089668
63	6	0	-2.864187	4.247484	3.067618
64	6	0	-4.103286	4.293152	3.712982
65	6	0	-5.282785	4.110114	2.984675
66	6	0	-5.219183	3.868035	1.608690
67	6	0	-3.983730	3.818158	0.958304
68	6	0	-2.799638	4.022576	1.683579
69	6	0	-1.064790	5.287245	0.189484
70	6	0	-1.476256	4.006331	0.974173
71	6	0	-0.354789	4.898741	1.480417
72	6	0	-1.141748	2.581427	0.520216
73	8	0	-1.490006	2.249480	-0.648734
74	8	0	-0.561280	1.851640	1.387259
75	6	0	3.376728	-0.283505	-5.962926
76	6	0	4.681808	-0.239773	-5.456044
77	6	0	4.927585	0.338308	-4.211702
78	6	0	3.870146	0.884889	-3.453431
79	6	0	2.570860	0.836683	-3.963610
80	6	0	2.327921	0.251762	-5.213910
81	6	0	7.279084	3.848154	-2.356083
82	6	0	6.736044	4.945050	-3.030886
83	6	0	5.389415	4.930732	-3.411265
84	6	0	4.588551	3.825077	-3.118424
85	6	0	5.131089	2.724885	-2.434229
86	6	0	6.481411	2.738912	-2.057982
87	6	0	4.348777	2.687697	1.228446
88	6	0	4.548420	3.813446	2.031887
89	6	0	4.008027	5.048489	1.659086
90	6	0	3.257333	5.151787	0.483797
91	6	0	3.052464	4.028988	-0.322793
92	6	0	3.609301	2.793263	0.039318
93	6	0	4.256308	1.531084	-2.154148

94	6	0	3.419964	1.590427	-0.841413
95	6	0	4.570366	0.607555	-0.986484
96	6	0	1.999010	1.040992	-0.663755
97	8	0	1.152582	1.273815	-1.570957
98	8	0	1.802046	0.418226	0.431778
99	1	0	-6.032526	4.302484	-2.951246
100	1	0	-7.842171	3.597295	-1.392429
101	1	0	-7.607669	1.510435	-0.081237
102	1	0	-3.699929	0.843972	-1.866877
103	1	0	-3.974946	2.907373	-3.161957
104	1	0	-9.901375	-2.082800	0.674189
105	1	0	-9.912399	-3.221071	-1.537325
106	1	0	-7.956645	-2.995743	-3.058030
107	1	0	-5.990918	-1.634145	-2.369555
108	1	0	-7.946193	-0.724937	1.367562
109	1	0	-5.378060	-2.535267	2.560563
110	1	0	-5.706640	-4.990393	2.640599
111	1	0	-5.087757	-6.400433	0.684928
112	1	0	-4.127020	-5.338156	-1.353774
113	1	0	-3.797713	-2.879302	-1.445908
114	1	0	-5.832083	-0.598551	2.176833
115	1	0	-4.776256	0.775688	1.742738
116	1	0	-4.922383	-3.814689	-4.821940
117	1	0	-4.180239	-6.092145	-4.143922
118	1	0	-1.981166	-6.404481	-3.040098
119	1	0	-1.271716	-2.128654	-3.261437
120	1	0	-3.455709	-1.850325	-4.366092
121	1	0	1.724811	-8.641851	-3.967664
122	1	0	2.651656	-7.585135	-6.019639
123	1	0	2.303355	-5.155951	-6.429706
124	1	0	1.031432	-3.783665	-4.789949
125	1	0	0.457336	-7.280698	-2.328458
126	1	0	2.525320	-5.344614	-0.325403
127	1	0	4.966574	-5.449882	-0.740528
128	1	0	6.028773	-3.886610	-2.360024
129	1	0	4.639558	-2.180607	-3.532609
130	1	0	2.192748	-2.060694	-3.114194
131	1	0	0.526704	-5.747447	-0.625539
132	1	0	-0.917965	-4.723182	-0.368917
133	1	0	1.955960	5.897752	-4.245753
134	1	0	1.884945	7.648386	-2.476261
135	1	0	0.486535	7.316100	-0.456575
136	1	0	-0.733495	3.424793	-1.955798
137	1	0	0.640646	3.797938	-3.957287
138	1	0	-2.833761	9.338059	1.752099
139	1	0	-4.666494	9.304398	0.070656
140	1	0	-4.834523	7.418248	-1.542876
141	1	0	-3.173014	5.568436	-1.477482
142	1	0	-1.177452	7.495920	1.827729
143	1	0	-1.950021	4.380885	3.642629
144	1	0	-4.148045	4.471431	4.785520
145	1	0	-6.246461	4.154202	3.486917
146	1	0	-6.134283	3.717196	1.035514
147	1	0	-3.937224	3.616028	-0.115467
148	1	0	-0.499088	5.481372	2.388080
149	1	0	0.675067	4.538014	1.421260
150	1	0	3.183805	-0.731063	-6.935140

151	1	0	5.504310	-0.651617	-6.037115
152	1	0	5.944927	0.382185	-3.824407
153	1	0	1.717805	1.239086	-3.387596
154	1	0	1.307888	0.216656	-5.596013
155	1	0	8.326130	3.855964	-2.059941
156	1	0	7.357724	5.807417	-3.260221
157	1	0	4.963849	5.783239	-3.937363
158	1	0	3.540113	3.811478	-3.419737
159	1	0	6.912146	1.888925	-1.531421
160	1	0	4.766775	1.725021	1.523065
161	1	0	5.130679	3.729509	2.946947
162	1	0	4.173864	5.926230	2.279493
163	1	0	2.831914	6.110342	0.186641
164	1	0	2.461542	4.115138	-1.238833
165	1	0	5.476787	0.743277	-0.395171
166	1	0	4.348375	-0.457478	-1.085340
167	6	0	1.103400	0.768972	4.810634
168	6	0	1.482833	0.115217	3.437799
169	6	0	0.338243	-0.557996	2.791867
170	6	0	-0.538529	-1.439675	3.602459
171	8	0	-0.194120	-2.719994	3.534412
172	6	0	-1.024620	-3.804272	4.137370
173	6	0	-2.381309	-3.822789	3.434836
174	6	0	-1.141185	-3.590722	5.649247
175	6	0	-0.206430	-5.055602	3.816716
176	8	0	-1.470959	-0.929500	4.197996
177	1	0	-2.966934	-4.678531	3.788528
178	1	0	-2.256506	-3.920167	2.350216
179	1	0	-2.945281	-2.908723	3.633149
180	1	0	-1.622639	-4.467632	6.096619
181	1	0	-1.738539	-2.707061	5.879373
182	1	0	-0.151159	-3.475003	6.100611
183	1	0	-0.726203	-5.943424	4.191472
184	1	0	0.779413	-5.004051	4.289549
185	1	0	-0.072748	-5.159589	2.735265
186	1	0	1.926267	0.839861	2.752451
187	6	0	3.646823	-3.056279	5.643127
188	6	0	3.917466	-4.171216	6.436737
189	6	0	3.347405	-4.305219	7.703131
190	6	0	2.501721	-3.298329	8.173583
191	6	0	2.222300	-2.175137	7.397119
192	6	0	2.789656	-2.047153	6.116480
193	6	0	2.562165	-0.969412	3.864136
194	7	0	2.564571	-0.880718	5.350505
195	8	0	1.311991	-0.279641	5.741616
196	1	0	4.119745	-2.961868	4.672930
197	1	0	4.583657	-4.939775	6.053691
198	1	0	3.561616	-5.176427	8.315025
199	1	0	2.050755	-3.382227	9.158944
200	1	0	1.567142	-1.398095	7.769051
201	1	0	2.240331	-1.967950	3.539856
202	1	0	0.034373	0.983914	4.870856
203	6	0	1.924665	2.021661	5.106519
204	1	0	1.716636	2.793850	4.357495
205	1	0	1.654835	2.410875	6.092951
206	1	0	2.996591	1.805443	5.101238
207	6	0	3.917393	-0.656702	3.301896

208	1	0	4.402452	0.219678	3.726320
209	6	0	4.494281	-1.373141	2.324005
210	1	0	3.944874	-2.229154	1.928278
211	6	0	5.797035	-1.131939	1.689292
212	6	0	6.162950	-1.917997	0.582030
213	6	0	6.703054	-0.148807	2.131987
214	6	0	7.379133	-1.722685	-0.070939
215	1	0	5.474633	-2.683973	0.225462
216	6	0	7.917899	0.045366	1.481643
217	1	0	6.462356	0.461034	2.998092
218	6	0	8.261549	-0.737953	0.374950
219	1	0	7.635800	-2.340302	-0.927263
220	1	0	8.603246	0.808264	1.841410
221	1	0	9.211714	-0.584608	-0.128870

7b-II

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.090802	4.565107	-3.955003
2	6	0	3.333925	5.602743	-3.046621
3	6	0	2.458457	5.819321	-1.982795
4	6	0	1.325857	4.997871	-1.811820
5	6	0	1.090212	3.959570	-2.718100
6	6	0	1.972066	3.746882	-3.785808
7	6	0	-0.487226	9.053171	-0.601788
8	6	0	-1.468243	9.122131	-1.595282
9	6	0	-1.844193	7.963638	-2.283861
10	6	0	-1.243116	6.739870	-1.980590
11	6	0	-0.262910	6.668351	-0.978394
12	6	0	0.116982	7.830757	-0.292565
13	6	0	-1.944735	5.439495	1.871104
14	6	0	-3.214683	5.879090	2.257496
15	6	0	-4.317383	5.662826	1.426133
16	6	0	-4.149806	4.993192	0.209121
17	6	0	-2.884830	4.549278	-0.181442
18	6	0	-1.771751	4.783353	0.643216
19	6	0	0.400514	5.348837	-0.684341
20	6	0	-0.410767	4.344072	0.186864
21	6	0	0.834199	5.023530	0.736668
22	6	0	-0.379753	2.823901	0.009907
23	8	0	-0.720884	2.360978	-1.123269
24	8	0	-0.050806	2.152772	1.036472
25	45	0	-0.585159	0.296202	-1.431243
26	45	0	-0.135297	0.062864	0.935623
27	6	0	-5.526720	3.451955	-3.453833
28	6	0	-6.421981	3.617743	-2.389836
29	6	0	-6.413484	2.718718	-1.323620
30	6	0	-5.507708	1.638836	-1.309318
31	6	0	-4.612884	1.480152	-2.371053
32	6	0	-4.623817	2.386974	-3.438604
33	6	0	-9.146526	-0.674549	0.452905
34	6	0	-9.329040	-1.488424	-0.668341

35	6	0	-8.307913	-1.602106	-1.618445
36	6	0	-7.109278	-0.906711	-1.447928
37	6	0	-6.920396	-0.094533	-0.317110
38	6	0	-7.947236	0.022913	0.629684
39	6	0	-4.812343	-1.626114	2.501178
40	6	0	-5.119688	-2.886439	3.018434
41	6	0	-5.356208	-3.960718	2.154061
42	6	0	-5.265480	-3.772428	0.771780
43	6	0	-4.956241	-2.513035	0.249119
44	6	0	-4.749367	-1.427897	1.112718
45	6	0	-5.630977	0.670981	-0.169027
46	6	0	-4.467707	-0.056098	0.565778
47	6	0	-5.168830	1.134164	1.205195
48	6	0	-2.975883	0.073332	0.239126
49	8	0	-2.623646	0.076794	-0.979841
50	8	0	-2.207390	0.132493	1.250684
51	6	0	2.881548	-1.981114	-5.905230
52	6	0	4.063159	-2.470960	-5.335375
53	6	0	4.545349	-1.921937	-4.147517
54	6	0	3.847995	-0.875538	-3.510597
55	6	0	2.666477	-0.393308	-4.080780
56	6	0	2.186803	-0.946881	-5.274799
57	6	0	8.139585	0.632487	-2.861233
58	6	0	8.013226	1.836684	-3.559607
59	6	0	6.741553	2.352290	-3.833322
60	6	0	5.599965	1.667458	-3.411306
61	6	0	5.725921	0.460837	-2.704584
62	6	0	7.000353	-0.056949	-2.434386
63	6	0	5.332546	1.235935	0.704652
64	6	0	5.959151	2.340137	1.289831
65	6	0	5.667292	3.632591	0.844168
66	6	0	4.737432	3.818415	-0.184124
67	6	0	4.105800	2.719369	-0.771798
68	6	0	4.408422	1.419733	-0.335471
69	6	0	4.484617	-0.285621	-2.287514
70	6	0	3.765388	0.239020	-1.007603
71	6	0	4.486976	-1.101948	-1.005041
72	6	0	2.254923	0.225351	-0.753436
73	8	0	1.476731	0.471778	-1.727489
74	8	0	1.905775	-0.016531	0.445016
75	6	0	-5.028886	-3.562037	-3.337473
76	6	0	-4.944992	-4.786343	-2.662796
77	6	0	-3.756947	-5.157066	-2.033567
78	6	0	-2.632258	-4.307601	-2.071740
79	6	0	-2.723698	-3.083059	-2.740109
80	6	0	-3.919782	-2.714532	-3.370020
81	6	0	-0.549778	-8.404328	-2.471912
82	6	0	-0.018622	-8.205374	-3.749473
83	6	0	0.076667	-6.909893	-4.269453
84	6	0	-0.355891	-5.816663	-3.515549
85	6	0	-0.882329	-6.014451	-2.229240
86	6	0	-0.982916	-7.313588	-1.711713
87	6	0	1.741542	-5.285852	0.068731
88	6	0	3.052631	-5.729363	-0.131041
89	6	0	3.766180	-5.329509	-1.264404
90	6	0	3.170074	-4.469386	-2.193132
91	6	0	1.864446	-4.015832	-1.995081

92	6	0	1.136699	-4.436747	-0.869216
93	6	0	-1.373969	-4.828292	-1.441332
94	6	0	-0.286960	-3.987139	-0.706438
95	6	0	-1.272807	-4.838503	0.076787
96	6	0	-0.339786	-2.466459	-0.533611
97	8	0	-0.415643	-1.775986	-1.597999
98	8	0	-0.262123	-2.025270	0.655214
99	1	0	3.769729	4.400157	-4.788973
100	1	0	4.204622	6.243571	-3.173814
101	1	0	2.641131	6.636276	-1.285425
102	1	0	0.223450	3.290077	-2.594543
103	1	0	1.778891	2.934254	-4.485356
104	1	0	-0.191523	9.953298	-0.065929
105	1	0	-1.938040	10.073996	-1.833055
106	1	0	-2.607092	8.014907	-3.058643
107	1	0	-1.532825	5.837561	-2.518428
108	1	0	0.882008	7.786413	0.479892
109	1	0	-1.091007	5.607240	2.527658
110	1	0	-3.340654	6.395112	3.207709
111	1	0	-5.302432	6.015890	1.722811
112	1	0	-5.006908	4.816906	-0.441502
113	1	0	-2.756515	4.013847	-1.126076
114	1	0	0.739238	5.763216	1.530709
115	1	0	1.733951	4.422390	0.892352
116	1	0	-5.536426	4.150099	-4.288055
117	1	0	-7.129527	4.444759	-2.398813
118	1	0	-7.118725	2.840682	-0.502344
119	1	0	-3.881163	0.657508	-2.364859
120	1	0	-3.919956	2.256601	-4.259311
121	1	0	-9.939298	-0.582310	1.193145
122	1	0	-10.261975	-2.031384	-0.803104
123	1	0	-8.448423	-2.233177	-2.494087
124	1	0	-6.317475	-0.989926	-2.192976
125	1	0	-7.815979	0.654970	1.505789
126	1	0	-4.597265	-0.792389	3.180261
127	1	0	-5.172248	-3.032244	4.095731
128	1	0	-5.606735	-4.939501	2.556982
129	1	0	-5.437454	-4.607267	0.093081
130	1	0	-4.877267	-2.377042	-0.831591
131	1	0	-5.796217	0.979381	2.081587
132	1	0	-4.636034	2.084342	1.285245
133	1	0	2.508520	-2.404595	-6.835007
134	1	0	4.609302	-3.275468	-5.824093
135	1	0	5.474246	-2.291131	-3.714269
136	1	0	2.095186	0.405656	-3.584229
137	1	0	1.263941	-0.565832	-5.709073
138	1	0	9.127453	0.229331	-2.646578
139	1	0	8.900807	2.372450	-3.888538
140	1	0	6.640707	3.290574	-4.375414
141	1	0	4.609015	2.069348	-3.624059
142	1	0	7.107637	-0.993512	-1.891282
143	1	0	5.562297	0.232767	1.069551
144	1	0	6.671177	2.185379	2.100563
145	1	0	6.160869	4.489975	1.295872
146	1	0	4.505087	4.822909	-0.535488
147	1	0	3.381762	2.873148	-1.574523
148	1	0	5.398554	-1.219112	-0.418380

149	1	0	3.896087	-2.020581	-0.964159
150	1	0	-5.952842	-3.275967	-3.835062
151	1	0	-5.805872	-5.451767	-2.635609
152	1	0	-3.689624	-6.115781	-1.520412
153	1	0	-1.866796	-2.388969	-2.768114
154	1	0	-3.977566	-1.757687	-3.887672
155	1	0	-0.626515	-9.411145	-2.065622
156	1	0	0.319850	-9.055114	-4.338283
157	1	0	0.489153	-6.752148	-5.264495
158	1	0	-0.285397	-4.807696	-3.921526
159	1	0	-1.397319	-7.478113	-0.719510
160	1	0	1.196722	-5.601426	0.958991
161	1	0	3.514725	-6.390636	0.600205
162	1	0	4.781073	-5.686335	-1.424741
163	1	0	3.721706	-4.152167	-3.078261
164	1	0	1.405279	-3.329426	-2.711490
165	1	0	-0.919016	-5.726518	0.599344
166	1	0	-2.051326	-4.339405	0.658922
167	6	0	2.877493	1.573185	4.351134
168	6	0	2.093047	0.280178	4.276479
169	6	0	0.628209	0.154402	4.092410
170	6	0	-0.252781	1.281077	4.634373
171	8	0	-1.506374	0.825783	4.764319
172	6	0	-2.638444	1.727791	5.076897
173	6	0	-2.780641	2.762976	3.959258
174	6	0	-2.439662	2.365331	6.456759
175	6	0	-3.831190	0.768485	5.091597
176	8	0	0.126881	2.408758	4.875127
177	1	0	-3.693775	3.349695	4.110197
178	1	0	-2.847504	2.262021	2.986899
179	1	0	-1.930268	3.448025	3.937774
180	1	0	-3.346273	2.914097	6.735631
181	1	0	-1.596241	3.056942	6.457376
182	1	0	-2.265130	1.592218	7.212949
183	1	0	-4.751428	1.321428	5.307257
184	1	0	-3.699451	-0.000015	5.860195
185	1	0	-3.938709	0.270030	4.115901
186	1	0	0.370428	0.119641	2.992393
187	6	0	5.437321	-1.745754	2.959110
188	6	0	6.622143	-2.107144	2.316387
189	6	0	7.799998	-1.390269	2.527054
190	6	0	7.782661	-0.299304	3.400910
191	6	0	6.614999	0.064048	4.064641
192	6	0	5.426933	-0.658182	3.848997
193	6	0	2.970272	-0.756764	4.362481
194	7	0	4.276537	-0.284452	4.583071
195	8	0	4.192907	1.129117	4.795528
196	1	0	4.527888	-2.299693	2.757719
197	1	0	6.611499	-2.952004	1.632411
198	1	0	8.716862	-1.674066	2.018603
199	1	0	8.690451	0.272519	3.575222
200	1	0	6.602585	0.906438	4.745510
201	1	0	0.260770	-0.802671	4.473582
202	1	0	2.510262	2.223711	5.148014
203	6	0	2.955867	2.356925	3.040494
204	1	0	1.969830	2.759388	2.789310
205	1	0	3.661891	3.188137	3.142404

206	1	0	3.285661	1.713287	2.216753
207	6	0	2.729586	-2.192868	4.443865
208	1	0	3.409563	-2.721010	5.109230
209	6	0	1.749245	-2.866428	3.802217
210	1	0	1.131204	-2.336092	3.081477
211	6	0	1.413844	-4.285987	3.953360
212	6	0	0.282582	-4.777029	3.273874
213	6	0	2.147870	-5.181628	4.755982
214	6	0	-0.108589	-6.109422	3.399618
215	1	0	-0.286685	-4.095681	2.643060
216	6	0	1.760663	-6.512703	4.874190
217	1	0	3.028205	-4.836906	5.290623
218	6	0	0.628636	-6.983226	4.200118
219	1	0	-0.993092	-6.464191	2.877327
220	1	0	2.341458	-7.187432	5.497325
221	1	0	0.326188	-8.021895	4.300647

3. Computed Energies

Sum of electronic and zero-point energies (E_0 , in Hartree), sum of electronic and thermal enthalpies (H , in Hartree), sum of electronic and thermal free energies (G , in Hartree), thermal correction to Gibbs free energy ($TCGFE$, in Hartree), total free energy in solution (E_{sol} , in Hartree, solvent = *n*-pentane), and thermo corrected Gibbs free energy in solvent (G_{sol} , which equals to E_{sol} + $TCGFE$, in Hartree). Reactive energies at 298.15K and 1atm are reported in kcal/mol.

Structure	TCGEF	E_0	H	G	E_{sol}	G_{sol}	ΔH_{gas}	ΔG	ΔG_{sol}
1	1.306786	-1584.901457	-1584.797339	-1585.056315	-1586.802494	-1585.495708			
TS-1	1.305132	-1584.888839	-1584.784853	-1585.043119	-1586.786095	-1585.480963	7.8	8.3	9.3
2-I (N ₂)	1.297802	-1475.408657	-1475.306748	-1475.562477	-1477.263113	-1475.965311			
2-I	1.297802	-1475.408657	-1475.306748	-1475.562477	-1477.263113	-1475.965311			
TS-2	1.297078	-1475.387492	-1475.286041	-1475.540806	-1477.239704	-1475.942626	13.3	13.6	14.2
2-II	1.295236	-1475.405882	-1475.303789	-1475.562303	-1477.260540	-1475.965304			
2-II+3a	1.489238	-2107.110048	-2106.994393	-2107.282575	-2109.354213	-2107.864975			
TS-3a-I	1.495032	-2107.106974	-2106.992759	-2107.274541	-2109.349952	-2107.854920	1.9	5.0	6.3
4a-I	1.500090	-2107.111016	-2106.997041	-2107.275324	-2109.351772	-2107.851682			
TS-4a-I	1.499716	-2107.105630	-2106.992417	-2107.270099	-2109.342924	-2107.843208	3.4	3.3	5.3
5a-I	1.498329	-2107.115997	-2107.002608	-2107.283893	-2109.353230	-2107.854901			
TS-5a-I	1.496883	-2107.091367	-2106.978310	-2107.256638	-2109.327765	-2107.830882	15.5	17.1	15.1
6a-I	1.499776	-2107.137546	-2107.024282	-2107.304197	-2109.379065	-2107.879289			
TS-6a-I	1.492454	-2107.089256	-2106.975466	-2107.256918	-2109.326491	-2107.834037	30.3	29.7	28.4
7a-I	1.495320	-2107.157299	-2107.043090	-2107.326527	-2109.399759	-2107.904439			
2-II+3a	1.491063	-2107.111609	-2106.996379	-2107.282547	-2109.353634	-2107.862571			
TS-3a-II	1.498324	-2107.105245	-2106.991510	-2107.270228	-2109.346819	-2107.848495	4.0	7.7	8.8
4a-II	1.501012	-2107.109558	-2106.995813	-2107.273499	-2109.349412	-2107.848400			
TS-4a-II	1.500301	-2107.105183	-2106.992212	-2107.269323	-2109.340950	-2107.840649	2.7	2.6	4.9
5a-II	1.499539	-2107.113844	-2107.000518	-2107.280617	-2109.350127	-2107.850588			
TS-5a-II	1.496522	-2107.095059	-2106.982084	-2107.260456	-2109.329387	-2107.832865	11.8	12.7	11.1
6a-II	1.500367	-2107.148079	-2107.034807	-2107.314376	-2109.389873	-2107.889506			
TS-6a-II	1.494340	-2107.091210	-2106.977691	-2107.257579	-2109.329296	-2107.834956	35.7	35.6	34.2
7a-II	1.494561	-2107.160821	-2107.046832	-2107.332393	-2109.403729	-2107.909168			
2-II+3b	1.519279	-2184.483371	-2184.365378	-2184.659215	-2186.783714	-2185.264435			
TS-3b-I	1.525087	-2184.482354	-2184.365724	-2184.653094	-2186.781882	-2185.256795	0.6	3.8	4.8
4b-I	1.530973	-2184.491219	-2184.375083	-2184.658990	-2186.791331	-2185.260358			
TS-4b-I	1.528144	-2184.474247	-2184.358674	-2184.643457	-2186.767220	-2185.239076	10.6	9.7	13.4
5b-I	1.527460	-2184.483125	-2184.367365	-2184.654964	-2186.776452	-2185.248992			
TS-5b-I	1.527348	-2184.457226	-2184.341879	-2184.625158	-2186.750441	-2185.223093	16.3	18.7	16.3
6b-I	1.530869	-2184.530438	-2184.414908	-2184.700145	-2186.826374	-2185.295505			
TS-6b-I	1.525046	-2184.459128	-2184.343288	-2184.628505	-2186.754101	-2185.229055	44.7	45.0	41.7
7b-I	1.523381	-2184.525674	-2184.409107	-2184.700507	-2186.824169	-2185.300788			
2-II+3b	1.521078	-2184.481884	-2184.364234	-2184.656331	-2186.780277	-2185.259199			
TS-3b-II	1.527509	-2184.480379	-2184.364220	-2184.649384	-2186.778767	-2185.251258	0.9	4.4	5.0
4b-II	1.530368	-2184.484825	-2184.368802	-2184.652918	-2186.781346	-2185.250978			

TS-4b-II	1. 530135	-2184. 476422	-2184. 361098	-2184. 644189	-2186. 768016	-2185. 237881	5. 3	5. 5	8. 2
5b-II	1. 527024	-2184. 481674	-2184. 365820	-2184. 653881	-2186. 774751	-2185. 247727			
TS-5b-II	1. 526216	-2184. 459855	-2184. 344494	-2184. 628563	-2186. 750100	-2185. 223884	13. 7	15. 9	15. 0
6b-II	1. 532498	-2184. 524733	-2184. 409367	-2184. 693125	-2186. 821474	-2185. 288976			
TS-6b-II	1. 523504	-2184. 464693	-2184. 348952	-2184. 635239	-2186. 757402	-2185. 233898	37. 7	36. 3	34. 6
7b-II	1. 526509	-2184. 527860	-2184. 411740	-2184. 699631	-2186. 825157	-2185. 298648			

4. Functional Effects and Basis Set effects

In consideration of the inadequacy of B3LYP to describe the vdW dispersion corrections, we compared the computed energy profiles of M06L, M062X and B3LYP-D3 with the BJ-damping (-D3(BJ)) methods. The initial step of metal catalyzed reaction is especially important for the dispersion force, thus the carbenoid formation of vinyl diazoacetate **2a-I** (the same below) can be adopted as example reaction to efficiently estimate the discrepancies induced by theoretical methods. The M06L, M062X calculations of geometries optimization and single-point energies in solvent (*n*-pentane) were performed using the same basis sets as original level using Gaussian'09. The B3LYP-D3 calculations were performed on the optimized geometries using the same level. In addition, a higher basis set was tested on the example reaction to evaluate the basis set effects, and the results were shown in Table S1.

Table S1. Test of M06L, M062X and B3LYP-D3 methods.

Structure	E_0	H	G	$TCGFE$	$E_{\text{sol}}^{\text{a}}$	$G_{\text{sol}}^{\text{a}}$	ΔH_{gas}	ΔG	$\Delta G_{\text{sol}}^{\text{a}}$
1 ^b	-1428.636083	-1428.539029	-1428.778833	1.368634	-1430.551440	-1429.182806	—	—	—
TS1 ^b	-1428.618521	-1428.521591	-1428.760007	1.367611	-1430.531064	-1429.163453	10.9	11.8	12.1
1 ^c	-1428.611148	-1428.513969	-1428.753432	1.368623	-1430.482275	-1429.113652	—	—	—
TS1 ^c	-1428.593861	-1428.496768	-1428.735424	1.366658	-1430.460268	-1429.093610	10.8	11.3	12.6
1 ^d	-1427.914491	-1427.817921	-1428.055849	1.373912	-1429.835117	-1428.461205	—	—	—
TS1 ^d	-1427.898217	-1427.801569	-1428.039007	1.371887	-1429.816017	-1428.444130	10.3	10.6	10.7
1 ^e	-1428.636083	-1428.539029	-1428.778833	1.368634	-5193.257698	-5191.889064	—	—	—
TS1 ^e	-1428.618521	-1428.521591	-1428.760007	1.367611	-5193.237497	-5191.869886	10.9	11.8	12.0
1 ^f	-1428.650348	-1428.553272	-1428.793127	1.368210	-1430.582878	-1429.214668	—	—	—
TS1 ^f	-1428.632738	-1428.535786	-1428.774266	1.367151	-1430.562527	-1429.195376	11.0	11.8	12.1

^a solvent = *n*-pentane

^b ONIOM(B3LYP/6-311+G(d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d)[Rh-LA2]:PM6

^c ONIOM(M06L/6-311+G(d,p)[Rh-LA2]:PM6)//M06L/6-31G(d)[Rh-LA2]:PM6

^d ONIOM(M062X/6-311+G(d,p)[Rh-LA2]:PM6)//M062X/6-31G(d)[Rh-LA2]:PM6

^e ONIOM(B3LYP-D3//6-31G(d) [Rh-LA2]:PM6)//B3LYP/6-31G(d)[Rh-LA2]:PM6

^f ONIOM(B3LYP/6-311+G(2d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d,p)[Rh-LA2]:PM6

As shown in Table S1, the energy barriers of the example reaction computed by M06L and B3LYP-D3 theoretical methods in the high level of ONIOM methodology are 12.6 and 12.0 kcal/mol, respectively. The discrepancies induced by these two functionals are subtle compared with the original data 12.1 kcal/mol computed by that of B3LYP basis sets. The energy barrier obtained by M062X method is lower 1.4 kcal/mol than the original result, the slight difference can be attributed the insufficiency of M062X to describe the ubiquitous long-rang dispersion corrections. Thus we believe that B3LYP method is suitable for studying the present system.

In addition, we used the bigger basis set of ONIOM(B3LYP/6-311+G(2d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d,p)[Rh-LA2]:PM6 and the discrepancy induced by this higher basis set compared with the original result is not more than 0.1 kcal/mol, this result suggested this present system is not sensitive to the basis sets used in calculations.

5. Solvent Effects

Except for the effect of solvent polarity illustrated in main text, we also supplement the theoretical tests of solvent model and the optimization in solvent of the structures of the example reactions above. The calculated results are shown in Table S2.

Table S2. The effect of solvent.

Structure	E_0	H	G	$TCGFE$	E_{sol}	G_{sol}	ΔH_{gas}	ΔG	ΔG_{sol}
1 ^a	-1428.636083	-1428.539029	-1428.778833	1.368634	-1430.602195	-1429.233561			
TS1 ^a	-1428.618521	-1428.521591	-1428.760007	1.367611	-1430.581567	-1429.213956	10.9	11.8	12.3
1 ^b	-1428.662635	-1428.565156	-1428.807546	1.363606	-1430.552786	-1429.189180			
TS1 ^b	-1428.645096	-1428.547738	-1428.788784	1.362334	-1430.532279	-1429.169945	10.9	11.8	12.1

^aSMD¹-ONIOM(B3LYP/6-311+G(d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d)[Rh-LA2]:PM6

^bCPCM-ONIOM(B3LYP/6-311+G(d,p)[Rh-LA2]:PM6)//B3LYP/6-31G(d)[Rh-LA2]:PM6, optimized in solvent

As shown in Table 2S, the energy barrier of example reactions with solvent method SMD in *n*-pentane which is also popular displays a barrier of 12.3 kcal/mol, this result suggests the chosen solvent method in this rhodium has a negligible influence on the single point energies of the structures. Besides, the geometries of the example reaction are optimized in the solvent *n*-pentane and obtained an energy barrier of 12.1 kcal/mol. This value is not more 0.1 kcal/mol than the computed energy barrier which geometries optimized in gas-phase, thus the geometries of this system optimized in gas-phase is reasonable.

Polar solvent has been reported to dramatically enhance the vinylogous reactivity. With an attempt to determine the influence of solvent polarity on vinylcarbenoid we conduct an array of tests on solvent polarity using hexane, dichloromethane (DCM), acetone. We adopt the initial step of carbenoid formation of vinyl diazoacetate **1** catalyzed by Rh₂(*S*-TPCP)₄ and the vinylogous reaction with aryl nitrene **3a** as example reactions. The calculated results are shown in Table 1.

Table S3. Effects of solvent polarity.

structure	1	TS2		2-II+3a (<i>Si</i>)	TS4a-I		2-II+3a (<i>Re</i>)	TS4a-II	
solvent	G_{sol}^a	ΔG_{sol}^b		G_{sol}^a	ΔG_{sol}^b		G_{sol}^a	ΔG_{sol}^b	
<i>n</i> -pentane($\epsilon=1.84$)	-1585.495708	-1585.480963	9.25	-2107.864975	-2107.854920	6.31	-2107.862571	-2107.848495	8.83
hexane($\epsilon=1.88$)	-1585.496187	-1585.481358	9.31	-2107.865419	-2107.855378	6.30	-2107.862985	-2107.848935	8.82
DCM($\epsilon=8.93$)	-1585.521820	-1585.502837	11.91	-2107.878240	-2107.872293	3.73	-2107.875308	-2107.865094	6.41
acetone($\epsilon=20.49$)	-1585.523999	-1585.504588	12.18	-2107.882649	-2107.873733	5.59	-2107.879267	-2107.865094	8.89

^a Gibbs free energies in solvent with thermal corrections of stationary points, in Hartree. ^b Relative energies, in kcal/mol.

As can be seen in the first column of Table. S3, along with the dielectric coefficient ϵ rising, the relative Gibbs free energies with thermal corrections gradually increase. That is to say, the decomposition of certain vinyl diazoacetate within polar solvent should overcome distinctly high energy barrier. As the competing pathway shown in column 2 and 3, this vinylogous reaction of

aryl nitrene all has a preference of the approach from the *Si*-face rather than that from the *Re*-face. the differences between competitive pathways with the opposite faces in vinylogous reaction also become large with the dielectric coefficient ϵ rising, are 2.52, 2.52, 2.71 and 3.30 kcal/mol, respectively. These comparative tests illuminate that weak polar solvent is favor of decomposition of vinyl diazoacetate to form rhodium vinylcarbenoid, while relatively the polar solvents support vinylogous reaction. This theoretical result of solvent polarity can provide a reliable guide for other analogous catalytic reactions.