Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Theoretical study on the mechanism and stereochemistry of cinchona-thiourea organocatalytic hydrophosphonylation of α-ketoester

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CONTENTS:

S1: Summarize energies of all species over actual reaction system.

Species	E_{zpe} (Hartree)	G_c[a] (Hartree)	SCF_{PCM}[b] (Hartree)	D_c[c] (Hartree)	$SCF_{PCM}+G_c+D_c$ (Hartree)	ΔG (kcal/mol)
α-ketoester	–573.31208	0.11472	–573.60978	–0.03589	–573.53095	-
DMHP	–647.40434	0.06705	–647.61797	–0.01717	–647.56809	-
(*S*)-CAT	–1611.08754	0.47672	–1625.13444	–0.14863	–1624.80635	-
Product	–1220.71924	0.20778	–1221.23674	–0.06921	–1221.10005	–0.6
s-**IM1**	–2258.50500	0.56264	–2272.76592	–0.17811	–2272.38139	–4.4
s-**TS1**	–2258.48843	0.56423	–2272.74824	-0.18423	–2272.36825	3.9
s-**IM2a**	–2258.48941	0.56980	–2272.75939	–0.18419	–2272.37489	–0.3
s-**TS**-ex	–2258.48723	0.57145	–2272.75734	–0.18643	–2272.37232	1.3
s-**IM2b**	–2258.49134	0.56813	–2272.75948	–0.17811	–2272.37614	–1.1
k-**IM0**	–2184.39063	0.61075	–2198.73375	–0.19604	–2198.31904	11.5
k-**IM1**	–2831.80304	0.70144	–2846.35761	–0.23544	–2845.89161	8.7
k-**TS1**	–2831.78298	0.70273	–2846.33705	–0.24431	–2845.87863	16.8
k-**IM2**	–2831.78400	0.70735	–2846.34617	–0.24292	–2845.88174	14.8
ds-**IM3**	–2831.81566	0.70522	–2846.37687	–0.23977	–2845.91141	–3.8
ds-**TS2**	–2831.81190	0.70944	–2846.37487	–0.24231	–2845.90783	–1.5
ds-**IM4**	–2831.81714	0.71124	–2846.37906	–0.24585	–2845.91367	–5.2
ds-**TS3**	–2831.81885	0.70607	–2846.37719	–0.24620	–2845.91731	–7.5
ds-**IM5**	–2831.82066	0.70807	–2846.38300	–0.23851	–2845.91343	–5.0
ms-**IM3**	–2831.81254	0.70469	–2272.76592	–0.24126	–2845.90854	–2.0
ms-**TS2**	–2831.81143	0.70912	–2272.74824	–0.24387	–2845.90518	0.1
ms-**IM4**	–2831.82153	0.70964	–2272.75939	–0.24585	–2845.91766	–7.7
ms-**TS3**	–2831.82432	0.70689	–2272.75734	–0.24620	–2845.92071	–9.6
ms-**IM5**	–2831.82750	0.70994	–2272.75948	–0.24396	–2845.92330	–11.2
dr-**IM3**	–2831.81195	0.70342	–2846.37244	–0.23573	–2845.90475	0.4
dr-**TS2**	–2831.80519	0.70828	–2846.36766	–0.24291	–2845.90229	1.9
dr-**IM4**	–2831.81306	0.71139	–2846.37408	–0.24841	–2845.91111	–3.6
dr-**TS3**	–2831.81310	0.70721	–2846.37048	–0.24726	–2845.91054	–3.2
dr-**IM5**	–2831.81382	0.70848	–2846.37498	–0.24361	–2845.91126	–3.7
mr-**IM3**	–2831.81368	0.70441	–2846.37502	–0.23647	–2845.90708	–1.1
mr-**TS2**	–2831.80430	0.70897	–2846.36490	–0.24089	–2845.89682	5.4
mr-**IM4**	–2831.82122	0.71085	–2846.38159	–0.24412	–2845.91486	–5.9
mr-**TS3**	–2831.82367	0.70679	–2846.38096	–0.24451	–2845.91868	–8.3
mr-**IM5**	–2831.82633	0.70931	–2846.38756	–0.24128	–2845.91954	–8.9

a: Thermal correction to Gibbs Free Energy.
b: Total electronic energy in solvent.
c: Dispersion effect correction energy.

S2. Cartesian coordinates of all optimized structures over actual reaction system.

α-ketoester

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.817205	-0.416616	-1.746857
2	6	0	-2.451159	-1.097046	-1.953702
3	8	0	-4.042187	-0.157687	-0.455073
4	6	0	-5.249143	0.576526	-0.154366
5	1	0	-5.219265	1.556766	-0.636349
6	1	0	-6.125625	0.023732	-0.502281
7	1	0	-5.258103	0.677113	0.930501
8	8	0	-4.553949	-0.109244	-2.662125
9	8	0	-1.460347	-0.507994	-1.552517
10	6	0	-2.400995	-2.396516	-2.671850
11	6	0	-3.557719	-3.049695	-3.130705
12	6	0	-1.142640	-2.994887	-2.866181
13	6	0	-3.454061	-4.284288	-3.773286
14	1	0	-4.531910	-2.589330	-3.004755
15	6	0	-1.044233	-4.225322	-3.509036
16	1	0	-0.258592	-2.479165	-2.504227
17	6	0	-2.200620	-4.872449	-3.963265
18	1	0	-4.350906	-4.783646	-4.129599
19	1	0	-0.069915	-4.683270	-3.657257
20	1	0	-2.122727	-5.833482	-4.465372

DMHP

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.209645	-0.655673	-1.151524
2	8	0	1.701245	0.752399	0.181151
3	15	0	1.532751	-0.324304	-0.829303
4	8	0	2.236793	-1.732341	-0.440187
5	6	0	2.356046	-2.132324	0.940771
6	1	0	3.093604	-2.936477	0.960401
7	1	0	2.689501	-1.294210	1.557746
8	1	0	1.394868	-2.507772	1.309266
9	8	0	2.084001	-0.072678	-2.317137
10	6	0	3.436437	0.384245	-2.531532
11	1	0	4.147532	-0.397905	-2.248606
12	1	0	3.626376	1.296214	-1.958429
13	1	0	3.516600	0.589843	-3.599713

(*S*)-CAT

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.699437	-0.253417	-0.699260
2	6	0	-1.509152	-0.090439	-0.013491

3	7	0	-0.477594	0.127241	-0.900826
4	16	0	-1.346005	-0.102356	1.653898
5	6	0	-3.990760	-0.704565	-0.300133
6	6	0	0.950733	0.318274	-0.579312
7	6	0	1.625594	-1.016063	-0.173913
8	6	0	3.169412	-0.928229	0.018239
9	6	0	3.811567	-2.179845	-0.619001
10	7	0	1.301173	-2.066234	-1.178329
11	6	0	1.603109	-3.376981	-0.572415
12	6	0	3.097830	-3.469074	-0.103957
13	6	0	2.098249	-1.925241	-2.414974
14	6	0	3.623001	-2.095054	-2.144204
15	1	0	-2.657061	0.036500	-1.673894
16	6	0	1.181036	1.538335	0.351788
17	1	0	1.387833	0.603484	-1.545475
18	1	0	3.426900	-0.869761	1.080920
19	1	0	3.581456	-0.026046	-0.458274
20	1	0	1.391202	-4.146515	-1.323554
21	1	0	0.902211	-3.534801	0.249986
22	6	0	3.368612	-3.691603	1.399621
23	1	0	3.575066	-4.319090	-0.620576
24	1	0	1.732925	-2.677138	-3.124155
25	1	0	1.887592	-0.948567	-2.864772
26	1	0	4.192479	-1.247778	-2.548592
27	1	0	4.878126	-2.222187	-0.369746
28	1	0	4.011843	-3.001463	-2.626549
29	1	0	-0.583783	-0.391036	-1.767017
30	6	0	-4.288876	-1.173946	0.977688
31	6	0	-5.570126	-1.615358	1.266127
32	6	0	-6.564739	-1.597388	0.302665
33	6	0	-6.268641	-1.130125	-0.969970
34	6	0	-4.995926	-0.688446	-1.273057
35	1	0	-5.790376	-1.977031	2.263047
36	1	0	-7.562162	-1.942424	0.538767
37	1	0	-7.035845	-1.110257	-1.733963
38	1	0	-4.767060	-0.327413	-2.266598
39	1	0	-3.511449	-1.172516	1.727059
40	6	0	0.916770	2.868672	-0.150411
41	6	0	1.173324	3.960400	0.696839
42	7	0	1.666276	3.829932	2.003473
43	6	0	1.875629	2.597345	2.407403
44	6	0	1.648120	1.428161	1.617235
45	6	0	0.407419	3.142389	-1.459079
46	1	0	1.847205	0.467732	2.067368
47	6	0	2.507146	-3.769899	2.380642
48	1	0	2.832600	-3.937009	3.397943
49	1	0	1.439430	-3.677363	2.247691
50	1	0	4.426373	-3.795652	1.619720
51	1	0	1.154339	-1.345752	0.754732
52	6	0	0.929825	5.292251	0.233581
53	6	0	0.450757	5.513560	-1.012668
54	6	0	0.183639	4.412838	-1.872867
55	1	0	2.252827	2.471506	3.420024
56	1	0	1.141290	6.106530	0.914958
57	1	0	0.264839	6.520140	-1.364755
58	1	0	-0.204368	4.601519	-2.865916
59	1	0	0.187411	2.317618	-2.120405

Product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.028285	0.017899	-1.602553
2	6	0	2.484354	1.243671	-2.723083
3	6	0	2.943968	0.019891	-1.900941
4	8	0	1.332514	1.632677	-2.676048
5	8	0	1.780385	-0.533306	-1.302633
6	8	0	3.441757	1.789671	-3.466522
7	6	0	3.049165	2.911755	-4.290025
8	1	0	2.263237	2.603793	-4.983238
9	1	0	2.691949	3.730656	-3.661257
10	1	0	3.952624	3.198664	-4.827159
11	6	0	3.979437	0.387795	-0.829154
12	6	0	5.207805	0.987458	-1.149129
13	6	0	6.113601	1.319272	-0.140434
14	6	0	5.812068	1.055416	1.198837
15	6	0	3.682465	0.123367	0.514717
16	6	0	4.593910	0.455081	1.520997
17	1	0	5.460640	1.187539	-2.183103
18	1	0	7.060263	1.783990	-0.404894
19	1	0	6.520801	1.314434	1.981415
20	1	0	4.346070	0.242321	2.557956
21	1	0	2.736230	-0.341167	0.764828
22	8	0	2.537470	-1.466917	-4.262047
23	15	0	3.453925	-1.347665	-3.093546
24	8	0	3.575543	-2.674174	-2.180640
25	6	0	2.462023	-3.583264	-2.028929
26	1	0	2.894590	-4.536697	-1.719066
27	1	0	1.931292	-3.696877	-2.977673
28	1	0	1.784679	-3.203776	-1.260778
29	8	0	4.997707	-1.027263	-3.413928
30	6	0	5.699357	-1.807817	-4.404053
31	1	0	5.845595	-2.830053	-4.041593
32	1	0	5.144695	-1.814982	-5.346796
33	1	0	6.666656	-1.321222	-4.539413

s-IM1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.049833	3.258378	-0.118422
2	6	0	-1.199382	2.911109	0.561951
3	7	0	-0.998980	1.808146	1.342023
4	16	0	-2.676711	3.723316	0.462257
5	6	0	0.268278	4.349481	-0.974522
6	6	0	-1.987110	1.048789	2.122028
7	6	0	-2.993857	0.280935	1.225856
8	6	0	-4.048676	-0.553933	2.012699
9	6	0	-4.259516	-1.895968	1.279176
10	7	0	-2.270667	-0.605795	0.268298
11	6	0	-3.216980	-0.964652	-0.806419
12	6	0	-4.512033	-1.645462	-0.240608
13	6	0	-1.796558	-1.848211	0.910403
14	6	0	-2.973682	-2.727111	1.428297
15	1	0	0.726112	2.603416	0.005915
16	6	0	-2.595014	1.907999	3.269066
17	1	0	-1.380374	0.281337	2.617401
18	1	0	-4.995616	-0.009973	2.087788

19	1	0	-3.715789	-0.752700	3.042655
20	1	0	-2.700188	-1.648323	-1.490952
21	1	0	-3.440321	-0.057641	-1.371780
22	6	0	-5.860527	-0.930283	-0.470696
23	1	0	-4.618290	-2.638962	-0.708628
24	1	0	-1.198681	-2.394902	0.169763
25	1	0	-1.117233	-1.582794	1.728154
26	1	0	-2.823639	-3.007197	2.479416
27	1	0	-5.111397	-2.432142	1.713101
28	1	0	-3.052338	-3.660719	0.855587
29	1	0	-0.118273	1.322320	1.191905
30	1	0	0.143962	-0.641952	-1.206207
31	6	0	-0.623849	5.365632	-1.313330
32	6	0	-0.215535	6.387950	-2.154419
33	6	0	1.070099	6.419464	-2.667984
34	6	0	1.960005	5.409528	-2.330641
35	6	0	1.567916	4.384228	-1.493452
36	1	0	2.263711	3.600227	-1.227708
37	1	0	2.969283	5.421929	-2.722759
38	1	0	1.378802	7.221998	-3.323854
39	1	0	-0.917925	7.171735	-2.410384
40	1	0	-1.623703	5.324245	-0.905181
41	6	0	-3.864731	2.376333	3.250503
42	6	0	-4.369034	3.143353	4.345947
43	7	0	-3.684703	3.454342	5.423578
44	6	0	-2.361235	2.991157	5.450762
45	6	0	-1.779408	2.234720	4.418275
46	6	0	-1.589625	3.329126	6.607522
47	6	0	-0.299735	2.935053	6.717781
48	6	0	0.298535	2.178532	5.672778
49	6	0	-0.411543	1.842010	4.569221
50	1	0	-4.521519	2.198193	2.412921
51	1	0	-5.395813	3.499719	4.298419
52	1	0	0.066980	1.277956	3.782608
53	1	0	1.333605	1.875179	5.766749
54	1	0	0.286295	3.191604	7.590912
55	1	0	-2.075317	3.909963	7.381335
56	1	0	-3.503534	1.022209	0.607678
57	6	0	-6.082767	0.228989	-1.034022
58	1	0	-6.703538	-1.506825	-0.103439
59	1	0	-7.086980	0.615612	-1.138548
60	1	0	-5.301447	0.864717	-1.423734
61	8	0	1.577128	0.736963	0.196104
62	15	0	1.457611	-0.322082	-0.857536
63	8	0	2.189541	-1.705954	-0.460898
64	6	0	2.401265	-2.092316	0.914917
65	1	0	3.177342	-2.858979	0.895367
66	1	0	2.727728	-1.235579	1.509050
67	1	0	1.479868	-2.511492	1.331182
68	8	0	2.059283	-0.004441	-2.305258
69	6	0	3.451906	0.337430	-2.488708
70	1	0	4.080220	-0.530753	-2.270630
71	1	0	3.727233	1.179239	-1.847217
72	1	0	3.552312	0.618932	-3.537261

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s-TS1

Standard orientation:

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

1	7	0	0.017695	3.302498	-0.140897
2	6	0	-1.119771	2.927278	0.529002
3	7	0	-0.869528	1.880990	1.379270
4	16	0	-2.655629	3.610155	0.332299
5	6	0	0.300198	4.403944	-0.995899
6	6	0	-1.825624	1.074559	2.146428
7	6	0	-2.765221	0.257820	1.215478
8	6	0	-3.966224	-0.458481	1.888082
9	6	0	-4.212279	-1.809763	1.182604
10	7	0	-1.977899	-0.800571	0.466804
11	6	0	-2.752777	-1.179847	-0.752810
12	6	0	-4.197510	-1.617265	-0.364999
13	6	0	-1.736994	-2.021770	1.295080
14	6	0	-3.067039	-2.764111	1.562434
15	1	0	0.791668	2.623723	-0.064006
16	6	0	-2.496937	1.894351	3.286513
17	1	0	-1.190660	0.335770	2.645741
18	1	0	-4.856342	0.172255	1.820397
19	1	0	-3.779031	-0.630933	2.957163
20	1	0	-2.205509	-1.992764	-1.239561
21	1	0	-2.727682	-0.324467	-1.428934
22	6	0	-5.363396	-0.722411	-0.834156
23	1	0	-4.379610	-2.609932	-0.807988
24	1	0	-1.011070	-2.636456	0.752756
25	1	0	-1.254920	-1.704441	2.223754
26	1	0	-3.137215	-3.048984	2.618816
27	1	0	-5.175736	-2.226911	1.494435
28	1	0	-3.125471	-3.688806	0.975176
29	1	0	0.089920	1.531460	1.357661
30	1	0	-0.771296	-0.501385	0.057792
31	6	0	-0.575276	5.463509	-1.226981
32	6	0	-0.194028	6.503102	-2.060264
33	6	0	1.048864	6.508940	-2.669492
34	6	0	1.923464	5.455872	-2.438140
35	6	0	1.558234	4.413161	-1.610773
36	1	0	2.240932	3.594454	-1.426392
37	1	0	2.899729	5.448286	-2.906518
38	1	0	1.336916	7.324696	-3.318467
39	1	0	-0.883692	7.320141	-2.232847
40	1	0	-1.546676	5.444751	-0.755466
41	6	0	-3.743304	2.412407	3.190956
42	6	0	-4.304372	3.150653	4.278954
43	7	0	-3.694027	3.386341	5.417860
44	6	0	-2.391492	2.876610	5.522949
45	6	0	-1.755795	2.145102	4.503658
46	6	0	-1.701125	3.141134	6.747827
47	6	0	-0.433947	2.704483	6.935627
48	6	0	0.221051	1.977841	5.903745
49	6	0	-0.412904	1.708753	4.736894
50	1	0	-4.335611	2.298508	2.296144
51	1	0	-5.311449	3.547279	4.170380
52	1	0	0.114565	1.168575	3.965017
53	1	0	1.239242	1.642923	6.057741
54	1	0	0.091759	2.906065	7.860135
55	1	0	-2.228436	3.703378	7.508073
56	1	0	-3.133276	0.941138	0.449155
57	6	0	-5.312390	0.376772	-1.540762
58	1	0	-6.327733	-1.108851	-0.522320
59	1	0	-6.215927	0.904203	-1.814328
60	1	0	-4.394324	0.825185	-1.892581
61	8	0	1.595114	0.911469	0.203482
62	15	0	0.906378	-0.307363	-0.421576

63	8	0	1.871658	-1.645644	-0.161661
64	6	0	2.763535	-1.699712	0.957818
65	1	0	3.474096	-2.505161	0.753471
66	1	0	3.295472	-0.752475	1.083351
67	1	0	2.217185	-1.933473	1.882309
68	8	0	0.924417	-0.284765	-2.062622
69	6	0	2.151763	-0.092903	-2.789429
70	1	0	2.815324	-0.951951	-2.646620
71	1	0	2.655138	0.823264	-2.463781
72	1	0	1.876070	-0.007656	-3.842854

s-IM2a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.696118	-1.731904	-0.253518
2	6	0	-0.490189	-1.245856	-0.679867
3	7	0	0.141430	-0.552316	0.321309
4	16	0	0.153071	-1.412218	-2.241591
5	6	0	-2.691259	-2.508344	-0.911939
6	6	0	1.392354	0.195251	0.251735
7	6	0	1.277807	1.419959	-0.690336
8	6	0	2.525972	2.323696	-0.811119
9	6	0	2.083695	3.798767	-0.933601
10	7	0	0.132754	2.330427	-0.241808
11	6	0	-0.296448	3.171446	-1.416692
12	6	0	0.936685	3.929588	-1.983698
13	6	0	0.509760	3.224300	0.917245
14	6	0	1.546762	4.258388	0.434277
15	1	0	-1.991110	-1.359597	0.667540
16	6	0	2.628207	-0.716098	0.002691
17	1	0	1.512345	0.597576	1.264594
18	1	0	3.106715	2.025298	-1.687460
19	1	0	3.182318	2.205065	0.061992
20	1	0	-1.066849	3.851739	-1.046078
21	1	0	-0.763432	2.494653	-2.131485
22	6	0	1.414084	3.542771	-3.398266
23	1	0	0.673512	4.997812	-2.029732
24	1	0	-0.419261	3.662003	1.288585
25	1	0	0.893113	2.578521	1.708515
26	1	0	2.362989	4.332582	1.161227
27	1	0	2.931302	4.421549	-1.236771
28	1	0	1.095901	5.254663	0.355172
29	1	0	-0.421218	-0.425950	1.181789
30	1	0	-0.713959	1.789649	0.086327
31	6	0	-2.465333	-3.247445	-2.071567
32	6	0	-3.492596	-3.998339	-2.621115
33	6	0	-4.743668	-4.031371	-2.030263
34	6	0	-4.968644	-3.300145	-0.871412
35	6	0	-3.956759	-2.544636	-0.313680
36	1	0	-4.131257	-1.971678	0.588205
37	1	0	-5.942809	-3.317807	-0.399067
38	1	0	-5.538872	-4.621098	-2.465769
39	1	0	-3.306164	-4.566743	-3.523830
40	1	0	-1.490146	-3.208933	-2.533341
41	6	0	3.268941	-0.793033	-1.186224
42	6	0	4.405729	-1.646954	-1.337129
43	7	0	4.908773	-2.399057	-0.385391
44	6	0	4.239909	-2.346472	0.846882

45	6	0	3.111822	-1.541957	1.086688
46	6	0	4.758962	-3.173826	1.891926
47	6	0	4.168459	-3.199202	3.109709
48	6	0	3.018777	-2.398662	3.354412
49	6	0	2.510638	-1.601252	2.383653
50	1	0	2.940054	-0.233945	-2.048787
51	1	0	4.901847	-1.681420	-2.304538
52	1	0	1.626127	-1.016734	2.589776
53	1	0	2.546288	-2.435461	4.328120
54	1	0	4.556794	-3.827226	3.901387
55	1	0	5.630929	-3.775335	1.668650
56	1	0	0.970032	1.053731	-1.670016
57	6	0	0.937620	2.621514	-4.194719
58	1	0	2.246725	4.154611	-3.726988
59	1	0	1.365232	2.462026	-5.175309
60	1	0	0.110223	1.972278	-3.944377
61	8	0	-1.922238	-0.091469	2.076839
62	15	0	-2.430514	1.281889	1.571595
63	8	0	-2.350050	2.363539	2.862470
64	6	0	-2.771081	1.942888	4.170148
65	1	0	-2.554746	2.769361	4.853527
66	1	0	-3.846184	1.728591	4.182827
67	1	0	-2.225744	1.045873	4.481933
68	8	0	-4.092956	1.027937	1.461731
69	6	0	-4.910241	2.095228	0.993582
70	1	0	-4.542237	2.500692	0.038893
71	1	0	-4.962134	2.911820	1.726477
72	1	0	-5.913460	1.687653	0.839136

s-**TS**-ex

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.322394	1.918962	-0.050572
2	6	0	0.146612	1.362180	-0.486622
3	7	0	-0.338145	0.457408	0.425369
4	16	0	-0.611398	1.679459	-1.967458
5	6	0	-1.347116	-0.575213	0.194210
6	6	0	-0.852922	-1.590686	-0.864717
7	6	0	-1.771772	-2.786028	-1.194674
8	6	0	-0.909897	-4.044614	-1.437071
9	7	0	0.485954	-2.189614	-0.408315
10	6	0	1.216620	-2.721417	-1.620141
11	6	0	0.286192	-3.707077	-2.380927
12	6	0	0.318976	-3.303327	0.607033
13	6	0	-0.347460	-4.509806	-0.083616
14	1	0	1.755610	1.407075	0.739037
15	1	0	-1.386065	-1.117652	1.146727
16	1	0	-2.364164	-2.551851	-2.082404
17	1	0	-2.480980	-2.974634	-0.377266
18	1	0	2.120528	-3.198975	-1.239399
19	1	0	1.513741	-1.855649	-2.210723
20	1	0	0.848238	-4.643518	-2.520479
21	1	0	1.315741	-3.512295	0.995787
22	1	0	-0.275971	-2.902119	1.428304
23	1	0	-1.150141	-4.901575	0.550687
24	1	0	-1.518680	-4.835045	-1.887127
25	1	0	0.375185	-5.321883	-0.224812

26	1	0	0.297038	0.263865	1.216972
27	1	0	-0.610130	-1.032900	-1.770364
28	1	0	1.076834	-1.463046	0.033416
29	6	0	2.074625	3.027103	-0.532057
30	6	0	1.621750	3.914514	-1.507349
31	6	0	3.331397	3.237755	0.047160
32	6	0	2.417567	4.981071	-1.893175
33	1	0	0.655446	3.744209	-1.957802
34	6	0	4.112895	4.305433	-0.347046
35	1	0	3.681630	2.556493	0.810194
36	6	0	3.661894	5.184707	-1.321786
37	1	0	2.054123	5.661944	-2.652936
38	1	0	5.082861	4.453440	0.111017
39	1	0	4.276066	6.019877	-1.629873
40	6	0	-2.775324	-0.004846	-0.026760
41	6	0	-3.477454	0.556339	1.105495
42	6	0	-3.402439	-0.001304	-1.225384
43	6	0	-4.780472	1.041556	0.896516
44	6	0	-2.927569	0.657575	2.422370
45	6	0	-4.728234	0.520518	-1.342210
46	1	0	-2.925429	-0.369821	-2.120529
47	6	0	-5.515911	1.598026	1.990089
48	1	0	-5.206116	0.504115	-2.319220
49	6	0	-0.199273	-3.282832	-3.782095
50	6	0	0.062163	-2.180185	-4.434656
51	1	0	-0.821625	-4.041516	-4.243457
52	1	0	-0.336725	-2.015253	-5.426353
53	1	0	0.676101	-1.378727	-4.048218
54	7	0	-5.426754	1.019957	-0.348449
55	6	0	-4.966353	1.671455	3.224932
56	6	0	-3.643793	1.194369	3.439765
57	1	0	-1.918732	0.318328	2.605429
58	1	0	-3.209561	1.268399	4.429029
59	1	0	-5.519343	2.094924	4.053696
60	1	0	-6.517256	1.957372	1.789582
61	8	0	1.891769	-0.116871	1.854645
62	15	0	2.673126	-1.384577	2.348208
63	8	0	3.326327	-2.018064	0.858929
64	6	0	4.337039	-1.304618	0.146581
65	1	0	4.542971	-1.848554	-0.782851
66	1	0	5.260772	-1.254173	0.735273
67	1	0	4.011276	-0.285404	-0.103605
68	8	0	4.083226	-0.808539	3.064761
69	6	0	4.467836	0.564867	3.087436
70	1	0	5.100504	0.809385	2.222918
71	1	0	3.591917	1.222872	3.087288
72	1	0	5.045767	0.722764	4.003667

s-IM2b

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.149912	1.948144	-0.212430
2	8	0	1.083024	2.516872	0.580020
3	8	0	-1.037926	2.331297	-0.228990
4	6	0	0.626831	0.799902	-0.970361
5	6	0	4.554830	-0.229705	-1.252828
6	6	0	3.185408	0.150820	-1.160233
7	6	0	2.017510	0.497693	-1.075187

8	1	0	0.066770	0.690830	-1.902230
9	6	0	0.791597	3.635695	1.488158
10	6	0	5.489521	0.184499	-0.276728
11	6	0	6.829161	-0.190680	-0.368720
12	6	0	7.274010	-0.986063	-1.430851
13	6	0	6.359233	-1.402194	-2.404572
14	6	0	5.017671	-1.031078	-2.321045
15	1	0	5.147756	0.802531	0.547774
16	1	0	7.530563	0.140189	0.392893
17	1	0	8.318560	-1.276245	-1.499413
18	1	0	6.693096	-2.018123	-3.235670
19	1	0	4.312037	-1.353103	-3.080962
20	1	0	-0.016404	-0.305109	-0.235915
21	6	0	-2.017791	-3.207858	0.179322
22	6	0	-0.586860	-2.614176	0.460348
23	7	0	-2.873886	-2.026643	0.316942
24	6	0	-2.063574	-0.935205	0.133412
25	7	0	-0.777787	-1.152100	0.275095
26	6	0	-4.152029	-1.747428	-0.341176
27	6	0	-4.194035	-0.185992	-0.303318
28	7	0	-2.758006	0.143206	-0.238997
29	1	0	-2.303569	-3.991366	0.884307
30	1	0	-2.083927	-3.618095	-0.840184
31	1	0	-4.991927	-2.193585	0.195894
32	1	0	-4.149657	-2.128486	-1.374138
33	1	0	-2.312608	1.073404	-0.286075
34	1	0	0.110638	-2.966397	-0.309223
35	1	0	-4.676954	0.121730	0.637260
36	6	0	-4.950090	0.522160	-1.459401
37	6	0	-4.939307	2.042266	-1.186758
38	1	0	-3.924646	2.453637	-1.198153
39	1	0	-5.516176	2.568518	-1.955066
40	1	0	-5.389619	2.274570	-0.214222
41	6	0	-6.409357	0.021154	-1.458229
42	1	0	-6.889160	0.183940	-0.485438
43	1	0	-6.995153	0.560478	-2.210206
44	1	0	-6.476372	-1.046806	-1.695709
45	6	0	-4.303693	0.252060	-2.832052
46	1	0	-3.262332	0.586541	-2.855525
47	1	0	-4.325552	-0.809644	-3.100878
48	1	0	-4.849209	0.795268	-3.611326
49	6	0	0.041666	-2.975720	1.839465
50	6	0	0.292612	-4.497317	1.889329
51	1	0	0.797542	-4.766664	2.823415
52	1	0	-0.636933	-5.076374	1.844863
53	1	0	0.934515	-4.822498	1.061584
54	6	0	-0.870514	-2.554188	3.007138
55	1	0	-1.064214	-1.477121	2.984706
56	1	0	-1.834678	-3.074639	2.988660
57	1	0	-0.389340	-2.787814	3.963510
58	6	0	1.395487	-2.246148	1.959526
59	1	0	1.888528	-2.516339	2.900221
60	1	0	2.070113	-2.513822	1.138367
61	1	0	1.268750	-1.160131	1.942084
62	6	0	0.335577	4.862310	0.687776
63	1	0	-0.630082	4.686375	0.211852
64	1	0	0.249089	5.725038	1.357878
65	1	0	1.072446	5.104214	-0.085182
66	6	0	2.153890	3.896313	2.139886
67	1	0	2.079812	4.728736	2.847437
68	1	0	2.499065	3.008814	2.679146
69	1	0	2.900323	4.147677	1.380546

70	6	0	-0.237365	3.217169	2.546458
71	1	0	0.089441	2.302863	3.053139
72	1	0	-0.328290	4.007965	3.299628
73	1	0	-1.217075	3.043875	2.099260

k-IM0

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.196111	-0.102822	-1.840878
2	6	0	-2.133348	-1.074611	-2.398664
3	8	0	-4.293171	-0.052723	-2.598667
4	6	0	-5.286210	0.939748	-2.231241
5	1	0	-5.670491	0.729166	-1.230578
6	1	0	-4.839417	1.936143	-2.253951
7	1	0	-6.070519	0.844898	-2.980941
8	8	0	-2.992405	0.581845	-0.859391
9	8	0	-1.020143	-0.594733	-2.564847
10	6	0	-2.465115	-2.488451	-2.675057
11	6	0	-3.689686	-3.060554	-2.287730
12	6	0	-1.493614	-3.287805	-3.307076
13	6	0	-3.937356	-4.411705	-2.529671
14	1	0	-4.448067	-2.457213	-1.799607
15	6	0	-1.749982	-4.631941	-3.557310
16	1	0	-0.549731	-2.835859	-3.594980
17	6	0	-2.971478	-5.196106	-3.166651
18	1	0	-4.882568	-4.851137	-2.223706
19	1	0	-1.001144	-5.243739	-4.052574
20	1	0	-3.168723	-6.247477	-3.359294
21	7	0	-0.836666	2.577845	0.317702
22	6	0	0.409622	2.690660	-0.264845
23	7	0	0.561434	1.814633	-1.304300
24	16	0	1.594292	3.801828	0.183340
25	6	0	1.804116	1.377319	-1.959130
26	6	0	2.389154	0.139194	-1.179779
27	6	0	3.691203	-0.504868	-1.745100
28	6	0	4.402372	-1.206002	-0.564778
29	7	0	2.443047	0.225147	0.295302
30	6	0	3.708386	0.783751	0.799897
31	6	0	4.927158	-0.140828	0.440040
32	6	0	2.310122	-1.149035	0.815732
33	6	0	3.380561	-2.093502	0.179430
34	1	0	-1.421066	1.825364	-0.046665
35	1	0	1.437552	0.895606	-2.877848
36	1	0	1.589391	-0.592875	-1.350024
37	1	0	4.364028	0.225989	-2.204311
38	1	0	3.440847	-1.233840	-2.528153
39	1	0	3.609720	0.893972	1.885510
40	1	0	3.812615	1.791618	0.402323
41	6	0	6.198103	0.585251	-0.052547
42	1	0	5.225591	-0.693817	1.349235
43	1	0	2.424278	-1.099316	1.904895
44	1	0	1.293041	-1.507116	0.614784
45	1	0	2.916977	-2.800198	-0.523016
46	1	0	5.235756	-1.814302	-0.935651
47	1	0	3.885122	-2.693248	0.948393
48	1	0	-0.199856	1.161774	-1.468484
49	6	0	-1.503106	3.345233	1.317492
50	6	0	-0.934432	4.433955	1.975717

51	6	0	-2.809499	2.959578	1.639775
52	6	0	-1.665772	5.117355	2.933803
53	1	0	0.075809	4.716719	1.716135
54	6	0	-3.524549	3.650061	2.597781
55	1	0	-3.251659	2.115672	1.128166
56	6	0	-2.957766	4.734863	3.252019
57	1	0	-1.213270	5.962288	3.438198
58	1	0	-4.534070	3.339672	2.836512
59	1	0	-3.519998	5.274314	4.002023
60	6	0	2.651135	2.563927	-2.510643
61	6	0	3.940153	2.816754	-2.185412
62	6	0	2.049325	3.411753	-3.524422
63	6	0	4.650868	3.892125	-2.802866
64	1	0	4.470882	2.237469	-1.450519
65	6	0	2.826571	4.444531	-4.077013
66	6	0	0.712296	3.257025	-4.009826
67	7	0	4.157513	4.699617	-3.712480
68	1	0	5.682776	4.063507	-2.503618
69	6	0	2.269214	5.299692	-5.079098
70	6	0	0.998453	5.124595	-5.510513
71	6	0	0.208262	4.078506	-4.962555
72	1	0	0.575544	5.770415	-6.269263
73	1	0	2.901714	6.083891	-5.475106
74	1	0	-0.806522	3.943558	-5.314632
75	1	0	0.091868	2.474594	-3.601097
76	6	0	6.584951	1.783164	0.305488
77	1	0	6.823476	-0.002595	-0.716455
78	1	0	7.511025	2.209902	-0.053827
79	1	0	6.010444	2.409090	0.973737

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k-**IM**1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.965487	2.524719	-0.630020
2	8	0	-0.152488	3.030865	0.355607
3	8	0	-2.192302	2.748840	-0.662740
4	6	0	-0.287122	1.676491	-1.557266
5	6	0	3.561053	0.487309	-1.415057
6	6	0	2.169369	0.780427	-1.378585
7	6	0	1.038184	1.272364	-1.472494
8	1	0	-0.853486	1.422991	-2.449983
9	6	0	-0.655813	3.924778	1.394033
10	6	0	4.100705	-0.389693	-2.388319
11	6	0	5.463662	-0.682394	-2.412993
12	6	0	6.332570	-0.121292	-1.469418
13	6	0	5.813959	0.747616	-0.501297
14	6	0	4.453832	1.049900	-0.469452
15	1	0	3.435851	-0.825103	-3.128944
16	1	0	5.851269	-1.351541	-3.177360
17	1	0	7.393835	-0.351143	-1.492026
18	1	0	6.476847	1.199587	0.232508
19	1	0	4.062365	1.733276	0.278060
20	6	0	-0.486467	-3.550797	0.591798
21	6	0	0.799644	-2.656354	0.564152
22	7	0	-1.558967	-2.553831	0.609468
23	6	0	-1.067786	-1.399597	0.081127
24	7	0	0.256076	-1.368724	0.061342
25	6	0	-2.955862	-2.687346	0.186359

26	6	0	-3.351933	-1.200126	-0.076199
27	7	0	-2.025296	-0.591823	-0.346162
28	1	0	-0.532040	-4.197518	1.469546
29	1	0	-0.555018	-4.178342	-0.309340
30	1	0	-3.569964	-3.144406	0.964476
31	1	0	-3.025333	-3.297251	-0.726575
32	1	0	-1.828080	0.361330	-0.666763
33	1	0	-3.743085	-0.773270	0.858005
34	1	0	1.504979	-3.041376	-0.179829
35	1	0	0.822172	-0.617021	-0.364194
36	6	0	-4.403431	-0.945069	-1.188611
37	6	0	1.568301	-2.527386	1.913809
38	6	0	2.726305	-1.526537	1.727028
39	1	0	2.362587	-0.517038	1.515479
40	1	0	3.329243	-1.477068	2.640097
41	1	0	3.389248	-1.819361	0.905657
42	6	0	2.161043	-3.908966	2.263762
43	1	0	2.811607	-4.279080	1.462360
44	1	0	2.767924	-3.835172	3.172125
45	1	0	1.388906	-4.664067	2.450934
46	6	0	0.653065	-2.042653	3.054565
47	1	0	0.218292	-1.063561	2.829767
48	1	0	-0.164676	-2.742476	3.258345
49	1	0	1.234236	-1.940295	3.977248
50	6	0	-4.788410	0.550338	-1.169683
51	1	0	-3.934343	1.215612	-1.334383
52	1	0	-5.530051	0.753160	-1.950163
53	1	0	-5.236371	0.825685	-0.207352
54	6	0	-5.654483	-1.789232	-0.862690
55	1	0	-6.036120	-1.568425	0.141495
56	1	0	-6.453594	-1.560438	-1.575232
57	1	0	-5.458448	-2.866083	-0.926147
58	6	0	-3.867161	-1.322615	-2.583301
59	1	0	-2.985917	-0.731628	-2.849622
60	1	0	-3.599696	-2.383155	-2.656348
61	1	0	-4.637544	-1.130200	-3.337243
62	6	0	-1.216739	5.212042	0.772784
63	1	0	-2.106375	5.002540	0.177258
64	1	0	-1.475976	5.923457	1.565687
65	1	0	-0.463013	5.678111	0.129277
66	6	0	0.603225	4.235946	2.212858
67	1	0	0.362404	4.914676	3.038184
68	1	0	1.028430	3.317078	2.629362
69	1	0	1.362098	4.708193	1.581584
70	6	0	-1.696677	3.212512	2.271391
71	1	0	-1.280908	2.278544	2.667062
72	1	0	-1.963848	3.850268	3.122146
73	1	0	-2.598031	2.987201	1.699698

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k-**TS1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.901859	-0.128630	-1.837641
2	6	0	-1.874186	-1.196068	-2.289890
3	8	0	-4.109903	-0.624964	-1.589649
4	6	0	-5.111654	0.312879	-1.143601
5	1	0	-4.809374	0.736039	-0.182726
6	1	0	-5.239752	1.108488	-1.881660

7	1	0	-6.025322	-0.272043	-1.039690
8	8	0	-2.630464	1.058284	-1.840618
9	8	0	-0.847381	-0.759643	-2.792238
10	6	0	-2.164202	-2.654111	-2.237745
11	6	0	-2.935844	-3.255531	-1.228756
12	6	0	-1.597484	-3.455137	-3.246449
13	6	0	-3.136757	-4.636065	-1.239264
14	1	0	-3.328957	-2.645935	-0.425280
15	6	0	-1.817940	-4.830980	-3.262113
16	1	0	-0.997292	-2.982904	-4.018601
17	6	0	-2.588638	-5.424141	-2.256164
18	1	0	-3.720133	-5.099352	-0.447769
19	1	0	-1.391228	-5.439621	-4.055122
20	1	0	-2.758214	-6.498099	-2.263424
21	7	0	-1.089907	2.912962	-0.077085
22	6	0	0.236809	2.596097	-0.243858
23	7	0	0.412429	1.685977	-1.256213
24	16	0	1.503836	3.208588	0.686880
25	6	0	1.631953	1.357084	-2.007174
26	6	0	2.217533	-0.069329	-1.643275
27	6	0	3.641733	-0.375280	-2.196545
28	6	0	4.357612	-1.344805	-1.235046
29	7	0	2.135742	-0.560804	-0.222346
30	6	0	3.248319	-0.067232	0.634446
31	6	0	4.604432	-0.671599	0.147878
32	6	0	2.181609	-2.063855	-0.260991
33	6	0	3.439641	-2.557993	-1.011922
34	1	0	-1.725808	2.423595	-0.709164
35	1	0	1.242380	1.123902	-3.004106
36	1	0	1.513529	-0.735467	-2.147875
37	1	0	4.234522	0.532464	-2.322175
38	1	0	3.555383	-0.831191	-3.190729
39	1	0	3.016632	-0.359104	1.663539
40	1	0	3.219482	1.020509	0.598790
41	6	0	5.793957	0.311781	0.149134
42	1	0	4.882926	-1.488400	0.836760
43	1	0	2.156595	-2.399037	0.778335
44	1	0	1.254324	-2.407916	-0.727292
45	1	0	3.169062	-3.008785	-1.974881
46	1	0	5.312331	-1.662408	-1.668687
47	1	0	3.951458	-3.331675	-0.427186
48	1	0	-0.434192	1.311468	-1.681682
49	6	0	-1.771192	3.782411	0.824442
50	6	0	-1.145050	4.539442	1.812333
51	6	0	-3.160571	3.868476	0.676957
52	6	0	-1.902409	5.360556	2.632827
53	1	0	-0.072341	4.465064	1.914630
54	6	0	-3.901151	4.691028	1.501627
55	1	0	-3.646954	3.283723	-0.091822
56	6	0	-3.276419	5.443504	2.486708
57	1	0	-1.404690	5.943704	3.397828
58	1	0	-4.975061	4.746771	1.374892
59	1	0	-3.858143	6.087702	3.131948
60	6	0	2.530033	2.604246	-2.269159
61	6	0	3.723943	2.844183	-1.679001
62	6	0	2.059637	3.578417	-3.234944
63	6	0	4.488434	4.001180	-2.024397
64	1	0	4.134500	2.188688	-0.929448
65	6	0	2.880956	4.686032	-3.512834
66	6	0	0.806116	3.495835	-3.921643
67	7	0	4.125552	4.905189	-2.904462
68	1	0	5.445652	4.152119	-1.530300

69	6	0	2.459242	5.669146	-4.462781
70	6	0	1.269380	5.553122	-5.096729
71	6	0	0.427964	4.442796	-4.813990
72	1	0	0.946791	6.296841	-5.814048
73	1	0	3.124839	6.502691	-4.647788
74	1	0	-0.526405	4.360878	-5.318913
75	1	0	0.139431	2.671289	-3.719559
76	6	0	5.943044	1.333681	0.952891
77	1	0	6.576227	0.064745	-0.560206
78	1	0	6.828923	1.952850	0.918120
79	1	0	5.203257	1.617666	1.688695
80	1	0	0.971621	-0.413207	0.368500
81	15	0	-0.542576	-0.716448	1.211678
82	8	0	-0.208913	-2.197494	1.916847
83	6	0	-1.162415	-2.829104	2.775904
84	1	0	-2.148655	-2.879742	2.300042
85	1	0	-1.241252	-2.288650	3.727529
86	1	0	-0.799764	-3.842788	2.969501
87	8	0	-0.655181	0.275618	2.534361
88	6	0	-1.898365	0.740959	3.066077
89	1	0	-2.669930	0.772435	2.290412
90	1	0	-2.231950	0.085354	3.880991
91	1	0	-1.722673	1.745530	3.461149
92	8	0	-1.895794	-0.775366	0.501102

k-IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.740563	-0.138779	-1.775506
2	6	0	-1.755138	-1.281482	-2.095770
3	8	0	-4.006315	-0.536893	-1.679780
4	6	0	-4.979097	0.477135	-1.362690
5	1	0	-4.779414	0.873089	-0.363837
6	1	0	-4.943446	1.282740	-2.100319
7	1	0	-5.942857	-0.031458	-1.389202
8	8	0	-2.389773	1.032124	-1.782285
9	8	0	-0.640729	-0.933475	-2.474806
10	6	0	-2.178141	-2.710002	-2.133725
11	6	0	-3.115392	-3.271153	-1.249958
12	6	0	-1.579252	-3.523323	-3.112660
13	6	0	-3.443441	-4.623140	-1.352882
14	1	0	-3.537033	-2.654175	-0.467140
15	6	0	-1.923671	-4.869945	-3.221783
16	1	0	-0.853650	-3.083132	-3.790342
17	6	0	-2.857111	-5.423036	-2.339254
18	1	0	-4.156811	-5.056145	-0.656187
19	1	0	-1.466820	-5.485944	-3.992250
20	1	0	-3.124692	-6.474002	-2.418469
21	7	0	-0.947230	2.958036	-0.030076
22	6	0	0.369825	2.687165	-0.279381
23	7	0	0.515147	1.764163	-1.286507
24	16	0	1.679117	3.369956	0.544915
25	6	0	1.710369	1.416006	-2.059463
26	6	0	2.306776	0.021914	-1.611880
27	6	0	3.716414	-0.370926	-2.122763
28	6	0	4.390380	-1.293040	-1.085617
29	7	0	2.237632	-0.327865	-0.131296
30	6	0	3.389253	0.206329	0.674161

31	6	0	4.695472	-0.510671	0.225855
32	6	0	2.197938	-1.840658	-0.010475
33	6	0	3.418874	-2.436335	-0.742841
34	1	0	-1.603681	2.438010	-0.616277
35	1	0	1.294885	1.115087	-3.028297
36	1	0	1.583317	-0.681078	-2.026642
37	1	0	4.342448	0.502630	-2.311510
38	1	0	3.611550	-0.895002	-3.079828
39	1	0	3.146048	0.026309	1.723996
40	1	0	3.396133	1.283192	0.520931
41	6	0	5.927108	0.411672	0.114743
42	1	0	4.944991	-1.272868	0.983593
43	1	0	2.175431	-2.060994	1.057865
44	1	0	1.243819	-2.167858	-0.423702
45	1	0	3.104640	-2.952156	-1.657780
46	1	0	5.320391	-1.697901	-1.497949
47	1	0	3.907885	-3.181518	-0.105641
48	1	0	-0.339918	1.321078	-1.627956
49	6	0	-1.601835	3.757427	0.956703
50	6	0	-0.942041	4.519012	1.917709
51	6	0	-3.000663	3.766218	0.919009
52	6	0	-1.676717	5.268484	2.823498
53	1	0	0.137481	4.506456	1.935905
54	6	0	-3.718484	4.518343	1.826783
55	1	0	-3.512812	3.175515	0.171856
56	6	0	-3.060128	5.275438	2.786404
57	1	0	-1.153317	5.855467	3.568049
58	1	0	-4.800466	4.514153	1.786253
59	1	0	-3.624042	5.864113	3.497321
60	6	0	2.597015	2.644880	-2.419015
61	6	0	3.824851	2.900597	-1.911158
62	6	0	2.074000	3.575994	-3.399284
63	6	0	4.572525	4.035861	-2.352610
64	1	0	4.276725	2.279363	-1.156349
65	6	0	2.882148	4.664520	-3.774045
66	6	0	0.782635	3.467937	-4.007038
67	7	0	4.161350	4.901492	-3.249512
68	1	0	5.557803	4.202301	-1.922987
69	6	0	2.409226	5.606415	-4.741195
70	6	0	1.183762	5.468137	-5.298693
71	6	0	0.356575	4.376366	-4.917901
72	1	0	0.821945	6.180798	-6.028855
73	1	0	3.065384	6.427051	-5.002094
74	1	0	-0.626009	4.277603	-5.362255
75	1	0	0.126175	2.657858	-3.727522
76	6	0	6.118666	1.524352	0.776047
77	1	0	6.699669	0.033283	-0.544997
78	1	0	7.033923	2.090331	0.667453
79	1	0	5.391527	1.940311	1.460274
80	1	0	1.317840	-0.008809	0.275843
81	15	0	-0.788853	-0.650918	1.260212
82	8	0	-0.319613	-2.120744	1.985922
83	6	0	-1.266966	-2.977867	2.621715
84	1	0	-2.190140	-3.051231	2.034729
85	1	0	-1.503302	-2.613469	3.630517
86	1	0	-0.812644	-3.971528	2.703583
87	8	0	-1.283539	0.240848	2.601776
88	6	0	-2.630744	0.262633	3.069564
89	1	0	-3.338672	0.143607	2.241598
90	1	0	-2.803882	-0.537338	3.802736
91	1	0	-2.789111	1.229606	3.559031
92	8	0	-2.079971	-0.961273	0.452316

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ds-**IM3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.250773	2.719199	-0.163153
2	6	0	-1.171115	1.729251	-0.386870
3	7	0	-0.861508	0.580865	0.289390
4	16	0	-2.531506	1.864586	-1.390737
5	6	0	-0.133665	4.057656	-0.644039
6	6	0	-1.681146	-0.622451	0.463045
7	6	0	-1.875555	-1.422360	-0.845434
8	6	0	-2.682744	-2.733403	-0.666195
9	6	0	-2.065239	-3.846861	-1.534742
10	7	0	-0.545696	-1.802034	-1.477623
11	6	0	-0.796116	-2.183129	-2.913598
12	6	0	-1.846389	-3.325699	-2.987082
13	6	0	0.139234	-2.941780	-0.769481
14	6	0	-0.699494	-4.228575	-0.935447
15	1	0	0.515715	2.452051	0.457331
16	6	0	-3.001985	-0.323551	1.233868
17	1	0	-1.069685	-1.248120	1.116765
18	1	0	-3.726148	-2.563609	-0.946091
19	1	0	-2.682925	-3.048079	0.386590
20	1	0	0.171457	-2.480898	-3.321545
21	1	0	-1.097903	-1.270649	-3.426082
22	6	0	-3.188065	-3.008940	-3.679910
23	1	0	-1.398992	-4.155989	-3.556412
24	1	0	1.134183	-3.018030	-1.212774
25	1	0	0.272526	-2.648273	0.272628
26	1	0	-0.835580	-4.716055	0.036671
27	1	0	-2.726728	-4.719528	-1.552452
28	1	0	-0.185611	-4.947056	-1.585353
29	1	0	-0.015851	0.592820	0.859233
30	6	0	-1.044068	4.664238	-1.505975
31	6	0	-0.840987	5.975007	-1.908432
32	6	0	0.255153	6.694856	-1.465702
33	6	0	1.162717	6.091043	-0.605977
34	6	0	0.974145	4.786455	-0.196400
35	1	0	-1.554923	6.436531	-2.579436
36	1	0	0.404689	7.717139	-1.785722
37	1	0	2.025139	6.641993	-0.252292
38	1	0	1.682049	4.315410	0.471937
39	1	0	-1.894139	4.089455	-1.843402
40	1	0	0.190370	-1.006624	-1.521284
41	6	0	-2.957903	-0.135076	2.667477
42	6	0	-4.165511	0.145031	3.331602
43	7	0	-5.403192	0.257106	2.680489
44	6	0	-5.376041	0.090181	1.378151
45	6	0	-4.200320	-0.199369	0.617651
46	6	0	-1.764585	-0.210113	3.453909
47	1	0	-4.303037	-0.299909	-0.452114
48	6	0	-3.590773	-1.875011	-4.191855
49	1	0	-4.560795	-1.791567	-4.662521
50	1	0	-3.003050	-0.968089	-4.185112
51	1	0	-3.838086	-3.875788	-3.729664
52	1	0	-2.349110	-0.770936	-1.578522
53	6	0	-4.171597	0.335630	4.749290
54	6	0	-3.023599	0.254694	5.461643

55	6	0	-1.798341	-0.022451	4.795546
56	1	0	-6.323632	0.180237	0.851547
57	1	0	-5.122129	0.547693	5.222135
58	1	0	-3.024641	0.400524	6.534289
59	1	0	-0.885130	-0.080978	5.374424
60	1	0	-0.818821	-0.414674	2.973354
61	6	0	2.698954	0.636587	1.791564
62	6	0	2.403151	-0.872458	1.947871
63	8	0	1.799786	1.443811	1.611952
64	8	0	1.214729	-1.178371	1.999958
65	8	0	3.970186	0.965840	2.007572
66	6	0	4.323172	2.350326	1.782286
67	1	0	4.167448	2.586234	0.726424
68	1	0	3.718009	3.001114	2.417894
69	1	0	5.377991	2.420253	2.047454
70	6	0	3.474036	-1.880226	2.191650
71	6	0	4.769823	-1.805660	1.652059
72	6	0	5.697942	-2.809914	1.925157
73	6	0	5.354431	-3.888019	2.747027
74	6	0	3.130677	-2.977592	3.003809
75	6	0	4.067344	-3.969365	3.288537
76	1	0	5.035098	-0.989810	0.992117
77	1	0	6.690768	-2.753467	1.486963
78	1	0	6.085525	-4.663753	2.961401
79	1	0	3.795211	-4.803080	3.930761
80	1	0	2.127589	-3.031463	3.416051
81	8	0	1.518526	-0.312620	-1.951837
82	15	0	2.856171	-0.187554	-1.163232
83	8	0	3.963807	-1.196537	-1.934475
84	6	0	4.143967	-1.169356	-3.351753
85	1	0	4.690799	-2.076737	-3.628177
86	1	0	4.735458	-0.293847	-3.648914
87	1	0	3.179678	-1.150866	-3.874450
88	8	0	3.456752	1.345975	-1.562042
89	6	0	2.950323	2.106260	-2.665056
90	1	0	3.449302	1.818273	-3.599698
91	1	0	1.871303	1.964436	-2.777642
92	1	0	3.168825	3.158998	-2.457360

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ds-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.242608	2.582350	-0.205563
2	6	0	-1.196398	1.623509	-0.406401
3	7	0	-0.897529	0.460708	0.245727
4	16	0	-2.591597	1.804130	-1.361957
5	6	0	-0.065905	3.894135	-0.738684
6	6	0	-1.754304	-0.706182	0.461943
7	6	0	-2.001497	-1.497495	-0.840494
8	6	0	-2.876682	-2.764525	-0.696521
9	6	0	-2.315364	-3.884272	-1.596529
10	7	0	-0.676360	-1.945563	-1.449176
11	6	0	-0.908060	-2.267495	-2.903015
12	6	0	-2.035151	-3.330072	-3.027879
13	6	0	-0.078729	-3.146596	-0.756352
14	6	0	-0.989187	-4.371781	-0.986427
15	1	0	0.511596	2.306460	0.431756
16	6	0	-3.028124	-0.361130	1.283426

17	1	0	-1.138662	-1.348867	1.096063
18	1	0	-3.907434	-2.528853	-0.974493
19	1	0	-2.897563	-3.107817	0.346986
20	1	0	0.046778	-2.623994	-3.293360
21	1	0	-1.134179	-1.323971	-3.397888
22	6	0	-3.339011	-2.897935	-3.729956
23	1	0	-1.635424	-4.170248	-3.617527
24	1	0	0.920717	-3.262111	-1.177959
25	1	0	0.049970	-2.880625	0.292795
26	1	0	-1.175365	-4.884017	-0.035678
27	1	0	-3.029695	-4.711885	-1.657625
28	1	0	-0.506651	-5.097482	-1.652300
29	1	0	0.005609	0.371366	0.724362
30	6	0	-0.951006	4.508253	-1.621254
31	6	0	-0.686920	5.789729	-2.079159
32	6	0	0.445152	6.472729	-1.670535
33	6	0	1.327175	5.861500	-0.789296
34	6	0	1.078832	4.585584	-0.325269
35	1	0	-1.381668	6.257646	-2.765637
36	1	0	0.642042	7.472638	-2.032849
37	1	0	2.216865	6.384616	-0.461938
38	1	0	1.765487	4.105999	0.359185
39	1	0	-1.831464	3.963143	-1.928802
40	1	0	0.075296	-1.205415	-1.418657
41	6	0	-2.904201	-0.155658	2.709682
42	6	0	-4.069568	0.155772	3.432097
43	7	0	-5.336776	0.286418	2.843719
44	6	0	-5.380461	0.108042	1.543321
45	6	0	-4.252277	-0.215246	0.726270
46	6	0	-1.670791	-0.241883	3.430862
47	1	0	-4.410352	-0.323792	-0.336046
48	6	0	-3.654649	-1.722124	-4.207331
49	1	0	-4.608462	-1.556896	-4.689499
50	1	0	-3.008190	-0.857286	-4.158918
51	1	0	-4.044611	-3.716521	-3.820614
52	1	0	-2.425742	-0.815319	-1.576834
53	6	0	-3.996912	0.361494	4.845766
54	6	0	-2.813867	0.266986	5.496599
55	6	0	-1.630050	-0.038028	4.770004
56	1	0	-6.351980	0.214020	1.065568
57	1	0	-4.916611	0.596645	5.366194
58	1	0	-2.755175	0.424715	6.565988
59	1	0	-0.687968	-0.103525	5.299835
60	1	0	-0.754335	-0.461759	2.901364
61	6	0	2.809537	0.846817	1.626561
62	6	0	2.488558	-0.632757	1.348649
63	8	0	1.953597	1.716883	1.582050
64	8	0	1.263983	-0.926248	1.388148
65	8	0	4.082901	1.090722	1.957030
66	6	0	4.441331	2.474760	2.143869
67	1	0	4.306053	3.019599	1.206000
68	1	0	3.826171	2.924327	2.927171
69	1	0	5.491711	2.460701	2.435800
70	6	0	3.506664	-1.699942	1.704562
71	6	0	4.878768	-1.635180	1.410633
72	6	0	5.735809	-2.664624	1.800907
73	6	0	5.242503	-3.776045	2.493427
74	6	0	3.020721	-2.821566	2.395777
75	6	0	3.879705	-3.849996	2.790549
76	1	0	5.276044	-0.790983	0.859922
77	1	0	6.793837	-2.600083	1.558295
78	1	0	5.915125	-4.574620	2.797076

79	1	0	3.483943	-4.704905	3.334017
80	1	0	1.961603	-2.866538	2.628258
81	8	0	1.669530	-0.746912	-1.821513
82	15	0	2.915706	-0.266906	-1.065525
83	8	0	4.259098	-0.928059	-1.816537
84	6	0	4.247597	-2.294184	-2.233599
85	1	0	5.195890	-2.470115	-2.749061
86	1	0	3.416505	-2.485209	-2.921797
87	1	0	4.178881	-2.973736	-1.374359
88	8	0	3.242535	1.315014	-1.385654
89	6	0	3.212202	1.811261	-2.736985
90	1	0	4.035290	1.381704	-3.317809
91	1	0	2.255098	1.572607	-3.211246
92	1	0	3.331281	2.895376	-2.669892

ds-**IM4**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.539457	2.946336	-0.867832
2	6	0	-1.422025	1.902105	-0.747294
3	7	0	-0.808950	0.763635	-0.319304
4	16	0	-3.082027	1.970755	-1.104776
5	6	0	-0.684210	4.283647	-1.340797
6	6	0	-1.402752	-0.515407	0.084909
7	6	0	-1.998475	-1.226309	-1.141136
8	6	0	-2.742833	-2.555678	-0.910724
9	6	0	-2.410213	-3.527864	-2.063042
10	7	0	-0.841692	-1.529620	-2.110085
11	6	0	-1.418318	-1.703932	-3.488262
12	6	0	-2.522422	-2.800652	-3.441666
13	6	0	-0.055660	-2.763091	-1.723631
14	6	0	-0.958282	-4.004289	-1.879700
15	1	0	0.420420	2.724949	-0.590071
16	6	0	-2.250102	-0.384265	1.371117
17	1	0	-0.528672	-1.099458	0.366168
18	1	0	-3.817705	-2.359004	-0.864773
19	1	0	-2.457297	-3.007298	0.048552
20	1	0	-0.590553	-1.981771	-4.144914
21	1	0	-1.785815	-0.728544	-3.804826
22	6	0	-3.970757	-2.355949	-3.730248
23	1	0	-2.273598	-3.550112	-4.209369
24	1	0	0.819366	-2.779782	-2.375135
25	1	0	0.311168	-2.600959	-0.709689
26	1	0	-0.874663	-4.637778	-0.989754
27	1	0	-3.093539	-4.383084	-2.046893
28	1	0	-0.643824	-4.611590	-2.737338
29	1	0	0.198055	0.762025	-0.156114
30	6	0	-1.885371	4.833427	-1.782572
31	6	0	-1.918872	6.146737	-2.224344
32	6	0	-0.774352	6.925069	-2.232725
33	6	0	0.422775	6.378295	-1.790462
34	6	0	0.472733	5.071658	-1.348278
35	1	0	-2.858223	6.564251	-2.565363
36	1	0	-0.811050	7.949212	-2.578508
37	1	0	1.325359	6.976488	-1.790272
38	1	0	1.404339	4.644464	-1.001988
39	1	0	-2.770090	4.213449	-1.766290
40	1	0	-0.149022	-0.749241	-2.115219

41	6	0	-1.544152	-0.264002	2.630215
42	6	0	-2.330200	-0.115062	3.788728
43	7	0	-3.734686	-0.081689	3.782249
44	6	0	-4.306182	-0.190041	2.605408
45	6	0	-3.601324	-0.339234	1.371493
46	6	0	-0.111348	-0.282959	2.756988
47	1	0	-4.172376	-0.397415	0.456973
48	6	0	-4.421941	-1.151368	-3.965769
49	1	0	-5.471568	-0.981542	-4.163417
50	1	0	-3.803520	-0.264954	-3.978909
51	1	0	-4.659442	-3.193539	-3.735345
52	1	0	-2.635090	-0.525931	-1.681742
53	6	0	-1.699175	0.012819	5.064255
54	6	0	-0.349618	-0.005805	5.160389
55	6	0	0.442962	-0.156559	3.989684
56	1	0	-5.393260	-0.160511	2.582312
57	1	0	-2.334730	0.124892	5.932537
58	1	0	0.135324	0.091762	6.123862
59	1	0	1.520840	-0.170588	4.093252
60	1	0	0.572154	-0.410119	1.872412
61	6	0	2.692712	1.290251	0.750555
62	6	0	2.726970	-0.194524	0.316391
63	8	0	2.226560	2.185525	0.049111
64	8	0	1.473753	-0.695343	0.560377
65	8	0	3.091509	1.484802	2.004386
66	6	0	2.876239	2.797156	2.562875
67	1	0	3.399960	3.552099	1.970738
68	1	0	1.806735	3.022813	2.588045
69	1	0	3.283101	2.744586	3.572741
70	6	0	3.882653	-0.960927	0.968516
71	6	0	5.213549	-0.543678	0.830778
72	6	0	6.245914	-1.255063	1.443589
73	6	0	5.957726	-2.394718	2.203469
74	6	0	3.598757	-2.098462	1.726612
75	6	0	4.631518	-2.811420	2.344028
76	1	0	5.449299	0.338567	0.238823
77	1	0	7.274631	-0.920326	1.329624
78	1	0	6.761090	-2.948731	2.683898
79	1	0	4.398017	-3.692652	2.937954
80	1	0	2.562408	-2.402308	1.829998
81	8	0	1.568377	-0.049554	-2.335872
82	15	0	2.858609	-0.243857	-1.576980
83	8	0	3.518883	-1.706620	-1.808084
84	6	0	3.967005	-2.105308	-3.112151
85	1	0	4.283927	-3.146130	-3.018366
86	1	0	4.813646	-1.487457	-3.427332
87	1	0	3.157718	-2.026774	-3.847740
88	8	0	4.041248	0.739022	-2.119661
89	6	0	3.753006	1.977056	-2.802725
90	1	0	2.921801	1.844979	-3.500091
91	1	0	3.505158	2.752320	-2.073524
92	1	0	4.665398	2.240359	-3.342794

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ds-**TS3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.287042	2.849966	-0.005286
2	6	0	-1.256677	1.900626	0.257567

3	7	0	-0.736627	0.634773	0.250330
4	16	0	-2.880426	2.261946	0.511012
5	6	0	-0.352988	4.261458	0.172027
6	6	0	-1.471334	-0.619267	0.006734
7	6	0	-1.949127	-0.652149	-1.478839
8	6	0	-3.096380	-1.605801	-1.897625
9	6	0	-2.821454	-2.134120	-3.321656
10	7	0	-0.748523	-0.968744	-2.362341
11	6	0	-1.023484	-0.434657	-3.732776
12	6	0	-2.390437	-0.966198	-4.260452
13	6	0	-0.513750	-2.450485	-2.454471
14	6	0	-1.659268	-3.135162	-3.233185
15	1	0	0.463521	2.539221	-0.627904
16	6	0	-2.464142	-0.964730	1.150973
17	1	0	-0.686372	-1.378735	0.070563
18	1	0	-4.045215	-1.063356	-1.870817
19	1	0	-3.190718	-2.453775	-1.206550
20	1	0	-0.193163	-0.757225	-4.365001
21	1	0	-0.987747	0.653741	-3.665529
22	6	0	-3.532645	0.054685	-4.449187
23	1	0	-2.216193	-1.411485	-5.253863
24	1	0	0.453087	-2.581057	-2.941052
25	1	0	-0.427489	-2.831671	-1.433709
26	1	0	-1.978264	-4.048847	-2.716787
27	1	0	-3.718855	-2.618174	-3.722407
28	1	0	-1.326580	-3.430016	-4.236296
29	1	0	0.248705	0.557276	-0.013269
30	6	0	-1.085075	4.858622	1.199350
31	6	0	-1.067074	6.234436	1.349449
32	6	0	-0.317692	7.032155	0.498465
33	6	0	0.422462	6.439670	-0.512771
34	6	0	0.407009	5.066929	-0.679054
35	1	0	-1.642200	6.687105	2.147616
36	1	0	-0.307694	8.106245	0.624819
37	1	0	1.015564	7.051651	-1.180797
38	1	0	0.982997	4.601728	-1.467457
39	1	0	-1.668979	4.242062	1.866367
40	1	0	0.377605	-0.525087	-1.929827
41	6	0	-1.931987	-1.469971	2.398513
42	6	0	-2.841106	-1.812268	3.415390
43	7	0	-4.231744	-1.680363	3.291609
44	6	0	-4.652697	-1.191301	2.147422
45	6	0	-3.806643	-0.821210	1.056867
46	6	0	-0.536232	-1.632423	2.670683
47	1	0	-4.272591	-0.412134	0.174623
48	6	0	-3.503531	1.350479	-4.275184
49	1	0	-4.379183	1.957504	-4.458916
50	1	0	-2.629101	1.892492	-3.945593
51	1	0	-4.451357	-0.412915	-4.787392
52	1	0	-2.240539	0.367882	-1.737691
53	6	0	-2.357627	-2.322489	4.661668
54	6	0	-1.030357	-2.470558	4.879781
55	6	0	-0.104325	-2.112429	3.861753
56	1	0	-5.727361	-1.068279	2.032322
57	1	0	-3.090807	-2.578404	5.415942
58	1	0	-0.662101	-2.853751	5.822789
59	1	0	0.956155	-2.224078	4.049502
60	1	0	0.187278	-1.352982	1.919432
61	6	0	2.327368	1.455604	-2.685787
62	6	0	2.591387	0.145179	-1.899786
63	8	0	1.443491	2.237871	-2.397079
64	8	0	1.425156	-0.290385	-1.308341

65	8	0	3.174127	1.655536	-3.709468
66	6	0	2.997136	2.881126	-4.455633
67	1	0	1.994665	2.915384	-4.888041
68	1	0	3.145716	3.743543	-3.801394
69	1	0	3.755320	2.853456	-5.238316
70	6	0	3.684334	0.430248	-0.843661
71	6	0	4.881737	1.090629	-1.157231
72	6	0	5.836951	1.334639	-0.167752
73	6	0	5.612561	0.918403	1.147125
74	6	0	3.468693	0.010234	0.474097
75	6	0	4.425418	0.252931	1.462338
76	1	0	5.078716	1.410161	-2.174953
77	1	0	6.758002	1.850655	-0.428035
78	1	0	6.355406	1.110656	1.917281
79	1	0	4.239547	-0.078252	2.481124
80	1	0	2.549626	-0.511123	0.711800
81	8	0	2.161765	-1.502562	-4.181347
82	15	0	3.144609	-1.227193	-3.084079
83	8	0	3.368736	-2.410810	-2.012248
84	6	0	3.906995	-3.679504	-2.423590
85	1	0	3.911452	-4.308026	-1.531283
86	1	0	4.929018	-3.556256	-2.795270
87	1	0	3.278215	-4.135678	-3.195640
88	8	0	4.659314	-0.996994	-3.623979
89	6	0	4.943563	-0.654665	-4.992410
90	1	0	4.118944	-0.950988	-5.645636
91	1	0	5.112046	0.423155	-5.064833
92	1	0	5.855203	-1.191545	-5.266413

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ds-**IM5**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.291510	2.852734	0.016549
2	6	0	-1.299849	1.920880	0.203563
3	7	0	-0.809461	0.645553	0.204346
4	16	0	-2.924677	2.318989	0.368052
5	6	0	-0.337529	4.260316	0.225922
6	6	0	-1.552216	-0.608531	-0.024974
7	6	0	-2.033442	-0.676311	-1.506207
8	6	0	-3.156723	-1.685831	-1.870857
9	6	0	-2.866321	-2.268241	-3.270465
10	7	0	-0.838857	-0.942015	-2.386792
11	6	0	-1.174871	-0.478120	-3.757120
12	6	0	-2.503534	-1.127822	-4.269554
13	6	0	-0.523654	-2.398975	-2.448513
14	6	0	-1.653980	-3.202672	-3.144300
15	1	0	0.477692	2.542378	-0.581412
16	6	0	-2.552627	-0.908999	1.127036
17	1	0	-0.776067	-1.374690	0.056838
18	1	0	-4.127761	-1.181831	-1.864526
19	1	0	-3.217856	-2.507544	-1.143824
20	1	0	-0.335010	-0.748566	-4.403615
21	1	0	-1.230876	0.612375	-3.733363
22	6	0	-3.711658	-0.198977	-4.518057
23	1	0	-2.297338	-1.614103	-5.238165
24	1	0	0.422689	-2.498395	-2.984681
25	1	0	-0.355528	-2.753989	-1.426784
26	1	0	-1.917725	-4.092419	-2.557649

27	1	0	-3.741056	-2.817586	-3.637255
28	1	0	-1.333653	-3.552695	-4.134369
29	1	0	0.194409	0.559403	0.069221
30	6	0	-1.106617	4.846544	1.232666
31	6	0	-1.068437	6.217099	1.420579
32	6	0	-0.262335	7.020733	0.628769
33	6	0	0.514100	6.439020	-0.360989
34	6	0	0.478973	5.071592	-0.564961
35	1	0	-1.672840	6.661009	2.201879
36	1	0	-0.237079	8.090696	0.784411
37	1	0	1.151217	7.055296	-0.982963
38	1	0	1.083051	4.615610	-1.337379
39	1	0	-1.734880	4.225638	1.853795
40	1	0	0.802885	-0.383779	-1.837020
41	6	0	-2.040959	-1.402032	2.388026
42	6	0	-2.963090	-1.692869	3.409207
43	7	0	-4.348633	-1.521865	3.277480
44	6	0	-4.750727	-1.048582	2.119723
45	6	0	-3.890267	-0.729243	1.024457
46	6	0	-0.651967	-1.602915	2.669773
47	1	0	-4.339483	-0.329513	0.129031
48	6	0	-3.785283	1.099324	-4.378591
49	1	0	-4.698323	1.634095	-4.600190
50	1	0	-2.963014	1.712777	-4.041188
51	1	0	-4.585709	-0.740925	-4.864753
52	1	0	-2.377890	0.327093	-1.767541
53	6	0	-2.499249	-2.188399	4.668964
54	6	0	-1.178086	-2.372730	4.895875
55	6	0	-0.238430	-2.068418	3.872942
56	1	0	-5.821001	-0.896967	1.997509
57	1	0	-3.242355	-2.403843	5.426202
58	1	0	-0.824926	-2.745111	5.848869
59	1	0	0.817302	-2.210215	4.066756
60	1	0	0.082346	-1.367400	1.914008
61	6	0	2.463252	1.500642	-2.631065
62	6	0	2.773352	0.174760	-1.897873
63	8	0	1.580754	2.258356	-2.287106
64	8	0	1.613560	-0.269906	-1.242870
65	8	0	3.276431	1.732960	-3.670810
66	6	0	3.054066	2.970196	-4.388811
67	1	0	2.036621	2.992655	-4.784751
68	1	0	3.211624	3.822057	-3.723278
69	1	0	3.785431	2.967728	-5.196696
70	6	0	3.872440	0.421030	-0.851233
71	6	0	5.053772	1.105255	-1.173004
72	6	0	6.034516	1.318689	-0.202329
73	6	0	5.851338	0.848638	1.100376
74	6	0	3.695826	-0.053614	0.454760
75	6	0	4.679529	0.160364	1.422773
76	1	0	5.217894	1.466645	-2.182348
77	1	0	6.942779	1.853693	-0.468087
78	1	0	6.614124	1.017330	1.856179
79	1	0	4.525205	-0.211946	2.432349
80	1	0	2.790832	-0.592330	0.706557
81	8	0	2.248593	-1.396697	-4.196960
82	15	0	3.265799	-1.177840	-3.125044
83	8	0	3.502691	-2.376458	-2.080111
84	6	0	3.935117	-3.673469	-2.534055
85	1	0	3.982206	-4.301729	-1.643279
86	1	0	4.926885	-3.603957	-2.991736
87	1	0	3.216733	-4.090369	-3.246824
88	8	0	4.764650	-0.921118	-3.680042

89	6	0	5.026797	-0.539418	-5.045010
90	1	0	4.179942	-0.792485	-5.687467
91	1	0	5.220999	0.535485	-5.081914
92	1	0	5.917676	-1.089506	-5.357033

ms-IM3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.627156	0.573423	-3.155134
2	6	0	0.975927	-1.875170	-2.298309
3	6	0	0.758936	-0.343605	-2.362191
4	8	0	-0.298175	0.061139	-1.877509
5	8	0	2.106921	-2.312135	-2.860187
6	6	0	2.365026	-3.727086	-2.745481
7	1	0	2.438131	-4.000184	-1.689606
8	1	0	1.566272	-4.298515	-3.224717
9	1	0	3.315896	-3.886064	-3.254007
10	8	0	0.116701	-2.612619	-1.850023
11	6	0	1.007607	1.735471	-3.655198
12	6	0	1.726455	2.648900	-4.423978
13	6	0	3.080910	2.424631	-4.689602
14	6	0	2.991226	0.357625	-3.424822
15	6	0	3.708877	1.281930	-4.182822
16	1	0	-0.040055	1.907792	-3.431598
17	1	0	1.232070	3.537375	-4.808050
18	1	0	3.645853	3.138728	-5.283739
19	1	0	4.765349	1.111851	-4.373530
20	1	0	3.492528	-0.511500	-3.020524
21	8	0	1.974011	0.697058	1.158529
22	15	0	2.452094	-0.513415	0.302520
23	8	0	2.180932	-1.907429	1.207904
24	6	0	2.721393	-2.027656	2.531489
25	1	0	2.281462	-2.926810	2.974910
26	1	0	3.810645	-2.133064	2.493389
27	1	0	2.466219	-1.152864	3.141937
28	8	0	4.142562	-0.528387	0.446236
29	6	0	4.863035	0.700648	0.416941
30	1	0	5.910883	0.459148	0.621523
31	1	0	4.491816	1.395451	1.178581
32	1	0	4.798628	1.181488	-0.570240
33	7	0	0.541573	2.985788	0.132528
34	6	0	-0.715028	2.591074	0.505858
35	7	0	-0.665061	1.437877	1.246510
36	16	0	-2.174142	3.360828	0.113210
37	6	0	1.005915	4.076731	-0.651469
38	6	0	-1.728529	0.845576	2.047718
39	6	0	-2.767167	0.108308	1.169704
40	6	0	-3.802908	-0.737049	1.955333
41	6	0	-3.782001	-2.197688	1.467044
42	7	0	-2.056054	-0.832802	0.202053
43	6	0	-3.057364	-1.368668	-0.792016
44	6	0	-4.095588	-2.260261	-0.056050
45	6	0	-1.349254	-1.987108	0.880840
46	6	0	-2.377788	-2.776938	1.718043
47	1	0	1.285425	2.334688	0.439822
48	6	0	-2.346829	1.826963	3.086081
49	1	0	-1.217212	0.072441	2.634907
50	1	0	-4.803423	-0.309768	1.832494

51	1	0	-3.576072	-0.708694	3.028637
52	1	0	-2.480801	-1.911406	-1.541982
53	1	0	-3.501272	-0.493204	-1.265672
54	6	0	-5.577863	-1.950498	-0.350267
55	1	0	-3.927640	-3.304185	-0.367842
56	1	0	-0.906122	-2.570864	0.075334
57	1	0	-0.522110	-1.584134	1.464131
58	1	0	-2.137929	-2.714337	2.785923
59	1	0	-4.527261	-2.780215	2.018504
60	1	0	-2.345290	-3.837635	1.444585
61	1	0	0.282976	1.035416	1.364822
62	1	0	-1.350683	-0.311691	-0.352640
63	6	0	0.178825	5.050935	-1.208344
64	6	0	0.731213	6.082411	-1.950734
65	6	0	2.098432	6.164335	-2.149332
66	6	0	2.924432	5.196373	-1.593607
67	6	0	2.389496	4.162384	-0.852398
68	1	0	3.033106	3.409419	-0.417714
69	1	0	3.996159	5.249015	-1.738975
70	1	0	2.520351	6.974032	-2.728942
71	1	0	0.077957	6.833395	-2.377664
72	1	0	-0.886038	4.974868	-1.042199
73	6	0	-3.607208	2.310185	2.995711
74	6	0	-4.112367	3.194765	3.998728
75	7	0	-3.436707	3.599510	5.049391
76	6	0	-2.123006	3.116397	5.148980
77	6	0	-1.539430	2.248033	4.209408
78	6	0	-1.364953	3.553158	6.280413
79	6	0	-0.086336	3.143750	6.453385
80	6	0	0.512457	2.272704	5.501891
81	6	0	-0.184558	1.840196	4.423062
82	1	0	-4.259998	2.057414	2.174310
83	1	0	-5.130698	3.563480	3.897542
84	1	0	0.300114	1.192360	3.707023
85	1	0	1.539003	1.958635	5.644136
86	1	0	0.490858	3.475081	7.307282
87	1	0	-1.850143	4.219504	6.982106
88	1	0	-3.246894	0.844302	0.524054
89	6	0	-6.064671	-1.202090	-1.305794
90	1	0	-6.253612	-2.466881	0.322389
91	1	0	-7.132279	-1.081331	-1.428793
92	1	0	-5.454401	-0.670835	-2.022315

ms-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.818905	0.360732	-2.932087
2	6	0	1.138559	-2.048359	-2.052321
3	6	0	1.023245	-0.511255	-1.987276
4	8	0	-0.061618	-0.070966	-1.540019
5	8	0	2.264346	-2.511530	-2.613379
6	6	0	2.418444	-3.943222	-2.643762
7	1	0	2.426406	-4.338972	-1.624848
8	1	0	1.604771	-4.401929	-3.211567
9	1	0	3.377083	-4.117250	-3.133194
10	8	0	0.242049	-2.777782	-1.663348
11	6	0	1.144411	1.476973	-3.455428
12	6	0	1.771706	2.328834	-4.366869

13	6	0	3.089476	2.085215	-4.760982
14	6	0	3.147739	0.127611	-3.328020
15	6	0	3.773717	0.984389	-4.233611
16	1	0	0.125545	1.664636	-3.134353
17	1	0	1.230043	3.184309	-4.763169
18	1	0	3.582211	2.748057	-5.468206
19	1	0	4.803730	0.793151	-4.525112
20	1	0	3.698158	-0.708207	-2.915327
21	8	0	2.015466	0.755402	0.955727
22	15	0	2.520491	-0.424218	0.101631
23	8	0	2.354133	-1.843340	0.954690
24	6	0	2.953596	-1.986252	2.253527
25	1	0	2.609914	-2.944208	2.653930
26	1	0	4.045272	-1.991106	2.171602
27	1	0	2.641832	-1.173107	2.919296
28	8	0	4.193722	-0.356672	0.083336
29	6	0	4.872163	0.904306	0.091492
30	1	0	5.929763	0.685649	0.264536
31	1	0	4.491404	1.548197	0.890621
32	1	0	4.764676	1.414558	-0.873789
33	7	0	0.420545	3.056510	0.031482
34	6	0	-0.796473	2.611352	0.474809
35	7	0	-0.660166	1.483426	1.237898
36	16	0	-2.303334	3.312466	0.136047
37	6	0	0.799155	4.163727	-0.777547
38	6	0	-1.675698	0.809816	2.037589
39	6	0	-2.693175	0.029222	1.170331
40	6	0	-3.716657	-0.813180	1.970998
41	6	0	-3.916489	-2.182821	1.291421
42	7	0	-1.970810	-0.932733	0.233617
43	6	0	-2.920988	-1.368747	-0.857414
44	6	0	-4.198543	-1.985557	-0.228655
45	6	0	-1.433506	-2.151067	0.949997
46	6	0	-2.622032	-3.000740	1.451095
47	1	0	1.203708	2.438226	0.287550
48	6	0	-2.314266	1.735779	3.114191
49	1	0	-1.109404	0.052962	2.592899
50	1	0	-4.666920	-0.276054	2.032054
51	1	0	-3.369800	-0.962938	3.002812
52	1	0	-2.364297	-2.082073	-1.466883
53	1	0	-3.110393	-0.486563	-1.467451
54	6	0	-5.530706	-1.244414	-0.464232
55	1	0	-4.327215	-2.991101	-0.658952
56	1	0	-0.796594	-2.666498	0.232039
57	1	0	-0.796702	-1.797574	1.761544
58	1	0	-2.472595	-3.271381	2.502612
59	1	0	-4.755908	-2.710737	1.755906
60	1	0	-2.689848	-3.937710	0.885616
61	1	0	0.293661	1.095387	1.287864
62	1	0	-1.171151	-0.476126	-0.272516
63	6	0	-0.094060	5.105853	-1.284513
64	6	0	0.376823	6.157150	-2.054821
65	6	0	1.726699	6.290061	-2.330096
66	6	0	2.618343	5.353808	-1.823982
67	6	0	2.164782	4.300832	-1.055578
68	1	0	2.859691	3.572287	-0.660243
69	1	0	3.677363	5.445933	-2.030045
70	1	0	2.084624	7.114519	-2.931563
71	1	0	-0.327173	6.882761	-2.443223
72	1	0	-1.144421	4.988661	-1.060252
73	6	0	-3.574377	2.220241	3.026295
74	6	0	-4.098473	3.055617	4.061413

75	7	0	-3.440541	3.413499	5.140101
76	6	0	-2.125210	2.934384	5.234936
77	6	0	-1.523644	2.113461	4.264588
78	6	0	-1.384227	3.326074	6.394027
79	6	0	-0.103541	2.921886	6.563358
80	6	0	0.514836	2.102059	5.579472
81	6	0	-0.166385	1.711986	4.474832
82	1	0	-4.210863	2.006145	2.181418
83	1	0	-5.116924	3.424569	3.962165
84	1	0	0.332545	1.103923	3.734420
85	1	0	1.543522	1.793672	5.718483
86	1	0	0.460780	3.219592	7.437930
87	1	0	-1.883940	3.955506	7.119302
88	1	0	-3.190377	0.738876	0.508717
89	6	0	-5.731708	-0.110238	-1.083283
90	1	0	-6.375532	-1.782443	-0.048516
91	1	0	-6.728225	0.297166	-1.185852
92	1	0	-4.944615	0.484120	-1.525369

ms-IM4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.963574	0.184519	-2.624004
2	6	0	1.374771	-2.089455	-1.620229
3	6	0	1.420425	-0.550831	-1.363302
4	8	0	0.237796	-0.061675	-0.958038
5	8	0	2.584535	-2.636075	-1.838156
6	6	0	2.613942	-4.053919	-2.084447
7	1	0	2.209243	-4.594904	-1.224738
8	1	0	2.030299	-4.296968	-2.976332
9	1	0	3.666095	-4.299007	-2.232811
10	8	0	0.346688	-2.737705	-1.622782
11	6	0	1.170190	1.215019	-3.144002
12	6	0	1.575327	1.922788	-4.279351
13	6	0	2.784822	1.615560	-4.907349
14	6	0	3.180383	-0.118215	-3.256699
15	6	0	3.585455	0.592648	-4.389883
16	1	0	0.238700	1.445726	-2.640025
17	1	0	0.943876	2.718089	-4.668797
18	1	0	3.101543	2.166077	-5.790050
19	1	0	4.529418	0.342859	-4.869350
20	1	0	3.812078	-0.909095	-2.869192
21	8	0	2.274555	1.092510	0.805455
22	15	0	2.591651	-0.210352	0.114506
23	8	0	2.328462	-1.515762	1.049873
24	6	0	3.004013	-1.641479	2.315359
25	1	0	2.592239	-2.531823	2.795131
26	1	0	4.079354	-1.770062	2.157514
27	1	0	2.821106	-0.761866	2.941151
28	8	0	4.182623	-0.345722	-0.202269
29	6	0	5.022952	0.820020	-0.339186
30	1	0	6.049911	0.461038	-0.242514
31	1	0	4.799755	1.548618	0.444109
32	1	0	4.878624	1.271905	-1.324870
33	7	0	0.362503	3.237262	0.002518
34	6	0	-0.816711	2.773060	0.525282
35	7	0	-0.613604	1.666739	1.300818
36	16	0	-2.350825	3.446437	0.260014

37	6	0	0.678143	4.368840	-0.800020
38	6	0	-1.598782	0.867207	2.028791
39	6	0	-2.569023	0.090272	1.097158
40	6	0	-3.709096	-0.673845	1.819926
41	6	0	-3.954867	-2.027589	1.123117
42	7	0	-1.820441	-0.932240	0.253438
43	6	0	-2.689584	-1.311566	-0.915674
44	6	0	-4.070178	-1.820962	-0.417326
45	6	0	-1.463923	-2.170494	1.028506
46	6	0	-2.749426	-2.940100	1.406113
47	1	0	1.170866	2.633947	0.195005
48	6	0	-2.270013	1.685473	3.172065
49	1	0	-0.991434	0.103088	2.524936
50	1	0	-4.620649	-0.070896	1.808734
51	1	0	-3.456730	-0.847233	2.875433
52	1	0	-2.135756	-2.073116	-1.466847
53	1	0	-2.750313	-0.429177	-1.551491
54	6	0	-5.312008	-0.980439	-0.780733
55	1	0	-4.238484	-2.817273	-0.857088
56	1	0	-0.793437	-2.745367	0.389396
57	1	0	-0.894997	-1.856893	1.906219
58	1	0	-2.726089	-3.221708	2.465596
59	1	0	-4.874530	-2.483468	1.505440
60	1	0	-2.828195	-3.868914	0.828146
61	1	0	0.325685	1.270747	1.248204
62	1	0	-0.867727	-0.554997	-0.206703
63	6	0	-0.249724	5.325947	-1.206740
64	6	0	0.162561	6.400506	-1.978447
65	6	0	1.487310	6.541983	-2.354063
66	6	0	2.413245	5.590448	-1.948543
67	6	0	2.018072	4.514538	-1.179615
68	1	0	2.739603	3.774056	-0.861976
69	1	0	3.453037	5.688658	-2.234270
70	1	0	1.799111	7.384282	-2.956458
71	1	0	-0.567912	7.137468	-2.288786
72	1	0	-1.280381	5.199336	-0.908271
73	6	0	-3.512154	2.213376	3.073763
74	6	0	-4.072661	2.949064	4.163786
75	7	0	-3.466311	3.172958	5.307242
76	6	0	-2.168065	2.652960	5.415023
77	6	0	-1.533014	1.923861	4.393768
78	6	0	-1.481056	2.903713	6.644667
79	6	0	-0.217931	2.456384	6.834431
80	6	0	0.436488	1.732607	5.800089
81	6	0	-0.194255	1.476173	4.628681
82	1	0	-4.102713	2.108163	2.176642
83	1	0	-5.076247	3.353850	4.052859
84	1	0	0.331460	0.939507	3.853076
85	1	0	1.451768	1.390186	5.956242
86	1	0	0.305237	2.647656	7.762557
87	1	0	-2.007318	3.464421	7.406745
88	1	0	-2.981949	0.801626	0.381132
89	6	0	-5.365974	0.146226	-1.442382
90	1	0	-6.231712	-1.433645	-0.426826
91	1	0	-6.312604	0.630407	-1.639473
92	1	0	-4.497316	0.659522	-1.829356

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ms-**TS3**

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	1.973493	0.247032	-2.651522
2	6	0	1.373675	-2.042498	-1.704685
3	6	0	1.432385	-0.515519	-1.408679
4	8	0	0.237479	-0.014051	-1.013011
5	8	0	2.584497	-2.592473	-1.902036
6	6	0	2.608284	-4.003255	-2.190813
7	1	0	2.171839	-4.565527	-1.361006
8	1	0	2.050287	-4.212171	-3.107274
9	1	0	3.662255	-4.253846	-2.313986
10	8	0	0.339968	-2.677479	-1.752403
11	6	0	1.193192	1.300714	-3.145026
12	6	0	1.606044	2.027132	-4.265655
13	6	0	2.808095	1.715707	-4.905325
14	6	0	3.183162	-0.060227	-3.295703
15	6	0	3.594649	0.669349	-4.414361
16	1	0	0.265968	1.536620	-2.636689
17	1	0	0.984877	2.840017	-4.634385
18	1	0	3.129519	2.280583	-5.777074
19	1	0	4.532311	0.414952	-4.903419
20	1	0	3.803800	-0.869380	-2.929125
21	8	0	2.305678	1.095696	0.772928
22	15	0	2.596274	-0.206427	0.073017
23	8	0	2.303091	-1.516524	0.987294
24	6	0	2.965142	-1.674829	2.257383
25	1	0	2.534139	-2.566423	2.716936
26	1	0	4.039496	-1.818271	2.106442
27	1	0	2.789673	-0.803171	2.895944
28	8	0	4.177135	-0.371025	-0.260443
29	6	0	5.044887	0.777858	-0.381804
30	1	0	6.062611	0.393419	-0.287636
31	1	0	4.836471	1.501596	0.409750
32	1	0	4.911399	1.243424	-1.362339
33	7	0	0.406595	3.275936	-0.020266
34	6	0	-0.772275	2.797109	0.496501
35	7	0	-0.559386	1.699593	1.279658
36	16	0	-2.310661	3.448839	0.210958
37	6	0	0.715393	4.414428	-0.815086
38	6	0	-1.536726	0.880395	1.998940
39	6	0	-2.484322	0.078613	1.064825
40	6	0	-3.615428	-0.688995	1.802338
41	6	0	-3.843093	-2.055158	1.126601
42	7	0	-1.720823	-0.932209	0.226812
43	6	0	-2.599844	-1.333985	-0.923224
44	6	0	-3.968729	-1.869583	-0.414815
45	6	0	-1.351243	-2.154499	1.011491
46	6	0	-2.620508	-2.942134	1.414639
47	1	0	1.219591	2.682139	0.175661
48	6	0	-2.229083	1.695164	3.132863
49	1	0	-0.918505	0.130296	2.502840
50	1	0	-4.536114	-0.099831	1.784567
51	1	0	-3.359407	-0.844201	2.860074
52	1	0	-2.044258	-2.088817	-1.481397
53	1	0	-2.688712	-0.457944	-1.565344
54	6	0	-5.232149	-1.062812	-0.781719
55	1	0	-4.117990	-2.874598	-0.842490
56	1	0	-0.681609	-2.738161	0.378922
57	1	0	-0.776603	-1.829423	1.881982
58	1	0	-2.584930	-3.206055	2.478768
59	1	0	-4.752979	-2.521433	1.520417
60	1	0	-2.688804	-3.881825	0.852530

61	1	0	0.389302	1.326272	1.250599
62	1	0	-0.693580	-0.523973	-0.315333
63	6	0	-0.221611	5.360140	-1.228023
64	6	0	0.183262	6.442600	-1.992339
65	6	0	1.509560	6.603512	-2.355014
66	6	0	2.444397	5.663569	-1.943469
67	6	0	2.056638	4.579916	-1.181529
68	1	0	2.785629	3.848871	-0.859220
69	1	0	3.485472	5.776927	-2.218767
70	1	0	1.815435	7.451852	-2.951911
71	1	0	-0.554315	7.170402	-2.307536
72	1	0	-1.253217	5.217586	-0.939820
73	6	0	-3.475098	2.210733	3.017712
74	6	0	-4.055000	2.948119	4.096262
75	7	0	-3.464070	3.186188	5.245016
76	6	0	-2.162471	2.679002	5.370841
77	6	0	-1.509207	1.948779	4.361935
78	6	0	-1.491779	2.944991	6.606375
79	6	0	-0.226912	2.510932	6.814064
80	6	0	0.445730	1.785470	5.792749
81	6	0	-0.169293	1.515045	4.616209
82	1	0	-4.054266	2.093401	2.114698
83	1	0	-5.061121	3.342447	3.971225
84	1	0	0.369597	0.976355	3.851193
85	1	0	1.461958	1.452970	5.963289
86	1	0	0.283712	2.713769	7.746677
87	1	0	-2.031914	3.506257	7.358271
88	1	0	-2.911411	0.779490	0.346895
89	6	0	-5.316203	0.056838	-1.452129
90	1	0	-6.140186	-1.534511	-0.421380
91	1	0	-6.274742	0.516371	-1.650256
92	1	0	-4.461142	0.587618	-1.845291

ms-IM5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.179562	0.291975	-2.746580
2	6	0	1.386939	-1.988868	-1.890632
3	6	0	1.527478	-0.476222	-1.575960
4	8	0	0.286511	0.096092	-1.330315
5	8	0	2.572557	-2.600854	-2.033566
6	6	0	2.527824	-4.013372	-2.323002
7	1	0	2.021133	-4.546007	-1.514280
8	1	0	2.001308	-4.188907	-3.264356
9	1	0	3.570157	-4.323464	-2.397669
10	8	0	0.318569	-2.550038	-1.984961
11	6	0	1.500883	1.399761	-3.275018
12	6	0	2.046803	2.120869	-4.340674
13	6	0	3.275432	1.750164	-4.890735
14	6	0	3.416133	-0.076305	-3.301317
15	6	0	3.956638	0.648268	-4.366054
16	1	0	0.547174	1.687034	-2.850341
17	1	0	1.504379	2.975309	-4.737568
18	1	0	3.697324	2.311046	-5.720936
19	1	0	4.912210	0.345113	-4.787227
20	1	0	3.956224	-0.929091	-2.908614
21	8	0	2.250122	1.064788	0.705757
22	15	0	2.553213	-0.228393	0.005511

23	8	0	2.148932	-1.554868	0.833420
24	6	0	2.693031	-1.796935	2.148298
25	1	0	2.186928	-2.687119	2.524845
26	1	0	3.769333	-1.980342	2.079189
27	1	0	2.496540	-0.946779	2.808491
28	8	0	4.133338	-0.438900	-0.255804
29	6	0	5.056483	0.676505	-0.284692
30	1	0	6.042393	0.249441	-0.092168
31	1	0	4.798908	1.406304	0.485940
32	1	0	5.036392	1.144843	-1.272203
33	7	0	0.330931	3.278514	-0.021647
34	6	0	-0.844376	2.786275	0.502330
35	7	0	-0.620594	1.680194	1.268994
36	16	0	-2.383672	3.435881	0.235782
37	6	0	0.627226	4.432719	-0.797692
38	6	0	-1.580175	0.867828	2.029228
39	6	0	-2.534461	0.039853	1.127482
40	6	0	-3.630295	-0.739849	1.911564
41	6	0	-3.845424	-2.111525	1.240698
42	7	0	-1.769826	-0.925510	0.268177
43	6	0	-2.673335	-1.341763	-0.838572
44	6	0	-4.017093	-1.931383	-0.297810
45	6	0	-1.361988	-2.138024	1.024489
46	6	0	-2.591717	-2.965028	1.491962
47	1	0	1.150106	2.693025	0.163616
48	6	0	-2.249474	1.705203	3.160344
49	1	0	-0.944425	0.131696	2.532544
50	1	0	-4.566043	-0.173041	1.925185
51	1	0	-3.337415	-0.891987	2.961193
52	1	0	-2.133396	-2.082781	-1.432796
53	1	0	-2.828306	-0.471185	-1.478353
54	6	0	-5.321275	-1.174219	-0.628451
55	1	0	-4.144590	-2.942443	-0.720565
56	1	0	-0.711555	-2.723951	0.369839
57	1	0	-0.751426	-1.822037	1.876120
58	1	0	-2.511341	-3.216540	2.557877
59	1	0	-4.732164	-2.600925	1.660026
60	1	0	-2.658790	-3.913287	0.942520
61	1	0	0.340103	1.345742	1.281207
62	1	0	-0.323340	-0.388852	-0.692960
63	6	0	-0.322540	5.369268	-1.203264
64	6	0	0.068822	6.467250	-1.951865
65	6	0	1.394150	6.653180	-2.307171
66	6	0	2.341315	5.722651	-1.903479
67	6	0	1.966991	4.623591	-1.156729
68	1	0	2.706426	3.900612	-0.840298
69	1	0	3.381733	5.855483	-2.172530
70	1	0	1.689298	7.513643	-2.891945
71	1	0	-0.678635	7.187586	-2.261029
72	1	0	-1.352682	5.206344	-0.919863
73	6	0	-3.506471	2.198465	3.066161
74	6	0	-4.068033	2.959184	4.138085
75	7	0	-3.450087	3.241869	5.262520
76	6	0	-2.138742	2.755875	5.367602
77	6	0	-1.503016	2.004321	4.363329
78	6	0	-1.438748	3.066937	6.576259
79	6	0	-0.163700	2.654091	6.763500
80	6	0	0.490366	1.904782	5.747442
81	6	0	-0.152203	1.592779	4.596325
82	1	0	-4.108842	2.043329	2.184223
83	1	0	-5.083266	3.334751	4.029488
84	1	0	0.370738	1.033655	3.835025

85	1	0	1.513857	1.587247	5.901966
86	1	0	0.368463	2.890705	7.675833
87	1	0	-1.965810	3.644065	7.325431
88	1	0	-3.008454	0.735558	0.433787
89	6	0	-5.468671	-0.052987	-1.285390
90	1	0	-6.202353	-1.683502	-0.251419
91	1	0	-6.449339	0.368967	-1.456134
92	1	0	-4.645219	0.515240	-1.692458

dr-**IM3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.334282	-1.899683	-5.641756
2	6	0	2.479306	0.677505	-3.535398
3	6	0	3.983402	0.717154	-3.185141
4	6	0	4.397114	-0.663732	-2.600102
5	6	0	3.850316	-1.738395	-3.575538
6	6	0	2.280024	-0.189009	-4.799803
7	6	0	4.666932	-0.280360	-5.373380
8	6	0	4.806877	0.964846	-4.466132
9	7	0	3.503202	-1.098682	-4.895060
10	1	0	5.544590	-0.931443	-5.331347
11	1	0	4.485120	-0.035059	-6.422778
12	1	0	5.862066	1.136577	-4.224605
13	1	0	4.445057	1.863682	-4.979845
14	1	0	5.500501	-0.702661	-2.611918
15	1	0	2.943695	-2.205590	-3.201912
16	1	0	2.362444	0.431974	-5.697363
17	1	0	2.094914	1.686162	-3.712030
18	1	0	4.176048	1.508695	-2.454016
19	1	0	1.905934	0.274911	-2.696904
20	7	0	-0.474633	-2.735354	-2.068935
21	6	0	-0.226282	-1.595356	-2.794539
22	7	0	0.608790	-1.857489	-3.854459
23	16	0	-0.829948	-0.058183	-2.456465
24	6	0	-1.198357	-2.970891	-0.862724
25	6	0	0.965190	-1.003221	-4.995534
26	1	0	-0.046691	-3.581937	-2.449634
27	6	0	-1.211899	-4.286110	-0.385102
28	6	0	-1.888514	-4.600058	0.776583
29	6	0	-2.562480	-3.614226	1.484136
30	6	0	-2.549979	-2.312712	1.012213
31	6	0	-1.875999	-1.982277	-0.152802
32	1	0	-1.890192	-5.622429	1.133375
33	1	0	-3.092245	-3.861882	2.393984
34	1	0	-3.073663	-1.536071	1.556009
35	1	0	-1.859466	-0.971777	-0.534818
36	1	0	-0.687294	-5.055478	-0.935193
37	6	0	-0.228548	1.166784	-5.658885
38	6	0	-0.221936	-0.184492	-5.584414
39	6	0	-1.334995	1.853204	-6.247705
40	7	0	-2.396492	1.269718	-6.754163
41	6	0	-2.396183	-0.132476	-6.703218
42	1	0	0.577101	1.766482	-5.266628
43	1	0	4.572487	-2.530695	-3.786796
44	1	0	0.818387	-2.842369	-4.003498
45	1	0	1.228936	-1.726956	-5.778190
46	6	0	3.965544	-0.841485	-1.131241

47	6	0	3.475723	-1.922590	-0.581595
48	1	0	3.230260	-1.947517	0.471371
49	1	0	3.291223	-2.839183	-1.125000
50	1	0	4.140480	0.040007	-0.524516
51	6	0	-1.351799	-0.892825	-6.147646
52	6	0	-1.467150	-2.318116	-6.190404
53	6	0	-3.533613	-0.790626	-7.267875
54	6	0	-3.612724	-2.141790	-7.282731
55	6	0	-2.553503	-2.916790	-6.736270
56	1	0	-1.309492	2.940226	-6.280982
57	1	0	-0.674290	-2.929988	-5.787363
58	1	0	-2.620654	-3.997061	-6.762672
59	1	0	-4.471668	-2.642317	-7.711242
60	1	0	-4.317807	-0.169153	-7.680970
61	8	0	4.124022	-4.981468	-7.814854
62	8	0	3.147660	-2.856583	-6.722645
63	15	0	3.060544	-4.422120	-6.610787
64	6	0	5.481176	-4.567811	-7.747872
65	1	0	5.575295	-3.485860	-7.907357
66	1	0	6.020512	-5.095956	-8.540479
67	1	0	5.940219	-4.827646	-6.780452
68	8	0	1.663558	-4.875388	-7.420212
69	6	0	1.385287	-4.380445	-8.738930
70	1	0	1.507665	-3.292532	-8.780474
71	1	0	2.050789	-4.849532	-9.470936
72	1	0	0.346160	-4.640417	-8.962913
73	6	0	1.433928	-5.800829	-4.024730
74	6	0	2.771150	-5.742694	-3.235765
75	8	0	0.629999	-4.883707	-3.976787
76	8	0	2.865308	-4.815527	-2.444936
77	8	0	1.211437	-6.955730	-4.636990
78	6	0	-0.001526	-7.046059	-5.428703
79	1	0	-0.871036	-6.835984	-4.801819
80	1	0	0.068568	-6.331815	-6.251950
81	1	0	-0.021008	-8.072329	-5.794503
82	6	0	3.820729	-6.792317	-3.348349
83	6	0	4.038060	-7.569526	-4.499900
84	6	0	5.069226	-8.508821	-4.522627
85	6	0	5.881545	-8.694741	-3.399962
86	6	0	4.655056	-6.973078	-2.228443
87	6	0	5.671355	-7.925183	-2.250133
88	1	0	3.426431	-7.419432	-5.380047
89	1	0	5.240058	-9.093634	-5.422427
90	1	0	6.678035	-9.434506	-3.421384
91	1	0	6.299467	-8.067087	-1.374576
92	1	0	4.486475	-6.363428	-1.346041

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dr-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.531925	-1.947356	-5.344216
2	6	0	2.602629	0.751348	-3.519217
3	6	0	4.106732	0.883954	-3.187243
4	6	0	4.578633	-0.417193	-2.480086
5	6	0	4.045816	-1.594718	-3.329029
6	6	0	2.438023	-0.205932	-4.718112
7	6	0	4.833259	-0.303202	-5.269931
8	6	0	4.916242	1.033650	-4.493379

9	7	0	3.685606	-1.101809	-4.714043
10	1	0	5.729908	-0.916966	-5.148519
11	1	0	4.656054	-0.173719	-6.340352
12	1	0	5.963574	1.272244	-4.276740
13	1	0	4.517347	1.858258	-5.095964
14	1	0	5.682301	-0.422166	-2.510358
15	1	0	3.145943	-2.035640	-2.917285
16	1	0	2.533690	0.347918	-5.657895
17	1	0	2.175675	1.727436	-3.763907
18	1	0	4.274025	1.750401	-2.539953
19	1	0	2.043934	0.380875	-2.654914
20	7	0	-0.502340	-2.880574	-2.185199
21	6	0	-0.122383	-1.688322	-2.752934
22	7	0	0.823257	-1.892846	-3.723877
23	16	0	-0.714977	-0.160349	-2.347791
24	6	0	-1.229866	-3.183437	-0.999261
25	6	0	1.146054	-1.057894	-4.881540
26	1	0	-0.223702	-3.708239	-2.722097
27	6	0	-1.471179	-4.536106	-0.733779
28	6	0	-2.153621	-4.912675	0.405790
29	6	0	-2.606004	-3.954506	1.302359
30	6	0	-2.367273	-2.615919	1.041132
31	6	0	-1.685523	-2.222199	-0.099058
32	1	0	-2.333916	-5.963187	0.596886
33	1	0	-3.140982	-4.251465	2.194130
34	1	0	-2.717840	-1.859907	1.732952
35	1	0	-1.506830	-1.180039	-0.319509
36	1	0	-1.118101	-5.282967	-1.431939
37	6	0	-0.092755	1.064045	-5.614330
38	6	0	-0.065372	-0.281971	-5.479093
39	6	0	-1.217595	1.708729	-6.216124
40	7	0	-2.276964	1.089176	-6.681019
41	6	0	-2.256032	-0.309672	-6.567611
42	1	0	0.710470	1.693118	-5.267484
43	1	0	4.771554	-2.398843	-3.464273
44	1	0	1.231604	-2.834704	-3.761430
45	1	0	1.421108	-1.787688	-5.655852
46	6	0	4.182221	-0.460834	-0.991644
47	6	0	3.644923	-1.462537	-0.344712
48	1	0	3.427522	-1.390980	0.712270
49	1	0	3.389747	-2.404988	-0.808559
50	1	0	4.424549	0.453778	-0.461937
51	6	0	-1.193673	-1.030496	-5.993283
52	6	0	-1.289972	-2.457139	-5.968797
53	6	0	-3.391261	-1.006841	-7.086665
54	6	0	-3.452048	-2.358416	-7.039119
55	6	0	-2.376085	-3.093481	-6.471555
56	1	0	-1.207230	2.793387	-6.297964
57	1	0	-0.487689	-3.041492	-5.543815
58	1	0	-2.429179	-4.174396	-6.443650
59	1	0	-4.310078	-2.888720	-7.432315
60	1	0	-4.189139	-0.414816	-7.516279
61	8	0	3.866556	-5.355668	-7.613825
62	8	0	3.373232	-3.086281	-6.466711
63	15	0	2.868796	-4.543540	-6.546180
64	6	0	5.283503	-5.164714	-7.563457
65	1	0	5.535000	-4.099895	-7.613218
66	1	0	5.696812	-5.681440	-8.434089
67	1	0	5.709663	-5.602418	-6.652091
68	8	0	1.478981	-4.618222	-7.433345
69	6	0	1.403912	-4.046186	-8.751196
70	1	0	1.736604	-3.002520	-8.740381

71	1	0	2.018751	-4.622045	-9.450131
72	1	0	0.354072	-4.094590	-9.050668
73	6	0	1.043648	-5.794750	-4.528391
74	6	0	2.471816	-5.307286	-4.198926
75	8	0	0.062664	-5.136162	-4.223692
76	8	0	2.516590	-4.229008	-3.558100
77	8	0	0.970807	-6.987047	-5.128430
78	6	0	-0.346559	-7.428833	-5.514183
79	1	0	-0.998173	-7.491572	-4.639123
80	1	0	-0.768983	-6.732322	-6.242463
81	1	0	-0.198851	-8.412978	-5.959491
82	6	0	3.587827	-6.317254	-4.014491
83	6	0	3.829817	-7.416431	-4.855629
84	6	0	4.872130	-8.301696	-4.578437
85	6	0	5.689899	-8.109440	-3.459481
86	6	0	4.417084	-6.129338	-2.896482
87	6	0	5.457465	-7.018734	-2.618296
88	1	0	3.218519	-7.570128	-5.736267
89	1	0	5.049106	-9.143454	-5.243673
90	1	0	6.499323	-8.803796	-3.247333
91	1	0	6.082136	-6.860959	-1.742187
92	1	0	4.224238	-5.282169	-2.246416

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dr-IM4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.362057	-2.450080	-4.499233
2	6	0	2.695493	0.787944	-3.731684
3	6	0	4.141577	0.818978	-3.180181
4	6	0	4.273567	-0.261451	-2.074413
5	6	0	3.652124	-1.545452	-2.665414
6	6	0	2.542703	-0.441832	-4.659612
7	6	0	4.934805	-1.016075	-4.699888
8	6	0	5.137609	0.468785	-4.309020
9	7	0	3.595767	-1.451630	-4.178075
10	1	0	5.678816	-1.674742	-4.242994
11	1	0	4.939125	-1.202397	-5.774793
12	1	0	6.169315	0.629306	-3.975846
13	1	0	4.976712	1.123217	-5.174432
14	1	0	5.351814	-0.427516	-1.904963
15	1	0	2.630383	-1.701372	-2.333572
16	1	0	2.882202	-0.169060	-5.664690
17	1	0	2.511965	1.702123	-4.301403
18	1	0	4.365028	1.810899	-2.774560
19	1	0	1.961638	0.760639	-2.920207
20	7	0	-0.432482	-3.006363	-2.160204
21	6	0	-0.101159	-1.821211	-2.781838
22	7	0	0.778105	-2.045844	-3.794574
23	16	0	-0.674524	-0.282794	-2.376719
24	6	0	-1.132625	-3.291365	-0.954424
25	6	0	1.185070	-1.181998	-4.898024
26	1	0	-0.118658	-3.841366	-2.663522
27	6	0	-1.272279	-4.640165	-0.607871
28	6	0	-1.928641	-4.996969	0.553114
29	6	0	-2.455339	-4.023048	1.390338
30	6	0	-2.317662	-2.688581	1.048075
31	6	0	-1.663518	-2.314279	-0.114584
32	1	0	-2.029736	-6.044514	0.808084

33	1	0	-2.969235	-4.305086	2.299161
34	1	0	-2.727131	-1.920909	1.693118
35	1	0	-1.557779	-1.277537	-0.400277
36	1	0	-0.860612	-5.398854	-1.259944
37	6	0	0.079439	0.977433	-5.739980
38	6	0	0.027245	-0.358508	-5.535890
39	6	0	-1.008313	1.660872	-6.367826
40	7	0	-2.107839	1.088030	-6.796122
41	6	0	-2.167244	-0.303983	-6.621885
42	1	0	0.921604	1.572480	-5.433516
43	1	0	4.222393	-2.447598	-2.438657
44	1	0	1.240250	-2.972304	-3.863525
45	1	0	1.461369	-1.913852	-5.670557
46	6	0	3.680179	0.187460	-0.725398
47	6	0	2.904681	-0.506333	0.066991
48	1	0	2.561836	-0.099889	1.008697
49	1	0	2.562632	-1.506684	-0.158028
50	1	0	3.996691	1.182411	-0.432793
51	6	0	-1.145096	-1.061474	-6.022638
52	6	0	-1.321242	-2.479307	-5.953187
53	6	0	-3.344408	-0.952796	-7.109018
54	6	0	-3.482804	-2.296006	-7.013125
55	6	0	-2.444725	-3.070424	-6.428859
56	1	0	-0.931306	2.737817	-6.500877
57	1	0	-0.544632	-3.089939	-5.518490
58	1	0	-2.557793	-4.145264	-6.366724
59	1	0	-4.372822	-2.789676	-7.382098
60	1	0	-4.109655	-0.331182	-7.555829
61	8	0	3.464553	-5.563765	-7.829974
62	8	0	3.879070	-3.198163	-6.831968
63	15	0	2.989489	-4.406053	-6.785431
64	6	0	4.829989	-5.639290	-8.288692
65	1	0	5.240297	-4.637987	-8.440917
66	1	0	4.802202	-6.186835	-9.233658
67	1	0	5.436833	-6.185706	-7.560362
68	8	0	1.462658	-4.138269	-7.269673
69	6	0	1.200528	-3.599898	-8.579064
70	1	0	1.742347	-2.659722	-8.724867
71	1	0	1.490661	-4.322711	-9.348089
72	1	0	0.125061	-3.419528	-8.624119
73	6	0	1.299952	-5.714278	-4.905505
74	6	0	2.700593	-5.026688	-4.999920
75	8	0	0.421517	-5.329154	-4.157075
76	8	0	2.699129	-3.902435	-4.251930
77	8	0	1.158698	-6.772771	-5.717119
78	6	0	-0.113387	-7.448068	-5.678442
79	1	0	-0.297523	-7.852261	-4.679531
80	1	0	-0.915234	-6.755109	-5.945664
81	1	0	-0.035168	-8.251107	-6.411895
82	6	0	3.802736	-6.044322	-4.590566
83	6	0	4.043718	-7.256595	-5.257669
84	6	0	5.050091	-8.121099	-4.818599
85	6	0	5.829370	-7.794201	-3.704612
86	6	0	4.586678	-5.727549	-3.474658
87	6	0	5.590039	-6.593855	-3.031837
88	1	0	3.444429	-7.528714	-6.118780
89	1	0	5.221506	-9.055591	-5.348262
90	1	0	6.609681	-8.470158	-3.363195
91	1	0	6.182262	-6.331034	-2.158041
92	1	0	4.380753	-4.797756	-2.956680

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dr-**TS3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.319376	-2.870587	-4.439105
2	6	0	2.751833	0.659237	-3.724612
3	6	0	4.190763	0.687241	-3.156468
4	6	0	4.297562	-0.376199	-2.034345
5	6	0	3.673936	-1.665260	-2.624002
6	6	0	2.602050	-0.598848	-4.619225
7	6	0	4.962181	-1.187540	-4.635098
8	6	0	5.193587	0.303465	-4.266929
9	7	0	3.625035	-1.615584	-4.128234
10	1	0	5.705628	-1.841911	-4.167467
11	1	0	4.987143	-1.377559	-5.709665
12	1	0	6.224276	0.455776	-3.924154
13	1	0	5.051676	0.947658	-5.144187
14	1	0	5.372465	-0.547709	-1.845968
15	1	0	2.652659	-1.808427	-2.280954
16	1	0	2.940410	-0.345391	-5.630558
17	1	0	2.587125	1.563715	-4.316535
18	1	0	4.419363	1.684327	-2.764873
19	1	0	2.010701	0.663695	-2.918977
20	7	0	-0.501443	-3.009742	-2.096005
21	6	0	-0.135583	-1.850687	-2.753397
22	7	0	0.765554	-2.122338	-3.735215
23	16	0	-0.700219	-0.296274	-2.418589
24	6	0	-1.242932	-3.242479	-0.903033
25	6	0	1.225031	-1.302414	-4.858749
26	1	0	-0.184778	-3.866711	-2.553254
27	6	0	-1.415733	-4.575743	-0.515094
28	6	0	-2.113997	-4.881963	0.636013
29	6	0	-2.650399	-3.871509	1.421811
30	6	0	-2.479473	-2.551883	1.038586
31	6	0	-1.783013	-2.228334	-0.114603
32	1	0	-2.240234	-5.918361	0.923295
33	1	0	-3.197185	-4.113624	2.322930
34	1	0	-2.895690	-1.755843	1.643725
35	1	0	-1.650226	-1.203915	-0.431856
36	1	0	-0.996411	-5.363669	-1.126224
37	6	0	0.176811	0.853041	-5.780090
38	6	0	0.094150	-0.475646	-5.541178
39	6	0	-0.882948	1.540596	-6.450115
40	7	0	-1.984665	0.978925	-6.888123
41	6	0	-2.075621	-0.406306	-6.678198
42	1	0	1.024636	1.438306	-5.470334
43	1	0	4.242681	-2.558942	-2.354098
44	1	0	1.169332	-3.063585	-3.774330
45	1	0	1.488919	-2.064998	-5.603234
46	6	0	3.691463	0.097293	-0.698501
47	6	0	2.933710	-0.593959	0.113191
48	1	0	2.579497	-0.173338	1.044135
49	1	0	2.618788	-1.607999	-0.087167
50	1	0	3.980703	1.107723	-0.430145
51	6	0	-1.082356	-1.166849	-6.036237
52	6	0	-1.290173	-2.578597	-5.934343
53	6	0	-3.254845	-1.044837	-7.174599
54	6	0	-3.423277	-2.381867	-7.047063
55	6	0	-2.414250	-3.160593	-6.419417
56	1	0	-0.781197	2.611905	-6.609941

57	1	0	-0.536050	-3.192639	-5.466691
58	1	0	-2.550690	-4.230928	-6.331745
59	1	0	-4.314805	-2.867400	-7.422904
60	1	0	-3.997247	-0.420230	-7.654679
61	8	0	3.529790	-5.613083	-7.889772
62	8	0	3.976317	-3.223071	-6.961600
63	15	0	3.089783	-4.423443	-6.877562
64	6	0	4.868358	-5.684154	-8.429787
65	1	0	5.290320	-4.683011	-8.543546
66	1	0	4.778169	-6.173219	-9.402247
67	1	0	5.497133	-6.284076	-7.765865
68	8	0	1.543859	-4.182701	-7.290705
69	6	0	1.213857	-3.638123	-8.584986
70	1	0	1.734570	-2.689102	-8.745455
71	1	0	1.479361	-4.352285	-9.370600
72	1	0	0.135233	-3.474767	-8.577345
73	6	0	1.500323	-5.773508	-4.952528
74	6	0	2.875023	-5.050153	-5.096817
75	8	0	0.628762	-5.400271	-4.193233
76	8	0	2.810011	-3.937958	-4.292381
77	8	0	1.382965	-6.846864	-5.744834
78	6	0	0.134371	-7.564469	-5.672385
79	1	0	-0.016436	-7.958583	-4.664121
80	1	0	-0.694362	-6.902465	-5.935342
81	1	0	0.227641	-8.375294	-6.395073
82	6	0	4.030399	-6.007321	-4.704638
83	6	0	4.282116	-7.227003	-5.354954
84	6	0	5.334290	-8.047979	-4.941983
85	6	0	6.151746	-7.669718	-3.872882
86	6	0	4.851787	-5.639842	-3.631570
87	6	0	5.903132	-6.462272	-3.217615
88	1	0	3.654950	-7.539572	-6.181116
89	1	0	5.511309	-8.989213	-5.457285
90	1	0	6.968521	-8.311602	-3.552239
91	1	0	6.524651	-6.157807	-2.378838
92	1	0	4.645049	-4.710133	-3.115531

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dr-IM5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.491299	-0.351065	1.148083
2	6	0	-1.962636	-0.242341	3.466669
3	6	0	-1.270048	-1.159790	4.502985
4	6	0	-0.754376	-2.422790	3.767477
5	6	0	0.000656	-1.891055	2.514684
6	6	0	-0.856093	0.436081	2.615637
7	6	0	1.006614	-0.254952	3.970021
8	6	0	-0.046190	-0.433466	5.104201
9	7	0	0.366858	-0.449091	2.646128
10	1	0	1.813086	-0.992702	4.055686
11	1	0	1.474336	0.734333	3.987686
12	1	0	0.374254	-1.013660	5.935645
13	1	0	-0.349185	0.538401	5.516215
14	1	0	-0.032660	-2.921771	4.439574
15	1	0	-0.611382	-1.992558	1.620665
16	1	0	-0.542002	1.352856	3.130932
17	1	0	-2.565029	0.506278	3.990029
18	1	0	-1.977347	-1.435819	5.293023

19	1	0	-2.652146	-0.814854	2.837838
20	7	0	-2.098297	-1.460165	-1.476477
21	6	0	-2.412626	-0.701466	-0.363509
22	7	0	-1.289902	-0.152425	0.177108
23	16	0	-3.958051	-0.456362	0.263109
24	6	0	-2.861374	-2.371351	-2.260062
25	6	0	-1.134170	0.926783	1.159952
26	1	0	-1.144165	-1.333374	-1.817782
27	6	0	-2.217266	-2.958575	-3.354688
28	6	0	-2.886259	-3.863389	-4.154888
29	6	0	-4.204024	-4.202084	-3.881923
30	6	0	-4.842086	-3.621983	-2.798324
31	6	0	-4.185023	-2.711487	-1.986857
32	1	0	-2.374680	-4.308982	-4.998873
33	1	0	-4.726413	-4.910613	-4.510135
34	1	0	-5.870957	-3.878232	-2.577205
35	1	0	-4.673866	-2.242312	-1.145127
36	1	0	-1.189535	-2.696513	-3.567044
37	6	0	-2.902964	2.588787	1.987337
38	6	0	-2.148790	2.096515	0.977681
39	6	0	-3.780636	3.696169	1.769314
40	7	0	-3.929292	4.324845	0.627063
41	6	0	-3.130642	3.850390	-0.425373
42	1	0	-2.879129	2.164678	2.976271
43	1	0	0.925781	-2.452550	2.344409
44	1	0	-0.392575	-0.445727	-0.208054
45	1	0	-0.163830	1.359619	0.878379
46	6	0	-1.868405	-3.451693	3.487550
47	6	0	-2.038130	-4.151806	2.395648
48	1	0	-2.839930	-4.871643	2.308063
49	1	0	-1.400980	-4.059023	1.528154
50	1	0	-2.538985	-3.603370	4.327023
51	6	0	-2.235670	2.772882	-0.303416
52	6	0	-1.451502	2.429704	-1.449602
53	6	0	-3.252227	4.539967	-1.672378
54	6	0	-2.503162	4.177267	-2.739848
55	6	0	-1.580574	3.103637	-2.618524
56	1	0	-4.379412	4.051024	2.605550
57	1	0	-0.740673	1.620936	-1.380326
58	1	0	-0.976822	2.826789	-3.473313
59	1	0	-2.593262	4.698534	-3.684237
60	1	0	-3.959076	5.358210	-1.724342
61	8	0	4.516445	1.993137	-0.518967
62	8	0	3.048408	1.544366	1.588518
63	15	0	3.104956	1.506772	0.099298
64	6	0	5.712012	2.068169	0.294454
65	1	0	5.454364	2.259981	1.338203
66	1	0	6.303444	2.891074	-0.112094
67	1	0	6.265125	1.129077	0.209687
68	8	0	2.034704	2.418575	-0.689377
69	6	0	1.929574	3.830607	-0.401395
70	1	0	1.771338	3.989007	0.669211
71	1	0	2.835069	4.347978	-0.732898
72	1	0	1.066712	4.187589	-0.964774
73	6	0	2.096905	-0.109165	-2.020531
74	6	0	2.641027	-0.197725	-0.569612
75	8	0	0.984368	-0.471649	-2.341003
76	8	0	1.543935	-0.636362	0.186057
77	8	0	2.992861	0.400029	-2.872043
78	6	0	2.571894	0.521080	-4.247732
79	1	0	2.338541	-0.464576	-4.657780
80	1	0	1.692068	1.165438	-4.313381

81	1	0	3.420089	0.966945	-4.766881
82	6	0	3.830793	-1.179820	-0.483527
83	6	0	5.013127	-1.006503	-1.222177
84	6	0	6.055347	-1.930190	-1.116129
85	6	0	5.936834	-3.039505	-0.274081
86	6	0	3.718365	-2.295974	0.355216
87	6	0	4.762629	-3.218709	0.459123
88	1	0	5.119740	-0.154735	-1.883278
89	1	0	6.961636	-1.781561	-1.698310
90	1	0	6.749169	-3.757414	-0.194845
91	1	0	4.652583	-4.079357	1.114047
92	1	0	2.803127	-2.446352	0.914616

mr-IM3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.831459	-0.616877	-2.375173
2	6	0	1.075255	-2.142721	-2.238268
3	8	0	0.086492	-2.791289	-1.914842
4	8	0	2.036646	0.911657	1.343650
5	15	0	2.486789	-0.419977	0.657320
6	8	0	1.944679	-1.672545	1.652650
7	6	0	2.347747	-1.739849	3.026929
8	1	0	1.728746	-2.506992	3.504790
9	1	0	3.402701	-2.021682	3.104508
10	1	0	2.196574	-0.778229	3.532574
11	8	0	4.130269	-0.578869	1.072159
12	6	0	4.986911	0.534548	0.859525
13	1	0	5.988210	0.238592	1.188528
14	1	0	4.655936	1.407151	1.435387
15	1	0	5.037930	0.811801	-0.206359
16	7	0	0.633957	3.074599	0.155151
17	6	0	-0.638444	2.673093	0.471559
18	7	0	-0.610397	1.540129	1.242018
19	16	0	-2.084851	3.407273	-0.023177
20	6	0	1.125285	4.149787	-0.631198
21	6	0	-1.689470	0.974976	2.043242
22	6	0	-2.726382	0.222849	1.177765
23	6	0	-3.737132	-0.633618	1.976435
24	6	0	-3.886870	-2.017930	1.315473
25	7	0	-2.017927	-0.710352	0.202912
26	6	0	-2.991569	-1.149354	-0.865167
27	6	0	-4.207243	-1.852813	-0.202051
28	6	0	-1.415211	-1.929970	0.866803
29	6	0	-2.557517	-2.780714	1.465829
30	1	0	1.369011	2.444553	0.534424
31	6	0	-2.315304	1.986232	3.048074
32	1	0	-1.188250	0.212230	2.651820
33	1	0	-4.703390	-0.122568	2.016104
34	1	0	-3.399344	-0.757309	3.014144
35	1	0	-2.431133	-1.812277	-1.525645
36	1	0	-3.253812	-0.254414	-1.427801
37	6	0	-5.592644	-1.210363	-0.418934
38	1	0	-4.271100	-2.868496	-0.621869
39	1	0	-0.858215	-2.449343	0.087530
40	1	0	-0.687743	-1.586863	1.601813
41	1	0	-2.360193	-2.985005	2.524219
42	1	0	-4.694570	-2.575862	1.800524

43	1	0	-2.615173	-3.750398	0.957987
44	1	0	0.343750	1.174295	1.434012
45	1	0	-1.254055	-0.205027	-0.278393
46	6	0	0.318092	5.100237	-1.255359
47	6	0	0.896929	6.113777	-2.001994
48	6	0	2.271490	6.201375	-2.140095
49	6	0	3.077734	5.257869	-1.517546
50	6	0	2.516435	4.241678	-0.771030
51	1	0	3.144478	3.508614	-0.282415
52	1	0	4.154685	5.315787	-1.614618
53	1	0	2.713901	6.996684	-2.724280
54	1	0	0.258934	6.845965	-2.481503
55	1	0	-0.752914	5.019106	-1.137429
56	6	0	-3.563863	2.489784	2.915491
57	6	0	-4.078493	3.403413	3.887379
58	7	0	-3.422924	3.817301	4.946945
59	6	0	-2.120257	3.314828	5.089131
60	6	0	-1.528007	2.418564	4.181655
61	6	0	-1.383402	3.762470	6.230056
62	6	0	-0.115638	3.337702	6.441996
63	6	0	0.492858	2.440194	5.521927
64	6	0	-0.184564	1.996255	4.435150
65	1	0	-4.200880	2.232092	2.083400
66	1	0	-5.087336	3.787226	3.752781
67	1	0	0.308978	1.329036	3.743229
68	1	0	1.511310	2.114950	5.694121
69	1	0	0.445711	3.677239	7.303215
70	1	0	-1.875164	4.449682	6.906562
71	1	0	-3.226831	0.947717	0.535904
72	6	0	-5.880387	-0.073707	-0.997952
73	1	0	-6.393140	-1.824870	-0.022036
74	1	0	-6.905269	0.259535	-1.087802
75	1	0	-5.141670	0.594271	-1.417815
76	6	0	2.363865	-2.793965	-2.584647
77	6	0	3.598386	-2.122513	-2.623153
78	6	0	2.323910	-4.174194	-2.861798
79	6	0	4.763966	-2.820006	-2.937031
80	1	0	3.650369	-1.069750	-2.379137
81	6	0	3.488355	-4.863934	-3.187373
82	1	0	1.368668	-4.687802	-2.821377
83	6	0	4.712784	-4.187138	-3.224114
84	1	0	5.715963	-2.296441	-2.946605
85	1	0	3.444676	-5.927041	-3.408826
86	1	0	5.624747	-4.725467	-3.470036
87	6	0	1.422769	1.386620	-3.479173
88	1	0	1.513491	1.946273	-2.546341
89	1	0	2.190906	1.680770	-4.193787
90	1	0	0.423569	1.528656	-3.897061
91	8	0	-0.122806	-0.064798	-1.857034
92	8	0	1.658620	-0.020703	-3.231602

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mr-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.012644	-0.395512	-1.933477
2	6	0	1.418975	-1.622981	-1.090729
3	8	0	0.508741	-2.019298	-0.325359
4	8	0	2.212932	1.162471	1.007011

5	15	0	2.836195	-0.148584	0.475302
6	8	0	2.909605	-1.252995	1.699163
7	6	0	3.558541	-0.927027	2.938156
8	1	0	3.318823	-1.733564	3.636747
9	1	0	4.642570	-0.870608	2.796183
10	1	0	3.190375	0.026873	3.332511
11	8	0	4.484968	0.092397	0.307383
12	6	0	4.967469	1.235935	-0.395002
13	1	0	6.057901	1.155397	-0.412756
14	1	0	4.678352	2.160166	0.118079
15	1	0	4.595973	1.259335	-1.428354
16	7	0	0.498445	3.173621	0.005993
17	6	0	-0.720837	2.668994	0.377767
18	7	0	-0.582161	1.507480	1.089636
19	16	0	-2.229423	3.352608	-0.001739
20	6	0	0.869999	4.327421	-0.738113
21	6	0	-1.598347	0.793227	1.866080
22	6	0	-2.674982	0.149965	0.952496
23	6	0	-3.952334	-0.387700	1.636609
24	6	0	-4.433315	-1.659082	0.906165
25	7	0	-2.079007	-1.028393	0.175001
26	6	0	-2.923563	-1.259429	-1.054720
27	6	0	-4.409384	-1.436317	-0.637413
28	6	0	-2.023315	-2.296401	0.998178
29	6	0	-3.459056	-2.799714	1.246993
30	1	0	1.299857	2.594949	0.315647
31	6	0	-2.131276	1.638182	3.060457
32	1	0	-1.043128	-0.042031	2.301794
33	1	0	-4.723358	0.385875	1.608877
34	1	0	-3.768882	-0.618884	2.694622
35	1	0	-2.520714	-2.152619	-1.536997
36	1	0	-2.741610	-0.415720	-1.716900
37	6	0	-5.401567	-0.337642	-1.070120
38	1	0	-4.769587	-2.371871	-1.093682
39	1	0	-1.394986	-2.992908	0.445591
40	1	0	-1.495527	-2.054364	1.921853
41	1	0	-3.571061	-3.099959	2.294949
42	1	0	-5.448594	-1.915636	1.225409
43	1	0	-3.672983	-3.684152	0.634868
44	1	0	0.391272	1.202128	1.233049
45	1	0	-1.107284	-0.840111	-0.157623
46	6	0	-0.030601	5.234389	-1.294620
47	6	0	0.440126	6.326849	-2.005660
48	6	0	1.797594	6.535878	-2.175313
49	6	0	2.697117	5.635102	-1.620829
50	6	0	2.243596	4.542633	-0.910030
51	1	0	2.943821	3.842692	-0.475018
52	1	0	3.762276	5.786738	-1.743185
53	1	0	2.155175	7.391574	-2.731671
54	1	0	-0.270568	7.023981	-2.432154
55	1	0	-1.086987	5.060039	-1.151865
56	6	0	-3.255559	2.387619	2.981805
57	6	0	-3.694296	3.150299	4.108212
58	7	0	-3.078966	3.193291	5.267589
59	6	0	-1.896893	2.442832	5.355424
60	6	0	-1.382408	1.670118	4.298150
61	6	0	-1.200166	2.497994	6.603403
62	6	0	-0.039484	1.823769	6.776962
63	6	0	0.496531	1.055897	5.707003
64	6	0	-0.147429	0.980733	4.516993
65	1	0	-3.833300	2.442455	2.071795
66	1	0	-4.605805	3.736286	4.013511

67	1	0	0.296308	0.405103	3.718050
68	1	0	1.433639	0.532059	5.848936
69	1	0	0.492190	1.867042	7.718955
70	1	0	-1.633288	3.099903	7.392123
71	1	0	-2.941528	0.882338	0.191780
72	6	0	-5.155849	0.767032	-1.725380
73	1	0	-6.419231	-0.570516	-0.777240
74	1	0	-5.954480	1.452091	-1.975849
75	1	0	-4.171189	1.070697	-2.052502
76	6	0	2.488029	-2.592062	-1.523461
77	6	0	3.217718	-2.501345	-2.720301
78	6	0	2.698930	-3.703663	-0.687797
79	6	0	4.131680	-3.499911	-3.068593
80	1	0	3.079962	-1.655238	-3.381158
81	6	0	3.618575	-4.690949	-1.032365
82	1	0	2.137637	-3.767508	0.237724
83	6	0	4.339395	-4.595155	-2.228107
84	1	0	4.683862	-3.415993	-4.001606
85	1	0	3.776194	-5.536495	-0.367075
86	1	0	5.056233	-5.366259	-2.499844
87	6	0	1.549212	1.299449	-3.489899
88	1	0	1.203100	2.090991	-2.821675
89	1	0	2.443640	1.608116	-4.031689
90	1	0	0.748975	1.031474	-4.184618
91	8	0	-0.125936	0.038984	-1.872367
92	8	0	1.952573	0.142280	-2.724158

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mr-IM4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.232053	-0.210566	-1.823659
2	6	0	1.689909	-0.973930	-0.547260
3	8	0	0.666895	-1.074377	0.334724
4	8	0	2.455007	1.399980	0.828063
5	15	0	2.975448	0.050715	0.395705
6	8	0	3.308779	-0.959741	1.607054
7	6	0	4.226445	-0.566597	2.640725
8	1	0	4.236957	-1.386077	3.361900
9	1	0	5.230757	-0.425977	2.227508
10	1	0	3.887355	0.353573	3.127912
11	8	0	4.428772	0.156887	-0.333617
12	6	0	4.931563	1.387616	-0.878294
13	1	0	5.995114	1.220639	-1.063908
14	1	0	4.798919	2.207979	-0.167862
15	1	0	4.422944	1.623017	-1.817258
16	7	0	0.431719	3.291824	0.071483
17	6	0	-0.754216	2.762902	0.519075
18	7	0	-0.561726	1.588661	1.187614
19	16	0	-2.290332	3.441557	0.268121
20	6	0	0.736025	4.457771	-0.685296
21	6	0	-1.549248	0.762462	1.893055
22	6	0	-2.559540	0.118102	0.899298
23	6	0	-3.910549	-0.397832	1.446694
24	6	0	-4.321786	-1.671329	0.676022
25	7	0	-1.891310	-1.063694	0.199335
26	6	0	-2.594187	-1.297733	-1.107082
27	6	0	-4.120921	-1.464933	-0.856057
28	6	0	-1.946486	-2.320032	1.029025

29	6	0	-3.402826	-2.817647	1.132025
30	1	0	1.263677	2.739766	0.323835
31	6	0	-2.116584	1.486476	3.147586
32	1	0	-0.944895	-0.067582	2.264163
33	1	0	-4.665545	0.383241	1.326622
34	1	0	-3.850605	-0.623128	2.519880
35	1	0	-2.150426	-2.194829	-1.544983
36	1	0	-2.338113	-0.464965	-1.756809
37	6	0	-5.052830	-0.364769	-1.406347
38	1	0	-4.437411	-2.402433	-1.341531
39	1	0	-1.275214	-3.033544	0.548336
40	1	0	-1.513861	-2.082297	2.002357
41	1	0	-3.629347	-3.105062	2.165358
42	1	0	-5.369316	-1.914611	0.882718
43	1	0	-3.559134	-3.706713	0.508759
44	1	0	0.381676	1.198926	1.172390
45	1	0	-0.809388	-0.906700	0.042164
46	6	0	-0.214028	5.355445	-1.169288
47	6	0	0.191215	6.459585	-1.902181
48	6	0	1.530817	6.689280	-2.164026
49	6	0	2.479043	5.797382	-1.681525
50	6	0	2.090930	4.693052	-0.950409
51	1	0	2.828510	3.998797	-0.571669
52	1	0	3.530777	5.965460	-1.876767
53	1	0	1.836930	7.554251	-2.736499
54	1	0	-0.556916	7.149786	-2.272281
55	1	0	-1.255272	5.164340	-0.953657
56	6	0	-3.276785	2.182962	3.136792
57	6	0	-3.742118	2.831756	4.322679
58	7	0	-3.118980	2.815756	5.478486
59	6	0	-1.902073	2.117750	5.500257
60	6	0	-1.361810	1.455440	4.382959
61	6	0	-1.198266	2.107805	6.745531
62	6	0	-0.007294	1.475516	6.861446
63	6	0	0.552827	0.816973	5.732893
64	6	0	-0.096043	0.806558	4.543265
65	1	0	-3.864758	2.281154	2.237353
66	1	0	-4.682159	3.377418	4.279031
67	1	0	0.362460	0.309735	3.700852
68	1	0	1.511302	0.322922	5.831182
69	1	0	0.528792	1.468854	7.801820
70	1	0	-1.652145	2.625777	7.580826
71	1	0	-2.750464	0.845776	0.111097
72	6	0	-4.733587	0.695105	-2.102715
73	1	0	-6.094709	-0.552977	-1.171325
74	1	0	-5.492313	1.386544	-2.442795
75	1	0	-3.720954	0.950073	-2.380491
76	6	0	2.299317	-2.332028	-0.984045
77	6	0	3.214789	-2.465985	-2.038170
78	6	0	1.910747	-3.474858	-0.276531
79	6	0	3.716553	-3.723348	-2.385259
80	1	0	3.546131	-1.590334	-2.587602
81	6	0	2.414819	-4.731494	-0.620081
82	1	0	1.219487	-3.349173	0.549768
83	6	0	3.317640	-4.861819	-1.679283
84	1	0	4.422489	-3.811207	-3.207915
85	1	0	2.105690	-5.609687	-0.057283
86	1	0	3.709884	-5.839286	-1.949672
87	6	0	1.822764	1.212436	-3.623931
88	1	0	1.040580	1.937045	-3.385527
89	1	0	2.727709	1.716990	-3.964176
90	1	0	1.460282	0.515360	-4.383585

91	8	0	0.091795	-0.245128	-2.236482
92	8	0	2.210279	0.492142	-2.432392

mr-**TS3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.194595	-0.120905	-1.757371
2	6	0	1.695789	-0.979021	-0.566823
3	8	0	0.696694	-1.174381	0.351047
4	8	0	2.480715	1.306280	0.937718
5	15	0	2.982798	-0.023657	0.434668
6	8	0	3.308292	-1.108093	1.577405
7	6	0	4.238798	-0.795133	2.628869
8	1	0	4.254790	-1.667561	3.284431
9	1	0	5.238299	-0.624317	2.215959
10	1	0	3.905393	0.085144	3.187832
11	8	0	4.421599	0.096826	-0.309973
12	6	0	4.934832	1.342126	-0.814460
13	1	0	5.995312	1.169728	-1.010672
14	1	0	4.813834	2.137490	-0.074447
15	1	0	4.422684	1.613247	-1.741124
16	7	0	0.530221	3.271513	0.056534
17	6	0	-0.671684	2.734796	0.462459
18	7	0	-0.489725	1.595693	1.188863
19	16	0	-2.200617	3.368233	0.093007
20	6	0	0.857028	4.444177	-0.679959
21	6	0	-1.487465	0.777463	1.894384
22	6	0	-2.457571	0.059613	0.906207
23	6	0	-3.835887	-0.388591	1.455294
24	6	0	-4.230990	-1.732471	0.809466
25	7	0	-1.777154	-1.166610	0.322640
26	6	0	-2.467274	-1.514545	-0.959117
27	6	0	-3.999263	-1.679677	-0.730046
28	6	0	-1.859124	-2.340570	1.253011
29	6	0	-3.320593	-2.824167	1.396016
30	1	0	1.353433	2.734981	0.357764
31	6	0	-2.099084	1.552190	3.098667
32	1	0	-0.879310	-0.021760	2.320345
33	1	0	-4.581011	0.379657	1.230983
34	1	0	-3.815929	-0.504170	2.547168
35	1	0	-2.014775	-2.443190	-1.318967
36	1	0	-2.213827	-0.739946	-1.677928
37	6	0	-4.932481	-0.651734	-1.404225
38	1	0	-4.297630	-2.664237	-1.126757
39	1	0	-1.198450	-3.109430	0.845642
40	1	0	-1.432434	-2.033520	2.210575
41	1	0	-3.561483	-2.998880	2.451654
42	1	0	-5.282542	-1.956622	1.019936
43	1	0	-3.473882	-3.774927	0.869987
44	1	0	0.471076	1.264065	1.275833
45	1	0	-0.537854	-1.045189	0.146120
46	6	0	-0.081078	5.318382	-1.226629
47	6	0	0.344084	6.432138	-1.932924
48	6	0	1.692058	6.694204	-2.108234
49	6	0	2.628058	5.825550	-1.564072
50	6	0	2.219951	4.712398	-0.857374
51	1	0	2.948975	4.037813	-0.429997
52	1	0	3.685931	6.018914	-1.690811

53	1	0	2.013631	7.566214	-2.661187
54	1	0	-0.394997	7.104013	-2.351804
55	1	0	-1.129073	5.101100	-1.078173
56	6	0	-3.242805	2.270357	3.004178
57	6	0	-3.752362	2.974263	4.138716
58	7	0	-3.188060	2.992161	5.324716
59	6	0	-1.989986	2.271112	5.434339
60	6	0	-1.408907	1.554824	4.371857
61	6	0	-1.350267	2.295962	6.713870
62	6	0	-0.181229	1.645109	6.915879
63	6	0	0.420500	0.931355	5.843732
64	6	0	-0.167404	0.887689	4.623802
65	1	0	-3.781814	2.342393	2.072048
66	1	0	-4.677034	3.536338	4.026993
67	1	0	0.321699	0.347537	3.826746
68	1	0	1.361196	0.421795	6.010432
69	1	0	0.305950	1.664537	7.882271
70	1	0	-1.834649	2.855399	7.504102
71	1	0	-2.615163	0.730374	0.062306
72	6	0	-4.610961	0.355811	-2.173343
73	1	0	-5.978798	-0.843356	-1.191224
74	1	0	-5.371077	0.999011	-2.594944
75	1	0	-3.594184	0.611668	-2.434344
76	6	0	2.295188	-2.293662	-1.123368
77	6	0	3.185371	-2.330166	-2.206731
78	6	0	1.932159	-3.494771	-0.503962
79	6	0	3.688586	-3.549060	-2.668458
80	1	0	3.494536	-1.409228	-2.690675
81	6	0	2.437306	-4.713111	-0.964160
82	1	0	1.258955	-3.450681	0.344697
83	6	0	3.315555	-4.745914	-2.050662
84	1	0	4.374332	-3.561133	-3.512319
85	1	0	2.146744	-5.637653	-0.470417
86	1	0	3.708120	-5.693634	-2.411072
87	6	0	1.736620	1.442189	-3.450657
88	1	0	0.950771	2.134373	-3.140617
89	1	0	2.629361	1.983251	-3.765807
90	1	0	1.368913	0.800353	-4.254942
91	8	0	0.048665	-0.140466	-2.148256
92	8	0	2.155593	0.635413	-2.324993

mr-IM5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.253890	-0.212413	-1.836003
2	6	0	1.827103	-1.185480	-0.782597
3	8	0	0.797078	-1.670634	0.032269
4	8	0	2.345983	0.926994	1.056892
5	15	0	2.963804	-0.293745	0.431765
6	8	0	3.283531	-1.506502	1.429831
7	6	0	4.111503	-1.304570	2.592070
8	1	0	4.117609	-2.258005	3.122116
9	1	0	5.130084	-1.040407	2.290793
10	1	0	3.688896	-0.523761	3.231698
11	8	0	4.414244	-0.003657	-0.223167
12	6	0	4.875872	1.321292	-0.550652
13	1	0	5.931150	1.210159	-0.806921
14	1	0	4.765994	1.988436	0.307872

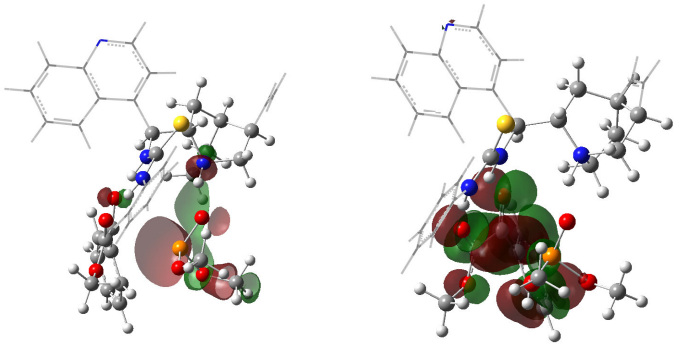
15	1	0	4.321228	1.714400	-1.405949
16	7	0	0.586141	3.101268	0.116045
17	6	0	-0.661466	2.634380	0.485464
18	7	0	-0.568419	1.510782	1.253390
19	16	0	-2.131287	3.336033	0.031956
20	6	0	0.998172	4.265890	-0.590708
21	6	0	-1.637091	0.802153	1.983633
22	6	0	-2.601590	0.043193	1.029183
23	6	0	-3.935469	-0.447733	1.660932
24	6	0	-4.297489	-1.817530	1.049792
25	7	0	-1.895288	-1.127545	0.413987
26	6	0	-2.643858	-1.503996	-0.810649
27	6	0	-4.155014	-1.770377	-0.502071
28	6	0	-1.873141	-2.297474	1.332785
29	6	0	-3.300024	-2.852590	1.593592
30	1	0	1.366884	2.540324	0.471412
31	6	0	-2.260821	1.722143	3.074633
32	1	0	-1.092087	0.019131	2.516796
33	1	0	-4.733103	0.276635	1.470508
34	1	0	-3.852840	-0.550356	2.752683
35	1	0	-2.170893	-2.403950	-1.217953
36	1	0	-2.495750	-0.712861	-1.545607
37	6	0	-5.196003	-0.818699	-1.130088
38	1	0	-4.412442	-2.778006	-0.870816
39	1	0	-1.221183	-3.053282	0.884464
40	1	0	-1.391090	-1.991635	2.266403
41	1	0	-3.464791	-3.013996	2.667031
42	1	0	-5.323381	-2.092148	1.321407
43	1	0	-3.444604	-3.821388	1.097239
44	1	0	0.374207	1.161435	1.417654
45	1	0	-0.079203	-1.188127	-0.056324
46	6	0	0.129757	5.124366	-1.263872
47	6	0	0.632861	6.225366	-1.937724
48	6	0	1.991969	6.489302	-1.959796
49	6	0	2.858477	5.636584	-1.290704
50	6	0	2.371326	4.537320	-0.612363
51	1	0	3.046745	3.878159	-0.085581
52	1	0	3.923560	5.831942	-1.295207
53	1	0	2.374734	7.350885	-2.489628
54	1	0	-0.053244	6.885303	-2.454395
55	1	0	-0.928711	4.909705	-1.229007
56	6	0	-3.418591	2.399278	2.890940
57	6	0	-3.939207	3.238917	3.923909
58	7	0	-3.372814	3.428239	5.093989
59	6	0	-2.161952	2.749254	5.294035
60	6	0	-1.571475	1.907396	4.334384
61	6	0	-1.519032	2.954894	6.555665
62	6	0	-0.339382	2.354767	6.837521
63	6	0	0.270403	1.512085	5.868438
64	6	0	-0.320149	1.297490	4.668139
65	1	0	-3.966459	2.333607	1.963687
66	1	0	-4.874907	3.763295	3.742162
67	1	0	0.171117	0.660658	3.947688
68	1	0	1.218288	1.042340	6.098830
69	1	0	0.149686	2.510626	7.790443
70	1	0	-2.009941	3.607188	7.266737
71	1	0	-2.830850	0.717171	0.203611
72	6	0	-4.991509	0.217418	-1.901507
73	1	0	-6.214848	-1.093608	-0.876594
74	1	0	-5.817864	0.799220	-2.285590
75	1	0	-4.010557	0.556635	-2.200179
76	6	0	2.545031	-2.349482	-1.493376

77	6	0	3.557479	-2.134009	-2.440300
78	6	0	2.169307	-3.662781	-1.184958
79	6	0	4.177330	-3.215506	-3.069560
80	1	0	3.867248	-1.125074	-2.688461
81	6	0	2.793195	-4.742116	-1.815201
82	1	0	1.389862	-3.827644	-0.451027
83	6	0	3.798316	-4.524332	-2.760168
84	1	0	4.957891	-3.031593	-3.803655
85	1	0	2.489749	-5.755721	-1.565010
86	1	0	4.281355	-5.365116	-3.251602
87	6	0	1.700216	1.543006	-3.352551
88	1	0	0.895722	2.163332	-2.952898
89	1	0	2.565771	2.149379	-3.620054
90	1	0	1.342053	0.975244	-4.214344
91	8	0	0.097016	-0.238893	-2.183842
92	8	0	2.174612	0.633904	-2.327659

Table S1 The calculated HOMO and LUMO energy, Electronic chemical potential μ, Chemical hardness η, global electrophilicity ω, and global nucleophilicity *N* for reactants, molecular complexes and intermediates at B3LYP/6-311++G(d,p)

	HOMO [a.u.]	LUMO [a.u.]	μ^a [a.u.]	η^b [a.u.]	ω^c [eV]	N^d [eV]
TCE	−0.34767	−0.19513	−0.27140	0.15254	6.6	-
DMHP	−0.30294	−0.01224	−0.15759	0.29070	1.2	1.2
phosphite	−0.25951	−0.01725	−0.13838	0.24226	1.1	2.4
α-ketoester	−0.26728	−0.09149	−0.17939	0.17579	2.5	2.2
s-**IM1**	−0.19507	−0.05498	−0.12503	0.14009	1.5	4.2
s-**IM2a**	−0.20525	−0.06625	−0.13575	0.13900	1.8	3.9
s-**IM2b**	−0.20879	−0.06884	−0.13882	0.13995	1.9	3.8
ds-**IM3**	−0.20355	−0.10014	−0.15185	0.10341	3.0	3.9
ms-**IM3**	−0.19908	−0.09718	−0.14813	0.10190	2.9	4.0
dr-**IM3**	−0.20086	−0.10752	−0.15419	0.09334	3.5	4.0
mr-**IM3**	−0.19662	−0.10316	−0.14989	0.09346	3.3	4.1

a: $\mu = (\varepsilon_{HOMO} + \varepsilon_{LUMO}) / 2$; *b*: $\eta = \varepsilon_{HOMO} - \varepsilon_{LUMO}$; *c*: $\omega\ [eV] = (\mu^2/2\eta)$; *d*: $N = \varepsilon_{HOMO(Nu)} - \varepsilon_{LUMO(TCE)}$



HOMO LUMO

Fig. S1 The visualization of HOMO and LUMO for the pre-transition complex *ds*-**IM3**

S3 Energies of C-P bond formation TSs over (R)-CAT, (S)-Py-CAT, (S)-Ac-CAT .

Species	E_{ZPE} (Hartree)	Gc[a] (Hartree)	SCF_{PCM}[b] (Hartree)	D_c[c] (Hartree)	$SCF_{PCM}+G_c+D_c$ (Hartree)	ΔG (kcal/mol)
(*R*)-CAT	−1611.08843	0.47694	−1625.13511	−0.14785	−1624.80603	-
(*R*)-*dr*-**TS2**	−2831.81254	0.71003	−2846.37413	−0.24079	−2845.90489	0.1
(*R*)-*mr*-**TS2**	−2831.81240	0.70889	−2846.37099	−0.24339	−2845.90549	-0.3
(*R*)-*ds*-**TS2**	−2831.79473	0.70860	−2846.35593	−0.24210	−2845.88943	9.8
(*R*)-*ms*-**TS2**	−2831.80489	0.70953	−2846.36526	−0.23953	−2845.89526	6.1
(*S*)-*Py*-CAT	−1460.34701	0.42608	−1471.46140	−0.12854	−1471.16387	-
(*S*)-*Py*-*ds*-**TS2**	−2681.07237	0.65742	−2692.69823	−0.22041	−2692.26121	1.0
(*S*)-*Py*-*ms*-**TS2**	−2681.07216	0.65753	−2692.69635	−0.22258	−2692.26141	0.9
(*S*)-*Py*-*dr*-**TS2**	−2681.06681	0.65566	−2692.69351	−0.21929	−2692.25715	3.6
(*S*)-*Py*-*mr*-**TS2**	−2681.06736	0.65620	−2692.69026	−0.21826	−2692.25231	6.6
(*S*)-*Ac*-CAT	−1761.80295	0.52740	−1778.79242	−0.17118	−1778.43620	-
(*S*)-*Ac*-*ds*-**TS2**	−2982.52815	0.76064	−3000.02885	−0.26526	−2999.53347	1.1
(*S*)-*Ac*-*ms*-**TS2**	−2982.52384	0.76063	−3000.02392	−0.26448	−2999.52777	4.7
(*S*)-*Ac*-*dr*-**TS2**	−2982.51325	0.76254	−3000.01893	−0.26883	−2999.52521	6.3
(*S*)-*Ac* -*mr*-**TS2**	−2982.52246	0.76016	−3000.02239	−0.26472	−2999.52695	5.2

a: Thermal correction to Gibbs Free Energy.
b: Total electronic energies in solvent.
c: Dispersion effect correction energy.

S4: Cartesian coordinates of C-P bond formation TSs over (R)-CAT, (S)-Py-CAT, (S)-Ac-CAT.

(*R*)-CAT

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.750490	-0.559635	-0.751499
2	6	0	1.694512	-0.236996	0.081466
3	7	0	0.527834	-0.146957	-0.646136
4	16	0	1.815705	0.052719	1.727350
5	6	0	4.093541	-0.962669	-0.497752
6	6	0	-0.822045	0.161333	-0.134496
7	6	0	-1.434953	-1.045364	0.619542
8	6	0	-2.921439	-0.856205	1.042199
9	6	0	-3.654364	-2.200868	0.836852
10	7	0	-1.305841	-2.273837	-0.214295
11	6	0	-2.336484	-2.329878	-1.271928
12	6	0	-3.778971	-2.481843	-0.685602
13	6	0	-1.477840	-3.439504	0.674998
14	6	0	-2.817538	-3.334257	1.468965
15	1	0	-1.414280	0.281481	-1.051158
16	6	0	-0.876472	1.541421	0.573103
17	1	0	-0.815680	-1.224299	1.501988
18	1	0	-3.410791	-0.072879	0.444481
19	1	0	-2.993572	-0.545245	2.090161
20	1	0	-2.089214	-3.166763	-1.935035
21	1	0	-2.258724	-1.419942	-1.873525
22	6	0	-4.875824	-1.629633	-1.359132
23	1	0	-4.097285	-3.534129	-0.794020
24	1	0	-1.456392	-4.339609	0.048906
25	1	0	-0.615042	-3.491434	1.347611
26	1	0	-2.630171	-3.113216	2.527964
27	1	0	-4.648611	-2.161414	1.295975
28	1	0	-3.370988	-4.281472	1.433902
29	1	0	2.543769	-0.446662	-1.741568
30	1	0	0.478440	-0.819105	-1.405065
31	6	0	-0.698646	2.743578	-0.211161
32	6	0	-0.795764	3.983272	0.444085
33	6	0	-1.111503	1.687450	1.897902
34	6	0	-1.189446	2.991288	2.478355
35	7	0	-1.049589	4.117885	1.816957
36	6	0	-0.427566	2.748574	-1.615955
37	6	0	-0.632393	5.194957	-0.299419
38	6	0	-4.845610	-1.120104	-2.563708
39	1	0	-5.762914	-1.497284	-0.748187
40	1	0	-4.001516	-1.227671	-3.229290
41	1	0	-5.681738	-0.561540	-2.960469
42	6	0	4.923065	-1.137968	-1.610571
43	6	0	4.602987	-1.209614	0.775605
44	6	0	6.231650	-1.548005	-1.448756
45	6	0	6.738427	-1.793118	-0.180384
46	6	0	5.917705	-1.621771	0.921804
47	1	0	6.861252	-1.677906	-2.320194
48	1	0	4.529779	-0.950080	-2.600463
49	1	0	7.763825	-2.113308	-0.055119
50	1	0	6.303089	-1.809307	1.916525
51	1	0	3.961063	-1.060760	1.630982

52	1	0	-1.231551	0.836153	2.550189
53	1	0	-1.381106	3.071192	3.546243
54	6	0	-0.274882	3.909995	-2.296515
55	6	0	-0.380753	5.161296	-1.628778
56	1	0	-0.331821	1.807160	-2.136127
57	1	0	-0.067962	3.895034	-3.359181
58	1	0	-0.255862	6.076644	-2.192941
59	1	0	-0.716258	6.129595	0.240446

(*R*)-*dr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.230475	3.374282	0.533247
2	6	0	-1.033533	2.930448	0.248499
3	7	0	-1.023298	1.935339	-0.684854
4	16	0	-2.465943	3.501326	0.963496
5	6	0	0.724949	4.364134	1.433555
6	6	0	-2.155476	1.345066	-1.399660
7	6	0	-3.022715	0.457308	-0.482405
8	6	0	-4.225030	-0.236766	-1.162839
9	6	0	-4.413058	-1.642494	-0.554675
10	7	0	-2.173304	-0.655057	0.130580
11	6	0	-1.941726	-1.802829	-0.825479
12	6	0	-3.269023	-2.565976	-1.058652
13	6	0	-2.872402	-1.156406	1.365832
14	6	0	-4.320418	-1.543318	0.982915
15	1	0	-1.671232	0.666663	-2.105867
16	6	0	-2.931658	2.387332	-2.252536
17	1	0	-3.348451	1.058657	0.367266
18	1	0	-4.067947	-0.317964	-2.246977
19	1	0	-5.125402	0.366332	-1.015660
20	1	0	-1.159308	-2.417302	-0.378531
21	1	0	-1.527867	-1.367938	-1.733640
22	6	0	-3.492231	-3.054216	-2.503962
23	1	0	-3.275186	-3.465731	-0.419799
24	1	0	-2.284380	-2.000318	1.732907
25	1	0	-2.822096	-0.358443	2.109736
26	1	0	-5.030266	-0.795531	1.354945
27	1	0	-5.384999	-2.053033	-0.846105
28	1	0	-4.586570	-2.499121	1.447848
29	1	0	0.974093	2.910622	0.001420
30	1	0	-0.125100	1.564841	-1.019356
31	1	0	-1.208078	-0.342426	0.421087
32	6	0	-2.351658	2.839257	-3.497947
33	6	0	-3.072868	3.779209	-4.255162
34	6	0	-4.119194	2.916106	-1.877785
35	6	0	-4.776330	3.872615	-2.713157
36	7	0	-4.312686	4.306391	-3.862797
37	6	0	-1.088316	2.395810	-4.004543
38	6	0	-2.542722	4.249465	-5.497697
39	6	0	-2.588569	-3.170198	-3.442404
40	1	0	-4.514714	-3.357422	-2.699833
41	1	0	-1.549819	-2.903381	-3.306107
42	1	0	-2.845341	-3.554991	-4.419933
43	6	0	2.108959	4.574452	1.431116
44	6	0	-0.076208	5.114713	2.290788
45	6	0	2.672108	5.514395	2.270536
46	6	0	1.873075	6.261620	3.125432

47	6	0	0.504562	6.054866	3.127468
48	1	0	3.744083	5.666617	2.258272
49	1	0	2.729331	3.991661	0.763631
50	1	0	2.316729	6.997818	3.781935
51	1	0	-0.127891	6.633112	3.789716
52	1	0	-1.142899	4.944009	2.277884
53	1	0	-4.592947	2.646795	-0.946000
54	1	0	-5.732059	4.275836	-2.385564
55	6	0	-0.608257	2.861455	-5.183216
56	6	0	-1.347255	3.804099	-5.949909
57	1	0	-0.500772	1.687728	-3.436381
58	1	0	0.350553	2.518363	-5.551334
59	1	0	-0.942259	4.159645	-6.888792
60	1	0	-3.129605	4.970269	-6.052641
61	8	0	0.313808	-0.718202	1.086276
62	15	0	1.723627	-1.037294	0.572474
63	8	0	2.818510	-0.573275	1.747070
64	6	0	2.522359	0.502568	2.649513
65	1	0	1.505467	0.414963	3.042072
66	1	0	2.634161	1.470357	2.148482
67	1	0	3.246763	0.428466	3.465544
68	8	0	2.002848	-2.664819	0.598749
69	6	0	1.860593	-3.417140	1.813498
70	1	0	2.612240	-3.106454	2.546487
71	1	0	0.858343	-3.286903	2.238545
72	1	0	2.014123	-4.466251	1.547735
73	6	0	2.849967	0.882032	-1.278275
74	6	0	1.869946	-0.210725	-1.742118
75	8	0	2.475011	1.938425	-0.788745
76	8	0	4.139548	0.598757	-1.490091
77	6	0	5.097399	1.577160	-1.038618
78	1	0	4.915870	2.537972	-1.526598
79	1	0	5.028971	1.694758	0.046053
80	1	0	6.070201	1.175462	-1.322773
81	6	0	2.402336	-1.399000	-2.517037
82	8	0	0.698222	0.192664	-1.979178
83	6	0	3.525333	-2.156940	-2.151413
84	6	0	3.956097	-3.215617	-2.950173
85	6	0	1.719669	-1.734475	-3.697022
86	6	0	2.152059	-2.793226	-4.498978
87	6	0	3.273581	-3.538504	-4.128240
88	1	0	4.050648	-1.935874	-1.229648
89	1	0	4.823362	-3.796980	-2.646495
90	1	0	3.613089	-4.364900	-4.748177
91	1	0	1.615415	-3.031029	-5.414611
92	1	0	0.854883	-1.143936	-3.982125

(*R*)-*mr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.056174	-0.446699	-0.339122
2	7	0	0.353307	3.348750	-0.627953
3	6	0	1.543087	2.703021	-0.420108
4	7	0	1.455570	1.837805	0.636459
5	16	0	2.960254	2.894053	-1.331779
6	6	0	-0.054614	4.321381	-1.582824
7	6	0	2.530463	1.100293	1.287621
8	6	0	3.039465	-0.087885	0.435271

9	6	0	4.072870	-0.995569	1.148172
10	6	0	3.786376	-2.473363	0.813511
11	7	0	1.879247	-0.988346	0.025632
12	6	0	1.392213	-1.850379	1.168907
13	6	0	2.469492	-2.910887	1.512898
14	6	0	2.314982	-1.867281	-1.121954
15	6	0	3.603298	-2.613477	-0.710962
16	1	0	-0.403748	3.028022	-0.008030
17	1	0	2.045210	0.655585	2.164109
18	6	0	3.651876	2.023176	1.849158
19	1	0	3.428927	0.308205	-0.503494
20	1	0	4.030884	-0.846841	2.235814
21	1	0	5.083304	-0.723538	0.829866
22	1	0	0.445089	-2.279611	0.845515
23	1	0	1.189046	-1.178946	2.001516
24	6	0	2.657871	-3.175109	3.020706
25	1	0	2.166883	-3.870136	1.059999
26	1	0	1.472895	-2.531780	-1.324789
27	1	0	2.450216	-1.213749	-1.986331
28	1	0	4.474205	-2.200329	-1.233118
29	1	0	4.617473	-3.100948	1.150886
30	1	0	3.528984	-3.669103	-0.995006
31	1	0	0.517701	1.740356	1.052633
32	6	0	-1.385430	4.751307	-1.513036
33	6	0	-1.858934	5.701438	-2.395135
34	6	0	-1.021832	6.242663	-3.361582
35	6	0	0.294303	5.819977	-3.430911
36	6	0	0.784798	4.867316	-2.552212
37	6	0	4.881881	2.121846	1.294492
38	6	0	5.867216	2.979477	1.875427
39	7	0	5.681674	3.714650	2.947618
40	6	0	4.404021	3.637153	3.522274
41	6	0	3.370969	2.827538	3.017575
42	6	0	4.174785	4.442530	4.681923
43	6	0	2.968145	4.441262	5.295282
44	6	0	1.915272	3.634574	4.782193
45	6	0	2.107399	2.857935	3.688409
46	1	0	-1.395093	6.987407	-4.051250
47	1	0	-2.890512	6.023680	-2.328313
48	1	0	-2.037353	4.330776	-0.759264
49	1	0	0.956311	6.236783	-4.179907
50	1	0	1.809560	4.527446	-2.593012
51	1	0	5.152255	1.575513	0.403916
52	1	0	6.847663	3.032187	1.407275
53	1	0	4.996340	5.048950	5.041393
54	1	0	2.790802	5.052268	6.171175
55	1	0	0.950199	3.649532	5.273135
56	1	0	1.285771	2.268150	3.308949
57	6	0	1.816844	-2.881117	3.978341
58	1	0	2.029880	-3.139146	5.006821
59	1	0	0.873228	-2.380436	3.810448
60	1	0	3.579732	-3.696504	3.252658
61	6	0	-1.570279	-0.267059	-1.263467
62	6	0	-1.985506	-1.700356	-0.870190
63	8	0	-3.301518	-1.946670	-0.936600
64	8	0	-0.335325	-0.049898	-1.291685
65	6	0	-2.467807	0.568471	-2.149920
66	8	0	-1.165136	-2.550718	-0.568524
67	6	0	-3.724622	-3.261348	-0.528140
68	1	0	-3.257154	-4.024342	-1.155973
69	1	0	-3.457617	-3.430737	0.518284
70	1	0	-4.807407	-3.265901	-0.656083

71	6	0	-1.827200	1.298424	-3.165567
72	6	0	-2.565018	2.074575	-4.062029
73	6	0	-3.955605	2.143282	-3.949823
74	6	0	-4.600531	1.430189	-2.933067
75	6	0	-3.867097	0.648536	-2.040322
76	1	0	-0.746092	1.248511	-3.238866
77	1	0	-2.050020	2.628403	-4.843307
78	1	0	-4.532816	2.749695	-4.643671
79	1	0	-5.681638	1.486429	-2.830308
80	1	0	-4.380213	0.119800	-1.246990
81	15	0	-2.215130	0.645062	1.031723
82	8	0	-3.757023	1.149404	1.443404
83	6	0	-4.141122	2.523653	1.317749
84	1	0	-3.381955	3.183568	1.748967
85	1	0	-5.081932	2.633531	1.864787
86	1	0	-4.304233	2.789543	0.265992
87	8	0	-2.038184	-0.542221	2.184918
88	6	0	-2.184136	-0.226633	3.579774
89	1	0	-3.217330	0.060183	3.800570
90	1	0	-1.927756	-1.133112	4.135314
91	1	0	-1.509963	0.588155	3.868261
92	8	0	-1.247452	1.805826	1.330198

(*R*)-*ds*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	18.933385	-0.748293	0.258994
2	6	0	17.620474	-0.493225	0.602865
3	7	0	16.826775	-0.464384	-0.498904
4	16	0	17.041359	-0.233442	2.168132
5	6	0	20.103278	-0.996919	1.033577
6	6	0	15.402394	-0.142575	-0.609113
7	6	0	14.581512	-1.458153	-0.350439
8	6	0	14.113722	-1.946708	1.044463
9	6	0	12.771324	-2.690693	0.884550
10	7	0	13.378228	-1.536169	-1.293490
11	6	0	12.163910	-0.862835	-0.724521
12	6	0	11.646803	-1.687738	0.488238
13	6	0	13.076190	-2.985591	-1.583565
14	6	0	12.903651	-3.733795	-0.242947
15	1	0	15.283817	-0.016457	-1.690586
16	6	0	15.067414	1.258979	-0.013679
17	1	0	15.248155	-2.207807	-0.774715
18	1	0	14.023238	-1.142813	1.771791
19	1	0	14.878996	-2.617069	1.447243
20	1	0	11.430566	-0.785326	-1.530879
21	1	0	12.465551	0.146968	-0.447078
22	6	0	11.140695	-0.843747	1.675384
23	1	0	10.790016	-2.295252	0.149014
24	1	0	12.166199	-2.993854	-2.190839
25	1	0	13.906865	-3.349864	-2.190454
26	1	0	13.765667	-4.383095	-0.051491
27	1	0	12.507121	-3.185839	1.824575
28	1	0	12.017215	-4.377370	-0.283337
29	1	0	19.098582	-0.791140	-0.746367
30	1	0	17.219800	-0.791551	-1.385445
31	6	0	15.699445	2.414297	-0.625428
32	6	0	15.396621	3.686308	-0.107097

33	6	0	14.210803	1.490832	1.007116
34	6	0	13.962177	2.823364	1.462820
35	7	0	14.511070	3.903286	0.960480
36	6	0	16.606149	2.347692	-1.730486
37	6	0	15.997774	4.852476	-0.675038
38	6	0	10.689196	0.382684	1.617337
39	1	0	11.134094	-1.377382	2.619255
40	1	0	10.655832	0.959024	0.703195
41	1	0	10.318297	0.886568	2.499325
42	6	0	21.280433	-1.273316	0.329863
43	6	0	20.129758	-0.980314	2.426432
44	6	0	22.455353	-1.527382	1.009235
45	6	0	22.481100	-1.512720	2.396810
46	6	0	21.316212	-1.239078	3.093663
47	1	0	23.358836	-1.739277	0.451201
48	1	0	21.261711	-1.285939	-0.751578
49	1	0	23.402444	-1.711934	2.927044
50	1	0	21.325984	-1.223638	4.176616
51	1	0	19.213183	-0.759626	2.954650
52	1	0	13.696084	0.698612	1.521098
53	1	0	13.269727	2.962374	2.290103
54	1	0	13.623022	-1.091224	-2.225295
55	6	0	16.856987	4.749420	-1.715835
56	6	0	17.161188	3.469249	-2.251935
57	1	0	16.858415	1.390488	-2.160483
58	1	0	17.844011	3.394624	-3.088763
59	1	0	17.313692	5.630679	-2.148028
60	1	0	15.738139	5.809990	-0.242110
61	6	0	17.635411	-1.268801	-4.119787
62	6	0	16.371470	-2.168595	-4.064766
63	8	0	18.109762	-0.750677	-3.118710
64	8	0	18.172357	-1.118062	-5.333830
65	6	0	19.305367	-0.233117	-5.434131
66	1	0	19.022253	0.771878	-5.111839
67	1	0	20.129668	-0.600652	-4.817522
68	1	0	19.580582	-0.239084	-6.489075
69	8	0	15.978039	-2.430950	-2.890200
70	6	0	16.252725	-3.260272	-5.129670
71	6	0	16.369537	-3.058585	-6.514483
72	6	0	16.022767	-4.562517	-4.659360
73	6	0	16.260104	-4.132969	-7.399131
74	1	0	16.531940	-2.061993	-6.907380
75	6	0	15.916722	-5.638485	-5.544491
76	1	0	15.940562	-4.715502	-3.588043
77	6	0	16.033940	-5.427865	-6.920279
78	1	0	16.347495	-3.955623	-8.468555
79	1	0	15.746708	-6.640610	-5.157400
80	1	0	15.950289	-6.261509	-7.613415
81	8	0	13.782122	-0.424157	-3.708842
82	15	0	14.870070	-0.534712	-4.785928
83	8	0	14.125953	-0.661509	-6.266849
84	6	0	12.994133	-1.524963	-6.431757
85	1	0	13.287447	-2.577462	-6.340959
86	1	0	12.613891	-1.344020	-7.440454
87	1	0	12.218063	-1.290544	-5.695930
88	8	0	15.627863	0.904065	-5.018801
89	6	0	14.870436	2.104371	-5.268566
90	1	0	14.133043	2.265643	-4.475539
91	1	0	15.590084	2.926006	-5.277008
92	1	0	14.367209	2.038730	-6.238154

(*R*)-*ms*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.264474	-0.557474	0.209105
2	7	0	0.635214	3.209086	-0.071826
3	6	0	-0.685584	2.873029	-0.227552
4	7	0	-0.824726	1.762326	-1.015087
5	16	0	-2.005229	3.687404	0.460349
6	6	0	1.276419	4.243097	0.665083
7	6	0	-2.051971	1.230299	-1.604017
8	6	0	-2.961808	0.563303	-0.538304
9	6	0	-4.361496	0.106340	-1.014750
10	6	0	-4.751948	-1.203884	-0.300326
11	7	0	-2.283494	-0.686820	0.031978
12	6	0	-2.431326	-1.882195	-0.887634
13	6	0	-3.901274	-2.364855	-0.883171
14	6	0	-2.899189	-0.996188	1.374917
15	6	0	-4.432642	-1.071779	1.203084
16	1	0	1.285694	2.559519	-0.542809
17	1	0	-1.698342	0.416350	-2.245133
18	6	0	-2.745721	2.252479	-2.552089
19	1	0	-3.045074	1.250298	0.304650
20	1	0	-4.377028	-0.043854	-2.102532
21	1	0	-5.090873	0.889000	-0.791892
22	1	0	-1.716211	-2.625630	-0.542878
23	1	0	-2.109434	-1.552019	-1.874561
24	6	0	-4.421258	-2.859557	-2.247758
25	1	0	-3.989267	-3.215530	-0.186007
26	1	0	-2.454992	-1.938847	1.701991
27	1	0	-2.572320	-0.211702	2.059077
28	1	0	-4.911741	-0.175203	1.612793
29	1	0	-5.818279	-1.405806	-0.442375
30	1	0	-4.826958	-1.930459	1.757762
31	1	0	0.058072	1.333109	-1.327762
32	6	0	0.606456	5.196228	1.430943
33	6	0	1.326545	6.162654	2.114567
34	6	0	2.708732	6.200339	2.050429
35	6	0	3.378291	5.254047	1.286579
36	6	0	2.674916	4.284796	0.600187
37	1	0	3.261853	6.958733	2.587553
38	1	0	4.459219	5.272201	1.225072
39	1	0	3.196762	3.549421	0.003295
40	1	0	0.793570	6.896795	2.706179
41	1	0	-0.472350	5.154718	1.469833
42	6	0	-3.817439	2.993273	-2.186573
43	6	0	-4.405222	3.915087	-3.107702
44	7	0	-3.980631	4.121521	-4.333002
45	6	0	-2.852602	3.380810	-4.716862
46	6	0	-2.203814	2.456827	-3.877814
47	6	0	-2.359508	3.610936	-6.039592
48	6	0	-1.263764	2.957278	-6.491409
49	6	0	-0.592603	2.034641	-5.642714
50	6	0	-1.043476	1.792494	-4.387862
51	6	0	-3.702744	-3.191038	-3.289264
52	1	0	-4.168062	-3.557113	-4.194376
53	1	0	-2.623509	-3.130394	-3.314047
54	1	0	-5.500124	-2.961518	-2.281276
55	1	0	-0.885573	3.132818	-7.490445
56	1	0	-2.890635	4.326332	-6.654477

57	1	0	0.291850	1.527219	-6.007365
58	1	0	-0.501173	1.101037	-3.759811
59	1	0	-4.245531	2.922794	-1.198705
60	1	0	-5.270660	4.489000	-2.783962
61	15	0	2.418595	-0.393602	-1.014809
62	8	0	4.080283	-0.316374	-1.219743
63	6	0	4.795616	0.859516	-0.843633
64	1	0	4.735365	1.037869	0.239111
65	1	0	4.414731	1.737101	-1.377079
66	1	0	5.841025	0.689364	-1.115812
67	8	0	2.100351	-1.521084	-2.172079
68	6	0	2.492715	-1.300782	-3.535740
69	1	0	3.582752	-1.339871	-3.629556
70	1	0	2.042667	-2.106499	-4.121994
71	1	0	2.128319	-0.332197	-3.896827
72	8	0	1.833210	0.972222	-1.433893
73	6	0	1.270963	-1.641890	0.864547
74	6	0	1.161894	-0.350336	1.700742
75	8	0	2.260065	0.009411	2.379607
76	8	0	0.181246	-1.989125	0.347707
77	8	0	0.112171	0.267742	1.752879
78	6	0	2.150766	1.205560	3.180174
79	1	0	1.892457	2.060151	2.550890
80	1	0	1.385275	1.075524	3.949205
81	1	0	3.134019	1.335880	3.633123
82	6	0	2.294390	-2.699003	1.210528
83	6	0	3.623148	-2.446093	1.588301
84	6	0	4.471207	-3.496823	1.938886
85	6	0	4.011338	-4.817619	1.919516
86	6	0	1.846913	-4.030284	1.179151
87	6	0	2.694534	-5.080489	1.534668
88	1	0	4.002059	-1.431954	1.592890
89	1	0	5.498991	-3.282935	2.221915
90	1	0	4.675589	-5.632813	2.196258
91	1	0	0.824068	-4.224174	0.874184
92	1	0	2.325385	-6.103170	1.511143

(*S*)-*Py-CAT*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.652509	-0.417443	-0.857441
2	6	0	-1.560931	-0.188227	-0.028140
3	7	0	-0.548545	0.418604	-0.710203
4	16	0	-1.514424	-0.619696	1.592527
5	6	0	-3.991079	-0.772719	-0.517219
6	6	0	0.892933	0.497574	-0.404023
7	6	0	1.524015	-0.870514	-0.057516
8	6	0	3.059644	-0.775908	0.190231
9	6	0	3.719979	-2.014836	-0.452363
10	7	0	1.227348	-1.884636	-1.096259
11	6	0	1.511936	-3.211822	-0.516707
12	6	0	2.987607	-3.314680	0.006941
13	6	0	2.062857	-1.704095	-2.298950
14	6	0	3.577969	-1.891895	-1.981868
15	1	0	-2.415078	-0.584110	-1.832862
16	6	0	1.233200	1.630766	0.606445
17	1	0	1.327220	0.820037	-1.357537
18	1	0	3.272587	-0.727715	1.264547

19	1	0	3.486393	0.133355	-0.259429
20	1	0	1.332757	-3.959061	-1.298247
21	1	0	0.779388	-3.395390	0.271997
22	6	0	3.200222	-3.569780	1.514733
23	1	0	3.485565	-4.152890	-0.509435
24	1	0	1.720262	-2.427059	-3.048526
25	1	0	1.869099	-0.710239	-2.717838
26	1	0	4.166964	-1.040445	-2.348320
27	1	0	4.778451	-2.066423	-0.172264
28	1	0	3.975688	-2.790209	-2.472177
29	1	0	-0.793136	0.751978	-1.634123
30	6	0	-4.603895	-0.353378	0.663757
31	6	0	-5.923423	-0.690525	0.911587
32	6	0	-6.652654	-1.430329	-0.006752
33	6	0	-6.049415	-1.834202	-1.187596
34	6	0	-4.729392	-1.511054	-1.443972
35	1	0	-6.388276	-0.363819	1.833574
36	1	0	-7.683878	-1.686962	0.194707
37	1	0	-6.609108	-2.408255	-1.915512
38	1	0	-4.260090	-1.826205	-2.366194
39	1	0	-4.040656	0.223461	1.382014
40	6	0	1.702638	2.850402	0.134883
41	6	0	2.004802	3.865039	1.031393
42	7	0	1.874904	3.757034	2.372840
43	6	0	1.414574	2.560579	2.809040
44	6	0	1.090895	1.495084	1.982518
45	1	0	1.838985	3.018129	-0.924946
46	1	0	0.705514	0.577950	2.406054
47	6	0	2.301692	-3.657956	2.461068
48	1	0	2.587345	-3.847737	3.486344
49	1	0	1.240574	-3.551474	2.290269
50	1	0	4.248020	-3.688483	1.771822
51	1	0	1.039063	-1.233108	0.849301
52	1	0	2.373157	4.819156	0.663901
53	1	0	1.302203	2.460410	3.885364

(*S*)-*Py*-*ds*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.319046	2.647150	-0.175128
2	6	0	-1.274058	1.682299	-0.355520
3	7	0	-0.950322	0.522363	0.284069
4	16	0	-2.694131	1.858465	-1.274526
5	6	0	-0.203749	3.989341	-0.644910
6	6	0	-1.762275	-0.681714	0.456181
7	6	0	-1.966963	-1.456842	-0.861989
8	6	0	-2.805216	-2.750428	-0.738020
9	6	0	-2.201478	-3.844378	-1.641406
10	7	0	-0.628283	-1.852594	-1.473997
11	6	0	-0.848476	-2.169848	-2.931001
12	6	0	-1.935805	-3.271473	-3.067820
13	6	0	0.010754	-3.037591	-0.791006
14	6	0	-0.860717	-4.289729	-1.029211
15	1	0	0.469698	2.361806	0.415497
16	6	0	-3.061851	-0.418231	1.268521
17	1	0	-1.132160	-1.302719	1.102808
18	1	0	-3.840602	-2.541236	-1.021514
19	1	0	-2.823973	-3.103539	0.302229

20	1	0	0.118748	-2.488323	-3.323842
21	1	0	-1.108118	-1.230586	-3.417487
22	6	0	-3.251464	-2.881186	-3.772450
23	1	0	-1.503942	-4.092787	-3.661324
24	1	0	1.013291	-3.121402	-1.214459
25	1	0	0.133781	-2.773108	0.259070
26	1	0	-1.032473	-4.812175	-0.081368
27	1	0	-2.885935	-4.696263	-1.710435
28	1	0	-0.353131	-4.996533	-1.696653
29	1	0	-0.014049	0.413588	0.701379
30	6	0	-1.145971	4.621467	-1.452735
31	6	0	-0.939922	5.932504	-1.852828
32	6	0	0.190816	6.627475	-1.460738
33	6	0	1.130039	5.998181	-0.654663
34	6	0	0.939658	4.692985	-0.248143
35	1	0	-1.679187	6.414241	-2.480782
36	1	0	0.342362	7.650391	-1.777752
37	1	0	2.018969	6.530603	-0.340411
38	1	0	1.669758	4.199887	0.379477
39	1	0	-2.023991	4.065820	-1.748549
40	1	0	0.094610	-1.083676	-1.439540
41	6	0	-2.962997	-0.338543	2.653322
42	6	0	-4.096964	-0.085694	3.409026
43	7	0	-5.333344	0.092850	2.887581
44	6	0	-5.403657	0.014239	1.539495
45	6	0	-4.318893	-0.232993	0.708535
46	1	0	-4.467584	-0.260771	-0.360777
47	6	0	-3.606968	-1.714086	-4.243124
48	1	0	-4.564202	-1.579455	-4.727995
49	1	0	-2.991790	-0.827255	-4.186366
50	1	0	-3.927196	-3.723666	-3.871425
51	1	0	-2.411323	-0.774343	-1.586933
52	1	0	-6.389302	0.160253	1.105644
53	1	0	-4.023130	-0.024175	4.491546
54	1	0	-2.008538	-0.472047	3.145009
55	6	0	2.916009	0.973893	1.450177
56	6	0	2.544332	-0.502300	1.188684
57	8	0	2.109049	1.883123	1.328837
58	8	0	1.300684	-0.747731	1.246844
59	8	0	4.180588	1.172527	1.835827
60	6	0	4.587424	2.542833	2.024364
61	1	0	4.512334	3.085714	1.078613
62	1	0	3.959964	3.024374	2.778419
63	1	0	5.623641	2.489341	2.359028
64	6	0	3.510056	-1.579223	1.660264
65	6	0	4.884178	-1.603460	1.377902
66	6	0	5.693942	-2.621005	1.882035
67	6	0	5.147333	-3.633758	2.677721
68	6	0	2.969458	-2.602268	2.454037
69	6	0	3.780089	-3.620595	2.962118
70	1	0	5.321264	-0.838199	0.747156
71	1	0	6.755427	-2.627156	1.646037
72	1	0	5.782149	-4.425206	3.069050
73	1	0	3.343186	-4.399396	3.583110
74	1	0	1.907295	-2.577883	2.675326
75	8	0	1.613251	-0.465289	-1.857602
76	15	0	2.948329	-0.284264	-1.130992
77	8	0	4.050224	-1.391948	-1.666725
78	6	0	4.380495	-1.476827	-3.060884
79	1	0	5.051838	-2.332194	-3.171484
80	1	0	4.893407	-0.565314	-3.388322
81	1	0	3.480971	-1.632969	-3.667724

82	8	0	3.631973	1.144719	-1.634690
83	6	0	2.997268	1.991335	-2.608574
84	1	0	3.162091	1.602822	-3.620381
85	1	0	1.922463	2.070075	-2.426338
86	1	0	3.467278	2.973811	-2.514496

(*S*)-*Py-ms*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.806639	0.334932	-2.943618
2	6	0	1.167453	-2.070304	-2.011194
3	6	0	1.019638	-0.535872	-1.994339
4	8	0	-0.066803	-0.105053	-1.547413
5	8	0	2.292024	-2.529040	-2.578028
6	6	0	2.477246	-3.957381	-2.558895
7	1	0	2.512761	-4.314063	-1.526238
8	1	0	1.663647	-4.454276	-3.093685
9	1	0	3.430396	-4.128704	-3.059824
10	8	0	0.290630	-2.803700	-1.586362
11	6	0	1.124011	1.444772	-3.471035
12	6	0	1.744243	2.296516	-4.386964
13	6	0	3.063068	2.059501	-4.781886
14	6	0	3.136745	0.108841	-3.340240
15	6	0	3.755422	0.965685	-4.250603
16	1	0	0.104526	1.627868	-3.149388
17	1	0	1.196607	3.146791	-4.786149
18	1	0	3.550438	2.722429	-5.492727
19	1	0	4.786420	0.780392	-4.542311
20	1	0	3.693952	-0.720052	-2.923114
21	8	0	2.036646	0.813916	0.936177
22	15	0	2.547422	-0.390124	0.117905
23	8	0	2.405554	-1.778895	1.025759
24	6	0	3.010075	-1.860490	2.327307
25	1	0	2.686260	-2.809156	2.764815
26	1	0	4.101569	-1.847237	2.242689
27	1	0	2.683554	-1.028814	2.962395
28	8	0	4.221280	-0.301542	0.085254
29	6	0	4.885822	0.966223	0.074062
30	1	0	5.946263	0.761890	0.247918
31	1	0	4.499775	1.617876	0.864296
32	1	0	4.771238	1.461787	-0.898222
33	7	0	0.408121	3.049542	0.016253
34	6	0	-0.802110	2.596308	0.467013
35	7	0	-0.654194	1.471865	1.232697
36	16	0	-2.317080	3.286552	0.136013
37	6	0	0.773665	4.162022	-0.791375
38	6	0	-1.665086	0.774076	2.017677
39	6	0	-2.687296	0.011376	1.144295
40	6	0	-3.741141	-0.793813	1.941960
41	6	0	-3.985158	-2.154085	1.257886
42	7	0	-1.983967	-0.974606	0.219218
43	6	0	-2.935938	-1.382413	-0.881311
44	6	0	-4.244356	-1.945050	-0.264836
45	6	0	-1.497381	-2.207040	0.947539
46	6	0	-2.721473	-3.017272	1.428325
47	1	0	1.197701	2.434156	0.265805
48	6	0	-2.296481	1.670654	3.122386
49	1	0	-1.083668	0.018424	2.562006

50	1	0	-4.669957	-0.219617	2.002107
51	1	0	-3.402044	-0.958591	2.974120
52	1	0	-2.400021	-2.122216	-1.477901
53	1	0	-3.083274	-0.498878	-1.500749
54	6	0	-5.542010	-1.148938	-0.513058
55	1	0	-4.410415	-2.944456	-0.696637
56	1	0	-0.862352	-2.743501	0.243566
57	1	0	-0.866053	-1.869906	1.770382
58	1	0	-2.594112	-3.299352	2.479675
59	1	0	-4.847220	-2.652936	1.712835
60	1	0	-2.815237	-3.947860	0.856068
61	1	0	0.307200	1.103997	1.298401
62	1	0	-1.166606	-0.541368	-0.279568
63	6	0	-0.128161	5.101274	-1.288389
64	6	0	0.331285	6.157642	-2.058726
65	6	0	1.678215	6.298375	-2.344085
66	6	0	2.578565	5.364991	-1.848042
67	6	0	2.136448	4.307199	-1.079653
68	1	0	2.838002	3.580952	-0.691855
69	1	0	3.635460	5.463309	-2.061994
70	1	0	2.027219	7.126642	-2.945567
71	1	0	-0.379421	6.880901	-2.439199
72	1	0	-1.176205	4.977947	-1.056866
73	6	0	-3.541626	2.278156	3.033243
74	6	0	-3.986586	3.072877	4.081459
75	7	0	-3.285364	3.311492	5.212587
76	6	0	-2.071837	2.714227	5.272262
77	6	0	-1.553167	1.904585	4.274036
78	1	0	-1.494005	2.898240	6.174072
79	1	0	-0.573256	1.462459	4.396133
80	1	0	-4.165472	2.159843	2.159785
81	1	0	-4.960556	3.550514	4.016158
82	1	0	-3.161671	0.731065	0.476574
83	6	0	-5.689777	-0.008493	-1.135584
84	1	0	-6.412175	-1.650380	-0.103988
85	1	0	-6.667449	0.440133	-1.247303
86	1	0	-4.874744	0.551865	-1.571494

(*S*)-*Py*-*dr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.624956	-1.984065	-5.230189
2	6	0	2.561612	0.773667	-3.562097
3	6	0	4.045498	0.947896	-3.168865
4	6	0	4.504972	-0.311559	-2.380230
5	6	0	4.043857	-1.541974	-3.199177
6	6	0	2.467170	-0.256496	-4.706624
7	6	0	4.883998	-0.316130	-5.161449
8	6	0	4.912013	1.054007	-4.441886
9	7	0	3.732313	-1.117163	-4.616229
10	1	0	5.786984	-0.905872	-4.981701
11	1	0	4.744231	-0.238199	-6.242218
12	1	0	5.944722	1.319331	-4.188837
13	1	0	4.529114	1.845181	-5.097496
14	1	0	5.608574	-0.292335	-2.354562
15	1	0	3.138065	-1.991463	-2.808269
16	1	0	2.578075	0.244798	-5.673856
17	1	0	2.129235	1.724179	-3.888441

18	1	0	4.169103	1.844831	-2.554033
19	1	0	1.968838	0.446767	-2.703401
20	7	0	-0.468884	-2.895041	-2.129348
21	6	0	-0.088892	-1.721858	-2.735655
22	7	0	0.864366	-1.955436	-3.690689
23	16	0	-0.700151	-0.184039	-2.397128
24	6	0	-1.200079	-3.158034	-0.936281
25	6	0	1.203391	-1.144711	-4.859106
26	1	0	-0.189017	-3.737643	-2.641586
27	6	0	-1.446418	-4.500551	-0.627922
28	6	0	-2.131344	-4.837953	0.522474
29	6	0	-2.581171	-3.849942	1.387312
30	6	0	-2.337269	-2.521215	1.083656
31	6	0	-1.652863	-2.166771	-0.067719
32	1	0	-2.315431	-5.881173	0.747013
33	1	0	-3.118052	-4.116227	2.287590
34	1	0	-2.685649	-1.742164	1.750577
35	1	0	-1.470496	-1.132720	-0.320883
36	1	0	-1.094902	-5.270904	-1.300895
37	6	0	-0.083125	0.902726	-5.842311
38	6	0	-0.026856	-0.438180	-5.497271
39	6	0	-1.220526	1.397970	-6.470891
40	7	0	-2.303693	0.659128	-6.788153
41	6	0	-2.220974	-0.651869	-6.448023
42	1	0	0.729375	1.580882	-5.632956
43	1	0	4.799327	-2.327015	-3.267573
44	1	0	1.266601	-2.900759	-3.709960
45	1	0	1.503591	-1.893390	-5.606723
46	6	0	4.033182	-0.296494	-0.913285
47	6	0	3.503838	-1.286752	-0.242614
48	1	0	3.229232	-1.172258	0.797108
49	1	0	3.311276	-2.261144	-0.669089
50	1	0	4.211141	0.652693	-0.420148
51	6	0	-1.129438	-1.226790	-5.823374
52	1	0	-1.134382	-2.283715	-5.592485
53	1	0	-3.082812	-1.263530	-6.701496
54	1	0	-1.266972	2.450474	-6.738384
55	8	0	3.814700	-5.306957	-7.697101
56	8	0	3.570370	-3.085731	-6.391309
57	15	0	2.926752	-4.481378	-6.547124
58	6	0	5.244795	-5.245846	-7.684402
59	1	0	5.589758	-4.207301	-7.647411
60	1	0	5.582895	-5.714246	-8.612937
61	1	0	5.655014	-5.801348	-6.832143
62	8	0	1.512744	-4.358777	-7.395320
63	6	0	1.471722	-3.736092	-8.691180
64	1	0	1.953819	-2.752402	-8.666248
65	1	0	1.969229	-4.369718	-9.432012
66	1	0	0.415480	-3.621625	-8.947786
67	6	0	1.049026	-5.751042	-4.562611
68	6	0	2.495201	-5.322874	-4.223130
69	8	0	0.091290	-5.094572	-4.188529
70	8	0	2.578243	-4.266892	-3.550979
71	8	0	0.931976	-6.888976	-5.254379
72	6	0	-0.405383	-7.264404	-5.643030
73	1	0	-1.037051	-7.388706	-4.759973
74	1	0	-0.827995	-6.497069	-6.296155
75	1	0	-0.293258	-8.208832	-6.176003
76	6	0	3.581570	-6.370777	-4.083814
77	6	0	3.759367	-7.470466	-4.940830
78	6	0	4.779870	-8.392179	-4.704132
79	6	0	5.639975	-8.236475	-3.611664

80	6	0	4.453088	-6.220052	-2.992519
81	6	0	5.471759	-7.145577	-2.755528
82	1	0	3.115134	-7.598057	-5.801812
83	1	0	4.906398	-9.234139	-5.380544
84	1	0	6.432159	-8.959091	-3.431248
85	1	0	6.130041	-7.015476	-1.899750
86	1	0	4.310260	-5.371918	-2.331020

(*S*)-*Py*-*mr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.003805	-0.558358	-1.940684
2	6	0	1.374441	-1.768346	-1.064136
3	8	0	0.470607	-2.113157	-0.274174
4	6	0	2.489442	-2.721724	-1.369937
5	6	0	3.216883	-2.742109	-2.571985
6	6	0	2.750523	-3.711714	-0.404286
7	6	0	4.179103	-3.729895	-2.797563
8	1	0	3.036975	-1.992698	-3.331587
9	6	0	3.719560	-4.685780	-0.627435
10	1	0	2.192402	-3.689506	0.525157
11	6	0	4.438023	-4.701131	-1.828598
12	1	0	4.728836	-3.735078	-3.735601
13	1	0	3.918672	-5.433084	0.136715
14	1	0	5.193616	-5.462746	-2.005263
15	6	0	1.561547	1.016975	-3.608536
16	1	0	1.356205	1.861411	-2.946416
17	1	0	2.430039	1.215551	-4.237008
18	1	0	0.679858	0.809807	-4.220390
19	8	0	-0.094989	-0.037929	-1.830699
20	8	0	1.916840	-0.148115	-2.832015
21	8	0	2.248302	1.392347	0.769563
22	15	0	2.816023	-0.002613	0.411534
23	8	0	2.822687	-0.947748	1.770566
24	6	0	3.454620	-0.485648	2.975678
25	1	0	3.167012	-1.183954	3.766685
26	1	0	4.543062	-0.487548	2.858210
27	1	0	3.115053	0.524380	3.231064
28	8	0	4.478908	0.163989	0.256423
29	6	0	5.001562	1.220209	-0.547034
30	1	0	6.091346	1.149425	-0.488882
31	1	0	4.677209	2.197083	-0.170731
32	1	0	4.694880	1.114075	-1.596969
33	7	0	0.397854	3.340350	-0.105685
34	6	0	-0.757112	2.810764	0.403747
35	7	0	-0.504835	1.680760	1.120014
36	16	0	-2.326647	3.452200	0.167113
37	6	0	0.666597	4.514932	-0.862062
38	6	0	-1.418397	0.763659	1.802473
39	6	0	-2.525553	0.211293	0.847652
40	6	0	-3.912195	-0.082652	1.461867
41	6	0	-4.520080	-1.331292	0.793345
42	7	0	-2.067792	-1.077954	0.163890
43	6	0	-2.878590	-1.271309	-1.095648
44	6	0	-4.392863	-1.233489	-0.756687
45	6	0	-2.220194	-2.282787	1.058905
46	6	0	-3.724089	-2.561560	1.271888
47	1	0	1.239785	2.776099	0.108853

48	6	0	-1.922261	1.296946	3.174502
49	1	0	-0.765980	-0.082367	2.050435
50	1	0	-4.542639	0.800382	1.320423
51	1	0	-3.841534	-0.252282	2.543231
52	1	0	-2.572879	-2.235696	-1.508305
53	1	0	-2.554888	-0.497405	-1.787412
54	6	0	-5.212878	-0.055190	-1.319837
55	1	0	-4.845703	-2.149493	-1.168143
56	1	0	-1.681215	-3.099214	0.576664
57	1	0	-1.697707	-2.056126	1.990015
58	1	0	-3.919400	-2.753847	2.332740
59	1	0	-5.574207	-1.432950	1.070987
60	1	0	-4.034767	-3.457439	0.720900
61	1	0	0.491914	1.416273	1.163210
62	1	0	-1.063184	-1.039025	-0.127633
63	6	0	-0.302801	5.423171	-1.283693
64	6	0	0.069472	6.537150	-2.019286
65	6	0	1.394911	6.764728	-2.346260
66	6	0	2.362559	5.861524	-1.926881
67	6	0	2.007639	4.747874	-1.192951
68	1	0	2.761174	4.045952	-0.861357
69	1	0	3.403695	6.028195	-2.173404
70	1	0	1.675491	7.636931	-2.920895
71	1	0	-0.693098	7.236089	-2.340122
72	1	0	-1.332981	5.231410	-1.020672
73	6	0	-2.660602	2.468560	3.297441
74	6	0	-3.054058	2.889136	4.557882
75	7	0	-2.772427	2.230075	5.708234
76	6	0	-2.048356	1.098578	5.560320
77	6	0	-1.611342	0.606446	4.337903
78	1	0	-1.808651	0.562566	6.474818
79	1	0	-1.028177	-0.304219	4.307414
80	1	0	-2.895812	3.040512	2.404522
81	1	0	-3.629659	3.804633	4.666423
82	1	0	-2.642750	0.928962	0.037589
83	6	0	-4.793830	0.960598	-2.028655
84	1	0	-6.265443	-0.137686	-1.073330
85	1	0	-5.483316	1.721205	-2.369138
86	1	0	-3.762752	1.114757	-2.314410

(*S*)-*Ac-CAT*

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.311857	2.840481	-0.562573
2	6	0	-1.293980	1.885589	-0.803690
3	7	0	-1.488444	1.109204	0.300529
4	16	0	-2.112394	1.773874	-2.267959
5	6	0	-0.009087	4.026707	-1.296103
6	6	0	-1.957974	-0.283152	0.517461
7	6	0	-1.987761	-1.191147	-0.735109
8	6	0	-2.580700	-2.602452	-0.446954
9	6	0	-1.770252	-3.627834	-1.271255
10	7	0	-0.630884	-1.317173	-1.323841
11	6	0	-0.796129	-1.809672	-2.705435
12	6	0	-1.619628	-3.144230	-2.748212
13	6	0	0.213481	-2.275425	-0.584658
14	6	0	-0.364001	-3.722474	-0.648718
15	1	0	0.429160	2.538022	0.065965

16	6	0	-3.240791	-0.335418	1.414371
17	1	0	-1.154579	-0.701545	1.119603
18	1	0	-3.644483	-2.627818	-0.712237
19	1	0	-2.510794	-2.868134	0.617730
20	1	0	0.205819	-1.967562	-3.120434
21	1	0	-1.259361	-1.013626	-3.290569
22	6	0	-2.984247	-3.125101	-3.470543
23	1	0	-1.019277	-3.910757	-3.267327
24	1	0	1.218896	-2.226873	-1.018614
25	1	0	0.312471	-1.937413	0.452813
26	1	0	-0.421711	-4.169545	0.352846
27	1	0	-2.264648	-4.605826	-1.247920
28	1	0	0.275877	-4.377141	-1.255082
29	1	0	-1.081481	1.499223	1.143400
30	6	0	-0.993763	4.790859	-1.923082
31	6	0	-0.645683	5.960430	-2.576161
32	6	0	0.671465	6.393581	-2.603464
33	6	0	1.647892	5.644285	-1.966386
34	6	0	1.314448	4.468670	-1.317874
35	1	0	-1.416856	6.543901	-3.063690
36	1	0	0.933734	7.310410	-3.113963
37	1	0	2.679173	5.974449	-1.975722
38	1	0	2.077339	3.884968	-0.820476
39	1	0	-2.021672	4.460485	-1.901952
40	6	0	-3.173564	-0.906422	2.700943
41	6	0	-4.368366	-0.965904	3.483189
42	7	0	-5.573752	-0.507572	3.069487
43	6	0	-5.611783	0.052467	1.835246
44	6	0	-4.477540	0.169766	0.975828
45	6	0	-1.973870	-1.452936	3.318754
46	6	0	-4.687285	0.814762	-0.307412
47	6	0	-3.593384	-2.113294	-4.032614
48	1	0	-4.552218	-2.237910	-4.516331
49	1	0	-3.192824	-1.110341	-4.052650
50	1	0	-3.456086	-4.102306	-3.493337
51	1	0	-2.591332	-0.715473	-1.503759
52	6	0	-4.333510	-1.554601	4.812730
53	6	0	-3.197814	-2.042590	5.326278
54	6	0	-1.984898	-1.984456	4.550037
55	6	0	-6.902775	0.548489	1.390794
56	1	0	-5.267791	-1.575485	5.359317
57	1	0	-3.169420	-2.480328	6.315772
58	1	0	-1.072647	-2.379120	4.979601
59	1	0	-1.039827	-1.430939	2.780047
60	6	0	-7.042205	1.123708	0.189266
61	6	0	-5.897275	1.263376	-0.675091
62	1	0	-3.846329	0.963335	-0.974823
63	1	0	-6.027106	1.747025	-1.635027
64	1	0	-8.002961	1.494844	-0.144989
65	1	0	-7.733741	0.430431	2.073941

(*S*)-*Ac*-*ds*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.246204	2.674267	-0.228450
2	6	0	-1.179935	1.700589	-0.455374
3	7	0	-0.937098	0.586427	0.292289
4	16	0	-2.460734	1.831044	-1.570622

5	6	0	-0.063136	3.987610	-0.759127
6	6	0	-1.714438	-0.641052	0.499289
7	6	0	-1.968208	-1.434899	-0.804418
8	6	0	-2.811214	-2.718903	-0.643264
9	6	0	-2.247187	-3.822268	-1.561858
10	7	0	-0.634038	-1.861685	-1.421774
11	6	0	-0.876934	-2.181668	-2.874835
12	6	0	-1.995816	-3.253593	-2.992546
13	6	0	-0.009805	-3.056271	-0.744344
14	6	0	-0.903240	-4.294138	-0.976627
15	1	0	0.484795	2.416365	0.442383
16	6	0	-2.885451	-0.520165	1.544567
17	1	0	-0.991922	-1.263416	1.023740
18	1	0	-3.853395	-2.496235	-0.889241
19	1	0	-2.796489	-3.068251	0.398164
20	1	0	0.076924	-2.530327	-3.274731
21	1	0	-1.114108	-1.238244	-3.364536
22	6	0	-3.314170	-2.827786	-3.671048
23	1	0	-1.596977	-4.084809	-3.595446
24	1	0	0.988994	-3.155125	-1.173527
25	1	0	0.123027	-2.800944	0.307003
26	1	0	-1.066100	-4.820921	-0.029603
27	1	0	-2.948997	-4.660796	-1.618523
28	1	0	-0.417827	-5.003139	-1.658094
29	1	0	-0.030488	0.528934	0.767319
30	6	0	-0.926567	4.599054	-1.664513
31	6	0	-0.659951	5.885388	-2.107562
32	6	0	0.453274	6.575877	-1.661720
33	6	0	1.313565	5.967482	-0.757351
34	6	0	1.062266	4.687123	-0.307517
35	1	0	-1.337865	6.350789	-2.812330
36	1	0	0.652377	7.579294	-2.013042
37	1	0	2.188132	6.496557	-0.400155
38	1	0	1.731102	4.210362	0.396346
39	1	0	-1.790436	4.047628	-2.005291
40	1	0	0.103878	-1.103837	-1.402166
41	6	0	-2.535237	-0.651988	2.906437
42	6	0	-3.578030	-0.698421	3.879101
43	7	0	-4.899928	-0.634775	3.578773
44	6	0	-5.209047	-0.446939	2.275345
45	6	0	-4.242413	-0.349011	1.225199
46	6	0	-1.172933	-0.737840	3.408723
47	6	0	-4.754791	-0.068245	-0.105044
48	6	0	-3.640302	-1.655635	-4.150385
49	1	0	-4.603319	-1.495142	-4.615491
50	1	0	-2.994491	-0.789458	-4.119565
51	1	0	-4.019962	-3.648033	-3.743379
52	1	0	-2.396852	-0.783005	-1.559159
53	6	0	-3.248028	-0.849486	5.285434
54	6	0	-1.974067	-0.928753	5.691241
55	6	0	-0.912852	-0.863976	4.719592
56	6	0	-6.625799	-0.356980	1.956843
57	1	0	-4.077753	-0.888350	5.979529
58	1	0	-1.723817	-1.035962	6.738994
59	1	0	0.111943	-0.913759	5.065937
60	1	0	-0.341169	-0.676668	2.721672
61	6	0	-7.040164	-0.143767	0.702241
62	6	0	-6.068922	0.030715	-0.350188
63	1	0	-4.043058	0.163654	-0.883415
64	1	0	-6.419764	0.268564	-1.346532
65	1	0	-8.093882	-0.072669	0.463943
66	1	0	-7.317597	-0.465195	2.782197

67	6	0	2.901611	0.985457	1.527141
68	6	0	2.534546	-0.498182	1.343551
69	8	0	2.075308	1.879614	1.421740
70	8	0	1.303424	-0.751243	1.377957
71	8	0	4.179627	1.206151	1.850775
72	6	0	4.585629	2.585553	1.958812
73	1	0	4.474632	3.079726	0.990135
74	1	0	3.983143	3.100807	2.710928
75	1	0	5.633421	2.551536	2.258004
76	6	0	3.518539	-1.570885	1.756207
77	6	0	4.884914	-1.574988	1.434844
78	6	0	5.716025	-2.596370	1.893569
79	6	0	5.200464	-3.630842	2.682038
80	6	0	3.007867	-2.617903	2.540658
81	6	0	3.841337	-3.638282	3.004083
82	1	0	5.294539	-0.795258	0.804310
83	1	0	6.769843	-2.589157	1.626008
84	1	0	5.852984	-4.424555	3.038022
85	1	0	3.428929	-4.434739	3.619216
86	1	0	1.952067	-2.611772	2.792146
87	8	0	1.598717	-0.482966	-1.818916
88	15	0	2.941860	-0.235365	-1.114646
89	8	0	4.074302	-1.307145	-1.684394
90	6	0	4.349249	-1.403342	-3.087917
91	1	0	5.034074	-2.245754	-3.217948
92	1	0	4.829813	-0.486131	-3.448441
93	1	0	3.429959	-1.585569	-3.657164
94	8	0	3.544172	1.221343	-1.663576
95	6	0	2.906795	1.972535	-2.708976
96	1	0	3.263916	1.636713	-3.690565
97	1	0	1.819751	1.865949	-2.666520
98	1	0	3.187903	3.018990	-2.560848

(*S*)-*Ac*-*ms*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.008208	3.385757	-0.533676
2	6	0	-1.073155	2.739542	0.025662
3	7	0	-0.678681	1.850407	0.978745
4	16	0	-2.686884	3.021668	-0.482224
5	6	0	0.035685	4.397502	-1.539367
6	6	0	-1.359994	0.815604	1.781397
7	6	0	-2.518505	0.106771	1.036528
8	6	0	-3.586033	-0.629564	1.868192
9	6	0	-4.078827	-1.858296	1.070086
10	7	0	-1.947806	-0.913864	0.047285
11	6	0	-2.961283	-1.089069	-1.054170
12	6	0	-4.330164	-1.496442	-0.429034
13	6	0	-1.649619	-2.249631	0.687346
14	6	0	-2.968615	-2.921880	1.117396
15	1	0	0.913194	2.987961	-0.279597
16	6	0	-1.639571	1.231227	3.266909
17	1	0	-0.588343	0.053089	1.850605
18	1	0	-4.404948	0.065917	2.076429
19	1	0	-3.192005	-0.960229	2.838616
20	1	0	-2.570363	-1.859766	-1.723029
21	1	0	-2.995524	-0.148104	-1.602420
22	6	0	-5.511198	-0.520164	-0.597424

23	1	0	-4.642838	-2.432417	-0.917398
24	1	0	-1.092121	-2.826601	-0.053435
25	1	0	-0.971210	-2.060756	1.517383
26	1	0	-2.863862	-3.326323	2.130459
27	1	0	-5.001294	-2.250523	1.510140
28	1	0	-3.214325	-3.763388	0.458343
29	1	0	0.343107	1.774118	1.054245
30	1	0	-1.030209	-0.586097	-0.359048
31	6	0	-0.929156	5.395458	-1.673675
32	6	0	-0.784231	6.369817	-2.647824
33	6	0	0.318551	6.376152	-3.485931
34	6	0	1.288604	5.394706	-3.343540
35	6	0	1.151966	4.412194	-2.381083
36	1	0	1.909317	3.647410	-2.268348
37	1	0	2.157904	5.392307	-3.988990
38	1	0	0.425133	7.142437	-4.241993
39	1	0	-1.541795	7.137302	-2.745313
40	1	0	-1.789728	5.393021	-1.021954
41	6	0	-2.698341	2.080362	3.631491
42	6	0	-2.937509	2.317905	5.018902
43	7	0	-2.182375	1.798893	6.017560
44	6	0	-1.129324	1.034142	5.641103
45	6	0	-0.809938	0.717645	4.283679
46	6	0	-0.306807	0.508949	6.718770
47	6	0	0.760232	-0.258088	6.464264
48	6	0	1.103107	-0.568407	5.099239
49	6	0	0.366820	-0.114131	4.074005
50	6	0	-3.578694	2.741770	2.686562
51	6	0	-4.057236	3.152216	5.419989
52	1	0	0.681557	-0.365886	3.072281
53	1	0	1.978475	-1.176267	4.907738
54	1	0	1.377375	-0.646757	7.264172
55	1	0	-0.599181	0.773966	7.726769
56	1	0	-3.011931	0.835173	0.400378
57	6	0	-5.500866	0.698661	-1.070777
58	1	0	-6.446961	-0.959945	-0.271378
59	1	0	-6.416376	1.270807	-1.138328
60	1	0	-4.610244	1.214712	-1.403571
61	6	0	-4.854612	3.719442	4.505468
62	6	0	-4.592655	3.515690	3.102508
63	1	0	-3.375465	2.662394	1.621293
64	1	0	-5.225251	4.014322	2.378809
65	1	0	-5.688128	4.344394	4.800604
66	1	0	-4.207252	3.291640	6.482691
67	8	0	2.134375	1.945351	0.566156
68	15	0	3.002052	0.878919	-0.114408
69	8	0	4.151967	0.373853	0.983071
70	6	0	4.383572	1.049182	2.229931
71	1	0	5.257783	1.705013	2.137525
72	1	0	3.512667	1.642019	2.522780
73	1	0	4.587415	0.282219	2.983275
74	8	0	3.903695	1.567807	-1.309676
75	6	0	4.763008	2.685424	-1.036823
76	1	0	5.105414	3.059007	-2.005032
77	1	0	5.628019	2.364094	-0.444813
78	1	0	4.222530	3.477193	-0.506070
79	6	0	2.373034	-1.174997	-2.392178
80	6	0	1.981708	-1.747058	0.166026
81	6	0	1.656512	-0.905514	-1.082866
82	8	0	0.468727	-0.467107	-1.134725
83	8	0	3.002496	-2.601430	0.015161
84	6	0	3.416344	-3.318871	1.193285

85	1	0	3.754899	-2.612909	1.955700
86	1	0	2.591412	-3.919527	1.585293
87	1	0	4.237232	-3.957558	0.865903
88	8	0	1.337905	-1.655076	1.200243
89	6	0	1.591359	-1.130495	-3.556866
90	6	0	2.154212	-1.386868	-4.809183
91	6	0	3.513537	-1.687207	-4.917322
92	6	0	3.742218	-1.462403	-2.513646
93	6	0	4.304142	-1.719342	-3.763390
94	1	0	0.539713	-0.880918	-3.464804
95	1	0	1.530170	-1.346448	-5.698908
96	1	0	3.957122	-1.883923	-5.890489
97	1	0	5.367598	-1.933632	-3.837681
98	1	0	4.377389	-1.464192	-1.635711

(*S*)-*Ac*-*dr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.520129	-1.533260	-5.778857
2	6	0	3.023002	0.517197	-3.161210
3	6	0	4.564738	0.556031	-3.070779
4	6	0	5.081733	-0.894192	-2.865796
5	6	0	4.407823	-1.749272	-3.960501
6	6	0	2.600524	-0.017441	-4.547374
7	6	0	4.865800	0.093794	-5.522303
8	6	0	5.154456	1.108530	-4.387474
9	7	0	3.810383	-0.855120	-5.032287
10	1	0	5.740762	-0.509634	-5.779623
11	1	0	4.497309	0.566907	-6.436474
12	1	0	6.235127	1.262881	-4.293861
13	1	0	4.709157	2.083010	-4.619711
14	1	0	6.170331	-0.883589	-3.041427
15	1	0	3.606797	-2.388670	-3.605453
16	1	0	2.564002	0.795939	-5.276515
17	1	0	2.617286	1.514230	-2.994930
18	1	0	4.871173	1.189733	-2.232557
19	1	0	2.608794	-0.118295	-2.373357
20	7	0	-0.427878	-2.618623	-2.039355
21	6	0	0.006410	-1.442234	-2.600922
22	7	0	0.928591	-1.681595	-3.582748
23	16	0	-0.494611	0.114025	-2.181713
24	6	0	-1.161638	-2.892766	-0.850693
25	6	0	1.274795	-0.842226	-4.727033
26	1	0	-0.187368	-3.456716	-2.578936
27	6	0	-1.456905	-4.234575	-0.584446
28	6	0	-2.151228	-4.582666	0.556965
29	6	0	-2.562191	-3.606683	1.454328
30	6	0	-2.270263	-2.278919	1.192017
31	6	0	-1.576089	-1.913441	0.049951
32	1	0	-2.373565	-5.624909	0.749004
33	1	0	-3.106438	-3.881537	2.347558
34	1	0	-2.588313	-1.509245	1.884470
35	1	0	-1.354917	-0.879656	-0.171984
36	1	0	-1.136101	-4.994827	-1.283790
37	6	0	-0.230179	1.215081	-5.509511
38	6	0	0.048028	-0.161938	-5.451357
39	6	0	-1.264439	1.669407	-6.388129
40	7	0	-2.040518	0.856153	-7.139095

41	6	0	-1.816440	-0.474929	-7.004022
42	6	0	0.430440	2.241296	-4.723171
43	1	0	5.115282	-2.397431	-4.482396
44	1	0	1.311786	-2.635351	-3.623052
45	1	0	1.578354	-1.584484	-5.471527
46	6	0	4.876479	-1.379198	-1.417661
47	6	0	4.094514	-2.339532	-0.996632
48	1	0	4.037870	-2.582590	0.055953
49	1	0	3.474015	-2.940338	-1.648210
50	1	0	5.472472	-0.818732	-0.706112
51	6	0	-0.788625	-1.031162	-6.185957
52	6	0	-0.683522	-2.479057	-6.174925
53	6	0	-2.679265	-1.350511	-7.776699
54	6	0	-2.535335	-2.681281	-7.726643
55	6	0	-1.508213	-3.254622	-6.895966
56	6	0	-1.527948	3.095006	-6.516850
57	1	0	0.058597	-2.952023	-5.553386
58	1	0	-1.403924	-4.331239	-6.859466
59	1	0	-3.179085	-3.337648	-8.298276
60	1	0	-3.437893	-0.874461	-8.384432
61	6	0	-0.850482	3.995279	-5.795352
62	6	0	0.142710	3.543797	-4.852793
63	1	0	0.642013	4.276051	-4.230857
64	1	0	-2.301663	3.382435	-7.217333
65	1	0	-1.049227	5.055370	-5.886066
66	1	0	1.123853	1.930631	-3.966731
67	8	0	3.925065	-5.336060	-7.320949
68	8	0	3.105474	-3.003392	-6.534585
69	15	0	2.761667	-4.500759	-6.462799
70	6	0	5.309155	-5.023037	-7.150066
71	1	0	5.495582	-3.962112	-7.351793
72	1	0	5.857074	-5.633736	-7.872659
73	1	0	5.650945	-5.275050	-6.138433
74	8	0	1.476939	-4.860854	-7.423825
75	6	0	1.457121	-4.456893	-8.806208
76	1	0	1.630323	-3.379404	-8.895259
77	1	0	2.217878	-5.004814	-9.370954
78	1	0	0.462696	-4.703215	-9.185317
79	6	0	0.939822	-5.670244	-4.382879
80	6	0	2.392551	-5.182886	-4.159911
81	8	0	-0.018385	-5.000283	-4.036523
82	8	0	2.468114	-4.111670	-3.490851
83	8	0	0.827378	-6.882124	-4.937630
84	6	0	-0.511473	-7.356932	-5.178843
85	1	0	-1.074137	-7.398504	-4.242766
86	1	0	-1.020136	-6.696114	-5.884490
87	1	0	-0.389352	-8.354121	-5.602578
88	6	0	3.480494	-6.232651	-3.976806
89	6	0	3.672388	-7.344287	-4.814451
90	6	0	4.681954	-8.268924	-4.544774
91	6	0	5.518268	-8.105160	-3.435264
92	6	0	4.327068	-6.075215	-2.867588
93	6	0	5.335773	-7.003274	-2.596522
94	1	0	3.047353	-7.480843	-5.687843
95	1	0	4.817902	-9.119513	-5.208507
96	1	0	6.302056	-8.829895	-3.228141
97	1	0	5.973181	-6.866674	-1.725947
98	1	0	4.173406	-5.222988	-2.215216

(*S*)-*Ac*-*mr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.146773	-0.754787	-1.631874
2	6	0	1.503473	-1.597473	-0.389976
3	8	0	0.565273	-1.725311	0.415751
4	6	0	2.648024	-2.577070	-0.380549
5	6	0	3.817485	-2.478741	-1.154865
6	6	0	2.500719	-3.681950	0.476426
7	6	0	4.798465	-3.467964	-1.080071
8	1	0	3.976137	-1.622659	-1.796793
9	6	0	3.481919	-4.669952	0.548030
10	1	0	1.606858	-3.744900	1.087579
11	6	0	4.636348	-4.568299	-0.232959
12	1	0	5.700500	-3.370614	-1.679201
13	1	0	3.347140	-5.516439	1.217141
14	1	0	5.406181	-5.334209	-0.177190
15	6	0	1.742307	0.165593	-3.725988
16	1	0	1.487097	1.182838	-3.418526
17	1	0	2.634431	0.159075	-4.352540
18	1	0	0.895479	-0.280189	-4.253653
19	8	0	0.024947	-0.278632	-1.771802
20	8	0	2.087764	-0.630609	-2.572366
21	8	0	2.068919	1.843292	0.836431
22	15	0	2.828998	0.516387	0.596079
23	8	0	3.114733	-0.222973	2.042425
24	6	0	3.709316	0.505736	3.127823
25	1	0	3.692099	-0.160172	3.994537
26	1	0	4.744129	0.771264	2.886920
27	1	0	3.136350	1.413700	3.346298
28	8	0	4.427977	0.901055	0.234343
29	6	0	4.720231	1.963215	-0.667208
30	1	0	5.800056	1.941397	-0.841575
31	1	0	4.440538	2.931069	-0.236448
32	1	0	4.203853	1.837019	-1.629897
33	7	0	0.221182	3.414826	-0.554609
34	6	0	-0.959089	2.829778	-0.184442
35	7	0	-0.758056	1.851745	0.739561
36	16	0	-2.485142	3.275787	-0.835979
37	6	0	0.535684	4.501444	-1.421053
38	6	0	-1.617616	0.899705	1.470274
39	6	0	-2.836956	0.379819	0.668900
40	6	0	-4.018763	-0.220059	1.454043
41	6	0	-4.663508	-1.341762	0.607913
42	7	0	-2.387779	-0.696644	-0.330208
43	6	0	-3.384432	-0.703947	-1.463491
44	6	0	-4.816241	-0.909340	-0.885069
45	6	0	-2.303184	-2.072548	0.294187
46	6	0	-3.722317	-2.557422	0.648254
47	1	0	1.055028	2.986447	-0.108428
48	6	0	-1.909135	1.316742	2.952025
49	1	0	-0.965826	0.032436	1.546349
50	1	0	-4.734149	0.579685	1.668930
51	1	0	-3.697967	-0.632318	2.419883
52	1	0	-3.092907	-1.517581	-2.132187
53	1	0	-3.258021	0.237959	-1.996021
54	6	0	-5.828594	0.240415	-1.055365
55	1	0	-5.253496	-1.774846	-1.406753
56	1	0	-1.787732	-2.711621	-0.424310

57	1	0	-1.650564	-1.988798	1.160122
58	1	0	-3.716216	-3.009594	1.646352
59	1	0	-5.645521	-1.604646	1.013834
60	1	0	-4.062571	-3.329331	-0.052623
61	1	0	0.238712	1.713765	0.968423
62	1	0	-1.442450	-0.471127	-0.713561
63	6	0	-0.384833	5.189626	-2.209096
64	6	0	0.041058	6.229781	-3.020548
65	6	0	1.373577	6.599027	-3.065414
66	6	0	2.293485	5.915762	-2.280918
67	6	0	1.883856	4.879738	-1.466805
68	1	0	2.598396	4.350342	-0.851572
69	1	0	3.339438	6.194953	-2.302967
70	1	0	1.696253	7.411474	-3.702262
71	1	0	-0.685767	6.756628	-3.626360
72	1	0	-1.422488	4.895223	-2.162246
73	6	0	-2.842043	2.313231	3.285987
74	6	0	-3.119615	2.552603	4.665348
75	7	0	-2.518657	1.890999	5.684775
76	6	0	-1.579390	0.977599	5.340483
77	6	0	-1.229453	0.653833	3.991912
78	6	0	-0.919999	0.293811	6.441179
79	6	0	0.027622	-0.624622	6.216750
80	6	0	0.409075	-0.938762	4.862292
81	6	0	-0.181322	-0.341707	3.816189
82	6	0	-3.554471	3.125370	2.317382
83	6	0	-4.111600	3.548023	5.033496
84	1	0	0.165770	-0.594652	2.825585
85	1	0	1.196687	-1.663091	4.695544
86	1	0	0.523993	-1.131512	7.034428
87	1	0	-1.230615	0.569599	7.440756
88	1	0	-3.204296	1.180487	0.035441
89	6	0	-5.622581	1.446928	-1.515203
90	1	0	-6.825675	-0.052439	-0.746521
91	1	0	-6.436936	2.155177	-1.587877
92	1	0	-4.657857	1.820676	-1.830835
93	6	0	-4.754966	4.257605	4.097085
94	6	0	-4.453545	4.043364	2.703780
95	1	0	-3.315649	3.030750	1.261946
96	1	0	-4.959924	4.650439	1.963748
97	1	0	-5.492123	5.002939	4.367929
98	1	0	-4.296897	3.686331	6.090832

S5 Energies of optimized structures with differnet R substituents.

Species	E_{ZPE} (Hartree)	Gc[a] (Hartree)	SCF_{PCM}[b] (Hartree)	D_c[c] (Hartree)	$SCF_{PCM}+G_c+D_c$ (Hartree)	ΔG (kcal/mol)
R=Me	-	-	-	-	-	-
Me-α-ketoester	−381.61897	0.06560	−381.82595	−0.01579	−381.77615	-
Me-product	-1029.03854	0.16063	-1029.46390	−0.04626	−1029.34953	−14.1
Me-*k*-**IM0**	−1992.70021	0.56181	−2006.95255	−0.17466	−2006.56540	10.7
Me-*k*-**IM1**	−2640.11504	0.65342	−2654.57789	−0.21270	−2654.13717	−2.4
Me-*k*-**TS1**	−2640.09559	0.65320	−2654.55789	−0.22126	−2654.12595	4.7
Me-*k*-**IM2**	−2640.09661	0.65734	−2654.56705	−0.21999	−2654.12971	2.3
Me-*ds*-**IM3**	−2640.12752	0.65604	−2654.59825	−0.21690	−2654.15911	−16.1
Me-*ds*-**TS2**	−2640.12609	0.66058	−2654.59720	−0.21782	−2654.15444	−13.2
Me-*ds*-**IM4**	−2640.13092	0.66225	−2654.60126	−0.21708	−2654.15609	−14.2
Me-*ds*-**TS3**	−2640.13346	0.65885	−2654.60046	−0.21698	−2654.15859	−15.8
Me-*ds*-**IM5**	−2640.13644	0.66088	−2654.60777	−0.21347	−2654.16036	−16.9
Me-*ms*-**TS2**	−2640.12413	0.66010	−2654.59333	−0.21696	−2654.15019	0.3
Me-*dr*-**TS2**	−2640.11760	0.65954	−2654.58893	−0.21869	−2654.14808	1.6
Me-*mr*-**TS2**	−2640.11854	0.66151	−2654.58831	−0.21747	−2654.14428	4.0
R=Et	-	-	-			-
Et-α-ketoester	−420.90548	0.09176	−421.15079	−0.02064	−421.07967	-
Et-*ds*-**TS2**	−2679.41112	0.68816	−2693.92023	−0.22541	−2693.45748	−2.1
Et-*ms*-**TS2**	−2679.40789	0.68770	−2693.91515	−0.22430	−2693.45175	1.5
Et-*dr*-**TS2**	−2679.40316	0.68682	−2693.91221	−0.22691	−2693.45230	1.1
Et-*mr*-**TS2**	−2679.40401	0.68769	−2693.91129	−0.22430	−2693.44791	3.9
R=*i*Pr	-	-	-			-
*i*Pr-α-ketoester	−460.19117	0.11891	−460.47388	−0.23349	−2732.76203	-
*i*Pr-*ds*-**TS2**	−2718.69642	0.71464	−2733.24318	−0.23204	−2732.75289	−3.4
*i*Pr-*ms*-**TS2**	−2718.68996	0.71387	−2733.23472	−0.23497	−2732.75651	2.3
*i*Pr-*dr*-**TS2**	−2718.68893	0.71410	−2733.23563	−0.23062	−2732.74859	0.0
*i*Pr-*mr*-**TS2**	−2718.69005	0.71457	−2733.23254	−0.23349	−2732.76203	5.0

a: Thermal correction to Gibbs Free Energy.
b: Total electronic energies in solvent.
c: Dispersion effect correction energy.

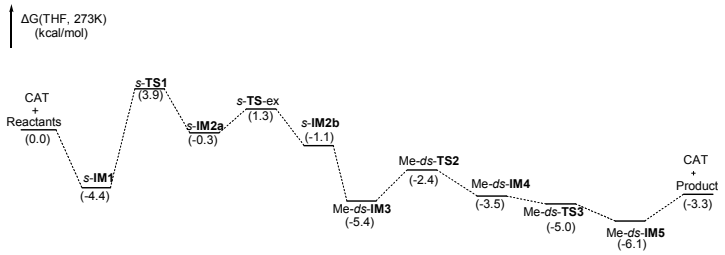


Fig S1. The energy profile of the catalytic cycle of hydrophosphonylation of methyl substituted α-ketoester.

S6: Cartesian coordinates of optimized structures with differnet R substituents.

Me-α-ketoester

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.272123	0.018295	-1.554649
2	6	0	-2.056033	-0.697107	-2.211837
3	8	0	-4.333393	-0.807933	-1.459871
4	6	0	-5.519971	-0.243031	-0.861353
5	1	0	-5.305314	0.083466	0.159305
6	1	0	-5.866547	0.609707	-1.450642
7	1	0	-6.256868	-1.045858	-0.867007
8	6	0	-2.220882	-2.129228	-2.659733
9	1	0	-3.034071	-2.211221	-3.390569
10	1	0	-1.284129	-2.477274	-3.100183
11	1	0	-2.498029	-2.766680	-1.811904
12	8	0	-3.256044	1.166108	-1.181098
13	8	0	-1.029584	-0.067140	-2.334071

Me-*k*-**IM0**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.190501	-0.166318	-1.642769
2	6	0	-2.195516	-0.776878	-2.670454
3	8	0	-4.404683	-0.713942	-1.735026
4	6	0	-5.411579	-0.210385	-0.821972
5	1	0	-5.093255	-0.379203	0.209253
6	1	0	-5.563517	0.857868	-0.992541
7	1	0	-6.313231	-0.776359	-1.051894
8	8	0	-2.874372	0.704292	-0.861290
9	8	0	-1.066728	-0.332053	-2.675013
10	7	0	-0.790421	2.798173	0.227583
11	6	0	0.480075	2.848073	-0.310818
12	7	0	0.625201	1.952218	-1.333880
13	16	0	1.699190	3.906088	0.170999
14	6	0	1.864481	1.463546	-1.957006
15	6	0	2.378056	0.201047	-1.165926
16	6	0	3.665968	-0.496122	-1.699845
17	6	0	4.315671	-1.229998	-0.504115
18	7	0	2.397647	0.281805	0.310511
19	6	0	3.672565	0.784860	0.848378
20	6	0	4.859494	-0.190400	0.517098
21	6	0	2.193839	-1.086832	0.823111
22	6	0	3.238119	-2.074635	0.210458
23	1	0	-1.393203	2.069337	-0.154041
24	1	0	1.502878	0.997650	-2.885934
25	1	0	1.553639	-0.497801	-1.358243
26	1	0	4.380611	0.207169	-2.138382
27	1	0	3.405319	-1.211086	-2.492213
28	1	0	3.551315	0.898027	1.931384
29	1	0	3.829818	1.787714	0.455478
30	6	0	6.172564	0.481555	0.059564

31	1	0	5.110462	-0.757468	1.431997
32	1	0	2.282232	-1.044490	1.915028
33	1	0	1.167631	-1.401022	0.595502
34	1	0	2.762854	-2.758576	-0.506497
35	1	0	5.131400	-1.872726	-0.855530
36	1	0	3.696887	-2.697452	0.989647
37	1	0	-0.158723	1.329418	-1.507907
38	6	0	-1.457222	3.607832	1.191816
39	6	0	-0.867155	4.684199	1.851882
40	6	0	-2.788434	3.281016	1.475495
41	6	0	-1.601860	5.412994	2.773103
42	1	0	0.162127	4.921170	1.622902
43	6	0	-3.506758	4.016346	2.396984
44	1	0	-3.246614	2.446253	0.963078
45	6	0	-2.918562	5.088667	3.052742
46	1	0	-1.132571	6.247764	3.279115
47	1	0	-4.535682	3.751363	2.605737
48	1	0	-3.483292	5.663507	3.773998
49	6	0	2.774762	2.613014	-2.485871
50	6	0	4.064566	2.811347	-2.127564
51	6	0	2.236098	3.483624	-3.515731
52	6	0	4.836439	3.853677	-2.727999
53	1	0	4.550804	2.211689	-1.378362
54	6	0	3.071116	4.480301	-4.049991
55	6	0	0.906148	3.385921	-4.034243
56	7	0	4.402023	4.678840	-3.651713
57	1	0	5.866670	3.981490	-2.402357
58	6	0	2.577009	5.355742	-5.067631
59	6	0	1.311156	5.234647	-5.530853
60	6	0	0.462472	4.225772	-5.000868
61	1	0	0.936030	5.895952	-6.301305
62	1	0	3.252776	6.110591	-5.448923
63	1	0	-0.548292	4.134561	-5.377689
64	1	0	0.241941	2.633060	-3.638986
65	6	0	6.599909	1.662073	0.429132
66	1	0	6.790059	-0.132146	-0.588119
67	1	0	7.552415	2.049310	0.095055
68	1	0	6.034786	2.311736	1.082559
69	6	0	-2.675289	-1.866953	-3.588917
70	1	0	-3.519831	-1.511963	-4.191526
71	1	0	-1.855825	-2.180596	-4.238532
72	1	0	-3.044824	-2.720187	-3.007621

Me-*k*-**IM1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.335221	-0.114130	-1.739748
2	6	0	-2.203791	-1.089438	-2.152438
3	8	0	-4.478044	-0.753279	-1.493644
4	6	0	-5.583055	0.056440	-1.034957
5	1	0	-5.328481	0.502869	-0.070859
6	1	0	-5.803873	0.839733	-1.763964
7	1	0	-6.421243	-0.632488	-0.934904
8	8	0	-3.184344	1.089607	-1.697094
9	8	0	-1.158688	-0.602326	-2.537513
10	7	0	-1.116255	2.745079	-0.218541
11	6	0	0.239508	2.547296	-0.387033
12	7	0	0.505856	1.722716	-1.439564

13	16	0	1.439219	3.209945	0.600643
14	6	0	1.794985	1.397849	-2.071698
15	6	0	2.327270	-0.015434	-1.619545
16	6	0	3.688246	-0.442234	-2.251779
17	6	0	4.363815	-1.436023	-1.282197
18	7	0	2.278752	-0.384564	-0.184460
19	6	0	3.481342	0.022964	0.564967
20	6	0	4.765879	-0.710234	0.033496
21	6	0	2.185890	-1.861728	-0.126222
22	6	0	3.346876	-2.536617	-0.919766
23	1	0	-1.718785	2.214698	-0.852041
24	1	0	1.501773	1.165441	-3.105903
25	1	0	1.560782	-0.666920	-2.054568
26	1	0	4.351467	0.408507	-2.435153
27	1	0	3.516077	-0.919738	-3.225813
28	1	0	3.308167	-0.217006	1.620304
29	1	0	3.559435	1.107256	0.509013
30	6	0	6.025787	0.170759	-0.114000
31	1	0	5.033456	-1.504747	0.753441
32	1	0	2.210443	-2.150074	0.930244
33	1	0	1.209667	-2.168963	-0.518744
34	1	0	2.973322	-3.017439	-1.834186
35	1	0	5.250915	-1.876030	-1.752646
36	1	0	3.827543	-3.320544	-0.320054
37	1	0	-0.284770	1.250529	-1.872101
38	6	0	-1.855953	3.649717	0.599912
39	6	0	-1.278053	4.566115	1.476258
40	6	0	-3.250670	3.599778	0.488824
41	6	0	-2.085540	5.408278	2.224111
42	1	0	-0.200465	4.592895	1.551801
43	6	0	-4.041358	4.445126	1.240847
44	1	0	-3.697860	2.893444	-0.196985
45	6	0	-3.464413	5.355483	2.115698
46	1	0	-1.623728	6.116278	2.901278
47	1	0	-5.118623	4.395130	1.143215
48	1	0	-4.086249	6.016510	2.703940
49	6	0	2.693457	2.660160	-2.256758
50	6	0	3.916983	2.833244	-1.706088
51	6	0	2.213874	3.707907	-3.139960
52	6	0	4.683474	4.007348	-1.983326
53	1	0	4.351423	2.110289	-1.038017
54	6	0	3.037233	4.827610	-3.353175
55	6	0	0.953891	3.676010	-3.818112
56	7	0	4.301303	4.989185	-2.766187
57	1	0	5.660493	4.105225	-1.514916
58	6	0	2.601558	5.881687	-4.216627
59	6	0	1.401456	5.816422	-4.838565
60	6	0	0.564412	4.686680	-4.632434
61	1	0	1.069971	6.613135	-5.492004
62	1	0	3.266914	6.725139	-4.350127
63	1	0	-0.394046	4.640561	-5.133852
64	1	0	0.295793	2.833243	-3.673800
65	6	0	6.340904	1.187338	0.647761
66	1	0	6.707314	-0.142427	-0.898047
67	1	0	7.262703	1.734893	0.509002
68	1	0	5.706795	1.535659	1.450949
69	1	0	0.189785	-0.388144	1.084521
70	15	0	-0.986223	-0.892571	1.658087
71	8	0	-0.504240	-2.378493	2.058522
72	6	0	-1.386052	-3.269217	2.770016
73	1	0	-2.341052	-3.368284	2.244342
74	1	0	-1.552764	-2.901635	3.786830

75	1	0	-0.878247	-4.234582	2.801985
76	8	0	-1.134144	-0.220293	3.119337
77	6	0	-1.615073	1.132298	3.278091
78	1	0	-2.587393	1.251037	2.791718
79	1	0	-1.711772	1.289173	4.353534
80	1	0	-0.893229	1.841630	2.862275
81	8	0	-2.203978	-0.805644	0.791425
82	6	0	-2.465166	-2.566888	-2.077586
83	1	0	-2.743959	-2.831646	-1.052410
84	1	0	-3.309811	-2.837130	-2.722611
85	1	0	-1.570353	-3.112159	-2.385064

Me-*k*-**TS1**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.044901	0.253301	-1.969397
2	6	0	-2.098648	-0.904060	-2.367019
3	8	0	-4.277723	-0.175432	-1.711145
4	6	0	-5.227103	0.810831	-1.256886
5	1	0	-4.904644	1.202605	-0.289271
6	1	0	-5.308422	1.622533	-1.984013
7	1	0	-6.172476	0.277332	-1.160979
8	8	0	-2.700070	1.421371	-1.977553
9	8	0	-1.004857	-0.602526	-2.809294
10	7	0	-1.096492	3.098411	-0.081242
11	6	0	0.216008	2.725785	-0.244896
12	7	0	0.360762	1.837976	-1.282127
13	16	0	1.499924	3.255521	0.711971
14	6	0	1.567862	1.496615	-2.048324
15	6	0	2.108274	0.039916	-1.737730
16	6	0	3.523469	-0.289754	-2.300399
17	6	0	4.208088	-1.313711	-1.373474
18	7	0	2.008605	-0.499950	-0.335581
19	6	0	3.133731	-0.072240	0.540195
20	6	0	4.472013	-0.699441	0.033533
21	6	0	2.009043	-2.000915	-0.428952
22	6	0	3.254027	-2.506289	-1.194496
23	1	0	-1.743961	2.677789	-0.749852
24	1	0	1.169693	1.312511	-3.052234
25	1	0	1.384647	-0.585170	-2.266177
26	1	0	4.143770	0.603371	-2.393498
27	1	0	3.425063	-0.707289	-3.310144
28	1	0	2.890686	-0.393788	1.557770
29	1	0	3.139060	1.016375	0.543967
30	6	0	5.690953	0.246362	0.072717
31	1	0	4.724042	-1.549303	0.691948
32	1	0	1.969195	-2.373703	0.597191
33	1	0	1.073444	-2.297353	-0.910850
34	1	0	2.973083	-2.914829	-2.173219
35	1	0	5.153637	-1.644234	-1.817325
36	1	0	3.741177	-3.314654	-0.636264
37	1	0	-0.498287	1.510532	-1.720571
38	6	0	-1.749591	3.954672	0.853472
39	6	0	-1.108665	4.606457	1.904921
40	6	0	-3.125761	4.137912	0.674935
41	6	0	-1.838776	5.420650	2.756398
42	1	0	-0.045810	4.460109	2.029531
43	6	0	-3.839292	4.952129	1.531188

44	1	0	-3.623475	3.635237	-0.143017
45	6	0	-3.199961	5.599689	2.579376
46	1	0	-1.329740	5.921612	3.570606
47	1	0	-4.903298	5.083903	1.379589
48	1	0	-3.760373	6.237615	3.249249
49	6	0	2.505499	2.722886	-2.266745
50	6	0	3.705296	2.903885	-1.667590
51	6	0	2.067570	3.745351	-3.197239
52	6	0	4.506832	4.047422	-1.971439
53	1	0	4.093501	2.209634	-0.941369
54	6	0	2.924206	4.835363	-3.435356
55	6	0	0.812719	3.727760	-3.886220
56	7	0	4.174300	4.992974	-2.819219
57	1	0	5.467552	4.150243	-1.471819
58	6	0	2.535336	5.864755	-4.349595
59	6	0	1.343025	5.809735	-4.987179
60	6	0	0.466069	4.717688	-4.744080
61	1	0	1.045222	6.588591	-5.677411
62	1	0	3.227541	6.682588	-4.504692
63	1	0	-0.490027	4.684642	-5.251298
64	1	0	0.119403	2.918640	-3.713525
65	6	0	5.869101	1.232998	0.913745
66	1	0	6.467099	0.001726	-0.644136
67	1	0	6.773572	1.825602	0.903055
68	1	0	5.136448	1.512292	1.658430
69	1	0	0.845307	-0.338220	0.252844
70	15	0	-0.693218	-0.612521	1.059513
71	8	0	-0.454199	-2.143543	1.694443
72	6	0	-1.470563	-2.768966	2.485167
73	1	0	-2.447872	-2.703045	1.993146
74	1	0	-1.526675	-2.303220	3.476985
75	1	0	-1.189245	-3.819827	2.599828
76	8	0	-0.779912	0.326107	2.421821
77	6	0	-2.011235	0.810065	2.965701
78	1	0	-2.772878	0.907033	2.185680
79	1	0	-2.376067	0.128658	3.745113
80	1	0	-1.803060	1.787287	3.410335
81	8	0	-2.034629	-0.571982	0.325246
82	6	0	-2.602559	-2.314898	-2.250423
83	1	0	-2.914655	-2.500972	-1.218861
84	1	0	-3.479173	-2.456578	-2.894510
85	1	0	-1.812189	-3.009044	-2.544822

Me-*k*-**IM2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.914046	0.346458	-1.980213
2	6	0	-2.042421	-0.902318	-2.205673
3	8	0	-4.211329	0.051930	-1.919236
4	6	0	-5.115257	1.139987	-1.649607
5	1	0	-4.938900	1.515429	-0.638476
6	1	0	-4.976051	1.942597	-2.378164
7	1	0	-6.114293	0.711282	-1.728711
8	8	0	-2.465897	1.484491	-1.985239
9	8	0	-0.875419	-0.722417	-2.526474
10	7	0	-0.962997	3.216711	-0.054784
11	6	0	0.338112	2.883272	-0.313587
12	7	0	0.437327	2.018363	-1.375904

13	16	0	1.678415	3.434662	0.556473
14	6	0	1.619968	1.637947	-2.152894
15	6	0	2.118091	0.186320	-1.775971
16	6	0	3.501008	-0.274843	-2.301038
17	6	0	4.100386	-1.296999	-1.312919
18	7	0	2.013185	-0.235423	-0.315973
19	6	0	3.192983	0.168563	0.524819
20	6	0	4.450468	-0.609786	0.039794
21	6	0	1.864465	-1.745999	-0.279671
22	6	0	3.048947	-2.386208	-1.034368
23	1	0	-1.643494	2.779078	-0.679479
24	1	0	1.201971	1.419056	-3.143006
25	1	0	1.352388	-0.443775	-2.228705
26	1	0	4.188866	0.561096	-2.438278
27	1	0	3.367786	-0.737092	-3.286063
28	1	0	2.928405	-0.056973	1.560561
29	1	0	3.277066	1.249412	0.438321
30	6	0	5.742185	0.231844	-0.019053
31	1	0	4.644067	-1.426780	0.755487
32	1	0	1.811842	-2.022620	0.774417
33	1	0	0.895490	-1.977675	-0.721138
34	1	0	2.708764	-2.831706	-1.976651
35	1	0	5.002648	-1.743861	-1.743132
36	1	0	3.480266	-3.194582	-0.433535
37	1	0	-0.439957	1.650058	-1.747970
38	6	0	-1.577483	3.986682	0.980459
39	6	0	-0.881941	4.633588	1.998588
40	6	0	-2.972120	4.089287	0.932559
41	6	0	-1.577939	5.363292	2.949868
42	1	0	0.194238	4.549915	2.024137
43	6	0	-3.651278	4.820374	1.886194
44	1	0	-3.512137	3.587710	0.141262
45	6	0	-2.957491	5.462991	2.902594
46	1	0	-1.027042	5.860575	3.738588
47	1	0	-4.730700	4.889461	1.837020
48	1	0	-3.491063	6.035236	3.649447
49	6	0	2.588717	2.825414	-2.431039
50	6	0	3.826533	2.966241	-1.903009
51	6	0	2.137726	3.847517	-3.354712
52	6	0	4.651995	4.073798	-2.269821
53	1	0	4.229320	2.270883	-1.186052
54	6	0	3.019736	4.900556	-3.657348
55	6	0	0.847888	3.862983	-3.974906
56	7	0	4.307142	5.018724	-3.113043
57	1	0	5.642422	4.147032	-1.826255
58	6	0	2.619087	5.929594	-4.566611
59	6	0	1.392333	5.907790	-5.137839
60	6	0	0.491311	4.852056	-4.829912
61	1	0	1.085190	6.686591	-5.824184
62	1	0	3.330481	6.719194	-4.772787
63	1	0	-0.491418	4.846384	-5.284754
64	1	0	0.136908	3.082625	-3.749487
65	6	0	6.007425	1.287698	0.706813
66	1	0	6.488671	-0.158265	-0.701586
67	1	0	6.959172	1.795769	0.630291
68	1	0	5.308717	1.710559	1.415980
69	1	0	1.116719	0.126452	0.103283
70	15	0	-1.045638	-0.444087	1.066077
71	8	0	-0.683693	-1.995504	1.679803
72	6	0	-1.700740	-2.838252	2.221549
73	1	0	-2.623972	-2.769866	1.633736
74	1	0	-1.912237	-2.568148	3.264850

75	1	0	-1.328961	-3.868771	2.194173
76	8	0	-1.500893	0.377153	2.463098
77	6	0	-2.847434	0.424348	2.934184
78	1	0	-3.558495	0.357848	2.103340
79	1	0	-3.041777	-0.396640	3.637975
80	1	0	-2.975492	1.376747	3.459806
81	8	0	-2.346311	-0.615356	0.229437
82	6	0	-2.700989	-2.254769	-2.187584
83	1	0	-3.333438	-2.359009	-1.305041
84	1	0	-3.332221	-2.361157	-3.080623
85	1	0	-1.930233	-3.029161	-2.202471

Me-*ds*-**IM3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.389077	2.883309	-0.207318
2	6	0	-1.265279	1.850952	-0.401303
3	7	0	-0.891998	0.726128	0.283349
4	16	0	-2.649793	1.907952	-1.381883
5	6	0	-0.326174	4.209394	-0.731348
6	6	0	-1.653370	-0.509579	0.488932
7	6	0	-1.830438	-1.328520	-0.809239
8	6	0	-2.582487	-2.669473	-0.623582
9	6	0	-1.932537	-3.754295	-1.505200
10	7	0	-0.487071	-1.658362	-1.444835
11	6	0	-0.725406	-2.042141	-2.882459
12	6	0	-1.740973	-3.215717	-2.955587
13	6	0	0.239428	-2.776316	-0.740810
14	6	0	-0.550389	-4.091721	-0.917140
15	1	0	0.393115	2.665722	0.415233
16	6	0	-2.969320	-0.263519	1.284324
17	1	0	-1.000577	-1.099169	1.136241
18	1	0	-3.634843	-2.538786	-0.890272
19	1	0	-2.557944	-2.987562	0.427907
20	1	0	0.250377	-2.309936	-3.291589
21	1	0	-1.056217	-1.138270	-3.392246
22	6	0	-3.097079	-2.935770	-3.635940
23	1	0	-1.272425	-4.027669	-3.534141
24	1	0	1.237541	-2.809731	-1.181934
25	1	0	0.358107	-2.480599	0.302513
26	1	0	-0.662881	-4.594477	0.050175
27	1	0	-2.562894	-4.649535	-1.525620
28	1	0	-0.013323	-4.783162	-1.577606
29	1	0	-0.030043	0.765405	0.826864
30	6	0	-1.270266	4.757510	-1.595974
31	6	0	-1.117979	6.060961	-2.042511
32	6	0	-0.040067	6.830385	-1.640591
33	6	0	0.900859	6.284719	-0.777622
34	6	0	0.763439	4.988127	-0.324794
35	1	0	-1.857630	6.477106	-2.715305
36	1	0	0.069644	7.846547	-1.994500
37	1	0	1.749330	6.875356	-0.455694
38	1	0	1.496383	4.561166	0.346378
39	1	0	-2.105788	4.144615	-1.901058
40	1	0	0.211579	-0.842783	-1.475264
41	6	0	-2.901854	-0.059550	2.714820
42	6	0	-4.106400	0.167952	3.403998
43	7	0	-5.362184	0.214840	2.780030

44	6	0	-5.356210	0.038671	1.478637
45	6	0	-4.185229	-0.201557	0.693896
46	6	0	-1.688618	-0.068793	3.473869
47	1	0	-4.306125	-0.316293	-0.372594
48	6	0	-3.538081	-1.811822	-4.138247
49	1	0	-4.513974	-1.755561	-4.600784
50	1	0	-2.978543	-0.887205	-4.130877
51	1	0	-3.720563	-3.821852	-3.685657
52	1	0	-2.332456	-0.700322	-1.543856
53	6	0	-4.089847	0.370497	4.819940
54	6	0	-2.923416	0.351655	5.506290
55	6	0	-1.701267	0.129092	4.814416
56	1	0	-6.318599	0.078716	0.973127
57	1	0	-5.038630	0.540413	5.312901
58	1	0	-2.907359	0.506725	6.577530
59	1	0	-0.773371	0.121040	5.372493
60	1	0	-0.744834	-0.229017	2.972868
61	6	0	2.747551	1.185834	1.675301
62	6	0	2.484067	-0.325893	1.755135
63	8	0	1.857156	2.009124	1.522656
64	8	0	1.312149	-0.694353	1.808582
65	8	0	4.028347	1.496290	1.893394
66	6	0	4.395440	2.880520	1.711615
67	1	0	4.241136	3.155578	0.665071
68	1	0	3.799258	3.520637	2.366430
69	1	0	5.452217	2.932516	1.973298
70	8	0	1.588894	-0.138729	-1.894812
71	15	0	2.903240	0.075633	-1.096768
72	8	0	4.012177	-1.066243	-1.640459
73	6	0	4.322143	-1.194628	-3.030757
74	1	0	4.905843	-2.112842	-3.148887
75	1	0	4.923173	-0.342443	-3.371376
76	1	0	3.409763	-1.261701	-3.636610
77	8	0	3.570834	1.505107	-1.688125
78	6	0	3.067836	2.166881	-2.855088
79	1	0	3.567216	1.790611	-3.757753
80	1	0	1.988405	2.020449	-2.955611
81	1	0	3.292562	3.232279	-2.742294
82	6	0	3.643136	-1.259635	2.008345
83	1	0	4.537603	-0.974348	1.454316
84	1	0	3.879027	-1.228985	3.082358
85	1	0	3.347601	-2.278889	1.748768

Me- *ds*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.307164	2.646885	-0.138879
2	6	0	-1.246914	1.674744	-0.351407
3	7	0	-0.917376	0.503136	0.267731
4	16	0	-2.655720	1.850526	-1.286095
5	6	0	-0.186366	3.990292	-0.605293
6	6	0	-1.740229	-0.693320	0.450614
7	6	0	-1.972959	-1.457548	-0.870808
8	6	0	-2.792437	-2.763461	-0.738494
9	6	0	-2.188601	-3.849225	-1.651641
10	7	0	-0.641950	-1.835167	-1.511913
11	6	0	-0.886727	-2.152161	-2.964716
12	6	0	-1.955770	-3.274018	-3.082599

13	6	0	0.027209	-3.012309	-0.844860
14	6	0	-0.832073	-4.276287	-1.062715
15	1	0	0.469188	2.366573	0.469894
16	6	0	-3.021828	-0.408476	1.283735
17	1	0	-1.105610	-1.336402	1.065552
18	1	0	-3.834014	-2.570163	-1.009234
19	1	0	-2.793659	-3.118089	0.301346
20	1	0	0.078230	-2.449604	-3.379034
21	1	0	-1.174642	-1.216285	-3.441714
22	6	0	-3.289501	-2.908551	-3.766337
23	1	0	-1.519152	-4.088527	-3.681981
24	1	0	1.019519	-3.081200	-1.293998
25	1	0	0.169941	-2.749450	0.203790
26	1	0	-0.980738	-4.797572	-0.110278
27	1	0	-2.862734	-4.710244	-1.708171
28	1	0	-0.327927	-4.978843	-1.737261
29	1	0	-0.007808	0.421105	0.735450
30	6	0	-1.111263	4.618719	-1.435471
31	6	0	-0.900476	5.930652	-1.830365
32	6	0	0.217669	6.629787	-1.410663
33	6	0	1.139568	6.003977	-0.582121
34	6	0	0.944379	4.697920	-0.180694
35	1	0	-1.626012	6.409615	-2.476186
36	1	0	0.373002	7.653332	-1.723846
37	1	0	2.018754	6.539567	-0.246590
38	1	0	1.661516	4.207380	0.463688
39	1	0	-1.979853	4.060322	-1.752862
40	1	0	0.077058	-1.059016	-1.491012
41	6	0	-2.900789	-0.234864	2.714442
42	6	0	-4.073389	0.022373	3.446457
43	7	0	-5.345575	0.127952	2.863901
44	6	0	-5.387216	-0.020610	1.559689
45	6	0	-4.251646	-0.288404	0.732889
46	6	0	-1.663726	-0.301925	3.431338
47	1	0	-4.409617	-0.376889	-0.331314
48	6	0	-3.675501	-1.747593	-4.228094
49	1	0	-4.642519	-1.630930	-4.697964
50	1	0	-3.077188	-0.848895	-4.178319
51	1	0	-3.949848	-3.764057	-3.857271
52	1	0	-2.436895	-0.775556	-1.583106
53	6	0	-4.003610	0.194987	4.864710
54	6	0	-2.816720	0.120260	5.511076
55	6	0	-1.626028	-0.130699	4.775119
56	1	0	-6.362869	0.066218	1.086517
57	1	0	-4.928828	0.388793	5.392355
58	1	0	-2.760299	0.252769	6.584000
59	1	0	-0.681263	-0.181560	5.301745
60	1	0	-0.742504	-0.481806	2.895187
61	6	0	2.877028	0.949372	1.512306
62	6	0	2.506767	-0.525062	1.315473
63	8	0	2.069004	1.864228	1.442518
64	8	0	1.289260	-0.816238	1.401343
65	8	0	4.171912	1.132847	1.804719
66	6	0	4.622404	2.499235	1.893737
67	1	0	4.497658	2.990636	0.925330
68	1	0	4.058237	3.037006	2.659803
69	1	0	5.677460	2.436094	2.160947
70	8	0	1.600641	-0.466593	-1.900375
71	15	0	2.907820	-0.221747	-1.127316
72	8	0	4.057810	-1.322891	-1.609392
73	6	0	4.433576	-1.432180	-2.988796
74	1	0	5.113564	-2.285043	-3.065116

75	1	0	4.952169	-0.523943	-3.317025
76	1	0	3.555756	-1.604645	-3.623020
77	8	0	3.566022	1.207798	-1.685401
78	6	0	2.948709	1.973351	-2.731514
79	1	0	3.171868	1.538576	-3.713407
80	1	0	1.863936	2.021861	-2.602381
81	1	0	3.377924	2.977544	-2.674354
82	6	0	3.565337	-1.569603	1.632111
83	1	0	4.555646	-1.305498	1.260435
84	1	0	3.614951	-1.678863	2.725068
85	1	0	3.260096	-2.529491	1.208079

Me-*ds*-**IM4**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.434676	2.927107	-0.179869
2	6	0	-1.354579	1.930704	0.061779
3	7	0	-0.773861	0.694513	0.093108
4	16	0	-3.014334	2.194119	0.241141
5	6	0	-0.579020	4.341250	-0.078477
6	6	0	-1.465082	-0.595423	-0.048906
7	6	0	-2.042472	-0.706248	-1.491550
8	6	0	-3.123683	-1.756621	-1.833153
9	6	0	-2.890808	-2.278505	-3.268605
10	7	0	-0.873253	-0.961903	-2.450592
11	6	0	-1.249297	-0.456014	-3.815500
12	6	0	-2.603708	-1.092925	-4.242276
13	6	0	-0.518793	-2.426835	-2.538814
14	6	0	-1.656142	-3.193108	-3.242822
15	1	0	0.422517	2.630068	-0.658429
16	6	0	-2.367933	-0.936429	1.167723
17	1	0	-0.642312	-1.315805	-0.007745
18	1	0	-4.108426	-1.289397	-1.754247
19	1	0	-3.108678	-2.598074	-1.128104
20	1	0	-0.425884	-0.724485	-4.480271
21	1	0	-1.283658	0.631481	-3.749898
22	6	0	-3.824162	-0.156599	-4.363672
23	1	0	-2.459514	-1.537226	-5.240292
24	1	0	0.427534	-2.472859	-3.075613
25	1	0	-0.341727	-2.774799	-1.519702
26	1	0	-1.876867	-4.120293	-2.701115
27	1	0	-3.770938	-2.831226	-3.613749
28	1	0	-1.363793	-3.475136	-4.261596
29	1	0	0.215336	0.624932	-0.195347
30	6	0	-1.483019	4.957504	0.787091
31	6	0	-1.533362	6.339328	0.862850
32	6	0	-0.686765	7.124563	0.097190
33	6	0	0.223045	6.513533	-0.752675
34	6	0	0.279832	5.135689	-0.843626
35	1	0	-2.242143	6.805949	1.535602
36	1	0	-0.732046	8.203081	0.164319
37	1	0	0.894085	7.115929	-1.352115
38	1	0	0.990801	4.654922	-1.501723
39	1	0	-2.146676	4.349362	1.382943
40	1	0	0.044896	-0.484864	-2.112154
41	6	0	-1.728603	-1.336660	2.402784
42	6	0	-2.551017	-1.672964	3.492679
43	7	0	-3.952485	-1.631536	3.450703

44	6	0	-4.472745	-1.236425	2.311298
45	6	0	-3.719663	-0.879702	1.150051
46	6	0	-0.311048	-1.400493	2.590476
47	1	0	-4.262817	-0.550034	0.278731
48	6	0	-3.872930	1.140802	-4.207546
49	1	0	-4.799811	1.682293	-4.338091
50	1	0	-3.018825	1.748729	-3.945604
51	1	0	-4.727088	-0.693626	-4.633176
52	1	0	-2.421902	0.280752	-1.760538
53	6	0	-1.961370	-2.080470	4.730801
54	6	0	-0.616361	-2.136699	4.869588
55	6	0	0.221476	-1.784564	3.775794
56	1	0	-5.558043	-1.184963	2.259055
57	1	0	-2.629242	-2.335042	5.543847
58	1	0	-0.167614	-2.441920	5.806233
59	1	0	1.296402	-1.822568	3.900266
60	1	0	0.346827	-1.122818	1.779894
61	6	0	2.659074	1.600056	-2.325945
62	6	0	2.616568	0.146510	-1.783741
63	8	0	1.863416	2.461887	-2.001859
64	8	0	1.375848	-0.176354	-1.331979
65	8	0	3.696744	1.850459	-3.146821
66	6	0	3.828549	3.208989	-3.616000
67	1	0	2.939652	3.502184	-4.179946
68	1	0	3.966321	3.888041	-2.770777
69	1	0	4.710738	3.209048	-4.256874
70	8	0	2.034884	-1.069944	-4.300748
71	15	0	3.025893	-1.067056	-3.172485
72	8	0	3.096818	-2.446516	-2.318133
73	6	0	3.519630	-3.663747	-2.953070
74	1	0	3.394142	-4.454438	-2.210360
75	1	0	4.571801	-3.595288	-3.246893
76	1	0	2.902567	-3.880549	-3.832282
77	8	0	4.572369	-0.966340	-3.679208
78	6	0	4.927409	-0.436000	-4.967362
79	1	0	4.100492	-0.546964	-5.674058
80	1	0	5.192805	0.619169	-4.863142
81	1	0	5.795320	-1.004665	-5.311443
82	6	0	3.693391	0.060322	-0.668163
83	1	0	3.432993	0.777572	0.118960
84	1	0	3.670572	-0.944739	-0.240191
85	1	0	4.702677	0.276068	-1.035156

Me-*ds*-**TS3**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.301689	2.823439	-0.076351
2	6	0	-1.262615	1.878696	0.243006
3	7	0	-0.740668	0.615132	0.247256
4	16	0	-2.876217	2.247903	0.542353
5	6	0	-0.368434	4.237318	0.079615
6	6	0	-1.477646	-0.639559	0.015155
7	6	0	-1.975372	-0.669047	-1.463617
8	6	0	-3.112774	-1.636614	-1.875868
9	6	0	-2.846983	-2.149793	-3.307313
10	7	0	-0.782072	-0.961185	-2.366686
11	6	0	-1.080304	-0.419019	-3.729705
12	6	0	-2.445450	-0.968727	-4.242942

13	6	0	-0.522939	-2.437960	-2.474804
14	6	0	-1.669514	-3.134626	-3.240703
15	1	0	0.409160	2.505187	-0.741188
16	6	0	-2.457002	-0.984026	1.170337
17	1	0	-0.691617	-1.398700	0.069580
18	1	0	-4.069011	-1.108298	-1.834292
19	1	0	-3.187047	-2.490617	-1.189660
20	1	0	-0.252170	-0.723457	-4.373937
21	1	0	-1.058150	0.668906	-3.653543
22	6	0	-3.605182	0.036152	-4.409117
23	1	0	-2.277249	-1.404283	-5.241635
24	1	0	0.437886	-2.546154	-2.978520
25	1	0	-0.411181	-2.824968	-1.459005
26	1	0	-1.968202	-4.055157	-2.724450
27	1	0	-3.741808	-2.644327	-3.700865
28	1	0	-1.347297	-3.419717	-4.249988
29	1	0	0.242300	0.534251	-0.030858
30	6	0	-1.041238	4.844543	1.141303
31	6	0	-1.026573	6.222406	1.269608
32	6	0	-0.337792	7.012872	0.362198
33	6	0	0.344066	6.410823	-0.683557
34	6	0	0.330609	5.035414	-0.828378
35	1	0	-1.555506	6.682811	2.094841
36	1	0	-0.329613	8.088820	0.471743
37	1	0	0.889434	7.017250	-1.395874
38	1	0	0.861043	4.562422	-1.643698
39	1	0	-1.576811	4.233859	1.852921
40	1	0	0.315371	-0.507660	-1.948040
41	6	0	-1.908061	-1.479803	2.414288
42	6	0	-2.804113	-1.822864	3.442321
43	7	0	-4.196850	-1.699758	3.332711
44	6	0	-4.633052	-1.218251	2.191046
45	6	0	-3.801092	-0.848401	1.089582
46	6	0	-0.508155	-1.631680	2.671420
47	1	0	-4.278897	-0.446371	0.210388
48	6	0	-3.591384	1.331578	-4.230610
49	1	0	-4.478381	1.926771	-4.398040
50	1	0	-2.719380	1.884815	-3.913331
51	1	0	-4.522320	-0.443393	-4.734508
52	1	0	-2.284890	0.348245	-1.712079
53	6	0	-2.303979	-2.324437	4.685493
54	6	0	-0.973437	-2.463033	4.889559
55	6	0	-0.060660	-2.103474	3.860068
56	1	0	-5.709622	-1.102055	2.087136
57	1	0	-3.027162	-2.581592	5.448918
58	1	0	-0.592531	-2.839637	5.830209
59	1	0	1.002469	-2.207159	4.037076
60	1	0	0.205697	-1.350405	1.911291
61	6	0	2.371662	1.478505	-2.680579
62	6	0	2.562659	0.147970	-1.914230
63	8	0	1.442789	2.239546	-2.485683
64	8	0	1.386438	-0.252523	-1.322552
65	8	0	3.362979	1.743556	-3.548693
66	6	0	3.280678	3.003418	-4.250448
67	1	0	2.360103	3.048823	-4.837056
68	1	0	3.304115	3.832396	-3.538854
69	1	0	4.155646	3.029087	-4.900196
70	8	0	2.163512	-1.429495	-4.248932
71	15	0	3.109204	-1.202655	-3.109001
72	8	0	3.273315	-2.426501	-2.065834
73	6	0	3.759270	-3.704042	-2.513740
74	1	0	3.735336	-4.359054	-1.640870

75	1	0	4.786352	-3.614033	-2.881684
76	1	0	3.113934	-4.110152	-3.299756
77	8	0	4.652733	-0.995937	-3.577880
78	6	0	5.006033	-0.601344	-4.916264
79	1	0	4.195164	-0.827849	-5.613331
80	1	0	5.224625	0.469427	-4.926637
81	1	0	5.902274	-1.166582	-5.184329
82	6	0	3.650075	0.387034	-0.838294
83	1	0	3.307203	1.179096	-0.162773
84	1	0	3.775626	-0.530408	-0.258319
85	1	0	4.611694	0.674478	-1.274217

Me-*ds*-**IM5**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.299412	2.819415	-0.051714
2	6	0	-1.305129	1.895326	0.199518
3	7	0	-0.817197	0.620115	0.213601
4	16	0	-2.918708	2.307440	0.418083
5	6	0	-0.340027	4.230002	0.138267
6	6	0	-1.563021	-0.633429	-0.009270
7	6	0	-2.059828	-0.694263	-1.485031
8	6	0	-3.167299	-1.722747	-1.845226
9	6	0	-2.882728	-2.284336	-3.254688
10	7	0	-0.872182	-0.925272	-2.383543
11	6	0	-1.235245	-0.453394	-3.743747
12	6	0	-2.556813	-1.125499	-4.245957
13	6	0	-0.526400	-2.373353	-2.466822
14	6	0	-1.649852	-3.194606	-3.153943
15	1	0	0.420733	2.502665	-0.705324
16	6	0	-2.555941	-0.932807	1.148871
17	1	0	-0.787311	-1.400911	0.064644
18	1	0	-4.148501	-1.239289	-1.821936
19	1	0	-3.202477	-2.552419	-1.125324
20	1	0	-0.398860	-0.699397	-4.404782
21	1	0	-1.311931	0.635371	-3.708267
22	6	0	-3.787302	-0.219608	-4.467854
23	1	0	-2.353751	-1.596993	-5.222524
24	1	0	0.412864	-2.446192	-3.020056
25	1	0	-0.331842	-2.736338	-1.452725
26	1	0	-1.887269	-4.094404	-2.571349
27	1	0	-3.750422	-2.848061	-3.616373
28	1	0	-1.336802	-3.529541	-4.151547
29	1	0	0.185530	0.532741	0.070592
30	6	0	-1.032954	4.822734	1.195576
31	6	0	-0.992997	6.195569	1.363566
32	6	0	-0.258597	6.995601	0.501020
33	6	0	0.442868	6.407841	-0.539506
34	6	0	0.404195	5.037416	-0.723956
35	1	0	-1.538087	6.644564	2.184584
36	1	0	-0.230958	8.067620	0.641401
37	1	0	1.023241	7.021496	-1.217141
38	1	0	0.949156	4.576507	-1.536423
39	1	0	-1.603815	4.204774	1.872745
40	1	0	0.777626	-0.336962	-1.838287
41	6	0	-2.036431	-1.424148	2.407181
42	6	0	-2.952393	-1.714533	3.433950
43	7	0	-4.338813	-1.544322	3.310000

44	6	0	-4.747955	-1.072171	2.154240
45	6	0	-3.894119	-0.753514	1.053597
46	6	0	-0.645491	-1.623501	2.680427
47	1	0	-4.348742	-0.355017	0.160261
48	6	0	-3.884891	1.075715	-4.315942
49	1	0	-4.811795	1.593707	-4.519113
50	1	0	-3.069953	1.702857	-3.985949
51	1	0	-4.655395	-0.776281	-4.806079
52	1	0	-2.427813	0.304773	-1.731154
53	6	0	-2.480686	-2.208587	4.691347
54	6	0	-1.157994	-2.391643	4.910368
55	6	0	-0.224576	-2.087506	3.881640
56	1	0	-5.819020	-0.921211	2.038264
57	1	0	-3.218986	-2.423927	5.453286
58	1	0	-0.798859	-2.762878	5.861589
59	1	0	0.832422	-2.228090	4.069367
60	1	0	0.084308	-1.387923	1.920146
61	6	0	2.495526	1.526646	-2.657218
62	6	0	2.753135	0.193256	-1.927659
63	8	0	1.553220	2.253191	-2.415473
64	8	0	1.592261	-0.220055	-1.253564
65	8	0	3.451274	1.821454	-3.549806
66	6	0	3.307657	3.081095	-4.246753
67	1	0	2.367469	3.095697	-4.802413
68	1	0	3.328555	3.908112	-3.533224
69	1	0	4.160276	3.132972	-4.923504
70	8	0	2.280182	-1.328460	-4.270287
71	15	0	3.248727	-1.147428	-3.148596
72	8	0	3.419495	-2.373317	-2.118273
73	6	0	3.791092	-3.681701	-2.594739
74	1	0	3.782170	-4.333031	-1.719452
75	1	0	4.795663	-3.656769	-3.028949
76	1	0	3.068089	-4.040103	-3.333784
77	8	0	4.780747	-0.910732	-3.620942
78	6	0	5.121961	-0.489844	-4.957489
79	1	0	4.299747	-0.692663	-5.648046
80	1	0	5.350859	0.578364	-4.943946
81	1	0	6.008651	-1.058415	-5.247511
82	6	0	3.847217	0.418492	-0.867497
83	1	0	3.516833	1.199777	-0.174298
84	1	0	3.994316	-0.506861	-0.305560
85	1	0	4.793578	0.716132	-1.325874

Me-*ms*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.160046	-1.983725	-2.078357
2	6	0	1.021738	-0.458323	-1.959032
3	8	0	-0.067925	-0.008967	-1.546097
4	8	0	2.300903	-2.362949	-2.678189
5	6	0	2.533047	-3.781038	-2.765644
6	1	0	2.571304	-4.214273	-1.762625
7	1	0	1.740266	-4.262797	-3.344229
8	1	0	3.495591	-3.884422	-3.267060
9	8	0	0.296322	-2.766901	-1.720703
10	8	0	2.017975	0.778479	0.994865
11	15	0	2.488628	-0.426847	0.154534
12	8	0	2.244968	-1.831582	1.011532

13	6	0	2.820575	-1.997839	2.318400
14	1	0	2.412531	-2.927757	2.724606
15	1	0	3.910322	-2.072763	2.248443
16	1	0	2.554653	-1.159431	2.972652
17	8	0	4.165877	-0.437880	0.187917
18	6	0	4.892478	0.789608	0.100843
19	1	0	5.942149	0.545071	0.286147
20	1	0	4.542158	1.507486	0.849903
21	1	0	4.804325	1.233916	-0.900071
22	7	0	0.419549	3.059043	0.065791
23	6	0	-0.800745	2.617549	0.507054
24	7	0	-0.665698	1.491135	1.273154
25	16	0	-2.304241	3.324230	0.172247
26	6	0	0.795181	4.122703	-0.800138
27	6	0	-1.684069	0.815723	2.067651
28	6	0	-2.701402	0.042742	1.193507
29	6	0	-3.705114	-0.829050	1.987438
30	6	0	-3.886871	-2.190750	1.286980
31	7	0	-1.979048	-0.887804	0.226335
32	6	0	-2.937812	-1.315241	-0.859979
33	6	0	-4.192283	-1.973406	-0.226110
34	6	0	-1.409611	-2.112885	0.904811
35	6	0	-2.575482	-2.986773	1.417823
36	1	0	1.200903	2.444121	0.337376
37	6	0	-2.326818	1.736865	3.146022
38	1	0	-1.120806	0.054971	2.621130
39	1	0	-4.663837	-0.308946	2.064052
40	1	0	-3.348136	-0.989733	3.014072
41	1	0	-2.377953	-2.003020	-1.495566
42	1	0	-3.154495	-0.422403	-1.444990
43	6	0	-5.544061	-1.259537	-0.432131
44	1	0	-4.302939	-2.974033	-0.672393
45	1	0	-0.784769	-2.606644	0.160767
46	1	0	-0.753684	-1.768298	1.704607
47	1	0	-2.404925	-3.264013	2.464397
48	1	0	-4.710352	-2.742288	1.752557
49	1	0	-2.636110	-3.919912	0.845316
50	1	0	0.288912	1.105558	1.328190
51	1	0	-1.193598	-0.407913	-0.278032
52	6	0	-0.098559	5.042210	-1.346741
53	6	0	0.369494	6.048239	-2.176660
54	6	0	1.717237	6.158875	-2.472724
55	6	0	2.609423	5.246314	-1.926434
56	6	0	2.158518	4.237812	-1.098790
57	1	0	2.854366	3.529288	-0.669973
58	1	0	3.666778	5.322078	-2.147371
59	1	0	2.072799	6.948120	-3.120990
60	1	0	-0.334863	6.756043	-2.596100
61	1	0	-1.147196	4.942423	-1.106440
62	6	0	-3.591346	2.210366	3.062437
63	6	0	-4.118961	3.041497	4.099214
64	7	0	-3.460410	3.405248	5.175512
65	6	0	-2.141071	2.936412	5.266516
66	6	0	-1.536072	2.119991	4.294530
67	6	0	-1.399797	3.333687	6.423481
68	6	0	-0.115844	2.938502	6.589473
69	6	0	0.505559	2.122403	5.604401
70	6	0	-0.175755	1.727441	4.501533
71	1	0	-4.229457	1.990806	2.220202
72	1	0	-5.140756	3.401964	4.003213
73	1	0	0.325125	1.121887	3.760400
74	1	0	1.536537	1.820679	5.741079

75	1	0	0.448674	3.240385	7.462493
76	1	0	-1.902018	3.959691	7.149985
77	1	0	-3.213719	0.760873	0.553045
78	6	0	-5.778163	-0.116190	-1.022003
79	1	0	-6.371591	-1.827226	-0.021105
80	1	0	-6.785086	0.269411	-1.105405
81	1	0	-5.009943	0.507131	-1.457357
82	6	0	1.896853	0.400629	-2.855361
83	1	0	2.921665	0.034911	-2.929280
84	1	0	1.452388	0.393640	-3.861580
85	1	0	1.880119	1.430804	-2.492240

Me-*dr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.539353	-1.927953	-5.358439
2	6	0	2.600068	0.754957	-3.511228
3	6	0	4.104232	0.893118	-3.182967
4	6	0	4.585041	-0.410195	-2.486170
5	6	0	4.058969	-1.585218	-3.343112
6	6	0	2.436068	-0.196964	-4.714355
7	6	0	4.829073	-0.274307	-5.277600
8	6	0	4.908431	1.056720	-4.490739
9	7	0	3.689299	-1.084476	-4.722729
10	1	0	5.730031	-0.883561	-5.165610
11	1	0	4.646050	-0.137165	-6.346110
12	1	0	5.955370	1.298833	-4.276032
13	1	0	4.503244	1.884044	-5.085344
14	1	0	5.688733	-0.407661	-2.517930
15	1	0	3.166024	-2.039351	-2.930736
16	1	0	2.522876	0.362059	-5.651859
17	1	0	2.167194	1.730056	-3.749482
18	1	0	4.268982	1.755864	-2.530087
19	1	0	2.045930	0.377108	-2.647212
20	7	0	-0.515252	-2.871620	-2.184801
21	6	0	-0.126435	-1.678973	-2.745584
22	7	0	0.826151	-1.883915	-3.710409
23	16	0	-0.717413	-0.150933	-2.340193
24	6	0	-1.243548	-3.175100	-0.999580
25	6	0	1.147158	-1.054509	-4.873042
26	1	0	-0.245036	-3.698190	-2.727634
27	6	0	-1.504851	-4.526396	-0.746472
28	6	0	-2.188180	-4.903692	0.392349
29	6	0	-2.621598	-3.947654	1.300449
30	6	0	-2.363008	-2.610386	1.051534
31	6	0	-1.680080	-2.215964	-0.087689
32	1	0	-2.384186	-5.953113	0.573728
33	1	0	-3.157349	-4.245127	2.191582
34	1	0	-2.698605	-1.855966	1.752453
35	1	0	-1.486775	-1.174377	-0.297966
36	1	0	-1.166623	-5.271547	-1.453750
37	6	0	-0.099965	1.062709	-5.605193
38	6	0	-0.066792	-0.283382	-5.471999
39	6	0	-1.226920	1.703276	-6.207439
40	7	0	-2.283027	1.079642	-6.674313
41	6	0	-2.256367	-0.319203	-6.562319
42	1	0	0.699950	1.694880	-5.256222
43	1	0	4.791943	-2.381217	-3.486802

44	1	0	1.237312	-2.824406	-3.739153
45	1	0	1.422507	-1.786968	-5.644614
46	6	0	4.190094	-0.469778	-0.997850
47	6	0	3.679100	-1.488870	-0.356743
48	1	0	3.460635	-1.429256	0.700774
49	1	0	3.448313	-2.434847	-0.826415
50	1	0	4.409758	0.447638	-0.463177
51	6	0	-1.191502	-1.036116	-5.987659
52	6	0	-1.282150	-2.463068	-5.963869
53	6	0	-3.388273	-1.020647	-7.082821
54	6	0	-3.443621	-2.372508	-7.036074
55	6	0	-2.365252	-3.103560	-6.467871
56	1	0	-1.221190	2.788065	-6.287870
57	1	0	-0.478137	-3.044764	-5.538579
58	1	0	-2.413809	-4.184718	-6.440380
59	1	0	-4.299167	-2.906032	-7.430339
60	1	0	-4.188178	-0.431599	-7.512752
61	8	0	3.849673	-5.372037	-7.583630
62	8	0	3.399197	-3.078883	-6.466387
63	15	0	2.858744	-4.526124	-6.528385
64	6	0	5.265898	-5.196222	-7.537070
65	1	0	5.532063	-4.135188	-7.593724
66	1	0	5.675749	-5.725482	-8.401846
67	1	0	5.691623	-5.630699	-6.622177
68	8	0	1.476428	-4.578346	-7.428949
69	6	0	1.427761	-4.027972	-8.756696
70	1	0	1.788013	-2.993356	-8.761528
71	1	0	2.032715	-4.632142	-9.440192
72	1	0	0.379568	-4.053650	-9.064705
73	6	0	1.034345	-5.775498	-4.514954
74	6	0	2.455087	-5.291208	-4.181257
75	8	0	0.036054	-5.133766	-4.228979
76	8	0	2.532823	-4.234554	-3.514744
77	8	0	1.001341	-6.979078	-5.101542
78	6	0	-0.293387	-7.447060	-5.528793
79	1	0	-0.975654	-7.511703	-4.677351
80	1	0	-0.699848	-6.763987	-6.278753
81	1	0	-0.114491	-8.432341	-5.959748
82	6	0	3.543843	-6.349006	-4.069513
83	1	0	3.402410	-6.878914	-3.116164
84	1	0	3.517406	-7.080052	-4.879164
85	1	0	4.519785	-5.857429	-4.035868

Me-*mr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.997953	-0.360661	-1.945135
2	6	0	1.439339	-1.604051	-1.161490
3	8	0	0.533352	-2.137394	-0.482261
4	8	0	2.180365	1.063249	1.074615
5	15	0	2.770335	-0.223631	0.458469
6	8	0	2.865916	-1.403355	1.605674
7	6	0	3.527659	-1.156257	2.856019
8	1	0	3.325559	-2.023430	3.490511
9	1	0	4.606817	-1.053111	2.702419
10	1	0	3.136841	-0.249668	3.331569
11	8	0	4.418919	0.008715	0.252635
12	6	0	4.907594	1.231200	-0.296906

13	1	0	5.997133	1.144549	-0.332836
14	1	0	4.629048	2.081874	0.334617
15	1	0	4.530919	1.393653	-1.316196
16	7	0	0.523940	3.163308	0.067575
17	6	0	-0.705097	2.679525	0.435967
18	7	0	-0.587291	1.520145	1.153710
19	16	0	-2.201815	3.384766	0.052563
20	6	0	0.915321	4.300812	-0.691600
21	6	0	-1.622250	0.816508	1.911545
22	6	0	-2.677896	0.165142	0.980646
23	6	0	-3.939287	-0.417163	1.658193
24	6	0	-4.378887	-1.699989	0.922719
25	7	0	-2.050226	-0.984550	0.184949
26	6	0	-2.895940	-1.232782	-1.041519
27	6	0	-4.371923	-1.464980	-0.618840
28	6	0	-1.945342	-2.259063	0.995222
29	6	0	-3.363693	-2.808431	1.250265
30	1	0	1.312334	2.569627	0.376295
31	6	0	-2.183110	1.674343	3.083624
32	1	0	-1.080494	-0.014432	2.372899
33	1	0	-4.735787	0.330294	1.633073
34	1	0	-3.749950	-0.646446	2.715628
35	1	0	-2.463405	-2.106344	-1.533518
36	1	0	-2.747648	-0.376090	-1.695826
37	6	0	-5.403945	-0.397795	-1.037162
38	1	0	-4.701696	-2.408692	-1.081136
39	1	0	-1.298956	-2.928364	0.431356
40	1	0	-1.419257	-2.008985	1.917611
41	1	0	-3.459109	-3.118200	2.297073
42	1	0	-5.382791	-1.993811	1.245972
43	1	0	-3.552302	-3.695992	0.634406
44	1	0	0.378706	1.189122	1.290754
45	1	0	-1.098301	-0.747760	-0.167466
46	6	0	0.028942	5.222003	-1.247711
47	6	0	0.516153	6.298225	-1.972023
48	6	0	1.876306	6.477394	-2.155025
49	6	0	2.761441	5.562632	-1.600730
50	6	0	2.291276	4.485657	-0.876923
51	1	0	2.980963	3.775488	-0.442114
52	1	0	3.828466	5.690760	-1.733305
53	1	0	2.246828	7.320852	-2.721505
54	1	0	-0.183503	7.006626	-2.398210
55	1	0	-1.029568	5.070264	-1.094735
56	6	0	-3.328926	2.388245	2.989946
57	6	0	-3.790006	3.160540	4.101041
58	7	0	-3.176238	3.245745	5.258851
59	6	0	-1.972395	2.532532	5.361499
60	6	0	-1.435636	1.754093	4.319890
61	6	0	-1.277260	2.633094	6.607510
62	6	0	-0.097254	1.996644	6.793385
63	6	0	0.460909	1.223547	5.738585
64	6	0	-0.180921	1.105643	4.550871
65	1	0	-3.910555	2.406672	2.081046
66	1	0	-4.718546	3.717072	3.994859
67	1	0	0.278732	0.527789	3.762570
68	1	0	1.413016	0.730422	5.890397
69	1	0	0.433103	2.074185	7.733929
70	1	0	-1.727524	3.237589	7.384566
71	1	0	-2.959283	0.904655	0.231824
72	6	0	-5.199413	0.723399	-1.678373
73	1	0	-6.412063	-0.670759	-0.745800
74	1	0	-6.022664	1.382200	-1.919317

75	1	0	-4.226940	1.066317	-2.003088
76	6	0	1.497644	1.243787	-3.609030
77	1	0	1.309485	2.084042	-2.936024
78	1	0	2.341818	1.451264	-4.267096
79	1	0	0.595888	1.036342	-4.191025
80	8	0	-0.099928	0.149259	-1.779376
81	8	0	1.883310	0.075813	-2.854135
82	6	0	2.586404	-2.436558	-1.707938
83	1	0	2.193498	-3.056448	-2.527696
84	1	0	3.410313	-1.832236	-2.091111
85	1	0	2.948576	-3.101501	-0.920427

Et-α-ketoester

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.880469	0.996479	1.399327
2	6	0	2.520288	-0.517330	1.334329
3	8	0	2.120166	1.880759	1.086801
4	8	0	1.380585	-0.810484	1.048715
5	8	0	4.138365	1.186940	1.846829
6	6	0	4.569081	2.561234	1.949033
7	1	0	4.538146	3.037567	0.965794
8	1	0	3.919765	3.107336	2.637980
9	1	0	5.589812	2.516809	2.328317
10	6	0	3.608978	-1.529969	1.624922
11	1	0	4.447094	-1.326432	0.942659
12	1	0	4.009854	-1.314354	2.625418
13	6	0	3.134926	-2.978384	1.511505
14	1	0	3.961248	-3.663673	1.729104
15	1	0	2.321250	-3.184876	2.214048
16	1	0	2.761973	-3.195821	0.505519

Et-*ds*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.330246	2.646561	-0.181365
2	6	0	-1.266990	1.669580	-0.387123
3	7	0	-0.920206	0.495771	0.216724
4	16	0	-2.690543	1.845359	-1.300794
5	6	0	-0.223364	3.993135	-0.641452
6	6	0	-1.738174	-0.702355	0.412643
7	6	0	-1.995914	-1.455011	-0.910216
8	6	0	-2.839993	-2.745481	-0.791701
9	6	0	-2.269103	-3.824321	-1.734694
10	7	0	-0.672012	-1.854190	-1.555792
11	6	0	-0.921151	-2.137317	-3.014661
12	6	0	-2.026110	-3.221303	-3.153089
13	6	0	-0.035915	-3.060893	-0.908792
14	6	0	-0.921707	-4.299154	-1.162167
15	1	0	0.452462	2.368303	0.420622
16	6	0	-2.996159	-0.423053	1.281373
17	1	0	-1.087360	-1.347891	1.007285
18	1	0	-3.880243	-2.524655	-1.045547

19	1	0	-2.835879	-3.121021	0.240750
20	1	0	0.034722	-2.459853	-3.431478
21	1	0	-1.177784	-1.184945	-3.476712
22	6	0	-3.351179	-2.798150	-3.820090
23	1	0	-1.617791	-4.034061	-3.774314
24	1	0	0.959376	-3.141484	-1.348085
25	1	0	0.101545	-2.823992	0.146399
26	1	0	-1.079308	-4.845069	-0.225159
27	1	0	-2.965474	-4.666002	-1.809123
28	1	0	-0.433738	-4.991997	-1.858383
29	1	0	-0.003067	0.410933	0.674048
30	6	0	-1.159286	4.619231	-1.461062
31	6	0	-0.960768	5.934383	-1.851554
32	6	0	0.156055	6.639220	-1.437973
33	6	0	1.088986	6.015862	-0.619979
34	6	0	0.906084	4.706681	-0.223038
35	1	0	-1.694998	6.411400	-2.488937
36	1	0	0.301762	7.665265	-1.747561
37	1	0	1.967180	6.555978	-0.289126
38	1	0	1.631606	4.217963	0.413289
39	1	0	-2.027028	4.056497	-1.773103
40	1	0	0.063423	-1.099149	-1.512650
41	6	0	-2.835305	-0.268287	2.710400
42	6	0	-3.986780	-0.016216	3.476908
43	7	0	-5.273634	0.102614	2.929976
44	6	0	-5.350901	-0.027242	1.625398
45	6	0	-4.239286	-0.289077	0.764822
46	6	0	-1.578936	-0.348247	3.392026
47	1	0	-4.425098	-0.361888	-0.296085
48	6	0	-3.702669	-1.615342	-4.253077
49	1	0	-4.668109	-1.457625	-4.714152
50	1	0	-3.076359	-0.737018	-4.186244
51	1	0	-4.038600	-3.630199	-3.926453
52	1	0	-2.448581	-0.758951	-1.616159
53	6	0	-3.878261	0.137102	4.894905
54	6	0	-2.674565	0.049708	5.507708
55	6	0	-1.505006	-0.194779	4.736501
56	1	0	-6.338465	0.070755	1.179931
57	1	0	-4.788090	0.327063	5.449942
58	1	0	-2.588708	0.167668	6.580394
59	1	0	-0.546535	-0.254871	5.236709
60	1	0	-0.672132	-0.522322	2.829125
61	6	0	2.869052	0.979063	1.456587
62	6	0	2.506464	-0.502846	1.266088
63	8	0	2.058789	1.889944	1.366796
64	8	0	1.280030	-0.789584	1.345737
65	8	0	4.161599	1.176903	1.750291
66	6	0	4.601359	2.547331	1.825110
67	1	0	4.471344	3.028686	0.852393
68	1	0	4.034423	3.088350	2.586914
69	1	0	5.657341	2.495186	2.091360
70	8	0	1.643407	-0.571964	-1.894864
71	15	0	2.929254	-0.298194	-1.103067
72	8	0	4.123513	-1.355774	-1.561099
73	6	0	4.547434	-1.432620	-2.929992
74	1	0	5.261586	-2.257924	-2.992447
75	1	0	5.040329	-0.500917	-3.229872
76	1	0	3.697064	-1.631384	-3.592888
77	8	0	3.559362	1.152891	-1.630276
78	6	0	2.927532	1.924727	-2.663842
79	1	0	3.138209	1.496420	-3.650994
80	1	0	1.844716	1.972631	-2.519972

81	1	0	3.357097	2.928483	-2.604536
82	6	0	3.563336	-1.517147	1.717005
83	1	0	4.539370	-1.266204	1.295401
84	1	0	3.649932	-1.388120	2.807835
85	6	0	3.192467	-2.967355	1.405777
86	1	0	3.941172	-3.647665	1.828360
87	1	0	2.216561	-3.222501	1.831053
88	1	0	3.159516	-3.138283	0.323970

Et-*ms*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327836	-2.352907	-1.719499
2	6	0	1.070203	-0.848864	-1.928050
3	8	0	-0.049329	-0.402994	-1.591374
4	8	0	2.523141	-2.751096	-2.185275
5	6	0	2.872840	-4.126416	-1.945322
6	1	0	2.896959	-4.318369	-0.869438
7	1	0	2.151177	-4.794100	-2.423769
8	1	0	3.864152	-4.251239	-2.381786
9	8	0	0.509260	-3.116772	-1.237739
10	8	0	1.990493	0.906395	0.871058
11	15	0	2.565119	-0.290541	0.084527
12	8	0	2.585058	-1.636123	1.058753
13	6	0	3.228345	-1.597247	2.343242
14	1	0	2.977883	-2.534898	2.847253
15	1	0	4.313872	-1.519900	2.223902
16	1	0	2.864895	-0.750091	2.935928
17	8	0	4.226415	-0.072455	-0.021014
18	6	0	4.771125	1.230855	-0.229203
19	1	0	5.858070	1.129031	-0.164347
20	1	0	4.419675	1.929915	0.537119
21	1	0	4.510701	1.619271	-1.223342
22	7	0	0.325914	3.159679	0.062466
23	6	0	-0.881309	2.658801	0.472834
24	7	0	-0.721707	1.478968	1.150206
25	16	0	-2.401469	3.355577	0.187961
26	6	0	0.678138	4.325810	-0.672986
27	6	0	-1.704672	0.779891	1.972921
28	6	0	-2.770650	0.061708	1.111381
29	6	0	-3.841066	-0.736879	1.892484
30	6	0	-4.154038	-2.052736	1.149304
31	7	0	-2.098389	-0.927155	0.164032
32	6	0	-3.054227	-1.258933	-0.956461
33	6	0	-4.396987	-1.765476	-0.363956
34	6	0	-1.674394	-2.202763	0.859133
35	6	0	-2.936105	-2.984455	1.281257
36	1	0	1.125705	2.554186	0.301974
37	6	0	-2.268067	1.660775	3.125721
38	1	0	-1.122519	-0.012409	2.456610
39	1	0	-4.745508	-0.131693	1.993871
40	1	0	-3.493132	-0.962813	2.910026
41	1	0	-2.554029	-2.014933	-1.564031
42	1	0	-3.148417	-0.356918	-1.559392
43	6	0	-5.643608	-0.883302	-0.581051
44	1	0	-4.621395	-2.734607	-0.836399
45	1	0	-1.033757	-2.734547	0.155311
46	1	0	-1.056431	-1.915347	1.711156

47	1	0	-2.831760	-3.331187	2.315576
48	1	0	-5.042588	-2.524843	1.581069
49	1	0	-3.065390	-3.875373	0.655402
50	1	0	0.245340	1.122384	1.190257
51	1	0	-1.247809	-0.530690	-0.302323
52	6	0	-0.242202	5.231929	-1.196874
53	6	0	0.204386	6.340362	-1.898580
54	6	0	1.556523	6.565521	-2.090001
55	6	0	2.475205	5.665506	-1.566968
56	6	0	2.045910	4.557388	-0.865040
57	1	0	2.762091	3.859162	-0.453679
58	1	0	3.536332	5.830187	-1.706290
59	1	0	1.895217	7.433594	-2.638963
60	1	0	-0.520861	7.037221	-2.300303
61	1	0	-1.293944	5.046061	-1.034719
62	6	0	-3.504420	2.209773	3.103590
63	6	0	-3.960656	3.001168	4.203480
64	7	0	-3.258975	3.256830	5.283623
65	6	0	-1.965878	2.712796	5.310020
66	6	0	-1.429124	1.929489	4.272700
67	6	0	-1.177379	2.995815	6.469317
68	6	0	0.087770	2.526213	6.574830
69	6	0	0.642154	1.746836	5.522418
70	6	0	-0.085539	1.458505	4.416125
71	1	0	-4.170601	2.079966	2.264496
72	1	0	-4.962049	3.423326	4.156707
73	1	0	0.367510	0.880653	3.623796
74	1	0	1.659857	1.387269	5.609954
75	1	0	0.688183	2.741816	7.449461
76	1	0	-1.628519	3.598375	7.247343
77	1	0	-3.232518	0.805078	0.461120
78	6	0	-5.723826	0.279271	-1.174360
79	1	0	-6.540955	-1.340433	-0.178907
80	1	0	-6.672470	0.790151	-1.267747
81	1	0	-4.878224	0.799380	-1.601965
82	6	0	1.853845	-0.187527	-3.059945
83	1	0	2.910293	-0.458879	-2.997689
84	1	0	1.472271	-0.652966	-3.984926
85	6	0	1.663759	1.326285	-3.137907
86	1	0	2.177431	1.728386	-4.018784
87	1	0	0.604533	1.591112	-3.199194
88	1	0	2.074428	1.819518	-2.250323

Et-*dr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.574741	-1.931790	-5.337546
2	6	0	2.589581	0.761153	-3.525691
3	6	0	4.088474	0.912277	-3.179625
4	6	0	4.569086	-0.381606	-2.465329
5	6	0	4.060101	-1.567767	-3.317236
6	6	0	2.446764	-0.202370	-4.722684
7	6	0	4.846939	-0.269395	-5.253654
8	6	0	4.907901	1.069400	-4.478581
9	7	0	3.704946	-1.082063	-4.706093
10	1	0	5.749841	-0.872289	-5.124800
11	1	0	4.676693	-0.143746	-6.325668
12	1	0	5.950498	1.320314	-4.253095

13	1	0	4.504844	1.888557	-5.085867
14	1	0	5.673032	-0.372664	-2.484281
15	1	0	3.164091	-2.022283	-2.911993
16	1	0	2.542854	0.348913	-5.663887
17	1	0	2.153299	1.731290	-3.777419
18	1	0	4.239077	1.781940	-2.532511
19	1	0	2.027040	0.386850	-2.665580
20	7	0	-0.500441	-2.879071	-2.197021
21	6	0	-0.120744	-1.687314	-2.766633
22	7	0	0.836825	-1.892094	-3.725639
23	16	0	-0.728665	-0.161586	-2.376538
24	6	0	-1.226767	-3.179063	-1.009938
25	6	0	1.162758	-1.066242	-4.888741
26	1	0	-0.222830	-3.707581	-2.733411
27	6	0	-1.475966	-4.530495	-0.745392
28	6	0	-2.156011	-4.904262	0.396550
29	6	0	-2.598144	-3.944573	1.296555
30	6	0	-2.351642	-2.607180	1.036310
31	6	0	-1.672165	-2.216272	-0.106154
32	1	0	-2.342496	-5.953842	0.586831
33	1	0	-3.131217	-4.239334	2.190181
34	1	0	-2.694113	-1.849930	1.730824
35	1	0	-1.488227	-1.174805	-0.325296
36	1	0	-1.130804	-5.278454	-1.446333
37	6	0	-0.081612	1.042714	-5.649825
38	6	0	-0.050372	-0.301561	-5.498810
39	6	0	-1.208587	1.677392	-6.258262
40	7	0	-2.267108	1.049858	-6.714096
41	6	0	-2.242218	-0.347564	-6.584649
42	1	0	0.719556	1.678441	-5.310586
43	1	0	4.798571	-2.361152	-3.445114
44	1	0	1.259045	-2.829318	-3.746319
45	1	0	1.445630	-1.801185	-5.655593
46	6	0	4.157488	-0.428934	-0.981084
47	6	0	3.639122	-1.442216	-0.336716
48	1	0	3.408651	-1.373126	0.717665
49	1	0	3.413366	-2.392307	-0.800413
50	1	0	4.370999	0.493190	-0.452028
51	6	0	-1.176689	-1.059096	-6.004445
52	6	0	-1.268555	-2.485638	-5.965231
53	6	0	-3.376931	-1.053306	-7.092967
54	6	0	-3.434214	-2.404424	-7.029973
55	6	0	-2.354432	-3.130262	-6.458003
56	1	0	-1.200983	2.761035	-6.352801
57	1	0	-0.462389	-3.063856	-5.539217
58	1	0	-2.403978	-4.210974	-6.418569
59	1	0	-4.292056	-2.941234	-7.414684
60	1	0	-4.177411	-0.468100	-7.527025
61	8	0	3.796582	-5.359313	-7.663308
62	8	0	3.508244	-3.086320	-6.452692
63	15	0	2.922196	-4.514359	-6.512511
64	6	0	5.200550	-5.150327	-7.823593
65	1	0	5.431560	-4.083571	-7.910243
66	1	0	5.489128	-5.668030	-8.742658
67	1	0	5.764366	-5.578321	-6.983992
68	8	0	1.468494	-4.493984	-7.298517
69	6	0	1.342315	-3.931532	-8.615380
70	1	0	1.766540	-2.921786	-8.649412
71	1	0	1.847556	-4.567656	-9.349052
72	1	0	0.272444	-3.887592	-8.833626
73	6	0	1.054586	-5.769448	-4.546870
74	6	0	2.476905	-5.277155	-4.211879

75	8	0	0.052351	-5.153675	-4.222405
76	8	0	2.541474	-4.212505	-3.550040
77	8	0	1.028721	-6.950371	-5.177565
78	6	0	-0.266876	-7.427917	-5.590302
79	1	0	-0.926078	-7.538288	-4.725389
80	1	0	-0.706138	-6.725865	-6.303289
81	1	0	-0.080182	-8.392638	-6.062603
82	6	0	3.533820	-6.368921	-4.027707
83	1	0	3.202397	-6.959626	-3.157709
84	1	0	3.531388	-7.051441	-4.881534
85	6	0	4.933063	-5.817007	-3.755556
86	1	0	4.934024	-5.173854	-2.870099
87	1	0	5.642007	-6.636420	-3.589634
88	1	0	5.295927	-5.221770	-4.602551

Et-*mr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.037148	-0.363247	-1.879694
2	6	0	1.465112	-1.596023	-1.064712
3	8	0	0.548991	-2.096693	-0.369634
4	8	0	2.206492	1.138139	1.006933
5	15	0	2.801653	-0.195672	0.511059
6	8	0	2.899228	-1.258223	1.769380
7	6	0	3.540488	-0.871266	2.996090
8	1	0	3.322172	-1.659349	3.721777
9	1	0	4.622750	-0.791561	2.850586
10	1	0	3.147795	0.085719	3.356892
11	8	0	4.447535	0.021124	0.278545
12	6	0	4.930402	1.188519	-0.386448
13	1	0	6.020048	1.102092	-0.417128
14	1	0	4.650613	2.094019	0.162873
15	1	0	4.548837	1.251646	-1.414405
16	7	0	0.502233	3.193297	0.030473
17	6	0	-0.717278	2.700840	0.417757
18	7	0	-0.579822	1.549024	1.143927
19	16	0	-2.224702	3.388517	0.042466
20	6	0	0.875762	4.337447	-0.727427
21	6	0	-1.600857	0.824981	1.903037
22	6	0	-2.656353	0.169085	0.973427
23	6	0	-3.933168	-0.387413	1.643743
24	6	0	-4.384941	-1.669806	0.914320
25	7	0	-2.034864	-1.000812	0.202677
26	6	0	-2.865719	-1.249563	-1.033307
27	6	0	-4.351669	-1.451384	-0.629455
28	6	0	-1.963606	-2.266066	1.029770
29	6	0	-3.393490	-2.791797	1.267611
30	1	0	1.300057	2.605188	0.325268
31	6	0	-2.161490	1.663119	3.089637
32	1	0	-1.044734	-0.004584	2.348329
33	1	0	-4.716647	0.373090	1.604052
34	1	0	-3.758229	-0.611111	2.704762
35	1	0	-2.441825	-2.136580	-1.508676
36	1	0	-2.692818	-0.403795	-1.695551
37	6	0	-5.358734	-0.371095	-1.074079
38	1	0	-4.691349	-2.394283	-1.086356
39	1	0	-1.317706	-2.951741	0.484745
40	1	0	-1.448938	-2.012581	1.957761

41	1	0	-3.509867	-3.090410	2.315547
42	1	0	-5.398284	-1.943057	1.225876
43	1	0	-3.586807	-3.681918	0.656850
44	1	0	0.390391	1.230300	1.272870
45	1	0	-1.069285	-0.791576	-0.132808
46	6	0	-0.022592	5.261580	-1.258747
47	6	0	0.449094	6.345254	-1.982337
48	6	0	1.805244	6.528836	-2.188883
49	6	0	2.702366	5.610943	-1.659428
50	6	0	2.247843	4.526619	-0.936699
51	1	0	2.946583	3.813737	-0.520769
52	1	0	3.766468	5.742619	-1.810689
53	1	0	2.163563	7.378085	-2.754562
54	1	0	-0.259669	7.055982	-2.389168
55	1	0	-1.077869	5.105881	-1.088513
56	6	0	-3.295002	2.396761	2.996468
57	6	0	-3.759510	3.152220	4.117420
58	7	0	-3.160607	3.202649	5.285092
59	6	0	-1.969896	2.468065	5.388521
60	6	0	-1.430511	1.703636	4.337691
61	6	0	-1.291561	2.530601	6.646288
62	6	0	-0.124869	1.871148	6.835548
63	6	0	0.436017	1.111595	5.772410
64	6	0	-0.189998	1.029927	4.573316
65	1	0	-3.861310	2.444272	2.078886
66	1	0	-4.677646	3.725677	4.010771
67	1	0	0.271657	0.460475	3.780176
68	1	0	1.377394	0.599193	5.927267
69	1	0	0.392684	1.919777	7.785105
70	1	0	-1.743660	3.125632	7.429574
71	1	0	-2.923249	0.899122	0.210363
72	6	0	-5.126268	0.736124	-1.729888
73	1	0	-6.374856	-0.620649	-0.789652
74	1	0	-5.934280	1.406673	-1.989327
75	1	0	-4.144125	1.055809	-2.049157
76	6	0	1.572477	1.224183	-3.549692
77	1	0	1.331484	2.070003	-2.901199
78	1	0	2.441245	1.442543	-4.171291
79	1	0	0.705167	0.983292	-4.170056
80	8	0	-0.072479	0.132439	-1.761550
81	8	0	1.951176	0.078382	-2.757653
82	6	0	2.567674	-2.469538	-1.662914
83	1	0	2.146805	-2.871250	-2.600773
84	1	0	3.425367	-1.855362	-1.950123
85	6	0	2.992885	-3.626536	-0.757215
86	1	0	2.134762	-4.253434	-0.495160
87	1	0	3.736555	-4.249966	-1.267443
88	1	0	3.430928	-3.254186	0.173811

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*i*Pr-α-ketoester

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.954445	1.004655	1.623215
2	6	0	2.611767	-0.475320	1.320931
3	8	0	2.149189	1.820744	2.006078
4	8	0	1.617050	-0.700548	0.664633
5	8	0	4.255734	1.258972	1.380346
6	6	0	4.678177	2.628738	1.565401

7	1	0	4.105308	3.289130	0.909770
8	1	0	4.530353	2.929519	2.605610
9	1	0	5.735720	2.641459	1.302749
10	6	0	3.528146	-1.544381	1.897877
11	1	0	4.545157	-1.288978	1.566981
12	6	0	3.153774	-2.939401	1.390437
13	1	0	3.853692	-3.682752	1.788837
14	1	0	2.141633	-3.214952	1.705456
15	1	0	3.183106	-2.988034	0.297209
16	6	0	3.508550	-1.460159	3.442078
17	1	0	4.211039	-2.189532	3.859790
18	1	0	3.801269	-0.469400	3.808088
19	1	0	2.509760	-1.687700	3.832802

*i*Pr-*ds*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.324882	2.638125	-0.163738
2	6	0	-1.261691	1.663048	-0.381527
3	7	0	-0.915576	0.483737	0.210504
4	16	0	-2.683259	1.848483	-1.296646
5	6	0	-0.214395	3.987655	-0.613779
6	6	0	-1.740124	-0.709613	0.407405
7	6	0	-2.001487	-1.459744	-0.916033
8	6	0	-2.865647	-2.737462	-0.805866
9	6	0	-2.305244	-3.822910	-1.747809
10	7	0	-0.677687	-1.880273	-1.549655
11	6	0	-0.916898	-2.156759	-3.011495
12	6	0	-2.040200	-3.219768	-3.162366
13	6	0	-0.068366	-3.098826	-0.898263
14	6	0	-0.970775	-4.321854	-1.165600
15	1	0	0.452275	2.355452	0.443519
16	6	0	-2.992956	-0.423094	1.280508
17	1	0	-1.091499	-1.358761	1.000386
18	1	0	-3.900576	-2.499972	-1.066088
19	1	0	-2.874038	-3.115280	0.225690
20	1	0	0.037113	-2.496286	-3.418851
21	1	0	-1.151607	-1.199352	-3.474821
22	6	0	-3.352071	-2.770873	-3.838493
23	1	0	-1.641431	-4.037707	-3.782972
24	1	0	0.931071	-3.192758	-1.324873
25	1	0	0.059797	-2.865990	0.158886
26	1	0	-1.145294	-4.869434	-0.232572
27	1	0	-3.015043	-4.652487	-1.830723
28	1	0	-0.487358	-5.019023	-1.860675
29	1	0	0.005035	0.387857	0.662562
30	6	0	-1.142552	4.618298	-1.438784
31	6	0	-0.940788	5.935768	-1.819595
32	6	0	0.171708	6.638546	-1.391080
33	6	0	1.096862	6.010696	-0.567714
34	6	0	0.910672	4.699128	-0.180275
35	1	0	-1.669037	6.416316	-2.461179
36	1	0	0.319961	7.666464	-1.693139
37	1	0	1.971523	6.549216	-0.225099
38	1	0	1.630075	4.206762	0.460188
39	1	0	-2.007360	4.057254	-1.761882
40	1	0	0.068271	-1.139074	-1.497112
41	6	0	-2.824117	-0.269217	2.708738

42	6	0	-3.970419	-0.010957	3.480857
43	7	0	-5.259229	0.115211	2.940094
44	6	0	-5.343465	-0.013305	1.635818
45	6	0	-4.237562	-0.281223	0.769751
46	6	0	-1.564536	-0.355398	3.383812
47	1	0	-4.428586	-0.352315	-0.290344
48	6	0	-3.678538	-1.580881	-4.271374
49	1	0	-4.637360	-1.404515	-4.739454
50	1	0	-3.036933	-0.714234	-4.197531
51	1	0	-4.053644	-3.590031	-3.952159
52	1	0	-2.437819	-0.757152	-1.625941
53	6	0	-3.854049	0.141592	4.898304
54	6	0	-2.647713	0.047993	5.504973
55	6	0	-1.483226	-0.202176	4.727908
56	1	0	-6.332584	0.090685	1.195185
57	1	0	-4.760041	0.336261	5.457946
58	1	0	-2.555856	0.165517	6.577216
59	1	0	-0.522525	-0.266548	5.223289
60	1	0	-0.661191	-0.533234	2.816245
61	6	0	2.882076	0.954543	1.423516
62	6	0	2.507345	-0.529791	1.240603
63	8	0	2.067577	1.864454	1.370628
64	8	0	1.271797	-0.798823	1.309408
65	8	0	4.189271	1.158786	1.639894
66	6	0	4.630002	2.529931	1.672401
67	1	0	4.446550	2.997560	0.701686
68	1	0	4.105335	3.081165	2.456958
69	1	0	5.699196	2.482346	1.880753
70	8	0	1.683286	-0.669889	-1.882074
71	15	0	2.954672	-0.357358	-1.085395
72	8	0	4.190863	-1.361074	-1.541402
73	6	0	4.629135	-1.409693	-2.907705
74	1	0	5.377177	-2.204361	-2.968469
75	1	0	5.085394	-0.456117	-3.196156
76	1	0	3.793198	-1.639262	-3.578704
77	8	0	3.532518	1.121405	-1.591221
78	6	0	2.869247	1.883252	-2.613187
79	1	0	3.046546	1.444761	-3.602036
80	1	0	1.792007	1.936739	-2.434452
81	1	0	3.303014	2.886196	-2.576736
82	6	0	3.533810	-1.559276	1.759905
83	1	0	4.527619	-1.279623	1.397689
84	6	0	3.208790	-2.979653	1.282875
85	1	0	3.938217	-3.688092	1.694307
86	1	0	2.211585	-3.282873	1.620798
87	1	0	3.250927	-3.055091	0.191650
88	6	0	3.539930	-1.506727	3.304024
89	1	0	4.272187	-2.221646	3.699031
90	1	0	3.809936	-0.514048	3.680158
91	1	0	2.554245	-1.771560	3.703985

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*i*Pr-*ms*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.186080	-2.037008	-2.039249
2	6	0	1.083592	-0.499685	-1.945528
3	8	0	0.012658	-0.054747	-1.472533
4	8	0	2.330287	-2.482244	-2.577422

5	6	0	2.497982	-3.911512	-2.626906
6	1	0	2.474303	-4.323869	-1.614811
7	1	0	1.708274	-4.368875	-3.229056
8	1	0	3.474925	-4.069807	-3.084458
9	8	0	0.280672	-2.776808	-1.692238
10	8	0	2.044807	0.791514	0.975947
11	15	0	2.566124	-0.398827	0.144843
12	8	0	2.259729	-1.819051	0.960731
13	6	0	2.746132	-2.010008	2.298624
14	1	0	2.335735	-2.961258	2.649656
15	1	0	3.839846	-2.056288	2.305279
16	1	0	2.413140	-1.198199	2.956203
17	8	0	4.238335	-0.409140	0.296954
18	6	0	4.964730	0.815588	0.425613
19	1	0	5.981280	0.545244	0.725477
20	1	0	4.512443	1.464027	1.182558
21	1	0	5.009547	1.351459	-0.532481
22	7	0	0.434557	3.048769	0.037608
23	6	0	-0.782482	2.603481	0.484234
24	7	0	-0.639745	1.484914	1.259097
25	16	0	-2.290544	3.299304	0.143671
26	6	0	0.804192	4.114724	-0.827555
27	6	0	-1.653749	0.803177	2.053650
28	6	0	-2.664726	0.021661	1.179768
29	6	0	-3.687216	-0.830540	1.970667
30	6	0	-3.888583	-2.190221	1.270985
31	7	0	-1.935626	-0.930722	0.238733
32	6	0	-2.878973	-1.353537	-0.862730
33	6	0	-4.163097	-1.971176	-0.247717
34	6	0	-1.404373	-2.157023	0.945189
35	6	0	-2.596769	-3.013528	1.424361
36	1	0	1.218976	2.436707	0.307546
37	6	0	-2.299387	1.723062	3.131173
38	1	0	-1.085247	0.046853	2.607561
39	1	0	-4.636858	-0.293427	2.040893
40	1	0	-3.338876	-0.995550	2.999727
41	1	0	-2.320807	-2.064279	-1.474038
42	1	0	-3.061335	-0.465396	-1.466348
43	6	0	-5.490132	-1.219522	-0.478953
44	1	0	-4.295566	-2.970284	-0.691694
45	1	0	-0.759045	-2.663053	0.227725
46	1	0	-0.775979	-1.811862	1.766698
47	1	0	-2.453829	-3.302574	2.471888
48	1	0	-4.731492	-2.722210	1.724355
49	1	0	-2.662959	-3.940394	0.842251
50	1	0	0.315413	1.100031	1.307235
51	1	0	-1.128647	-0.471733	-0.255846
52	6	0	-0.093019	5.036137	-1.365311
53	6	0	0.369679	6.045434	-2.194260
54	6	0	1.715529	6.157562	-2.498158
55	6	0	2.611241	5.243090	-1.960845
56	6	0	2.165724	4.231367	-1.134285
57	1	0	2.864315	3.521199	-0.712613
58	1	0	3.667197	5.320024	-2.187965
59	1	0	2.066936	6.949387	-3.145531
60	1	0	-0.337392	6.754681	-2.606637
61	1	0	-1.140196	4.934727	-1.119320
62	6	0	-3.560858	2.203379	3.040606
63	6	0	-4.091316	3.033442	4.076818
64	7	0	-3.438308	3.389993	5.158915
65	6	0	-2.121493	2.915417	5.256455
66	6	0	-1.513802	2.100024	4.285301

67	6	0	-1.385624	3.305983	6.419170
68	6	0	-0.103898	2.906162	6.591097
69	6	0	0.520734	2.092195	5.606320
70	6	0	-0.155620	1.703230	4.498294
71	1	0	-4.193750	1.989879	2.192878
72	1	0	-5.110759	3.399071	3.975464
73	1	0	0.347947	1.099891	3.757187
74	1	0	1.550230	1.787449	5.747363
75	1	0	0.456562	3.203058	7.468427
76	1	0	-1.889962	3.931018	7.145042
77	1	0	-3.163671	0.732907	0.521278
78	6	0	-5.682649	-0.077138	-1.085496
79	1	0	-6.339402	-1.757430	-0.072229
80	1	0	-6.676505	0.337127	-1.186419
81	1	0	-4.890799	0.517913	-1.518081
82	6	0	1.832539	0.409779	-2.940408
83	1	0	1.746867	1.402525	-2.483109
84	6	0	1.002641	0.435174	-4.245533
85	1	0	1.437993	1.155788	-4.948150
86	1	0	1.005230	-0.547581	-4.735848
87	1	0	-0.033628	0.726232	-4.049406
88	6	0	3.311350	0.141209	-3.253550
89	1	0	3.905142	-0.024489	-2.350488
90	1	0	3.440981	-0.732320	-3.898421
91	1	0	3.721891	1.011859	-3.780614

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*i*Pr-*dr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.584429	-1.947873	-5.319771
2	6	0	2.581661	0.753136	-3.527768
3	6	0	4.077862	0.907025	-3.171604
4	6	0	4.554346	-0.383175	-2.448058
5	6	0	4.052643	-1.573647	-3.298254
6	6	0	2.447947	-0.216011	-4.721440
7	6	0	4.851765	-0.283257	-5.234902
8	6	0	4.906470	1.058958	-4.465314
9	7	0	3.706453	-1.094548	-4.691797
10	1	0	5.753980	-0.885215	-5.097395
11	1	0	4.688880	-0.162387	-6.308614
12	1	0	5.947302	1.311396	-4.233464
13	1	0	4.507377	1.875244	-5.079066
14	1	0	5.658385	-0.373379	-2.458972
15	1	0	3.154524	-2.027786	-2.897354
16	1	0	2.550462	0.330997	-5.664459
17	1	0	2.146312	1.721749	-3.786777
18	1	0	4.223065	1.779743	-2.527370
19	1	0	2.013326	0.382093	-2.670043
20	7	0	-0.507733	-2.882590	-2.197789
21	6	0	-0.129304	-1.693221	-2.773175
22	7	0	0.832360	-1.901318	-3.727173
23	16	0	-0.742723	-0.166559	-2.394789
24	6	0	-1.239133	-3.177305	-1.012496
25	6	0	1.164271	-1.079800	-4.891374
26	1	0	-0.224751	-3.713872	-2.727292
27	6	0	-1.483730	-4.527942	-0.739642
28	6	0	-2.168438	-4.896556	0.401179
29	6	0	-2.619877	-3.932445	1.291811

30	6	0	-2.377936	-2.595862	1.023332
31	6	0	-1.693874	-2.210090	-0.118145
32	1	0	-2.351265	-5.945574	0.597984
33	1	0	-3.156585	-4.223208	2.184571
34	1	0	-2.727670	-1.835212	1.710469
35	1	0	-1.513292	-1.169428	-0.343848
36	1	0	-1.131265	-5.279303	-1.433287
37	6	0	-0.070897	1.027745	-5.671467
38	6	0	-0.045350	-0.315387	-5.509391
39	6	0	-1.194707	1.662231	-6.285912
40	7	0	-2.255680	1.035601	-6.737166
41	6	0	-2.236593	-0.360859	-6.596656
42	1	0	0.732444	1.663084	-5.336796
43	1	0	4.793068	-2.366398	-3.418129
44	1	0	1.257568	-2.837824	-3.740416
45	1	0	1.449267	-1.817682	-5.654767
46	6	0	4.132009	-0.423986	-0.966628
47	6	0	3.608482	-1.434174	-0.321579
48	1	0	3.370385	-1.360315	0.730783
49	1	0	3.385583	-2.386175	-0.782716
50	1	0	4.342099	0.500359	-0.440084
51	6	0	-1.174194	-1.072294	-6.010575
52	6	0	-1.271692	-2.498149	-5.961186
53	6	0	-3.374145	-1.065705	-7.099795
54	6	0	-3.437118	-2.416043	-7.026428
55	6	0	-2.360239	-3.141949	-6.449178
56	1	0	-1.182374	2.745033	-6.389208
57	1	0	-0.467253	-3.076437	-5.532014
58	1	0	-2.414196	-4.222119	-6.401832
59	1	0	-4.297195	-2.952192	-7.407051
60	1	0	-4.172090	-0.480468	-7.538442
61	8	0	3.769124	-5.387546	-7.654603
62	8	0	3.555067	-3.117384	-6.423685
63	15	0	2.932358	-4.529363	-6.487209
64	6	0	5.168059	-5.187880	-7.866957
65	1	0	5.407242	-4.121644	-7.933813
66	1	0	5.413005	-5.682943	-8.810912
67	1	0	5.759501	-5.645096	-7.062915
68	8	0	1.467959	-4.461457	-7.252961
69	6	0	1.342866	-3.888275	-8.565090
70	1	0	1.806022	-2.895808	-8.602182
71	1	0	1.811043	-4.540243	-9.309420
72	1	0	0.272272	-3.801277	-8.766287
73	6	0	1.052902	-5.773444	-4.549195
74	6	0	2.473797	-5.282832	-4.195674
75	8	0	0.047610	-5.171381	-4.209151
76	8	0	2.527372	-4.215356	-3.535534
77	8	0	1.031983	-6.929234	-5.225825
78	6	0	-0.259284	-7.388337	-5.670891
79	1	0	-0.932443	-7.520765	-4.819899
80	1	0	-0.683953	-6.663319	-6.369640
81	1	0	-0.070009	-8.339562	-6.168916
82	6	0	3.536979	-6.376371	-3.984609
83	1	0	3.512145	-7.057515	-4.841306
84	6	0	4.939846	-5.775286	-3.845761
85	1	0	4.993715	-5.117558	-2.971475
86	1	0	5.683098	-6.572202	-3.722399
87	1	0	5.217376	-5.184814	-4.726467
88	6	0	3.170950	-7.179647	-2.715975
89	1	0	2.190587	-7.661157	-2.804630
90	1	0	3.912579	-7.969760	-2.546798
91	1	0	3.157830	-6.529438	-1.833554

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*i*Pr-*mr*-**TS2**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.164315	-0.459096	-1.788644
2	6	0	1.504653	-1.633849	-0.858873
3	8	0	0.577289	-1.993080	-0.108212
4	8	0	2.381069	1.571787	0.762418
5	15	0	2.927830	0.142347	0.545088
6	8	0	2.990957	-0.638377	2.004819
7	6	0	3.621068	-0.011871	3.135357
8	1	0	3.421052	-0.653899	3.997389
9	1	0	4.701264	0.065897	2.973985
10	1	0	3.203439	0.985694	3.309972
11	8	0	4.585764	0.275435	0.294722
12	6	0	5.090587	1.297499	-0.563604
13	1	0	6.181222	1.219921	-0.536723
14	1	0	4.784682	2.289617	-0.213901
15	1	0	4.749367	1.155544	-1.598476
16	7	0	0.562280	3.494168	-0.239815
17	6	0	-0.605882	3.013413	0.287124
18	7	0	-0.377613	1.934688	1.084928
19	16	0	-2.162864	3.657476	-0.026534
20	6	0	0.858281	4.611176	-1.070292
21	6	0	-1.300157	1.062403	1.821349
22	6	0	-2.413918	0.473365	0.896986
23	6	0	-3.792548	0.186917	1.531434
24	6	0	-4.410274	-1.065640	0.877872
25	7	0	-1.958293	-0.832742	0.241025
26	6	0	-2.770281	-1.045800	-1.014305
27	6	0	-4.284020	-0.988624	-0.673882
28	6	0	-2.116107	-2.020365	1.159411
29	6	0	-3.620537	-2.294006	1.369835
30	1	0	1.392747	2.932253	0.017486
31	6	0	-1.817491	1.693627	3.149271
32	1	0	-0.654173	0.225643	2.091367
33	1	0	-4.424147	1.069076	1.390015
34	1	0	-3.710243	0.025204	2.613541
35	1	0	-2.473071	-2.021222	-1.406619
36	1	0	-2.441598	-0.288540	-1.722363
37	6	0	-5.094694	0.188568	-1.252488
38	1	0	-4.745388	-1.906305	-1.072025
39	1	0	-1.573378	-2.845350	0.697565
40	1	0	-1.599887	-1.775142	2.088634
41	1	0	-3.818876	-2.476502	2.431850
42	1	0	-5.464767	-1.156914	1.157513
43	1	0	-3.932098	-3.193786	0.825629
44	1	0	0.614987	1.664027	1.154470
45	1	0	-0.955549	-0.802031	-0.051246
46	6	0	-0.090125	5.507131	-1.560228
47	6	0	0.309548	6.563846	-2.362937
48	6	0	1.641921	6.745950	-2.690126
49	6	0	2.588756	5.855001	-2.202611
50	6	0	2.206411	4.798233	-1.401436
51	1	0	2.943748	4.106359	-1.016663
52	1	0	3.635070	5.986608	-2.448408
53	1	0	1.943889	7.573594	-3.317425
54	1	0	-0.437004	7.253767	-2.736600

55	1	0	-1.126172	5.351183	-1.296836
56	6	0	-2.559886	2.825742	3.117868
57	6	0	-3.038101	3.404869	4.331336
58	7	0	-2.820478	2.912035	5.530869
59	6	0	-2.040543	1.748390	5.577244
60	6	0	-1.514597	1.110214	4.437310
61	6	0	-1.783497	1.211792	6.879125
62	6	0	-1.030407	0.098579	7.033596
63	6	0	-0.483026	-0.543668	5.888979
64	6	0	-0.715801	-0.060165	4.645263
65	1	0	-2.771798	3.298313	2.162091
66	1	0	-3.633559	4.313728	4.276372
67	1	0	-0.267785	-0.563594	3.801767
68	1	0	0.131206	-1.425822	6.020454
69	1	0	-0.831895	-0.306959	8.017320
70	1	0	-2.210352	1.732934	7.726750
71	1	0	-2.547109	1.166620	0.068334
72	6	0	-4.670916	1.183025	-1.988236
73	1	0	-6.145491	0.124559	-0.993346
74	1	0	-5.354755	1.944650	-2.337761
75	1	0	-3.641230	1.318509	-2.288196
76	6	0	1.820071	0.951204	-3.567983
77	1	0	1.640361	1.856566	-2.983114
78	1	0	2.705583	1.059736	-4.194643
79	1	0	0.939906	0.731590	-4.178134
80	8	0	0.084668	0.108679	-1.729750
81	8	0	2.109497	-0.158350	-2.691552
82	6	0	2.632544	-2.589026	-1.249722
83	1	0	3.485622	-1.996791	-1.593666
84	6	0	3.061887	-3.470695	-0.071502
85	1	0	2.226241	-4.087388	0.276852
86	1	0	3.875877	-4.136477	-0.382718
87	1	0	3.408570	-2.866560	0.771507
88	6	0	2.139630	-3.455986	-2.433574
89	1	0	1.849800	-2.848259	-3.298562
90	1	0	2.942446	-4.129741	-2.755455
91	1	0	1.281685	-4.070605	-2.135439

S7: Reference 24 details.

24 M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Jr. Montgomery, T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian 03, B05; 105 Gaussian, Inc.: Wallingford, CT, 2003.