Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supporting Information

Computational investigation on the mechanism and stereochemistry of guanidine-catalyzed enantioselective isomerization of 3-alkynoates to allenoates

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Part I: Model system

Part II: Actual system

Part I: Model system

S1: Summarize energies of all optimized stationary points over model reaction system. (a.u.)

Species	B3LYP/6-31+G(d,p)					
	ZPE	E_{ZPE}	G_c[a]	E_{PCM}[b]	G[c]	
Reactant	0.181252	−575.434572	0.139312	−575.628546	−575.489234	
Cat.	0.147311	−360.058238	0.117003	−360.216473	−360.099470	
cis-COM	0.329802	−935.503328	0.273605	−935.853084	−935.579479	0.0
cis-TS1	0.325445	−935.486876	0.273901	−935.833160	−935.559259	53.1
cis-IM1	0.329353	−935.490612	0.277327	−935.841760	−935.564433	39.5
cis-TSR	0.328403	−935.489907	0.276956	−935.840637	−935.563681	41.5
cis-IM2	0.328489	−935.491882	0.275394	−935.843446	−935.568052	30.0
cis-TS2	0.325110	−935.489572	0.273455	−935.836559	−935.563104	43.0
cis-IM3	0.329371	−935.511965	0.274559	−935.861149	−935.586590	–18.7
Product	0.180937	−575.442305	0.140377	−575.635898	−575.495521	
trans-COM	0.329851	−935.503649	0.274345	−935.853780	−935.579435	0.1
trans-TS1	0.325265	−935.485686	0.272891	−935.833183	−935.560292	50.3
trans-IM1	0.328458	−935.486706	0.275195	−935.839419	−935.564224	40.0
trans-TSR	0.329012	−935.477560	0.277008	−935.831639	−935.554631	65.2
trans-IM2	0.328482	−935.479252	0.274491	−935.832846	−935.558355	55.4
trans-TS2	0.324708	−935.479332	0.271294	−935.827758	−935.556464	60.4
trans-IM3	0.329167	−935.506791	0.273075	−935.856734	−935.583659	–11.0
cis-COM'	0.329329	−935.498739	0.272869	−935.849239	−935.576370	8.2
cis-TS1'	0.325176	−935.477004	0.272431	−935.826861	−935.554430	65.7
cis-IM1'	0.328871	−935.475346	0.274743	−935.830545	−935.555802	62.1
trans-COM'	0.329686	−935.500043	0.274042	−935.850481	−935.576439	8.0
trans-TS1'	0.325176	−935.477004	0.272431	−935.827575	−935.555144	63.9
trans-IM1'	0.328871	−935.475346	0.274743	−935.832601	−935.557858	56.7

a: Thermal correction to Gibbs Free Energy
b: total electronic energies in solvent.
c:$G=E_{PCM}+Gc$.

S2. Cartesian coordinates and energies of all optimized stationary points of model reaction system.

Catalyst

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.174651	-0.185097	-0.090443
2	7	0	0.035733	0.663801	-0.293356
3	6	0	0.059912	-0.710168	-0.017053
4	7	0	1.201329	-1.284810	0.103390
5	6	0	-2.156284	-0.049280	-0.130720
6	7	0	-1.233321	-1.152916	0.165101
7	1	0	-1.463511	-2.106448	-0.074725
8	1	0	-2.493253	-0.058633	-1.177512
9	1	0	3.001679	-0.271595	0.620459
10	1	0	-3.031740	-0.076037	0.524011
11	1	0	2.599305	-0.230409	-1.103853
12	6	0	-1.257376	1.182835	0.134558
13	6	0	1.363478	1.134889	0.101887
14	1	0	-1.568167	2.058085	-0.442447
15	1	0	-1.258144	1.443529	1.207503
16	1	0	1.713614	1.959240	-0.525578
17	1	0	1.367738	1.460666	1.156827

Reactant

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.976985	0.021719	0.000654
2	8	0	4.256572	-0.415507	-0.001832
3	8	0	2.661655	1.189435	0.000654
4	6	0	2.031342	-1.178895	0.003897
5	6	0	-1.952767	-0.208082	0.001160
6	6	0	-0.565250	-0.557550	0.002913
7	6	0	0.617002	-0.827681	0.002990
8	1	0	2.283324	-1.797514	-0.867754
9	1	0	2.283377	-1.792185	0.879375
10	6	0	5.271564	0.608343	-0.004173
11	6	0	-2.947646	-1.206172	-0.001993
12	6	0	-4.297667	-0.855488	-0.003751
13	6	0	-4.676822	0.490821	-0.002335
14	6	0	-3.695649	1.487946	0.000908
15	6	0	-2.343540	1.146352	0.002700
16	1	0	-2.651205	-2.250517	-0.003074
17	1	0	-5.054866	-1.634482	-0.006227
18	1	0	-5.728922	0.760992	-0.003710
19	1	0	-3.984162	2.535300	0.002054
20	1	0	-1.579064	1.916759	0.005191
21	1	0	5.177847	1.234011	-0.895079
22	1	0	5.181441	1.234520	0.886754
23	1	0	6.221105	0.073812	-0.005933

Product

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.780259	-0.089546	0.102031
2	8	0	3.933416	0.226744	-0.538592
3	8	0	2.627813	0.019320	1.302502
4	6	0	1.772459	-0.575116	-0.879590
5	6	0	-1.850626	-0.503977	-0.072875
6	6	0	-0.636743	-1.338404	-0.164198
7	6	0	0.564628	-0.947359	-0.518289
8	1	0	2.083250	-0.611556	-1.922216
9	6	0	4.999075	0.709200	0.299783
10	6	0	-1.837236	0.876085	-0.346382
11	6	0	-3.006908	1.626961	-0.250779
12	6	0	-4.211756	1.017186	0.120732
13	6	0	-4.235491	-0.351989	0.396643
14	6	0	-3.063974	-1.106069	0.300546
15	1	0	-0.905157	1.356719	-0.629330
16	1	0	-2.980151	2.691944	-0.463658
17	1	0	-5.121371	1.605981	0.195496
18	1	0	-5.164298	-0.834521	0.687416
19	1	0	-3.086979	-2.171061	0.517596
20	1	0	-0.755327	-2.391574	0.095365
21	1	0	5.269395	-0.044469	1.043670
22	1	0	4.695417	1.625219	0.812931
23	1	0	5.833258	0.902983	-0.374277

cis-COM

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.755988	2.543540	0.010556
2	8	0	1.212264	3.758735	-0.337755
3	8	0	0.875169	2.085212	1.133604
4	6	0	0.141003	1.818410	-1.175575
5	6	0	-3.398134	-0.070010	-0.307877
6	6	0	-2.164760	0.591154	-0.605044
7	6	0	-1.116130	1.149236	-0.853113
8	1	0	0.012435	2.523015	-2.003158
9	1	0	0.900605	1.072246	-1.478583
10	6	0	1.902197	4.498610	0.690530
11	6	0	-4.070043	-0.815642	-1.297811
12	6	0	-5.272775	-1.457847	-1.003788
13	6	0	-5.825826	-1.369906	0.278006
14	6	0	-5.166096	-0.633008	1.267193
15	6	0	-3.963582	0.013082	0.980945
16	1	0	-3.639023	-0.884085	-2.291744
17	1	0	-5.779209	-2.028679	-1.777155
18	1	0	-6.762643	-1.871119	0.504060
19	1	0	-5.589938	-0.560191	2.264957
20	1	0	-3.450525	0.586010	1.747006
21	1	0	1.236104	4.681737	1.536859
22	1	0	2.778671	3.942902	1.031988
23	1	0	2.197687	5.436243	0.220819
24	6	0	3.557870	-1.202515	-1.922661

25	7	0	3.404021	-2.069931	0.212885
26	6	0	2.555404	-0.973585	0.010942
27	7	0	2.576498	-0.407440	-1.149979
28	6	0	2.190763	-1.739921	2.157959
29	7	0	1.785729	-0.786057	1.122733
30	1	0	1.374555	0.120773	1.325366
31	1	0	2.916789	-1.303329	2.859602
32	1	0	3.205885	-1.367148	-2.945767
33	1	0	1.329343	-2.103542	2.725211
34	1	0	4.518631	-0.669752	-1.982586
35	6	0	2.853546	-2.855756	1.312554
36	6	0	3.725741	-2.537810	-1.134930
37	1	0	3.626422	-3.397813	1.864299
38	1	0	2.097838	-3.576698	0.954760
39	1	0	4.733259	-2.958619	-1.197562
40	1	0	2.998908	-3.297733	-1.471954

cis-TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.268201	-1.906755	-0.000077
2	8	0	-3.362175	-2.578266	-0.450123
3	8	0	-2.165379	-1.595297	1.195757
4	6	0	-1.364404	-1.525595	-1.075928
5	6	0	2.595926	-1.022608	-0.270819
6	6	0	1.213066	-1.215532	-0.555646
7	6	0	0.027776	-1.409709	-0.777811
8	1	0	-1.598604	-1.998939	-2.030121
9	6	0	-4.382349	-2.853364	0.521294
10	6	0	3.071092	-1.049021	1.060285
11	6	0	4.423809	-0.855074	1.337952
12	6	0	5.338025	-0.634251	0.301639
13	6	0	4.881621	-0.611403	-1.020950
14	6	0	3.530022	-0.800575	-1.307735
15	1	0	2.366767	-1.235148	1.865519
16	1	0	4.767747	-0.883980	2.368648
17	1	0	6.391658	-0.487865	0.521192
18	1	0	5.582919	-0.446894	-1.834852
19	1	0	3.181120	-0.785314	-2.335900
20	1	0	-3.989551	-3.475024	1.330090
21	1	0	-4.775987	-1.925090	0.945255
22	1	0	-5.164089	-3.384591	-0.023036
23	1	0	-1.733140	-0.106304	-1.183892
24	6	0	-0.650920	3.182034	-1.324786
25	6	0	-1.574701	2.164275	-2.057933
26	7	0	-1.012632	2.928023	0.077060
27	6	0	-1.480485	1.629063	0.112000
28	7	0	-1.870587	1.132738	-1.040856
29	6	0	-0.126468	3.095227	1.237188
30	6	0	-0.701379	2.042427	2.226924
31	7	0	-1.375371	1.095687	1.330169
32	1	0	-0.845219	4.217795	-1.613647
33	1	0	0.413838	2.956711	-1.492594
34	1	0	-0.166196	4.110782	1.637951
35	1	0	0.913619	2.857957	0.964339
36	1	0	-1.578975	0.102449	1.509644
37	1	0	-1.090084	1.714885	-2.929264

38	1	0	0.082126	1.547283	2.805810
39	1	0	-1.417911	2.497163	2.922075
40	1	0	-2.504043	2.642658	-2.390486

cis-IM1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.947956	-1.259850	-0.027356
2	8	0	4.208725	-1.627263	0.366503
3	8	0	2.808533	-0.654066	-1.127106
4	6	0	1.949999	-1.597087	0.916220
5	6	0	-2.011466	-1.424080	0.111651
6	6	0	-0.624189	-1.504119	0.391712
7	6	0	0.582837	-1.572063	0.613498
8	1	0	2.277933	-2.111493	1.814784
9	6	0	5.283114	-1.246222	-0.496523
10	6	0	-2.979056	-1.557833	1.139438
11	6	0	-4.341209	-1.464791	0.858976
12	6	0	-4.789180	-1.230070	-0.446899
13	6	0	-3.847500	-1.101393	-1.475154
14	6	0	-2.482767	-1.199025	-1.207201
15	1	0	-2.642075	-1.746289	2.154609
16	1	0	-5.060334	-1.578753	1.666298
17	1	0	-5.851625	-1.160984	-0.660870
18	1	0	-4.180295	-0.938106	-2.497358
19	1	0	-1.760388	-1.130209	-2.015548
20	6	0	-0.958715	2.504029	-1.244046
21	6	0	0.201743	1.922625	-2.104245
22	7	0	-0.315883	2.629124	0.075908
23	6	0	0.723789	1.741222	0.092075
24	7	0	1.098071	1.328492	-1.098228
25	6	0	-0.988457	2.531534	1.381715
26	6	0	0.156260	1.988655	2.288051
27	7	0	1.127650	1.427609	1.325455
28	1	0	-1.804574	1.804869	-1.187045
29	1	0	-1.310934	3.469563	-1.613281
30	1	0	-1.828242	1.824996	1.325052
31	1	0	-1.357883	3.503322	1.716489
32	1	0	1.774113	0.510381	-1.225980
33	1	0	0.724385	2.708356	-2.661869
34	1	0	-0.193931	1.212444	2.971900
35	1	0	1.589826	0.517945	1.472751
36	1	0	5.338929	-0.158112	-0.603785
37	1	0	5.168610	-1.691607	-1.488931
38	1	0	6.187599	-1.623231	-0.015731
39	1	0	-0.142048	1.162405	-2.809198
40	1	0	0.625041	2.789363	2.869117

cis-TSR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.086687	-1.243983	-0.077352
2	8	0	4.355699	-1.644906	0.253650

3	8	0	2.955863	-0.281593	-0.893537
4	6	0	2.082628	-1.983657	0.572299
5	6	0	-1.861247	-1.609565	-0.215211
6	6	0	-0.479738	-1.776627	0.037919
7	6	0	0.727007	-1.874574	0.263240
8	1	0	2.404695	-2.748879	1.271261
9	6	0	-2.842761	-2.228770	0.602104
10	6	0	-4.201533	-2.044143	0.355718
11	6	0	-4.636223	-1.239177	-0.705426
12	6	0	-3.681580	-0.627292	-1.527266
13	6	0	-2.318952	-0.806908	-1.293256
14	1	0	-2.517084	-2.860106	1.423611
15	1	0	-4.929919	-2.536222	0.995490
16	1	0	-5.696645	-1.102971	-0.895802
17	1	0	-4.002728	-0.016972	-2.368232
18	1	0	-1.584971	-0.354004	-1.953788
19	6	0	-0.562739	3.120489	-0.994404
20	6	0	0.784522	2.595019	-1.566911
21	7	0	-0.446089	2.734599	0.420238
22	6	0	0.427756	1.679728	0.466438
23	7	0	1.156230	1.535045	-0.614133
24	6	0	-1.554624	2.421709	1.335989
25	6	0	-0.869588	1.447012	2.338181
26	7	0	0.319462	0.977693	1.597535
27	1	0	-1.422782	2.613221	-1.456061
28	1	0	-0.678494	4.200059	-1.111501
29	1	0	-2.372400	1.927810	0.792253
30	1	0	-1.937102	3.319791	1.825683
31	1	0	1.891662	0.745328	-0.764571
32	1	0	1.549052	3.381103	-1.579142
33	1	0	-1.515152	0.606159	2.600206
34	1	0	0.644631	0.013288	1.625505
35	6	0	5.432698	-0.906847	-0.325494
36	1	0	6.342063	-1.374040	0.057211
37	1	0	5.410174	-0.964530	-1.417836
38	1	0	5.397823	0.146526	-0.028445
39	1	0	0.685263	2.189672	-2.576244
40	1	0	-0.561663	1.960904	3.254608

cis-IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.633011	-1.950862	-0.055387
2	8	0	-3.794006	-2.616055	-0.361731
3	8	0	-2.690690	-0.989708	0.767905
4	6	0	-1.510704	-2.455746	-0.734210
5	6	0	2.305676	-1.434606	0.091486
6	6	0	0.961369	-1.708453	-0.275851
7	6	0	-0.210308	-2.053595	-0.464210
8	1	0	-1.678035	-3.249217	-1.455140
9	6	0	-4.988993	-2.137195	0.254100
10	6	0	3.391473	-1.911098	-0.685956
11	6	0	4.707350	-1.620050	-0.331551
12	6	0	4.990290	-0.841497	0.797972
13	6	0	3.929169	-0.364141	1.576712
14	6	0	2.608438	-0.652938	1.235830
15	1	0	3.182136	-2.515934	-1.563195
16	1	0	5.520318	-2.005947	-0.941497

17	1	0	6.017802	-0.619933	1.071148
18	1	0	4.132633	0.228244	2.465620
19	1	0	1.792372	-0.299161	1.859317
20	6	0	-1.292552	3.669037	0.751961
21	6	0	-2.286979	2.520882	1.073817
22	7	0	-0.599726	3.116213	-0.418530
23	6	0	-0.682118	1.748224	-0.316843
24	7	0	-1.600525	1.334456	0.531280
25	6	0	0.753006	3.436199	-0.893245
26	6	0	1.117220	2.139948	-1.671734
27	7	0	0.237955	1.135904	-1.050716
28	1	0	-0.584348	3.831670	1.579616
29	1	0	-1.793014	4.611641	0.520515
30	1	0	1.433974	3.598859	-0.043608
31	1	0	0.759705	4.322979	-1.530345
32	1	0	-1.971647	0.321042	0.624871
33	1	0	-3.248347	2.671545	0.567467
34	1	0	2.166027	1.859781	-1.554052
35	1	0	0.410497	0.119583	-1.009266
36	1	0	-5.199533	-1.102498	-0.037237
37	1	0	-4.921593	-2.187974	1.345048
38	1	0	-5.783532	-2.794356	-0.104654
39	1	0	-2.469628	2.407109	2.144279
40	1	0	0.891895	2.238024	-2.739853

cis-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.381959	2.727886	0.164556
2	8	0	-2.055205	3.873088	0.468569
3	8	0	-1.716808	2.045918	-0.819834
4	6	0	-0.332338	2.444072	1.109108
5	6	0	2.671550	0.264100	0.137490
6	6	0	1.327233	0.460258	0.679548
7	6	0	0.581567	1.473315	0.883058
8	1	0	-0.286382	3.059332	2.003208
9	6	0	-3.145129	4.218898	-0.393696
10	6	0	3.733043	1.133348	0.467347
11	6	0	5.019401	0.914820	-0.026399
12	6	0	5.281641	-0.171811	-0.868511
13	6	0	4.239907	-1.041741	-1.205097
14	6	0	2.954734	-0.833199	-0.700656
15	1	0	3.535134	1.978589	1.120065
16	1	0	5.820135	1.598882	0.243287
17	1	0	6.283347	-0.338545	-1.254481
18	1	0	4.428994	-1.888629	-1.860030
19	1	0	2.152312	-1.516542	-0.965178
20	6	0	-3.169103	-2.706926	-0.886590
21	6	0	-3.234948	-1.194896	-1.220609
22	7	0	-2.256011	-2.689809	0.258020
23	6	0	-1.426983	-1.597712	0.109736
24	7	0	-1.916819	-0.717366	-0.770537
25	6	0	-1.422196	-3.778904	0.775490
26	6	0	-0.322941	-2.963899	1.514388
27	7	0	-0.302229	-1.682774	0.783385
28	1	0	-2.741378	-3.282815	-1.723210
29	1	0	-4.144004	-3.125739	-0.627001
30	1	0	-0.997731	-4.372313	-0.050521

31	1	0	-1.981888	-4.441213	1.439869
32	1	0	-1.661999	0.288033	-0.798363
33	1	0	-4.040965	-0.701200	-0.662746
34	1	0	0.655893	-3.448093	1.478587
35	1	0	0.468090	-0.764369	0.855710
36	1	0	-3.915445	3.441793	-0.380621
37	1	0	-2.799841	4.357689	-1.421942
38	1	0	-3.544018	5.153479	0.003131
39	1	0	-3.376476	-1.004149	-2.286558
40	1	0	-0.593158	-2.802242	2.565854

cis-IM3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.839191	-0.988296	1.497854
2	6	0	2.976321	0.280397	1.694821
3	7	0	3.553974	-1.289241	0.099759
4	6	0	2.243164	-0.869466	-0.167836
5	7	0	1.847112	0.018811	0.795190
6	6	0	3.673197	-2.583615	-0.568408
7	6	0	2.623163	-2.386303	-1.702429
8	7	0	1.635015	-1.424628	-1.163882
9	1	0	3.500168	-1.801839	2.163148
10	1	0	4.902615	-0.806256	1.676149
11	1	0	3.384239	-3.405736	0.110376
12	1	0	4.686143	-2.768068	-0.937248
13	1	0	1.160374	0.744946	0.609719
14	1	0	3.535648	1.179204	1.397604
15	1	0	2.138270	-3.325145	-1.987849
16	1	0	2.640360	0.402567	2.728116
17	1	0	3.105176	-1.974148	-2.601515
18	6	0	-0.422501	3.117787	-0.287251
19	8	0	-0.553146	4.448413	-0.482609
20	8	0	0.274317	2.643955	0.599224
21	6	0	-1.208565	2.356512	-1.284641
22	6	0	-2.449181	-1.017902	-0.330399
23	6	0	-1.406813	-0.250524	-1.038731
24	6	0	-1.346292	1.050179	-1.179662
25	1	0	-1.653125	2.922082	-2.100764
26	6	0	0.183919	5.296163	0.417094
27	6	0	-3.629465	-0.425744	0.155100
28	6	0	-4.584749	-1.193218	0.819042
29	6	0	-4.380786	-2.565594	1.009522
30	6	0	-3.212424	-3.163221	0.529391
31	6	0	-2.254327	-2.396260	-0.137022
32	1	0	-3.795824	0.637547	0.005339
33	1	0	-5.492370	-0.722541	1.186880
34	1	0	-5.127923	-3.161706	1.525783
35	1	0	-3.045753	-4.227224	0.672942
36	1	0	-1.341543	-2.856401	-0.504803
37	1	0	-0.557936	-0.815964	-1.441948
38	1	0	1.256145	5.102924	0.329766
39	1	0	-0.130156	5.121434	1.449092
40	1	0	-0.049689	6.315404	0.110154

trans-COM

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.299912	1.939537	-0.159684
2	8	0	0.603911	2.554247	0.610038
3	8	0	-1.409297	2.402417	-0.383672
4	6	0	0.157976	0.599270	-0.711332
5	6	0	4.096402	-0.445014	-0.235846
6	6	0	2.725429	-0.071929	-0.403010
7	6	0	1.563449	0.253331	-0.533313
8	1	0	-0.111542	0.595281	-1.774687
9	1	0	-0.502945	-0.156031	-0.244476
10	6	0	0.201007	3.810700	1.190927
11	6	0	4.660002	-0.542254	1.052908
12	6	0	5.997387	-0.903893	1.213715
13	6	0	6.794780	-1.176937	0.097324
14	6	0	6.244664	-1.084982	-1.185449
15	6	0	4.908683	-0.721712	-1.354419
16	1	0	4.038858	-0.331483	1.917781
17	1	0	6.417985	-0.974126	2.213036
18	1	0	7.835722	-1.459583	0.225922
19	1	0	6.857926	-1.296246	-2.057068
20	1	0	4.480815	-0.648980	-2.349460
21	1	0	-0.045901	4.529505	0.406101
22	1	0	-0.667981	3.667514	1.837534
23	1	0	1.061489	4.147996	1.767805
24	6	0	-4.331570	-2.626725	0.604692
25	6	0	-2.847092	-2.451445	1.049994
26	7	0	-4.681364	-1.227262	0.363239
27	6	0	-3.467087	-0.612145	0.036616
28	7	0	-2.379487	-1.211792	0.388278
29	6	0	-5.697866	-0.708074	-0.545170
30	6	0	-5.158597	0.723976	-0.783798
31	7	0	-3.709522	0.513097	-0.703673
32	1	0	-4.965548	-3.086234	1.368160
33	1	0	-4.405926	-3.217215	-0.325408
34	1	0	-6.696279	-0.712047	-0.099326
35	1	0	-5.726402	-1.279075	-1.489798
36	1	0	-3.040759	1.279711	-0.692580
37	1	0	-2.224322	-3.303969	0.762556
38	1	0	-5.450914	1.122552	-1.759353
39	1	0	-5.519576	1.406832	-0.000713
40	1	0	-2.784931	-2.346242	2.143209

trans-TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.671766	2.042270	-0.453401
2	8	0	0.111690	2.736613	0.407445
3	8	0	-1.825976	2.438084	-0.714411
4	6	0	-0.104210	0.799422	-0.936035
5	6	0	3.757672	-0.290816	-0.259473
6	6	0	2.410769	0.100143	-0.507268
7	6	0	1.265364	0.468174	-0.717696

8	1	0	-0.495538	0.538303	-1.921513
9	6	0	-0.466996	3.909002	0.995496
10	6	0	4.508638	0.318522	0.771492
11	6	0	5.827408	-0.063729	1.013063
12	6	0	6.432991	-1.059699	0.238436
13	6	0	5.700736	-1.670637	-0.785636
14	6	0	4.381214	-1.294476	-1.034678
15	1	0	4.042250	1.093399	1.372020
16	1	0	6.386752	0.419642	1.809944
17	1	0	7.461091	-1.354169	0.428970
18	1	0	6.160721	-2.443862	-1.395629
19	1	0	3.817924	-1.768740	-1.832746
20	1	0	-0.753627	4.629883	0.225179
21	1	0	-1.350049	3.653627	1.588797
22	1	0	0.312331	4.324911	1.635422
23	1	0	-0.918888	-0.175045	-0.146261
24	6	0	-3.135769	-2.832553	0.679813
25	6	0	-1.721126	-2.241484	0.963082
26	7	0	-3.925865	-1.600672	0.550410
27	6	0	-3.040984	-0.626845	0.139453
28	7	0	-1.777865	-0.890251	0.367000
29	6	0	-5.166976	-1.402140	-0.205576
30	6	0	-5.106341	0.125790	-0.480286
31	7	0	-3.659041	0.375488	-0.492670
32	1	0	-3.502243	-3.468638	1.488810
33	1	0	-3.152571	-3.404900	-0.261727
34	1	0	-6.048877	-1.691224	0.370467
35	1	0	-5.148909	-1.975274	-1.146685
36	1	0	-3.166291	1.262235	-0.694217
37	1	0	-0.921031	-2.831099	0.509270
38	1	0	-5.563761	0.396996	-1.434590
39	1	0	-1.530073	-2.172184	2.040847
40	1	0	-5.599285	0.690934	0.321479

trans-IM1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.707590	2.086578	-0.453981
2	8	0	0.034433	2.821436	0.424034
3	8	0	-1.919889	2.416146	-0.656496
4	6	0	-0.057302	0.980924	-1.037101
5	6	0	3.731257	-0.234136	-0.274206
6	6	0	2.405032	0.197410	-0.539481
7	6	0	1.271527	0.597112	-0.781113
8	1	0	-0.561264	0.552681	-1.900713
9	6	0	-0.627379	3.910811	1.070879
10	6	0	4.333710	-1.265045	-1.034524
11	6	0	5.636063	-1.683439	-0.765910
12	6	0	6.377817	-1.091147	0.262958
13	6	0	5.795502	-0.068831	1.021900
14	6	0	4.493902	0.356270	0.762335
15	1	0	3.766369	-1.724723	-1.838438
16	1	0	6.076859	-2.475555	-1.366152
17	1	0	7.393131	-1.418434	0.467802
18	1	0	6.361251	0.402620	1.821661
19	1	0	4.048376	1.151996	1.351479
20	1	0	-0.992021	4.640089	0.341771
21	1	0	-1.473176	3.562537	1.672737

22	1	0	0.128321	4.365614	1.713842
23	6	0	-3.167660	-2.916344	0.636275
24	6	0	-1.722378	-2.436055	0.960097
25	7	0	-3.876478	-1.634214	0.517279
26	6	0	-2.950495	-0.696855	0.136634
27	7	0	-1.706160	-1.076979	0.393146
28	6	0	-5.102299	-1.341242	-0.237714
29	6	0	-4.933253	0.183042	-0.493031
30	7	0	-3.469289	0.353347	-0.468731
31	1	0	-3.589132	-3.541139	1.426352
32	1	0	-3.202911	-3.468808	-0.315545
33	1	0	-6.000434	-1.578006	0.336428
34	1	0	-5.119323	-1.905864	-1.182999
35	1	0	-2.897725	1.260403	-0.639359
36	1	0	-5.403369	0.774451	0.302420
37	1	0	-0.957250	-3.061813	0.496221
38	1	0	-5.347157	0.496040	-1.453855
39	1	0	-1.544279	-2.402897	2.040887
40	1	0	-0.897844	-0.499241	0.089201

trans-TSR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.580045	2.540080	-0.437909
2	8	0	-1.041720	2.858481	0.790360
3	8	0	-2.777325	2.776800	-0.681210
4	6	0	-0.682175	1.867885	-1.321523
5	6	0	2.931815	0.368979	-0.325011
6	6	0	1.624094	0.817583	-0.657380
7	6	0	0.573847	1.389859	-0.972643
8	1	0	-1.004757	1.806483	-2.357559
9	6	0	3.745460	-0.293598	-1.277612
10	6	0	5.018441	-0.748963	-0.937989
11	6	0	5.521921	-0.567456	0.355824
12	6	0	4.729576	0.085889	1.307890
13	6	0	3.455721	0.546828	0.980064
14	1	0	3.366641	-0.432037	-2.286123
15	1	0	5.624756	-1.246053	-1.691239
16	1	0	6.515414	-0.921507	0.615073
17	1	0	5.110325	0.244048	2.313940
18	1	0	2.851916	1.063188	1.720486
19	6	0	-1.414916	-3.420146	0.662711
20	6	0	-0.085561	-2.617377	0.663513
21	7	0	-2.388452	-2.332478	0.512420
22	6	0	-1.762737	-1.303653	-0.129349
23	7	0	-0.442665	-1.419222	-0.120739
24	6	0	-3.780682	-2.369095	0.047811
25	6	0	-3.990133	-0.883430	-0.353995
26	7	0	-2.618692	-0.464402	-0.696917
27	1	0	-1.570624	-3.979072	1.587476
28	1	0	-1.468064	-4.112416	-0.191390
29	1	0	-4.462361	-2.693976	0.836334
30	1	0	-3.884650	-3.039554	-0.818939
31	1	0	-2.331134	0.474678	-0.998724
32	1	0	-4.372764	-0.287351	0.481918
33	1	0	0.737351	-3.157668	0.192479
34	1	0	0.218449	-0.645850	-0.339363
35	1	0	-4.657125	-0.764167	-1.209179

36	1	0	0.210376	-2.334531	1.680374
37	6	0	-1.929965	3.498323	1.707995
38	1	0	-1.336705	3.688411	2.604771
39	1	0	-2.308760	4.439709	1.299005
40	1	0	-2.785236	2.857880	1.949747

trans-IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.670653	2.699498	-0.398942
2	8	0	-1.185674	2.753147	0.892996
3	8	0	-2.740903	3.239258	-0.692775
4	6	0	-0.853786	1.913903	-1.287693
5	6	0	2.780563	0.423091	-0.346706
6	6	0	1.444974	0.811473	-0.657315
7	6	0	0.394756	1.396135	-0.952079
8	1	0	-1.113745	2.005914	-2.339611
9	6	0	-1.969063	3.518587	1.811136
10	6	0	3.616063	-0.178648	-1.319557
11	6	0	4.913988	-0.575432	-1.000540
12	6	0	5.419487	-0.395962	0.292624
13	6	0	4.604324	0.195297	1.265436
14	6	0	3.305660	0.598097	0.957789
15	1	0	3.234107	-0.316460	-2.326909
16	1	0	5.537568	-1.025221	-1.769189
17	1	0	6.432001	-0.704629	0.535799
18	1	0	4.985857	0.351008	2.271522
19	1	0	2.683542	1.068271	1.713686
20	1	0	-2.059985	4.557495	1.480171
21	1	0	-2.975936	3.101963	1.920297
22	1	0	-1.435024	3.471229	2.762416
23	6	0	-1.356536	-3.605703	0.676776
24	6	0	-0.005755	-2.848164	0.816560
25	7	0	-2.281567	-2.483999	0.472891
26	6	0	-1.569093	-1.463244	-0.087451
27	7	0	-0.258804	-1.620438	0.041440
28	6	0	-3.619640	-2.464182	-0.133189
29	6	0	-3.737846	-0.964100	-0.526386
30	7	0	-2.325959	-0.578237	-0.711751
31	1	0	-1.608737	-4.184014	1.567861
32	1	0	-1.353921	-4.273480	-0.198359
33	1	0	-4.389925	-2.777557	0.574316
34	1	0	-3.655791	-3.116602	-1.019168
35	1	0	-1.944052	0.367593	-0.992359
36	1	0	-4.194221	-0.372887	0.275686
37	1	0	0.835626	-3.405707	0.401109
38	1	0	-4.306970	-0.811333	-1.444979
39	1	0	0.209349	-2.605952	1.863974
40	1	0	0.412536	-0.854037	-0.158874

trans-TS2

Standard orientation:

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

1	6	0	-0.917598	3.076309	-0.272953
2	8	0	-0.515823	2.985279	1.032052
3	8	0	-1.733025	3.918558	-0.638914
4	6	0	-0.316033	2.073162	-1.140284
5	6	0	2.691075	-0.184239	-0.203473
6	6	0	1.277261	0.146315	-0.358575
7	6	0	0.596891	1.147927	-0.748983
8	1	0	-0.546218	2.200424	-2.195979
9	1	0	0.233558	-0.962718	-0.054722
10	6	0	-1.074680	3.960063	1.920003
11	6	0	3.637246	0.128059	-1.202190
12	6	0	4.977627	-0.229898	-1.057018
13	6	0	5.412942	-0.901826	0.090391
14	6	0	4.487859	-1.216496	1.090134
15	6	0	3.143244	-0.872622	0.940086
16	1	0	3.305435	0.652891	-2.093030
17	1	0	5.687402	0.022673	-1.840537
18	1	0	6.457909	-1.176067	0.202932
19	1	0	4.813139	-1.734196	1.988804
20	1	0	2.430242	-1.119078	1.722438
21	6	0	-2.178951	-3.513365	0.420434
22	6	0	-0.724026	-3.045360	0.712296
23	7	0	-2.862963	-2.218020	0.321445
24	6	0	-1.911208	-1.309645	-0.076859
25	7	0	-0.673535	-1.701467	0.103319
26	6	0	-4.105688	-1.892367	-0.386172
27	6	0	-3.929300	-0.365193	-0.600241
28	7	0	-2.464361	-0.235663	-0.647573
29	1	0	-2.595974	-4.134291	1.216205
30	1	0	-2.241316	-4.059821	-0.533799
31	1	0	-4.989304	-2.134170	0.208040
32	1	0	-4.160859	-2.425515	-1.348343
33	1	0	-1.933653	0.620421	-0.844642
34	1	0	-4.346744	0.205279	0.238283
35	1	0	0.025912	-3.702449	0.266778
36	1	0	-4.385060	-0.015129	-1.528486
37	1	0	-0.539120	-2.983760	1.792013
38	1	0	-0.812226	4.973069	1.602168
39	1	0	-2.165107	3.877784	1.959024
40	1	0	-0.641191	3.745055	2.897830

trans-IM3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.649361	3.243895	-0.218022
2	8	0	0.933343	2.960026	1.071100
3	8	0	0.335913	4.355237	-0.609443
4	6	0	0.751931	2.064827	-1.116018
5	6	0	2.603668	-1.039017	-0.239381
6	6	0	1.281048	-0.394699	-0.352448
7	6	0	1.043050	0.839741	-0.724821
8	1	0	0.576287	2.295207	-2.165844
9	6	0	0.851513	4.065041	1.988398
10	6	0	3.804177	-0.360418	-0.519415
11	6	0	5.030103	-1.012090	-0.400630
12	6	0	5.082647	-2.352669	0.001508
13	6	0	3.896512	-3.035256	0.283219
14	6	0	2.666780	-2.383924	0.163734

15	1	0	3.771150	0.680143	-0.830234
16	1	0	5.948315	-0.474583	-0.620899
17	1	0	6.039910	-2.857751	0.093632
18	1	0	3.926749	-4.075274	0.596033
19	1	0	1.744210	-2.914814	0.381796
20	1	0	1.555676	4.851249	1.704172
21	1	0	-0.160154	4.478933	2.001466
22	1	0	1.110221	3.650388	2.962515
23	6	0	-4.015664	-2.544689	0.598367
24	6	0	-2.517457	-2.787997	0.958117
25	7	0	-3.973834	-1.105322	0.340363
26	6	0	-2.656908	-0.857822	-0.059484
27	7	0	-1.760829	-1.731396	0.245769
28	6	0	-4.858080	-0.326802	-0.519820
29	6	0	-3.960001	0.899799	-0.811888
30	7	0	-2.623786	0.289865	-0.812959
31	1	0	-4.706061	-2.799903	1.406926
32	1	0	-4.307378	-3.099270	-0.310399
33	1	0	-5.790308	-0.052473	-0.018956
34	1	0	-5.098447	-0.868034	-1.451270
35	1	0	-1.783238	0.850809	-0.847432
36	1	0	-4.068024	1.653916	-0.019434
37	1	0	-2.174967	-3.781707	0.654196
38	1	0	-4.185866	1.363945	-1.775519
39	1	0	-2.363498	-2.698282	2.043304
40	1	0	0.404462	-1.004147	-0.098016

cis-COM'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.034386	0.867259	-1.621904
2	6	0	1.834179	3.699439	0.390072
3	8	0	1.373717	2.477013	-0.222533
4	6	0	0.105422	2.096749	0.120067
5	8	0	-0.583504	2.740482	0.875811
6	6	0	-0.250635	0.787645	-0.564704
7	6	0	-4.185232	-0.307433	-0.197030
8	6	0	-2.812862	0.073901	-0.329493
9	6	0	-1.652868	0.413676	-0.431226
10	1	0	0.407694	0.006536	-0.141282
11	6	0	-4.689340	-1.433525	-0.878755
12	6	0	-6.028796	-1.798874	-0.744581
13	6	0	-6.886693	-1.051641	0.069132
14	6	0	-6.395016	0.067085	0.750153
15	6	0	-5.057205	0.439639	0.621121
16	1	0	-4.022013	-2.013114	-1.509021
17	1	0	-6.403506	-2.669203	-1.276204
18	1	0	-7.929273	-1.338811	0.172000
19	1	0	-7.055585	0.651723	1.384427
20	1	0	-4.672253	1.306847	1.148258
21	6	0	4.114874	-2.611990	0.996792
22	6	0	2.555911	-2.588564	0.985617
23	7	0	4.400932	-1.677749	-0.095835
24	6	0	3.263615	-0.859177	-0.153963
25	7	0	2.185787	-1.274369	0.414914
26	6	0	5.567287	-0.798971	-0.165925
27	6	0	5.022642	0.376441	-1.024600
28	7	0	3.572485	0.298956	-0.809867

29	1	0	4.538413	-3.603286	0.813361
30	1	0	4.514368	-2.225443	1.950721
31	1	0	6.428011	-1.288295	-0.629773
32	1	0	5.861013	-0.451176	0.840306
33	1	0	2.969601	1.107341	-0.727412
34	1	0	5.267575	0.235500	-2.084844
35	1	0	2.132069	-2.711488	1.986680
36	1	0	2.160525	-3.397823	0.355126
37	1	0	5.430036	1.340176	-0.703428
38	1	0	2.836090	3.867427	-0.006143
39	1	0	1.174038	4.528315	0.125224
40	1	0	1.860980	3.593295	1.477140

cis-TS1'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.410497	1.131532	-1.821302
2	6	0	2.511132	3.686072	0.188846
3	8	0	1.917168	2.561042	-0.475918
4	6	0	0.633455	2.202987	0.015206
5	8	0	0.216058	2.730650	1.033035
6	6	0	0.059096	1.145773	-0.788051
7	6	0	-3.791153	-0.020979	-0.200229
8	6	0	-2.447119	0.394780	-0.417501
9	6	0	-1.305268	0.792921	-0.593814
10	1	0	0.773187	-0.115601	-0.240944
11	6	0	-4.493444	-0.765950	-1.174838
12	6	0	-5.810275	-1.167723	-0.953007
13	6	0	-6.462297	-0.840069	0.241049
14	6	0	-5.778280	-0.101889	1.213982
15	6	0	-4.461618	0.303953	1.001531
16	1	0	-3.993689	-1.018348	-2.105336
17	1	0	-6.331662	-1.737494	-1.718042
18	1	0	-7.488820	-1.152891	0.409822
19	1	0	-6.274796	0.161924	2.144289
20	1	0	-3.934756	0.880602	1.755490
21	6	0	2.614147	-3.027947	0.663341
22	6	0	1.209347	-2.451995	0.312264
23	7	0	3.483067	-2.063876	-0.027028
24	6	0	2.767782	-0.894221	-0.101896
25	7	0	1.479339	-1.015038	0.091383
26	6	0	4.876118	-1.707423	0.260587
27	6	0	4.958539	-0.294462	-0.383830
28	7	0	3.564877	0.163634	-0.289978
29	1	0	2.763511	-4.045228	0.294881
30	1	0	2.796452	-3.006764	1.749159
31	1	0	5.580009	-2.412403	-0.186680
32	1	0	5.054662	-1.660363	1.346491
33	1	0	3.190717	1.095859	-0.486044
34	1	0	5.285125	-0.355647	-1.429602
35	1	0	0.484745	-2.589483	1.117039
36	1	0	0.809053	-2.909431	-0.600700
37	1	0	5.632601	0.371614	0.159620
38	1	0	3.453086	3.877536	-0.330925
39	1	0	1.861387	4.562219	0.116654
40	1	0	2.690950	3.472838	1.246722

cis-IM1'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.539791	1.672945	-1.944154
2	6	0	3.046582	3.493357	0.318584
3	8	0	2.296299	2.542356	-0.446268
4	6	0	0.967749	2.281339	0.070399
5	8	0	0.736895	2.558697	1.244217
6	6	0	0.177973	1.649828	-0.920067
7	6	0	-3.550210	0.246510	-0.198689
8	6	0	-2.245602	0.740886	-0.459005
9	6	0	-1.133528	1.217125	-0.669600
10	1	0	0.483537	-0.267252	-0.373569
11	6	0	-4.345208	-0.309001	-1.230546
12	6	0	-5.623475	-0.796969	-0.963866
13	6	0	-6.149994	-0.748687	0.332399
14	6	0	-5.376146	-0.199443	1.362238
15	6	0	-4.097020	0.291451	1.107273
16	1	0	-3.946280	-0.343466	-2.240112
17	1	0	-6.215232	-1.214412	-1.774836
18	1	0	-7.147673	-1.127232	0.535567
19	1	0	-5.774724	-0.149183	2.372505
20	1	0	-3.504225	0.723549	1.907784
21	6	0	1.951068	-3.175134	0.532495
22	6	0	0.634310	-2.496398	0.058201
23	7	0	2.961495	-2.288871	-0.066591
24	6	0	2.377921	-1.060356	-0.216428
25	7	0	1.061802	-1.101164	-0.146273
26	6	0	4.346297	-2.060624	0.365659
27	6	0	4.617736	-0.652175	-0.234660
28	7	0	3.262903	-0.079609	-0.326256
29	1	0	2.049899	-4.201145	0.172857
30	1	0	2.033620	-3.167292	1.629804
31	1	0	5.024610	-2.820884	-0.026499
32	1	0	4.413858	-2.049159	1.464258
33	1	0	3.011159	0.920242	-0.451761
34	1	0	5.073567	-0.723816	-1.229184
35	1	0	-0.163148	-2.550279	0.800937
36	1	0	0.273889	-2.928084	-0.882368
37	1	0	5.257940	-0.041256	0.405207
38	1	0	4.022958	3.572183	-0.166940
39	1	0	2.551265	4.469460	0.305210
40	1	0	3.155528	3.173903	1.359217

trans-COM'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.966902	3.047818	-0.422353
2	8	0	-0.955435	2.550417	0.838646
3	8	0	-1.373507	4.156668	-0.693222
4	6	0	-0.472161	2.035485	-1.445713
5	6	0	2.943502	-0.004930	-0.429650
6	6	0	1.757184	0.716239	-0.777157
7	6	0	0.746501	1.322291	-1.069293

8	1	0	-0.338102	2.578318	-2.386339
9	6	0	-1.480566	3.425001	1.859004
10	6	0	3.043088	-1.387081	-0.691020
11	6	0	4.200611	-2.087998	-0.352941
12	6	0	5.275686	-1.427212	0.250734
13	6	0	5.186640	-0.056303	0.514034
14	6	0	4.033100	0.652012	0.177567
15	1	0	2.208059	-1.897220	-1.161149
16	1	0	4.264277	-3.152133	-0.562550
17	1	0	6.176093	-1.975655	0.512221
18	1	0	6.018658	0.463362	0.980929
19	1	0	3.963487	1.716547	0.378300
20	1	0	-1.291414	1.306334	-1.586350
21	6	0	-3.337198	-2.779232	-0.848715
22	6	0	-3.190693	-1.593882	-1.852973
23	7	0	-2.313132	-2.400495	0.124504
24	6	0	-2.225645	-1.008796	0.020384
25	7	0	-2.674236	-0.457222	-1.054902
26	6	0	-2.244437	-2.748970	1.538679
27	6	0	-1.334283	-1.610987	2.062655
28	7	0	-1.726767	-0.496138	1.191419
29	1	0	-3.141242	-3.757595	-1.296157
30	1	0	-4.338156	-2.792371	-0.383137
31	1	0	-2.478152	-1.853162	-2.649828
32	1	0	-1.812665	-3.739893	1.703211
33	1	0	-3.238768	-2.708597	2.016812
34	1	0	-1.520648	-1.379467	3.115050
35	1	0	-1.216534	0.379158	1.174029
36	1	0	-0.274887	-1.876896	1.938916
37	1	0	-4.140943	-1.332995	-2.328216
38	1	0	-2.527282	3.659631	1.652704
39	1	0	-0.901500	4.350341	1.898192
40	1	0	-1.386361	2.871881	2.793374

trans-TS1'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.037613	-2.383568	-0.550362
2	8	0	1.716965	-2.208765	0.799075
3	8	0	3.026117	-3.030198	-0.865924
4	6	0	1.158593	-1.642183	-1.440873
5	6	0	-2.645156	-0.641274	-0.400311
6	6	0	-1.319243	-1.009897	-0.765283
7	6	0	-0.187284	-1.361183	-1.069114
8	1	0	1.311219	-1.930742	-2.481230
9	6	0	2.556678	-2.926901	1.716455
10	6	0	-3.121062	-0.846057	0.915806
11	6	0	-4.418029	-0.477723	1.271751
12	6	0	-5.277774	0.099063	0.330087
13	6	0	-4.822181	0.301833	-0.977572
14	6	0	-3.525528	-0.059356	-1.341346
15	1	0	-2.463846	-1.309278	1.645874
16	1	0	-4.762953	-0.649747	2.288178
17	1	0	-6.288984	0.380615	0.609287
18	1	0	-5.481971	0.743330	-1.720014
19	1	0	-3.178259	0.098379	-2.357982
20	1	0	1.761880	-0.244541	-1.344078
21	6	0	1.882492	3.285344	-0.983313

22	6	0	1.979089	2.072289	-1.955350
23	7	0	1.246860	2.639108	0.167473
24	6	0	1.576606	1.314020	0.106301
25	7	0	2.045165	0.901210	-1.050288
26	6	0	1.172356	3.028051	1.575458
27	6	0	0.790645	1.667301	2.220032
28	7	0	1.420239	0.708330	1.295561
29	1	0	1.275468	4.103180	-1.378309
30	1	0	2.879593	3.670766	-0.717874
31	1	0	1.086317	2.008351	-2.590483
32	1	0	0.418121	3.798706	1.748708
33	1	0	2.147024	3.386712	1.942856
34	1	0	1.186670	1.558302	3.232001
35	1	0	1.318941	-0.306777	1.343606
36	1	0	-0.298413	1.536374	2.240440
37	1	0	2.862897	2.119490	-2.595185
38	1	0	3.591836	-2.579411	1.654944
39	1	0	2.531799	-3.998034	1.501321
40	1	0	2.145276	-2.733052	2.709314

trans-IM1'

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.741888	-1.816218	-0.588976
2	8	0	2.355123	-1.696128	0.775591
3	8	0	3.906159	-2.110066	-0.848042
4	6	0	1.687929	-1.506567	-1.499673
5	6	0	-2.202885	-1.129807	-0.451925
6	6	0	-0.846182	-1.266437	-0.839636
7	6	0	0.335319	-1.426482	-1.141845
8	1	0	1.943148	-1.660467	-2.545029
9	6	0	3.358359	-2.103257	1.715702
10	6	0	-2.609128	-1.368121	0.886124
11	6	0	-3.940374	-1.215728	1.270580
12	6	0	-4.913455	-0.829341	0.340810
13	6	0	-4.531291	-0.603122	-0.987328
14	6	0	-3.202213	-0.746476	-1.381215
15	1	0	-1.866802	-1.698621	1.607361
16	1	0	-4.223971	-1.413462	2.301582
17	1	0	-5.950808	-0.718537	0.642645
18	1	0	-5.276907	-0.314126	-1.723918
19	1	0	-2.917121	-0.572410	-2.414622
20	1	0	1.846719	0.500585	-1.427003
21	6	0	0.474873	3.523331	-0.855629
22	6	0	1.035040	2.526686	-1.909064
23	7	0	0.207350	2.605604	0.253679
24	6	0	1.022210	1.532904	0.122460
25	7	0	1.618727	1.459982	-1.065350
26	6	0	-0.057223	2.816635	1.678460
27	6	0	0.170858	1.376631	2.218999
28	7	0	1.133412	0.825568	1.243044
29	1	0	-0.432661	4.027878	-1.193406
30	1	0	1.224762	4.276851	-0.571355
31	1	0	0.230944	2.118319	-2.532155
32	1	0	-1.074231	3.172309	1.854553
33	1	0	0.658966	3.531907	2.110508
34	1	0	0.588081	1.369147	3.227745
35	1	0	1.466225	-0.151296	1.215666

36	1	0	-0.760732	0.799855	2.202375
37	1	0	1.795580	2.976827	-2.549460
38	1	0	4.257502	-1.486545	1.628592
39	1	0	3.634827	-3.148505	1.554443
40	1	0	2.907436	-1.986032	2.704415

S3: Comparsion of the energies of all optimized stationary points along cis-path at the B3LTP/6-31+G(d,p) and B3LYP/6-311++G(d,p) levels

Species	B3LYP/6-311++G(d,p)			B3LYP/6-31+G(d,p)		
	ZPE (a.u.)	E_{ZPE} (a.u.)	E_r (kJ/mol)	ZPE (a.u.)	E_{ZPE} (a.u.)	E_r (kJ/mol)
cis-COM	0.328726	−935.718267	0.0	0.329802	−935.503328	0.0
cis-TS1	0.324355	−935.701109	45.0	0.325445	−935.486876	43.2
cis-IM1	0.328498	−935.705105	34.5	0.329353	−935.490612	33.4
cis-TSR	0.327673	−935.704358	36.5	0.328403	-935.489907	35.2
cis-IM2	0.327657	−935.706202	31.6	0.328489	−935.491882	30.0
cis-TS2	0.323915	−935.702749	40.7	0.325110	−935.489572	36.1
cis-IM3	0.328122	−935.725407	−18.7	0.329371	−935.511965	−22.7

S4. Preliminary results and discussion of model system

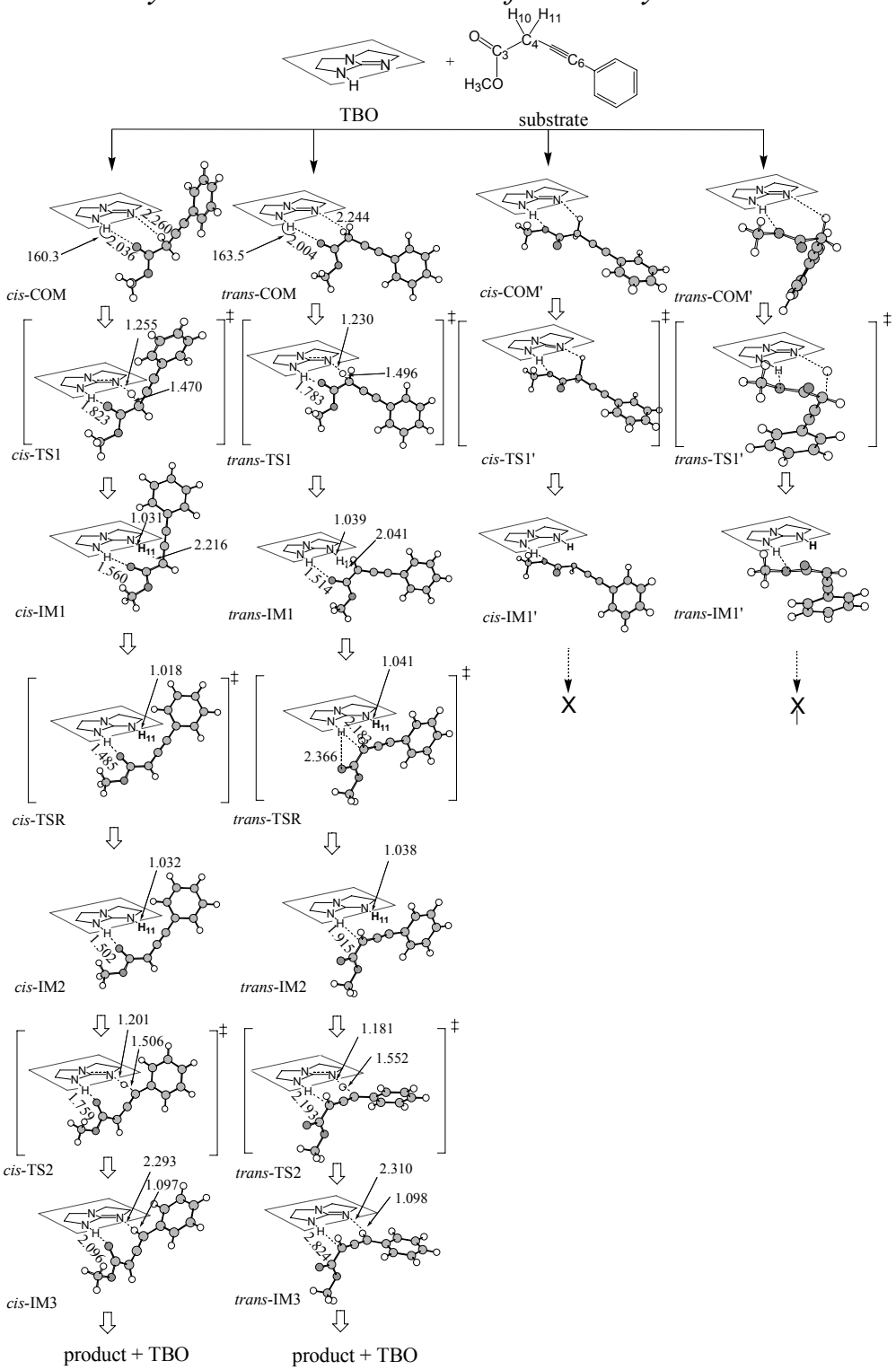

Figure S1. Predicted reaction mechanism of the model system. The bond lengths are in angstroms and the angles are in degrees.

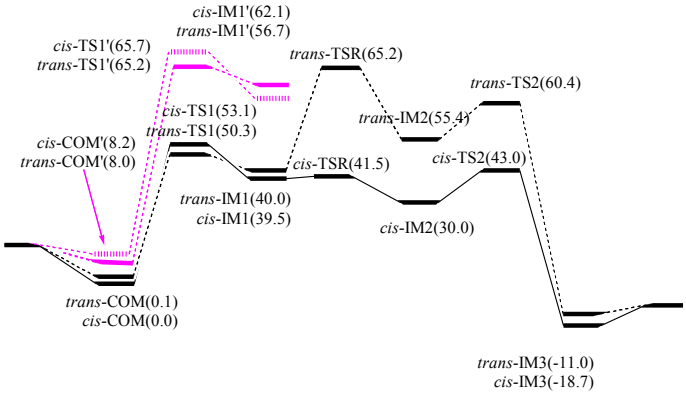

Figure S2. The potential energy profile calculated at the B3LYP/6-31+G(d,p) level. The relative Gibbs free energies (in kJ/mol) are listed in parentheses.

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The optimized structures and the reaction routes are depicted in Figure S1. The potential energy surfaces (PES) of the calculated reaction pathways are shown in Figure S2.

The predicted energy-favored reaction paths (*cis*-path & *trans*-path) are composed of three reaction steps: 1) deprotonation of the substrate, corresponding to the migration of the hydrogen atom (H_{11}) atom form C_4 to guanidine moiety; 2) conformational change step, corresponding to the rotation (*cis*-path) or parallel move (*trans*-path) of the substrate with respect to the guanidine moiety; 3) hydrogen transfer from the guanidine moiety to the substrate with the of recovery of the catalyst.

As shown in Figure 2S, the largest energy barrier lies in the step from COM to TS1, which means that the deprotonation of the substrate might be the RDS for overall reaction.

On the other hand, apart from *cis*-COM and *trans*-COM, the calculations identified other two catalyst-substrate complexes *cis*-COM' and *trans*-COM' in the entrance of the reaction. From either *cis*-COM' or *trans*-COM, the deprotonation of the substrate could occur along the reaction path marked as *cis*-path' or *trans*-path', respectively. However, the calculations met the failure to locate subsequent steps connecting *cis*-IM1' or *trans*-IM1' to the final product, suggesting that these incomplete reaction routes might be the dead paths in reaction mechanism. For these reasons, *cis*-path' and *trans*-path' will not be taken into account for the following discussion.

Part II: Actual system

S5: Summarize energies of all species over actual reaction system.

Species	E_{zpe}	E_r	G_c[a]	SCF[b]$_{PCM}$	SCF$_{PCM}$+G_c	G_r
sub + cat	–1367.679028	30.7	0.550836	–1368.344477	–1367.793641	–11.6
anti-cis-COM	–1367.690739	0.0	0.564703	–1368.353938	–1367.789235	0.0
anti-cis-TS1	–1367.674315	43.1	0.564203	–1368.333639	–1367.769436	52.0
anti-cis-IM1	–1367.677804	33.9	0.567177	–1368.341972	–1367.774795	37.9
anti-cis-TSR	–1367.677891	33.7	0.568611	–1368.341682	–1367.773071	42.4
anti-cis-IM2	–1367.679618	29.2	0.567189	–1368.343987	–1367.776798	32.6
anti-cis-TS2	–1367.676769	36.7	0.563963	–1368.336434	–1367.772471	44.0
anti-cis-IM3	–1367.698060	–19.2	0.565375	–1368.360811	–1367.795436	–16.3
pro + cat	–1367.687842	7.6	0.547395	–1368.352896	–1367.805501	–42.7
anti-trans-COM	–1367.690620	0.3	0.565116	–1368.354314	–1367.789198	0.1
anti-trans-TS1	–1367.673836	44.4	0.562657	–1368.333626	–1367.770969	47.9
anti-trans-IM1	–1367.676094	38.4	0.565414	–1368.340912	–1367.775498	36.0
anti-trans-TSR	–1367.665446	66.4	0.568532	–1368.331163	–1367.762631	69.8
anti-trans-IM2	–1367.667525	60.9	0.565728	–1368.332570	–1367.766842	58.8
anti-trans-TS2	–1367.667474	61.0	0.563019	–1368.327869	–1367.764850	64.0
anti-trans-IM3	–1367.693550	–7.4	0.562717	–1368.356720	–1367.794003	–12.5
syn-cis-COM	–1367.689608	3.0	0.564936	–1368.353275	–1367.788339	2.4
syn-cis-TS1	–1367.672572	47.7	0.563573	–1368.332035	–1367.768462	54.5
syn-cis-IM1	–1367.677096	35.8	0.567691	–1368.341930	–1367.774239	39.4
syn-cis-TSR	–1367.674465	42.7	0.569632	–1368.339178	–1367.769546	51.7
syn-cis-IM2	–1367.672041	49.1	0.566911	–1368.337339	-1367.770428	49.3
syn-cis-TS2	–1367.671165	51.4	0.564067	–1368.330832	–1367.766765	59.0
syn-cis-IM3	–1367.694655	–10.3	0.564776	–1368.357608	–1367.792832	–9.4
syn-trans-COM	–1367.689763	2.6	0.564336	–1368.353451	–1367.789115	0.3
syn-trans-TS1	–1367.671122	51.5	0.563158	–1368.331108	–1367.767950	55.9
syn-trans-IM1	–1367.674498	43.6	0.566758	–1368.339747	–1367.772989	42.6
syn-trans-TSR	–1367.663289	72.1	0.569518	–1368.329584	–1367.760066	76.5
syn-trans-IM2	–1367.665813	65.4	0.566475	–1368.331282	–1367.764807	64.1
syn-trans-TS2	–1367.666022	64.9	0.563437	–1368.326401	–1367.762964	68.9
syn-trans-IM3	–1367.692824	–5.5	0.564201	–1368.356213	–1367.792012	–7.3

a: Thermal correction to Gibbs Free Energy.
b: Total electronic energies in solvent.

S6. Cartesian coordinates and energies of all optimized TSs over actual reaction system.

anti-cis-COM

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.142607	2.410634	0.056510
2	8	0	0.734625	3.602801	-0.077985
3	8	0	-0.039071	1.831433	1.115766
4	6	0	-0.241186	1.836138	-1.304408
5	6	0	-4.103162	0.450695	-1.441337
6	6	0	-2.757975	0.935608	-1.390045
7	6	0	-1.614271	1.339615	-1.343256
8	1	0	-0.077289	2.593024	-2.077540
9	1	0	0.468099	1.006328	-1.484496
10	6	0	1.277858	4.362418	1.076801
11	6	0	-4.533245	-0.362227	-2.509912
12	6	0	-5.845126	-0.833705	-2.555267
13	6	0	-6.749309	-0.506431	-1.539425
14	6	0	-6.332165	0.299497	-0.474917
15	6	0	-5.022543	0.776473	-0.423270
16	1	0	-3.829914	-0.616784	-3.296602
17	1	0	-6.162195	-1.458800	-3.385407
18	1	0	-7.770244	-0.875484	-1.577354
19	1	0	-7.029154	0.558424	0.317315
20	1	0	-4.697272	1.402455	0.401819
21	6	0	2.841869	-1.622929	-1.665240
22	7	0	1.999353	-2.620702	0.278992
23	6	0	1.435203	-1.374849	0.022875
24	7	0	1.864006	-0.720380	-1.005765
25	6	0	0.364829	-2.239734	1.893047
26	7	0	0.437909	-1.136249	0.923414
27	1	0	0.156251	-0.183397	1.138182
28	1	0	0.982827	-2.007007	2.777080
29	1	0	2.567809	-1.706797	-2.725579
30	6	0	1.073761	-3.382111	1.106527
31	6	0	2.636709	-3.021889	-0.969405
32	1	0	1.593598	-4.076722	1.771747
33	1	0	0.359137	-3.952991	0.490294
34	1	0	3.566122	-3.569568	-0.790586
35	1	0	1.968073	-3.663587	-1.567495
36	6	0	4.302129	-1.069224	-1.642402
37	6	0	4.842372	-0.942426	-0.205598
38	1	0	4.202943	-0.287231	0.394208
39	1	0	4.897625	-1.913745	0.297616
40	1	0	5.852164	-0.514687	-0.215690
41	6	0	4.300234	0.322975	-2.307103
42	1	0	5.316374	0.734493	-2.339314
43	1	0	3.927798	0.268633	-3.337741
44	1	0	3.659341	1.015899	-1.755737
45	6	0	5.216307	-2.002675	-2.463205
46	1	0	4.840909	-2.125855	-3.486855
47	1	0	6.227885	-1.585376	-2.529540
48	1	0	5.304814	-2.998869	-2.015299
49	6	0	-1.071584	-2.532128	2.406760
50	6	0	-1.556386	-1.308684	3.214879
51	1	0	-1.647403	-0.416109	2.587156

52	1	0	-2.542451	-1.506230	3.650366
53	1	0	-0.867736	-1.078098	4.036973
54	6	0	-1.013315	-3.756658	3.343357
55	1	0	-1.997299	-3.943215	3.787595
56	1	0	-0.717227	-4.665753	2.807679
57	1	0	-0.302713	-3.599836	4.164409
58	6	0	-2.061032	-2.797246	1.255830
59	1	0	-2.084847	-1.959277	0.553632
60	1	0	-1.807401	-3.702531	0.693477
61	1	0	-3.071202	-2.935774	1.657412
62	6	0	1.858215	5.608937	0.404146
63	1	0	2.294866	6.270023	1.159331
64	1	0	2.639760	5.334047	-0.310596
65	1	0	1.077949	6.159225	-0.130238
66	6	0	2.380642	3.551045	1.764609
67	1	0	1.979253	2.668588	2.264745
68	1	0	3.133662	3.234162	1.036114
69	1	0	2.875456	4.180850	2.511738
70	6	0	0.138013	4.735886	2.029840
71	1	0	0.525179	5.397977	2.811798
72	1	0	-0.650105	5.272343	1.491350
73	1	0	-0.293451	3.852661	2.502957

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anti-cis-TS1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.272221	-2.063088	-0.503382
2	8	0	-2.455928	-2.597175	-0.901686
3	8	0	-0.850307	-2.169084	0.659664
4	6	0	-0.652221	-1.275554	-1.563281
5	6	0	3.401978	-0.939631	-1.794897
6	6	0	1.985515	-1.063803	-1.690489
7	6	0	0.774741	-1.205614	-1.613017
8	1	0	-1.131887	-1.406759	-2.534542
9	6	0	-3.350728	-3.322846	0.011653
10	6	0	4.261316	-1.625371	-0.907051
11	6	0	5.645841	-1.498191	-1.014358
12	6	0	6.211100	-0.693690	-2.010073
13	6	0	5.371986	-0.014836	-2.900650
14	6	0	3.986326	-0.131177	-2.795994
15	1	0	3.826946	-2.261626	-0.142139
16	1	0	6.287694	-2.036051	-0.321381
17	1	0	7.290142	-0.600813	-2.093612
18	1	0	5.799200	0.609232	-3.681327
19	1	0	3.338476	0.397380	-3.488852
20	1	0	-1.012368	0.070902	-1.112303
21	6	0	-0.410140	3.431211	-0.139116
22	6	0	-1.198248	2.533554	-1.162830
23	7	0	-0.427008	2.605134	1.070280
24	6	0	-0.649051	1.314751	0.657038
25	7	0	-1.165811	1.184615	-0.542845
26	6	0	0.564725	2.566333	2.147892
27	6	0	0.363063	1.125672	2.718996
28	7	0	-0.227338	0.428963	1.560782
29	1	0	-0.881838	4.401182	0.033978
30	1	0	0.623107	3.603141	-0.476827
31	1	0	0.374328	3.334348	2.900960
32	1	0	1.580061	2.706818	1.747091

33	1	0	-0.335376	-0.583929	1.421535
34	1	0	-0.640992	2.487644	-2.106933
35	1	0	-0.386372	1.175890	3.523950
36	6	0	1.618458	0.424092	3.303094
37	6	0	1.193272	-0.956169	3.850903
38	1	0	0.847766	-1.625093	3.055895
39	1	0	2.041893	-1.444056	4.342673
40	1	0	0.389077	-0.860982	4.590649
41	6	0	2.148041	1.284871	4.469109
42	1	0	1.378204	1.443739	5.234346
43	1	0	2.996321	0.787409	4.951347
44	1	0	2.496217	2.266595	4.127928
45	6	0	2.722164	0.230744	2.246210
46	1	0	2.359642	-0.333013	1.382241
47	1	0	3.121934	1.183058	1.881802
48	1	0	3.560045	-0.323152	2.683091
49	6	0	-2.641342	3.006704	-1.512351
50	6	0	-3.273296	1.966332	-2.460013
51	1	0	-3.350662	0.986518	-1.980192
52	1	0	-4.280412	2.282052	-2.754823
53	1	0	-2.679689	1.848967	-3.374807
54	6	0	-3.515102	3.142561	-0.251038
55	1	0	-3.574588	2.192433	0.288897
56	1	0	-3.129491	3.901621	0.438545
57	1	0	-4.534066	3.436260	-0.527291
58	6	0	-2.561990	4.360707	-2.247431
59	1	0	-1.936856	4.290011	-3.145957
60	1	0	-3.561383	4.678791	-2.564256
61	1	0	-2.153777	5.156622	-1.614406
62	6	0	-2.663183	-4.594233	0.525556
63	1	0	-1.812974	-4.353417	1.165215
64	1	0	-3.380281	-5.191920	1.099546
65	1	0	-2.311300	-5.200541	-0.315674
66	6	0	-3.815000	-2.411204	1.155160
67	1	0	-4.231036	-1.480571	0.754683
68	1	0	-4.602054	-2.916318	1.726266
69	1	0	-2.992982	-2.169726	1.830044
70	6	0	-4.532276	-3.681775	-0.896419
71	1	0	-5.281922	-4.247513	-0.333517
72	1	0	-5.003724	-2.776613	-1.291914
73	1	0	-4.196409	-4.291538	-1.740584

anti-cis-IM1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.271852	0.006972	-1.553072
2	8	0	-3.442861	0.599937	-1.953611
3	8	0	-2.282959	-0.917546	-0.688516
4	6	0	-1.147602	0.575299	-2.193900
5	6	0	2.643594	-0.827470	-2.315654
6	6	0	1.295417	-0.393639	-2.235726
7	6	0	0.133404	0.006503	-2.203317
8	1	0	-1.350364	1.372709	-2.903350
9	6	0	-4.749926	0.234874	-1.416087
10	6	0	3.612517	-0.054007	-3.004417
11	6	0	4.939263	-0.472360	-3.084867
12	6	0	5.350324	-1.668495	-2.483679
13	6	0	4.405031	-2.446471	-1.804905

14	6	0	3.074278	-2.039401	-1.721192
15	1	0	3.301835	0.871622	-3.479993
16	1	0	5.658650	0.138700	-3.624404
17	1	0	6.384881	-1.992141	-2.551036
18	1	0	4.705154	-3.384917	-1.344895
19	1	0	2.346048	-2.660225	-1.209934
20	6	0	1.076495	-0.872651	2.934524
21	6	0	-0.307544	-1.469917	2.520673
22	7	0	0.985094	0.489917	2.393643
23	6	0	0.085797	0.455827	1.370060
24	7	0	-0.673434	-0.618368	1.365123
25	6	0	2.083966	1.377179	1.993281
26	6	0	1.444553	2.237800	0.844629
27	7	0	0.188564	1.501953	0.553963
28	1	0	1.914932	-1.412191	2.470032
29	1	0	1.213789	-0.867249	4.017550
30	1	0	2.933714	0.790131	1.618477
31	1	0	2.425992	1.983843	2.834136
32	1	0	-1.347564	-0.826526	0.567733
33	1	0	-1.022171	-1.269541	3.332800
34	1	0	2.081660	2.183010	-0.045120
35	1	0	-0.236757	1.458445	-0.382492
36	6	0	1.205342	3.741056	1.163756
37	6	0	0.332297	3.924283	2.419404
38	1	0	-0.641122	3.438670	2.298023
39	1	0	0.807923	3.515298	3.317732
40	1	0	0.153720	4.989753	2.600699
41	6	0	0.499776	4.386946	-0.047246
42	1	0	0.367223	5.461264	0.120395
43	1	0	1.086267	4.262362	-0.965215
44	1	0	-0.490720	3.952597	-0.215463
45	6	0	2.574956	4.422702	1.363010
46	1	0	3.213707	4.300443	0.480156
47	1	0	2.441474	5.496897	1.529491
48	1	0	3.115797	4.024576	2.228796
49	6	0	-0.360031	-2.991391	2.225600
50	6	0	-1.826594	-3.383719	1.940669
51	1	0	-2.211337	-2.898878	1.038244
52	1	0	-1.902011	-4.466465	1.792501
53	1	0	-2.479089	-3.116707	2.780913
54	6	0	0.127198	-3.737313	3.485527
55	1	0	-0.466143	-3.467036	4.367657
56	1	0	0.032277	-4.818731	3.341928
57	1	0	1.180623	-3.528665	3.705569
58	6	0	0.510494	-3.375728	1.014662
59	1	0	0.187435	-2.855358	0.108273
60	1	0	1.570208	-3.151591	1.178959
61	1	0	0.430940	-4.452631	0.830835
62	6	0	-5.082023	-1.227752	-1.745715
63	1	0	-4.412876	-1.910478	-1.220798
64	1	0	-6.116260	-1.446461	-1.455826
65	1	0	-4.985752	-1.401137	-2.822664
66	6	0	-4.824347	0.517385	0.091959
67	1	0	-4.526205	1.551259	0.298299
68	1	0	-5.854933	0.385286	0.440819
69	1	0	-4.175228	-0.156767	0.652029
70	6	0	-5.696921	1.174731	-2.173636
71	1	0	-6.733570	0.995088	-1.869550
72	1	0	-5.448364	2.220578	-1.966984
73	1	0	-5.615956	1.010057	-3.252465

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anti-cis-TSR

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.494024	-1.560015	-0.603202
2	8	0	3.628531	-2.278149	-0.302520
3	8	0	2.501432	-0.290746	-0.538726
4	6	0	1.421829	-2.398581	-0.953175
5	6	0	-2.186832	-1.187245	-2.296025
6	6	0	-0.907258	-1.585098	-1.844640
7	6	0	0.202360	-1.938462	-1.440411
8	1	0	1.600981	-3.468006	-0.921293
9	6	0	4.887404	-1.656801	0.106617
10	6	0	-3.228073	-2.133632	-2.482520
11	6	0	-4.494680	-1.731288	-2.899692
12	6	0	-4.776090	-0.380280	-3.144006
13	6	0	-3.759206	0.565905	-2.970873
14	6	0	-2.486544	0.176299	-2.555970
15	1	0	-3.018936	-3.183494	-2.299788
16	1	0	-5.270769	-2.479150	-3.038933
17	1	0	-5.764309	-0.073502	-3.473025
18	1	0	-3.956592	1.615979	-3.174404
19	1	0	-1.696938	0.912837	-2.445319
20	6	0	-0.765674	3.036354	0.999828
21	6	0	0.740026	2.700945	0.736973
22	7	0	-1.267682	1.763108	1.534505
23	6	0	-0.436355	0.777666	1.086989
24	7	0	0.717602	1.217516	0.636700
25	6	0	-2.645375	1.253697	1.496944
26	6	0	-2.443045	-0.303485	1.469363
27	7	0	-0.990392	-0.433748	1.163496
28	1	0	-1.297978	3.295574	0.072682
29	1	0	-0.884349	3.850387	1.717380
30	1	0	-3.156567	1.597567	0.587144
31	1	0	-3.212410	1.587367	2.367659
32	1	0	1.449597	0.598600	0.154364
33	1	0	1.314471	2.975090	1.633700
34	1	0	-3.003445	-0.727207	0.629645
35	1	0	-0.640415	-1.185656	0.568449
36	6	0	-2.852358	-1.068943	2.758999
37	6	0	-2.115844	-0.526670	3.998419
38	1	0	-1.031767	-0.621032	3.882603
39	1	0	-2.349113	0.526965	4.189113
40	1	0	-2.410152	-1.094558	4.887769
41	6	0	-2.503139	-2.560501	2.567871
42	1	0	-2.827523	-3.138548	3.439866
43	1	0	-3.001555	-2.976253	1.684390
44	1	0	-1.424717	-2.706915	2.453150
45	6	0	-4.378738	-0.935054	2.942857
46	1	0	-4.918443	-1.306094	2.063626
47	1	0	-4.705149	-1.522372	3.807559
48	1	0	-4.686439	0.102020	3.117365
49	6	0	1.405772	3.398987	-0.478823
50	6	0	2.917404	3.082313	-0.462895
51	1	0	3.105227	2.014254	-0.599937
52	1	0	3.418317	3.619194	-1.276040
53	1	0	3.376421	3.400890	0.480779
54	6	0	1.208067	4.922328	-0.323623
55	1	0	1.611080	5.282229	0.630829
56	1	0	1.733849	5.450594	-1.125775

57	1	0	0.152230	5.209871	-0.379629
58	6	0	0.805970	2.915737	-1.814168
59	1	0	0.963426	1.842291	-1.952872
60	1	0	-0.267643	3.121456	-1.883859
61	1	0	1.290404	3.437081	-2.646627
62	6	0	5.446937	-0.780350	-1.023374
63	1	0	4.786913	0.064635	-1.221010
64	1	0	6.438744	-0.405342	-0.746228
65	1	0	5.546506	-1.370358	-1.940387
66	6	0	4.714853	-0.872120	1.416016
67	1	0	4.273752	-1.515534	2.184869
68	1	0	5.693231	-0.532129	1.774037
69	1	0	4.069930	-0.005600	1.268284
70	6	0	5.797423	-2.870554	0.335989
71	1	0	6.796841	-2.543500	0.641053
72	1	0	5.384438	-3.515232	1.117750
73	1	0	5.885296	-3.458279	-0.582674

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anti-cis-IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.456884	-1.778799	-0.143989
2	8	0	3.607439	-2.386725	0.291619
3	8	0	2.442623	-0.537708	-0.393314
4	6	0	1.388085	-2.691114	-0.248945
5	6	0	-2.206293	-1.850486	-1.881055
6	6	0	-0.974648	-2.118368	-1.231071
7	6	0	0.152881	-2.366483	-0.789757
8	1	0	1.573511	-3.714975	0.058240
9	6	0	4.865607	-1.677512	0.490119
10	6	0	-3.253181	-2.808143	-1.892981
11	6	0	-4.469713	-2.532211	-2.513307
12	6	0	-4.694186	-1.297745	-3.136678
13	6	0	-3.670315	-0.342743	-3.137150
14	6	0	-2.446541	-0.608363	-2.524094
15	1	0	-3.088744	-3.768911	-1.414379
16	1	0	-5.250538	-3.288699	-2.512582
17	1	0	-5.643739	-1.088796	-3.620481
18	1	0	-3.822016	0.613892	-3.631685
19	1	0	-1.649895	0.129382	-2.553315
20	6	0	-0.535408	3.327228	0.458190
21	6	0	0.863802	2.741970	0.082513
22	7	0	-1.154983	2.196699	1.153111
23	6	0	-0.535514	1.061513	0.726135
24	7	0	0.601068	1.281275	0.095211
25	6	0	-2.578427	1.902118	1.337452
26	6	0	-2.591922	0.338064	1.474242
27	7	0	-1.238180	-0.037120	0.992735
28	1	0	-1.120324	3.595142	-0.434173
29	1	0	-0.455892	4.204528	1.103296
30	1	0	-3.158563	2.229695	0.462813
31	1	0	-2.973303	2.405258	2.222294
32	1	0	1.305285	0.512319	-0.135343
33	1	0	1.566783	2.974000	0.896111
34	1	0	-3.325827	-0.083091	0.778651
35	1	0	-1.059655	-0.904264	0.466300
36	6	0	1.491597	3.263776	-1.239057
37	6	0	0.678518	2.827957	-2.473313

38	1	0	-0.346359	3.216407	-2.457553
39	1	0	1.154571	3.209931	-3.382619
40	1	0	0.630193	1.738106	-2.553112
41	6	0	2.928480	2.712996	-1.355925
42	1	0	3.401789	3.094224	-2.267490
43	1	0	3.541866	3.031827	-0.504438
44	1	0	2.947080	1.620453	-1.395992
45	6	0	1.552099	4.804380	-1.164095
46	1	0	2.099002	5.141049	-0.274910
47	1	0	2.073525	5.201202	-2.041432
48	1	0	0.555004	5.259335	-1.144158
49	6	0	-2.908052	-0.224507	2.890380
50	6	0	-2.792997	-1.762112	2.836167
51	1	0	-1.772755	-2.082216	2.603680
52	1	0	-3.065216	-2.195052	3.804811
53	1	0	-3.463561	-2.186220	2.079641
54	6	0	-4.358938	0.152242	3.254006
55	1	0	-5.068046	-0.225764	2.507881
56	1	0	-4.630026	-0.286201	4.220186
57	1	0	-4.501291	1.235605	3.337897
58	6	0	-1.933356	0.323261	3.949908
59	1	0	-0.898679	0.062714	3.706070
60	1	0	-1.997141	1.412628	4.048772
61	1	0	-2.163495	-0.107736	4.930216
62	6	0	5.804481	-2.789228	0.977389
63	1	0	6.804601	-2.385737	1.167681
64	1	0	5.424783	-3.233841	1.902698
65	1	0	5.883901	-3.580400	0.225459
66	6	0	5.378162	-1.100750	-0.837656
67	1	0	5.431067	-1.890693	-1.594214
68	1	0	4.721298	-0.311314	-1.204275
69	1	0	6.385573	-0.691272	-0.699499
70	6	0	4.723942	-0.597922	1.573443
71	1	0	4.314558	-1.035240	2.490575
72	1	0	5.709083	-0.177737	1.806783
73	1	0	4.065463	0.205840	1.242514

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anti-cis-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.007316	-3.195148	1.284898
2	6	0	0.392622	-2.511541	1.375336
3	7	0	-1.579639	-2.545880	0.108000
4	6	0	-0.974940	-1.326619	-0.046636
5	7	0	0.152430	-1.233405	0.667842
6	6	0	-2.985988	-2.386424	-0.259786
7	6	0	-2.944206	-1.090685	-1.148526
8	7	0	-1.644005	-0.473542	-0.791523
9	1	0	-1.618254	-2.990985	2.177581
10	1	0	-0.929172	-4.276992	1.155243
11	6	0	0.975544	-2.343875	2.806196
12	1	0	-3.610277	-2.238843	0.635090
13	1	0	-3.357999	-3.261915	-0.796818
14	6	0	-3.112429	-1.310298	-2.682266
15	1	0	0.897452	-0.549483	0.454882
16	6	0	-2.053614	-2.282199	-3.236251
17	6	0	-2.967724	0.056553	-3.382918
18	6	0	-4.528109	-1.859544	-2.954551

19	6	0	0.127049	-1.387324	3.666223
20	6	0	2.410240	-1.786017	2.694364
21	6	0	1.032688	-3.737286	3.467781
22	1	0	-2.176385	-2.394391	-4.319265
23	1	0	-1.042011	-1.907701	-3.051807
24	1	0	-2.135334	-3.280050	-2.790820
25	1	0	-3.115071	-0.053980	-4.463093
26	1	0	-3.712634	0.772775	-3.015928
27	1	0	-1.976877	0.489048	-3.217356
28	1	0	-4.695974	-1.955244	-4.032805
29	1	0	-4.685131	-2.850561	-2.513254
30	1	0	-5.299329	-1.187352	-2.558799
31	1	0	0.582402	-1.278272	4.656496
32	1	0	0.063013	-0.394227	3.212460
33	1	0	-0.893242	-1.757277	3.818243
34	1	0	2.853369	-1.687424	3.691578
35	1	0	3.050262	-2.458211	2.110168
36	1	0	2.433369	-0.803164	2.215757
37	1	0	1.520154	-3.669590	4.446262
38	1	0	0.034181	-4.159762	3.628749
39	1	0	1.608882	-4.445956	2.860151
40	6	0	2.509371	1.201219	-0.921895
41	8	0	3.686039	1.387669	-1.576824
42	8	0	2.387298	0.384221	0.007490
43	6	0	1.468491	2.041867	-1.468654
44	6	0	-1.639951	2.910818	0.594920
45	6	0	-0.906399	2.079842	-0.360956
46	6	0	0.259399	2.147041	-0.877117
47	1	0	1.700643	2.598238	-2.372352
48	6	0	4.905757	0.635879	-1.261689
49	6	0	5.914826	1.198401	-2.269281
50	6	0	4.690447	-0.864186	-1.503766
51	6	0	5.359691	0.933944	0.173257
52	6	0	-1.420450	4.301848	0.691632
53	6	0	-2.145448	5.083509	1.590935
54	6	0	-3.106910	4.499775	2.424342
55	6	0	-3.338386	3.123607	2.340797
56	6	0	-2.621261	2.342952	1.431667
57	1	0	6.888871	0.716045	-2.136907
58	1	0	5.574546	1.022250	-3.294440
59	1	0	6.037634	2.276616	-2.128675
60	1	0	5.645606	-1.391716	-1.402525
61	1	0	3.980412	-1.281921	-0.789011
62	1	0	4.314089	-1.034828	-2.518044
63	1	0	6.337884	0.473154	0.351516
64	1	0	5.460147	2.014173	0.321763
65	1	0	4.647671	0.544549	0.901916
66	1	0	-0.675676	4.760390	0.047535
67	1	0	-1.957838	6.152980	1.644533
68	1	0	-3.669526	5.110059	3.125232
69	1	0	-4.083458	2.657389	2.980609
70	1	0	-2.812506	1.275138	1.368908
71	1	0	-1.397283	0.702869	-0.705309
72	1	0	1.110535	-3.111286	0.795372
73	1	0	-3.743300	-0.406542	-0.836730

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anti-cis-IM3

Standard orientation:

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

1	6	0	-2.263261	-1.869515	2.261190
2	6	0	-0.739230	-1.554126	2.226122
3	7	0	-2.630302	-1.648018	0.872182
4	6	0	-1.774531	-0.695163	0.330117
5	7	0	-0.657832	-0.579667	1.120500
6	6	0	-3.946268	-1.360257	0.318099
7	6	0	-3.553271	-0.556578	-0.977878
8	7	0	-2.181539	-0.053426	-0.714374
9	1	0	-2.804145	-1.183969	2.934888
10	1	0	-2.461553	-2.896311	2.580482
11	1	0	-4.538654	-0.734011	1.006437
12	1	0	-4.510299	-2.275700	0.119004
13	1	0	0.242650	-0.375912	0.693618
14	1	0	-0.207578	-2.478992	1.948090
15	1	0	-4.220667	0.309856	-1.079245
16	6	0	2.702640	-0.264788	-1.138597
17	8	0	3.772525	-0.837313	-1.722664
18	8	0	2.275849	-0.548776	-0.026867
19	6	0	2.110208	0.749875	-2.048055
20	6	0	0.145293	3.552869	-0.575248
21	6	0	0.103710	2.227000	-1.219873
22	6	0	1.122487	1.524291	-1.649734
23	1	0	2.518021	0.809835	-3.054835
24	6	0	4.553562	-1.914940	-1.075682
25	6	0	1.336557	4.286802	-0.425780
26	6	0	1.325479	5.536793	0.190312
27	6	0	0.125877	6.078966	0.668483
28	6	0	-1.062815	5.358803	0.523991
29	6	0	-1.053466	4.106229	-0.093726
30	1	0	2.269792	3.872826	-0.797791
31	1	0	2.253240	6.092238	0.297172
32	1	0	0.120170	7.054321	1.146705
33	1	0	-1.998437	5.771178	0.891445
34	1	0	-1.976196	3.543036	-0.202646
35	1	0	-0.873240	1.737257	-1.311538
36	6	0	-0.115084	-1.051354	3.558052
37	6	0	1.403245	-0.867770	3.352127
38	1	0	1.622381	-0.082958	2.622337
39	1	0	1.883157	-0.590371	4.297749
40	1	0	1.870533	-1.793125	2.995103
41	6	0	-0.722087	0.288702	4.017305
42	1	0	-1.783892	0.197502	4.271048
43	1	0	-0.202236	0.644168	4.914251
44	1	0	-0.624370	1.051230	3.239294
45	6	0	-0.344686	-2.128314	4.639046
46	1	0	0.074197	-3.095751	4.335313
47	1	0	0.141922	-1.835854	5.576141
48	1	0	-1.409790	-2.272092	4.853410
49	6	0	-3.670789	-1.346027	-2.320860
50	6	0	-5.151182	-1.697111	-2.578252
51	1	0	-5.262369	-2.192748	-3.549720
52	1	0	-5.557228	-2.375538	-1.819329
53	1	0	-5.776077	-0.795302	-2.592557
54	6	0	-3.177788	-0.433690	-3.462945
55	1	0	-3.280775	-0.940521	-4.430088
56	1	0	-3.761980	0.493946	-3.507348
57	1	0	-2.128562	-0.163036	-3.320471
58	6	0	-2.825476	-2.633733	-2.303627
59	1	0	-1.771721	-2.405554	-2.115562
60	1	0	-3.162890	-3.336087	-1.533685
61	1	0	-2.893890	-3.144048	-3.271790

62	6	0	5.625705	-2.220771	-2.124848
63	1	0	6.286339	-3.015622	-1.763979
64	1	0	5.167079	-2.549302	-3.062401
65	1	0	6.230984	-1.332349	-2.328919
66	6	0	5.189622	-1.395450	0.218363
67	1	0	5.779751	-0.494848	0.019781
68	1	0	4.433367	-1.164321	0.969769
69	1	0	5.862832	-2.159580	0.621937
70	6	0	3.658097	-3.136435	-0.839774
71	1	0	3.175734	-3.442864	-1.773599
72	1	0	4.271581	-3.971580	-0.484814
73	1	0	2.888257	-2.928386	-0.095538

anti-trans-COM

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.716407	-1.682184	0.272254
2	8	0	-1.693329	-1.904275	1.147410
3	8	0	0.401122	-2.181614	0.320444
4	6	0	-1.097827	-0.691980	-0.824439
5	6	0	-5.051966	0.321118	-1.234844
6	6	0	-3.675366	-0.040859	-1.089755
7	6	0	-2.509009	-0.347217	-0.951394
8	1	0	-0.715298	-1.111268	-1.762945
9	1	0	-0.484487	0.209171	-0.636545
10	6	0	-1.535288	-2.797556	2.323237
11	6	0	-5.581457	1.421442	-0.529701
12	6	0	-6.923889	1.772137	-0.671156
13	6	0	-7.761108	1.036296	-1.516356
14	6	0	-7.245663	-0.056473	-2.221251
15	6	0	-5.904303	-0.413580	-2.084299
16	1	0	-4.929691	1.991722	0.124690
17	1	0	-7.317436	2.622336	-0.120960
18	1	0	-8.806083	1.312289	-1.625110
19	1	0	-7.889994	-0.632100	-2.880007
20	1	0	-5.502815	-1.261130	-2.631078
21	6	0	3.303706	2.931550	-0.402131
22	6	0	1.757093	2.935158	-0.094691
23	7	0	3.632654	1.533384	-0.153439
24	6	0	2.435090	0.839686	-0.286045
25	7	0	1.337143	1.515765	-0.222243
26	6	0	4.698002	0.730737	-0.736342
27	6	0	4.151132	-0.707498	-0.495055
28	7	0	2.697617	-0.477647	-0.549524
29	1	0	3.883568	3.603246	0.236767
30	1	0	3.496075	3.203833	-1.453405
31	1	0	5.656502	0.893975	-0.236404
32	1	0	4.822288	0.942736	-1.811687
33	1	0	2.022221	-1.184792	-0.267428
34	1	0	1.239543	3.513873	-0.871265
35	1	0	4.446986	-1.011276	0.523447
36	6	0	-2.908573	-2.700814	2.991664
37	1	0	-3.694618	-3.039175	2.310315
38	1	0	-2.930641	-3.326926	3.889316
39	1	0	-3.125600	-1.668356	3.280917
40	6	0	-0.437956	-2.255208	3.244177
41	1	0	-0.427111	-2.838359	4.171322
42	1	0	0.546088	-2.323440	2.778397

43	1	0	-0.637242	-1.210439	3.502948
44	6	0	-1.254604	-4.227600	1.850675
45	1	0	-1.268754	-4.901338	2.714122
46	1	0	-2.029184	-4.557474	1.150826
47	1	0	-0.280580	-4.304196	1.365155
48	6	0	4.648422	-1.816360	-1.462404
49	6	0	4.055801	-3.165484	-1.000649
50	1	0	2.962632	-3.173403	-1.063963
51	1	0	4.429473	-3.981745	-1.629218
52	1	0	4.336001	-3.387451	0.036347
53	6	0	6.186621	-1.889966	-1.371777
54	1	0	6.519534	-2.052262	-0.339220
55	1	0	6.564803	-2.721482	-1.976719
56	1	0	6.660557	-0.973220	-1.740375
57	6	0	4.222179	-1.552988	-2.919620
58	1	0	4.535907	-2.387273	-3.557318
59	1	0	3.136194	-1.449601	-2.999402
60	1	0	4.677619	-0.643211	-3.325160
61	6	0	1.343378	3.578043	1.267155
62	6	0	-0.185145	3.439243	1.422376
63	1	0	-0.481703	2.387568	1.440625
64	1	0	-0.520288	3.914281	2.352357
65	1	0	-0.712760	3.921275	0.590120
66	6	0	1.700136	5.079031	1.252542
67	1	0	1.226252	5.590995	0.405678
68	1	0	1.349318	5.563968	2.170956
69	1	0	2.780605	5.249501	1.186984
70	6	0	2.037200	2.888450	2.457152
71	1	0	1.807909	1.818373	2.473890
72	1	0	3.126244	3.000728	2.418019
73	1	0	1.692528	3.323908	3.402681

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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

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.023775	2.023123	-0.268533
2	8	0	0.878562	2.653088	0.584399
3	8	0	-1.224067	2.277446	-0.246654
4	6	0	0.622751	1.068387	-1.118179

5	6	0	4.530340	0.009206	-1.208755
6	6	0	3.163960	0.391259	-1.179472
7	6	0	1.990277	0.745872	-1.147489
8	1	0	-0.001749	0.731200	-1.942590
9	6	0	0.451196	3.668204	1.545395
10	6	0	5.030660	-0.851918	-2.215343
11	6	0	6.373601	-1.225187	-2.234910
12	6	0	7.259685	-0.754576	-1.258657
13	6	0	6.779975	0.099954	-0.258591
14	6	0	5.439083	0.478426	-0.229107
15	1	0	4.350901	-1.215879	-2.980203
16	1	0	6.732499	-1.885623	-3.020507
17	1	0	8.305870	-1.046149	-1.278468
18	1	0	7.457117	0.476190	0.504263
19	1	0	5.073899	1.143678	0.547334
20	6	0	-1.939544	-3.327611	0.121128
21	6	0	-0.476205	-2.796605	0.342521
22	7	0	-2.753611	-2.120020	0.291648
23	6	0	-1.946362	-1.040540	0.089654
24	7	0	-0.655513	-1.330204	0.211783
25	6	0	-4.060718	-1.801084	-0.292771
26	6	0	-4.046170	-0.237425	-0.263880
27	7	0	-2.594713	0.056909	-0.243664
28	1	0	-2.220469	-4.098624	0.840923
29	1	0	-2.062677	-3.737449	-0.892260
30	1	0	-4.879401	-2.216967	0.297865
31	1	0	-4.129298	-2.192234	-1.318951
32	1	0	-2.109779	1.017327	-0.294351
33	1	0	-4.482807	0.093508	0.690224
34	1	0	0.165203	-3.139575	-0.477218
35	1	0	0.049169	-0.645583	-0.118826
36	6	0	-4.813258	0.489269	-1.400290
37	6	0	0.212954	-3.211673	1.674742
38	6	0	1.594877	-2.527682	1.738125
39	1	0	1.508846	-1.437547	1.771840
40	1	0	2.132169	-2.846643	2.637714
41	1	0	2.213654	-2.786612	0.871372
42	6	0	0.414518	-4.741333	1.665349
43	1	0	1.002503	-5.061885	0.796875
44	1	0	0.957004	-5.054175	2.563613
45	1	0	-0.534949	-5.288859	1.653058
46	6	0	-0.622895	-2.794519	2.899470
47	1	0	-0.778203	-1.711339	2.921341
48	1	0	-1.604683	-3.280854	2.917165
49	1	0	-0.101904	-3.074835	3.821249
50	6	0	-4.771669	2.007627	-1.121061
51	1	0	-3.749628	2.398734	-1.129441
52	1	0	-5.341840	2.545957	-1.886004
53	1	0	-5.217683	2.242531	-0.147068
54	6	0	-6.279909	0.010269	-1.372782
55	1	0	-6.737128	0.172718	-0.389131
56	1	0	-6.871218	0.566883	-2.107403
57	1	0	-6.371302	-1.054026	-1.619564
58	6	0	-4.195525	0.212602	-2.784721
59	1	0	-3.155556	0.548683	-2.831704
60	1	0	-4.223515	-0.850244	-3.050294
61	1	0	-4.757099	0.753025	-3.554227
62	6	0	-0.138023	4.883902	0.816359
63	1	0	-1.070167	4.624895	0.312298
64	1	0	-0.332662	5.687151	1.536419
65	1	0	0.573259	5.257751	0.072414
66	6	0	1.767996	4.047927	2.234173

67	1	0	1.593233	4.827347	2.983387
68	1	0	2.206581	3.176882	2.731121
69	1	0	2.488691	4.421353	1.500635
70	6	0	-0.530093	3.079750	2.569690
71	1	0	-0.104725	2.179083	3.026107
72	1	0	-0.711179	3.809915	3.366955
73	1	0	-1.481730	2.825489	2.101315

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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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anti-trans-IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.464107	2.620845	-0.544026
2	8	0	-0.676512	2.993492	0.519000
3	8	0	-2.640100	2.983641	-0.664695
4	6	0	-0.794727	1.726270	-1.456458
5	6	0	3.142864	0.912595	-1.477266
6	6	0	1.722548	0.990530	-1.349687
7	6	0	0.556395	1.407856	-1.413734
8	1	0	-1.330584	1.562328	-2.389217
9	6	0	-1.147982	3.927013	1.539363
10	6	0	3.743737	0.153779	-2.510731
11	6	0	5.131033	0.067434	-2.623273
12	6	0	5.963813	0.722691	-1.708703
13	6	0	5.383810	1.475292	-0.680139
14	6	0	3.998191	1.570996	-0.560930
15	1	0	3.105607	-0.352636	-3.229477
16	1	0	5.565032	-0.512913	-3.433817
17	1	0	7.043935	0.654171	-1.799633
18	1	0	6.016911	1.998637	0.032161
19	1	0	3.556608	2.165814	0.232993
20	6	0	0.039463	-3.717768	0.601284
21	6	0	1.252755	-2.723242	0.569611
22	7	0	-1.113499	-2.813408	0.629906
23	6	0	-0.714070	-1.616573	0.116176
24	7	0	0.602505	-1.470802	0.112172
25	6	0	-2.483433	-3.056805	0.166238
26	6	0	-2.993951	-1.603057	-0.093660
27	7	0	-1.717828	-0.881119	-0.325971
28	1	0	0.052073	-4.372145	1.474663

29	1	0	0.016901	-4.344184	-0.302987
30	1	0	-3.079274	-3.572917	0.921322
31	1	0	-2.475815	-3.658971	-0.754716
32	1	0	-1.568308	0.092935	-0.687345
33	1	0	-3.441940	-1.222205	0.835185
34	1	0	1.967895	-3.038598	-0.198121
35	1	0	1.070490	-0.657312	-0.332000
36	6	0	-4.040126	-1.425324	-1.225642
37	6	0	-3.444653	-1.734149	-2.613004
38	1	0	-4.213856	-1.603078	-3.381234
39	1	0	-2.615544	-1.062268	-2.853377
40	1	0	-3.079713	-2.764833	-2.691270
41	6	0	-5.219238	-2.380028	-0.937755
42	1	0	-5.638355	-2.209088	0.061270
43	1	0	-6.021322	-2.211427	-1.663690
44	1	0	-4.929043	-3.434723	-1.011361
45	6	0	-4.558879	0.028586	-1.195101
46	1	0	-5.308082	0.174476	-1.980879
47	1	0	-5.038181	0.253978	-0.235203
48	1	0	-3.772634	0.774319	-1.348546
49	6	0	2.043145	-2.565434	1.902682
50	6	0	3.115689	-1.474212	1.708984
51	1	0	2.669271	-0.491367	1.534243
52	1	0	3.740588	-1.398648	2.605276
53	1	0	3.773802	-1.698037	0.861889
54	6	0	2.747799	-3.904089	2.207902
55	1	0	3.410615	-4.202640	1.386838
56	1	0	3.362884	-3.806818	3.108538
57	1	0	2.039511	-4.721140	2.386697
58	6	0	1.121484	-2.174049	3.073369
59	1	0	0.603545	-1.230584	2.874321
60	1	0	0.367546	-2.940478	3.283572
61	1	0	1.714490	-2.039860	3.984439
62	6	0	-1.488711	5.285396	0.909854
63	1	0	-2.350253	5.203384	0.245826
64	1	0	-1.714284	6.012536	1.698555
65	1	0	-0.634392	5.659110	0.335412
66	6	0	-2.339974	3.338231	2.308582
67	1	0	-2.079795	2.353053	2.712540
68	1	0	-2.596489	3.991747	3.150636
69	1	0	-3.210525	3.237271	1.659159
70	6	0	0.067526	4.059815	2.464899
71	1	0	0.336917	3.086479	2.887917
72	1	0	0.930196	4.443303	1.911460
73	1	0	-0.154190	4.747980	3.287748

anti-trans-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.991206	-3.691922	0.653099
2	6	0	0.441675	-3.047603	0.621313
3	7	0	-1.853455	-2.510198	0.599175
4	6	0	-1.113183	-1.502746	0.043388
5	7	0	0.182478	-1.699068	0.056334
6	6	0	-3.228161	-2.388553	0.113296
7	6	0	-3.314510	-0.861621	-0.194263
8	7	0	-1.895142	-0.544391	-0.468566
9	1	0	-1.176681	-4.280444	1.553858

10	1	0	-1.157199	-4.335725	-0.224319
11	6	0	1.200407	-3.011863	1.982663
12	1	0	-3.954215	-2.695589	0.868950
13	1	0	-3.378909	-2.996803	-0.791784
14	6	0	-4.291118	-0.429835	-1.320038
15	6	0	-3.878007	-0.989073	-2.695170
16	6	0	-4.317442	1.112764	-1.381515
17	6	0	-5.700629	-0.938238	-0.949677
18	6	0	2.529465	-2.255682	1.780619
19	6	0	1.514942	-4.461647	2.408170
20	6	0	0.378277	-2.308798	3.079711
21	1	0	-4.577627	-0.638028	-3.461166
22	1	0	-2.875002	-0.657086	-2.979175
23	1	0	-3.891326	-2.084361	-2.720544
24	1	0	-5.036800	1.448432	-2.136229
25	1	0	-4.617951	1.545045	-0.420162
26	1	0	-3.345532	1.540817	-1.646508
27	1	0	-6.434254	-0.574499	-1.676648
28	1	0	-5.756887	-2.032919	-0.948052
29	1	0	-6.009574	-0.579028	0.039429
30	1	0	3.113969	-2.265849	2.707216
31	1	0	3.139727	-2.718060	0.996353
32	1	0	2.361689	-1.212014	1.500149
33	1	0	2.101818	-4.464315	3.332944
34	1	0	0.609814	-5.050132	2.598073
35	1	0	2.102930	-4.982829	1.642839
36	1	0	0.951547	-2.276659	4.012862
37	1	0	0.144935	-1.277132	2.798452
38	1	0	-0.563390	-2.827662	3.290784
39	1	0	0.914356	-0.934171	-0.497345
40	1	0	-3.623352	-0.343052	0.726000
41	1	0	1.075019	-3.598761	-0.083749
42	1	0	-1.524917	0.372199	-0.734229
43	6	0	-0.528300	3.056382	-0.484882
44	8	0	0.283004	3.057175	0.611085
45	8	0	-1.469397	3.832520	-0.636319
46	6	0	-0.180260	2.018409	-1.452546
47	6	0	3.106026	0.019376	-1.484788
48	6	0	1.677990	0.187282	-1.210391
49	6	0	0.855985	1.154197	-1.345345
50	1	0	-0.753820	2.068804	-2.376393
51	6	0	0.117848	4.028427	1.697663
52	6	0	4.039460	1.039214	-1.202405
53	6	0	5.401181	0.851374	-1.442220
54	6	0	5.868572	-0.355015	-1.976137
55	6	0	4.955914	-1.374940	-2.262590
56	6	0	3.594468	-1.193770	-2.009504
57	1	0	3.680287	1.977298	-0.789717
58	1	0	6.100711	1.652269	-1.216178
59	1	0	6.928814	-0.497540	-2.165409
60	1	0	5.305015	-2.315651	-2.681006
61	1	0	2.890472	-1.991077	-2.234154
62	6	0	1.242113	3.644002	2.666023
63	6	0	-1.250459	3.855259	2.371474
64	6	0	0.325524	5.456010	1.174266
65	1	0	1.232157	4.305627	3.538645
66	1	0	1.118958	2.611997	3.009278
67	1	0	2.216974	3.727577	2.176076
68	1	0	-1.304269	4.492943	3.261192
69	1	0	-2.060358	4.126724	1.693014
70	1	0	-1.385743	2.816097	2.691564
71	1	0	0.331894	6.158249	2.015632

72	1	0	1.289000	5.533486	0.659376
73	1	0	-0.467742	5.741531	0.482067

anti-trans-IM3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.306657	-2.613838	-0.022315
2	8	0	-2.746562	-1.858180	0.999082
3	8	0	-2.323601	-3.833697	-0.063044
4	6	0	-1.771879	-1.795671	-1.148323
5	6	0	-2.584415	1.792098	-1.656387
6	6	0	-1.576540	0.825809	-1.178003
7	6	0	-1.696790	-0.480335	-1.162883
8	1	0	-1.448516	-2.388320	-2.002963
9	6	0	-3.323960	-2.449073	2.224793
10	6	0	-3.842869	1.395898	-2.146084
11	6	0	-4.761638	2.345333	-2.589196
12	6	0	-4.443953	3.708933	-2.551064
13	6	0	-3.197589	4.113127	-2.065909
14	6	0	-2.275274	3.162695	-1.622229
15	1	0	-4.096392	0.339796	-2.176396
16	1	0	-5.729095	2.023218	-2.964633
17	1	0	-5.162478	4.446818	-2.896431
18	1	0	-2.941702	5.168532	-2.032030
19	1	0	-1.305945	3.476746	-1.245291
20	6	0	3.842423	1.980594	0.514667
21	6	0	2.389109	2.579211	0.638179
22	7	0	3.546464	0.556715	0.404389
23	6	0	2.232995	0.483853	-0.040248
24	7	0	1.493675	1.532071	0.078692
25	6	0	4.320729	-0.487913	-0.249612
26	6	0	3.229330	-1.576181	-0.469405
27	7	0	2.021605	-0.742067	-0.624261
28	1	0	4.482784	2.194162	1.374629
29	1	0	4.346304	2.351963	-0.392900
30	1	0	5.136955	-0.850449	0.380640
31	1	0	4.743067	-0.138899	-1.206381
32	1	0	1.097167	-1.150457	-0.594203
33	1	0	3.158222	-2.172231	0.455339
34	1	0	2.312234	3.467199	-0.003083
35	1	0	-0.635801	1.237263	-0.791426
36	6	0	3.460273	-2.569488	-1.640378
37	6	0	2.301432	-3.589822	-1.649987
38	1	0	1.341148	-3.113205	-1.875217
39	1	0	2.470395	-4.354306	-2.416317
40	1	0	2.208578	-4.101514	-0.684564
41	6	0	4.783073	-3.321929	-1.386023
42	1	0	4.776498	-3.827054	-0.412417
43	1	0	4.939442	-4.086443	-2.154840
44	1	0	5.646717	-2.647968	-1.413021
45	6	0	3.515617	-1.859800	-3.007128
46	1	0	3.594347	-2.601979	-3.809399
47	1	0	2.614903	-1.263439	-3.179740
48	1	0	4.381719	-1.195090	-3.092688
49	6	0	1.973349	3.042788	2.069515
50	6	0	0.511644	3.532384	2.015684
51	1	0	-0.161273	2.724943	1.716383
52	1	0	0.195700	3.903714	2.997809

53	1	0	0.396498	4.352883	1.296373
54	6	0	2.869633	4.221738	2.502925
55	1	0	2.817151	5.046599	1.781278
56	1	0	2.543894	4.611023	3.474390
57	1	0	3.921369	3.931406	2.605394
58	6	0	2.084645	1.898441	3.095011
59	1	0	1.454062	1.052416	2.804450
60	1	0	3.113525	1.535871	3.195348
61	1	0	1.755744	2.240992	4.083216
62	6	0	-4.592302	-3.237469	1.878351
63	1	0	-4.364015	-4.120142	1.278978
64	1	0	-5.081458	-3.559943	2.803937
65	1	0	-5.295306	-2.604634	1.326701
66	6	0	-2.275210	-3.313213	2.934605
67	1	0	-2.667370	-3.631564	3.906635
68	1	0	-2.026939	-4.201052	2.351006
69	1	0	-1.362116	-2.735172	3.111506
70	6	0	-3.663858	-1.211653	3.059836
71	1	0	-2.763152	-0.626634	3.268293
72	1	0	-4.374590	-0.570966	2.529392
73	1	0	-4.111105	-1.515200	4.011842

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.177460	2.314260	-1.056624
2	8	0	-0.487794	3.290385	-1.917002
3	8	0	-0.617280	2.208008	0.077154
4	6	0	0.776335	1.306883	-1.692561
5	6	0	4.089071	0.573688	0.618883
6	6	0	2.933218	0.830680	-0.184214
7	6	0	1.950669	1.046735	-0.863396
8	1	0	1.070625	1.659078	-2.685553
9	6	0	-1.452082	4.371489	-1.588788
10	6	0	4.103895	0.921321	1.985087
11	6	0	5.233408	0.672888	2.764667
12	6	0	6.365010	0.075610	2.199522
13	6	0	6.359651	-0.273094	0.844957
14	6	0	5.234262	-0.027742	0.058400
15	1	0	3.225357	1.386124	2.421493
16	1	0	5.230382	0.946847	3.816048
17	1	0	7.243236	-0.116342	2.809257
18	1	0	7.234659	-0.737797	0.399095
19	1	0	5.228877	-0.298489	-0.992795
20	1	0	0.193502	0.374277	-1.817477
21	6	0	-2.010970	-3.608678	-0.726348
22	6	0	-1.248453	-2.852912	-1.880069
23	7	0	-1.694366	-2.762648	0.417520
24	6	0	-1.371593	-1.519962	-0.119925
25	7	0	-1.061243	-1.468443	-1.372849
26	6	0	-2.473648	-2.553059	1.629070
27	6	0	-1.905075	-1.187376	2.115868
28	7	0	-1.539811	-0.560868	0.836524
29	1	0	-1.675363	-4.637848	-0.573363
30	1	0	-2.315171	-3.347663	2.363026
31	1	0	-1.078291	0.341064	0.763600
32	6	0	-2.835813	-0.317148	3.003910
33	6	0	-4.109626	0.124768	2.258169

34	1	0	-3.861487	0.669189	1.342387
35	1	0	-4.707280	0.783732	2.898390
36	1	0	-4.742809	-0.725350	1.982580
37	6	0	-3.218816	-1.133894	4.255493
38	1	0	-3.824846	-2.010803	4.001269
39	1	0	-3.805209	-0.518463	4.946735
40	1	0	-2.328586	-1.481208	4.793992
41	6	0	-2.052001	0.937288	3.448787
42	1	0	-1.775956	1.570110	2.598964
43	1	0	-1.132107	0.661746	3.978779
44	1	0	-2.659807	1.544647	4.129268
45	6	0	0.078741	-3.524844	-2.355481
46	6	0	0.712290	-2.634844	-3.444448
47	1	0	0.017788	-2.475763	-4.278753
48	1	0	1.617300	-3.106481	-3.845899
49	1	0	0.983921	-1.656126	-3.041761
50	6	0	-0.241150	-4.900351	-2.977988
51	1	0	-0.963778	-4.807530	-3.798571
52	1	0	-0.652835	-5.603831	-2.245676
53	1	0	0.668685	-5.354005	-3.387983
54	6	0	1.079569	-3.696298	-1.196944
55	1	0	1.319700	-2.730570	-0.742050
56	1	0	2.013520	-4.138426	-1.564304
57	1	0	0.688400	-4.352813	-0.412081
58	1	0	-1.897130	-2.805091	-2.765090
59	1	0	-0.996971	-1.394449	2.707124
60	1	0	-3.097130	-3.624962	-0.918324
61	1	0	-3.552842	-2.487333	1.409027
62	6	0	-0.920916	5.198660	-0.413756
63	1	0	-1.568898	6.069189	-0.265561
64	1	0	-0.901352	4.617133	0.508991
65	1	0	0.089988	5.560949	-0.626997
66	6	0	-2.832766	3.768820	-1.310264
67	1	0	-3.565090	4.577727	-1.215272
68	1	0	-3.143660	3.125066	-2.139331
69	1	0	-2.837780	3.184826	-0.389007
70	6	0	-1.467637	5.199118	-2.876296
71	1	0	-1.803691	4.592636	-3.722718
72	1	0	-2.149724	6.047761	-2.764132
73	1	0	-0.468301	5.583778	-3.101190

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.503231	-1.921425	-0.583161
2	8	0	2.490369	-2.410317	-1.377697
3	8	0	1.688476	-1.617035	0.605507
4	6	0	0.265106	-1.713058	-1.327686
5	6	0	-3.276060	-1.981893	0.669767
6	6	0	-2.036602	-1.897307	-0.028229
7	6	0	-0.964543	-1.853735	-0.611785
8	1	0	0.275440	-2.177429	-2.314774
9	6	0	3.868489	-2.611238	-0.909399
10	6	0	-3.313664	-1.964723	2.082423
11	6	0	-4.527305	-2.047996	2.763716
12	6	0	-5.732399	-2.151582	2.059835
13	6	0	-5.708752	-2.172649	0.660954
14	6	0	-4.499718	-2.088477	-0.028761

15	1	0	-2.379665	-1.893503	2.631398
16	1	0	-4.532457	-2.036351	3.850623
17	1	0	-6.675899	-2.218900	2.593870
18	1	0	-6.637779	-2.256794	0.103094
19	1	0	-4.486152	-2.108018	-1.114282
20	1	0	0.313292	-0.259570	-1.548474
21	6	0	0.064271	3.381664	-1.467052
22	6	0	-0.082975	2.103689	-2.370848
23	7	0	-0.046881	2.813171	-0.124847
24	6	0	0.311174	1.493109	-0.230391
25	7	0	0.294730	1.000670	-1.446474
26	6	0	0.479214	3.324837	1.139952
27	6	0	0.543413	2.020834	1.997507
28	7	0	0.681197	0.991601	0.951266
29	1	0	-0.707598	4.132258	-1.650135
30	1	0	-0.182361	4.073469	1.581287
31	1	0	0.916871	-0.001457	1.072226
32	6	0	1.637739	1.958572	3.096374
33	6	0	3.060929	2.041859	2.511277
34	1	0	3.246843	1.234655	1.796663
35	1	0	3.797890	1.954764	3.317157
36	1	0	3.246655	2.994526	2.003490
37	6	0	1.402905	3.128877	4.073973
38	1	0	1.547084	4.102220	3.591055
39	1	0	2.108364	3.070444	4.909705
40	1	0	0.389723	3.103329	4.492879
41	6	0	1.483215	0.625561	3.861562
42	1	0	1.669899	-0.240854	3.218692
43	1	0	0.476550	0.525572	4.284372
44	1	0	2.198723	0.579883	4.690059
45	6	0	-1.473112	1.916293	-3.052416
46	6	0	-1.460377	0.586849	-3.835334
47	1	0	-0.633032	0.555912	-4.555109
48	1	0	-2.394309	0.471038	-4.396741
49	1	0	-1.365593	-0.272886	-3.167445
50	6	0	-1.689092	3.069516	-4.055721
51	1	0	-0.878230	3.114818	-4.793386
52	1	0	-1.754184	4.046788	-3.564410
53	1	0	-2.625902	2.920426	-4.603525
54	6	0	-2.620631	1.890060	-2.024912
55	1	0	-2.488277	1.079764	-1.301907
56	1	0	-3.576368	1.726782	-2.535693
57	1	0	-2.700457	2.832936	-1.472938
58	1	0	0.660266	2.144364	-3.176298
59	1	0	-0.428881	1.894238	2.498245
60	1	0	1.049464	3.853210	-1.610905
61	1	0	1.476355	3.770875	0.999308
62	6	0	3.898808	-3.653937	0.215316
63	1	0	4.938660	-3.885631	0.472039
64	1	0	3.387773	-3.288316	1.107015
65	1	0	3.415223	-4.579621	-0.113700
66	6	0	4.494809	-1.277663	-0.481510
67	1	0	5.563749	-1.421736	-0.287881
68	1	0	4.391675	-0.535423	-1.280388
69	1	0	4.024142	-0.891702	0.423469
70	6	0	4.569333	-3.151552	-2.160992
71	1	0	4.517902	-2.423395	-2.976548
72	1	0	5.622396	-3.358900	-1.944167
73	1	0	4.093682	-4.077985	-2.496779

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.079391	-1.235187	-1.225485
2	8	0	-3.195012	-2.032505	-1.166279
3	8	0	-2.180941	0.023720	-1.166799
4	6	0	-0.885593	-1.988547	-1.320738
5	6	0	2.661815	-0.335543	-2.354923
6	6	0	1.425006	-0.911892	-1.968480
7	6	0	0.337052	-1.403613	-1.679014
8	1	0	-0.989473	-3.067175	-1.395226
9	6	0	-4.550628	-1.500946	-1.067683
10	6	0	2.795393	1.064492	-2.529484
11	6	0	4.013750	1.627020	-2.905652
12	6	0	5.137293	0.820031	-3.121865
13	6	0	5.020145	-0.565652	-2.958879
14	6	0	3.807111	-1.138528	-2.581250
15	1	0	1.923956	1.695383	-2.380906
16	1	0	4.086189	2.703779	-3.038804
17	1	0	6.084180	1.261762	-3.418385
18	1	0	5.881526	-1.206463	-3.130365
19	1	0	3.724648	-2.214829	-2.462761
20	1	0	-0.339876	-1.587190	0.825003
21	6	0	1.074962	0.084294	3.386856
22	6	0	0.797494	-1.325235	2.755005
23	7	0	0.890984	0.982293	2.246686
24	6	0	0.101235	0.353384	1.336267
25	7	0	-0.000586	-0.953908	1.561782
26	6	0	0.565604	2.410173	2.208698
27	6	0	-0.028052	2.554192	0.766790
28	7	0	-0.466744	1.171106	0.476149
29	1	0	2.080812	0.168039	3.802416
30	1	0	1.454287	3.028601	2.349048
31	1	0	-1.081811	0.813232	-0.311327
32	6	0	-1.141637	3.616125	0.571759
33	6	0	-2.394554	3.303430	1.412760
34	1	0	-2.808999	2.323153	1.159579
35	1	0	-3.167052	4.055060	1.218070
36	1	0	-2.189940	3.321010	2.489148
37	6	0	-0.567163	4.991148	0.972618
38	1	0	-0.322652	5.040424	2.040219
39	1	0	-1.299529	5.779442	0.768993
40	1	0	0.340300	5.227692	0.404074
41	6	0	-1.529641	3.646080	-0.923106
42	1	0	-1.974707	2.701704	-1.251240
43	1	0	-0.656862	3.848336	-1.555136
44	1	0	-2.262338	4.440131	-1.104497
45	6	0	2.049786	-2.199426	2.448030
46	6	0	1.586166	-3.483785	1.726827
47	1	0	0.828017	-4.020887	2.310446
48	1	0	2.435769	-4.160372	1.586029
49	1	0	1.173719	-3.270901	0.735836
50	6	0	2.694976	-2.598023	3.792475
51	1	0	1.983401	-3.124575	4.440564
52	1	0	3.080301	-1.733272	4.344564
53	1	0	3.540972	-3.270253	3.615435
54	6	0	3.073150	-1.459318	1.566754
55	1	0	2.637951	-1.160962	0.608611
56	1	0	3.921834	-2.117419	1.351461

57	1	0	3.471204	-0.565149	2.059172
58	1	0	0.156307	-1.904166	3.429529
59	1	0	0.794656	2.807261	0.082486
60	1	0	0.347551	0.308738	4.181545
61	1	0	-0.170037	2.662292	2.987233
62	6	0	-4.886312	-0.642581	-2.295875
63	1	0	-5.947040	-0.366819	-2.275563
64	1	0	-4.282383	0.265386	-2.317827
65	1	0	-4.699096	-1.210411	-3.213337
66	6	0	-4.742664	-0.727654	0.245684
67	1	0	-5.798302	-0.457537	0.364938
68	1	0	-4.454358	-1.352751	1.098225
69	1	0	-4.142466	0.182997	0.255151
70	6	0	-5.409918	-2.771772	-1.059343
71	1	0	-5.147494	-3.407582	-0.207745
72	1	0	-6.471341	-2.511822	-0.987465
73	1	0	-5.252074	-3.346054	-1.977353

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.616009	-0.706854	1.420883
2	6	0	-2.243639	-1.799809	0.234882
3	8	0	-3.343495	-2.331084	0.865920
4	8	0	-2.335281	-0.703228	-0.398474
5	6	0	-1.096690	-2.593702	0.411945
6	6	0	2.384568	-1.969511	-1.543358
7	6	0	1.174365	-2.184388	-0.842180
8	6	0	0.106691	-2.356801	-0.253311
9	1	0	-1.203643	-3.500733	0.997793
10	6	0	-4.706470	-1.880613	0.617725
11	6	0	-4.931070	-0.473295	1.189314
12	6	0	-5.546616	-2.902489	1.395194
13	6	0	-5.040320	-1.951957	-0.879599
14	6	0	2.505620	-0.930304	-2.501344
15	6	0	3.701582	-0.723044	-3.185825
16	6	0	4.814283	-1.539413	-2.947393
17	6	0	4.707949	-2.575740	-2.011011
18	6	0	3.518765	-2.791040	-1.318091
19	1	0	-5.992661	-0.208000	1.121524
20	1	0	-4.638148	-0.443533	2.244457
21	1	0	-4.346594	0.264930	0.640450
22	1	0	-6.612065	-2.664094	1.307807
23	1	0	-5.380592	-3.911491	1.005546
24	1	0	-5.272972	-2.895132	2.455048
25	1	0	-6.105377	-1.742054	-1.031127
26	1	0	-4.452999	-1.230271	-1.449148
27	1	0	-4.831961	-2.955492	-1.265198
28	1	0	1.642331	-0.303296	-2.704265
29	1	0	3.764925	0.078196	-3.918255
30	1	0	5.742759	-1.377233	-3.487018
31	1	0	5.559744	-3.224342	-1.821453
32	1	0	3.444022	-3.600486	-0.597949
33	6	0	1.599105	2.419483	2.107439
34	6	0	1.736167	0.903521	2.482708
35	7	0	1.032451	2.366347	0.759184
36	6	0	0.405545	1.166964	0.608337
37	7	0	0.765921	0.289806	1.545087

38	6	0	0.240052	3.369646	0.044425
39	6	0	-0.491664	2.481277	-1.014097
40	7	0	-0.476391	1.144053	-0.366766
41	1	0	2.556831	2.942518	2.115639
42	1	0	0.913727	2.935376	2.796393
43	6	0	3.174566	0.310313	2.413683
44	1	0	0.874992	4.124661	-0.423065
45	1	0	-0.463773	3.867934	0.728000
46	6	0	-1.891075	2.961008	-1.475407
47	1	0	-1.168735	0.334406	-0.490268
48	6	0	3.848313	0.572410	1.053789
49	6	0	3.094463	-1.211551	2.663571
50	6	0	4.005117	0.951012	3.546447
51	6	0	-2.906477	2.989002	-0.316997
52	6	0	-2.398633	2.007853	-2.579785
53	6	0	-1.731237	4.377461	-2.068410
54	1	0	4.843313	0.115925	1.039468
55	1	0	3.281728	0.136371	0.226887
56	1	0	3.977004	1.642504	0.857138
57	1	0	4.103285	-1.633019	2.726570
58	1	0	2.582157	-1.438254	3.606909
59	1	0	2.578046	-1.735050	1.852526
60	1	0	5.011574	0.520179	3.560812
61	1	0	4.118863	2.033877	3.420928
62	1	0	3.553085	0.769177	4.529224
63	1	0	-3.009142	2.004129	0.145997
64	1	0	-2.631068	3.710092	0.461102
65	1	0	-3.890628	3.284063	-0.696528
66	1	0	-3.352915	2.371441	-2.976842
67	1	0	-1.689183	1.957996	-3.414605
68	1	0	-2.558218	0.993901	-2.202355
69	1	0	-2.687592	4.724382	-2.473436
70	1	0	-1.411709	5.107173	-1.315087
71	1	0	-1.001065	4.389651	-2.886708
72	1	0	0.145666	2.428257	-1.908702
73	1	0	1.367768	0.747511	3.502894

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.202344	-0.267908	-1.051567
2	6	0	2.178821	-1.728892	-0.705139
3	8	0	3.311428	-2.104353	-1.395415
4	8	0	2.245143	-0.867705	0.219818
5	6	0	1.031977	-2.390119	-1.183215
6	6	0	-2.479624	-2.463558	0.765344
7	6	0	-1.318992	-2.254264	-0.028137
8	6	0	-0.203368	-2.307502	-0.558044
9	1	0	1.161619	-3.089285	-2.002475
10	6	0	4.643604	-2.082981	-0.803539
11	6	0	5.172842	-0.648409	-0.676052
12	6	0	5.481282	-2.864017	-1.824273
13	6	0	4.637969	-2.807559	0.550076
14	6	0	-2.656032	-1.789644	1.999720
15	6	0	-3.801038	-1.991916	2.768917
16	6	0	-4.807172	-2.865023	2.338347
17	6	0	-4.645381	-3.540529	1.122189
18	6	0	-3.506059	-3.345377	0.343983

19	1	0	6.232335	-0.665618	-0.394215
20	1	0	5.082048	-0.126089	-1.634618
21	1	0	4.614905	-0.095749	0.078803
22	1	0	6.525309	-2.920196	-1.497751
23	1	0	5.094611	-3.881169	-1.939225
24	1	0	5.447714	-2.372307	-2.801825
25	1	0	5.661000	-2.883420	0.935406
26	1	0	4.028578	-2.271235	1.280569
27	1	0	4.238663	-3.820854	0.437392
28	1	0	-1.872910	-1.123964	2.351194
29	1	0	-3.905914	-1.468375	3.716112
30	1	0	-5.696588	-3.021563	2.941641
31	1	0	-5.413027	-4.229427	0.778403
32	1	0	-3.387610	-3.877579	-0.595164
33	6	0	-1.611086	3.058946	-1.391989
34	6	0	-2.124692	1.640075	-1.812337
35	7	0	-0.855179	2.778348	-0.171160
36	6	0	-0.467728	1.470201	-0.208653
37	7	0	-1.187738	0.758706	-1.070443
38	6	0	0.237684	3.551966	0.416584
39	6	0	0.961604	2.461847	1.266153
40	7	0	0.572214	1.208277	0.561923
41	1	0	-2.424016	3.762397	-1.204318
42	1	0	-0.951846	3.485461	-2.162791
43	6	0	-3.635765	1.367728	-1.552304
44	1	0	-0.137303	4.370891	1.033388
45	1	0	0.887943	3.964998	-0.369049
46	6	0	2.484309	2.658893	1.475153
47	1	0	1.135336	0.311488	0.510348
48	6	0	-4.032377	1.646065	-0.089976
49	6	0	-3.943944	-0.106579	-1.887895
50	6	0	-4.447039	2.273646	-2.503793
51	6	0	3.263097	2.595269	0.147399
52	6	0	2.998962	1.564785	2.436004
53	6	0	2.691084	4.039135	2.136801
54	1	0	-5.091861	1.411505	0.057936
55	1	0	-3.461554	1.022067	0.604213
56	1	0	-3.886659	2.695769	0.188087
57	1	0	-5.027152	-0.268164	-1.899269
58	1	0	-3.553282	-0.390956	-2.872261
59	1	0	-3.527410	-0.778955	-1.134342
60	1	0	-5.517833	2.086656	-2.372598
61	1	0	-4.279055	3.340401	-2.316373
62	1	0	-4.202207	2.071503	-3.553674
63	1	0	3.115043	1.637437	-0.357206
64	1	0	2.976508	3.399785	-0.539584
65	1	0	4.334949	2.707141	0.343068
66	1	0	4.060706	1.728018	2.652045
67	1	0	2.458275	1.595086	3.389904
68	1	0	2.895172	0.564235	2.008500
69	1	0	3.750007	4.182172	2.375798
70	1	0	2.391416	4.863305	1.479073
71	1	0	2.126183	4.125001	3.073064
72	1	0	0.495518	2.442113	2.261919
73	1	0	-1.950548	1.491407	-2.883974

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Standard orientation:

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

1	1	0	-1.431135	-0.506487	-0.861542
2	6	0	2.473310	-1.578054	-0.737116
3	8	0	3.657852	-2.048537	-1.209957
4	8	0	2.393335	-0.700046	0.135753
5	6	0	1.360729	-2.228265	-1.401521
6	6	0	-1.906189	-2.605170	0.494768
7	6	0	-1.057409	-1.883766	-0.460552
8	6	0	0.110880	-2.122160	-0.916022
9	1	0	1.582633	-2.849787	-2.263674
10	6	0	4.963911	-1.629182	-0.690095
11	6	0	5.197915	-0.139510	-0.968398
12	6	0	5.938388	-2.484552	-1.507737
13	6	0	5.076709	-1.966594	0.802205
14	6	0	-2.195958	-2.058057	1.760806
15	6	0	-3.028668	-2.727774	2.659730
16	6	0	-3.608293	-3.952253	2.312331
17	6	0	-3.336641	-4.502130	1.055091
18	6	0	-2.497327	-3.839519	0.157321
19	1	0	6.229726	0.125251	-0.710890
20	1	0	5.046759	0.076642	-2.031371
21	1	0	4.520413	0.481389	-0.382624
22	1	0	6.970285	-2.267395	-1.212889
23	1	0	5.745399	-3.549071	-1.344044
24	1	0	5.829860	-2.275996	-2.576635
25	1	0	6.097280	-1.764979	1.146278
26	1	0	4.380728	-1.373447	1.396868
27	1	0	4.864638	-3.027875	0.967909
28	1	0	-1.745281	-1.110519	2.043514
29	1	0	-3.224742	-2.290810	3.635753
30	1	0	-4.259867	-4.470138	3.010380
31	1	0	-3.776427	-5.455184	0.771938
32	1	0	-2.289119	-4.273227	-0.816531
33	6	0	-2.356988	2.966160	-1.123441
34	6	0	-2.700984	1.495391	-1.556855
35	7	0	-1.417998	2.754838	-0.024652
36	6	0	-0.894963	1.494718	-0.176410
37	7	0	-1.590665	0.702343	-0.960269
38	6	0	-0.357298	3.641381	0.440342
39	6	0	0.579738	2.638633	1.178299
40	7	0	0.265875	1.368286	0.479743
41	1	0	-3.230336	3.534007	-0.795777
42	1	0	-1.873960	3.517218	-1.945116
43	6	0	-4.130418	1.000108	-1.183083
44	1	0	-0.739838	4.412987	1.112055
45	1	0	0.148578	4.129296	-0.407783
46	6	0	2.083224	3.017222	1.224110
47	1	0	0.869370	0.538766	0.439832
48	6	0	-4.377684	1.053492	0.335613
49	6	0	-4.298631	-0.448711	-1.685910
50	6	0	-5.162236	1.885865	-1.915564
51	6	0	2.723914	3.015143	-0.177206
52	6	0	2.821818	2.012851	2.135270
53	6	0	2.197597	4.425284	1.848087
54	1	0	-5.389119	0.699559	0.563967
55	1	0	-3.675515	0.410882	0.874080
56	1	0	-4.286065	2.071703	0.730203
57	1	0	-5.317879	-0.799579	-1.489363
58	1	0	-4.125697	-0.514380	-2.767223
59	1	0	-3.610465	-1.136925	-1.190431
60	1	0	-6.172295	1.494295	-1.753790
61	1	0	-5.156847	2.922441	-1.560543

62	1	0	-4.982372	1.897365	-2.997805
63	1	0	2.645602	2.033568	-0.651737
64	1	0	2.265518	3.755266	-0.842689
65	1	0	3.787239	3.266171	-0.097357
66	1	0	3.875573	2.298526	2.230237
67	1	0	2.388581	2.005895	3.142892
68	1	0	2.788186	0.996256	1.735871
69	1	0	3.251956	4.690058	1.980793
70	1	0	1.743801	5.196981	1.215884
71	1	0	1.719867	4.466629	2.834571
72	1	0	0.234217	2.556623	2.219949
73	1	0	-2.619892	1.415114	-2.647653

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.235838	1.598526	-0.874535
2	6	0	-2.866414	1.002900	-0.900879
3	8	0	-4.079098	1.114231	-1.477272
4	8	0	-2.584498	0.231876	0.005402
5	6	0	-1.916749	1.953491	-1.536893
6	6	0	0.886450	3.325101	0.466738
7	6	0	0.481732	2.314523	-0.530898
8	6	0	-0.718395	2.155426	-1.033021
9	1	0	-2.257413	2.473474	-2.429709
10	6	0	-5.241835	0.302141	-1.057381
11	6	0	-4.956237	-1.183633	-1.300547
12	6	0	-6.348751	0.801885	-1.989926
13	6	0	-5.586224	0.602340	0.405669
14	6	0	2.224401	3.364642	0.894194
15	6	0	2.646899	4.309083	1.832609
16	6	0	1.738326	5.229908	2.359824
17	6	0	0.402106	5.198790	1.941081
18	6	0	-0.020611	4.256839	1.005390
19	1	0	-5.867672	-1.762123	-1.114635
20	1	0	-4.655443	-1.349666	-2.340149
21	1	0	-4.169386	-1.552263	-0.641647
22	1	0	-7.281791	0.268968	-1.781010
23	1	0	-6.520786	1.873028	-1.847320
24	1	0	-6.078441	0.631579	-3.036476
25	1	0	-6.522770	0.097951	0.666939
26	1	0	-4.802839	0.254980	1.080586
27	1	0	-5.728742	1.678200	0.551051
28	1	0	2.933790	2.650726	0.486511
29	1	0	3.685761	4.324046	2.150218
30	1	0	2.065253	5.965636	3.089068
31	1	0	-0.310955	5.911437	2.346453
32	1	0	-1.058779	4.238120	0.685489
33	6	0	3.228727	-2.732798	-0.847006
34	6	0	3.202484	-1.348081	-1.597454
35	7	0	2.279312	-2.487473	0.230633
36	6	0	1.476339	-1.437513	-0.216732
37	7	0	1.932247	-0.700533	-1.174844
38	6	0	1.435278	-3.460965	0.905706
39	6	0	0.310597	-2.544966	1.468317
40	7	0	0.288960	-1.477121	0.455005
41	1	0	4.213564	-3.010578	-0.461879
42	1	0	2.876781	-3.544133	-1.506352

43	6	0	4.464548	-0.454010	-1.384755
44	1	0	1.970251	-3.987332	1.700591
45	1	0	1.033285	-4.206774	0.198351
46	6	0	-1.060921	-3.222201	1.737714
47	1	0	-0.381898	-0.718882	0.438244
48	6	0	4.694321	-0.144062	0.106255
49	6	0	4.266924	0.864324	-2.160186
50	6	0	5.702815	-1.170505	-1.964263
51	6	0	-1.736455	-3.704820	0.439952
52	6	0	-1.984166	-2.207225	2.446602
53	6	0	-0.829043	-4.420563	2.682517
54	1	0	5.552377	0.527746	0.229871
55	1	0	3.815726	0.339755	0.544076
56	1	0	4.897682	-1.050964	0.686200
57	1	0	5.150048	1.506500	-2.058112
58	1	0	4.112441	0.673394	-3.229105
59	1	0	3.395765	1.412669	-1.794572
60	1	0	6.584677	-0.522793	-1.896258
61	1	0	5.938914	-2.097107	-1.429299
62	1	0	5.556565	-1.420735	-3.022497
63	1	0	-1.889320	-2.876719	-0.257440
64	1	0	-1.145377	-4.471805	-0.072188
65	1	0	-2.713677	-4.144552	0.670572
66	1	0	-2.935612	-2.683436	2.711309
67	1	0	-1.527194	-1.841261	3.374252
68	1	0	-2.211570	-1.346456	1.811881
69	1	0	-1.787819	-4.864311	2.972630
70	1	0	-0.232414	-5.207945	2.208558
71	1	0	-0.315992	-4.111455	3.601567
72	1	0	0.662284	-2.138244	2.431432
73	1	0	3.143149	-1.530470	-2.679003

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.644433	-1.775577	-0.578568
2	8	0	1.571374	-2.575363	-0.057499
3	8	0	-0.514441	-2.095204	-0.811487
4	6	0	1.151452	-0.366523	-0.872040
5	6	0	5.101355	0.489312	-0.170069
6	6	0	3.727500	0.176949	-0.418507
7	6	0	2.561620	-0.094380	-0.619379
8	1	0	0.904945	-0.171039	-1.923794
9	6	0	1.298381	-3.982299	0.329639
10	6	0	5.590357	0.572190	1.149889
11	6	0	6.929654	0.878926	1.389579
12	6	0	7.803716	1.109698	0.322120
13	6	0	7.328485	1.030649	-0.991132
14	6	0	5.990893	0.722741	-1.238715
15	1	0	4.909679	0.395612	1.976836
16	1	0	7.291681	0.939672	2.412181
17	1	0	8.845897	1.349986	0.512081
18	1	0	8.001458	1.209552	-1.825110
19	1	0	5.620718	0.661382	-2.257360
20	6	0	0.888016	-4.790180	-0.905786
21	1	0	-0.078382	-4.465832	-1.294431
22	1	0	0.819691	-5.849445	-0.635717
23	1	0	1.640783	-4.690140	-1.694498

24	6	0	2.657924	-4.444845	0.858815
25	1	0	2.594043	-5.487023	1.187531
26	1	0	2.971728	-3.829838	1.707333
27	1	0	3.421892	-4.370878	0.079388
28	6	0	0.239657	-4.017086	1.436327
29	1	0	0.541530	-3.380549	2.274229
30	1	0	0.141193	-5.042780	1.807769
31	1	0	-0.732787	-3.684120	1.071104
32	1	0	0.505959	0.320687	-0.294471
33	6	0	-3.147571	3.005512	0.994587
34	6	0	-1.577224	2.972685	0.861958
35	7	0	-3.523743	1.877730	0.150416
36	6	0	-2.393711	1.065533	0.097328
37	7	0	-1.258892	1.589484	0.421075
38	6	0	-4.697754	1.023380	0.261084
39	6	0	-4.214439	-0.251225	-0.493646
40	7	0	-2.768884	-0.203777	-0.232844
41	1	0	-3.601880	3.938148	0.649327
42	1	0	-5.577283	1.469970	-0.210366
43	1	0	-2.097891	-0.869790	-0.604893
44	6	0	-4.885794	-1.595162	-0.097520
45	6	0	-6.405082	-1.467711	-0.333073
46	1	0	-6.626010	-1.176469	-1.367276
47	1	0	-6.859578	-0.725299	0.332586
48	1	0	-6.902000	-2.425880	-0.145071
49	6	0	-4.614388	-1.973812	1.371068
50	1	0	-5.047941	-2.956591	1.588722
51	1	0	-5.059686	-1.258594	2.070813
52	1	0	-3.540776	-2.019526	1.575259
53	6	0	-4.330439	-2.705798	-1.016028
54	1	0	-4.498404	-2.465962	-2.073081
55	1	0	-4.830444	-3.658512	-0.807155
56	1	0	-3.255935	-2.857632	-0.870202
57	6	0	-0.960202	4.075531	-0.055362
58	6	0	-1.237259	5.463268	0.560677
59	1	0	-0.748674	6.247040	-0.029831
60	1	0	-0.846683	5.527629	1.584051
61	1	0	-2.306672	5.700074	0.593587
62	6	0	0.566412	3.864482	-0.112132
63	1	0	1.008648	3.894185	0.891188
64	1	0	1.039851	4.652089	-0.710559
65	1	0	0.815143	2.897541	-0.555839
66	6	0	-1.532897	4.017426	-1.484204
67	1	0	-2.612724	4.201489	-1.501202
68	1	0	-1.350348	3.038383	-1.938207
69	1	0	-1.056362	4.776879	-2.115578
70	1	0	-1.132008	3.122855	1.854574
71	1	0	-4.410336	-0.098960	-1.568887
72	1	0	-4.938137	0.802256	1.314971
73	1	0	-3.457299	2.837799	2.039887

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.305086	-2.132001	0.382314
2	8	0	-2.178086	-2.840100	1.151487
3	8	0	-1.665142	-1.654633	-0.703710
4	6	0	-0.024756	-1.922715	1.043046

5	6	0	3.387050	-1.555570	-1.157259
6	6	0	2.182560	-1.682761	-0.404307
7	6	0	1.149262	-1.822549	0.230901
8	1	0	0.096661	-2.529808	1.941641
9	6	0	-3.515156	-2.963480	0.646015
10	6	0	3.380814	-1.678880	-2.564821
11	6	0	4.561383	-1.552120	-3.296216
12	6	0	5.776605	-1.307299	-2.647385
13	6	0	5.798239	-1.190276	-1.253248
14	6	0	4.621179	-1.309223	-0.514854
15	1	0	2.441801	-1.881145	-3.070167
16	1	0	4.533738	-1.651848	-4.378189
17	1	0	6.695054	-1.213658	-3.220033
18	1	0	6.737002	-1.004696	-0.737937
19	1	0	4.641629	-1.217903	0.566951
20	1	0	-0.216220	-0.553794	1.495712
21	6	0	0.014183	3.042651	2.069008
22	6	0	0.296005	1.579852	2.648671
23	7	0	-0.337254	2.754667	0.697439
24	6	0	-0.605302	1.412758	0.585241
25	7	0	-0.365744	0.694700	1.657296
26	6	0	-0.751720	3.478860	-0.481535
27	6	0	-1.020592	2.292998	-1.504257
28	7	0	-1.010061	1.094475	-0.645579
29	1	0	0.875744	3.702774	2.118201
30	1	0	0.038438	4.137584	-0.838940
31	1	0	-1.287639	0.138808	-0.898378
32	6	0	-2.322763	2.427301	-2.368012
33	6	0	-3.613539	2.339264	-1.495309
34	1	0	-3.649911	1.386178	-0.964777
35	1	0	-4.498853	2.416212	-2.129881
36	1	0	-3.642404	3.148166	-0.764845
37	6	0	-2.312505	3.781848	-3.143750
38	1	0	-2.359692	4.622713	-2.450607
39	1	0	-3.173004	3.839328	-3.813178
40	1	0	-1.400740	3.867567	-3.737932
41	6	0	-2.360611	1.274829	-3.422207
42	1	0	-2.419061	0.304212	-2.928160
43	1	0	-1.461905	1.299782	-4.041283
44	1	0	-3.232864	1.384744	-4.069672
45	6	0	1.819232	1.283652	2.912098
46	6	0	1.999990	-0.157677	3.483766
47	1	0	1.341118	-0.310937	4.340350
48	1	0	3.032227	-0.309622	3.806491
49	1	0	1.773102	-0.903338	2.727386
50	6	0	2.373588	2.260382	4.000506
51	1	0	1.777848	2.184160	4.912097
52	1	0	2.347432	3.292511	3.651215
53	1	0	3.409244	2.008948	4.239325
54	6	0	2.677823	1.431288	1.618143
55	1	0	2.275609	0.805965	0.822537
56	1	0	3.707989	1.127558	1.813963
57	1	0	2.683241	2.466988	1.275822
58	1	0	-0.245638	1.480429	3.594042
59	1	0	-0.155110	2.227193	-2.171428
60	1	0	-0.835352	3.492047	2.585587
61	1	0	-1.653732	4.047573	-0.263862
62	6	0	-3.521142	-3.691707	-0.710911
63	1	0	-4.384139	-4.321105	-0.774110
64	1	0	-3.546119	-2.971679	-1.502009
65	1	0	-2.637328	-4.288313	-0.799415
66	6	0	-4.167731	-1.579331	0.473159

67	1	0	-5.211115	-1.645997	0.700765
68	1	0	-3.702060	-0.880191	1.135921
69	1	0	-4.043429	-1.250091	-0.537311
70	6	0	-4.276388	-3.787177	1.701311
71	1	0	-4.255557	-3.272034	2.638911
72	1	0	-5.291273	-3.917172	1.388249
73	1	0	-3.811239	-4.744634	1.809998

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013524	1.885390	-0.574898
2	8	0	-0.719737	2.772533	0.179410
3	8	0	1.240084	2.032958	-0.750415
4	6	0	-0.768062	0.814967	-1.097776
5	6	0	-4.736680	0.186317	-0.594359
6	6	0	-3.348283	0.416675	-0.775819
7	6	0	-2.151187	0.637914	-0.925206
8	1	0	-0.272176	0.239541	-1.876624
9	6	0	-0.118412	3.925822	0.843437
10	6	0	-5.477948	0.921142	0.362920
11	6	0	-6.841037	0.692169	0.540723
12	6	0	-7.509386	-0.272852	-0.222515
13	6	0	-6.790285	-1.006273	-1.173613
14	6	0	-5.427097	-0.783196	-1.361510
15	1	0	-4.965951	1.671908	0.957026
16	1	0	-7.386999	1.272056	1.280814
17	1	0	-8.572014	-0.447887	-0.080747
18	1	0	-7.296455	-1.755558	-1.777370
19	1	0	-4.878490	-1.350708	-2.107498
20	6	0	0.487638	4.889804	-0.186222
21	1	0	1.342736	4.438980	-0.691392
22	1	0	0.811567	5.809060	0.315464
23	1	0	-0.263107	5.157271	-0.937120
24	6	0	-1.322892	4.577255	1.534667
25	1	0	-1.008645	5.474405	2.078557
26	1	0	-1.781832	3.880497	2.242944
27	1	0	-2.078694	4.861118	0.796359
28	6	0	0.911355	3.477169	1.890710
29	1	0	0.459657	2.754255	2.579006
30	1	0	1.243803	4.341766	2.476782
31	1	0	1.779718	3.019441	1.415092
32	1	0	-0.064782	-0.709227	0.255602
33	6	0	2.076012	-3.108100	1.290044
34	6	0	0.571648	-2.665613	1.213897
35	7	0	2.701003	-2.300889	0.240574
36	6	0	1.912247	-1.211058	0.024905
37	7	0	0.692607	-1.352112	0.535913
38	6	0	4.094314	-1.868056	0.099891
39	6	0	3.937805	-0.612556	-0.822573
40	7	0	2.529836	-0.218248	-0.579742
41	1	0	2.212178	-4.175284	1.106045
42	1	0	4.711609	-2.641647	-0.361038
43	1	0	2.047270	0.728779	-0.768801
44	6	0	4.957204	0.537937	-0.611722
45	6	0	6.374410	-0.035822	-0.821260
46	1	0	6.475308	-0.504300	-1.807780
47	1	0	6.634044	-0.781945	-0.061060

48	1	0	7.118084	0.765522	-0.758942
49	6	0	4.844894	1.161641	0.792899
50	1	0	5.559287	1.986418	0.888229
51	1	0	5.072971	0.443236	1.588572
52	1	0	3.844090	1.565165	0.971610
53	6	0	4.691001	1.627801	-1.673623
54	1	0	4.758731	1.216611	-2.687985
55	1	0	5.438711	2.423869	-1.587670
56	1	0	3.703737	2.084233	-1.554770
57	6	0	-0.409457	-3.656035	0.518452
58	6	0	-0.468704	-4.949495	1.358834
59	1	0	-1.215438	-5.632182	0.940394
60	1	0	-0.759245	-4.739400	2.395320
61	1	0	0.486869	-5.485421	1.375656
62	6	0	-1.815333	-3.019484	0.501403
63	1	0	-2.152284	-2.769871	1.514627
64	1	0	-2.540565	-3.722514	0.078269
65	1	0	-1.860507	-2.106797	-0.100297
66	6	0	0.028358	-3.983909	-0.921610
67	1	0	1.010925	-4.467780	-0.955665
68	1	0	0.070138	-3.083555	-1.542690
69	1	0	-0.691865	-4.668103	-1.382861
70	1	0	0.193071	-2.496011	2.228031
71	1	0	4.028627	-0.942223	-1.867889
72	1	0	4.521848	-1.610303	1.080500
73	1	0	2.505577	-2.865900	2.273669

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.219896	2.213379	-1.018785
2	8	0	0.763442	3.001650	0.011083
3	8	0	2.422407	2.185393	-1.351020
4	6	0	0.201825	1.411486	-1.618842
5	6	0	-3.631849	1.310352	-0.371543
6	6	0	-2.261430	1.209975	-0.739253
7	6	0	-1.117527	1.356245	-1.183744
8	1	0	0.467343	0.960657	-2.572078
9	6	0	1.582994	4.042051	0.622766
10	6	0	-4.010171	1.833433	0.889901
11	6	0	-5.352539	1.927680	1.253158
12	6	0	-6.361406	1.498296	0.381997
13	6	0	-6.003574	0.979420	-0.868127
14	6	0	-4.664330	0.885896	-1.243660
15	1	0	-3.234146	2.172699	1.569667
16	1	0	-5.613997	2.341214	2.224132
17	1	0	-7.406272	1.572823	0.669070
18	1	0	-6.775204	0.651709	-1.560536
19	1	0	-4.398325	0.495503	-2.221613
20	6	0	2.037419	5.056966	-0.436179
21	1	0	2.722717	4.596958	-1.150083
22	1	0	2.543650	5.898813	0.050297
23	1	0	1.170738	5.447433	-0.979843
24	6	0	0.610735	4.701202	1.609334
25	1	0	1.107513	5.516851	2.145879
26	1	0	0.252362	3.969708	2.340889
27	1	0	-0.256176	5.106287	1.078893
28	6	0	2.775186	3.438512	1.379101

29	1	0	2.427125	2.679244	2.088901
30	1	0	3.288492	4.222575	1.948204
31	1	0	3.482984	2.981375	0.686816
32	1	0	-0.957226	-0.567418	-0.124625
33	6	0	0.107633	-3.368055	1.391969
34	6	0	-1.135381	-2.553857	0.900446
35	7	0	1.151115	-2.923193	0.467823
36	6	0	0.803421	-1.694150	-0.001376
37	7	0	-0.482626	-1.429404	0.178553
38	6	0	2.606531	-2.960590	0.618094
39	6	0	3.051874	-1.891042	-0.424121
40	7	0	1.844169	-1.022200	-0.474189
41	1	0	-0.044105	-4.446753	1.329967
42	1	0	3.008496	-3.949083	0.388854
43	1	0	1.734053	-0.131723	-0.968359
44	6	0	4.383590	-1.152826	-0.134873
45	6	0	5.483768	-2.224435	0.028645
46	1	0	5.543121	-2.877413	-0.850777
47	1	0	5.324700	-2.853130	0.912772
48	1	0	6.458504	-1.739792	0.144495
49	6	0	4.301010	-0.286713	1.135800
50	1	0	5.259230	0.217964	1.298156
51	1	0	4.091208	-0.880028	2.033383
52	1	0	3.533560	0.485379	1.043406
53	6	0	4.727280	-0.258840	-1.346409
54	1	0	4.797532	-0.854238	-2.265396
55	1	0	5.700680	0.219015	-1.188961
56	1	0	3.992174	0.538494	-1.497376
57	6	0	-2.165339	-3.350832	0.043028
58	6	0	-2.830906	-4.405067	0.953714
59	1	0	-3.601750	-4.946705	0.395778
60	1	0	-3.318353	-3.935595	1.816495
61	1	0	-2.120082	-5.150001	1.329163
62	6	0	-3.252107	-2.380936	-0.459748
63	1	0	-3.735378	-1.846956	0.365360
64	1	0	-4.029057	-2.935811	-0.996252
65	1	0	-2.846772	-1.631496	-1.144901
66	6	0	-1.500977	-4.041339	-1.163731
67	1	0	-0.753213	-4.782922	-0.861840
68	1	0	-1.015181	-3.314391	-1.822458
69	1	0	-2.260119	-4.564261	-1.755009
70	1	0	-1.673073	-2.138917	1.759202
71	1	0	3.153823	-2.386026	-1.400918
72	1	0	2.898459	-2.682843	1.641628
73	1	0	0.370814	-3.109244	2.428428

syn-cis-IM2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.568988	-3.366178	1.475974
2	6	0	-1.685365	-2.321303	1.131336
3	7	0	0.426303	-3.115695	0.432225
4	6	0	0.259332	-1.836829	-0.003763
5	7	0	-0.924544	-1.336807	0.320198
6	6	0	1.861792	-3.407615	0.425490
7	6	0	2.374596	-2.412771	-0.662662
8	7	0	1.334247	-1.352043	-0.602194
9	1	0	-0.930055	-4.395376	1.443137

10	1	0	-0.142421	-3.176553	2.472317
11	6	0	-2.950977	-2.891292	0.421997
12	1	0	2.058686	-4.447232	0.157346
13	1	0	2.304478	-3.201463	1.411156
14	6	0	3.833615	-1.911030	-0.511378
15	6	0	4.036937	-1.091034	0.776515
16	6	0	4.191943	-1.040791	-1.735887
17	6	0	4.750646	-3.153748	-0.491604
18	6	0	-3.891516	-1.721812	0.071424
19	6	0	-3.677939	-3.826775	1.411820
20	6	0	-2.592405	-3.661253	-0.863579
21	1	0	5.070297	-0.732184	0.823547
22	1	0	3.386063	-0.213528	0.802685
23	1	0	3.857044	-1.683625	1.681098
24	1	0	5.255522	-0.780323	-1.706265
25	1	0	4.009983	-1.583251	-2.672000
26	1	0	3.640056	-0.095714	-1.759357
27	1	0	5.799445	-2.841728	-0.460585
28	1	0	4.571878	-3.786385	0.385807
29	1	0	4.615043	-3.767392	-1.390566
30	1	0	-4.823632	-2.104854	-0.357207
31	1	0	-4.152220	-1.131485	0.957232
32	1	0	-3.448808	-1.042586	-0.661384
33	1	0	-4.608101	-4.192242	0.964528
34	1	0	-3.080560	-4.705523	1.679707
35	1	0	-3.942183	-3.300968	2.337232
36	1	0	-3.506277	-4.024602	-1.345627
37	1	0	-2.074429	-3.018128	-1.582194
38	1	0	-1.957638	-4.531936	-0.665379
39	1	0	-1.246583	-0.400333	0.010202
40	1	0	2.297430	-2.907839	-1.641746
41	1	0	-2.019986	-1.824220	2.048259
42	1	0	1.338725	-0.399605	-1.036517
43	6	0	1.925520	2.147777	-0.907309
44	8	0	1.518041	2.694019	0.286431
45	8	0	3.093880	2.217705	-1.306889
46	6	0	0.865010	1.457372	-1.602203
47	6	0	-3.002368	1.865589	-0.630842
48	6	0	-1.647720	1.457020	-0.839204
49	6	0	-0.469606	1.516995	-1.225343
50	1	0	1.104306	1.192785	-2.630235
51	6	0	2.370986	3.595391	1.058030
52	6	0	-3.971588	1.742743	-1.655056
53	6	0	-5.294246	2.128243	-1.439833
54	6	0	-5.695790	2.645551	-0.202565
55	6	0	-4.747859	2.774311	0.819565
56	6	0	-3.423843	2.386992	0.615652
57	1	0	-3.667066	1.351989	-2.621678
58	1	0	-6.015866	2.030729	-2.247247
59	1	0	-6.726194	2.948160	-0.040110
60	1	0	-5.041317	3.182594	1.783595
61	1	0	-2.693710	2.495342	1.412466
62	6	0	1.458570	4.016469	2.216707
63	6	0	2.758242	4.818869	0.214799
64	6	0	3.607415	2.861090	1.596159
65	1	0	1.985353	4.708966	2.881958
66	1	0	0.559696	4.511038	1.836363
67	1	0	1.148510	3.142114	2.798463
68	1	0	3.283477	5.547959	0.842495
69	1	0	3.407421	4.535043	-0.614930
70	1	0	1.859832	5.299216	-0.187060
71	1	0	4.166153	3.522963	2.268337

72	1	0	3.303630	1.977518	2.168687
73	1	0	4.260257	2.548796	0.780086

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syn-cis-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.651264	-3.286721	1.279569
2	6	0	-2.449379	-1.986861	0.906671
3	7	0	-0.527963	-3.223440	0.344739
4	6	0	-0.374567	-1.909627	-0.005135
5	7	0	-1.416759	-1.152252	0.237706
6	6	0	0.797633	-3.831398	0.445463
7	6	0	1.621269	-2.938079	-0.531776
8	7	0	0.858775	-1.669215	-0.468974
9	1	0	-2.232143	-4.201296	1.144273
10	1	0	-1.295054	-3.249932	2.320714
11	6	0	-3.730853	-2.208756	0.044662
12	1	0	0.787420	-4.877837	0.133351
13	1	0	1.180874	-3.771394	1.475644
14	6	0	3.136657	-2.794576	-0.233722
15	6	0	3.399242	-2.094427	1.113032
16	6	0	3.790456	-1.980828	-1.371713
17	6	0	3.751951	-4.210432	-0.217360
18	6	0	-4.326448	-0.833799	-0.317128
19	6	0	-4.761853	-2.985055	0.891718
20	6	0	-3.425705	-2.984890	-1.250784
21	1	0	4.477434	-1.975153	1.262848
22	1	0	2.945004	-1.100187	1.141105
23	1	0	3.014052	-2.669161	1.962689
24	1	0	4.875048	-1.936084	-1.225981
25	1	0	3.606443	-2.446996	-2.347278
26	1	0	3.435408	-0.946512	-1.414872
27	1	0	4.837584	-4.145414	-0.090987
28	1	0	3.362481	-4.820321	0.605989
29	1	0	3.560515	-4.742728	-1.157111
30	1	0	-5.264348	-0.963364	-0.868408
31	1	0	-4.544914	-0.240428	0.577918
32	1	0	-3.646910	-0.250684	-0.944258
33	1	0	-5.699741	-3.093088	0.336443
34	1	0	-4.420331	-3.993925	1.149844
35	1	0	-4.990539	-2.455892	1.824879
36	1	0	-4.342265	-3.103431	-1.839265
37	1	0	-2.701070	-2.448851	-1.871762
38	1	0	-3.030219	-3.986658	-1.051294
39	1	0	-1.391947	0.020754	0.001833
40	1	0	1.523690	-3.359464	-1.543911
41	1	0	-2.763727	-1.472969	1.822437
42	1	0	1.101301	-0.799082	-0.947878
43	6	0	2.393822	1.816049	-1.072444
44	8	0	2.252390	2.308036	0.189979
45	8	0	3.474809	1.730603	-1.652331
46	6	0	1.126146	1.392297	-1.666113
47	6	0	-2.293249	2.429979	-0.277625
48	6	0	-1.203609	1.468016	-0.465620
49	6	0	-0.085760	1.524975	-1.079302
50	1	0	1.202288	1.111609	-2.714926
51	6	0	3.356697	2.965413	0.897597
52	6	0	-2.784331	3.213722	-1.342674

53	6	0	-3.841533	4.104541	-1.151027
54	6	0	-4.432013	4.243862	0.109968
55	6	0	-3.954641	3.475641	1.176654
56	6	0	-2.907599	2.572272	0.982377
57	1	0	-2.326271	3.113610	-2.322505
58	1	0	-4.201855	4.697085	-1.988250
59	1	0	-5.252335	4.940458	0.258472
60	1	0	-4.401028	3.577395	2.162698
61	1	0	-2.541731	1.977542	1.815355
62	6	0	2.696823	3.413003	2.206620
63	6	0	3.844180	4.182008	0.099005
64	6	0	4.492715	1.973768	1.181750
65	1	0	3.426144	3.929501	2.839595
66	1	0	1.863866	4.092918	2.004490
67	1	0	2.307546	2.549862	2.755912
68	1	0	4.571756	4.744483	0.694916
69	1	0	4.316805	3.877553	-0.836148
70	1	0	3.004035	4.846463	-0.128518
71	1	0	5.248670	2.454645	1.813198
72	1	0	4.109135	1.101114	1.720928
73	1	0	4.964256	1.640510	0.256375

syn-cis-IM3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.187183	-0.789504	1.121359
2	6	0	-3.591556	0.656104	0.928200
3	7	0	-3.331001	-1.560145	0.228257
4	6	0	-2.169838	-0.810413	0.090284
5	7	0	-2.212977	0.436955	0.411528
6	6	0	-2.975365	-2.969236	0.294931
7	6	0	-1.680314	-2.988549	-0.567969
8	7	0	-1.147160	-1.637119	-0.307914
9	1	0	-5.241188	-0.875248	0.844428
10	1	0	-4.075352	-1.125650	2.165605
11	6	0	-4.440936	1.614114	0.033794
12	1	0	-3.755145	-3.609991	-0.124900
13	1	0	-2.776735	-3.289093	1.331408
14	6	0	-0.671113	-4.134144	-0.286179
15	6	0	-0.106328	-4.075662	1.146401
16	6	0	0.492886	-4.020044	-1.293847
17	6	0	-1.391818	-5.480154	-0.509399
18	6	0	-3.690196	2.955092	-0.091380
19	6	0	-5.800011	1.876611	0.716119
20	6	0	-4.668153	1.031432	-1.374217
21	1	0	0.652127	-4.855214	1.279356
22	1	0	0.358784	-3.106469	1.348534
23	1	0	-0.880528	-4.241414	1.903067
24	1	0	1.188377	-4.857910	-1.174111
25	1	0	0.127919	-4.036703	-2.327949
26	1	0	1.072250	-3.101830	-1.152061
27	1	0	-0.687553	-6.311331	-0.394819
28	1	0	-2.201576	-5.633641	0.212734
29	1	0	-1.819052	-5.544119	-1.517640
30	1	0	-4.274778	3.668442	-0.684347
31	1	0	-3.518021	3.403753	0.895217
32	1	0	-2.720231	2.816890	-0.575085
33	1	0	-6.377775	2.611483	0.143813

34	1	0	-6.411943	0.970650	0.791423
35	1	0	-5.665467	2.276898	1.728838
36	1	0	-5.236498	1.738457	-1.989946
37	1	0	-3.713884	0.840635	-1.875061
38	1	0	-5.229342	0.091110	-1.344808
39	1	0	-0.178829	1.579707	0.013937
40	1	0	-1.984467	-3.074989	-1.624376
41	1	0	-3.512256	1.144743	1.908105
42	1	0	-0.384741	-1.258365	-0.853024
43	6	0	3.275096	-0.703049	-1.078410
44	8	0	3.505747	-0.377037	0.205240
45	8	0	3.865219	-1.565425	-1.709729
46	6	0	2.193586	0.120191	-1.692146
47	6	0	1.088288	3.360115	-0.277479
48	6	0	0.760545	1.928579	-0.431549
49	6	0	1.487052	1.035159	-1.060195
50	1	0	2.038987	-0.081387	-2.751216
51	6	0	4.556706	-1.035734	1.009591
52	6	0	2.236781	3.939224	-0.848920
53	6	0	2.506923	5.295431	-0.677525
54	6	0	1.637655	6.101316	0.068701
55	6	0	0.495406	5.536250	0.641353
56	6	0	0.222623	4.177116	0.469612
57	1	0	2.914974	3.320659	-1.430285
58	1	0	3.397034	5.727262	-1.126914
59	1	0	1.850416	7.158411	0.200143
60	1	0	-0.185788	6.152509	1.221638
61	1	0	-0.666618	3.739382	0.913797
62	6	0	4.426003	-0.332329	2.363314
63	6	0	5.932101	-0.768988	0.387106
64	6	0	4.258224	-2.533200	1.143311
65	1	0	5.164251	-0.733595	3.065020
66	1	0	4.594096	0.743560	2.257714
67	1	0	3.427069	-0.484255	2.783111
68	1	0	6.712026	-1.146433	1.057329
69	1	0	6.034852	-1.262835	-0.580376
70	1	0	6.089036	0.306777	0.256834
71	1	0	4.964377	-2.979964	1.851697
72	1	0	3.246261	-2.687263	1.531817
73	1	0	4.352775	-3.046141	0.185007

S7 Energies of anti-cis- and syn-cis-TS2 with different R_1 group.

Species	B3LYP/6-31+G(d,p)				
	ZPE	E_{ZPE}	Gc[a]	SCF_{PCM}[b]	$SCF_{PCM}+G_c$
R_1 = Me					
anti-cis-Me-TS2	0.463770	−1131.950113	0.403348	−1132.437969	−1132.034621
syn-cis-Me-TS2	0.463832	−1131.948529	0.403800	−1132.436664	−1132.032864
R_1 =Et					
anti-cis-Et-TS2	0.520689	−1210.525501	0.455822	−1211.071314	−1210.615492
syn-cis-Et-TS2	0.520589	−1210.524109	0.456277	−1211.070065	−1210.613788
R_1 = *i*Pr					
*anti-cis-i*Pr-TS2	0.576711	−1289.100774	0.508546	−1289.703402	−1289.194856
*syn-cis-i*Pr-TS2	0.576900	−1289.098092	0.510560	−1289.701312	−1289.190752

a: Thermal correction to Gibbs Free Energy.
b: Total electronic energies in solvent.

S8: Cartesian coordinates and energies of anti-cis- and syn-cis-TS2 with different R_1 group.

anti-cis- Me-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.563307	3.913485	-1.113363
2	6	0	0.624103	2.932486	-1.324250
3	7	0	-1.183636	3.357532	0.089584
4	6	0	-0.902380	2.009982	0.116085
5	7	0	0.098706	1.694537	-0.711894
6	6	0	-2.560775	3.509000	0.563923
7	6	0	-2.723281	2.224076	1.444093
8	7	0	-1.710806	1.305510	0.873796
9	1	0	-1.257724	3.877178	-1.969752
10	1	0	-0.233467	4.944827	-0.966652
11	6	0	1.039314	2.734225	-2.777298
12	1	0	-3.267513	3.513108	-0.281164
13	1	0	-2.692756	4.429073	1.139881
14	6	0	-2.487956	2.470632	2.937373
15	1	0	0.671282	0.833036	-0.638497
16	1	0	1.488258	3.284908	-0.741763
17	1	0	-3.717631	1.787912	1.301140
18	6	0	2.188749	-1.070079	0.436156
19	8	0	3.430421	-1.443501	0.844981
20	8	0	2.007937	-0.326768	-0.545144
21	6	0	1.165557	-1.623653	1.293047
22	6	0	-2.406408	-2.163106	0.030309
23	6	0	-1.372465	-1.361680	0.686557
24	6	0	-0.145170	-1.564279	0.970038
25	1	0	1.494147	-2.124927	2.199094
26	6	0	4.657758	-1.013639	0.166453
27	6	0	5.753981	-1.688434	0.998908
28	6	0	4.804789	0.512786	0.231265
29	6	0	4.680161	-1.539081	-1.275070
30	6	0	-2.508352	-3.554645	0.242800
31	6	0	-3.517630	-4.302315	-0.364061
32	6	0	-4.449926	-3.685145	-1.206115
33	6	0	-4.362879	-2.307224	-1.427226
34	6	0	-3.361699	-1.555270	-0.809124
35	1	0	6.740414	-1.451730	0.586675
36	1	0	5.717546	-1.342911	2.036770
37	1	0	5.625440	-2.775078	0.993834
38	1	0	5.792232	0.800712	-0.146598
39	1	0	4.040530	1.009172	-0.368115
40	1	0	4.723478	0.858018	1.267497
41	1	0	5.652278	-1.319413	-1.730761
42	1	0	4.537902	-2.624731	-1.283949
43	1	0	3.894990	-1.078051	-1.875762
44	1	0	-1.786960	-4.039173	0.894365
45	1	0	-3.574429	-5.372798	-0.183049
46	1	0	-5.233471	-4.269501	-1.680280
47	1	0	-5.079590	-1.815027	-2.079956
48	1	0	-3.304434	-0.484261	-0.983657
49	1	0	-1.633610	0.111049	0.916912
50	1	0	1.410824	3.674742	-3.199182
51	1	0	0.194056	2.386722	-3.379906

52	1	0	1.838992	1.991160	-2.847664
53	1	0	-3.268846	3.120584	3.348675
54	1	0	-1.514296	2.942676	3.106117
55	1	0	-2.507460	1.523096	3.483648

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.226763	-1.100498	-0.402591
2	8	0	3.460667	-1.549824	-0.752174
3	8	0	2.042168	-0.321007	0.547462
4	6	0	1.209866	-1.630030	-1.286788
5	6	0	-2.378178	-2.106436	-0.067287
6	6	0	-1.329088	-1.319462	-0.718130
7	6	0	-0.102595	-1.540803	-0.990285
8	1	0	1.547073	-2.147351	-2.180279
9	6	0	4.683863	-1.182398	-0.030119
10	6	0	4.935854	0.327097	-0.135338
11	6	0	5.766002	-1.957710	-0.790144
12	6	0	4.605899	-1.658847	1.426257
13	6	0	-3.055036	-1.612038	1.066012
14	6	0	-4.073633	-2.348541	1.674249
15	6	0	-4.458126	-3.588983	1.155362
16	6	0	-3.803800	-4.086609	0.023148
17	6	0	-2.777158	-3.358399	-0.580132
18	1	0	5.920157	0.564160	0.283847
19	1	0	4.927502	0.641485	-1.184422
20	1	0	4.177455	0.891514	0.408021
21	1	0	6.748070	-1.772030	-0.342877
22	1	0	5.564318	-3.032553	-0.754437
23	1	0	5.796489	-1.648585	-1.839578
24	1	0	5.571356	-1.494800	1.918171
25	1	0	3.832151	-1.122453	1.977148
26	1	0	4.383758	-2.730416	1.462229
27	1	0	-2.761742	-0.651211	1.479802
28	1	0	-4.568950	-1.951182	2.556733
29	1	0	-5.254419	-4.159011	1.625548
30	1	0	-4.090005	-5.050558	-0.390158
31	1	0	-2.271586	-3.751150	-1.457488
32	6	0	-2.383742	3.612170	-0.956010
33	6	0	-2.850753	2.171345	-1.345414
34	7	0	-1.417767	3.320059	0.104262
35	6	0	-0.941018	2.049597	-0.141504
36	7	0	-1.689771	1.335042	-0.951402
37	6	0	-0.291461	4.134001	0.558728
38	6	0	0.621068	3.055472	1.209628
39	7	0	0.236767	1.846917	0.453283
40	1	0	-3.205739	4.237084	-0.596084
41	1	0	-1.893185	4.118476	-1.802619
42	6	0	-4.141916	1.738881	-0.643424
43	1	0	-0.600535	4.902755	1.271094
44	1	0	0.218443	4.617585	-0.292037
45	6	0	2.113230	3.354194	1.132397
46	1	0	0.759515	0.955057	0.485858
47	1	0	0.329762	2.929449	2.262868
48	1	0	-2.985699	2.097116	-2.429395
49	1	0	-1.592941	0.121313	-0.965561
50	1	0	-4.988149	2.338299	-0.998198

51	1	0	-4.058685	1.862507	0.441556
52	1	0	-4.356606	0.686511	-0.849173
53	1	0	2.344810	4.267223	1.691937
54	1	0	2.432485	3.487286	0.093785
55	1	0	2.691391	2.533979	1.566714

anti-cis-Et-TS2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.641485	-3.616025	-1.066219
2	6	0	-0.638992	-2.737471	-1.175346
3	7	0	1.335937	-2.974622	0.050367
4	6	0	0.945370	-1.655753	0.083240
5	7	0	-0.162435	-1.448204	-0.635065
6	6	0	2.763545	-2.999891	0.376585
7	6	0	2.912435	-1.677688	1.204372
8	7	0	1.765706	-0.865735	0.736133
9	1	0	1.238030	-3.553066	-1.992457
10	1	0	0.418172	-4.664973	-0.859149
11	6	0	-1.213602	-2.597275	-2.585839
12	1	0	3.374892	-2.975353	-0.539402
13	1	0	3.029650	-3.890284	0.952004
14	1	0	-0.790858	-0.631874	-0.522498
15	1	0	-1.414162	-3.147141	-0.509250
16	1	0	3.843858	-1.164519	0.937715
17	1	0	1.603820	0.326942	0.741362
18	6	0	-2.317298	1.223934	0.636037
19	8	0	-3.531990	1.533377	1.162456
20	8	0	-2.188019	0.445822	-0.325834
21	6	0	-1.251417	1.888068	1.351386
22	6	0	2.125746	2.583840	-0.314835
23	6	0	1.219331	1.757674	0.483409
24	6	0	0.018324	1.898031	0.890585
25	1	0	-1.516809	2.410752	2.265973
26	6	0	-4.790047	0.979990	0.649712
27	6	0	-5.836174	1.622979	1.567402
28	6	0	-4.811154	-0.546515	0.807061
29	6	0	-5.010886	1.417174	-0.804291
30	6	0	2.188588	3.984045	-0.150320
31	6	0	3.082678	4.755272	-0.893527
32	6	0	3.934277	4.153407	-1.826966
33	6	0	3.883953	2.767043	-2.002299
34	6	0	2.999586	1.992166	-1.249239
35	1	0	-6.841028	1.293032	1.283924
36	1	0	-5.658167	1.342371	2.610222
37	1	0	-5.793318	2.713826	1.493173
38	1	0	-5.810052	-0.925287	0.562843
39	1	0	-4.083984	-1.021682	0.147448
40	1	0	-4.586046	-0.824402	1.842289
41	1	0	-6.008549	1.105412	-1.133804
42	1	0	-4.951417	2.507586	-0.884628
43	1	0	-4.265170	0.976063	-1.467032
44	1	0	1.529707	4.456727	0.572301
45	1	0	3.111850	5.832116	-0.746957
46	1	0	4.627888	4.756000	-2.406637
47	1	0	4.538633	2.286341	-2.725007
48	1	0	2.970532	0.914987	-1.389309
49	6	0	-1.767689	-3.915653	-3.140487

50	6	0	2.875354	-1.880750	2.728319
51	6	0	4.152212	-2.514966	3.293168
52	1	0	-2.008985	-1.843624	-2.555213
53	1	0	-0.432638	-2.200425	-3.246454
54	1	0	-2.200613	-3.765402	-4.134201
55	1	0	-0.987090	-4.679595	-3.235365
56	1	0	-2.555107	-4.320727	-2.493997
57	1	0	2.718666	-0.897948	3.187431
58	1	0	1.997650	-2.487844	2.985191
59	1	0	4.084837	-2.620434	4.380586
60	1	0	4.336275	-3.513736	2.880243
61	1	0	5.031399	-1.897314	3.074191

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.322980	-1.407390	-0.477185
2	8	0	3.536916	-1.873829	-0.872114
3	8	0	2.189835	-0.575997	0.436413
4	6	0	1.260231	-1.987236	-1.271643
5	6	0	-2.264282	-2.381783	0.145217
6	6	0	-1.246232	-1.633492	-0.594726
7	6	0	-0.034891	-1.876488	-0.913864
8	1	0	1.549758	-2.552927	-2.152483
9	6	0	4.800382	-1.437845	-0.267533
10	6	0	5.018684	0.060488	-0.515407
11	6	0	5.840372	-2.262066	-1.034942
12	6	0	4.833149	-1.791713	1.225099
13	6	0	-2.907829	-1.815794	1.264424
14	6	0	-3.899328	-2.516093	1.954779
15	6	0	-4.289377	-3.791619	1.534568
16	6	0	-3.667462	-4.361488	0.418210
17	6	0	-2.667878	-3.669042	-0.266867
18	1	0	6.020725	0.347351	-0.177126
19	1	0	4.943789	0.283309	-1.585095
20	1	0	4.282063	0.659144	0.021510
21	1	0	6.847660	-2.027628	-0.675240
22	1	0	5.660768	-3.332383	-0.895414
23	1	0	5.792223	-2.042533	-2.106048
24	1	0	5.830743	-1.582704	1.627443
25	1	0	4.096400	-1.215269	1.785877
26	1	0	4.625838	-2.857584	1.365684
27	1	0	-2.610695	-0.826692	1.601753
28	1	0	-4.369299	-2.062745	2.824060
29	1	0	-5.064988	-4.333337	2.068507
30	1	0	-3.957991	-5.353542	0.081542
31	1	0	-2.187808	-4.117267	-1.131888
32	6	0	-2.303246	3.282281	-1.034787
33	6	0	-2.780231	1.826717	-1.355232
34	7	0	-1.307639	3.032600	0.008782
35	6	0	-0.839895	1.752653	-0.195494
36	7	0	-1.611679	1.005553	-0.952602
37	6	0	-0.171051	3.865531	0.397603
38	6	0	0.768574	2.813872	1.058669
39	7	0	0.352216	1.572488	0.376707
40	1	0	-3.111621	3.925060	-0.676662
41	1	0	-1.837113	3.754834	-1.913959
42	6	0	-4.062749	1.410580	-0.615294

43	1	0	-0.464735	4.659526	1.087757
44	1	0	0.310039	4.319428	-0.486177
45	6	0	2.263646	3.096671	0.907527
46	1	0	0.884566	0.687242	0.411491
47	1	0	0.524953	2.738589	2.129623
48	1	0	-2.939340	1.709554	-2.433325
49	1	0	-1.517713	-0.211099	-0.908126
50	6	0	2.709898	4.356013	1.661018
51	6	0	-5.328543	2.071341	-1.174842
52	1	0	-4.156040	0.321513	-0.687618
53	1	0	-3.950609	1.641505	0.452008
54	1	0	2.814966	2.226190	1.280139
55	1	0	2.501250	3.184361	-0.160087
56	1	0	3.790170	4.501411	1.564568
57	1	0	2.222186	5.258546	1.274585
58	1	0	2.479609	4.282967	2.730472
59	1	0	-6.215192	1.732550	-0.629796
60	1	0	-5.295186	3.164477	-1.096559
61	1	0	-5.473191	1.817693	-2.231809

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.908329	-3.319652	1.227368
2	6	0	0.469068	-2.589686	1.246290
3	7	0	-1.558186	-2.673254	0.086826
4	6	0	-1.011545	-1.422752	-0.063692
5	7	0	0.136826	-1.300726	0.607241
6	6	0	-2.985085	-2.561975	-0.217658
7	6	0	-3.025615	-1.256767	-1.091156
8	7	0	-1.745452	-0.587715	-0.764455
9	1	0	-1.476360	-3.143348	2.154214
10	1	0	-0.803597	-4.396745	1.078496
11	6	0	1.148844	-2.420479	2.620404
12	1	0	-3.574895	-2.445905	0.704828
13	1	0	-3.350495	-3.443072	-0.751683
14	1	0	0.845174	-0.564382	0.437469
15	1	0	1.163152	-3.143370	0.595707
16	1	0	-3.847748	-0.614325	-0.753645
17	1	0	-1.486044	0.589000	-0.767934
18	6	0	2.492408	1.136319	-0.790624
19	8	0	3.709422	1.330488	-1.363867
20	8	0	2.328349	0.378600	0.182009
21	6	0	1.464895	1.891490	-1.471778
22	6	0	-1.769247	2.894309	0.306835
23	6	0	-0.976932	1.981621	-0.519454
24	6	0	0.218431	2.014772	-0.966605
25	1	0	1.742378	2.384315	-2.399348
26	6	0	4.928752	0.660551	-0.897912
27	6	0	5.994081	1.199743	-1.859300
28	6	0	4.797036	-0.861116	-1.048021
29	6	0	5.247450	1.077137	0.543996
30	6	0	-1.630232	4.295061	0.204464
31	6	0	-2.413240	5.153604	0.976170
32	6	0	-3.352808	4.640076	1.877735
33	6	0	-3.503261	3.254753	1.991767
34	6	0	-2.729414	2.394888	1.209581
35	1	0	6.974064	0.778737	-1.611750

36	1	0	5.750948	0.933318	-2.892606
37	1	0	6.055752	2.290083	-1.791196
38	1	0	5.763495	-1.334104	-0.840731
39	1	0	4.053657	-1.263219	-0.358559
40	1	0	4.505686	-1.117174	-2.072237
41	1	0	6.222501	0.671060	0.835979
42	1	0	5.296288	2.168349	0.620654
43	1	0	4.489037	0.711043	1.237234
44	1	0	-0.902584	4.699413	-0.493211
45	1	0	-2.287301	6.228874	0.877000
46	1	0	-3.960098	5.310326	2.479574
47	1	0	-4.228997	2.841930	2.688050
48	1	0	-2.856804	1.319617	1.301658
49	6	0	1.533537	-3.793150	3.196325
50	6	0	-3.203242	-1.470573	-2.613604
51	6	0	-4.627837	-1.947983	-2.938221
52	1	0	2.076579	-1.868220	2.417683
53	1	0	2.113985	-3.675319	4.116992
54	1	0	0.645069	-4.387323	3.444255
55	1	0	2.141029	-4.372610	2.491267
56	1	0	-3.076823	-0.472357	-3.055143
57	1	0	-4.780699	-1.995903	-4.021434
58	1	0	-4.821846	-2.951431	-2.539042
59	1	0	-5.384034	-1.270062	-2.525111
60	6	0	-2.140802	-2.389179	-3.233604
61	1	0	-1.130151	-2.030408	-3.017994
62	1	0	-2.225060	-3.417721	-2.862858
63	1	0	-2.258275	-2.422889	-4.322082
64	6	0	0.331362	-1.592932	3.623324
65	1	0	0.044939	-0.624219	3.204330
66	1	0	-0.580926	-2.113848	3.938233
67	1	0	0.924887	-1.407424	4.524740

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Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.326652	1.564832	-0.416494
2	8	0	-3.536565	2.071060	-0.773500
3	8	0	-2.177543	0.795900	0.547374
4	6	0	-1.285088	2.021436	-1.314783
5	6	0	2.264965	2.571569	-0.051108
6	6	0	1.238669	1.728807	-0.669962
7	6	0	0.019291	1.933783	-0.986495
8	1	0	-1.597893	2.502824	-2.236995
9	6	0	-4.769311	1.820122	-0.018200
10	6	0	-5.129760	0.329829	-0.057934
11	6	0	-5.807767	2.640263	-0.791903
12	6	0	-4.630639	2.344993	1.416570
13	6	0	2.921255	2.166472	1.128515
14	6	0	3.919351	2.955537	1.704126
15	6	0	4.303095	4.160367	1.106782
16	6	0	3.668532	4.569560	-0.071196
17	6	0	2.662608	3.788763	-0.642698
18	1	0	-6.124966	0.180777	0.375948
19	1	0	-5.152175	-0.027641	-1.092801
20	1	0	-4.408663	-0.262855	0.505730
21	1	0	-6.792215	2.541735	-0.322762
22	1	0	-5.530666	3.698699	-0.802062

23	1	0	-5.878708	2.293799	-1.827686
24	1	0	-5.595479	2.264689	1.929810
25	1	0	-3.884808	1.777670	1.975094
26	1	0	-4.336442	3.399571	1.407109
27	1	0	2.626587	1.235451	1.603927
28	1	0	4.398403	2.627657	2.623385
29	1	0	5.083380	4.771079	1.552099
30	1	0	3.954085	5.505206	-0.545520
31	1	0	2.172666	4.112782	-1.556275
32	6	0	2.238019	-3.233133	-0.912627
33	6	0	2.790243	-1.783404	-1.140304
34	7	0	1.158892	-2.991307	0.044730
35	6	0	0.773874	-1.679135	-0.108949
36	7	0	1.650772	-0.927754	-0.732646
37	6	0	-0.036880	-3.794464	0.289386
38	6	0	-0.998771	-2.735475	0.910498
39	7	0	-0.459677	-1.475173	0.361136
40	1	0	2.987911	-3.919178	-0.510264
41	1	0	1.841948	-3.658685	-1.847994
42	6	0	4.099332	-1.437526	-0.389566
43	1	0	0.162444	-4.620411	0.976083
44	1	0	-0.433636	-4.205665	-0.651988
45	6	0	-2.503095	-2.927539	0.630189
46	1	0	-0.934409	-0.562599	0.446671
47	1	0	-0.859422	-2.736978	2.001825
48	1	0	2.974114	-1.623852	-2.208938
49	1	0	1.531108	0.284691	-0.803675
50	6	0	-3.011124	-4.207014	1.315144
51	6	0	5.301770	-2.138744	-1.042430
52	1	0	4.230951	-0.355312	-0.523240
53	1	0	-2.999036	-2.072173	1.107773
54	1	0	-4.098205	-4.290229	1.215708
55	1	0	-2.572931	-5.106069	0.864023
56	1	0	-2.772945	-4.215639	2.385189
57	1	0	6.236834	-1.816237	-0.572767
58	1	0	5.244360	-3.229582	-0.935940
59	1	0	5.370287	-1.908650	-2.112108
60	6	0	-2.870174	-2.899839	-0.860776
61	1	0	-2.494419	-1.997552	-1.351399
62	1	0	-2.475705	-3.770976	-1.397105
63	1	0	-3.958877	-2.915338	-0.976157
64	6	0	4.041965	-1.714776	1.119739
65	1	0	3.187788	-1.217868	1.588537
66	1	0	3.969054	-2.787531	1.334319
67	1	0	4.950385	-1.343367	1.605769

S9: Reference 14 details.

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