Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Mechanism of *N*-Heterocyclic Carbenes-Catalyzed Chemical Fixation of CO_2 with Aziridines：A Theoretical Study

Weiyi Li*[a], Dongfeng Huang*[b] and Yajing Lv[a]

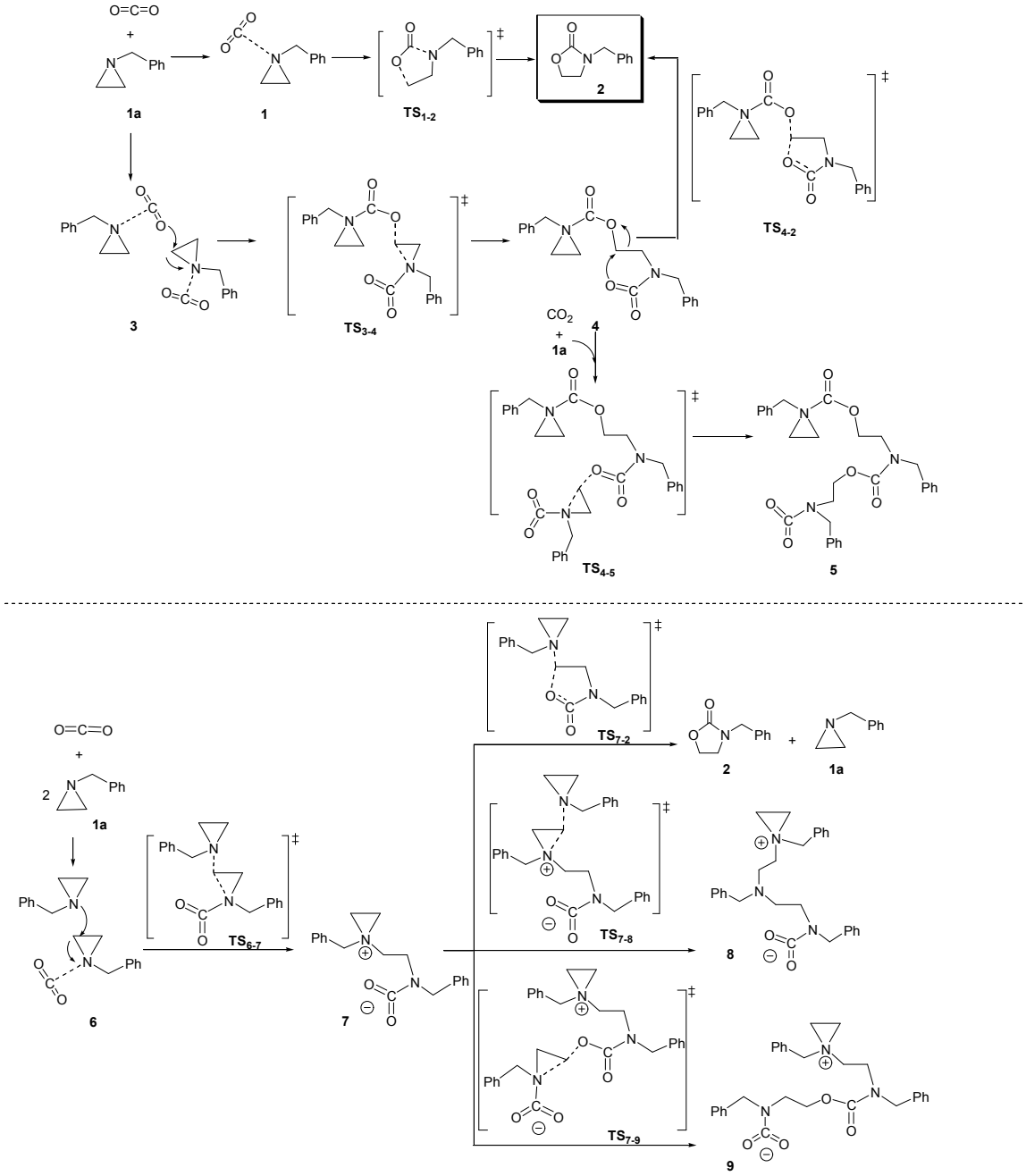
[a] *Research Center for Advanced Computation, School of Physics and Chemistry, Xihua University, Chengdu, Sichuan, 610039, P. R. China.*

E-mail: weiyili@mail.xhu.edu.cn ;Fax:+86-028-87648043; Tel: +86-028-87648043

[b]*College of Chemistry and Chemical Engineering, Anyang Normal University, Anyang, Henan 455000, P. R. China*

CONTENTS:

S1: The mechanism of background reaction.



Scheme S1. Proposed mechanism for cycloaddition of **1a** and CO_2 without NHC-CO_2 adduct.

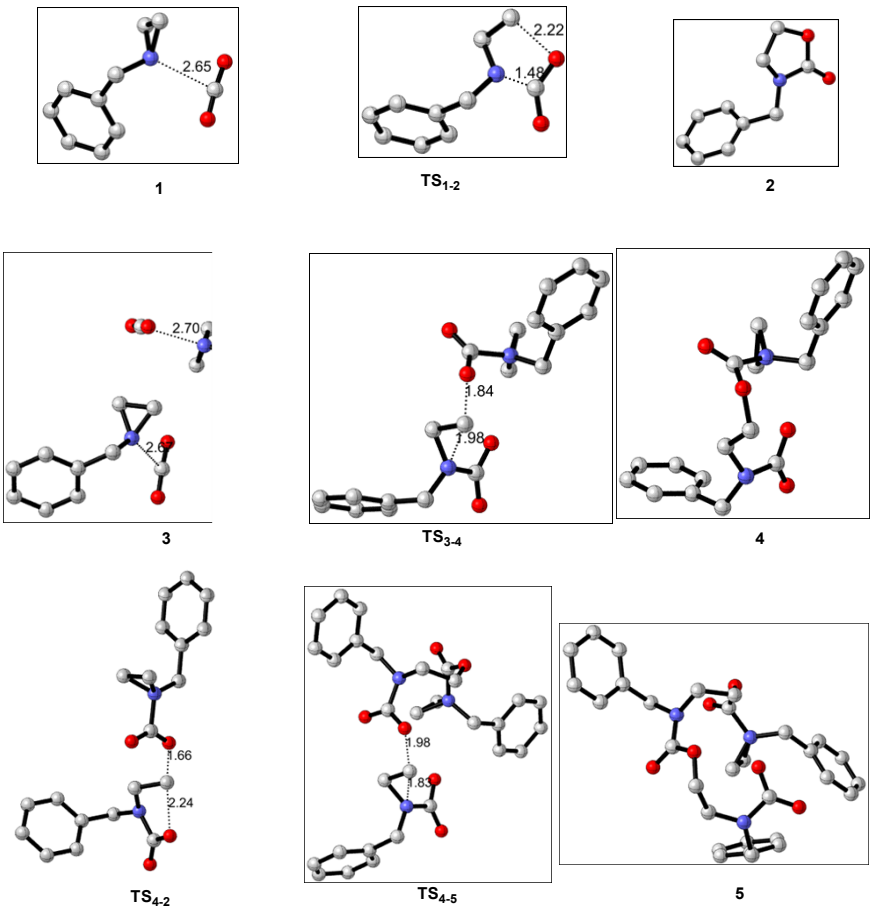


Figure S1. Optimized structures of the species along the unfavorable reaction pathways in the absence of NHC-CO_2 adduct.

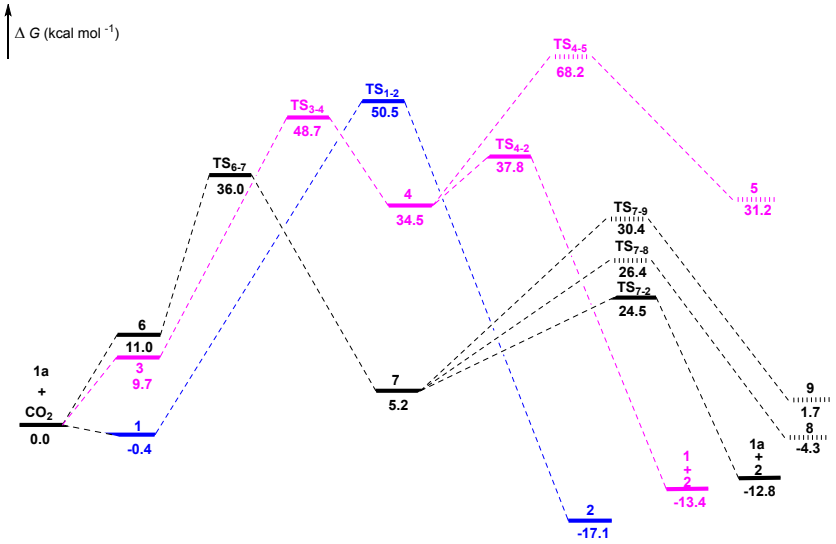
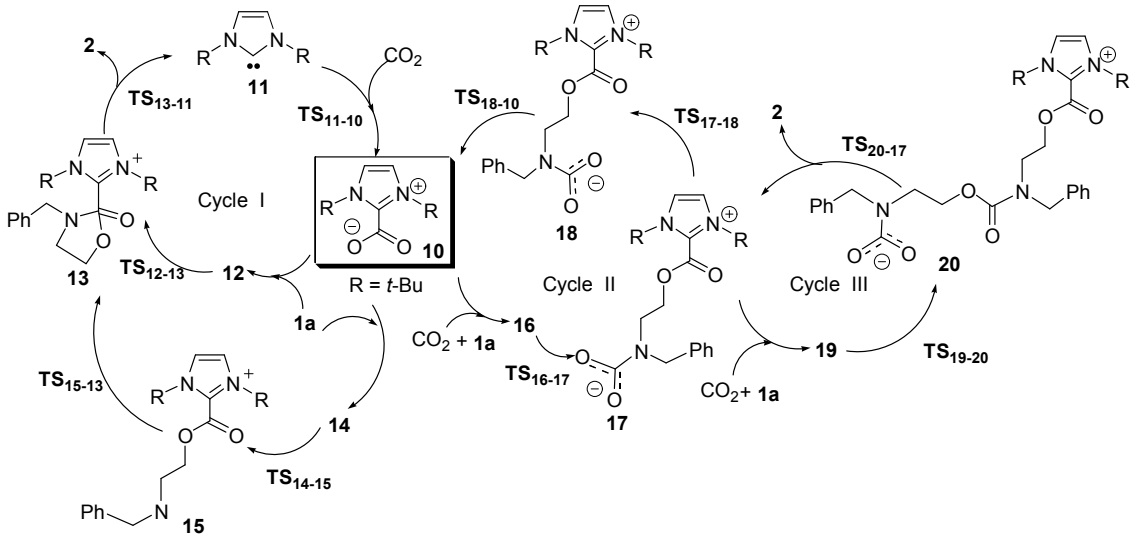


Figure S2. Potential energy profile for cycloaddition of **2a** and **CO_2** without NHC-CO_2 adduct.

S2 The reaction mechanism catalyzed by NHC-CO_2 adduct or free NHC.



Scheme S2. Proposed mechanism for cycloaddition of **1a** and **CO_2** catalyzed by NHC-CO_2 adduct.

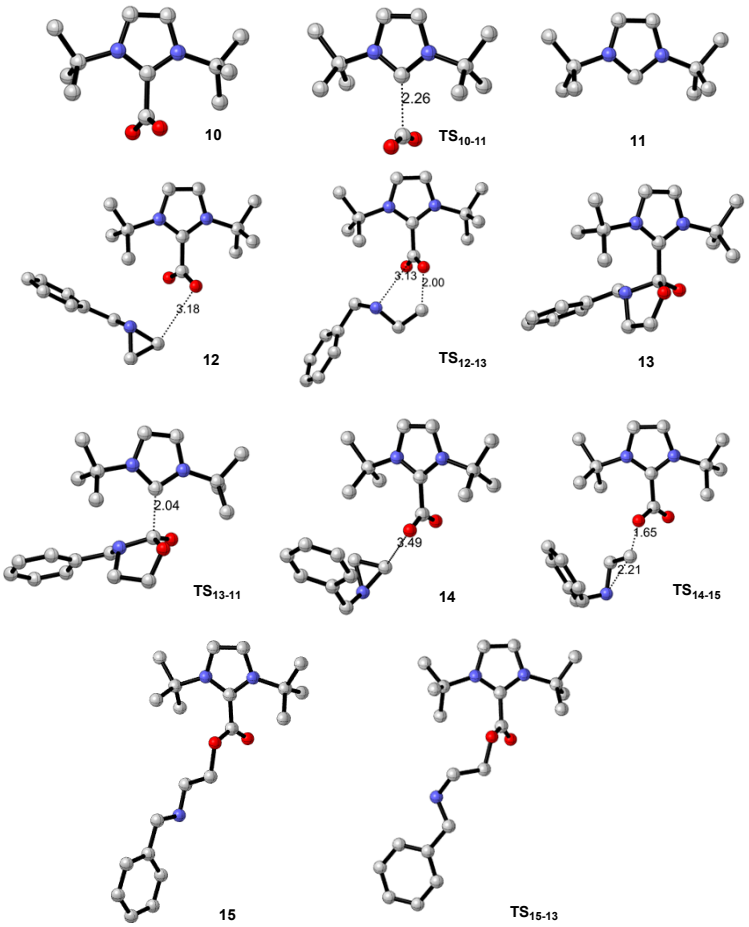


Figure S3. Optimized structures of the species along the unfavorable reaction pathways catalyzed by NHC-CO_2 adduct.

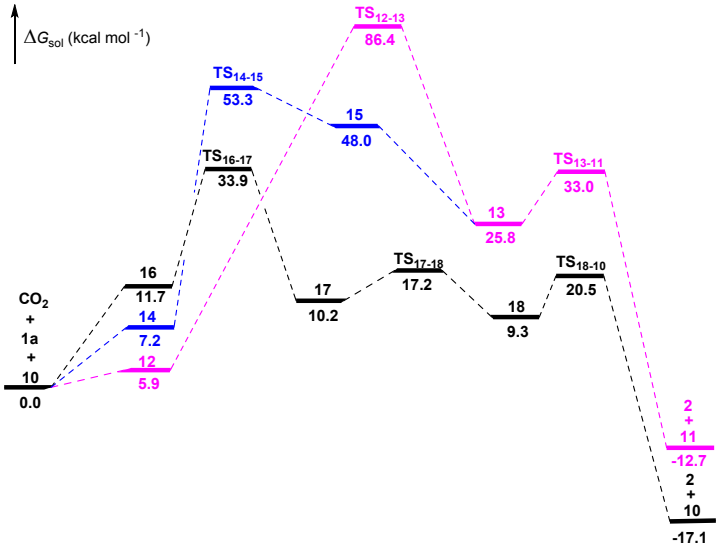


Figure S4. Potential energy profile for cycloaddition of **1a** and CO_2 without NHC-CO2 adduct.

S3: Comparison of the geometrics and energies of the key transition states and intermediates at the M06-2X/6-31G and M06-2X /6-311++G** levels.**

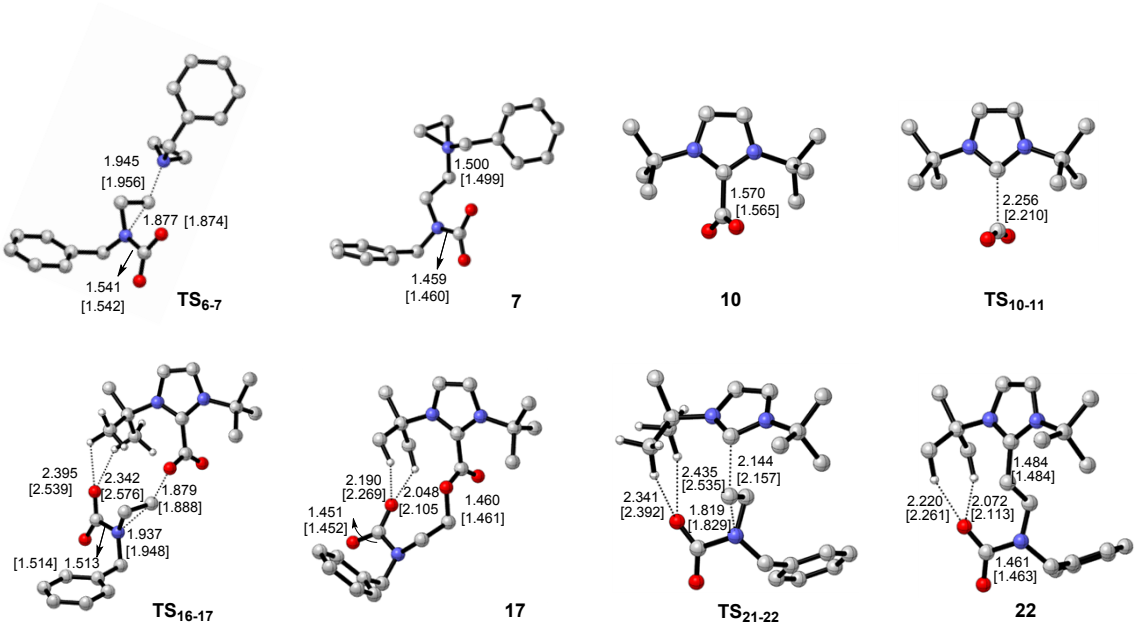


Figure S5. Geometric structures of key transition states and intermediates optimized at M06-2X/6-31G** and M06-2X/6-311++G** (bond length in square brackets) level, respectively.

Table S1 The relative Gibbs free energy of the key transition states and intermediates calculated at M06-2X/6-31G** and M06-2X/6-311++G**, respectively.

Species	M06-2X/6-31G**		M06-2X/6-311G++**	
	G_{gas}[a]	ΔG_{gas}	G_{gas}	ΔG_{gas}
TS_{6-7}	−996.63077	48.3	−996.635056	46.3
7	−996.67086	23.3	−996.673758	22.0
TS_{10-11}	−728.89068	7.0	−728.892535	7.5
TS_{16-17}	−1321.47524	44.8	-1321.4812	42.9
17	−1321.50460	26.4	−1321.512963	25.9
TS_{21-22}	−1132.90172	43.9	−1132.905514	43.0
22	−1132.97467	−1.9	−1132.977866	−2.4

a: G_{gas} is obtained by the combination of the Gibbs free energy corrections calculated at M06-2X /6-1G** level and the single point energy calculated at M06-2X /6-311++G** level.

S4: Cartesian coordinates of optimized structures.

CO_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000015	-0.000355	-0.000628
2	8	0	-1.096881	0.334458	-0.191886
3	8	0	1.096893	-0.334192	0.192357

1a

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.080805	0.813349	-0.520856
2	6	0	0.338928	0.362949	-0.257640
3	6	0	0.706823	-0.976755	-0.386029
4	6	0	2.024092	-1.368548	-0.161163
5	6	0	2.987573	-0.427614	0.189891
6	6	0	2.626350	0.911402	0.319496
7	6	0	1.309096	1.300615	0.100696
8	1	0	-0.051642	-1.702814	-0.659649
9	1	0	2.298519	-2.414210	-0.260973
10	1	0	4.013525	-0.735155	0.365403
11	1	0	3.370012	1.651597	0.597897
12	1	0	1.027689	2.345321	0.211816
13	7	0	-2.027670	-0.284168	-0.399323
14	6	0	-2.464721	-0.562992	0.956048
15	6	0	-3.375273	0.091387	-0.021254
16	1	0	-2.059375	0.060531	1.751492
17	1	0	-2.590860	-1.610962	1.208554
18	1	0	-3.582622	1.149756	0.129739
19	1	0	-4.173935	-0.472966	-0.491864
20	1	0	-1.162600	1.212300	-1.539633
21	1	0	-1.327399	1.643015	0.167342

1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.095322	-1.059598	-1.084550
2	6	0	-1.145154	-0.400880	-0.534184
3	6	0	-1.230184	0.992723	-0.474817
4	6	0	-2.359829	1.605591	0.054829
5	6	0	-3.417801	0.833109	0.532865
6	6	0	-3.338668	-0.554113	0.480812
7	6	0	-2.204523	-1.166140	-0.049479
8	1	0	-0.400640	1.589694	-0.843319
9	1	0	-2.418234	2.688906	0.093485
10	1	0	-4.300221	1.313256	0.943754
11	1	0	-4.158155	-1.161104	0.852498
12	1	0	-2.143433	-2.251094	-0.091738

13	7	0	1.246254	-0.794167	-0.220842
14	6	0	1.338662	-1.633903	0.959611
15	6	0	2.262205	-1.833881	-0.186762
16	1	0	0.554463	-2.374376	1.107484
17	1	0	1.693737	-1.138926	1.857653
18	1	0	2.102118	-2.710043	-0.812050
19	1	0	3.288945	-1.488191	-0.119035
20	1	0	0.333670	-0.662689	-2.077648
21	1	0	-0.082064	-2.143489	-1.191894
22	6	0	2.560108	1.480456	0.160381
23	8	0	2.009936	2.090406	-0.663869
24	8	0	3.170715	0.949223	0.998177

TS_{1-2}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.221833	0.847574	0.090447
2	8	0	-1.884052	1.876135	0.652076
3	8	0	-3.197650	0.515133	-0.625317
4	6	0	-2.598472	-1.623938	-0.512301
5	1	0	-3.474541	-1.522717	-1.134004
6	1	0	-2.681617	-2.232374	0.382460
7	6	0	-0.265314	-0.340651	1.258423
8	6	0	1.080850	-0.121210	0.612547
9	6	0	2.078768	-1.093153	0.654174
10	6	0	3.524622	0.316222	-0.662364
11	6	0	3.301201	-0.874524	0.020663
12	6	0	1.308266	1.074492	-0.078204
13	6	0	2.526221	1.289861	-0.711129
14	1	0	1.903628	-2.021761	1.192880
15	1	0	4.075553	-1.633973	0.060807
16	1	0	4.475628	0.488289	-1.156283
17	1	0	2.701279	2.220443	-1.241463
18	1	0	0.517932	1.822029	-0.099905
19	7	0	-1.337556	-0.331777	0.268730
20	6	0	-1.249995	-1.216622	-0.886659
21	1	0	-1.143787	-0.706481	-1.842993
22	1	0	-0.463100	-1.956660	-0.727481
23	1	0	-0.515508	0.473767	1.943316
24	1	0	-0.284839	-1.286557	1.813899

2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.140259	-1.143000	0.308242
2	6	0	2.415222	-0.548437	-0.397007
3	8	0	2.667881	-1.552973	-1.005737
4	8	0	3.323786	0.433147	-0.142635
5	6	0	1.372461	0.939521	1.050686
6	6	0	2.667992	1.533811	0.488892
7	7	0	1.204952	-0.178057	0.147236
8	1	0	2.460195	2.299396	-0.265507
9	1	0	3.330448	1.941633	1.252363

10	1	0	0.529192	1.632869	0.995052
11	1	0	1.483843	0.599168	2.090648
12	1	0	0.182522	-1.600266	1.308267
13	1	0	0.334173	-1.933420	-0.424010
14	6	0	-1.222208	-0.521479	0.091334
15	6	0	-2.299356	-0.876055	0.901699
16	6	0	-1.420726	0.403043	-0.936233
17	6	0	-3.560506	-0.326055	0.684341
18	1	0	-2.150038	-1.588568	1.709182
19	6	0	-2.677412	0.958254	-1.151153
20	1	0	-0.577823	0.685647	-1.561253
21	6	0	-3.751885	0.593205	-0.342204
22	1	0	-4.390984	-0.612099	1.321960
23	1	0	-2.820138	1.676870	-1.952124
24	1	0	-4.732429	1.026926	-0.509828

3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.379619	0.599048	0.767321
2	6	0	2.927176	1.200342	1.972566
3	6	0	1.149429	-1.686982	1.492020
4	8	0	0.898851	-1.169121	2.504691
5	8	0	1.354044	-2.289298	0.516955
6	6	0	1.620429	1.650128	1.431039
7	6	0	3.051395	0.997593	-0.470819
8	1	0	2.363006	0.789811	-1.299356
9	1	0	2.955473	0.556961	2.845882
10	1	0	3.780925	1.864616	1.851466
11	1	0	1.580122	2.623315	0.945824
12	1	0	0.697564	1.332665	1.905879
13	1	0	3.261621	2.080636	-0.481291
14	6	0	4.342527	0.238786	-0.654990
15	6	0	5.558851	0.912675	-0.750068
16	6	0	6.750877	0.208249	-0.908912
17	6	0	6.733197	-1.180799	-0.967175
18	6	0	5.520760	-1.862165	-0.865989
19	6	0	4.332749	-1.157529	-0.711217
20	1	0	5.573326	1.998898	-0.702563
21	1	0	7.690830	0.745978	-0.983897
22	1	0	7.659620	-1.732796	-1.090371
23	1	0	5.503105	-2.946730	-0.908920
24	1	0	3.386743	-1.684062	-0.625245
25	6	0	-0.640919	-0.043838	-0.546689
26	6	0	-1.506108	-0.354901	0.623739
27	1	0	-0.291829	-0.882467	-1.145865
28	1	0	0.024844	0.812876	-0.505535
29	1	0	-1.752867	-1.401055	0.802821
30	7	0	-2.062347	0.259927	-0.568438
31	1	0	-1.472944	0.274469	1.507699
32	6	0	-2.887320	-0.625175	-1.392396
33	1	0	-2.433335	-1.626868	-1.478689
34	1	0	-2.926036	-0.192080	-2.398246
35	6	0	-4.275030	-0.751480	-0.814066
36	6	0	-4.756101	-1.983235	-0.373890
37	6	0	-5.085761	0.379914	-0.687364
38	6	0	-6.031472	-2.091611	0.177915
39	1	0	-4.128809	-2.866478	-0.467212

40	6	0	-6.356827	0.274693	-0.134734
41	1	0	-4.707072	1.342328	-1.019582
42	6	0	-6.833417	-0.962197	0.298566
43	1	0	-6.395316	-3.057371	0.514140
44	1	0	-6.979537	1.158881	-0.040870
45	1	0	-7.826369	-1.042816	0.729413
46	6	0	-2.162309	2.896589	-0.179762
47	8	0	-1.298077	2.776966	0.593460
48	8	0	-3.016906	3.116966	-0.936897

$TS_{3\text{-}4}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.109557	0.537683	0.766920
2	6	0	2.640334	1.173805	1.986368
3	6	0	1.460765	-0.881330	0.939181
4	8	0	1.375764	-1.250552	2.077062
5	8	0	1.110026	-1.365691	-0.174936
6	6	0	1.359801	1.644753	1.427157
7	6	0	2.837235	0.803249	-0.508633
8	1	0	2.205234	0.433115	-1.314618
9	1	0	2.620655	0.515210	2.845972
10	1	0	3.548243	1.741496	1.815238
11	1	0	1.276447	2.546926	0.833569
12	1	0	0.428048	1.331902	1.880336
13	1	0	2.931398	1.888201	-0.601092
14	6	0	4.185456	0.132261	-0.503585
15	6	0	5.338523	0.879578	-0.257910
16	6	0	6.584754	0.260557	-0.220474
17	6	0	6.682858	-1.112168	-0.426997
18	6	0	5.536097	-1.862302	-0.678703
19	6	0	4.290649	-1.244797	-0.720527
20	1	0	5.263557	1.954779	-0.111037
21	1	0	7.476306	0.850103	-0.034427
22	1	0	7.653420	-1.596533	-0.398937
23	1	0	5.611990	-2.931119	-0.848578
24	1	0	3.394433	-1.825006	-0.920566
25	6	0	-0.329981	-0.476852	-0.888767
26	6	0	-1.462291	-0.496340	0.050281
27	1	0	-0.395947	-1.114659	-1.761707
28	1	0	0.145033	0.490325	-0.986184
29	1	0	-1.973570	-1.454807	0.141596
30	7	0	-2.108622	0.395308	-0.895648
31	1	0	-1.289623	-0.035043	1.022300
32	6	0	-3.286970	-0.088208	-1.607085
33	1	0	-3.019100	-0.979256	-2.189498
34	1	0	-3.561146	0.713598	-2.294761
35	6	0	-4.432366	-0.412671	-0.674252
36	6	0	-4.889059	-1.721008	-0.523273
37	6	0	-5.021385	0.609673	0.078402
38	6	0	-5.924967	-2.014298	0.362409
39	1	0	-4.433943	-2.517339	-1.108742
40	6	0	-6.052596	0.316338	0.963088
41	1	0	-4.656607	1.625851	-0.050373
42	6	0	-6.506715	-0.994786	1.107796
43	1	0	-6.273168	-3.037004	0.469497
44	1	0	-6.508722	1.113560	1.542014
45	1	0	-7.312658	-1.219069	1.799628

46	6	0	-1.927836	1.869984	-0.667012
47	8	0	-0.922947	2.122311	0.032669
48	8	0	-2.766678	2.576583	-1.216460

4

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.056110	-1.098474	0.875562
2	8	0	-0.913435	-2.275311	0.999297
3	8	0	-1.007945	-0.199934	1.830465
4	7	0	-1.432043	-0.577550	-0.481022
5	6	0	-1.704541	-1.617159	-1.511620
6	6	0	-0.439519	-0.866509	-1.561480
7	6	0	-2.266588	0.671983	-0.564932
8	1	0	-1.835167	1.388936	0.125320
9	1	0	-1.708158	-2.624405	-1.114580
10	1	0	-2.524049	-1.340638	-2.165412
11	1	0	-0.278135	-0.009556	-2.204019
12	1	0	0.461414	-1.346865	-1.195461
13	1	0	-2.096445	1.075929	-1.563706
14	6	0	-3.711006	0.348670	-0.295890
15	6	0	-4.621894	0.269191	-1.351180
16	6	0	-5.954557	-0.055497	-1.111708
17	6	0	-6.384400	-0.305444	0.188173
18	6	0	-5.483409	-0.220473	1.247289
19	6	0	-4.153429	0.109354	1.008852
20	1	0	-4.289728	0.481800	-2.364920
21	1	0	-6.655677	-0.108997	-1.937972
22	1	0	-7.422376	-0.558307	0.377628
23	1	0	-5.819062	-0.403364	2.262615
24	1	0	-3.454629	0.190566	1.836757
25	6	0	-0.007952	0.884167	1.872354
26	6	0	1.351315	0.439123	1.333144
27	1	0	0.022247	1.130502	2.933391
28	1	0	-0.364987	1.728030	1.289640
29	1	0	1.971823	0.059616	2.151145
30	7	0	2.015602	1.554935	0.709343
31	1	0	1.214202	-0.408906	0.638725
32	6	0	3.466701	1.575208	0.852513
33	1	0	3.721319	1.674687	1.915198
34	1	0	3.808442	2.465161	0.323193
35	6	0	4.129323	0.332881	0.286984
36	6	0	4.697990	-0.627700	1.123466
37	6	0	4.119801	0.105064	-1.095777
38	6	0	5.252652	-1.795217	0.600474
39	1	0	4.711292	-0.456598	2.198133
40	6	0	4.671340	-1.059998	-1.617810
41	1	0	3.678419	0.860483	-1.740748
42	6	0	5.238730	-2.014148	-0.772682
43	1	0	5.695376	-2.530904	1.265205
44	1	0	4.669303	-1.222478	-2.691826
45	1	0	5.673513	-2.919652	-1.184847
46	6	0	1.490097	1.963451	-0.587826
47	8	0	0.314911	1.544680	-0.816270
48	8	0	2.222580	2.655868	-1.295884

TS_{4-2}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.987728	-0.460052	1.138584
2	8	0	0.440831	0.022125	2.089063
3	8	0	0.661617	-1.297875	0.248968
4	7	0	2.437557	0.016816	0.875368
5	6	0	3.178447	0.384842	2.104194
6	6	0	2.661596	1.441972	1.217394
7	1	0	3.352917	1.948827	0.554492
8	1	0	1.751942	1.954192	1.507808
9	1	0	4.234727	0.146425	2.069176
10	1	0	2.625738	0.163362	3.009208
11	6	0	-1.755239	-0.714617	-0.116675
12	1	0	-1.135228	-0.010558	-0.690459
13	1	0	-2.140723	-0.176153	0.763832
14	6	0	-3.530857	-0.216098	-1.735113
15	6	0	-4.156170	0.867347	-0.876023
16	6	0	-5.154954	0.529463	0.045516
17	6	0	-5.285656	2.832357	0.771401
18	6	0	-5.712945	1.507282	0.861396
19	6	0	-3.730391	2.192653	-0.954411
20	6	0	-4.292284	3.174757	-0.139357
21	1	0	-5.477846	-0.507591	0.098187
22	1	0	-6.490380	1.236693	1.569818
23	1	0	-5.727333	3.592659	1.408635
24	1	0	-3.954264	4.204276	-0.216651
25	1	0	-2.953094	2.458930	-1.668686
26	7	0	-2.791891	-1.212959	-0.984854
27	6	0	-0.890323	-1.874012	0.344805
28	1	0	-0.932946	-2.162639	1.385684
29	1	0	-2.866484	0.249494	-2.477281
30	1	0	-4.310908	-0.770863	-2.261014
31	6	0	-3.545734	-2.302997	-0.381895
32	8	0	-4.674835	-2.529341	-0.825173
33	8	0	-2.888514	-2.879445	0.529807
34	1	0	-0.779989	-2.686697	-0.359237
35	6	0	3.134179	-0.621415	-0.298857
36	6	0	4.536340	-0.129435	-0.521052
37	1	0	2.492060	-0.419334	-1.157037
38	1	0	3.104948	-1.693853	-0.101354
39	6	0	5.617535	-0.771162	0.090376
40	6	0	6.916070	-0.318530	-0.121286
41	6	0	7.143969	0.774732	-0.953529
42	6	0	6.074524	1.409411	-1.580706
43	6	0	4.776289	0.956327	-1.368202
44	1	0	5.440536	-1.639701	0.720890
45	1	0	7.748990	-0.825294	0.354068
46	1	0	8.156662	1.124751	-1.123448
47	1	0	6.252151	2.248890	-2.244311
48	1	0	3.943326	1.436510	-1.876607

TS_{4-5}

Standard orientation:

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

1	6	0	-2.428775	2.057254	-0.417105
2	8	0	-3.096552	2.082803	-1.403964
3	8	0	-2.875134	2.135231	0.823875
4	7	0	-0.939194	2.134758	-0.553952
5	6	0	-0.464388	2.398175	-1.948110
6	6	0	-0.329279	1.043543	-1.408487
7	6	0	-0.112475	2.735786	0.568939
8	1	0	-0.728506	2.689744	1.463188
9	1	0	-1.273694	2.623176	-2.630578
10	1	0	0.408570	3.040119	-1.965116
11	1	0	0.647892	0.747364	-1.029751
12	1	0	-1.035038	0.270311	-1.687976
13	1	0	0.772340	2.103271	0.671191
14	6	0	0.298044	4.150035	0.270774
15	6	0	1.630469	4.408779	-0.059640
16	6	0	2.025288	5.713278	-0.350140
17	6	0	1.095822	6.749088	-0.316767
18	6	0	-0.234126	6.488758	0.011933
19	6	0	-0.632759	5.190367	0.309607
20	1	0	2.337604	3.579667	-0.088484
21	1	0	3.060481	5.918415	-0.602115
22	1	0	1.406643	7.763737	-0.544204
23	1	0	-0.956087	7.298255	0.042361
24	1	0	-1.665938	4.982451	0.581471
25	6	0	-2.623578	1.070216	1.787547
26	6	0	-3.251927	-0.222468	1.307753
27	1	0	-3.077216	1.443610	2.705881
28	1	0	-1.552524	0.914887	1.925020
29	1	0	-3.164138	-0.964666	2.109151
30	7	0	-2.597266	-0.660791	0.086018
31	1	0	-4.313566	-0.058175	1.100991
32	6	0	-3.474902	-1.097930	-1.001160
33	1	0	-2.822530	-1.371825	-1.832689
34	6	0	-1.334761	-1.320395	0.224881
35	8	0	-0.852689	-1.874424	-0.769273
36	8	0	-0.807510	-1.185623	1.381387
37	1	0	-4.092536	-0.246290	-1.309012
38	6	0	-4.354255	-2.269426	-0.620599
39	6	0	-3.775729	-3.512003	-0.340071
40	6	0	-5.736600	-2.123570	-0.513054
41	6	0	-4.573020	-4.584945	0.041056
42	1	0	-2.698391	-3.623405	-0.434523
43	6	0	-6.537323	-3.199732	-0.134034
44	1	0	-6.190025	-1.159702	-0.733735
45	6	0	-5.955812	-4.431498	0.145080
46	1	0	-4.117241	-5.547095	0.253216
47	1	0	-7.612753	-3.073945	-0.056290
48	1	0	-6.575852	-5.271879	0.440863
49	6	0	3.929273	-1.735984	1.502496
50	7	0	2.922337	-0.878386	0.872418
51	6	0	1.165679	-0.980352	1.367021
52	6	0	1.807286	-1.524504	0.173039
53	6	0	3.311035	0.513123	0.467459
54	1	0	1.573817	-1.086201	-0.788496
55	1	0	1.904015	-2.606633	0.121290
56	1	0	1.216583	-1.543062	2.288500
57	1	0	0.973885	0.079309	1.402733
58	6	0	4.713822	-2.542755	0.493860
59	8	0	4.432828	0.858289	0.810260
60	8	0	2.392044	1.121746	-0.135382
61	6	0	5.610801	-1.901643	-0.367070

62	6	0	4.534486	-3.921807	0.389381
63	6	0	5.241392	-4.659343	-0.558364
64	6	0	6.315333	-2.637994	-1.312663
65	6	0	6.132792	-4.017109	-1.410855
66	1	0	4.583324	-1.067789	2.064155
67	1	0	3.420342	-2.409270	2.202726
68	1	0	3.839996	-4.424320	1.059370
69	1	0	5.740296	-0.826468	-0.278320
70	1	0	7.013777	-2.135683	-1.974767
71	1	0	6.686172	-4.588317	-2.149619
72	1	0	5.094399	-5.732480	-0.629275

5

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.569993	-2.293299	0.398453
2	8	0	-0.990715	-2.607989	1.470717
3	8	0	-1.134015	-2.569412	-0.754303
4	7	0	0.770993	-1.645850	0.300876
5	6	0	1.416858	-1.393424	1.628237
6	6	0	0.844067	-0.262522	0.896014
7	6	0	1.598118	-1.990536	-0.940754
8	1	0	1.166703	-2.927352	-1.298784
9	1	0	0.871356	-1.836898	2.450612
10	1	0	2.491976	-1.515397	1.600727
11	1	0	1.503165	0.392900	0.337275
12	1	0	-0.125547	0.135899	1.184338
13	1	0	1.416750	-1.173427	-1.648951
14	6	0	3.064792	-2.149609	-0.658621
15	6	0	3.957858	-1.205367	-1.165159
16	6	0	5.325709	-1.362022	-0.932854
17	6	0	5.797446	-2.441465	-0.193966
18	6	0	4.903052	-3.389737	0.307455
19	6	0	3.542945	-3.249580	0.065263
20	1	0	3.582414	-0.353221	-1.737920
21	1	0	6.020031	-0.628550	-1.331329
22	1	0	6.861793	-2.555506	-0.013322
23	1	0	5.269263	-4.241649	0.871139
24	1	0	2.844335	-3.995121	0.441326
25	6	0	-1.386219	-1.527371	-1.753010
26	6	0	-2.744160	-0.931726	-1.432584
27	1	0	-1.382404	-2.056398	-2.706642
28	1	0	-0.610622	-0.753860	-1.741024
29	1	0	-3.039907	-0.263515	-2.245016
30	7	0	-2.692395	-0.222378	-0.159120
31	1	0	-3.493148	-1.723959	-1.347793
32	6	0	-3.519791	-0.713734	0.946543
33	1	0	-3.204458	-0.169020	1.838604
34	6	0	-2.282331	1.093504	-0.123271
35	8	0	-2.327634	1.794845	0.873101
36	8	0	-1.800643	1.470767	-1.306214
37	1	0	-3.291094	-1.773262	1.094882
38	6	0	-4.998052	-0.519507	0.692666
39	6	0	-5.538903	0.770476	0.676843
40	6	0	-5.830460	-1.609057	0.441413
41	6	0	-6.889428	0.960522	0.409568
42	1	0	-4.889883	1.617816	0.883152
43	6	0	-7.185540	-1.419578	0.174469

44	1	0	-5.415886	-2.614537	0.461553
45	6	0	-7.715638	-0.134208	0.156825
46	1	0	-7.302345	1.964335	0.402426
47	1	0	-7.823993	-2.275549	-0.019923
48	1	0	-8.770175	0.016770	-0.050740
49	6	0	2.460880	3.480112	-0.571025
50	7	0	1.331977	2.831460	-1.237712
51	6	0	-1.178718	2.763290	-1.371450
52	6	0	0.077350	2.917634	-0.510435
53	6	0	1.662797	1.577554	-1.854984
54	1	0	0.010191	2.223245	0.336534
55	1	0	0.039379	3.921256	-0.070838
56	1	0	-1.930491	3.497477	-1.069143
57	1	0	-0.928543	2.893506	-2.423715
58	6	0	2.890410	2.700720	0.660946
59	8	0	2.824378	1.453666	-2.283852
60	8	0	0.734089	0.719476	-1.869346
61	6	0	3.862681	1.698272	0.559319
62	6	0	2.235368	2.871880	1.885124
63	6	0	2.527209	2.054772	2.975762
64	6	0	4.160433	0.881043	1.648788
65	6	0	3.491159	1.055088	2.859548
66	1	0	3.278427	3.532508	-1.289352
67	1	0	2.165008	4.497575	-0.291547
68	1	0	1.485130	3.652984	1.984192
69	1	0	4.358107	1.554083	-0.395288
70	1	0	4.912424	0.102367	1.545702
71	1	0	3.725938	0.422704	3.711049
72	1	0	2.008996	2.205604	3.917954

6

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.637392	-1.094927	0.881901
2	6	0	-3.864463	-0.743615	0.077877
3	6	0	-4.527889	0.464272	0.310789
4	6	0	-5.647786	0.806280	-0.438108
5	6	0	-6.116945	-0.053585	-1.430674
6	6	0	-5.458600	-1.254361	-1.671719
7	6	0	-4.335055	-1.594640	-0.920114
8	1	0	-4.151748	1.135150	1.078124
9	1	0	-6.157782	1.745556	-0.248307
10	1	0	-6.992527	0.214106	-2.013508
11	1	0	-5.816870	-1.927582	-2.444110
12	1	0	-3.821020	-2.534140	-1.108256
13	7	0	-1.569912	-0.123578	0.639665
14	6	0	-0.213708	-0.629917	0.758143
15	6	0	-0.805754	-0.339231	-0.575864
16	1	0	-0.066689	-1.675348	1.025826
17	1	0	0.508221	0.059523	1.186951
18	1	0	-1.082789	-1.192199	-1.193557
19	1	0	-0.520097	0.557828	-1.117075
20	1	0	-2.311215	-2.118142	0.630139
21	1	0	-2.860744	-1.074135	1.954372
22	6	0	-1.301368	2.468593	1.243554
23	8	0	-2.276002	2.570800	1.869170
24	8	0	-0.303030	2.461440	0.641318
25	6	0	2.736403	-1.601401	-0.547646

26	6	0	3.580154	-0.371906	-0.798052
27	6	0	4.934543	-0.479746	-1.123546
28	6	0	5.712848	0.657261	-1.323509
29	6	0	5.142138	1.921262	-1.202650
30	6	0	3.791197	2.043038	-0.885392
31	6	0	3.017583	0.903690	-0.686274
32	1	0	5.377601	-1.467011	-1.233610
33	1	0	6.762781	0.556420	-1.579949
34	1	0	5.746138	2.808887	-1.362046
35	1	0	3.337307	3.024969	-0.796083
36	1	0	1.960394	1.000948	-0.446302
37	7	0	2.661803	-2.106442	0.833662
38	6	0	2.823075	-1.186920	1.944854
39	6	0	3.880873	-2.177786	1.614468
40	1	0	2.155454	-1.354076	2.785655
41	1	0	3.054431	-0.144943	1.732177
42	1	0	4.001241	-3.077470	2.210595
43	1	0	3.104336	-2.433199	-1.157668
44	1	0	1.706305	-1.396342	-0.856058
45	1	0	4.797172	-1.774752	1.187260

TS_{6-7}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.982533	0.564830	1.219930
2	6	0	-3.907713	-0.320559	0.416286
3	6	0	-4.550260	0.197991	-0.713541
4	6	0	-5.382546	-0.615303	-1.474127
5	6	0	-5.582678	-1.949576	-1.118970
6	6	0	-4.945578	-2.470072	0.002063
7	6	0	-4.108866	-1.655678	0.764018
8	1	0	-4.383330	1.240934	-0.971494
9	1	0	-5.881062	-0.207307	-2.347965
10	1	0	-6.235316	-2.579747	-1.715172
11	1	0	-5.098049	-3.507274	0.284270
12	1	0	-3.614573	-2.059314	1.645584
13	7	0	-1.813442	0.989683	0.459615
14	6	0	-0.053952	0.611270	0.993683
15	6	0	-0.894296	-0.026966	-0.026367
16	1	0	-0.228270	0.344266	2.032630
17	1	0	0.311631	1.600286	0.745083
18	1	0	-1.230680	-1.044793	0.175633
19	1	0	-0.608259	0.142748	-1.062427
20	1	0	-2.656771	0.034198	2.125775
21	1	0	-3.486150	1.487921	1.512979
22	6	0	-1.856523	2.297705	-0.354532
23	8	0	-2.893562	2.930896	-0.185232
24	8	0	-0.816830	2.458978	-1.002962
25	6	0	2.270922	-0.001867	-0.436201
26	6	0	3.755463	-0.206877	-0.585784
27	6	0	4.277619	-1.480656	-0.824346
28	6	0	5.652110	-1.675005	-0.929867
29	6	0	6.518694	-0.593428	-0.800519
30	6	0	6.008142	0.682505	-0.571712
31	6	0	4.634064	0.873879	-0.466987
32	1	0	3.599441	-2.322253	-0.945857
33	1	0	6.044380	-2.668437	-1.120855
34	1	0	7.590071	-0.741692	-0.887721

35	1	0	6.679993	1.530024	-0.483637
36	1	0	4.233825	1.871398	-0.302210
37	7	0	1.754466	-0.103913	0.947433
38	6	0	2.571945	0.214084	2.103396
39	6	0	2.150360	-1.185757	1.826337
40	1	0	2.062957	0.789860	2.871939
41	1	0	3.611444	0.470580	1.924337
42	1	0	1.341707	-1.633748	2.397505
43	1	0	1.720914	-0.748214	-1.017224
44	1	0	1.965940	0.986948	-0.797669
45	1	0	2.909887	-1.868889	1.456158

7

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.661328	-0.850983	-1.494436
2	6	0	-3.676087	-0.314337	-0.504198
3	6	0	-3.852702	-0.956080	0.727985
4	6	0	-4.750799	-0.446122	1.659150
5	6	0	-5.482745	0.708058	1.377084
6	6	0	-5.311948	1.351129	0.156191
7	6	0	-4.409820	0.839809	-0.776426
8	1	0	-3.277898	-1.856898	0.929370
9	1	0	-4.886520	-0.952952	2.609891
10	1	0	-6.185671	1.099997	2.105887
11	1	0	-5.880615	2.247476	-0.073249
12	1	0	-4.279666	1.338227	-1.735361
13	7	0	-1.287886	-0.761879	-1.023944
14	6	0	0.627213	0.733267	-1.164128
15	6	0	-0.812242	0.546049	-0.662045
16	1	0	0.668719	1.250400	-2.126777
17	1	0	1.117978	-0.235224	-1.233781
18	1	0	-1.463988	1.301791	-1.117453
19	1	0	-0.836930	0.712433	0.427699
20	1	0	-2.757319	-0.306483	-2.443624
21	1	0	-2.838033	-1.911500	-1.680902
22	6	0	-0.788433	-1.847806	-0.187419
23	8	0	-1.415219	-2.907321	-0.217972
24	8	0	0.258510	-1.538065	0.454465
25	6	0	1.966338	0.783973	0.999096
26	6	0	3.257399	0.094017	0.652222
27	6	0	4.478896	0.749235	0.844176
28	6	0	5.675179	0.128376	0.502258
29	6	0	5.655995	-1.159572	-0.027821
30	6	0	4.445328	-1.827394	-0.192073
31	6	0	3.243562	-1.211923	0.151019
32	1	0	4.500159	1.739163	1.297521
33	1	0	6.618523	0.640581	0.661182
34	1	0	6.587685	-1.649210	-0.293080
35	1	0	4.433180	-2.841839	-0.576972
36	1	0	2.288715	-1.733027	0.075217
37	7	0	1.423940	1.553393	-0.193675
38	6	0	2.226123	2.672666	-0.703742
39	6	0	0.956526	2.932799	0.016662
40	1	0	2.254092	2.757003	-1.783194
41	1	0	3.169309	2.817955	-0.191943
42	1	0	0.068642	3.195326	-0.546916
43	1	0	2.112708	1.524805	1.790149

44	1	0	1.181740	0.060931	1.251459
45	1	0	0.987763	3.272574	1.044933

$TS_{7\text{-}2}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.907135	-0.346477	1.457830
2	6	0	3.388337	0.836245	0.640379
3	6	0	4.221350	0.623182	-0.464693
4	6	0	4.635452	1.697168	-1.244822
5	6	0	4.225874	2.994182	-0.935284
6	6	0	3.396716	3.212793	0.159690
7	6	0	2.978975	2.135150	0.939249
8	1	0	4.534776	-0.392864	-0.691868
9	1	0	5.285455	1.524256	-2.097169
10	1	0	4.555620	3.830038	-1.544584
11	1	0	3.075427	4.219925	0.408483
12	1	0	2.332073	2.304418	1.797963
13	7	0	2.016146	-1.233561	0.732387
14	6	0	0.006964	-1.784910	-0.433123
15	6	0	0.853261	-0.648252	0.116224
16	1	0	0.301858	-0.077541	0.877793
17	1	0	1.106136	0.049121	-0.700390
18	1	0	2.399550	0.015491	2.362030
19	1	0	3.753171	-0.968569	1.758159
20	6	0	2.602752	-2.229158	-0.123491
21	8	0	3.770277	-2.563503	0.047491
22	8	0	1.751716	-2.649571	-0.980356
23	6	0	-2.072616	-0.002953	-0.795924
24	6	0	-3.441916	0.533360	-0.472379
25	6	0	-3.605251	1.497672	0.525959
26	6	0	-4.872067	1.978732	0.842971
27	6	0	-5.988298	1.502064	0.160235
28	6	0	-5.834955	0.549615	-0.844062
29	6	0	-4.567116	0.070245	-1.159491
30	1	0	-2.731540	1.881207	1.047905
31	1	0	-4.986712	2.730950	1.616267
32	1	0	-6.975849	1.879051	0.404490
33	1	0	-6.700879	0.185989	-1.387142
34	1	0	-4.445602	-0.661830	-1.954515
35	7	0	-1.658733	-1.197183	-0.021575
36	6	0	-2.609137	-2.245393	0.315769
37	6	0	-2.029992	-1.374193	1.372975
38	1	0	-2.228630	-3.253880	0.184060
39	1	0	-3.643369	-2.077746	0.034122
40	1	0	-1.224690	-1.751366	1.997981
41	1	0	-1.307415	0.756401	-0.609691
42	1	0	-2.008463	-0.295969	-1.848551
43	1	0	-2.671490	-0.615957	1.810138
44	1	0	-0.191190	-1.871855	-1.493500
45	1	0	-0.078883	-2.683905	0.167185

$TS_{7\text{-}8}$

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	7	0	-1.764453	3.240680	-2.622684
2	6	0	-2.579717	3.237887	-3.826090
3	6	0	-1.161650	3.679937	-3.871112
4	6	0	-2.026657	4.180431	-1.512554
5	6	0	-2.449260	5.569615	-1.917592
6	6	0	-1.491960	6.565672	-2.128468
7	6	0	-1.875521	7.841140	-2.531830
8	6	0	-3.223274	8.133711	-2.724650
9	6	0	-4.185947	7.151101	-2.507483
10	6	0	-3.799709	5.876425	-2.103685
11	1	0	-1.123667	8.607749	-2.686670
12	1	0	-0.440731	6.341452	-1.962915
13	1	0	-3.524024	9.128956	-3.034500
14	1	0	-5.237787	7.379087	-2.644468
15	1	0	-2.798339	3.711369	-0.893408
16	1	0	-1.103374	4.220490	-0.925625
17	1	0	-2.842019	2.250568	-4.197866
18	1	0	-3.348310	4.000403	-3.906067
19	1	0	-0.405348	3.006501	-4.273137
20	1	0	-0.971961	4.743024	-3.981651
21	1	0	-4.552960	5.113822	-1.919351
22	6	0	2.406317	-0.896960	2.695059
23	6	0	3.594347	0.046625	2.660093
24	6	0	4.768603	-0.337413	1.999304
25	6	0	5.847273	0.536759	1.924415
26	6	0	5.774331	1.803830	2.504802
27	6	0	4.612073	2.192527	3.161822
28	6	0	3.529649	1.316053	3.233645
29	1	0	4.808750	-1.331380	1.559440
30	1	0	6.755380	0.227394	1.414942
31	1	0	6.621725	2.480665	2.447819
32	1	0	4.546215	3.175548	3.619814
33	1	0	2.620434	1.618395	3.750405
34	7	0	1.839210	-1.172698	1.386911
35	6	0	0.150232	-0.342676	-0.197034
36	6	0	1.413431	-0.024676	0.627480
37	1	0	-0.752736	0.055815	0.284651
38	1	0	0.063608	-1.422803	-0.294150
39	1	0	1.205442	0.796664	1.326477
40	1	0	2.199981	0.333108	-0.061020
41	1	0	1.631832	-0.473298	3.350176
42	1	0	2.711613	-1.866819	3.091617
43	6	0	2.482343	-2.227372	0.592242
44	8	0	3.191142	-3.025100	1.219257
45	8	0	2.205620	-2.168116	-0.632425
46	6	0	1.020883	-0.537902	-2.540504
47	6	0	0.835567	-0.029666	-3.949673
48	6	0	1.753822	0.857643	-4.515949
49	6	0	1.552062	1.378255	-5.794061
50	6	0	0.425272	1.011690	-6.524835
51	6	0	-0.485777	0.104852	-5.982502
52	6	0	-0.275202	-0.416431	-4.709597
53	1	0	2.642064	1.130873	-3.951377
54	1	0	2.279241	2.062247	-6.220085
55	1	0	0.266738	1.414057	-7.520180
56	1	0	-1.351526	-0.205479	-6.559242
57	1	0	-0.979412	-1.130322	-4.288091
58	7	0	0.201090	0.222741	-1.559481
59	6	0	-1.053692	1.490053	-2.093467
60	6	0	0.318917	1.678235	-1.602081

61	1	0	-1.831638	1.280379	-1.367272
62	1	0	-1.183296	1.135806	-3.107378
63	1	0	0.442118	2.132825	-0.619625
64	1	0	2.068072	-0.507871	-2.225305
65	1	0	0.726539	-1.583925	-2.443123
66	1	0	1.047652	2.057529	-2.317460

8

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.821424	-0.089166	-0.972152
2	6	0	4.151199	-0.728114	-0.982238
3	6	0	3.357761	-0.688637	0.267780
4	6	0	2.687525	1.404059	-1.107653
5	6	0	3.780623	2.198099	-0.452008
6	6	0	3.636196	2.633854	0.868227
7	6	0	4.645370	3.373397	1.477190
8	6	0	5.802356	3.687196	0.768185
9	6	0	5.947377	3.270256	-0.552858
10	6	0	4.937733	2.531984	-1.161939
11	1	0	4.523289	3.713421	2.499844
12	1	0	2.723275	2.406764	1.413961
13	1	0	6.586672	4.267993	1.241891
14	1	0	6.839755	3.529755	-1.112047
15	1	0	2.648917	1.589904	-2.184706
16	1	0	1.713984	1.646272	-0.675420
17	1	0	4.190948	-1.649547	-1.551487
18	1	0	4.982684	-0.041521	-1.089381
19	1	0	2.824859	-1.577402	0.594240
20	1	0	3.641776	0.029688	1.028208
21	1	0	5.039330	2.227258	-2.201194
22	6	0	-4.823344	0.731474	-1.270387
23	6	0	-4.594868	1.806775	-0.222619
24	6	0	-4.876723	1.536583	1.123520
25	6	0	-4.632152	2.498635	2.097168
26	6	0	-4.105224	3.743131	1.748541
27	6	0	-3.822725	4.019275	0.415138
28	6	0	-4.064888	3.051844	-0.560351
29	1	0	-5.293607	0.563210	1.373158
30	1	0	-4.860791	2.280990	3.136711
31	1	0	-3.924323	4.493872	2.512500
32	1	0	-3.418068	4.987311	0.131798
33	1	0	-3.845993	3.267942	-1.604741
34	7	0	-3.984147	-0.439899	-1.101350
35	6	0	-1.782647	-1.340688	-1.784112
36	6	0	-2.560364	-0.201909	-1.090922
37	1	0	-1.543481	-1.072027	-2.822020
38	1	0	-2.422914	-2.221007	-1.793432
39	1	0	-2.371055	0.750269	-1.607652
40	1	0	-2.175736	-0.086010	-0.061649
41	1	0	-4.656930	1.164829	-2.267218
42	1	0	-5.850844	0.368486	-1.209646
43	6	0	-4.444005	-1.445075	-0.133206
44	8	0	-5.649688	-1.404312	0.157990
45	8	0	-3.536353	-2.213947	0.264080
46	6	0	-0.734938	-2.490147	0.110438
47	6	0	0.564558	-3.052249	0.643173
48	6	0	0.970650	-2.795203	1.954582

49	6	0	2.173327	-3.304325	2.449553
50	6	0	2.996200	-4.071713	1.629527
51	6	0	2.598167	-4.345713	0.318799
52	6	0	1.391152	-3.847127	-0.163225
53	1	0	0.328500	-2.195161	2.594106
54	1	0	2.464507	-3.100472	3.475551
55	1	0	3.931559	-4.469112	2.010672
56	1	0	3.221857	-4.966497	-0.318036
57	1	0	1.067202	-4.064451	-1.178702
58	7	0	-0.519912	-1.716671	-1.122848
59	6	0	1.696186	-0.840693	-1.611069
60	6	0	0.357759	-0.578869	-0.907911
61	1	0	1.678195	-0.558990	-2.667825
62	1	0	1.939892	-1.898775	-1.529238
63	1	0	-0.095587	0.339107	-1.297260
64	1	0	-1.241302	-1.899918	0.886092
65	1	0	-1.441250	-3.290768	-0.122311
66	1	0	0.547877	-0.405793	0.165187

$TS_{7\text{-}9}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.648660	-1.860394	3.263337
2	6	0	1.469363	-1.906671	4.535687
3	6	0	2.535411	-2.806759	4.640977
4	6	0	3.315647	-2.835539	5.790803
5	6	0	3.044167	-1.966177	6.847675
6	6	0	1.986677	-1.069034	6.749943
7	6	0	1.204848	-1.040750	5.595477
8	1	0	2.732523	-3.483628	3.813538
9	1	0	4.137637	-3.540438	5.867189
10	1	0	3.655728	-1.990965	7.743970
11	1	0	1.769550	-0.389922	7.568516
12	1	0	0.375324	-0.340715	5.519565
13	7	0	1.427847	-1.485276	2.087613
14	6	0	1.504973	0.838689	1.134105
15	6	0	2.076581	-0.193283	2.105799
16	1	0	2.010041	1.796841	1.288843
17	1	0	0.432757	0.982145	1.295946
18	1	0	1.970260	0.243720	3.106296
19	1	0	3.147771	-0.314082	1.918517
20	1	0	-0.175177	-1.145398	3.385255
21	1	0	0.219551	-2.839827	3.047289
22	6	0	2.046671	-2.479165	1.288275
23	8	0	1.728911	-3.682262	1.553294
24	8	0	2.798027	-2.071271	0.385048
25	6	0	0.551439	-0.393104	-0.842970
26	6	0	0.701853	-0.788199	-2.281962
27	6	0	0.007030	-0.086441	-3.274244
28	6	0	0.126868	-0.462174	-4.607814
29	6	0	0.938464	-1.542389	-4.953385
30	6	0	1.627206	-2.250018	-3.970917
31	6	0	1.506656	-1.876001	-2.634034
32	1	0	-0.640719	0.743586	-2.997797
33	1	0	-0.418459	0.079514	-5.374055
34	1	0	1.025630	-1.837755	-5.994367
35	1	0	2.260489	-3.102666	-4.195610
36	1	0	2.056880	-2.439789	-1.882080

37	7	0	1.664235	0.489820	-0.311626
38	6	0	2.218395	1.526626	-1.214787
39	6	0	3.035377	0.356686	-0.823085
40	1	0	2.381989	2.489774	-0.745902
41	1	0	1.769966	1.530502	-2.202309
42	1	0	3.795881	0.460655	-0.059728
43	1	0	0.534463	-1.254859	-0.179922
44	1	0	-0.355709	0.200844	-0.693488
45	1	0	3.177948	-0.460225	-1.519163
46	6	0	3.713374	-7.300640	-0.663178
47	6	0	5.187088	-7.594312	-0.491163
48	6	0	5.703344	-7.979609	0.745373
49	6	0	7.066582	-8.226203	0.901554
50	6	0	7.923984	-8.083532	-0.183759
51	6	0	7.414350	-7.695869	-1.423008
52	6	0	6.054713	-7.451872	-1.579746
53	1	0	5.030403	-8.092853	1.592909
54	1	0	7.455521	-8.528613	1.869124
55	1	0	8.986301	-8.274813	-0.066835
56	1	0	8.082196	-7.587058	-2.272177
57	1	0	5.637970	-7.149206	-2.537134
58	7	0	3.450524	-5.895627	-0.959140
59	6	0	3.788641	-4.906632	0.062422
60	6	0	2.332395	-4.906229	0.158034
61	1	0	4.220357	-4.001674	-0.352272
62	1	0	4.345367	-5.331878	0.897503
63	1	0	1.806524	-4.358350	-0.611320
64	1	0	3.303335	-7.861206	-1.504838
65	1	0	1.836489	-5.709279	0.685858
66	1	0	3.172971	-7.581270	0.250371
67	6	0	3.429839	-5.440963	-2.401387
68	8	0	3.303900	-4.210248	-2.507849
69	8	0	3.517538	-6.357870	-3.216253

9

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.554850	2.500782	-1.313320
2	6	0	2.191644	3.854851	-0.742861
3	6	0	0.863137	4.134538	-0.407451
4	6	0	0.523938	5.367785	0.135331
5	6	0	1.507174	6.333978	0.350251
6	6	0	2.830075	6.061733	0.020256
7	6	0	3.169592	4.823177	-0.522143
8	1	0	0.097719	3.383019	-0.584341
9	1	0	-0.510019	5.579067	0.388127
10	1	0	1.238881	7.296793	0.772926
11	1	0	3.598785	6.810007	0.184315
12	1	0	4.203903	4.610228	-0.783762
13	7	0	2.239887	1.399488	-0.401131
14	6	0	3.930771	0.239063	1.072090
15	6	0	2.915538	1.367370	0.882655
16	1	0	4.453179	0.401180	2.019107
17	1	0	4.670503	0.235954	0.266603
18	1	0	3.471172	2.304867	0.995760
19	1	0	2.173373	1.334263	1.685721
20	1	0	3.627948	2.465633	-1.534877
21	1	0	2.017727	2.309542	-2.242806

22	6	0	1.050371	0.698943	-0.455326
23	8	0	0.312430	0.991074	-1.514431
24	8	0	0.780569	-0.130859	0.396514
25	6	0	3.242620	-1.797273	-0.251120
26	6	0	2.585013	-3.144343	-0.243178
27	6	0	3.365274	-4.307927	-0.242511
28	6	0	2.749783	-5.554685	-0.251243
29	6	0	1.356657	-5.643724	-0.266125
30	6	0	0.576220	-4.490266	-0.275521
31	6	0	1.191274	-3.239948	-0.267189
32	1	0	4.451634	-4.235367	-0.256065
33	1	0	3.355211	-6.455407	-0.258032
34	1	0	0.882119	-6.620118	-0.279873
35	1	0	-0.510414	-4.496124	-0.299108
36	1	0	0.541956	-2.366083	-0.269554
37	7	0	3.357337	-1.141443	1.117405
38	6	0	3.737568	-2.013079	2.256379
39	6	0	2.377081	-1.441268	2.175775
40	1	0	4.471203	-1.583304	2.928264
41	1	0	3.871435	-3.053493	1.980059
42	1	0	2.117844	-0.584974	2.786060
43	1	0	2.695094	-1.083351	-0.863624
44	1	0	4.277293	-1.860334	-0.602704
45	1	0	1.547937	-2.060595	1.853730
46	6	0	-4.298487	-0.388881	-1.438399
47	6	0	-4.930293	0.182888	-0.183096
48	6	0	-5.305213	1.522972	-0.099392
49	6	0	-5.855954	2.041191	1.072819
50	6	0	-6.033489	1.215946	2.177503
51	6	0	-5.658855	-0.126441	2.103141
52	6	0	-5.110111	-0.641778	0.934734
53	1	0	-5.167976	2.167889	-0.965538
54	1	0	-6.145008	3.087339	1.120864
55	1	0	-6.463087	1.613488	3.092354
56	1	0	-5.800639	-0.775306	2.962810
57	1	0	-4.813852	-1.685146	0.853225
58	7	0	-2.929737	-0.830591	-1.253531
59	6	0	-1.960084	0.169531	-0.860894
60	6	0	-0.776586	0.056359	-1.810555
61	1	0	-1.615638	0.017376	0.166624
62	1	0	-2.407901	1.168057	-0.941443
63	1	0	-0.394960	-0.964013	-1.757706
64	1	0	-4.853863	-1.270717	-1.762929
65	1	0	-1.066698	0.309721	-2.830542
66	1	0	-4.337675	0.365784	-2.236673
67	6	0	-2.704854	-2.183355	-0.770612
68	8	0	-1.519939	-2.404912	-0.403774
69	8	0	-3.680247	-2.948664	-0.791579

10

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.802965	-0.172375	1.707375
2	6	0	-0.672287	-0.766121	1.285813
3	7	0	-0.880328	-2.094795	1.285038
4	6	0	-2.743908	-1.148188	1.980211
5	6	0	-2.170920	-2.344255	1.714257
6	6	0	0.651646	-0.035179	0.863863

7	8	0	1.225517	0.506727	1.813452
8	8	0	0.885599	-0.128554	-0.345042
9	6	0	-1.998659	1.298998	1.939757
10	6	0	-3.502107	1.578279	1.985481
11	6	0	-1.346079	1.653802	3.277251
12	6	0	-1.376174	2.097036	0.788552
13	1	0	-0.289630	2.122353	0.859269
14	1	0	-1.743131	3.124825	0.850125
15	1	0	-1.663527	1.681645	-0.180833
16	1	0	-3.985565	1.109496	2.846962
17	1	0	-3.643287	2.656188	2.085673
18	1	0	-3.999759	1.252592	1.066938
19	1	0	-1.827380	1.106560	4.094061
20	1	0	-0.282407	1.407675	3.242882
21	1	0	-1.465158	2.725356	3.462119
22	1	0	-3.735879	-0.924008	2.328985
23	1	0	-2.576466	-3.335798	1.805587
24	6	0	0.084801	-3.143617	0.810714
25	6	0	1.493654	-2.825374	1.322897
26	1	0	1.482670	-2.596613	2.391737
27	1	0	2.120443	-3.706320	1.161367
28	1	0	1.940282	-1.991795	0.782199
29	6	0	-0.359810	-4.493279	1.377219
30	1	0	-1.318095	-4.821189	0.964999
31	1	0	-0.422314	-4.471097	2.469497
32	1	0	0.383947	-5.240568	1.093666
33	6	0	0.041596	-3.164321	-0.718509
34	1	0	0.742756	-3.917960	-1.088644
35	1	0	0.324799	-2.183478	-1.106562
36	1	0	-0.962426	-3.424527	-1.068461

$TS_{10\text{-}11}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.018760	-0.308517	1.774213
2	6	0	-0.854046	-0.869291	1.353411
3	7	0	-1.114791	-2.203408	1.355040
4	6	0	-2.982167	-1.270515	2.028644
5	6	0	-2.411294	-2.466824	1.764562
6	6	0	1.047395	0.175270	0.733798
7	8	0	1.651378	0.231622	1.748739
8	8	0	0.866407	0.351889	-0.421463
9	6	0	-2.215707	1.159507	1.927586
10	6	0	-3.627327	1.437003	2.444869
11	6	0	-1.198987	1.687828	2.942014
12	6	0	-2.043095	1.822887	0.559542
13	1	0	-1.052448	1.633809	0.144888
14	1	0	-2.186439	2.903098	0.655724
15	1	0	-2.786132	1.435023	-0.143524
16	1	0	-3.797414	0.978288	3.423500
17	1	0	-3.747502	2.517061	2.557214
18	1	0	-4.391653	1.087320	1.744576
19	1	0	-1.354772	1.211304	3.914367
20	1	0	-0.174535	1.487918	2.626723
21	1	0	-1.327831	2.767704	3.060064
22	1	0	-3.977042	-1.045858	2.371225
23	1	0	-2.826084	-3.456625	1.840765
24	6	0	-0.116589	-3.236161	0.962009

25	6	0	1.090721	-3.128963	1.895853
26	1	0	0.784902	-3.317719	2.929232
27	1	0	1.840054	-3.874422	1.613844
28	1	0	1.544221	-2.138405	1.850980
29	6	0	-0.734719	-4.627700	1.099465
30	1	0	-1.599739	-4.753007	0.441467
31	1	0	-1.032158	-4.839314	2.130870
32	1	0	0.014839	-5.367638	0.809145
33	6	0	0.277537	-3.005943	-0.498629
34	1	0	1.009883	-3.759034	-0.803907
35	1	0	0.708079	-2.015321	-0.647476
36	1	0	-0.601481	-3.094962	-1.143952

11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.570762	0.614491	1.114851
2	6	0	-0.364578	-0.172659	0.021484
3	7	0	0.027594	-1.352503	0.579942
4	6	0	-0.317207	-0.048220	2.306081
5	6	0	0.062784	-1.302300	1.965325
6	6	0	-1.011850	2.020902	0.965057
7	6	0	-2.342281	2.023949	0.208727
8	6	0	-1.188805	2.666756	2.336986
9	6	0	0.055100	2.771395	0.164636
10	1	0	1.005729	2.775420	0.706428
11	1	0	-0.256867	3.806572	-0.004105
12	1	0	0.204940	2.275371	-0.796183
13	1	0	-3.107336	1.490677	0.780938
14	1	0	-2.680505	3.051305	0.042951
15	1	0	-2.216170	1.522738	-0.752571
16	1	0	-1.946231	2.145450	2.930370
17	1	0	-0.248617	2.686429	2.896538
18	1	0	-1.520460	3.699294	2.201218
19	1	0	-0.421755	0.399221	3.280298
20	1	0	0.346186	-2.130449	2.592909
21	6	0	0.345716	-2.524838	-0.268382
22	6	0	1.473998	-2.129205	-1.223502
23	1	0	2.376083	-1.870897	-0.660804
24	1	0	1.706342	-2.959433	-1.897336
25	1	0	1.169416	-1.259374	-1.808122
26	6	0	0.785592	-3.700043	0.601055
27	1	0	-0.009708	-4.015918	1.283122
28	1	0	1.678665	-3.454623	1.183910
29	1	0	1.028240	-4.546837	-0.045719
30	6	0	-0.912647	-2.894993	-1.057139
31	1	0	-0.707318	-3.736480	-1.725742
32	1	0	-1.238899	-2.034338	-1.644113
33	1	0	-1.720290	-3.177361	-0.375107

12

Standard orientation:

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

1	7	0	1.338225	-1.577712	-0.312954
2	6	0	1.907653	-0.385438	-0.068512
3	7	0	3.212677	-0.593788	0.186495
4	6	0	2.303949	-2.560708	-0.207379
5	6	0	3.471115	-1.949147	0.099007
6	6	0	1.201019	1.009951	-0.038539
7	8	0	0.516785	1.175863	0.977950
8	8	0	1.482341	1.723901	-1.008628
9	6	0	-0.116871	-1.821089	-0.608472
10	6	0	-0.257161	-3.228269	-1.190651
11	6	0	-0.898943	-1.718604	0.701433
12	6	0	-0.599245	-0.799144	-1.640934
13	1	0	-0.732252	0.203566	-1.225861
14	1	0	-1.579314	-1.125909	-1.999049
15	1	0	0.088199	-0.754612	-2.490830
16	1	0	0.006237	-4.005134	-0.466945
17	1	0	-1.306710	-3.375124	-1.453490
18	1	0	0.343949	-3.353913	-2.096656
19	1	0	-0.550125	-2.475817	1.411723
20	1	0	-0.769038	-0.726667	1.139712
21	1	0	-1.962116	-1.886107	0.501408
22	1	0	2.094563	-3.603597	-0.363585
23	1	0	4.445882	-2.371259	0.264888
24	6	0	4.252222	0.466434	0.411954
25	6	0	3.717198	1.534460	1.372762
26	1	0	3.250711	1.080026	2.250222
27	1	0	4.561385	2.146518	1.700916
28	1	0	2.995773	2.189776	0.886515
29	6	0	5.482489	-0.195044	1.035913
30	1	0	5.964664	-0.899228	0.352462
31	1	0	5.234841	-0.706810	1.970878
32	1	0	6.211235	0.586890	1.258555
33	6	0	4.604993	1.072895	-0.947981
34	1	0	5.357354	1.854805	-0.809548
35	1	0	3.710839	1.506380	-1.401859
36	1	0	5.019492	0.307556	-1.611637
37	6	0	-1.192185	3.373153	-0.499595
38	1	0	-0.258877	3.345693	-1.051028
39	1	0	-1.156707	3.906309	0.449294
40	6	0	-2.532574	1.748736	0.744388
41	6	0	-3.470801	0.572217	0.600192
42	6	0	-3.947823	-0.075155	1.743263
43	6	0	-5.106172	-1.697568	0.384436
44	6	0	-4.757234	-1.200799	1.639863
45	6	0	-3.837355	0.079218	-0.651650
46	6	0	-4.647977	-1.050326	-0.759194
47	1	0	-3.661729	0.299003	2.723786
48	1	0	-5.111021	-1.696864	2.538656
49	1	0	-5.733839	-2.579433	0.301979
50	1	0	-4.921643	-1.425010	-1.741425
51	1	0	-3.459023	0.576349	-1.538883
52	7	0	-1.945543	2.139291	-0.524082
53	6	0	-2.513247	3.306523	-1.181755
54	1	0	-2.573335	3.258185	-2.265178
55	1	0	-3.355435	3.796236	-0.694217
56	1	0	-1.699090	1.471224	1.399261
57	1	0	-3.063693	2.590558	1.227862

$TS_{12\text{-}13}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.936777	-0.239780	1.730482
2	6	0	-0.396171	-1.147848	0.904530
3	7	0	-0.954182	-2.343986	1.165120
4	6	0	-1.861228	-0.875228	2.534268
5	6	0	-1.876736	-2.181781	2.180629
6	6	0	0.686933	-0.894787	-0.167433
7	8	0	1.845820	-0.871419	0.214167
8	8	0	0.170754	-0.799271	-1.314631
9	6	0	-0.585029	1.226596	1.785603
10	6	0	-1.574980	1.917210	2.723416
11	6	0	0.830370	1.348091	2.352466
12	6	0	-0.720357	1.820186	0.381123
13	1	0	0.004078	1.447160	-0.354628
14	1	0	-0.566663	2.900734	0.456455
15	1	0	-1.732409	1.646430	0.001605
16	1	0	-1.495475	1.553076	3.752235
17	1	0	-1.332660	2.981484	2.733609
18	1	0	-2.606638	1.811635	2.374182
19	1	0	0.865910	0.943048	3.368973
20	1	0	1.554572	0.820788	1.729596
21	1	0	1.107237	2.405119	2.389190
22	1	0	-2.429766	-0.359136	3.286776
23	1	0	-2.457727	-2.995084	2.576522
24	6	0	-0.749186	-3.618641	0.393699
25	6	0	0.735312	-3.810275	0.065600
26	1	0	1.365512	-3.629829	0.939532
27	1	0	0.877259	-4.842443	-0.263694
28	1	0	1.063202	-3.156657	-0.741987
29	6	0	-1.221700	-4.783690	1.265270
30	1	0	-2.300883	-4.761604	1.437294
31	1	0	-0.699368	-4.803866	2.226291
32	1	0	-1.000418	-5.713556	0.737929
33	6	0	-1.589448	-3.529427	-0.882041
34	1	0	-1.455921	-4.444865	-1.465308
35	1	0	-1.273648	-2.672424	-1.480876
36	1	0	-2.650836	-3.426695	-0.636739
37	6	0	1.417435	-0.234725	-2.770305
38	1	0	0.565537	0.161318	-3.309053
39	1	0	1.572956	-1.307711	-2.845743
40	6	0	2.530913	2.071032	-0.667069
41	6	0	3.661266	2.998496	-1.114217
42	6	0	4.821118	3.159048	-0.353926
43	6	0	5.702358	4.728224	-1.960650
44	6	0	5.832909	4.021594	-0.767051
45	6	0	3.542833	3.706564	-2.311845
46	6	0	4.554595	4.564865	-2.732909
47	1	0	4.930239	2.596267	0.571357
48	1	0	6.728674	4.136485	-0.162892
49	1	0	6.493586	5.395407	-2.289455
50	1	0	4.450698	5.106567	-3.669073
51	1	0	2.636619	3.552111	-2.892434
52	7	0	1.726733	1.594974	-1.761428
53	6	0	2.530116	0.693313	-2.567180
54	1	0	2.993166	1.104419	-3.495734
55	1	0	3.342732	0.190008	-2.010598
56	1	0	1.892380	2.641236	0.028354
57	1	0	2.997981	1.260329	-0.069475

13

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.327172	1.408540	-2.970746
2	6	0	1.720407	2.722740	-3.611809
3	6	0	2.949484	2.805447	-4.273358
4	6	0	2.572616	5.132567	-4.780167
5	6	0	3.376751	3.996591	-4.848232
6	6	0	0.922019	3.867178	-3.552354
7	6	0	1.343699	5.061882	-4.132846
8	1	0	3.574563	1.917895	-4.337234
9	1	0	4.334904	4.038050	-5.357227
10	1	0	2.900421	6.062684	-5.233561
11	1	0	0.706039	5.939315	-4.081457
12	1	0	-0.039097	3.814769	-3.048881
13	7	0	-0.327838	0.975661	0.413164
14	6	0	-0.163607	-0.035016	-0.487335
15	7	0	0.325460	-1.104120	0.202007
16	6	0	0.131816	0.549805	1.641667
17	6	0	0.527237	-0.729738	1.511530
18	6	0	-0.393328	-0.059177	-2.066849
19	8	0	0.211465	-1.015414	-2.646560
20	8	0	-1.843769	-0.074481	-2.149932
21	6	0	-0.890188	2.380300	0.291658
22	6	0	-2.076453	2.448333	-0.670959
23	6	0	-1.416109	2.807720	1.673535
24	6	0	0.249265	3.312714	-0.114284
25	1	0	1.046201	3.291676	0.636115
26	1	0	-0.128576	4.337287	-0.185559
27	1	0	0.655481	3.024625	-1.081165
28	1	0	-2.794177	1.650911	-0.467085
29	1	0	-2.565117	3.415558	-0.523975
30	1	0	-1.743411	2.368722	-1.699583
31	1	0	-2.128005	2.081942	2.076729
32	1	0	-0.621338	2.982990	2.402176
33	1	0	-1.936379	3.758518	1.545640
34	1	0	0.139456	1.170546	2.516995
35	1	0	0.922280	-1.390053	2.259188
36	6	0	0.551252	-2.554649	-0.216392
37	6	0	1.843482	-2.658623	-1.028733
38	1	0	2.690362	-2.331832	-0.415251
39	1	0	2.004208	-3.708200	-1.293510
40	1	0	1.770420	-2.056528	-1.930691
41	6	0	0.729607	-3.404418	1.051763
42	1	0	-0.123194	-3.323853	1.732407
43	1	0	1.654480	-3.180187	1.591040
44	1	0	0.796251	-4.444328	0.726180
45	6	0	-0.697339	-3.084381	-0.927381
46	1	0	-0.533555	-4.142699	-1.151704
47	1	0	-0.883254	-2.545366	-1.852467
48	1	0	-1.562714	-3.008588	-0.260823
49	6	0	-0.919214	1.244665	-3.873318
50	6	0	-2.182459	0.499866	-3.397377
51	7	0	-0.089681	1.301705	-2.660867
52	1	0	-3.028629	1.180803	-3.242741
53	1	0	-2.482731	-0.269807	-4.116659
54	1	0	-1.141008	2.245793	-4.254263
55	1	0	-0.410896	0.674046	-4.662861
56	1	0	1.882714	1.296763	-2.025416

57	1	0	1.645252	0.571547	-3.609579

$TS_{13\text{-}11}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.372825	1.427067	-3.392462
2	6	0	1.577393	2.852233	-3.857704
3	6	0	2.693258	3.141691	-4.649349
4	6	0	2.081031	5.472130	-4.735663
5	6	0	2.948425	4.437604	-5.081138
6	6	0	0.713251	3.895243	-3.520836
7	6	0	0.962862	5.195184	-3.956837
8	1	0	3.367593	2.335325	-4.928302
9	1	0	3.821831	4.641616	-5.692790
10	1	0	2.274289	6.484385	-5.076112
11	1	0	0.277846	5.993279	-3.686888
12	1	0	-0.158146	3.684103	-2.908422
13	7	0	-0.208843	0.958147	0.635765
14	6	0	-0.139358	-0.073510	-0.255496
15	7	0	0.199207	-1.155831	0.512636
16	6	0	0.134223	0.545442	1.908248
17	6	0	0.387894	-0.774127	1.829805
18	6	0	-0.070042	-0.168275	-2.294760
19	8	0	0.821991	-0.986977	-2.509414
20	8	0	-1.442276	-0.498519	-2.446879
21	6	0	-0.561770	2.374633	0.335817
22	6	0	-1.784148	2.390457	-0.583934
23	6	0	-0.946051	3.099721	1.631168
24	6	0	0.672549	3.056159	-0.254463
25	1	0	1.492372	3.019481	0.469935
26	1	0	0.457257	4.105256	-0.479386
27	1	0	0.982770	2.559747	-1.170823
28	1	0	-2.679329	2.124420	-0.013429
29	1	0	-1.921872	3.396613	-0.993241
30	1	0	-1.676462	1.680841	-1.397974
31	1	0	-1.729918	2.564401	2.174714
32	1	0	-0.090127	3.258508	2.292893
33	1	0	-1.334748	4.084670	1.360124
34	1	0	0.157887	1.200306	2.760718
35	1	0	0.666857	-1.455696	2.611669
36	6	0	0.347096	-2.605433	0.124976
37	6	0	1.773738	-2.846221	-0.373880
38	1	0	2.492506	-2.597326	0.414375
39	1	0	1.893405	-3.906007	-0.620454
40	1	0	1.972514	-2.245013	-1.258984
41	6	0	0.109182	-3.472998	1.372232
42	1	0	-0.848715	-3.243024	1.848522
43	1	0	0.910512	-3.387371	2.110791
44	1	0	0.086892	-4.516489	1.051545
45	6	0	-0.710396	-3.005075	-0.905086
46	1	0	-0.694570	-4.094790	-1.001247
47	1	0	-0.515891	-2.564943	-1.877036
48	1	0	-1.705377	-2.700943	-0.567628
49	6	0	-1.057617	1.340976	-3.805890
50	6	0	-1.800980	0.002899	-3.722209
51	7	0	0.046277	1.174053	-2.848776
52	1	0	-2.887106	0.103503	-3.762487
53	1	0	-1.469264	-0.686066	-4.510084

54	1	0	-1.705958	2.178957	-3.522655
55	1	0	-0.675689	1.537595	-4.813013
56	1	0	2.097938	1.184916	-2.606774
57	1	0	1.599106	0.735565	-4.219404

14

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.896040	0.221959	-0.137579
2	7	0	3.184026	0.079014	0.229488
3	7	0	1.629926	1.540071	-0.201233
4	6	0	3.739329	1.333121	0.402419
5	6	0	2.773306	2.240576	0.134104
6	6	0	3.913864	-1.224032	0.405297
7	6	0	0.316379	2.166200	-0.594049
8	1	0	4.761045	1.485692	0.699249
9	1	0	2.814350	3.314141	0.160783
10	6	0	0.893085	-0.945573	-0.458626
11	8	0	0.895697	-1.269140	-1.651184
12	8	0	0.265124	-1.344787	0.531276
13	6	0	5.351179	-0.925571	0.832125
14	1	0	5.865420	-1.880123	0.961611
15	1	0	5.894267	-0.356530	0.071864
16	1	0	5.392851	-0.393857	1.787405
17	6	0	3.931361	-1.963635	-0.934844
18	1	0	4.475599	-2.903613	-0.809109
19	1	0	2.926076	-2.179255	-1.297914
20	1	0	4.448034	-1.363231	-1.689534
21	6	0	3.222771	-2.034888	1.504218
22	1	0	2.184177	-2.257341	1.258616
23	1	0	3.766913	-2.973416	1.640542
24	1	0	3.243135	-1.482874	2.448596
25	6	0	0.446145	3.683715	-0.462949
26	1	0	-0.513891	4.123339	-0.740635
27	1	0	0.667825	3.987136	0.564761
28	1	0	1.203853	4.092164	-1.138171
29	6	0	-0.774912	1.672299	0.356588
30	1	0	-1.705848	2.205539	0.140752
31	1	0	-0.963605	0.602833	0.260069
32	1	0	-0.499683	1.874443	1.396192
33	6	0	0.016479	1.803881	-2.049945
34	1	0	-0.938846	2.255706	-2.332626
35	1	0	0.796583	2.198668	-2.708256
36	1	0	-0.051068	0.724172	-2.192786
37	6	0	-2.155824	-1.210796	-1.979278
38	6	0	-3.056321	-0.041234	-2.177541
39	1	0	-1.617581	-1.279096	-1.036184
40	1	0	-1.630712	-1.648534	-2.822249
41	1	0	-3.118798	0.672151	-1.357079
42	7	0	-3.597609	-1.372230	-1.978004
43	1	0	-3.204333	0.377951	-3.169231
44	6	0	-4.253848	-1.687741	-0.700896
45	6	0	-3.830587	-0.900204	0.521963
46	6	0	-4.527896	0.258251	0.880595
47	6	0	-2.730406	-1.283435	1.293121
48	6	0	-4.144460	1.012826	1.984844
49	6	0	-3.045654	0.618356	2.747027
50	6	0	-2.336151	-0.526383	2.394632

51	1	0	-5.384930	0.564341	0.284659
52	1	0	-4.704108	1.903544	2.254181
53	1	0	-2.743373	1.204713	3.609769
54	1	0	-5.328987	-1.545713	-0.857559
55	1	0	-4.087011	-2.755582	-0.525173
56	1	0	-2.152820	-2.161652	1.020265
57	1	0	-1.458794	-0.828431	2.957352

$TS_{14\text{-}15}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.900485	0.365583	0.372321
2	7	0	-1.954860	-0.216392	-0.226056
3	7	0	-1.156591	1.677655	0.517470
4	6	0	-2.903540	0.755498	-0.465794
5	6	0	-2.407171	1.929131	-0.006275
6	6	0	-2.112002	-1.681954	-0.543563
7	6	0	-0.260289	2.719819	1.148230
8	1	0	-3.843770	0.548909	-0.944199
9	1	0	-2.851264	2.908324	-0.005667
10	6	0	0.392675	-0.354960	0.741351
11	8	0	0.401139	-1.176968	1.634625
12	8	0	1.327486	0.038038	-0.045183
13	6	0	-3.281809	-1.833505	-1.516470
14	1	0	-3.359446	-2.888412	-1.785787
15	1	0	-4.234827	-1.545631	-1.064410
16	1	0	-3.122444	-1.260052	-2.434447
17	6	0	-2.413020	-2.420790	0.761857
18	1	0	-2.533773	-3.486063	0.546967
19	1	0	-1.596073	-2.293851	1.474237
20	1	0	-3.342914	-2.050351	1.203404
21	6	0	-0.834919	-2.206156	-1.210744
22	1	0	-0.023543	-2.344180	-0.496553
23	1	0	-1.055471	-3.184386	-1.644574
24	1	0	-0.504255	-1.539900	-2.011744
25	6	0	-1.119062	3.944619	1.469581
26	1	0	-0.492672	4.657375	2.009084
27	1	0	-1.475752	4.447799	0.566559
28	1	0	-1.969508	3.689752	2.108864
29	6	0	0.838427	3.109281	0.156265
30	1	0	1.447287	3.899263	0.605138
31	1	0	1.490871	2.270202	-0.085310
32	1	0	0.398173	3.497357	-0.767370
33	6	0	0.304011	2.159392	2.454580
34	1	0	0.880604	2.948368	2.943580
35	1	0	-0.503894	1.851627	3.124738
36	1	0	0.984532	1.321698	2.306080
37	6	0	2.894679	-0.278043	0.356951
38	6	0	3.368416	0.369008	1.629372
39	1	0	3.352313	0.126353	-0.538636
40	1	0	2.924197	-1.362767	0.410330
41	1	0	3.170438	1.463237	1.609578
42	7	0	4.734646	-0.031826	1.553838
43	1	0	2.827698	-0.046912	2.499260
44	6	0	5.574271	1.078866	1.180616
45	6	0	5.318429	1.639863	-0.216486
46	6	0	4.577958	2.805681	-0.419799
47	6	0	5.708124	0.907191	-1.345609

48	6	0	4.224215	3.227025	-1.703703
49	6	0	4.623826	2.490095	-2.812782
50	6	0	5.376587	1.327722	-2.627383
51	1	0	4.279395	3.392262	0.447707
52	1	0	3.643370	4.137016	-1.835754
53	1	0	4.357749	2.816125	-3.813812
54	1	0	5.496397	1.944298	1.879531
55	1	0	6.620589	0.743671	1.219033
56	1	0	6.255968	-0.019959	-1.193390
57	1	0	5.697905	0.749247	-3.489295

15

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.749406	0.378416	0.505055
2	7	0	-1.765563	-0.245878	-0.119000
3	7	0	-1.013132	1.696020	0.553643
4	6	0	-2.695296	0.706495	-0.475900
5	6	0	-2.227425	1.909061	-0.061425
6	6	0	-1.907748	-1.728495	-0.363116
7	6	0	-0.153691	2.781282	1.164636
8	1	0	-3.603430	0.466799	-0.998645
9	1	0	-2.669172	2.885084	-0.152191
10	6	0	0.478514	-0.327473	1.036261
11	8	0	0.405066	-1.091304	1.972348
12	8	0	1.507873	-0.019979	0.301892
13	6	0	-2.983406	-1.929261	-1.432383
14	1	0	-3.042224	-2.996746	-1.651861
15	1	0	-3.972850	-1.617671	-1.087625
16	1	0	-2.735730	-1.404998	-2.359989
17	6	0	-2.340107	-2.387330	0.948305
18	1	0	-2.463823	-3.460731	0.781264
19	1	0	-1.589275	-2.235744	1.725270
20	1	0	-3.297672	-1.978863	1.284522
21	6	0	-0.581220	-2.300322	-0.878008
22	1	0	0.161072	-2.408042	-0.087344
23	1	0	-0.775480	-3.298936	-1.275872
24	1	0	-0.170453	-1.684743	-1.682605
25	6	0	-1.042021	4.002838	1.406184
26	1	0	-0.440292	4.755112	1.919335
27	1	0	-1.391450	4.453941	0.473507
28	1	0	-1.899134	3.761981	2.042043
29	6	0	0.960343	3.130063	0.177204
30	1	0	1.588081	3.910402	0.615318
31	1	0	1.589776	2.264921	-0.031944
32	1	0	0.537371	3.507551	-0.758651
33	6	0	0.394416	2.293462	2.507221
34	1	0	0.871337	3.140042	3.006476
35	1	0	-0.410204	1.921377	3.147728
36	1	0	1.162980	1.528226	2.402585
37	6	0	2.864660	-0.475095	0.759391
38	6	0	3.508705	0.436688	1.829106
39	1	0	3.443557	-0.451615	-0.162056
40	1	0	2.755191	-1.492423	1.133822
41	1	0	3.302761	1.500094	1.522709
42	7	0	4.857653	0.076942	1.931818
43	1	0	2.959635	0.265531	2.773388
44	6	0	5.623460	0.745598	0.938823

45	1	0	5.516902	1.862612	0.975759
46	1	0	5.354119	0.519363	-0.130838
47	6	0	7.105510	0.442300	1.049107
48	6	0	7.583867	-0.399718	2.051797
49	6	0	8.018431	1.001805	0.151108
50	6	0	8.946703	-0.674670	2.152746
51	1	0	6.849032	-0.815852	2.732645
52	6	0	9.379312	0.732000	0.249737
53	1	0	7.650830	1.659500	-0.635426
54	6	0	9.849998	-0.111389	1.255238
55	1	0	9.307456	-1.333944	2.938129
56	1	0	10.074795	1.176842	-0.456997
57	1	0	10.911740	-0.326264	1.336109

$TS_{15\text{-}13}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.123491	0.014373	0.403911
2	7	0	0.382320	0.463865	1.645184
3	6	0	1.732905	0.722836	1.729020
4	6	0	1.451231	-0.406690	-1.750086
5	6	0	0.014434	1.558820	3.813470
6	1	0	-0.512013	-1.253799	-2.316856
7	1	0	-3.724353	0.356987	-1.385413
8	7	0	1.268985	-0.021318	-0.296134
9	1	0	2.198278	1.101654	2.621135
10	6	0	-1.232059	-0.431291	-0.079920
11	1	0	-0.726431	1.728247	4.596855
12	1	0	0.894066	1.122128	4.293563
13	1	0	0.276744	2.527202	3.377474
14	1	0	-1.260880	-1.445759	2.646635
15	1	0	-2.503668	0.537892	1.678162
16	1	0	3.621136	-0.065177	-1.775951
17	1	0	3.137037	-1.706451	-1.261155
18	1	0	1.925109	1.619336	-2.367970
19	1	0	0.528170	-2.346206	-1.356154
20	7	0	-3.033563	-0.751310	-4.169829
21	1	0	-4.897944	0.255241	-4.391943
22	6	0	-4.977624	-1.651019	-5.345691
23	6	0	-6.829489	-2.684393	-6.527139
24	6	0	2.280662	0.426099	0.524583
25	6	0	-0.604049	0.620544	2.775946
26	1	0	3.303688	0.493676	0.200658
27	1	0	0.083224	-1.172498	3.785781
28	1	0	-1.695377	2.126751	1.634331
29	1	0	0.875916	-1.998189	-3.055429
30	6	0	-2.823978	-0.088643	-1.817823
31	6	0	-2.585660	0.266433	-3.323023
32	1	0	-3.044018	1.278771	-3.474220
33	1	0	-1.494720	0.407840	-3.430471
34	6	0	-4.454636	-0.763687	-4.229958
35	1	0	-4.985447	-1.115696	-3.303431
36	6	0	-6.347031	-1.882563	-5.498000
37	1	0	-3.039624	-2.047972	-6.094016
38	1	0	-7.041636	-1.425785	-4.794414
39	8	0	-1.746659	-1.426648	0.376955
40	8	0	-1.691376	0.388662	-0.987065
41	6	0	-0.848754	-0.759910	3.388530

42	1	0	-1.560567	-0.660666	4.212331
43	6	0	-1.900958	1.245389	2.247948
44	6	0	2.898884	-0.871481	-1.926596
45	6	0	1.183600	0.844440	-2.586423
46	1	0	-2.862555	-1.176698	-1.726368
47	6	0	-4.573568	-3.054771	-7.275807
48	1	0	-3.875060	-3.514925	-7.970429
49	1	0	-7.898370	-2.850919	-6.631404
50	1	0	-2.499121	1.558515	3.106734
51	1	0	3.015623	-1.213057	-2.956508
52	1	0	0.182462	1.232578	-2.392028
53	6	0	-4.095394	-2.247348	-6.245494
54	1	0	1.246554	0.587008	-3.647021
55	6	0	0.514863	-1.564272	-2.120747
56	6	0	-5.940291	-3.276729	-7.423103
57	1	0	-6.311566	-3.906501	-8.226636

16

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.059750	0.013793	-0.146764
2	7	0	-3.074001	1.324022	-0.454814
3	7	0	-4.317348	-0.450705	-0.259081
4	6	0	-4.367597	1.690781	-0.770419
5	6	0	-5.142645	0.588762	-0.646276
6	6	0	-1.886599	2.251881	-0.409148
7	6	0	-4.787384	-1.824523	0.126921
8	1	0	-4.634788	2.691761	-1.058182
9	1	0	-6.197393	0.466617	-0.813366
10	6	0	-1.820829	-0.861443	0.249539
11	8	0	-1.179276	-1.272225	-0.723772
12	8	0	-1.688716	-1.021874	1.471068
13	6	0	-2.349303	3.664118	-0.762935
14	1	0	-1.476234	4.317595	-0.703959
15	1	0	-2.743217	3.725109	-1.782047
16	1	0	-3.095663	4.040275	-0.056919
17	6	0	-0.857163	1.791707	-1.443950
18	1	0	0.042708	2.402565	-1.337665
19	1	0	-0.590972	0.743197	-1.308294
20	1	0	-1.265486	1.912406	-2.452414
21	6	0	-1.336226	2.254329	1.020492
22	1	0	-1.193512	1.244454	1.408551
23	1	0	-0.374168	2.773236	1.030727
24	1	0	-2.035039	2.767009	1.688983
25	6	0	-6.190365	-2.029754	-0.445970
26	1	0	-6.505036	-3.049188	-0.214598
27	1	0	-6.923342	-1.355559	0.005269
28	1	0	-6.203621	-1.908069	-1.533323
29	6	0	-4.819861	-1.890347	1.655765
30	1	0	-5.150876	-2.885494	1.966492
31	1	0	-3.823002	-1.699041	2.060661
32	1	0	-5.521698	-1.151660	2.055035
33	6	0	-3.849466	-2.889074	-0.452594
34	1	0	-4.342417	-3.860118	-0.357498
35	1	0	-3.641407	-2.701353	-1.508510
36	1	0	-2.902599	-2.940540	0.083525
37	6	0	1.287453	-0.498166	0.552584
38	6	0	2.100653	-0.374915	-0.666857

39	1	0	1.105102	-1.473028	0.988427
40	1	0	0.535932	0.255054	0.744420
41	1	0	2.541411	-1.264610	-1.103642
42	7	0	2.665499	0.023516	0.627784
43	1	0	1.913510	0.463919	-1.327173
44	6	0	3.730946	-0.804547	1.231560
45	1	0	3.329722	-1.807109	1.410706
46	1	0	3.959153	-0.330522	2.188040
47	6	0	4.951083	-0.882375	0.348561
48	6	0	5.221374	-2.051126	-0.364777
49	6	0	5.810072	0.212990	0.218008
50	6	0	6.332109	-2.131800	-1.200995
51	1	0	4.561016	-2.908942	-0.257268
52	6	0	6.918480	0.131807	-0.618764
53	1	0	5.595002	1.120366	0.774334
54	6	0	7.181742	-1.037719	-1.329295
55	1	0	6.532821	-3.047597	-1.747816
56	1	0	7.582506	0.985082	-0.714464
57	1	0	8.049213	-1.095612	-1.979092
58	6	0	2.744318	1.708202	0.929885
59	8	0	1.884603	2.253887	0.271946
60	8	0	3.619273	1.927272	1.731562

$TS_{16\text{-}17}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.548068	1.538823	-1.324243
2	7	0	-1.373798	0.495665	-1.130080
3	7	0	-1.266165	2.672693	-1.254324
4	6	0	-2.645270	0.986213	-0.929608
5	6	0	-2.582055	2.337564	-1.008215
6	6	0	-0.991602	-0.974700	-1.096922
7	6	0	-0.765022	4.069628	-1.505301
8	1	0	-3.489064	0.344958	-0.747603
9	1	0	-3.360070	3.070907	-0.896783
10	6	0	0.955731	1.469228	-1.644505
11	8	0	1.673604	1.166364	-0.642595
12	8	0	1.279502	1.692231	-2.801604
13	6	0	-2.272749	-1.806452	-1.052763
14	1	0	-1.973814	-2.856039	-1.092692
15	1	0	-2.831905	-1.658682	-0.124240
16	1	0	-2.920932	-1.607943	-1.911617
17	6	0	-0.183673	-1.228970	0.176656
18	1	0	0.233050	-2.238089	0.138447
19	1	0	0.646986	-0.531063	0.258174
20	1	0	-0.828134	-1.115923	1.054609
21	6	0	-0.233481	-1.325680	-2.380047
22	1	0	0.542690	-0.605987	-2.633214
23	1	0	0.262017	-2.290317	-2.244004
24	1	0	-0.926554	-1.366886	-3.225710
25	6	0	-1.773631	5.051270	-0.905927
26	1	0	-1.375580	6.060429	-1.027108
27	1	0	-2.736379	5.021612	-1.422731
28	1	0	-1.926830	4.870358	0.162025
29	6	0	-0.663669	4.267350	-3.019368
30	1	0	-0.301648	5.278817	-3.223935
31	1	0	0.030881	3.544866	-3.452742
32	1	0	-1.645804	4.150674	-3.487103

33	6	0	0.592538	4.268525	-0.822654
34	1	0	0.813984	5.338413	-0.814563
35	1	0	0.574046	3.910357	0.209819
36	1	0	1.400403	3.772532	-1.359680
37	6	0	3.037295	-0.040991	-1.104788
38	6	0	3.452088	-0.717754	0.128093
39	1	0	3.720922	0.664591	-1.560881
40	1	0	2.381166	-0.614532	-1.743593
41	1	0	4.116069	-0.153591	0.783634
42	7	0	4.172859	-1.579632	-0.796242
43	1	0	2.672484	-1.248304	0.669791
44	6	0	5.629796	-1.532261	-0.801211
45	1	0	5.957351	-0.507831	-1.021381
46	1	0	5.941193	-2.185562	-1.618117
47	6	0	6.232688	-1.989282	0.509042
48	6	0	6.931662	-1.103391	1.327980
49	6	0	6.063501	-3.315081	0.924012
50	6	0	7.463354	-1.527989	2.545000
51	1	0	7.067253	-0.072583	1.006704
52	6	0	6.592335	-3.737477	2.138140
53	1	0	5.515540	-3.994846	0.276224
54	6	0	7.293482	-2.846805	2.951336
55	1	0	8.008237	-0.829105	3.172403
56	1	0	6.460992	-4.768376	2.452609
57	1	0	7.705599	-3.182745	3.897940
58	6	0	3.463504	-2.842515	-1.232909
59	8	0	2.230209	-2.772703	-1.070830
60	8	0	4.211972	-3.703563	-1.688408

17

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.428826	1.202332	-1.319726
2	7	0	-1.236263	0.194697	-0.970697
3	7	0	-0.990339	2.367383	-0.947363
4	6	0	-2.339943	0.732429	-0.351584
5	6	0	-2.192042	2.080847	-0.339214
6	6	0	-0.983258	-1.295402	-1.151972
7	6	0	-0.479063	3.757909	-1.231035
8	1	0	-3.141828	0.124350	0.026669
9	1	0	-2.840705	2.840443	0.058034
10	6	0	0.887790	1.120252	-2.069513
11	8	0	1.857702	0.814443	-1.254799
12	8	0	0.947540	1.400077	-3.241290
13	6	0	-2.329969	-2.007735	-1.023962
14	1	0	-2.158521	-3.064220	-1.236235
15	1	0	-2.742467	-1.948236	-0.012470
16	1	0	-3.062582	-1.631909	-1.745126
17	6	0	-0.033886	-1.736531	-0.040103
18	1	0	0.156868	-2.806324	-0.150783
19	1	0	0.938548	-1.251724	-0.137602
20	1	0	-0.487704	-1.546874	0.938656
21	6	0	-0.412465	-1.528353	-2.550151
22	1	0	0.633831	-1.229536	-2.626821
23	1	0	-0.400887	-2.605968	-2.727532
24	1	0	-1.038527	-1.049904	-3.309964
25	6	0	-1.191587	4.725299	-0.284499
26	1	0	-0.770846	5.720300	-0.440210

27	1	0	-2.262320	4.794105	-0.492419
28	1	0	-1.038320	4.450771	0.763185
29	6	0	-0.814000	4.092002	-2.686340
30	1	0	-0.454110	5.099326	-2.912530
31	1	0	-0.334558	3.385065	-3.366599
32	1	0	-1.895699	4.067703	-2.846298
33	6	0	1.030386	3.829019	-0.972833
34	1	0	1.315902	4.882411	-0.928845
35	1	0	1.297434	3.358074	-0.023469
36	1	0	1.608621	3.375781	-1.778702
37	6	0	3.191777	0.718231	-1.841018
38	6	0	4.103012	-0.030232	-0.870107
39	1	0	3.509158	1.754685	-2.009582
40	1	0	3.113860	0.186823	-2.787028
41	1	0	4.994713	0.581049	-0.686184
42	7	0	4.546498	-1.301293	-1.395068
43	1	0	3.577815	-0.117274	0.095726
44	6	0	5.842717	-1.751439	-0.919425
45	1	0	6.617118	-1.051152	-1.262566
46	1	0	6.010759	-2.721013	-1.390676
47	6	0	5.930431	-1.886873	0.589774
48	6	0	6.759200	-1.056735	1.343917
49	6	0	5.137721	-2.833082	1.251520
50	6	0	6.810141	-1.165500	2.733149
51	1	0	7.375946	-0.318374	0.835035
52	6	0	5.185695	-2.940506	2.637028
53	1	0	4.498450	-3.475851	0.651123
54	6	0	6.021740	-2.108587	3.382864
55	1	0	7.464180	-0.514315	3.305953
56	1	0	4.573089	-3.682619	3.140999
57	1	0	6.059055	-2.199438	4.464398
58	6	0	3.522262	-2.310249	-1.588434
59	8	0	2.360081	-1.828288	-1.701621
60	8	0	3.891760	-3.489847	-1.633236

$TS_{17\text{-}18}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.678695	0.431780	0.720802
2	7	0	-1.871737	0.014576	0.267374
3	7	0	-0.791478	1.695961	1.159521
4	6	0	-2.768669	1.046949	0.422859
5	6	0	-2.097331	2.088819	0.974884
6	6	0	-2.220589	-1.361164	-0.253537
7	6	0	0.306657	2.579352	1.732745
8	1	0	-3.799465	0.972709	0.126302
9	1	0	-2.452002	3.066272	1.248219
10	6	0	0.550376	-0.456313	0.797059
11	8	0	0.606783	-1.351303	1.599057
12	8	0	1.423866	-0.118975	-0.117119
13	6	0	-3.503694	-1.239025	-1.077034
14	1	0	-3.716509	-2.216071	-1.514425
15	1	0	-4.366417	-0.969378	-0.462951
16	1	0	-3.393275	-0.517751	-1.891889
17	6	0	-2.443757	-2.275612	0.952547
18	1	0	-2.701146	-3.276380	0.595729
19	1	0	-1.542180	-2.342553	1.564252
20	1	0	-3.269456	-1.906608	1.567762

21	6	0	-1.095217	-1.879239	-1.155907
22	1	0	-0.232874	-2.228545	-0.587675
23	1	0	-1.477225	-2.738150	-1.711834
24	1	0	-0.776967	-1.119580	-1.874721
25	6	0	-0.347138	3.827735	2.324393
26	1	0	0.445257	4.417478	2.789247
27	1	0	-0.813355	4.454855	1.559197
28	1	0	-1.078754	3.579448	3.098842
29	6	0	1.240957	2.989706	0.594403
30	1	0	2.045765	3.607070	1.003673
31	1	0	1.699694	2.128898	0.109705
32	1	0	0.692850	3.571067	-0.153503
33	6	0	1.020747	1.824719	2.854908
34	1	0	1.831555	2.457083	3.227313
35	1	0	0.330086	1.612020	3.675462
36	1	0	1.484621	0.893220	2.536506
37	6	0	2.767485	-0.721206	-0.014727
38	6	0	3.495998	-0.115227	1.180042
39	1	0	3.235830	-0.458179	-0.963179
40	1	0	2.662181	-1.803964	0.079369
41	1	0	3.245439	0.959280	1.214349
42	7	0	4.906734	-0.319397	1.086557
43	1	0	3.159642	-0.608494	2.097541
44	6	0	5.660842	0.740804	0.447287
45	1	0	5.425269	0.797702	-0.627467
46	1	0	6.709961	0.458654	0.560263
47	6	0	5.419880	2.102708	1.074528
48	6	0	4.924301	3.178904	0.340025
49	6	0	5.631240	2.263014	2.450804
50	6	0	4.642613	4.400435	0.956384
51	1	0	4.757266	3.059882	-0.729278
52	6	0	5.336723	3.472934	3.069002
53	1	0	6.037604	1.418811	3.004754
54	6	0	4.837441	4.545972	2.326309
55	1	0	4.269981	5.233743	0.365826
56	1	0	5.508054	3.587964	4.135463
57	1	0	4.621829	5.493471	2.811870
58	6	0	5.539021	-1.025140	2.245513
59	8	0	6.746843	-0.775375	2.390707
60	8	0	4.751056	-1.744341	2.877803

18

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.634868	0.478421	0.676002
2	7	0	-1.838166	0.031311	0.284187
3	7	0	-0.728385	1.781418	0.984814
4	6	0	-2.722317	1.085576	0.343353
5	6	0	-2.032453	2.170567	0.775830
6	6	0	-2.210750	-1.393982	-0.054230
7	6	0	0.388045	2.697781	1.456195
8	1	0	-3.758408	0.992477	0.071300
9	1	0	-2.372546	3.175416	0.952033
10	6	0	0.588714	-0.409932	0.827200
11	8	0	0.670678	-1.164830	1.760013
12	8	0	1.413294	-0.230454	-0.172053
13	6	0	-3.518019	-1.362016	-0.846957
14	1	0	-3.751761	-2.384052	-1.150377

15	1	0	-4.359150	-1.008079	-0.245480
16	1	0	-3.428834	-0.750864	-1.749790
17	6	0	-2.402082	-2.149793	1.262220
18	1	0	-2.677324	-3.184014	1.039793
19	1	0	-1.482393	-2.151539	1.850488
20	1	0	-3.205411	-1.697343	1.850815
21	6	0	-1.116559	-2.031181	-0.917616
22	1	0	-0.233427	-2.306931	-0.340829
23	1	0	-1.518300	-2.954684	-1.340227
24	1	0	-0.823612	-1.375667	-1.741793
25	6	0	-0.244365	3.972821	2.011716
26	1	0	0.566548	4.595968	2.394344
27	1	0	-0.762881	4.552039	1.242653
28	1	0	-0.926655	3.760691	2.840035
29	6	0	1.267355	3.032332	0.251249
30	1	0	2.140129	3.590606	0.602354
31	1	0	1.621167	2.126982	-0.243053
32	1	0	0.717784	3.642198	-0.471909
33	6	0	1.172700	2.006276	2.570650
34	1	0	1.882996	2.723313	2.991889
35	1	0	0.505872	1.656699	3.363631
36	1	0	1.772721	1.172035	2.213038
37	6	0	2.742945	-0.885458	-0.073300
38	6	0	3.604272	0.031464	0.774630
39	1	0	3.094064	-0.939379	-1.102938
40	1	0	2.642659	-1.869564	0.378077
41	1	0	3.408568	1.060630	0.444209
42	7	0	5.015333	-0.222955	0.656488
43	1	0	3.260065	-0.063778	1.818558
44	6	0	5.840694	0.967128	0.800392
45	1	0	5.818712	1.557307	-0.127463
46	1	0	6.854285	0.595886	0.965522
47	6	0	5.406121	1.851006	1.954694
48	6	0	4.909033	3.138322	1.744250
49	6	0	5.406586	1.332828	3.256215
50	6	0	4.426881	3.906431	2.806029
51	1	0	4.909072	3.545765	0.734293
52	6	0	4.917114	2.091816	4.314149
53	1	0	5.800064	0.328741	3.404859
54	6	0	4.426067	3.380952	4.095473
55	1	0	4.062069	4.915331	2.626723
56	1	0	4.925202	1.681002	5.319441
57	1	0	4.058014	3.973616	4.928107
58	6	0	5.444794	-1.432152	1.403890
59	8	0	6.603365	-1.404134	1.845442
60	8	0	4.548082	-2.296048	1.474988

$TS_{18\text{-}10}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.878903	0.597675	0.546881
2	7	0	-2.041575	0.036401	0.182412
3	7	0	-1.035686	1.929771	0.591562
4	6	0	-2.963620	1.044004	-0.009673
5	6	0	-2.338124	2.219512	0.241759
6	6	0	-2.340398	-1.440287	0.086878
7	6	0	0.027660	2.958403	0.900881
8	1	0	-3.977499	0.855242	-0.313674

9	1	0	-2.719579	3.223954	0.203167
10	6	0	0.387125	-0.181187	0.908677
11	8	0	0.397992	-0.778798	1.966549
12	8	0	1.271715	-0.087972	-0.011164
13	6	0	-3.589742	-1.611458	-0.778335
14	1	0	-3.765154	-2.680738	-0.909343
15	1	0	-4.482796	-1.196334	-0.304012
16	1	0	-3.459281	-1.164485	-1.768272
17	6	0	-2.593622	-1.956503	1.504597
18	1	0	-2.815489	-3.026087	1.459736
19	1	0	-1.712455	-1.803640	2.131185
20	1	0	-3.450584	-1.444838	1.952697
21	6	0	-1.165925	-2.169168	-0.575835
22	1	0	-0.327358	-2.306895	0.106817
23	1	0	-1.508102	-3.163792	-0.870001
24	1	0	-0.823217	-1.643919	-1.470917
25	6	0	-0.671012	4.277579	1.231442
26	1	0	0.096227	4.998772	1.519230
27	1	0	-1.197733	4.695381	0.369245
28	1	0	-1.365862	4.169323	2.069421
29	6	0	0.899629	3.118936	-0.345257
30	1	0	1.704920	3.826484	-0.129100
31	1	0	1.340558	2.163927	-0.635856
32	1	0	0.309118	3.509381	-1.179523
33	6	0	0.840962	2.506064	2.116184
34	1	0	1.488320	3.330893	2.423916
35	1	0	0.188721	2.244578	2.953461
36	1	0	1.496122	1.664066	1.898800
37	6	0	2.790883	-0.868514	0.306347
38	6	0	3.554844	0.318146	0.857403
39	1	0	2.979744	-1.154883	-0.718575
40	1	0	2.424887	-1.628952	0.976864
41	1	0	3.163996	1.238917	0.403459
42	7	0	4.950252	0.212791	0.529041
43	1	0	3.370669	0.382834	1.945760
44	6	0	5.773554	1.354888	0.867547
45	1	0	5.522905	2.197575	0.206923
46	1	0	6.801155	1.042788	0.668563
47	6	0	5.624804	1.790922	2.311892
48	6	0	5.003761	2.992844	2.649167
49	6	0	6.049095	0.935650	3.335310
50	6	0	4.815629	3.350796	3.983912
51	1	0	4.669225	3.657630	1.853854
52	6	0	5.859873	1.289825	4.666528
53	1	0	6.521290	-0.004317	3.057511
54	6	0	5.243686	2.497629	4.995660
55	1	0	4.338131	4.294720	4.232492
56	1	0	6.195290	0.621746	5.454116
57	1	0	5.100049	2.770711	6.036677
58	6	0	5.478611	-1.113023	0.751829
59	8	0	6.690018	-1.239379	0.936363
60	8	0	4.560288	-1.986996	0.705572

19

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.163419	0.613403	-0.051366
2	7	0	6.474781	0.393972	0.170915

3	7	0	4.866099	1.870783	0.304521
4	6	0	7.016070	1.550614	0.685865
5	6	0	6.017901	2.463030	0.769083
6	6	0	7.289827	-0.818961	-0.213476
7	6	0	3.521097	2.573528	0.188425
8	1	0	8.051197	1.638929	0.960880
9	1	0	6.044907	3.477115	1.123465
10	6	0	7.586356	-0.720845	-1.711725
11	1	0	8.148399	0.191042	-1.932936
12	1	0	8.191024	-1.580849	-2.011924
13	1	0	6.661362	-0.720958	-2.291364
14	6	0	6.538790	-2.112083	0.123274
15	1	0	7.255596	-2.934756	0.075045
16	1	0	6.115229	-2.080622	1.130151
17	1	0	5.750468	-2.331504	-0.596843
18	6	0	8.592997	-0.784137	0.588701
19	1	0	9.149763	-1.695853	0.365126
20	1	0	9.231564	0.056444	0.306782
21	1	0	8.403523	-0.755433	1.665614
22	6	0	3.102299	2.551003	-1.282245
23	1	0	2.192220	3.148508	-1.381293
24	1	0	3.884161	3.000777	-1.902537
25	1	0	2.836300	1.548692	-1.624711
26	6	0	2.529954	1.862524	1.107544
27	1	0	2.309003	0.856831	0.746784
28	1	0	2.904207	1.850502	2.136204
29	1	0	1.587911	2.417239	1.082962
30	6	0	3.707953	4.018343	0.649422
31	1	0	4.421010	4.564426	0.024151
32	1	0	2.739943	4.512564	0.551892
33	1	0	4.006818	4.084396	1.700248
34	6	0	4.271423	-0.449645	-0.677551
35	8	0	3.658101	-1.127547	0.262161
36	8	0	4.330683	-0.657118	-1.859343
37	6	0	2.795025	-2.225206	-0.154494
38	1	0	3.330297	-3.123139	0.172510
39	6	0	1.424451	-2.099598	0.515636
40	1	0	2.695582	-2.207592	-1.237563
41	6	0	-4.883899	-1.828958	-0.519921
42	8	0	-5.656735	-2.182312	0.342956
43	8	0	-4.165993	-2.250038	-1.393852
44	6	0	-4.608605	0.528644	-1.807331
45	6	0	-3.447077	0.430867	-0.903525
46	7	0	-4.754452	-0.115113	-0.494644
47	6	0	-5.536330	0.585569	0.548095
48	6	0	-6.918090	0.965726	0.076983
49	6	0	-7.236741	2.305312	-0.151051
50	6	0	-7.889233	-0.014514	-0.151740
51	6	0	-9.153492	0.349199	-0.603621
52	6	0	-9.464699	1.689055	-0.828680
53	6	0	-8.504064	2.668929	-0.600505
54	1	0	-5.142823	1.466913	-1.914866
55	1	0	-2.668618	-0.291206	-1.126192
56	1	0	-3.132451	1.306695	-0.345962
57	1	0	-5.579848	-0.108559	1.389035
58	1	0	-4.980918	1.476487	0.857608
59	1	0	-6.485715	3.071399	0.028810
60	1	0	-8.738335	3.714839	-0.772314
61	1	0	-10.453557	1.967915	-1.178979
62	1	0	-9.902063	-0.417451	-0.777549
63	1	0	-7.634748	-1.054992	0.026666
64	1	0	-4.661124	-0.171746	-2.633107

65	7	0	0.370383	-1.800584	-0.425274
66	6	0	-0.949337	-2.285641	-0.093457
67	6	0	0.447902	-0.541034	-1.123185
68	8	0	-0.577663	-0.146920	-1.692207
69	8	0	1.584910	0.009671	-1.053149
70	1	0	-1.573543	-2.203009	-0.988239
71	1	0	-0.890478	-3.353101	0.155560
72	6	0	-1.641189	-1.551997	1.044999
73	6	0	-2.798224	-2.093580	1.607893
74	6	0	-1.190254	-0.311802	1.505397
75	6	0	-3.499380	-1.413431	2.599207
76	1	0	-3.173900	-3.046853	1.243820
77	6	0	-1.884911	0.367922	2.504000
78	1	0	-0.298538	0.130113	1.068939
79	6	0	-3.043101	-0.177344	3.053414
80	1	0	-4.411158	-1.846915	2.999034
81	1	0	-1.520874	1.330748	2.852336
82	1	0	-3.586125	0.355780	3.828368
83	1	0	1.181376	-3.058610	0.986144
84	1	0	1.517833	-1.363868	1.332691

$TS_{19\text{-}20}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.475061	0.676394	0.896173
2	7	0	-1.788642	0.683114	1.184890
3	7	0	-0.158123	1.808717	0.257133
4	6	0	-2.317362	1.861003	0.707491
5	6	0	-1.305151	2.555884	0.129916
6	6	0	-2.557490	-0.352342	1.969739
7	6	0	1.200181	2.203161	-0.303794
8	1	0	-3.357986	2.113318	0.803516
9	1	0	-1.318130	3.517133	-0.352060
10	6	0	-2.271807	-0.125163	3.455703
11	1	0	-2.594914	0.874275	3.760384
12	1	0	-2.830007	-0.860930	4.040697
13	1	0	-1.207880	-0.238509	3.671902
14	6	0	-2.144900	-1.759434	1.522990
15	1	0	-2.876072	-2.467719	1.918537
16	1	0	-2.137211	-1.846706	0.433341
17	1	0	-1.172845	-2.052936	1.920774
18	6	0	-4.046260	-0.155509	1.678604
19	1	0	-4.596370	-0.946570	2.191278
20	1	0	-4.421234	0.795976	2.063667
21	1	0	-4.262333	-0.229132	0.608846
22	6	0	2.281814	1.818706	0.704429
23	1	0	3.222861	2.257519	0.366093
24	1	0	2.046033	2.205813	1.700294
25	1	0	2.472583	0.745472	0.717611
26	6	0	1.367136	1.489710	-1.643908
27	1	0	1.387022	0.407574	-1.512567
28	1	0	0.573644	1.792877	-2.334890
29	1	0	2.337787	1.760506	-2.065069
30	6	0	1.195598	3.719582	-0.496594
31	1	0	0.968347	4.249616	0.433415
32	1	0	2.197862	4.010391	-0.815314
33	1	0	0.505853	4.039917	-1.282552
34	6	0	0.465305	-0.435258	1.311872

35	8	0	0.768563	-1.190699	0.288368
36	8	0	0.795256	-0.573355	2.462328
37	6	0	1.669817	-2.303430	0.560217
38	1	0	1.086208	-3.034477	1.130686
39	6	0	2.186831	-2.853423	-0.772707
40	1	0	2.492089	-1.936749	1.173786
41	6	0	8.063849	-4.626139	0.589777
42	8	0	9.162239	-5.059575	0.929609
43	8	0	7.087530	-5.107062	-0.002756
44	6	0	6.475571	-2.683008	1.042461
45	6	0	6.849685	-2.253489	-0.301396
46	7	0	7.852983	-3.159843	0.955635
47	6	0	8.867527	-2.469716	1.744911
48	6	0	8.625448	-2.583651	3.233326
49	6	0	8.303084	-1.461979	3.996594
50	6	0	8.696482	-3.835682	3.854738
51	6	0	8.450833	-3.951117	5.218226
52	6	0	8.131948	-2.824415	5.976621
53	6	0	8.058583	-1.578193	5.364118
54	1	0	6.340500	-1.898965	1.787312
55	1	0	6.883330	-2.993021	-1.087669
56	1	0	7.419626	-1.341052	-0.404135
57	1	0	9.816644	-2.934197	1.471983
58	1	0	8.889397	-1.411277	1.454353
59	1	0	8.247262	-0.487337	3.516025
60	1	0	7.810126	-0.696582	5.947341
61	1	0	7.943388	-2.919908	7.041638
62	1	0	8.512513	-4.924887	5.694708
63	1	0	8.948163	-4.701158	3.246880
64	1	0	5.753204	-3.490813	1.128671
65	7	0	3.628337	-2.767837	-0.866018
66	6	0	4.376715	-3.910755	-1.379803
67	6	0	4.141010	-1.452789	-0.929698
68	8	0	5.379315	-1.289070	-1.143154
69	8	0	3.300879	-0.539324	-0.768961
70	1	0	5.208552	-4.181516	-0.724336
71	1	0	3.699702	-4.772154	-1.349434
72	6	0	4.903434	-3.771623	-2.793269
73	6	0	6.034838	-4.507342	-3.155238
74	6	0	4.278832	-2.964830	-3.743229
75	6	0	6.519800	-4.448419	-4.459500
76	1	0	6.539258	-5.104098	-2.395670
77	6	0	4.766399	-2.905115	-5.044948
78	1	0	3.420008	-2.363303	-3.453752
79	6	0	5.885167	-3.651496	-5.408519
80	1	0	7.402595	-5.019361	-4.730641
81	1	0	4.277893	-2.268316	-5.776735
82	1	0	6.267220	-3.601147	-6.423536
83	1	0	1.905029	-3.904908	-0.861334
84	1	0	1.684036	-2.298051	-1.577421

20

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.066159	-0.118369	1.600536
2	7	0	0.191369	-0.267707	2.611571
3	7	0	1.381042	1.176772	1.477450
4	6	0	-0.039102	0.976533	3.152059

5	6	0	0.700989	1.871172	2.448504
6	6	0	-0.439389	-1.551686	3.108914
7	6	0	2.314193	1.790164	0.454503
8	1	0	-0.710772	1.137888	3.975913
9	1	0	0.795498	2.935260	2.571516
10	6	0	0.522657	-2.240829	4.079054
11	1	0	0.727094	-1.598675	4.940948
12	1	0	0.048772	-3.156065	4.444502
13	1	0	1.461882	-2.510988	3.592817
14	6	0	-0.784837	-2.459099	1.920101
15	1	0	-1.488185	-3.217383	2.270660
16	1	0	-1.264978	-1.896149	1.114088
17	1	0	0.086257	-2.990536	1.535179
18	6	0	-1.734888	-1.175564	3.833134
19	1	0	-2.238277	-2.099932	4.121550
20	1	0	-1.546484	-0.616614	4.753208
21	1	0	-2.409609	-0.604195	3.188803
22	6	0	3.551131	0.906699	0.341141
23	1	0	4.328701	1.450970	-0.200034
24	1	0	3.932711	0.621428	1.324929
25	1	0	3.347852	0.027060	-0.266555
26	6	0	1.566713	1.867407	-0.876468
27	1	0	1.253819	0.872303	-1.199108
28	1	0	0.693348	2.522766	-0.803374
29	1	0	2.247328	2.261253	-1.635159
30	6	0	2.703842	3.181818	0.945529
31	1	0	3.190497	3.129185	1.923864
32	1	0	3.419839	3.592898	0.231722
33	1	0	1.852463	3.868114	0.982192
34	6	0	1.680746	-1.312722	0.904926
35	8	0	1.314352	-1.419505	-0.359952
36	8	0	2.344315	-2.071664	1.548899
37	6	0	1.648149	-2.683338	-1.029038
38	1	0	0.700524	-3.230241	-1.056423
39	6	0	2.156360	-2.385344	-2.444854
40	1	0	2.393515	-3.227992	-0.427091
41	6	0	4.596870	-3.694748	1.515440
42	8	0	4.394280	-4.085609	2.675705
43	8	0	4.061132	-4.064344	0.434897
44	6	0	5.448249	-1.823949	0.173051
45	6	0	6.122860	-2.433245	-1.050125
46	7	0	5.595575	-2.652770	1.344123
47	6	0	6.199596	-2.058709	2.518291
48	6	0	5.447775	-0.858299	3.069089
49	6	0	5.986501	0.428586	3.033851
50	6	0	4.160708	-1.036933	3.595604
51	6	0	3.433787	0.055780	4.057497
52	6	0	3.980190	1.341428	4.015046
53	6	0	5.262690	1.525468	3.506074
54	1	0	5.851272	-0.820132	0.359378
55	1	0	5.885384	-3.495732	-1.082670
56	1	0	7.207240	-2.312038	-1.018476
57	1	0	6.224062	-2.847349	3.273063
58	1	0	7.231429	-1.756833	2.291522
59	1	0	6.985866	0.574099	2.629546
60	1	0	5.701014	2.519101	3.475540
61	1	0	3.415660	2.188958	4.396967
62	1	0	2.440364	-0.089784	4.477537
63	1	0	3.768934	-2.051273	3.616330
64	1	0	4.380308	-1.715264	-0.057297
65	7	0	3.585050	-2.597517	-2.590292
66	6	0	4.018670	-3.999623	-2.633359

67	6	0	4.399456	-1.506307	-2.424779
68	8	0	5.718537	-1.752670	-2.258933
69	8	0	3.975694	-0.363445	-2.472126
70	1	0	4.186299	-4.376712	-1.617343
71	1	0	3.159717	-4.549204	-3.039788
72	6	0	5.200193	-4.283399	-3.532341
73	6	0	6.117898	-5.256911	-3.141456
74	6	0	5.358769	-3.657389	-4.769769
75	6	0	7.175637	-5.609848	-3.976214
76	1	0	6.000185	-5.735903	-2.172241
77	6	0	6.417870	-4.003156	-5.601353
78	1	0	4.653455	-2.887831	-5.072857
79	6	0	7.328028	-4.983136	-5.208527
80	1	0	7.883708	-6.368410	-3.657475
81	1	0	6.536097	-3.506088	-6.559331
82	1	0	8.154955	-5.251091	-5.858547
83	1	0	1.640968	-3.041523	-3.152993
84	1	0	1.931410	-1.351538	-2.711421

$TS_{20\text{-}17}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.013344	-0.195371	1.066722
2	7	0	0.054412	-0.396289	1.992561
3	7	0	1.469600	1.060330	1.172529
4	6	0	-0.072806	0.764086	2.719103
5	6	0	0.808736	1.662926	2.212188
6	6	0	-0.788058	-1.634850	2.209470
7	6	0	2.534407	1.737825	0.326759
8	1	0	-0.774418	0.873073	3.526010
9	1	0	1.018315	2.671312	2.521522
10	6	0	0.027212	-2.659538	3.000007
11	1	0	0.252420	-2.282216	4.001451
12	1	0	-0.566133	-3.571825	3.106996
13	1	0	0.958427	-2.904265	2.488667
14	6	0	-1.251671	-2.185555	0.854591
15	1	0	-2.052580	-2.905290	1.036865
16	1	0	-1.649694	-1.387727	0.221022
17	1	0	-0.461016	-2.716187	0.325091
18	6	0	-2.025022	-1.227235	3.014110
19	1	0	-2.662787	-2.107561	3.112506
20	1	0	-1.771852	-0.902296	4.026123
21	1	0	-2.599190	-0.444991	2.509382
22	6	0	3.682031	0.758671	0.129760
23	1	0	4.507170	1.264855	-0.375783
24	1	0	4.030689	0.390036	1.097522
25	1	0	3.433042	-0.080668	-0.520975
26	6	0	1.893860	2.178398	-0.989641
27	1	0	1.523828	1.326287	-1.559128
28	1	0	1.072570	2.878880	-0.809435
29	1	0	2.656670	2.684225	-1.586658
30	6	0	3.038573	2.960282	1.093186
31	1	0	3.413886	2.679640	2.080614
32	1	0	3.870550	3.380487	0.525125
33	1	0	2.278632	3.742377	1.183014
34	6	0	1.457755	-1.270476	0.098340
35	8	0	1.185194	-0.911066	-1.141701
36	8	0	1.887894	-2.323235	0.483386

37	6	0	1.434863	-1.864559	-2.213381
38	1	0	0.697400	-1.596407	-2.971247
39	6	0	2.839412	-1.752108	-2.779955
40	1	0	1.220620	-2.867189	-1.833271
41	6	0	9.001529	-0.498994	1.242801
42	8	0	9.745685	-0.182106	2.164095
43	8	0	9.275347	-0.829850	0.040937
44	6	0	6.874523	-0.476354	0.205218
45	6	0	7.543878	-1.466746	-0.720548
46	7	0	7.574056	-0.523564	1.469482
47	6	0	7.093025	0.339199	2.515546
48	6	0	5.702911	-0.017602	2.997732
49	6	0	4.910866	0.953629	3.618637
50	6	0	5.162121	-1.291638	2.802869
51	6	0	3.850868	-1.574894	3.180551
52	6	0	3.064387	-0.592224	3.779814
53	6	0	3.605685	0.671675	4.013630
54	1	0	6.899692	0.526195	-0.253280
55	1	0	7.853631	-2.423849	-0.333091
56	1	0	7.906978	-1.153678	-1.685852
57	1	0	7.824875	0.266621	3.326895
58	1	0	7.078557	1.401100	2.201791
59	1	0	5.325936	1.946288	3.781997
60	1	0	3.011105	1.437524	4.506592
61	1	0	2.044675	-0.812346	4.085721
62	1	0	3.443912	-2.565550	3.000119
63	1	0	5.780633	-2.043755	2.321503
64	1	0	5.829347	-0.755546	0.352477
65	7	0	3.856035	-2.275535	-1.898295
66	6	0	3.814121	-3.711582	-1.639299
67	6	0	5.108939	-1.597783	-1.873712
68	8	0	6.066628	-2.314936	-1.404416
69	8	0	5.161465	-0.421441	-2.234700
70	1	0	4.671215	-3.933101	-1.004322
71	1	0	2.909717	-3.948687	-1.067253
72	6	0	3.857075	-4.547636	-2.900854
73	6	0	2.787662	-5.367264	-3.257730
74	6	0	4.969121	-4.475774	-3.746805
75	6	0	2.821377	-6.113413	-4.434789
76	1	0	1.921644	-5.429385	-2.601156
77	6	0	5.004051	-5.216499	-4.922721
78	1	0	5.804368	-3.841628	-3.459447
79	6	0	3.930381	-6.037024	-5.270161
80	1	0	1.982231	-6.749819	-4.698737
81	1	0	5.873855	-5.160180	-5.569787
82	1	0	3.961506	-6.615485	-6.188056
83	1	0	2.821816	-2.290725	-3.742230
84	1	0	3.083960	-0.707020	-2.982871

21

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.104043	0.165253	0.517918
2	7	0	-2.793255	1.191617	-0.323059
3	7	0	-2.782305	-0.931641	-0.232615
4	6	0	-2.310939	0.752856	-1.548633
5	6	0	-2.296830	-0.598778	-1.487894
6	6	0	-3.026170	2.615917	-0.005430

7	6	0	-2.928668	-2.300407	0.317414
8	1	0	-2.019072	1.411726	-2.350842
9	1	0	-1.964395	-1.318899	-2.216578
10	6	0	-1.780254	3.424383	-0.380101
11	1	0	-1.589589	3.406836	-1.457075
12	1	0	-1.917701	4.468519	-0.085418
13	1	0	-0.900531	3.024352	0.131859
14	6	0	-3.296004	2.758738	1.490347
15	1	0	-3.470571	3.814378	1.718429
16	1	0	-4.163320	2.169793	1.788567
17	1	0	-2.441375	2.402703	2.071269
18	6	0	-4.239309	3.095936	-0.808156
19	1	0	-4.441560	4.150433	-0.598506
20	1	0	-4.065232	2.986094	-1.882997
21	1	0	-5.120806	2.507829	-0.539304
22	6	0	-2.628937	-3.335643	-0.763909
23	1	0	-2.764287	-4.334937	-0.342448
24	1	0	-3.311461	-3.230893	-1.612912
25	1	0	-1.599435	-3.255912	-1.124741
26	6	0	-1.950142	-2.454970	1.484655
27	1	0	-0.915044	-2.363937	1.138608
28	1	0	-2.137757	-1.672331	2.223461
29	1	0	-2.070587	-3.435129	1.955540
30	6	0	-4.367331	-2.464535	0.812454
31	1	0	-5.069713	-2.359759	-0.019749
32	1	0	-4.498600	-3.454265	1.259945
33	1	0	-4.591379	-1.695527	1.553413
34	6	0	0.323287	0.601314	0.745160
35	6	0	1.138561	1.133512	-0.377752
36	1	0	-0.524735	-0.042769	0.535255
37	1	0	0.230057	1.217564	1.638665
38	1	0	0.879588	0.862611	-1.396745
39	1	0	1.601958	2.111049	-0.250575
40	7	0	1.637702	0.050335	0.449808
41	6	0	2.704101	0.413703	1.382815
42	6	0	1.274240	-2.333651	-0.553800
43	8	0	1.936650	-2.878006	0.233263
44	8	0	0.578057	-1.894781	-1.379711
45	1	0	2.511082	1.396829	1.845363
46	1	0	2.705004	-0.335553	2.182386
47	6	0	4.039328	0.439607	0.681448
48	6	0	4.619118	-0.751619	0.236632
49	6	0	4.695743	1.644520	0.435167
50	6	0	5.834477	-0.734611	-0.437841
51	1	0	4.107775	-1.691677	0.424648
52	6	0	5.914955	1.664671	-0.239530
53	1	0	4.251999	2.575206	0.781018
54	6	0	6.485961	0.474633	-0.677308
55	1	0	6.277612	-1.666101	-0.776219
56	1	0	6.416747	2.609915	-0.421223
57	1	0	7.435815	0.486994	-1.202378

$TS_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.665686	0.269800	-0.888870
2	7	0	-1.410722	-0.760616	-0.394760
3	7	0	-1.212219	1.375046	-0.314323

4	6	0	-2.368542	-0.309086	0.499187
5	6	0	-2.242842	1.035287	0.546480
6	6	0	-1.240895	-2.186501	-0.777157
7	6	0	-0.914375	2.808012	-0.628342
8	1	0	-3.064565	-0.954987	1.007176
9	1	0	-2.810073	1.762957	1.103588
10	6	0	-0.245190	-2.867485	0.168127
11	1	0	-0.548422	-2.731416	1.211034
12	1	0	-0.208358	-3.940140	-0.042796
13	1	0	0.763401	-2.465659	0.046283
14	6	0	-0.762961	-2.260097	-2.228035
15	1	0	-0.637238	-3.309287	-2.508916
16	1	0	-1.499624	-1.803892	-2.894378
17	1	0	0.184934	-1.742866	-2.374399
18	6	0	-2.596487	-2.894562	-0.674338
19	1	0	-2.503630	-3.897316	-1.098355
20	1	0	-2.925414	-3.008821	0.362110
21	1	0	-3.364204	-2.353016	-1.233704
22	6	0	-0.431060	3.513649	0.641019
23	1	0	-0.317342	4.581375	0.432850
24	1	0	-1.145688	3.406020	1.463087
25	1	0	0.549050	3.132369	0.941597
26	6	0	0.156469	2.929163	-1.714060
27	1	0	1.158272	2.821368	-1.292502
28	1	0	-0.006357	2.203128	-2.514438
29	1	0	0.093898	3.933786	-2.140356
30	6	0	-2.220129	3.430742	-1.141090
31	1	0	-3.017917	3.392896	-0.394588
32	1	0	-2.045864	4.480373	-1.389747
33	1	0	-2.561494	2.910465	-2.040816
34	6	0	1.451757	0.107522	-0.595318
35	6	0	1.508532	0.151776	0.869845
36	1	0	1.645533	1.013695	-1.140881
37	1	0	1.571997	-0.843784	-1.097194
38	1	0	1.195577	1.080851	1.338531
39	1	0	1.196129	-0.740214	1.413053
40	7	0	2.909170	0.144739	0.492292
41	6	0	3.692993	-1.061690	0.753558
42	6	0	3.616609	1.525615	0.467664
43	8	0	4.832590	1.434832	0.571117
44	8	0	2.803366	2.445073	0.329530
45	1	0	3.258079	-1.902219	0.195488
46	1	0	4.689029	-0.852221	0.359632
47	6	0	3.748349	-1.396925	2.225273
48	6	0	4.426847	-0.544378	3.102624
49	6	0	3.098784	-2.522547	2.730990
50	6	0	4.452856	-0.825152	4.463940
51	1	0	4.923327	0.332537	2.694428
52	6	0	3.126749	-2.804034	4.096068
53	1	0	2.574228	-3.190241	2.049322
54	6	0	3.804131	-1.954196	4.963755
55	1	0	4.984311	-0.162235	5.139634
56	1	0	2.622132	-3.685833	4.478843
57	1	0	3.828993	-2.170450	6.027206

22

Standard orientation:

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

1	6	0	-0.527704	0.174651	-0.596196
2	7	0	-1.444171	-0.826925	-0.601503
3	7	0	-1.183614	1.333648	-0.361105
4	6	0	-2.687201	-0.283394	-0.348859
5	6	0	-2.522953	1.048246	-0.193852
6	6	0	-1.239753	-2.260963	-1.019322
7	6	0	-0.631569	2.755439	-0.319385
8	1	0	-3.586449	-0.868620	-0.296262
9	1	0	-3.261277	1.799950	0.012335
10	6	0	-0.128996	-2.932620	-0.205821
11	1	0	-0.287221	-2.784951	0.865842
12	1	0	-0.161599	-4.005649	-0.410252
13	1	0	0.867639	-2.580771	-0.468028
14	6	0	-0.943322	-2.282978	-2.521966
15	1	0	-0.841985	-3.319853	-2.853163
16	1	0	-1.764313	-1.820607	-3.077071
17	1	0	-0.018880	-1.758737	-2.768907
18	6	0	-2.539694	-3.029543	-0.760839
19	1	0	-2.367534	-4.075347	-1.021330
20	1	0	-2.830119	-2.989565	0.292931
21	1	0	-3.364149	-2.671813	-1.382658
22	6	0	0.190898	2.952574	0.954684
23	1	0	0.368354	4.025092	1.078359
24	1	0	-0.358969	2.595360	1.831271
25	1	0	1.172999	2.477969	0.868817
26	6	0	0.211906	3.041086	-1.573568
27	1	0	1.252520	2.733985	-1.444000
28	1	0	-0.228868	2.578740	-2.462126
29	1	0	0.219938	4.122319	-1.732640
30	6	0	-1.830806	3.709137	-0.303226
31	1	0	-2.423749	3.615895	0.611229
32	1	0	-1.434955	4.725207	-0.324909
33	1	0	-2.474963	3.581735	-1.179058
34	6	0	0.941039	0.011703	-0.728855
35	6	0	1.689424	-0.225027	0.609850
36	1	0	1.390149	0.918302	-1.125943
37	1	0	1.173568	-0.802766	-1.414121
38	1	0	1.387310	0.545987	1.329299
39	1	0	1.406687	-1.187459	1.046683
40	7	0	3.101752	-0.220267	0.347531
41	6	0	3.886276	-1.269410	0.972405
42	6	0	3.725437	1.086317	0.150539
43	8	0	4.950398	1.134556	0.295909
44	8	0	2.906253	1.996272	-0.159311
45	1	0	3.564986	-2.249704	0.589434
46	1	0	4.916519	-1.092661	0.658342
47	6	0	3.793708	-1.273016	2.485235
48	6	0	4.278662	-0.175417	3.206999
49	6	0	3.191616	-2.323889	3.175563
50	6	0	4.162960	-0.143948	4.591764
51	1	0	4.746923	0.636362	2.654875
52	6	0	3.076121	-2.293945	4.565267
53	1	0	2.814253	-3.179383	2.617107
54	6	0	3.562122	-1.202134	5.275598
55	1	0	4.546576	0.708456	5.144766
56	1	0	2.607348	-3.121629	5.089709
57	1	0	3.476215	-1.173661	6.357655

$TS_{22\text{-}11}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.772978	0.472460	-0.496703
2	7	0	-1.457120	-0.560588	0.063820
3	7	0	-1.516518	1.574753	-0.208551
4	6	0	-2.593014	-0.104143	0.709683
5	6	0	-2.631870	1.234789	0.539063
6	6	0	-1.119973	-2.010914	-0.105091
7	6	0	-1.257818	2.946015	-0.745444
8	1	0	-3.280841	-0.746072	1.230369
9	1	0	-3.357459	1.947327	0.888611
10	6	0	0.189754	-2.348147	0.609163
11	1	0	0.146730	-2.056646	1.664407
12	1	0	0.345053	-3.430409	0.572317
13	1	0	1.067376	-1.879497	0.159929
14	6	0	-1.049435	-2.311868	-1.604625
15	1	0	-0.799126	-3.365799	-1.752088
16	1	0	-2.015075	-2.113044	-2.078680
17	1	0	-0.292129	-1.708613	-2.106124
18	6	0	-2.235538	-2.859834	0.509389
19	1	0	-1.995331	-3.910611	0.334986
20	1	0	-2.307104	-2.713103	1.591034
21	1	0	-3.206643	-2.657797	0.048123
22	6	0	0.039697	3.514028	-0.164748
23	1	0	0.118828	4.571339	-0.432175
24	1	0	0.038614	3.433852	0.926066
25	1	0	0.924237	3.009931	-0.552698
26	6	0	-1.201879	2.861195	-2.272982
27	1	0	-0.419570	2.180650	-2.611792
28	1	0	-2.158202	2.506087	-2.667220
29	1	0	-0.999715	3.852340	-2.688106
30	6	0	-2.411391	3.870016	-0.347229
31	1	0	-2.475525	3.996676	0.737499
32	1	0	-2.228025	4.853153	-0.785661
33	1	0	-3.370685	3.508470	-0.727600
34	6	0	1.230472	0.455144	-1.005601
35	6	0	1.751263	0.552964	0.423909
36	1	0	1.139083	-0.515015	-1.466201
37	1	0	1.946046	1.609770	0.673307
38	1	0	1.032192	0.170571	1.154763
39	7	0	2.954368	-0.238116	0.479134
40	6	0	3.600863	-0.386013	1.764733
41	6	0	3.759561	-0.033234	-0.683304
42	8	0	4.938060	-0.352158	-0.688638
43	8	0	3.048502	0.480815	-1.626313
44	1	0	4.622219	-0.708626	1.545686
45	1	0	3.656578	0.578789	2.297008
46	6	0	2.879866	-1.400843	2.621807
47	6	0	2.051069	-1.011100	3.672505
48	6	0	2.990661	-2.761549	2.319498
49	6	0	1.338589	-1.958439	4.409057
50	1	0	1.963897	0.045795	3.915213
51	6	0	2.289988	-3.710051	3.054970
52	1	0	3.626115	-3.061910	1.489870
53	6	0	1.456955	-3.309620	4.100729
54	1	0	0.697772	-1.640120	5.225789
55	1	0	2.390930	-4.764406	2.815253
56	1	0	0.909836	-4.050533	4.675369
57	1	0	1.098418	1.315881	-1.635846

23

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.679764	-1.831805	-1.606113
2	8	0	-3.475470	-2.219456	-2.430663
3	8	0	-1.518210	-1.518105	-1.472979
4	6	0	2.234389	1.861392	-0.021952
5	7	0	3.207887	2.011992	-0.955301
6	7	0	1.607346	3.054236	0.113930
7	6	0	3.173143	3.309551	-1.419974
8	6	0	2.182309	3.950326	-0.763468
9	6	0	4.288618	1.027469	-1.334480
10	6	0	0.503497	3.443045	1.086881
11	1	0	3.839958	3.681535	-2.175280
12	1	0	1.855764	4.968302	-0.860687
13	6	0	3.687924	-0.310290	-1.763869
14	1	0	2.894858	-0.165794	-2.502980
15	1	0	4.478250	-0.912802	-2.218732
16	1	0	3.302006	-0.889001	-0.926832
17	6	0	5.238617	0.862088	-0.144665
18	1	0	6.034881	0.166676	-0.424439
19	1	0	5.688405	1.822033	0.125407
20	1	0	4.737972	0.445871	0.730920
21	6	0	5.071953	1.605653	-2.516605
22	1	0	5.820324	0.867957	-2.811290
23	1	0	4.424592	1.789006	-3.379107
24	1	0	5.605206	2.523420	-2.255003
25	6	0	-0.784139	2.698800	0.733567
26	1	0	-1.608276	3.166102	1.280838
27	1	0	-0.998185	2.772312	-0.337099
28	1	0	-0.730141	1.659043	1.066685
29	6	0	0.935312	3.140010	2.531385
30	1	0	0.720723	2.106890	2.815323
31	1	0	1.991708	3.378506	2.686929
32	1	0	0.348210	3.776561	3.198516
33	6	0	0.273404	4.950821	0.945060
34	1	0	-0.088646	5.222068	-0.050929
35	1	0	-0.504498	5.227581	1.657906
36	1	0	1.168298	5.532848	1.186344
37	6	0	1.895856	0.606180	0.694825
38	6	0	0.808828	-0.300446	0.040284
39	1	0	1.494048	0.843384	1.677384
40	1	0	2.797589	0.012681	0.836519
41	1	0	-0.068900	0.299837	-0.215373
42	1	0	1.166482	-0.725998	-0.900574
43	7	0	0.486366	-1.375400	0.934566
44	6	0	0.811786	-2.724428	0.536475
45	6	0	-0.137691	-1.102642	2.206815
46	8	0	-0.383964	-2.083022	2.922015
47	8	0	-0.372111	0.124736	2.409999
48	1	0	0.444934	-3.362193	1.346761
49	1	0	0.285928	-2.988422	-0.393275
50	6	0	2.300577	-2.940254	0.344721
51	6	0	2.810879	-3.537966	-0.807525
52	6	0	3.195863	-2.502290	1.328034
53	6	0	4.186882	-3.684118	-0.987193
54	1	0	2.121614	-3.879491	-1.576010
55	6	0	4.569117	-2.634097	1.147410
56	1	0	2.788575	-2.054176	2.232103

57	6	0	5.070099	-3.221363	-0.016306
58	1	0	4.567776	-4.149254	-1.891779
59	1	0	5.252649	-2.290777	1.919108
60	1	0	6.141648	-3.328836	-0.156057
61	6	0	-2.841294	-0.813240	0.897659
62	6	0	-2.689820	-2.268804	1.036248
63	7	0	-3.461869	-1.704509	-0.091813
64	6	0	-4.931690	-1.843808	-0.104680
65	6	0	-5.617548	-0.534267	-0.406691
66	6	0	-6.263225	0.167355	0.612729
67	6	0	-5.599631	0.001028	-1.698234
68	6	0	-6.217237	1.220690	-1.955734
69	6	0	-6.859658	1.916060	-0.932924
70	6	0	-6.883593	1.386946	0.353376
71	1	0	-3.532267	-0.284950	1.545564
72	1	0	-1.743783	-2.708100	0.750029
73	1	0	-3.269963	-2.794136	1.785952
74	1	0	-5.148269	-2.592694	-0.868804
75	1	0	-5.253820	-2.218298	0.872403
76	1	0	-6.287565	-0.248604	1.617467
77	1	0	-7.385880	1.919328	1.154834
78	1	0	-7.343964	2.865391	-1.139366
79	1	0	-6.201156	1.628342	-2.961719
80	1	0	-5.095831	-0.547612	-2.488141
81	1	0	-1.993908	-0.257580	0.519484

$TS_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.856145	-0.764752	3.170411
2	8	0	6.218375	-1.008956	4.319247
3	8	0	4.839791	-1.035750	2.509796
4	6	0	0.708495	0.456315	-0.298575
5	7	0	-0.428372	-0.164407	0.103530
6	7	0	0.589602	1.771348	0.001232
7	6	0	-1.257310	0.773340	0.681142
8	6	0	-0.626558	1.966170	0.621687
9	6	0	-0.852251	-1.592542	-0.155317
10	6	0	1.547789	2.915150	-0.303644
11	1	0	-2.220061	0.534153	1.092546
12	1	0	-0.960087	2.924350	0.972266
13	6	0	0.187676	-2.579496	0.374446
14	1	0	0.453107	-2.351792	1.410736
15	1	0	-0.242403	-3.583683	0.341955
16	1	0	1.090521	-2.611025	-0.232713
17	6	0	-1.085816	-1.766742	-1.658816
18	1	0	-1.438905	-2.784923	-1.843589
19	1	0	-1.844074	-1.063428	-2.014858
20	1	0	-0.173243	-1.627364	-2.240372
21	6	0	-2.171681	-1.843970	0.580486
22	1	0	-2.447109	-2.887119	0.416580
23	1	0	-2.069207	-1.690814	1.658595
24	1	0	-2.988481	-1.227197	0.196245
25	6	0	2.808310	2.781293	0.551505
26	1	0	3.358048	3.725372	0.499542
27	1	0	2.556711	2.588549	1.598569
28	1	0	3.468824	2.007952	0.156805
29	6	0	1.893834	2.934742	-1.801218

30	1	0	2.720478	2.263549	-2.040306
31	1	0	1.016994	2.706074	-2.414223
32	1	0	2.226685	3.943609	-2.057496
33	6	0	0.834376	4.223278	0.053053
34	1	0	0.624810	4.301252	1.123584
35	1	0	1.509801	5.040689	-0.202245
36	1	0	-0.088989	4.362158	-0.517740
37	6	0	1.895811	-0.202919	-0.905562
38	6	0	2.975005	-0.674203	0.104330
39	1	0	2.403679	0.489257	-1.572361
40	1	0	1.577092	-1.059935	-1.497903
41	1	0	3.235841	0.129179	0.797532
42	1	0	2.605590	-1.491450	0.727268
43	7	0	4.141642	-1.140584	-0.607263
44	6	0	4.529683	-2.522957	-0.401708
45	6	0	5.021084	-0.175420	-1.146664
46	8	0	6.235788	-0.537045	-1.308555
47	8	0	4.547280	0.957026	-1.358099
48	1	0	5.466461	-2.669530	-0.946638
49	1	0	4.708089	-2.715192	0.666214
50	6	0	3.466252	-3.479561	-0.905423
51	6	0	3.045409	-4.553957	-0.120971
52	6	0	2.865351	-3.283585	-2.154038
53	6	0	2.043439	-5.414851	-0.568217
54	1	0	3.500592	-4.707023	0.854221
55	6	0	1.855598	-4.132410	-2.598479
56	1	0	3.195620	-2.447237	-2.765559
57	6	0	1.438951	-5.201006	-1.803647
58	1	0	1.729426	-6.246907	0.054769
59	1	0	1.399904	-3.969409	-3.571149
60	1	0	0.655447	-5.867209	-2.151639
61	6	0	6.368349	0.725160	1.191308
62	6	0	6.852198	-0.509590	0.577767
63	7	0	6.883126	0.020617	2.360823
64	6	0	8.069666	0.546420	3.027960
65	6	0	7.841231	1.917544	3.625080
66	6	0	8.467065	3.044526	3.093258
67	6	0	6.966709	2.068944	4.707304
68	6	0	6.734005	3.330455	5.243574
69	6	0	7.365989	4.453095	4.708856
70	6	0	8.233653	4.309017	3.631752
71	1	0	6.919592	1.633128	0.951558
72	1	0	6.290160	-1.405427	0.772625
73	1	0	7.894121	-0.573000	0.291743
74	1	0	8.316176	-0.177908	3.806127
75	1	0	8.894609	0.590686	2.305750
76	1	0	9.149675	2.930746	2.253747
77	1	0	8.729694	5.177671	3.209559
78	1	0	7.184622	5.435628	5.134036
79	1	0	6.058555	3.439693	6.086849
80	1	0	6.482580	1.182281	5.108821
81	1	0	5.292668	0.871370	1.227096

24

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	5.899878	-0.067117	2.355049
2	8	0	5.372602	0.540184	3.304970

3	8	0	5.547797	-1.166181	1.838447
4	6	0	0.963598	0.522018	0.262946
5	7	0	-0.266061	-0.051626	0.201361
6	7	0	0.898788	1.540876	1.146215
7	6	0	-1.099359	0.613584	1.075349
8	6	0	-0.376462	1.595261	1.659162
9	6	0	-0.758434	-1.102101	-0.764833
10	6	0	1.956056	2.599733	1.442816
11	1	0	-2.127807	0.344070	1.226167
12	1	0	-0.676175	2.313441	2.399503
13	6	0	0.080987	-2.375108	-0.669344
14	1	0	0.150631	-2.717650	0.366681
15	1	0	-0.405131	-3.163089	-1.250309
16	1	0	1.087156	-2.266682	-1.072266
17	6	0	-0.749428	-0.501432	-2.173831
18	1	0	-1.151684	-1.236324	-2.875715
19	1	0	-1.377386	0.393219	-2.210128
20	1	0	0.253788	-0.234723	-2.508530
21	6	0	-2.202232	-1.460773	-0.398264
22	1	0	-2.532078	-2.243708	-1.083436
23	1	0	-2.275458	-1.855660	0.618966
24	1	0	-2.885123	-0.615349	-0.515357
25	6	0	3.255353	1.962371	1.923062
26	1	0	3.891919	2.746110	2.340964
27	1	0	3.096546	1.233534	2.720929
28	1	0	3.835305	1.494207	1.126207
29	6	0	2.131282	3.434038	0.171985
30	1	0	2.605000	2.870120	-0.634050
31	1	0	1.168159	3.821878	-0.175542
32	1	0	2.789081	4.273467	0.406016
33	6	0	1.425557	3.508301	2.553906
34	1	0	1.235330	2.951189	3.475848
35	1	0	2.213390	4.234756	2.764204
36	1	0	0.529371	4.063471	2.259541
37	6	0	2.192918	0.049884	-0.444185
38	6	0	2.978755	-0.993516	0.376110
39	1	0	2.856071	0.887858	-0.646921
40	1	0	1.924305	-0.387882	-1.406240
41	1	0	3.380512	-0.569021	1.302540
42	1	0	2.313361	-1.818138	0.643660
43	7	0	4.084947	-1.566875	-0.388697
44	6	0	4.338163	-2.967076	-0.035396
45	6	0	5.170977	-0.710683	-0.501831
46	8	0	6.315787	-1.335268	-0.851859
47	8	0	5.051835	0.500751	-0.490899
48	1	0	5.327261	-3.226917	-0.411274
49	1	0	4.365253	-3.063772	1.056210
50	6	0	3.299137	-3.867526	-0.661370
51	6	0	2.521392	-4.729312	0.110802
52	6	0	3.099944	-3.837912	-2.046226
53	6	0	1.563843	-5.551090	-0.484900
54	1	0	2.669714	-4.754953	1.187665
55	6	0	2.148310	-4.655322	-2.644258
56	1	0	3.700719	-3.157138	-2.643933
57	6	0	1.375320	-5.516251	-1.863004
58	1	0	0.966621	-6.218070	0.129620
59	1	0	2.010260	-4.628944	-3.721052
60	1	0	0.634901	-6.159468	-2.328745
61	6	0	7.746036	0.185457	0.573687
62	6	0	7.477631	-1.193760	-0.011619
63	7	0	7.044515	0.568188	1.783120
64	6	0	7.471941	1.797023	2.409546

65	6	0	6.612270	3.011674	2.107471
66	6	0	6.195617	3.297217	0.803925
67	6	0	6.239479	3.881908	3.132216
68	6	0	5.484596	5.023353	2.867866
69	6	0	5.098041	5.315133	1.561406
70	6	0	5.456971	4.444452	0.531817
71	1	0	8.827036	0.188590	0.790167
72	1	0	7.419795	-1.939414	0.781159
73	1	0	8.301629	-1.423880	-0.692805
74	1	0	7.487972	1.654842	3.493623
75	1	0	8.499209	2.009773	2.081411
76	1	0	6.415550	2.595272	0.006240
77	1	0	5.153857	4.658119	-0.489998
78	1	0	4.526175	6.213873	1.345665
79	1	0	5.201722	5.685582	3.681288
80	1	0	6.527441	3.644861	4.152877
81	1	0	7.591700	0.914005	-0.236372

NMe-11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000462	-1.642129	-0.007178
2	7	0	1.069114	-0.795417	-0.018431
3	7	0	-1.068176	-0.795827	0.007088
4	6	0	0.684838	0.549253	-0.015185
5	6	0	-0.683868	0.549533	0.011027
6	6	0	2.462584	-1.294916	0.102010
7	6	0	-2.462606	-1.295234	-0.101201
8	6	0	3.047230	-0.809515	1.433411
9	1	0	4.053286	-1.218932	1.567819
10	1	0	3.110676	0.280368	1.456125
11	1	0	2.420806	-1.151291	2.262654
12	6	0	3.321496	-0.807621	-1.070309
13	1	0	4.282616	-1.330280	-1.055540
14	1	0	2.827601	-1.031276	-2.021121
15	1	0	3.517295	0.263205	-1.006888
16	6	0	2.440778	-2.824437	0.089695
17	1	0	2.020189	-3.203815	-0.843374
18	1	0	3.470352	-3.180349	0.194530
19	1	0	1.833067	-3.218399	0.904411
20	6	0	-3.062737	-0.804858	-1.423726
21	1	0	-4.069823	-1.214721	-1.548410
22	1	0	-3.128141	0.284980	-1.441201
23	1	0	-2.445709	-1.142078	-2.261768
24	6	0	-3.307613	-0.812556	1.083227
25	1	0	-4.266812	-1.338915	1.080946
26	1	0	-2.800181	-1.035145	2.027121
27	1	0	-3.507814	0.257536	1.023319
28	6	0	-2.439800	-2.824831	-0.095536
29	1	0	-3.469843	-3.181853	-0.191528
30	1	0	-1.839725	-3.214273	-0.918173
31	1	0	-2.009510	-3.208400	0.831349
32	7	0	1.619162	1.600001	-0.070706
33	7	0	-1.617328	1.600151	0.072096
34	6	0	1.568679	2.593754	0.984566
35	1	0	2.545449	3.085121	1.066645
36	1	0	0.816880	3.379580	0.802441

37	1	0	1.343479	2.107822	1.936603
38	6	0	1.858189	2.182769	-1.383779
39	1	0	1.123289	2.957785	-1.649839
40	1	0	2.853927	2.641783	-1.402161
41	1	0	1.826982	1.399892	-2.143599
42	6	0	-1.577400	2.588572	-0.988210
43	1	0	-2.554760	3.079831	-1.064506
44	1	0	-0.823014	3.374401	-0.817720
45	1	0	-1.361052	2.096710	-1.939372
46	6	0	-1.851696	2.184454	1.384713
47	1	0	-1.124879	2.969848	1.641658
48	1	0	-2.852952	2.630748	1.411885
49	1	0	-1.802311	1.404355	2.146203

NMe-TS$_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.333022	0.554743	1.267018
2	7	0	1.615809	-0.764457	1.082455
3	7	0	1.831881	1.186866	0.169629
4	6	0	2.231207	-0.974020	-0.168435
5	6	0	2.360534	0.264243	-0.728875
6	6	0	1.295180	-1.795299	2.108985
7	6	0	1.991254	2.675249	0.026497
8	6	0	-0.067217	-2.434828	1.816241
9	1	0	-0.094878	-2.848036	0.803820
10	1	0	-0.248486	-3.251423	2.521546
11	1	0	-0.883051	-1.715613	1.917330
12	6	0	1.300420	-1.134382	3.491432
13	1	0	1.057326	-1.891154	4.242519
14	1	0	2.291491	-0.728512	3.710977
15	1	0	0.584917	-0.318149	3.570650
16	6	0	2.366267	-2.891493	2.120449
17	1	0	2.245439	-3.483622	3.031528
18	1	0	2.272422	-3.567763	1.270478
19	1	0	3.370967	-2.459059	2.125519
20	6	0	1.283088	3.184296	-1.232030
21	1	0	1.389954	4.273088	-1.265668
22	1	0	1.725531	2.770274	-2.138337
23	1	0	0.210362	2.973126	-1.181067
24	6	0	1.399246	3.407759	1.235138
25	1	0	0.319577	3.534005	1.126582
26	1	0	1.636277	2.903550	2.174399
27	1	0	1.835323	4.409864	1.259465
28	6	0	3.498457	2.957265	-0.031958
29	1	0	3.957611	2.487454	-0.902702
30	1	0	3.658824	4.036557	-0.102175
31	1	0	3.986866	2.595091	0.878444
32	7	0	2.603322	-2.177506	-0.756868
33	7	0	2.846430	0.613362	-2.002033
34	6	0	1.613245	-3.054017	-1.341074
35	1	0	1.964837	-3.421478	-2.314533
36	1	0	1.395905	-3.935327	-0.714493
37	1	0	0.683636	-2.502679	-1.502092
38	6	0	3.937482	-2.722616	-0.631656
39	1	0	3.965973	-3.627677	-0.006420
40	1	0	4.336089	-2.990970	-1.619330
41	1	0	4.597884	-1.976773	-0.185254

42	6	0	1.909299	0.278658	-3.070548
43	1	0	2.240490	0.752890	-3.999767
44	1	0	1.839180	-0.808426	-3.235976
45	1	0	0.917578	0.664827	-2.823109
46	6	0	4.198313	0.163604	-2.304925
47	1	0	4.851935	0.365649	-1.452768
48	1	0	4.246717	-0.908904	-2.543544
49	1	0	4.572911	0.724703	-3.167257
50	6	0	-0.757156	0.965448	1.524146
51	6	0	-1.248160	0.535218	0.211196
52	1	0	-0.594621	2.016260	1.683674
53	1	0	-0.907386	0.319728	2.378985
54	1	0	-0.919051	1.125701	-0.640602
55	1	0	-1.291035	-0.537377	0.016358
56	7	0	-2.442800	1.063447	0.841256
57	6	0	-3.484138	0.124188	1.254193
58	6	0	-2.832588	2.518568	0.458969
59	8	0	-4.020644	2.749969	0.641968
60	8	0	-1.853387	3.155009	0.060153
61	1	0	-3.075805	-0.561637	2.008974
62	1	0	-4.260726	0.737000	1.715254
63	6	0	-4.033421	-0.663887	0.088509
64	6	0	-4.749488	-0.002487	-0.914872
65	6	0	-3.803527	-2.034629	-0.025417
66	6	0	-5.228478	-0.712084	-2.010218
67	1	0	-4.916381	1.067237	-0.813750
68	6	0	-4.285983	-2.745662	-1.123363
69	1	0	-3.250790	-2.552093	0.757067
70	6	0	-4.998778	-2.083751	-2.117271
71	1	0	-5.787795	-0.194570	-2.783430
72	1	0	-4.107214	-3.813918	-1.199314
73	1	0	-5.377522	-2.634140	-2.972829

NMe-22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.960039	0.245193	-1.004047
2	7	0	-1.586544	-0.956159	-0.887323
3	7	0	-1.546996	1.136529	-0.175091
4	6	0	-2.526823	-0.848001	0.139731
5	6	0	-2.506937	0.440026	0.589442
6	6	0	-1.395792	-2.111056	-1.853843
7	6	0	-1.299391	2.645763	-0.125092
8	6	0	0.000007	-2.729363	-1.698601
9	1	0	0.187513	-2.978853	-0.650096
10	1	0	0.027336	-3.657240	-2.275925
11	1	0	0.808862	-2.094460	-2.056421
12	6	0	-1.664527	-1.585119	-3.272571
13	1	0	-1.504110	-2.398212	-3.985162
14	1	0	-2.706326	-1.261162	-3.353604
15	1	0	-1.025111	-0.753605	-3.564254
16	6	0	-2.411987	-3.236783	-1.614872
17	1	0	-2.268330	-3.950561	-2.430720
18	1	0	-2.256668	-3.751462	-0.668140
19	1	0	-3.442857	-2.881863	-1.657951
20	6	0	-0.192163	2.961676	0.881915
21	1	0	-0.188201	4.043154	1.050471
22	1	0	-0.380159	2.470617	1.841257

23	1	0	0.790776	2.694347	0.482007
24	6	0	-0.927748	3.194262	-1.517262
25	1	0	0.149453	3.164960	-1.692420
26	1	0	-1.473133	2.678346	-2.313749
27	1	0	-1.224347	4.244755	-1.547372
28	6	0	-2.606519	3.332792	0.295865
29	1	0	-2.834146	3.198725	1.350758
30	1	0	-2.475675	4.402990	0.128279
31	1	0	-3.455800	2.998210	-0.308899
32	6	0	0.365348	0.427919	-1.656416
33	6	0	1.504026	0.127242	-0.639218
34	1	0	0.542140	1.446813	-1.973843
35	1	0	0.487916	-0.219336	-2.519403
36	1	0	1.319495	0.712900	0.270667
37	1	0	1.483654	-0.929494	-0.349557
38	7	0	2.764516	0.436486	-1.245634
39	6	0	3.812151	-0.562212	-1.155025
40	6	0	3.142022	1.847150	-1.275989
41	8	0	4.341113	2.087127	-1.451251
42	8	0	2.165421	2.630933	-1.124270
43	1	0	3.498978	-1.479934	-1.675296
44	1	0	4.667902	-0.137381	-1.683007
45	6	0	4.198616	-0.905853	0.269682
46	6	0	4.751582	0.086640	1.088736
47	6	0	3.978895	-2.176327	0.799793
48	6	0	5.081380	-0.200377	2.408084
49	1	0	4.916365	1.072283	0.658961
50	6	0	4.310485	-2.465567	2.123609
51	1	0	3.550673	-2.950550	0.164885
52	6	0	4.862794	-1.476614	2.929889
53	1	0	5.515614	0.572681	3.035187
54	1	0	4.139899	-3.461520	2.522343
55	1	0	5.125267	-1.697152	3.960237
56	7	0	-3.226178	-1.929265	0.675960
57	7	0	-3.232702	0.897931	1.674115
58	6	0	-2.787366	-2.328116	2.007056
59	1	0	-3.135536	-1.635203	2.788456
60	1	0	-3.181042	-3.325683	2.226424
61	1	0	-1.696346	-2.374764	2.034987
62	6	0	-4.672596	-1.923065	0.528190
63	1	0	-5.044747	-2.951998	0.585833
64	1	0	-5.176548	-1.330849	1.305834
65	1	0	-4.943663	-1.515916	-0.449001
66	6	0	-2.578891	1.161217	2.940066
67	1	0	-2.453979	2.236315	3.140590
68	1	0	-3.173926	0.735057	3.757942
69	1	0	-1.592819	0.692005	2.951307
70	6	0	-4.619386	1.299443	1.572702
71	1	0	-5.223360	0.776660	2.325965
72	1	0	-4.750374	2.380074	1.728747
73	1	0	-5.004411	1.047942	0.582729

NMe-TS$_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.033065	-1.338385	-1.932312
2	8	0	-3.674306	-1.261122	-2.978421
3	8	0	-1.823069	-1.303929	-1.656643

4	6	0	-3.295509	-1.203808	0.582697
5	6	0	-3.067139	-2.645919	0.538629
6	7	0	-3.906399	-1.546347	-0.697676
7	6	0	-5.357433	-1.461967	-0.826503
8	6	0	-5.877351	-0.049692	-0.671554
9	6	0	-6.613595	0.322059	0.453252
10	6	0	-5.597359	0.909009	-1.651853
11	6	0	-6.058147	2.212474	-1.502834
12	6	0	-6.797671	2.576281	-0.377167
13	6	0	-7.074331	1.629090	0.602534
14	1	0	-4.007004	-0.845407	1.324918
15	1	0	-2.326967	-3.006893	-0.152518
16	1	0	-3.849785	-3.306529	0.888107
17	1	0	-5.587988	-1.851332	-1.819440
18	1	0	-5.819739	-2.110408	-0.071686
19	1	0	-6.833957	-0.421199	1.216671
20	1	0	-7.649596	1.903874	1.481347
21	1	0	-7.159733	3.594041	-0.267696
22	1	0	-5.846366	2.949683	-2.271725
23	1	0	-5.016315	0.606076	-2.519129
24	1	0	-2.425645	-0.563205	0.470839
25	6	0	2.133473	0.726579	0.855926
26	7	0	3.019325	0.935102	-0.151658
27	7	0	1.484774	1.883320	1.122626
28	6	0	2.821494	2.229802	-0.633855
29	6	0	1.878378	2.828702	0.149793
30	6	0	4.129627	-0.030517	-0.537378
31	6	0	0.562070	2.173371	2.303731
32	6	0	3.556489	-1.241625	-1.274773
33	1	0	2.934452	-0.917431	-2.114613
34	1	0	4.386188	-1.830976	-1.674710
35	1	0	2.973700	-1.907506	-0.640532
36	6	0	4.890438	-0.419126	0.741035
37	1	0	5.665628	-1.141217	0.472468
38	1	0	5.375743	0.463209	1.168696
39	1	0	4.271103	-0.877333	1.509805
40	6	0	5.165346	0.632051	-1.457094
41	1	0	5.997847	-0.073167	-1.529869
42	1	0	4.781152	0.820723	-2.457574
43	1	0	5.549227	1.567358	-1.043741
44	6	0	-0.892950	1.898782	1.920795
45	1	0	-1.534269	2.299980	2.711620
46	1	0	-1.159866	2.393756	0.983810
47	1	0	-1.084404	0.825805	1.862436
48	6	0	0.953088	1.330253	3.532159
49	1	0	0.457959	0.358672	3.532300
50	1	0	2.038368	1.218914	3.618670
51	1	0	0.605826	1.859880	4.421637
52	6	0	0.728085	3.649967	2.691238
53	1	0	0.235733	4.322034	1.991907
54	1	0	0.251526	3.788050	3.663152
55	1	0	1.781973	3.929783	2.788016
56	6	0	1.688412	-0.631321	1.291985
57	6	0	0.506431	-1.086310	0.389671
58	1	0	1.325795	-0.647303	2.311779
59	1	0	2.488346	-1.360119	1.205435
60	1	0	-0.238791	-0.287161	0.333195
61	1	0	0.850653	-1.255062	-0.635401
62	7	0	-0.088464	-2.302454	0.879501
63	6	0	-0.005596	-3.474636	0.030313
64	6	0	-1.000792	-2.199273	1.954066
65	8	0	-1.873673	-3.127130	2.053536

66	8	0	-0.909625	-1.181850	2.664583
67	1	0	-0.602926	-4.252211	0.515190
68	1	0	-0.438961	-3.259862	-0.957456
69	6	0	1.424470	-3.946612	-0.144751
70	6	0	1.905463	-4.312506	-1.402239
71	6	0	2.292735	-4.005418	0.950256
72	6	0	3.227184	-4.725137	-1.567632
73	1	0	1.239051	-4.261618	-2.259655
74	6	0	3.616190	-4.404052	0.787383
75	1	0	1.915600	-3.719859	1.929318
76	6	0	4.088462	-4.764380	-0.474841
77	1	0	3.585341	-5.006467	-2.553331
78	1	0	4.278608	-4.443783	1.647279
79	1	0	5.119471	-5.079576	-0.602581
80	7	0	3.379441	2.700276	-1.820256
81	7	0	1.354749	4.087781	-0.075525
82	6	0	4.182784	3.908535	-1.757914
83	1	0	4.859825	3.931029	-2.618794
84	1	0	3.575904	4.825123	-1.774428
85	1	0	4.788242	3.904727	-0.848206
86	6	0	2.459735	2.672271	-2.952388
87	1	0	1.713829	3.480693	-2.903800
88	1	0	3.031798	2.781368	-3.879078
89	1	0	1.937486	1.713106	-2.980041
90	6	0	0.026711	4.247356	-0.635176
91	1	0	-0.708372	4.590049	0.109280
92	1	0	0.054099	4.989119	-1.443487
93	1	0	-0.317219	3.298335	-1.051684
94	6	0	2.015604	5.298661	0.362238
95	1	0	2.113065	6.003075	-0.473572
96	1	0	1.461599	5.807711	1.164229
97	1	0	3.013772	5.060614	0.734499

OMe-11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000299	-1.378796	-0.003101
2	7	0	1.070213	-0.528075	-0.046222
3	7	0	-1.070174	-0.528678	0.041723
4	6	0	0.677284	0.803379	-0.025289
5	6	0	-0.677151	0.803174	0.024631
6	6	0	2.477223	-0.976722	-0.139869
7	6	0	-2.476965	-0.977511	0.140081
8	6	0	3.254944	-0.444366	1.069246
9	1	0	4.273873	-0.842400	1.057343
10	1	0	3.316025	0.645837	1.051293
11	1	0	2.770085	-0.762203	1.997114
12	6	0	3.077345	-0.446680	-1.446442
13	1	0	4.115991	-0.778219	-1.538567
14	1	0	2.512983	-0.832772	-2.300010
15	1	0	3.057002	0.645091	-1.472746
16	6	0	2.510743	-2.502987	-0.135686
17	1	0	1.943513	-2.909464	-0.974113
18	1	0	3.553882	-2.824626	-0.210505
19	1	0	2.072631	-2.902360	0.780586
20	6	0	-3.259898	-0.440308	-1.063662
21	1	0	-4.279205	-0.837064	-1.048171
22	1	0	-3.319295	0.649986	-1.041043

23	1	0	-2.779829	-0.755461	-1.994844
24	6	0	-3.070730	-0.451257	1.450945
25	1	0	-4.109824	-0.780736	1.545420
26	1	0	-2.504474	-0.842808	2.300746
27	1	0	-3.046702	0.640454	1.481991
28	6	0	-2.510655	-2.503692	0.131217
29	1	0	-3.553361	-2.825750	0.210138
30	1	0	-2.076804	-2.900439	-0.788259
31	1	0	-1.939957	-2.912806	0.965989
32	6	0	1.431395	2.697962	1.090378
33	1	0	2.147374	3.508131	0.948027
34	1	0	0.419711	3.105492	1.185907
35	1	0	1.680349	2.133986	1.995768
36	8	0	1.531982	1.860460	-0.061525
37	6	0	-1.433617	2.696262	-1.091109
38	1	0	-2.148614	3.506988	-0.947534
39	1	0	-0.421753	3.102456	-1.189985
40	1	0	-1.685644	2.131229	-1.995154
41	8	0	-1.531923	1.860038	0.062031

OMe-$TS_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.671840	0.299004	-1.092098
2	7	0	-1.847436	-1.016372	-0.766543
3	7	0	-2.058767	0.990893	0.017025
4	6	0	-2.266918	-1.142527	0.549113
5	6	0	-2.407548	0.117107	1.036424
6	6	0	-1.650300	-2.155944	-1.704006
7	6	0	-2.285604	2.471335	0.105313
8	6	0	-0.336077	-2.863159	-1.362253
9	1	0	-0.329430	-3.166975	-0.311286
10	1	0	-0.220622	-3.756560	-1.982682
11	1	0	0.521998	-2.208945	-1.545850
12	6	0	-1.648210	-1.634614	-3.142065
13	1	0	-1.536986	-2.489162	-3.814894
14	1	0	-2.590612	-1.129807	-3.367112
15	1	0	-0.839445	-0.935181	-3.343133
16	6	0	-2.827650	-3.134247	-1.571856
17	1	0	-2.778256	-3.855036	-2.392243
18	1	0	-2.798724	-3.684952	-0.632578
19	1	0	-3.778136	-2.597057	-1.649800
20	6	0	-1.479554	3.065675	1.263530
21	1	0	-1.665743	4.143500	1.291611
22	1	0	-1.782909	2.649076	2.225427
23	1	0	-0.406931	2.930558	1.094436
24	6	0	-1.857878	3.163038	-1.190549
25	1	0	-0.777045	3.321770	-1.211034
26	1	0	-2.182503	2.606051	-2.072277
27	1	0	-2.329547	4.149120	-1.210359
28	6	0	-3.792843	2.666545	0.316270
29	1	0	-4.139096	2.166998	1.223788
30	1	0	-4.008261	3.734480	0.407548
31	1	0	-4.345975	2.273988	-0.542574
32	6	0	-3.744381	-2.523931	1.708653
33	1	0	-4.472358	-2.560668	0.891721
34	1	0	-3.723479	-3.479878	2.231319
35	1	0	-4.011177	-1.720760	2.401581

36	6	0	-1.867809	0.154016	3.292046
37	1	0	-2.284914	0.518868	4.230450
38	1	0	-1.728651	-0.930850	3.336993
39	1	0	-0.906765	0.640608	3.095910
40	6	0	0.354135	0.736014	-1.528151
41	6	0	0.975463	0.446245	-0.228585
42	1	0	0.156005	1.764488	-1.775181
43	1	0	0.481312	0.017784	-2.326554
44	1	0	0.688202	1.094598	0.595683
45	1	0	1.075154	-0.602689	0.054577
46	7	0	2.101379	0.955583	-0.983309
47	6	0	3.147801	0.021289	-1.391333
48	6	0	2.446553	2.449974	-0.775262
49	8	0	3.601142	2.716129	-1.083863
50	8	0	1.473861	3.083675	-0.351751
51	1	0	2.708475	-0.756308	-2.031341
52	1	0	3.850740	0.611514	-1.981785
53	6	0	3.835275	-0.618381	-0.207646
54	6	0	4.605373	0.171031	0.653201
55	6	0	3.685195	-1.978177	0.062310
56	6	0	5.216088	-0.402470	1.762569
57	1	0	4.709694	1.230290	0.431589
58	6	0	4.299423	-2.552719	1.174098
59	1	0	3.090381	-2.595657	-0.608599
60	6	0	5.065454	-1.764058	2.025556
61	1	0	5.816934	0.213711	2.424285
62	1	0	4.180581	-3.613526	1.372204
63	1	0	5.546854	-2.207910	2.891349
64	8	0	-2.426050	-2.322435	1.189084
65	8	0	-2.813939	0.493571	2.271145

OMe-22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.251597	0.110111	-0.681827
2	7	0	-1.895271	-1.068443	-0.444375
3	7	0	-1.838722	1.093814	0.040330
4	6	0	-2.881689	-0.818246	0.501414
5	6	0	-2.838517	0.501148	0.807592
6	6	0	-1.718669	-2.342944	-1.251364
7	6	0	-1.543295	2.600087	-0.026721
8	6	0	-0.285250	-2.877903	-1.139590
9	1	0	0.014209	-2.957691	-0.091099
10	1	0	-0.268115	-3.881174	-1.572526
11	1	0	0.451960	-2.280844	-1.672670
12	6	0	-2.119819	-2.038119	-2.699558
13	1	0	-2.017381	-2.950010	-3.293622
14	1	0	-3.165559	-1.719022	-2.738868
15	1	0	-1.504964	-1.265013	-3.160592
16	6	0	-2.647617	-3.448497	-0.733825
17	1	0	-2.457974	-4.327884	-1.353372
18	1	0	-2.446259	-3.705823	0.306273
19	1	0	-3.701924	-3.189606	-0.838782
20	6	0	-0.302462	2.914225	0.809744
21	1	0	-0.244423	4.000743	0.926063
22	1	0	-0.380241	2.471537	1.808375
23	1	0	0.613882	2.599365	0.301290
24	6	0	-1.343702	3.037139	-1.493010

25	1	0	-0.294053	2.995139	-1.792000
26	1	0	-1.967394	2.450942	-2.174491
27	1	0	-1.657915	4.079410	-1.579286
28	6	0	-2.748888	3.370173	0.531915
29	1	0	-2.856852	3.267827	1.610806
30	1	0	-2.564585	4.424323	0.318256
31	1	0	-3.687355	3.080763	0.051790
32	6	0	0.021298	0.243554	-1.434403
33	6	0	1.271668	0.014560	-0.540678
34	1	0	0.158292	1.247762	-1.821009
35	1	0	0.058148	-0.442634	-2.277267
36	1	0	1.200382	0.669981	0.336689
37	1	0	1.297822	-1.012691	-0.164275
38	7	0	2.446417	0.265580	-1.326125
39	6	0	3.521113	-0.705034	-1.233419
40	6	0	2.792801	1.667038	-1.550636
41	8	0	3.960582	1.895370	-1.880561
42	8	0	1.824288	2.458885	-1.381030
43	1	0	3.175751	-1.678524	-1.612631
44	1	0	4.308834	-0.334019	-1.891616
45	6	0	4.056203	-0.882642	0.173253
46	6	0	4.677215	0.196247	0.814768
47	6	0	3.903270	-2.083783	0.863596
48	6	0	5.139530	0.060803	2.118685
49	1	0	4.787647	1.127130	0.262808
50	6	0	4.367355	-2.221006	2.171816
51	1	0	3.420557	-2.924122	0.366868
52	6	0	4.986803	-1.147046	2.801297
53	1	0	5.627006	0.899388	2.607098
54	1	0	4.245669	-3.164822	2.695466
55	1	0	5.353462	-1.248783	3.818267
56	6	0	-5.074596	-1.545147	0.816711
57	1	0	-5.588874	-2.355952	1.330978
58	1	0	-5.401209	-0.579025	1.208303
59	1	0	-5.277565	-1.598468	-0.258443
60	6	0	-3.139497	0.994687	3.057313
61	1	0	-2.171269	1.496369	3.153266
62	1	0	-3.876753	1.488201	3.689632
63	1	0	-3.043882	-0.058150	3.337898
64	8	0	-3.677370	-1.738767	1.070264
65	8	0	-3.629495	1.102300	1.713222

OMe-TS$_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.615371	0.112501	-1.464118
2	8	0	-3.130267	0.671733	-2.430666
3	8	0	-1.576201	0.349856	-0.814939
4	6	0	-3.131309	-1.493339	0.429048
5	6	0	-2.227921	-2.397139	-0.267004
6	7	0	-3.352203	-1.101235	-0.968191
7	6	0	-4.627579	-1.457117	-1.589864
8	6	0	-5.812730	-0.794831	-0.923921
9	6	0	-6.713137	-1.543102	-0.166103
10	6	0	-6.002816	0.586247	-1.042847
11	6	0	-7.081780	1.197430	-0.413744
12	6	0	-7.979662	0.442718	0.340625
13	6	0	-7.794092	-0.929850	0.464781

14	1	0	-4.010305	-1.944175	0.885781
15	1	0	-1.313964	-1.977083	-0.663162
16	1	0	-2.609188	-3.326460	-0.669223
17	1	0	-4.546615	-1.149051	-2.633200
18	1	0	-4.744265	-2.546950	-1.548159
19	1	0	-6.569915	-2.617625	-0.072793
20	1	0	-8.487050	-1.524504	1.051813
21	1	0	-8.820800	0.924806	0.829020
22	1	0	-7.227019	2.268841	-0.514232
23	1	0	-5.291551	1.158594	-1.632187
24	1	0	-2.670153	-0.725893	1.040231
25	6	0	2.136762	1.156881	0.911669
26	7	0	2.868446	1.598609	-0.150950
27	7	0	1.093455	1.995331	1.095601
28	6	0	2.193978	2.680924	-0.704542
29	6	0	1.088246	2.908131	0.051741
30	6	0	4.245474	1.090962	-0.528731
31	6	0	0.162511	2.172919	2.290760
32	6	0	4.155723	-0.270857	-1.220665
33	1	0	3.462277	-0.226114	-2.065244
34	1	0	5.145337	-0.530540	-1.607266
35	1	0	3.851664	-1.078366	-0.554276
36	6	0	5.099481	1.038813	0.745555
37	1	0	6.097987	0.684363	0.477743
38	1	0	5.193415	2.038932	1.178033
39	1	0	4.704623	0.367584	1.506648
40	6	0	4.935700	2.070780	-1.486183
41	1	0	5.965376	1.723346	-1.600042
42	1	0	4.466136	2.094544	-2.468070
43	1	0	4.965454	3.085221	-1.079909
44	6	0	-1.270759	1.895353	1.849112
45	1	0	-1.917893	1.974176	2.727627
46	1	0	-1.612832	2.608291	1.097451
47	1	0	-1.344274	0.886554	1.440926
48	6	0	0.524568	1.248996	3.452854
49	1	0	0.205956	0.221027	3.269829
50	1	0	1.590211	1.302520	3.698633
51	1	0	-0.028496	1.616739	4.320935
52	6	0	0.358963	3.622036	2.762308
53	1	0	0.100958	4.348982	1.993019
54	1	0	-0.294642	3.788074	3.622151
55	1	0	1.392813	3.782258	3.085059
56	6	0	2.130339	-0.277150	1.350107
57	6	0	1.177870	-0.990895	0.352895
58	1	0	1.724395	-0.409159	2.345404
59	1	0	3.119875	-0.728570	1.318502
60	1	0	0.278786	-0.376855	0.230428
61	1	0	1.667552	-1.046505	-0.625712
62	7	0	0.804677	-2.328555	0.765057
63	6	0	1.147411	-3.404388	-0.146973
64	6	0	-0.428359	-2.390304	1.479526
65	8	0	-1.204208	-3.359911	1.170110
66	8	0	-0.663033	-1.453995	2.253823
67	1	0	0.738665	-4.323972	0.277341
68	1	0	0.679565	-3.279087	-1.138317
69	6	0	2.648185	-3.506769	-0.320440
70	6	0	3.222460	-3.643002	-1.584096
71	6	0	3.489394	-3.447047	0.796592
72	6	0	4.606774	-3.720621	-1.734882
73	1	0	2.578695	-3.679269	-2.459421
74	6	0	4.871125	-3.516192	0.649884
75	1	0	3.040007	-3.331261	1.779444

76	6	0	5.435173	-3.652841	-0.618872
77	1	0	5.036754	-3.827017	-2.726201
78	1	0	5.510577	-3.471254	1.526502
79	1	0	6.513084	-3.709139	-0.734442
80	6	0	2.673127	4.729009	-1.709195
81	1	0	2.975266	5.092805	-2.690209
82	1	0	1.713810	5.165989	-1.420490
83	1	0	3.433649	4.985021	-0.963899
84	6	0	-0.720905	3.454441	-1.301425
85	1	0	-1.558465	4.150190	-1.269915
86	1	0	-0.149045	3.598651	-2.223369
87	1	0	-1.066157	2.417134	-1.220101
88	8	0	2.560908	3.306736	-1.832741
89	8	0	0.116306	3.805455	-0.162640

Triazol -11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.056497	-0.232112	-0.000159
2	6	0	0.018985	0.670617	-0.000187
3	7	0	-1.032578	-0.168669	-0.000168
4	6	0	0.564817	-1.510979	-0.000061
5	6	0	2.473392	0.194282	0.000010
6	6	0	2.713965	1.032743	1.256827
7	6	0	3.382128	-1.032457	-0.000355
8	6	0	2.714092	1.033534	-1.256261
9	1	0	2.545086	0.433304	-2.155309
10	1	0	3.743637	1.402950	-1.270020
11	1	0	2.025072	1.880310	-1.269421
12	1	0	2.544783	0.431975	2.155483
13	1	0	3.743535	1.402079	1.270955
14	1	0	2.025009	1.879567	1.270396
15	1	0	3.224986	-1.647990	0.890840
16	1	0	3.225007	-1.647404	-0.891953
17	1	0	4.423283	-0.701315	-0.000231
18	1	0	1.163722	-2.408103	0.000041
19	6	0	-2.462210	0.201290	0.000003
20	6	0	-2.575660	1.721680	-0.000538
21	1	0	-2.095222	2.149337	-0.882565
22	1	0	-3.635397	1.993114	-0.000301
23	1	0	-2.094628	2.150054	0.880803
24	6	0	-3.105665	-0.387602	-1.257424
25	1	0	-2.987876	-1.473275	-1.272846
26	1	0	-2.637447	0.029380	-2.153654
27	1	0	-4.172128	-0.146049	-1.276524
28	6	0	-3.105091	-0.386642	1.258166
29	1	0	-4.171533	-0.145051	1.277576
30	1	0	-2.636439	0.031030	2.153851
31	1	0	-2.987293	-1.472306	1.274368
32	7	0	-0.732302	-1.507848	-0.000039

Triazol -$TS_{21\text{-}22}$

Standard orientation:

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

1	6	0	2.123994	0.261630	-0.401136
2	7	0	2.218259	1.529318	0.114746
3	7	0	2.692294	-0.483506	0.561909
4	6	0	2.807358	1.454116	1.350903
5	6	0	1.813295	2.781381	-0.578605
6	6	0	3.024818	-1.942716	0.577413
7	1	0	3.011662	2.297245	1.990984
8	6	0	0.309027	3.012731	-0.407515
9	1	0	0.032280	3.001876	0.651083
10	1	0	0.039987	3.987404	-0.824377
11	1	0	-0.276687	2.252270	-0.928235
12	6	0	2.187571	2.656864	-2.055997
13	1	0	1.885989	3.565802	-2.583114
14	1	0	3.267730	2.529129	-2.166527
15	1	0	1.697146	1.801547	-2.522496
16	6	0	2.576600	3.957374	0.036336
17	1	0	2.368189	4.854331	-0.551230
18	1	0	2.260497	4.159637	1.063735
19	1	0	3.655825	3.781091	0.020853
20	6	0	2.205458	-2.615813	1.679357
21	1	0	2.537685	-3.652340	1.784858
22	1	0	2.347730	-2.105398	2.635122
23	1	0	1.145327	-2.637472	1.410684
24	6	0	2.714611	-2.584421	-0.773981
25	1	0	1.650281	-2.808935	-0.877063
26	1	0	3.062679	-1.960716	-1.602223
27	1	0	3.247411	-3.537653	-0.820046
28	6	0	4.526073	-2.042716	0.869401
29	1	0	4.771981	-1.593849	1.832756
30	1	0	4.814216	-3.096619	0.886500
31	1	0	5.101221	-1.539020	0.086300
32	6	0	0.262584	-0.392119	-1.188718
33	6	0	-0.570282	-0.385740	0.020175
34	1	0	0.669067	-1.333040	-1.515768
35	1	0	0.150426	0.406356	-1.911340
36	1	0	-0.303501	-1.104895	0.790265
37	1	0	-0.885626	0.580763	0.413124
38	7	0	-1.471503	-0.933003	-0.974574
39	6	0	-2.583544	-0.104821	-1.436779
40	6	0	-1.609127	-2.479116	-0.985794
41	8	0	-2.656428	-2.855048	-1.495106
42	8	0	-0.618032	-3.020459	-0.486175
43	1	0	-2.186473	0.793153	-1.930329
44	1	0	-3.107378	-0.712944	-2.176499
45	6	0	-3.505727	0.295943	-0.309900
46	6	0	-4.247707	-0.684495	0.357450
47	6	0	-3.600880	1.624620	0.102540
48	6	0	-5.073929	-0.329187	1.417509
49	1	0	-4.161190	-1.716771	0.026947
50	6	0	-4.431060	1.980277	1.164380
51	1	0	-3.029027	2.390108	-0.419559
52	6	0	-5.168287	1.002161	1.823100
53	1	0	-5.649617	-1.093681	1.929794
54	1	0	-4.501178	3.018304	1.474610
55	1	0	-5.815155	1.274578	2.651055
56	7	0	3.107968	0.231202	1.650709

Triazol -22

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		

Number	Number	Type	X	Y	Z
1	6	0	1.916938	0.052995	-0.118131
2	7	0	2.534907	1.214684	0.236425
3	7	0	2.446871	-0.898114	0.661919
4	6	0	3.401255	0.887049	1.242374
5	6	0	2.460145	2.562847	-0.430440
6	6	0	2.212860	-2.405619	0.703933
7	1	0	4.042134	1.587418	1.749822
8	6	0	1.015511	3.065884	-0.485188
9	1	0	0.548854	3.019853	0.502529
10	1	0	1.030816	4.109686	-0.808187
11	1	0	0.399543	2.511550	-1.192563
12	6	0	3.079408	2.441316	-1.825525
13	1	0	3.067819	3.422715	-2.306571
14	1	0	4.116500	2.101835	-1.756162
15	1	0	2.527897	1.748296	-2.462961
16	6	0	3.285846	3.547429	0.402277
17	1	0	3.203708	4.531550	-0.062337
18	1	0	2.907903	3.627868	1.425609
19	1	0	4.346595	3.283466	0.421824
20	6	0	0.857923	-2.684689	1.355614
21	1	0	0.811768	-3.753496	1.583336
22	1	0	0.758821	-2.133474	2.295813
23	1	0	0.036440	-2.466714	0.666447
24	6	0	2.275547	-2.984173	-0.716092
25	1	0	1.323164	-2.888305	-1.243001
26	1	0	3.095454	-2.539665	-1.289003
27	1	0	2.479864	-4.053794	-0.623322
28	6	0	3.342737	-2.996519	1.550134
29	1	0	3.322543	-2.628423	2.576238
30	1	0	3.195683	-4.078083	1.563856
31	1	0	4.325044	-2.784018	1.120710
32	6	0	0.799834	-0.094423	-1.078620
33	6	0	-0.603226	0.062803	-0.425742
34	1	0	0.785073	-1.099388	-1.497370
35	1	0	0.902482	0.621762	-1.893297
36	1	0	-0.646268	-0.570133	0.469267
37	1	0	-0.762244	1.093859	-0.094006
38	7	0	-1.595153	-0.282502	-1.402564
39	6	0	-2.750586	0.591937	-1.498680
40	6	0	-1.787250	-1.712101	-1.648716
41	8	0	-2.849386	-2.035040	-2.187009
42	8	0	-0.810973	-2.420772	-1.276986
43	1	0	-2.428207	1.596410	-1.810904
44	1	0	-3.376020	0.166325	-2.285444
45	6	0	-3.536720	0.699931	-0.207165
46	6	0	-4.154896	-0.441165	0.319141
47	6	0	-3.625647	1.901493	0.494444
48	6	0	-4.848863	-0.368386	1.521018
49	1	0	-4.080989	-1.370922	-0.240312
50	6	0	-4.323758	1.975935	1.699660
51	1	0	-3.149222	2.791991	0.087069
52	6	0	-4.936403	0.839314	2.215172
53	1	0	-5.329901	-1.256830	1.919197
54	1	0	-4.389223	2.920212	2.232482
55	1	0	-5.482741	0.891790	3.152023
56	7	0	3.358468	-0.378067	1.517701

Triazol -$TS_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.629260	-1.782942	-1.500939
2	8	0	-3.303745	-2.143684	-2.462524
3	8	0	-1.430416	-1.490789	-1.349633
4	6	0	2.274579	1.845002	0.065970
5	7	0	3.194851	1.980358	-0.927083
6	7	0	1.635096	3.020420	0.139540
7	6	0	3.036098	3.247585	-1.413804
8	6	0	4.290278	1.028868	-1.346462
9	6	0	0.536998	3.504269	1.077360
10	1	0	3.611675	3.668657	-2.219874
11	6	0	3.709005	-0.334212	-1.717618
12	1	0	2.882629	-0.232025	-2.426456
13	1	0	4.497072	-0.925460	-2.190760
14	1	0	3.375823	-0.900583	-0.848510
15	6	0	5.299592	0.916860	-0.201169
16	1	0	6.116394	0.263487	-0.519003
17	1	0	5.714251	1.897259	0.049939
18	1	0	4.859528	0.475866	0.695056
19	6	0	4.981709	1.625491	-2.574875
20	1	0	5.750999	0.922361	-2.898304
21	1	0	4.282517	1.760451	-3.405308
22	1	0	5.478731	2.574251	-2.353959
23	6	0	-0.772853	2.803906	0.716262
24	1	0	-1.585281	3.312631	1.242290
25	1	0	-0.969440	2.865625	-0.357865
26	1	0	-0.767633	1.767254	1.057944
27	6	0	0.930211	3.223067	2.533680
28	1	0	0.701729	2.198565	2.833991
29	1	0	1.983122	3.459555	2.714271
30	1	0	0.329332	3.877967	3.169437
31	6	0	0.409080	5.013779	0.862673
32	1	0	0.110181	5.256566	-0.157365
33	1	0	-0.362814	5.368869	1.548177
34	1	0	1.342794	5.535063	1.086548
35	6	0	1.986124	0.615737	0.844249
36	6	0	0.898789	-0.294421	0.208609
37	1	0	1.607285	0.881518	1.828632
38	1	0	2.901850	0.038980	0.973142
39	1	0	0.017466	0.293253	-0.060006
40	1	0	1.251978	-0.744845	-0.720896
41	7	0	0.556438	-1.351088	1.125641
42	6	0	0.788414	-2.711532	0.676460
43	6	0	-0.313814	-1.030641	2.193895
44	8	0	-1.003054	-1.991017	2.677313
45	8	0	-0.369398	0.169180	2.522137
46	1	0	0.421702	-3.369988	1.468944
47	1	0	0.222352	-2.912534	-0.244631
48	6	0	2.260446	-2.960722	0.409807
49	6	0	2.675003	-3.562082	-0.779081
50	6	0	3.231801	-2.561560	1.334717
51	6	0	4.029875	-3.761747	-1.043631
52	1	0	1.926841	-3.865925	-1.506947
53	6	0	4.585778	-2.747359	1.069192
54	1	0	2.906606	-2.095388	2.262012
55	6	0	4.989360	-3.347630	-0.124535
56	1	0	4.334157	-4.233476	-1.973214
57	1	0	5.328152	-2.435937	1.798797
58	1	0	6.044695	-3.499328	-0.329628

59	6	0	-2.821975	-0.880896	0.853219
60	6	0	-2.347494	-2.208934	1.237640
61	7	0	-3.417291	-1.697593	-0.198949
62	6	0	-4.867969	-1.855710	-0.228392
63	6	0	-5.588668	-0.550734	-0.485885
64	6	0	-6.338889	0.064384	0.515966
65	6	0	-5.477713	0.071047	-1.734934
66	6	0	-6.113080	1.285706	-1.967587
67	6	0	-6.863506	1.894412	-0.961715
68	6	0	-6.976175	1.281992	0.281708
69	1	0	-3.554772	-0.420837	1.514339
70	1	0	-1.599354	-2.662029	0.613361
71	1	0	-2.986050	-2.828651	1.853580
72	1	0	-5.070009	-2.573816	-1.024753
73	1	0	-5.199413	-2.279430	0.727843
74	1	0	-6.430732	-0.416734	1.487513
75	1	0	-7.558667	1.749042	1.070025
76	1	0	-7.359787	2.841825	-1.148665
77	1	0	-6.026123	1.759697	-2.940727
78	1	0	-4.886346	-0.416671	-2.505552
79	1	0	-2.084505	-0.178226	0.476696
80	7	0	2.099979	3.889006	-0.788168

Thiazol -11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.751917	-1.079738	-0.000190
2	7	0	0.032990	0.060478	-0.000342
3	6	0	2.053177	1.115318	-0.000013
4	6	0	0.716543	1.279797	-0.000144
5	1	0	2.805969	1.888993	0.000074
6	1	0	0.180599	2.215894	-0.000226
7	6	0	-1.464793	-0.048515	0.000014
8	6	0	-1.875663	-0.813259	1.258926
9	1	0	-1.574454	-0.263972	2.156020
10	1	0	-2.961493	-0.943647	1.277531
11	1	0	-1.392324	-1.791604	1.269441
12	6	0	-2.111803	1.334793	-0.001866
13	1	0	-1.845678	1.908842	-0.894526
14	1	0	-1.846521	1.910929	0.889697
15	1	0	-3.196841	1.205840	-0.002180
16	6	0	-1.876174	-0.816801	-1.256581
17	1	0	-2.962017	-0.947182	-1.274245
18	1	0	-1.392842	-1.795160	-1.264592
19	1	0	-1.575383	-0.270014	-2.155336
20	16	0	2.398177	-0.585740	-0.000009

Thiazol -$TS_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.223681	0.789072	-0.904689
2	7	0	2.969631	0.505177	0.171361
3	6	0	2.920847	2.770970	0.495304

4	6	0	3.351729	1.588405	0.969270
5	6	0	3.452297	-0.878748	0.550283
6	1	0	3.092409	3.749367	0.917609
7	1	0	3.931071	1.423843	1.865329
8	6	0	2.735418	-1.307319	1.831928
9	1	0	3.150468	-2.262098	2.167014
10	1	0	2.868732	-0.579681	2.638663
11	1	0	1.670436	-1.464305	1.635746
12	6	0	3.154516	-1.886121	-0.560847
13	1	0	2.122675	-2.239783	-0.507354
14	1	0	3.372060	-1.469598	-1.547635
15	1	0	3.796701	-2.756585	-0.405296
16	6	0	4.971090	-0.793004	0.752005
17	1	0	5.257670	-0.161571	1.596152
18	1	0	5.352602	-1.796005	0.955327
19	1	0	5.458860	-0.415208	-0.151301
20	6	0	0.413653	-0.213449	-1.359478
21	6	0	-0.394828	0.112820	-0.175781
22	1	0	0.901003	-1.169851	-1.401310
23	1	0	0.212476	0.317077	-2.282977
24	1	0	-0.031584	-0.246156	0.784011
25	1	0	-0.818924	1.116521	-0.138259
26	7	0	-1.236503	-0.844863	-0.864129
27	6	0	-2.482493	-0.378487	-1.472744
28	6	0	-1.130736	-2.307674	-0.368640
29	8	0	-2.107941	-2.981889	-0.663848
30	8	0	-0.059600	-2.511063	0.216856
31	1	0	-2.250078	0.379717	-2.231146
32	1	0	-2.909840	-1.254433	-1.963657
33	6	0	-3.438054	0.191487	-0.449738
34	6	0	-3.996587	-0.648149	0.520232
35	6	0	-3.743113	1.552206	-0.432929
36	6	0	-4.847051	-0.124347	1.487239
37	1	0	-3.749584	-1.706471	0.497433
38	6	0	-4.598274	2.075809	0.535507
39	1	0	-3.314949	2.207347	-1.188896
40	6	0	-5.149904	1.237159	1.497860
41	1	0	-5.279320	-0.781775	2.235140
42	1	0	-4.831939	3.135979	0.536137
43	1	0	-5.817393	1.640743	2.252770
44	16	0	2.023234	2.498161	-0.957931

Thiazol -22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.031467	0.775019	-0.701027
2	7	0	2.904110	0.401322	0.238715
3	6	0	3.372145	2.650391	0.160942
4	6	0	3.658476	1.463333	0.729978
5	6	0	3.077345	-1.018349	0.811590
6	1	0	3.831202	3.605171	0.366154
7	1	0	4.400548	1.293591	1.489952
8	6	0	1.921045	-1.271761	1.778005
9	1	0	2.124852	-2.207552	2.306911
10	1	0	1.849162	-0.467847	2.517818
11	1	0	0.980467	-1.414464	1.235857
12	6	0	3.107762	-2.057552	-0.321728
13	1	0	2.105707	-2.423366	-0.559124

14	1	0	3.606460	-1.665340	-1.213165
15	1	0	3.687217	-2.915577	0.026417
16	6	0	4.411547	-1.066072	1.563655
17	1	0	4.410921	-0.453596	2.469399
18	1	0	4.556599	-2.098042	1.885729
19	1	0	5.258974	-0.791880	0.927385
20	6	0	0.965949	0.001628	-1.380174
21	6	0	-0.422892	0.190833	-0.692499
22	1	0	1.144777	-1.068159	-1.346941
23	1	0	0.892747	0.334196	-2.419116
24	1	0	-0.293496	0.096613	0.395250
25	1	0	-0.794718	1.203657	-0.893006
26	7	0	-1.333921	-0.772454	-1.232241
27	6	0	-2.666217	-0.303890	-1.573241
28	6	0	-1.179921	-2.148656	-0.769960
29	8	0	-2.144994	-2.896702	-0.941621
30	8	0	-0.046687	-2.385318	-0.261188
31	1	0	-2.595385	0.465794	-2.354317
32	1	0	-3.186249	-1.171541	-1.982956
33	6	0	-3.429319	0.252503	-0.387432
34	6	0	-3.759472	-0.593817	0.678540
35	6	0	-3.773090	1.601381	-0.311484
36	6	0	-4.422839	-0.089914	1.791088
37	1	0	-3.487023	-1.644131	0.605045
38	6	0	-4.439341	2.107655	0.804248
39	1	0	-3.521538	2.261775	-1.139406
40	6	0	-4.764399	1.261560	1.858625
41	1	0	-4.680836	-0.753767	2.610923
42	1	0	-4.703862	3.160219	0.847574
43	1	0	-5.284303	1.650143	2.729148
44	16	0	2.131902	2.458277	-1.010195

Thiazol -$TS_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.467418	-1.765802	-1.444755
2	8	0	-3.245958	-2.155520	-2.312320
3	8	0	-1.259877	-1.477022	-1.434703
4	6	0	2.767365	1.678998	-0.427009
5	7	0	2.381356	2.944134	-0.234234
6	6	0	3.319562	3.140386	-2.321557
7	6	0	2.689492	3.770653	-1.311340
8	6	0	1.627878	3.487930	0.990755
9	1	0	3.664077	3.570519	-3.249416
10	1	0	2.433231	4.815170	-1.283643
11	6	0	0.164176	3.063000	0.873131
12	1	0	-0.401536	3.583846	1.651095
13	1	0	-0.249834	3.344289	-0.099924
14	1	0	0.047199	1.992714	1.060140
15	6	0	2.258184	2.961955	2.291591
16	1	0	1.796325	2.025382	2.609924
17	1	0	3.342196	2.848137	2.199901
18	1	0	2.070166	3.695176	3.078810
19	6	0	1.731607	5.016699	0.972419
20	1	0	1.177152	5.468151	0.145697
21	1	0	1.271273	5.379333	1.892393
22	1	0	2.770264	5.361292	0.958595
23	6	0	2.505047	0.469113	0.382890

24	6	0	1.224138	-0.276605	-0.111967
25	1	0	2.333109	0.698840	1.428542
26	1	0	3.358076	-0.211802	0.296835
27	1	0	0.399738	0.432583	-0.223852
28	1	0	1.394759	-0.717481	-1.098366
29	7	0	0.879322	-1.308542	0.813893
30	6	0	1.125469	-2.682855	0.409359
31	6	0	0.217858	-0.939402	2.002482
32	8	0	-0.450500	-1.856947	2.586915
33	8	0	0.291373	0.261683	2.329712
34	1	0	0.806609	-3.315728	1.241002
35	1	0	0.525109	-2.919072	-0.480161
36	6	0	2.596403	-2.881889	0.107184
37	6	0	3.045321	-2.996239	-1.208235
38	6	0	3.536974	-2.850996	1.141875
39	6	0	4.409708	-3.072167	-1.490480
40	1	0	2.316175	-3.023635	-2.014943
41	6	0	4.897382	-2.932210	0.865691
42	1	0	3.187612	-2.749925	2.166930
43	6	0	5.337645	-3.038385	-0.454540
44	1	0	4.745250	-3.163094	-2.519130
45	1	0	5.617349	-2.914021	1.678262
46	1	0	6.399561	-3.101753	-0.670582
47	6	0	-2.403229	-0.789198	0.891484
48	6	0	-1.916402	-2.111616	1.279553
49	7	0	-3.112680	-1.627607	-0.068106
50	6	0	-4.561472	-1.755210	0.054755
51	6	0	-5.281082	-0.444200	-0.175563
52	6	0	-5.925276	0.215054	0.871322
53	6	0	-5.276847	0.137510	-1.448505
54	6	0	-5.911855	1.356162	-1.660164
55	6	0	-6.555883	2.009086	-0.609022
56	6	0	-6.562434	1.436681	0.658099
57	1	0	-3.061462	-0.289652	1.600925
58	1	0	-1.231861	-2.596716	0.607118
59	1	0	-2.507819	-2.700378	1.968883
60	1	0	-4.856609	-2.494148	-0.692054
61	1	0	-4.802283	-2.139686	1.053785
62	1	0	-5.933854	-0.235082	1.861872
63	1	0	-7.062771	1.937696	1.481231
64	1	0	-7.052521	2.959441	-0.779625
65	1	0	-5.909298	1.798610	-2.651905
66	1	0	-4.767730	-0.384647	-2.254414
67	1	0	-1.690462	-0.119229	0.418752
68	16	0	3.537666	1.480794	-1.943570

ImBicar-11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.034266	-0.791282	-0.057818
2	6	0	0.000013	-1.680204	-0.022296
3	7	0	1.034270	-0.791255	-0.059203
4	6	0	-0.676316	0.555891	-0.114617
5	6	0	0.676481	0.555773	-0.116291
6	6	0	-2.477380	-0.976113	-0.061493
7	6	0	-2.984808	0.418209	0.357434
8	6	0	-1.904740	1.410244	-0.148595
9	6	0	1.905036	1.410304	-0.147855

10	6	0	2.477283	-0.975841	-0.062820
11	6	0	2.984482	0.417714	0.358910
12	1	0	-2.764432	-1.770647	0.628636
13	1	0	-2.819606	-1.246017	-1.066968
14	1	0	-3.978834	0.637374	-0.036493
15	1	0	-2.126208	1.739234	-1.170840
16	1	0	-1.834975	2.302271	0.477837
17	1	0	1.833835	2.301376	0.479773
18	1	0	3.979110	0.637457	-0.033303
19	1	0	3.030395	0.466804	1.450487
20	1	0	2.819695	-1.242719	-1.069031
21	1	0	2.764526	-1.772278	0.625013
22	1	0	-3.032211	0.468407	1.448983
23	1	0	2.128364	1.740630	-1.169213

ImBicar-TS$_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.094379	0.047109	-1.013849
2	7	0	2.718909	1.183714	-0.623777
3	7	0	2.622042	-0.844956	-0.143199
4	6	0	3.597765	1.016515	0.443673
5	6	0	3.529356	-0.300732	0.757026
6	6	0	2.652266	2.566673	-1.078803
7	6	0	2.392911	-2.276811	0.074402
8	6	0	4.226133	2.329338	0.794061
9	6	0	4.007292	-1.357641	1.703289
10	6	0	3.945848	3.160363	-0.485591
11	1	0	3.856660	4.229013	-0.284995
12	1	0	4.764163	3.013014	-1.195540
13	1	0	1.758329	3.050137	-0.669528
14	1	0	2.611293	2.613237	-2.167782
15	1	0	2.392613	-2.808638	-0.878923
16	1	0	1.418567	-2.435426	0.548738
17	6	0	3.593417	-2.658363	0.965551
18	1	0	3.736352	2.776037	1.666840
19	1	0	5.292981	2.255567	1.013419
20	1	0	3.490467	-1.269979	2.665233
21	1	0	5.080825	-1.313714	1.897072
22	1	0	3.346907	-3.467762	1.653445
23	1	0	4.422101	-2.990240	0.334317
24	6	0	0.023136	-0.510959	-1.411295
25	6	0	-0.639399	-0.104509	-0.171602
26	1	0	0.374873	-1.528473	-1.483764
27	1	0	-0.098940	0.085331	-2.304575
28	1	0	-0.314985	-0.593180	0.743804
29	1	0	-0.880595	0.951535	-0.054843
30	7	0	-1.654418	-0.861129	-0.889243
31	6	0	-2.799044	-0.138930	-1.445208
32	6	0	-1.831756	-2.347988	-0.458081
33	8	0	-2.928977	-2.796667	-0.762140
34	8	0	-0.814885	-2.782086	0.088454
35	1	0	-2.437623	0.599251	-2.172533
36	1	0	-3.391684	-0.892624	-1.966585
37	6	0	-3.618306	0.550466	-0.378705
38	6	0	-4.289932	-0.212534	0.582940
39	6	0	-3.693937	1.941859	-0.320110
40	6	0	-5.022777	0.416500	1.582709
41	1	0	-4.226292	-1.296014	0.524974

42	6	0	-4.432342	2.571609	0.680415
43	1	0	-3.177652	2.538159	-1.069726
44	6	0	-5.096588	1.808457	1.634528
45	1	0	-5.543743	-0.181488	2.323934
46	1	0	-4.487112	3.655436	0.712601
47	1	0	-5.672865	2.294911	2.415367

ImBicar-22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.691956	-0.283242	1.283565
2	7	0	2.584358	-1.045760	0.643934
3	7	0	1.945777	0.967247	0.893528
4	6	0	3.338396	-0.289035	-0.234848
5	6	0	2.942026	0.997972	-0.067565
6	6	0	2.588563	-2.466055	0.289430
7	6	0	1.314330	2.274664	1.097479
8	6	0	4.057883	-1.191492	-1.186279
9	6	0	3.074092	2.384846	-0.611934
10	1	0	1.712881	-2.622584	-0.349464
11	1	0	2.556069	-3.098661	1.178315
12	6	0	3.905259	-2.569788	-0.499701
13	1	0	0.236735	2.152414	1.203735
14	6	0	1.708954	2.996051	-0.207295
15	6	0	0.520397	-0.746131	2.071663
16	6	0	-0.656883	-1.044917	1.090956
17	1	0	0.227245	0.047883	2.765383
18	1	0	0.788266	-1.628789	2.661254
19	1	0	-0.412360	-1.929514	0.498807
20	1	0	-1.553325	-1.262053	1.683441
21	7	0	-0.887676	0.067444	0.218436
22	6	0	-1.999109	0.952835	0.492425
23	6	0	-0.183868	0.137316	-1.048913
24	8	0	-0.438551	1.140407	-1.744693
25	8	0	0.624946	-0.799552	-1.251352
26	1	0	-1.994400	1.250625	1.553715
27	1	0	-1.830536	1.843959	-0.118722
28	6	0	-3.343980	0.346472	0.150272
29	6	0	-3.611710	0.012868	-1.182216
30	6	0	-4.304620	0.084437	1.123925
31	6	0	-4.825447	-0.568474	-1.525944
32	1	0	-2.850623	0.224368	-1.930315
33	6	0	-5.523511	-0.500890	0.780246
34	1	0	-4.099223	0.343585	2.160813
35	6	0	-5.784831	-0.827682	-0.545287
36	1	0	-5.029496	-0.820250	-2.562321
37	1	0	-6.265318	-0.700020	1.547892
38	1	0	-6.732279	-1.282801	-0.817310
39	1	0	3.881216	-3.392504	-1.214611
40	1	0	4.736654	-2.735322	0.191549
41	1	0	3.510569	-1.172061	-2.134737
42	1	0	5.099019	-0.919839	-1.366605
43	1	0	1.737046	2.743495	1.992379
44	1	0	3.216977	2.386747	-1.693410
45	1	0	3.914843	2.914664	-0.149520
46	1	0	1.749541	4.078451	-0.077671
47	1	0	0.964731	2.730312	-0.965407

ImBicar-$TS_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.061992	-1.652184	0.183201
2	8	0	-4.053215	-2.267219	0.569013
3	8	0	-2.109792	-1.954240	-0.559905
4	6	0	-2.067627	0.695394	0.055055
5	6	0	-1.203823	0.205661	1.119991
6	7	0	-2.933474	-0.261328	0.750370
7	6	0	-4.020113	0.271696	1.569694
8	6	0	-5.056562	1.008626	0.752399
9	6	0	-5.223238	2.386781	0.882293
10	6	0	-5.844085	0.308133	-0.167728
11	6	0	-6.781610	0.985185	-0.939134
12	6	0	-6.945271	2.363537	-0.802401
13	6	0	-6.164975	3.064745	0.110299
14	1	0	-2.429333	1.720140	0.124775
15	1	0	-0.740116	-0.754847	0.944978
16	1	0	-1.303375	0.605348	2.119506
17	1	0	-4.463487	-0.588783	2.072842
18	1	0	-3.595883	0.948107	2.322587
19	1	0	-4.613774	2.934122	1.598342
20	1	0	-6.286691	4.137766	0.222414
21	1	0	-7.680442	2.887564	-1.405252
22	1	0	-7.391475	0.435227	-1.649338
23	1	0	-5.703331	-0.765726	-0.259859
24	1	0	-1.791825	0.380702	-0.945274
25	6	0	2.434470	-1.926507	-0.994235
26	7	0	2.881282	-2.380042	0.182140
27	7	0	1.332834	-2.635862	-1.246457
28	6	0	2.041385	-3.357768	0.693625
29	6	0	1.050408	-3.523145	-0.224861
30	6	0	4.008640	-2.073709	1.058630
31	6	0	0.250610	-2.551921	-2.239365
32	6	0	2.554582	-3.804511	2.027554
33	6	0	-0.231106	-4.243671	-0.508917
34	1	0	4.181583	-0.998074	1.077917
35	1	0	4.902700	-2.595191	0.701491
36	6	0	3.499154	-2.633886	2.401771
37	1	0	-0.354920	-1.681368	-1.980236
38	1	0	0.667063	-2.463106	-3.244272
39	6	0	-0.499195	-3.874479	-1.991213
40	6	0	3.033303	-0.874927	-1.863276
41	6	0	3.352264	0.461108	-1.144398
42	1	0	2.309930	-0.692127	-2.656034
43	1	0	3.951200	-1.268546	-2.316964
44	1	0	4.417468	0.480739	-0.883682
45	1	0	3.190535	1.273264	-1.866022
46	7	0	2.620998	0.675845	0.092015
47	6	0	3.233070	1.635276	1.008377
48	6	0	1.198863	0.660235	0.003527
49	8	0	0.582986	1.074333	1.039840
50	8	0	0.700684	0.200795	-1.035287
51	1	0	2.613477	1.644372	1.905774
52	1	0	4.235008	1.273019	1.279290
53	6	0	3.350244	3.030527	0.427649
54	6	0	4.583294	3.546264	0.030931
55	6	0	2.197899	3.800864	0.237687

56	6	0	4.673291	4.812704	-0.544178
57	1	0	5.483476	2.952401	0.177205
58	6	0	2.286170	5.063436	-0.337675
59	1	0	1.239188	3.392956	0.547200
60	6	0	3.523585	5.572732	-0.729697
61	1	0	5.639825	5.202956	-0.847682
62	1	0	1.386882	5.654931	-0.479298
63	1	0	3.590341	6.559464	-1.177083
64	1	0	2.922240	-1.852860	2.903811
65	1	0	1.759950	-3.945612	2.761375
66	1	0	3.105232	-4.747707	1.940065
67	1	0	4.316799	-2.938566	3.055912
68	1	0	-1.038118	-3.837328	0.105910
69	1	0	-0.149145	-5.320635	-0.349573
70	1	0	-1.565719	-3.733953	-2.158129
71	1	0	-0.111872	-4.655467	-2.652085

ImCylm-11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.052694	0.896314	-0.004524
2	6	0	0.000012	1.764413	0.000013
3	7	0	-1.052686	0.896344	0.004526
4	6	0	0.678606	-0.445954	0.001132
5	6	0	-0.678644	-0.445936	-0.001159
6	6	0	2.436643	1.340513	0.093154
7	6	0	3.387344	0.241514	-0.369127
8	6	0	1.675928	-1.564232	-0.047249
9	6	0	-1.675940	-1.564234	0.047240
10	6	0	-2.436638	1.340506	-0.093183
11	6	0	-3.387313	0.241529	0.369167
12	1	0	2.656445	1.596828	1.137049
13	1	0	2.533432	2.251453	-0.500397
14	1	0	3.286699	0.095305	-1.451943
15	1	0	1.726746	-1.968187	-1.067852
16	1	0	1.352563	-2.387140	0.598833
17	1	0	-1.726795	-1.968187	1.067840
18	1	0	-4.416851	0.556289	0.175395
19	1	0	-3.286535	0.095329	1.451975
20	1	0	-2.656448	1.596737	-1.137102
21	1	0	-2.533451	2.251514	0.500264
22	1	0	4.416868	0.556243	-0.175222
23	1	0	-1.352503	-2.387127	-0.598829
24	6	0	-3.069711	-1.068832	-0.354742
25	6	0	3.069685	-1.068826	0.354744
26	1	0	3.104010	-0.896880	1.437829
27	1	0	3.817029	-1.833349	0.124372
28	1	0	-3.104050	-0.896859	-1.437818
29	1	0	-3.817057	-1.833344	-0.124359

ImCylm-$TS_{21\text{-}22}$

Standard orientation:

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

1	6	0	-0.201647	-0.667788	-1.608177
2	6	0	-0.748314	-0.295003	-0.301020
3	1	0	0.089774	-1.695034	-1.763589
4	1	0	-0.351840	-0.016128	-2.458548
5	1	0	-0.391708	-0.855025	0.560332
6	1	0	-0.915453	0.764247	-0.106482
7	7	0	-1.853049	-0.946492	-0.985608
8	6	0	-2.983061	-0.125259	-1.422141
9	1	0	-2.621389	0.634683	-2.126779
10	1	0	-3.652738	-0.809032	-1.946488
11	6	0	-3.686497	0.541240	-0.262619
12	6	0	-4.394204	-0.236587	0.660016
13	6	0	-3.611008	1.921408	-0.076292
14	6	0	-5.015253	0.367417	1.747500
15	1	0	-4.442081	-1.311387	0.505563
16	6	0	-4.235320	2.526360	1.013383
17	1	0	-3.066080	2.529356	-0.796125
18	6	0	-4.937761	1.748324	1.927222
19	1	0	-5.566497	-0.240977	2.457712
20	1	0	-4.173463	3.602160	1.145816
21	1	0	-5.426393	2.215615	2.776439
22	6	0	-2.099687	-2.444677	-0.619343
23	8	0	-3.239096	-2.805900	-0.880125
24	8	0	-1.082764	-2.965911	-0.157780
25	6	0	2.832732	3.538689	0.407231
26	6	0	1.882075	-0.149860	-1.290681
27	7	0	2.257101	1.087279	-0.883479
28	7	0	2.446298	-0.962052	-0.364986
29	6	0	3.024232	1.058351	0.277516
30	6	0	3.143584	-0.255545	0.608660
31	6	0	1.789807	2.314779	-1.519064
32	6	0	2.216409	-2.412228	-0.321023
33	6	0	3.600116	2.300474	0.883731
34	6	0	3.871076	-0.941107	1.722960
35	6	0	2.666304	3.495084	-1.113400
36	1	0	2.210483	4.416478	-1.485773
37	1	0	3.650970	3.401779	-1.587454
38	1	0	0.753409	2.500641	-1.205935
39	1	0	1.792099	2.154362	-2.599104
40	1	0	2.311862	-2.792363	-1.340814
41	1	0	1.186107	-2.598545	0.010130
42	6	0	3.213806	-3.085694	0.615589
43	1	0	3.583384	2.221821	1.975577
44	1	0	4.653837	2.401056	0.591274
45	1	0	3.810744	-0.332136	2.630894
46	1	0	4.936521	-1.029722	1.471944
47	1	0	2.897164	-4.121177	0.763377
48	6	0	3.294222	-2.342316	1.950037
49	1	0	3.363709	4.444502	0.711038
50	1	0	1.842885	3.567239	0.879496
51	1	0	2.290451	-2.266532	2.385090
52	1	0	3.918399	-2.890321	2.660681
53	1	0	4.208608	-3.108590	0.152993

ImCylm-22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.440552	-2.460847	-1.250673

2	6	0	1.445078	-0.151068	1.419941
3	7	0	2.331392	-0.994773	0.876344
4	7	0	1.657952	1.056772	0.886636
5	6	0	3.062541	-0.324930	-0.089859
6	6	0	2.644766	0.968838	-0.081147
7	6	0	2.167241	-2.454824	0.909257
8	6	0	0.954927	2.302347	1.220175
9	6	0	3.979023	-1.046093	-1.021578
10	6	0	2.911906	2.086977	-1.041170
11	1	0	1.194943	-2.641003	0.442528
12	1	0	2.165244	-2.785181	1.951386
13	6	0	3.265745	-3.143008	0.106692
14	1	0	-0.055043	2.040100	1.529999
15	6	0	0.932310	3.210156	-0.003353
16	6	0	0.272816	-0.523073	2.257850
17	6	0	-0.956386	-0.826550	1.333256
18	1	0	0.036532	0.307496	2.928658
19	1	0	0.514965	-1.387228	2.883054
20	1	0	-0.831729	-1.815853	0.887559
21	1	0	-1.853410	-0.845793	1.961832
22	7	0	-1.092240	0.166359	0.303743
23	6	0	-2.244064	1.046206	0.334197
24	6	0	-0.376084	-0.038977	-0.947587
25	8	0	-0.521846	0.854270	-1.804517
26	8	0	0.338832	-1.068343	-0.973713
27	1	0	-2.326388	1.525447	1.322532
28	1	0	-2.050998	1.822824	-0.410074
29	6	0	-3.544510	0.338581	0.012497
30	6	0	-3.710398	-0.222988	-1.258898
31	6	0	-4.560491	0.198396	0.955133
32	6	0	-4.876486	-0.909557	-1.572843
33	1	0	-2.911160	-0.103055	-1.986975
34	6	0	-5.731948	-0.491268	0.641260
35	1	0	-4.435701	0.635443	1.944032
36	6	0	-5.890442	-1.046680	-0.623256
37	1	0	-4.999904	-1.339858	-2.562079
38	1	0	-6.516012	-0.595792	1.385175
39	1	0	-6.799809	-1.585074	-0.871694
40	1	0	2.978973	-4.191353	-0.011688
41	1	0	4.213303	-3.124546	0.659571
42	1	0	4.030026	-0.482978	-1.957511
43	1	0	4.995885	-1.094551	-0.610316
44	1	0	1.485713	2.778307	2.053635
45	1	0	2.391126	1.824855	-1.971523
46	1	0	3.981704	2.157332	-1.256864
47	1	0	0.476098	4.161234	0.285464
48	1	0	0.310160	2.734285	-0.773138
49	6	0	2.354038	3.417421	-0.527154
50	1	0	2.468296	-2.387409	-1.751155
51	1	0	4.126497	-3.029533	-1.883486
52	1	0	2.360776	4.148389	-1.339263
53	1	0	2.993482	3.813219	0.272675

ImCylm-$TS_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.879202	-0.736837	-0.102161
2	8	0	3.779443	-1.435564	-0.574168

3	8	0	2.025641	-0.945341	0.775564
4	6	0	1.870576	1.589484	-0.054910
5	6	0	0.977243	0.988818	-1.034340
6	7	0	2.727741	0.613817	-0.739311
7	6	0	3.765640	1.099445	-1.645714
8	6	0	4.865621	1.833742	-0.913883
9	6	0	5.032727	3.209866	-1.061345
10	6	0	5.710627	1.130378	-0.048801
11	6	0	6.704458	1.802198	0.653545
12	6	0	6.867718	3.178817	0.500436
13	6	0	6.031152	3.882700	-0.358813
14	1	0	2.187217	2.617366	-0.222555
15	1	0	0.584221	0.015693	-0.777498
16	1	0	0.974427	1.346834	-2.054967
17	1	0	4.156556	0.214381	-2.150544
18	1	0	3.304572	1.762290	-2.388282
19	1	0	4.379072	3.760089	-1.734902
20	1	0	6.152873	4.954299	-0.483271
21	1	0	7.646836	3.699348	1.048522
22	1	0	7.358067	1.249699	1.321574
23	1	0	5.569144	0.057970	0.058999
24	1	0	1.662398	1.331117	0.977842
25	6	0	-1.928111	-4.033099	-2.756439
26	6	0	-1.685274	-1.990693	0.852023
27	7	0	-1.833307	-2.473054	-0.390602
28	7	0	-0.499073	-2.420135	1.302077
29	6	0	-0.714127	-3.222938	-0.734534
30	6	0	0.125627	-3.187713	0.337081
31	6	0	-3.051515	-2.403945	-1.202972
32	6	0	0.088352	-2.071764	2.608885
33	6	0	-0.564892	-3.851241	-2.083511
34	6	0	1.420594	-3.876565	0.611818
35	1	0	-3.455323	-1.397202	-1.110549
36	1	0	-3.771489	-3.125945	-0.798929
37	6	0	-2.730315	-2.735192	-2.655749
38	1	0	0.256576	-0.992274	2.579882
39	1	0	-0.666101	-2.315051	3.362941
40	6	0	1.394539	-2.831818	2.888956
41	6	0	-2.695005	-1.252914	1.671697
42	6	0	-3.405256	-0.038255	1.022935
43	1	0	-2.163151	-0.902473	2.552741
44	1	0	-3.456798	-1.972671	2.002183
45	1	0	-4.388348	-0.352177	0.651776
46	1	0	-3.593157	0.693040	1.820973
47	7	0	-2.706236	0.555001	-0.099972
48	6	0	-3.543108	1.321990	-1.017003
49	6	0	-1.379497	1.012369	0.136950
50	8	0	-0.869045	1.712057	-0.801648
51	8	0	-0.825041	0.631108	1.177863
52	1	0	-2.891379	1.644236	-1.830029
53	1	0	-4.315671	0.657652	-1.430402
54	6	0	-4.209979	2.516307	-0.364800
55	6	0	-5.584265	2.541342	-0.133802
56	6	0	-3.428967	3.598816	0.055169
57	6	0	-6.179552	3.630632	0.500539
58	1	0	-6.195780	1.701107	-0.456468
59	6	0	-4.021132	4.684347	0.690521
60	1	0	-2.357549	3.573454	-0.127804
61	6	0	-5.397595	4.703596	0.914390
62	1	0	-7.251489	3.638730	0.672300
63	1	0	-3.408500	5.521874	1.009486
64	1	0	-5.857657	5.553472	1.408598

65	1	0	-2.158372	-1.908250	-3.093290
66	1	0	0.067014	-3.211772	-2.711937
67	1	0	-0.040198	-4.805770	-1.980281
68	1	0	-3.672963	-2.808332	-3.204661
69	1	0	2.257364	-3.243450	0.294857
70	1	0	1.449100	-4.809412	0.038939
71	1	0	2.226593	-2.191189	2.599393
72	1	0	1.448989	-3.017806	3.965456
73	1	0	-2.482604	-4.843347	-2.267098
74	1	0	-1.789977	-4.319310	-3.801937
75	6	0	1.508833	-4.147788	2.117916
76	1	0	2.464055	-4.624520	2.351406
77	1	0	0.713657	-4.843688	2.416807

ImDpylm-11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.050532	-0.856292	0.000020
2	6	0	0.000002	-1.740353	-0.001379
3	7	0	-1.050530	-0.856291	-0.001097
4	6	0	0.690612	0.504633	0.000741
5	6	0	-0.690615	0.504634	-0.000355
6	6	0	2.384425	-1.225001	0.000614
7	6	0	3.351210	-0.279429	0.001841
8	6	0	1.704665	1.498374	0.002060
9	6	0	-1.704665	1.498374	-0.000332
10	6	0	-2.384425	-1.225000	-0.001887
11	6	0	-3.351211	-0.279428	-0.001940
12	1	0	2.552044	-2.294061	-0.000021
13	1	0	4.389212	-0.588768	0.002224
14	1	0	1.415734	2.543897	0.002522
15	1	0	-1.415735	2.543897	0.000452
16	1	0	-4.389214	-0.588763	-0.002676
17	1	0	-2.552040	-2.294061	-0.002515
18	6	0	-3.010744	1.117183	-0.001094
19	6	0	3.010744	1.117182	0.002568
20	1	0	3.800423	1.859463	0.003457
21	1	0	-3.800422	1.859468	-0.000950

ImDpylm-$TS_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.243991	0.006086	-1.286297
2	6	0	1.015526	0.042193	-0.045652
3	1	0	-0.055431	0.936305	-1.742206
4	1	0	0.246600	-0.898998	-1.879108
5	1	0	0.814649	0.849542	0.654406
6	1	0	1.220148	-0.914366	0.433299
7	7	0	1.987463	0.398464	-1.070428
8	6	0	3.060294	-0.547604	-1.379788
9	1	0	2.616649	-1.482935	-1.744337
10	1	0	3.629174	-0.084470	-2.187670
11	6	0	3.942462	-0.830061	-0.186044
12	6	0	4.746086	0.185794	0.342918

13	6	0	3.942356	-2.085963	0.419840
14	6	0	5.535492	-0.063221	1.460033
15	1	0	4.735319	1.161064	-0.137105
16	6	0	4.735596	-2.335247	1.538323
17	1	0	3.322010	-2.879090	0.007204
18	6	0	5.532834	-1.322236	2.059901
19	1	0	6.159593	0.727655	1.864316
20	1	0	4.729630	-3.318080	1.999441
21	1	0	6.152355	-1.512565	2.930773
22	6	0	2.243188	1.915127	-1.254447
23	8	0	3.327817	2.157682	-1.765620
24	8	0	1.281411	2.588306	-0.864315
25	6	0	-5.011827	-2.771220	0.008546
26	6	0	-1.853487	-0.183175	-0.634174
27	7	0	-2.840182	-1.105179	-0.477113
28	7	0	-2.348760	0.890959	0.051091
29	6	0	-3.933638	-0.644462	0.275389
30	6	0	-3.611021	0.658171	0.618380
31	6	0	-2.833633	-2.393871	-0.988447
32	6	0	-1.716392	2.121798	0.210442
33	6	0	-5.033246	-1.507295	0.513855
34	6	0	-4.255298	1.684642	1.355154
35	6	0	-3.882770	-3.214909	-0.758799
36	1	0	-3.859524	-4.218427	-1.165635
37	1	0	-1.952570	-2.656269	-1.558981
38	1	0	-0.733146	2.241625	-0.241326
39	6	0	-2.338516	3.094415	0.917314
40	1	0	-5.870777	-1.139945	1.096598
41	1	0	-5.231621	1.489662	1.784541
42	1	0	-1.832461	4.044913	1.032626
43	6	0	-3.629862	2.884293	1.501779
44	1	0	-5.840577	-3.447601	0.179524
45	1	0	-4.102294	3.684842	2.058927

ImDpylm-22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.416808	-2.299783	-0.905110
2	6	0	1.489310	-0.352907	1.204630
3	7	0	2.419090	-1.111777	0.593067
4	7	0	1.724362	0.920588	0.818991
5	6	0	3.246627	-0.330891	-0.208389
6	6	0	2.799797	0.978034	-0.061763
7	6	0	2.523242	-2.489753	0.595200
8	6	0	0.994324	2.056095	1.129361
9	6	0	4.279693	-0.944380	-0.949324
10	6	0	3.197752	2.220966	-0.602779
11	1	0	1.785250	-3.026422	1.174383
12	6	0	3.507202	-3.078043	-0.125743
13	6	0	1.374804	3.244789	0.605081
14	6	0	0.302936	-0.842510	1.947950
15	6	0	-0.870571	-1.065329	0.948416
16	1	0	0.014598	-0.094883	2.693988
17	1	0	0.558234	-1.753330	2.500254
18	1	0	-0.601750	-1.879124	0.269490
19	1	0	-1.763565	-1.353915	1.515995
20	7	0	-1.109193	0.130649	0.196091
21	6	0	-2.268692	0.934207	0.515732

22	6	0	-0.433907	0.296338	-1.092960
23	8	0	-0.812699	1.265352	-1.767380
24	8	0	0.472360	-0.546603	-1.295943
25	1	0	-2.280317	1.172974	1.592876
26	1	0	-2.145087	1.864101	-0.045628
27	6	0	-3.581814	0.278216	0.142143
28	6	0	-3.832929	-0.011012	-1.204353
29	6	0	-4.528976	-0.071413	1.101512
30	6	0	-5.018379	-0.634308	-1.573772
31	1	0	-3.081040	0.270687	-1.938632
32	6	0	-5.718885	-0.698836	0.731462
33	1	0	-4.336135	0.152620	2.149061
34	6	0	-5.964501	-0.980422	-0.607453
35	1	0	-5.210360	-0.851278	-2.620336
36	1	0	-6.449676	-0.967186	1.488733
37	1	0	-6.889220	-1.468189	-0.900585
38	1	0	3.579839	-4.158465	-0.117147
39	1	0	4.927781	-0.321031	-1.553966
40	1	0	0.123156	1.909043	1.750167
41	1	0	4.038024	2.247295	-1.286081
42	1	0	0.788766	4.123295	0.843120
43	6	0	2.496364	3.340838	-0.273524
44	1	0	5.194765	-2.794483	-1.473419
45	1	0	2.768402	4.302705	-0.690643

ImDpylm-TS$_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.752108	-1.586297	-1.442778
2	8	0	4.787374	-1.790606	-2.071211
3	8	0	2.837487	-2.326745	-1.040126
4	6	0	2.566653	0.209745	-0.047941
5	6	0	1.738079	0.384330	-1.237397
6	7	0	3.508948	-0.130804	-1.114123
7	6	0	4.550759	0.844342	-1.427935
8	6	0	5.551284	1.008035	-0.305433
9	6	0	5.584320	2.172259	0.462062
10	6	0	6.441093	-0.030509	-0.009476
11	6	0	7.348544	0.105714	1.035011
12	6	0	7.378116	1.273829	1.796654
13	6	0	6.493586	2.307761	1.509852
14	1	0	2.841360	1.100734	0.512885
15	1	0	1.338270	-0.515280	-1.683688
16	1	0	1.854516	1.279037	-1.831551
17	1	0	5.040176	0.480950	-2.332503
18	1	0	4.075646	1.810690	-1.641220
19	1	0	4.895665	2.983168	0.233764
20	1	0	6.509619	3.219576	2.098963
21	1	0	8.090408	1.376674	2.609508
22	1	0	8.039809	-0.702065	1.255493
23	1	0	6.398971	-0.934975	-0.610367
24	1	0	2.318845	-0.632570	0.586589
25	6	0	-5.498508	-2.671376	-0.913830
26	6	0	-2.430419	-1.538682	1.568055
27	7	0	-3.524708	-1.841264	0.842397
28	7	0	-1.401139	-2.216988	0.999243
29	6	0	-3.208371	-2.711864	-0.202975
30	6	0	-1.836771	-2.948432	-0.100345

31	6	0	-4.817348	-1.368820	1.016089
32	6	0	-0.067413	-2.230024	1.386776
33	6	0	-4.225740	-3.132909	-1.086241
34	6	0	-0.906842	-3.690651	-0.867087
35	1	0	-4.970487	-0.692729	1.846206
36	6	0	-5.786514	-1.773205	0.159463
37	1	0	0.196912	-1.592155	2.215741
38	6	0	0.815325	-2.948433	0.655556
39	6	0	-2.345199	-0.416412	2.535317
40	6	0	-2.499138	0.937850	1.776270
41	1	0	-1.364368	-0.433410	3.007203
42	1	0	-3.104821	-0.521500	3.318067
43	1	0	-3.558643	1.199121	1.681616
44	1	0	-2.019289	1.712184	2.383304
45	7	0	-1.943834	0.882030	0.445253
46	6	0	-2.786524	1.242462	-0.681371
47	6	0	-0.536414	0.832409	0.332010
48	8	0	-0.083019	1.009591	-0.845222
49	8	0	0.095482	0.599110	1.377590
50	1	0	-2.205153	1.021120	-1.577933
51	1	0	-3.682084	0.603424	-0.689046
52	6	0	-3.208220	2.696161	-0.671612
53	6	0	-4.549479	3.063690	-0.596045
54	6	0	-2.227918	3.692571	-0.712951
55	6	0	-4.916539	4.408919	-0.570103
56	1	0	-5.313503	2.288929	-0.560586
57	6	0	-2.591159	5.033180	-0.686345
58	1	0	-1.184223	3.393187	-0.774435
59	6	0	-3.937235	5.394561	-0.614917
60	1	0	-5.965093	4.684644	-0.512935
61	1	0	-1.825386	5.801790	-0.725199
62	1	0	-4.218777	6.442663	-0.595156
63	1	0	-6.792217	-1.397732	0.304032
64	1	0	1.866986	-2.927793	0.905673
65	1	0	-6.291879	-2.977884	-1.583948
66	6	0	0.406710	-3.671118	-0.506165
67	1	0	1.176199	-4.150488	-1.098401
68	1	0	-3.966419	-3.811218	-1.890868
69	1	0	-1.259456	-4.224235	-1.741862

ImPhen-11

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.064475	1.306184	-0.068931
2	6	0	-0.000030	2.175898	0.000056
3	7	0	1.064473	1.306173	0.068234
4	6	0	-0.685529	-0.020943	-0.046722
5	6	0	0.685558	-0.020950	0.045314
6	6	0	-2.483995	1.594204	-0.210723
7	6	0	-3.297952	0.434988	0.395604
8	6	0	-1.445183	-1.177811	-0.089840
9	6	0	1.445126	-1.177841	0.089309
10	6	0	2.483899	1.594189	0.211049
11	6	0	3.298309	0.434967	-0.394651
12	1	0	-2.728619	1.712002	-1.273642
13	1	0	-2.700128	2.537521	0.294445
14	1	0	-3.124303	0.422598	1.477295
15	6	0	-0.706169	-2.361333	-0.039435

16	1	0	4.361259	0.636648	-0.235895
17	1	0	3.125573	0.422683	-1.476492
18	1	0	2.727712	1.712083	1.274139
19	1	0	2.700483	2.537450	-0.294038
20	1	0	-4.361029	0.636694	0.237736
21	6	0	0.706054	-2.361351	0.039428
22	6	0	2.937375	-0.955542	0.180276
23	6	0	-2.937488	-0.955465	-0.179791
24	1	0	-3.259067	-1.011968	-1.227883
25	1	0	-3.486078	-1.733215	0.360329
26	1	0	3.258209	-1.012263	1.228585
27	1	0	3.486334	-1.733210	-0.359596
28	1	0	-1.225021	-3.315772	-0.063930
29	1	0	1.224842	-3.315808	0.064584

ImPhen-TS$_{21\text{-}22}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.696158	-0.657965	-1.623586
2	6	0	-1.194018	-0.199216	-0.322955
3	1	0	-0.422074	-1.697506	-1.714958
4	1	0	-0.898597	-0.072785	-2.510357
5	1	0	-0.784350	-0.687461	0.558335
6	1	0	-1.366596	0.870137	-0.202017
7	7	0	-2.324075	-0.911284	-0.894933
8	6	0	-3.490286	-0.141060	-1.327555
9	1	0	-3.183754	0.563810	-2.111114
10	1	0	-4.177367	-0.873251	-1.754987
11	6	0	-4.138670	0.609300	-0.187220
12	6	0	-4.734633	-0.100071	0.861218
13	6	0	-4.125188	2.003150	-0.148215
14	6	0	-5.307034	0.585107	1.926772
15	1	0	-4.738784	-1.186142	0.817940
16	6	0	-4.702193	2.689320	0.919139
17	1	0	-3.666672	2.556634	-0.965376
18	6	0	-5.292986	1.979429	1.958757
19	1	0	-5.772186	0.030226	2.735601
20	1	0	-4.689988	3.774710	0.936515
21	1	0	-5.745333	2.509058	2.791371
22	6	0	-2.517266	-2.382804	-0.417217
23	8	0	-3.663974	-2.779092	-0.575048
24	8	0	-1.461472	-2.858536	0.007210
25	6	0	3.505946	3.226392	0.044275
26	6	0	1.393291	-0.185505	-1.437688
27	7	0	1.954224	1.010569	-1.092923
28	7	0	1.984154	-1.080450	-0.596631
29	6	0	2.870568	0.868630	-0.068881
30	6	0	2.883510	-0.467473	0.252317
31	6	0	1.709346	2.353399	-1.605148
32	6	0	1.753206	-2.520412	-0.436636
33	6	0	3.666820	1.814019	0.556736
34	6	0	3.678888	-1.002310	1.253841
35	6	0	2.979129	3.203989	-1.409894
36	1	0	2.765128	4.222869	-1.743221
37	1	0	3.762119	2.803718	-2.062940
38	1	0	0.866032	2.798271	-1.062531
39	1	0	1.441083	2.283869	-2.661330
40	1	0	1.556184	-2.952418	-1.420411

41	1	0	0.859769	-2.679257	0.178681
42	6	0	3.012403	-3.160953	0.175870
43	6	0	4.489071	1.301317	1.558962
44	6	0	4.491079	-0.072757	1.901631
45	1	0	2.793556	-4.214203	0.367273
46	6	0	3.512791	-2.487162	1.474669
47	1	0	4.454703	3.769571	0.082285
48	1	0	2.801667	3.775462	0.682254
49	1	0	2.786233	-2.657070	2.278982
50	1	0	4.453074	-2.946920	1.792984
51	1	0	3.816895	-3.123682	-0.567305
52	1	0	5.153541	1.970533	2.098264
53	1	0	5.153473	-0.407173	2.695014

ImPhen-22

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.913314	-2.378589	-1.013589
2	6	0	1.032450	-0.487533	1.445510
3	7	0	1.950812	-1.291680	0.882127
4	7	0	1.371636	0.788353	1.204642
5	6	0	2.831334	-0.509759	0.161782
6	6	0	2.476557	0.801198	0.374844
7	6	0	1.848169	-2.699875	0.499025
8	6	0	0.721283	2.065575	1.525441
9	6	0	3.800762	-0.896160	-0.749766
10	6	0	3.061634	1.873638	-0.279909
11	1	0	1.150431	-2.727759	-0.346666
12	1	0	1.446723	-3.277591	1.335397
13	6	0	3.254269	-3.192175	0.120543
14	1	0	-0.343169	1.881455	1.669275
15	6	0	0.941772	3.028993	0.346637
16	6	0	-0.201272	-0.932177	2.142833
17	6	0	-1.361255	-1.085404	1.111089
18	1	0	-0.471564	-0.178002	2.887991
19	1	0	-0.008280	-1.871790	2.670042
20	1	0	-1.156859	-1.952886	0.478730
21	1	0	-2.287434	-1.268649	1.667359
22	7	0	-1.482780	0.095071	0.306281
23	6	0	-2.625500	0.963792	0.502986
24	6	0	-0.715120	0.165729	-0.927260
25	8	0	-0.936386	1.162816	-1.638975
26	8	0	0.106589	-0.770460	-1.073344
27	1	0	-2.719186	1.225652	1.569069
28	1	0	-2.406157	1.874874	-0.060100
29	6	0	-3.930093	0.364127	0.020827
30	6	0	-4.083725	0.084605	-1.342153
31	6	0	-4.966194	0.055839	0.899480
32	6	0	-5.259436	-0.490154	-1.808290
33	1	0	-3.266470	0.333663	-2.015586
34	6	0	-6.146999	-0.521770	0.432192
35	1	0	-4.850582	0.273801	1.959521
36	6	0	-6.294492	-0.795151	-0.922733
37	1	0	-5.374547	-0.699526	-2.867518
38	1	0	-6.948022	-0.756846	1.126730
39	1	0	-7.212598	-1.242405	-1.291274
40	1	0	3.178458	-4.241116	-0.176410
41	1	0	3.888382	-3.152092	1.013230
42	6	0	4.438698	0.164366	-1.387694

43	1	0	1.163535	2.453050	2.450642
44	6	0	4.078322	1.513484	-1.159674
45	1	0	0.499927	3.991129	0.620134
46	1	0	0.389815	2.629923	-0.514608
47	6	0	2.430386	3.220246	-0.020018
48	1	0	3.405865	-2.598310	-1.960379
49	1	0	4.957290	-2.685321	-1.129450
50	1	0	2.510209	3.854709	-0.906674
51	1	0	2.958156	3.734845	0.793721
52	1	0	5.205821	-0.046475	-2.127258
53	1	0	4.581787	2.287540	-1.731336

ImPhen-$TS_{23\text{-}24}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.152463	-0.840138	-0.717510
2	8	0	-4.123713	-1.502582	-0.333013
3	8	0	-2.375661	-0.953404	-1.673478
4	6	0	-1.804519	1.274552	-0.257698
5	6	0	-1.003551	0.418164	0.612020
6	7	0	-2.806950	0.309504	0.192935
7	6	0	-3.780377	0.744361	1.189287
8	6	0	-4.764337	1.749410	0.633799
9	6	0	-4.760708	3.075624	1.063733
10	6	0	-5.675969	1.351658	-0.350192
11	6	0	-6.566291	2.273461	-0.888686
12	6	0	-6.559417	3.598315	-0.452343
13	6	0	-5.655964	3.999205	0.525588
14	1	0	-2.009672	2.291693	0.074304
15	1	0	-0.683781	-0.521229	0.178223
16	1	0	-1.077569	0.540806	1.685207
17	1	0	-4.293268	-0.161110	1.517466
18	1	0	-3.246094	1.183461	2.041976
19	1	0	-4.054717	3.388261	1.830472
20	1	0	-5.644771	5.028863	0.869681
21	1	0	-7.258056	4.314433	-0.873801
22	1	0	-7.271821	1.957395	-1.650970
23	1	0	-5.668213	0.315177	-0.677686
24	1	0	-1.591459	1.178378	-1.318469
25	6	0	0.395529	-2.265929	3.311044
26	6	0	2.561146	-2.307449	-0.322600
27	7	0	2.113402	-2.331114	0.945645
28	7	0	1.603664	-2.795392	-1.124282
29	6	0	0.803117	-2.773149	0.944691
30	6	0	0.482221	-3.064310	-0.361046
31	6	0	2.700369	-1.893807	2.214610
32	6	0	1.466006	-2.721001	-2.587598
33	6	0	-0.123088	-2.755016	1.979544
34	6	0	-0.807138	-3.363897	-0.780838
35	1	0	3.462690	-1.142209	2.009784
36	1	0	3.162796	-2.761397	2.699021
37	6	0	1.579716	-1.298907	3.084367
38	1	0	2.068184	-1.878969	-2.934077
39	1	0	1.847147	-3.653906	-3.016473
40	6	0	-0.012164	-2.484953	-2.946128
41	6	0	3.861933	-1.711054	-0.736647
42	6	0	3.741409	-0.172598	-0.965069
43	1	0	4.221534	-2.204560	-1.643891

44	1	0	4.590545	-1.911627	0.054829
45	1	0	4.748256	0.255888	-0.956184
46	1	0	3.298145	0.010541	-1.945675
47	7	0	2.939477	0.458190	0.058025
48	6	0	3.569471	1.389561	0.981511
49	6	0	1.544367	0.491494	-0.177564
50	8	0	0.842230	1.073888	0.722889
51	8	0	1.125910	-0.092108	-1.186726
52	1	0	2.842988	1.581426	1.774605
53	1	0	4.449173	0.908934	1.432552
54	6	0	3.986743	2.688547	0.325018
55	6	0	5.329167	3.028587	0.173449
56	6	0	3.002765	3.549756	-0.171618
57	6	0	5.692857	4.214688	-0.463557
58	1	0	6.097206	2.362701	0.561708
59	6	0	3.363603	4.731837	-0.806160
60	1	0	1.956978	3.278105	-0.048180
61	6	0	4.709955	5.066687	-0.954092
62	1	0	6.741994	4.469582	-0.576441
63	1	0	2.595117	5.397426	-1.186462
64	1	0	4.989046	5.990379	-1.451014
65	1	0	1.225239	-0.389934	2.582585
66	6	0	-1.418457	-3.072641	1.582934
67	1	0	2.017939	-1.009289	4.043327
68	6	0	-1.753390	-3.371892	0.238142
69	1	0	-0.287289	-1.473616	-2.633634
70	1	0	-0.098760	-2.552429	-4.034098
71	1	0	0.719377	-3.112696	3.929823
72	1	0	-0.396237	-1.753074	3.864384
73	6	0	-0.998614	-3.459907	-2.271268
74	1	0	-2.015372	-3.152768	-2.520546
75	1	0	-0.831617	-4.489880	-2.614072
76	1	0	-2.223928	-3.028215	2.310721
77	1	0	-2.802564	-3.486773	-0.017357

S5: Reference 24 details.

24. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.