Electronic Supplementary Material (ESI) for Dalton Transactions.

2-Quinoxalinol Diamine Cu(II) Complex: Facilitating Catalytic Oxidation Through Dual Mechanisms

Yuancheng Li, TaeBum Lee, Kushan Weerasiri, Tanyu Wang, Emily E. Buss, Michael L. McKee, Anne E. V. Gorden*

Department of Chemistry and Biochemistry, College of Science and Mathematics, Auburn University, Auburn, Alabama 36849-5319, United States

gordeae@auburn.edu

SUPPORTING INFORMATION

Table of Contents

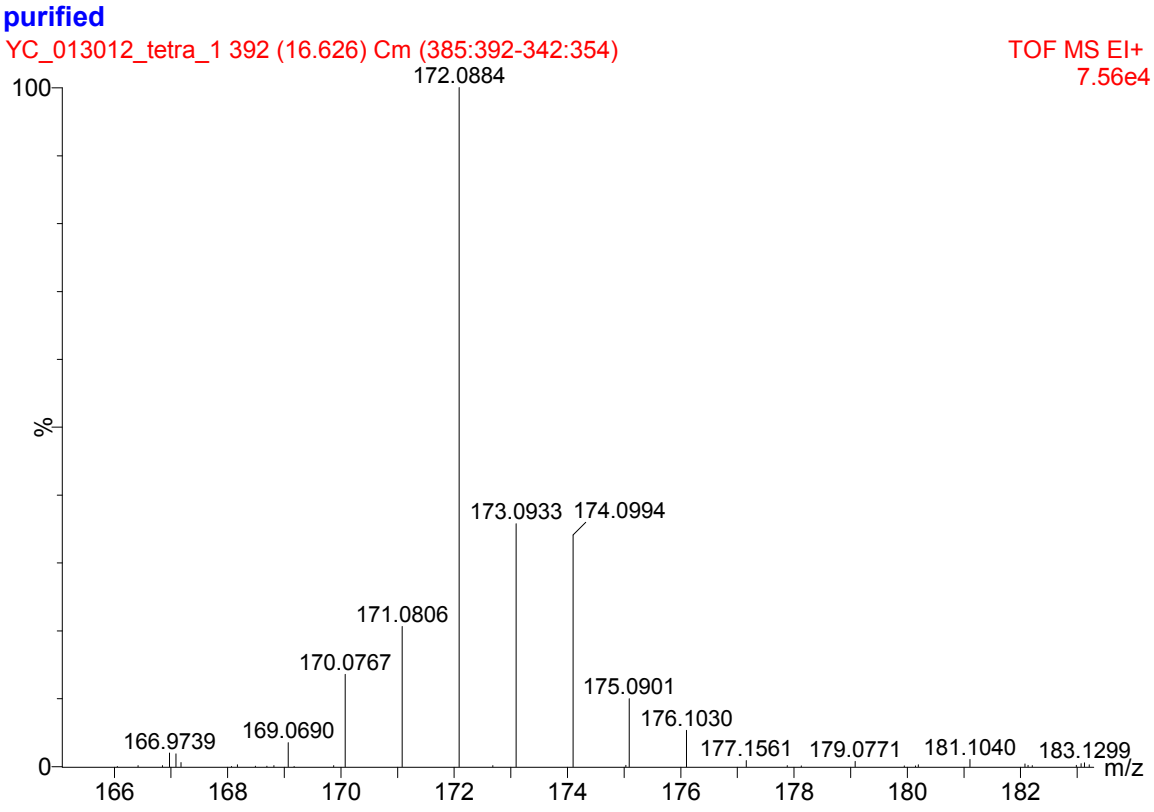

Figure S1. ESI-MS of reaction solution using regular TBHP as the oxidant under $^{18}O_2$ atmosphere.

Theoretical Calculation

Point groups, Electronic States, Total Energies (hartrees) at B3LYP/6-311+G(2df,p), Zero-Point Energies (kcal/mol), Thermal Corrections (kcal/mol), Entropies (cal/mol·K) at B3LYP/6-31G(d) and Solvation Free Energies (kcal/mol) at B3LYP/6-311+G(2df,p)

	PG[a]	ES[b]	SCF Energy	ZPE[c] (NIF)	TC[d]	S[e]	Solvation Free Energy[f]
4	C_1	^2A	-2896.86773	233.53(0)	17.54	182.47	-26.54
7	C_2	^1A	-234.72318	92.26(0)	4.03	72.37	-4.22
4,7TS9,14	C_1	^2A	-3131.54240	321.89(1)	22.13	220.21	-24.50
9	C_S	$^2A''$	-234.08297	83.47(0)	4.04	74.98	-4.40
14	C_1	^1A	-2897.51628	239.88(0)	18.21	186.70	-24.04
9,14TS15	C_1	^2A	-3131.59951	323.35(1)	22.68	227.84	-27.76
15	C_1	^2A	-3131.66672	326.69(0)	22.37	221.44	-26.43
16	C_1	^2A	-3131.67303	327.02(0)	22.15	220.45	-21.99
16TS17	C_1	^2A	-3131.65941	326.09(1)	21.96	218.80	-20.86
17	C_1	^2A	-3131.67667	326.78(0)	22.35	222.84	-24.07
17TS18	C_1	^2A	-3131.67855	326.60(1)	21.96	221.07	-24.48
18	C_1	^2A	-3131.68971	327.31(0)	21.99	223.11	-25.31
19	C_1	^1A	-309.96884	95.00(0)	4.71	79.31	-7.11
20	C_1	^2A	-2821.69973	230.93(0)	17.07	178.55	-23.16
4TS5,6	C_1	^2A	-2896.79585	230.05(1)	18.22	189.72	-29.47
5	C_1	^2A	-115.09697	23.10(0)	2.48	56.57	-3.30
^{3}6	C_1	^3A	-2781.70645	206.23(0)	15.70	168.16	-28.49
6[g]	C_1	^1A	-2781.70155	206.20(0)	15.71	166.19	-29.18
5,7TS8,9	C_1	^2A	-349.81611	113.96(1)	6.35	96.94	-6.69
8	C_S	$^1A'$	-115.76963	32.30(0)	2.66	56.74	-3.62
9	C_S	$^2A''$	-234.08297	83.47(0)	4.04	74.98	-4.40
^{3}6,7TS9,10	C_1	^3A	-3016.42769	295.57(1)	19.99	206.76	-28.56
6,7TS9,10[g]	C_1	^1A	-3016.42390	295.99(1)	19.99	205.40	-29.25
10	C_1	^2A	-2782.39162	213.34(0)	15.96	168.97	-25.88
^{3}O$_2$	$D_{\infty h}$	$^3\Sigma_g^-$	-150.37835	2.37(0)	2.08	49.01	-2.40
11	C_1	^2A	-384.48870	89.67(0)	5.23	86.27	-8.69
11TS12	C_1	^2A	-384.42030	85.62(0)	5.18	86.06	-10.08
12	C_1	^2A	-384.53981	87.62(0)	5.93	92.50	-13.55
13	C_1	^1A	-308.76956	80.29(0)	4.41	77.73	-8.86
OH	$C_{\infty V}$	$^2\Pi$	-75.76403	5.21(0)	2.07	42.61	-3.79

[a]Point group. [b]Electronic state. [c]Zero-point energies and number of imaginary frequencies. [d]Thermal corrections to 298K. [e]Entropies (cal/mol·K). [f]Solvation free energies are computed as the difference between the B3LYP and SMD(acetonitrile)/B3LYP energies. [g]Result from the open shell singlet state (broken symmetry).

Geometry at B3LYP/6-31G(d) level of calculation **4** C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.308570	1.519379	-0.242579
2	6	0	-5.354226	-1.797293	0.355398
3	6	0	-3.217317	-0.987638	0.070552
4	6	0	-3.732774	0.272663	-0.351161
5	6	0	-5.848396	-0.512639	-0.080572
6	1	0	-1.482529	-2.157127	0.503960
7	6	0	-1.823618	-1.193322	0.142790
8	6	0	-2.828965	1.303695	-0.694985
9	6	0	-1.473283	1.082683	-0.620228
10	6	0	-0.941937	-0.181259	-0.209336
11	1	0	-3.226776	2.262624	-1.013697
12	6	0	1.115021	-1.379676	-0.088039
13	6	0	2.522897	-1.527647	-0.030844
14	6	0	3.433515	-0.409958	-0.103528
15	6	0	3.038778	-2.854108	0.077596
16	6	0	4.843475	-0.695013	-0.054887
17	6	0	4.386351	-3.114052	0.127839
18	1	0	2.326785	-3.676924	0.126124
19	6	0	5.270336	-2.000245	0.059219
20	1	0	6.342514	-2.190898	0.097404
21	1	0	0.540423	-2.310369	-0.088978
22	7	0	0.463622	-0.240446	-0.155666
23	8	0	3.070108	0.824307	-0.228019
24	6	0	5.801227	0.463707	-0.131291
25	1	0	5.615954	1.181372	0.676150
26	1	0	6.839131	0.121664	-0.067803
27	1	0	5.672216	1.021051	-1.066590
28	6	0	4.935411	-4.514742	0.252202
29	1	0	5.527533	-4.637149	1.168657
30	1	0	4.130560	-5.256618	0.276457
31	1	0	5.594718	-4.766557	-0.588734
32	7	0	-4.061886	-2.009060	0.423541
33	7	0	-5.080448	0.487082	-0.420164
34	8	0	-7.189932	-0.360269	-0.130516
35	1	0	-7.351524	0.551428	-0.436795
36	6	0	-6.311376	-2.891157	0.731621
37	1	0	-5.749579	-3.777001	1.033936
38	1	0	-6.964466	-2.574980	1.553730
39	1	0	-6.967481	-3.144538	-0.109649
40	7	0	-0.491826	2.093060	-0.949991

41	1	0	-0.617578	2.995005	-0.470924
42	1	0	-0.458821	2.279546	-1.953086
43	8	0	1.853022	3.237646	0.203639
44	8	0	0.710606	4.136844	0.367987
45	6	0	0.677157	4.478569	1.737636
46	1	0	0.494635	3.597621	2.371423
47	1	0	1.620877	4.946357	2.042216
48	1	0	-0.145457	5.195407	1.852327

7 C_2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.005187	1.503056	0.047817
2	6	0	-0.371449	0.671579	-1.192338
3	6	0	0.371449	-0.671579	-1.192338
4	6	0	0.005187	-1.503056	0.047817
5	6	0	-0.005187	-0.668485	1.306185
6	6	0	0.005187	0.668485	1.306185
7	1	0	0.983277	1.970244	-0.089870
8	1	0	-1.454055	0.482516	-1.192849
9	1	0	0.149634	-1.236805	-2.105944
10	1	0	0.708859	-2.339186	0.163919
11	1	0	-0.019119	-1.204621	2.254763
12	1	0	0.019119	1.204621	2.254763
13	1	0	1.454055	-0.482516	-1.192849
14	1	0	-0.149634	1.236805	-2.105944
15	1	0	-0.708859	2.339186	0.163919
16	1	0	-0.983277	-1.970244	-0.089870

4,7TS9,14 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.911597	-0.383565	0.188246
2	6	0	-6.610100	0.080816	-0.367472
3	6	0	-4.318461	0.112883	-0.146239
4	6	0	-4.286133	-1.310518	-0.080067
5	6	0	-6.549116	-1.358596	-0.290505
6	1	0	-3.197158	1.924495	-0.177954

7	6	0	-3.117264	0.848167	-0.076450
8	6	0	-3.041289	-1.960359	0.067383
9	6	0	-1.878284	-1.226374	0.150075
10	6	0	-1.897247	0.203872	0.075732
11	1	0	-3.022969	-3.044886	0.122975
12	6	0	-0.499076	2.126003	0.174992
13	6	0	0.711566	2.858323	0.053156
14	6	0	1.974715	2.237925	-0.254636
15	6	0	0.632804	4.275056	0.187944
16	6	0	3.107378	3.101344	-0.448321
17	6	0	1.727075	5.090945	0.022152
18	1	0	-0.335615	4.712957	0.425976
19	6	0	2.960910	4.465398	-0.303203
20	1	0	3.838167	5.096587	-0.443320
21	1	0	-1.395085	2.731704	0.332433
22	7	0	-0.630138	0.822820	0.098082
23	8	0	2.146093	0.959770	-0.380527
24	6	0	4.431690	2.471263	-0.787915
25	1	0	5.211543	3.230293	-0.906408
26	1	0	4.743681	1.769104	-0.005195
27	1	0	4.367142	1.891731	-1.717172
28	6	0	1.646822	6.591320	0.170584
29	1	0	0.627226	6.913020	0.406660
30	1	0	2.302635	6.954361	0.972885
31	1	0	1.953197	7.106796	-0.749104
32	7	0	-5.504763	0.783610	-0.296311
33	7	0	-5.441522	-2.036790	-0.156132
34	8	0	-7.723321	-2.025153	-0.366923
35	1	0	-7.502841	-2.972667	-0.298862
36	6	0	-7.930288	0.778286	-0.529954
37	1	0	-7.767980	1.857206	-0.569588
38	1	0	-8.436609	0.451956	-1.446248
39	1	0	-8.604519	0.541602	0.301829
40	7	0	-0.583655	-1.828566	0.274005
41	1	0	-0.495401	-2.686674	-0.265086
42	1	0	-0.293915	-2.029537	1.250091
43	8	0	2.199750	-1.687562	0.618585
44	8	0	1.032867	-1.295697	2.229161
45	6	0	1.933297	-1.382482	3.280013
46	1	0	2.357646	-2.395067	3.389902
47	1	0	2.769991	-0.673002	3.180582
48	1	0	1.406624	-1.141162	4.222707
49	6	0	5.722487	-4.010833	-0.364336
50	6	0	4.212430	-4.302391	-0.364364
51	6	0	3.481951	-3.456051	-1.416465
52	6	0	3.733341	-1.982758	-1.177726

53	6	0	5.105478	-1.619264	-0.833425
54	6	0	6.022564	-2.539627	-0.463685
55	1	0	6.191025	-4.422597	0.540263
56	1	0	4.034417	-5.370401	-0.536042
57	1	0	3.848860	-3.713521	-2.424299
58	1	0	3.225246	-1.291498	-1.850091
59	1	0	5.373062	-0.566072	-0.865871
60	1	0	7.040331	-2.220087	-0.244576
61	1	0	3.125696	-1.635757	-0.017496
62	1	0	2.408055	-3.663765	-1.403710
63	1	0	3.792103	-4.054676	0.617503
64	1	0	6.213074	-4.529514	-1.205386

9 C_s

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.108186	-0.694320	1.274119
2	6	0	0.502718	-1.305691	0.000000
3	6	0	-0.108186	-0.694320	-1.274119
4	6	0	-0.108186	0.809006	-1.218098
5	6	0	-0.098409	1.478107	0.000000
6	6	0	-0.108186	0.809006	1.218098
7	1	0	-1.141713	-1.062139	1.400211
8	1	0	1.582547	-1.108573	0.000000
9	1	0	0.437306	-1.045154	-2.160460
10	1	0	-0.098916	2.567160	0.000000
11	1	0	-0.139485	1.370009	2.148664
12	1	0	-1.141713	-1.062139	-1.400211
13	1	0	0.374759	-2.394745	0.000000
14	1	0	0.437306	-1.045154	2.160460
15	1	0	-0.139485	1.370009	-2.148664

14 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.372345	-1.621649	-0.381425
2	6	0	-5.271570	1.446290	-0.742210
3	6	0	-3.149919	0.751758	-0.190531

4	6	0	-3.659655	-0.076295	0.853994
5	6	0	-5.764490	0.606332	0.318451
6	1	0	-1.377463	1.377501	-1.242777
7	6	0	-1.756040	0.780700	-0.419229
8	6	0	-2.772868	-0.831761	1.646026
9	6	0	-1.405220	-0.795160	1.416619
10	6	0	-0.900903	0.034709	0.361095
11	1	0	-3.186274	-1.443320	2.442937
12	6	0	1.158114	1.161640	0.177340
13	6	0	2.574355	1.311234	0.068040
14	6	0	3.432161	0.177947	0.177066
15	6	0	3.122202	2.615578	-0.022944
16	6	0	4.840653	0.396345	0.212172
17	6	0	4.485953	2.828528	-0.024022
18	1	0	2.439760	3.460240	-0.098217
19	6	0	5.320333	1.691678	0.099995
20	1	0	6.399300	1.840642	0.109840
21	1	0	0.577418	2.071941	0.344968
22	7	0	0.505571	0.032886	0.145032
23	8	0	2.987128	-1.051670	0.320227
24	6	0	5.759240	-0.788180	0.357552
25	1	0	5.613314	-1.505151	-0.459301
26	1	0	6.807529	-0.474640	0.357108
27	1	0	5.561566	-1.332867	1.288440
28	6	0	5.083969	4.209598	-0.148302
29	1	0	5.675728	4.311545	-1.067091
30	1	0	4.305709	4.979059	-0.169885
31	1	0	5.753634	4.435948	0.690861
32	7	0	-3.979387	1.502522	-0.973372
33	7	0	-5.006439	-0.125433	1.091380
34	8	0	-7.103348	0.588063	0.513526
35	1	0	-7.257786	-0.026345	1.254994
36	6	0	-6.218979	2.255411	-1.581869
37	1	0	-5.651281	2.822687	-2.322433
38	1	0	-6.940727	1.609547	-2.096350
39	1	0	-6.803022	2.948028	-0.963781
40	7	0	-0.513362	-1.555539	2.157297
41	1	0	-0.880920	-1.966939	3.004914
42	1	0	0.419712	-1.181270	2.269591
43	8	0	2.151341	-3.152432	-0.837448
44	8	0	-0.166717	-2.110415	-1.128071
45	6	0	-0.367613	-3.406616	-1.619243
46	1	0	0.347558	-3.684821	-2.403093
47	1	0	-0.336790	-4.170879	-0.830352
48	1	0	-1.379111	-3.401017	-2.056160
49	1	0	3.063876	-3.029892	-0.521134

9,14TS15 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.225231	-0.060533	-0.151628
2	6	0	-6.054488	-0.239692	-1.001256
3	6	0	-3.891905	0.089474	-0.290856
4	6	0	-4.088894	-0.792708	0.813585
5	6	0	-6.232310	-1.122942	0.119777
6	1	0	-2.473578	1.341724	-1.319087
7	6	0	-2.627873	0.699649	-0.457803
8	6	0	-3.033720	-1.030179	1.715169
9	6	0	-1.794788	-0.429043	1.540583
10	6	0	-1.600733	0.457507	0.427829
11	1	0	-3.212231	-1.697256	2.553871
12	6	0	-0.280856	2.375471	0.232346
13	6	0	0.874590	3.195140	0.070889
14	6	0	2.186961	2.642047	-0.030114
15	6	0	0.695519	4.604805	0.070483
16	6	0	3.294589	3.544692	-0.111189
17	6	0	1.759931	5.474802	-0.025850
18	1	0	-0.318063	4.994568	0.148941
19	6	0	3.056058	4.906824	-0.113759
20	1	0	3.911051	5.578166	-0.187421
21	1	0	-1.227148	2.906750	0.366950
22	7	0	-0.323428	1.068814	0.270032
23	8	0	2.435095	1.360855	-0.044475
24	6	0	4.684765	2.973829	-0.206167
25	1	0	4.791501	2.336169	-1.092086
26	1	0	5.434243	3.769517	-0.260520
27	1	0	4.913718	2.341541	0.660418
28	6	0	1.577611	6.973866	-0.036453
29	1	0	1.951966	7.420100	-0.966912
30	1	0	0.521481	7.245999	0.058700
31	1	0	2.119934	7.453454	0.788627
32	7	0	-4.892122	0.347643	-1.182464
33	7	0	-5.303304	-1.396225	0.997704
34	8	0	-7.449888	-1.699778	0.261591
35	1	0	-7.387425	-2.258324	1.058486
36	6	0	-7.180763	0.017822	-1.962322
37	1	0	-6.844079	0.712930	-2.734453

38	1	0	-7.517751	-0.912379	-2.435748
39	1	0	-8.052136	0.441632	-1.448346
40	7	0	-0.743303	-0.670270	2.406101
41	1	0	-0.981343	-1.065669	3.305079
42	1	0	-0.015882	0.029528	2.445855
43	8	0	2.652597	-1.191599	-0.025968
44	8	0	0.108261	-1.324399	-0.765621
45	6	0	0.485461	-2.654897	-0.932094
46	1	0	1.197459	-2.802917	-1.760448
47	1	0	0.926418	-3.095196	-0.024626
48	1	0	-0.431093	-3.222583	-1.164924
49	1	0	3.392039	-0.558927	0.004652
50	6	0	3.362635	-5.446702	-0.681419
51	6	0	4.659905	-4.819434	-1.220204
52	6	0	4.710143	-3.306386	-0.943253
53	6	0	4.384876	-2.991716	0.487589
54	6	0	3.628614	-3.876299	1.265384
55	6	0	3.100430	-5.034753	0.739147
56	1	0	2.510846	-5.135190	-1.309073
57	1	0	5.514902	-5.302782	-0.729255
58	1	0	5.693974	-2.899902	-1.211557
59	1	0	3.422043	-3.617244	2.301162
60	1	0	2.471564	-5.671538	1.357065
61	1	0	3.976995	-2.782500	-1.573763
62	1	0	4.757309	-5.010324	-2.295097
63	1	0	3.403801	-6.541161	-0.758616
64	1	0	4.829809	-2.120164	0.955265

---

15 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.196157	0.303290	0.695463
2	6	0	-5.972414	-1.024257	0.544217
3	6	0	-3.732954	-0.814990	0.062076
4	6	0	-3.991009	0.306849	-0.780551
5	6	0	-6.209717	0.106452	-0.312791
6	1	0	-2.206717	-2.072384	0.914965
7	6	0	-2.399412	-1.252260	0.231042
8	6	0	-2.922030	0.941025	-1.445994
9	6	0	-1.619968	0.501632	-1.274075
10	6	0	-1.361166	-0.613812	-0.411728
11	1	0	-3.146576	1.777741	-2.101765

12	6	0	0.344811	-2.221764	-0.426019
13	6	0	1.654664	-2.784548	-0.283208
14	6	0	2.803541	-2.003655	0.061288
15	6	0	1.799657	-4.171521	-0.548931
16	6	0	4.071940	-2.659765	0.110492
17	6	0	3.022408	-4.807922	-0.487243
18	1	0	0.908204	-4.740410	-0.808637
19	6	0	4.147692	-4.016408	-0.153963
20	1	0	5.123725	-4.498028	-0.102709
21	1	0	-0.432623	-2.911540	-0.771323
22	7	0	-0.004303	-0.981661	-0.216961
23	8	0	2.747751	-0.720368	0.311432
24	6	0	5.290291	-1.846576	0.461570
25	1	0	5.176639	-1.362998	1.439332
26	1	0	6.187947	-2.472169	0.487698
27	1	0	5.455957	-1.041624	-0.266064
28	6	0	3.175296	-6.285426	-0.760877
29	1	0	3.565820	-6.820903	0.114246
30	1	0	2.215712	-6.741444	-1.025223
31	1	0	3.871754	-6.474503	-1.588002
32	7	0	-4.744370	-1.461289	0.712956
33	7	0	-5.272589	0.752122	-0.955457
34	8	0	-7.494070	0.513561	-0.452895
35	1	0	-7.465693	1.280819	-1.054034
36	6	0	-7.112181	-1.708107	1.245323
37	1	0	-6.725073	-2.542932	1.833399
38	1	0	-7.641534	-1.013621	1.908990
39	1	0	-7.852391	-2.081921	0.527555
40	7	0	-0.538040	1.120578	-1.904592
41	1	0	-0.799691	1.755906	-2.648893
42	1	0	0.195969	0.485232	-2.193620
43	8	0	2.605009	1.825004	0.595148
44	8	0	-0.122073	1.134400	1.641680
45	6	0	0.256041	1.743621	2.842854
46	1	0	0.759561	1.054551	3.548770
47	1	0	0.927259	2.610586	2.701371
48	1	0	-0.642548	2.117662	3.361477
49	1	0	3.352688	1.261581	0.317786
50	6	0	2.287459	5.917242	-0.422316
51	6	0	3.438105	5.126697	-1.068308
52	6	0	3.702711	3.819789	-0.307154
53	6	0	2.457585	2.934769	-0.336489
54	6	0	1.216003	3.689953	0.050069
55	6	0	1.147994	5.023910	0.003869
56	1	0	2.657079	6.467951	0.457139
57	1	0	3.178668	4.891507	-2.110038

58	1	0	4.561640	3.285765	-0.735474
59	1	0	0.374581	3.078447	0.369861
60	1	0	0.222283	5.515503	0.300170
61	1	0	3.940329	4.035841	0.742148
62	1	0	4.348785	5.735677	-1.103322
63	1	0	1.921644	6.687232	-1.115521
64	1	0	2.328152	2.502481	-1.342152

16 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.459952	-0.216569	0.410934
2	6	0	6.188136	0.173955	0.553340
3	6	0	3.918545	0.053840	0.208401
4	6	0	4.066090	-1.145118	-0.547343
5	6	0	6.315134	-1.034231	-0.219658
6	1	0	2.530648	1.500951	0.963668
7	6	0	2.623949	0.587915	0.384447
8	6	0	2.919113	-1.792490	-1.040715
9	6	0	1.639567	-1.285208	-0.837208
10	6	0	1.502984	-0.018790	-0.158521
11	1	0	3.050532	-2.732004	-1.570708
12	6	0	0.241712	1.918255	-0.348137
13	6	0	-0.819142	2.873363	-0.247355
14	6	0	-2.148181	2.548166	0.163441
15	6	0	-0.499628	4.218760	-0.578244
16	6	0	-3.110341	3.600409	0.250115
17	6	0	-1.427592	5.235826	-0.500387
18	1	0	0.517836	4.441876	-0.894703
19	6	0	-2.734040	4.891256	-0.076092
20	1	0	-3.481528	5.680658	-0.004159
21	1	0	1.188016	2.333818	-0.702682
22	7	0	0.233904	0.634887	-0.074362
23	8	0	-2.521386	1.328825	0.452887
24	6	0	-4.509962	3.263003	0.692435
25	1	0	-4.508461	2.763952	1.668640
26	1	0	-5.128714	4.162926	0.763254
27	1	0	-4.995317	2.571621	-0.008925
28	6	0	-1.084716	6.665383	-0.846824
29	1	0	-1.240446	7.337308	0.007070
30	1	0	-0.038436	6.758984	-1.154965
31	1	0	-1.707310	7.042759	-1.668348

32	7	0	4.996620	0.692084	0.752133
33	7	0	5.310281	-1.678128	-0.751841
34	8	0	7.566462	-1.520054	-0.396720
35	1	0	7.465103	-2.327247	-0.934528
36	6	0	7.401991	0.844781	1.131620
37	1	0	7.094086	1.737046	1.680876
38	1	0	7.941784	0.171349	1.808365
39	1	0	8.109623	1.130649	0.343862
40	7	0	0.513755	-1.943360	-1.319001
41	1	0	0.747980	-2.834206	-1.745402
42	1	0	-0.199358	-2.076716	-0.585431
43	8	0	-3.175197	-0.903722	-0.643289
44	8	0	-1.045757	-1.887085	1.039254
45	6	0	-0.177822	-2.062734	2.128506
46	1	0	0.771528	-1.511822	2.017651
47	1	0	-0.631460	-1.742449	3.082560
48	1	0	0.081395	-3.128395	2.234707
49	1	0	-3.737897	-0.131864	-0.454787
50	6	0	-3.861335	-5.015603	0.072653
51	6	0	-4.886848	-4.036024	0.666869
52	6	0	-4.313772	-2.613079	0.727535
53	6	0	-3.967931	-2.120487	-0.679260
54	6	0	-3.196955	-3.146259	-1.464433
55	6	0	-3.156851	-4.439391	-1.130379
56	1	0	-3.107692	-5.276268	0.831833
57	1	0	-5.795189	-4.042441	0.047473
58	1	0	-5.025283	-1.924838	1.202626
59	1	0	-2.674835	-2.775889	-2.344384
60	1	0	-2.581775	-5.130325	-1.745847
61	1	0	-3.386871	-2.600577	1.311522
62	1	0	-5.189410	-4.364606	1.667981
63	1	0	-4.349434	-5.961781	-0.198443
64	1	0	-4.888025	-1.867046	-1.230230

16TS17 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.259523	-0.289071	0.505518
2	6	0	6.257391	0.641997	0.103382
3	6	0	3.964213	0.453155	0.101669
4	6	0	4.054528	-0.922591	-0.257659
5	6	0	6.321866	-0.750004	-0.268527

6	1	0	2.669652	2.091665	0.550791
7	6	0	2.694955	1.044357	0.270342
8	6	0	2.869535	-1.679065	-0.375602
9	6	0	1.629234	-1.100694	-0.180288
10	6	0	1.534254	0.309340	0.079249
11	1	0	2.953061	-2.740026	-0.592807
12	6	0	0.073630	2.142561	-0.188067
13	6	0	-1.144561	2.885696	-0.192770
14	6	0	-2.427582	2.300146	0.063306
15	6	0	-1.053145	4.273465	-0.493247
16	6	0	-3.577040	3.152438	0.020357
17	6	0	-2.159963	5.092815	-0.530204
18	1	0	-0.067134	4.691001	-0.690895
19	6	0	-3.418054	4.495616	-0.264758
20	1	0	-4.306266	5.126252	-0.288412
21	1	0	0.959046	2.710089	-0.484218
22	7	0	0.234889	0.878525	0.111413
23	8	0	-2.603519	1.033640	0.316616
24	6	0	-4.929379	2.547142	0.290149
25	1	0	-4.950689	2.042094	1.262930
26	1	0	-5.712829	3.311225	0.276323
27	1	0	-5.183157	1.785990	-0.459168
28	6	0	-2.060859	6.568118	-0.837047
29	1	0	-2.655308	6.838752	-1.719298
30	1	0	-2.429170	7.180560	-0.003724
31	1	0	-1.025126	6.864374	-1.032268
32	7	0	5.089332	1.213304	0.280891
33	7	0	5.275040	-1.510947	-0.442901
34	8	0	7.554153	-1.279916	-0.442031
35	1	0	7.414991	-2.214099	-0.685002
36	6	0	7.516173	1.440350	0.288419
37	1	0	7.258162	2.463556	0.568816
38	1	0	8.151065	0.999217	1.066140
39	1	0	8.112300	1.454604	-0.631929
40	7	0	0.417430	-1.835202	-0.258118
41	1	0	0.473312	-2.627370	-0.892697
42	1	0	0.079911	-2.161848	0.663411
43	8	0	-2.727628	-1.232716	-0.995067
44	8	0	-1.254009	-1.624654	1.833540
45	6	0	-1.279698	-1.405345	3.213563
46	1	0	-2.204873	-0.897337	3.540012
47	1	0	-1.226030	-2.358957	3.766697
48	1	0	-0.435707	-0.783275	3.566734
49	1	0	-3.399798	-0.566557	-0.765870
50	6	0	-2.905051	-5.385425	-0.301572
51	6	0	-4.152513	-4.580196	0.098078

52	6	0	-3.827242	-3.084463	0.213853
53	6	0	-3.338972	-2.533600	-1.130577
54	6	0	-2.320187	-3.438423	-1.773082
55	6	0	-2.126917	-4.708965	-1.403750
56	1	0	-2.248003	-5.519465	0.571846
57	1	0	-4.935682	-4.731674	-0.658690
58	1	0	-4.709594	-2.521548	0.546903
59	1	0	-1.747502	-2.997910	-2.587372
60	1	0	-1.375910	-5.306761	-1.920182
61	1	0	-3.033424	-2.914473	0.951540
62	1	0	-4.556734	-4.954511	1.045864
63	1	0	-3.188098	-6.399099	-0.617083
64	1	0	-4.190816	-2.422544	-1.823162

---

17 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.952784	-0.275556	1.000622
2	6	0	6.314003	0.869727	-0.181655
3	6	0	4.023452	0.673185	-0.056668
4	6	0	4.133554	-0.739824	0.096157
5	6	0	6.396577	-0.562877	-0.032433
6	1	0	2.717651	2.366798	-0.115900
7	6	0	2.751066	1.284731	-0.049268
8	6	0	2.958266	-1.513030	0.236135
9	6	0	1.726060	-0.900561	0.231261
10	6	0	1.604764	0.519122	0.087019
11	1	0	3.051899	-2.589626	0.342597
12	6	0	-0.056575	2.182951	-0.279037
13	6	0	-1.368028	2.741517	-0.254571
14	6	0	-2.531995	1.999012	0.148068
15	6	0	-1.508119	4.086708	-0.698512
16	6	0	-3.799808	2.665561	0.092280
17	6	0	-2.727693	4.724248	-0.739449
18	1	0	-0.610069	4.620621	-1.005887
19	6	0	-3.864120	3.978557	-0.333204
20	1	0	-4.838747	4.465002	-0.360214
21	1	0	0.714349	2.808997	-0.737928
22	7	0	0.283753	1.006211	0.179024
23	8	0	-2.509528	0.751203	0.529183
24	6	0	-5.027358	1.897670	0.506149
25	1	0	-5.185848	1.024081	-0.138485

26	1	0	-4.924726	1.509180	1.525722
27	1	0	-5.921231	2.527535	0.457677
28	6	0	-2.874432	6.156364	-1.194905
29	1	0	-3.289698	6.792205	-0.402161
30	1	0	-1.908878	6.581301	-1.487852
31	1	0	-3.549152	6.239569	-2.056807
32	7	0	5.140311	1.455911	-0.189888
33	7	0	5.358888	-1.344137	0.103194
34	8	0	7.633559	-1.107180	-0.034730
35	1	0	7.509441	-2.068018	0.077170
36	6	0	7.561655	1.692785	-0.325985
37	1	0	7.291941	2.746068	-0.424638
38	1	0	8.218748	1.564685	0.542458
39	1	0	8.138955	1.380478	-1.204440
40	7	0	0.488734	-1.607859	0.402085
41	1	0	0.562698	-2.426307	1.002107
42	1	0	0.041997	-1.877375	-0.480201
43	8	0	-1.892952	-1.334865	-1.456267
44	8	0	-1.570121	-1.438572	2.265571
45	6	0	-2.743607	-1.201169	2.983526
46	1	0	-2.782758	-1.869184	3.861288
47	1	0	-2.826600	-0.167490	3.364447
48	1	0	-3.656887	-1.397947	2.391752
49	6	0	-2.841125	-5.341066	-0.607535
50	6	0	-3.987326	-4.330970	-0.436402
51	6	0	-3.446977	-2.897745	-0.344082
52	6	0	-2.696595	-2.517662	-1.626748
53	6	0	-1.760609	-3.612861	-2.070925
54	6	0	-1.816878	-4.866403	-1.609137
55	1	0	-2.345152	-5.515343	0.360348
56	1	0	-4.669675	-4.412257	-1.294469
57	1	0	-4.264813	-2.186115	-0.171901
58	1	0	-2.434389	-0.646863	-1.021206
59	1	0	-1.016839	-3.325810	-2.813476
60	1	0	-1.097334	-5.601198	-1.969890
61	1	0	-2.758396	-2.799913	0.505118
62	1	0	-4.575328	-4.572726	0.456421
63	1	0	-3.234332	-6.319267	-0.916933
64	1	0	-3.424454	-2.323355	-2.434193

17TS18 C_1

Standard orientation:

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

1	29	0	-1.291632	0.477067	-0.660176
2	6	0	5.354223	-2.923294	-0.097908
3	6	0	3.228035	-2.039023	-0.096320
4	6	0	3.758392	-0.715644	-0.112261
5	6	0	5.863932	-1.573682	-0.106625
6	1	0	1.475920	-3.263301	-0.133399
7	6	0	1.830979	-2.239131	-0.100463
8	6	0	2.868378	0.382295	-0.128152
9	6	0	1.509006	0.167382	-0.127105
10	6	0	0.965921	-1.155589	-0.102364
11	1	0	3.276215	1.388520	-0.140744
12	6	0	-1.091625	-2.294446	0.222991
13	6	0	-2.500707	-2.465018	0.224465
14	6	0	-3.415257	-1.409499	-0.126283
15	6	0	-3.005814	-3.737418	0.621947
16	6	0	-4.821887	-1.701369	-0.067445
17	6	0	-4.352616	-4.008520	0.671705
18	1	0	-2.288106	-4.512683	0.886701
19	6	0	-5.242023	-2.957865	0.316522
20	1	0	-6.313143	-3.155313	0.351176
21	1	0	-0.512807	-3.150454	0.581230
22	7	0	-0.443194	-1.214645	-0.144526
23	8	0	-3.052391	-0.215608	-0.474728
24	6	0	-5.790992	-0.608755	-0.432554
25	1	0	-5.665987	0.264895	0.218411
26	1	0	-5.619392	-0.253697	-1.455527
27	1	0	-6.825717	-0.957071	-0.352790
28	6	0	-4.890862	-5.357767	1.083154
29	1	0	-5.483675	-5.818614	0.282127
30	1	0	-4.079990	-6.049316	1.334241
31	1	0	-5.546082	-5.281658	1.960787
32	7	0	4.058710	-3.129489	-0.094187
33	7	0	5.109142	-0.508238	-0.115860
34	8	0	7.208051	-1.427864	-0.106799
35	1	0	7.377945	-0.467612	-0.115249
36	6	0	6.296904	-4.092301	-0.093831
37	1	0	5.722982	-5.021004	-0.088772
38	1	0	6.950531	-4.072581	-0.974063
39	1	0	6.953097	-4.064487	0.784296
40	7	0	0.538820	1.226883	-0.174135
41	1	0	0.783330	1.961883	-0.836472
42	1	0	0.376234	1.701278	0.729296
43	8	0	-0.491481	2.860688	1.979803
44	8	0	-1.669949	2.130079	-1.367478
45	6	0	-2.894479	2.453880	-1.958879

46	1	0	-2.927799	2.195431	-3.033896
47	1	0	-3.748983	1.950840	-1.479917
48	1	0	-3.074302	3.542045	-1.888652
49	6	0	0.931582	5.979945	-0.460482
50	6	0	-0.494308	6.155881	0.086032
51	6	0	-1.060877	4.821290	0.589085
52	6	0	-0.199407	4.258641	1.725333
53	6	0	1.273545	4.353073	1.419378
54	6	0	1.776313	5.112723	0.440353
55	1	0	0.897262	5.531294	-1.465589
56	1	0	-0.475604	6.882271	0.910742
57	1	0	-2.091783	4.955594	0.944944
58	1	0	-1.424089	2.715694	1.748534
59	1	0	1.929345	3.761853	2.057272
60	1	0	2.853542	5.125338	0.275327
61	1	0	-1.097464	4.080603	-0.222175
62	1	0	-1.148008	6.574343	-0.687504
63	1	0	1.415158	6.957681	-0.590779
64	1	0	-0.407619	4.808622	2.658322

---

18 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.072897	0.247366	-0.887574
2	6	0	-6.349160	-0.101442	0.327157
3	6	0	-4.071652	0.152846	0.103011
4	6	0	-3.940903	-1.208217	-0.299538
5	6	0	-6.186976	-1.477509	-0.077534
6	1	0	-3.092110	2.017702	0.443386
7	6	0	-2.931398	0.979804	0.174400
8	6	0	-2.659010	-1.708984	-0.618457
9	6	0	-1.556868	-0.888705	-0.534073
10	6	0	-1.673656	0.476322	-0.127033
11	1	0	-2.565919	-2.746328	-0.926162
12	6	0	-0.377252	2.393136	0.412500
13	6	0	0.743329	3.259858	0.354689
14	6	0	1.943732	2.931028	-0.368018
15	6	0	0.639863	4.515412	1.022667
16	6	0	2.988375	3.916712	-0.411229
17	6	0	1.650331	5.446482	0.989765
18	1	0	-0.278335	4.731984	1.566757
19	6	0	2.820596	5.113686	0.253521

20	1	0	3.628829	5.843390	0.213552
21	1	0	-1.238339	2.774640	0.967310
22	7	0	-0.465318	1.202392	-0.135017
23	8	0	2.134858	1.808831	-0.988104
24	6	0	4.240861	3.593040	-1.180920
25	1	0	4.729320	2.696462	-0.781482
26	1	0	4.013321	3.374007	-2.230900
27	1	0	4.952122	4.424304	-1.143984
28	6	0	1.546312	6.777402	1.694891
29	1	0	1.640857	7.615837	0.992512
30	1	0	0.584588	6.881570	2.207694
31	1	0	2.337669	6.899986	2.445936
32	7	0	-5.299865	0.681176	0.407834
33	7	0	-5.038478	-2.018174	-0.382640
34	8	0	-7.306798	-2.231718	-0.138946
35	1	0	-7.022771	-3.119925	-0.424512
36	6	0	-7.711417	0.438467	0.655249
37	1	0	-7.627362	1.490666	0.933966
38	1	0	-8.388969	0.341028	-0.201366
39	1	0	-8.167126	-0.121955	1.480304
40	7	0	-0.224537	-1.326442	-0.862863
41	1	0	-0.200202	-1.868852	-1.725654
42	1	0	0.208614	-1.923714	-0.130562
43	8	0	1.682205	-2.421476	0.849628
44	8	0	2.427746	-0.989821	-1.220178
45	6	0	3.754244	-0.616650	-1.488369
46	1	0	4.363236	-1.522278	-1.643132
47	1	0	3.837227	-0.004315	-2.399078
48	1	0	4.212659	-0.038996	-0.668415
49	6	0	4.660812	-5.445719	0.568020
50	6	0	4.395903	-4.828955	1.951906
51	6	0	3.656958	-3.490026	1.826537
52	6	0	2.290018	-3.677448	1.152731
53	6	0	2.406711	-4.552561	-0.076082
54	6	0	3.462522	-5.328593	-0.341583
55	1	0	5.523104	-4.951110	0.092933
56	1	0	3.785694	-5.524431	2.545451
57	1	0	3.519631	-3.014481	2.804331
58	1	0	2.184079	-1.962082	0.105352
59	1	0	1.564244	-4.517624	-0.766149
60	1	0	3.480124	-5.913573	-1.260935
61	1	0	4.250178	-2.797630	1.212936
62	1	0	5.338936	-4.697910	2.496171
63	1	0	4.949135	-6.501369	0.669339
64	1	0	1.603204	-4.154121	1.868388

---

19 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.365379	-0.010639	-0.199102
2	6	0	-1.885342	0.157494	-0.238553
3	6	0	-1.232820	-1.144287	0.256769
4	6	0	0.230619	-1.232857	-0.195451
5	6	0	1.055590	-0.071611	0.376176
6	6	0	0.329647	1.244950	0.219844
7	6	0	-0.971657	1.347445	-0.071963
8	1	0	-2.163660	0.060846	-1.300435
9	1	0	-1.272912	-1.172512	1.354585
10	1	0	0.685679	-2.185879	0.096556
11	1	0	2.249039	0.216698	-1.136266
12	1	0	0.941871	2.136301	0.350968
13	1	0	-1.417435	2.334236	-0.195620
14	1	0	0.275730	-1.180626	-1.294074
15	1	0	-1.799104	-2.013008	-0.099526
16	1	0	-2.829281	0.338353	0.293945
17	1	0	1.250817	-0.256102	1.441747

20 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.289297	-1.688267	-0.036604
2	6	0	-5.430383	1.537636	0.345196
3	6	0	-3.281986	0.750586	0.084950
4	6	0	-3.778674	-0.536910	-0.271944
5	6	0	-5.905497	0.225791	-0.025994
6	1	0	-1.562424	1.964373	0.458132
7	6	0	-1.891340	0.981265	0.140014
8	6	0	-2.859786	-1.568397	-0.572078
9	6	0	-1.507551	-1.322756	-0.515736
10	6	0	-0.995192	-0.032273	-0.167928
11	1	0	-3.244604	-2.547536	-0.841722
12	6	0	1.036965	1.206463	-0.145724
13	6	0	2.442611	1.388070	-0.090163
14	6	0	3.377100	0.289801	-0.042037

15	6	0	2.928269	2.729392	-0.109199
16	6	0	4.779325	0.611007	-0.011405
17	6	0	4.269565	3.024838	-0.073882
18	1	0	2.197881	3.536429	-0.148530
19	6	0	5.177582	1.930701	-0.024628
20	1	0	6.245075	2.147883	0.002614
21	1	0	0.444214	2.121176	-0.238729
22	7	0	0.408800	0.054161	-0.114404
23	8	0	3.041454	-0.960038	-0.040271
24	6	0	5.764330	-0.526301	0.036408
25	1	0	5.597421	-1.155795	0.918326
26	1	0	5.649670	-1.184796	-0.832751
27	1	0	6.793864	-0.155257	0.060625
28	6	0	4.785462	4.443526	-0.085273
29	1	0	5.441131	4.628678	-0.946184
30	1	0	3.963312	5.164973	-0.133560
31	1	0	5.371697	4.667979	0.815485
32	7	0	-4.141371	1.773630	0.394441
33	7	0	-5.122906	-0.776370	-0.322341
34	8	0	-7.244562	0.049160	-0.060286
35	1	0	-7.392402	-0.879081	-0.320317
36	6	0	-6.403499	2.632129	0.675868
37	1	0	-5.854838	3.539954	0.933833
38	1	0	-7.067803	2.835828	-0.172468
39	1	0	-7.047238	2.343652	1.515339
40	7	0	-0.507283	-2.329360	-0.796526
41	1	0	-0.434443	-2.528253	-1.794618
42	1	0	-0.665667	-3.216753	-0.317509
43	8	0	1.542315	-3.391896	0.559874
44	6	0	2.766136	-3.895551	1.001632
45	1	0	2.595763	-4.707555	1.730330
46	1	0	3.372019	-4.325128	0.181810
47	1	0	3.392817	-3.137361	1.500235

4TS5,6 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.200810	-1.427701	-0.464240
2	6	0	5.676640	1.384269	-0.087090
3	6	0	3.475380	0.707619	-0.008230
4	6	0	3.879910	-0.649401	0.151290
5	6	0	6.059230	0.000339	0.083860

6	1	0	1.838260	2.072099	-0.231870
7	6	0	2.103720	1.034349	-0.063120
8	6	0	2.892810	-1.655521	0.262830
9	6	0	1.561820	-1.313151	0.212590
10	6	0	1.143820	0.041279	0.054700
11	1	0	3.204140	-2.687871	0.389410
12	6	0	-0.814910	1.382179	0.184010
13	6	0	-2.206680	1.666449	0.093000
14	6	0	-3.193020	0.665129	-0.209400
15	6	0	-2.610690	3.011089	0.334860
16	6	0	-4.565820	1.079929	-0.266680
17	6	0	-3.930090	3.401799	0.277530
18	1	0	-1.838950	3.743009	0.566020
19	6	0	-4.890840	2.402469	-0.029160
20	1	0	-5.939750	2.692289	-0.078990
21	1	0	-0.177910	2.219449	0.477510
22	7	0	-0.253140	0.220589	-0.040470
23	8	0	-2.921450	-0.591531	-0.418970
24	6	0	-5.617430	0.049219	-0.585600
25	1	0	-5.611580	-0.766971	0.147010
26	1	0	-6.615550	0.497549	-0.594200
27	1	0	-5.438870	-0.413111	-1.564350
28	6	0	-4.361500	4.827679	0.526040
29	1	0	-5.062560	4.895429	1.367800
30	1	0	-3.503130	5.467459	0.753920
31	1	0	-4.872560	5.252089	-0.347690
32	7	0	4.406590	1.708389	-0.131020
33	7	0	5.205320	-0.981661	0.196230
34	8	0	7.381090	-0.258671	0.123960
35	1	0	7.485840	-1.222051	0.240920
36	6	0	6.726480	2.449249	-0.214350
37	1	0	6.248930	3.423009	-0.339720
38	1	0	7.368490	2.473249	0.674110
39	1	0	7.380150	2.253509	-1.072490
40	7	0	0.493840	-2.286671	0.308830
41	1	0	0.277130	-2.491141	1.287650
42	1	0	0.761140	-3.174101	-0.116110
43	8	0	-1.734550	-2.939511	-1.297900
44	8	0	-3.647950	-4.325681	0.414820
45	6	0	-3.369190	-3.562651	1.521600
46	1	0	-2.425940	-3.829261	2.026170
47	1	0	-3.401750	-2.485041	1.297560
48	1	0	-4.195200	-3.751541	2.237910

---

5 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.575017	0.000209	-0.012882
2	1	0	0.871214	-0.007846	1.057348
3	1	0	1.014774	0.911965	-0.451469
4	1	0	1.014129	-0.906015	-0.463614
5	8	0	-0.793778	0.000080	-0.008121

6 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.320290	-1.921576	0.171316
2	8	0	-1.603361	-3.557840	0.807821
3	6	0	5.248143	1.614351	0.245887
4	6	0	3.132555	0.725049	0.055011
5	6	0	3.680410	-0.560416	-0.225633
6	6	0	5.775134	0.302234	-0.047024
7	1	0	1.365993	1.886730	0.372559
8	6	0	1.733868	0.900963	0.110215
9	6	0	2.803396	-1.644733	-0.456523
10	6	0	1.443283	-1.448928	-0.403661
11	6	0	0.877588	-0.165704	-0.124234
12	1	0	3.227806	-2.620744	-0.673694
13	6	0	-1.208093	0.977872	-0.142246
14	6	0	-2.617835	1.098804	-0.082081
15	6	0	-3.499960	-0.040037	0.014662
16	6	0	-3.166126	2.414858	-0.155129
17	6	0	-4.916744	0.216451	0.038366
18	6	0	-4.519058	2.647497	-0.124836
19	1	0	-2.474532	3.252900	-0.231179
20	6	0	-5.375211	1.514074	-0.026505
21	1	0	-6.451493	1.682711	-0.002616
22	1	0	-0.657996	1.911072	-0.293537
23	7	0	-0.526280	-0.142328	-0.053655
24	8	0	-3.108144	-1.270266	0.058514
25	6	0	-5.845736	-0.963836	0.135702
26	1	0	-6.891660	-0.641540	0.155880
27	1	0	-5.705555	-1.646774	-0.710471
28	1	0	-5.641125	-1.552825	1.037278

29	6	0	-5.102265	4.038242	-0.191350
30	1	0	-5.764850	4.158174	-1.058542
31	1	0	-5.699937	4.268939	0.700247
32	1	0	-4.315610	4.795935	-0.267926
33	7	0	3.950766	1.799767	0.292234
34	7	0	5.032705	-0.747805	-0.273237
35	8	0	7.119761	0.179053	-0.082230
36	1	0	7.305259	-0.756631	-0.285213
37	6	0	6.177142	2.766346	0.498608
38	1	0	6.837697	2.557439	1.348461
39	1	0	6.826772	2.943334	-0.366891
40	1	0	5.593177	3.665390	0.704480
41	7	0	0.488259	-2.518145	-0.616629
42	1	0	0.800642	-3.401065	-0.214626
43	1	0	0.326675	-2.683874	-1.611561

---

6 C_1 open shell singlet (broken symmetry)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.321057	-1.925220	0.158739
2	8	0	-1.631368	-3.583944	0.753504
3	6	0	5.240713	1.617626	0.257645
4	6	0	3.128814	0.721872	0.056977
5	6	0	3.681699	-0.561266	-0.224215
6	6	0	5.772969	0.307794	-0.036159
7	1	0	1.357674	1.876826	0.373081
8	6	0	1.729335	0.893254	0.107977
9	6	0	2.808971	-1.647972	-0.459967
10	6	0	1.448017	-1.456453	-0.412032
11	6	0	0.877796	-0.175771	-0.132327
12	1	0	3.236874	-2.622449	-0.676996
13	6	0	-1.205923	0.968255	-0.161498
14	6	0	-2.613356	1.099064	-0.092908
15	6	0	-3.498375	-0.033712	0.034772
16	6	0	-3.156598	2.416252	-0.183188
17	6	0	-4.913799	0.228081	0.073478
18	6	0	-4.508132	2.654354	-0.140734
19	1	0	-2.462671	3.249866	-0.282587
20	6	0	-5.367474	1.526256	-0.010178
21	1	0	-6.442634	1.700070	0.024190
22	1	0	-0.650474	1.895769	-0.325366
23	7	0	-0.527492	-0.154405	-0.065583

24	8	0	-3.107980	-1.263231	0.095879
25	6	0	-5.845672	-0.946455	0.205264
26	1	0	-6.889951	-0.619594	0.234195
27	1	0	-5.720002	-1.645288	-0.630141
28	1	0	-5.630625	-1.519810	1.114445
29	6	0	-5.087294	4.045744	-0.226168
30	1	0	-5.759950	4.151784	-1.087375
31	1	0	-5.673233	4.295192	0.668142
32	1	0	-4.298995	4.798929	-0.326497
33	7	0	3.942568	1.798705	0.299661
34	7	0	5.034773	-0.744165	-0.267229
35	8	0	7.118048	0.189010	-0.066518
36	1	0	7.307411	-0.745654	-0.270678
37	6	0	6.165041	2.772000	0.516490
38	1	0	6.823234	2.563191	1.368197
39	1	0	6.817185	2.953177	-0.346250
40	1	0	5.577427	3.668652	0.722420
41	7	0	0.494786	-2.525294	-0.627039
42	1	0	0.802550	-3.408254	-0.221424
43	1	0	0.334404	-2.693140	-1.621747

5,7TS8,9 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	2.104349	0.208368	-0.862662
2	6	0	-2.280219	-0.461156	-0.514978
3	6	0	-1.059778	-1.360241	-0.256985
4	6	0	-0.285572	-0.903092	0.987135
5	6	0	0.177715	0.540857	0.817116
6	6	0	-0.841081	1.447955	0.258377
7	6	0	-1.960426	1.001252	-0.346562
8	1	0	-2.676659	-0.638350	-1.524372
9	1	0	-1.375744	-2.405228	-0.155017
10	1	0	-0.928061	-0.974497	1.878480
11	1	0	0.683422	0.949925	1.700256
12	1	0	-0.659479	2.519008	0.328927
13	1	0	-2.688411	1.718778	-0.722735
14	1	0	1.085417	0.499679	-0.005018
15	1	0	0.574534	-1.559230	1.165950
16	1	0	-0.380718	-1.308985	-1.117199
17	1	0	-3.102183	-0.727470	0.170342
18	6	0	3.233046	-0.114798	-0.113271

19	1	0	4.030132	-0.350442	-0.838041
20	1	0	3.599754	0.714866	0.515157
21	1	0	3.101101	-1.009661	0.519589

8 C_s

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.046868	-0.757690	0.000000
2	6	0	0.046868	0.660853	0.000000
3	1	0	-0.437012	1.086274	0.893285
4	1	0	1.094153	0.974885	0.000000
5	1	0	-0.437012	1.086274	-0.893285
6	1	0	-0.876287	-1.051030	0.000000

9 C_s

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.108186	-0.694320	1.274119
2	6	0	0.502718	-1.305691	0.000000
3	6	0	-0.108186	-0.694320	-1.274119
4	6	0	-0.108186	0.809006	-1.218098
5	6	0	-0.098409	1.478107	0.000000
6	6	0	-0.108186	0.809006	1.218098
7	1	0	-1.141713	-1.062139	1.400211
8	1	0	1.582547	-1.108573	0.000000
9	1	0	0.437306	-1.045154	-2.160460
10	1	0	-0.098916	2.567160	0.000000
11	1	0	-0.139485	1.370009	2.148664
12	1	0	-1.141713	-1.062139	-1.400211
13	1	0	0.374759	-2.394745	0.000000
14	1	0	0.437306	-1.045154	2.160460
15	1	0	-0.139485	1.370009	-2.148664

6,7TS9,10 C_1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	29	0	0.910958	-0.591486	-0.956359
2	6	0	-6.210046	0.452720	0.966887
3	6	0	-4.008634	0.405867	0.292871
4	6	0	-4.260475	-0.746515	-0.507316
5	6	0	-6.437934	-0.710570	0.142926
6	1	0	-2.555302	1.801377	1.011957
7	6	0	-2.709965	0.954481	0.352498
8	6	0	-3.196763	-1.319319	-1.241767
9	6	0	-1.939512	-0.765871	-1.173684
10	6	0	-1.672862	0.391967	-0.377060
11	1	0	-3.396749	-2.196025	-1.850871
12	6	0	0.018419	2.023662	-0.019514
13	6	0	1.341415	2.533141	0.011408
14	6	0	2.489128	1.763615	-0.404554
15	6	0	1.509916	3.883665	0.439036
16	6	0	3.770633	2.419146	-0.377575
17	6	0	2.740247	4.493696	0.475410
18	1	0	0.623122	4.436319	0.746435
19	6	0	3.860608	3.725839	0.052473
20	1	0	4.842784	4.197632	0.065770
21	1	0	-0.769972	2.731521	0.253330
22	7	0	-0.328835	0.807040	-0.368729
23	8	0	2.441726	0.538559	-0.818009
24	6	0	4.977144	1.641447	-0.831658
25	1	0	5.878883	2.261267	-0.800674
26	1	0	5.142034	0.758161	-0.203264
27	1	0	4.842884	1.267898	-1.853516
28	6	0	2.923255	5.919453	0.936609
29	1	0	1.965696	6.375075	1.209156
30	1	0	3.580803	5.979762	1.813800
31	1	0	3.377316	6.542448	0.154928
32	7	0	-5.012337	0.983683	1.027023
33	7	0	-5.510477	-1.294526	-0.566846
34	8	0	-7.694284	-1.206957	0.122250
35	1	0	-7.673921	-1.981611	-0.469852
36	6	0	-7.335742	1.057126	1.755410
37	1	0	-6.966860	1.921705	2.310527
38	1	0	-8.153850	1.368998	1.095245
39	1	0	-7.759303	0.327528	2.455846
40	7	0	-0.798864	-1.307543	-1.880312
41	1	0	-0.784961	-1.019239	-2.859550
42	1	0	-0.766106	-2.326167	-1.860363
43	8	0	1.607482	-2.246005	-1.082388
44	6	0	3.792487	-4.236119	2.318617

45	6	0	3.408616	-4.694725	0.901889
46	6	0	4.213090	-3.936822	-0.163420
47	6	0	3.958226	-2.435408	-0.049501
48	6	0	3.965168	-1.929494	1.343951
49	6	0	3.894871	-2.734319	2.419174
50	1	0	3.059621	-4.607621	3.049145
51	1	0	3.553007	-5.778028	0.803106
52	1	0	5.287662	-4.140414	-0.031578
53	1	0	4.591052	-1.838711	-0.715798
54	1	0	4.010632	-0.850487	1.482925
55	1	0	3.919665	-2.301376	3.418914
56	1	0	2.860612	-2.260177	-0.503257
57	1	0	3.942156	-4.283921	-1.167160
58	1	0	2.343919	-4.490605	0.731361
59	1	0	4.753856	-4.687523	2.616413

6,17TS9,10 C_1 open shell singlet (broken symmetry)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.952545	-0.602388	-1.069722
2	6	0	-6.098583	0.681946	0.957713
3	6	0	-3.903905	0.553993	0.272276
4	6	0	-4.208263	-0.571203	-0.547954
5	6	0	-6.379404	-0.455115	0.113301
6	1	0	-2.392466	1.875418	1.007991
7	6	0	-2.583345	1.046615	0.335320
8	6	0	-3.172431	-1.175066	-1.296913
9	6	0	-1.892883	-0.676280	-1.224107
10	6	0	-1.573144	0.455090	-0.409561
11	1	0	-3.410855	-2.031929	-1.920235
12	6	0	0.187468	2.004056	-0.009851
13	6	0	1.529087	2.457542	0.028302
14	6	0	2.640168	1.656853	-0.427824
15	6	0	1.759204	3.780767	0.510682
16	6	0	3.950615	2.252094	-0.379058
17	6	0	3.015573	4.332925	0.564570
18	1	0	0.899429	4.358743	0.846903
19	6	0	4.099944	3.533880	0.104618
20	1	0	5.102196	3.960585	0.133904
21	1	0	-0.568593	2.730155	0.302587
22	7	0	-0.213309	0.817080	-0.405257
23	8	0	2.535652	0.455430	-0.892687

24	6	0	5.117846	1.438035	-0.870175
25	1	0	6.050679	2.006761	-0.802225
26	1	0	5.230360	0.514034	-0.290656
27	1	0	4.970804	1.127205	-1.911118
28	6	0	3.264498	5.728636	1.083129
29	1	0	2.329975	6.213866	1.383124
30	1	0	3.930498	5.723064	1.955982
31	1	0	3.739947	6.363443	0.323978
32	7	0	-4.879202	1.160222	1.021992
33	7	0	-5.480624	-1.064542	-0.611672
34	8	0	-7.655823	-0.896784	0.089739
35	1	0	-7.671527	-1.660279	-0.516834
36	6	0	-7.194376	1.318741	1.762591
37	1	0	-6.786896	2.156190	2.332097
38	1	0	-8.000891	1.677486	1.112052
39	1	0	-7.646022	0.594642	2.451076
40	7	0	-0.780354	-1.252743	-1.950914
41	1	0	-0.786784	-0.983091	-2.935528
42	1	0	-0.763353	-2.271850	-1.912702
43	8	0	1.608547	-2.268001	-1.304048
44	6	0	2.944658	-4.204851	2.490054
45	6	0	2.686321	-4.734297	1.069528
46	6	0	3.766850	-4.249559	0.093135
47	6	0	3.781032	-2.722346	0.041633
48	6	0	3.697355	-2.082574	1.380958
49	6	0	3.325388	-2.744714	2.489766
50	1	0	2.055551	-4.355922	3.119057
51	1	0	2.629858	-5.830187	1.079054
52	1	0	4.752804	-4.618583	0.416885
53	1	0	4.610398	-2.324453	-0.555479
54	1	0	3.935185	-1.021884	1.443747
55	1	0	3.299312	-2.222439	3.445966
56	1	0	2.825702	-2.406230	-0.579507
57	1	0	3.586128	-4.653063	-0.909703
58	1	0	1.719021	-4.359095	0.711965
59	1	0	3.745101	-4.789613	2.973673

---

10 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.323196	-1.899009	0.097644
2	6	0	-5.260015	1.617971	0.259015

3	6	0	-3.145268	0.728596	0.059037
4	6	0	-3.693938	-0.558395	-0.213413
5	6	0	-5.788049	0.304727	-0.025626
6	1	0	-1.378319	1.893409	0.358417
7	6	0	-1.746419	0.905617	0.104002
8	6	0	-2.817758	-1.643728	-0.442639
9	6	0	-1.456771	-1.449523	-0.398933
10	6	0	-0.891791	-0.161654	-0.133206
11	1	0	-3.241874	-2.621955	-0.649372
12	6	0	1.188845	0.992279	-0.163253
13	6	0	2.599195	1.124302	-0.093147
14	6	0	3.490674	-0.002034	0.044942
15	6	0	3.135424	2.443258	-0.185300
16	6	0	4.902963	0.270596	0.090639
17	6	0	4.485682	2.692062	-0.137432
18	1	0	2.436864	3.272102	-0.292232
19	6	0	5.350716	1.571286	0.002889
20	1	0	6.424796	1.751092	0.041298
21	1	0	0.634133	1.922304	-0.317178
22	7	0	0.514337	-0.130888	-0.076574
23	8	0	3.107046	-1.235334	0.114818
24	6	0	5.844087	-0.895675	0.233014
25	1	0	6.886187	-0.561251	0.252674
26	1	0	5.640345	-1.457769	1.152241
27	1	0	5.720180	-1.606095	-0.592933
28	6	0	5.054231	4.087663	-0.227503
29	1	0	4.260312	4.833630	-0.337243
30	1	0	5.632438	4.347746	0.668853
31	1	0	5.731197	4.194534	-1.085244
32	7	0	-3.962435	1.804049	0.296955
33	7	0	-5.046736	-0.745875	-0.252171
34	8	0	-7.133191	0.180535	-0.052444
35	1	0	-7.318312	-0.756190	-0.250916
36	6	0	-6.187895	2.770766	0.512914
37	1	0	-5.602854	3.670715	0.711829
38	1	0	-6.842747	2.944470	-0.349324
39	1	0	-6.843317	2.565143	1.367547
40	7	0	-0.498438	-2.511532	-0.610789
41	1	0	-0.411534	-2.759910	-1.596725
42	1	0	-0.713274	-3.367801	-0.099671
43	8	0	1.608307	-3.592867	0.686823
44	1	0	2.525233	-3.710550	0.974767

O_2 $D_{\infty h}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.607259
2	8	0	0.000000	0.000000	-0.607259

11 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.140517	-0.314116	-0.254179
2	6	0	0.992166	-1.331498	-0.325953
3	6	0	-0.070601	-1.026902	0.736016
4	6	0	-0.647926	0.376111	0.557720
5	6	0	0.383914	1.414861	0.231135
6	6	0	1.636735	1.099433	-0.116573
7	1	0	2.801072	-0.542392	0.597974
8	1	0	0.526697	-1.282577	-1.318287
9	1	0	-0.895344	-1.746487	0.705721
10	1	0	0.072857	2.455205	0.292647
11	1	0	2.350853	1.899925	-0.306588
12	1	0	0.372298	-1.084995	1.739843
13	1	0	1.376542	-2.350110	-0.201609
14	1	0	2.776946	-0.390151	-1.145762
15	1	0	-1.252076	0.663660	1.423760
16	8	0	-1.611260	0.378942	-0.581688
17	8	0	-2.731074	-0.245119	-0.262899

11TS12 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.244386	0.050862	-0.171634
2	6	0	-1.464553	-1.170557	0.340516
3	6	0	-0.069606	-1.236614	-0.306232
4	6	0	0.695335	0.066375	-0.075620
5	6	0	-0.083655	1.306035	0.041654
6	6	0	-1.427153	1.311838	-0.055833
7	1	0	-2.542772	-0.104660	-1.221288

8	1	0	-1.356896	-1.095966	1.430030
9	1	0	0.527092	-2.060534	0.094885
10	1	0	0.479534	2.221353	0.203382
11	1	0	-1.960122	2.259747	-0.005907
12	1	0	-0.189290	-1.411174	-1.383818
13	1	0	-2.016681	-2.094029	0.131729
14	1	0	-3.181268	0.168360	0.387559
15	1	0	1.557743	0.180923	-1.051310
16	8	0	1.812160	-0.005643	0.770804
17	8	0	2.718686	0.001687	-0.423599

---

12 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.247656	-0.711840	0.082087
2	6	0	0.963480	-1.461333	-0.301059
3	6	0	-0.268101	-0.828754	0.361154
4	6	0	-0.368485	0.660874	0.073614
5	6	0	0.897294	1.399725	-0.079605
6	6	0	2.090207	0.778482	-0.051229
7	1	0	2.529314	-0.942418	1.122949
8	1	0	0.843600	-1.426792	-1.391763
9	1	0	-1.205530	-1.305873	0.060923
10	1	0	0.811884	2.476713	-0.196404
11	1	0	3.000716	1.372375	-0.123441
12	1	0	-0.195743	-0.934190	1.455650
13	1	0	1.040725	-2.518488	-0.024556
14	1	0	3.092812	-1.049280	-0.531217
15	1	0	-2.955606	0.155291	-0.039924
16	8	0	-1.448750	1.247870	0.011389
17	8	0	-3.593060	-0.604152	-0.116638

---

13 C_1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.819134	0.093660	0.131885
2	6	0	-1.075866	-1.163638	-0.342485
3	6	0	0.328718	-1.243373	0.271427

4	6	0	1.143295	0.022378	0.017904
5	6	0	0.380531	1.289621	-0.051952
6	6	0	-0.960786	1.326041	0.025528
7	1	0	-2.743244	0.236084	-0.443072
8	1	0	-1.652489	-2.063132	-0.098050
9	1	0	0.974024	2.195331	-0.147430
10	1	0	-1.471135	2.288807	0.014823
11	1	0	-0.988027	-1.130393	-1.436480
12	1	0	-2.140484	-0.025425	1.179885
13	1	0	0.898714	-2.099017	-0.103304
14	1	0	0.251538	-1.365250	1.363325
15	8	0	2.361320	0.001858	-0.080443

OH $C_{\infty v}$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.109192
2	1	0	0.000000	0.000000	-0.873537

Reference

(1) Wu, X.; Gorden, A. E. V.; Tonks, S. A.; Vilseck, J. Z. *J. Org. Chem.* **2007**, *72*, 8691-8699.