

## 反式双氧锰(V)卟咯配合物的稳定性

章小慧<sup>1</sup>      徐志广<sup>1,\*</sup>      龚丽珍<sup>1</sup>      许旋<sup>1</sup>      沈桂贤<sup>1</sup>  
陈华彬<sup>1</sup>      刘海洋<sup>2,\*</sup>

<sup>1</sup> 华南师范大学化学与环境学院, 教育部环境理论化学重点实验室, 广州 510006;

<sup>2</sup> 华南理工大学化学系, 广州 510641)

## Stability of *trans*-Dioxo Manganese(V) Corrole Complex

ZHANG Xiao-Hui<sup>1</sup>      XU Zhi-Guang<sup>1,\*</sup>      GONG Li-Zhen<sup>1</sup>      XU Xuan<sup>1</sup>  
SHEN Gui-Xian<sup>1</sup>      CHEN Hua-Bin<sup>1</sup>      LIU Hai-Yang<sup>2,\*</sup>

<sup>1</sup>*School of Chemistry and Environment, Key Laboratory of Theoretical Chemistry of Environment,  
Ministry of Education, South China Normal University, Guangzhou 510006, P. R. China;*

<sup>2</sup>*Department of Chemistry, South China University of Technology, Guangzhou 510641, P. R. China)*

\*Corresponding authors. XU Zhi-Guang, Email: chzgxu@scnu.edu.cn; Tel: +86-20-39310187.

LIU Hai-Yang, Email: chhyliu@scut.edu.cn; Tel: +86-20-22236805.

表 S1 不同自旋态下分子[1-OMnO]<sup>2-</sup>优化的能量和部分几何结构参数

Table S1 Optimized energy and selected structure parameters of [1-OMnO]<sup>2-</sup> in different spin multiplicities

[1-OMnO] <sup>2-</sup>	Singlet	Triplet	Quintet
$d_{C-N}^a/\text{nm}$	0.1357	0.1359	0.3608
$d_{N-Mn}^a/\text{nm}$	0.1961	0.1969	0.1949
$d_{ca-ca}^a/\text{nm}$	0.2255	0.2266	0.2251
$d_{c\beta-c\beta}^a/\text{nm}$	0.3097	0.3104	0.3900
$d_{c_{meso-ca}}^a/\text{nm}$	0.1418	0.1425	0.1414
$d_{N-N}^a/\text{nm}$	0.2771	0.2782	0.2752

<sup>a</sup>representing average values

### Cartesian Coordinates of Optimized Geometries

#### [1-OMnO]<sup>2-</sup>(Singlet)

Number	Atomic Type	X	Y	Z
1	Mn	0.000000	0.000000	0.003641
2	O	1.637750	0.000000	0.049967
3	N	0.000000	1.253178	-1.477445
4	N	0.000000	-1.460989	1.342000
5	N	0.000000	-1.253178	-1.477445
6	N	0.000000	1.460989	1.342000
7	C	0.000000	-2.585989	3.307359
8	H	0.000000	-2.776493	4.376840
9	C	0.000000	2.606625	-1.488947
10	C	0.000000	2.999873	-2.877647
11	H	0.000000	4.018156	-3.256286
12	C	0.000000	1.269342	2.681963
13	C	0.000000	2.794731	1.034372
14	C	0.000000	3.339030	-0.267953
15	C	0.000000	0.727651	-2.725057
16	C	0.000000	0.000000	3.313051
17	C	0.000000	1.829555	-3.643055
18	H	0.000000	1.768471	-4.727050
19	C	0.000000	2.585989	3.307359

20	H	0.000000	2.776493	4.376840
21	C	0.000000	-0.727651	-2.725057
22	C	0.000000	3.517786	2.296452
23	H	0.000000	4.599275	2.400268
24	C	0.000000	-3.339030	-0.267953
25	C	0.000000	-1.829555	-3.643055
26	H	0.000000	-1.768471	-4.727050
27	C	0.000000	-3.517786	2.296452
28	H	0.000000	-4.599275	2.400268
29	C	0.000000	-2.794731	1.034372
30	C	0.000000	-2.606625	-1.488947
31	C	0.000000	-2.999873	-2.877647
32	H	0.000000	-4.018156	-3.256286
33	C	0.000000	-1.269342	2.681963
34	O	-1.637750	0.000000	0.049967
35	H	0.000000	4.426791	-0.336225
36	H	0.000000	-4.426791	-0.336225
37	H	0.000000	0.000000	4.402510

[1-OMnO]<sup>2-</sup>(Triplet)

Number	Atomic Type	X	Y	Z
1	Mn	0.000000	0.000000	0.008005
2	O	-1.637100	0.000000	-0.047975
3	N	0.000000	1.256004	1.486955
4	N	0.000000	-1.473039	-1.340005
5	N	0.000000	-1.256004	1.486955
6	N	0.000000	1.473039	-1.340005
7	C	0.000000	-2.572583	-3.327624
8	H	0.000000	-2.757447	-4.397800
9	C	0.000000	2.617806	1.499068
10	C	0.000000	3.012049	2.877577
11	H	0.000000	4.031250	3.252900
12	C	0.000000	1.277121	-2.698848
13	C	0.000000	2.794747	-1.053407
14	C	0.000000	3.346570	0.273619
15	C	0.000000	0.741762	2.735438
16	C	0.000000	0.000000	-3.303599
17	C	0.000000	1.830084	3.650839
18	H	0.000000	1.765698	4.734126
19	C	0.000000	2.572583	-3.327624
20	H	0.000000	2.757447	-4.397800
21	C	0.000000	-0.741762	2.735438
22	C	0.000000	3.514411	-2.313657

23	H	0.000000	4.594873	-2.421071
24	C	0.000000	-3.346570	0.273619
25	C	0.000000	-1.830084	3.650839
26	H	0.000000	-1.765698	4.734126
27	C	0.000000	-3.514411	-2.313657
28	H	0.000000	-4.594873	-2.421071
29	C	0.000000	-2.794747	-1.053407
30	C	0.000000	-2.617806	1.499068
31	C	0.000000	-3.012049	2.877577
32	H	0.000000	-4.031250	3.252900
33	C	0.000000	-1.277121	-2.698848
34	O	1.637100	0.000000	-0.047975
35	H	0.000000	4.434184	0.337087
36	H	0.000000	-4.434184	0.337087
37	H	0.000000	0.000000	-4.394807

[1-OMnO]<sup>2-</sup>( Quintet)

Number	Atomic Type	X	Y	Z
1	Mn	0.000000	0.000000	0.033412
2	O	1.804977	0.000000	0.103797
3	N	0.000000	1.248318	-1.462611
4	N	0.000000	-1.477881	1.306160
5	N	0.000000	-1.248318	-1.462611
6	N	0.000000	1.477881	1.306160
7	C	0.000000	-2.579586	3.283439
8	H	0.000000	-2.755329	4.354999
9	C	0.000000	2.607445	-1.488306
10	C	0.000000	2.992627	-2.876398
11	H	0.000000	4.009988	-3.255957
12	C	0.000000	1.270257	2.648217
13	C	0.000000	2.817587	1.015964
14	C	0.000000	3.358383	-0.282646
15	C	0.000000	0.725217	-2.712623
16	C	0.000000	0.000000	3.272595
17	C	0.000000	1.818594	-3.634493
18	H	0.000000	1.747610	-4.717535
19	C	0.000000	2.579586	3.283439
20	H	0.000000	2.755329	4.354999
21	C	0.000000	-0.725217	-2.712623
22	C	0.000000	3.523895	2.285183
23	H	0.000000	4.603649	2.400123
24	C	0.000000	-3.358383	-0.282646

25	C	0.000000	-1.818594	-3.634493
26	H	0.000000	-1.747610	-4.717535
27	C	0.000000	-3.523895	2.285183
28	H	0.000000	-4.603649	2.400123
29	C	0.000000	-2.817587	1.015964
30	C	0.000000	-2.607445	-1.488306
31	C	0.000000	-2.992627	-2.876398
32	H	0.000000	-4.009988	-3.255957
33	C	0.000000	-1.270257	2.648217
34	O	-1.804977	0.000000	0.103797
35	H	0.000000	4.444622	-0.363168
36	H	0.000000	-4.444622	-0.363168
37	H	0.000000	0.000000	4.361746

[2-OMnO]<sup>2-</sup>(Singlet)

Number	Atomic Type	X	Y	Z
1	Mn	0.006294	-0.653865	-0.073843
2	O	0.043473	-0.710250	1.562100
3	N	1.276301	-2.120591	-0.168048
4	N	-1.472815	0.662358	0.039693
5	N	-1.248663	-2.134795	-0.130175
6	N	1.470083	0.678902	-0.027094
7	C	-2.601203	2.617728	-0.152118
8	H	-2.802708	3.674350	-0.267027
9	C	2.622435	-2.143781	-0.064568
10	C	-4.840953	-1.099392	0.064824
11	C	3.000715	-3.537912	0.051764
12	H	4.006931	-3.922207	0.162428
13	C	4.853758	-1.053878	0.101949
14	C	-0.053159	6.992429	-0.166148
15	C	5.574435	-1.874107	-0.793853
16	C	1.269505	2.019720	-0.044201
17	C	-5.619774	-0.391891	1.007632
18	C	2.806588	0.383593	0.011483
19	C	3.380157	-0.927286	0.008378
20	C	-0.025020	4.145910	-0.091940
21	C	5.601679	-0.388005	1.097859
22	C	-7.006405	-0.527478	1.059480
23	C	-6.919659	-2.105185	-0.755415
24	C	0.743477	-3.365087	-0.105590
25	C	-5.534450	-1.961066	-0.814110
26	C	-0.012941	2.661041	-0.054336
27	C	1.830582	-4.290396	0.018243

28	H	1.755445	-5.370081	0.089474
29	C	2.579671	2.653025	-0.006720
30	H	2.773898	3.716897	0.012318
31	C	-0.701087	-3.373585	-0.088881
32	C	6.987052	-0.521091	1.182288
33	C	6.958337	-2.016362	-0.703173
34	C	3.516570	1.652386	0.007464
35	H	4.590943	1.778893	0.005329
36	C	-7.671008	-1.387096	0.180009
37	C	7.679693	-1.337632	0.283506
38	C	0.663834	6.262429	-1.118796
39	C	-3.367264	-0.965399	0.007593
40	C	-0.738231	4.905345	0.861386
41	C	-0.757511	6.299262	0.822565
42	C	-1.776585	-4.312467	0.031362
43	H	-1.688997	-5.391884	0.091833
44	C	-3.526726	1.607047	-0.130879
45	H	-4.598730	1.714274	-0.230398
46	C	-2.805540	0.351024	-0.000710
47	C	0.671706	4.868372	-1.085491
48	C	-2.594516	-2.174662	-0.034560
49	C	-2.955738	-3.573998	0.073932
50	H	-3.956719	-3.971737	0.184264
51	C	-1.286639	2.003913	-0.032551
52	O	-0.031400	-0.503192	-1.702834
53	H	7.479365	-2.652390	-1.416873
54	H	5.023797	-2.391463	-1.572867
55	H	5.070132	0.225861	1.817510
56	H	7.528251	0.004521	1.967204
57	H	8.760203	-1.445314	0.352598
58	H	-7.571062	0.031226	1.804031
59	H	-8.752637	-1.496750	0.223762
60	H	-7.418414	-2.773552	-1.455380
61	H	-4.961483	-2.507566	-1.556030
62	H	-5.111224	0.258299	1.711880
63	H	1.209070	6.782571	-1.904669
64	H	-0.063660	8.080094	-0.194454
65	H	1.212138	4.310565	-1.843607
66	H	-1.315111	6.848772	1.579272
67	H	-1.272432	4.376864	1.644658

[2-OMnO]<sup>2-</sup>(Triplet)

Number Atomic Type

X

Y

Z

1	Mn	0.006835	-0.664790	-0.071278
2	O	0.030311	-0.769095	1.560815
3	N	1.284272	-2.121925	-0.206982
4	7	-1.487711	0.652323	0.067832
5	N	-1.256587	-2.136804	-0.185222
6	N	1.484174	0.668479	0.029690
7	C	-2.583362	2.630606	-0.157239
8	H	-2.774029	3.689124	-0.274676
9	C	2.639993	-2.152821	-0.083005
10	C	-4.853545	-1.094060	0.087243
11	C	3.007587	-3.540532	0.019065
12	H	4.008134	-3.931625	0.149498
13	C	4.866626	-1.049038	0.123640
14	C	-0.055315	6.956590	-0.217279
15	C	5.599689	-1.933370	-0.706740
16	C	1.272930	2.024638	-0.009300
17	C	-5.626098	-0.318597	0.988809
18	C	2.809868	0.397909	0.033312
19	C	3.402966	-0.936928	0.020063
20	C	-0.025467	4.131055	-0.098745
21	C	5.618805	-0.305426	1.067482
22	C	-7.009501	-0.448530	1.069606
23	C	-6.952620	-2.139514	-0.640838
24	C	0.757504	-3.364304	-0.168876
25	C	-5.569107	-2.010960	-0.723714
26	C	-0.012549	2.637993	-0.034654
27	C	1.825326	-4.293166	-0.041717
28	H	1.741853	-5.372685	0.014403
29	C	2.563549	2.666662	-0.017631
30	H	2.748004	3.732586	-0.026532
31	C	-0.715669	-3.372893	-0.160509
32	C	7.001691	-0.431643	1.166587
33	C	6.982308	-2.059175	-0.605200
34	C	3.511052	1.667380	-0.009629
35	H	4.583251	1.799880	-0.048594
36	C	-7.693135	-1.360384	0.256149
37	C	7.703377	-1.309108	0.331488
38	C	0.532467	6.212633	-1.243375
39	C	-3.389859	-0.975519	0.008043
40	C	-0.615241	4.894514	0.924275
41	C	-0.629913	6.289344	0.867154
42	C	-1.772654	-4.315149	-0.039057
43	H	-1.676884	-5.394033	0.009028

44	C	-3.519549	1.620841	-0.143844
45	H	-4.588334	1.733356	-0.262608
46	C	-2.808483	0.365416	0.005989
47	C	0.546587	4.817931	-1.184356
48	C	-2.612500	-2.184135	-0.070124
49	C	-2.963731	-3.576763	0.025277
50	H	-3.959492	-3.980788	0.152394
51	C	-1.290435	2.008530	-0.018835
52	O	-0.017665	-0.442677	-1.692137
53	H	7.505880	-2.741304	-1.273489
54	H	5.056393	-2.507966	-1.449409
55	H	5.090109	0.359283	1.742560
56	H	7.537233	0.150146	1.915385
57	H	8.783892	-1.407666	0.410496
58	H	-7.560370	0.158489	1.786626
59	H	-8.774336	-1.461828	0.320674
60	H	-7.461733	-2.847288	-1.293514
61	H	-5.011527	-2.607680	-1.437639
62	H	-5.112265	0.376164	1.644966
63	H	0.976500	6.719331	-2.097768
64	H	-0.066366	8.043617	-0.262848
65	H	0.998688	4.238898	-1.983199
66	H	-1.087208	6.856382	1.675455
67	H	-1.060028	4.374877	1.767008

[2-OMnO]<sup>2-</sup> (Quintet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.010086	-0.624171	-0.125767
2	O	-0.056788	-0.649319	-1.823356
3	N	-1.269805	-2.097762	0.043994
4	N	1.485362	0.636117	-0.106388
5	N	1.236942	-2.106243	0.063314
6	N	-1.473084	0.653977	-0.010580
7	C	2.595942	2.596514	0.148410
8	H	2.783495	3.652171	0.289485
9	C	-2.622680	-2.134590	0.017449
10	C	4.854810	-1.111457	-0.036349
11	C	-3.000096	-3.532661	0.011849
12	H	-4.009571	-3.921536	-0.024281
13	C	-4.868751	-1.054340	-0.077266
14	C	0.070202	6.960611	0.224409
15	C	-5.564800	-1.847652	0.859917
16	C	-1.262032	1.998053	0.030853

17	C	5.657754	-0.420441	-0.970402
18	C	-2.815867	0.373129	-0.036823
19	C	-3.391973	-0.931081	-0.034239
20	C	0.034096	4.118989	0.100857
21	C	-5.640771	-0.402902	-1.063122
22	C	7.045585	-0.554241	-0.980000
23	C	6.909476	-2.093821	0.864995
24	C	-0.743386	-3.345497	0.067247
25	C	5.522826	-1.951874	0.881199
26	C	0.018787	2.633874	0.036259
27	C	-1.828481	-4.278799	0.053012
28	H	-1.748752	-5.360073	0.065222
29	C	-2.566034	2.636784	0.018482
30	H	-2.749308	3.702337	0.024382
31	C	0.693607	-3.351923	0.070570
32	C	-7.029155	-0.527757	-1.102102
33	C	-6.952006	-1.981323	0.815055
34	C	-3.511505	1.644399	-0.003558
35	H	-4.584789	1.776183	0.015315
36	C	7.685523	-1.394283	-0.064195
37	C	-7.698176	-1.319781	-0.164577
38	C	-0.619773	6.215784	1.185253
39	C	3.380916	-0.972578	-0.025316
40	C	0.721659	4.891677	-0.859260
41	C	0.744400	6.284879	-0.796739
42	C	1.764354	-4.296456	0.030351
43	H	1.669932	-5.376547	0.024876
44	C	3.529302	1.594786	0.122910
45	H	4.598540	1.703645	0.244978
46	C	2.820701	0.338576	-0.039587
47	C	-0.631721	4.822321	1.127451
48	C	2.590902	-2.164135	0.017940
49	C	2.946579	-3.565092	-0.012488
50	H	3.949666	-3.967471	-0.069772
51	C	1.288803	1.978560	-0.000373
52	O	-0.009619	-0.460199	1.845355
53	H	-7.455381	-2.596487	1.558981
54	H	-4.993612	-2.349363	1.634293
55	H	-5.126519	0.193255	-1.809963
56	H	-7.591321	-0.014472	-1.880327
57	H	-8.781009	-1.421078	-0.197945
58	H	7.630716	-0.009236	-1.718810
59	H	8.768129	-1.502592	-0.074807

60	H	7.389463	-2.745265	1.593401
61	H	4.929848	-2.481816	1.619341
62	H	5.167311	0.215341	-1.700353
63	H	-1.140403	6.723132	1.995720
64	H	0.083485	8.047638	0.271448
65	H	-1.150628	4.250710	1.890407
66	H	1.281139	6.847210	-1.559003
67	H	1.232989	4.374610	-1.665223

[3-OMnO]<sup>2-</sup>(Singlet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.004358	-0.991886	0.006424
2	O	-0.016044	-0.933267	-1.628692
3	N	-1.264695	-2.462946	-0.009309
4	N	1.468393	0.332179	0.007005
5	N	1.246586	-2.470005	-0.014414
6	F	-4.952374	-2.603798	1.911232
7	N	-1.468873	0.340250	0.025263
8	F	-4.998916	-0.206833	-2.205792
9	F	-7.615697	-2.881249	1.760502
10	F	-7.668609	-0.445068	-2.294329
11	F	-9.009308	-1.794553	-0.328404
12	F	5.064911	-0.200081	-2.068745
13	F	9.003533	-1.836982	-0.084675
14	F	1.113675	4.036710	-1.892975
15	F	7.735151	-0.447644	-2.070880
16	F	1.143669	6.714823	-1.729067
17	F	7.535789	-2.952512	1.937329
18	F	0.025949	7.986652	0.420140
19	F	-1.088348	3.831196	2.324676
20	F	4.870747	-2.665747	2.003598
21	C	2.595142	2.288995	0.198641
22	H	2.797284	3.347210	0.305387
23	C	-2.610523	-2.484157	-0.074419
24	F	-1.099780	6.512235	2.431300
25	C	4.828304	-1.416497	-0.029402
26	C	-2.996892	-3.874617	-0.198398
27	H	-4.007659	-4.257043	-0.276710
28	C	-4.837163	-1.386972	-0.137895
29	C	0.021537	6.639413	0.352121
30	C	-5.569958	-2.077308	0.844231
31	C	-1.275645	1.677792	0.094170
32	C	5.625671	-0.860812	-1.046107

33	C	-2.801700	0.046116	-0.022715
34	C	-3.360447	-1.265819	-0.074079
35	C	0.010727	3.794606	0.207789
36	C	-5.596790	-0.847632	-1.191317
37	C	7.012679	-0.986855	-1.067680
38	C	6.909559	-2.277240	0.951707
39	C	-0.734618	-3.706493	-0.093197
40	C	5.525182	-2.125642	0.965722
41	C	0.005329	2.311780	0.131471
42	C	-1.829671	-4.628972	-0.206065
43	H	-1.759555	-5.707699	-0.287925
44	C	-2.586041	2.310631	0.086744
45	H	-2.783889	3.374499	0.117206
46	C	0.709496	-3.710908	-0.090885
47	C	-6.982797	-0.969192	-1.257919
48	C	-6.953690	-2.224467	0.785934
49	C	-3.518805	1.309272	0.024704
50	H	-4.594549	1.431736	0.017985
51	C	7.661563	-1.702675	-0.067358
52	C	-7.668191	-1.664927	-0.267858
53	C	-0.559779	5.885245	1.365794
54	C	3.351388	-1.288166	-0.014869
55	C	0.579357	4.596197	-0.798136
56	C	0.598365	5.987399	-0.732476
57	C	1.800039	-4.641623	-0.176199
58	H	1.724121	-5.720585	-0.249334
59	C	3.522416	1.281500	0.154565
60	H	4.597570	1.392611	0.219785
61	C	2.799418	0.027175	0.028519
62	C	-0.550663	4.494403	1.290795
63	C	2.593320	-2.501212	-0.046023
64	C	2.972173	-3.895178	-0.152678
65	H	3.981463	-4.285408	-0.207632
66	C	1.282266	1.669608	0.098211
67	O	0.005721	-0.951167	1.641563

[3-OMnO]<sup>2-</sup>(Triplet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.005678	-1.005916	0.027199
2	O	-0.005468	-1.023485	-1.607490
3	N	-1.273705	-2.471350	0.072148
4	N	1.482062	0.317640	-0.020588
5	N	1.252724	-2.479550	0.078208

6	F	-5.005759	-2.750158	1.819381
7	N	-1.483202	0.326790	-0.022531
8	F	-4.996991	-0.059258	-2.122352
9	F	-7.663279	-2.988368	1.627170
10	F	-7.666151	-0.251065	-2.234894
11	F	-9.040137	-1.729689	-0.379966
12	F	5.034312	-0.072505	-2.029926
13	F	9.032203	-1.776983	-0.217304
14	F	0.726543	4.048210	-2.035384
15	F	7.704376	-0.276391	-2.088157
16	F	0.753589	6.734197	-1.829974
17	F	7.607531	-3.044428	1.750779
18	F	0.036579	7.942730	0.514143
19	F	-0.701956	3.734704	2.485250
20	F	4.948108	-2.794691	1.889522
21	C	2.578499	2.298398	0.183327
22	H	2.771020	3.358883	0.286720
23	C	-2.630514	-2.497436	-0.028575
24	F	-0.696729	6.422871	2.662140
25	C	4.839999	-1.416717	-0.063221
26	C	-3.006026	-3.880420	-0.156258
27	H	-4.012645	-4.265991	-0.258574
28	C	-4.850738	-1.386669	-0.139963
29	C	0.028730	6.599823	0.417868
30	C	-5.605748	-2.145665	0.781848
31	C	-1.278389	1.680126	0.064290
32	C	5.622766	-0.783165	-1.054122
33	C	-2.804892	0.055976	-0.027681
34	C	-3.384794	-1.280817	-0.062958
35	C	0.011410	3.776946	0.216671
36	C	-5.609224	-0.758537	-1.152773
37	C	7.007989	-0.886807	-1.105658
38	C	6.955376	-2.317621	0.818229
39	C	-0.751616	-3.711328	0.003227
40	C	5.572175	-2.185808	0.868815
41	C	0.005099	2.284585	0.109948
42	C	-1.828345	-4.636105	-0.131472
43	H	-1.749313	-5.714128	-0.207889
44	C	-2.569818	2.318703	0.109825
45	H	-2.757655	3.383520	0.167065
46	C	0.723397	-3.716123	0.009480
47	C	-6.993577	-0.856301	-1.232757
48	C	-6.988193	-2.271718	0.703179

49	C	-3.513115	1.317849	0.062507
50	H	-4.587062	1.444232	0.098781
51	C	7.687188	-1.663088	-0.169592
52	C	-7.695922	-1.621708	-0.304999
53	C	-0.347938	5.822852	1.507960
54	C	3.373509	-1.303548	-0.016791
55	C	0.382579	4.589833	-0.860829
56	C	0.396802	5.981288	-0.771806
57	C	1.795824	-4.648752	-0.106820
58	H	1.710671	-5.726556	-0.179612
59	C	3.515555	1.291214	0.147479
60	H	4.588518	1.407572	0.225226
61	C	2.801303	0.036744	0.013423
62	C	-0.350440	4.432725	1.399376
63	C	2.610775	-2.515090	-0.000217
64	C	2.978699	-3.901119	-0.118127
65	H	3.984038	-4.293920	-0.204018
66	C	1.284841	1.671119	0.078894
67	O	-0.004564	-0.875871	1.657172

[3-OMnO]<sup>2-</sup> (Quintet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.002766	-0.953869	-0.184622
2	O	-0.034443	-0.891487	1.786451
3	N	1.248615	-2.427282	-0.019793
4	N	-1.470434	0.320774	-0.043201
5	N	-1.248116	-2.441781	-0.076092
6	F	4.968520	-2.640283	-1.889745
7	N	1.478161	0.321228	-0.094285
8	F	4.988856	-0.202776	2.202281
9	F	7.628129	-2.941705	-1.704474
10	F	7.655241	-0.466409	2.326426
11	F	9.005988	-1.847657	0.390265
12	F	-5.050192	-0.169763	2.059608
13	F	-9.010176	-1.850234	0.157145
14	F	-1.075778	4.006143	1.902034
15	F	-7.718390	-0.429493	2.105387
16	F	-1.092149	6.686602	1.769800
17	F	-7.568520	-2.986089	-1.871755
18	F	0.007381	7.976340	-0.377585
19	F	1.080752	3.837075	-2.339178
20	F	-4.905826	-2.688589	-1.982029
21	C	-2.579943	2.290882	-0.196804

22	H	-2.771303	3.352383	-0.284082
23	C	2.598680	-2.463473	0.069833
24	F	1.102942	6.519863	-2.417573
25	C	-4.839309	-1.409365	0.031138
26	C	2.972407	-3.848190	0.246234
27	H	3.980449	-4.227957	0.359617
28	C	4.842493	-1.399949	0.143551
29	C	0.005373	6.628769	-0.324925
30	C	5.579481	-2.107580	-0.822737
31	C	1.277958	1.663369	-0.130811
32	C	-5.623097	-0.845503	1.053915
33	C	2.813872	0.042227	-0.014391
34	C	3.368857	-1.264250	0.056574
35	C	0.001732	3.783993	-0.213430
36	C	5.593253	-0.859157	1.202075
37	C	-7.009020	-0.978039	1.098276
38	C	-6.930653	-2.294144	-0.905771
39	C	0.718541	-3.672248	0.099766
40	C	-5.547473	-2.136313	-0.943306
41	C	0.001721	2.299921	-0.155903
42	C	1.801979	-4.594525	0.261829
43	H	1.718910	-5.667964	0.384838
44	C	2.581906	2.302280	-0.085571
45	H	2.768102	3.368327	-0.083023
46	C	-0.716507	-3.678728	0.074652
47	C	6.977184	-0.993762	1.287011
48	C	6.960882	-2.267940	-0.745727
49	C	3.521078	1.308203	-0.024907
50	H	4.595106	1.435563	0.014307
51	C	-7.669619	-1.709709	0.117303
52	C	7.667499	-1.705340	0.311791
53	C	0.570567	5.883555	-1.354209
54	C	-3.364772	-1.275974	-0.011898
55	C	-0.549732	4.575760	0.809023
56	C	-0.561791	5.967871	0.759333
57	C	-1.799692	-4.603690	0.241728
58	H	-1.715087	-5.674509	0.385471
59	C	-3.516630	1.292037	-0.156001
60	H	-4.591299	1.412360	-0.202619
61	C	-2.808430	0.032502	-0.053055
62	C	0.555172	4.491863	-1.294856
63	C	-2.596370	-2.476668	0.009015
64	C	-2.970722	-3.860927	0.203446

65	H	-3.978975	-4.240688	0.315684
66	C	-1.273790	1.663435	-0.119172
67	O	-0.023538	-0.887981	-1.880779

[4-OMnO]<sup>2-</sup>(Singlet)

Number	Atomic Type	X	Y	Z
1	Mn	0.005111	-0.809778	-0.047447
2	O	0.019222	-0.783870	1.586168
3	N	1.273141	-2.283957	-0.067589
4	N	-1.478156	0.515143	-0.015927
5	N	-1.252309	-2.292783	-0.056576
6	F	4.975693	-2.383783	-1.966227
7	N	1.478265	0.525398	-0.040638
8	F	4.990073	-0.095940	2.199391
9	F	7.641641	-2.684837	-1.798451
10	F	7.660027	-0.382849	2.334943
11	F	9.012369	-1.683155	0.346237
12	F	-5.048989	-0.072573	2.081710
13	F	-9.006195	-1.730525	0.152109
14	F	-1.023822	4.185152	1.978370
15	F	-7.719798	-0.371218	2.145438
16	F	-1.041657	6.874246	1.874982
17	F	-7.567127	-2.778434	-1.924718
18	F	-0.039193	8.176825	-0.310989
19	F	0.990760	4.048284	-2.320399
20	F	-4.899970	-2.466240	-2.022144
21	C	-2.590935	2.457238	-0.183239
22	C	2.622040	-2.293525	0.005529
23	F	0.978208	6.738060	-2.402188
24	C	-4.850068	-1.255520	0.026436
25	C	2.985512	-3.687030	0.108434
26	C	4.860209	-1.222831	0.107705
27	C	-0.031657	6.830436	-0.264396
28	C	5.593472	-1.887322	-0.885847
29	C	1.265800	1.866211	-0.083164
30	C	-5.627941	-0.734436	1.070855
31	C	2.813046	0.216144	-0.002338
32	C	3.380452	-1.087692	0.029200
33	C	-0.014389	3.995968	-0.166081
34	C	5.602976	-0.727010	1.188977
35	C	-7.010705	-0.882023	1.119879
36	C	-6.932300	-2.115164	-0.938519

37	C	0.730974	-3.526630	-0.003942
38	C	-5.550831	-1.948039	-0.971847
39	C	-0.007048	2.505153	-0.113060
40	C	1.826522	-4.437013	0.098974
41	C	2.578872	2.480953	-0.067245
42	C	-0.701296	-3.531726	-0.000159
43	C	6.984456	-0.869777	1.275687
44	C	6.974221	-2.049228	-0.815594
45	C	3.507772	1.485942	-0.030322
46	C	-7.668375	-1.578526	0.111692
47	C	7.675564	-1.536533	0.269767
48	C	0.488878	6.095101	-1.323517
49	C	-3.369937	-1.112905	-0.010306
50	C	-0.526539	4.773088	0.881436
51	C	-0.544215	6.164191	0.843206
52	C	-1.790834	-4.450970	0.086869
53	C	-3.512921	1.455617	-0.150784
54	C	-2.810516	0.194587	-0.041554
55	C	0.487690	4.704523	-1.265698
56	C	-2.601953	-2.313165	-0.004561
57	C	-2.955590	-3.709836	0.089166
58	C	-1.274750	1.855855	-0.093388
59	O	-0.009525	-0.728193	-1.678672
60	F	2.868304	3.802392	-0.081406
61	F	4.845684	1.682051	-0.028471
62	F	4.238601	-4.195866	0.197313
63	F	1.754922	-5.783344	0.177596
64	F	-1.709820	-5.797201	0.157958
65	F	-4.205451	-4.228820	0.163215
66	F	-4.850474	1.636549	-0.232686
67	F	-2.886665	3.772306	-0.299158

[4-OMnO]<sup>2-</sup>(Triplet)

Number	Atomic Type	X	Y	Z
1	Mn	0.006822	-0.826864	-0.099577
2	O	0.009912	-0.910031	1.530559
3	N	1.285067	-2.293978	-0.205954
4	N	-1.490290	0.499288	0.005057
5	N	-1.258974	-2.304399	-0.207480
6	F	5.051280	-2.524922	-1.856936
7	N	1.491457	0.511274	0.001407
8	F	4.951612	0.058512	2.138913

9	F	7.708871	-2.795333	-1.600690
10	F	7.619621	-0.184830	2.346260
11	F	9.028996	-1.621622	0.490130
12	F	-4.992227	0.050390	2.050680
13	F	-9.020895	-1.682941	0.338120
14	F	-0.768528	4.191567	2.065675
15	F	-7.662093	-0.209505	2.203450
16	F	-0.788357	6.885149	1.922535
17	F	-7.647299	-2.874672	-1.707838
18	F	-0.055884	8.142198	-0.391239
19	F	0.732681	3.973910	-2.428453
20	F	-4.987615	-2.587548	-1.911246
21	C	-2.576914	2.463954	-0.173586
22	C	2.641105	-2.308540	-0.061513
23	F	0.702147	6.667783	-2.562584
24	C	-4.856272	-1.257741	0.063949
25	C	2.991202	-3.690510	0.071036
26	C	4.869117	-1.220507	0.130544
27	C	-0.043438	6.798795	-0.321474
28	C	5.635896	-1.955850	-0.792962
29	C	1.269399	1.869672	-0.063164
30	C	-5.607996	-0.660404	1.093528
31	C	2.813730	0.225233	-0.002063
32	C	3.402119	-1.101278	0.014412
33	C	-0.015874	3.979089	-0.175725
34	C	5.593389	-0.633523	1.185142
35	C	-6.988063	-0.789137	1.189589
36	C	-6.977435	-2.161072	-0.780371
37	C	0.750429	-3.533696	-0.153381
38	C	-5.598279	-2.010231	-0.866455
39	C	-0.006820	2.482146	-0.097461
40	C	1.822514	-4.442661	0.009001
41	C	2.565633	2.487690	-0.102037
42	C	-0.714748	-3.539651	-0.155812
43	C	6.971956	-0.754332	1.309729
44	C	7.013979	-2.098513	-0.678968
45	C	3.502668	1.492758	-0.076926
46	C	-7.682183	-1.547258	0.250856
47	C	7.691592	-1.494167	0.375735
48	C	0.343122	6.045595	-1.424610
49	C	-3.388477	-1.129177	-0.022029
50	C	-0.399905	4.765492	0.913457
51	C	-0.416408	6.156455	0.853953

52	C	-1.780848	-4.457934	-0.005516
53	C	-3.506184	1.461427	-0.156851
54	C	-2.809509	0.201940	-0.036699
55	C	0.353334	4.655808	-1.341141
56	C	-2.616364	-2.330413	-0.079015
57	C	-2.956156	-3.715547	0.048139
58	C	-1.277952	1.858250	-0.076820
59	O	0.002689	-0.624314	-1.719681
60	F	2.843006	3.810956	-0.155918
61	F	4.838795	1.692679	-0.135224
62	F	4.235678	-4.206660	0.227751
63	F	1.743654	-5.790658	0.092851
64	F	-1.691675	-5.805504	0.074996
65	F	-4.197572	-4.242342	0.192635
66	F	-4.841362	1.647272	-0.263541
67	F	-2.861760	3.782578	-0.278743

[1-OMnOH]<sup>-</sup> (Singlet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.012846	0.051050	-0.218259
2	O	0.040016	-0.010301	1.668812
3	N	-1.082736	-1.560583	-0.042624
4	N	0.858211	1.745600	-0.066058
5	N	-1.712075	0.848649	-0.117996
6	N	1.651533	-1.055670	-0.005732
7	C	2.488047	3.319347	0.115984
8	H	3.475703	3.758125	0.195660
9	C	-0.750144	-2.876191	0.010745
10	C	-1.995237	-3.603464	0.094974
11	H	-2.093908	-4.681482	0.148442
12	C	2.900105	-0.526337	0.028907
13	C	1.713941	-2.426124	0.002025
14	C	0.599951	-3.289571	0.016434
15	C	-2.424105	-1.377566	0.004969
16	C	3.161434	0.859692	0.047251
17	C	-3.028902	-2.675987	0.091983
18	H	-4.089505	-2.886748	0.151788
19	C	3.845192	-1.624773	0.064467
20	H	4.923527	-1.522738	0.099775
21	C	-2.792986	0.008494	-0.014562
22	C	3.116140	-2.788204	0.047311
23	H	3.495663	-3.803229	0.074010

24	C	-1.142461	3.186695	-0.018266
25	C	-3.954147	0.822340	0.098070
26	H	-4.974284	0.470053	0.189767
27	C	1.283404	3.974572	0.088066
28	H	1.112964	5.043290	0.145565
29	C	0.243023	2.978105	-0.015247
30	C	-2.103452	2.154664	-0.035677
31	C	-3.531271	2.151702	0.081323
32	H	-4.159311	3.031100	0.160530
33	C	2.218071	1.900766	0.030637
34	O	0.173604	-0.197880	-1.752483
35	H	0.804728	-4.356460	0.052758
36	H	-1.491286	4.214057	0.043911
37	H	4.205403	1.158438	0.100099
38	H	0.318341	-0.890156	1.954042

[1-OMnOH]<sup>-</sup> (Triplet)

Number	Atomic Type	X	Y	Z
1	Mn	0.001642	-0.000051	0.246423
2	O	0.101205	0.000717	1.866095
3	N	-1.471143	-1.238253	0.145261
4	N	1.328848	1.439229	0.044511
5	N	-1.471978	1.237302	0.144981
6	N	1.329843	-1.438518	0.045718
7	C	3.297150	2.574575	-0.109607
8	H	4.361882	2.764656	-0.174835
9	C	-1.483142	-2.594769	0.016092
10	C	-2.867800	-2.987118	-0.136572
11	H	-3.233242	-4.000364	-0.254612
12	C	2.680103	-1.268033	-0.014661
13	C	1.035237	-2.768339	-0.017050
14	C	-0.280132	-3.312798	-0.030320
15	C	-2.706824	-0.730953	0.042851
16	C	3.303942	0.000986	-0.027021
17	C	-3.626600	-1.827674	-0.125767
18	H	-4.701634	-1.754675	-0.234382
19	C	3.298797	-2.572584	-0.109383
20	H	4.363630	-2.761992	-0.174911
21	C	-2.707323	0.729213	0.042895
22	C	2.281857	-3.497359	-0.112373
23	H	2.373142	-4.575185	-0.179576
24	C	-0.282280	3.312624	-0.030383

25	C	-3.627854	1.825400	-0.125232
26	H	-4.702871	1.751730	-0.233559
27	C	2.279626	3.498740	-0.112512
28	H	2.370265	4.576648	-0.179307
29	C	1.033446	2.768954	-0.017658
30	C	-1.484840	2.593854	0.016264
31	C	-2.869817	2.985338	-0.135959
32	H	-3.235941	3.998382	-0.253612
33	C	2.679262	1.269623	-0.015394
34	O	-0.087181	-0.001217	-1.711953
35	H	0.827989	0.008499	-2.021223
36	H	4.390449	0.001342	-0.085833
37	H	-0.344971	-4.394786	-0.127401
38	H	-0.347794	4.394612	-0.127010

[1-OMnOH]<sup>-</sup> (Quintet)

Number	Atomic Type		X	Y	Z
1	Mn		0	0.019882	0.014728
0.089522					
2	O	0	0.010354	-0.007421	1.954241
3	N	0	-1.078972	-1.555708	-0.080464
4	N	0	0.886350	1.724936	-0.052711
5	N	0	-1.725231	0.841114	0.109986
6	N	0	1.634184	-1.087755	0.101532
7	C	0	2.514995	3.297342	-0.068728
8	H	0	3.503789	3.740257	-0.072827
9	C	0	-0.765208	-2.879365	-0.074801
10	C	0	-2.012833	-3.591805	-0.075827
11	H	0	-2.120092	-4.670162	-0.071025
12	C	0	2.890001	-0.554775	0.006238
13	C	0	1.691893	-2.461642	-0.004835
14	C	0	0.579221	-3.313843	-0.053661
15	C	0	-2.434986	-1.366800	-0.054603
16	C	0	3.177630	0.823219	-0.027614
17	C	0	-3.043614	-2.654628	-0.061868
18	H	0	-4.106718	-2.859254	-0.053283
19	C	0	3.819924	-1.657505	-0.095826
20	H	0	4.896010	-1.556298	-0.171967
21	C	0	-2.803680	0.015662	0.008378
22	C	0	3.087939	-2.819109	-0.103360
23	H	0	3.462735	-3.832539	-0.185790
24	C	0	-1.121356	3.170635	-0.017427

25	C	0	-3.966335	0.839914	-0.089483
26	H	0	-4.989723	0.495961	-0.172059
27	C	0	1.307549	3.953114	-0.066423
28	H	0	1.141682	5.023868	-0.072297
29	C	0	0.262041	2.960896	-0.049726
30	C	0	-2.092901	2.144424	0.026813
31	C	0	-3.528496	2.160028	-0.073448
32	H	0	-4.145144	3.048044	-0.145454
33	C	0	2.247424	1.878392	-0.052762
34	O	0	0.078643	0.104498	-1.738317
35	H	0	0.772267	-4.381902	-0.101612
36	H	0	-1.464961	4.200897	-0.049229
37	H	0	4.227273	1.100978	-0.066096
38	H	0	0.744295	-0.577708	2.221552

[1-OMnH<sub>2</sub>O] (Singlet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.034031	0.001474	-0.600247
2	O	0.021269	0.003098	-2.137758
3	N	-1.419161	1.180996	-0.064106
4	N	1.230141	-1.359249	-0.048316
5	N	-1.382108	-1.221333	-0.066085
6	N	1.187293	1.399391	-0.047967
7	C	3.248165	-2.465409	0.026770
8	H	4.318765	-2.616252	0.064933
9	C	-1.502837	2.556984	0.002763
10	C	-2.883326	2.902583	0.140948
11	H	-3.264093	3.912538	0.215498
12	C	2.572116	1.268381	-0.008172
13	C	0.917606	2.769698	-0.036186
14	C	-0.355402	3.335306	-0.017798
15	C	-2.687394	0.660773	0.053680
16	C	3.239039	0.051287	-0.002686
17	C	-3.615146	1.728639	0.176118
18	H	-4.685347	1.627735	0.293619
19	C	3.170134	2.566683	0.035136
20	H	4.235547	2.750032	0.076263
21	C	-2.665748	-0.740740	0.052694
22	C	2.155708	3.485724	0.012552
23	H	2.235022	4.564400	0.045615
24	C	-0.252285	-3.341927	-0.022555
25	C	-3.560034	-1.836880	0.174051

26	H	-4.632833	-1.769279	0.291709
27	C	2.262359	-3.415125	0.003246
28	H	2.374964	-4.490933	0.032596
29	C	1.002758	-2.737597	-0.040759
30	C	-1.423117	-2.599278	-0.000365
31	C	-2.792211	-2.987544	0.137736
32	H	-3.141501	-4.008867	0.211489
33	C	2.610718	-1.186024	-0.011187
34	O	0.519015	-0.025772	2.943523
35	H	0.786443	-0.739660	2.350034
36	H	0.759210	0.763316	2.441135
37	H	4.323185	0.068381	0.031728
38	H	-0.438451	4.415904	0.020643
39	H	-0.302183	-4.424607	0.014216

[1-OMnH<sub>2</sub>O] (Triplet)

Number	Atomic Type	X	Y	Z
1	Mn	-0.010980	-0.004570	-0.535686
2	O	0.055553	0.017433	-2.109410
3	N	-1.892237	0.381533	-0.199529
4	N	1.822593	-0.625879	-0.097083
5	N	-0.651401	-1.734779	-0.056921
6	N	0.394913	1.819533	-0.007591
7	C	4.107165	-0.641445	0.058267
8	H	5.123656	-0.277836	0.132045
9	C	-2.597291	1.549099	-0.066172
10	C	-3.983591	1.196547	0.144999
11	H	-4.798310	1.894452	0.286546
12	C	1.672756	2.349211	0.029908
13	C	-0.496285	2.873204	0.007775
14	C	-1.914774	2.755283	-0.007896
15	C	-2.716038	-0.664263	-0.017833
16	C	2.849787	1.581406	0.010901
17	C	-4.053812	-0.181717	0.185519
18	H	-4.933425	-0.785953	0.360320
19	C	1.579851	3.774738	0.094781
20	H	2.421647	4.452755	0.144586
21	C	-1.992365	-1.916113	0.027532
22	C	0.239797	4.096705	0.082231
23	H	-0.200764	5.084098	0.126002
24	C	1.370797	-3.044110	0.002215
25	C	-2.264735	-3.308544	0.171016

26	H	-3.240978	-3.761905	0.273843
27	C	3.680641	-1.948441	0.052833
28	H	4.288645	-2.840984	0.122727
29	C	2.245676	-1.927294	-0.037792
30	C	-0.017355	-2.954075	0.021211
31	C	-1.039377	-3.956095	0.161649
32	H	-0.865892	-5.020162	0.255116
33	C	2.931601	0.181030	-0.027724
34	O	0.279577	0.126691	2.634899
35	H	1.029075	-0.332199	2.232475
36	H	0.307313	0.996594	2.213957
37	H	3.786280	2.129617	0.059010
38	H		-2.480769	3.677504
0.083818				
39	H		1.825217	-4.028337
0.065136				

[1-OMnH<sub>2</sub>O] (Quintet)

Number	Atomic Type		X	Y	Z
1	Mn	0	0.013734	0.000126	-0.276613
2	O	0	0.119038	0.000278	-1.917747
3	N	0	-1.453341	1.236747	-0.082703
4	N	0	1.294764	-1.449546	0.012288
5	N	0	-1.452619	-1.237391	-0.082724
6	N	0	1.293880	1.450458	0.012590
7	C	0	3.278253	-2.564416	0.017663
8	H	0	4.344844	-2.746629	0.029620
9	C	0	-1.484341	2.605101	-0.036026
10	C	0	-2.877250	2.982826	0.046736
11	H	0	-3.252955	3.996067	0.103618
12	C	0	2.654790	1.268771	0.013692
13	C	0	1.016864	2.790235	-0.005861
14	C	0	-0.298328	3.340652	-0.019269
15	C	0	-2.696800	0.727208	-0.020918
16	C	0	3.275570	0.001038	0.013583
17	C	0	-3.625918	1.819601	0.059663
18	H	0	-4.702463	1.740190	0.124691
19	C	0	3.276753	2.566471	0.017956
20	H	0	4.343238	2.749307	0.029930
21	C	0	-2.696409	-0.728560	-0.020977
22	C	0	2.267381	3.502407	0.006141
23	H	0	2.371212	4.579638	0.007574

24	C	0	-0.296370	-3.340669	-0.019638
25	C	0	-3.624868	-1.821484	0.059368
26	H	0	-4.701468	-1.742722	0.124279
27	C	0	2.269440	-3.500965	0.005921
28	H	0	2.373927	-4.578133	0.007372
29	C	0	1.018505	-2.789550	-0.006232
30	C	0	-1.482846	-2.605779	-0.036261
31	C	0	-2.875503	-2.984297	0.046556
32	H	0	-3.250644	-3.997751	0.103387
33	C	0	2.655526	-1.267096	0.013520
34	O	0	0.008405	-0.001028	2.166980
35	H	0	0.585226	-0.770965	2.271504
36	H	0	0.594431	0.761718	2.273067
37	H	0	4.362066	0.001358	0.012707
38	H	0	-0.369164	4.424306	0.002133
39	H	0	-0.366620	-4.424363	0.001704