CHEMISTRY
A EUROPEAN JOURNAL

Supporting Information

Aromatic Hydroxylation in a Copper Bis(imine) Complex Mediated by a μ-η²:η² Peroxo Dicopper Core:

A Mechanistic Scenario

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Supplementary Material:

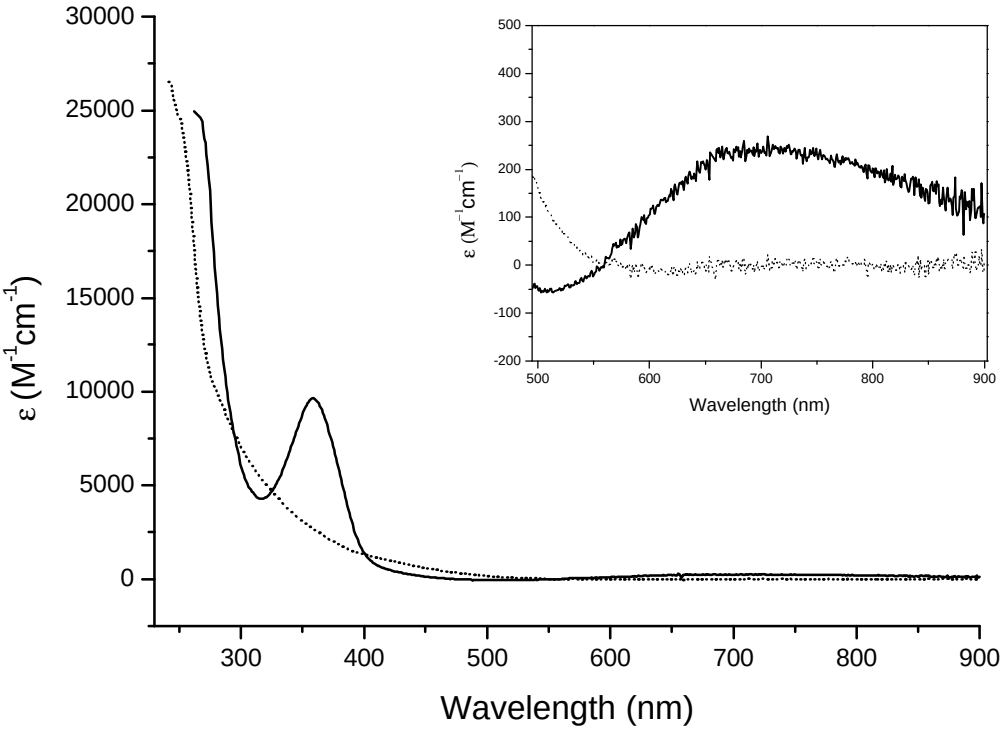

Fig. S1: UV-Vis spectra showing the oxygenation of Ib to II (solid line) by bubbling O_2 through the solution of Ib (dotted line, $2.9*10^{-4}$ mol/l) in methanol.

Table S1: Computed energy contributions (in atomic units) used to obtain relative free energies G_{rel} (in kcal mol^{-1}) and magnetic properties of all species discussed in the text.

Species	$G_{B3LYP/SVP}$/au	DG_{corr}/au[a]	$E_{B3LYP/TZVP}$/au[b]	$G^*_{B3LYP/TZVP}$/au[c]	G_{rel}/kcal mol^{-1}	J/cm^{-1} [d]	<a|b>[e]
1	-4195.60056	0.31044	-4197.35914	-4197.04870	0.0	25.0	0.24
TS1	-4195.56551	0.31172	-4197.33120	-4197.01949	18.3	-1325.4	0.54
2	-4195.60553	0.31473	-4197.37254	-4197.05781	-5.7	-23.5	0.13
TS2	-4195.58272	0.30871	-4197.34045	-4197.03175	10.6	251.1	0.15
3	-4195.75172	0.31483	-4197.51234	-4197.19750	-93.4	-521.8	0.23
TS3	-4195.59967	0.30969	-4197.36128	-4197.05159	-1.8	-84.5	0.21
4	-4195.64395	0.31271	-4197.40890	-4197.09619	-29.8	-307.2	0.26
TS4	-4195.56457	0.30689	-4197.32116	-4197.01427	21.6	-38.0	0.21
5	-4195.66128	0.31292	-4197.42523	-4197.11231	-39.9	530.1	0.04
TS5	-4195.57355	0.30669	-4197.33293	-4197.02623	14.1	-516.6	0.31
6	-4195.59091	0.30904	-4197.34809	-4197.03906	6.1	534.1	0.24
TS6	-4195.63820	0.31198	-4197.39824	-4197.08625	-23.6	-166.0	0.22
TS7	-4195.55689	0.30944	-4197.30342	-4196.99398	34.3	-241.6	0.62
7	-4195.56043	0.30960	-4197.31375	-4197.00415	28.0	-332.1	0.35
TS8	-4195.53386	0.30495	-4197.28254	-4196.97760	44.6	-3366.1[f]	1.00[f]
TS9	-4195.60805	0.30862	-4197.36248	-4197.05385	-3.2	285.1	0.04
4•ClO_4	-4195.66999	0.31918	-4958.43118	-4958.11200	0.0		
TS9•ClO_4	-4955.17452	0.31666	-4958.41677	-4958.10011	7.5		

[a] Thermal corrections to G(298.15) computed at the B3LYP/SVP+COSMO level; [b] Total energies of single point calculations at the B3LYP/TZVP+COSMO level; [c] $E_{B3LYP/TZVP} + \Delta G_{corr}$; [d] Spin coupling constant computed according to eq. 2 (see text); [e] Overlap integral of the magnetic orbitals; [f] magnetic coupling constant involving a closed-shell singlet solution, no bs wave function found.

Cartesian coordinates of stationary points optimized at the B3LYP/SVP+COSMO level

1

```
Cu  1.61461 -0.85358 -0.31123
Cu -1.61266 -0.85748 -0.30229
O  -0.00278 -0.14430 -1.24580
O  -0.00038 -1.57309 -1.24782
N  -2.77387 -2.48741 -0.17821
N   2.74820  0.58117  0.53775
N  -2.75382  0.58236  0.52760
N   2.78545 -2.47855 -0.20727
C   0.00177  4.34899 -0.75866
C  -0.00259  1.86593  0.53872
C   1.20974  3.72877 -0.43479
C  -1.20830  3.72892 -0.44242
C  -1.21883  2.46971  0.18956
C   1.21581  2.46922  0.19646
C  -2.50806  1.84545  0.51015
C   2.50238  1.84425  0.52662
C   4.05562  0.15618  1.07548
C  -4.06286 -2.35915  0.54590
C  -4.72257 -1.00338  0.31185
C   4.06804 -2.35720  0.52931
C   4.72422 -0.99501  0.32417
C  -4.06778  0.16205  1.05328
H  -0.00420  0.95052  1.13128
H   2.15684  4.21885 -0.67373
H   0.00337  5.32382 -1.25026
H  -2.15373  4.21956 -0.68672
H   3.31796  2.53551  0.79311
H  -3.32493  2.53770  0.76997
H  -5.75881 -1.06855  0.67910
H  -4.79351 -0.78643 -0.76851
H  -3.90792 -0.12746  2.10641
H  -4.74396  1.03194  1.05625
H   3.88178 -0.15083  2.12143
H   4.72911  1.02775  1.10208
H   4.80685 -0.76113 -0.75180
H   5.75631 -1.06157  0.70267
H   2.97311 -2.71345 -1.18792
H  -2.95251 -2.74114 -1.15581
H  -4.73774 -3.16989  0.22981
H  -3.86018 -2.49890  1.61813
H   3.85743 -2.51627  1.59732
H   4.74910 -3.15938  0.20475
H   2.24553 -3.27153  0.15147
H  -2.23238 -3.27051  0.19934
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TS1

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Cu  1.56615 -0.84142 -0.25651
Cu -1.57616 -0.85056 -0.25671
O  -0.00222  0.20117 -0.54928
O   0.00176 -1.65663 -0.98222
N  -2.87571 -2.35226 -0.46547
N   2.76498  0.53240  0.61567
N  -2.75939  0.54753  0.61387
N   2.86343 -2.34173 -0.48744
C   0.01594  4.14975 -0.98248
C   0.00825  1.79930  0.57253
C   1.22908  3.56583 -0.60045
C  -1.20155  3.57124 -0.60106
C  -1.22180  2.39905  0.16219
C   1.24096  2.39295  0.16395
C  -2.51452  1.80872  0.53383
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C	2.52780	1.79528	0.54244
C	4.06682	0.10253	1.14834
C	-4.12914	-2.31186	0.32441
C	-4.78176	-0.93365	0.29775
C	4.11315	-2.32996	0.30826
C	4.77975	-0.95844	0.30874
C	-4.07176	0.13310	1.13315
H	0.00556	1.14763	1.44633
H	2.17279	4.02727	-0.90039
H	0.01812	5.06475	-1.57796
H	-2.14213	4.03857	-0.90181
H	3.34268	2.50033	0.77304
H	-3.32804	2.51998	0.75030
H	-5.79709	-1.03531	0.71187
H	-4.90651	-0.58672	-0.74286
H	-3.89758	-0.26149	2.14931
H	-4.71709	1.02083	1.23358
H	3.87594	-0.30252	2.15731
H	4.71592	0.98490	1.26814
H	4.92128	-0.59847	-0.72519
H	5.78826	-1.07519	0.73527
H	3.08996	-2.34420	-1.48797
H	-3.09884	-2.37510	-1.46642
H	-4.82847	-3.06637	-0.06930
H	-3.88440	-2.59767	1.35845
H	3.86046	-2.63147	1.33590
H	4.80609	-3.08481	-0.09596
H	2.34735	-3.21293	-0.33269
H	-2.37081	-3.22588	-0.28940

2

H	-2.05899	4.39188	0.01333
C	-1.13275	3.81677	0.09001
C	1.33077	2.40452	0.13884
C	-1.20230	2.43199	0.10369
C	0.09526	4.50648	0.13838
C	1.30678	3.79186	0.12202
C	0.05601	1.60892	0.32575
H	0.10617	5.59751	0.12710
H	2.24968	4.34092	0.05971
C	-2.51561	1.84267	-0.02668
H	-3.33746	2.57319	-0.07602
C	2.60928	1.76293	0.00159
H	3.46847	2.44607	-0.06286
N	-2.81730	0.58692	-0.10839
N	2.85053	0.49066	-0.08318
C	-4.22808	0.23251	-0.30758
H	-4.36544	0.02189	-1.38376
H	-4.86010	1.10179	-0.06467
C	-4.68070	-0.98464	0.50038
H	-5.77649	-1.04463	0.40775
H	-4.46664	-0.83070	1.57234
C	-4.10136	-2.31403	0.02719
H	-4.24552	-2.42434	-1.05842
H	-4.63016	-3.14869	0.51546
N	-2.65183	-2.42399	0.30264
H	-2.25533	-3.24812	-0.15675
C	4.23138	0.06082	-0.33782
H	4.32142	-0.14016	-1.42040
H	4.91072	0.89526	-0.10426
C	4.64742	-1.18263	0.44272
H	4.52486	-1.01497	1.52632
H	5.72266	-1.33803	0.26664
C	3.91441	-2.44605	0.01355
H	3.98985	-2.59267	-1.07395
H	4.35742	-3.32937	0.50192
N	2.48260	-2.40031	0.36630
H	1.94972	-3.17871	-0.03395

H	2.35187	-2.46626	1.38225
H	-2.49324	-2.57560	1.30408
Cu	1.40744	-0.84535	-0.13690
O	0.04690	0.44088	-0.47912
Cu	-1.44954	-0.86746	-0.16350
H	0.03027	1.31515	1.40349
O	0.04010	-2.02155	-0.22934

TS2

C	-1.42714	2.28471	0.19520
C	-0.13934	1.54737	0.25364
C	1.07975	2.36022	0.03645
C	0.96999	3.71130	-0.30737
C	-0.27461	4.33582	-0.40665
C	-1.46066	3.62759	-0.15862
O	-0.08825	0.39606	0.92431
Cu	1.51906	-0.97996	-0.41480
N	2.78453	0.58619	-0.10722
C	4.21521	0.26363	-0.12711
C	4.59402	-0.85551	0.84940
C	4.07187	-2.24146	0.48780
N	2.59516	-2.33707	0.60566
C	2.44150	1.80692	0.06796
C	-2.70313	1.62420	0.49639
N	-2.86904	0.35436	0.58738
C	-4.21216	-0.17227	0.86934
C	-4.30629	-1.69060	0.72876
C	-3.88746	-2.24080	-0.63552
N	-2.41177	-2.35215	-0.75921
Cu	-1.32008	-0.78676	-0.10866
O	0.03838	-0.77368	-1.44933
H	-2.41994	4.14636	-0.21907
H	-0.32566	5.39225	-0.67730
H	1.87750	4.28733	-0.49963
H	-3.56147	2.30314	0.62174
H	3.22690	2.56743	0.20382
H	5.69400	-0.90556	0.86413
H	4.28199	-0.58210	1.87203
H	4.45736	-0.05138	-1.15705
H	4.80308	1.16970	0.09170
H	-4.93573	0.31910	0.19637
H	-4.47961	0.12056	1.89859
H	-3.72003	-2.18635	1.52260
H	-5.35686	-1.96515	0.90971
H	-2.08613	-3.17471	-0.24130
H	2.32934	-2.26583	1.59362
H	4.54200	-2.99344	1.14159
H	4.34117	-2.49268	-0.54939
H	-4.24597	-1.58527	-1.44389
H	-4.33986	-3.23219	-0.79526
H	-2.14476	-2.52888	-1.73153
H	2.29235	-3.27341	0.32136
H	-0.06266	1.26102	-0.92681

3

H	-2.14973	4.34940	0.30183
C	-1.19949	3.81167	0.24907
C	1.22836	2.41536	0.06047
C	-1.22996	2.41455	0.05877
C	-0.00170	4.51324	0.35613
C	1.19665	3.81272	0.24863
C	-0.00051	1.68985	-0.01588
H	-0.00217	5.59430	0.50255
H	2.14644	4.35123	0.30162
C	-2.53854	1.80908	-0.11079
H	-3.36415	2.53626	-0.15045

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C   2.53763  1.81060 -0.10633
H   3.36300  2.53818 -0.14326
N  -2.84674  0.56213 -0.24857
N   2.84683  0.56397 -0.24482
O   0.00003  0.38824 -0.17259
C  -4.25106  0.22898 -0.53009
H  -4.31288 -0.06887 -1.59150
H  -4.86548  1.13581 -0.41104
C  -4.81205 -0.89492  0.34046
H  -5.89748 -0.93789  0.15874
H  -4.68376 -0.64860  1.40891
C  -4.23399 -2.27191  0.03820
H  -4.30245 -2.48512 -1.03939
H  -4.81106 -3.04859  0.56549
N  -2.80989 -2.37383  0.42809
H  -2.41331 -3.25940  0.10282
C   4.25196  0.23253 -0.52462
H   4.31602 -0.06119 -1.58706
H   4.86575  1.13915 -0.40087
C   4.81191 -0.89453  0.34237
H   4.68096 -0.65287  1.41155
H   5.89778 -0.93587  0.16292
C   4.23559 -2.27064  0.03295
H   4.30598 -2.47891 -1.04550
H   4.81246 -3.04923  0.55760
N   2.81098 -2.37539  0.42030
H   2.41544 -3.25947  0.08979
H   2.73173 -2.41868  1.44231
H  -2.73193 -2.41154  1.45043
Cu  1.52106 -0.90267 -0.09036
Cu -1.52044 -0.90324 -0.08927
O   0.00043 -2.10887 -0.00189
H   0.00008 -2.86911 -0.60346
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TS3

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H  -2.14372  4.36228  0.38058
C  -1.20718  3.80767  0.29119
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C  -1.25254  2.44074  0.04023
C   0.01406  4.49777  0.41246
C   1.22320  3.82684  0.30360
C   0.00253  1.67949 -0.06622
H   0.00645  5.57208  0.60352
H   2.16503  4.36892  0.40682
C  -2.57212  1.82034 -0.11620
H  -3.40415  2.54148 -0.12026
C   2.58635  1.81024 -0.11328
H   3.41709  2.53237 -0.12807
N  -2.83090  0.56938 -0.25431
N   2.83279  0.55991 -0.25601
C  -4.23463  0.19461 -0.47147
H  -4.31186 -0.12611 -1.52554
H  -4.87919  1.08035 -0.34899
C  -4.72989 -0.93966  0.43182
H  -5.81934 -1.00482  0.28538
H  -4.57522 -0.67531  1.49200
C  -4.13642 -2.31388  0.13560
H  -4.22652 -2.53920 -0.93808
H  -4.70359 -3.08637  0.68092
N  -2.70673 -2.39063  0.49617
H  -2.27980 -3.25907  0.16392
C   4.23061  0.17201 -0.48926
H   4.28701 -0.15948 -1.54118
H   4.88418  1.05320 -0.38471
C   4.72542 -0.95833  0.41938
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H   5.81283 -1.03288  0.26281
C   4.11887 -2.33091  0.14226
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H	4.19862	-2.56823	-0.92958
H	4.68513	-3.10127	0.69141
N	2.69163	-2.39441	0.51511
H	2.25859	-3.26660	0.20112
H	2.59179	-2.39875	1.53475
H	-2.59925	-2.41344	1.51475
Cu	1.43080	-0.95245	-0.14973
O	0.00024	0.45532	-0.54140
Cu	-1.44041	-0.94131	-0.14842
H	0.29205	1.75458	1.11983
O	-0.00808	-2.12131	-0.14907

4

H	1.99486	4.43843	0.27501
C	1.08776	3.86029	0.07706
C	-1.31554	2.42542	-0.52552
C	1.18972	2.48165	0.00244
C	-0.14782	4.57378	-0.06149
C	-1.29946	3.90433	-0.30463
C	-0.00825	1.71721	-0.25508
H	-0.14530	5.65911	0.04661
H	-2.24971	4.43648	-0.39690
C	2.49884	1.86333	0.23575
H	3.30542	2.59589	0.39938
C	-2.58506	1.76991	0.00389
H	-3.40769	2.48198	0.17695
N	2.79243	0.61152	0.28658
N	-2.77947	0.52953	0.21878
C	4.18590	0.26495	0.61171
H	4.20321	-0.04121	1.67255
H	4.81899	1.16310	0.52337
C	4.76772	-0.86662	-0.24140
H	5.85067	-0.88943	-0.04280
H	4.65585	-0.63345	-1.31444
C	4.21446	-2.25732	0.06109
H	4.24485	-2.44416	1.14528
H	4.84586	-3.02182	-0.42060
N	2.81445	-2.41438	-0.38540
H	2.39380	-3.26843	-0.01060
C	-4.09664	0.12737	0.74670
H	-3.94340	-0.16336	1.79994
H	-4.77591	0.99536	0.73972
C	-4.73140	-1.04072	-0.01531
H	-4.77203	-0.81341	-1.09442
H	-5.77654	-1.10980	0.32451
C	-4.08097	-2.40234	0.21799
H	-3.98177	-2.58887	1.29809
H	-4.72731	-3.19489	-0.19317
N	-2.73319	-2.49761	-0.38269
H	-2.24878	-3.34598	-0.07798
H	-2.80437	-2.57831	-1.40170
H	2.77679	-2.52299	-1.40346
Cu	-1.42405	-1.00186	-0.02939
O	0.01514	0.47010	-0.31744
Cu	1.48945	-0.94538	0.02977
H	-1.40440	2.33088	-1.63738
O	0.04929	-2.11337	0.08005

TS4

H	2.09313	4.42583	0.34745
C	1.17768	3.86404	0.14320
C	-1.21007	2.45400	-0.35254
C	1.24252	2.46259	0.14126
C	-0.00490	4.57020	-0.15775
C	-1.18180	3.88689	-0.38899
C	0.04857	1.77669	-0.17261
H	0.00907	5.66072	-0.17031

H	-2.11991	4.42951	-0.52875
C	2.52636	1.80129	0.38774
H	3.34978	2.49449	0.62048
C	-2.52900	1.80785	-0.10534
H	-3.36038	2.52827	-0.12582
N	2.76208	0.53766	0.38754
N	-2.77460	0.57563	0.14772
C	4.11906	0.10154	0.75250
H	4.05359	-0.34457	1.76063
H	4.77928	0.98086	0.82639
C	4.72358	-0.92267	-0.21328
H	5.79179	-1.00848	0.04133
H	4.68191	-0.53735	-1.24692
C	4.11793	-2.32222	-0.14191
H	4.09545	-2.66979	0.90245
H	4.74845	-3.02758	-0.70806
N	2.73455	-2.36366	-0.66079
H	2.28179	-3.25711	-0.45253
C	-4.16042	0.23401	0.51811
H	-4.16652	0.07512	1.61043
H	-4.81563	1.09522	0.31068
C	-4.70887	-1.01573	-0.17443
H	-4.60610	-0.92125	-1.26949
H	-5.79040	-1.04208	0.03248
C	-4.11191	-2.33575	0.30561
H	-4.12527	-2.37761	1.40552
H	-4.72322	-3.17646	-0.06168
N	-2.71360	-2.50898	-0.13709
H	-2.25894	-3.29480	0.33457
H	-2.68075	-2.73853	-1.13515
H	2.73615	-2.28892	-1.68271
Cu	-1.42594	-0.96347	0.07767
O	-0.00919	0.51802	-0.63188
Cu	1.43999	-0.95697	0.00995
H	-0.80443	1.45371	-1.31807
O	0.01822	-2.09646	0.20126

5

H	-2.14897	4.35388	-0.28841
C	-1.20278	3.82595	-0.14783
C	1.23096	2.45153	0.17415
C	-1.22656	2.45207	0.16970
C	0.00377	4.50834	-0.29603
C	1.20941	3.82543	-0.14302
C	0.00163	1.80264	0.38244
H	0.00467	5.57218	-0.53972
H	2.15644	4.35290	-0.27975
C	-2.54586	1.79838	0.21347
H	-3.38869	2.49134	0.36267
C	2.54927	1.79619	0.21934
H	3.39299	2.48788	0.36960
N	-2.80828	0.55530	0.01562
N	2.80970	0.55286	0.01985
C	-4.22149	0.14711	-0.02149
H	-4.48016	-0.01742	-1.08229
H	-4.85180	0.97275	0.34593
C	-4.51810	-1.12874	0.77195
H	-5.61403	-1.23043	0.81259
H	-4.17953	-1.01413	1.81636
C	-3.95918	-2.41610	0.17104
H	-4.22902	-2.48657	-0.89376
H	-4.40438	-3.28621	0.68070
N	-2.48398	-2.49268	0.26783
H	-2.12157	-3.29210	-0.25848
C	4.22235	0.14273	-0.01791
H	4.48173	-0.01681	-1.07925
H	4.85339	0.96575	0.35406

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C   4.51703 -1.13756  0.76907
H   4.18018 -1.02763  1.81455
H   5.61281 -1.24179  0.80759
C   3.95452 -2.42072  0.16249
H   4.22142 -2.48577 -0.90339
H   4.39949 -3.29439  0.66616
N   2.47950 -2.49523  0.26243
H   2.11388 -3.29088 -0.26729
H   2.19996 -2.66153  1.23433
H  -2.20282 -2.65428  1.24002
Cu  1.45110 -0.87946 -0.37978
O   0.00050  0.48016  0.80234
Cu -1.45358 -0.88079 -0.38190
O  -0.00057 -1.64246 -1.17791
H   0.00803  0.42375  1.77697
```

TS5

```
H  -2.15408  4.43806 -0.16023
C  -1.21333  3.88950 -0.07912
C   1.25282  2.49662  0.05650
C  -1.24950  2.49469  0.05600
C  -0.00014  4.58224 -0.12952
C   1.21432  3.89163 -0.07916
C   0.00196  1.80580  0.23748
H  -0.00094  5.66867 -0.22963
H   2.15402  4.44194 -0.16156
C  -2.55991  1.84170  0.00772
H  -3.39823  2.55381 -0.04032
C   2.56438  1.84452  0.01712
H   3.40321  2.55672 -0.01747
N  -2.82503  0.58271 -0.04121
N   2.82841  0.58522 -0.03312
C  -4.24135  0.22051 -0.23029
H  -4.39218  0.09432 -1.31737
H  -4.87745  1.06188  0.08771
C  -4.67409 -1.06142  0.48225
H  -5.77363 -1.09481  0.43184
H  -4.41537 -1.01268  1.55417
C  -4.14164 -2.35125 -0.13769
H  -4.30404 -2.33825 -1.22593
H  -4.69236 -3.21598  0.26658
N  -2.69485 -2.52806  0.10096
H  -2.29889 -3.25689 -0.49797
C   4.24633  0.21839 -0.19890
H   4.41930  0.10444 -1.28404
H   4.87964  1.05266  0.14283
C   4.65623 -1.07386  0.50923
H   4.36456 -1.03924  1.57309
H   5.75695 -1.10685  0.49424
C   4.14438 -2.35544 -0.14394
H   4.35201 -2.33243 -1.22411
H   4.67546 -3.22530  0.27484
N   2.68813 -2.53198  0.03263
H   2.30918 -3.22157 -0.62059
H   2.48231 -2.90852  0.96279
H  -2.52924 -2.85303  1.05849
Cu  1.46087 -0.93317 -0.09502
O   0.00287  0.42140  0.45206
Cu -1.46002 -0.93901 -0.08116
O   0.00116 -2.04019 -0.32555
H   0.00331  1.45968  1.40881
```

TS6

```
C   0.07145  1.78993 -0.16426
C  -1.13882  2.50332 -0.19750
```

C	-1.05680	3.91106	-0.24440
C	0.17703	4.56147	-0.20728
C	1.35277	3.82245	-0.07331
C	1.32615	2.41239	-0.03196
C	-2.47568	1.89894	-0.07241
N	-2.80920	0.66966	0.13023
Cu	-1.57971	-0.95502	0.00265
O	-0.04719	-1.83491	-0.71631
Cu	1.48237	-1.06975	0.11019
O	0.01389	0.42670	-0.15835
C	2.58425	1.70944	0.27124
N	2.78537	0.44733	0.43041
C	4.09820	-0.01801	0.88990
C	4.82744	-0.94890	-0.09588
C	3.98874	-2.02276	-0.80856
N	2.84855	-2.52332	-0.00042
C	-4.23330	0.39600	0.39228
C	-4.75559	-0.90064	-0.23122
C	-4.24396	-2.18910	0.41246
N	-2.84079	-2.49352	0.04422
H	2.31226	4.33713	0.01832
H	0.21980	5.65116	-0.24546
H	-1.97942	4.49495	-0.28722
H	3.43457	2.38966	0.43680
H	-3.28419	2.64652	-0.09724
H	3.91676	-0.55304	1.83695
H	4.74932	0.83914	1.12539
H	5.63476	-1.42793	0.48036
H	5.31719	-0.34638	-0.87638
H	4.64329	-2.86223	-1.09114
H	3.56289	-1.62378	-1.74135
H	3.15462	-2.88446	0.90862
H	-4.34998	0.33819	1.48895
H	-4.83959	1.24871	0.04632
H	-4.56368	-0.91054	-1.31853
H	-5.85060	-0.88608	-0.11444
H	-4.29309	-2.10936	1.50884
H	-4.88469	-3.03465	0.11570
H	-2.45145	-3.21888	0.65299
H	-2.79417	-2.88701	-0.90101
H	2.39006	-3.30721	-0.47274
H	0.02572	-0.16421	-1.01443

6

Cu	1.96742	-0.94279	0.12443
Cu	-1.84248	-0.96667	-0.36484
O	-0.39475	-1.87611	-1.30642
O	0.14879	-1.36355	-0.18415
N	-3.55167	-1.54794	-1.24682
N	2.95938	0.80087	0.13285
N	-2.67149	0.30148	0.92908
N	3.37335	-2.37052	0.35618
C	-0.44554	4.18904	-0.80016
C	0.02746	1.70843	0.42610
C	0.84486	3.65943	-0.76362
C	-1.49764	3.49492	-0.20413
C	-1.27155	2.23844	0.39308
C	1.09749	2.41414	-0.15359
C	-2.41745	1.55570	1.02136
C	2.50057	1.98111	-0.08812
C	4.42166	0.68109	0.30817
C	-4.64877	-1.83389	-0.28748
C	-4.96561	-0.64522	0.61521
C	4.75480	-1.86858	0.56334
C	5.04365	-0.60341	-0.24380
C	-3.86383	-0.23747	1.60312
H	1.67453	4.22169	-1.19922

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H  -0.62688  5.15627 -1.27291
H  -2.50277  3.92363 -0.20000
H   3.22809  2.79591 -0.23381
H  -3.11246  2.19428  1.59016
H  -5.85168 -0.91046  1.21312
H  -5.25269  0.22862  0.00494
H  -3.54448 -1.11122  2.19460
H  -4.25916  0.51486  2.30375
H   4.61624  0.73303  1.39394
H   4.91015  1.55753 -0.14807
H   4.76232 -0.74655 -1.30221
H   6.13437 -0.44889 -0.23797
H   3.33801 -2.92986 -0.50193
H  -3.84418 -0.82408 -1.91165
H  -5.55450 -2.11965 -0.84613
H  -4.34652 -2.70471  0.31440
H   4.87906 -1.66194  1.63712
H   5.47719 -2.65656  0.29683
H   3.11875 -3.02316  1.10268
H  -3.36011 -2.37601 -1.81810
H   0.21352  0.78930  0.98099
```

TS7

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Cu  1.86139 -1.10219 -0.11746
Cu -1.86893 -1.10344 -0.11521
O   0.00059  0.29264 -1.27697
O  -0.00247 -0.89930 -0.65584
N  -3.40560 -2.23307 -0.68479
N   2.73895  0.47642  0.79495
N  -2.74352  0.49514  0.77647
N   3.39990 -2.22743 -0.69609
C   0.01694  4.14587 -0.90195
C   0.00313  1.60252  0.27908
C   1.22852  3.53078 -0.56461
C  -1.20166  3.53800 -0.57752
C  -1.22730  2.27775  0.03640
C   1.24003  2.27085  0.05037
C  -2.51057  1.72664  0.47052
C   2.51546  1.71188  0.49760
C   4.06696  0.14507  1.33566
C  -4.64679 -2.05751  0.10843
C  -4.99874 -0.59441  0.35585
C   4.65328 -2.05531  0.07967
C   4.99192 -0.59416  0.35547
C  -4.07900  0.18277  1.31132
H   2.17171  4.04690 -0.75917
H   0.02236  5.12917 -1.37675
H  -2.13970  4.05907 -0.78369
H   3.33110  2.44425  0.61387
H  -3.32445  2.46354  0.56918
H  -6.00023 -0.57810  0.81520
H  -5.09199 -0.05126 -0.60091
H  -3.93343 -0.40165  2.23509
H  -4.58154  1.12350  1.59045
H   3.91051 -0.47837  2.23153
H   4.56563  1.07310  1.65997
H   5.06287 -0.02920 -0.59050
H   5.99908 -0.57282  0.80186
H   3.57185 -2.01772 -1.68465
H  -3.59016 -2.01899 -1.67018
H  -5.48559 -2.54892 -0.41131
H  -4.50760 -2.57914  1.06766
H   4.53660 -2.60074  1.02846
H   5.48801 -2.52414 -0.46658
H   3.12232 -3.21325 -0.68603
H  -3.13186 -3.21997 -0.68108
H  -0.00327  0.74953  0.95582
```

7

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Cu  1.79722 -1.04534  0.06602
Cu -1.94338 -1.13353 -0.24112
O   0.10831  0.49397 -0.96004
O  -0.08916 -0.80359 -0.37483
N  -3.52550 -2.24687 -0.68335
N   2.99138  0.51119  0.50351
N  -2.73411  0.54379  0.62591
N   2.98581 -2.59803 -0.36143
C   0.14661  4.32205 -0.57739
C   0.16798  1.50837  0.10257
C   1.37816  3.64937 -0.43025
C  -1.06433  3.66129 -0.30011
C  -1.10347  2.31920  0.05343
C   1.43843  2.31497 -0.06981
C  -2.40081  1.77646  0.40951
C   2.74673  1.73913  0.17953
C   4.37328  0.13799  0.82212
C  -4.72894 -1.98584  0.14662
C  -5.03159 -0.49620  0.26739
C   4.33718 -2.41041  0.22898
C   4.92396 -1.02011 -0.02848
C  -4.08474  0.31382  1.16483
H   2.30741  4.20655 -0.57270
H   0.13564  5.37406 -0.86759
H  -1.99906  4.22472 -0.35581
H   3.58612  2.45078  0.11981
H  -3.17498  2.54781  0.55373
H  -6.03539 -0.39896  0.71067
H  -5.09295 -0.03397 -0.73340
H  -3.96042 -0.21442  2.12594
H  -4.55379  1.28703  1.38545
H   4.39279 -0.15996  1.88523
H   5.03429  1.01479  0.71351
H   4.84797 -0.76788 -1.10086
H   6.00158 -1.07720  0.19385
H   3.06324 -2.67866 -1.37996
H  -3.75191 -2.08149 -1.66983
H  -5.59548 -2.50795 -0.28951
H  -4.55050 -2.42002  1.14206
H   4.25750 -2.59247  1.31190
H   5.02384 -3.17109 -0.17809
H   2.59286 -3.49220 -0.05577
H  -3.28058 -3.24082 -0.63731
H   0.22370  0.94446  1.04967
```

TS8

```
C  -1.22591  3.56347 -0.63530
C  -1.27198  2.28821 -0.06473
C  -0.00637  1.58784  0.14724
C   1.26032  2.28757 -0.05362
C   1.21427  3.56434 -0.62042
C  -0.00424  4.18912 -0.90847
C  -2.59244  1.75420  0.27813
N  -2.87520  0.53760  0.58858
Cu -1.88519 -1.10190 -0.24000
N  -3.30516 -2.38473 -0.72847
C  -4.65322 -1.83956 -0.42122
C  -4.69278 -1.18392  0.96318
C  -4.25614  0.28015  1.02602
O  -0.00710  0.46447  0.95334
O  -0.00049 -0.55106 -0.21145
Cu  1.88854 -1.08534 -0.23454
N   3.30373 -2.36921 -0.73646
C   4.66215 -1.86117 -0.40913
```

```
C   4.70249 -1.17803  0.96127
C   4.26776  0.28824  1.00344
N   2.87317  0.54143  0.60542
C   2.58462  1.75237  0.27397
H  -2.15962  4.09571 -0.83277
H  -0.00283  5.19668 -1.32860
H   2.14998  4.09269 -0.81410
H  -3.38984  2.51717  0.26064
H   3.38531  2.50830  0.21226
H   5.74072 -1.20121  1.32837
H   4.11527 -1.77171  1.68374
H   4.95158  0.90677  0.39418
H   4.36625  0.64201  2.04462
H  -4.95530  0.91355  0.45094
H  -4.32049  0.61294  2.07667
H  -4.10172 -1.78898  1.67338
H  -5.72837 -1.21282  1.33569
H  -3.15767 -3.24261 -0.18840
H   3.13623 -3.24238 -0.22791
H   5.38338 -2.69379 -0.43167
H   4.95899 -1.15438 -1.19905
H  -4.90738 -1.10469 -1.20085
H  -5.40274 -2.64529 -0.47789
H  -3.25871 -2.68143 -1.70653
H   3.25680 -2.63158 -1.72433
H  -0.00313  0.77511 -0.84747
```

TS9

```
C  -1.13661  1.96939 -0.41674
C  -0.18041  1.52478  0.63697
C   1.12755  2.14286  0.63259
C   1.32436  3.33058 -0.04290
C   0.31609  3.91352 -0.87234
C  -0.86237  3.25703 -1.06489
O  -0.43729  0.51855  1.34662
Cu  1.63840 -0.67955 -0.70891
N   2.51620  0.19999  0.92875
C   3.61833 -0.48650  1.63096
C   4.13715 -1.73020  0.91148
C   4.50715 -1.50976 -0.55388
N   3.29906 -1.55764 -1.41744
C   2.25403  1.41373  1.25015
C  -2.58766  1.64017 -0.21124
N  -2.98665  0.52055  0.25582
C  -4.40223  0.19292  0.43818
C  -4.61395 -1.31379  0.61433
C  -3.97743 -2.19250 -0.46654
N  -2.52818 -2.43540 -0.22231
Cu -1.46835 -0.82670  0.26552
O  -0.10963 -0.47360 -1.11324
H  -1.62644  3.67016 -1.72850
H   0.51988  4.85872 -1.37750
H   2.30564  3.81214  0.00609
H  -3.31569  2.41310 -0.50608
H   2.90061  1.94285  1.96969
H   5.02706 -2.07220  1.46195
H   3.40258 -2.55194  0.98236
H   4.43930  0.23280  1.78863
H   3.24274 -0.77742  2.62550
H  -4.97436  0.56726 -0.42754
H  -4.77216  0.72141  1.33179
H  -4.24812 -1.63285  1.60635
H  -5.69948 -1.49578  0.61818
H  -2.41582 -3.11479  0.53829
H   3.04687 -2.53584 -1.59346
H   5.22508 -2.27415 -0.88877
H   4.98540 -0.52828 -0.69231
```

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H  -4.07625 -1.72671 -1.45870
H  -4.49266 -3.16447 -0.50948
H  -2.10204 -2.87773 -1.04181
H   3.51170 -1.17387 -2.34353
H  -0.68710  1.02322 -1.10044
```

4*ClO4

```
H   2.16802  4.49416  1.06960
C   1.25242  4.02965  0.69255
C  -1.16839  2.91423 -0.35307
C   1.31988  2.72887  0.22347
C   0.04119  4.79490  0.73979
C  -1.11977  4.26455  0.28763
C   0.11054  2.11341 -0.27102
H   0.06927  5.80180  1.15811
H  -2.05218  4.83309  0.33282
C   2.60418  2.02472  0.29612
H   3.42453  2.65035  0.68292
C  -2.47075  2.17781 -0.06464
H  -3.27909  2.83732  0.28940
N   2.86259  0.80237 -0.01193
N  -2.70472  0.93578 -0.22315
C   4.23557  0.32871  0.22926
H   4.21176 -0.27163  1.15578
H   4.89480  1.19162  0.41921
C   4.81324 -0.52708 -0.90241
H   5.88851 -0.64371 -0.69519
H   4.74100  0.01022 -1.86386
C   4.21400 -1.92588 -1.02860
H   4.20572 -2.41927 -0.04484
H   4.83946 -2.53967 -1.69734
N   2.82484 -1.89867 -1.53214
H   2.37015 -2.80958 -1.43055
C  -4.04789  0.44380  0.13630
H  -3.93523 -0.14427  1.06302
H  -4.70325  1.29960  0.36647
C  -4.68958 -0.43131 -0.94556
H  -4.69061  0.09968 -1.91295
H  -5.74624 -0.55964 -0.66347
C  -4.08322 -1.82380 -1.10303
H  -4.02261 -2.31809 -0.12158
H  -4.73737 -2.44075 -1.74054
N  -2.72045 -1.78768 -1.67572
H  -2.26852 -2.70411 -1.61964
H  -2.76208 -1.56767 -2.67563
H   2.81593 -1.70679 -2.53850
Cu -1.38353 -0.50417 -0.87501
O   0.10262  0.93762 -0.69194
Cu  1.52720 -0.56776 -0.73793
H  -1.22517  3.14847 -1.44622
O   0.05556 -1.64996 -1.06033
Cl -0.25694 -1.67765  2.21372
O  -0.27963 -3.07088  2.61650
O  -0.37716 -0.88266  3.42170
O   0.94993 -1.35766  1.49332
O  -1.44002 -1.43560  1.41257
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TS9*ClO4

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C   1.68035  2.41655 -0.05353
C   0.52680  1.87982 -0.84993
C  -0.65501  2.72562 -0.92673
C  -0.54766  4.07371 -0.66424
C   0.65700  4.66741 -0.15994
C   1.72096  3.87845  0.14549
O   0.52247  0.70375 -1.26778
Cu -1.43820  0.30367  1.07656
```

```
N  -2.37149  1.04849 -0.62597
C  -3.66052  0.48360 -1.07079
C  -4.32207 -0.46960 -0.07517
C  -4.41820  0.05333  1.35717
N  -3.13916 -0.15529  2.07869
C  -1.96123  2.10856 -1.22048
C   3.01820  1.75653 -0.24606
N   3.15171  0.49500 -0.37161
C   4.46717 -0.12800 -0.50697
C   4.47744 -1.55110  0.06799
C   3.83270 -1.68980  1.45125
N   2.35507 -1.80259  1.36864
Cu  1.40989 -0.55897  0.09379
O   0.33480  0.47377  1.41044
H   2.62956  4.31072  0.57376
H   0.68825  5.74423  0.01447
H  -1.42910  4.71014 -0.79160
H   3.90098  2.41800 -0.23791
H  -2.61427  2.61238 -1.95351
H  -5.33609 -0.67303 -0.45382
H  -3.79115 -1.43537 -0.07166
H  -4.34537  1.31345 -1.31694
H  -3.46285 -0.06922 -2.00306
H   5.23031  0.49904 -0.01342
H   4.72029 -0.17090 -1.57961
H   3.98011 -2.24537 -0.63197
H   5.52674 -1.87904  0.12777
H   2.08492 -2.74237  1.06293
H  -3.04705 -1.14642  2.32215
H  -5.23463 -0.45499  1.89516
H  -4.64350  1.13150  1.36739
H   4.06994 -0.81845  2.08113
H   4.23191 -2.57937  1.96423
H   1.92973 -1.66750  2.28953
H  -3.15707  0.33819  2.97575
H   1.22378  1.88063  0.91212
Cl -0.79839 -2.64737 -0.91152
O  -1.30672 -2.14048  0.40727
O  -1.53037 -2.01397 -2.02681
O   0.68312 -2.28020 -1.01136
O  -0.90709 -4.11749 -0.96350
```