Note Added after Publication: The original version of this Supporting Information appeared with the Article published on Articles ASAP on September 15, 2006, and printed in the October 12, 2006, issue. The Supporting Information was replaced with a corrected version on May 18, 2007. The corrected Supporting Information is also linked to an Addition and Correction published on Articles ASAP on May 15, 2007, and printed in the June 7, 2007, issue.

Theoretical Characterization of End-on and Side-on Peroxide Coordination in Ligated Cu_2O_2 Models

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(correction to original version dated *July 5, 2006*; correction is new 100% geometries for isomers **0** and **2** on pp. S-2 and S-4, respectively)

Contents

Cartesian Coordinates (0% and 100%)

Note that all other structures may be determined using eq. 2 of the manuscript

$Cu_2O_2^{2+}$ (**0**)

0%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-2.380000	-0.410000	0.000000
2	29	0	2.380000	0.410000	0.000000
3	8	0	-0.530000	0.410000	0.000000
4	8	0	0.530000	-0.410000	0.000000

100%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.800000	0.000000	0.000000
2	29	0	1.800000	0.000000	0.000000
3	8	0	0.000000	0.700000	0.000000
4	8	0	0.000000	-0.700000	0.000000

$\{(NH_3)Cu\}_2O_2^{2+}$ (**1**)

0%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.593891	2.340449	0.000000
2	29	0	-0.593891	-2.340449	0.000000
3	8	0	0.593891	0.314449	0.000000
4	8	0	-0.593891	-0.314449	0.000000
5	7	0	0.593891	4.440449	0.000000
6	7	0	-0.593891	-4.440449	0.000000
7	1	0	-0.345802	4.782469	0.000000
8	1	0	0.345802	-4.782469	0.000000
9	1	0	1.063737	4.782469	0.813798
10	1	0	-1.063737	-4.782469	-0.813798
11	1	0	1.063737	4.782469	-0.813798
12	1	0	-1.063737	-4.782469	0.813798

100%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	1.800000	0.000000
2	29	0	0.000000	-1.800000	0.000000
3	8	0	0.000000	0.000000	0.700000
4	8	0	0.000000	0.000000	-0.700000
5	7	0	0.000000	3.800000	0.000000
6	7	0	0.000000	-3.800000	0.000000
7	1	0	-0.939693	4.142020	0.000000
8	1	0	0.939693	-4.142020	0.000000
9	1	0	0.469846	4.142020	0.813798
10	1	0	-0.469846	-4.142020	-0.813798
11	1	0	0.469846	4.142020	-0.813798
12	1	0	-0.469846	-4.142020	0.813798

$\{(NH_3)_2Cu\}_2O_2^{2+}$ (**2**)

0%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.451897	2.203097	0.093215
2	29	0	-1.451897	-2.203097	-0.093215
3	8	0	0.562652	0.192151	-0.257954
4	8	0	-0.562652	-0.192151	0.257954
5	7	0	3.015496	1.885742	-1.059336
6	7	0	0.191645	3.085434	1.315301
7	7	0	-3.015496	-1.885742	1.059336
8	7	0	-0.191645	-3.085434	-1.315301
9	1	0	3.591514	1.090828	-0.742332
10	1	0	0.076925	2.580102	2.207074
11	1	0	-3.591514	-1.090828	0.742332
12	1	0	0.750033	-3.197954	-0.909807
13	1	0	3.641906	2.706025	-1.078320
14	1	0	-0.750033	3.197954	0.909807
15	1	0	-2.758967	-1.696618	2.040454
16	1	0	-0.076925	-2.580102	-2.207074
17	1	0	2.758967	1.696618	-2.040454
18	1	0	0.514919	4.034607	1.561292
19	1	0	-3.641906	-2.706025	1.078320
20	1	0	-0.514919	-4.034607	-1.561292

100%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.000000	1.800000	-0.000000
2	29	0	0.000000	-1.800000	-0.000000
3	8	0	0.700000	0.000000	0.000000
4	8	0	-0.700000	-0.000000	0.000000
5	7	0	1.414214	3.214214	0.000000
6	7	0	-1.414214	3.214214	-0.000000
7	7	0	-1.414214	-3.214214	0.000000
8	7	0	1.414214	-3.214214	-0.000000
9	1	0	2.320521	2.791595	0.000000
10	1	0	-2.320521	2.791595	-0.000000
11	1	0	-2.320521	-2.791595	0.000000
12	1	0	2.320521	-2.791595	-0.000000
13	1	0	1.323827	3.788290	0.813798
14	1	0	-1.323827	3.788290	-0.813798
15	1	0	-1.323827	-3.788290	0.813798
16	1	0	1.323827	-3.788290	-0.813798
17	1	0	1.323827	3.788290	-0.813798
18	1	0	-1.323827	3.788290	0.813798
19	1	0	-1.323827	-3.788290	-0.813798
20	1	0	1.323827	-3.788290	0.813798

$\{(NH_3)_3Cu\}_2O_2^{2+}$ (3)

0%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.003940	0.496472	0.452986
2	8	0	0.003940	-0.496472	-0.452986
3	29	0	-0.003612	2.404409	-0.230002
4	29	0	0.003612	-2.404409	0.230002
5	7	0	1.190098	2.088821	-1.928357
6	7	0	0.551959	3.211850	1.640773
7	7	0	-0.551959	-3.211850	-1.640773
8	7	0	-1.190098	-2.088821	1.928357
9	7	0	-1.660242	3.573354	-0.878350
10	7	0	1.660242	-3.573354	0.878350
11	1	0	-1.386347	4.519536	-1.181113
12	1	0	1.386347	-4.519536	1.181113
13	1	0	-2.371992	3.708222	-0.146259

14	1	0	2.371992	-3.708222	0.146259
15	1	0	-2.157125	3.154410	-1.677345
16	1	0	2.157125	-3.154410	1.677345
17	1	0	2.158182	2.420139	-1.812378
18	1	0	1.254298	2.622711	2.109147
19	1	0	-2.158182	-2.420139	1.812378
20	1	0	-1.254298	-2.622711	-2.109147
21	1	0	0.847713	2.507842	-2.803969
22	1	0	0.971890	4.149146	1.562455
23	1	0	-0.847713	-2.507842	2.803969
24	1	0	-0.971890	-4.149146	-1.562455
25	1	0	1.240054	1.072341	-2.084322
26	1	0	-0.230707	3.305888	2.303239
27	1	0	-1.240054	-1.072341	2.084322
28	1	0	0.230707	-3.305888	-2.303239

100%

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	0.730662
2	8	0	0.000000	0.000000	-0.730662
3	29	0	-0.411730	1.807560	0.000000
4	29	0	0.411730	-1.807560	0.000000
5	7	0	0.000000	3.032672	-1.605648
6	7	0	0.000000	3.032672	1.605648
7	7	0	0.000000	-3.032672	1.605648
8	7	0	0.000000	-3.032672	-1.605648
9	7	0	-2.633478	1.684278	0.000000
10	7	0	2.633478	-1.684278	0.000000
11	1	0	-3.183738	2.544750	0.000000
12	1	0	3.183738	-2.544750	0.000000
13	1	0	-2.943994	1.151207	0.813577
14	1	0	2.943994	-1.151207	-0.813577
15	1	0	-2.943994	1.151207	-0.813577
16	1	0	2.943994	-1.151207	0.813577
17	1	0	0.993345	3.260483	-1.683210
18	1	0	0.993345	3.260483	1.683210
19	1	0	-0.993345	-3.260483	1.683210
20	1	0	-0.993345	-3.260483	-1.683210
21	1	0	-0.501839	3.922784	-1.603432
22	1	0	-0.501839	3.922784	1.603432
23	1	0	0.501839	-3.922784	1.603432
24	1	0	0.501839	-3.922784	-1.603432
25	1	0	-0.251567	2.561760	-2.477161
26	1	0	-0.251567	2.561760	2.477161
27	1	0	0.251567	-2.561760	2.477161
28	1	0	0.251567	-2.561760	-2.477161

$\{(Imid)_3Cu\}_2O_2^{2+}$ **(4 BLYP)**

bis(μ-oxo)

Cu	1.175232	0.760040	-0.408035
Cu	-1.175232	-0.760040	0.408035
O	-0.578995	0.419067	-0.890793
O	0.578995	-0.419067	0.890793
C	2.673782	-0.782913	-3.100037
N	2.309341	-0.842834	-1.803986
C	2.373306	-2.202637	-1.451370
C	2.780945	-2.958145	-2.537186
N	2.966995	-2.043427	-3.575989
H	3.278397	-2.279037	-4.543488
H	2.731293	0.118057	-3.713440
H	2.117615	-2.528519	-0.441818
H	2.956451	-4.027100	-2.668716
C	-2.673782	0.782913	3.100037
N	-2.309341	0.842834	1.803986
C	-2.373306	2.202637	1.451370
C	-2.780945	2.958145	2.537186
N	-2.966995	2.043427	3.575989
H	-3.278397	2.279037	4.543488
H	-2.731293	-0.118057	3.713440
H	-2.117615	2.528519	0.441818
H	-2.956451	4.027100	2.668716
C	4.047394	0.624649	0.477554
N	2.827621	1.187576	0.621658
C	2.874023	2.006958	1.762100
C	4.141708	1.944336	2.305817
N	4.862717	1.071945	1.484300
H	5.862473	0.798355	1.619736
H	4.337326	-0.080521	-0.301849
H	1.997314	2.559647	2.103485
H	4.587509	2.424515	3.178909
C	2.275391	3.217500	-1.804626
N	1.335693	2.248703	-1.716843
C	0.393204	2.483521	-2.729202
C	0.769547	3.607483	-3.437103
N	1.953979	4.053345	-2.841965
H	2.501053	4.895157	-3.133041
H	3.147446	3.336136	-1.162048
H	-0.470383	1.827087	-2.849350
H	0.317505	4.120956	-4.287643
C	-2.275391	-3.217500	1.804626

N	-1.335693	-2.248703	1.716843
C	-0.393204	-2.483521	2.729202
C	-0.769547	-3.607483	3.437103
N	-1.953979	-4.053345	2.841965
H	-2.501053	-4.895157	3.133041
H	-3.147446	-3.336136	1.162048
H	0.470383	-1.827087	2.849350
H	-0.317505	-4.120956	4.287643
C	-4.047394	-0.624649	-0.477554
N	-2.827621	-1.187576	-0.621658
C	-2.874023	-2.006958	-1.762100
C	-4.141708	-1.944336	-2.305817
N	-4.862717	-1.071945	-1.484300
H	-5.862473	-0.798355	-1.619736
H	-4.337326	0.080521	0.301849
H	-1.997314	-2.559647	-2.103485
H	-4.587509	-2.424515	-3.178909

side-on peroxo

Cu	-1.511444	-0.778793	0.834946
Cu	1.511444	0.778793	-0.834946
O	0.421753	-0.231125	0.544937
O	-0.421753	0.231125	-0.544937
C	-2.574234	0.985306	3.292038
N	-2.178909	0.936478	2.003021
C	-2.184418	2.263916	1.541168
C	-2.586563	3.112228	2.556625
N	-2.828857	2.287537	3.657654
H	-3.150391	2.608154	4.597519
H	-2.679581	0.133728	3.966873
H	-1.893097	2.497772	0.516190
H	-2.722641	4.193924	2.602509
C	2.574234	-0.985306	-3.292038
N	2.178909	-0.936478	-2.003021
C	2.184418	-2.263916	-1.541168
C	2.586563	-3.112228	-2.556625
N	2.828857	-2.287537	-3.657654
H	3.150391	-2.608154	-4.597519
H	2.679581	-0.133728	-3.966873
H	1.893097	-2.497772	-0.516190
H	2.722641	-4.193924	-2.602509
C	-4.389664	-0.772171	-0.115082
N	-3.148636	-1.292755	-0.237488
C	-3.194458	-2.205124	-1.306564
C	-4.473541	-2.234924	-1.827362
N	-5.211746	-1.326691	-1.063980
H	-6.224258	-1.105560	-1.195557

H	-4.703537	-0.023041	0.613312
H	-2.306198	-2.755951	-1.619431
H	-4.917816	-2.799835	-2.648758
C	-2.086868	-3.356094	2.338821
N	-1.290131	-2.278030	2.164505
C	-0.235855	-2.398605	3.087051
C	-0.401657	-3.556671	3.821167
N	-1.572220	-4.146057	3.336258
H	-1.986084	-5.043000	3.676025
H	-2.997086	-3.582153	1.781647
H	0.552246	-1.646332	3.142044
H	0.187042	-4.007950	4.621811
C	2.086868	3.356094	-2.338821
N	1.290131	2.278030	-2.164505
C	0.235855	2.398605	-3.087051
C	0.401657	3.556671	-3.821167
N	1.572220	4.146057	-3.336258
H	1.986084	5.043000	-3.676025
H	2.997086	3.582153	-1.781647
H	-0.552246	1.646332	-3.142044
H	-0.187042	4.007950	-4.621811
C	4.389664	0.772171	0.115082
N	3.148636	1.292755	0.237488
C	3.194458	2.205124	1.306564
C	4.473541	2.234924	1.827362
N	5.211746	1.326691	1.063980
H	6.224258	1.105560	1.195557
H	4.703537	0.023041	-0.613312
H	2.306198	2.755951	1.619431
H	4.917816	2.799835	2.648758

end-on peroxo

Cu	-1.751587	-1.499634	-0.702774
Cu	1.751587	1.499634	0.702774
O	0.594406	-0.112076	0.274124
O	-0.594406	0.112076	-0.274124
C	-1.035980	-3.750671	-2.650436
N	-0.590317	-2.756317	-1.851852
C	0.807755	-2.729034	-1.989197
C	1.203979	-3.714096	-2.873611
N	0.028381	-4.349335	-3.280884
H	-0.031555	-5.144531	-3.954697
H	-2.076309	-4.049561	-2.791367
H	1.408218	-2.000443	-1.441757
H	2.184082	-4.018585	-3.243286
C	1.035980	3.750671	2.650436
N	0.590317	2.756317	1.851852

C	-0.807755	2.729034	1.989197
C	-1.203979	3.714096	2.873611
N	-0.028381	4.349335	3.280884
H	0.031555	5.144531	3.954697
H	2.076309	4.049561	2.791367
H	-1.408218	2.000443	1.441757
H	-2.184082	4.018585	3.243286
C	-4.455032	-0.754211	-1.969803
N	-3.178589	-0.402710	-1.692886
C	-2.959824	0.829453	-2.332809
C	-4.107651	1.221436	-2.993042
N	-5.041153	0.209808	-2.754364
H	-6.020828	0.188965	-3.115768
H	-4.963440	-1.660324	-1.634506
H	-1.993134	1.330719	-2.266068
H	-4.344100	2.098053	-3.597946
C	-3.304108	-2.203217	1.845093
N	-2.340302	-2.538895	0.957748
C	-1.801376	-3.760788	1.400360
C	-2.445908	-4.160965	2.554230
N	-3.389832	-3.165771	2.820800
H	-4.055771	-3.161804	3.625275
H	-3.927612	-1.307922	1.810760
H	-0.998398	-4.254440	0.852051
H	-2.328018	-5.036118	3.195251
C	3.304108	2.203217	-1.845093
N	2.340302	2.538895	-0.957748
C	1.801376	3.760788	-1.400360
C	2.445908	4.160965	-2.554230
N	3.389832	3.165771	-2.820800
H	4.055771	3.161804	-3.625275
H	3.927612	1.307922	-1.810760
H	0.998398	4.254440	-0.852051
H	2.328018	5.036118	-3.195251
C	4.455032	0.754211	1.969803
N	3.178589	0.402710	1.692886
C	2.959824	-0.829453	2.332809
C	4.107651	-1.221436	2.993042
N	5.041153	-0.209808	2.754364
H	6.020828	-0.188965	3.115768
H	4.963440	1.660324	1.634506
H	1.993134	-1.330719	2.266068
H	4.344100	-2.098053	3.597946

Singlet and Broken-symmetry Absolute (E_h) and Relative (kcal mol^{-1}) Electronic Energies

$Cu_2O_2^{2+}$ (**0**)

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-541.293 16	-541.314 16	-541.306 41	-541.280 90	-541.251 18	-541.217 34
MP2	-542.182 61	-542.177 51	-542.162 52	-542.141 18	-542.151 20	-542.176 75
CCSD	-542.107 30	-542.111 82	-542.099 36	-542.076 98	-542.067 11	-542.066 20
CCSD(T)	-542.159 99	-542.159 92	-542.146 11	-542.124 49	-542.128 10	-542.137 33
CR-CCSD(T)	-542.141 83	-542.143 86	-542.130 64	-542.108 58	-542.107 32	-542.112 21
CR-CC(2,3),A	-542.160 82	-542.161 86	-542.148 30	-542.126 52	-542.127 90	-542.133 04
CR-CC(2,3),D	-542.163 04	-542.164 10	-542.150 72	-542.129 11	-542.130 51	-542.136 69
CCSD(TQ)	-542.148 77	-542.148 51	-542.134 74	-542.112 84	-542.111 45	-542.122 44
CR-CCSD(TQ)	-542.147 73	-542.149 03	-542.135 64	-542.113 80	-542.113 22	-542.118 73
CR-CC(2,3)+Q[a]	-542.168 94	-542.169 27	-542.155 72	-542.134 34	-542.136 41	-542.143 21
CAS(16,14)	-541.502 74	-541.502 00	-541.488 31	-541.464 66	-541.450 12	-541.421 89
CASPT2(16,14)	-542.408 75	-542.406 88	-542.392 54	-542.378 37	-542.391 08	-542.396 64
MSCASPT2(16,14)	-542.432 52	-542.427 41	-542.410 94	-542.390 47	-542.396 74	-542.396 70
bs-BLYP	-544.251 69	-544.248 59	-544.235 66	-544.222 83	-544.217 38	-544.211 83
bs-B3LYP	-544.318 60	-544.322 09	-544.312 27	-544.299 86	-544.290 95	-544.278 44
bs-mPWPW91	-544.509 21	-544.508 48	-544.496 91	-544.485 00	-544.479 84	-544.473 85
bs-mPW1PW91	-544.287 20	-544.293 93	-544.285 56	-544.273 45	-544.263 45	-544.248 39
bs-MPW1K	-544.142 30	-544.154 07	-544.147 12	-544.133 45	-544.118 60	-544.095 46
bs-TPSS	-544.202 65	-544.201 37	-544.190 21	-544.179 73	-544.176 21	-544.172 32
bs-TPSSh	-544.133 02	-544.134 81	-544.125 02	-544.114 52	-544.109 11	-544.101 60
BLYP/BS1d	-3430.972 10					-3430.922 25
BLYP/BS1t	-3430.985 11					-3430.933 09

[a] Computed as CR-CC(2,3),D + {CR-CCSD(TQ) – CR-CCSD(T)}

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-47.6	-60.8	-55.9	-39.9	-21.2	0.0
MP2	-3.7	-0.5	8.9	22.3	16.0	0.0
CCSD	-25.8	-28.6	-20.8	-6.8	-0.6	0.0
CCSD(T)	-14.2	-14.2	-5.5	8.1	5.8	0.0
CR-CCSD(T)	-18.6	-19.9	-11.6	2.3	3.1	0.0
CR-CC(2,3),A	-17.4	-18.1	-9.6	4.1	3.2	0.0
CR-CC(2,3),D	-16.5	-17.2	-8.8	4.8	3.9	0.0
CCSD(TQ)	-16.5	-16.4	-7.7	6.0	6.9	0.0
CR-CCSD(TQ)	-18.2	-19.0	-10.6	3.1	3.5	0.0
CR-CC(2,3)+Q[a]	-16.2	-16.4	-7.9	5.6	4.3	0.0
CAS(16,14)	-50.7	-50.3	-41.7	-26.8	-17.7	0.0
CASPT2(16,14)	-7.6	-6.4	2.6	11.5	3.5	0.0
MSCASPT2(16,14)	-22.5	-19.3	-8.9	3.9	0.0	0.0
bs-BLYP	-25.0	-23.1	-15.0	-6.9	-3.5	0.0
bs-B3LYP	-25.2	-27.4	-21.2	-13.4	-7.8	0.0
bs-mPWPW91	-22.2	-21.7	-14.5	-7.0	-3.8	0.0
bs-mPW1PW91	-24.4	-28.6	-23.3	-15.7	-9.5	0.0
bs-MPW1K	-29.4	-36.8	-32.4	-23.8	-14.5	0.0
bs-TPSS	-19.0	-18.2	-11.2	-4.7	-2.4	0.0
bs-TPSSh	-19.7	-20.8	-14.7	-8.1	-4.7	0.0
sumbs-BLYP	-21.9	-19.5	-10.3	-1.6	0.2	0.0
sumbs-B3LYP	-21.4	-23.2	-16.1	-7.5	-3.2	0.0
sumbs-mPWPW91	-18.9	-18.1	-9.8	-1.8	-0.2	0.0
sumbs-mPW1PW91	-21.0	-24.8	-18.7	-10.2	-4.9	0.0
sumbs-mPW1K	-27.7	-34.9	-29.7	-19.8	-10.3	0.0
sumbs-TPSS	-15.4	-14.1	-6.2	0.6	1.1	0.0
sumbs-TPSSh	-15.8	-16.4	-9.5	-2.5	-0.6	0.0
BLYP/BS1d	-31.3					0.0
BLYP/BS1t	-32.6					0.0

[a] Computed as CR-CC(2,3),D + {CR-CCSD(TQ) – CR-CCSD(T)}

$\{(NH_3)Cu\}_2O_2^{2+}$ (**1**)

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-653.892 95	-653.893 04	-653.881 82	-653.867 52	-653.861 48	-653.852 36
MP2	-655.241 52	-655.243 25	-655.235 72	-655.248 02	-655.269 46	-655.295 41
CCSD	-655.183 58	-655.185 77	-655.177 76	-655.168 49	-655.175 98	-655.184 90
CCSD(T)	-655.259 38	-655.263 37	-655.257 77	-655.257 69	-655.267 71	-655.280 25
CR-CCSD(T)	-655.224 88	-655.227 55	-655.220 16	-655.217 64	-655.227 09	-655.238 10
CR-CC(2,3),A	-655.261 79	-655.265 75	-655.259 45	-655.253 52	-655.263 10	-655.273 33
CR-CC(2,3),D	-655.262 00	-655.266 08	-655.259 83	-655.255 70	-655.266 05	-655.275 75
CCSD(TQ)	-655.235 62	-655.236 49	-655.227 69	-655.233 97	-655.245 72	-655.261 14
CR-CCSD(TQ)	-655.231 66	-655.234 69	-655.227 73	-655.223 48	-655.233 07	-655.244 14
CR-CC(2,3),D+Q[a]	-655.268 77	-655.273 21	-655.267 39	-655.261 54	-655.272 03	-655.281 78
CAS(16,14),Ci	-654.061 11					-654.215 06
PT2(16,14),Ci	-655.210 78					-655.184 70
MSPT2(16,14),Ci	-655.211 26					-655.184 70
PT2(12,12) 4root	-655.167 17	-655.189 92	-655.135 56	-655.144 57	-655.160 07	-655.185 24
MS(12,12) 4root	-655.182 76	-655.195 53	-655.163 74	-655.176 22	-655.188 03	-655.196 39
PT2(12,12) 5root	-655.183 83	-655.157 52	-655.142 92	-655.154 18	-655.164 30	-655.197 01
MS(12,12) 5root	-655.196 54	-655.192 01	-655.182 18	-655.187 24	-655.205 06	-655.230 61
MS(12,12) 6root	-655.205 35	-655.190 27	-655.173 72	-655.188 88	-655.197 86	-655.223 98
PT2(12,14) 6root	-655.158 61	-655.145 74	-655.161 48	-655.166 62	-655.154 78	-655.197 35
MS(12,14) 6root	-655.194 66	-655.176 73	-655.181 30	-655.182 49	-655.175 50	-655.227 28
PT2(16,14) 4root	-655.113 83	-655.196 61	-655.139 40	-655.150 44	-655.169 95	-655.193 09
MS(16,14) 4root	-655.141 04	-655.200 92	-655.179 59	-655.193 78	-655.212 99	-655.201 40
bs-BLYP	-657.608 31	-657.611 62	-657.607 73	-657.600 24	-657.594 73	-657.591 09
bs-B3LYP	-657.718 02	-657.722 57	-657.720 18	-657.713 84	-657.708 26	-657.704 33
bs-mPWPW91	-657.896 22	-657.900 84	-657.898 21	-657.891 87	-657.887 38	-657.885 01

bs-mPW1PW91	-657.643 79	-657.649 24	-657.647 82	-657.642 30	-657.637 12	-657.633 34
bs-MPW1K	-657.479 13	-657.484 34	-657.482 73	-657.476 66	-657.469 94	-657.464 09
bs-TPSS	-657.609 69	-657.614 30	-657.612 15	-657.606 84	-657.603 75	-657.602 97
bs-TPSSh	-657.522 02	-657.527 07	-657.525 49	-657.520 55	-657.517 15	-657.515 76
BLYP/BS1d	-3544.318 82					-3544.301 28
BLYP/BS1t	-3544.335 47					-3544.316 77

[a] Computed as CR-CC(2,3),D + {CR-CCSD(TQ) – CR-CCSD(T)}

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-25.5	-25.5	-18.5	-9.5	-5.7	0.0
MP2	33.8	32.7	37.5	29.7	16.3	0.0
CCSD	0.8	-0.5	4.5	10.3	5.6	0.0
CCSD(T)	13.1	10.6	14.1	14.2	7.9	0.0
CR-CCSD(T)	8.3	6.6	11.3	12.8	6.9	0.0
CR-CC(2,3),A	7.2	4.8	8.7	12.4	6.4	0.0
CR-CC(2,3),D	8.6	6.1	10.0	12.6	6.1	0.0
CCSD(TQ)	16.0	15.5	21.0	17.1	9.7	0.0
CR-CCSD(TQ)	7.8	5.9	10.3	13.0	6.9	0.0
CR-CC(2,3),D+Q[a]	8.2	5.4	9.0	12.7	6.1	0.0
CAS(16,14),Ci	96.6					0.0
PT2(16,14),Ci	-16.4					0.0
MSPT2(16,14),Ci	-16.7					0.0
PT2(12,12) 4root	11.3	-2.9	31.2	25.5	15.8	0.0
MS(12,12) 4root	8.6	0.5	20.5	12.7	5.2	0.0
PT2(12,12) 5root	8.3	24.8	33.9	26.9	20.5	0.0
MS(12,12) 5root	21.4	24.2	30.4	27.2	16.0	0.0
MS(12,12) 6root	11.7	21.2	31.5	22.0	16.4	0.0
PT2(12,14) 6root	24.3	32.4	22.5	19.3	26.7	0.0
MS(12,14) 6root	20.5	31.7	28.8	28.1	32.5	0.0
PT2(16,14) 4root	49.7	-2.2	33.7	26.8	14.5	0.0

MS(16,14) 4root	37.9	0.3	13.7	4.8	-7.3	0.0
BLYP	-10.8	-12.9	-10.4	-5.7	-2.3	0.0
bs-BLYP	-8.6	-11.4	-10.0	-6.0	-2.5	0.0
B3LYP	-7.0	-9.9	-8.3	-4.3	-1.5	0.0
bs-B3LYP	-6.6	-10.0	-9.1	-5.6	-2.4	0.0
mPWPW91	-9.4	-12.7	-11.7	-7.9	-3.7	0.0
bs-mPWPW91	-4.2	-7.1	-5.8	-2.4	-0.5	0.0
mPW1PW91	-3.9	-7.1	-6.1	-3.0	-0.9	0.0
bs-mPW1PW91	-6.6	-8.1	-4.7	0.0	0.8	0.0
MPW1K	-1.0	-2.8	-0.3	3.1	3.0	0.0
bs-MPW1K	-2.7	-5.1	-2.5	1.3	1.6	0.0
TPSS	0.0	-2.2	-0.2	2.7	2.5	0.0
bs-TPSS	-4.0	-5.5	-2.6	1.4	2.3	0.0
TPSSh	0.7	-1.6	0.5	3.3	2.5	0.0
bs-TPSSh	2.2	-0.1	1.5	3.9	2.9	0.0
BLYP/BS1d	-11.0					0.0
BLYP/BS1t	-11.7					0.0

[a] Computed as CR-CC(2,3),D + {CR-CCSD(TQ) – CR-CCSD(T)}

$\{(NH_3)_2Cu\}_2O_2^{2+}$ (**2**)

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-766.454 28	-766.403 11	-766.327 11	-766.318 45	-766.376 97	-766.416 15
MP2	-768.249 27	-768.236 83	-768.200 70	-768.228 65	-768.300 54	-768.335 06
CCSD	-768.207 27	-768.177 96	-768.122 45	-768.128 83	-768.192 56	-768.226 08
CCSD(T)	-768.299 84	-768.283 65	-768.233 35	-768.242 38	-768.306 26	-768.340 21
CR-CCSD(T)	-768.245 57	-768.223 95	-768.176 22	-768.185 23	-768.250 01	-768.283 93
CR-CC(2,3),A	-768.298 87	-768.283 28	-768.230 62	-768.235 74	-768.296 71	-768.328 35
CR-CC(2,3),D	-768.299 08	-768.281 37	-768.231 11	-768.237 93	-768.300 07	-768.332 35
CAS(14,13)	-766.621 37					-766.737 65

CASPT2(14,13)	-768.417 77					-768.416 12
MSPT2(14,13)	-768.420284					-768.416 12
bs-BLYP	-770.877 38	-770.846 03	-770.786 54	-770.777 95	-770.827 47	-770.853 48
bs-B3LYP	-771.048 20	-771.018 12	-770.964 74	-770.950 80	-771.007 83	-771.036 77
bs-mPWPW91	-771.204 33	-771.179 35	-771.124 90	-771.117 49	-771.164 40	-771.187 40
bs-mPW1PW91	-770.942 50	-770.916 32	-770.867 91	-770.851 17	-770.898 82	-770.940 63
bs-MPW1K	-770.772 02	-770.743 63	-770.698 27	-770.673 97	-770.759 44	-770.792 87
bs-TPSS	-770.942 71	-770.917 23	-770.862 86	-770.856 51	-770.906 87	-770.933 55
bs-TPSSh	-770.844 74	-770.818 96	-770.767 11	-770.757 35	-770.807 55	-770.837 75

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-23.9	8.2	55.9	61.3	24.6	0.0
MP2	53.8	61.6	84.3	66.8	21.7	0.0
CCSD	11.8	30.2	65.0	61.0	21.0	0.0
CCSD(T)	25.3	35.5	67.1	61.4	21.3	0.0
CR-CCSD(T)	24.1	37.6	67.6	61.9	21.3	0.0
CR-CC(2,3),A	18.5	28.3	61.3	58.1	19.9	0.0
CR-CC(2,3),D	20.9	32.0	63.5	59.3	20.3	0.0
CAS(14,13)	73.0					0.0
CASPT2(14,13)	-1.0					0.0
MSPT2(14,13)	-2.6					0.0
bs-BLYP	-15.0	4.7	42.0	47.4	16.3	0.0
bs-B3LYP	-7.2	11.7	45.2	54.0	18.2	0.0
bs-mPWPW91	-10.6	5.1	39.2	43.9	14.4	0.0
bs-mPW1PW91	-1.2	15.3	45.6	56.1	26.2	0.0
bs-MPW1K	13.1	30.9	59.4	74.6	21.0	0.0
bs-TPSS	-5.7	10.2	44.4	48.3	16.7	0.0
bs-TPSSh	-4.4	11.8	44.3	50.5	19.0	0.0
sumbs-BLYP	-9.9	8.8	44.4	46.4	16.3	0.0
sumbs-B3LYP	7.9	26.0	56.0	62.3	18.6	0.0
sumbs-mPWPW91	-5.4	9.3	41.8	43.0	12.7	0.0

sumbs-mPW1PW91	15.1	31.1	57.0	65.8	33.2	0.0
sumbs-mPW1K	30.5	48.6	70.4	86.5	8.6	0.0
sumbs-TPSS	-0.9	14.2	46.8	47.5	16.7	0.0
sumbs-TPSSh	6.6	22.1	52.1	55.3	23.2	0.0

$\{(NH_3)_3Cu\}_2O_2^{2+}$ (**3**)

Data in blue are with BS2, data in black are with BS1, data in green are extrapolated assuming changes computed with BS2 can be added to values computed with BS1.

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	-878.802 79	-878.800 73	-878.784 27	-878.784 94	-878.799 78	-878.802 84
MP2	-880.853 02	-880.844 28	-880.833 55	-880.864 20	-880.917 67	-880.951 11
CCSD	-880.826 56	-880.822 84	-880.804 74	-880.819 26	-880.851 40	-880.867 67
CCSD(T)	-880.943 63	-880.935 90	-880.913 14	-880.924 12	-880.959 53	-880.980 33
CR-CCSD(T)	-880.875 02	-880.869 32	-880.848 90	-880.866 77	-880.901 13	-880.918 99
CR-CC(2,3),A	-880.930 70	-880.924 85	-880.904 15	-880.917 15	-880.948 48	-880.964 34
CR-CC(2,3),D	-880.931 41	-880.925 66	-880.905 09	-880.920 75	-880.952 78	-880.969 31
HF	-878.904 67	-878.901 69	-878.885 09	-878.885 90	-878.901 20	-878.907 29
MP2	-881.182 87	-881.173 56	-881.163 06	-881.193 21	-881.246 66	-881.284 50
CCSD	-881.148 43	-881.143 58	-881.126 24	-881.139 86	-881.171 66	-881.192 07
CCSD(T)	-881.292 20	-881.281 62	-881.257 07	-881.269 44	-881.304 54	-881.329 53
CR-CCSD(T)	-881.205 50	-881.199 12	-881.180 74	-881.197 29	-881.231 78	-881.253 91
CR-CC(2,3),A	-881.261 19	-881.254 66	-881.235 99	-881.247 67	-881.279 13	-881.299 26
CR-CC(2,3),D	-881.261 89	-881.255 47	-881.236 93	-881.251 27	-881.283 43	-881.304 23
CAS(16,14)	-879.154 76					-879.312 59
PT2(16,14)	-881.304 61					-881.367 46
MSPT2(16,14)	-881.305 78					-881.367 47
bs-BLYP	-884.055 43	-884.041 73	-884.018 66	-884.015 05	-884.035 37	-884.049 84
bs-B3LYP	-884.275 44	-884.267 85	-884.248 04	-884.245 05	-884.262 87	-884.289 24

bs-mPWPW91	-884.418 62	-884.410 04	-884.390 31	-884.387 15	-884.405 03	-884.416 36
bs-mPW1PW91	-884.133 34	-884.130 70	-884.114 00	-884.111 16	-884.126 13	-884.156 88
bs-MPW1K	-883.946 14	-883.947 73	-883.933 06	-883.929 36	-883.940 86	-884.002 98
bs-TPSS	-884.186 36	-884.177 57	-884.158 13	-884.156 31	-884.176 12	-884.189 72
bs-TPSSh	-884.072 45	-884.065 98	-884.047 68	-884.046 10	-884.064 57	-884.082 46
BLYP/BS1d	-3770.768 27					-3770.761 90
BLYP/BS1t	-3770.783 60					-3770.776 28

	Isomer					
	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
HF	0.0	1.3	11.7	11.2	1.9	0.0
MP2	61.6	67.0	73.8	54.5	21.0	0.0
CCSD	25.8	28.1	39.5	30.4	10.2	0.0
CCSD(T)	23.0	27.9	42.2	35.3	13.1	0.0
CR-CCSD(T)	27.6	31.2	44.0	32.8	11.2	0.0
CR-CC(2,3),A	21.1	24.8	37.8	29.6	10.0	0.0
CR-CC(2,3),D	23.8	27.4	40.3	30.5	10.4	0.0
HF	1.6	3.5	13.9	13.4	3.8	0.0
MP2	63.8	69.6	76.2	57.3	23.7	0.0
CCSD	27.4	30.4	41.3	32.8	12.8	0.0
CCSD(T)	23.4	30.1	45.5	37.7	15.7	0.0
CR-CCSD(T)	30.4	34.4	45.9	35.5	13.9	0.0
CR-CC(2,3),A	23.9	28.0	39.7	32.4	12.6	0.0
CR-CC(2,3),D	26.6	30.6	42.2	33.2	13.1	0.0
CAS(16,14)	99.0					0.0
PT2(16,14)	39.4					0.0
MSPT2(16,14)	38.7					0.0
bs-BLYP	-3.5	5.1	19.6	21.8	9.1	0.0
bs-B3LYP	8.7	13.4	25.9	27.7	16.5	0.0
bs-mPWPW91	-1.4	4.0	16.3	18.3	7.1	0.0
bs-mPW1PW91	14.8	16.4	26.9	28.7	19.3	0.0
bs-MPW1K	35.7	34.7	43.9	46.2	39.0	0.0

bs-TPSS	2.1	7.6	19.8	21.0	8.5	0.0
bs-TPSSh	6.3	10.3	21.8	22.8	11.2	0.0
sumbs-BLYP	1.0	9.8	24.1	23.1	8.1	0.0
sumbs-B3LYP	22.9	27.8	39.5	37.6	22.5	0.0
sumbs-mPWPW91	3.1	8.6	20.9	19.8	6.0	0.0
sumbs-mPW1PW91	30.3	31.9	41.7	39.9	25.6	0.0
sumbs-mPW1K	53.9	52.4	60.7	59.6	45.2	0.0
sumbs-TPSS	7.1	12.8	24.8	23.0	8.0	0.0
sumbs-TPSSh	17.4	21.6	32.5	30.7	15.6	0.0
BLYP/DZ/allelec	-4.0					0.0
BLYP/TZ/allelec	-4.6					0.0

Triplet Electronic Energies (E_h) and $\langle S^2 \rangle$ Values (for Computing Sum-bs Energies)

$Cu_2O_2^{2+}$ **(0)**

	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
bs-BLYP	0.9579	0.9602	0.9894	0.9989	0.9418	0.7959
	-544.260 82	-544.258 34	-544.246 63	-544.234 66	-544.227 69	-544.216 95
bs-B3LYP	0.9925	0.9909	1.0023	1.0004	0.942	0.7741
	-544.332 28	-544.336 37	-544.327 72	-544.316 69	-544.307 55	-544.290 13
bs-mPWPW91	0.9667	0.9685	0.9925	0.9982	0.9432	0.8041
	-544.518 40	-544.518 33	-544.507 88	-544.496 71	-544.490 02	-544.478 90
bs-mPW1PW91	0.999	0.9971	1.005	1.0018	0.9478	0.7868
	-544.301 53	-544.308 88	-544.301 64	-544.291 08	-544.281 41	-544.262 13
bs-MPW1K	1.0055	1.0018	1.0079	1.0099	0.9673	0.8023
	-544.158 79	-544.171 02	-544.165 10	-544.153 44	-544.140 67	-544.116 28
bs-TPSS	0.9831	0.9842	1.0001	0.9956	0.9345	0.7878
	-544.211 41	-544.210 94	-544.200 77	-544.190 78	-544.185 63	-544.176 36
bs-TPSSh	0.9954	0.9951	1.0045	0.9963	0.935	0.7795
	-544.144 00	-544.146 60	-544.137 84	-544.128 20	-544.121 81	-544.108 89

$\{(NH_3)Cu\}_2O_2^{2+}$ (**1**)

	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
bs-BLYP	0.9499	0.9625	0.9951	0.9891	0.8793	0.6975
	-657.616 94	-657.620 94	-657.618 08	-657.610 72	-657.602 41	-657.593 09
bs-B3LYP	0.9902	0.9972	1.0066	0.9761	0.8547	0.4645
	-657.732 69	-657.738 73	-657.737 69	-657.731 48	-657.723 09	-657.712 10
bs-mPWPW91	0.9592	0.9698	0.9970	0.9889	0.8860	0.7157
	-657.905 01	-657.910 30	-657.908 60	-657.902 28	-657.895 03	-657.887 13
bs-mPW1PW91	0.9981	1.0031	1.0076	0.9763	0.8635	0.6700
	-657.659 62	-657.666 83	-657.666 93	-657.661 75	-657.654 16	-657.643 76
bs-MPW1K	1.0066	1.0105	1.0124	0.9824	0.8745	0.6688
	-657.497 00	-657.504 93	-657.506 13	-657.501 84	-657.494 30	-657.482 94
bs-TPSS	0.9764	0.9849	1.0024	0.9827	0.8744	0.7016
	-657.618 63	-657.624 09	-657.622 71	-657.617 03	-657.610 85	-657.604 28
bs-TPSSh	0.9918	0.9978	1.0057	0.9760	0.8632	0.6815
	-657.534 06	-657.540 33	-657.539 65	-657.534 33	-657.527 79	-657.519 87

$\{(NH_3)_2Cu\}_2O_2^{2+}$ (**2**)

	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
bs-BLYP	0.943	0.912	0.870	0.514	0.000	0.000
	-770.886 56	-770.853 89	-770.791 46	-770.773 53	-770.802 06	-770.809 15
bs-B3LYP	0.967	0.932	1.004	0.801	0.578	0.602
	-771.062 54	-771.032 14	-770.971 30	-770.955 05	-770.983 49	-771.012 33
bs-mPWPW91	0.947	0.918	0.893	0.549	0.046	0.000
	-771.213 53	-771.187 30	-771.129 96	-771.113 73	-771.047 22	-771.142 49
bs-mPW1PW91	0.978	0.947	1.008	0.619	0.059	0.697
	-770.957 76	-770.931 73	-770.874 59	-770.860 02	-770.887 42	-770.919 40
bs-MPW1K	0.999	0.977	1.020	0.653	0.872	0.883

	-770.789 81	-770.762 81	-770.705 64	-770.692 62	-770.721 14	-770.780 30
bs-TPSS	0.949	0.917	0.943	0.553	0.000	0.000
	-770.951 20	-770.924 73	-770.867 29	-770.852 93	-770.874 78	-770.891 17
bs-TPSSh	0.960	0.927	0.999	0.602	0.055	0.386
	-770.855 91	-770.829 57	-770.772 22	-770.758 30	-770.787 99	-770.807 41

$\{(NH_3)_3Cu\}_2O_2^{2+}$ (**3**)

	F = 0	*F* = 20	*F* = 40	*F* = 60	*F* = 80	*F* = 100
bs-BLYP	0.982	0.992	0.997	0.785	0.233	0.000
	-884.062 85	-884.049 33	-884.025 97	-884.018 24	-884.023 62	-883.969 18
bs-B3LYP	0.962	0.985	0.990	0.775	0.249	0.687
	-884.288 84	-884.280 86	-884.259 86	-884.253 61	-884.257 45	-884.269 68
bs-mPWPW91	0.983	0.994	0.998	0.811	0.295	0.000
	-884.425 99	-884.417 60	-884.397 58	-884.390 64	-884.394 34	-884.336 56
bs-mPW1PW91	0.969	0.989	0.992	0.805	0.340	0.766
	-884.148 63	-884.145 41	-884.127 44	-884.122 32	-884.124 88	-884.140 28
bs-MPW1K	0.985	0.998	0.993	0.826	0.375	0.923
	-883.968 31	-883.968 50	-883.952 61	-883.948 96	-883.951 09	-883.994 21
bs-TPSS	0.978	0.992	0.998	0.815	0.310	0.029
	-884.193 39	-884.184 74	-884.164 85	-884.159 33	-884.165 15	-884.111 37
bs-TPSSh	0.968	0.988	0.995	0.881	0.319	0.511
	-884.082 23	-884.075 63	-884.056 37	-884.051 29	-884.056 33	-884.057 78

Software

All DFT calculations were carried out using Gaussian03 [1]. All CASSCF, CASPT2, and MS-CASPT2 calculations were carried out using MOLCAS6.2 [2]. All CC and MBPT(2)=MP2 calculations performed in this work, except CR-CC(2,3), were carried out with the routines from the Michigan State University package of CC computer codes [3] that form an integral part of the GAMESS package [4]. The CR-CC(2,3) calculations were performed with the computer programs described in references [5] and [6] that form part of GAMESS as well.

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