

Dioxygen reactivity of new bispidine-copper complexes

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Supporting Information

1. Time-resolved low-temperature electronic spectra

Apart from the experiments described in the text, further time-dependent spectra were recorded in different solvents. These and some of the spectra not shown in the main part of the manuscript are presented and discussed here. In diethyl ether as the solvent, a spectrum similar to that in acetone (see main part of the paper) results from oxygenation of $[\text{Cu}^{\text{I}}(\text{L}^1)]^+$, with transitions at 615, 521 and 454 nm (Figure S1). The small shift to lower wavelengths is a not unexpected solvatochromism. After 10 min a new band at 371 nm starts to develop in this reaction in Et_2O , and this dominates the spectrum after 2 h; there is no isosbestic point in this reaction.

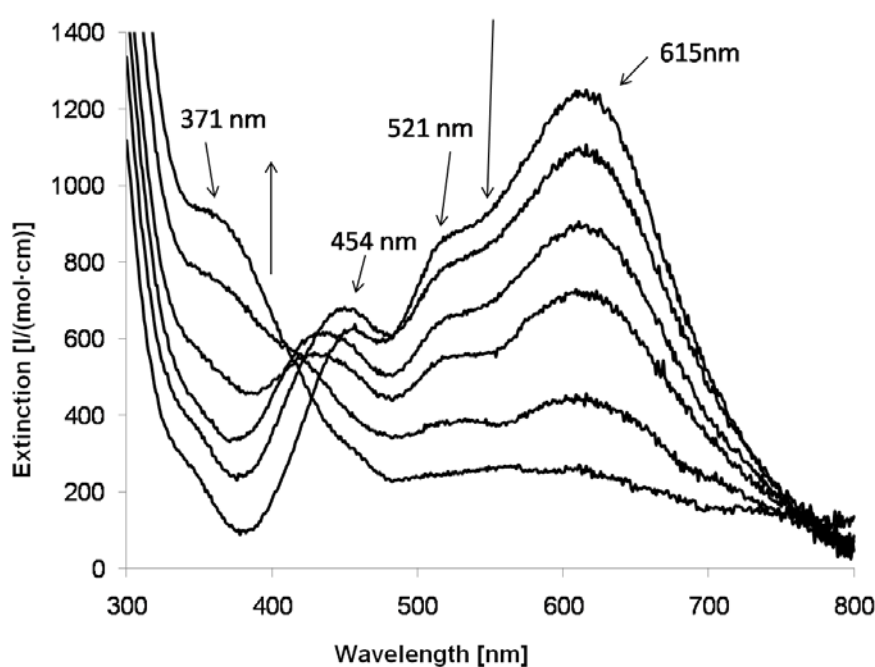


Figure S1. Oxidation of $[\text{Cu}^{\text{I}}(\text{L}^1)]^+$ (diethyl ether, -80°C , $c = 2.7 \cdot 10^{-4} \text{ M}$), recorded within 120 min; the values for extinction coefficients are based on 100% conversion.

Mononuclear $\text{Cu}^{\text{II}}-\eta^1$ -hydroperoxo compounds have transitions at approx. 350 nm. It is conceivable that a short-lived and therefore, in the experiments described here, undetected $\text{Cu}^{\text{II}}-\eta^1$ -superoxo compound is the precursor for $[\text{Cu}^{\text{II}}(\text{L}^1)(\text{OOH})]^+$. The more likely interpretation is that the *trans*- $[(\text{Cu}^{\text{II}}(\text{L}^1))_2\text{O}_2]^{2+}$ precursor is protonated and then splits into $[\text{Cu}^{\text{II}}(\text{L}^1)\text{OOH}]^{2+}$ and $[\text{Cu}^{\text{II}}(\text{L}^1)]^{2+}$. The identity of this putative hydroperoxo $[\text{Cu}^{\text{II}}(\text{L}^1)\text{OOH}]^+$ complex was further established by reaction of $[\text{Cu}^{\text{II}}(\text{L}^1)]^{2+}$ with H_2O_2 under basic conditions in MeOH at -80°C (ligand exchange), because this reproduced the high-energy transition at 357 nm, and also showed several weak dd-transitions at lower energy (Figure S2).

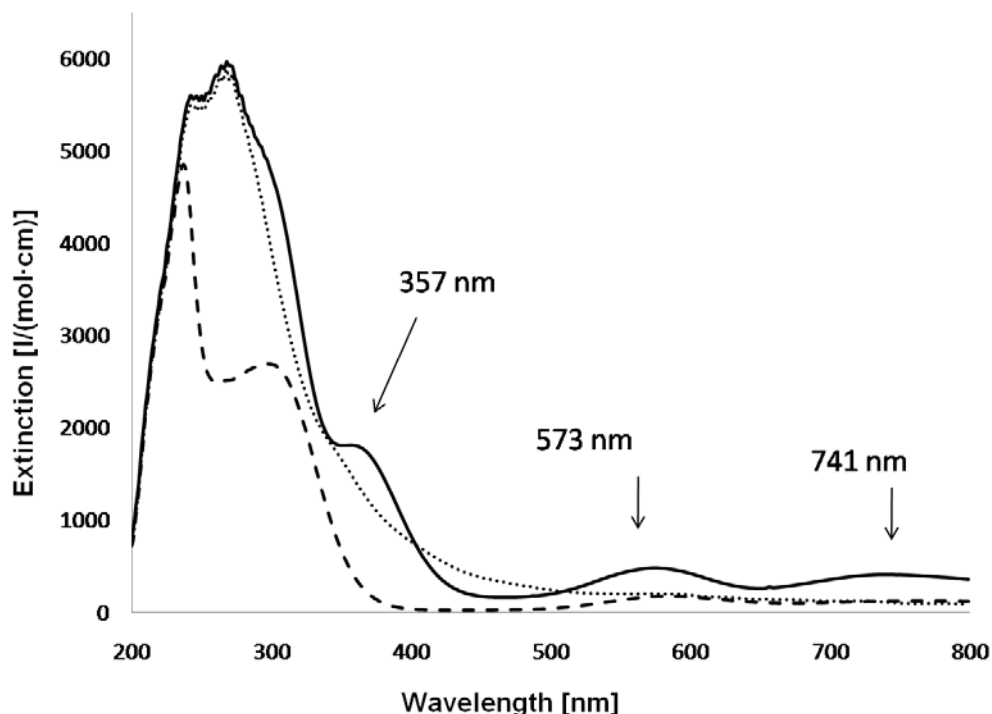


Figure S2. Product of the reaction of $[\text{Cu}^{\text{II}}(\text{L}^1)]^{2+}$ with H_2O_2 (MeOH, -80°C , $c = 5.5 \cdot 10^{-4} \text{ M}$); dashed line: $[\text{Cu}^{\text{II}}(\text{L}^1)]^{2+} + \text{NEt}_3$; full line: $[\text{Cu}^{\text{II}}(\text{L}^1)]^{2+} + \text{H}_2\text{O}_2 + \text{NEt}_3$; dotted line: spectrum of the hydroperoxo complex after warming up to ambient temperature; the values for extinction coefficients are based on 100% conversion.

In THF as the solvent (Figure S3), there is formation of an additional and new complex. Two of the three bands of *trans*- $[(\text{Cu}^{\text{II}}(\text{L}^1))_2\text{O}_2]^{2+}$, observed in acetone, are shifted in THF to 635 and 524 nm. The third transition (expected at around 450 nm) is partially obscured by a new strong band at 414 nm, which forms immediately and persists; its first signs of decay only occur after more than 1.5 h). The new oxygenated species, which coexists with the putative *trans*- $[(\text{Cu}^{\text{II}}(\text{L}^1))_2\text{O}_2]^{2+}$ peroxy-complex, is tentatively assigned to a mononuclear η^1 -superoxo Cu^{II} complex.

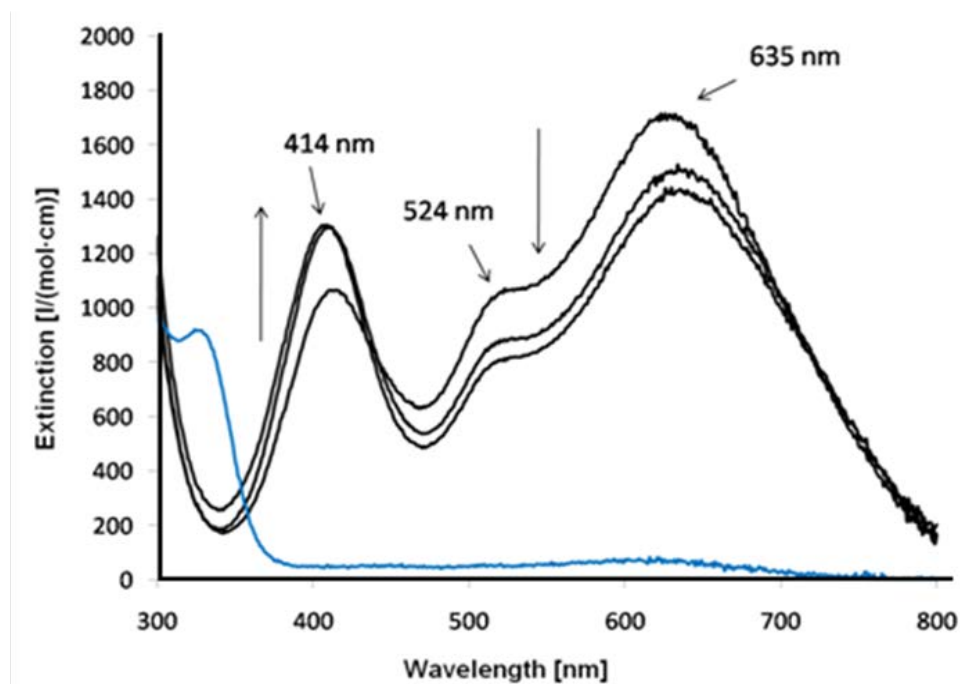


Figure S3. Oxidation of $[\text{Cu}^{\text{I}}(\text{L}^1)]^+$ (THF, -80°C , $c = 2.7 \cdot 10^{-4} \text{ M}$), recorded within 90 min; blue (for comparison): $[\text{Cu}^{\text{I}}(\text{L}^1)]^+$; black: oxygenated complex; the values for extinction coefficients are based on 100% conversion.

An intensely green solution is obtained at -120°C in MeTHF (see Figure S4). In addition to the two bands at 613 and 515 nm, assigned to $\text{trans}-[(\text{Cu}^{\text{II}}(\text{L}^1))_2\text{O}_2]^{2+}$, there again is a strong additional transition, in this solvent at 452 nm, which we also assign to $[\text{Cu}^{\text{II}}(\text{L}^1)\text{O}_2]^+$, *i.e.* a mononuclear η^1 -superoxo- Cu^{II} complex (solvatochromism, see experiment in THF, Figure S3). Moreover, there is another new transition at 340 nm, which is due to a third complex, probably a hydroperoxo complex ($[\text{Cu}^{\text{II}}(\text{L}^1)\text{OOH}]^{2+}$, see also experiment in diethyl ether above). This putative hydroperoxo complex forms relatively slowly (see below for further characterization of this species). The changing transition energies are proposed to be due to the change in solvent and temperature.

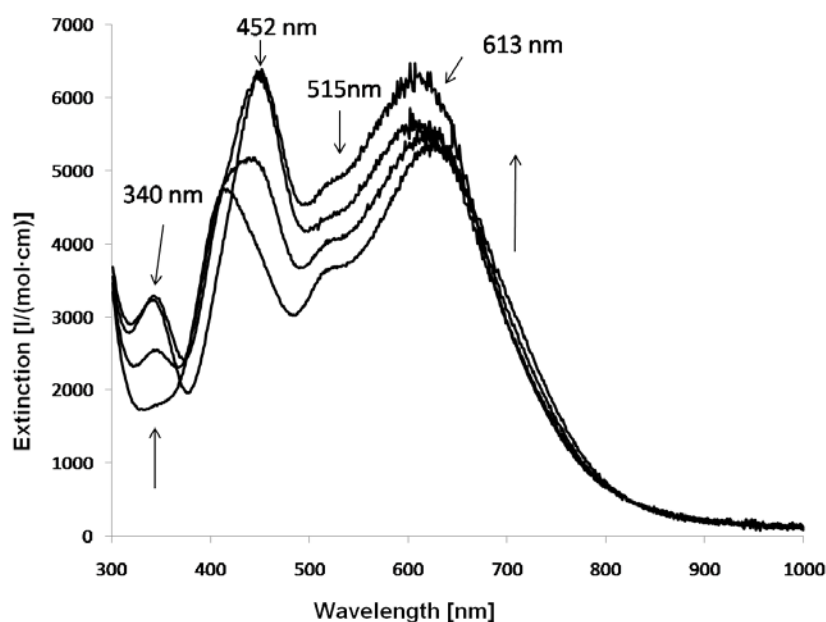


Figure S4. Oxidation of $[\text{Cu}^{\text{I}}(\text{L}^1)]^+$ (MeTHF, -120°C , $c = 4.5 \cdot 10^{-4} \text{ M}$), recorded within 85 min; the values for extinction coefficients are based on 100% conversion.

The ligand L^3 with its *meta*-xylene bridge provides the possibility to form both *trans*-peroxo complexes ($\text{Cu} : \text{O}_2$ ratio of 2 : 1) and complexes which are oxygenated at both copper centers ($\text{Cu} : \text{O}_2$ ratio of 1 : 1). The electronic spectrum generated at -80°C in acetone ($c = 1.3 \cdot 10^{-3} \text{ M}$) has two bands at 334 nm and 406 nm, as well as a weak band at 637 nm (see Figure S5). The oxygenation product is not stable, *i.e.* the band at 406 nm decays within 60 min at -80°C . The assignment of the spectra to specific oxygenated complexes is not unambiguous. The UV-vis spectrum of oxygenated $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}$ at -120°C in MeTHF has three bands at 412 nm, 563 nm and 678 nm (see Figure S6). These electronic transitions are typical for an *end-on* superoxo complex. Although the structure of $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}$ allows for both *trans*-peroxo and *end-on* superoxo, the *end-on* superoxo complex seems to be preferred due to the steric strain induced by a potential *trans*-peroxo bridge. After warming to -80°C the three bands decrease in intensity, and a new band at 398 nm is formed. This is very similar to the spectrum observed in acetone. A solution of the oxygenated complex (-120°C) was allowed to warm up to ambient temperature and was then analyzed by ESI mass spectrometry. Interestingly, a partially oxidized ligand was characterized (see Figure S10). The main fragment is a bispidine-derived aldehyde, which is proposed to be formed by attack at the CH-benzylic position near to the *meta*-xylene group (see Scheme 3 in the main text). This is not an unexpected reaction, and similar pathways have been described before. However, at this time we cannot be sure about

what species is effecting the oxidative N-dealkylation reaction, a superoxo, $(\text{Cu}^{\text{II}})_2$ -peroxo or another $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}/\text{O}_2$ derived species.

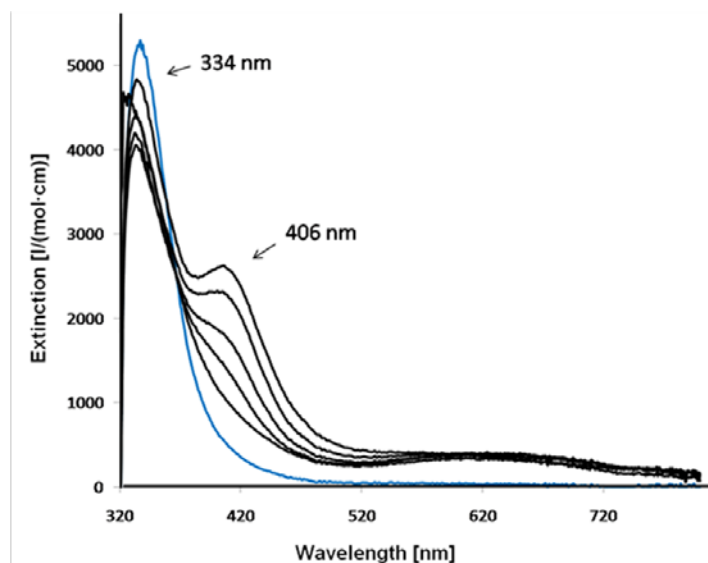


Figure S5. Oxidation of $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}$ (acetone, -80°C , $c = 1.3 \cdot 10^{-3} \text{ M}$), recorded over 60 min, while warming to ambient temperature (decrease of the 406 nm band); blue (for comparison): $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}$; black: oxygenated complex; the values for extinction coefficients are based on 100% conversion.

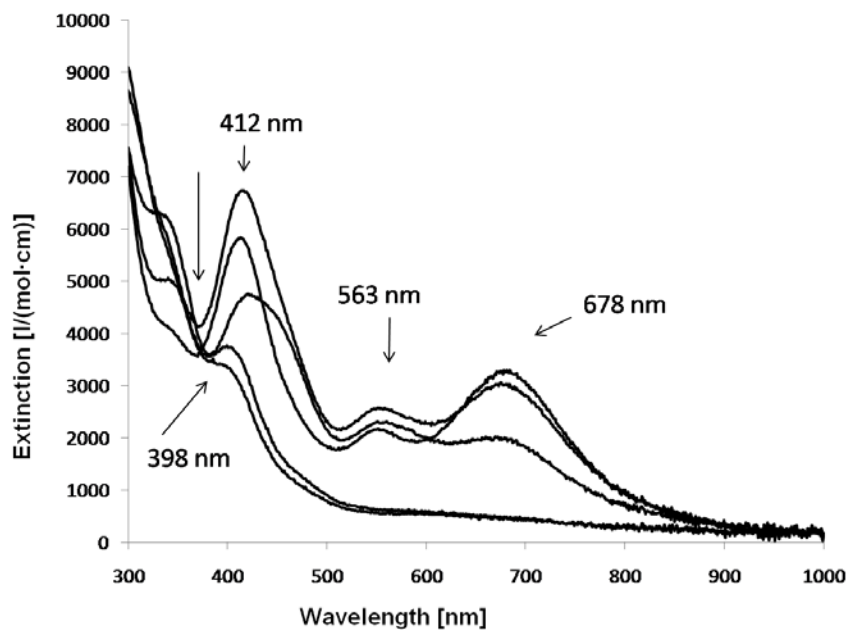


Figure S6. Oxidation of $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}$ (MeTHF, -120°C , $c = 1.0 \cdot 10^{-4} \text{ M}$), recorded for 120 min, while warming up to -80°C after 10 min; the values for extinction coefficients are based on 100% conversion.

2. Reversible dioxygen binding

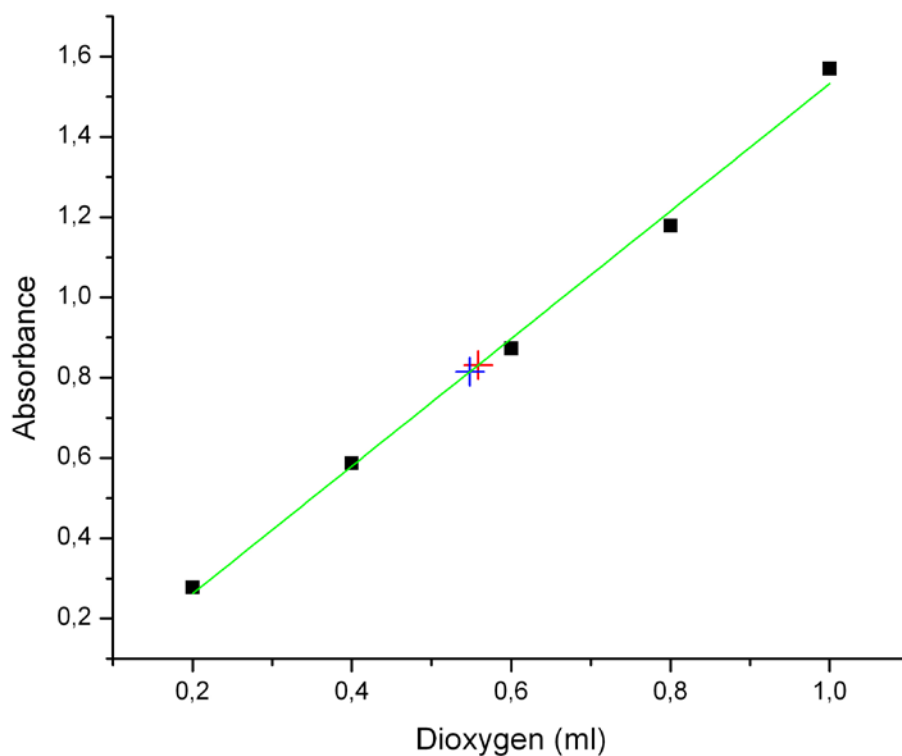


Figure S7. Determination of molecular dioxygen recovered from $[\text{Cu}^{\text{II}}(\text{L}^2)\text{O}_2]^+$, THF, $c = 1.0 \cdot 10^{-3}$ mol/l, $\lambda = 400$ nm. The plot shows the amount of added oxygen vs. the spectrophotometrically determined absorption of a basic pyrogallol solution. Red and blue crosses represent measurements 1 and 2, respectively (75% and 76% recovery).

3. EPR spectroscopy

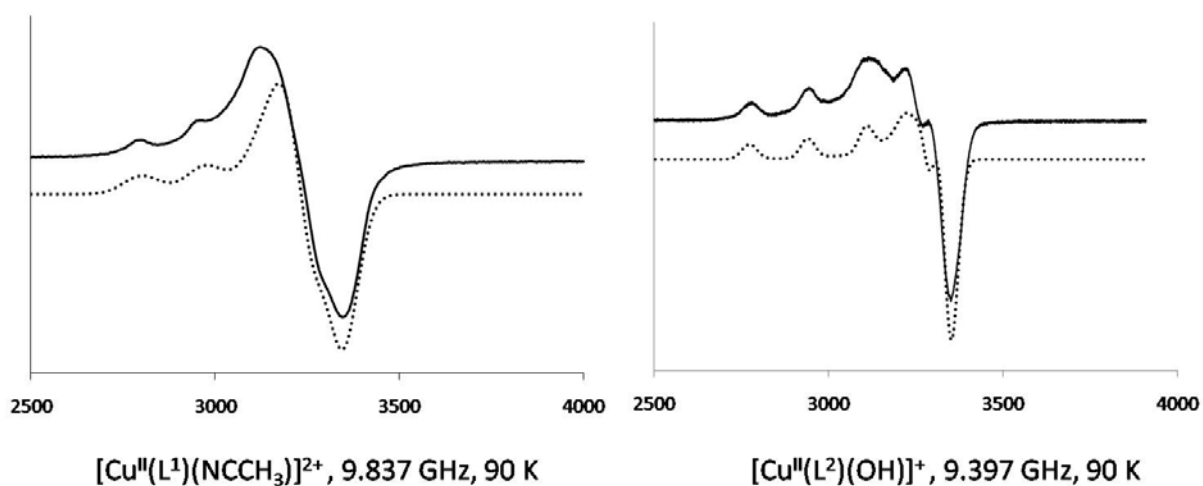


Figure S8. EPR-Spectra of $[\text{Cu}^{\text{II}}(\text{L}^1)(\text{NCCH}_3)]^{2+}$ (left) and $[\text{Cu}^{\text{II}}(\text{L}^2)(\text{OH})]^+$ (right); frozen solutions (90K, MeCN/toluene for $[\text{Cu}^{\text{II}}(\text{L}^1)(\text{NCCH}_3)]^{2+}$, MeOH for $[\text{Cu}^{\text{II}}(\text{L}^2)(\text{OH})]^+$); continuous lines: experimental spectra, dotted lines: X-Sophe⁶⁴ simulations.

4. Electrochemistry

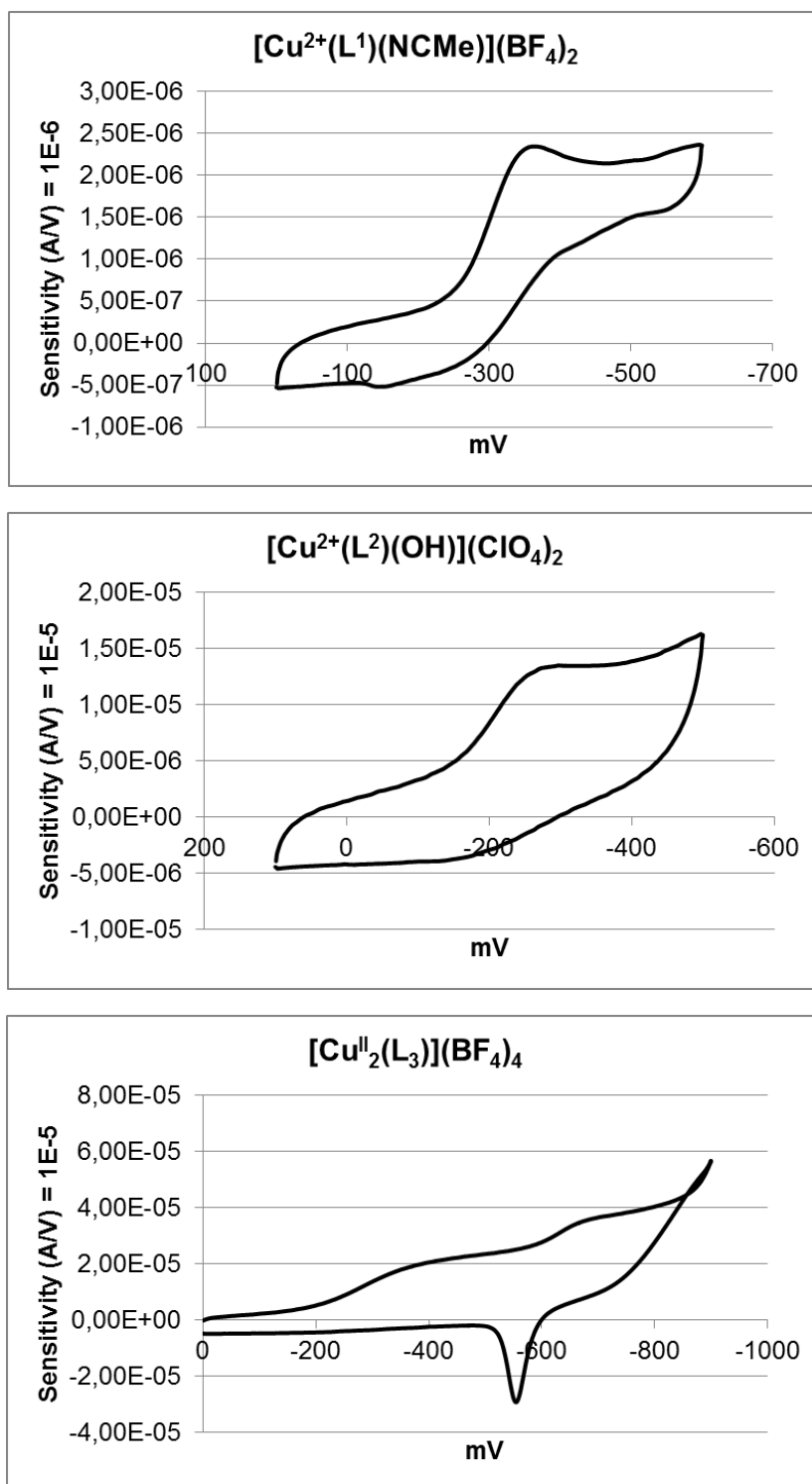


Figure S9. Electrochemical traces for $[\text{Cu}^{\text{II}}(\text{L}^1)(\text{NCMe})](\text{BF}_4)_2$, $[\text{Cu}^{\text{II}}(\text{L}^2)(\text{OH})](\text{ClO}_4)_2$ and $[\text{Cu}^{\text{II}}_2(\text{L}^3)](\text{BF}_4)_4$, solvent: MeCN, 100mV/s.

5. MS spectrometry

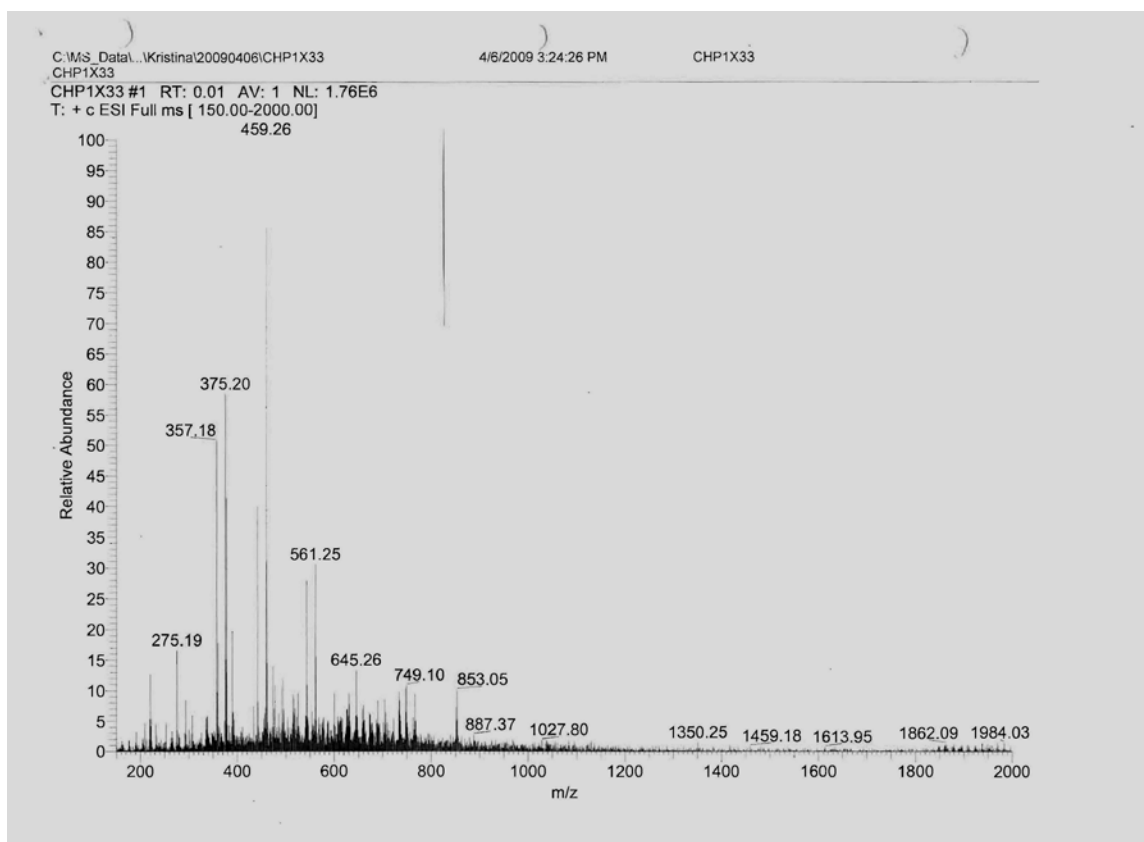


Figure S10. ESI-MS of a solution of $[\text{Cu}^{\text{I}}_2(\text{L}^3)]^{2+}$, oxygenated in MeTHF at -120° and then allowed to warm to ambient temperature, before recording the spectrum. The signal at 459.26 corresponds to L^3 with one cleaved bispidine unit, see text.

6. DFT calculations

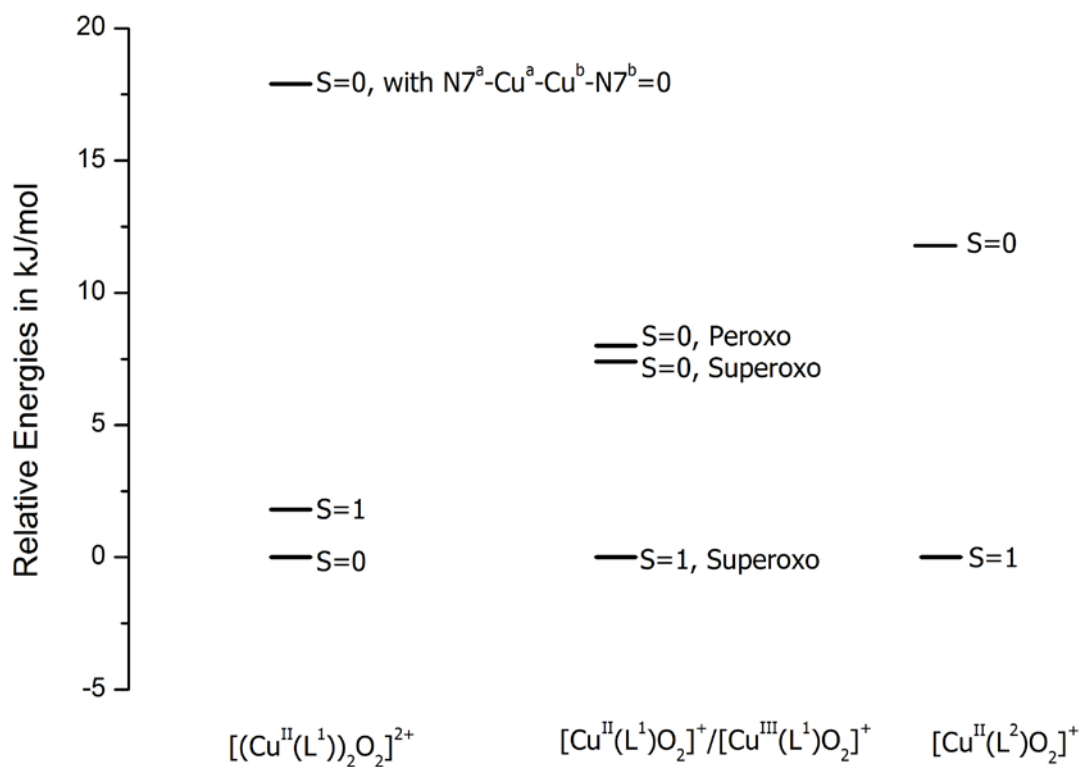


Figure S11. Relative energies (kJ/mol; calculated with the B2 basis set), for all relevant spin states of the oxygenated complexes $[(\text{Cu}^{\text{II}}(\text{L}^1))_2\text{O}_2]^{2+}$, $[\text{Cu}^{\text{II}}(\text{L}^1)\text{O}_2]^+ / [\text{Cu}^{\text{III}}(\text{L}^1)\text{O}_2]^+$ and $[\text{Cu}^{\text{II}}(\text{L}^2)\text{O}_2]^+$ (as usual, S is the spin state considered; note that more appropriately, the nomenclature of these states should be $M_S = 0, 1$).

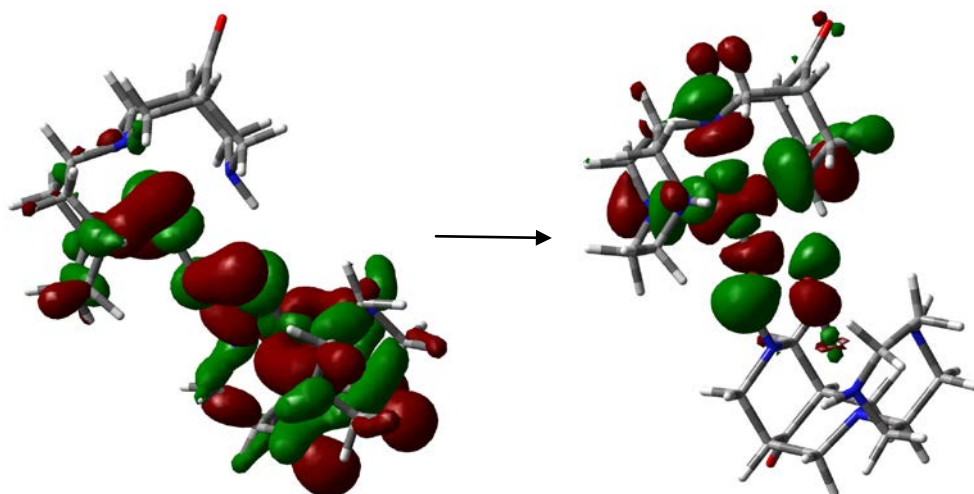
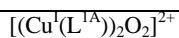


Figure S12. The charge transfer transition involved at 490 nm of $[(\text{Cu}^{\text{II}}(\text{L}^{\text{1A}}))_2\text{O}_2]^{2+}$.

Table S1: Key structural parameters and spin densities of all optimized oxygen adducts, computed with at the B2 level (kJ/mol).

Complex	Structural parameters				Spin Densities		
	Cu-O _a	Cu-O _b	O _a -O _b	Cu-N _{avg}	Cu	O _a	O _b
[Cu ^{II} (L ¹)O ₂] ⁺	1.97	1.36	-	2.15	0.45	-0.17	-0.55
[Cu ^{II} (L ¹)O ₂ H] ⁺	1.91	-	1.53	2.40	0.50	0.22	-0.01
[(Cu ^{II} (L ¹)) ₂ O ₂] ⁺	1.94	1.94	1.52	2.17	0.46	0.0	0.2
[Cu ^{II} (L ²)O ₂] ⁺	1.96	-	1.37	2.19	0.38	0.67	0.78
[(Cu ^{II} (L ²)) ₂ O ₂] ⁺	1.98	1.96	1.48	2.22	0.45	0.0	0.19
[(Cu ^{II} (tmpa)) ₂ O ₂] ⁺	1.96	1.95	1.48	2.20	0.48	0.21	-0.2

Optimized Coordinates for complexes mentioned in the paper:



S=0 (Open-Shell Singlet)				S=1			
C	0.6194101418	3.9089584430	-0.8449656400	C	0.1646520146	3.9663940868	-1.2972050826
C	-0.1058403266	5.1258193177	-0.2025537991	C	-0.4697286140	5.1476448503	-0.5090794336
C	0.6726913648	5.5265146046	1.0401935493	C	0.5528185525	5.6312168208	0.5068769195
C	0.6611992601	4.3915758837	2.0512009267	C	0.8657486291	4.5230464911	1.4990540888
C	1.3768400840	3.1702576693	1.4172578239	C	1.4918213644	3.3361633933	0.7240365172
C	-1.5754236919	4.8519503472	0.2134607445	C	-1.7743792258	4.7903912783	0.2528667079
C	-0.8049644164	4.1028770359	2.4495234433	C	-0.4380520803	4.1468010580	2.2396279430
C	-3.1063904226	3.4593300500	1.6736384209	C	-2.8036558303	3.3359445553	2.0552724452
C	-3.0975373635	2.3628026230	2.7649001678	C	-2.4486574103	2.2745836316	3.1258234175
C	-3.0154247266	0.0601667555	1.7426629650	C	-2.3922008971	-0.0491229784	2.1378513258
C	-3.7166891133	0.4477682613	0.4124945429	C	-3.4852198720	0.2579645174	1.0837688131
C	-3.8940245522	2.9612151353	0.4486988412	C	-3.8295022737	2.7515334865	1.0697136902
Cu	-1.1261995319	1.9560025164	0.3992901738	Cu	-1.1030226870	1.9332763969	0.3289135906
N	0.7267114598	2.7779716256	0.1296838295	N	0.5837528816	2.8698331423	-0.3672860411
N	-1.6803664182	3.7746231481	1.2650633037	N	-1.5478551922	3.7314153530	1.3043484974
N	-2.2694159117	1.2058444692	2.3211115323	N	-1.6464569870	1.1781205055	2.5129779372
N	-3.2289509736	1.7524589726	-0.1346850082	N	-3.2507170934	1.5567135628	0.3752907746
O	1.2353238442	6.6106079061	1.2044490867	O	1.0558952174	6.7558565983	0.5268263437
O	-0.6871930991	0.2662494565	-0.4423499097	O	-0.7463330509	0.2670172422	-0.5883013964
O	0.7914967995	-0.0007124897	-0.2433922328	O	0.7555920905	0.0537778345	-0.4590714861
C	-0.6494360425	-3.0334921812	-2.3170802939	C	-0.2851999007	-2.8573346617	-2.6927618321
C	0.0814153108	-4.4043702309	-2.3756811313	C	0.4478814064	-4.2285002908	-2.6782923254
C	-0.6046084555	-5.3378875427	-1.3914490382	C	-0.4424635812	-5.2198907658	-1.9473073775
C	-0.4687294772	-4.7965897251	0.0223845764	C	-0.6378617499	-4.7812958281	-0.5046399197
C	-1.1979660739	-3.4277908317	0.0876970229	C	-1.3632868074	-3.4099134498	-0.5093754659

C	1.5895835867	-4.3432860715	-2.0153750994	C	1.8324604896	-4.2125669860	-1.9776582576
C	1.0355535375	-4.7113564007	0.3761309597	C	0.7442696232	-4.7417296766	0.1885398998
C	3.2893205859	-3.7605481023	-0.2320594122	C	3.0680925646	-3.7871419106	0.1938697011
C	3.4179193401	-3.3117220550	1.2411565098	C	2.8479671420	-3.4046825546	1.6775851043
C	3.3534927945	-0.8002154502	1.4214146072	C	2.6938178913	-0.9035801503	1.9722314869
C	3.8423738770	-0.4715951078	-0.0173095827	C	3.6177190616	-0.5752872666	0.7694514114
C	3.9718693435	-2.7262575608	-1.1466786129	C	3.9657715597	-2.7339232856	-0.4787484024
Cu	1.2410714112	-1.8739248599	-0.4599132574	Cu	1.1536198380	-1.8430279208	-0.4151238666
N	-0.6437075994	-2.4796216265	-0.9257740785	N	-0.5964741657	-2.4019868690	-1.3007210125
N	1.8210719333	-3.8720430079	-0.6014215438	N	1.7298554999	-3.8431839509	-0.5170460107
N	2.6089721232	-2.0829654742	1.4730628613	N	1.9824187274	-2.1933387318	1.7759710758
N	3.2780917008	-1.4031109195	-1.0425770941	N	3.2970267821	-1.3958406691	-0.4386985300
O	-1.1920904624	-6.3783756245	-1.6928157377	O	-0.9396841447	-6.2293402801	-2.4493355186
H	0.0802009829	3.5521476862	-1.7281121082	H	-0.5438386324	3.5512097723	-2.0208910444
H	1.6183254568	4.2347264861	-1.1685280254	H	1.0303717187	4.3491593876	-1.8559069808
H	-0.1013865926	5.9564741520	-0.9148358189	H	-0.6947983726	5.9579570771	-1.2090330052
H	1.2067591511	4.7003420883	2.9485866901	H	1.5869245780	4.8902237173	2.2362660816
H	2.4316410153	3.4334256819	1.2509663697	H	2.4567030857	3.6602303093	0.3076110391
H	1.3445745631	2.3079375267	2.0914391942	H	1.6784678976	2.4894886419	1.3929222203
H	-2.0208828465	5.7845507463	0.5928361328	H	-2.1751745404	5.7012254331	0.7239246118
H	-2.1439180489	4.5440126613	-0.6661037701	H	-2.5176606736	4.4282193314	-0.4599692331
H	-0.8158150420	3.2579043476	3.1379143245	H	-0.2234020464	3.3209658131	2.9174506396
H	-1.2165507909	4.9766049152	2.9781278176	H	-0.7729412278	5.0037930024	2.8444169080
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H	-4.9211688415	2.7269796318	0.7584060288	H	-4.7374067269	2.4768487806	1.6231725358
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H	1.1449096964	1.9180736184	-0.2641360024	H	0.9735297913	2.0435204223	-0.8423248521
H	-1.6494805053	0.8811751764	3.0593833454	H	-0.8366726674	0.9398058601	3.0800836175
H	-3.3144987195	1.7460587575	-1.1497140117	H	-3.5987649685	1.4904096000	-0.5797600245
H	-0.1711233207	-2.3037610606	-2.9780663229	H	0.3253060550	-2.0877541892	-3.1753191059
H	-1.6817299085	-3.1772776668	-2.6667037756	H	-1.2108573035	-2.9659827412	-3.2754285606
H	-0.0118980866	-4.8117315694	-3.3869144810	H	0.5911248937	-4.5631328282	-3.7101762836
H	-0.9467858575	-5.4887247512	0.7227886147	H	-1.2622663117	-5.5147873242	0.0151925684
H	-2.2702724683	-3.5968157015	-0.0881753339	H	-2.3683654427	-3.5486602145	-0.9335420739
H	-1.0832938637	-2.9774704252	1.0795388569	H	-1.4772497309	-3.0322601047	0.5126402224
H	2.0318722795	-5.3423784338	-2.1496289070	H	2.2969710093	-5.2055860069	-2.0776124011
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H	1.1322240684	-4.2734214963	1.3695574900	H	0.6103739542	-4.3817372721	1.2086224829
H	1.4574976097	-5.7276073363	0.4099703651	H	1.1535426119	-5.7625341670	0.2403449433
H	3.7845117251	-4.7356201480	-0.3575385465	H	3.5621675307	-4.7696400819	0.1444724337
H	4.4794815969	-3.1361727979	1.4635302361	H	3.8263092229	-3.2317328028	2.1457375402
H	3.0964769436	-4.1000145239	1.9245545981	H	2.3923796634	-4.2268692248	2.2326097858
H	4.2111110112	-0.8086238897	2.1092920370	H	3.2876968856	-0.9055324505	2.8977673405
H	2.6553633226	-0.0280907479	1.7517089869	H	1.9188560082	-0.1375723180	2.0544703673
H	3.5183912750	0.5344692549	-0.2901355090	H	3.4939101917	0.4748437017	0.4972437935
H	4.9390709347	-0.4941928629	-0.0632506544	H	4.6708618565	-0.7239977109	1.0419455302
H	5.0266519961	-2.6362001439	-0.8548540847	H	4.9307400882	-2.7033385058	0.0447561174
H	3.9643511299	-3.0462849007	-2.1901751949	H	4.1831979399	-2.9912655179	-1.5167441626
H	-1.0592010319	-1.5301332148	-0.8622227925	H	-1.0237180895	-1.4573158989	-1.2663130894
H	2.0760021414	-2.1403906820	2.3374820776	H	1.2643407084	-2.3080492026	2.4875895391
H	3.2629971800	-0.9323368475	-1.9458910205	H	3.4982181671	-0.8588282667	-1.2800956542

S=0 (Open-Shell Singlet)

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C	0.1037210181	4.4692740967	2.9008509753	C	0.2327755397	4.4345933409	2.8610161034
C	-0.4303984634	3.6868161505	4.0868961214	C	-0.3207067465	3.7161469131	4.0780922883
C	-1.1029057711	2.4169497830	3.5979092509	C	-1.0903638668	2.4845420471	3.6356383243
C	-0.0321529675	1.5415721337	2.9053029606	C	-0.0980736527	1.5234321817	2.9407058571
C	-1.0764480099	4.8444805210	1.9803816380	C	-0.9449759119	4.8678868552	1.9619650771
C	-2.2843891501	2.8055322557	2.6791435374	C	-2.2655076984	2.9292735869	2.7346018553
C	-2.9949909823	4.0497412394	0.6046966954	C	-2.9414456173	4.1605149563	0.6430668015
C	-3.8359385434	2.8247688369	0.2217439244	C	-3.8497153981	2.9743809051	0.2870060416
C	-2.9714078327	2.0245226452	-1.9521092485	C	-3.0504937549	2.0792098982	-1.8786676548
C	-1.9450190773	3.0792674840	-2.4346930502	C	-2.0021784315	3.0966202514	-2.3959414441
C	-2.4364829160	4.7510320921	-0.6517445595	C	-2.3685213358	4.8156810433	-0.6304550520
Cu	-0.7663883718	2.3773716268	0.1633585894	Cu	-0.8050529004	2.3664757891	0.1919944953
N	0.6719848210	2.2499746351	1.7734225702	N	0.6284537375	2.1557506605	1.7766504103
N	-1.8446892637	3.6394336533	1.5007902458	N	-1.8005523615	3.7059356665	1.5294869668
N	-2.9895800408	1.8088218934	-0.4725060791	N	-3.0674247389	1.9022289472	-0.3948363538
N	-1.3831301623	3.9221336350	-1.3352446838	N	-1.3726854760	3.9242566067	-1.3208017406
O	-0.3268666209	4.0253024942	5.2674073728	O	-0.1608919715	4.0719800660	5.2470153754
O	-0.0741858919	1.0113314898	-1.0257629829	O	-0.2785127151	0.9495579243	-1.0677121844
H	1.5532065862	4.1170517481	1.3033943555	H	1.6199083410	3.9499163000	1.2417228088
H	2.0229157232	3.4742955323	2.8859692586	H	2.0819638656	3.3150707236	2.8304824193
H	0.5742941488	5.3913088096	3.2570922153	H	0.7724759443	5.3307575246	3.1838864451
H	-1.5008802559	1.8645763754	4.4554521387	H	-1.5019963635	1.9794860877	4.5155956043
H	0.7126151641	1.2436839039	3.6605609230	H	0.6427269980	1.1928662085	3.6860789964
H	-0.4743329862	0.6297915333	2.4912229788	H	-0.6115124941	0.6343175859	2.5603123901
H	-1.7587899979	5.5193667552	2.5209356531	H	-1.5657686901	5.5982417289	2.5048769808
H	-0.6895362203	5.3844640284	1.1160940322	H	-0.5462740894	5.3632734842	1.0767879138
H	-2.7512797468	1.8927040324	2.3101465213	H	-2.7994663563	2.0413082890	2.3974204217

H	-3.0333261780	3.3581769990	3.2680394487	H	-2.9628900684	3.5416374629	3.3279330904
H	-3.6395236923	4.7631528438	1.1437527210	H	-3.5423721887	4.9129452903	1.1797144367
H	-4.6673667803	3.1534098933	-0.4191061220	H	-4.6682488796	3.3375646713	-0.3522441909
H	-4.2953896116	2.3730673908	1.1022278462	H	-4.3252555966	2.5637844715	1.1792002724
H	-3.9842381313	2.2899297427	-2.2902657640	H	-4.0583426684	2.3577943908	-2.2218585197
H	-2.7185614690	1.0701578379	-2.4153615027	H	-2.8156535491	1.1068604927	-2.3133601018
H	-1.0930976915	2.5695135765	-2.8881787779	H	-1.1854666599	2.5529089723	-2.8739939775
H	-2.4031011146	3.7245190145	-3.2003008209	H	-2.4585566971	3.7562325949	-3.1502087790
H	-3.2654401769	4.9646586811	-1.3403796701	H	-3.1972266968	5.0631943284	-1.3080000417
H	-2.0045177575	5.7187048320	-0.3910535746	H	-1.8827941033	5.7630775879	-0.3904850002
O	-0.1138988620	-0.3265772899	-0.3666235355	O	-0.3160246118	-0.3967323053	-0.4810081116
C	-0.6088888761	-4.2362880625	-0.3735362371	C	-0.5454350674	-4.3586453703	-0.4678556245
C	0.2275165700	-5.2002993818	-1.2462822849	C	0.3946029594	-5.2753328378	-1.2842089454
C	1.2923295045	-5.8376391307	-0.3711032387	C	1.4539488025	-5.8307857446	-0.3490281782
C	2.2181199290	-4.7634235339	0.1694680266	C	2.2798911498	-4.6911995259	0.2186977545
C	1.3942460057	-3.8040285293	1.0538067519	C	1.3498925654	-3.7836680592	1.0528236647
C	0.9277053340	-4.5166961719	-2.4419596345	C	1.1064357921	-4.5620620768	-2.4552105169
C	2.9040385102	-4.0582534866	-1.0186072832	C	2.9737695329	-3.9537328275	-0.9453509195
C	2.6256237128	-2.8212937287	-3.1708177395	C	2.7184889963	-2.7641856585	-3.1269733585
C	3.6540785001	-1.7963565422	-2.6523405851	C	3.6554382169	-1.6737788687	-2.5746481876
C	2.5899166181	0.4429704303	-2.3524937044	C	2.4468843334	0.5007011408	-2.3770439473
C	1.4694933489	0.2407606520	-3.4000101120	C	1.3763815463	0.2176073441	-3.4593389343
C	1.5912935459	-2.1409003814	-4.0795492463	C	1.6901947577	-2.1574964233	-4.0952707693
Cu	0.9071536174	-1.7921856090	-1.1734306567	Cu	0.8502061632	-1.8237225863	-1.2149844325
N	0.2207243936	-3.1848113794	0.3311558689	N	0.1755595026	-3.2497721413	0.2670132588
N	1.9186980456	-3.4707879905	-1.9990235256	N	2.0011819146	-3.4469664896	-1.9814837936
N	2.9955157048	-0.8385622123	-1.7173866978	N	2.8937561260	-0.7410861548	-1.6928337156
N	0.8069948975	-1.1054805523	-3.3259989715	N	0.8024779357	-1.1673318724	-3.3995050005
O	1.3948904804	-7.0437320057	-0.1412637435	O	1.6209124745	-7.0241812194	-0.0922554315
H	-1.3605775683	-3.7163319487	-0.9767669310	H	-1.2954876520	-3.8930676306	-1.1159022235
H	-1.1435361010	-4.8308324093	0.3831159740	H	-1.0808715215	-4.9801358137	0.2662767208
H	-0.4363707613	-5.9790811596	-1.6349376174	H	-0.1970935789	-6.1009694566	-1.6922305777

H	2.9922647796	-5.2284253533	0.7883280017	H	3.0531372800	-5.0971081522	0.8790350076
H	1.0207062365	-4.3644787460	1.9245081010	H	0.9734541181	-4.3632059941	1.9099171304
H	2.0213679442	-2.9883615816	1.4290950588	H	1.9022580324	-2.9255647428	1.4505552677
H	1.4401883922	-5.2801091700	-3.0481398989	H	1.6978527914	-5.2977509596	-3.0228560370
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H	3.5285180797	-3.2553177725	-0.6268062950	H	3.5228851257	-3.1055101508	-0.5356609955
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H	2.1962289971	1.0797074981	-1.5614445570	H	1.9939139384	1.1362599750	-1.6168843174
H	0.6999045156	0.9843678578	-3.2007215367	H	0.5520483760	0.9095293028	-3.2924453845
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C	1.8354400070	1.4244633881	1.3257530489	C	1.7205312196	1.2398360119	1.3276773776
H	1.4532876064	0.4917192931	0.9090413053	H	1.2686501576	0.3317978817	0.9253850139
H	2.3776273325	1.9710137792	0.5520939161	H	2.2936149629	1.7349386387	0.5414303537
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C	-0.6394882227	-2.4809936367	1.3324647639	C	-0.7817851941	-2.5949014616	1.2119077609
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C	-0.6016193304	-1.0066697923	-3.8100699761	C	-0.5845722008	-1.1695579998	-3.9521613706
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C	-0.2751037825	4.7721797950	-1.8669585248	C	-0.2393566396	4.7128561623	-1.8922937411
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C	-1.7123179133	1.0801885334	1.8624699138
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C	-3.4932655527	-3.1981190514	1.4467533974
C	-4.2828760622	-2.9609870194	0.1339926467
C	-4.7088451717	-0.4776301300	-0.0020099969
Cu	-1.8662096743	-1.1857088969	-0.0388722705
N	-0.0990928363	-0.2422864754	-0.4063319417
N	-2.5765218121	0.6029263356	0.7221615844
N	-2.8887660838	-1.9381648179	1.9510750444
N	-3.9403057366	-1.6534595987	-0.5153768658
O	0.0782665860	3.6711438329	0.4134875107
O	-1.3040667306	-2.8710383350	-0.7440779807
H	-0.8475320881	0.3423246230	-2.2918204557
H	0.6308189048	1.1968935345	-1.8155885426
H	-1.2348157801	2.7691459333	-1.6259534290
H	0.2473412978	1.8825259692	2.2776289350
H	1.5578038409	0.6188269888	0.6387294701
H	0.5894476662	-0.5415499911	1.5633242602
H	-3.1071960646	2.5240570776	-0.0740761061
H	-3.1353194459	1.1937426936	-1.2447426268
H	-1.6362307399	0.2818654595	2.6001415569

H	-2.1901438626	1.9469269200	2.3449218708
H	-4.5266485814	1.0485931706	1.5289289939
H	-4.8276336507	-1.2486467936	2.5594243113
H	-3.4831599602	-0.3669406935	3.2479137987
H	-4.1583773727	-3.6534284945	2.1949976736
H	-2.6627653132	-3.8782245488	1.2500709226
H	-4.0391385182	-3.7546201262	-0.5750401097
H	-5.3649487676	-2.9963466698	0.3199326024
H	-5.7060003672	-0.7842640947	0.3421040565
H	-4.8641469232	0.2287913131	-0.8198672863
H	0.4016750326	-1.0764087179	-0.7570977090
H	-2.2157661854	-2.1438223403	2.6851446149
H	-4.0372538586	-1.7431476494	-1.5251485261
O	0.2219643313	-2.9288916005	-0.6439507460
H	0.4175924949	-3.6240190489	-1.3088060026

S=1

S=0 (Open-Shell Singlet)

			C	-0.0413017943	0.4172613761	-1.5570328864	
C	-0.0258944742	0.4204886292	-1.5513187284	C	-0.8063685621	1.7029064833	-1.1628825424
C	-0.7956213157	1.7030372305	-1.1558281098	C	-0.0888772533	2.3413447861	0.0081554735
C	-0.0840384081	2.3378186405	0.0213694632	C	-0.1301750695	1.4017610632	1.1972681775
C	-0.1284509207	1.3932223295	1.2066544352	C	0.6257945643	0.1023448975	0.8255713907
C	0.6273403087	0.0945530594	0.8341143291	C	-2.2829619269	1.4625812856	-0.7728079093
C	-2.2733892638	1.4576227992	-0.7734331000	C	-1.6100957427	1.1845117193	1.5899429050
C	-1.6084408164	1.1705727740	1.5926662481	C	-3.8632751992	0.3535636244	0.8261944757
C	-3.8632626239	0.3506155884	0.8230346315	C	-3.9377872617	-0.4915101522	2.1130032477
C	-3.9369316776	-0.4971487393	2.1084492132	C	-4.0367477075	-2.9223909633	1.5051957915
C	-4.0067409154	-2.9291367741	1.4963715846	C	-4.3570721754	-2.8928262062	-0.0178427621
C	-4.3452288136	-2.8934658413	-0.0226917608	C	-4.5679730011	-0.3932809260	-0.3293769754
C	-4.5693782086	-0.3917489851	-0.3336887466	Cu	-1.8086938849	-1.4037503724	0.1273099781
Cu	-1.8095084842	-1.3900427589	0.1083901628	N	0.1079508367	-0.5767678364	-0.4271213947
N	0.1128348714	-0.5773089596	-0.4238224501	N	-2.4199462453	0.6096479739	0.4584167160
N	-2.4148287021	0.5978199519	0.4547879430	N	-3.1973430851	-1.7688878681	1.9293134656
N	-3.1841314553	-1.7639030012	1.9169088894	N	-3.8439868004	-1.6556701969	-0.6809718407
N	-3.8427124600	-1.6517852917	-0.6883628691	O	0.4511704345	3.4510602370	-0.0037056996
O	0.4542984309	3.4481898288	0.0160727302	O	-1.3075951011	-3.3215202203	0.1728852478
O	-1.3024343655	-3.2851615975	0.1448498611	O	-0.5894120102	-3.5072087170	1.2949279117
O	-0.6114629086	-3.4355686516	1.3116378983	H	-0.5386652947	-0.0817550874	-2.3898691080
H	-0.5148148122	-0.0756403862	-2.3908577592	H	0.9592299000	0.7062784122	-1.9110514858
H	0.9778003748	0.7111277142	-1.8945252178	H	-0.7854623213	2.3862276337	-2.0182265053
H	-0.7729249946	2.3901830570	-2.0079832207	H	0.3842779884	1.8663042505	2.0449833070
H	0.3816361383	1.8547487179	2.0586254136	H	1.6861136694	0.3595137349	0.6773668733
H	1.6886204483	0.3490991510	0.6906634431	H	0.5748026854	-0.6277595841	1.6405745985
H	0.5701272810	-0.6400263867	1.6444693891	H	-2.7766505668	2.4340403937	-0.6076473554
H	-2.7697337947	2.4261543274	-0.6025235223	H	-2.7865581117	0.9684006666	-1.6052706526
H	-2.7743421087	0.9665045878	-1.6092877925	H	-1.6442006960	0.4983463834	2.4363898215

H	-1.6444247079	0.4807017748	2.4357630019	H	-2.0439081426	2.1451742057	1.9118802835
H	-2.0485921173	2.1277683408	1.9146693216	H	-4.3822511651	1.3113114846	0.9956161469
H	-4.3725327695	1.3128367638	0.9923841239	H	-4.9950647209	-0.6808269430	2.3447643481
H	-4.9929977595	-0.6970797695	2.3357720347	H	-3.5306285281	0.0508516610	2.9683267187
H	-3.5382688501	0.0460315150	2.9673234300	H	-4.9699558999	-2.9413753133	2.0848363870
H	-4.9322307837	-2.9697541144	2.0869965606	H	-3.4806036994	-3.8317935425	1.7391435083
H	-3.4289163856	-3.8281974766	1.7155305110	H	-3.8682429687	-3.7359737663	-0.5108372064
H	-3.8580876738	-3.7328152348	-0.5234447162	H	-5.4402991647	-2.9850628555	-0.1745567554
H	-5.4295867075	-2.9865271708	-0.1692785423	H	-5.6010544711	-0.6111577916	-0.0268713282
H	-5.6018556316	-0.6113906358	-0.0308720147	H	-4.6331214033	0.2355241818	-1.2195579886
H	-4.6350995120	0.2395602146	-1.2220954644	H	-2.6409022312	-2.0166142464	2.7444151661
H	-2.6026868028	-2.0065090730	2.7156357280	H	-3.8356554804	-1.7959354806	-1.6898311321
H	-3.8393781492	-1.7930634424	-1.6971972367	C	1.1088418575	-1.6583797427	-0.7959468086
C	1.1112085048	-1.6660389196	-0.7858569783	H	1.1576748864	-2.3229423340	0.0692572497
H	1.1517841103	-2.3278804315	0.0813168136	H	2.0927779365	-1.1769590533	-0.9056295365
H	2.0958322021	-1.1854995678	-0.8919178769	C	0.7902070256	-2.4854032139	-2.0572055629
C	0.7983385411	-2.4977444186	-2.0444401735	H	1.3537274837	-3.4228203388	-1.9451805064
H	1.3721397711	-3.4285681117	-1.9289404411	H	-0.2647461976	-2.7824228102	-2.0402915508
H	-0.2522166428	-2.8076412876	-2.0231055367	C	1.1352032465	-1.8574697863	-3.4008894262
C	1.1360797250	-1.8696255374	-3.3889839412	C	2.4291343104	-1.3855303628	-3.6817110107
C	2.4285990528	-1.3975141184	-3.6762297101	C	0.1696595044	-1.7698928680	-4.4216685302
C	0.1646382918	-1.7803651256	-4.4038407367	C	2.7457515568	-0.8253827288	-4.9235687396
C	2.7380361680	-0.8355988026	-4.9189233297	H	3.2130237931	-1.4644504797	-2.9332591824
H	3.2163823455	-1.4781125570	-2.9319376935	C	0.4700588203	-1.2169118797	-5.6668673403
C	0.4575721259	-1.2246938177	-5.6495761133	H	-0.8312623315	-2.1563362971	-4.2436415762
H	-0.8347897646	-2.1681906742	-4.2206377271	C	1.7620518035	-0.7379674716	-5.9173887406
C	1.7481076532	-0.7457464801	-5.9064320655	H	3.7537654366	-0.4689404910	-5.1168132897
H	3.7451978327	-0.4800627940	-5.1181469000	H	-0.2701311934	-1.1538814619	-6.4554880632
H	-0.2870359573	-1.1610327820	-6.4339679117	O	1.9897859614	-0.1895770310	-7.1693824899
O	1.9692541276	-0.1967699065	-7.1591979758	H	2.9164872437	0.0911636547	-7.2962397831
H	2.8970939065	0.0768128782	-7.2927255005				

$[(\text{Cu}^{\text{II}}(\text{L}^2))_2\text{O}_2]^+$ (Trans End-On Peroxo Structure)

S=0 (Open-Shell Singlet)

C	1.400032	4.278187	0.265065
C	0.361775	5.200623	0.939645
C	0.504590	5.081741	2.446016
C	0.196752	3.658084	2.875405
C	1.257277	2.729543	2.225992
C	-1.087263	4.853037	0.545709
C	-1.276007	3.349506	2.501261
C	-2.935134	3.193455	0.596996
C	-3.299147	1.753586	0.985203
C	-2.765601	0.286274	-0.998937
C	-2.476032	1.277482	-2.157425
C	-3.066801	3.375908	-0.932306
Cu	-0.501413	1.840704	0.118459
N	1.310433	2.844542	0.718670
N	-1.513103	3.490034	1.019304
N	-2.342656	0.808884	0.336416
N	-2.021110	2.593037	-1.647456
O	0.819360	6.002498	3.203992
O	0.434092	0.188014	-0.435630
H	1.271431	4.289246	-0.822943
H	2.401773	4.670575	0.486207
H	0.565143	6.232505	0.635471
H	0.294444	3.577640	3.962676
H	2.232177	2.997836	2.654321
H	1.064220	1.679498	2.471445
H	-1.772645	5.611771	0.955726
H	-1.160237	4.885161	-0.541288

H	-1.532649	2.337667	2.820378
H	-1.931635	4.043775	3.051041
H	-3.624558	3.892188	1.097605
H	-4.328687	1.544407	0.664460
H	-3.271162	1.608463	2.065868
H	-3.835137	0.038941	-0.965800
H	-2.191844	-0.629255	-1.144489
H	-1.673520	0.887491	-2.788479
H	-3.372591	1.383132	-2.786872
H	-4.072725	3.052379	-1.234388
H	-2.992975	4.428285	-1.213011
H	-2.119542	0.013937	0.935149
H	-1.594759	3.135540	-2.395192
O	-0.213314	-1.108242	-0.112575
C	-1.407049	-5.090867	-0.265599
C	-0.444099	-6.166361	-0.812885
C	0.383749	-6.700964	0.340318
C	1.235248	-5.585298	0.917626
C	0.278939	-4.511771	1.493158
C	0.502361	-5.630811	-1.904325
C	2.194067	-5.074048	-0.181893
C	2.370114	-4.111197	-2.511001
C	3.308445	-3.014631	-1.991949
C	2.217904	-0.857282	-2.607876
C	0.897392	-1.150752	-3.348221
C	1.508859	-3.571734	-3.681582
Cu	0.536241	-2.744394	-0.881198
N	-0.706392	-3.982045	0.477196
N	1.453847	-4.577135	-1.398066
N	2.497157	-1.854308	-1.530113
N	0.508005	-2.576853	-3.191078
O	0.357032	-7.861724	0.754894

H	-1.974743	-4.632013	-1.082561
H	-2.126546	-5.586524	0.400422
H	-1.039286	-6.980138	-1.239818
H	1.839849	-5.981364	1.739939
H	-0.258413	-4.973319	2.331808
H	0.838508	-3.656419	1.887341
H	1.079501	-6.467174	-2.329049
H	-0.103639	-5.200863	-2.702379
H	2.791364	-4.257962	0.227006
H	2.880190	-5.887264	-0.466643
H	2.970145	-4.961136	-2.872934
H	4.000466	-2.721121	-2.792371
H	3.931170	-3.370252	-1.170291
H	3.063807	-0.838922	-3.308037
H	2.142662	0.123991	-2.144198
H	0.103788	-0.556007	-2.891736
H	0.996353	-0.871790	-4.407501
H	2.176557	-3.123283	-4.428644
H	0.991085	-4.386170	-4.191845
H	2.933207	-1.384328	-0.738264
H	-0.408649	-2.741014	-3.602251
C	2.438055	2.035752	0.122621
H	2.210416	0.991742	0.343159
H	2.345427	2.153551	-0.963214
C	3.896777	2.364310	0.529088
H	4.033680	2.265997	1.612191
H	4.168555	3.390535	0.257835
C	-1.724946	-3.066961	1.114863
H	-1.177478	-2.174856	1.423481
H	-2.404823	-2.763902	0.312099
C	-2.557620	-3.624923	2.297318
H	-3.073452	-4.551326	2.022698

H	-1.901799	-3.864010	3.143251
C	4.806748	1.385089	-0.193044
C	5.343928	1.689066	-1.455139
C	5.065893	0.110680	0.349864
C	6.100225	0.752096	-2.168188
H	5.180340	2.671915	-1.888192
C	5.822142	-0.833373	-0.348649
H	4.700742	-0.131923	1.344950
C	6.329349	-0.514549	-1.616611
H	6.511334	1.011491	-3.139516
H	6.063783	-1.799475	0.080063
C	-3.585937	-2.595380	2.739453
C	-3.161283	-1.380081	3.303580
C	-4.963264	-2.833020	2.591269
C	-4.101740	-0.432988	3.714759
H	-2.109705	-1.176729	3.481256
C	-5.896563	-1.880811	3.018710
H	-5.307887	-3.770205	2.166249
C	-5.473570	-0.671215	3.579408
H	-6.957704	-2.080994	2.916740
H	-6.200375	0.065207	3.909758
O	-3.593790	0.774938	4.217802
H	-4.251089	1.252759	4.761094
O	7.025136	-1.520085	-2.273171
H	7.515480	-1.197712	-3.054192
