

Supporting Information

For

X-ray Absorption Spectroscopic and Computational Investigation of a Possible S···S Interaction in the [Cu₃S₂]³⁺ Core

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Title Running Head: Electronic Structure of [(LCu)₃S₂]³⁺.

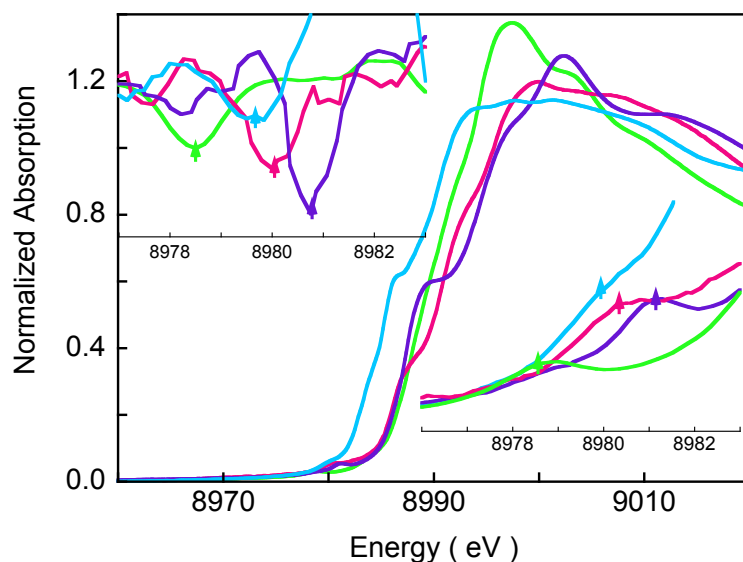


Figure S1. Cu K pre-edge XAS data for $[\text{Cu}^{\text{II}}(\text{TMPA})(\text{OH}_2)](\text{ClO}_4)_2$ (—, 8978.5 eV), **5** (Cu^{II} complex) (—, 8979.7 eV), $[\text{Cu}_2^{\text{III}}(\mu\text{-O})_2(\text{LMe}_3\text{-TACN})_2]^{2+}$ (—, 8980.1 eV) and $[\text{Cu}^{\text{III}}(\text{H-3Aib}_3)]$ (—, 8980.8 eV). The pre-edge energy positions have been measured from the second derivative data obtained in KaleidaGraph.

Cu K-pre-edge energy position dominantly reflects the ligand field strength felt by the Cu center and the charge on the Cu center. These are generally coupled and the pre-edge energy position has been used as a marker of oxidation state. Cu(II) complexes typically have pre-edge energy position at ~ 8979 eV, while the pre-edge energy positions of Cu(III) complexes occur 1.5 to 2 eV to higher energy. However, both Cu(II) and Cu(III) complexes exhibit a range of energies. Figure S1 shows the Cu K-edge XAS spectra of two Cu(II) and two Cu(III) complexes indicating that depending on the type and number of ligands the pre-edge energy difference between a Cu(II) and Cu(III) complex can be small. In particular, **5** is a Cu(II) complex with a pre-edge at 8979.7 eV, only 0.4 eV lower than that of $[\text{Cu}_2^{\text{III}}(\mu\text{-O})_2(\text{LMe}_3\text{-TACN})_2]^{2+}$, a Cu(III) complex with highly covalent oxo ligation.

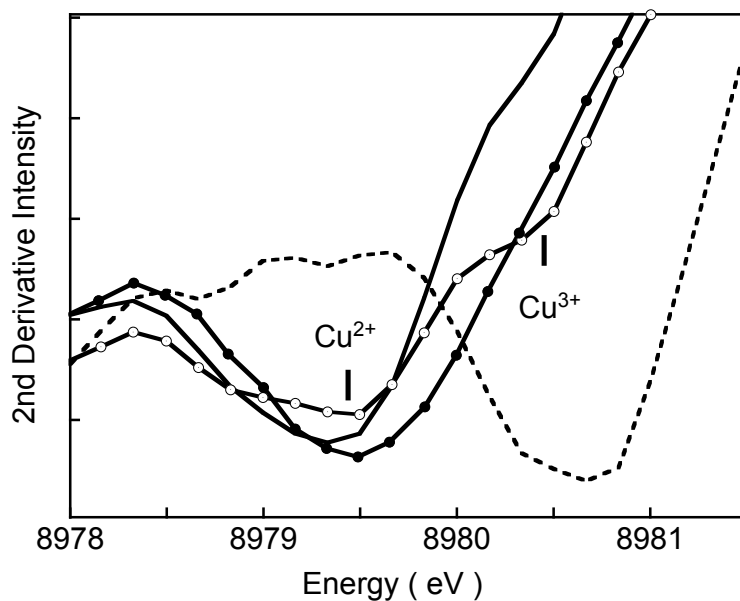


Figure S2. The second derivative of the Cu K-edge XAS spectra for **1** (—,•), $[\text{Cu}(\text{MNT})_2](\text{Bu}_4\text{N})$ (**3b**) (—) and $[\text{Cu}(\text{MNT})_2](\text{Bu}_4\text{N})_2$ (**3a**). A simulated spectrum representing a species containing two Cu^{2+} and one Cu^{3+} centers was constructed using the spectra for **3a** and **3b** (—,◦). The simulated spectrum for a localized ($\text{Cu}^{3+}\text{Cu}^{2+}\text{Cu}^{2+}$) species has two pre-edge features separated by ~ 2 eV. Since there is only one pre-edge feature in the Cu K-pre-edge of **1**, the data confirm that **1** is not a localized ($\text{Cu}^{3+}\text{Cu}^{2+}\text{Cu}^{2+}$) species.

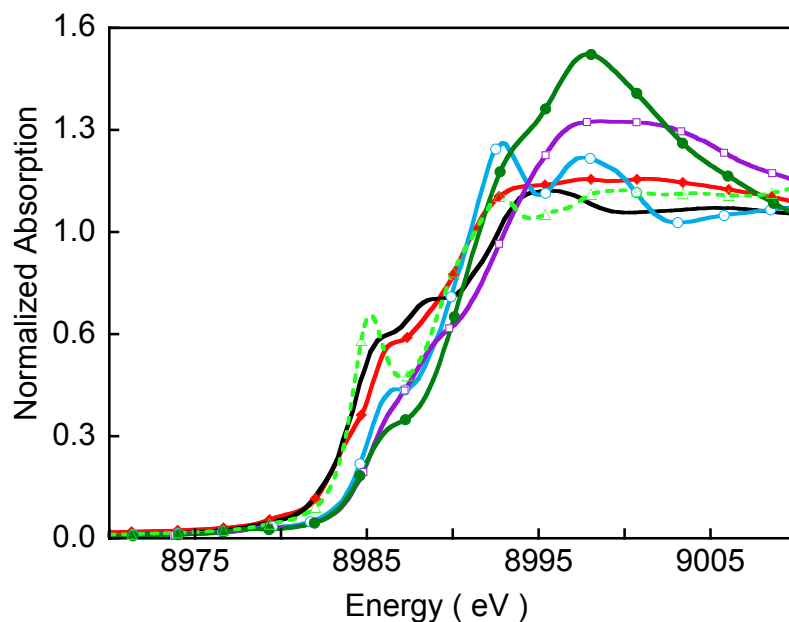


Figure S3. Cu K-edge XAS spectra tetragonal Cu(II) complexes. $[\text{Cu}(\text{MNT})_2](\text{Bu}_4\text{N})_2$ (S4 ligation)(**3a**) (---), $[\text{LCu}_2(\mu\text{-}1,2\text{-S}_2)_2](\text{OTf})_2$ (S_2N_2 ligation) (**5**) (—,◊), $[\text{Cu}(\text{2,5-dithiahexane})_2](\text{ClO}_4)_4$ (S_4 ligation) (—), $[\text{Cu}(\text{Cl})_4](\text{creatinium})_2$ (Cl_4 ligation) (—,◦), $[\text{Cu}(\text{acetylacetonate})_2]$ (O_4 ligation) (—,◻), $[\text{Cu}(\text{succinate})_2(\text{H}_2\text{O})_2]$ (O_4 ligation) (—,•). See *J. Am. Chem. Soc.*, 109, 21, 1987 for details.

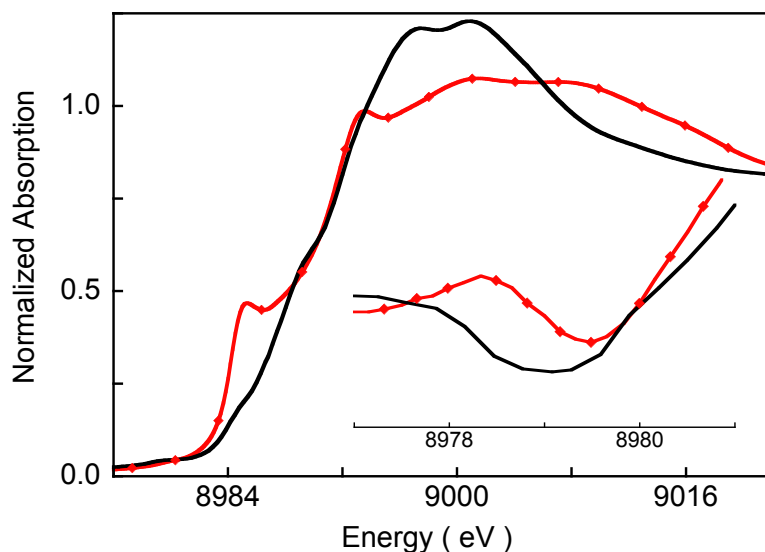


Figure S4. The normalized Cu K-edge XAS spectra for **1** (—,♦) and **4** (—) (bottom energy axis). The inset shows the second derivative spectrum of the pre-edge region.

Table S1. Selected DFT Parameters.			
		1	2
Bond Distance (Å) ^b	Cu-Cu	3.13	2.73
	Cu-S/O	2.28	1.98
	Cu-N	2.07	2.03
	S-S/O-O	2.77	2.35
Average Mayer Bond Order	Cu-Cu	0.20	0.36
	Cu-S/O	0.54	0.47
	Cu-N	0.43	0.44
	S-S/O-O	0.20	0.08
Mulliken Charge ^c	Cu	0.59	0.62
	S/O	-0.52	-0.65
	N	-0.23	-0.21

^aThe calculations were performed on the cation of **1** and **2**. ^bAverage Cu-S/O and Cu-N distance are listed (variation ≤ 0.002 Å). ^cAverage over all six N atoms.

Table S2. Cu 1s→4p + shakedown transition energy position.	
Complex	Energy (eV)
[Cu(MNT) ₂](Bu ₄ N) ₂	8985.0 eV
[(LCu) ₂ (μ-1,2-S ₂) ₂](OTf) ₂	8985.1 eV
[Cu(2,5-dithiahexane) ₂](ClO) ₄	8985.6 eV
[Cu(Cl) ₄](creatinium) ₂	8985. 8 eV
[Cu(acetylacetonate) ₂]	8986.0 eV
[Cu(succinate) ₂ (H ₂ O) ₂]	8985. 8 eV

Cu-S compounds	Type of Ligand	S K pre-edge energy (eV)		S K pre-edge intensity	
		absolute	Relative to 1	absolute	Relative to 1
1	--	2469.5	-	2.13	-
4	disulfide	2470.9	1.4	1.87	-0.3
5	supersulfide	2471.1	1.6	3.04	0.9
{Cu(TMPA)} ₂ S ₂ (ClO ₄) ₂ ^a	disulfide	2469.9	0.4	0.77	-1.4
3a	dithiolato	2470.4	0.9	0.63	-1.5
3b *	dithiolato	2470.1	0.6	1.41	-0.7
Covellite	sulfide/disulfide	2469.9	0.4	0.33	-1.8
Oxidized Chalcocite	sulfide	2470.1	0.6	0.52	-1.6
Plastocyanin	thiolate	2469.0	-0.5	1.08	-1.1
[ML(SC ₆ F ₅)] ^b	aromatic thiolate	2469.7	0.2	0.79	-1.3
[L ^{N³S} Cu] ₂ (ClO ₄) ₂ ^c	aliphatic thiolate	2470.4	0.9	0.69	-1.4
[Cu(L1)(pyridine)]	thioether	2472.1	2.6	0.34	-1.7

^a*J. Am. Chem. Soc.* **2008**, 130, 676-686, ^b*Inorg. Chem.*, **2005**, 44, 4947-4960, ^c*J. Am. Chem. Soc.*, **2001**, 123, 5757-5767. ^d*J. Am. Chem. Soc.* **2008**, 130, 3866-3877. A comparison of the S K-edge XAS data of Covellite and oxidized chalcocite with **1** is presented in Figure S5. ***3b** is the only Cu(III) complex in the list.

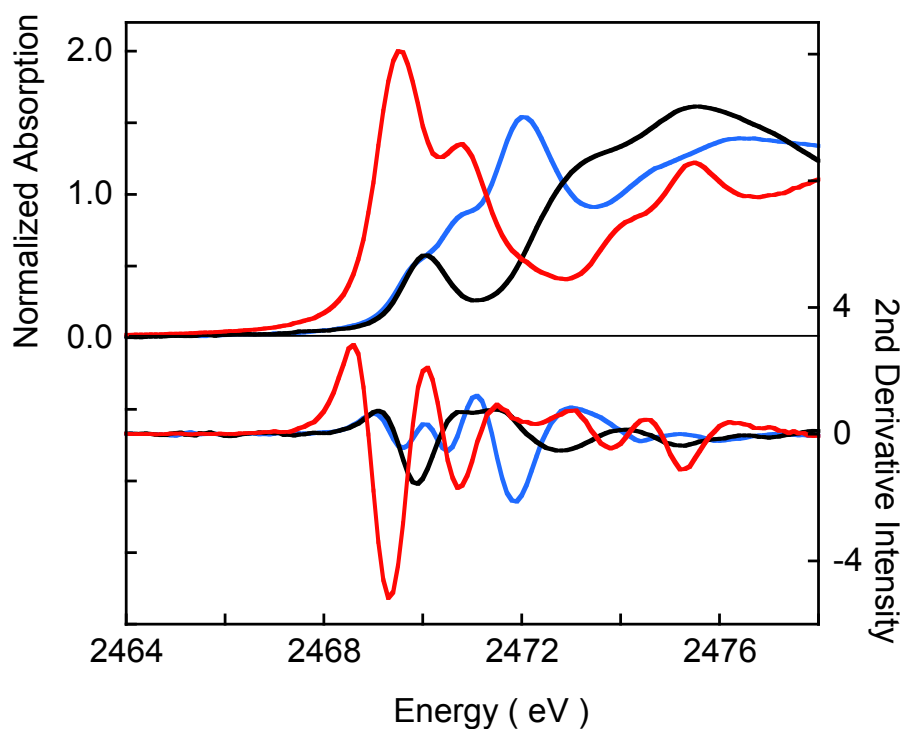


Figure S5. Top Panel: A comparison of the S K-edge XAS near-edge data for **1** (—), Covellite (—) and oxidized Chalcocite (—), Bottom Panel: Second Derivative Spectra.

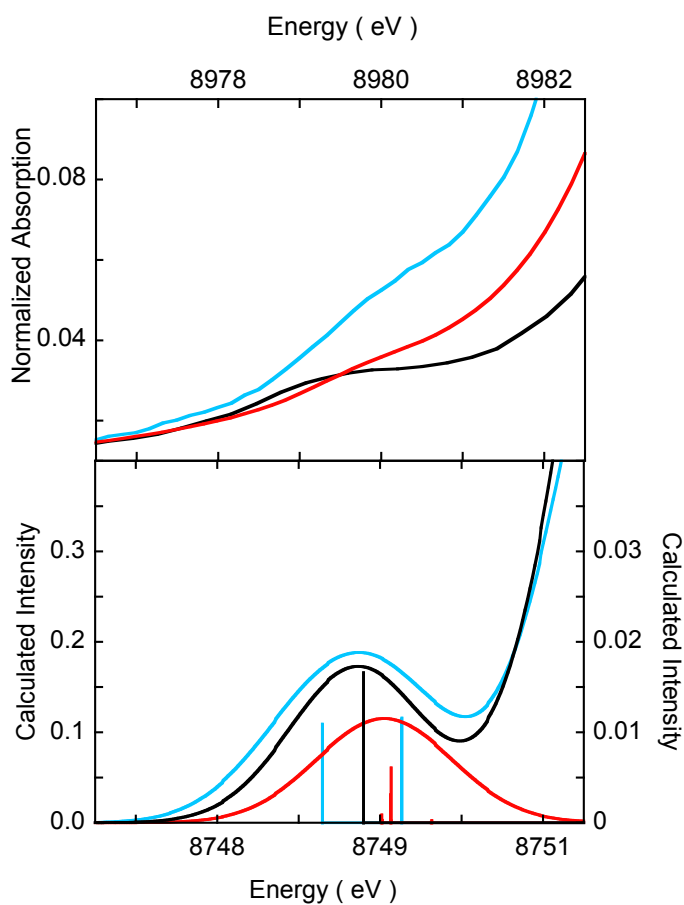


Figure S6. Top Panel: A comparison of the Cu K-pre-edge XAS data for **1** (—), **4** (—) and **5** (—).

Bottom Panel: TD-DFT calculated spectra using ORCA.¹

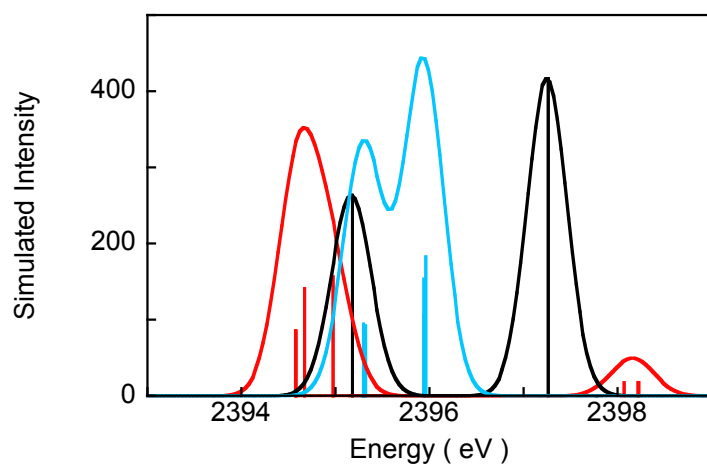


Figure S7. A comparison of the TD-DFT calculated S K-pre-edge spectra for **1** (—), **4** (—) and **5** (—).

Calculation performed in ORCA.¹

Table S4. TD-DFT calculated energies and intensities						
	Cu K-edge		S K-edge ^a			
			Pre-edge 1		Pre-edge 2	
1	8749.2		2394.60		2394.95	
4	8749.2		2395.17		2397.25	
5	8749.4		2395.29		2395.94	
Intensities ^{b,c}						
	Exp	Calc	Exp	Calc	Exp	Calc
1	1	1	1	1	0.48 ^d	0.54
4	6.8	15.8	0.88	1.14	0.96 ^d	1.35
5	7	19.3	1.26	1.43	1.68 ^d	1.44
^a Pre-edge 1 and 2 refer to the lower and higher energy pre-edge peaks in the main text. ^b Exp =experimental, Calc = calculated. ^c Relative intensities (w.r.t the pre-edge transition of 1 are reported). ^d Total intensity.						

The Cu K-pre-edge calculations for **1**, **4** and **5** are shown in Figure S6 and the energies and relative intensities are reported in Table S4. The energies do not accurately reproduce the experimental data but are within the error previously reported¹ for TD-DFT calculations for several related Fe complexes. Interestingly, the calculated pre-edge for **1** is very weak due to the absence of a dipole contribution to the pre-edge feature. A dipole component is present in **4** and **5**, which significantly increases their intensities. This increase in intensity is experimentally observed (Table S4), although not to the extent predicted by DFT.

The S K-pre-edge calculations for **1**, **4** and **5** are shown in Figure S7 and the energies and relative intensities are reported in Table S4. The calculations do not accurately reproduce the pre-edge energy splitting in any of the complexes. In **4** and **5**, this is likely because the higher energy pre-edge transition (peak 2) is to a purely ligand based diffuse orbital. To our knowledge successful calculations of the higher lying ligand based orbitals have not been reported. The relative energy and intensity of the lower energy pre-edge transition in **4** and **5** is reasonably reproduced by TD-DFT. However, both the energy

splitting and the relative energy position of **1** is not well predicted. The lower energy pre-edge feature in **1** is only 0.6 eV lower than **4**, compared to the experimental value of 1.4 eV.

The final geometry optimized xyz coordinates obtained from the DFT calculation on **1** (UBP86, basis sets: CP(PPP) on Cu, TZVPP on S and TZVP on the rest of the atoms, Conductor like screening model with CH₂Cl₂ as dielectric.)

Cu	-1.582372	0.888966	1.358614
S	-0.009524	0.001243	-0.039262
N	-2.882789	1.624955	2.787459
C	-3.867015	2.525107	2.061499
H	-3.328532	3.475678	1.919066
Cu	-0.000201	-1.816062	1.347254
N	-2.905327	1.617795	-0.053652
C	-5.152511	2.816628	2.858776
H	-5.681060	1.873121	3.065722
H	-4.898420	3.269986	3.827637
N	-0.020130	-3.320566	2.767816
C	-6.094136	3.737307	2.067618
H	-7.007735	3.906451	2.656516
H	-5.622263	4.723666	1.921745
C	-6.433798	3.118719	0.708822
H	-7.087173	3.787763	0.129579
H	-6.991336	2.178146	0.855496
C	-5.153591	2.848704	-0.096370
H	-5.400844	2.391095	-1.064877
H	-4.661711	3.811834	-0.303781
C	-4.191668	1.935481	0.687045
H	-4.682800	0.959356	0.829338
C	-3.520068	0.422811	3.399278
H	-4.176431	0.707396	4.234045
H	-2.729070	-0.227807	3.791195
H	-4.105404	-0.126603	2.652302
C	-2.166638	2.390354	3.843800
H	-2.872073	2.745712	4.610069
H	-1.657689	3.252353	3.395644
H	-1.431181	1.737302	4.328977
C	-3.163379	0.629812	-1.135406
H	-3.835849	1.054129	-1.895987
H	-3.622507	-0.271523	-0.711360
H	-2.215199	0.369683	-1.621256
C	-2.239503	2.819537	-0.635433
H	-2.839154	3.243634	-1.453612
H	-1.268284	2.515024	-1.043602
H	-2.085400	3.586727	0.132697
C	-0.341570	-4.609088	2.031669
H	-1.432769	-4.582991	1.880732
C	0.004323	-5.883851	2.824239
H	1.084301	-5.904021	3.038346
H	-0.521708	-5.880299	3.789633
C	-0.356193	-7.144657	2.023986
H	-0.077693	-8.032852	2.610042
H	-1.447575	-7.193872	1.870489
C	1.341843	-3.309085	3.376632
H	1.409901	-4.032086	4.202037
H	1.533153	-2.307740	3.780654
H	2.103741	-3.548050	2.625054

C	-1.032188	-3.068091	3.828684
H	-1.002192	-3.861839	4.590231
H	-2.034249	-3.034802	3.383878
H	-0.811948	-2.112151	4.319023
Cu	1.582276	0.889018	1.335853
S	0.009455	0.001303	2.733806
N	2.882525	1.625022	-0.093076
C	3.867338	2.524669	0.632763
H	3.329364	3.475538	0.775064
N	2.905197	1.618284	2.747977
C	5.152951	2.815423	-0.164575
H	5.681139	1.871638	-0.371182
H	4.899089	3.268565	-1.133600
N	0.019777	-3.320319	-0.073529
C	6.094855	3.736038	0.626345
H	7.008567	3.904641	0.037469
H	5.623316	4.722619	0.771800
C	6.434177	3.117863	1.985420
H	7.087668	3.786949	2.564480
H	6.991471	2.177080	1.839177
C	5.153808	2.848484	2.790582
H	5.400837	2.391119	3.759264
H	4.662157	3.811807	2.997627
C	4.191765	1.935219	2.007360
H	4.682700	0.958942	1.865449
C	3.519285	0.423009	-0.705587
H	4.175138	0.707690	-1.540723
H	2.728031	-0.227544	-1.097127
H	4.105032	-0.126682	0.040873
C	2.166068	2.391090	-1.148738
H	2.871088	2.745912	-1.915633
H	1.658332	3.253491	-0.699974
H	1.429295	1.738925	-1.633081
C	3.162700	0.630944	3.830453
H	3.835019	1.055570	4.590978
H	3.621562	-0.270897	3.407212
H	2.214342	0.371273	4.316294
C	2.239725	2.820708	3.328691
H	2.838376	3.244290	4.147846
H	1.267382	2.517420	3.735148
H	2.087457	3.587979	2.560293
C	0.341967	-4.608798	0.662420
H	1.433162	-4.582126	0.813293
C	-0.003295	-5.883593	-0.130369
H	-1.083279	-5.904333	-0.344386
H	0.522648	-5.879570	-1.095808
C	0.357985	-7.144336	0.669643
H	0.080009	-8.032598	0.083440
H	1.449398	-7.192925	0.823120
C	-1.342375	-3.309345	-0.681968
H	-1.410179	-4.032107	-1.507604
H	-1.534492	-2.308005	-1.085592
H	-2.103934	-3.549073	0.069711
C	1.031355	-3.067389	-1.134716
H	1.001402	-3.861087	-1.896318
H	2.033590	-3.033561	-0.690351
H	0.810364	-2.111574	-1.624960

The final geometry optimized xyz coordinates obtained from the DFT calculation on D_{3h} $[\text{Cu}_3-(\mu\text{-O})_2]^{3+}$ (UBP86, basis sets: CP(PPP) on Cu, TZVPP on O and TZVP on the rest of the atoms, Conductor like screening model with CH_2Cl_2 as dielectric.)

Cu	1.197018	-0.993231	1.337498
O	-0.031543	-0.016122	2.543143
N	2.251334	-2.009529	-0.065611
C	3.510895	-2.516113	0.612821
H	4.183681	-1.644080	0.643905
Cu	-1.501131	-0.586254	1.342279
N	2.417659	-1.815811	2.732904
C	4.226283	-3.648294	-0.145074
H	3.552811	-4.514699	-0.238609
H	4.481908	-3.317815	-1.162161
N	-2.907754	-0.990027	-0.061483
C	5.491355	-4.088873	0.609005
H	5.968159	-4.912471	0.057444
H	6.219113	-3.260116	0.635318
C	5.149624	-4.523689	2.037480
H	6.060965	-4.808743	2.583439
H	4.501932	-5.416328	2.011202
C	4.445179	-3.389191	2.798770
H	4.181072	-3.715109	3.815221
H	5.144946	-2.544219	2.894064
C	3.181657	-2.933756	2.047308
H	2.476191	-3.779533	2.015951
C	1.334358	-3.094846	-0.516238
H	1.786900	-3.673633	-1.334456
H	0.415674	-2.630200	-0.891566
H	1.094149	-3.771296	0.312611
C	2.583925	-1.138343	-1.226310
H	3.068256	-1.724720	-2.021932
H	3.267268	-0.343522	-0.903787
H	1.656875	-0.701876	-1.614528
C	1.640830	-2.331419	3.891501
H	2.317645	-2.664682	4.693005
H	1.024307	-3.179760	3.570851
H	1.002203	-1.526244	4.273204
C	3.286396	-0.690254	3.186314
H	3.960414	-1.017288	3.991036
H	2.641693	0.103715	3.577876
H	3.885269	-0.301413	2.353941
C	-3.957196	-1.849383	0.625254
H	-3.521605	-2.861094	0.647292
C	-5.299474	-1.918955	-0.125395
H	-5.727948	-0.908411	-0.213176
H	-5.141178	-2.300167	-1.144403
C	-6.298736	-2.809406	0.630568
H	-7.252667	-2.819231	0.083056
H	-5.933004	-3.849919	0.651937
C	-3.419595	0.344027	-0.491982
H	-4.162992	0.233231	-1.294405
H	-2.577825	0.926704	-0.880290
H	-3.877824	0.875044	0.350700
C	-2.330790	-1.698188	-1.237979
H	-3.098223	-1.838836	-2.014077
H	-1.956616	-2.680524	-0.926103
H	-1.511493	-1.097115	-1.646423
Cu	0.197326	1.549378	1.353647
O	-0.033635	-0.001582	0.145820

N	0.279973	3.008501	2.759740
C	0.858314	4.237563	2.082905
H	1.944165	4.053878	2.045763
N	0.523012	2.987250	-0.039218
C	0.619610	5.551442	2.847724
H	-0.462437	5.728137	2.952234
H	1.041411	5.479013	3.860545
N	-2.800659	-1.252046	2.749416
C	1.240352	6.737925	2.092819
H	1.032850	7.663874	2.649097
H	2.337413	6.626701	2.057934
C	0.683152	6.828380	0.668844
H	1.150972	7.660590	0.122564
H	-0.399150	7.039176	0.704250
C	0.935965	5.521117	-0.099489
H	0.514027	5.583558	-1.113024
H	2.023211	5.379700	-0.202271
C	0.325513	4.324502	0.651340
H	-0.766783	4.463784	0.688840
C	-1.130398	3.179037	3.211142
H	-1.191810	3.907139	4.032959
H	-1.488432	2.211894	3.581844
H	-1.766173	3.516162	2.383848
C	1.116533	2.592768	3.918931
H	1.073521	3.349521	4.716951
H	2.157948	2.475490	3.595643
H	0.732932	1.641529	4.304561
C	-0.405438	2.837575	-1.191018
H	-0.144353	3.545293	-1.992597
H	-1.432441	3.036362	-0.861563
H	-0.325181	1.814181	-1.575889
C	1.922626	2.754678	-0.502188
H	2.188757	3.454663	-1.307233
H	1.987492	1.734734	-0.895684
H	2.630953	2.875933	0.326299
C	-4.152232	-1.365334	2.063139
H	-4.542506	-0.335275	2.039956
C	-5.165364	-2.247119	2.815491
H	-4.771333	-3.271509	2.904228
H	-5.315552	-1.861796	3.834205
C	-6.503241	-2.301361	2.060614
H	-7.195831	-2.956613	2.609107
H	-6.962896	-1.298777	2.039041
C	-2.244494	-2.563713	3.193320
H	-2.857939	-2.993094	3.998331
H	-1.234736	-2.393887	3.581291
H	-2.203736	-3.271346	2.356781
C	-2.875684	-0.328819	3.915839
H	-3.528780	-0.749065	4.695562
H	-3.283946	0.636169	3.592474
H	-1.868841	-0.192160	4.324638

The final geometry optimized xyz coordinates obtained from the non-constrained fully optimized DFT calculation on $[\text{Cu}_3-(\mu\text{-O})_2]^{3+}$ (UBP86, basis sets: CP(PPP) on Cu, TZVPP on O and TZVP on the rest of the atoms, Conductor like screening model with CH_2Cl_2 as dielectric.)

Cu	1.142088	-0.976674	1.335315
O	-0.175756	-0.082841	2.517801
N	2.222478	-1.978160	-0.078018
C	3.499464	-2.441490	0.597988

H	4.145489	-1.548936	0.620404
Cu	-1.565055	-0.611995	1.342052
N	2.406682	-1.763985	2.732552
C	4.245187	-3.555758	-0.158059
H	3.597410	-4.442253	-0.244514
H	4.484279	-3.222458	-1.178324
N	-2.943977	-1.016420	-0.049159
C	5.527410	-3.958582	0.587394
H	6.024069	-4.769596	0.034689
H	6.231578	-3.109437	0.607677
C	5.206362	-4.399030	2.018872
H	6.128107	-4.658557	2.560111
H	4.582250	-5.308553	1.998310
C	4.476444	-3.280981	2.779729
H	4.230352	-3.609000	3.800124
H	5.154736	-2.417734	2.865939
C	3.194020	-2.860931	2.039106
H	2.512060	-3.726168	2.015992
C	1.335148	-3.096834	-0.507282
H	1.800626	-3.678954	-1.315941
H	0.402091	-2.666520	-0.887578
H	1.115132	-3.765147	0.333979
C	2.526255	-1.121599	-1.256580
H	3.015219	-1.709345	-2.048598
H	3.196292	-0.307815	-0.954524
H	1.587768	-0.710867	-1.645884
C	1.655823	-2.306762	3.897118
H	2.348538	-2.644910	4.682967
H	1.043546	-3.157717	3.574448
H	1.011660	-1.518303	4.302343
C	3.253839	-0.623062	3.185180
H	3.944362	-0.937267	3.981217
H	2.597169	0.154291	3.589830
H	3.833257	-0.213733	2.348928
C	-4.000097	-1.875499	0.632598
H	-3.562845	-2.885988	0.662907
C	-5.336641	-1.950184	-0.126212
H	-5.765112	-0.940751	-0.224316
H	-5.173627	-2.342012	-1.140156
C	-6.334927	-2.836378	0.637604
H	-7.287919	-2.850870	0.088784
H	-5.967709	-3.876026	0.665889
C	-3.448382	0.320267	-0.485519
H	-4.186411	0.205503	-1.291537
H	-2.600978	0.897294	-0.869957
H	-3.911556	0.854093	0.352547
C	-2.356394	-1.728043	-1.219300
H	-3.118257	-1.858039	-2.001925
H	-1.995899	-2.714031	-0.903664
H	-1.527765	-1.131453	-1.614834
Cu	0.164746	1.496058	1.352996
O	-0.181915	-0.064766	0.166968
N	0.269961	2.967774	2.768518
C	0.896631	4.174598	2.096706
H	1.976403	3.954854	2.073528
N	0.552851	2.941659	-0.040929
C	0.691979	5.497078	2.857534
H	-0.384903	5.709479	2.948431
H	1.096873	5.410412	3.876241
N	-2.843961	-1.253338	2.739995
C	1.359206	6.665330	2.114826

H	1.174188	7.596492	2.670374
H	2.452668	6.519732	2.092975
C	0.822983	6.774905	0.684156
H	1.322135	7.593547	0.145119
H	-0.252988	7.017903	0.706759
C	1.046245	5.460861	-0.080936
H	0.643532	5.537957	-1.101404
H	2.130316	5.287396	-0.167042
C	0.388358	4.280130	0.655420
H	-0.699298	4.454867	0.678407
C	-1.144313	3.186450	3.186547
H	-1.205580	3.928731	3.995764
H	-1.540573	2.236560	3.562465
H	-1.751985	3.528561	2.340082
C	1.065841	2.544868	3.952457
H	1.018447	3.305854	4.746495
H	2.112997	2.405156	3.658311
H	0.654415	1.604473	4.336755
C	-0.371677	2.830451	-1.201313
H	-0.101192	3.553567	-1.986098
H	-1.398561	3.032184	-0.872326
H	-0.305013	1.816073	-1.610727
C	1.947912	2.681394	-0.498943
H	2.238247	3.381622	-1.295694
H	1.992911	1.664937	-0.904051
H	2.653792	2.774863	0.335271
C	-4.200751	-1.377928	2.061155
H	-4.594318	-0.349663	2.029928
C	-5.207823	-2.256395	2.823934
H	-4.809864	-3.278186	2.922471
H	-5.361652	-1.860583	3.837831
C	-6.543136	-2.319218	2.063800
H	-7.234354	-2.973333	2.615172
H	-7.005713	-1.318335	2.035632
C	-2.277881	-2.558439	3.196241
H	-2.888549	-2.977306	4.008121
H	-1.268213	-2.376025	3.578491
H	-2.239137	-3.275921	2.368266
C	-2.915058	-0.315477	3.896072
H	-3.558133	-0.736221	4.683060
H	-3.335475	0.641410	3.565034
H	-1.905131	-0.168760	4.293046

References

1. DeBeer George, S.; Petrenko, T.; Neese, F. *J. Phys. Chem. A.*, **2008**, *112*, 12936–12943