Supporting Information

Experimental and Computational Investigation of Heteroatom Substitution in Nucleolytic Cu(II) Cyclen Complexes for Balancing Stability and Redox Activity

Jan Hormann,[a] Olga Verbitsky,[b] Xiaoyu Zhou,[c] Beatrice Battistella,[a,d] Margarete van der Meer,[a] Biprajit Sarkar,[a,e] Cunyuan Zhao,[c] Nora Kulak[a,b]**

a Institut für Chemie und Biochemie, Freie Universität Berlin, Fabeckstr. 34/36, 14195 Berlin, Germany

b Institut für Chemie, Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

c MOE Key Laboratory of Bioinorganic and Synthetic Chemistry, School of Chemistry, Sun Yat-Sen University, XinGang Rd. W., Guangzhou 510275, China

d Department of Chemistry, Humboldt Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany

e Institut für Anorganische Chemie, Universität Stuttgart, Pfaffenwaldring 55, 70569 Stuttgart, Germany.

S-1 Synthesis of ligands and complexes

[Cu([12]aneN$_4$)NO$_3$]NO$_3$ (CuL^1)

This complex was synthesized according to a procedure previously published by our lab.[1]

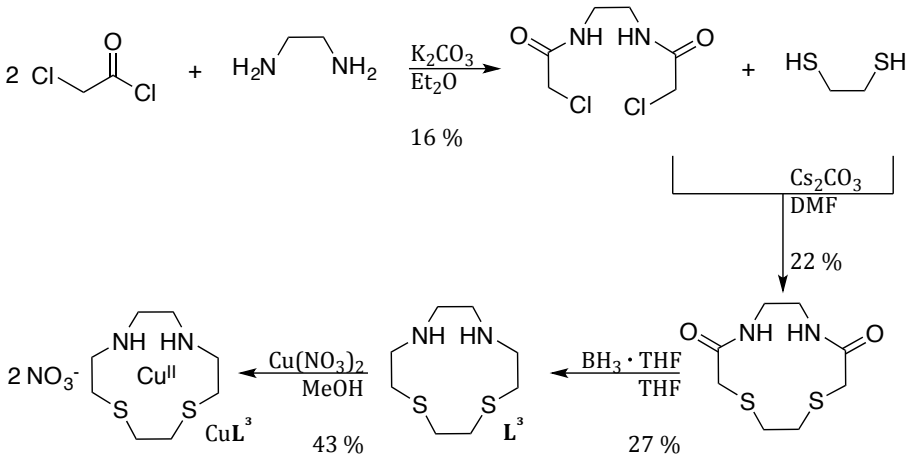
[Cu([12]aneN$_3$S)NO$_3$]NO$_3$ (CuL^2)

This complex was synthesized according to a procedure previously published by our lab.[1]

[Cu([12]aneN$_2$S$_2$)(NO$_3$)]NO$_3$ (CuL^3)

N,N'-(Ethane-1,2-diyl)bis(2-chloroacetamide) (CAS 2620-09-9),[2] 1,4-dithia-7,10-diazacyclododecane-6,11-dione (CAS 90777-30-3)[3] and 1,4-dithia-7,10-diazacyclododecane (CAS 88439-31-0, **L^3**)[3] were synthesized as previously described.

[12]aneN$_2$S$_2$ (**L^3**) (152.0 mg, 0.7 mmol) was dissolved in 3.5 mL methanol and heated under reflux. A solution of Cu(NO$_3$)$_2$ · 3 H$_2$O (174.0 mg, 0.7 mmol) in 3.5 mL methanol was added and heated under reflux for another 10 min. The solution was cooled down to -18 °C, the precipitated dark blue solid was filtered and dried *in vacuo*. Crystals suitable for X-ray analysis were obtained by slow diffusion of diethyl ether into a methanolic solution of the complex. Yield: 122.0 mg (0.3 mmol, 43%). Elemental analysis (Cu(C$_8$H$_{18}$N$_2$S$_2$)(NO$_3$)$_2$ · 0.25 CH$_3$OH) calcd. C 24.65, H 4.76, N 13.94 and S 15.95%; found C 24.31, H 4.61, N 13.60 and S 16.29%; max. deviation [%] 0.34. UV/VIS (50 mM Tris-HCl, pH 7.4): λ_{max} (ε) = 650 nm (575 L mol^{-1} cm^{-1}). MS (ESI+) (m/z): calcd. for [M – 2NO$_3$ + Cl]$^+$ 303.9896; found 303.9925.

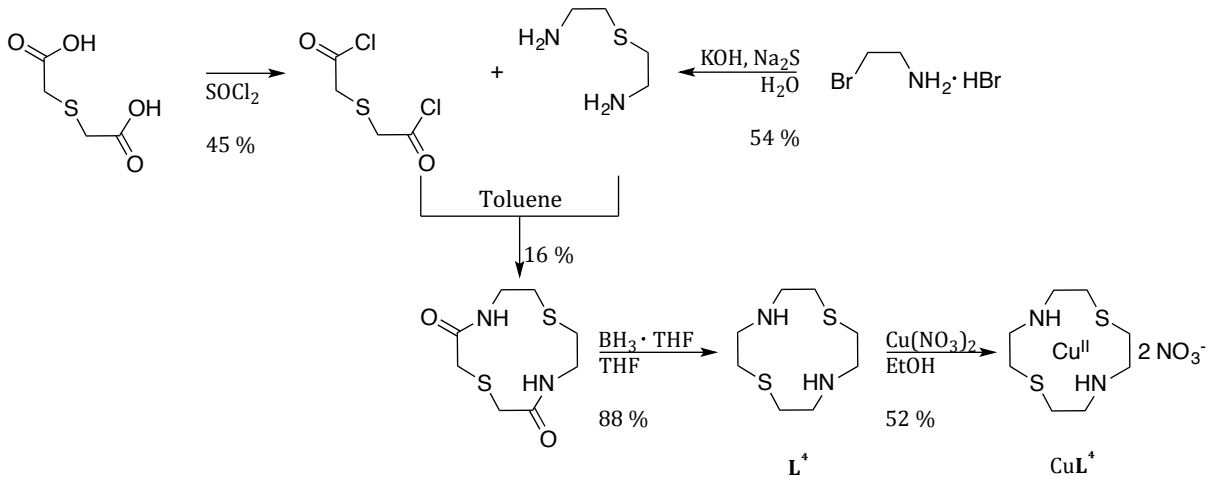


Scheme S-1.1 Synthesis of Cu**L^3**.

[Cu([12]aneNSNS)(NO$_3$)]NO$_3$ (CuL^4)

2,2'-Thiodiacetylchloride (CAS 7646-91-5)[4], bis(2-aminoethyl)sulfide (CAS 871-76-1)[3], 1,7-dithia-4,10-diazacyclododecan-3,11-dione (CAS 90777-32-5)[5] and 1,7-dithia-4,10-diazacyclododecane (CAS 65113-45-3, **L^4**)[6] were synthesized as previously described.

[12]aneNSNS (**L⁴**) (95.0 mg, 0.46 mmol) was dissolved in 1.5 mL ethanol and heated under reflux. A solution of $Cu(NO_3)_2 \cdot 3\ H_2O$ (111.2 mg, 0.46 mmol) in 1.5 mL ethanol was added and heated under reflux for another 30 min. The solution was cooled down to room temperature, the precipitated dark-green needles were filtered off and dried *in vacuo*. Yield: 94.0 mg (0.24 mmol, 52%). Elemental analysis calcd. C 24.39, H 4.61, N 14.22 and S 16.28%; found C 24.50, H 4.65, N 14.28 and S 16.40%; max. deviation [%] 0.12. UV/VIS (50 mM Tris-HCl, pH 7.4): λ_{max} (ε) = 651 nm (214 L mol^{-1} cm^{-1}). MS (ESI+) (m/z): calcd. for $[M - 2NO_3 + Cl]^+$ 303.9896; found 303.9919.

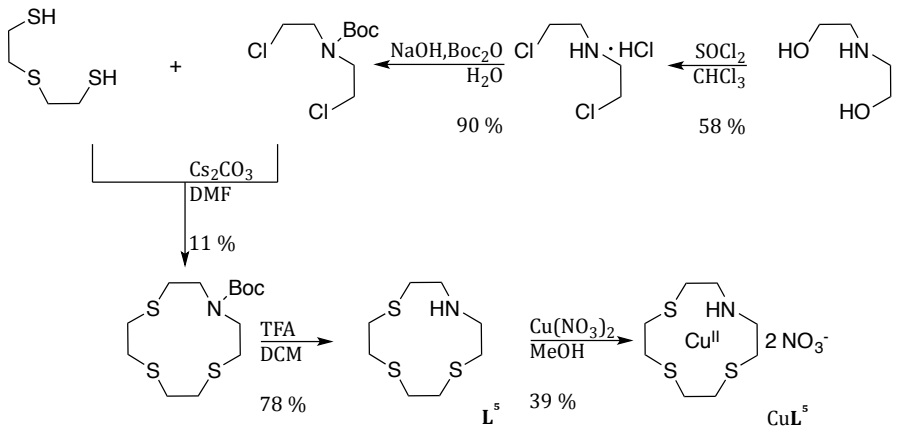


Scheme S-1.2 Synthesis of Cu**L⁴** (note: the yield of the cyclization step is low in comparison to the literature[6] since 1.5 instead of 2 equivalents of the amine were used inadvertently).

[Cu([12]aneNS₃)(NO₃)]NO₃ (CuL⁵)

Bis(2-chloroethyl)amine hydrochloride (CAS 821-48-7) was obtained from Merck. *N*-Boc-bis(2-chloroethyl)amine (CAS 118753-70-1)[6], *N*-Boc-1,4,7-trithia-10-azacyclododecane (CAS 878673-76-8)[3] and 1,4,7-trithia-10-azacyclododecane (**L⁵**, CAS 122011-96-5)[3] were synthesized as previously described.

[12]aneNS₃ (**L⁵**) (110.3 mg, 0.5 mmol) was dissolved in 5 mL acetonitrile and heated to reflux. A solution of $Cu(NO_3)_2 \cdot 3\ H_2O$ (119.3 mg, 0.5 mmol) in 1 mL acetonitrile was added and heated under reflux for another 10 min. The solution was cooled down to -18 °C, the precipitated dark green powder was filtered off and dried *in vacuo*. Yield: 80.0 mg (0.2 mmol, 39%). Elemental analysis calcd. C 23.38, H 4.17, N 10.22 and S 23.40%; found C 23.44, H 4.15, N 10.24 and S 23.40%; max. deviation [%] 0.06. UV/VIS (50 mM Tris-HCl, pH 7.4): λ_{max} (ε) = 659 nm (497 L mol^{-1} cm^{-1}). MS (ESI+) (m/z): calcd. for $[Cu^{I}[12]aneNS_3]^+$ 285.9819; found 285.9928.

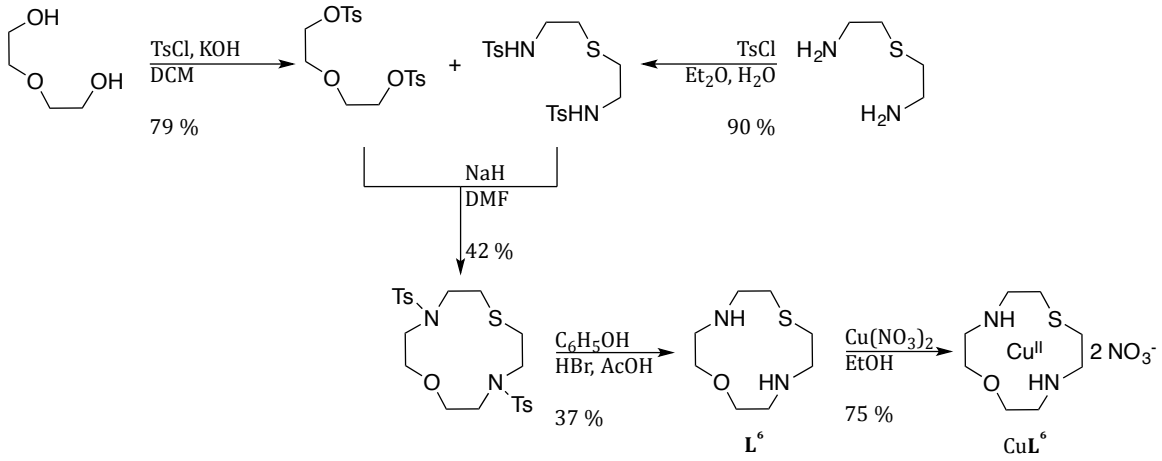


Scheme S-1.3 Synthesis of Cu**L**[5].

[Cu([12]aneNONS)(NO$_3$)]NO$_3$ (CuL^6)

1,5-Bis(tolylsulfonyloxy)-3-oxapentane (CAS 7460-82-4),[7] bis[(*p*-tolylsulfonylamino)ethyl]sulfide (CAS 85775-49-1)[3], 4,10-bis(*p*-tolylsulfonyl)-1-oxa-7-thia-4,10-diazacyclododecane (CAS 221055-19-2)[8], and 1-oxa-7-thia-4,10-diazacyclododecane (CAS 124775-44-6, **L^6**)[9] were synthesized as previously described with slight modifications (see caption of Scheme S-1.4) .

Freshly sublimed [12]aneNONS (**L^6**) (163.6 mg, 0.9 mmol) was dissolved in 3 mL ethanol and heated under reflux. A solution of $Cu(NO_3)_2 \cdot 3\,H_2O$ (208.0 mg, 0.9 mmol) in 3 mL ethanol was added and heated under reflux for another 20 min. The solution was cooled down to room temperature, the precipitated light-blue crystalline solid was filtered off and dried *in vacuo*. Crystals suitable for X-ray analysis were obtained by slow diffusion of diethyl ether into a methanolic solution of the complex, however, the obtained data were not of sufficient quality. Yield: 240.0 mg (0.6 mmol, 75%). Elemental analysis calcd. C 25.43, H 4.80, N 14.83 and S 8.48%; found C 25.53, H 4.62, N 14.63 and S 8.65%; max. deviation [%] 0.2. UV/VIS (50 mM Tris-HCl, pH 7.4): λ_{max} (ε) = 658 nm (58 L mol^{-1} cm^{-1}). MS (ESI+) (m/z): calcd. for $[Cu(C_8H_{18}N_2OS)–H]^+$ 252.0363; found 252.0390.



Scheme S-1.4 Synthesis of Cu**L^6** (note: the yield of the cyclization step might be lower than the literature[9] since the thioether as a starting material was prepared only *in situ* instead of isolating and purifying it; on the other hand the yield was twice as high than in that literature for the deprotection step).

S-2 UV/VIS, IR and EPR spectroscopy

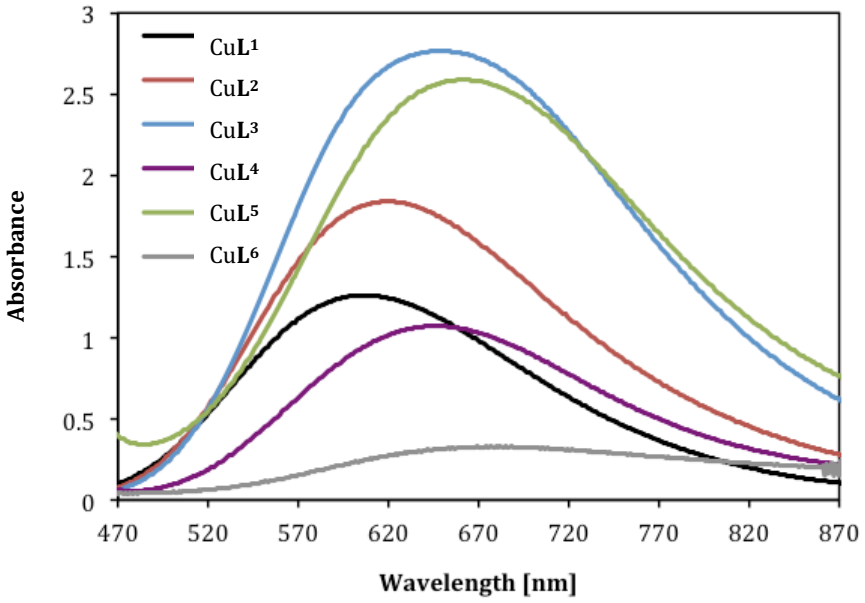


Figure S-2.1 UV/VIS spectra of complexes Cu**L**¹-Cu**L**⁶ (5 mM) in 50 mM Tris-HCl buffer (pH 7.4).

Table S-2 Maximum absorption wavelengths λ_{max} with corresponding extintion coefficients ε for complexes Cu**L**¹-Cu**L**⁶.

	λ_{max} [nm]	ε [L mol^{-1}cm^{-1}]
Cu**L**¹	601	235.9
Cu**L**²	619	377.0
Cu**L**³	652	575.0
Cu**L**⁴	647	208.4
Cu**L**⁵	659	497.2
Cu**L**⁶	658	57.9

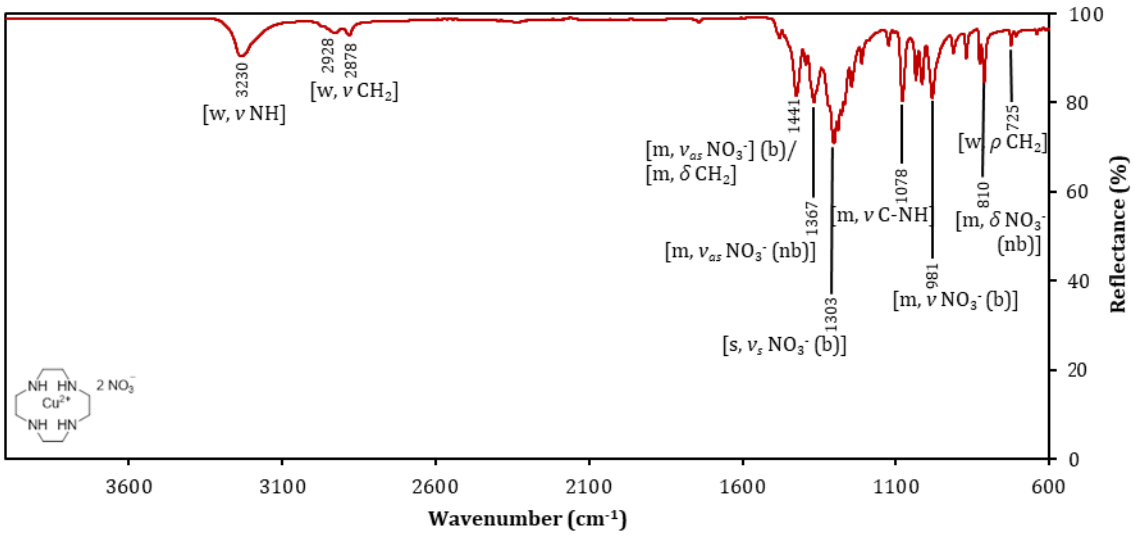


Figure S-2.2a IR spectrum of complex Cu**L**[1] (for nitrate, nb=not bound/ionic, b=bound).

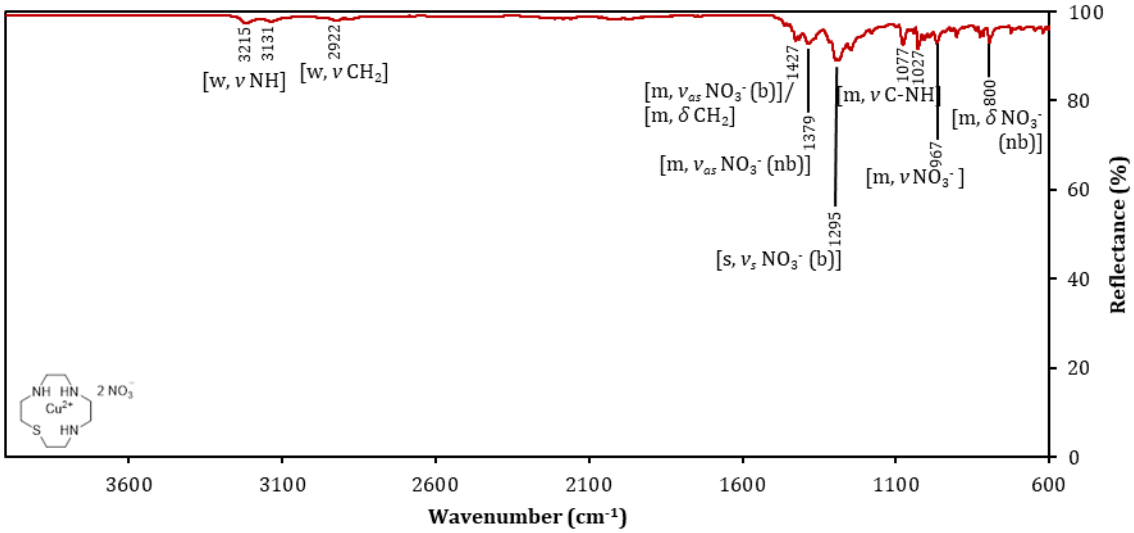


Figure S-2.2b IR spectrum of complex Cu**L**[2].

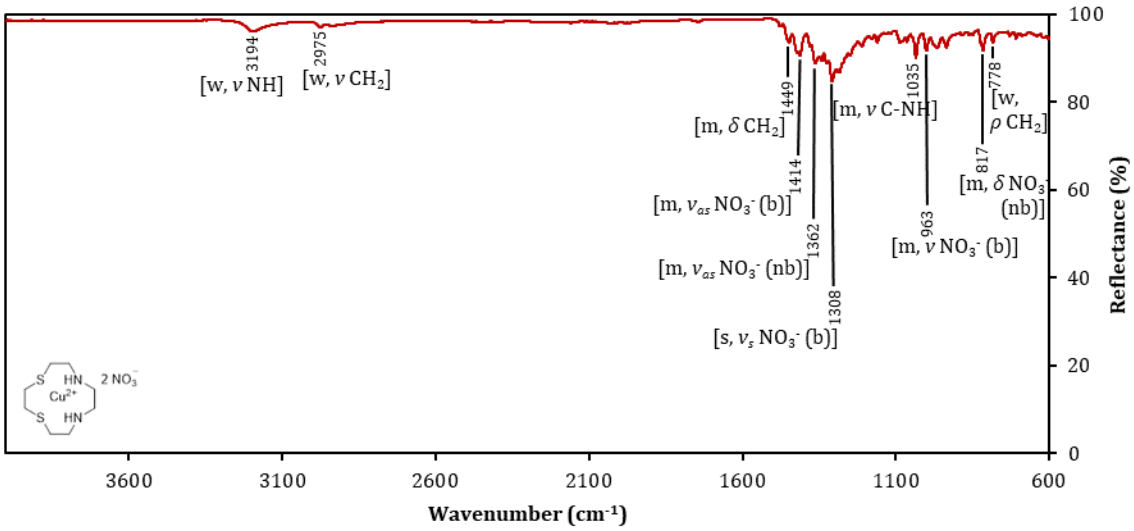


Figure S-2.2c IR spectrum of complex Cu**L**³.

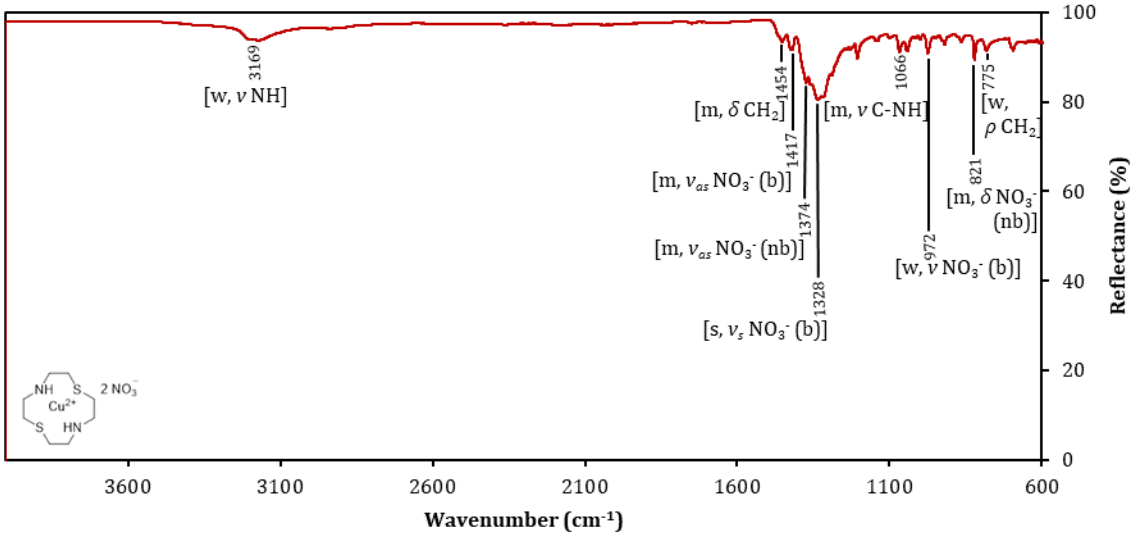


Figure S-2.2d IR spectrum of complex Cu**L**⁴.

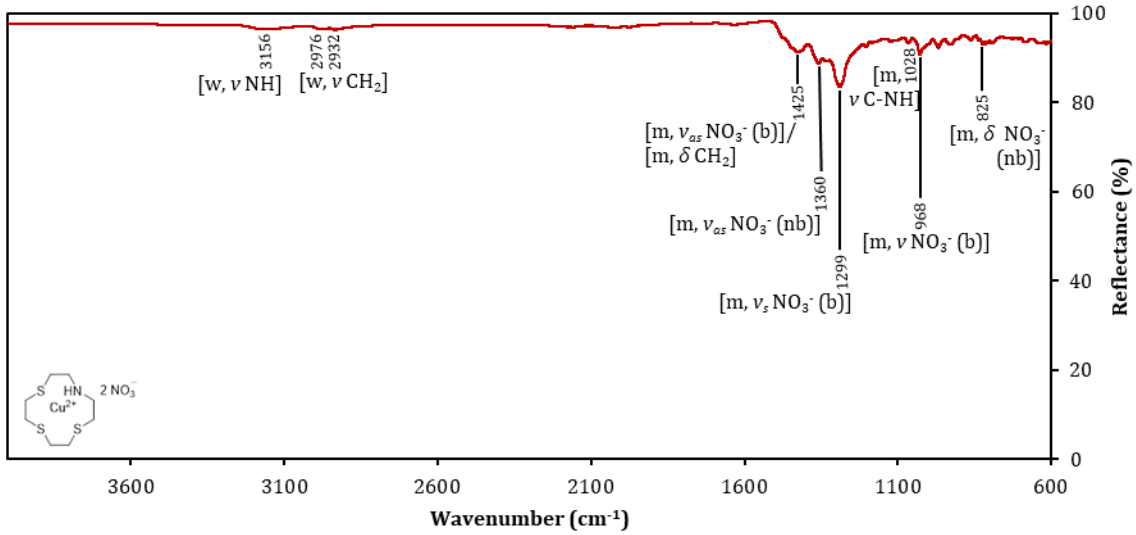


Figure S-2.2e IR spectrum of complex Cu**L**[5].

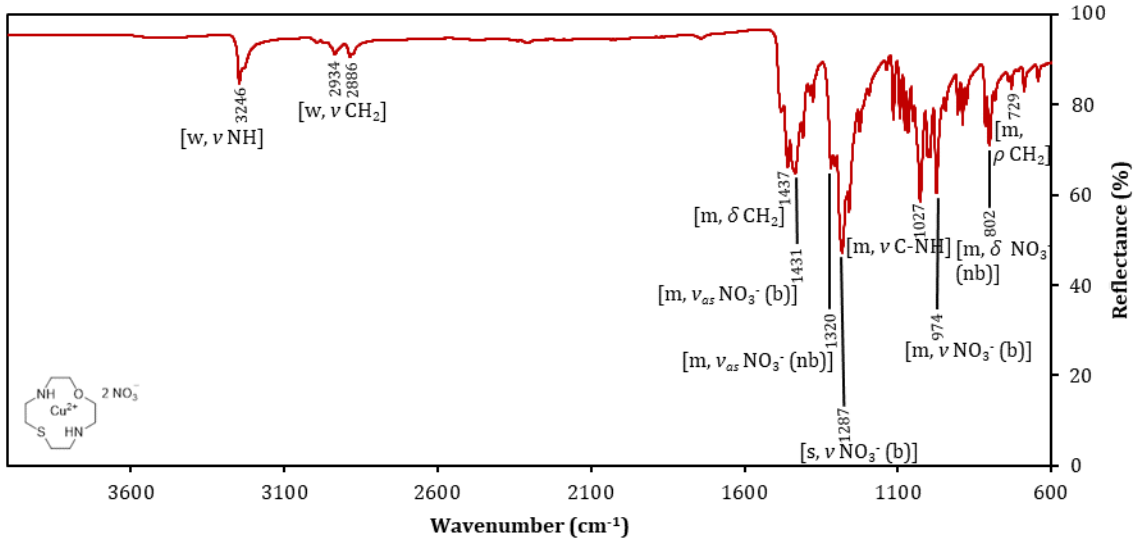


Figure S-2.2f IR spectrum of complex Cu**L**[6].

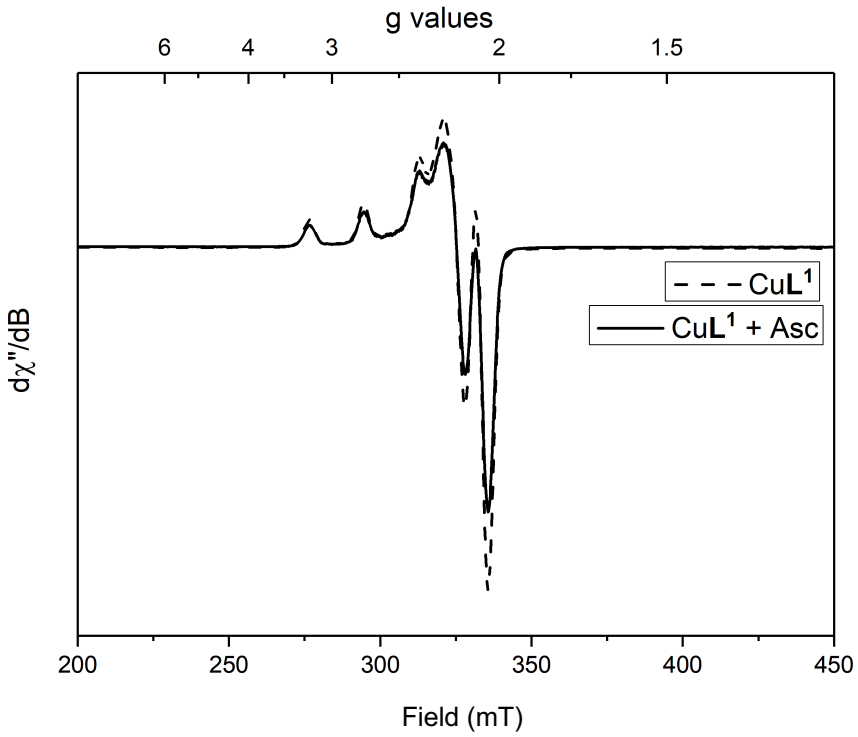


Figure S-2.3a Measured EPR spectra of complex Cu**L**^{1} (1 mM) in 50 mM Tris-HCl buffer (pH 7.4) before (dashed line) and after (solid line) addition of ascorbic acid (8 mM).

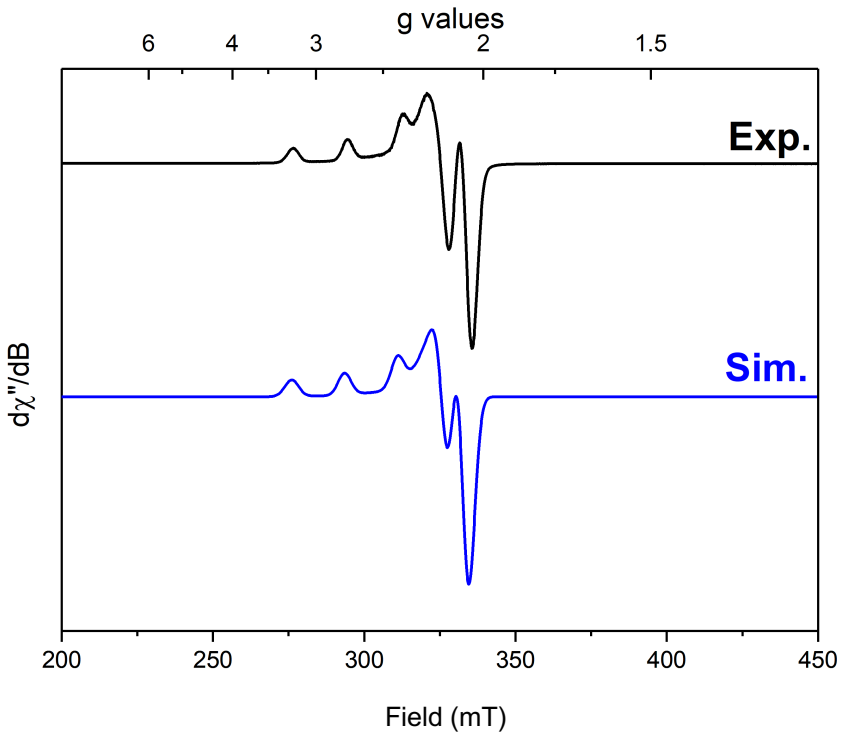


Figure S-2.3b Simulated EPR spectrum of complex Cu**L**^{1} (blue line) in comparison to the measured spectrum (black line). Simulated parameters: g = 2.21, 2.06, 2.03, A = 528, 51, 2 MHz.

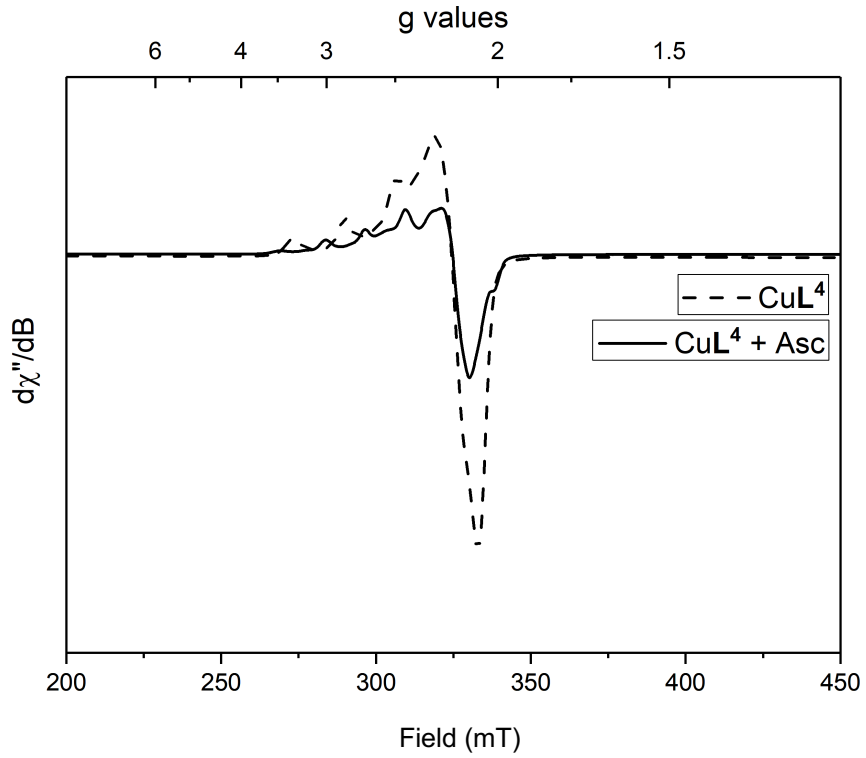


Figure S-2.4a Measured EPR spectra of complex Cu**L**⁴ (1 mM) in 50 mM Tris-HCl buffer (pH 7.4) before (dashed line) and after (solid line) addition of ascorbic acid (8 mM).

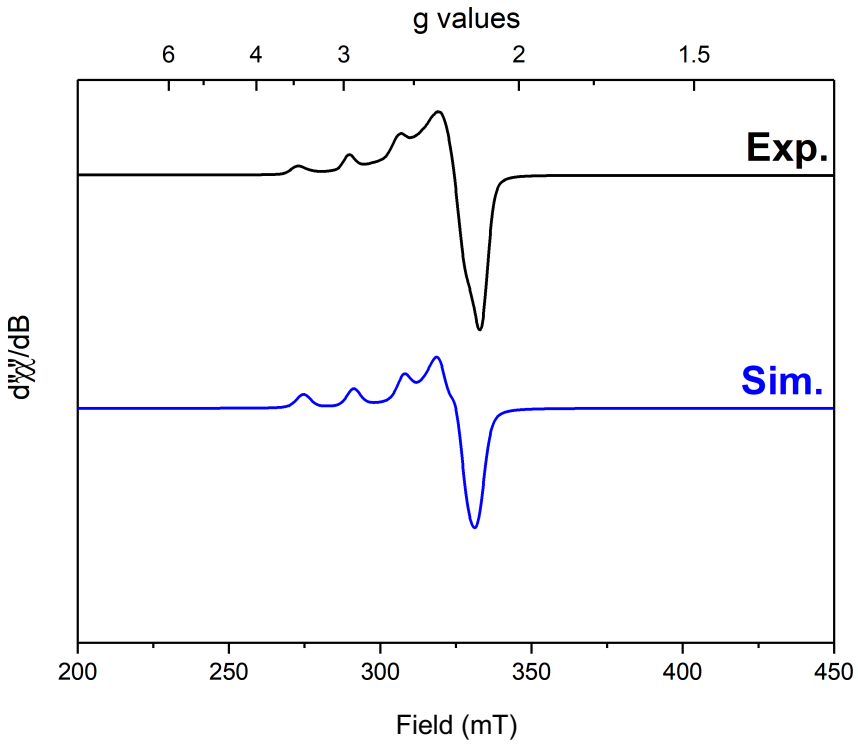


Figure S-2.4b Simulated EPR spectrum of complex Cu**L**⁴ (blue) in comparison to the measured spectrum (black) in absence of ascorbic acid. Simulating parameters: *g* = 2.23, 2.09, 2.05; A = 507, 31, 7 MHz.

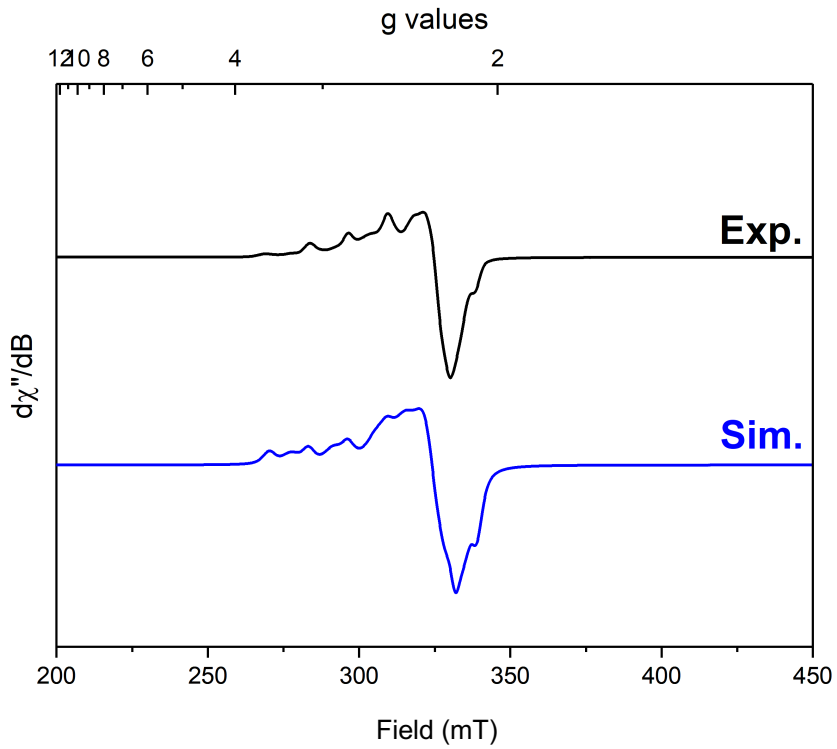


Figure S-2.4c Simulated EPR spectrum of complex Cu**L**^{4} (blue) in comparison to the measured spectrum (black) in the presence of ascorbic acid.

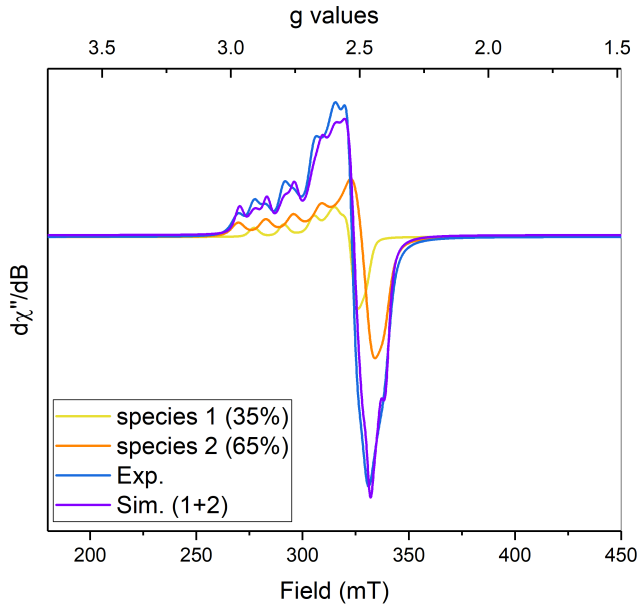


Figure S-2.4d Superimposition of the experimental EPR spectrum of complex Cu**L**^{4} (blue) in the presence of ascorbate (8 mM), the overall simulated curve (purple) and the single components of the overall simulated curve, corresponding to two different species. Simulated parameters: species 1: g = 2.24, 2.11, 2.05, A= 430, 30, 6 MHz, 35% (yellow); species 2: g = 2.31, 2.04, 2.00, A= 410, 50, 88 MHz, 65% (orange).

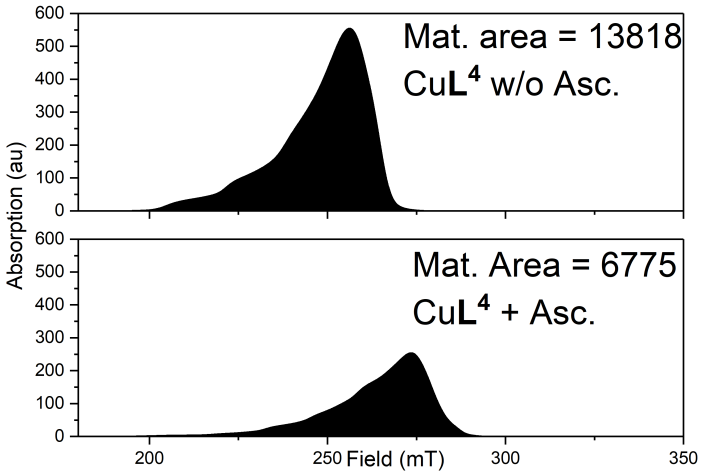


Figure S-2.4e Spin quantification of the EPR signal of Cu**L⁴** (1 mM) before (top) and after (bottom) the addition of ascorbic acid. The halved spin quantity after addition of ascorbic acid suggests the formation of an EPR silent species under the experimental conditions (perpendicular mode) such as the dimeric species predicted by DFT calculations (see main text).

S-3 X-ray crystallography

Table S-3 Crystallographic data for complex Cu**L**^{3}.

Name	Cu([12]aneN$_2$S$_2$)
CCDC deposition number	1569176
Empirical formula	$C_8H_{18}CuN_4O_6S_2$
M [g mol^{-1}]	393.92
Appearance	darkblue needles
Crystal system	monoclinic
Space group	$P2_1/n$
a [Å]	9.1896(2)
b [Å]	12.3669(3)
c [Å]	12.9821(3)
α; β; γ [°]	90; 100.1510(7); 90
Volume [Å^3]	1452.28(6)
Z	4
Density [g cm^{-3}]	1.802
Temperature [K]	99.93
θ *range* [°]	4.584 – 56.636
F(000)	812.0
μ [mm^{-1}]	1.824
Reflections collected	11688
Independent reflections	3568 (R_{int} = 0.0184)
***R*$_1$ / *wR*$_2$ [all data]**	0.0244 / 0.0714
***R*$_1$ / *wR*$_2$ [I > 2σ(I)]**	0.0223 / 0.0714
goodness of fit	1.180

S-4 Summary of stability constants

Table S-4 Stability constants of complexes Cu**L**^{1}–Cu**L**^{6}.

Complex	log*K*	Method	T [°C]	Conditions	Reference
Cu**L**^{1} (Cu^{II})	23.3	Potentiometry	25	H_2O, 0.1 M $NaNO_3$	[10]
Cu**L**^{2} (Cu^{II})	18.0	Potentiometry	25	H_2O, 0.2 $NaClO_4$	[11]
Cu**L**^{2} (Cu^{I})	17.5	Calculation (*vide infra*)			
Cu**L**^{3} (Cu^{II})	14.0	Potentiometry	20	H_2O, 0.2 M Na_2SO_4	[12]
Cu**L**^{3} (Cu^{I})	13.1	Potentiometry	20	2% v/v MeCN, 0.2 M Na_2SO_4	[12]
Cu**L**^{4} (Cu^{II})	11.7	Potentiometry	20	H_2O, 0.2 M Na_2SO_4	[12]
Cu**L**^{4} (Cu^{I})	12.3	Potentiometry	20	2% v/v MeCN, 0.2 M Na_2SO_4	[12]
Cu**L**^{5} (Cu^{II})	7.9	Potentiometry	25	H_2O, 0.1 M NMe_4NO_3	[13]
Cu**L**^{5} (Cu^{I})	15.2	Calculation (*vide infra*)			
Cu**L**^{6} (Cu^{II})	9.8	Potentiometry	25	H_2O, 0.1 M NMe_4NO_3	[13]
Cu**L**^{6} (Cu^{I})	13.5	Calculation (*vide infra*)			
Cu^{II}(tetrathiacyclen)	3.4	Spectroscopy	25	H_2O, 0.1 M $HClO_4$	[14]
Cu^{I}(tetrathiacyclen)	12.9	Calculation	25	H_2O, 0.1 M $HClO_4$	[14]
Cu-Tris system	5.3–6.3*	Potentiometry	25	H_2O, 0.1 M KNO_3	[15]

*For [Cu] = 100 µM and [Tris] = 0.01–0.1 M.[15]

For complexes Cu**L**^{1}, Cu**L**^{2}, Cu**L**^{5} and Cu**L**^{6}, no stability constants have been reported in the literature in the case of Cu(I). According to Osella *et al.*,[16] stability constants can be derived from electrochemical potentials by application of the Nernst equation:

$$E^{0}_{complex} - E^{o}_{free} = -0.059\ log\left(\frac{K_{ox}}{K_{red}}\right)$$

$$\rightarrow\ logK_{red} = logK_{ox} + \frac{E^{0}_{complex} - E^{o}_{free}}{0.059}$$

Using the respective stability constants tabulated in Table S-4 for Cu(II), and the experimentally determined potentials (Table 2 in the manuscript and $E_{1/2}$ = -0.57 V for free Cu(II)[1] measured under the same conditions). For Cu**L**^{1}, no calculation could be carried out, because of the redox process being irreversible and $E_{1/2}$ thus not being available.[1]

S-5 Further DNA cleavage studies and ROS detection

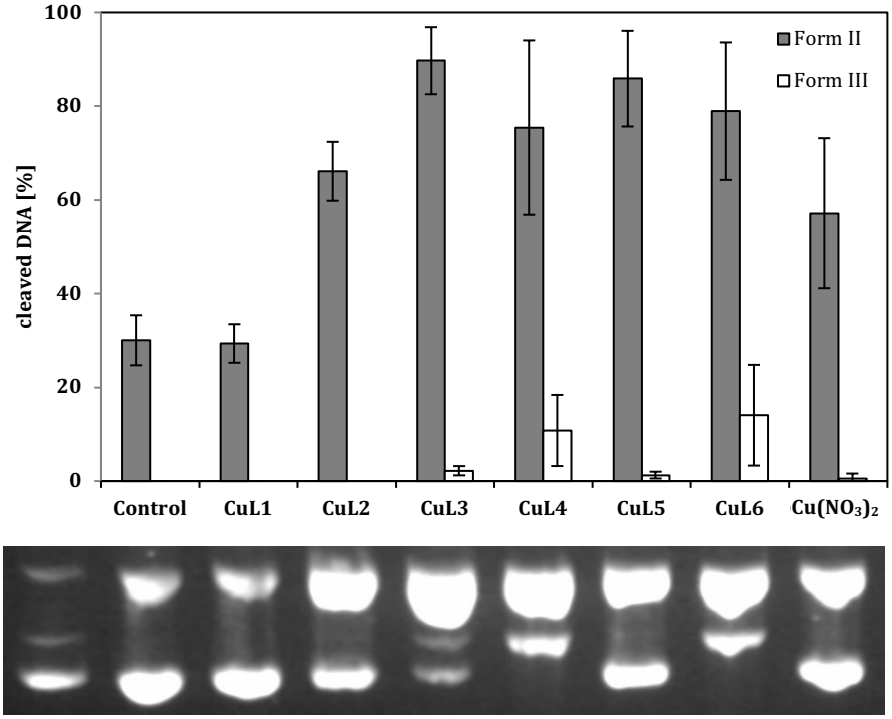


Figure S-5.1 Cleavage activities of complexes Cu**L**^{1}–Cu**L**^{6} and $Cu(NO_3)_2$ (0.04 mM) on pBR322 plasmid DNA (0.025 μg μL^{-1}) in Tris-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

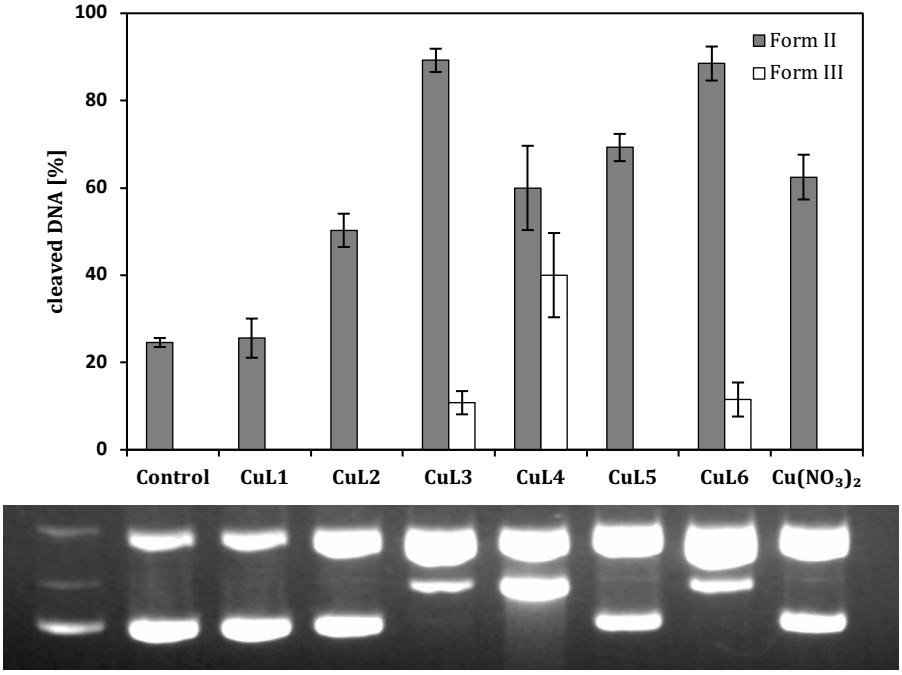


Figure S-5.2 Cleavage activities of complexes Cu**L**^{1}–Cu**L**^{6} and $Cu(NO_3)_2$ (0.04 mM) on pBR322 plasmid DNA (0.025 μg μL^{-1}) in MOPS buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

Table S-5 Quench assay for oxidative DNA cleavage: Summary of the quench experiments for Cu**L**^{1}–Cu**L**^{6} (0 no inhibition, + enhanced cleavage, - small inhibition, -- medium inhibition, --- strong inhibition).

	ROS	Cu**L**^{1}	Cu**L**^{2}	Cu**L**^{3}	Cu**L**^{4}	Cu**L**^{5}	Cu**L**^{6}
DMSO	$^{\cdot}$**OH**	0	––	0	–	–––	0
NaN_3	^{1}**O**$_2$	0	–	0	-	--	0
Pyruvate	**O**$_2^{2-}$	0	––	––	–	–––	–
SOD	**O**$_2^{\cdot-}$	0	0	0	0	-	(+)*

* For complex Cu**L**^{6}, the cleavage activity seems enhanced in the presence of the superoxide scavenger SOD. This effect is not significant, however, when the error bars of this experiment are compared with the ones from the experiments for complexes Cu**L**^{1}-Cu**L**^{5}.

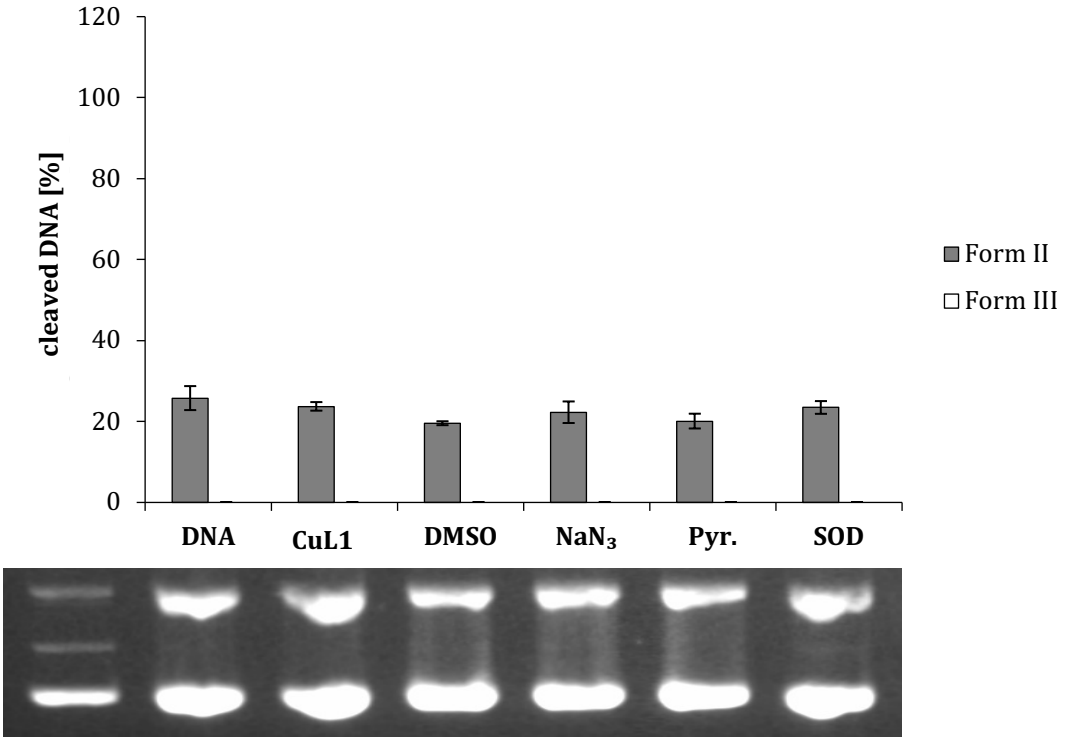


Figure S-5.3 Cleavage activities of complex Cu**L**^{1} (0.04 mM) on pBR322 plasmid DNA (0.025 μg μL^{-1}) in TRIS-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h in the presence of the indicated ROS scavengers. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

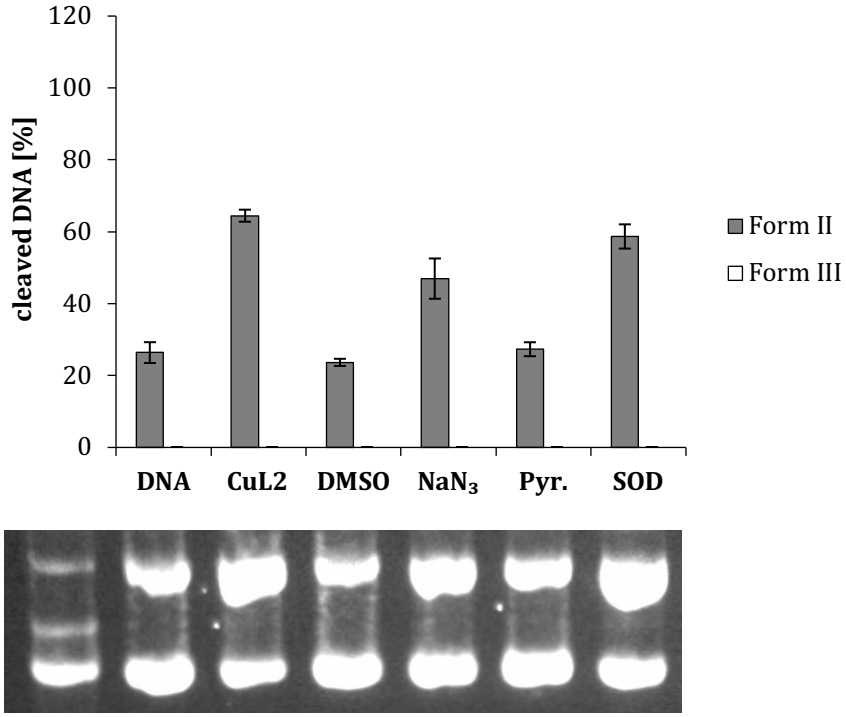


Figure S-5.4 Cleavage activities of complex Cu**L²** (0.04 mM) on pBR322 plasmid DNA (0.025 µg µL^{-1}) in TRIS-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h in the presence of the indicated ROS scavengers. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

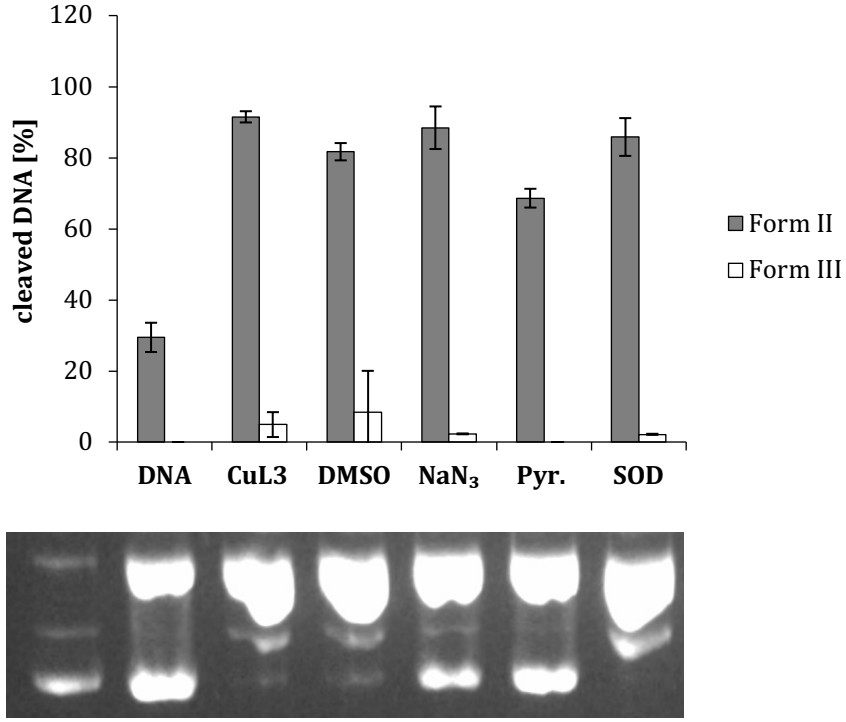


Figure S-5.5 Cleavage activities of complex Cu**L³** (0.04 mM) on pBR322 plasmid DNA (0.025 µg µL^{-1}) in TRIS-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h in the presence of the indicated ROS scavengers. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

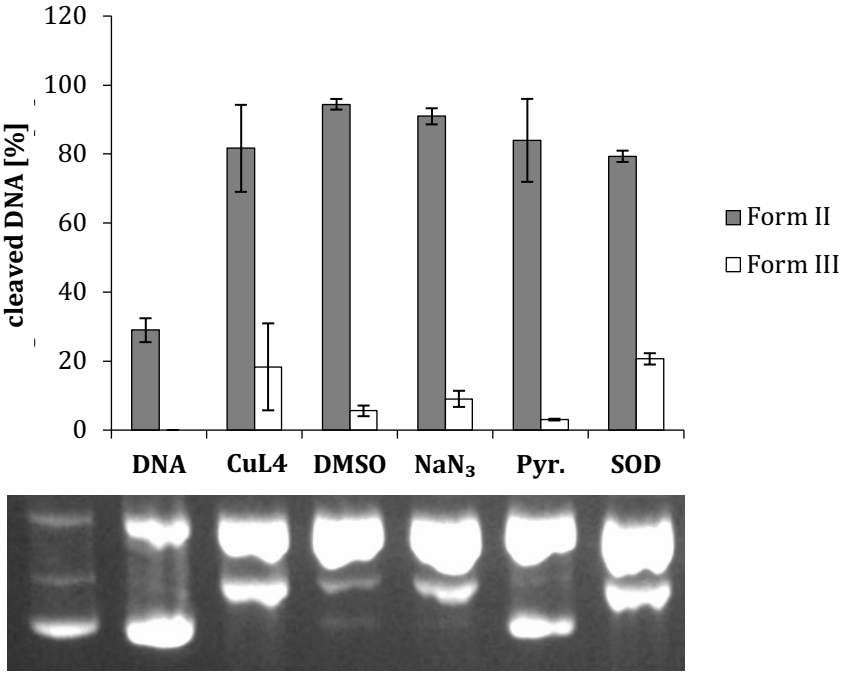


Figure S-5.6 Cleavage activities of complex Cu**L**[4] (0.04 mM) on pBR322 plasmid DNA (0.025 μg μL^{-1}) in TRIS-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h in the presence of the indicated ROS scavengers. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

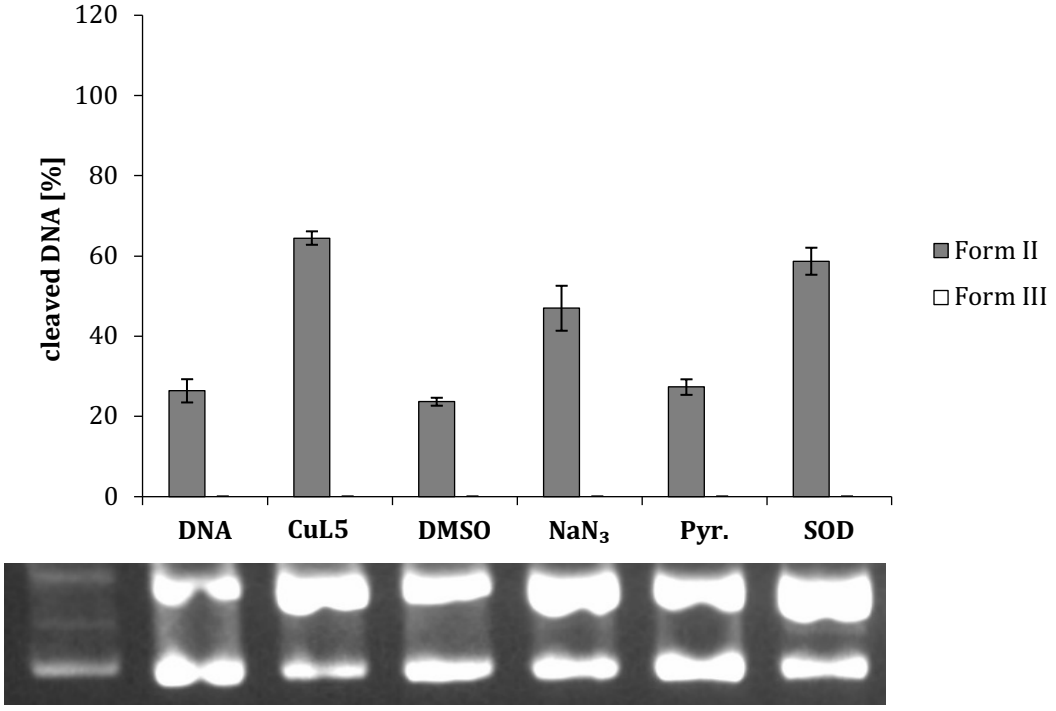


Figure S-5.7 Cleavage activities of complex Cu**L**[5] (0.04 mM) on pBR322 plasmid DNA (0.025 μg μL^{-1}) in TRIS-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h in the presence of the indicated ROS scavengers. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

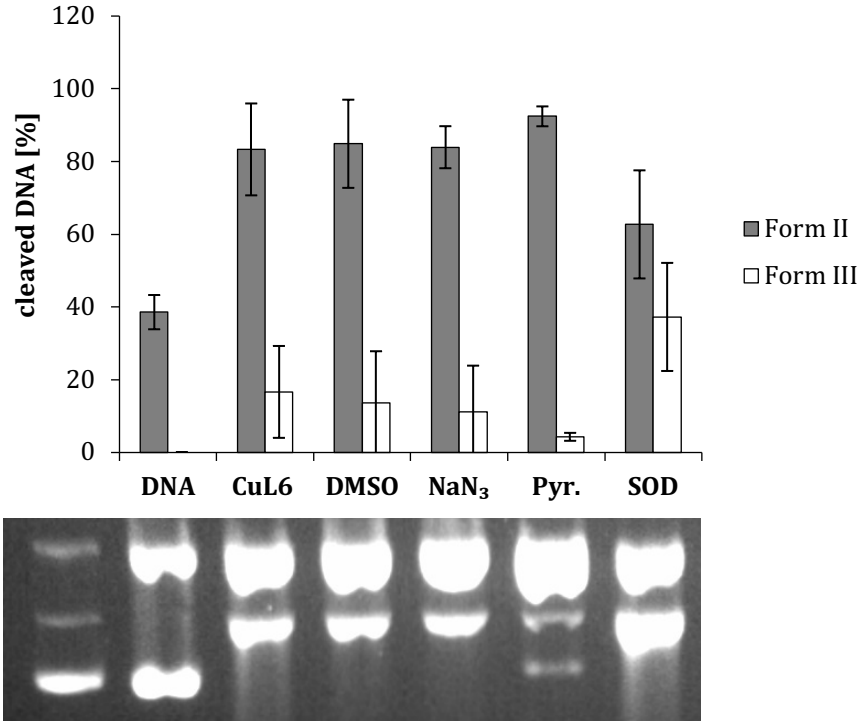


Figure S-5.8 Cleavage activities of complex Cu**L**^{6} (0.04 mM) on pBR322 plasmid DNA (0.025 µg µL^{-1}) in TRIS-HCl buffer (50 mM, pH 7.4) and ascorbic acid (0.32 mM) at 37 °C for 2 h in the presence of the indicated ROS scavengers. Illustrated is the average of three experiments, the standard deviations are shown as error bars (top) and a representative agarose gel (bottom).

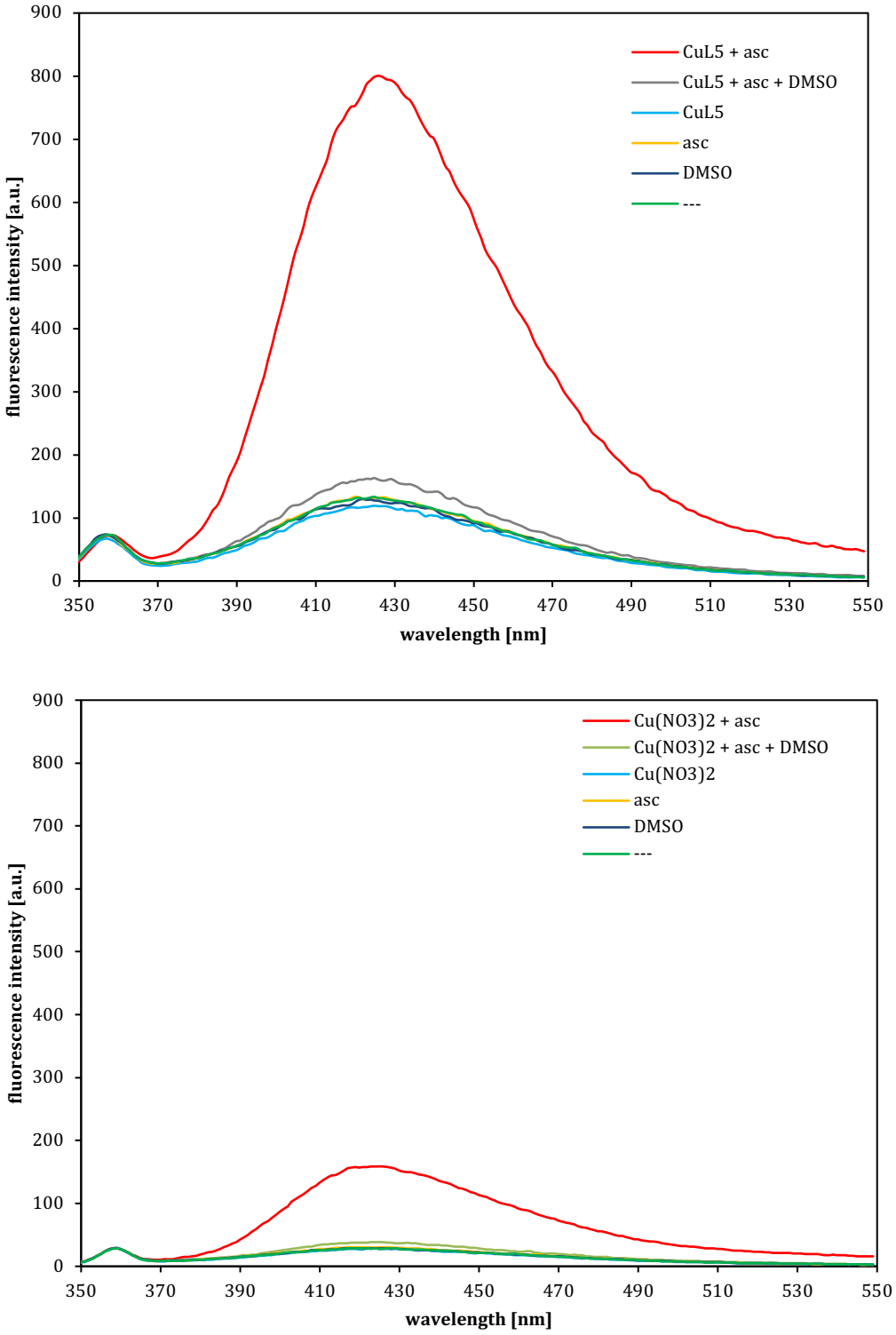


Figure S-5.9 Fluorescence spectra (λ_{ex}=320 nm) of TPA[17] (50 µM) in the presence of 40 µM Cu**L**[5] (top) and $Cu(NO_3)_2$ (bottom), respectively, ascorbic acid as reducing agent (0.25 mM) and with (grey line) or without (red line) DMSO (200 mM) as a scavenger for hydroxyl radicals in Tris-HCl buffer (50 mM, pH 7.4) after incubation for 2.5 h at 37 °C. Activation of TPA just by interacting with the Cu(II) complex/salt can be excluded (blue line).

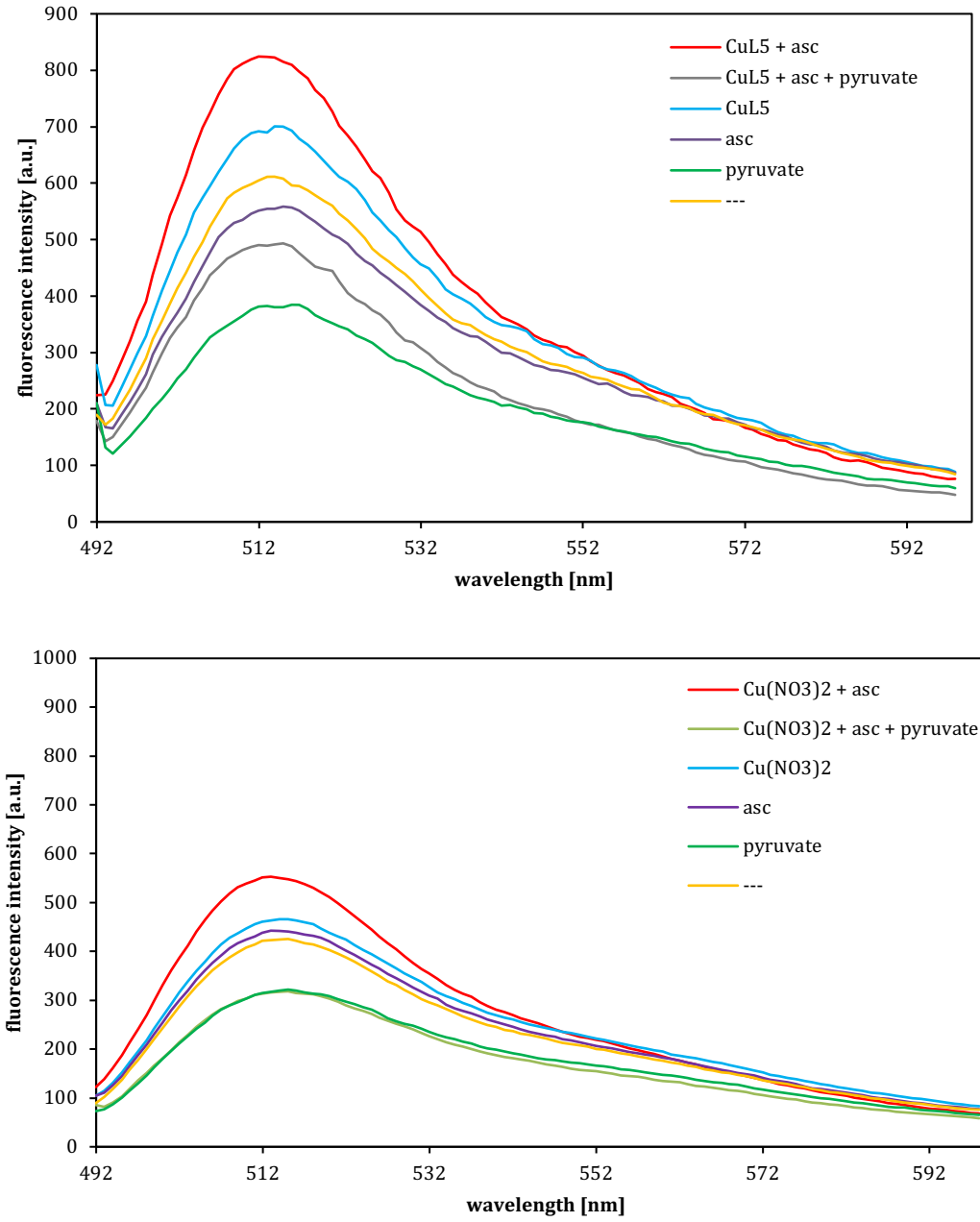


Figure S-5.10a Fluorescence spectra (λ_{ex}=485 nm) of PBSF[17] (25 µM) in the presence of 40 µM Cu**L**[5] (top) and $Cu(NO_3)_2$ (bottom), respectively, ascorbic acid (0.25 mM) and with (grey line) or without (red line) pyruvate (2 mM) as a scavenger for hydrogen peroxide in **Tris-HCl buffer** (50 mM, pH 7.4) after incubation for 2.5 h at 37 °C. Activation of PBSF just by interacting with the Cu(II) complex/salt (background reaction, blue line) is possible, but the intensity is increased in the presence of the reducing agent, which initiates the generation of hydrogen peroxide.

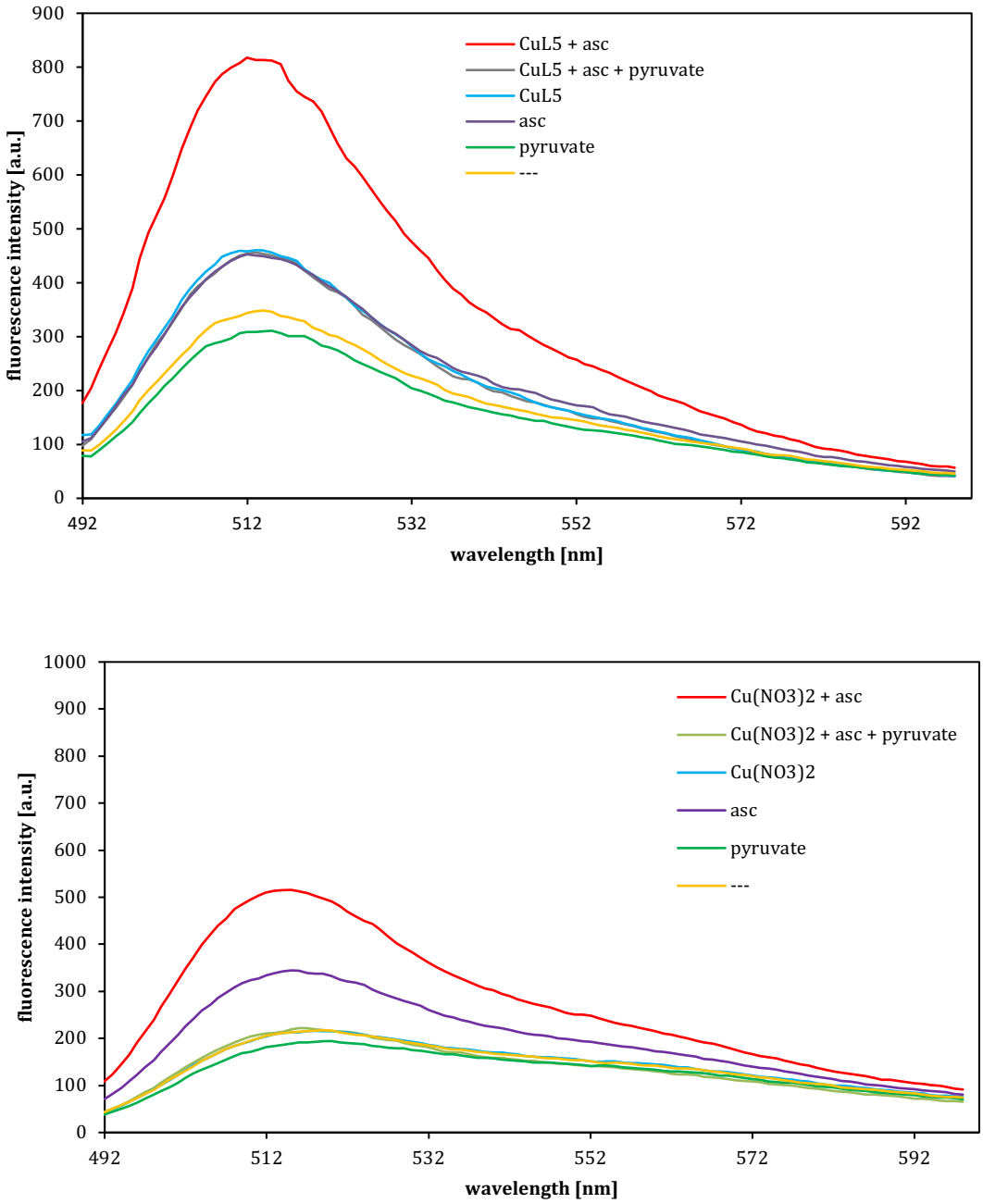


Figure S-5.10b Fluorescence spectra (λ_{ex}=485 nm) of PBSF[17] (25 µM) in the presence of 40 µM Cu**L**[5] (top) and $Cu(NO_3)_2$ (bottom), respectively, ascorbic acid (0.25 mM) and with (grey line) or without (red line) pyruvate (2 mM) as a scavenger for hydrogen peroxide in **MOPS buffer** (50 mM, pH 7.4) after incubation for 2.5 h at 37 °C. Activation of PBSF just by interacting with the Cu(II) complex/salt (background reaction, blue line) is possible, but the intensity is significantly increased in the presence of the reducing agent, which initiates the generation of hydrogen peroxide.

S-6 BNPP assay

BNPP (bis(4-nitrophenyl) phosphate) cleavage activity of the complexes was measured by UV/VIS spectroscopy. First BNPP (Sigma Aldrich, 0.08 mM) and Tris-HCl buffer (50 mM, pH 7.5, Fisher Scientific) were mixed with the complexes (0.4 mM) or with phosphodiesterase (Crotalus atrox, 0.05 U, Sigma). Deionized water (Millipore system) was added up to a total reaction volume of 1 mL before the samples were incubated for up to 8 d at 37 °C. After incubation, samples were analyzed by UV/VIS spectroscopy: 500 µL of the incubation solution were diluted with 500 µL of deionized water, the solution was filled in precision cells made of quartz (1 cm) and measured using a Varian Cary 100 spectrophotometer at 25 °C.

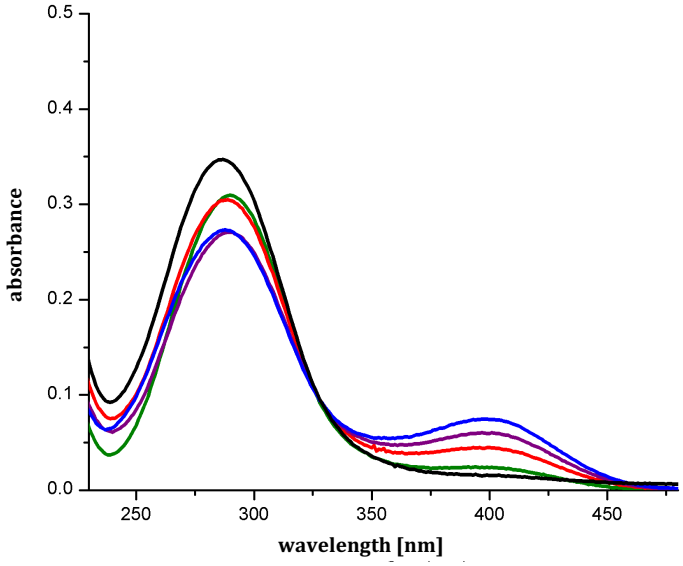


Figure S-6.1 UV/VIS spectra of BNPP (0.08 mM) in the absence (black line) and presence of complex Cu**L**^{6} (1 mM) in 50 mM Tris-HCl buffer (pH 7.5) after an incubation for 2 (green line), 4 (red line), 6 (purple line) and 8 d (blue line) at 37 °C. The absorbance of the complexes at the respective concentration were subtracted.

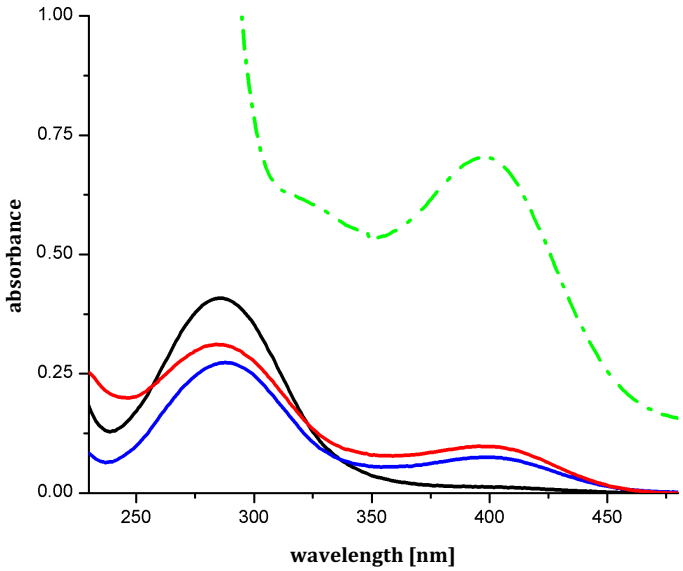


Figure S-6.2 UV/VIS spectra of BNPP (0.08 mM) in the absence (black line) and presence of complex Cu**L**^{6} (0.4 mM – black line, 1 mM – blue line, 2 mM – red line) and phosphodiesterase (0.05 U – green line), respectively, in 50 mM Tris-HCl buffer (pH 7.5) after an incubation of 8 d (for phosphodiesterase only 2 d) at 37 °C. The absorbance of the complexes at the respective concentration were subtracted.

For comparison, the background spectra (no addition of BNPP) are given here:

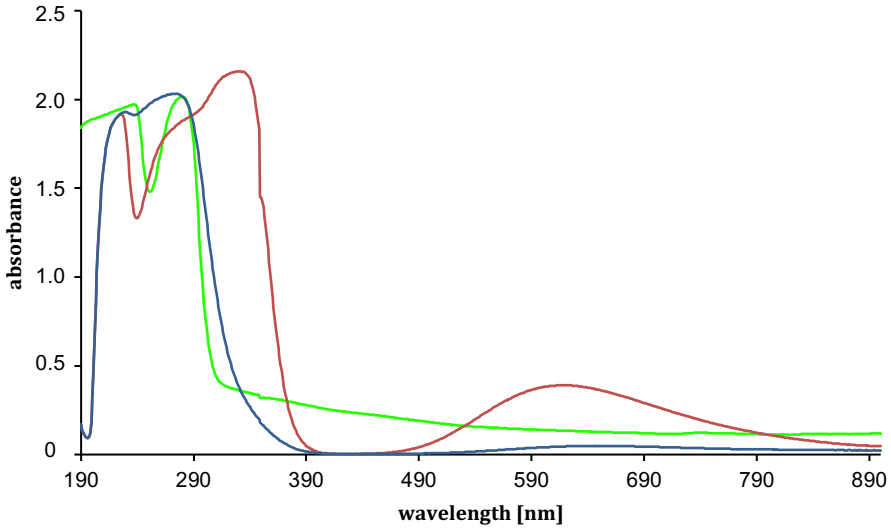


Figure S-6.3 UV/VIS spectra of complexes Cu**L**^{2} and Cu**L**^{6} (1 mM – red and blue line, respectively) and phosphodiesterase (0.05 U – green line) in Tris-HCl buffer (pH 7.5, 50 mM).

S-7 Computational studies: Intrinsic reaction coordinates, structural parameters and cartesian coordinates of optimized structures

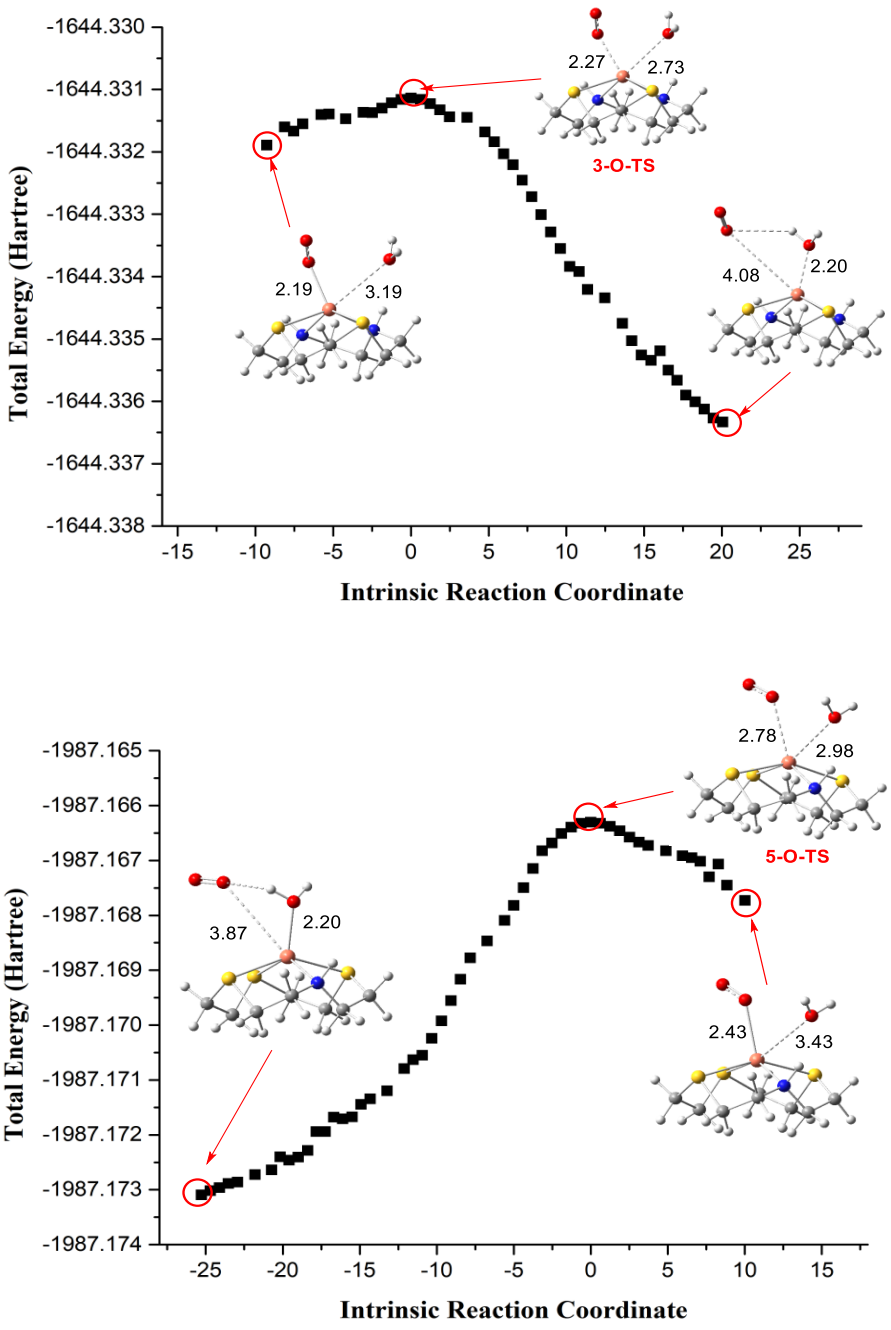


Figure S-7 Intrinsic reaction coordinates for n-O-TS (n=3 top, n=5 bottom).

Table S-7.1 Structural parameters of optimized stationary structures in the generation of ROS mediated by Cu(I)**L**^{n} complexes.

Structural parameters	B(Cu-O1)[a]	B(O2-O3)[b]	B(Cu-O2)	B(Cu-O3)	A(O3-O2-Cu)[c]	A(O1-Cu-O2)	B(Cu-N1)	B(Cu-N2)	B(Cu-N3)	B(Cu-N4)
1-O-RC	2.21	1.21	4.42	5.63	171.54	42.83	2.26	2.28	2.26	2.28
1-O-TS1	2.18	1.23	2.93	3.63	115.48	70.82	2.27	2.28	2.22	2.42
1-O-IM	2.21	1.27	2.14	2.96	118.21	81.74	2.23	2.28	2.27	2.42
1-O-TS2	2.43	1.27	2.06	2.78	111.04	81.57	2.19	2.26	2.34	2.34
1-O-PC	4.09	1.24	2.03	2.88	120.78	73.05	2.19	2.26	2.24	2.27
Structural parameters	B(Cu-O1)	B(O2-O3)	B(Cu-O2)	B(Cu-O3)	A(O3-O2-Cu)	A(O1-Cu-O2)	B(Cu-S1)	B(Cu-N2)	B(Cu-N3)	B(Cu-N4)
2-O-RC	2.20	1.21	4.64	5.82	165.13	37.43	2.55	2.27	2.28	2.26
2-O-TS1	2.19	1.23	2.76	3.51	117.90	74.19	2.69	2.27	2.26	2.23
2-O-IM	2.19	1.26	2.16	2.97	118.18	82.67	2.79	2.24	2.28	2.26
2-O-TS2	2.70	1.26	2.05	2.75	109.87	79.52	2.58	2.18	2.25	2.35
2-O-PC	3.80	1.26	2.03	2.56	99.53	87.22	2.59	2.15	2.26	2.27
Structural parameters	B(Cu-O1)	B(O2-O3)	B(Cu-O2)	B(Cu-O3)	A(O3-O2-Cu)	A(O1-Cu-O2)	B(Cu-S1)	B(Cu-S2)	B(Cu-N3)	B(Cu-N4)
3-O-RC	2.20	1.21	4.47	5.66	166.86	41.11	2.60	2.50	2.27	2.29
3-O-TS	2.73	1.23	2.27	2.73	119.39	74.18	2.58	2.56	2.24	2.28
3-O-PC	4.13	1.23	2.13	2.99	123.61	68.53	2.57	2.52	2.20	2.27
Structural parameters	B(Cu-O1)	B(O2-O3)	B(Cu-O2)	B(Cu-O3)	A(O3-O2-Cu)	A(O1-Cu-O2)	B(Cu-S1)	B(Cu-N2)	B(Cu-S3)	B(Cu-N4)
4-O-RC	2.20	1.21	4.72	5.54	127.13	34.98	2.58	2.25	2.56	2.25
4-O-TS1	2.30	1.23	2.47	3.33	124.41	72.61	2.59	2.25	2.63	2.24
4-O-IM	2.44	1.24	2.19	3.07	124.63	75.17	2.60	2.22	2.62	2.28
4-O-TS2	2.85	1.24	2.13	3.00	123.90	74.36	2.56	2.22	2.55	2.30
4-O-PC	4.08	1.23	2.15	3.02	123.91	69.27	2.55	2.21	2.53	2.24
Structural parameters	B(Cu-O1)	B(O2-O3)	B(Cu-O2)	B(Cu-O3)	A(O3-O2-Cu)	A(O1-Cu-O2)	B(Cu-S1)	B(Cu-S2)	B(Cu-S3)	B(Cu-N4)
5-O-RC	2.18	1.21	4.58	5.73	158.35	38.28	2.63	2.48	2.59	2.25
5-O-TS	2.98	1.22	2.78	3.67	129.36	66.62	2.57	2.48	2.56	2.19
5-O-PC	4.11	1.23	2.20	3.06	124.41	68.97	2.64	2.54	2.60	2.20
Structural parameters	B(Cu-O1)	B(O2-O3)	B(Cu-O2)	B(Cu-O3)	A(O3-O2-Cu)	A(O1-Cu-O2)	B(Cu-S1)	B(Cu-N2)	B(Cu-O3)	B(Cu-N4)
6-O-RC	2.17	1.21	4.64	5.07	103.98	59.12	2.45	2.19	2.55	2.20
6-O-TS1	2.17	1.23	2.51	3.30	119.23	76.75	2.61	2.52	2.26	2.14
6-O-IM	2.17	1.25	2.27	3.08	119.41	80.38	2.64	2.52	2.26	2.15
6-O-TS2	2.80	1.24	2.09	2.86	115.55	75.75	2.55	2.48	2.16	2.22
6-O-PC	4.07	1.23	2.09	2.91	120.01	70.76	2.51	2.43	2.14	2.17

[a]Bond length (in Å), and O1 is the oxygen atom in the water molecule. [b]O2 and O3 are the oxygen atoms in the O_2 molecule, O2 is closer to the metal center and O3 is farther away from the metal center. [c]Bond angle (in degrees).

Table S-7.2 Cartesian coordinates of optimized structures

$[Cu^{I}\mathbf{L^{1}}(H_2O)]^{+}$

H	1.550349	-2.295331	0.722034
H	-2.347406	-1.574548	0.689913
H	-1.550111	2.295123	0.723669
Cu	0.000195	-0.000204	0.944028
C	1.267973	1.904961	-1.013815
H	2.016313	2.614974	-1.398360
H	0.958258	1.288327	-1.864005
C	0.063958	2.691278	-0.474321
H	0.388505	3.317941	0.364754
H	-0.300265	3.370378	-1.260784
C	-1.904879	1.264590	-1.007986
H	-1.296141	0.961799	-1.866358
H	-2.607703	2.027730	-1.376456
C	-2.705389	0.062462	-0.485563
H	-3.338558	0.386210	0.349060
H	-3.379297	-0.288445	-1.282676
C	-1.268474	-1.904506	-1.014061
H	-0.959143	-1.287502	-1.864125
H	-2.016999	-2.614345	-1.398567
C	-0.064212	-2.691054	-0.475458
H	-0.388370	-3.318068	0.363506
H	0.299643	-3.369826	-1.262375
C	1.904397	-1.264145	-1.009402
H	1.295292	-0.961002	-1.867392
H	2.607071	-2.027125	-1.378492
C	2.705133	-0.062236	-0.486816
H	3.378696	0.289008	-1.284073
H	3.338665	-0.386343	0.347391
N	-0.999419	1.797121	0.026629
N	-1.827515	-1.012556	0.018498
N	0.999383	-1.797101	0.025373
O	0.001502	-0.001674	3.171423
H	-0.684265	-0.364811	3.754376
H	0.686449	0.363539	3.754043
N	1.827490	1.012575	0.018101
H	2.347701	1.574279	0.689509

$[Cu^{I}\mathbf{L^{1}}(OH)]$

H	-1.616093	2.117070	0.990508
H	2.340809	1.720706	0.651085
H	1.382243	-1.748443	0.646446
Cu	-0.074816	0.125150	1.254456
C	-1.292516	-1.880543	-1.164486
H	-1.976107	-2.648561	-1.573679
H	-1.081261	-1.182670	-1.983871
C	0.028047	-2.542330	-0.720822
H	-0.180868	-3.211810	0.122250
H	0.399424	-3.175858	-1.547790
C	1.934813	-1.021363	-1.239400
H	1.380312	-0.703222	-2.135274
H	2.687946	-1.753381	-1.599251
C	2.710506	0.172072	-0.649883
H	3.344917	-0.199180	0.163123
H	3.383035	0.570613	-1.433092
C	1.111233	2.071843	-0.958590
H	0.758935	1.475717	-1.807291
H	1.723756	2.888104	-1.386979

C -0.090901 2.704509 -0.237815
H 0.269027 3.256812 0.638106
H -0.576276 3.431353 -0.910489
C -1.985548 1.226899 -0.810303
H -1.384590 0.993690 -1.694256
H -2.687755 2.025121 -1.103061
C -2.774794 -0.023501 -0.393599
H -3.490186 -0.257844 -1.204899
H -3.371776 0.206528 0.497968
N 1.000221 -1.562002 -0.282254
N 1.845651 1.195655 -0.063394
N -1.061488 1.694315 0.247286
O 0.748061 -1.119186 2.451252
H 0.721530 -0.929184 3.398389
N -1.884156 -1.124261 -0.064545
H -2.267718 -1.734774 0.649330

$[Cu^{I}\mathbf{L}^{2}(H_2O)]^{+}$
H -0.078971 2.718388 0.757892
H 2.961256 0.121642 0.710328
H 0.373670 -2.726577 0.484533
Cu 0.144097 -0.036115 0.860101
S -2.315152 0.049912 0.148775
C -1.988164 -1.122439 -1.241068
H -2.943258 -1.441480 -1.668870
H -1.429109 -0.598811 -2.022883
C -1.217840 -2.353769 -0.742428
H -1.788790 -2.836969 0.057682
H -1.153700 -3.076981 -1.570311
C 1.188067 -1.941683 -1.217214
H 0.834680 -1.302291 -2.033629
H 1.413924 -2.923916 -1.660606
C 2.473983 -1.364576 -0.610782
H 2.828224 -2.032585 0.183271
H 3.256114 -1.342794 -1.384958
C 2.276845 1.093512 -0.953797
H 1.754069 0.783127 -1.864062
H 3.301394 1.358090 -1.256148
C 1.595461 2.331306 -0.356238
H 2.133131 2.638355 0.548278
H 1.666479 3.163269 -1.073528
C -0.774364 2.135854 -1.071061
H -0.415205 1.498804 -1.885933
H -0.841562 3.158596 -1.477388
C -2.183439 1.703920 -0.648190
H -2.859352 1.747115 -1.507935
H -2.587026 2.390578 0.105260
N 0.117437 -2.023358 -0.206976
N 2.252984 -0.035348 -0.004354
N 0.196298 2.055307 0.034621
O 0.048212 -0.417564 3.040507
H 0.683872 -0.146677 3.722528
H -0.822235 -0.428601 3.470725

$[Cu^{I}\mathbf{L}^{2}(OH)]$
H 0.076933 2.654991 0.764642
H 3.069212 -0.174719 0.323800
H 0.229350 -2.061044 0.561392
Cu 0.452665 0.196332 1.248633
S -2.666019 0.240694 0.348317

C -2.454527 -1.024210 -0.981611
H -3.444297 -1.430318 -1.221353
H -2.078702 -0.526205 -1.882204
C -1.510437 -2.166913 -0.558293
H -1.888023 -2.603322 0.373759
H -1.581443 -2.959127 -1.328052
C 0.795328 -1.875813 -1.438223
H 0.475064 -1.232291 -2.274263
H 0.840282 -2.903798 -1.852983
C 2.223710 -1.504183 -1.002306
H 2.555812 -2.237432 -0.259431
H 2.890594 -1.598737 -1.879130
C 2.282558 0.998764 -1.183368
H 1.678607 0.785798 -2.071866
H 3.275595 1.308411 -1.556917
C 1.679277 2.189462 -0.415309
H 2.314981 2.425793 0.445008
H 1.663613 3.072383 -1.076313
C -0.696325 1.885080 -0.961956
H -0.471351 1.037205 -1.612991
H -0.604303 2.800062 -1.574101
C -2.145368 1.791508 -0.481860
H -2.798552 1.978977 -1.342362
H -2.359948 2.580140 0.250718
N -0.141683 -1.741890 -0.340832
N 2.316091 -0.194522 -0.356095
N 0.318059 1.905160 0.115816
O 0.834598 -1.335136 2.302400
H 0.516255 -1.323821 3.215357

$[Cu^{I}\mathbf{L^{3}}(H_2O)]^{+}$
H -2.823338 0.859751 0.623194
H 0.533378 2.821811 0.478288
Cu -0.090654 0.209990 0.874098
S 2.250488 -0.612186 0.129432
C 2.267651 0.581037 -1.277268
H 3.264899 0.590804 -1.727161
H 1.555927 0.251337 -2.040774
C 1.922008 1.989069 -0.771390
H 2.622436 2.269815 0.022507
H 2.074049 2.700409 -1.597507
C -0.489280 2.358604 -1.229351
H -0.340443 1.670783 -2.068529
H -0.406295 3.377046 -1.638880
C -1.891055 2.176719 -0.635562
H -2.029446 2.889565 0.185692
H -2.640163 2.421007 -1.404138
C -2.444486 -0.200871 -1.079427
H -1.734454 -0.128202 -1.909360
H -3.445319 -0.021473 -1.505083
C -2.422740 -1.617633 -0.494845
H -3.182322 -1.725860 0.288024
H -2.661396 -2.350888 -1.271619
C 0.295465 -2.334795 -1.088110
H 0.051731 -1.608892 -1.869524
H 0.142434 -3.338563 -1.499441
C 1.760966 -2.202832 -0.654965
H 2.411214 -2.384967 -1.516976
H 2.010037 -2.959745 0.096216
N 0.553223 2.082490 -0.223032

N -2.087178 0.820834 -0.080464
O 0.145438 0.759896 2.999278
H -0.538964 0.558512 3.658264
H 0.986997 0.495662 3.406304
S -0.852924 -2.098804 0.336656

[Cu^{I}**L**^{3}(OH)]
H 3.084400 -0.101596 0.069256
H 0.335163 -2.279005 0.445299
Cu 0.603778 -0.085916 1.225053
S -2.760224 0.018276 0.428599
C -2.467421 -1.184055 -0.943145
H -3.430674 -1.629128 -1.217514
H -2.098787 -0.637775 -1.818299
C -1.480849 -2.296745 -0.544507
H -1.813404 -2.740875 0.400595
H -1.552731 -3.093397 -1.310095
C 0.739929 -1.855997 -1.544053
H 0.320516 -1.183711 -2.308358
H 0.794711 -2.855908 -2.019172
C 2.179369 -1.439258 -1.199487
H 2.588726 -2.170532 -0.494953
H 2.787551 -1.483935 -2.120684
C 2.146466 1.059051 -1.352379
H 1.405861 0.865776 -2.135398
H 3.084360 1.325924 -1.874406
C 1.716489 2.281057 -0.520794
H 2.484871 2.528761 0.220044
H 1.585569 3.158518 -1.164612
C -1.053027 1.917289 -0.882771
H -0.732292 1.137736 -1.578668
H -1.047237 2.877401 -1.414345
C -2.473176 1.635454 -0.387397
H -3.157994 1.739764 -1.237828
H -2.775165 2.380227 0.357555
N -0.113609 -1.836085 -0.366970
N 2.265927 -0.135186 -0.532038
O 1.224837 -1.684443 2.076039
H 1.140349 -1.754076 3.036417
S 0.183665 2.043039 0.482063

[Cu^{I}**L**^{4}(H_2O)]$^{+}$
H -0.020368 -2.678403 0.747007
H -0.641103 2.698000 0.398038
Cu -0.368702 0.030039 0.847587
S 2.161092 -0.001055 0.538892
C 2.067205 1.202610 -0.858450
H 3.075457 1.563464 -1.082224
H 1.690822 0.688600 -1.748322
C 1.173504 2.393278 -0.486345
H 1.558471 2.862077 0.425428
H 1.246672 3.143261 -1.289013
C -1.068602 1.927923 -1.442867
H -0.615258 1.198131 -2.122258
H -1.095984 2.889182 -1.982118
C -2.513351 1.530366 -1.122557
H -2.998425 2.303312 -0.514783
H -3.092461 1.446414 -2.047252
C -2.265540 -1.336864 -1.330944
H -1.651248 -0.906109 -2.127835

H -3.178179 -1.730440 -1.788170
C -1.525954 -2.474794 -0.615740
H -2.151814 -2.857496 0.197437
H -1.388623 -3.300355 -1.331065
C 0.895100 -2.074884 -0.972544
H 0.649324 -1.420152 -1.815557
H 1.051968 -3.083226 -1.389620
C 2.206674 -1.628896 -0.318518
H 3.011580 -1.624374 -1.059943
H 2.504736 -2.334169 0.466248
N -0.231414 2.010238 -0.233431
N -0.236440 -2.052133 -0.028076
O -0.688202 0.301959 3.015036
H -1.533362 0.177505 3.476457
H 0.004721 0.290112 3.695066
S -2.721536 -0.007928 -0.134137

[Cu^{I}**L^{4}**(OH)]
H 0.115272 -1.997400 0.520829
H -0.492130 2.615633 0.868227
Cu -0.165664 0.215234 1.363275
S 2.573546 -0.129425 -0.011205
C 2.052930 1.345937 -0.977723
H 2.947121 1.860151 -1.346628
H 1.486701 1.022881 -1.855437
C 1.252163 2.352548 -0.138647
H 1.786045 2.559404 0.794348
H 1.197368 3.296531 -0.707787
C -1.010096 1.874274 -0.960624
H -0.685371 1.046218 -1.594929
H -0.887263 2.803640 -1.543922
C -2.494996 1.715553 -0.636687
H -2.829196 2.513635 0.038750
H -3.061903 1.836468 -1.567409
C -2.622601 -1.121596 -1.073235
H -2.261777 -0.624880 -1.981330
H -3.566368 -1.617210 -1.328150
C -1.612884 -2.170738 -0.573789
H -1.963834 -2.568073 0.384019
H -1.620286 -3.008872 -1.297358
C 0.651435 -1.745868 -1.482146
H 0.379112 -1.006562 -2.252899
H 0.600741 -2.730850 -1.991074
C 2.120624 -1.558648 -1.081003
H 2.741122 -1.553524 -1.984164
H 2.444290 -2.410958 -0.471830
N -0.121427 1.912991 0.225692
N -0.268154 -1.653121 -0.365689
O -0.136794 -1.367482 2.390133
H 0.229577 -1.301211 3.282152
S -2.998383 0.164594 0.198497

[Cu^{I}**L^{5}**(H_2O)]$^{+}$
H 0.239719 -2.792311 0.519169
Cu 0.016617 -0.162200 0.947384
S -2.509442 -0.036134 0.212832
C -2.203783 -1.243512 -1.148519
H -3.165487 -1.582461 -1.544841
H -1.663310 -0.744548 -1.959225
C -1.419032 -2.449974 -0.619578

H -1.948701 -2.880562 0.236838
H -1.398145 -3.221583 -1.404178
C 0.943225 -2.095755 -1.265208
H 0.617770 -1.368966 -2.017125
H 0.990709 -3.074145 -1.770548
C 2.352709 -1.757373 -0.771228
H 2.718083 -2.533474 -0.088523
H 3.047270 -1.728475 -1.616509
C 2.273487 1.092052 -1.096014
H 1.625015 0.698064 -1.884334
H 3.246707 1.319702 -1.544175
C 1.693867 2.381473 -0.502964
H 2.353368 2.780822 0.274612
H 1.623174 3.146452 -1.283525
C -1.098885 2.089021 -1.110957
H -0.667993 1.421671 -1.863815
H -1.220251 3.079579 -1.562983
C -2.473577 1.588493 -0.651794
H -3.150158 1.543613 -1.511459
H -2.916504 2.286951 0.065908
N -0.050563 -2.103686 -0.175319
O -0.074356 -0.720102 3.064243
H 0.653119 -0.482050 3.662236
H -0.893986 -0.543817 3.554798
S 0.055465 2.229714 0.319484
S 2.507852 -0.202092 0.197841

[Cu^{I}**L**^{5}(OH)]
H 0.748426 -2.125604 0.464667
Cu 0.139687 -0.036244 1.399081
S -2.821473 -0.519179 0.175526
C -2.138521 -1.662986 -1.105931
H -2.949003 -2.328400 -1.423591
H -1.840277 -1.073988 -1.980148
C -0.964899 -2.507055 -0.582232
H -1.245098 -2.955348 0.376402
H -0.811487 -3.338143 -1.297589
C 1.143244 -1.618852 -1.512819
H 0.687211 -0.934051 -2.244001
H 1.281502 -2.578704 -2.051597
C 2.552803 -1.133927 -1.148088
H 3.055226 -1.894095 -0.538564
H 3.141630 -1.012993 -2.064185
C 1.953427 1.693287 -1.132145
H 1.338715 1.236620 -1.912480
H 2.740278 2.269362 -1.634024
C 1.127523 2.667993 -0.280517
H 1.726855 3.055664 0.549813
H 0.823553 3.527283 -0.890709
C -1.394953 1.664337 -0.996035
H -0.844542 0.972103 -1.639005
H -1.506601 2.617446 -1.528438
C -2.780873 1.103091 -0.676976
H -3.352458 1.041479 -1.611023
H -3.326025 1.782026 -0.011868
N 0.266257 -1.756031 -0.362527
O 0.593995 -1.620903 2.335127
H 0.769959 -1.566566 3.283487
S -0.394312 1.999396 0.518680
S 2.717153 0.375028 -0.107217

[Cu^{I}**L**^{6}(H_2O)]$^{+}$
H 0.081844 -2.637045 0.785534
H -0.495481 2.612279 0.501343
Cu 0.002310 0.030283 0.932436
S 2.376124 -0.013449 0.385349
C 2.130402 1.194867 -0.996855
H 3.108773 1.578430 -1.300903
H 1.696539 0.669724 -1.853361
C 1.240924 2.364541 -0.550822
H 1.692992 2.849874 0.320474
H 1.220248 3.110142 -1.360208
C -1.071319 1.853218 -1.305088
H -0.616872 1.226158 -2.079494
H -1.255938 2.838746 -1.762133
C -2.413211 1.261494 -0.863001
H -2.872203 1.894601 -0.095835
H -3.102095 1.222551 -1.717707
C -2.156839 -1.119585 -1.174700
H -1.562334 -0.826102 -2.050431
H -3.150923 -1.421166 -1.533318
C -1.506241 -2.291450 -0.447492
H -2.116489 -2.544962 0.425393
H -1.504612 -3.165482 -1.116865
C 0.910163 -2.063896 -0.987493
H 0.621027 -1.420828 -1.824663
H 0.993833 -3.086956 -1.388539
C 2.288753 -1.652304 -0.457559
H 3.022980 -1.679654 -1.268612
H 2.635911 -2.356112 0.307915
N -0.126257 1.942603 -0.173183
N -0.143366 -1.974561 0.043271
O -1.222892 0.409055 2.669086
H -2.139898 0.104831 2.569615
H -0.976165 0.263562 3.596550
O -2.278926 -0.028210 -0.263277

[Cu^{I}**L**^{6}(OH)]
H 0.090210 -2.091887 0.544033
H -0.466010 2.566240 0.893602
Cu -0.104414 0.178238 1.320484
S 2.577682 -0.114105 -0.030856
C 2.016693 1.316659 -1.041040
H 2.893867 1.826966 -1.453776
H 1.430241 0.954986 -1.890328
C 1.225165 2.342298 -0.214343
H 1.783618 2.585780 0.695247
H 1.140013 3.267435 -0.809892
C -1.080163 1.901725 -0.933169
H -0.686348 1.232545 -1.701832
H -1.130676 2.911549 -1.375727
C -2.498733 1.462823 -0.560879
H -2.879964 2.070258 0.269057
H -3.151781 1.646341 -1.430679
C -2.469657 -0.887104 -1.126321
H -2.010020 -0.481169 -2.039252
H -3.475436 -1.246366 -1.393466
C -1.635485 -2.043055 -0.571822
H -2.067096 -2.341259 0.388654
H -1.729395 -2.901042 -1.265516

C 0.673504 -1.805511 -1.437364
H 0.396096 -1.089971 -2.227077
H 0.628172 -2.806033 -1.917025
C 2.140028 -1.593889 -1.038011
H 2.765913 -1.627157 -1.936788
H 2.465358 -2.414871 -0.387932
N -0.128651 1.891688 0.204743
N -0.246742 -1.673491 -0.327382
O -0.142063 -1.356767 2.411169
H 0.045067 -1.236880 3.351542
O -2.590073 0.124301 -0.125797

$[Cu^{II}\mathbf{L^1}(H_2O)]^{2+}$
H 1.462013 -2.171631 0.812438
H -2.188753 -1.485978 0.788105
H -1.461857 2.171558 0.813774
Cu 0.000034 -0.000043 0.589084
C 1.287480 1.942596 -1.004990
H 2.089685 2.639194 -1.276690
H 1.024421 1.382566 -1.908356
C 0.078194 2.706417 -0.459500
H 0.377272 3.328602 0.390365
H -0.330588 3.376053 -1.225154
C -1.957232 1.296757 -0.989090
H -1.412575 1.047176 -1.905620
H -2.658664 2.102105 -1.238409
C -2.714749 0.080526 -0.451201
H -3.332600 0.370960 0.404798
H -3.387562 -0.322655 -1.217110
C -1.288000 -1.942131 -1.005190
H -1.025296 -1.381782 -1.908459
H -2.090320 -2.638632 -1.276805
C -0.078512 -2.706128 -0.460412
H -0.377277 -3.328543 0.389396
H 0.329948 -3.375566 -1.226412
C 1.956732 -1.296271 -0.990332
H 1.411753 -1.046304 -1.906564
H 2.658051 -2.101542 -1.240216
C 2.714468 -0.080258 -0.452246
H 3.386987 0.323230 -1.218250
H 3.332632 -0.371028 0.403412
N -0.961807 1.747886 0.030163
N -1.753232 -0.963695 0.025975
N 0.961683 -1.747750 0.029120
O 0.001402 -0.001329 2.859096
H -0.676765 -0.369975 3.451709
H 0.679862 0.367411 3.451312
N 1.753108 0.963808 0.025669
H 2.188889 1.485865 0.787811

$[Cu^{II}\mathbf{L^1}(OH)]^{+}$
H -1.579964 2.079441 0.967232
H 2.216304 1.642948 0.781876
H 1.541990 -2.077712 0.498324
Cu 0.000812 0.050692 0.949655
C -1.274421 -1.834842 -1.136599
H -2.032455 -2.551090 -1.485670
H -1.089819 -1.140479 -1.963941
C 0.022091 -2.579871 -0.790125
H -0.181973 -3.310641 -0.000351

H 0.359239 -3.144133 -1.672239
C 1.965557 -1.033730 -1.226507
H 1.393530 -0.685236 -2.094791
H 2.731686 -1.724038 -1.613827
C 2.680396 0.142616 -0.539579
H 3.303018 -0.241374 0.275718
H 3.348198 0.641289 -1.255598
C 1.131142 2.061038 -0.909074
H 0.847304 1.495526 -1.801994
H 1.855770 2.822874 -1.228076
C -0.100840 2.731781 -0.301386
H 0.192710 3.330790 0.567870
H -0.560993 3.414385 -1.027517
C -2.062259 1.248627 -0.835898
H -1.528410 1.046212 -1.769563
H -2.800737 2.033359 -1.046780
C -2.762021 -0.017708 -0.327476
H -3.482840 -0.365159 -1.081741
H -3.330467 0.215530 0.580287
N 1.044048 -1.658071 -0.282962
N 1.725812 1.111906 0.062408
N -1.067595 1.703917 0.167614
O 0.338052 -0.960836 2.459859
H 1.024512 -0.666633 3.080300
N -1.762424 -1.047937 0.016059
H -2.131335 -1.675399 0.729665

$[Cu^{II}\mathbf{L}^{2}(H_2O)]^{2+}$
H -0.146667 2.599648 0.777758
H 2.772074 0.227133 0.814066
H 0.419096 -2.592911 0.767532
Cu 0.155091 -0.003470 0.611953
S -2.214296 -0.012374 0.246153
C -2.003904 -1.285521 -1.089896
H -2.996300 -1.629495 -1.395428
H -1.515956 -0.830809 -1.957242
C -1.192048 -2.444887 -0.507053
H -1.724640 -2.886274 0.340690
H -1.081828 -3.230238 -1.265133
C 1.241820 -2.042787 -1.038776
H 0.885431 -1.529403 -1.938020
H 1.470170 -3.077363 -1.322808
C 2.488848 -1.362624 -0.473021
H 2.879704 -1.938723 0.372073
H 3.279612 -1.317213 -1.230953
C 2.238298 1.109806 -0.966296
H 1.767904 0.767071 -1.893535
H 3.283610 1.345067 -1.200242
C 1.525736 2.342393 -0.408665
H 2.046808 2.708533 0.481894
H 1.526716 3.154227 -1.145392
C -0.889029 2.115456 -1.082897
H -0.539211 1.535853 -1.942797
H -0.974471 3.160468 -1.410076
C -2.260045 1.624521 -0.615297
H -2.966113 1.569095 -1.449255
H -2.696347 2.298436 0.130138
N 0.150184 -1.996895 -0.018345
N 2.150253 0.003688 0.034806
N 0.128428 1.991768 0.003315

O 0.144411 -0.033483 2.856199
H 0.862091 0.018883 3.511333
H -0.675971 -0.113585 3.373694

$[Cu^{II}\mathbf{L}^{2}(OH)]^{+}$
H 0.371737 -2.548631 0.940955
H -2.917896 -0.453170 0.627087
H -0.558097 2.398459 0.466435
Cu -0.296959 -0.058635 0.961783
S 2.349989 0.196101 0.396371
C 2.054167 1.235623 -1.104515
H 3.011070 1.653507 -1.431378
H 1.673742 0.597024 -1.908219
C 1.063931 2.368245 -0.796893
H 1.476277 3.003908 -0.006915
H 0.968818 2.997783 -1.693795
C -1.308171 1.745682 -1.335570
H -0.932373 1.164741 -2.186934
H -1.635668 2.717020 -1.738704
C -2.531587 1.061574 -0.704443
H -2.942417 1.708099 0.077429
H -3.311758 0.923228 -1.465191
C -2.048183 -1.378405 -0.989961
H -1.523427 -1.022021 -1.881209
H -3.025292 -1.755578 -1.320044
C -1.250768 -2.495650 -0.318295
H -1.792060 -2.862042 0.560964
H -1.127121 -3.343369 -1.004685
C 1.140213 -2.034275 -0.876215
H 0.806426 -1.460032 -1.745773
H 1.293023 -3.070330 -1.211856
C 2.462189 -1.485231 -0.336717
H 3.219023 -1.495926 -1.127090
H 2.842184 -2.117945 0.473919
N -0.240217 1.866498 -0.343664
N -2.192448 -0.235554 -0.055861
N 0.067568 -1.979803 0.148226
O -0.561520 1.113589 2.366573
H -1.327086 0.956000 2.943506

$[Cu^{II}\mathbf{L}^{3}(H_2O)]^{2+}$
H -1.716995 2.187990 0.739340
H 2.003255 1.906997 0.640894
Cu 0.044537 0.225901 0.644518
S 1.408485 -1.725830 0.231200
C 2.251359 -0.856005 -1.174193
H 3.088192 -1.475769 -1.509679
H 1.553509 -0.737208 -2.008904
C 2.758488 0.488334 -0.647641
H 3.464934 0.327539 0.172151
H 3.300029 1.011806 -1.445335
C 1.016209 2.244962 -1.134907
H 0.783571 1.653830 -2.026706
H 1.715313 3.033126 -1.440787
C -0.245527 2.865490 -0.537776
H 0.015942 3.505423 0.311388
H -0.751315 3.495738 -1.278795
C -2.106931 1.251821 -1.047451
H -1.521585 0.937792 -1.916983
H -2.796649 2.036332 -1.386887

C -2.914032 0.083333 -0.481792
H -3.607545 0.411542 0.300300
H -3.514350 -0.396770 -1.260657
C -1.108793 -2.144316 -1.051330
H -0.904464 -1.466949 -1.885670
H -1.833943 -2.894371 -1.385079
C 0.160806 -2.841833 -0.558831
H 0.649527 -3.374355 -1.381315
H -0.064321 -3.581058 0.216590
N 1.642143 1.337800 -0.128089
N -1.163831 1.797484 -0.026598
O 0.406305 0.527451 2.824753
H -0.092381 1.057617 3.470747
H 0.901849 -0.122630 3.353406
S -1.873000 -1.198237 0.351254

$[Cu^{II}\mathbf{L}^{3}(OH)]^{+}$
H -2.466998 -1.585124 0.465609
H -1.580834 2.136907 0.464144
Cu -0.386636 -0.048105 0.990895
S 1.978797 1.284328 0.394465
C 1.278076 2.057878 -1.128563
H 1.984718 2.804236 -1.504025
H 1.150116 1.292105 -1.901425
C -0.065284 2.723849 -0.801284
H 0.082347 3.472254 -0.015998
H -0.413403 3.264758 -1.693408
C -1.992981 1.220105 -1.327406
H -1.415540 0.897599 -2.201890
H -2.713503 1.970534 -1.688211
C -2.789496 0.047800 -0.735930
H -3.414357 0.410285 0.085852
H -3.453075 -0.373082 -1.503346
C -1.299234 -1.895507 -1.194438
H -0.829101 -1.257429 -1.947637
H -2.073363 -2.485212 -1.707332
C -0.264873 -2.842310 -0.586818
H -0.729157 -3.538712 0.120338
H 0.212951 -3.446195 -1.364111
C 2.149329 -1.267253 -0.884284
H 1.554152 -0.947647 -1.744429
H 2.831140 -2.058341 -1.213087
C 2.959307 -0.105362 -0.297475
H 3.637684 0.280552 -1.065600
H 3.583002 -0.450377 0.533727
N -1.065327 1.754621 -0.328586
N -1.908171 -1.013967 -0.169644
O -1.264307 0.868244 2.338340
H -1.782668 0.355691 2.981584
S 1.029216 -1.978921 0.398120

$[Cu^{II}\mathbf{L}^{4}(H_2O)]^{2+}$
H 0.074321 2.586314 0.793868
H 0.341534 -2.626679 0.737600
Cu 0.203788 -0.017908 0.689075
S -2.170664 0.158973 0.409140
C -2.149083 -1.149992 -0.904259
H -3.183514 -1.429203 -1.125229
H -1.699549 -0.747688 -1.816956
C -1.378520 -2.351302 -0.354685

H -1.857758 -2.719431 0.557485
H -1.403677 -3.167397 -1.087508
C 0.991862 -2.140657 -1.153735
H 0.647986 -1.491350 -1.965021
H 0.981773 -3.170727 -1.535100
C 2.417532 -1.783281 -0.732905
H 2.829321 -2.524594 -0.039175
H 3.087269 -1.746787 -1.597348
C 2.403647 1.141613 -1.092217
H 1.872742 0.753137 -1.966112
H 3.413913 1.424864 -1.401941
C 1.686172 2.333341 -0.457110
H 2.246645 2.689564 0.412444
H 1.643968 3.159774 -1.177488
C -0.747992 2.137997 -1.038256
H -0.481034 1.507535 -1.892390
H -0.772268 3.176124 -1.396469
C -2.128893 1.770676 -0.494681
H -2.875681 1.750493 -1.294106
H -2.474130 2.498187 0.248276
N 0.037466 -2.000798 -0.012069
N 0.307259 1.975102 0.007515
O 0.322250 -0.024740 2.902522
H 1.133438 -0.025561 3.440310
H -0.418447 -0.032384 3.533948
S 2.543335 -0.188904 0.192736

$[Cu^{II}\mathbf{L^4}(OH)]^+$
H -0.255952 -2.310571 0.585411
H -0.220645 2.704745 0.783172
Cu -0.311037 0.174379 1.013985
S 2.249970 -0.243021 0.466505
C 2.222702 1.086793 -0.808507
H 3.248855 1.360449 -1.071362
H 1.731596 0.721348 -1.715723
C 1.501685 2.306953 -0.236558
H 1.979022 2.609362 0.700960
H 1.588973 3.150223 -0.934814
C -0.834668 2.239818 -1.102096
H -0.547467 1.526298 -1.880195
H -0.700253 3.247991 -1.520149
C -2.302314 2.063183 -0.713659
H -2.615984 2.838348 -0.005039
H -2.943779 2.158104 -1.594909
C -2.491683 -0.753188 -1.237374
H -1.939783 -0.280640 -2.055795
H -3.494118 -0.997686 -1.600546
C -1.781373 -2.025734 -0.753009
H -2.358200 -2.474871 0.061903
H -1.783516 -2.750481 -1.580372
C 0.675225 -1.953497 -1.215053
H 0.551409 -1.241295 -2.040341
H 0.664712 -2.960388 -1.663513
C 2.039087 -1.771783 -0.536796
H 2.841854 -1.823847 -1.278268
H 2.215725 -2.577243 0.184924
N 0.063617 2.036718 0.062726
N -0.421307 -1.766137 -0.261810
O -0.474863 -0.961058 2.460948
H -1.318704 -0.911282 2.941034

S -2.675482 0.473734 0.137224

$[Cu^{II}\mathbf{L}^5(H_2O)]^{2+}$

H 0.202697 -2.752200 0.584078
Cu -0.008384 -0.175529 0.688692
S -2.372843 -0.034402 0.209655
C -2.216908 -1.275320 -1.158990
H -3.224291 -1.576542 -1.461691
H -1.721452 -0.818587 -2.020936
C -1.446269 -2.477567 -0.611851
H -1.973053 -2.901217 0.248582
H -1.399804 -3.259485 -1.380180
C 0.962490 -2.180712 -1.240600
H 0.646843 -1.526133 -2.058997
H 1.016966 -3.200891 -1.644606
C 2.343221 -1.783945 -0.720161
H 2.729729 -2.517954 -0.004458
H 3.069232 -1.719412 -1.536406
C 2.283240 1.120323 -1.086335
H 1.689249 0.764475 -1.932694
H 3.305379 1.302363 -1.435859
C 1.712098 2.404272 -0.482457
H 2.354377 2.792331 0.314637
H 1.636941 3.186102 -1.245580
C -1.130464 2.174644 -1.105566
H -0.708677 1.583834 -1.923603
H -1.270036 3.202436 -1.458283
C -2.470878 1.612993 -0.627108
H -3.172172 1.530447 -1.463904
H -2.933128 2.265607 0.120282
N -0.066834 -2.105947 -0.161894
O -0.035134 -0.605832 2.849527
H 0.719585 -0.522030 3.458392
H -0.830249 -0.598368 3.410883
S 0.054715 2.219183 0.319811
S 2.357798 -0.192548 0.220143

$[Cu^{II}\mathbf{L}^5(OH)]^{+}$

H 0.648156 -2.517983 0.394334
Cu 0.143254 -0.137252 1.042906
S -2.461369 -0.518984 0.318421
C -2.029030 -1.490660 -1.191287
H -2.938377 -1.964831 -1.572630
H -1.650380 -0.812508 -1.963341
C -0.985733 -2.560637 -0.848561
H -1.369036 -3.199048 -0.046153
H -0.846756 -3.205101 -1.728908
C 1.327510 -1.826195 -1.418990
H 0.935688 -1.195219 -2.225734
H 1.607531 -2.787185 -1.881447
C 2.613232 -1.227962 -0.833096
H 3.071153 -1.921731 -0.119895
H 3.346883 -1.041754 -1.623243
C 1.901332 1.544119 -1.141699
H 1.313198 1.032122 -1.908211
H 2.803531 1.946359 -1.615237
C 1.107892 2.687085 -0.506390
H 1.707698 3.216439 0.240803
H 0.821706 3.419677 -1.268033
C -1.650700 1.914386 -0.941137

H -1.178772 1.401016 -1.783994
H -1.984463 2.900527 -1.280649
C -2.849111 1.129137 -0.397516
H -3.591252 1.007463 -1.193346
H -3.336650 1.680951 0.412808
N 0.291708 -1.982353 -0.398411
O 0.484977 -1.429158 2.327998
H 1.173074 -1.207851 2.979104
S -0.409384 2.165067 0.398070
S 2.419413 0.324108 0.144538

$[Cu^{II}\mathbf{L}^{6}(H_2O)]^{2+}$
H 0.058358 2.581652 0.820301
H 0.247617 -2.601085 0.796991
Cu 0.127263 -0.014428 0.617434
S -2.221748 0.164165 0.332790
C -2.156694 -1.146599 -0.984071
H -3.184119 -1.419433 -1.242613
H -1.671172 -0.744934 -1.878460
C -1.411753 -2.352177 -0.403276
H -1.937733 -2.729423 0.478787
H -1.394378 -3.161525 -1.143359
C 1.012382 -2.137230 -1.063408
H 0.626009 -1.648065 -1.963468
H 1.177818 -3.194538 -1.307209
C 2.319692 -1.487801 -0.615589
H 2.771608 -2.019788 0.226578
H 3.047458 -1.453613 -1.431330
C 2.274632 0.962142 -1.050577
H 1.798990 0.739536 -2.013566
H 3.350725 1.086108 -1.207982
C 1.688541 2.199470 -0.382293
H 2.256547 2.429737 0.523194
H 1.760984 3.062330 -1.055734
C -0.753411 2.175800 -1.034942
H -0.466257 1.575789 -1.903964
H -0.758915 3.226700 -1.353947
C -2.152736 1.793900 -0.545917
H -2.872817 1.784871 -1.369673
H -2.526444 2.503097 0.200835
N -0.017395 -1.996405 0.015998
N 0.267810 1.961369 0.034882
O 0.620665 -0.088989 2.761649
H 1.512225 -0.072613 3.151731
H -0.001230 -0.112679 3.509886
O 2.052489 -0.141030 -0.129518

$[Cu^{II}\mathbf{L}^{6}(OH)]^{+}$
H -0.193724 -2.612062 0.525509
H -0.197218 2.584148 0.925634
Cu -0.020930 -0.126734 1.010263
S 2.326284 -0.281126 0.292688
C 2.237417 1.155708 -0.865047
H 3.256366 1.456314 -1.123384
H 1.730436 0.851015 -1.785434
C 1.510479 2.314694 -0.169647
H 2.026770 2.562881 0.763633
H 1.568081 3.201487 -0.817572
C -0.822391 2.172979 -0.980471
H -0.431691 1.606159 -1.832347

H -0.861142 3.229125 -1.287725
C -2.235046 1.695941 -0.641409
H -2.650300 2.280608 0.186779
H -2.894377 1.832666 -1.508568
C -2.304072 -0.667325 -1.198776
H -1.719168 -0.378238 -2.083825
H -3.343518 -0.817028 -1.521139
C -1.783049 -1.962903 -0.584304
H -2.371786 -2.193963 0.307128
H -1.908099 -2.783392 -1.304503
C 0.623679 -1.962583 -1.249947
H 0.373695 -1.201183 -1.995005
H 0.549352 -2.938749 -1.752146
C 2.060826 -1.771960 -0.759710
H 2.755266 -1.747990 -1.604656
H 2.370575 -2.601743 -0.114356
N 0.105005 1.979684 0.160587
N -0.361813 -1.862160 -0.147853
O -1.089485 -0.443383 2.467976
H -1.962622 -0.017381 2.477139
O -2.240497 0.342216 -0.196608

[Cu^{I} **L^{1}**(NO_3)]
H 1.515844 -0.620379 1.565934
H 0.577486 2.886604 0.503383
H -1.470801 1.169482 -2.306328
Cu 0.274693 0.249559 -0.426901
C -2.274957 -1.469038 -0.435976
H -2.895917 -2.362525 -0.625632
H -2.653722 -1.019508 0.488658
C -2.459220 -0.485931 -1.604352
H -2.080022 -0.950893 -2.522025
H -3.537031 -0.303385 -1.753665
C -2.369849 1.772289 -0.567460
H -2.788370 1.262697 0.307155
H -3.216994 2.254146 -1.085519
C -1.384111 2.860072 -0.108316
H -0.991139 3.380712 -0.990148
H -1.939653 3.607240 0.485162
C -0.454024 1.982849 2.033083
H -1.453112 1.543871 2.136165
H -0.436989 2.883893 2.670453
C 0.598411 0.976407 2.535893
H 1.595418 1.422016 2.435701
H 0.434066 0.797527 3.612654
C -0.350306 -1.296641 2.158049
H -1.325709 -0.833897 2.358591
H -0.046867 -1.801148 3.093213
C -0.487334 -2.364872 1.059102
H -1.199566 -3.136519 1.399376
H 0.484948 -2.849870 0.922436
N -1.705667 0.763360 -1.403195
N -0.241420 2.294151 0.614646
N 0.580694 -0.251877 1.748279
N 3.016917 -0.520655 -1.004133
O 2.026481 0.161471 -1.482383
O 2.884498 -1.097582 0.112895
O 4.064855 -0.591517 -1.655086
N -0.861360 -1.786245 -0.239301
H -0.519760 -2.376705 -0.993591

$[Cu^{II}\mathbf{L^1}(NO_3)]^+$

H	-0.143501	-0.058338	-2.503596
H	-1.504378	2.634990	0.056465
H	-0.333213	0.101292	2.521606
Cu	-0.493415	-0.111707	-0.003712
C	2.276994	-1.187830	0.951758
H	3.004775	-1.973391	1.198341
H	2.854431	-0.314193	0.632087
C	1.458984	-0.840189	2.197832
H	0.899960	-1.721743	2.528828
H	2.127860	-0.547304	3.018302
C	0.956233	1.613570	2.047657
H	1.869164	1.718829	1.452016
H	1.224401	1.837018	3.089653
C	-0.122640	2.595339	1.574283
H	-0.997694	2.516784	2.229668
H	0.257978	3.623129	1.665809
C	0.325159	2.776465	-0.864147
H	1.359062	2.713241	-0.508800
H	0.137791	3.833379	-1.100108
C	0.159218	1.934330	-2.131089
H	-0.870039	2.017624	-2.495624
H	0.821022	2.308801	-2.923495
C	1.822133	0.061546	-1.959259
H	2.432443	0.722260	-1.334696
H	2.193072	0.159616	-2.988911
C	1.951144	-1.397298	-1.504006
H	3.006273	-1.702067	-1.562864
H	1.391356	-2.043198	-2.190145
N	0.471318	0.225905	1.904948
N	-0.562542	2.275342	0.202318
N	0.414694	0.499580	-1.855057
N	-2.704376	-1.224687	-0.045602
O	-2.017671	-1.026011	1.035029
O	-2.107655	-0.775682	-1.103653
O	-3.776093	-1.765896	-0.063559
N	1.383270	-1.581951	-0.154156
H	1.105902	-2.554841	-0.034504

$[Cu^{I}\mathbf{L^2}(NO_3)]$

H	1.450641	-0.767197	1.479884
H	0.691778	2.744934	0.368163
H	-1.481332	1.115709	-2.304614
Cu	0.222552	0.115065	-0.482282
S	-0.873312	-2.234171	-0.480787
C	-2.552287	-1.477397	-0.504358
H	-3.306775	-2.253601	-0.671643
H	-2.755234	-1.014764	0.466650
C	-2.637120	-0.435642	-1.631819
H	-2.341450	-0.904718	-2.576771
H	-3.689606	-0.124426	-1.741406
C	-2.342152	1.781063	-0.571250
H	-2.756887	1.307311	0.325482
H	-3.180847	2.287465	-1.078732
C	-1.295264	2.830544	-0.165765
H	-0.904919	3.314705	-1.069316
H	-1.799265	3.615065	0.425719
C	-0.339203	1.947763	1.962069
H	-1.360275	1.578320	2.114977

H -0.234001 2.852467 2.585841
C 0.667010 0.883490 2.431755
H 1.685192 1.254058 2.267158
H 0.549966 0.731304 3.518048
C -0.410988 -1.338842 2.213108
H -1.383605 -0.846732 2.346272
H -0.112741 -1.709811 3.211683
C -0.562236 -2.566097 1.303033
H -1.338284 -3.231099 1.696806
H 0.374097 -3.135808 1.285060
N -1.753278 0.721436 -1.405873
N -0.164427 2.222614 0.533967
N 0.530437 -0.365447 1.677621
N 3.115424 -0.077409 -0.862199
O 2.037842 0.389428 -1.406262
O 3.034598 -0.686514 0.242662
O 4.196171 0.089461 -1.435868

$[Cu^{II}\mathbf{L}^{2}(NO_3)]^{+}$
H -0.050082 -0.158043 -2.467966
H -1.544111 2.608928 0.112257
H -0.316650 0.116426 2.470933
Cu -0.525533 -0.110711 -0.003289
S 1.422731 -2.099550 -0.214956
C 2.388698 -1.311490 1.144661
H 3.100941 -2.042978 1.536995
H 2.966663 -0.473575 0.742705
C 1.462189 -0.860437 2.276237
H 0.875937 -1.714271 2.629914
H 2.072104 -0.512070 3.121519
C 1.009285 1.583376 1.974402
H 1.894530 1.675278 1.336030
H 1.327709 1.806715 3.002054
C -0.080260 2.575620 1.552525
H -0.921058 2.509770 2.252680
H 0.316317 3.598899 1.621319
C 0.232334 2.762058 -0.909119
H 1.278489 2.777425 -0.586000
H -0.026616 3.794031 -1.182240
C 0.074804 1.858502 -2.132965
H -0.971911 1.851143 -2.453745
H 0.676567 2.241198 -2.968074
C 1.888753 0.151604 -1.904616
H 2.413001 0.747691 -1.150815
H 2.282658 0.457058 -2.885271
C 2.168092 -1.340897 -1.714523
H 3.247291 -1.521225 -1.718383
H 1.748184 -1.919756 -2.545423
N 0.503560 0.196431 1.866070
N -0.593027 2.256972 0.205896
N 0.444359 0.453353 -1.814558
N -2.806456 -1.053623 -0.028620
O -2.103211 -0.888932 1.047997
O -2.182968 -0.659697 -1.093623
O -3.913273 -1.516516 -0.036242

$[Cu^{I}\mathbf{L}^{3}(NO_3)]$
H 1.797863 -0.595948 1.281931
H 0.427731 2.796398 0.535074
Cu 0.261430 0.186408 -0.476896

S -1.948983 0.620131 -1.497175
C -2.622642 1.645981 -0.120242
H -3.559308 2.113883 -0.441105
H -2.840953 0.996233 0.733737
C -1.609018 2.734233 0.270500
H -1.392346 3.354290 -0.606524
H -2.087709 3.390969 1.017790
C -0.307897 1.774961 2.159845
H -1.233285 1.230549 2.383864
H -0.275653 2.642511 2.841741
C 0.898995 0.864045 2.430898
H 1.820520 1.401915 2.178628
H 0.944798 0.638778 3.509420
C 0.169267 -1.489048 2.207991
H -0.842591 -1.176736 2.498400
H 0.662673 -1.838133 3.134082
C 0.099690 -2.688599 1.254418
H 1.107240 -3.075014 1.063700
H -0.480073 -3.497953 1.710946
C -2.289140 -1.870559 -0.120134
H -2.357851 -1.352976 0.841598
H -2.909690 -2.772942 -0.062693
C -2.822168 -0.981886 -1.251926
H -3.887682 -0.779938 -1.095153
H -2.731762 -1.494721 -2.215537
N -0.345848 2.171428 0.749098
N 0.857867 -0.350929 1.613126
N 3.161568 0.237772 -1.035581
O 2.017154 0.707210 -1.413859
O 3.216829 -0.511156 -0.016026
O 4.172542 0.536349 -1.675498
S -0.539344 -2.344437 -0.434791

$[Cu^{II}\mathbf{L^3}(NO_3)]^+$
H -1.392838 2.447176 0.944405
H -1.003444 -1.077462 2.147203
Cu -0.629419 -0.112747 -0.088110
S 1.388873 -2.001372 -0.788001
C 1.971385 -2.008833 0.960258
H 2.590552 -2.894818 1.127756
H 2.594107 -1.127756 1.144832
C 0.772591 -2.048568 1.908440
H 0.126984 -2.894311 1.651738
H 1.128184 -2.210156 2.935404
C 0.400326 0.285242 2.723063
H 1.440046 0.513098 2.467134
H 0.387823 -0.023267 3.777383
C -0.494678 1.513911 2.538407
H -1.519213 1.268702 2.840493
H -0.146366 2.319102 3.201230
C 0.620065 2.760381 0.717748
H 1.522827 2.324182 1.156063
H 0.538271 3.782837 1.116487
C 0.774286 2.843761 -0.802820
H -0.091513 3.333416 -1.262038
H 1.657380 3.432934 -1.068916
C 2.536789 0.584685 -1.239120
H 2.761233 0.756688 -0.181863
H 3.268000 1.139653 -1.836796
C 2.620778 -0.904056 -1.599730

H 3.626407 -1.276454 -1.379450
H 2.452773 -1.049307 -2.671792
N -0.060243 -0.818709 1.848740
N -0.531364 1.930775 1.120281
N -2.917969 -0.619545 -0.884241
O -2.413280 -1.125334 0.196621
O -2.092745 0.171179 -1.491864
O -4.026778 -0.856447 -1.276010
S 0.856887 1.212837 -1.637936

[Cu^{I}**L**^{4}(NO_3)]
H 1.413643 0.109147 1.545961
H -1.559543 0.395401 -2.461897
Cu 0.237084 0.271738 -0.551697
S -0.169371 -2.352575 0.035503
C -1.966586 -2.127791 -0.291756
H -2.446147 -3.107849 -0.386879
H -2.432921 -1.615746 0.555698
C -2.180623 -1.344750 -1.594648
H -1.613054 -1.823960 -2.399426
H -3.247906 -1.403497 -1.867127
C -2.725257 0.950660 -0.880619
H -2.868086 0.616170 0.152227
H -3.707303 0.871079 -1.379863
C -2.308371 2.423532 -0.900291
H -2.242314 2.785209 -1.933965
H -3.079036 3.023977 -0.404804
C -0.899098 2.492494 1.612972
H -1.831831 1.936763 1.758146
H -0.999643 3.452978 2.129220
C 0.294216 1.715249 2.192385
H 1.220594 2.255187 1.968227
H 0.190954 1.699591 3.291021
C -0.321075 -0.671114 2.364860
H -1.395960 -0.457878 2.286332
H -0.082872 -0.667393 3.444566
C -0.019911 -2.082528 1.847460
H -0.638009 -2.810751 2.383380
H 1.028073 -2.334824 2.044701
N -1.735750 0.062387 -1.514302
N 0.422428 0.362284 1.645870
N 3.137835 -0.034113 -0.700537
O 2.100565 0.291494 -1.398829
O 3.008659 -0.234985 0.544470
O 4.230256 -0.140833 -1.261803
S -0.660243 2.809167 -0.189821

[Cu^{II}**L**^{4}(NO_3)]$^{+}$
H -0.050274 -0.106726 -2.423449
H -0.339188 0.240503 2.442724
Cu -0.580303 -0.097307 -0.001976
S 1.245928 -2.171181 -0.288516
C 2.190284 -1.553095 1.172905
H 2.764220 -2.386790 1.587099
H 2.907196 -0.793834 0.846279
C 1.248626 -1.017370 2.252089
H 0.522085 -1.789882 2.521996
H 1.831573 -0.784719 3.154226
C 1.212681 1.461989 1.930906
H 1.991298 1.479291 1.161611

H 1.721366 1.528728 2.903832
C 0.278125 2.666327 1.794736
H -0.404581 2.718621 2.651011
H 0.860330 3.592725 1.800015
C 0.335765 2.932438 -1.065170
H 1.362428 2.912361 -0.687268
H 0.154773 3.933603 -1.466310
C 0.122678 1.906866 -2.179048
H -0.923643 1.922292 -2.499338
H 0.735745 2.186486 -3.047293
C 1.875466 0.165867 -1.804559
H 2.379750 0.701346 -0.993983
H 2.324918 0.511665 -2.746973
C 2.100280 -1.343456 -1.690165
H 3.172152 -1.558308 -1.643373
H 1.715258 -1.855874 -2.579633
N 0.475303 0.180652 1.826587
N 0.435061 0.511015 -1.768070
N -2.837991 -1.073387 -0.063715
O -2.140392 -0.935725 1.020510
O -2.213497 -0.637056 -1.112386
O -3.937097 -1.550748 -0.092734
S -0.836314 2.648493 0.332831

[Cu^{I} **L**^{5}(NO_3)]
H 0.825460 2.060986 0.395352
Cu 0.468796 -0.176907 -0.387380
S -2.028784 0.474838 -1.728494
C -2.400501 1.655473 -0.361345
H -3.202555 2.328345 -0.682439
H -2.761904 1.096483 0.508116
C -1.154859 2.476435 0.004989
H -0.733316 2.922860 -0.902253
H -1.474169 3.311387 0.651905
C -0.221643 1.570463 2.099926
H -1.145845 1.029361 2.342883
H -0.310878 2.564617 2.574485
C 0.987815 0.879767 2.739828
H 1.888743 1.481889 2.579191
H 0.835536 0.793609 3.820940
C 0.020286 -1.816943 2.494130
H -0.870853 -1.192246 2.608468
H 0.209829 -2.306689 3.456544
C -0.209907 -2.901257 1.433293
H 0.698746 -3.494687 1.286668
H -0.995291 -3.590108 1.765085
C -2.394316 -1.781508 0.005722
H -2.459548 -1.157003 0.902146
H -3.000973 -2.680107 0.171135
C -2.939307 -1.036154 -1.217208
H -3.991999 -0.786945 -1.041440
H -2.906383 -1.683306 -2.100516
N -0.099887 1.683252 0.644997
N 2.838400 1.297640 -1.300452
O 2.035228 0.333255 -1.606058
O 2.556530 2.049750 -0.317290
O 3.857362 1.467387 -1.969995
S -0.643728 -2.297126 -0.250128
S 1.458276 -0.757795 2.050911

$[Cu^{II}\mathbf{L^5}(NO_3)]^+$

H	-1.031179	-0.920841	2.170752
Cu	-0.671261	-0.157526	-0.142864
S	1.346541	-2.010163	-0.836514
C	1.841074	-2.134074	0.935880
H	2.345741	-3.092044	1.090650
H	2.559119	-1.343187	1.174027
C	0.612345	-2.072642	1.842828
H	-0.114668	-2.829704	1.532752
H	0.913669	-2.309651	2.872674
C	0.538040	0.285520	2.660935
H	1.501208	0.559710	2.219424
H	0.746323	-0.118145	3.662741
C	-0.365978	1.509877	2.814030
H	-1.293022	1.241189	3.334062
H	0.131511	2.265665	3.429354
C	0.640503	3.048908	0.643389
H	1.487343	2.597017	1.167743
H	0.619058	4.111994	0.904705
C	0.803637	2.926763	-0.873726
H	-0.034958	3.397649	-1.396890
H	1.714344	3.441941	-1.197692
C	2.512626	0.592731	-1.101856
H	2.693724	0.722188	-0.030403
H	3.258354	1.180843	-1.647960
C	2.624198	-0.877505	-1.522225
H	3.615385	-1.259992	-1.258379
H	2.520240	-0.973836	-2.607675
N	-0.086231	-0.757634	1.813570
N	-2.863636	-0.864427	-1.017357
O	-2.388545	-1.247852	0.128893
O	-2.053395	-0.077754	-1.646112
O	-3.932207	-1.205045	-1.439932
S	0.843598	1.220348	-1.547893
S	-0.923946	2.273920	1.239664

$[Cu^{I}\mathbf{L^6}(NO_3)]$

H	1.424520	0.096738	1.558749
H	-1.497710	0.340838	-2.440606
Cu	0.273212	0.004801	-0.561703
S	-0.258316	-2.413180	0.070738
C	-2.052287	-2.113937	-0.233545
H	-2.573304	-3.074375	-0.306478
H	-2.479149	-1.569933	0.614793
C	-2.250352	-1.336469	-1.544184
H	-1.739489	-1.864615	-2.356338
H	-3.326072	-1.327098	-1.786609
C	-2.645348	1.007567	-0.888335
H	-2.944376	0.621965	0.091878
H	-3.567838	1.098958	-1.487903
C	-2.025577	2.401102	-0.737379
H	-1.724247	2.786560	-1.718387
H	-2.784923	3.087004	-0.329148
C	-1.025480	2.326726	1.457873
H	-1.913280	1.726895	1.706076
H	-1.175681	3.333909	1.876235
C	0.228639	1.695608	2.057990
H	1.098263	2.271604	1.726302
H	0.174607	1.775660	3.157684
C	-0.302560	-0.698563	2.384369

H -1.375513 -0.469446 2.341986
H -0.024402 -0.681485 3.454520
C -0.050132 -2.124518 1.878348
H -0.670058 -2.832713 2.438177
H 0.996555 -2.402789 2.045832
N -1.708418 0.038517 -1.490028
N 0.422117 0.309571 1.615001
N 3.145286 0.219882 -0.734603
O 2.064704 0.408750 -1.423007
O 3.050414 -0.115230 0.482208
O 4.237970 0.372543 -1.283999
O -0.848376 2.413073 0.048227

$[Cu^{II}\mathbf{L^6}(NO_3)]^+$
H -0.083836 -0.075843 -2.463950
H -0.333066 0.125059 2.450227
Cu -0.524374 -0.152072 -0.017873
S 1.285032 -2.170701 -0.258525
C 2.284155 -1.466723 1.126598
H 2.941478 -2.250732 1.512864
H 2.919958 -0.662945 0.742718
C 1.374491 -0.973997 2.255148
H 0.727107 -1.791741 2.586701
H 1.994254 -0.680072 3.113446
C 1.102763 1.498222 1.991530
H 2.011690 1.531504 1.381934
H 1.401020 1.686176 3.032891
C 0.103508 2.567325 1.544755
H -0.779270 2.566812 2.192820
H 0.558109 3.563959 1.597653
C 0.431282 2.782114 -0.842157
H 1.494070 2.747920 -0.566602
H 0.171108 3.824847 -1.063358
C 0.150066 1.912310 -2.057983
H -0.912017 1.981071 -2.310427
H 0.730282 2.272771 -2.917933
C 1.869664 0.097598 -1.891360
H 2.429771 0.642520 -1.125249
H 2.274190 0.407389 -2.866121
C 2.066840 -1.412834 -1.741734
H 3.134295 -1.652517 -1.753840
H 1.613242 -1.947249 -2.584602
N 0.494722 0.153859 1.850359
N 0.443596 0.477510 -1.784325
N -2.882086 -0.854519 -0.030161
O -2.151212 -0.779763 1.039805
O -2.228589 -0.519404 -1.097306
O -4.030628 -1.195688 -0.028852
O -0.381606 2.293646 0.228312

$[Cu_2^{II}(\mathbf{L^1})_2(\mu\text{-}OH)]^{3+}$
H 1.892410 -0.982640 -2.456270
H 2.327619 2.542026 -1.246953
H 2.221260 1.306047 2.306868
Cu 2.114714 0.147442 -0.069596
C 3.705527 -1.564505 1.625098
H 3.912245 -2.482178 2.189467
H 4.620675 -1.307557 1.082691
C 3.297013 -0.434957 2.569466
H 2.421909 -0.733851 3.156296

H 4.104782 -0.216679 3.278438
C 4.051909 1.688130 1.446158
H 4.885331 1.075721 1.087708
H 4.407158 2.226399 2.333611
C 3.599563 2.674601 0.371178
H 2.824336 3.337050 0.771290
H 4.436642 3.309121 0.055550
C 3.991986 1.486823 -1.814853
H 4.838997 1.026817 -1.296416
H 4.386059 2.335868 -2.386967
C 3.312716 0.484758 -2.746094
H 2.507483 0.976036 -3.302483
H 4.027579 0.096646 -3.481711
C 3.618460 -1.755788 -1.642390
H 4.573868 -1.337695 -1.310596
H 3.823751 -2.355407 -2.537840
C 2.997131 -2.624187 -0.549341
H 3.685182 -3.427184 -0.258565
H 2.083175 -3.098184 -0.923217
N 2.920159 0.776996 1.784161
N 3.009708 1.938054 -0.786501
N 2.700609 -0.620855 -1.949201
H -1.892447 -0.984361 2.455733
H -2.327053 2.541397 1.249357
H -2.220603 1.308360 -2.305393
Cu -2.114464 0.147727 0.070038
C -3.705369 -1.562549 -1.626283
H -3.912081 -2.479738 -2.191437
H -4.620522 -1.305991 -1.083711
C -3.296598 -0.432244 -2.569617
H -2.421463 -0.730766 -3.156589
H -4.104255 -0.213253 -3.278498
C -4.051294 1.690009 -1.444584
H -4.884867 1.077436 -1.086758
H -4.406349 2.229093 -2.331620
C -3.598906 2.675502 -0.368725
H -2.823578 3.338210 -0.768211
H -4.435937 3.309851 -0.052623
C -3.991603 1.485975 1.816307
H -4.838649 1.026512 1.297448
H -4.385591 2.334600 2.389104
C -3.312506 0.483051 2.746747
H -2.507202 0.973754 3.303538
H -4.027433 0.094451 3.482044
C -3.618630 -1.756492 1.641158
H -4.573954 -1.337931 1.309714
H -3.824047 -2.356830 2.536097
C -2.997444 -2.624062 0.547355
H -3.685642 -3.426688 0.255905
H -2.083598 -3.098554 0.920873
N -2.919657 0.778976 -1.783232
N -3.009217 1.937915 0.788374
N -2.700570 -0.622003 1.948952
O 0.000146 0.521931 0.000448
H 0.000251 1.492679 0.000837
N -2.619112 -1.779630 -0.625122
H -1.828459 -2.212098 -1.103322
N 2.619031 -1.780692 0.623746
H 1.828300 -2.213392 1.101609

$[Cu_2^{II}(\mathbf{L^2})_2(\mu\text{-}OH)]^{3+}$

H	1.682073	0.914160	-2.347110
H	2.513834	2.640528	-1.266572
H	2.383702	1.539743	2.272311
Cu	2.008043	0.353959	-0.048806
S	1.986942	1.902006	0.862548
C	3.474028	1.574792	1.921913
H	3.604469	2.416824	2.607731
H	4.361302	1.512800	1.284934
C	3.231928	0.280304	2.698019
H	2.351973	0.388775	3.339376
H	4.088877	0.087686	3.356196
C	4.225561	1.607141	1.370515
H	4.940572	0.872477	0.986455
H	4.700738	2.106595	2.224245
C	3.860218	2.629654	0.297381
H	3.194028	3.391638	0.716123
H	4.757585	3.145824	-0.064415
C	4.015193	1.381289	-1.881234
H	4.840590	0.858017	-1.388772
H	4.458324	2.171900	-2.499165
C	3.198648	0.423393	-2.742804
H	2.410033	0.970063	-3.270467
H	3.834978	0.046593	-3.502580
C	3.376595	1.796103	-1.592795
H	4.323488	1.451691	-1.166578
H	3.618138	2.334790	-2.519581
C	2.664873	2.747920	-0.633683
H	3.326302	3.559677	-0.316098
H	1.790492	3.210550	-1.104159
N	2.993290	0.878384	1.788350
N	3.134703	1.961153	-0.824107
N	2.535232	0.601613	-1.881126
H	-1.682693	0.915980	2.346734
H	-2.514132	2.639554	1.268728
H	-2.383103	1.541459	-2.271001
Cu	-2.008036	0.353917	0.049303
S	-1.986744	1.901366	-0.863818
C	-3.473584	1.573309	-1.923267
H	-3.603894	2.414811	-2.609759
H	-4.360993	1.511788	-1.286431
C	-3.231297	0.278226	-2.698321
H	-2.351208	0.386218	-3.339577
H	-4.088103	0.085092	-3.356535
C	-4.225187	1.608239	-1.369623
H	-4.940324	0.873307	-0.986305
H	-4.700134	2.108369	-2.223085
C	-3.860071	2.629910	-0.295611
H	-3.193745	3.392191	-0.713597
H	-4.757508	3.145836	0.066358
C	-4.015669	1.379829	1.881962
H	-4.840904	0.856928	1.388837
H	-4.458998	2.169956	2.500368
C	-3.199375	0.421274	2.743031
H	-2.410910	0.967533	3.271344
H	-3.835921	0.049301	3.502262
C	-3.377010	1.797325	1.591259
H	-4.323790	1.452578	1.165060
H	-3.618803	2.336726	2.517565
C	-2.665047	2.748416	0.631611

H -3.326398 3.559930 0.313243
H -1.790781 3.211403 1.101951
N -2.992842 0.879752 -1.787707
N -3.134865 1.960518 0.825550
N -2.535715 0.603067 1.880745
O 0.000001 0.975470 0.000572
H 0.000011 1.945364 0.001242

$[Cu_2^{II}(\mathbf{L^3})_2(\mu\text{-}OH)]^{3+}$
H -2.769345 0.145686 -2.876374
H -1.739747 -2.683115 -0.622741
Cu -1.987985 -0.129920 -0.357065
S -1.944264 -0.147894 2.095252
C -3.124619 -1.572852 2.178780
H -3.164731 -1.934499 3.210416
H -4.125621 -1.236129 1.893354
C -2.599627 -2.664137 1.246119
H -1.599981 -2.977625 1.561962
H -3.252026 -3.544223 1.312996
C -3.744280 -2.382193 -0.969145
H -4.590639 -1.996604 -0.391835
H -3.933790 -3.448340 -1.146807
C -3.603704 -1.644619 -2.297025
H -2.785368 -2.078176 -2.881589
H -4.519650 -1.747899 -2.891464
C -4.465449 0.664949 -1.852007
H -5.074942 0.225044 -1.057311
H -5.086649 0.688461 -2.758028
C -4.046560 2.088651 -1.494260
H -3.545029 2.584840 -2.332249
H -4.913409 2.702844 -1.231599
C -3.856515 1.841645 1.387908
H -4.650095 1.130748 1.142099
H -4.324392 2.786695 1.684522
C -2.969301 1.330863 2.522669
H -3.574754 1.085716 3.401505
H -2.242653 2.088477 2.831676
N -2.504730 -2.185561 -0.163824
N -3.273547 -0.206300 -2.060372
H 2.649480 -1.413140 -2.495908
H 2.031110 2.234333 -1.828465
Cu 1.980524 0.060127 -0.408602
S 2.017084 1.201961 1.765409
C 3.347170 2.367095 1.216239
H 3.454330 3.154239 1.968284
H 4.297559 1.830304 1.142163
C 2.916011 2.960870 -0.124101
H 1.964186 3.488629 -0.011632
H 3.659898 3.698078 -0.452196
C 3.972203 1.566322 -1.921498
H 4.775400 1.389696 -1.199295
H 4.286109 2.405268 -2.555235
C 3.721661 0.325647 -2.773158
H 2.954761 0.534331 -3.526858
H 4.634186 0.039695 -3.310360
C 4.304883 -1.614981 -1.302713
H 4.986530 -0.940527 -0.776366
H 4.892333 -2.123109 -2.079986
C 3.727532 -2.658255 -0.350939
H 3.137997 -3.410261 -0.886404

H 4.521136 -3.192063 0.180893
C 3.669617 -1.096995 2.094338
H 4.530714 -0.677895 1.566408
H 4.036319 -1.847866 2.802591
C 2.885359 -0.021195 2.845923
H 3.544916 0.527239 3.526517
H 2.089368 -0.462162 3.453726
N 2.732670 1.904106 -1.163237
N 3.223931 -0.795358 -1.919641
O -0.007256 -0.124382 -1.028414
H -0.020748 -0.110193 -1.997849
S -2.821061 2.159938 -0.115048
S 2.554035 -1.943292 0.882304

$[Cu_2^{II}(\mathbf{L^4})_2(\mu\text{-}OH)]^{3+}$
H -1.981093 0.495528 -2.455558
H -2.357015 -1.340159 2.468319
Cu -2.016322 -0.443638 0.000871
S -2.092532 1.912405 0.562965
C -3.490300 1.700591 1.761905
H -3.594607 2.627388 2.333689
H -4.419170 1.536779 1.207618
C -3.159899 0.532196 2.687400
H -2.224637 0.730112 3.220092
H -3.948545 0.437490 3.445313
C -4.262552 -1.499265 1.736389
H -4.959621 -0.861163 1.184406
H -4.732186 -1.729644 2.702908
C -4.006385 -2.807058 0.990385
H -3.424972 -3.508738 1.598556
H -4.944402 -3.308504 0.733057
C -4.208860 -1.864938 -1.756944
H -5.010436 -1.357884 -1.212264
H -4.651678 -2.684765 -2.330412
C -3.447918 -0.916113 -2.678690
H -2.660044 -1.461395 -3.207343
H -4.134437 -0.521080 -3.438727
C -3.672118 1.387112 -1.722393
H -4.561429 1.072630 -1.167624
H -4.018305 1.782489 -2.687659
C -2.924198 2.492853 -0.979870
H -3.591470 3.323257 -0.729751
H -2.113390 2.905328 -1.590189
N -2.993077 -0.744909 1.934109
N -2.799372 0.197187 -1.921829
H 1.981025 0.494808 2.455713
H 2.357046 -1.339420 -2.468693
Cu 2.016337 -0.443633 -0.001002
S 2.092680 1.912512 -0.562306
C 3.490408 1.701088 -1.761360
H 3.594695 2.628064 -2.332857
H 4.419295 1.537100 -1.207155
C 3.159963 0.532987 -2.687206
H 2.224699 0.731092 -3.219822
H 3.948596 0.438485 -3.445158
C 4.262564 -1.498770 -1.736773
H 4.959631 -0.860843 -1.184585
H 4.732217 -1.728877 -2.703349
C 4.006336 -2.806768 -0.991159
H 3.424965 -3.508273 -1.599572

H 4.944328 -3.308293 -0.733893
C 4.208628 -1.865626 1.756523
H 5.010323 -1.358481 1.212104
H 4.651288 -2.685703 2.329754
C 3.447694 -0.917036 2.678512
H 2.659720 -1.462421 3.206907
H 4.134178 -0.522310 3.438741
C 3.672176 1.386457 1.722924
H 4.561489 1.072063 1.168105
H 4.018348 1.781514 2.688326
C 2.924381 2.492474 0.980695
H 3.591735 3.322884 0.730814
H 2.113598 2.904857 1.591111
N 2.993106 -0.744337 -1.934294
N 2.799310 0.196553 1.921946
O 0.000005 -0.954538 -0.000120
H 0.000012 -1.924811 -0.000252
S -3.008773 -2.590902 -0.547212
S 3.008583 -2.591020 0.546406

$[Cu_2^{II}(\mathbf{L^5})_2(\mu\text{-}OH)]^{3+}$
H 1.913542 0.597977 -2.577585
Cu 2.009707 0.162722 -0.013447
S 2.232247 -2.175142 -0.671789
C 3.737262 -2.567639 0.334046
H 3.972997 -3.627425 0.187881
H 4.580198 -1.975480 -0.032095
C 3.458461 -2.298179 1.811222
H 2.662738 -2.944947 2.193452
H 4.352204 -2.499147 2.411374
C 4.449888 0.410858 2.153878
H 5.090477 0.075264 1.333104
H 4.978693 0.235584 3.097129
C 4.096620 1.892391 2.032892
H 3.529344 2.240404 2.901657
H 5.005749 2.500154 1.975189
C 4.197194 2.288337 -0.856407
H 4.998641 1.567386 -0.669355
H 4.644820 3.282131 -0.952840
C 3.391032 1.941513 -2.106354
H 2.591126 2.674278 -2.251140
H 4.044969 1.999429 -2.986086
C 3.633227 -0.515768 -2.482091
H 4.560574 -0.498363 -1.901444
H 3.911638 -0.364167 -3.534560
C 2.931336 -1.864640 -2.352123
H 3.605770 -2.687384 -2.609035
H 2.069624 -1.933176 -3.024847
N 2.760588 0.591270 -2.005738
H -1.913913 0.595851 2.578195
Cu -2.009756 0.162634 0.013584
S -2.232024 -2.175772 0.670094
C -3.736804 -2.567846 -0.336269
H -3.972289 -3.627807 -0.190969
H -4.579948 -1.976200 0.030221
C -3.457869 -2.297168 -1.813198
H -2.661948 -2.943457 -2.195824
H -4.351487 -2.497872 -2.413624
C -4.449807 0.411986 -2.153688
H -5.090345 0.075599 -1.333200

H -4.978562 0.237375 -3.097089
C -4.096821 1.893494 -2.031505
H -3.529589 2.242303 -2.899979
H -5.006069 2.501036 -1.973354
C -4.197595 2.287293 0.858082
H -4.998945 1.566395 0.670437
H -4.645340 3.280963 0.955241
C -3.391444 1.939628 2.107802
H -2.591615 2.672365 2.253150
H -4.045421 1.996820 2.987553
C -3.633481 -0.517977 2.481473
H -4.560698 -0.500203 1.900631
H -3.912138 -0.367255 3.534003
C -2.931421 -1.866671 2.350563
H -3.605803 -2.689693 2.606717
H -2.069813 -1.935633 3.023377
N -2.760859 0.589533 2.006193
O -0.000041 0.667254 0.000285
H -0.000063 1.637389 0.000716
S 3.033371 2.312980 0.581526
S 2.887469 -0.581053 2.178834
S -2.887209 -0.579628 -2.179423
S -3.033709 2.313156 -0.579773

$[Cu_2^{II}(\mathbf{L^6})_2(\mu\text{-}OH)]^{3+}$
H -1.981645 0.395459 -2.582417
H -2.040924 -0.647889 2.562211
Cu -1.994117 -0.088625 -0.007012
S -2.611036 2.220305 0.167540
C -3.906637 1.883539 1.448667
H -4.224933 2.839686 1.874216
H -4.773774 1.412215 0.977564
C -3.274130 0.999419 2.524909
H -2.417875 1.512099 2.974087
H -4.004306 0.823315 3.325100
C -3.850212 -1.346381 1.876307
H -4.722057 -0.905973 1.382170
H -4.165843 -1.658992 2.880453
C -3.340303 -2.545412 1.084871
H -2.512699 -3.045252 1.597880
H -4.135578 -3.281034 0.928963
C -3.694615 -2.170450 -1.325418
H -4.682886 -1.775377 -1.058930
H -3.811402 -3.214874 -1.634210
C -3.030134 -1.366066 -2.433006
H -2.082710 -1.839192 -2.704975
H -3.671352 -1.349881 -3.323384
C -3.879391 0.958767 -2.014961
H -4.694741 0.511161 -1.439833
H -4.240324 1.080530 -3.045428
C -3.507473 2.326457 -1.446029
H -4.390296 2.961216 -1.323096
H -2.813817 2.864288 -2.101401
N -2.786975 -0.296169 1.959623
N -2.715129 0.024635 -1.975813
H 1.981207 0.394746 2.582374
H 2.041322 -0.647182 -2.562568
Cu 1.994072 -0.088584 0.006824
S 2.611273 2.220329 -0.166932
C 3.906974 1.883881 -1.448021

H 4.225368 2.840131 -1.873264
H 4.774048 1.412359 -0.976996
C 3.274475 1.000139 -2.524574
H 2.418266 1.513002 -2.973630
H 4.004679 0.824241 -3.324784
C 3.850506 -1.345791 -1.876498
H 4.722216 -0.905479 -1.382038
H 4.166365 -1.658055 -2.880679
C 3.340515 -2.545107 -1.085541
H 2.513049 -3.044838 -1.598879
H 4.135812 -3.280726 -0.929723
C 3.694223 -2.170982 1.324978
H 4.682606 -1.775930 1.058868
H 3.810839 -3.215502 1.633515
C 3.029524 -1.366859 2.432636
H 2.081999 -1.839989 2.704243
H 3.670528 -1.350986 3.323174
C 3.879120 0.957976 2.015369
H 4.694479 0.510429 1.440210
H 4.239934 1.079369 3.045921
C 3.507478 2.325889 1.446793
H 4.390406 2.960566 1.324198
H 2.813790 2.863614 2.102220
N 2.787225 -0.295603 -1.959715
N 2.714740 0.024002 1.975781
O -0.000025 -0.643610 -0.000225
H -0.000011 -1.614347 -0.000499
O -2.808702 -2.098769 -0.184906
O 2.808627 -2.098897 0.184263

$[Cu_2^{II}(\mathbf{L^1})_2(\mu\text{-}OH)_2]^{2+}$
H -2.313622 -0.743349 -2.412496
H -2.411137 -3.045597 0.915228
H -1.412338 0.290779 2.354036
Cu -1.520866 -0.779055 -0.007059
C -3.099632 2.495755 0.484045
H -3.280464 3.572585 0.602122
H -4.091073 2.033970 0.437610
C -2.354242 1.995336 1.725039
H -1.341115 2.412791 1.721712
H -2.858787 2.381440 2.624207
C -3.391745 -0.183484 2.335810
H -4.281913 0.119430 1.773974
H -3.580506 0.083951 3.386459
C -3.185980 -1.698529 2.250790
H -2.332946 -1.987068 2.873312
H -4.070633 -2.221681 2.635516
C -4.057904 -2.272760 -0.037283
H -4.798092 -1.526674 0.262492
H -4.530044 -3.255626 0.076646
C -3.627189 -2.045362 -1.486073
H -2.927997 -2.828991 -1.799027
H -4.496610 -2.092831 -2.155261
C -3.864475 0.408096 -1.727064
H -4.517381 0.408789 -0.850293
H -4.513503 0.239283 -2.598055
C -3.203099 1.776517 -1.906511
H -4.018401 2.487759 -2.116053
H -2.564759 1.758903 -2.798243
N -2.222435 0.522070 1.778089

N	-2.873932	-2.138163	0.859330
N	-2.923188	-0.737163	-1.593289
H	2.166316	-1.044481	2.205325
H	2.370025	-2.879464	-1.465526
H	1.630496	0.663748	-2.273344
Cu	1.462786	-0.245784	-0.023647
C	3.225554	2.477177	-0.009943
H	3.366102	3.556237	0.141297
H	4.223719	2.030017	0.025120
C	2.601818	2.232518	-1.384236
H	1.609637	2.695159	-1.423458
H	3.213472	2.705616	-2.164520
C	3.602346	0.115989	-2.246295
H	4.456677	0.250414	-1.575110
H	3.873999	0.581845	-3.204007
C	3.308504	-1.368727	-2.473154
H	2.501476	-1.470327	-3.208479
H	4.199847	-1.847187	-2.906041
C	3.948130	-2.329136	-0.278922
H	4.752637	-1.600397	-0.418123
H	4.392202	-3.317214	-0.462208
C	3.440796	-2.261244	1.161859
H	2.649643	-3.005727	1.307633
H	4.251185	-2.513288	1.859158
C	3.853933	0.070789	1.938232
H	4.623525	0.182775	1.167744
H	4.363503	-0.276130	2.848056
C	3.163468	1.405981	2.223841
H	3.918440	2.135392	2.553448
H	2.457846	1.279794	3.053829
N	2.429497	0.785754	-1.648842
N	2.860696	-2.019826	-1.227413
N	2.868671	-0.928574	1.473103
O	0.106548	-1.289432	1.082599
O	-0.208290	0.234285	-1.049916
H	0.305769	-2.238404	1.050343
H	-0.623473	1.116796	-0.925344
N	-2.364198	2.214271	-0.772377
H	-1.903649	3.074513	-1.065422
N	2.397863	1.868949	1.051088
H	1.702180	2.545343	1.358295

$[Cu_2^{II}(\mathbf{L^2})_2(\mu\text{-}OH)_2]^{2+}$

H	-2.488927	-0.655757	-2.465241
H	-2.394780	-3.049043	0.871029
H	-1.341493	0.207028	2.274493
Cu	-1.525178	-0.804485	-0.096839
S	-2.200113	2.552790	-0.940685
C	-3.017133	2.667018	0.711269
H	-3.109492	3.730629	0.950209
H	-4.035435	2.274619	0.632010
C	-2.227407	1.985525	1.832979
H	-1.198389	2.358362	1.822385
H	-2.669869	2.297297	2.792420
C	-3.335601	-0.186994	2.308629
H	-4.227849	0.130003	1.757465
H	-3.510085	0.075742	3.363155
C	-3.150328	-1.703199	2.216938
H	-2.291109	-2.002754	2.825662
H	-4.034334	-2.216299	2.616063

C -4.071402 -2.302709 -0.046769
H -4.828636 -1.588439 0.285913
H -4.506969 -3.302962 0.059782
C -3.682849 -2.036401 -1.499730
H -2.961493 -2.786832 -1.842600
H -4.564523 -2.104147 -2.150748
C -4.024524 0.408124 -1.610368
H -4.488906 0.457491 -0.622334
H -4.824878 0.160010 -2.323726
C -3.477358 1.777782 -2.008172
H -4.325799 2.464595 -2.092773
H -3.012446 1.738223 -3.000533
N -2.161822 0.508780 1.746731
N -2.868189 -2.146946 0.820688
N -3.030629 -0.699680 -1.600155
H 2.133600 -0.990178 2.182609
H 2.472453 -2.900492 -1.502349
H 1.760567 0.556663 -2.350217
Cu 1.472141 -0.362341 -0.123114
S 2.023390 2.154229 1.220886
C 3.130610 2.672744 -0.160624
H 3.209909 3.763370 -0.150384
H 4.132131 2.271319 0.019239
C 2.582822 2.223675 -1.515413
H 1.574994 2.628990 -1.652941
H 3.209984 2.651584 -2.310147
C 3.739131 0.105620 -2.156065
H 4.524215 0.250061 -1.406642
H 4.089336 0.581511 -3.082593
C 3.489110 -1.380850 -2.417885
H 2.746750 -1.487143 -3.217756
H 4.418806 -1.844746 -2.778282
C 3.975999 -2.384685 -0.204333
H 4.819820 -1.696598 -0.316300
H 4.381986 -3.394857 -0.347048
C 3.396294 -2.266972 1.204514
H 2.576261 -2.983261 1.325981
H 4.160924 -2.522044 1.950524
C 3.853393 0.078487 1.893156
H 4.537597 0.272472 1.061655
H 4.460320 -0.334853 2.712491
C 3.210809 1.374600 2.385693
H 3.988120 2.098131 2.649329
H 2.627273 1.194296 3.296131
N 2.499087 0.750503 -1.670745
N 2.951827 -2.049415 -1.215602
N 2.844625 -0.910455 1.453407
O 0.093613 -1.378555 0.977401
O -0.151739 0.031940 -1.230097
H 0.254083 -2.334115 0.924377
H -0.426765 0.970587 -1.186497

$[Cu_2^{II}(\mathbf{L^3})_2(\mu\text{-}OH)_2]^{2+}$
H -2.564422 -3.071024 0.185978
H -0.775684 -0.351675 2.202335
Cu -1.515211 -0.796312 -0.245780
S -2.120838 2.702421 -0.202770
C -2.631647 2.382655 1.541712
H -2.688037 3.344033 2.061011
H -3.638787 1.955541 1.556133

C -1.635027 1.486657 2.285537
H -0.617733 1.851386 2.112367
H -1.829172 1.584134 3.364899
C -2.752867 -0.709613 2.530450
H -3.699343 -0.200926 2.319988
H -2.649193 -0.740097 3.625067
C -2.778539 -2.141501 1.998411
H -1.839077 -2.644678 2.245173
H -3.597117 -2.705373 2.463414
C -4.300460 -1.998709 0.021465
H -4.770917 -1.207413 0.609209
H -4.875791 -2.916661 0.202731
C -4.335607 -1.649958 -1.464453
H -3.923863 -2.458572 -2.078519
H -5.364113 -1.483063 -1.799587
C -4.361889 1.163806 -1.127959
H -4.648869 0.879052 -0.112183
H -5.273099 1.210152 -1.735350
C -3.685724 2.535199 -1.143757
H -4.407107 3.274813 -0.779359
H -3.422309 2.827895 -2.165452
N -1.660100 0.055950 1.892457
N -2.903817 -2.164097 0.509879
H 2.591562 -3.076043 -0.238068
H 2.145694 -0.344959 -2.878102
Cu 1.482981 -0.778572 -0.547064
S 2.082283 2.686606 0.033188
C 3.395708 2.310124 -1.205548
H 3.771585 3.256560 -1.605474
H 4.237229 1.818055 -0.709410
C 2.865771 1.476273 -2.376149
H 1.885046 1.845822 -2.688753
H 3.545800 1.604633 -3.230183
C 4.004727 -0.726165 -2.113825
H 4.694172 -0.211688 -1.439279
H 4.464517 -0.717385 -3.110813
C 3.779292 -2.165573 -1.655545
H 3.157224 -2.700147 -2.382474
H 4.736228 -2.698916 -1.589595
C 3.951043 -1.985975 0.825858
H 4.653500 -1.183151 0.589260
H 4.547558 -2.894927 0.985441
C 3.177087 -1.654755 2.101859
H 2.455210 -2.442160 2.341823
H 3.867807 -1.576699 2.947176
C 3.501296 1.173794 2.022291
H 4.321584 0.876064 1.362340
H 3.896185 1.218373 3.043123
C 2.967165 2.555990 1.636444
H 3.795937 3.271845 1.656340
H 2.235139 2.904584 2.372703
N 2.715481 0.013889 -2.107533
N 3.057764 -2.175490 -0.351070
O 0.084951 -2.015844 0.246983
O -0.103785 0.174660 -1.171950
H 0.060388 -2.877946 -0.198366
H -0.156594 1.114399 -0.919873
S -3.312228 -0.170252 -1.862015
S 2.184340 -0.116147 1.965326

$[Cu_2^{II}(\mathbf{L^4})_2(\mu\text{-}OH)_2]^{2+}$

H	-2.044807	-0.096072	-2.396146
H	-2.046923	-0.607191	2.359358
Cu	-1.494280	-0.334611	-0.018582
S	-2.617754	2.323825	-0.323138
C	-3.716283	2.028046	1.128568
H	-3.949863	2.997983	1.576724
H	-4.659785	1.599538	0.778306
C	-3.043559	1.148717	2.180155
H	-2.086558	1.592886	2.471687
H	-3.677318	1.121845	3.078052
C	-3.930255	-1.145419	1.768436
H	-4.611319	-0.877347	0.955665
H	-4.483364	-1.002390	2.708220
C	-3.526044	-2.617405	1.677590
H	-2.969897	-2.919530	2.573023
H	-4.420453	-3.246512	1.639975
C	-3.526480	-2.846478	-1.181597
H	-4.500977	-2.486346	-0.838939
H	-3.685279	-3.831535	-1.629394
C	-2.912065	-1.920456	-2.228388
H	-1.922717	-2.292560	-2.512565
H	-3.538554	-1.940179	-3.131523
C	-3.968944	0.301445	-1.826382
H	-4.637221	-0.016419	-1.021033
H	-4.500365	0.119243	-2.771996
C	-3.674813	1.799039	-1.732272
H	-4.613933	2.359886	-1.705634
H	-3.133148	2.140849	-2.622287
N	-2.758232	-0.239783	1.723785
N	-2.734377	-0.515511	-1.768869
H	2.089806	-0.100084	2.356240
H	2.069201	-0.323251	-2.404815
Cu	1.538605	-0.226879	-0.020999
S	2.435582	2.455492	0.397161
C	3.590419	2.325974	-1.036252
H	3.767690	3.333264	-1.423619
H	4.553131	1.940642	-0.687723
C	3.006284	1.461970	-2.152865
H	2.041387	1.873579	-2.465668
H	3.671285	1.512156	-3.026318
C	3.984357	-0.811913	-1.880977
H	4.669217	-0.564168	-1.064266
H	4.516316	-0.596361	-2.819284
C	3.629212	-2.298230	-1.868605
H	3.043204	-2.561421	-2.756999
H	4.542410	-2.899781	-1.905273
C	3.755811	-2.650652	0.965926
H	4.687226	-2.204932	0.605032
H	4.002150	-3.644120	1.351253
C	3.131561	-1.825142	2.089999
H	2.198237	-2.296738	2.413792
H	3.809004	-1.832626	2.955236
C	3.963451	0.504607	1.804809
H	4.648807	0.300307	0.976840
H	4.521640	0.320451	2.734385
C	3.517574	1.965877	1.799684
H	4.392051	2.622907	1.825715
H	2.927019	2.191797	2.695317
N	2.779907	0.044021	-1.768158

N 2.812081 -0.423871 1.708996
O 0.033065 -0.639539 1.255832
O 0.005487 0.089145 -1.290829
H 0.042678 -1.604312 1.382877
H -0.056471 1.053746 -1.404370
S -2.418894 -3.057619 0.278603
S 2.595926 -2.854535 -0.454122

$[Cu_2^{II}(\mathbf{L^5})_2(\mu\text{-}OH)_2]^{2+}$
H -2.457607 -0.586439 -2.286068
Cu -1.493605 -0.823805 0.020270
S -2.359610 2.620901 -0.711378
C -3.368814 2.832014 0.818417
H -3.598639 3.897976 0.921340
H -4.321851 2.312861 0.685624
C -2.656391 2.373986 2.093218
H -1.710698 2.911167 2.217949
H -3.272713 2.615965 2.966591
C -3.769449 -0.246794 2.558163
H -4.524928 0.030192 1.815588
H -4.137310 0.065191 3.542036
C -3.556805 -1.760887 2.596251
H -2.835171 -2.034617 3.372192
H -4.496197 -2.272642 2.828756
C -4.252235 -2.465202 -0.160178
H -5.014615 -1.768954 0.199244
H -4.706218 -3.457208 -0.231612
C -3.683904 -2.045296 -1.516486
H -2.926289 -2.764400 -1.845994
H -4.489918 -2.057292 -2.263108
C -4.054247 0.394051 -1.448089
H -4.518614 0.425727 -0.459077
H -4.849881 0.137284 -2.163339
C -3.533623 1.776622 -1.842164
H -4.399376 2.429849 -1.992308
H -3.010388 1.734855 -2.804909
N -3.042377 -0.700512 -1.454765
H 2.145515 -0.998951 2.023778
Cu 1.464891 -0.377543 -0.205837
S 2.122316 2.161449 0.964645
C 3.363315 2.742536 -0.271545
H 3.512520 3.817338 -0.126339
H 4.317574 2.248306 -0.069434
C 2.915473 2.504273 -1.715816
H 1.985613 3.041628 -1.928667
H 3.670015 2.892430 -2.408660
C 4.214967 0.010263 -2.406917
H 4.820697 0.137868 -1.504780
H 4.718519 0.527254 -3.231285
C 4.040875 -1.468106 -2.769726
H 3.509963 -1.569474 -3.721448
H 5.023186 -1.933999 -2.897248
C 4.192051 -2.557579 -0.129624
H 5.008710 -1.841973 -0.262128
H 4.638868 -3.555407 -0.095570
C 3.439272 -2.312558 1.176739
H 2.605136 -3.016316 1.259608
H 4.114236 -2.518488 2.019186
C 3.872594 0.064371 1.750963
H 4.573426 0.246937 0.930645

H 4.461632 -0.333901 2.590342
C 3.212906 1.363599 2.209250
H 3.977540 2.078476 2.527612
H 2.566539 1.184825 3.076327
N 2.876939 -0.940901 1.310223
O 0.175900 -1.473669 0.902140
O -0.217749 0.117493 -1.132740
H 0.269194 -2.427426 0.739723
H -0.436646 1.062684 -1.023396
S -2.174286 0.603914 2.214352
S -2.874506 -2.546279 1.067758
S 2.554650 0.765668 -2.181805
S 3.058413 -2.470894 -1.579941

$[Cu_2^{II}(\mathbf{L^6})_2(\mu\text{-}OH)_2]^{2+}$
H -1.737148 -0.522856 -2.333571
H -2.122730 0.386828 2.516668
Cu -1.525067 0.408721 0.095402
S -3.012558 2.157623 -0.797334
C -4.283427 1.997628 0.533728
H -4.819601 2.947113 0.613614
H -5.003566 1.226255 0.247554
C -3.586366 1.671209 1.854142
H -2.876746 2.465588 2.107769
H -4.333077 1.631080 2.658817
C -3.698415 -0.801653 1.979222
H -4.438028 -0.824921 1.174024
H -4.252275 -0.697944 2.923465
C -2.910638 -2.110708 2.021930
H -2.170739 -2.085134 2.829090
H -3.600621 -2.937883 2.234104
C -2.934693 -2.866471 -0.277913
H -3.993197 -2.597301 -0.172413
H -2.871192 -3.962020 -0.286367
C -2.356331 -2.311966 -1.573171
H -1.298119 -2.587417 -1.630949
H -2.868389 -2.791327 -2.421345
C -3.746433 -0.305324 -2.050367
H -4.482403 -0.591105 -1.291687
H -4.093327 -0.735711 -3.003518
C -3.716034 1.215083 -2.219686
H -4.716312 1.605823 -2.428328
H -3.076977 1.503399 -3.061684
N -2.828262 0.389998 1.776729
N -2.431368 -0.834768 -1.653150
H 1.959542 -0.606785 2.285859
H 1.962524 0.457038 -2.370609
Cu 1.470673 0.065290 0.002535
S 2.781728 2.314229 0.977211
C 3.951877 2.329710 -0.449396
H 4.328898 3.348927 -0.572017
H 4.810182 1.693535 -0.215277
C 3.263231 1.894384 -1.744223
H 2.418083 2.560530 -1.946896
H 3.968115 2.013643 -2.578718
C 3.729556 -0.527337 -2.102648
H 4.550673 -0.518230 -1.378982
H 4.163426 -0.296582 -3.086438
C 3.061628 -1.901192 -2.159688
H 2.274762 -1.912449 -2.921885

H 3.795737 -2.670315 -2.430140
C 3.282003 -2.729759 0.089956
H 4.306362 -2.364563 -0.056447
H 3.307942 -3.825711 0.041603
C 2.735954 -2.289346 1.438538
H 1.726885 -2.691736 1.566636
H 3.362556 -2.700079 2.241839
C 3.914692 -0.136883 1.890576
H 4.603511 -0.250020 1.048208
H 4.384498 -0.628517 2.755253
C 3.706624 1.338443 2.231845
H 4.671527 1.817805 2.421927
H 3.115028 1.444358 3.148546
N 2.740779 0.503956 -1.709710
N 2.640161 -0.808799 1.550038
O -0.086347 -0.467202 1.150360
O 0.003859 0.844861 -1.135971
H -0.342928 -1.403088 1.043836
H 0.094285 1.809135 -1.210833
O -2.177206 -2.352435 0.824602
O 2.414069 -2.219338 -0.926910

$[Cu_2^{I}(\mathbf{L^1})_2(\mu\text{-}OH)]^+$
H -2.242334 2.748051 -1.169499
H -2.957258 -0.696958 -3.016211
H -2.332657 -2.395464 0.391382
Cu -1.890705 0.158051 -0.432981
C -3.585960 0.072255 2.219066
H -3.754830 0.220723 3.298726
H -4.539134 0.286678 1.724428
C -3.194644 -1.391060 1.964821
H -2.236139 -1.594754 2.457530
H -3.944930 -2.048027 2.436788
C -4.246915 -1.964972 -0.211029
H -5.010851 -1.234958 0.079175
H -4.660147 -2.958975 0.032667
C -4.007948 -1.891921 -1.726476
H -3.271468 -2.654846 -2.006898
H -4.948303 -2.148262 -2.243721
C -4.440689 0.497235 -2.272244
H -5.144255 0.427880 -1.435913
H -5.044619 0.423974 -3.192475
C -3.742051 1.864092 -2.246508
H -3.028355 1.916920 -3.077234
H -4.492457 2.654524 -2.412590
C -3.791916 2.522088 0.143664
H -4.699823 1.910813 0.175396
H -4.122314 3.568429 0.036024
C -3.023086 2.373338 1.463704
H -3.655084 2.748675 2.286106
H -2.129530 3.009095 1.431803
N -3.022866 -1.662184 0.533866
N -3.467795 -0.590850 -2.142851
N -2.983469 2.071459 -0.999343
H 1.701698 -1.265991 2.490875
H 2.733672 -2.797468 -0.948525
H 2.944492 0.782632 -2.539732
Cu 1.896046 -0.251541 -0.110247
C 3.863451 2.126423 0.362245
H 4.121631 3.153011 0.671985

H 4.696203 1.488800 0.677460
C 3.731276 2.084388 -1.166703
H 2.899017 2.730518 -1.471442
H 4.647340 2.507854 -1.612360
C 4.593929 -0.164233 -1.780500
H 5.231481 -0.022913 -0.901187
H 5.218299 0.072462 -2.658476
C 4.151514 -1.632507 -1.864863
H 3.523745 -1.766192 -2.754363
H 5.044164 -2.265347 -2.004237
C 4.121075 -2.393382 0.499012
H 4.916412 -1.651644 0.630065
H 4.621256 -3.372028 0.402913
C 3.223040 -2.416198 1.743708
H 2.434608 -3.164851 1.600435
H 3.823003 -2.740514 2.610424
C 3.379732 -0.102672 2.637760
H 4.385380 -0.138243 2.206321
H 3.496994 -0.293364 3.717717
C 2.784800 1.299301 2.440049
H 3.403481 2.030329 2.987051
H 1.783629 1.328121 2.887524
N 3.437974 0.729726 -1.651889
N 3.353796 -2.031167 -0.697050
N 2.562450 -1.121255 1.968660
O -0.000231 -0.455886 -0.765892
H 0.050457 -0.740047 -1.689594
N -2.575199 0.990365 1.677244
H -1.753295 0.982640 2.275878
N 2.642581 1.634612 1.015146
H 1.898221 2.317653 0.895720

$[Cu_2^{I}(\mathbf{L^2})_2(\mu\text{-}OH)]^+$
H -1.474937 2.317756 -0.756389
H -3.050038 -0.608108 -3.039870
H -2.735187 -2.736632 0.071763
Cu -1.734383 -0.329882 -0.503823
S -1.735844 0.390402 2.131073
C -3.310658 -0.503155 2.475385
H -3.456751 -0.577747 3.557536
H -4.141556 0.079562 2.065657
C -3.278483 -1.911330 1.862890
H -2.397319 -2.445496 2.235080
H -4.162584 -2.461875 2.226549
C -4.507697 -1.775799 -0.280735
H -5.026119 -0.903763 0.134311
H -5.159544 -2.645975 -0.093478
C -4.333430 -1.611417 -1.796079
H -3.842799 -2.506971 -2.196538
H -5.331394 -1.557647 -2.262208
C -4.148087 0.850253 -2.113799
H -4.861247 0.860608 -1.282917
H -4.732947 1.044254 -3.027677
C -3.122307 1.976834 -1.929402
H -2.400826 1.944233 -2.753920
H -3.639517 2.948774 -1.985276
C -3.073402 2.327730 0.512747
H -4.038822 1.814873 0.575192
H -3.296107 3.406111 0.429243
C -2.285048 2.114473 1.807624

H -2.866571 2.482724 2.659038
H -1.352773 2.691412 1.782679
N -3.209700 -1.895952 0.395590
N -3.486556 -0.459030 -2.133489
N -2.364118 1.827092 -0.672404
H 1.213889 -0.929713 2.048177
H 3.032988 -2.901785 -0.927308
H 3.111564 0.404845 -2.738444
Cu 1.795505 -0.389345 -0.542439
S 1.716748 2.084290 0.522394
C 3.367624 2.525175 -0.165917
H 3.506497 3.609664 -0.114676
H 4.140890 2.062433 0.454702
C 3.494379 2.069375 -1.626471
H 2.680862 2.510341 -2.213101
H 4.437699 2.473893 -2.029700
C 4.692843 -0.097848 -1.554218
H 5.071841 0.204773 -0.571779
H 5.461584 0.185756 -2.291867
C 4.497995 -1.619672 -1.592865
H 4.133095 -1.907940 -2.586553
H 5.479297 -2.105138 -1.460973
C 3.995585 -2.246155 0.761680
H 4.741551 -1.470151 0.965178
H 4.508319 -3.212196 0.900221
C 2.847010 -2.141253 1.774404
H 2.100283 -2.910481 1.547165
H 3.239004 -2.351028 2.783945
C 2.844590 0.251361 2.403912
H 3.861985 0.336917 2.006594
H 2.947373 0.051179 3.485938
C 2.108934 1.586437 2.249697
H 2.673162 2.384604 2.742900
H 1.130160 1.533837 2.740218
N 3.420003 0.606818 -1.788861
N 3.505185 -2.060222 -0.607756
N 2.166815 -0.838877 1.700232
O 0.009598 -1.176747 -1.028612
H -0.009284 -1.468266 -1.950664

$[Cu_2^{I}(\mathbf{L^3})_2(\mu\text{-}OH)]^+$
H 2.174034 -1.206405 2.365990
H 0.822244 -2.166355 -1.168729
Cu 1.629476 0.145624 0.187807
S 2.441730 1.241164 -1.809588
C 3.130849 -0.259923 -2.631570
H 3.360011 -0.028709 -3.676689
H 4.064146 -0.543276 -2.134072
C 2.109734 -1.405587 -2.568870
H 1.189656 -1.094724 -3.076285
H 2.517136 -2.257913 -3.137510
C 2.697485 -2.702695 -0.537838
H 3.717542 -2.384017 -0.779283
H 2.591922 -3.733731 -0.913216
C 2.504115 -2.691566 0.983871
H 1.465087 -2.954242 1.213852
H 3.142621 -3.469372 1.434365
C 4.165521 -1.096196 1.875919
H 4.761882 -1.252419 0.969717
H 4.557764 -1.804329 2.628264

C 4.393356 0.319477 2.417935
H 3.887272 0.440947 3.383277
H 5.462089 0.473886 2.600524
C 4.734476 1.597296 -0.126765
H 5.017617 0.555174 -0.300555
H 5.655285 2.178118 -0.000005
C 3.967855 2.154153 -1.331402
H 4.629374 2.198768 -2.203563
H 3.628390 3.176806 -1.136042
N 1.761941 -1.774944 -1.189995
N 2.763449 -1.360059 1.549730
H -2.083400 -0.998734 2.460797
H -2.782636 2.756803 1.630424
Cu -1.675677 0.427610 0.335135
S -2.440644 1.115466 -1.826265
C -4.040707 1.891915 -1.332821
H -4.432154 2.470190 -2.175594
H -4.761933 1.102946 -1.096936
C -3.828662 2.818136 -0.126884
H -3.115292 3.604391 -0.397012
H -4.788565 3.315696 0.090311
C -4.288435 1.388392 1.852053
H -4.985123 0.884405 1.172927
H -4.891942 2.071971 2.471307
C -3.608937 0.349934 2.753512
H -2.861462 0.852403 3.378188
H -4.359101 -0.083776 3.434764
C -3.750245 -1.814674 1.574107
H -4.617807 -1.428219 1.027077
H -4.155337 -2.357050 2.447775
C -3.001101 -2.839531 0.715129
H -2.204840 -3.314479 1.300593
H -3.687182 -3.635388 0.407401
C -3.482347 -1.556595 -1.815768
H -4.310123 -1.237521 -1.175929
H -3.847590 -2.366372 -2.457468
C -3.009963 -0.399550 -2.703751
H -3.809605 -0.116307 -3.396944
H -2.155237 -0.706469 -3.315882
N -3.293863 2.104242 1.040317
N -2.914945 -0.680294 1.965697
O 0.026785 0.337751 1.406582
H 0.155114 1.172242 1.881536
S 3.728212 1.702453 1.408866
S -2.116696 -2.182913 -0.755311

$[Cu_2^{I}(\mathbf{L^4})_2(\mu\text{-}OH)]^+$
H 2.696935 0.266473 -2.699413
H 1.840940 0.586220 2.202064
Cu 1.844416 0.590185 -0.301273
S 1.806156 -2.212083 -0.462502
C 2.747787 -2.416232 1.112533
H 2.599757 -3.438288 1.475315
H 3.814347 -2.294822 0.898139
C 2.281222 -1.416229 2.180971
H 1.198105 -1.508159 2.311391
H 2.746193 -1.705394 3.139582
C 3.900185 0.453334 2.223679
H 4.651711 -0.081372 1.628347
H 4.127708 0.226365 3.281512

C 4.067609 1.966755 2.047004
H 3.423057 2.499663 2.756335
H 5.098507 2.250419 2.282821
C 4.826171 1.989547 -0.741667
H 5.377053 1.183216 -0.248137
H 5.551983 2.768570 -0.995352
C 4.166519 1.503669 -2.037791
H 3.559646 2.311143 -2.460245
H 4.961818 1.275805 -2.765750
C 4.025551 -0.939511 -1.736025
H 4.607254 -0.899623 -0.810212
H 4.747264 -1.048156 -2.563087
C 3.124914 -2.176311 -1.737430
H 3.744663 -3.074803 -1.651244
H 2.586010 -2.256599 -2.689564
N 2.572304 -0.022317 1.835341
N 3.276133 0.329128 -1.861591
H -1.373615 -1.532369 -1.400248
H -2.887152 1.932695 2.246967
Cu -1.698393 0.341691 0.440942
S -3.014147 1.479845 -1.653049
C -4.536580 1.760522 -0.654971
H -5.189306 2.463431 -1.182017
H -5.079797 0.815917 -0.554318
C -4.180616 2.337210 0.721325
H -3.565564 3.233757 0.588247
H -5.113803 2.657422 1.213555
C -4.268669 0.433600 2.288504
H -4.810955 -0.168298 1.550772
H -5.033122 0.943538 2.900701
C -3.461314 -0.474627 3.219605
H -2.987737 0.116650 4.012581
H -4.129003 -1.188452 3.712601
C -2.912659 -2.602386 1.360729
H -3.946884 -2.281205 1.203969
H -2.940386 -3.572140 1.867352
C -2.174678 -2.749975 0.024334
H -1.128876 -3.014428 0.210755
H -2.626011 -3.591875 -0.526245
C -3.400514 -1.354890 -1.596121
H -4.259447 -1.301138 -0.918085
H -3.568843 -2.232047 -2.245314
C -3.360951 -0.115232 -2.493050
H -4.297209 -0.041449 -3.056076
H -2.555506 -0.204799 -3.232090
N -3.423525 1.395621 1.566783
N -2.184785 -1.515959 -0.783142
O 0.123594 1.213049 0.491986
H 0.007013 2.140282 0.238888
S -2.061768 -1.376202 2.440729
S 3.585845 2.686410 0.425662

$[Cu_2^{I}(\mathbf{L^5})_2(\mu\text{-}OH)]^+$
H -1.188217 1.575713 -0.934745
Cu -1.846564 -0.682836 0.082448
S -2.045284 0.891229 2.249613
C -3.769831 0.390486 2.664079
H -4.026855 0.785842 3.652956
H -4.451891 0.841616 1.937585
C -3.928965 -1.134046 2.686971

H -3.245399 -1.583094 3.415179
H -4.946040 -1.393512 3.001446
C -5.060656 -1.591561 0.112798
H -5.237954 -0.512226 0.152694
H -5.924901 -2.096193 0.560195
C -4.905251 -2.066642 -1.335796
H -4.784134 -3.154721 -1.368158
H -5.820824 -1.831011 -1.889298
C -3.883886 0.356242 -2.498483
H -4.681741 0.634305 -1.802414
H -4.273279 0.488745 -3.512864
C -2.654943 1.255538 -2.314593
H -1.830946 0.870291 -2.924192
H -2.902705 2.257850 -2.702544
C -2.906349 2.297428 -0.090379
H -3.950046 1.971159 -0.019405
H -2.923336 3.300796 -0.551761
C -2.300614 2.449343 1.308024
H -2.908000 3.139007 1.903008
H -1.294835 2.880510 1.245311
N -2.177955 1.330095 -0.921116
H 1.459561 -1.434846 1.520300
Cu 1.812851 -0.227838 -0.624809
S 1.734121 1.899464 1.218513
C 3.369198 2.531319 0.663676
H 3.580145 3.483339 1.163400
H 4.144497 1.819330 0.959986
C 3.390601 2.755926 -0.852387
H 2.585655 3.433589 -1.155717
H 4.333794 3.230411 -1.144811
C 4.828722 0.474584 -1.746706
H 5.135004 0.477569 -0.696021
H 5.541511 1.085717 -2.312153
C 4.833475 -0.947723 -2.314625
H 4.579678 -0.935050 -3.379980
H 5.844602 -1.360939 -2.231741
C 4.307926 -2.388240 0.123472
H 4.973441 -1.558659 0.383414
H 4.901752 -3.307763 0.128953
C 3.164788 -2.505242 1.141160
H 2.441649 -3.248820 0.789853
H 3.582508 -2.888431 2.086749
C 3.002055 -0.391116 2.404192
H 4.023832 -0.109728 2.120966
H 3.087505 -0.931462 3.364267
C 2.161246 0.861162 2.674361
H 2.656238 1.479400 3.430272
H 1.181458 0.582150 3.079177
N 2.445846 -1.238386 1.347717
O 0.028645 -1.129562 -0.481928
H -0.027770 -1.844179 -1.132662
S -3.564745 -2.004016 1.108631
S -3.453442 -1.419887 -2.254992
S 3.161025 1.253134 -1.890893
S 3.633523 -2.122685 -1.572828

$[Cu_2^{I}(\mathbf{L^6})_2(\mu\text{-}OH)]^+$
H 3.081724 0.244667 -2.712021
H 1.411801 0.651683 1.946239
Cu 1.784361 0.422784 -0.513215

S 1.865584 -2.225849 -0.509740
C 2.608673 -2.337631 1.179471
H 2.463868 -3.354479 1.557732
H 3.686220 -2.164329 1.097171
C 1.960031 -1.324572 2.137526
H 0.875393 -1.476842 2.141972
H 2.322729 -1.543692 3.156595
C 3.441455 0.656896 2.306506
H 4.296031 0.038828 2.003491
H 3.444033 0.667377 3.411967
C 3.630230 2.101861 1.827052
H 2.808911 2.725613 2.195827
H 4.567628 2.505753 2.237974
C 4.759342 1.853107 -0.291301
H 5.263102 1.017481 0.213397
H 5.474862 2.688140 -0.335818
C 4.364488 1.469074 -1.713767
H 3.812547 2.302659 -2.158497
H 5.280965 1.313084 -2.304832
C 4.219330 -0.992224 -1.559198
H 4.701657 -0.937991 -0.579125
H 5.024025 -1.110255 -2.303944
C 3.324677 -2.232069 -1.627911
H 3.928186 -3.126756 -1.443171
H 2.892837 -2.342627 -2.629986
N 2.222478 0.064823 1.752873
N 3.484115 0.272481 -1.774567
H -1.821148 -1.624826 -1.901725
H -2.237448 1.808028 1.839984
Cu -1.682357 0.407508 -0.322868
S -3.506450 1.436797 -1.799981
C -4.688121 1.743483 -0.412941
H -5.431312 2.476699 -0.741084
H -5.218291 0.813318 -0.186252
C -3.955998 2.275479 0.827955
H -3.399786 3.178985 0.555870
H -4.714326 2.577681 1.569511
C -3.587791 0.356729 2.343206
H -4.410442 -0.168846 1.844869
H -4.028772 0.863003 3.220461
C -2.548918 -0.646931 2.853769
H -1.745518 -0.115945 3.376841
H -3.023586 -1.327014 3.576966
C -2.661644 -2.429778 1.237593
H -3.733457 -2.191021 1.250284
H -2.526192 -3.356546 1.815449
C -2.176095 -2.660765 -0.188937
H -1.097168 -2.839942 -0.169549
H -2.661741 -3.570207 -0.579371
C -3.812694 -1.391212 -1.536989
H -4.451433 -1.309244 -0.652182
H -4.129419 -2.302051 -2.072794
C -4.047741 -0.192557 -2.459269
H -5.105401 -0.144281 -2.737840
H -3.479302 -0.303000 -3.390492
N -3.001510 1.306906 1.389710
N -2.413694 -1.500866 -1.080594
O 0.072422 1.295088 0.007569
H 0.049333 2.185565 -0.371107
O 3.591905 2.246239 0.411934

O -1.900634 -1.378710 1.819319

1-O-RC
H 0.322006 -1.867679 1.941905
H 1.718701 1.713774 0.962724
H -0.403087 1.574156 -2.356945
Cu 0.139424 -0.245429 -0.328136
C -2.814504 -0.239072 -0.943346
H -3.771524 -0.637498 -1.314013
H -3.041327 0.312730 -0.025225
C -2.229622 0.716524 -1.993269
H -2.021812 0.157869 -2.913456
H -2.984884 1.478057 -2.242642
C -1.093198 2.486485 -0.659254
H -1.879675 2.269983 0.071308
H -1.413412 3.386882 -1.206307
C 0.224966 2.789503 0.067832
H 0.996161 3.034345 -0.671983
H 0.087330 3.682559 0.697248
C 0.087804 1.452705 2.166857
H -0.986336 1.639228 2.064885
H 0.462607 2.180141 2.903470
C 0.322274 0.033382 2.704641
H 1.399429 -0.133861 2.822293
H -0.127729 -0.048382 3.706243
C -1.632280 -1.270440 1.879507
H -2.151262 -0.309928 1.962092
H -1.885280 -1.842545 2.785508
C -2.143099 -2.034200 0.649401
H -3.217230 -2.239271 0.778743
H -1.636022 -3.004620 0.591061
N -0.958479 1.315766 -1.543504
N 0.711030 1.629844 0.842729
N -0.185995 -1.000095 1.779674
O 1.847883 -0.991419 -1.513963
H 1.822058 -1.797634 -2.053325
H 2.761308 -0.909303 -1.193333
O 5.762740 -0.234011 -0.143261
O 4.553006 -0.171853 -0.058253
N -1.859873 -1.312422 -0.607138
H -1.838239 -1.982486 -1.373602

1-O-TS1
H 1.606495 1.927713 0.757489
H -1.420685 1.899311 -1.824738
H -1.515087 -1.993632 -1.456984
Cu 0.241498 -0.050235 -0.530735
C -0.515181 -1.968718 1.716462
H -0.340502 -2.762659 2.458402
H -1.185624 -1.243041 2.188683
C -1.192366 -2.575335 0.480161
H -0.519140 -3.309874 0.023346
H -2.096695 -3.118203 0.795851
C -2.724295 -0.784695 -0.330244
H -2.770398 -0.498725 0.725912
H -3.625411 -1.384497 -0.531782
C -2.754718 0.469807 -1.214330
H -2.747725 0.167321 -2.268483
H -3.700761 1.006026 -1.042070
C -1.662247 2.223332 0.177630

H -2.114674 1.660820 1.000688
H -2.317451 3.088242 -0.006631
C -0.272887 2.726217 0.590696
H 0.164636 3.301621 -0.233441
H -0.376373 3.411937 1.445168
C 0.519084 1.045677 2.247612
H -0.547655 0.928601 2.464412
H 0.923422 1.726370 3.011689
C 1.228203 -0.311379 2.356804
H 1.114605 -0.690682 3.383817
H 2.300944 -0.175882 2.181868
N -1.484525 -1.550132 -0.540648
N -1.575789 1.331432 -0.993716
N 0.648148 1.608769 0.888313
N 0.730276 -1.269027 1.350078
H 1.454702 -1.958901 1.159928
O 3.161367 0.114721 -0.392953
O 3.758988 -0.249681 -1.401139
O 1.084806 -0.626976 -2.461237
H 2.055247 -0.651227 -2.549522
H 0.747660 -0.280564 -3.302862

1-O-IM
H 1.579624 1.985818 -0.762005
H -1.690216 0.496024 -2.376868
H -1.309450 -2.335401 0.210733
Cu 0.346599 -0.386450 -0.411088
C -0.017158 -0.482960 2.624212
H 0.317675 -0.682600 3.652388
H -0.674381 0.391450 2.670430
C -0.795529 -1.689976 2.090639
H -0.138794 -2.567103 2.068498
H -1.627197 -1.925262 2.770422
C -2.559178 -0.758264 0.590499
H -2.547558 0.106401 1.262421
H -3.394319 -1.397389 0.913534
C -2.801802 -0.305533 -0.854900
H -2.876292 -1.187860 -1.501949
H -3.771285 0.213129 -0.909218
C -1.731271 1.934339 -0.927050
H -2.040291 1.961593 0.123039
H -2.477144 2.517759 -1.487320
C -0.354855 2.590186 -1.077554
H -0.056487 2.573344 -2.132129
H -0.418813 3.646477 -0.777034
C 0.793467 2.233455 1.107523
H -0.214002 2.281550 1.534728
H 1.236628 3.232531 1.232845
C 1.648142 1.209511 1.867271
H 1.724946 1.514785 2.921192
H 2.662942 1.206399 1.455224
N -1.262421 -1.447382 0.708637
N -1.690313 0.524505 -1.358541
N 0.673634 1.858737 -0.312928
N 1.111034 -0.160761 1.727729
H 1.864847 -0.828432 1.884018
O 2.374668 -0.219414 -1.070564
O 2.935693 -1.249163 -1.546974
O 0.422695 -2.204372 -1.667748
H 1.384165 -2.296057 -1.849666

H -0.021739 -2.274857 -2.528342

1-O-TS2
H 2.086326 -1.187121 1.379230
H -0.968575 -2.479012 -0.657796
H -2.199201 1.159441 -0.764189
Cu -0.265361 0.034752 0.529983
C 0.801860 2.537081 -0.801714
H 1.173813 3.571693 -0.808909
H 1.346914 2.000114 -1.584890
C -0.698996 2.524767 -1.113384
H -1.235368 3.101340 -0.351184
H -0.881194 3.016896 -2.079436
C -1.146070 0.392095 -2.347906
H -0.138961 0.525497 -2.757282
H -1.848496 0.774720 -3.102793
C -1.430404 -1.095311 -2.099270
H -2.460958 -1.211985 -1.744671
H -1.353476 -1.641451 -3.051336
C 0.809119 -2.015602 -1.558435
H 1.146900 -1.223282 -2.234584
H 0.789508 -2.944096 -2.147959
C 1.804529 -2.166339 -0.401932
H 1.483219 -2.986765 0.250205
H 2.788927 -2.445446 -0.807294
C 2.772206 0.110940 -0.043912
H 2.642379 0.229681 -1.125293
H 3.829251 -0.149919 0.118172
C 2.472919 1.432899 0.678120
H 3.183235 2.200460 0.337578
H 2.629507 1.300739 1.754406
N -1.231674 1.146379 -1.084546
N -0.534007 -1.651246 -1.062967
N 1.859176 -0.944728 0.416569
N 1.069588 1.862994 0.486382
H 0.809654 2.486494 1.250006
O 0.089747 -0.363904 2.523959
O -0.613530 0.380101 3.268327
O -2.568436 -0.011575 1.299388
H -2.433442 0.294297 2.216118
H -3.172264 -0.769417 1.366872

1-O-PC
H 2.523654 -0.513770 1.700604
H -0.333613 -2.756111 0.157800
H -2.311884 0.485723 -0.702287
Cu 0.016847 -0.009921 0.604285
C 0.447310 2.302880 -1.228610
H 0.611326 3.352983 -1.512004
H 1.037945 1.695242 -1.922852
C -1.045952 1.966666 -1.373845
H -1.629319 2.606048 -0.701085
H -1.367163 2.201293 -2.399665
C -1.102667 -0.417776 -2.088550
H -0.150602 -0.176901 -2.574852
H -1.877809 -0.359815 -2.866902
C -1.064866 -1.848963 -1.531915
H -2.040179 -2.085174 -1.093751
H -0.894408 -2.554277 -2.358714
C 1.333130 -2.224063 -0.907364

H 1.526056 -1.566142 -1.761196
H 1.491953 -3.253458 -1.261302
C 2.329319 -1.925580 0.224275
H 2.140508 -2.607465 1.061325
H 3.350703 -2.124912 -0.131825
C 2.884999 0.493284 -0.047069
H 2.704151 0.291216 -1.108240
H 3.974181 0.452180 0.100242
C 2.380911 1.899244 0.312305
H 2.932107 2.639890 -0.286134
H 2.605681 2.105866 1.365089
N -1.339201 0.564674 -1.011512
N -0.054143 -1.996730 -0.460725
N 2.185052 -0.544608 0.740009
N 0.918657 2.019462 0.141724
H 0.565769 2.738671 0.770454
O -0.810113 -0.043218 2.462000
O -2.033843 -0.198708 2.610528
O -4.042212 0.002031 0.103256
H -4.057689 -0.066282 1.071850
H -4.966740 0.112307 -0.169985

2-O-RC
H 0.296773 -1.804787 1.986340
H 1.661707 1.829887 1.047192
H -0.336819 1.633961 -2.247495
Cu 0.182695 -0.177121 -0.262196
S -1.778342 -1.689090 -0.879645
C -2.879537 -0.233609 -1.164233
H -3.805731 -0.575191 -1.635972
H -3.139544 0.210581 -0.198146
C -2.192722 0.793622 -2.076626
H -1.924561 0.311950 -3.023054
H -2.923186 1.582378 -2.315522
C -1.162271 2.503842 -0.592778
H -1.949228 2.240425 0.122454
H -1.514115 3.395903 -1.134192
C 0.133429 2.855005 0.150258
H 0.900422 3.138739 -0.580112
H -0.045896 3.735262 0.786449
C 0.032897 1.510170 2.241238
H -1.043213 1.682894 2.136889
H 0.395853 2.236304 2.984380
C 0.285719 0.090049 2.763677
H 1.364734 -0.067684 2.875421
H -0.161345 -0.010213 3.764712
C -1.657443 -1.216635 1.941309
H -2.192929 -0.264196 1.874047
H -1.910807 -1.652381 2.921966
C -2.156026 -2.176271 0.855170
H -3.233966 -2.332868 0.961678
H -1.681698 -3.159024 0.961184
N -0.959612 1.353638 -1.491415
N 0.658555 1.708585 0.920422
N -0.215694 -0.938379 1.827624
O 1.864832 -0.876928 -1.500471
H 1.731220 -1.673977 -2.038130
H 2.799285 -0.880993 -1.233536
O 5.961403 -0.742148 -0.637341
O 4.806435 -0.510794 -0.342569

2-O-TS1
H 1.116139 -2.009060 1.279071
H 2.232616 1.748957 0.498660
H -0.813806 1.946257 -1.810516
Cu 0.351424 -0.070949 -0.482014
S -1.896280 -1.539414 -0.529894
C -2.917584 -0.044981 -0.168021
H -3.973740 -0.295295 -0.304863
H -2.775531 0.239934 0.878901
C -2.541213 1.108793 -1.107793
H -2.649943 0.779129 -2.146668
H -3.262760 1.926628 -0.956897
C -0.972803 2.597831 0.120292
H -1.457228 2.238429 1.035015
H -1.462563 3.548018 -0.142968
C 0.516846 2.862902 0.374509
H 0.972294 3.266542 -0.537447
H 0.616231 3.634086 1.153216
C 1.124815 1.210234 2.133036
H 0.092306 1.386667 2.450468
H 1.764642 1.811725 2.795447
C 1.477718 -0.272173 2.301670
H 2.515531 -0.436751 1.994228
H 1.407213 -0.543026 3.365662
C -0.686008 -1.455481 2.064603
H -1.171685 -0.513022 2.337351
H -0.563914 -2.027920 2.998453
C -1.592702 -2.264540 1.132497
H -2.551769 -2.453926 1.624541
H -1.150286 -3.244032 0.916013
N -1.152664 1.573737 -0.924230
N 1.246607 1.625204 0.721552
N 0.620053 -1.136674 1.458948
O 0.775275 -0.432745 -2.597412
H 0.212645 -1.120551 -2.990565
H 1.685501 -0.636236 -2.877836
O 2.971198 -0.939807 -0.586830
O 3.492892 -1.058669 -1.690909

2-O-IM
H -0.708212 -2.429895 -0.620673
H -2.668477 1.071048 -0.655542
H 0.364462 2.354955 1.161795
Cu -0.423124 -0.034964 0.570459
S 2.185031 -1.017390 0.656314
C 2.819226 0.524441 -0.134279
H 3.908148 0.552937 -0.033301
H 2.585565 0.501434 -1.203130
C 2.213529 1.763828 0.532491
H 2.421229 1.737855 1.607500
H 2.715617 2.658025 0.133836
C 0.311837 2.545245 -0.872331
H 0.797355 2.058161 -1.725043
H 0.628110 3.598887 -0.885341
C -1.213094 2.476551 -1.009120
H -1.677410 3.017765 -0.176380
H -1.518186 2.985517 -1.935206
C -1.577814 0.341838 -2.231411
H -0.651655 0.656362 -2.723162

H -2.398267 0.589293 -2.919721
C -1.556307 -1.171172 -1.992101
H -2.492422 -1.480272 -1.516268
H -1.494082 -1.691371 -2.959099
C 0.847350 -1.752841 -1.758232
H 1.106481 -0.822212 -2.273666
H 0.786884 -2.535282 -2.531675
C 1.955787 -2.143981 -0.777086
H 2.905264 -2.246853 -1.311367
H 1.742680 -3.117766 -0.320772
N 0.748086 1.856966 0.358061
N -1.695036 1.079953 -0.955783
N -0.449878 -1.561540 -1.089751
O -0.374796 0.387309 2.718126
H 0.338805 -0.056509 3.206771
H -1.213373 0.028413 3.076437
O -2.125588 -1.244836 1.127756
O -2.648831 -1.051147 2.257165

2-O-TS2
H 0.135029 2.496474 -1.194475
H -2.757471 0.559345 0.639936
H -0.499945 -2.467169 0.573417
Cu -0.340620 -0.174352 -0.495737
S 2.212843 -0.271149 -0.848719
C 2.457043 -1.011091 0.827005
H 3.483092 -1.382575 0.904034
H 2.322985 -0.232056 1.583709
C 1.469525 -2.163541 1.044722
H 1.614195 -2.919099 0.265632
H 1.697542 -2.647554 2.005473
C -0.533648 -1.313614 2.275142
H 0.142245 -0.594500 2.751051
H -0.636041 -2.161631 2.967878
C -1.913541 -0.685064 2.040306
H -2.590140 -1.441106 1.625693
H -2.336834 -0.363814 3.003130
C -1.387840 1.711413 1.644123
H -0.564833 1.498747 2.334091
H -2.180939 2.189043 2.237383
C -0.915515 2.681351 0.554908
H -1.748506 2.903448 -0.121562
H -0.621901 3.632055 1.025090
C 1.527911 2.267415 0.282590
H 1.535935 1.903290 1.315872
H 1.831754 3.326496 0.321416
C 2.565734 1.512506 -0.557361
H 3.559399 1.609750 -0.109424
H 2.628291 1.937455 -1.565813
N 0.060481 -1.722360 0.989107
N -1.840982 0.427672 1.066324
N 0.172567 2.102395 -0.255488
O -0.937755 -2.540198 -1.658339
H -0.373149 -2.980737 -2.314607
H -1.786588 -2.399749 -2.111082
O -1.252765 0.474940 -2.216919
O -2.402493 -0.024956 -2.305888

2-O-PC
H -2.261704 1.216506 1.362189

H 1.156422 2.673742 -0.030145
H 2.222754 -0.921902 -0.521894
Cu 0.135297 0.132603 0.576379
S -1.314948 -2.011151 0.499590
C -0.707491 -2.353876 -1.212520
H -0.998312 -3.370636 -1.491945
H -1.191825 -1.662494 -1.909351
C 0.819504 -2.217559 -1.272184
H 1.275460 -2.906486 -0.553314
H 1.158967 -2.526221 -2.271800
C 1.377872 0.069624 -2.098240
H 0.421267 0.049666 -2.633061
H 2.149822 -0.250109 -2.813222
C 1.702151 1.490398 -1.617595
H 2.685869 1.488155 -1.136855
H 1.758209 2.164074 -2.485007
C -0.536713 2.496908 -1.174824
H -0.819613 1.873954 -2.029674
H -0.408952 3.518787 -1.560001
C -1.657969 2.489276 -0.127674
H -1.374911 3.133823 0.711992
H -2.569953 2.915874 -0.570540
C -2.795373 0.283735 -0.375326
H -2.417470 0.246589 -1.402622
H -3.810674 0.708605 -0.427312
C -2.905954 -1.131762 0.204823
H -3.543125 -1.749888 -0.434995
H -3.379196 -1.106384 1.193299
N 1.292032 -0.854814 -0.947905
N 0.720623 1.961064 -0.613316
N -1.891094 1.133720 0.415905
O 3.846321 -0.694486 0.559201
H 4.756534 -1.014557 0.454064
H 3.718948 -0.569642 1.513986
O 0.369779 0.690711 2.517517
O 1.528895 0.251426 2.721560

3-O-RC
H -1.621773 -0.783989 2.021492
H 0.445944 -2.836712 -0.568639
Cu -0.216064 -0.207211 -0.343077
S 1.783333 0.554335 -1.812209
C 2.912115 -0.631419 -0.962437
H 3.869027 -0.659631 -1.492144
H 3.100245 -0.284117 0.058667
C 2.286117 -2.033438 -0.960384
H 2.057917 -2.328634 -1.990208
H 3.034699 -2.746541 -0.582305
C 1.222037 -2.353666 1.259249
H 1.998777 -1.673035 1.624937
H 1.582290 -3.375507 1.454061
C -0.083379 -2.133774 2.032704
H -0.841133 -2.837586 1.669086
H 0.087018 -2.363166 3.095747
C 0.002345 0.252968 2.696832
H 1.088995 0.157768 2.605703
H -0.239441 0.093425 3.760429
C -0.431848 1.672648 2.318178
H -1.508092 1.805340 2.478290
H 0.075618 2.405176 2.953691

C 1.647512 2.328951 0.445874
H 2.128595 1.608448 1.114006
H 1.907699 3.335865 0.790169
C 2.148862 2.160189 -0.993845
H 3.229888 2.332612 -1.023124
H 1.690540 2.906875 -1.650922
N 1.033409 -2.099620 -0.180887
N -0.619214 -0.769903 1.838939
O -1.789276 -0.774242 -1.768104
H -1.610379 -0.531977 -2.691316
H -2.711719 -0.517192 -1.600143
O -5.825391 -0.023447 -1.069699
O -4.662415 0.044993 -0.727559
S -0.183591 2.122863 0.551037

3-O-TS
H -1.666015 -2.348441 0.511520
H 2.158477 -1.755102 0.350999
Cu 0.059994 -0.395258 -0.484325
S 1.332694 1.853642 -0.516253
C 2.123848 1.472876 1.106384
H 2.906241 2.211473 1.304346
H 1.375293 1.551125 1.901509
C 2.739904 0.067376 1.063890
H 3.447740 0.004833 0.231597
H 3.316568 -0.086208 1.988295
C 1.136063 -1.511967 2.120205
H 0.845421 -0.655372 2.738526
H 1.855974 -2.097895 2.711317
C -0.087381 -2.387096 1.818601
H 0.227778 -3.263627 1.240760
H -0.506606 -2.758507 2.765763
C -1.985413 -0.790055 1.794109
H -1.362324 -0.151329 2.428647
H -2.629833 -1.372540 2.472348
C -2.889586 0.072315 0.906702
H -3.566295 -0.555656 0.315878
H -3.518388 0.718497 1.527194
C -1.228644 2.414093 0.657950
H -0.936457 2.003584 1.629332
H -1.960235 3.209649 0.836036
C -0.020860 3.016732 -0.072276
H 0.398720 3.830717 0.527879
H -0.327161 3.451647 -1.029468
N 1.731212 -0.993875 0.876450
N -1.096158 -1.666539 1.011202
O 2.080496 -1.197610 -2.139339
H 2.390767 -0.427801 -2.644385
H 2.123846 -1.939335 -2.765130
O -0.934980 -1.559519 -2.154794
O -0.952608 -1.090187 -3.288361
S -2.022042 1.094393 -0.354031

3-O-PC
H -0.413910 -2.861756 0.292881
H -2.506597 0.268481 -0.616509
Cu -0.117278 -0.092961 0.569343
S 0.711332 2.307548 0.147005
C 0.036581 2.224373 -1.569697
H 0.081454 3.221253 -2.017818

H 0.659062 1.554977 -2.172275
C -1.421359 1.742659 -1.534232
H -2.008220 2.404660 -0.888582
H -1.838111 1.833637 -2.548796
C -1.390485 -0.688105 -2.035920
H -0.476733 -0.474701 -2.602636
H -2.218404 -0.692063 -2.760517
C -1.302348 -2.071289 -1.378975
H -2.233717 -2.267110 -0.837093
H -1.207162 -2.839756 -2.160240
C 1.126811 -2.433364 -0.980891
H 1.281052 -1.755149 -1.826460
H 1.176049 -3.456640 -1.386154
C 2.260863 -2.272376 0.039146
H 2.161061 -3.004948 0.848270
H 3.227779 -2.457043 -0.439135
C 2.884597 0.504959 -0.404370
H 2.458387 0.198639 -1.364544
H 3.975181 0.438211 -0.481523
C 2.504267 1.954112 -0.072955
H 2.900164 2.618552 -0.848024
H 2.956955 2.264730 0.874479
N -1.568820 0.366750 -1.017178
N -0.195394 -2.144645 -0.397761
O -4.235325 -0.117894 0.257084
H -5.136028 -0.112343 -0.104530
H -4.337379 0.033490 1.210866
O -1.044681 -0.186929 2.486996
O -2.143431 0.305627 2.736669
S 2.316394 -0.654187 0.915704

4-O-RC
H -0.070409 -2.678150 -0.325218
H 0.165243 2.703435 -0.073112
Cu 0.209522 0.022625 -0.422012
S -2.226549 -0.144761 -1.256573
C -2.778360 1.127971 -0.038237
H -3.794050 1.444609 -0.293062
H -2.808754 0.676587 0.958138
C -1.845181 2.345105 -0.064705
H -1.798014 2.743568 -1.083629
H -2.285422 3.131508 0.567771
C -0.255087 2.052102 1.814728
H -0.941053 1.330643 2.272013
H -0.503549 3.038082 2.240972
C 1.192499 1.730202 2.199455
H 1.869751 2.509468 1.830533
H 1.295224 1.713279 3.288839
C 1.003698 -1.142920 2.442736
H 0.088970 -0.723197 2.871876
H 1.639219 -1.472635 3.269935
C 0.692443 -2.340949 1.536856
H 1.623315 -2.711416 1.094549
H 0.289043 -3.151543 2.163279
C -1.656640 -2.058870 0.795663
H -1.823274 -1.351897 1.615436
H -1.940502 -3.054869 1.173395
C -2.573610 -1.728882 -0.386277
H -3.618788 -1.742010 -0.062092
H -2.477601 -2.488848 -1.170739

N -0.464838 2.026553 0.356520
N -0.229119 -2.010079 0.428633
O 1.334177 0.270680 -2.292222
H 0.928313 0.171701 -3.168272
H 2.283935 0.094833 -2.401905
O 5.438797 0.236275 -2.240662
O 4.437794 -0.407566 -2.480784
S 1.887777 0.175094 1.499863

4-O-TS1
H -1.561891 0.798377 1.776075
H 2.344894 -0.605915 -1.454676
Cu 0.623014 0.035421 0.414097
S -0.697943 -2.186083 0.317873
C -0.506397 -2.319329 -1.515449
H -0.760090 -3.338999 -1.819669
H -1.218143 -1.640906 -1.995943
C 0.932624 -2.001685 -1.938621
H 1.619852 -2.679138 -1.420861
H 1.031793 -2.207253 -3.015496
C 1.006007 0.378284 -2.646399
H -0.083214 0.405312 -2.762528
H 1.421744 0.098666 -3.628315
C 1.543011 1.768144 -2.292563
H 2.639321 1.764323 -2.285918
H 1.234884 2.493357 -3.051861
C -0.719262 2.738799 -0.809576
H -1.095437 2.189548 -1.678255
H -0.862376 3.805618 -1.004222
C -1.481308 2.353191 0.462810
H -1.060483 2.894007 1.316930
H -2.524838 2.686132 0.354841
C -2.414999 0.088365 0.067565
H -2.248476 0.191103 -1.010117
H -3.437263 0.448248 0.266973
C -2.346542 -1.383339 0.484768
H -3.084761 -1.966578 -0.074004
H -2.593851 -1.494063 1.546982
N 1.338021 -0.618771 -1.615894
N -1.413182 0.908527 0.772376
O 2.787382 -0.396412 1.051632
H 2.934163 -1.132321 1.669444
H 3.257081 0.360194 1.441055
O 0.734088 0.288122 2.869976
O -0.231870 0.546849 3.586580
S 1.087433 2.409230 -0.627858

4-O-IM
H -1.609493 0.800045 1.757405
H 2.322558 -0.592904 -1.342757
Cu 0.605105 0.043145 0.456657
S -0.739332 -2.175011 0.345967
C -0.518528 -2.309373 -1.483364
H -0.765443 -3.329426 -1.791692
H -1.221512 -1.631252 -1.977063
C 0.927658 -1.989347 -1.875608
H 1.605831 -2.665630 -1.344624
H 1.052692 -2.189557 -2.950291
C 1.026482 0.390053 -2.586045
H -0.058146 0.421171 -2.738040

H 1.473637 0.102231 -3.551067
C 1.560308 1.776954 -2.218019
H 2.655819 1.767645 -2.179187
H 1.277118 2.504664 -2.984520
C -0.744766 2.744330 -0.806032
H -1.091695 2.194169 -1.686192
H -0.879293 3.811301 -1.005649
C -1.547259 2.356355 0.441001
H -1.158041 2.900519 1.307841
H -2.587808 2.685280 0.297732
C -2.472920 0.084500 0.051371
H -2.304424 0.177698 -1.027377
H -3.499487 0.436750 0.243021
C -2.395819 -1.382013 0.485712
H -3.122133 -1.979648 -0.073382
H -2.651906 -1.482393 1.546793
N 1.321777 -0.604683 -1.540718
N -1.479608 0.914199 0.751196
O 2.944612 -0.460943 0.932726
H 3.105891 -1.213403 1.526581
H 3.429876 0.279895 1.333457
O 0.808574 0.317973 2.614753
O -0.133293 0.560574 3.387170
S 1.055956 2.415159 -0.566004

4-O-TS2
H 0.005318 0.001822 0.008336
H 0.002448 0.020543 5.251905
Cu 0.268695 0.018080 2.717463
S -0.316191 2.477078 2.370459
C -1.660190 2.393044 3.635194
H -1.967232 3.411616 3.889920
H -2.524822 1.878941 3.204153
C -1.159943 1.673270 4.893373
H -0.281636 2.196223 5.286109
H -1.940373 1.733943 5.666141
C -1.860882 -0.709060 4.785081
H -2.660080 -0.448216 4.082010
H -2.301093 -0.668364 5.794182
C -1.376788 -2.142941 4.544271
H -0.673910 -2.446001 5.328629
H -2.220418 -2.838339 4.587886
C -1.760623 -2.260933 1.692121
H -2.598301 -1.692724 2.107763
H -2.125623 -3.260887 1.440288
C -1.205935 -1.587358 0.430473
H -0.352490 -2.163216 0.057640
H -1.981799 -1.623895 -0.349284
C -1.785836 0.827698 0.542544
H -2.585508 0.599025 1.255990
H -2.245228 0.821807 -0.459346
C -1.229790 2.234511 0.789698
H -2.034626 2.973359 0.728812
H -0.497665 2.498990 0.018005
N -0.771804 0.270943 4.634673
N -0.745125 -0.204860 0.667944
O 2.159006 -0.226249 4.829836
H 2.819977 0.473130 4.962578
H 2.668447 -1.053192 4.843505
O 2.174867 -0.101752 1.771555

O 2.345248 -0.017566 0.546881
S -0.445603 -2.422057 2.980027

4-O-PC
H -2.357639 0.924177 1.614786
H 2.239744 -0.654136 -0.705408
Cu 0.045914 0.118632 0.627086
S -1.194460 -2.096458 0.407756
C -0.630964 -2.243501 -1.346347
H -0.859375 -3.252116 -1.702893
H -1.192503 -1.534569 -1.962676
C 0.879514 -1.991526 -1.451134
H 1.411040 -2.693600 -0.799977
H 1.192791 -2.211978 -2.482934
C 1.207645 0.373130 -2.133512
H 0.186185 0.394840 -2.531103
H 1.866573 0.097541 -2.972878
C 1.631592 1.766268 -1.654034
H 2.681822 1.755347 -1.344023
H 1.537754 2.491492 -2.467945
C -0.956067 2.739097 -0.807466
H -1.122159 2.141934 -1.709411
H -1.031601 3.794369 -1.085663
C -2.000568 2.421324 0.270073
H -1.781344 3.004426 1.170549
H -2.986642 2.747286 -0.092753
C -2.877480 0.141938 -0.196169
H -2.531193 0.236372 -1.231044
H -3.923608 0.486794 -0.178912
C -2.859228 -1.325848 0.244050
H -3.468684 -1.927262 -0.437298
H -3.299916 -1.434240 1.241994
N 1.275763 -0.625950 -1.051922
N -2.020210 0.990834 0.654482
O 4.047756 -0.397584 0.054799
H 4.147982 -0.268077 1.012258
H 4.917559 -0.690359 -0.261226
O 1.053593 -0.174718 2.508171
O 2.216009 0.163882 2.723954
S 0.747393 2.411269 -0.171482

5-O-RC
H 0.329408 -2.753739 -0.53164800
Cu -0.236238 -0.138848 -0.37002800
S 1.811783 0.601876 -1.84190900
C 2.885929 -0.672537 -1.05180100
H 3.814604 -0.759706 -1.62354000
H 3.144167 -0.350581 -0.03800000
C 2.169945 -2.028607 -1.03509800
H 1.858607 -2.287175 -2.05273400
H 2.890093 -2.797175 -0.71536500
C 1.244403 -2.322248 1.24112400
H 1.949144 -1.568160 1.60807600
H 1.737703 -3.300397 1.36326900
C -0.024246 -2.329537 2.09963400
H -0.689538 -3.146124 1.79550500
H 0.235496 -2.508241 3.14771300
C -0.072987 0.437850 2.86374500
H 0.988055 0.200342 2.74342700
H -0.309150 0.392202 3.93237800

C -0.379953 1.850999 2.35413500
H -1.440173 2.089018 2.48939400
H 0.188042 2.584107 2.93659900
C 1.770109 2.270653 0.49529800
H 2.209807 1.495594 1.13067500
H 2.075686 3.247103 0.88701400
C 2.266297 2.145420 -0.94994800
H 3.355387 2.256266 -0.97178900
H 1.851860 2.947995 -1.56906100
N 0.963793 -2.037194 -0.17842400
O -1.777944 -0.599995 -1.84539200
H -1.682305 -0.225752 -2.73628200
H -2.716062 -0.500061 -1.60925000
O -5.866486 -0.656713 -1.28353300
O -4.785097 -0.258758 -0.90083700
S -0.068588 2.153226 0.56700000
S -1.080508 -0.829467 1.98025300

5-O-TS
H 1.890870 -1.896570 0.432208
Cu 0.005763 -0.161945 0.481967
S -1.705641 -1.602887 -0.779731
C -0.392306 -2.120160 -1.971356
H -0.775083 -2.939606 -2.586683
H -0.153169 -1.281822 -2.633666
C 0.852850 -2.588092 -1.203748
H 0.570926 -3.386261 -0.508868
H 1.560522 -3.026650 -1.922917
C 2.505265 -0.740271 -1.153303
H 2.039729 -0.313832 -2.049220
H 3.323500 -1.390249 -1.503537
C 3.131877 0.365455 -0.295113
H 3.714381 -0.071685 0.523734
H 3.826831 0.959091 -0.896950
C 1.267862 2.485244 -0.837983
H 1.251623 1.868007 -1.741128
H 1.933439 3.335246 -1.022681
C -0.132076 3.023320 -0.515590
H -0.107016 3.657427 0.376737
H -0.483217 3.650332 -1.341869
C -1.840191 1.086780 -1.804552
H -0.925151 0.977402 -2.395076
H -2.494888 1.797202 -2.320893
C -2.580573 -0.251608 -1.674699
H -2.852331 -0.613006 -2.671850
H -3.514436 -0.120671 -1.118136
N 1.485420 -1.507540 -0.420609
O 1.366447 -1.833579 2.545233
H 0.940818 -2.582296 2.994256
H 1.816369 -1.343779 3.253033
O -1.404154 -0.331150 2.868402
O -2.483888 0.145768 3.161909
S -1.425829 1.768829 -0.141189
S 1.954453 1.493971 0.560571

5-O-PC
H 2.472963 0.293956 0.592001
Cu 0.102007 -0.006178 -0.602773
S -0.769192 2.368540 -0.066291
C -0.045745 2.242274 1.627334

H -0.075715 3.229117 2.098359
H -0.653757 1.561942 2.232261
C 1.408477 1.759717 1.543661
H 1.976533 2.425848 0.885532
H 1.856552 1.841177 2.545515
C 1.402619 -0.666448 2.037453
H 0.430291 -0.550646 2.529708
H 2.168420 -0.556181 2.821971
C 1.546346 -2.073194 1.446851
H 2.549871 -2.206251 1.028720
H 1.415405 -2.826859 2.229328
C -1.221884 -2.595989 0.850165
H -1.248008 -1.938488 1.724247
H -1.356034 -3.624845 1.201082
C -2.357018 -2.262332 -0.125553
H -2.340516 -2.940821 -0.984842
H -3.322649 -2.401667 0.371786
C -2.882454 0.503137 0.503790
H -2.421325 0.175334 1.440787
H -3.968737 0.407303 0.607162
C -2.546208 1.969989 0.205596
H -2.925942 2.601796 1.015110
H -3.040468 2.298445 -0.714589
N 1.542430 0.386080 1.012135
O 4.200587 -0.137867 -0.270763
H 5.105442 -0.014063 0.058158
H 4.282721 -0.201074 -1.236483
O 1.061479 0.300435 -2.555647
O 2.123269 -0.209033 -2.892900
S -2.323691 -0.583716 -0.878011
S 0.430045 -2.465507 0.036669

6-O-RC
H -1.012635 0.731086 1.774709
H 2.428743 -0.535363 -2.038552
Cu 0.939181 0.292550 0.020605
C -0.490590 -2.089659 -1.584502
H -0.818149 -3.121927 -1.771499
H -1.209611 -1.418489 -2.073698
C 0.909022 -1.892742 -2.156767
H 1.598183 -2.566629 -1.637789
H 0.901062 -2.179606 -3.219566
C 0.903514 0.460308 -2.956103
H -0.190035 0.416941 -2.942666
H 1.218300 0.192758 -3.977778
C 1.377522 1.891631 -2.677394
H 2.464605 1.970151 -2.795542
H 0.930380 2.578659 -3.402481
C -0.762399 2.718383 -0.897389
H -1.213251 2.135813 -1.706852
H -1.010399 3.770591 -1.064941
C -1.301532 2.279971 0.472423
H -0.812543 2.866777 1.257028
H -2.374993 2.519822 0.513209
C -2.099641 -0.059743 0.237525
H -2.239059 0.160559 -0.826266
H -3.072718 0.106787 0.726933
C -1.699681 -1.526067 0.428562
H -2.492811 -2.182340 0.045343
H -1.569967 -1.747244 1.493428

N 1.411576 -0.510700 -1.965984
N -1.060036 0.848892 0.762917
O 1.927885 -0.607290 1.727160
H 1.915838 -1.577626 1.764742
H 2.783173 -0.324912 2.089274
O -0.845997 0.679438 4.280870
O 0.128067 0.710676 5.005422
S 1.077930 2.527412 -0.972292
O -0.445943 -1.839839 -0.180341

6-O-TS1
H 0.524459 -1.583163 -2.064927
Cu -0.301142 0.353991 -0.479110
S 2.042245 1.467588 -0.177264
C 2.891356 -0.174176 -0.187640
H 3.962689 -0.009736 -0.334920
H 2.759853 -0.647696 0.789728
C 2.352337 -1.067550 -1.312581
H 2.457823 -0.547497 -2.270790
H 2.981617 -1.968910 -1.369567
C 0.690164 -2.615699 -0.310648
H 1.194079 -2.469244 0.650953
H 1.123385 -3.521852 -0.763199
C -0.809751 -2.836106 -0.097757
H -1.309896 -3.013012 -1.056221
H -0.975824 -3.719178 0.533378
C -1.343176 -1.551161 1.874226
H -0.359537 -1.892212 2.225921
H -2.106177 -2.168670 2.367745
C -1.574397 -0.087678 2.229118
H -2.562611 0.211394 1.869526
H -1.565157 0.024138 3.323154
C 0.723971 0.853349 2.291215
H 1.114860 -0.167588 2.337442
H 0.596577 1.191756 3.331400
C 1.736568 1.779267 1.611342
H 2.687956 1.743981 2.150941
H 1.393529 2.820080 1.642299
N 0.926922 -1.419296 -1.142080
O -0.716745 0.738943 -2.574066
H -0.171509 1.421555 -3.000105
H -1.643666 0.986342 -2.755504
O -2.572345 1.427152 -0.427944
O -3.203452 1.551640 -1.480326
N -0.577898 0.813033 1.589989
H -0.970097 1.755773 1.595703
O -1.447554 -1.686615 0.458391

6-O-IM
H -0.843344 -1.746830 -1.676146
H 0.385228 1.495495 2.114054
Cu -0.319588 -0.421259 0.474465
S 2.140451 -1.298600 0.060364
C 2.848166 0.406042 0.153361
H 3.930531 0.325240 0.288649
H 2.670537 0.918064 -0.796942
C 2.242769 1.186537 1.326270
H 2.403217 0.628310 2.254772
H 2.787745 2.137112 1.429220
C 0.442348 2.635536 0.420532

H 0.940387 2.585316 -0.554058
H 0.807502 3.546879 0.919702
C -1.074012 2.737399 0.241795
H -1.569375 2.819099 1.215461
H -1.329422 3.633262 -0.339193
C -1.532714 1.515178 -1.788162
H -0.594407 1.967233 -2.138041
H -2.362801 2.080740 -2.232748
C -1.631061 0.056203 -2.213739
H -2.577419 -0.355113 -1.852263
H -1.633464 -0.003025 -3.311677
C 0.746817 -0.662096 -2.355589
H 1.051689 0.388790 -2.350117
H 0.629000 -0.952725 -3.411073
C 1.841770 -1.537231 -1.739767
H 2.780264 -1.393103 -2.283714
H 1.585438 -2.599563 -1.826633
N 0.789768 1.418286 1.180573
N -0.539469 -0.772460 -1.635477
O -0.512826 -0.887050 2.581219
H 0.115946 -1.534310 2.942968
H -1.404349 -1.259451 2.740537
O -2.249207 -1.607893 0.424524
O -2.847692 -1.849014 1.491653
O -1.616357 1.564770 -0.365139

6-O-TS2
H 0.333744 2.639972 -0.185159
H -0.794001 -2.400098 -0.376511
Cu -0.216995 0.052963 -0.603247
S 2.319256 -0.165619 -0.862967
C 2.345014 -1.548658 0.364547
H 3.306276 -2.064399 0.288257
H 2.268243 -1.131990 1.373463
C 1.206198 -2.538537 0.085347
H 1.286883 -2.903123 -0.943928
H 1.328157 -3.408785 0.746077
C -0.665131 -1.981107 1.624091
H 0.074151 -1.529240 2.294430
H -0.817474 -3.016941 1.963101
C -1.993165 -1.225339 1.710796
H -2.742445 -1.697400 1.067447
H -2.374272 -1.242951 2.739496
C -1.381897 1.059436 2.195998
H -0.599381 0.603556 2.817792
H -2.197784 1.374544 2.859410
C -0.843230 2.268753 1.442009
H -1.649437 2.694300 0.836810
H -0.528029 3.032737 2.167787
C 1.573789 1.735319 1.159628
H 1.476214 0.979369 1.945306
H 1.899375 2.664751 1.652544
C 2.664757 1.325975 0.163994
H 3.613142 1.185207 0.691094
H 2.828897 2.116835 -0.577156
N -0.133673 -1.931990 0.246361
N 0.256114 1.903517 0.516704
O -2.032595 -1.559506 -2.004056
H -1.879043 -1.778638 -2.937974
H -2.956800 -1.262436 -1.966478

O -0.694583 1.174157 -2.306168
O -1.797229 1.742309 -2.280782
O -1.871653 0.118395 1.238454

6-O-PC
H -2.258248 0.952467 1.639122
H 2.239184 -0.592640 -0.688105
Cu 0.031918 0.022294 0.616654
S -1.196577 -2.158444 0.364741
C -0.597482 -2.235768 -1.385141
H -0.796029 -3.237446 -1.776334
H -1.163884 -1.521281 -1.990350
C 0.910546 -1.949913 -1.448220
H 1.442305 -2.648261 -0.794002
H 1.254950 -2.142857 -2.474430
C 1.166857 0.429688 -2.102969
H 0.181723 0.334092 -2.573008
H 1.916870 0.248949 -2.887455
C 1.354620 1.845815 -1.552738
H 2.343464 1.948011 -1.095907
H 1.274605 2.581102 -2.363174
C -0.870626 2.582372 -0.922562
H -1.210863 2.018983 -1.802697
H -0.835590 3.644989 -1.196478
C -1.824775 2.393766 0.252782
H -1.444314 2.962941 1.106168
H -2.811137 2.800162 -0.012586
C -2.827682 0.151859 -0.154418
H -2.514767 0.253532 -1.198385
H -3.861024 0.526685 -0.095992
C -2.838692 -1.326941 0.250126
H -3.483354 -1.890366 -0.431004
H -3.255644 -1.450793 1.256347
N 1.269131 -0.576818 -1.020578
N -1.918139 0.971715 0.677188
O 4.011152 -0.593447 0.122106
H 4.100982 -0.512229 1.085546
H 4.895260 -0.820308 -0.207293
O 1.017485 0.546849 2.378317
O 2.069326 -0.021113 2.684976
O 0.421437 2.141382 -0.508505

References

(1) Hormann, J.; Perera, C.; Deibel, N.; Lentz, D.; Sarkar, B.; Kulak, N. Straightforward Approach to Efficient Oxidative DNA Cleaving Agents Based on Cu(II) Complexes of Heterosubstituted Cyclens. *Dalton Trans.* **2013**, *42*, 4357–4360.

(2) Johnson, M. R.; Jones, N. F.; Sutherland, I. O.; Newton, R. F. Formation of Complexes between Aza Derivatives of Crown Ethers and Primary Alkylammonium Salts. Part 8. 12-Crown-4, 15-Crown-5, 21-Crown-7, and 24-Crown-8 Derivatives. *J. Chem. Soc. Perkin Trans. 1* **1985**, 1637–1643.

(3) Glenny, M. W.; van de Water, L. G. A.; Vere, J. M.; Blake, A. J.; Wilson, C.; Driessen, W. L.; Reedijk, J.; Schröder, M. Improved Synthetic Methods to Mixed-Donor Thiacrown Ethers. *Polyhedron* **2006**, *25*, 599–612.

(4) Zhang, X.; Huang, D.; Chen, Y.-S.; Holm, R. H. Synthesis of Binucleating Macrocycles and Their Nickel(II) Hydroxo- and Cyano-Bridged Complexes with Divalent Ions: Anatomical Variation of Ligand Features. *Inorg. Chem.* **2012**, *51*, 11017–11029.

(5) Gahan, L. R.; Grillo, V. A.; Hambley, T. W.; Hanson, G. R.; Hawkins, C. J.; Proudfoot, E. M.; Moubaraki, B.; Murray, K. S.; Wang, D. Synthetic, X-Ray Structure, Electron Paramagnetic Resonance, and Magnetic Studies of the Manganese(II) Complex of 1-Thia-4,7-diazacyclononane ([9]aneN_2S). *Inorg. Chem.* **1996**, *35*, 1039–1044.

(6) Alberts, A. H.; Lehn, J.-M.; Parker, D. Synthesis and Cryptate Complexes of Azathia Macropolycyclic Ligands Based on 12-Membered N_2S_2 and 15-Membered N_2S_3 Macrocyclic Subunits. *J. Chem. Soc. Dalton Trans.* **1985**, 2311–2317.

(7) Bonger, K. M.; van den Berg, R. J. B. H. N.; Heitman, L. H.; IJzerman, A. P.; Oosterom, J.; Timmers, C. M.; Overkleeft, H. S.; van der Marel, G. A. Synthesis and Evaluation of Homo-Bivalent GnRHR Ligands. *Bioorg. Med. Chem.* **2007**, *15*, 4841–4856.

(8) Hoffmann, P.; Steinhoff, A.; Mattes, R. Complexes of Acyclic and Cyclic Diazathiaalkanes. Crystal Structures of 1,7-Diaza-4-thiaheptane-tricarbonyl-molybdenum(0), 1-Thia-4,7-diazacyclononane-tricarbonyl-molybdenum(0) and 1-Thia-4,7-diazacyclononane-tricarbonyl-rhenium(I) bromide. *Zeitschrift für Naturforsch.* **1987**, *42b*, 867–873.

(9) Afshar, S.; Marcus, S. T.; Gahan, L. R.; Hambley, T. W. Mercury(II) and Lead(II) Complexes of 1-Oxa-7-Thia-4,10-Diazacyclododecane ([12]aneN_2OS). *Aust. J. Chem.* **1999**, *52*, 1–6.

(10) Hancock, R. D.; Dobson, S. M.; Evers, A.; Wade, P. W.; Ngwenya, M. P.; Boeyens, J. C. A.; Wainwright, K. P. More Rigid Macrocyclic Ligands That Show Metal Ion Size-Based Selectivity. A Crystallographic, Molecular Mechanics, and Formation Constant Study of the Complexes of Bridged Cyclen. *J. Am. Chem. Soc.* **1988**, *110*, 2788–2794.

(11) Kodama, M.; Koike, T.; Hoshiga, N.; Machida, R.; Kimura, E. Metal Chelates of Sulphur-Containing Polyamine Macrocycles and Oxygenation of the Corresponding Cobalt(II) Complexes. *Dalton Trans.* **1984**, 673–678.

(12) Balakrishnan, K. P.; Kaden, T. A.; Siegfried, L.; Zuberbühler, A. D. Stabilities and Redox Properties of Cu(I) and Cu(II) Complexes with Macrocyclic Ligands Containing the N_2S_2 Donor Set. *Helv. Chim. Acta* **1984**, *67*, 1060–1069.

(13) Aragoni, M. C.; Arca, M.; Bencini, A.; Blake, A. J.; Caltagirone, C.; Decortes, A.; Demartin, F.; Devillanova, F. A.; Faggi, E.; Dolci, L. S.; Garau, A.; Isaia, F.; Lippolis, V.; Prodi, L.; Wilson, C.; Valtancoli, B.; Zaccheroni, N. Coordination Chemistry of *N*-Aminopropyl Pendant Arm Derivatives of Mixed N/S-, and N/S/O-Donor Macrocycles, and Construction of Selective Fluorimetric Chemosensors for Heavy Metal Ions. *Dalton Trans.* **2005**, 2994–3004.

(14) Bernardo, M. M.; Schroeder, R. R.; Rorabacher, D. B. Electrochemical Properties of Copper(II)/Copper(I)-Macrocyclic Polythia Ether Complexes: Determination of Formal Potential Values and Cyclic Voltammetric Behavior. *Inorg. Chem.* **1991**, *30*, 1241–1247.

(15) Nagaj, J.; Stokowa-Sołtys, K.; Kurowska, E.; Frączyk, T.; Jeżowska-Bojczuk, M.; Bal, W. Revised Coordination Model and Stability Constants of Cu(II) Complexes of Tris Buffer. *Inorg. Chem.* **2013**, *52*, 13927–13933.

(16) Botta, M.; Ravera, M.; Barge, A.; Bottaro, M.; Osella, D. Relationship between Ligand Structure and Electrochemical and Relaxometric Properties of Acyclic Poly(Aminocarboxylate) Complexes of Eu(II). *Dalton Trans.* **2003**, 1628–1633.

(17) Leichnitz, S.; Heinrich, J.; Kulak, N. A Fluorescence Assay for the Detection of Hydrogen Peroxide and Hydroxyl Radicals Generated by Metallonucleases. *Chem. Commun.* **2018**, *54*, 13411–13414.