Supplementary materials

Cu/Zn heterometallic complex with solvent-binding cavity, catalytic activity for oxidation of 1-phenylethanol and unusual magnetic properties

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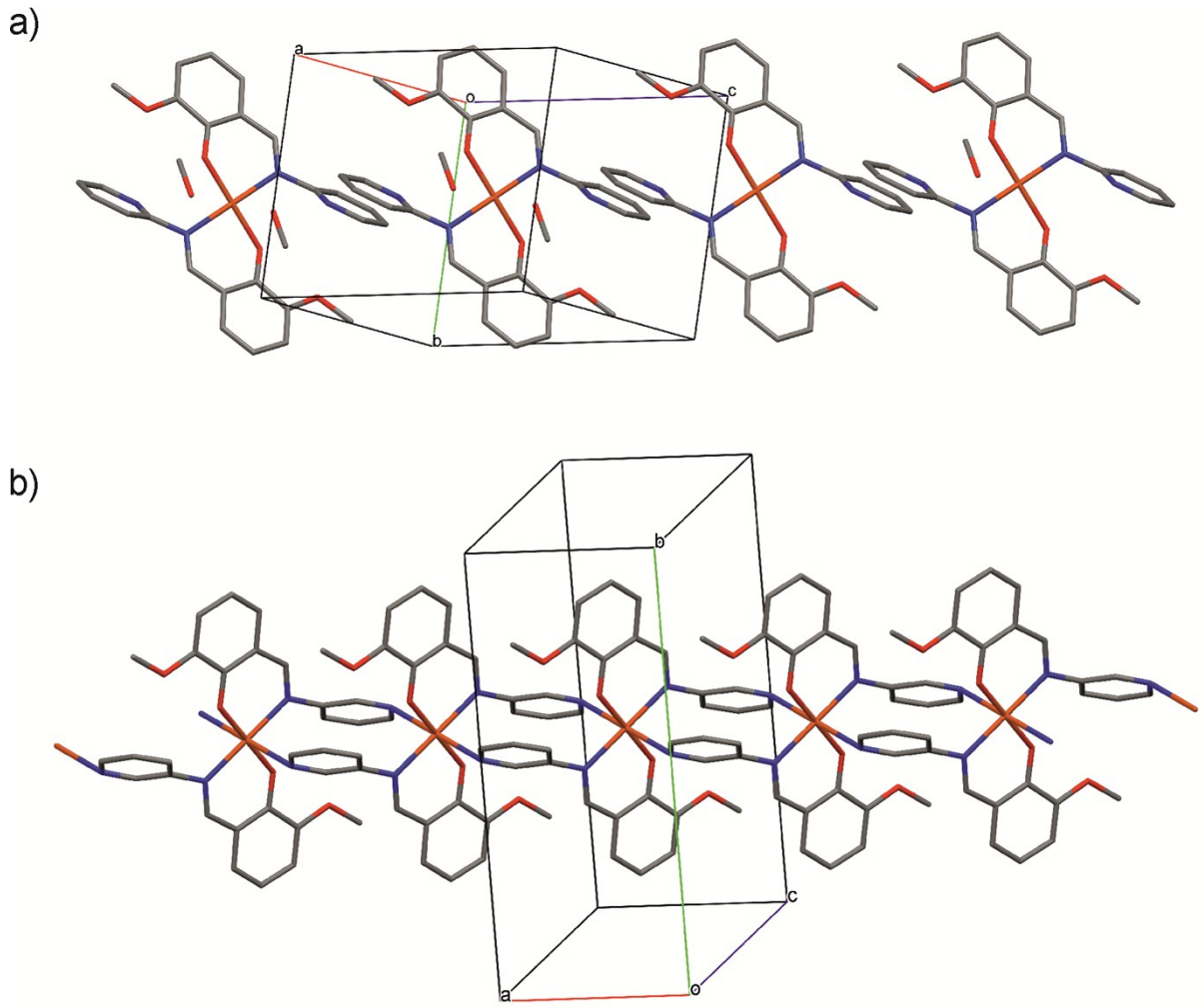

Fig. 1S Crystal packing of: a) complex **2**; b) complex **4**.

Table 1S. Crystal data and structure refinement for **2S** and **4S**.

Identification code	**2S**	**4S**
Empirical formula	$C_{26}H_{22}N_4O_4Cu$	$C_{26}H_{22}N_4O_4Cu$
Formula weight [u]	518.01	518.01
Temperature [K]	120(0)	
Wavelength [Å]	0.71073	
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/n$	P-1
Unit cell dimensions		
a [Å]	13.678(2)	7.1880(5)
b [Å]	12.3462(17)	11.6234(9)
c [Å]	14.989(3)	14.5327(10)
α [°]	90	73.227(5)
β [°]	116.006(13)	80.921(5)
γ [°]	90	74.794(6)
Volume [[Å^3]	2274.9(7)	1117.40(15)
Z	4	2
Density (calcd.) [Mg/m^3]	1.512	1.54
Absorption coefficient [mm^{-1}]	1.002	1.02
Absorption corr. method	integration	
F(000)	1068	534
Crystal size [mm]	0.10×0.08×0.07	0.10×0.08×0.06
θ range for data collect. [°]	3.024 to 25.998	1.88 to 25.997
Reflections collected	16509	11777
Independent reflections	4446	4389
Data/restraints/ parameters	4446 / 0 / 318	4389 / 0 / 334
R(int)	0.0925	0.0793
Completeness to θ=25.242°	0.996	1
Goodness-of-fit on F^2	1.008	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0517 wR2 = 0.1033	R1 = 0.0767 wR2 = 0.2075
R indices (all data)	R1 = 0.1038 wR2 = 0.1227	R1 = 0.1014 wR2 = 0.2278
Largest diff. peak/hole [e·Å^{-3}]	0.596 and -0.457	2.156 and -1.181
CCDC deposition number	**1903320**	**1946386**

The coordination geometries of the metal ion in the molecular complex **2S** is neither tetrahedral nor square planar. The τ' value is 0.42 indicating high degree of distortion from the ideal square planar geometry expected for d^9 copper(II) complex. In the coordination polymer 4S copper centre features CN=5.

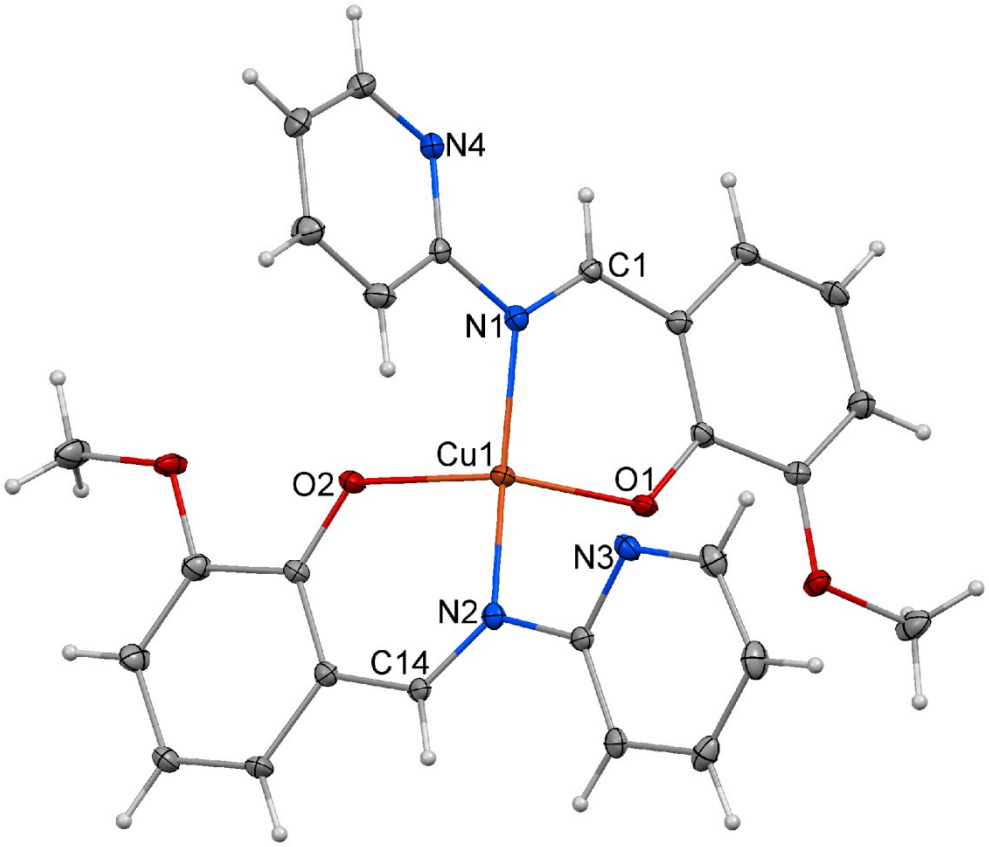

Fig. 2S X-ray molecular structure of complex **2S** drawn with thermal ellipsoids at the 50% probability level. Selected bond distances (Å): Cu1–O1 1.919(3), Cu1–O2 1.925(3), Cu1–N1 1.946(4), Cu1–N2 1.947(4), N1–C1 1.309(5), N2–C14 1.309(5); selected angles (deg): O1–Cu1–O2 138.67(14), N2–Cu1–N1 131.0(1), O2–Cu1–N1 96.07(14), O1–Cu1–N1 95.18(13), O1–Cu1–N2 93.93(14), O2–Cu1–N2 92.36(13).

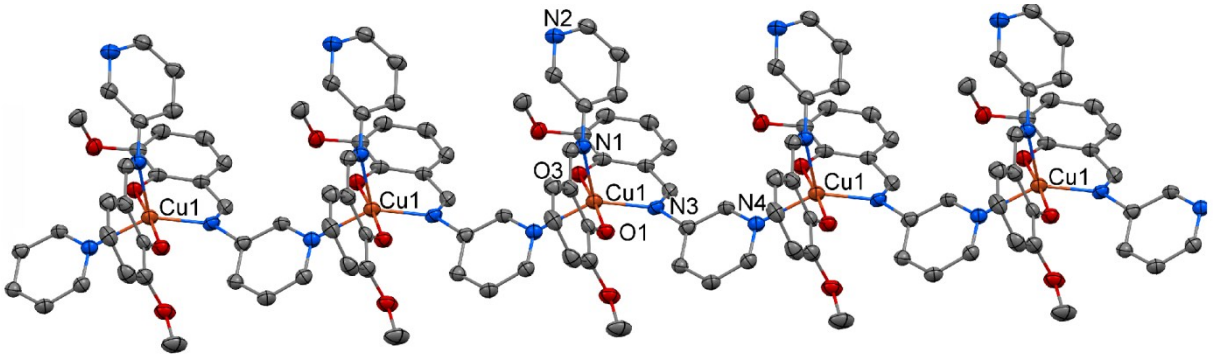

Fig. 3S X-ray molecular structure of CP **4S** drawn with thermal ellipsoids at the 50% probability level. Selected bond distances (Å): Cu1–O1 1.892(3), Cu1–O3 1.889(3), Cu1–N1 2.162(4), Cu1–N3 2.080(4), Cu1–N4^{i} 2.151(4), N1–C8 1.296(7), N3–C21 1.302(6); selected angles (deg): O1–Cu1–O3 175.01(13), N1–Cu1–N3 114.66(16), O1–Cu1–N1 88.50(15), O1–Cu1–N3 91.87(15), O1–Cu1–N4^{i} 89.91(15), O3–Cu1–N1 93.95(15). Symmetry operations: ^{i} x-1,y,z