Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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Synthesis, crystal structures, photoluminescence, magnetic and antioxidant properties, and theoretical analysis of Zn(II) and Cu(II) complexes of an aminoalcohol ligand supported by benzoate counter anions

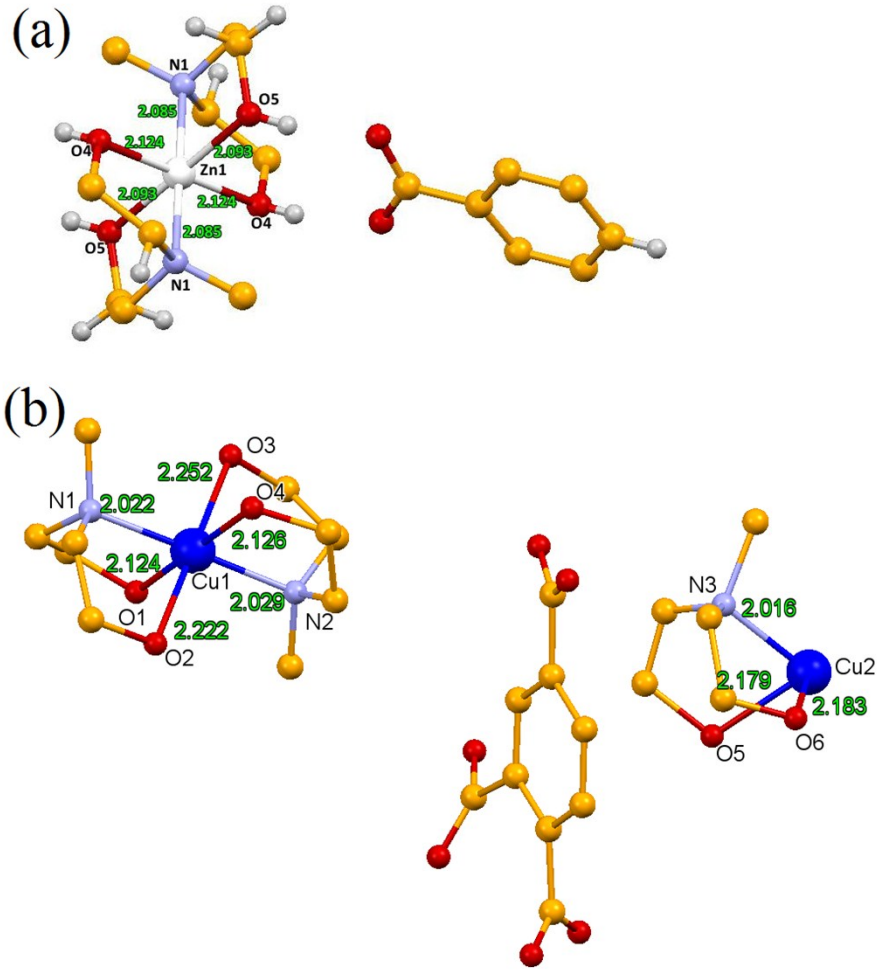

Fig. 1S. Geometric arrangements and selected bond lengths of **1** (a) and **2** (b).

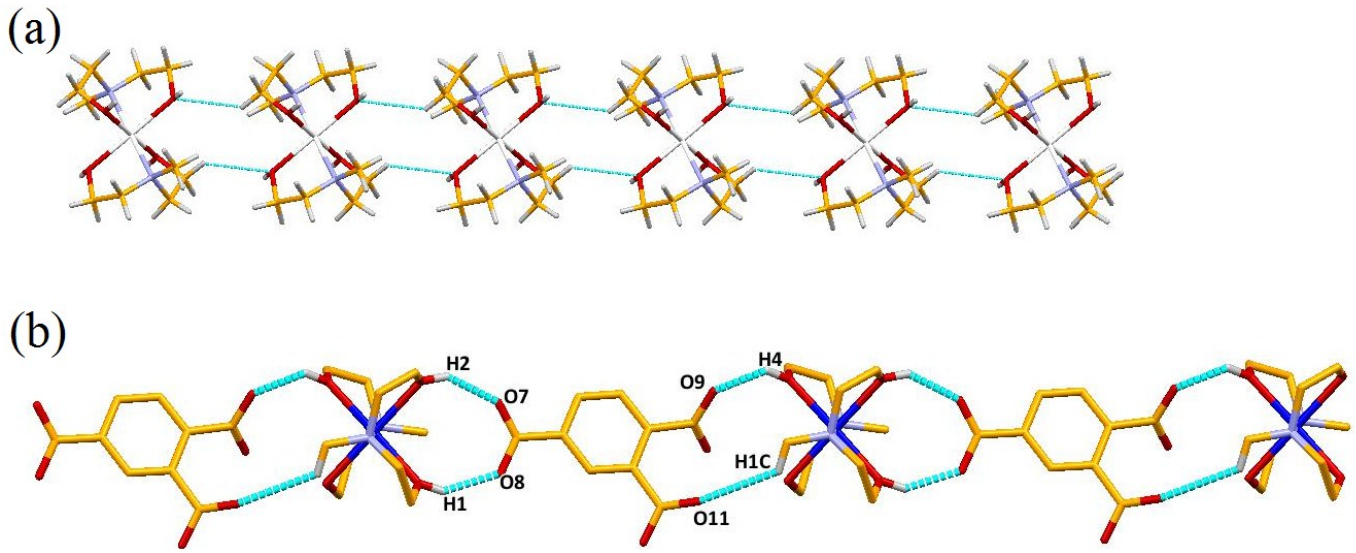

Fig. 2S. (a) 1D chain of **1** through C–H···O contacts (b) 1D chain of **2** through O–H···O contacts.

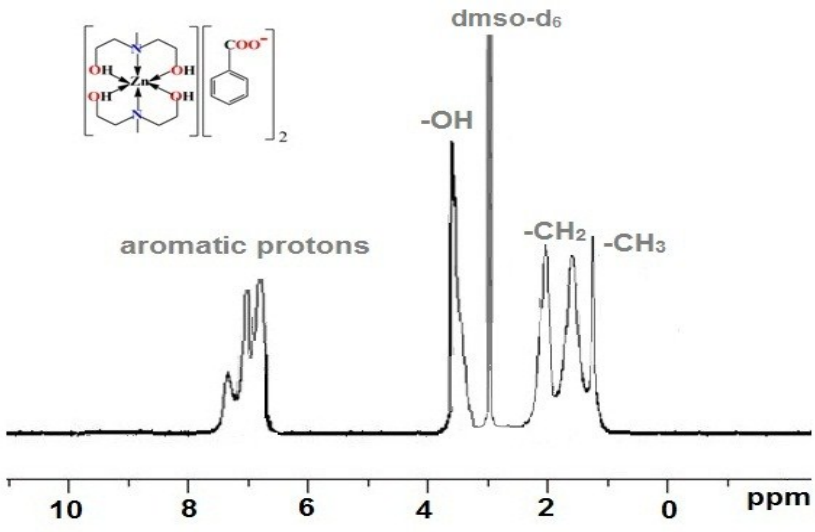

Fig. 3S. ^{1}H NMR spectrum of **1**.

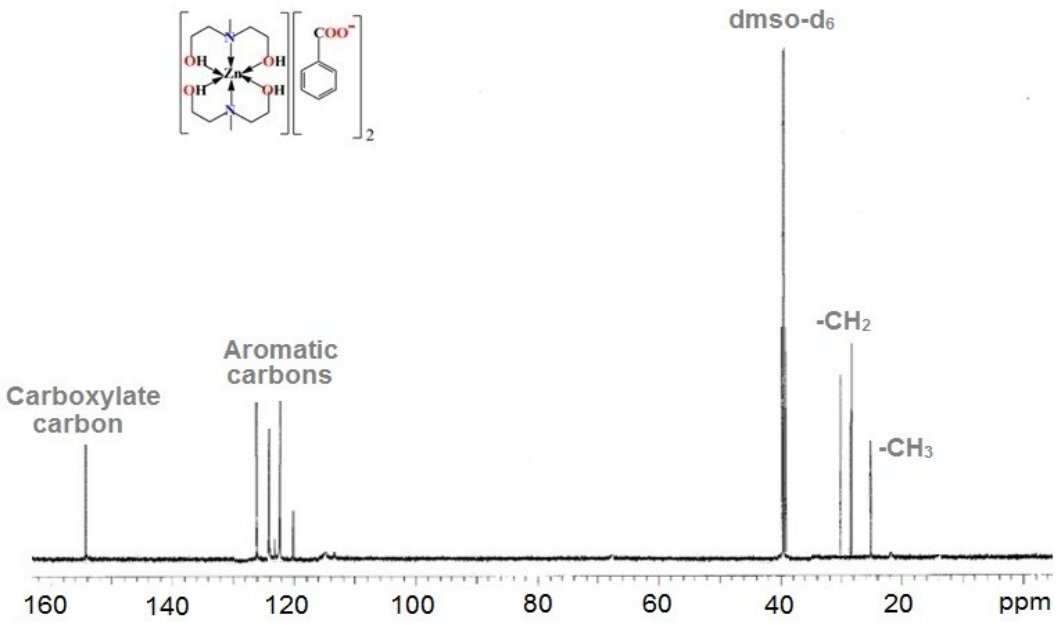

Fig. 4S. ^{13}C NMR spectrum of **1**.

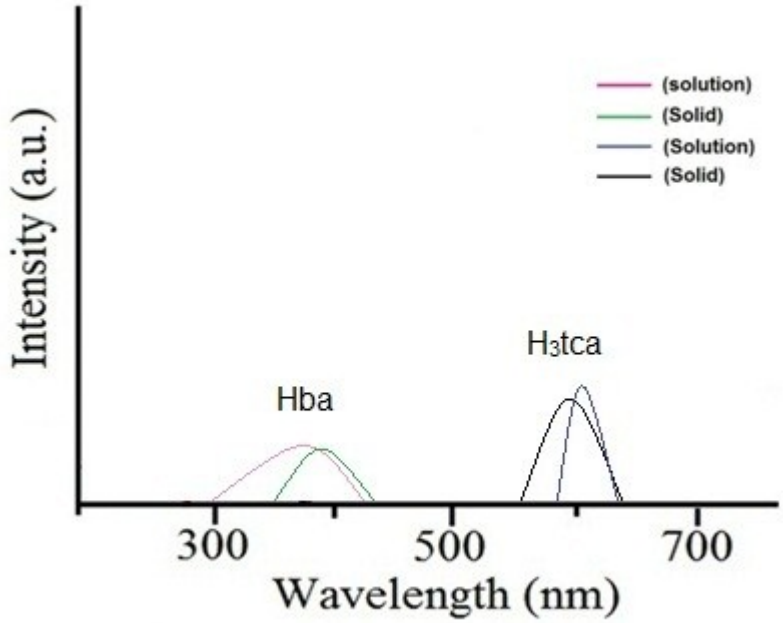

Fig. 5S. Fluorescence spectra of the free ligands [λ_{ex} = 270 nm (Hba) and 240 nm (H_3tca)].

Table 1S. Selected bond lengths and bond angles of **1** and **2**.

Bond lengths (Å)	
1	**2**
Zn1−N1=2.085(5) Zn1−O4=2.124(5) Zn1−O5=2.093(4) C1−O2=1.229(5) C1− O1=1.230(5) C1−C2=1.471(6) C2− C6=1.376(6) C2− C3=1.380(6) C3− C7=1.349(7)	Cu1−N1=2.022(4) Cu1−N2=2.030(4) Cu2−N3=2.015(6) Cu1−O1=2.124 (4) Cu1−O2=2.221 (4) Cu1−O3=2.253(4) Cu1−O4=2.125 (4) Cu2−O5=2.179(7) Cu2−O6=2.184(4)
Bond Angles (˚)	
1	**2**
N1 Zn1 N1 =180.0(2) N1 Zn1 O5 =82.6(2) N1 Zn1 O5 =97.4(2) N1 Zn1 O5 =97.4(2) N1 Zn1 O5= 82.6(2) O5 Zn1 O5 =180.0(2) N1 Zn1 O4 =99.49(18) N1 Zn1 O4= 80.51(18) O5 Zn1 O4 =87.31(19) O5 Zn1 O4 =92.69(19) N1 Zn1 O4= 80.51(18)	N1 Cu1 N2 =179.12(18) N1 Cu1 O1 =83.60(18) N2 Cu1 O1 =96.08(16) N1 Cu1 O4 =97.58(17) N2 Cu1 O4 =82.76(15) O1 Cu1 O4 =178.27(15) N1 Cu1 O2 =81.20(17) N2 Cu1 O2 =98.02(17) O1 Cu1 O2 =94.25(16) O4 Cu1 O2 =87.19(15) N1 Cu1 O3 =98.54(17) N2 Cu1 O3 =82.25(17) O1 Cu1 O3 =85.75(15) O4 Cu1 O3 =92.82(14)