Electronic Supplementary Information

Dicopper(II) complexes of a new pyrazolate-containing Schiff-base macrocycle and related acyclic ligand

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Table S1. Table of selected angles [°] for the four crystallographically characterised dicopper(II) complexes.

$[Cu_2(L1)(OAc)_2]\cdot 2MeOH\cdot H_2O$		$[Cu_2(L1)(NCS)_2]DMF$		$[Cu_2(L2)(H_2O)_2(OAc)_3]$		$[Cu_2(L2)(NCS)_2(DMF)]BF_4$	
N(1)-Cu(1)-N(3)	80.21(17)	N(1)-Cu(1)-N(3)	80.28(19)	N(1)-Cu(1)-N(3)	79.77(8)	N(1)-Cu(1)-N(3)	81.8(2)
N(1)-Cu(1)-N(4)	152.73(16)	N(1)-Cu(1)-N(4)	153.57(18)	N(1)-Cu(1)-N(4)	171.48(8)	N(2)-Cu(2)-N(6)	169.5(2)
N(1)-Cu(1)-O(30)	92.49(15)	N(1)-Cu(1)-N(5)	93.21(18)	N(1)-Cu(1)-O(30)	91.82(7)	N(2)-Cu(2)-O(70)	95.84(19)
N(2)-Cu(2)-N(7)	153.29(15)	N(1)-Cu(1)-N(50)	110.82(18)	N(1)-Cu(1)-O(40)	94.04(7)	N(4)-Cu(1)-N(1)	155.5(2)
N(2)-Cu(2)-N(8)	80.28(16)	N(2)-Cu(2)-N(6)	92.53(18)	N(2)-Cu(2)-N(6)	171.65(8)	N(4)-Cu(1)-N(3)	91.5(2)
N(2)-Cu(2)-O(40)	102.68(14)	N(2)-Cu(2)-N(7)	151.29(18)	N(2)-Cu(2)-O(60)	89.97(7)	N(5)-Cu(2)-N(2)	81.4(2)
N(3)-Cu(1)-N(4)	93.98(18)	N(2)-Cu(2)-N(8)	79.89(19)	N(2)-Cu(2)-O(70)	92.15(7)	N(5)-Cu(2)-N(6)	89.7(2)
N(3)-Cu(1)-O(30)	98.86(15)	N(2)-Cu(2)-N(60)	113.25(18)	N(3)-Cu(1)-N(4)	92.85(8)	N(5)-Cu(2)-O(70)	89.2(2)
N(4)-Cu(1)-O(30)	114.76(16)	N(3)-Cu(1)-N(50)	92.87(18)	N(3)-Cu(1)-O(30)	134.79(7)	N(6)-Cu(2)-O(70)	89.63(19)
N(5)-Cu(1)-N(1)	93.15(16)	N(4)-Cu(1)-N(3)	93.3(2)	N(3)-Cu(1)-O(40)	129.01(7)	N(50)-Cu(1)-N(1)	99.5(2)
N(5)-Cu(1)-N(3)	153.07(16)	N(4)-Cu(1)-N(50)	95.00(18)	N(4)-Cu(1)-O(30)	90.38(7)	N(50)-Cu(1)-N(3)	166.3(2)
N(5)-Cu(1)-N(4)	79.98(16)	N(5)-Cu(1)-N(3)	152.67(19)	N(4)-Cu(1)-O(40)	93.93(7)	N(50)-Cu(1)-N(4)	92.6(2)
N(5)-Cu(1)-O(30)	107.53(14)	N(5)-Cu(1)-N(4)	80.79(19)	N(5)-Cu(2)-N(2)	80.10(8)	N(60)-Cu(2)-N(2)	94.2(2)
N(6)-Cu(2)-N(2)	92.64(16)	N(5)-Cu(1)-N(50)	114.14(18)	N(5)-Cu(2)-N(6)	92.22(8)	N(60)-Cu(2)-N(5)	169.8(2)
N(6)-Cu(2)-N(7)	80.90(16)	N(6)-Cu(2)-N(7)	80.01(19)	N(5)-Cu(2)-O(60)	107.87(7)	N(60)-Cu(2)-N(6)	93.6(2)
N(6)-Cu(2)-N(8)	153.59(15)	N(6)-Cu(2)-N(8)	151.83(18)	N(5)-Cu(2)-O(70)	81.83(7)	N(60)-Cu(2)-O(70)	100.4(2)
N(6)-Cu(2)-O(40)	95.43(14)	N(6)-Cu(2)-N(60)	108.51(19)	N(6)-Cu(2)-O(60)	89.27(7)	Cu(1)-N(1)-N(2)	136.84(15)
N(7)-Cu(2)-N(8)	94.02(17)	N(7)-Cu(2)-N(8)	93.64(19)	N(6)-Cu(2)-O(70)	89.99(7)	Cu(2)-N(2)-N(1)	139.38(15)
N(7)-Cu(2)-O(40)	103.71(14)	Cu(1)-N(1)-N(2)	132.92(34)	O(30)-Cu(1)-O(40)	95.64(6)		
N(8)-Cu(2)-O(40)	110.92(14)	Cu(1)-N(5)-N(6)	132.89(35)	O(50)-Cu(2)-N(2)	97.43(7)		
Cu(1)-N(1)-N(2)	133.04(29)	Cu(2)-N(1)-N(2)	132.93(34)	O(50)-Cu(2)-N(5)	163.81(7)		
Cu(1)-N(5)-N(6)	132.38(29)	Cu(2)-N(5)-N(6)	133.18(34)	O(50)-Cu(2)-N(6)	90.86(7)		
Cu(2)-N(1)-N(2)	133.23(29)			O(50)-Cu(2)-O(60)	88.05(7)		
Cu(2)-N(5)-N(6)	134.10(29)			O(50)-Cu(2)-O(70)	82.28(6)		
				O(60)-Cu(2)-O(70)	170.29(6)		
				Cu(1)-N(1)-N(2)	140.95(36)		
				Cu(2)-N(2)-N(1)	138.00(38)		

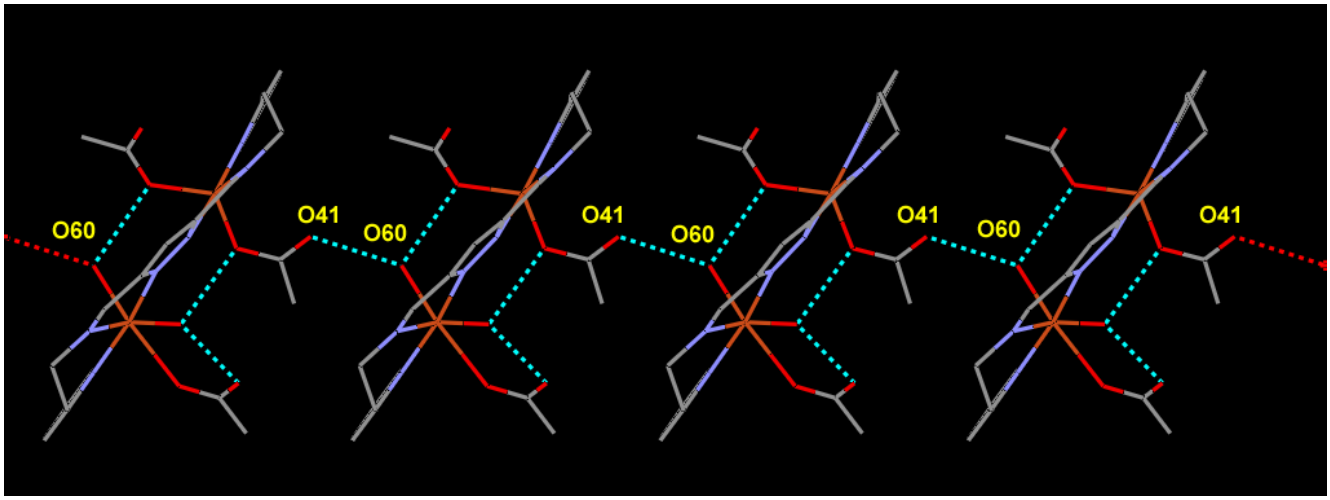

Figure S1 Inter- and intramolecular hydrogen bonding framework for the crystal structure of the complex $[Cu^{II}_2(L2)(H_2O)_2(OAc)_3]$.

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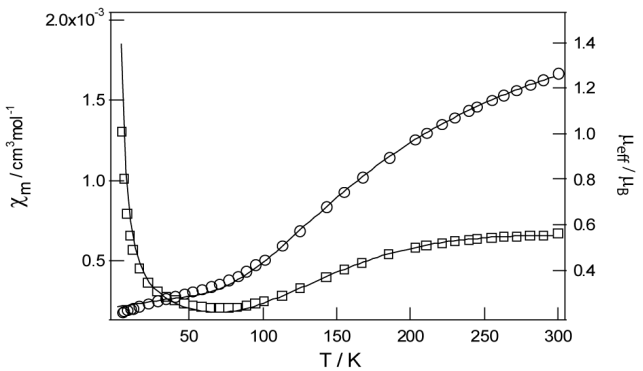

Figure S2. Thermal variation of μ_{eff} (○○) and χ_m (□□) for $[Cu_2(L1)(OAc)_2].2H_2O$ The solid lines represent the best fits and the parameters given in the text.