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SUPPLEMENTARY MATERIAL TO

Synthesis and crystal structure of Cu(II) and Co(II) complexes with 1,3-dimethyl-pyrazole-5-carboxylic acid ligand

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TABLE S-I. Crystallographic data for Cu(II) and Co(II) complexes

Parameter	$[CuL_2(H_2O)_2]$	$[CoL_2(MeOH)_4]$
Molecular formula	$C_{12}H_{18}N_4O_6Cu$	$C_{16}H_{30}N_4O_8Co$
Formula weight	377.84	465.37
Temperature, K	200(1)	150(1)
Wavelength, Å	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	P-1
Unit cell dimensions		
a / Å	3.8258(8)	8.3416(17)
b / Å	15.3819(15)	9.6067(19)
c / Å	13.1874(12)	14.497(3)
α / °	90	102.83(3)
β / °	97.337(3)	91.81(3)
γ / °	90	103.97(3)
V / Å^3	769.70(19)	1094.7(4)
Z	2	2
μ / mm^{-1}	1.456	1.412
F(000)	390	490
D_{calc} / g cm^{-3}	1.630	0.831
Crystal size / mm^3	0.42 × 0.24 × 0.22	0.28 × 0.15 × 0.13
θ range for data collection, °	4.09–30.03	3.67–30.39
Reflections collected	4368/116	12527/289

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TABLE S-I. Continued

Parameter	$[CuL_2(H_2O)_2]$	$[CoL_2(MeOH)_4]$
Independent reflections/parameters	2251	6484
Reflections for $I > 2\sigma(I)$	1835	4590
R_{int}	0.0144	0.0357
Goodness-of-fit on F^2	1.046	1.037
R_1, wR_2 [$I > 2\sigma(I)$]	0.0288, 0.0772	0.0420, 0.0933
Largest ΔF peak and hole, e Å^{-3}	0.36 / −0. 35	0.37 / −0.49

TABLE S-II. Selected bond lengths (Å) and angles (°) for the Cu(II) and Co(II) complexes

Bond	HL[1]	$[CuL_2(H_2O)_2]$	$[CoL_2(MeOH)_2]$	
			A	B
Cu1−O1/Co1−O1	–	1.950(1)	2.075(1)	2.072(1)
Cu1−O1w	–	1.953(2)	–	–
Co1−O3	–	–	2.066(2)	2.121(2)
Co1−O4	–	–	2.071(2)	2.104(1)
C1−O1	1.331	1.273(2)	1.270(2)	1.267(2)
C1−O2	1.205	1.245(2)	1.244(2)	1.252(2)
C1−C2	1.471	1.493(2)	1.496(3)	1.494(2)
C2−C3	1.401	1.377(2)	1.375(3)	1.387(3)
C3−C4	1.382	1.392(2)	1.400(3)	1.389(3)
N2−C4	1.353	1.337(2)	1.334(3)	1.340(2)
N1−N2	1.350	1.347(2)	1.360(2)	1.359(2)
N1−C6	1.470	1.458(2)	1.454(3)	1.458(2)
N1−C2	1.355	1.361(2)	1.361(2)	1.354(2)
C4−C5	1.501	1.500(2)	1.498(3)	1.501(3)
Angle, °				
O1−Cu−O1w	–	88.91(6)	–	–
O1−Co−O3	–	–	90.55(7)	93.22(6)
O1−Co−O4	–	–	88.38(7)	91.29(6)
O3−Co−O4	–	–	92.07(9)	91.43(6)
Cu1−O1−C1/Co1−O1−C1	–	120.36(12)	130.7(12)	128.34(12)
O1−C1−O2	124.7	126.54(16)	126.67(17)	126.01(17)
O1−C1−C2	110.9	114.44(15)	113.51(16)	114.79(16)
O2−C1−C2	124.4	119.02(15)	119.82(16)	119.20(16)
C1−C2−C3	129.2	129.74(15)	128.49(17)	128.37(17)
C1−C2−N1	124.4	123.69(15)	124.83(17)	125.22(16)

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