Electronic Supplementary Information (ESI)

Metal-ligand ratio-controlled assembly of two pairs of Co(II) complexes: syntheses, structures and magnetic properties

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Table S1. Selected bond lengths (Å) and bond angles (°) for complexes **1-4**

			1		
Co(1)-O(1)	2.0487(15)	O(1)-Co(1)-O(2)	107.91(6)	O(2)-Co(1)-N(1)	91.56(7)
Co(1)-O(2)	2.0296(16)	O(1)-Co(1)-O(4)	147.62(7)	O(2)-Co(1)-N(4)	85.60(7)
Co(1)-O(4)	2.1096(17)	O(1)-Co(1)-N(1)	96.17(7)	O(4)-Co(1)-N(1)	88.04(7)
Co(1)-N(1)	2.1054(19)	O(1)-Co(1)-N(3)	87.34(7)	O(4)-Co(1)-N(4)	89.97(7)
Co(1)-N(4)	2.120(2)	O(2)-Co(1)-O(4)	104.03(7)	N(1)-Co(1)-N(4)	176.04(7)
			2		
Co(1)-O(2)	1.9978(16)	Co(1)-O(1)	2.4503(15)	O(3)#1-Co(1)-N(1)	102.89(8)
Co(1)-O(3)#1	1.9524(16)	O(2)-Co(1)-N(1)	127.94(8)	O(3)#1-Co(1)-N(3)#2	114.31(7)
Co(1)-N(1)	2.0249(19)	O(2)-Co(1)-N(3)#2	105.47(7)	N(1)-Co(1)-N(3)#2	107.47(7)
Co(1)-N(3)	2.0923(19)	O(3)#1-Co(1)-O(2)	98.78(7)		
			3		
Co(1)-O(1)	2.390(4)	O(4)#1-Co(1)-O(2)	99.91(14)	N(1)-Co(1)-N(4)	129.93(19)
Co(1)-O(2)	2.006(4)	O(4)#1-Co(1)-N(1)	100.87(18)	O(4)#1-Co(1)-O(1)	158.79(14)
Co(1)-O(4)#1	1.993(4)	O(2)-Co(1)-N(1)	111.05(18)	O(2)-Co(1)-O(1)	59.06(14)
Co(1)-N(1)	2.011(5)	O(4)#1-Co(1)-N(4)	99.86(19)	N(1)-Co(1)-O(1)	90.45(17)
Co(1)-N(4)	2.044(5)	O(2)-Co(1)-N(4)	109.5(2)	N(4)-Co(1)-O(1)	86.03(19)
			4		
Co(1)-O(1)#1	2.1380(15)	O(2)-Co(1)#1	2.3345(16)	N(1)-Co(1)-O(2)#1	94.57(7)
Co(1)-O(2)#1	2.3345(17)	O(1)#4-Co(1)-O(2)#1	58.43(6)	N(3)-Co(1)-N(1)	175.27(8)
Co(1)-O(4)	2.0675(16)	O(4)-Co(1)-N(1)	90.80(7)	N(3)-Co(1)-O(1)#1	91.48(7)
Co(1)-O(7)	2.0448(15)	O(4)-Co(1)-N(3)	85.12(7)	N(3)-Co(1)-O(2)#1	88.61(7)
Co(1)-N(1)	2.115(2)	O(4)-Co(1)-O(1)#1	104.39(6)	O(3)-Co(2)-O(5)	121.02(7)
Co(1)-N(3)	2.097(2)	O(4)-Co(1)-O(2)#1	161.60(6)	O(3)-Co(2)-N(6)	118.54(9)
Co(2)-O(3)	1.9537(16)	O(7)-Co(1)-N(1)	92.61(7)	O(5)-Co(2)-N(6)	95.16(9)
Co(2)-O(5)	1.9761(17)	O(7)-Co(1)-O(1)#1	151.86(6)	O(7)-Co(1)-O(2)#1	93.58(6)
Co(1)-O(7)	2.0448(15)	O(7)-Co(1)-O(2)#1	93.58(6)	O(8)-Co(2)-O(3)	107.56(8)
Co(2)-O(8)	1.9464(17)	O(7)-Co(1)-O(4)	103.75(6)	O(8)-Co(2)-O(5)	106.35(8)
Co(2)-N(6)	2.023(2)	O(7)-Co(1)-N(3)	90.68(7)	O(8)-Co(2)-N(6)	106.81(9)
O(1)-Co(1)#1	2.1380(15)	N(1)-Co(1)-O(1)#1	87.22(7)		

Symmetry code: for **2**, #1 x,-y+1/2,z+1/2; #2 x,y-1,z; for **3**, #1 x+1,y,z; for **4**, #1 -x+1,-y+1,-z.

Table S2. Hydrogen bond lengths (Å) and bond angles (°) for complexes **1-4**

	D–H···A	d(D–H)	d(H···A)	d(D···A)	∠(D–H···A)
1	N(5)-H(5A)...O(3)#1	0.82	1.91	2.681(2)	156.3
	N(3)-H(3A) ...O(1)#3	0.86	2.59	3.045(3)	114.3
2	N(3)-H(3A) ...O(4)#2	0.86	2.24	2.981(2)	144.6
	N(3)-H(3B)...O(2)#1	0.86	2.47	3.031(2)	123.5
	O(5)-H(5A)...O(3)#2	0.86	2.03	2.842(6)	157.6
3	O(5)-H(5B)...O(3)#1	0.85	2.20	2.969(7)	149.9
	N(5)-H(5C)...O(5)#3	0.88	1.83	2.661(6)	157.3
4	N(7)-H(7B)...O(6)#2	0.81	1.86	2.651(2)	165.3

	N(8)-H(8A)...O(2)#1	0.82	1.95	2.738(2)	160.4

Symmetry code: for **1**, #1 -x+1, -y+2, -z; for **2**, #1 -x+1, y+1/2, -z+1/2, #2 -x+1, -y+2, -z, #3 x, y+1, z; for **3**,#1 -x+1, -y+1, -z+1 #2 x+1,y, z, #3 x, y+1, z; for **4**, #1 x, y+1, z+1, #2 -x, -y, -z.

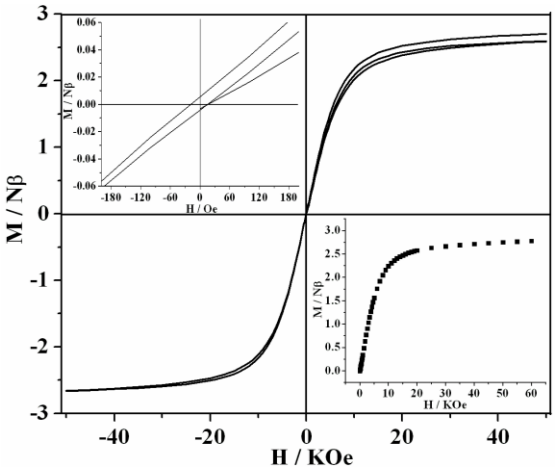
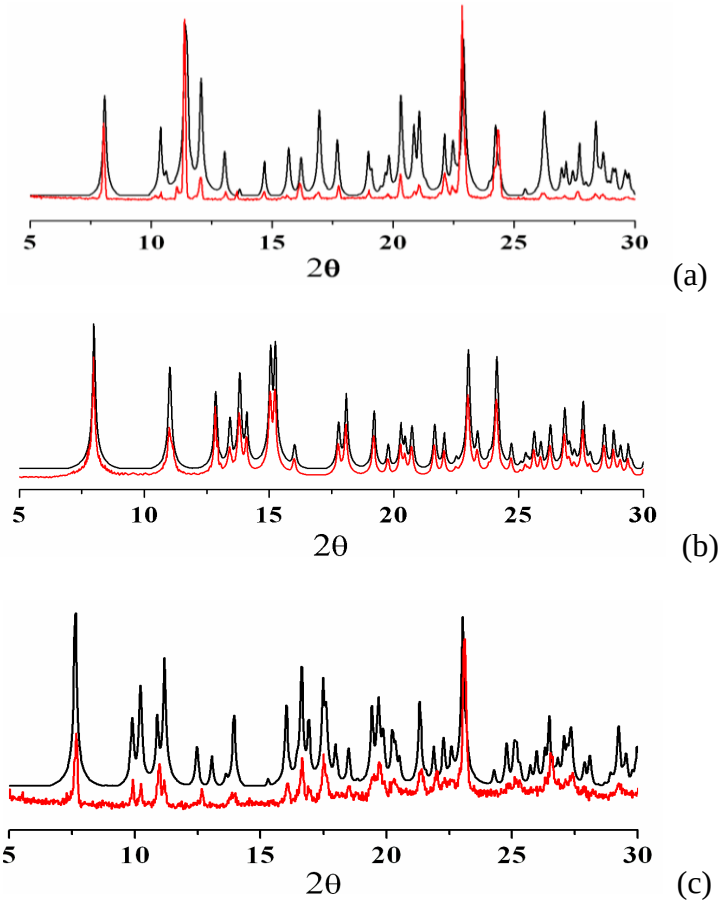
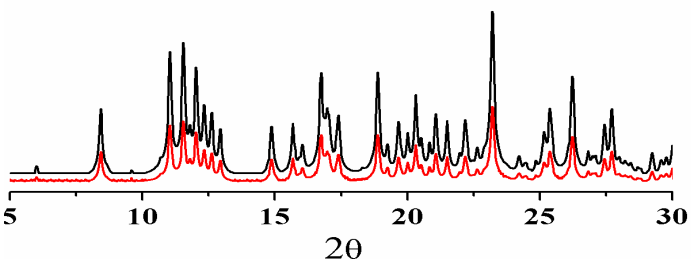


Fig. S1 The hysteresis loop for **1** at 2.0 K; The inset gives a blown-up view of the hysteresis loop below 200 Oe (left) and field dependence of magnetization **(**right**)**.





(d)

Fig. S2 The simulated (Black) and experimental (Red) PXRD of the three compounds ((a) for **1**, (b) for **2**, (c) for **3** and (d) for **4**.