Supporting Information

Synthesis, Structure, Fluorescent and Magnetic Properties of a Series of Coordination Polymers Based on a Long and Flexible Bis-triazole Ligand

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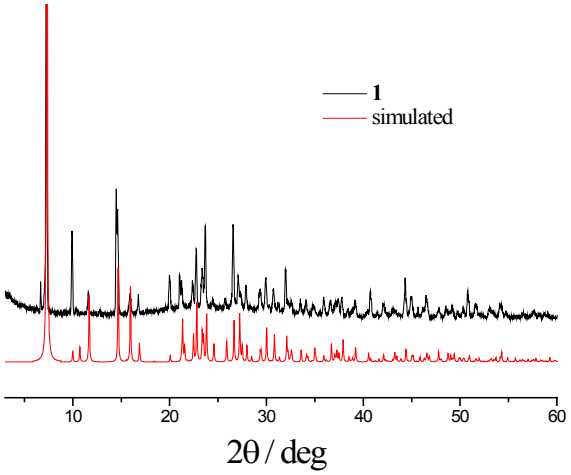
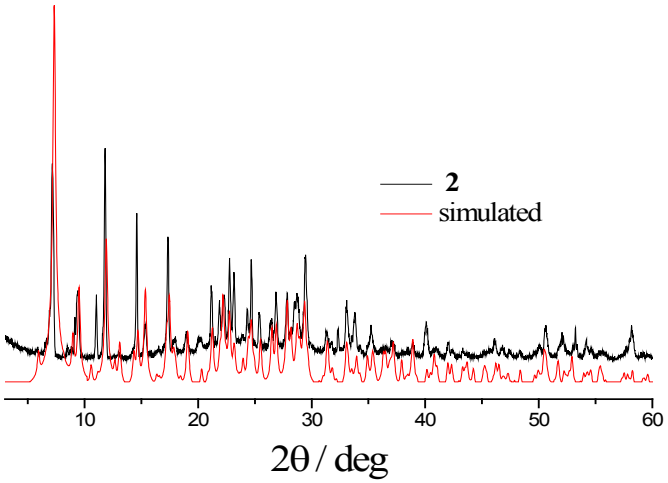
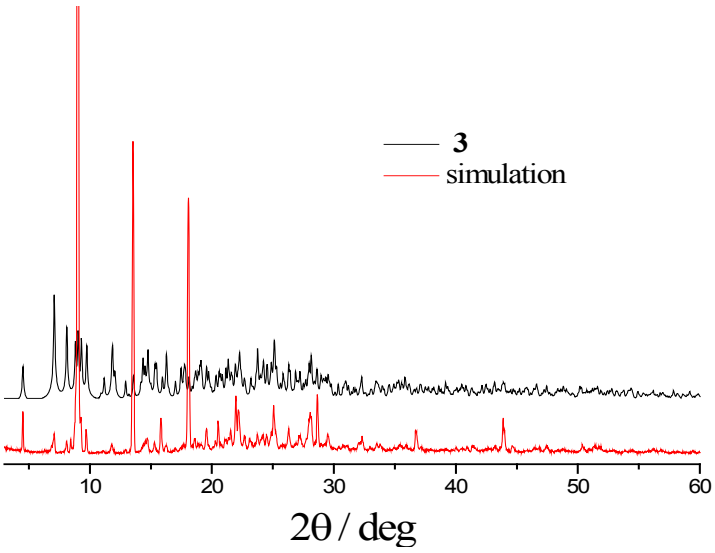






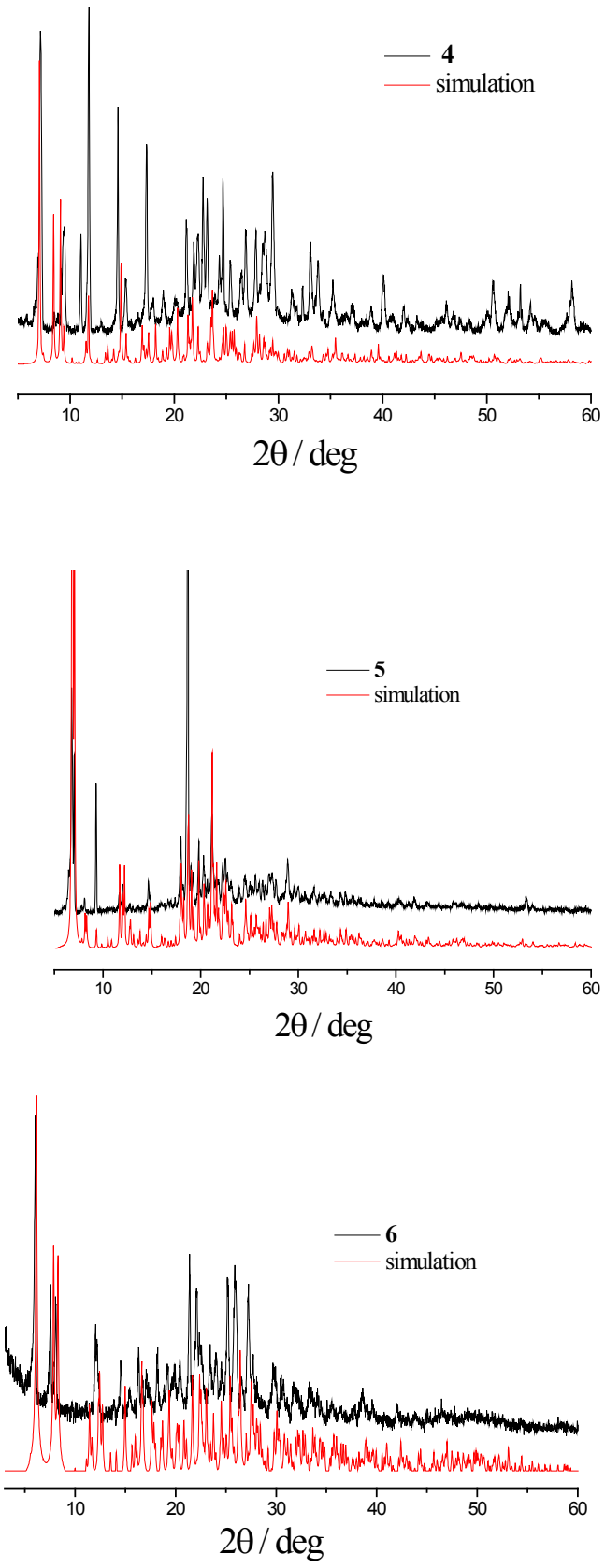


Fig. S1 The PXRD patterns of compounds **1**-**6**.

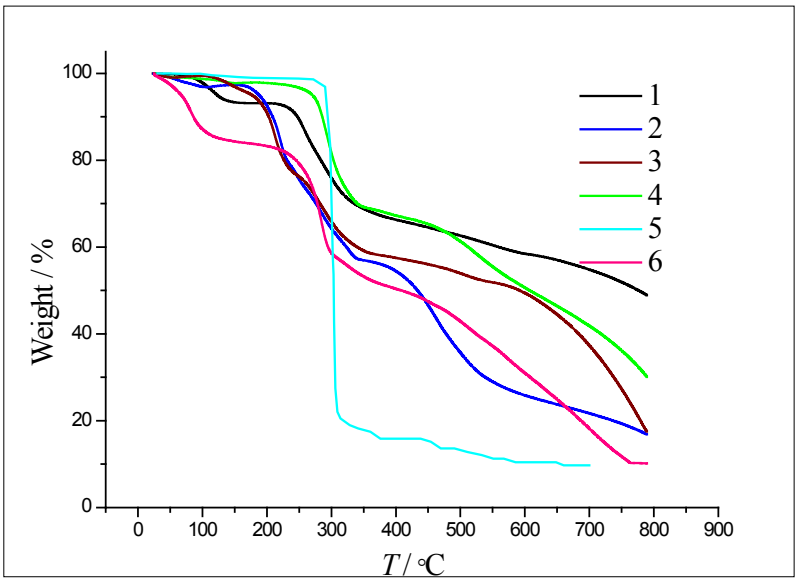
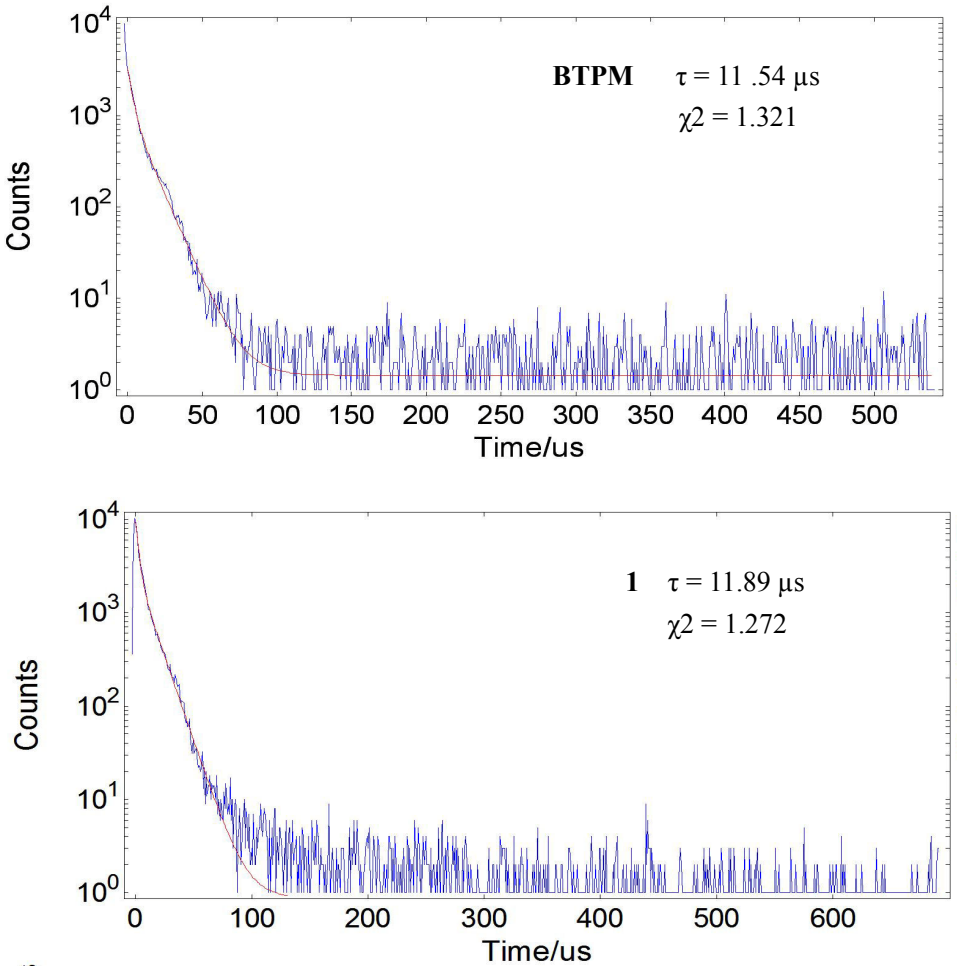


Fig. S2 The plots of TGA for compounds **1**-**6**.



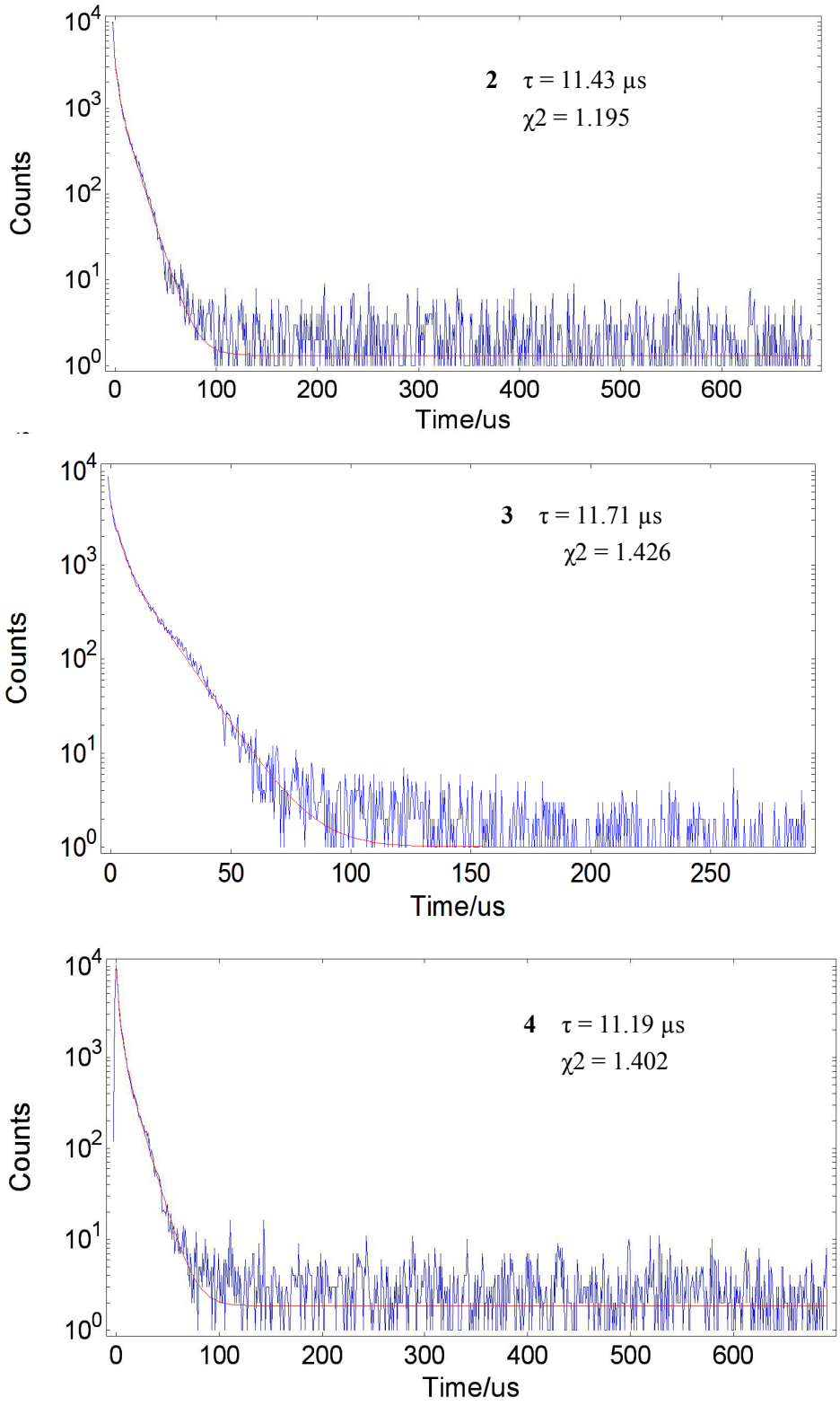


Fig. S3 The decay curves for BTPM and compounds **1**-**4**.

Table S1 Selected bond lengths (Å) and angles (°) for compounds **1-6**.

		1	
Zn1—O4	2.028(6)	Zn2—N5^{i}	2.171(4)
Zn1—O1	2.127(7)	Zn2—N5^{ii}	2.171(4)
Zn1—N4	2.163(5)	Zn2—N5	2.171(4)
Zn1—N4^{i}	2.163(5)	Zn3—O2^{iv}	2.081(6)
Zn1—N2^{i}	2.185(5)	Zn3—O2	2.081(6)
Zn1—N2	2.185(5)	Zn3—N1^{i}	2.184(4)
Zn2—O3^{ii}	2.081(6)	Zn3—N1^{v}	2.184(4)
Zn2—O3	2.081(6)	Zn3—N1	2.184(4)
Zn2—N5^{iii}	2.171(4)	Zn3—N1^{iv}	2.184(4)
O4—Zn1—O1	180	N5^{iii}—Zn2—N5^{i}	180
O4—Zn1—N4	94.76(9)	O3^{ii}—Zn2—N5^{ii}	93.13(11)
O1—Zn1—N4	84.73(9)	O3—Zn2—N5^{ii}	86.87(11)
O4—Zn1—N4^{i}	94.76(9)	N5^{iii}—Zn2—N5^{ii}	89.53(13)
O1—Zn1—N4^{i}	84.73(9)	N5^{i}—Zn2—N5^{ii}	90.47(13)
N4—Zn1—N4^{i}	91.00(16)	O3^{ii}—Zn2—N5	86.87(11)
O4—Zn1—N2^{i}	88.60(9)	O3—Zn2—N5	93.13(11)
O1—Zn1—N2^{i}	91.94(9)	N5^{iii}—Zn2—N5	90.47(13)
N4—Zn1—N2^{i}	90.28(16)	N5^{i}—Zn2—N5	89.53(13)
N4^{i}—Zn1—N2^{i}	176.30(15)	N5^{ii}—Zn2—N5	180
O4—Zn1—N2	88.60(9)	O2^{iv}—Zn3—O2	179.99(18)
O1—Zn1—N2	91.94(9)	O2^{iv}—Zn3—N^{1i}	86.27(11)
N4—Zn1—N2	176.30(15)	O2—Zn3—N1^{i}	93.73(11)
N4^{i}—Zn1—N2	90.28(16)	O2^{iv}—Zn3—N1^{v}	93.73(11)
N2^{i}—Zn1—N2	88.23(15)	O2—Zn3—N1^{v}	86.27(11)
O3^{ii}—Zn2—O3	180	N1^{i}—Zn3—N1^{v}	180
O3^{ii}—Zn2—N5^{iii}	93.13(11)	O2^{iv}—Zn3—N1	86.27(11)
O3—Zn2—N5^{iii}	86.87(11)	O2—Zn3—N1	93.73(11)
O3^{ii}—Zn2—N5^{i}	86.87(11)	N1^{i}—Zn3—N1	90.34(13)
O3—Zn2—N5^{i}	93.13(11)		
		2	
Cd1—O1	2.224(5)	Cd1—N1^{i}	2.354(3)
Cd1—O1^{i}	2.224(5)	Cd1—N1	2.354(3)
Cd1—N1^{iii}	2.354(3)		

O1—Cd1—O1^{i}	179.98(20)	N1^{ii}—Cd1—N1^{i}	37.65(8)
O1—Cd1—N1^{ii}	89.47(1)	N1^{iii}—Cd1—N1^{i}	87.90(12)
O1^{i}—Cd1—N1^{ii}	90.53(1)	O1—Cd1—N1	93.35(9)
O1—Cd1—N1^{iii}	93.35(9)	O1^{i}—Cd1—N1	86.65(9)
O1^{i}—Cd1—N1^{iii}	86.65(9)	N1^{ii}—Cd1—N1	142.35(8)
N1^{ii}—Cd1—N1^{iii}	50.26(8)	N1^{iii}—Cd1—N1	92.10(12)
O1—Cd1—N1^{i}	86.65(9)	N1^{i}—Cd1—N1	180.00(12)
O1^{i}—Cd1—N1^{i}	93.35(9)		

3

Zn1—N7	2.093(7)	Zn2—O3	2.119(7)
Zn1—O2	2.135(7)	Zn2—N10^{i}	2.118(7)
Zn1—N2	2.146(6)	Zn2—N1	2.145(7)
Zn1—N13	2.160(7)	Zn2—N14	2.157(7)
Zn1—N4	2.175(7)	Zn2—O4	2.176(5)
Zn1—O1	2.217(6)	Zn2—N5	2.177(7)
N7—Zn1—O2	89.93(23)	O3—Zn2—N10^{i}	91.42(23)
N7—Zn1—N2	93.76(23)	O3—Zn2—N1	86.87(23)
O2—Zn1—N2	89.11(23)	N10^{i}—Zn2—N1	95.47(23)
N7—Zn1—N13	94.63(23)	O3—Zn2—N14	174.83(23)
O2—Zn1—N13	173.78(23)	N10^{i}—Zn2—N14	90.15(23)
N2—Zn1—N13	94.79(23)	N1—Zn2—N14	97.89(23)
N7—Zn1—N4	176.67(23)	O3—Zn2—O4	86.02(23)
O2—Zn1—N4	88.32(23)	N10^{i}—Zn2—O4	87.31(22)
N2—Zn1—N4	89.04(23)	N1—Zn2—O4	172.42(22)
N13—Zn1—N4	86.91(23)	N14—Zn2—O4	89.14(22)
N7—Zn1—O1	89.13(23)	O3—Zn2—N5	94.03(23)
O2—Zn1—O1	88.01(23)	N10^{i}—Zn2—N5	173.24(23)
N2—Zn1—O1	175.91(23)	N1—Zn2—N5	88.84(23)
N13—Zn1—O1	87.84(23)	N14—Zn2—N5	84.08(23)
N4—Zn1—O1	87.98(23)	O4—Zn2—N5	89.06(22)

4

Cd1—N7	2.266(9)	Cd2—O4	2.267(8)
Cd1—O1	2.300(8)	Cd2—N10^{ii}	2.274(8)
Cd1—N4^{i}	2.335(8)	Cd2—N2	2.333(8)
Cd1—N13	2.347(8)	Cd2—O3	2.334(8)
Cd1—N1	2.350(8)	Cd2—N14	2.340(8)
Cd1—O2	2.369(7)	Cd2—N5^{i}	2.347(8)
N7—Cd1—O1	89.58(29)	O4—Cd2—N10^{ii}	90.96(27)
N7—Cd1—N4^{i}	177.38(29)	O4—Cd2—N2	90.14(26)
O1—Cd1—N4^{i}	87.80(28)	N10^{ii}—Cd2—N2	96.03(28)
N7—Cd1—N13	98.99(29)	O4—Cd2—O3	79.60(26)
O1—Cd1—N13	168.91(27)	N10^{ii}—Cd2—O3	87.92(28)

N4^{i}—Cd1—N13	83.59(27)	N2—Cd2—O3	169.09(28)
N7—Cd1—N1	91.33(29)	O4—Cd2—N14	169.10(27)
O1—Cd1—N1	88.62(28)	N10^{ii}—Cd2—N14	88.42(28)
N4^{i}—Cd1—N1	88.72(28)	N2—Cd2—N14	100.75(28)
N13—Cd1—N1	98.13(27)	O3—Cd2—N14	89.50(27)
N7—Cd1—O2	94.27(27)	O4—Cd2—N5^{i}	98.31(26)
O1—Cd1—O2	87.85(27)	N10^{ii}—Cd2—N5^{i}	169.27(28)
N4^{i}—Cd1—O2	85.53(26)	N2—Cd2—N5^{i}	89.38(28)
N13—Cd1—O2	84.53(27)	O3—Cd2—N5^{i}	88.45(28)
N1—Cd1—O2	173.36(26)	N14—Cd2—N5^{i}	81.45(27)
	5		
Cu1—N13	1.997(7)	Cu3—N29	1.958(7)
Cu1—O1	2.035(7)	Cu3—N28	2.218(7)
Cu1—N2	2.332(10)	Cu3—N4	1.999(7)
Cu1—N7	2.026(10)	Cu3—N10	2.072(7)
Cu1—N32	2.051(10)	Cu3—N35	2.197(13)
Cu1—N8	2.523(10)	Cu3—O2	2.571(10)
Cu2—N25	2.016(7)	Cu4—N34	2.020(13)
Cu2—O1	2.004(7)	Cu4—N5	2.116(7)
Cu2—N20	1.692(7)	Cu4—N23	2.150(7)
Cu2—N31	1.970(7)	Cu4—N17	2.061(7)
Cu2—N19	2.540(7)	Cu4—N16	2.167(7)
Cu2—N1	2.541(7)	Cu4—O2	2.601(10)
N13—Cu1—O1	174.28(29)	N29—Cu3—N10	95.52(29)
N13—Cu1—N2	92.24(29)	N4—Cu3—N10	90.04(29)
O1—Cu1—N2	82.04(27)	N29—Cu3—N35	91.02(38)
N34—Cu2—N5	86.64(39)	N4—Cu3—N35	86.70(38)
N34—Cu2—N23	89.24(36)	N10—Cu3—N35	91.28(35)
N5—Cu2—N23	91.06(28)	N29—Cu3—O2	85.71(21)
N34—Cu2—O2	93.83(31)	N4—Cu3—O2	88.84(21)
N5—Cu2—O2	87.88(20)	N10—Cu3—O2	176.92(21)
N23—Cu2—O2	176.69(20)	N35—Cu3—O2	91.52(28)
N29—Cu3—N4	174.04(30)		
	6		
Co1—N8	2.111(5)	Co2—O3	2.099(5)
Co1—N5^{i}	58.100(5)	Co2—N2	2.108(5)
Co1—N3	2.160(5)	Co2—N6^{i}	58.017(5)
Co2—O2	2.081(5)	Co2—O1	2.130(4)
Co2—N9	2.095(5)		
N8—Co1—N5^{i}	101.23(13)	O2—Co2—N6^{i}	57.07(13)
N8—Co1—N3	90.57(18)	N9—Co2—N6^{i}	125.73(13)
N5^{i}—Co1—N3	14.03(13)	O3—Co2—N6^{i}	57.39(13)
O2—Co2—N9	175.81(19)	N2—Co2—N6^{i}	51.38(13)
O2—Co2—O3	88.95(19)	O2—Co2—O1	88.21(18)

N9—Co2—O3	90.47(18)	N9—Co2—O1	87.62(18)
O2—Co2—N2	92.70(19)	O3—Co2—O1	89.01(18)
N9—Co2—N2	91.45(19)	N2—Co2—O1	178.76(18)
O3—Co2—N2	90.17(19)	N6^{i}—Co2—O1	128.71(11)

Symmetry transformations used to generate equivalent atoms:
(1) (i) x, -y, z; (ii) 1-x, -y, 2-z; (iii) 1-x, y, 2-z; (iv) 1-x, -y, 1-z; (v) 1-x, y, 1-z;
(2) (i) 1.5-x, 2.5-y, 1.5-z; (ii) 1.5-x, 1+y, 1.5-z; (iii) x, 2.5-y, z; (iv) 2-x, y, z;
(3) (i) x, y, -1+z;
(4) (i) 1+x, y, z; (ii) x, 1+y, z; (iii) -1+x, y, z;
(6) (i) -1-x, -y, z;

Table S2 The overall formula, formula weight, density and F(000) for **1** and **2**.

compounds	**1**	**2**
Formula	$C_{18}H_{20.5}N_7O_{7.25}Zn$	$C_{18}H_{20}N_7O_6Cd$
formula weight	516.30	542.82
crystal system	monoclinic	orthorhombic
space group	*C*2/*m*	*Imma*
a (Å)	20.264(2)	8.3699(14)
b (Å)	15.8241(16)	16.482(3)
c (Å)	16.1914(16)	17.686(3)
α (°)	90	90
ß (°)	113.573(3)	90
γ (°)	90	90
V (Å^3)	4758.7(8)	2439.8(7)
Z	8	4
D_c, g/cm^3	1.441	1.478
μ, mm^{-1}	1.085	0.940
F(000)	2123	1092