

Four metal-organic frameworks based on the 5-(1H-tetrazol-5-yl)isophthalic acid ligand: Luminescence and magnetic properties

Wei Gao, Peng Li, Feng Liu, Xiu-Mei Zhang,* and Jie-Ping Liu

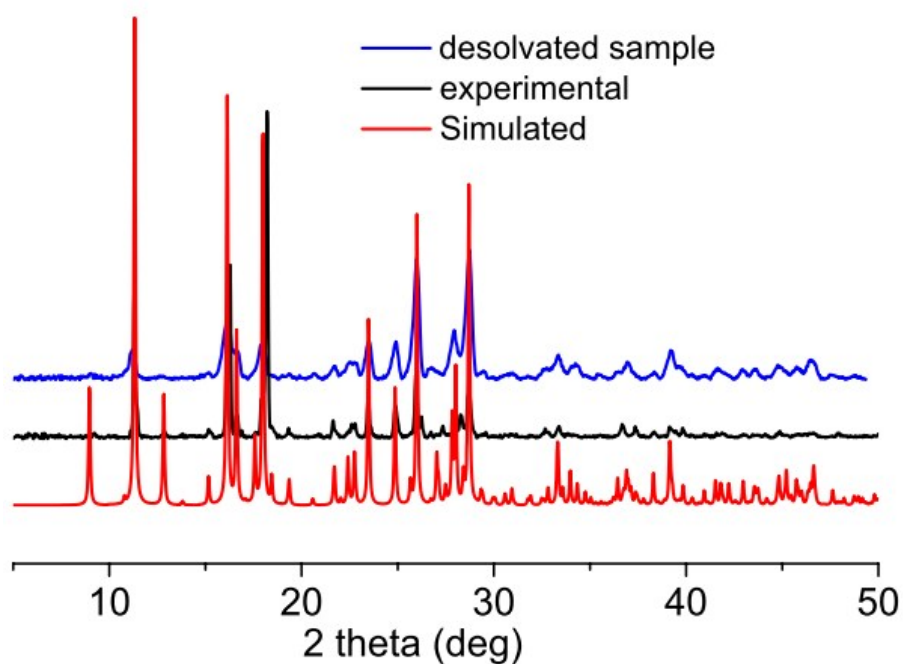


Fig. S1. PXRD patterns for **1** (simulated: red; experimental: black; desolvated sample: blue).

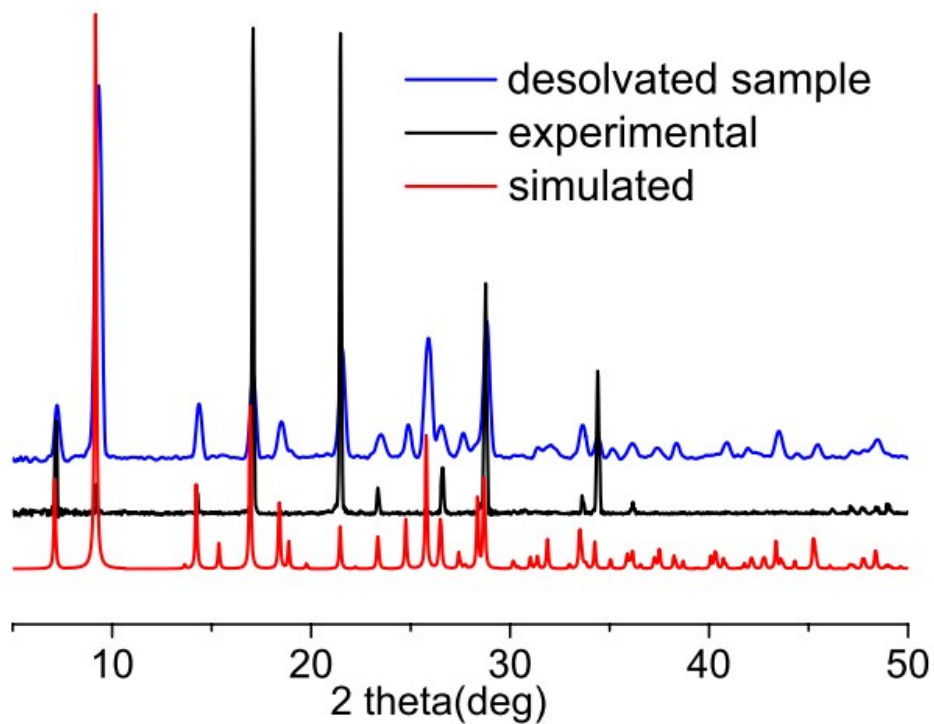


Fig. S2. PXRD patterns for 2 (simulated: red; experimental: black; desolvated sample: blue).

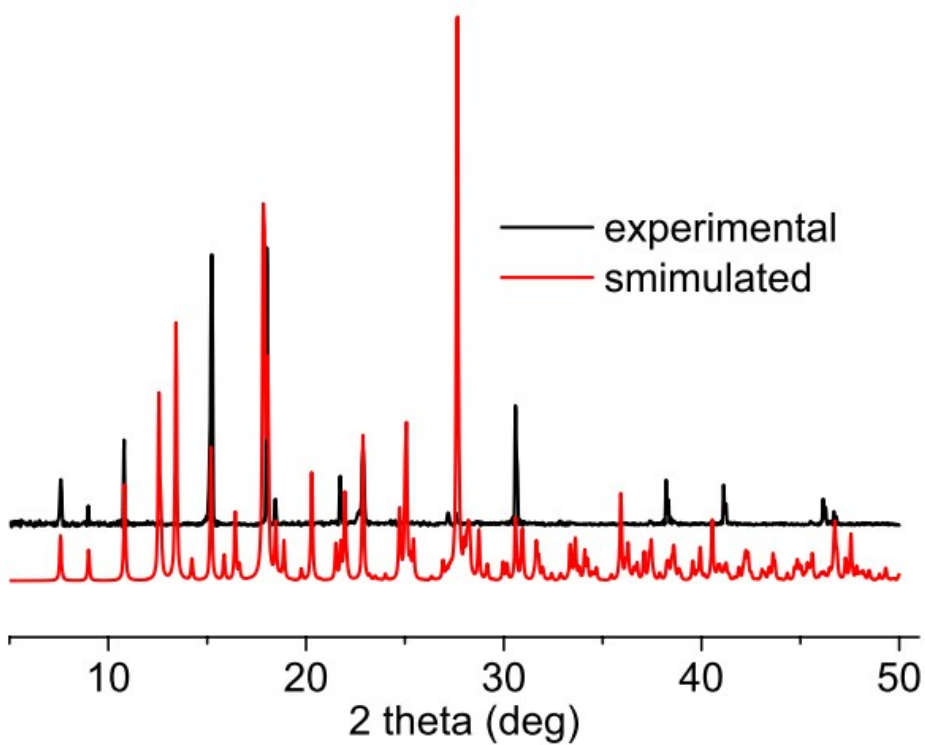


Fig. S3. PXRD patterns for 4 (simulated: red; experimental: black).

Table 2 Selected bond lengths [Å] and angles [°] for **1 - 4**.

Compound 1			
Zn1-O1A	2.000(2)	Zn1-N4B	2.001(2)
Zn1-O4	2.022(2)	Zn1-N1C	2.003(2)
O1A-Zn1-N4B	101.55(9)	O1A-Zn1-O4	93.78(8)
N4B-Zn1-O4	115.65(9)	O1A-Zn1-N1C	111.71(9)
N4B-Zn1-N1C	125.22(10)	O4-Zn1-N1C	104.47(10)
A x+1, y, z; B -x+1, y-1/2, -z+1/2; C -x+1, -y+1, -z+1			
Compound 2			
Cd1-O1	2.181(11)	Cd1-O4A	2.191(13)
Cd1-O5	2.236(12)	Cd1-N1B	2.507(14)
Cd1-N1C	2.507(14)	Cd1-O3A	2.535(15)
Cd2-O5D	2.228(7)	Cd2-N2B	2.319(10)
Cd2-O6	2.336(11)		
O1-Cd1-O4A	100.4(5)	O1-Cd1-O5	114.3(5)
O4A-Cd1-O5	145.2(5)	O1-Cd1-N1B	92.5(2)
O4A-Cd1-N1B	92.5(2)	O5-Cd1-N1B	86.3(2)
O1-Cd1-N1C	92.5(2)	O4A-Cd1-N1C	92.47(9)
O5-Cd1-N1C	86.34(7)	N1B-Cd1-N1C	172.2(4)
O1-Cd1-O3A	155.0(5)	O4A-Cd1-O3A	54.6(5)
O5-Cd1-O3A	90.7(5)	N1B-Cd1-O3A	89.0(2)
N1C-Cd1-O3A	89.0(2)	O5B-Cd2-O5D	180
O5D-Cd2-N2B	95.0(4)	O5-Cd2-N2B	85.0(4))
O5-Cd2-N2E	95.0(4)	N2E-Cd2-N2B	180
O5D-Cd2-O6	90.7(5)	O5-Cd2-O6	89.3(5)
N2E-Cd2-O6	86.0(4)	N2B-Cd2-O6	94.0(4)
O6-Cd2-O6D	180		
A x+1, y, z; B --x+1,-y,-z+1; C -x+1,y+1/2,-z+1 ; D -x+2,-y,-z+2; E x+1,y,z+1.			

Compound 3			
Mn1-O3A	2.049(5)	Mn1-O6	2.161(5)
Mn1-N2	2.179(6)	Mn1-O1B	2.206(5)
Mn1-O2B	2.340(5)	Mn1-O5	2.357(5)
Na1-O4C	2.374(7)	Na1-O1B	2.397(6)
Na1-O5D	2.444(6)	Na1-N1	2.452(7)
Na1-O2E	2.595(6)		
O3A-Mn1-O6	92.0(2)	O3A-Mn1-N2	102.3(2)
O6-Mn1-N2	99.5(2)	O3A-Mn1-O1B	164.6(2)
O6-Mn1-O1B	92.9(2)	N2-Mn1-O1B	91.3(2)
O3A-Mn1-O2B	107.5(2)	O6-Mn1-O2B	89.80(19)
N2-Mn1-O2B	148.4(2)	O1B-Mn1-O2B	57.91(17)
O3A-Mn1-O5	85.7(2)	O6-Mn1-O5	167.2(2)
N2-Mn1-O5	93.3(2)	O1B-Mn1-O5	86.30(19)
O2B-Mn1-O5	78.99(18)	O4C-Na1-O1B	81.3(2)
O4C-Na1-O5D	107.4(2)	O1B-Na1-O5D	115.3(2)
O4C-Na1-N1	127.8(2)	O1B-Na1-N1	82.0(2)
O5D-Na1-N1	124.4(2)	O4C-Na1-O2E	86.3(2)
O1B-Na1-O2E	166.9(2)	O5D-Na1-O2E	72.64(18)
N1-Na1-O2E	102.3(2)		

Hydrogen bond lengths (Å) and angles (°) for Compound 3^a.

D	A[Transformation]	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O5	O4[-x+1/2, y-1/2, -z+1/2]	0.85	1.94	2.785(8)	171
O5	N4[-x+1, -y+1, -z+1]	0.85	2.04	2.860(6)	161
O6	O2[-x+1, y-1, -z+1/2]	0.85	2.02	2.815(7)	155
O6	N3[-x+1, y, -z+1/2]	0.85	1.98	2.771(10)	156

^a D, donor; A, acceptor. A x, y-1, z; B x-1/2, -y+3/2, z-1/2; C -x+1/2, y-1/2, -z+1/2; D-x+1/2, y+1/2, -z+1/2; E -x+1, -y+2, -z+1.

Compound 4

Mn1-O4A	2.092(5)	Mn1-O2	2.154(4)
Mn1-O9	2.197(6)	Mn1-O6	2.201(6)
Mn1-O7	2.214(5)	Mn1-O5	2.217(6)
Mn2-O10	2.155(7)	Mn2-O8	2.223(5)
Mn2-N1	2.264(5)		
O4A-Mn1-O2	174.68(19)	O4A-Mn1-O9	89.8(2)
O2-Mn1-O9	84.8(2)	O4A-Mn1-O6	87.4(2)
O2-Mn1-O6	92.7(2)	O6-Mn1-O9	89.7(3)
O4A-Mn1-O7	98.7(2)	O2-Mn1-O7	86.62(19)
O6-Mn1-O7	89.0(2)	O9-Mn1-O7	171.3(2)
O4A-Mn1-O5	91.1(2)	O2-Mn1-O5	88.7(2)
O9-Mn1-O5	90.1(3)	O6-Mn1-O5	178.5(2)
O7-Mn1-O5	91.3(2)	O10-Mn2-O10B	180
O10-Mn2-O8B	91.3(2)	O10-Mn2-O8	88.8(3)
O10B-Mn2-O8	91.2(3)	O8B-Mn2-O8	180
O10-Mn2-N1B	88.8(3)	O10-Mn2-N1	91.2(3)
O8-Mn2-N1	94.38(19)	O8-Mn2-N1B	85.62(19)
N1B-Mn2-N1	180		

Hydrogen bond lengths (Å) and angles (°) for Compound 4^a.

D	A[Transformation]	d(D-H)	d(H···A)	d(D···A)	<(DHA)
O5	O11	0.86	2.02	2.855(11)	165
O5	N2[-x+1,-y+1,-z+1]	0.86	1.94	2.790(7)	169
O6	O11[x-1, y, z]	0.85	1.93	2.785(11)	176
O6	N3[-x+1, -y, -z+1]	0.85	1.89	2.734(7)	173
O7	O1	0.85	1.92	2.728(7)	158
O7	O8[-x+1, -y+1, -z+1]	0.85	2.16	2.905(8)	147
O8	O3[-x+2, -y, -z+1]	0.85	1.81	2.655(7)	173
O8	O1[x, y, z+1]	0.85	2.01	2.807(7)	158
O9	O6[-x, -y+1, -z+1]	0.85	2.14	2.859(8)	142

O10 O12' 0.71 2.25 2.96(2) 175

^aD, donor; A, acceptor. A $x-1, y+1, z$; B $-x+1, -y, -z+2$; C $x+1, y-1, z$.

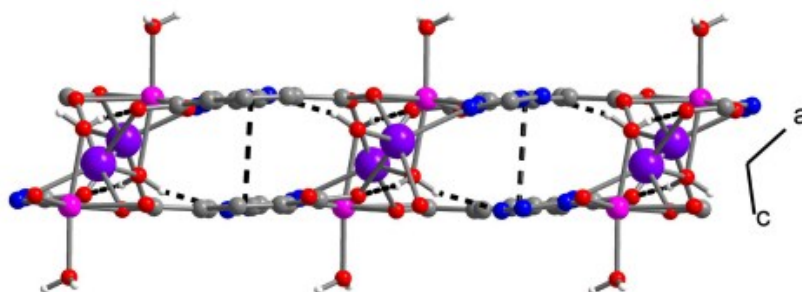


Fig. S4 Side views of the 2D layer in **3**.

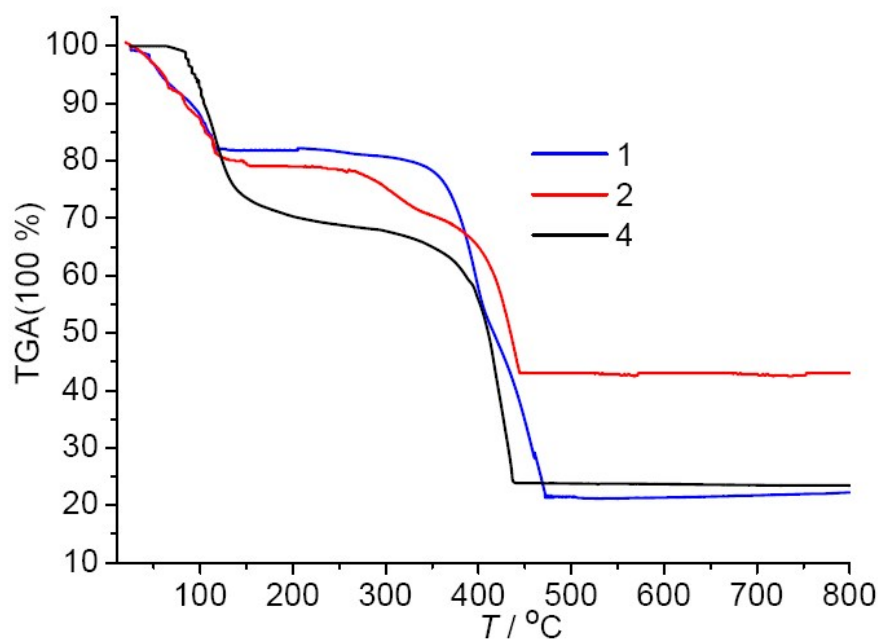


Fig. S5 The TGA curves for **1**, **2** and **4**.