Supplementary Material (ESI) for CrystEngComm

Supporting Information

Ancillary ligand-mediated syntheses and fluorescence properties of zinc(II) complexes based on flexible benzene dicarboxylic acid

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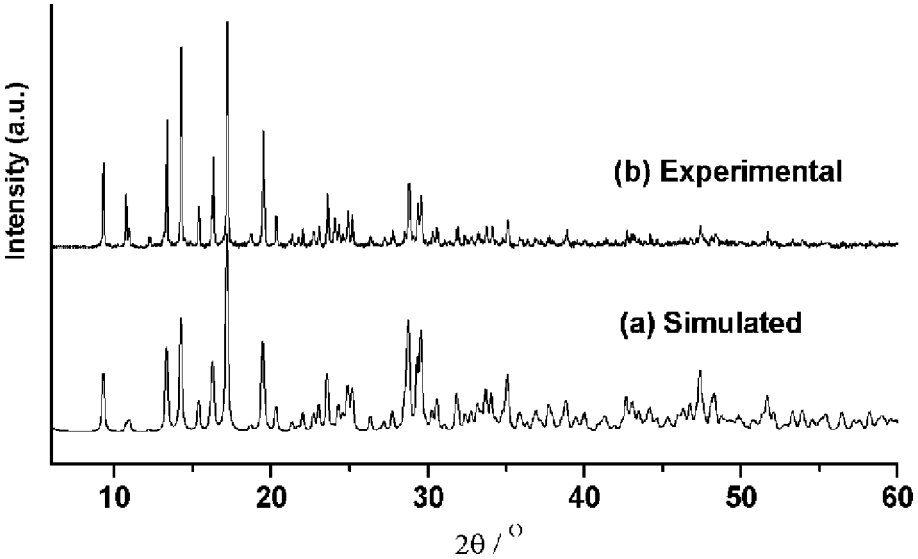

Fig. S1 Powder X-ray diffraction patterns for **1** with (a) simulated, (b) experimental.

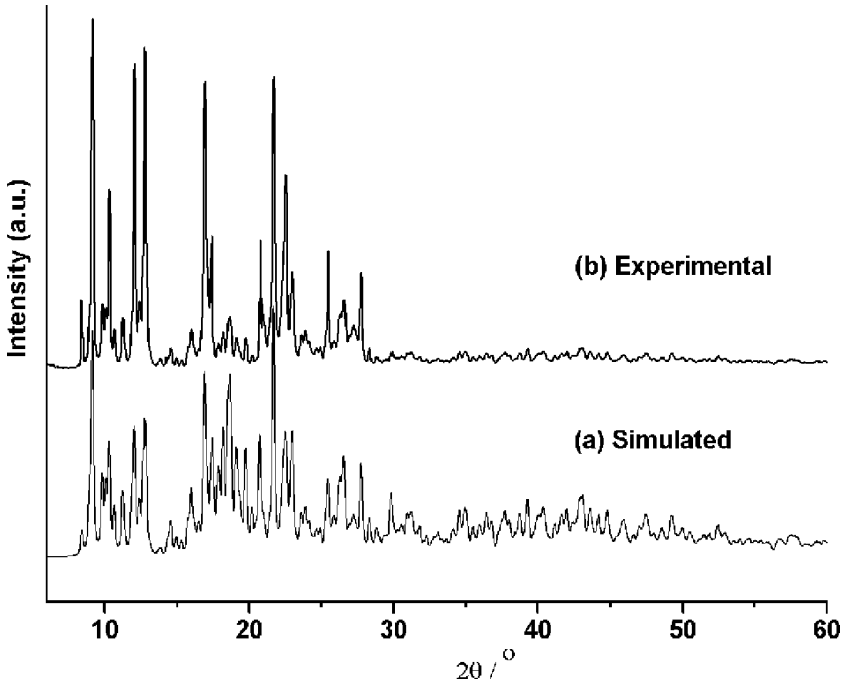

Fig. S2 Powder X-ray diffraction patterns for **2** with (a) simulated, (b) experimental.

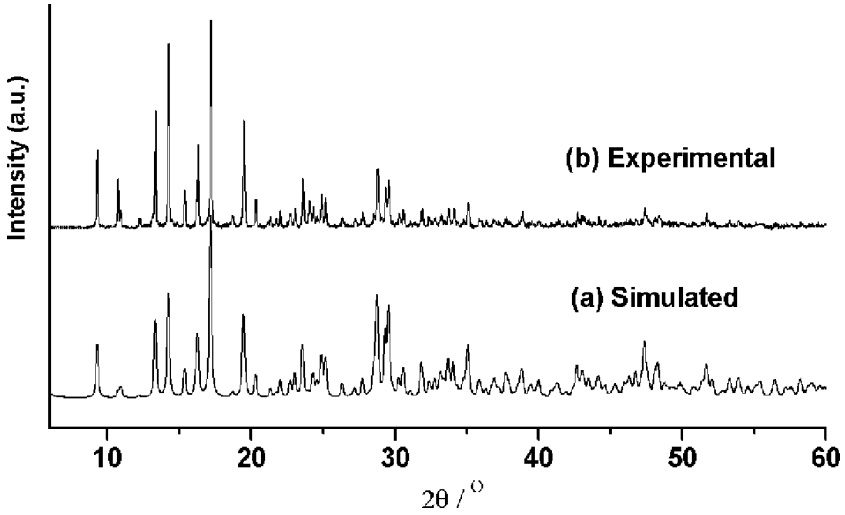

Fig. S3 Powder X-ray diffraction patterns for **3** with (a) simulated, (b) experimental.

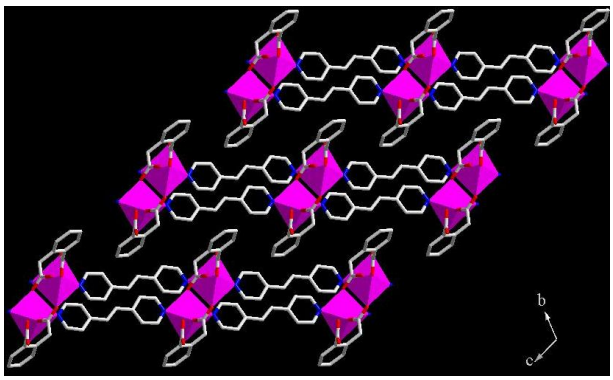

Fig. S4 View of the packing structure of **1** along the *a*-axis. ZnO_4N_2, purple octahedra.

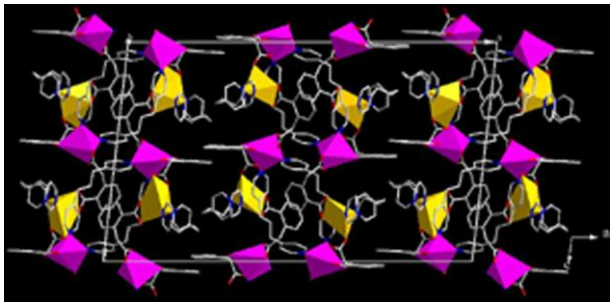

Fig. S5 View of the packing structure of **2** along the *b*-axis. ZnO_3N_2, yellow tetragonal pyramids; ZnO_4N_2, purple octahedra.

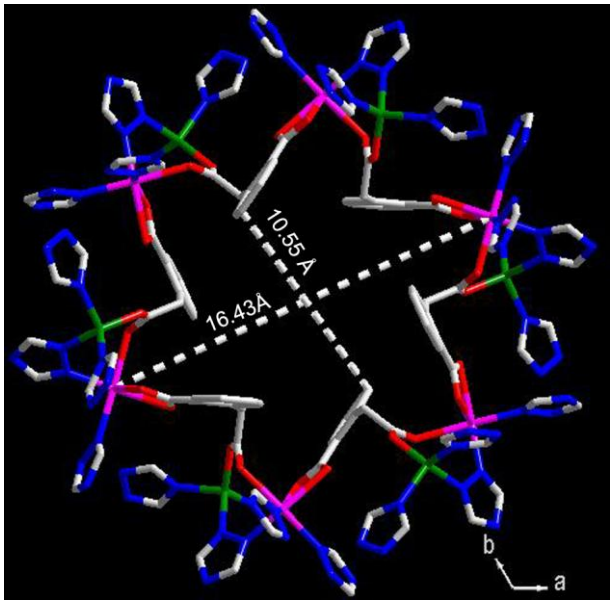

Fig. S6 The 48-MR opening with an approximate pore diameter of 10.55 × 16.43 Å in **3**.

Table S1 Selected Bond lengths (Å) and angles (°) for **1**[a]

Zn(1)-O(5)#1	1.999(2)	Zn(1)-N(1)	2.142(3)
Zn(1)-O(6)#2	2.008(2)	Zn(1)-N(2)#3	2.154(3)
Zn(1)-O(1)	2.027(3)		
O(5)#1-Zn(1)-O(6)#2	123.51(11)	O(1)-Zn(1)-N(1)	93.78(11)
O(5)#1-Zn(1)-O(1)	98.65(11)	O(5)#1-Zn(1)-N(2)#3	94.11(11)
O(6)#2-Zn(1)-O(1)	137.83(11)	O(6)#2-Zn(1)-N(2)#3	89.01(11)
O(5)#1-Zn(1)-N(1)	90.32(11)	O(1)-Zn(1)-N(2)#3	89.00(11)
O(6)#2-Zn(1)-N(1)	85.64(11)	N(1)-Zn(1)-N(2)#3	174.37(10)

[a] Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z; #2 x+1, y, z; #3 x-1, y-1, z-1; #4 x+1, y+1, z+1; #5 x-1, y, z.

Table S2 Selected Bond lengths (Å) and angles (°) for **2**[a]

Zn(1)-O(7)	1.995(3)	Zn(3)-N(5)	2.092(3)
Zn(1)-O(2)	2.031(3)	Zn(3)-O(14)	2.479(4)
Zn(1)-N(2)#1	2.071(3)	Zn(3)-O(10)	1.991(3)
Zn(1)-N(1)	2.107(3)	Zn(3)-O(13)	2.019(3)
Zn(1)-O(1)	2.469(4)	Zn(3)-N(6)#4	2.056(3)
Zn(2)-O(4)#2	1.956(3)	Zn(4)-O(15)	1.946(3)
Zn(2)-O(5)	1.965(3)	Zn(4)-O(11)#5	1.950(3)
Zn(2)-N(4)#3	2.029(3)	Zn(4)-N(7)	2.025(3)
Zn(2)-N(3)	2.092(3)	Zn(4)-N(8)#6	2.106(3)
O(7)-Zn(1)-O(2)	111.63(12)	O(10)-Zn(3)-N(6)#4	103.92(12)
O(7)-Zn(1)-N(2)#1	101.55(12)	O(13)-Zn(3)-N(6)#4	143.18(14)
O(2)-Zn(1)-N(2)#1	144.66(12)	O(10)-Zn(3)-N(5)	95.38(12)
O(7)-Zn(1)-N(1)	95.19(12)	O(13)-Zn(3)-N(5)	94.69(13)
O(2)-Zn(1)-N(1)	95.09(12)	N(6)#4-Zn(3)-N(5)	94.62(12)
N(2)#1-Zn(1)-N(1)	93.67(12)	O(10)-Zn(3)-O(14)	158.41(12)
O(7)-Zn(1)-O(1)	159.96(11)	O(13)-Zn(3)-O(14)	54.91(13)
O(2)-Zn(1)-O(1)	55.95(11)	N(6)#4-Zn(3)-O(14)	88.32(11)
N(2)#1-Zn(1)-O(1)	88.76(11)	N(5)-Zn(3)-O(14)	101.37(12)
N(1)-Zn(1)-O(1)	101.31(11)	O(10)-Zn(3)-C(61)	136.64(15)
O(4)#2-Zn(2)-O(5)	106.48(12)	O(13)-Zn(3)-C(61)	27.07(15)
O(4)#2-Zn(2)-N(4)#3	129.87(13)	N(6)#4-Zn(3)-C(61)	116.29(15)
O(5)-Zn(2)-N(4)#3	106.96(12)	N(5)-Zn(3)-C(61)	96.82(15)
O(4)#2-Zn(2)-N(3)	109.94(11)	O(14)-Zn(3)-C(61)	28.00(14)
O(5)-Zn(2)-N(3)	94.17(12)	O(15)-Zn(4)-O(11)#5	108.97(11)
N(4)#3-Zn(2)-N(3)	103.68(13)	O(15)-Zn(4)-N(7)	128.09(12)
O(4)#2-Zn(2)-C(9)#2	28.80(11)	O(11)#5-Zn(4)-N(7)	106.55(12)
O(5)-Zn(2)-C(9)#2	134.92(13)	O(15)-Zn(4)-N(8)#6	110.06(12)
N(4)#3-Zn(2)-C(9)#2	111.43(13)	O(11)#5-Zn(4)-N(8)#6	92.97(12)
N(3)-Zn(2)-C(9)#2	98.79(12)	N(7)-Zn(4)-N(8)#6	104.52(12)
O(10)-Zn(3)-O(13)	110.54(14)		

[a] Symmetry transformations used to generate equivalent atoms: #1 -x+1, y+1/2, -z+1/2; #2 x, -y+3/2, z+1/2; #3 x, y-1, z; #4 -x, y-1/2, -z+3/2; #5 x, -y+1/2, z-1/2; #6 x, y+1, z; #7 x, -y+3/2, z-1/2; #8 x, -y+1/2, z+1/2; #9 -x+1, y-1/2, -z+1/2; #10 -x, y+1/2, -z+3/2.

Table S3 Selected Bond lengths (Å) and angles (°) for **3**[a]

Zn(1)-N(4)#1	2.022(3)	Zn(1)-O(2)#2	2.401(4)
Zn(1)-O(1)#2	2.028(3)	Zn(2)-O(3)	1.925(3)
Zn(1)-N(2)	2.069(3)	Zn(2)-N(6)	1.991(3)
Zn(1)-N(5)#3	2.144(3)	Zn(2)-N(3)#4	2.030(3)
Zn(1)-O(4)	2.319(3)	Zn(2)-N(1)	2.035(3)
N(4)#1-Zn(1)-O(1)#2	152.12(13)	O(4)-Zn(1)-O(2)#2	93.74(13)
N(4)#1-Zn(1)-N(2)	101.80(11)	N(4)#1-Zn(1)-C(7)#2	124.52(14)
O(1)#2-Zn(1)-N(2)	102.62(12)	O(1)#2-Zn(1)-C(7)#2	29.59(13)
N(4)#1-Zn(1)-N(5)#3	103.14(11)	N(2)-Zn(1)-C(7)#2	132.21(13)
O(1)#2-Zn(1)-N(5)#3	90.23(11)	N(5)#3-Zn(1)-C(7)#2	90.48(12)
N(2)-Zn(1)-N(5)#3	89.75(12)	O(4)-Zn(1)-C(7)#2	87.36(12)
N(4)#1-Zn(1)-O(4)	84.57(10)	O(2)#2-Zn(1)-C(7)#2	28.80(12)
O(1)#2-Zn(1)-O(4)	83.98(11)	O(3)-Zn(2)-N(6)	120.36(12)
N(2)-Zn(1)-O(4)	85.85(11)	O(3)-Zn(2)-N(3)#4	101.30(12)
N(5)#3-Zn(1)-O(4)	171.79(10)	N(6)-Zn(2)-N(3)#4	105.29(12)
N(4)#1-Zn(1)-O(2)#2	97.26(11)	O(3)-Zn(2)-N(1)	120.09(11)
O(1)#2-Zn(1)-O(2)#2	58.32(11)	N(6)-Zn(2)-N(1)	104.71(12)
N(2)-Zn(1)-O(2)#2	160.80(11)	N(3)#4-Zn(2)-N(1)	102.53(13)
N(5)#3-Zn(1)-O(2)#2	88.14(13)		

[a] Symmetry transformations used to generate equivalent atoms: #1 x, y, z+1; #2 x-y, x-1, -z+2; #3 -x+5/3, -y+1/3, -z+4/3; #4 -y+4/3, x-y-1/3, z-1/3; #5 y+1, -x+y+1, -z+2; #6 -x+y+5/3, -x+4/3, z+1/3; #7 x, y, z-1.