Supplementary Material (ESI) for CrystEngComm

The construction of coordination frameworks based on imidazole-based dicarboxylate ligand containing hydroxymethyl group

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Supporting information

Table S1 Selected bond lengths [Å] and angles[°] for the complexes.[a]

Complex **1**

Cd(1)-N(1)	2.266(3)	Cd(1)-O(4)#1	2.355(3)
Cd(1)-N(2)#1	2.307(3)	Cd(1)-N(3)	2.366(3)
Cd(1)-N(4)#2	2.347(3)	Cd(1)-O(1)	2.446(2)
N(1)-Cd(1)-N(2)#1	168.40(10)	N(1)-Cd(1)-N(4)#2	89.93(11)
N(2)#1-Cd(1)-N(4)#2	92.14(11)	N(1)-Cd(1)-O(4)#1	118.42(9)
N(2)#1-Cd(1)-O(4)#1	72.87(9)	N(4)#2-Cd(1)-O(4)#1	93.11(11)
N(1)-Cd(1)-N(3)	90.83(11)	N(2)#1-Cd(1)-N(3)	86.71(11)
N(4)#2-Cd(1)-N(3)	177.83(13)	O(4)#1-Cd(1)-N(3)	88.31(11)
N(1)-Cd(1)-O(1)	72.05(9)	N(2)#1-Cd(1)-O(1)	96.43(9)
N(4)#2-Cd(1)-O(1)	93.34(12)	O(4)#1-Cd(1)-O(1)	167.70(9)
N(3)-Cd(1)-O(1)	84.96(11)		

Complex **2**

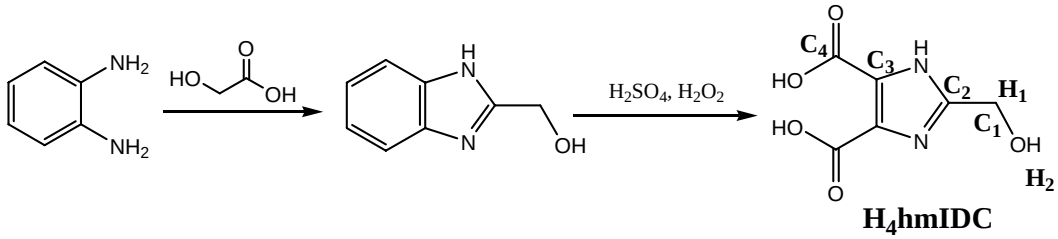
Fe(1)-O(1)#1	2.080(4)	Fe(2)-O(4)	2.072(4)
Fe(1)-O(2)	2.090(4)	Fe(2)-N(2)	2.151(4)
Fe(1)-O(3)	2.107(4)	Fe(2)-O(5)#2	2.240(5)
O(1)#1-Fe(1)-O(1)#2	87.7(3)	O(1)#2-Fe(1)-O(2)	172.34(16)
O(1)#1-Fe(1)-O(2)	84.95(18)	O(2)#3-Fe(1)-O(2)	102.5(2)
O(1)#1-Fe(1)-O(3)	88.74(18)	O(1)#2-Fe(1)-O(3)	95.68(18)
O(2)#3-Fe(1)-O(3)	89.96(16)	O(2)-Fe(1)-O(3)	86.21(15)
O(3)-Fe(1)-O(3)#3	173.9(2)	O(4)#4-Fe(2)-O(4)	180.0(3)
O(4)-Fe(2)-N(2)	78.42(16)	O(4)-Fe(2)-N(2)#4	101.58(16)
N(2)-Fe(2)-N(2)#4	180.00(18)	O(4)-Fe(2)-O(5)#2	85.24(18)
O(4)-Fe(2)-O(5)#5	94.76(18)	N(2)-Fe(2)-O(5)#5	90.26(18)

Complex **3**

Cu(1)-O(1)	1.9733(11)	Cu(1)-N(1)	1.9912(13)
Cu(1)-O(1W)	2.2852(14)	Cu(1)-O(2W)	1.9645(12)
Cu(1)-N(4)#2	1.9983(13)	Cu(2)-N(2)	1.9968(13)
Cu(2)-N(3)	2.0290(13)	Cu(2)-O(6)	1.9756(12)
Cu(2)-O(3)#1	1.9543(11)		
O(3)#1-Cu(2)-O(6)	171.33(5)	O(3)#1-Cu(2)-N(2)	94.35(5)
O(6)-Cu(2)-N(2)	81.72(5)	O(3)#1-Cu(2)-N(3)	94.62(5)
O(6)-Cu(2)-N(3)	88.65(5)	N(2)-Cu(2)-N(3)	169.50(5)
O(3)#1-Cu(2)-O(3W)	90.66(5)	O(6)-Cu(2)-O(3W)	97.46(5)
N(2)-Cu(2)-O(3W)	96.82(5)	N(3)-Cu(2)-O(3W)	88.54(5)
O(2W)-Cu(1)-O(1)	163.17(6)	O(2W)-Cu(1)-N(1)	92.05(5)
O(1)-Cu(1)-N(1)	83.27(5)	O(2W)-Cu(1)-N(4)#2	91.50(5)
O(1)-Cu(1)-N(4)#2	90.55(5)	N(1)-Cu(1)-N(4)#2	169.59(5)
O(2W)-Cu(1)-O(1W)	104.68(5)	O(1)-Cu(1)-O(1W)	91.72(5)
N(1)-Cu(1)-O(1W)	92.70(5)	N(4)#2-Cu(1)-O(1W)	95.85(5)

[a]Symmetry transformations used to generate equivalentatoms: #1 x-1/4,-y+1/4,z-1/4 #2 x-1/4,-y+1/4,z+3/4 for complex **1**; #1 -x+5/2,y+1/2,-z+1/2 #2 x-1/2,y+1/2,z #3 -x+2,y,-z+1/2 #4 -x+3/2,-y+1/2,-z #5 -x+2,-y,-z for complex **2**; #1 -x+1,-y,-z #2 x-3/2,-y+1/2,z+1/2 for complex **3**.

Scheme S1: Synthetic Route of Ligand H_4hmIDC



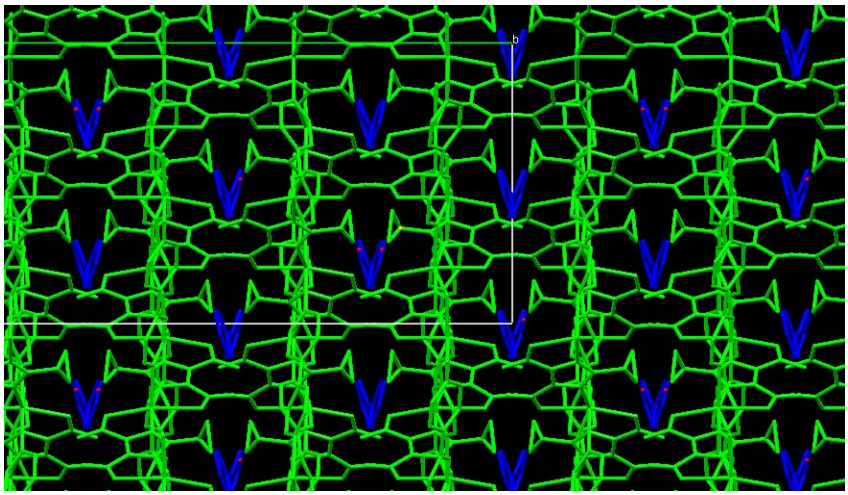


Fig. S1 The small channels in **1**

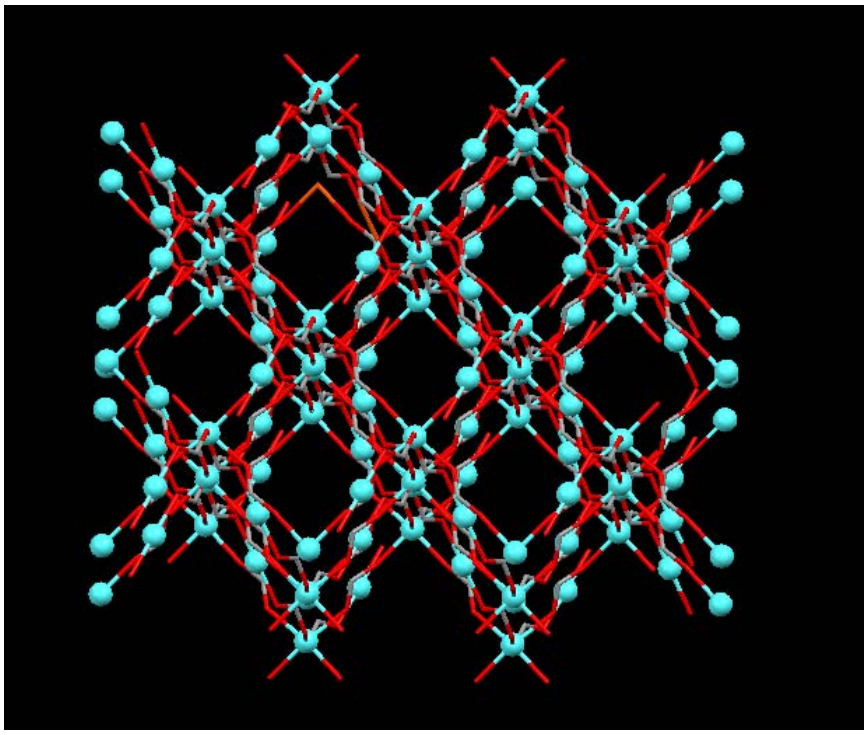


Fig. S2 The link of Fe(III) ions in **2**

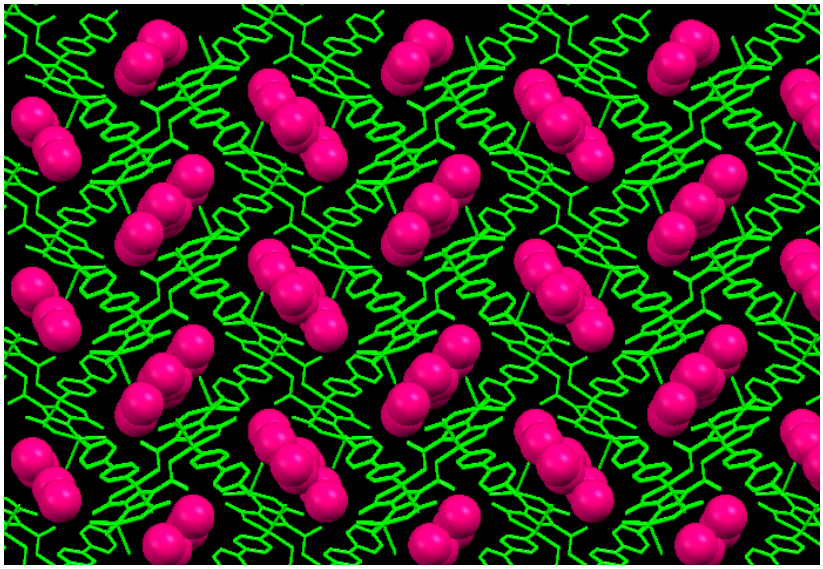


Fig. S3 The small channels in **3**

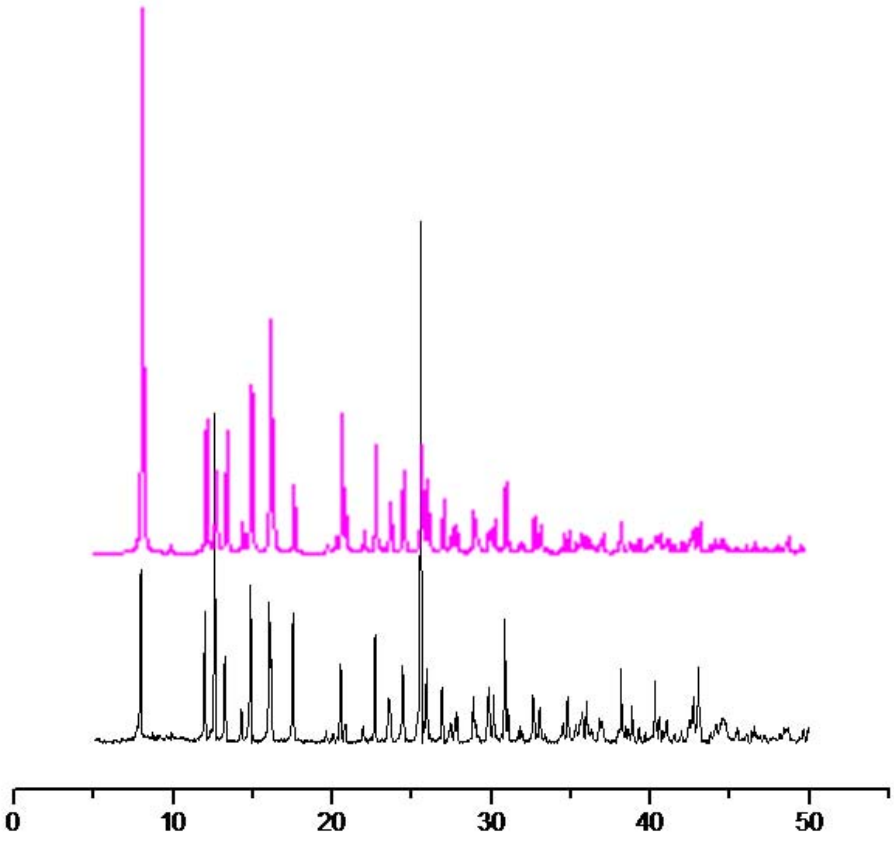


Fig. S4 The simulated X-ray powder diffraction patterns (upper) and the measured one (lower) of complex **1**

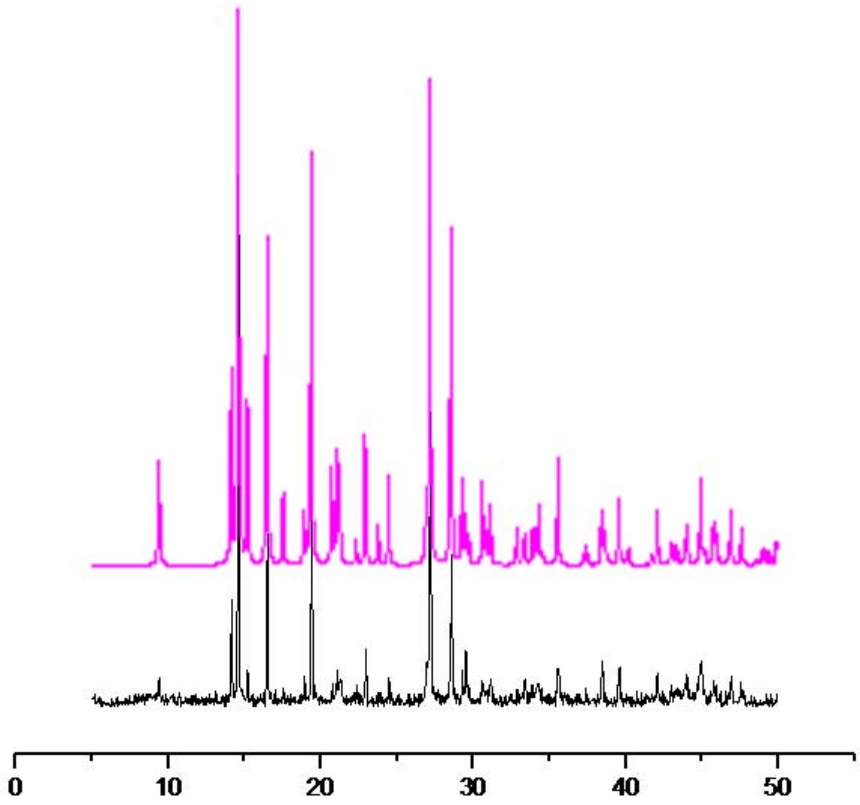


Fig. S5 The simulated X-ray powder diffraction patterns (upper) and the measured one (lower) of complex **2**

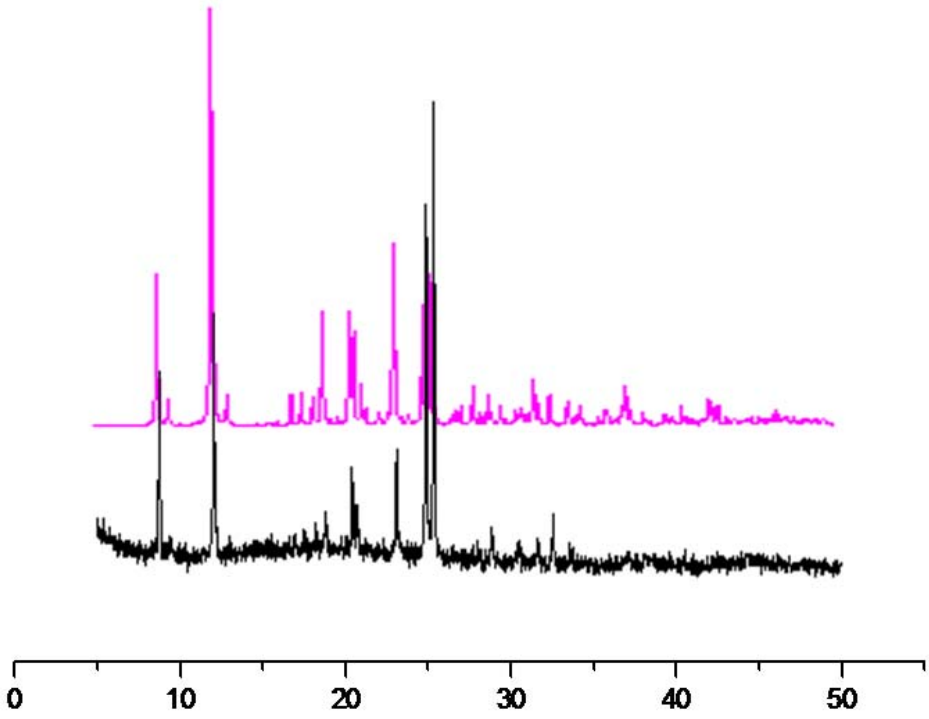


Fig. S6 The simulated X-ray powder diffraction patterns (upper) and the measured one (lower) of complex **3**