Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Functionalities and Architectures of Coordination Polymers with Multi−Dimensionalities *via* Transition Metal−Dicarboxylate Ligands

Xinyu Cao, Ling Li, Changxia Li, Lei, Lv, Rudan Huang*

Key Laboratory of Cluster Science of Ministry of Education, School of Chemistry, Beijing Institute of Technology, Beijing 100081, PR China E-mail: huangrudan1@bit.edu.cn

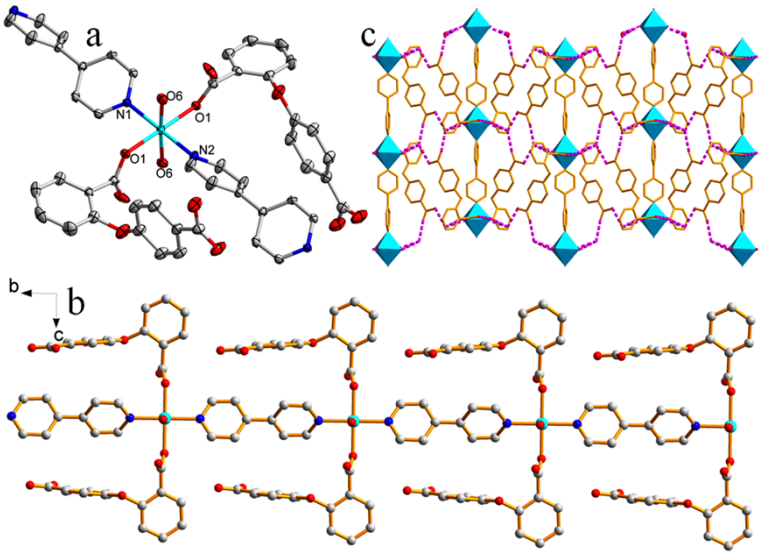

Figure S1. (a) The coordination environment of Ni(II) with the ellipsoids drawn at the 30% probability level. (b) 1D linear chain of **5**, viewed along the *a* axis. (c) 2D supramolecular layer of **5** formed through hydrogen bonding. Hydrogen atoms are omitted for clarity.

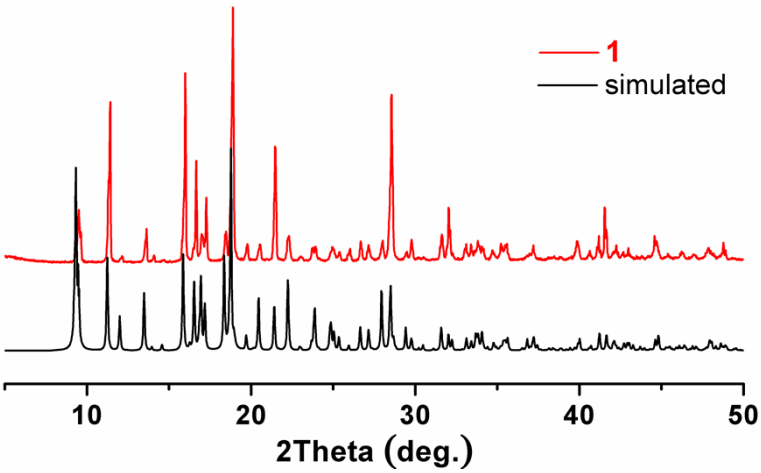

Figure S2. XRPD experimental and calculated patterns for complex **1**.

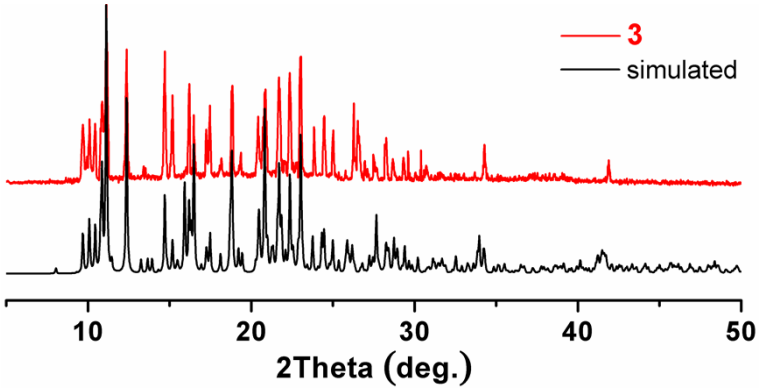

Figure S3. XRPD experimental and calculated patterns for complex **3**.

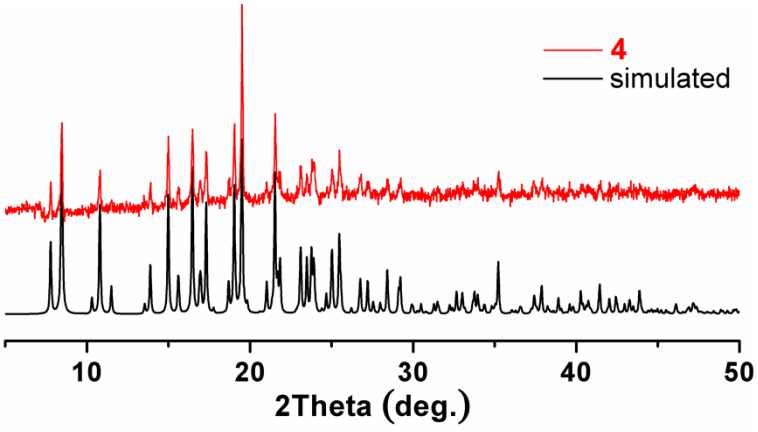

Figure S4. XRPD experimental and calculated patterns for complex **4**.

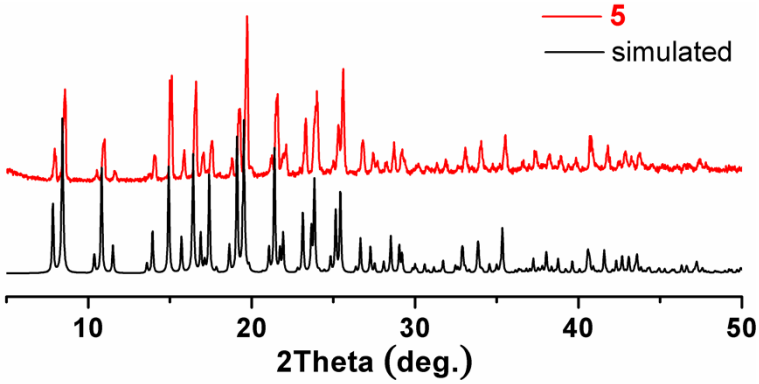

Figure S5. XRPD experimental and calculated patterns for complex **5**.

Proton Conductivity Studies

The presence of many interstitial and coordinated water molecules in the 2D ladder structure of complex **3** suggests the possibility of proton conductivity behaviour. Thus, the AC impedance measurements were carried out by two-probe method using Pt-pressed electrodes in the frequency range above 0.01Hz-1MHz (Figure S6). The solvent molecules in complex **3** were removed above 110 °C. The PXRD studies revealed that no structural change was observed after the removal of water molecules (Figure S7). There is no obvious change of the protonconductivity behaviour before and after the desorption coordination polymers.

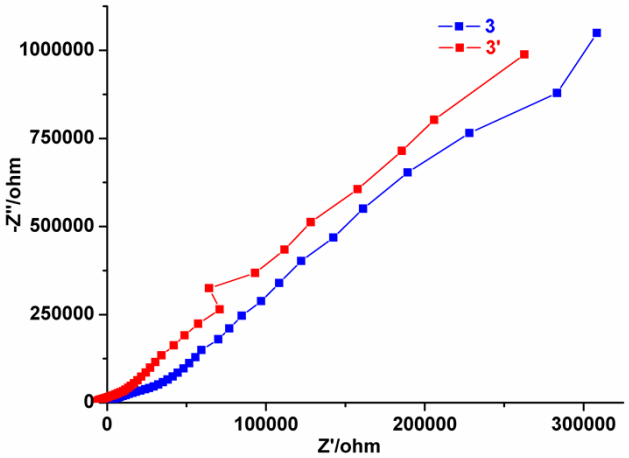

Figure S6. Proton conductivities for complexes **3** and **3'**.

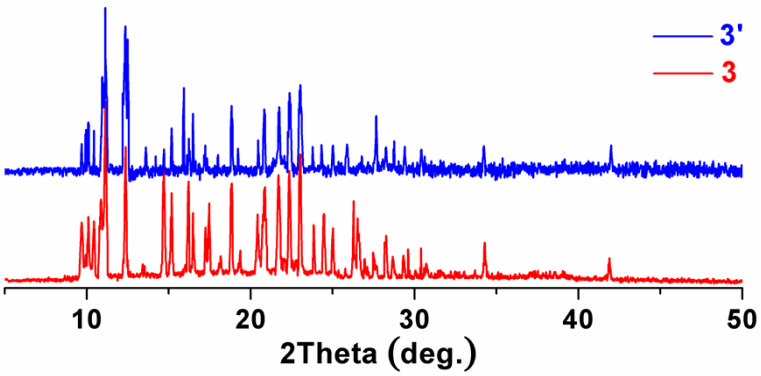

Figure S7. XRPD patterns for complexes **3** and **3'**.

Table S1. Selected Bond Lengths (Å) and Angles (deg) for **1-5**.

1			
Zn(1)-O(3)	1.930(3)	Zn(1)-O(2)#1	1.949(2)
Zn(1)-O(1)	1.974(3)	Zn(1)-N(1)	2.003(3)
Zn(1)-O(4)	2.559(3)		
O(3)-Zn(1)-O(2)#1	116.29(11)	O(3)-Zn(1)-O(1)	102.80(12)
O(2)#1-Zn(1)-O(1)	116.14(11)	O(3)-Zn(1)-N(1)	127.43(12)
O(2)#1-Zn(1)-N(1)	98.93(12)	O(1)-Zn(1)-N(1)	94.05(11)
O(3)-Zn(1)-O(4)	56.13(10)	O(2)#1-Zn(1)-O(4)	86.67(10)
O(1)-Zn(1)-O(4)	155.45(10)	N(1)-Zn(1)-O(4)	90.96(11)
2			
Zn(1)-O(6)	1.956(3)	Zn(1)-N(3)	2.095(4)
Zn(1)-N(1)	2.096(4)	Zn(1)-O(1)	2.155(4)
Zn(1)-O(2)	2.167(4)		
O(6)-Zn(1)-N(3)	98.83(16)	O(6)-Zn(1)-N(1)	100.17(16)
N(3)-Zn(1)-N(1)	94.98(15)	O(6)-Zn(1)-O(1)	159.43(14)
N(3)-Zn(1)-O(1)	91.65(16)	N(1)-Zn(1)-O(1)	96.47(15)
O(6)-Zn(1)-O(2)	104.68(15)	N(3)-Zn(1)-O(2)	149.47(17)
N(1)-Zn(1)-O(2)	99.67(16)	O(1)-Zn(1)-O(2)	60.30(14)
3			
Co(1)-O(1)	2.042(2)	Co(1)-N(3)	2.100(2)
Co(1)-N(1)	2.104(2)	Co(1)-O(6)	2.109(2)
Co(1)-O(7)	2.237(2)	Co(1)-O(2)	2.255(2)
Co(2)-O(8)#1	2.0719(19)	Co(2)-O(8)#2	2.0719(19)
Co(2)-O(11)#3	2.092(2)	Co(2)-O(11)	2.092(2)
Co(2)-N(2)#3	2.191(2)	Co(2)-N(2)	2.191(2)
O(1)-Co(1)-N(3)	100.50(9	O(1)-Co(1)-N(1)	101.62(9)
N(3)-Co(1)-N(1)	95.74(10)	O(1)-Co(1)-O(6)	99.74(9)
N(3)-Co(1)-O(6)	92.31(10)	N(1)-Co(1)-O(6)	155.35(9)
O(1)-Co(1)-O(7)	157.80(8)	N(3)-Co(1)-O(7)	90.08(9)
N(1)-Co(1)-O(7)	96.62(9)	O(6)-Co(1)-O(7)	60.04(8)
O(1)-Co(1)-O(2)	61.07(8)	N(3)-Co(1)-O(2)	161.57(9)
N(1)-Co(1)-O(2)	88.24(9)	O(6)-Co(1)-O(2)	91.43(9)
O(7)-Co(1)-O(2)	107.38(8)	O(8)#1-Co(2)-O(8)#2	180.00(7)
O(8)#1-Co(2)-O(11)#3	88.54(8)	O(8)#2-Co(2)-O(11)#3	91.46(8)
O(8)#1-Co(2)-O(11)	91.46(8)	O(8)#2-Co(2)-O(11)	88.54(8)
O(11)#3-Co(2)-O(11)	180.00(10)	O(8)#1-Co(2)-N(2)#3	90.09(9)
O(8)#2-Co(2)-N(2)#3	89.91(9)	O(11)#3-Co(2)-N(2)#3	94.41(9)
O(11)-Co(2)-N(2)#3	85.59(9)	O(8)#1-Co(2)-N(2)	89.91(9)
O(8)#2-Co(2)-N(2)	90.09(9)	O(11)#3-Co(2)-N(2)	85.59(9)
O(11)-Co(2)-N(2)	94.41(9)	N(2)#3-Co(2)-N(2)	180.00(12)
4			
Co(1)-O(6)	2.1035(17)	Co(1)-O(6)#1	2.1035(17)
Co(1)-O(1)	2.1127(17)	Co(1)-O(1)#1	2.1127(17)

Co(1)-N(2)	2.139(3)	Co(1)-N(1)	2.153(3)
O(6)-Co(1)-O(6)#1	174.92(10)	O(6)-Co(1)-O(1)	88.05(7)
O(6)#1-Co(1)-O(1)	91.95(7)	O(6)-Co(1)-O(1)#1	91.95(7)
O(6)#1-Co(1)-O(1)#1	88.05(7)	O(1)-Co(1)-O(1)#1	179.96(9)
O(6)-Co(1)-N(2)	87.46(5)	O(6)#1-Co(1)-N(2)	87.46(5)
O(1)-Co(1)-N(2)	90.02(5)	O(1)#1-Co(1)-N(2)	90.02(5)
O(6)-Co(1)-N(1)	92.54(5)	O(6)#1-Co(1)-N(1)	92.54(5)
O(1)-Co(1)-N(1)	89.98(5)	O(1)#1-Co(1)-N(1)	89.98(5)
N(2)-Co(1)-N(1)	180.0		
5			
Ni(1)-O(6)#1	2.062(2)	Ni(1)-O(6)	2.062(2)
Ni(1)-N(2)#2	2.083(4)	Ni(1)-O(1)#1	2.084(2)
Ni(1)-O(1)	2.084(2)	Ni(1)-N(1)	2.110(4)
O(6)#1-Ni(1)-O(6)	174.74(14)	O(6)#1-Ni(1)-N(2)#2	87.37(7)
O(6)-Ni(1)-N(2)#2	87.37(7)	O(6)#1-Ni(1)-O(1)#1	87.61(10)
O(6)-Ni(1)-O(1)#1	92.40(10)	N(2)#2-Ni(1)-O(1)#1	90.08(7)
O(6)#1-Ni(1)-O(1)	92.40(10)	O(6)-Ni(1)-O(1)	87.61(10)
N(2)#2-Ni(1)-O(1)	90.08(7)	O(1)#1-Ni(1)-O(1)	179.85(13)
O(6)#1-Ni(1)-N(1)	92.63(7)	O(6)-Ni(1)-N(1)	92.63(7)
N(2)#2-Ni(1)-N(1)	180.000(1)	O(1)#1-Ni(1)-N(1)	89.92(7)
O(1)-Ni(1)-N(1)	89.92(7)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z #2 -x+3/2,y-1/2,-z+1/2 #3 -x+3/2,y+1/2,-z+1/2 #4 -x,-y-1,-z for **1**; #1 -x+1,-y+1,-z+1 #2 x+1,y,z-1#3 -x+2,-y+1,-z #4 x-1,y,z+1 #5 -x,-y+1,-z+1 for **3**; #1 -x+1/2,y,-z+1/2 #2 x,y+1,z #3 x,y-1,z for **4**; #1 -x+3/2,y,-z+3/2 #2 x,y+1,z #3 x,y-1,z for **5**.

Table S2 Hydrogen bonding interactions in H_2dpd and **1**−**5**

D−H···A	d(D···A) (Å)	∠D-H···A(°)
2		
O(4)−H(4)···O(11)	2.5598	170
O(8)−H(8)···N(2)	2.6909	173
O(11)−H(11C)···O(7)	2.7658	178
O(11)−H(11D)···N(4)	2.8186	177
3		
O(3)−H(3)···O(7)	2.6150	141
O(12)−H(12C)···O(1)	2.9938	178
O(12)−H(12D)···O(9)	2.8240	178
4		
O(4)−H(4)···O(7)	2.6507	174
O(6)−H(6C)···O(7)	2.9363	148
O(7)−H(7C)···O(1)	2.7387	177
O(7)−H(7D)···O(3)	2.8772	177
5		
O(4)−H(4)···O(7)	2.6423	173
O(6)−H(6B)···O(7)	2.9166	149

O(7)−H(7C)···O(1)	2.7468	177
O(7)−H(7C)···O(6)	2.9166	104
O(7)−H(7D)···O(3)	2.8486	177