Electronic Supplementary Material for CrystEngComm

Supporting information

Cadmium(II) coordination polymers with flexible tetradentate ligand 1,2,4,5-tetrakis(imidazol-1-ylmethyl)benzene: anion effect and reversible anion exchange property

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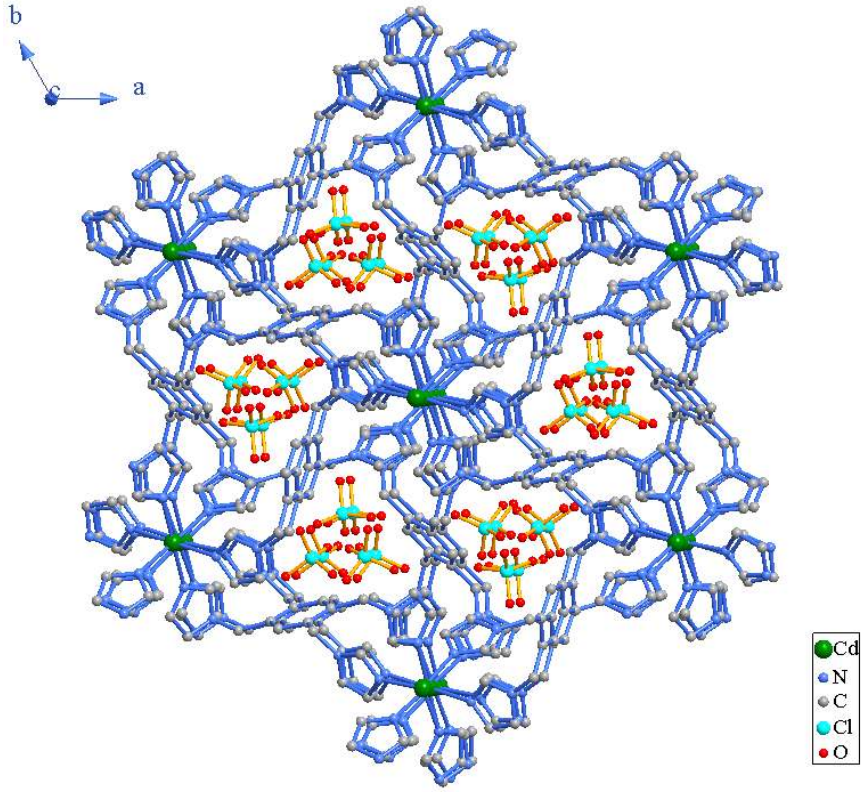


Figure S1. The 3D framework structure of **2** with the perchlorate anions filled in the 1D channels.

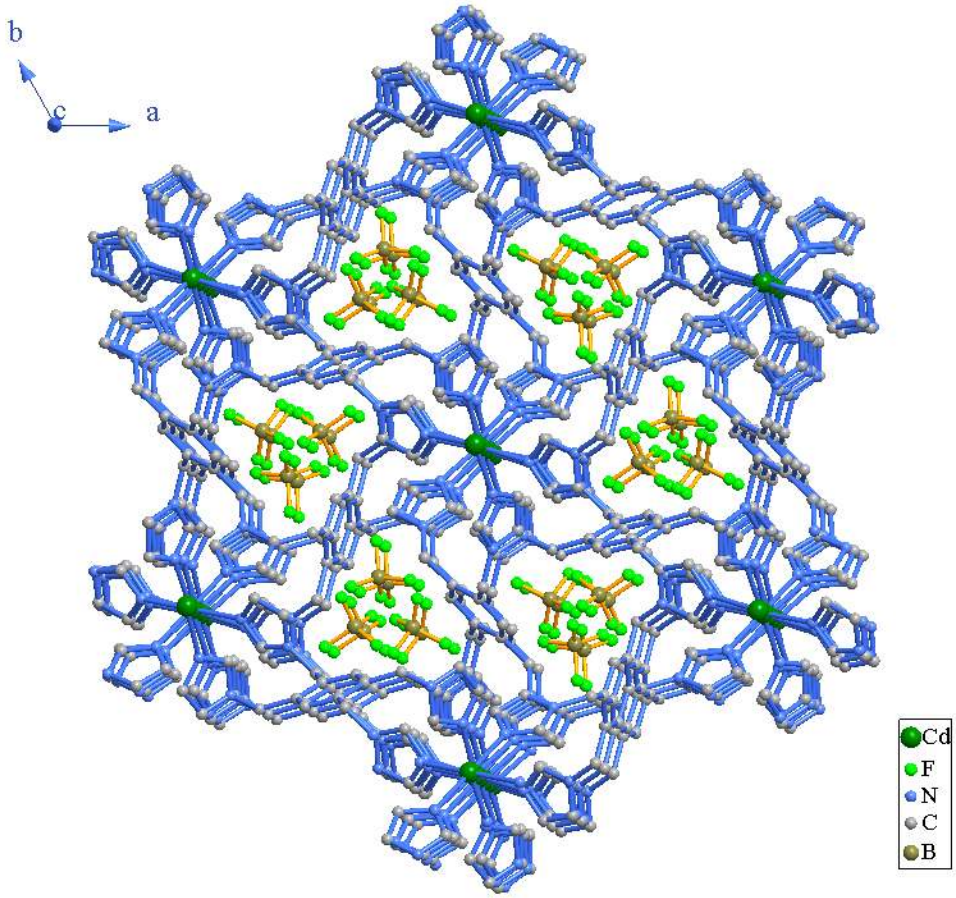


Figure S2. The 3D framework structure of **3** with the tetrafluoroborate anions filled in the 1D channels.

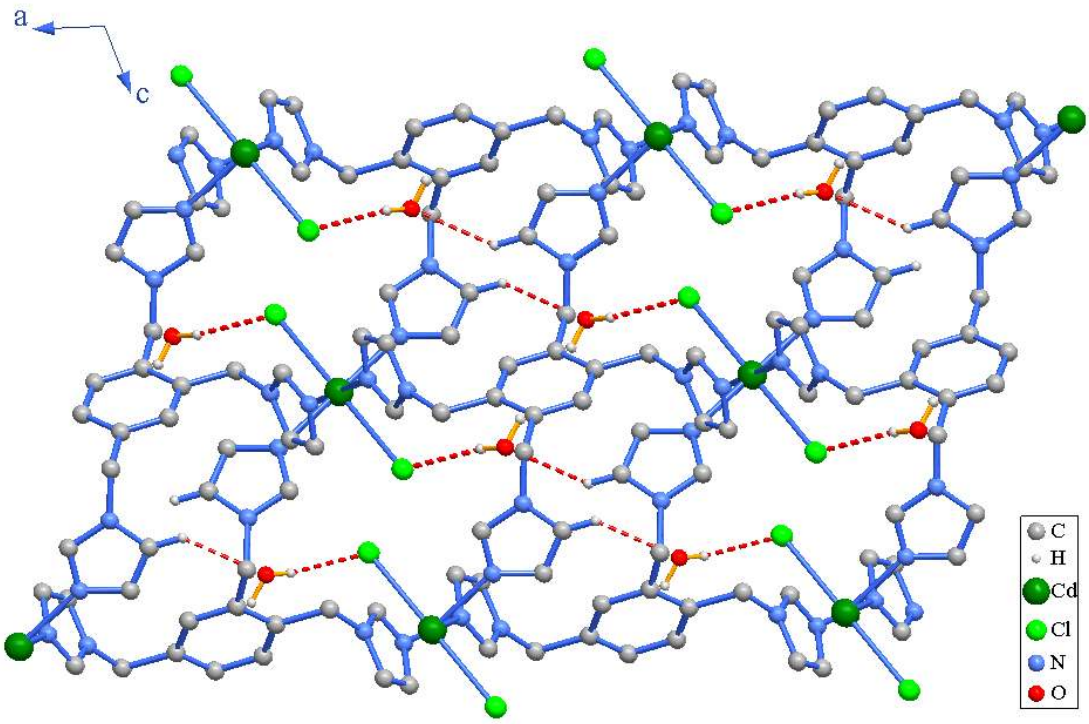


Figure S3. The intermolecular hydrogen bonds in the 3D framework of **4** indicated in the red dashed lines.

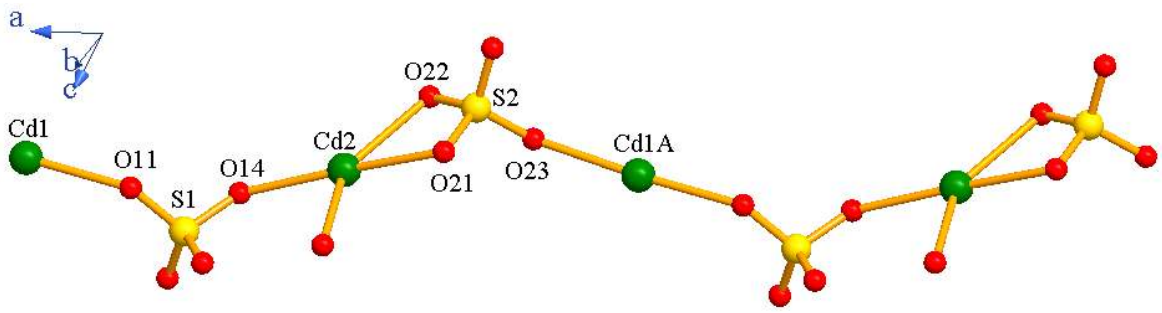
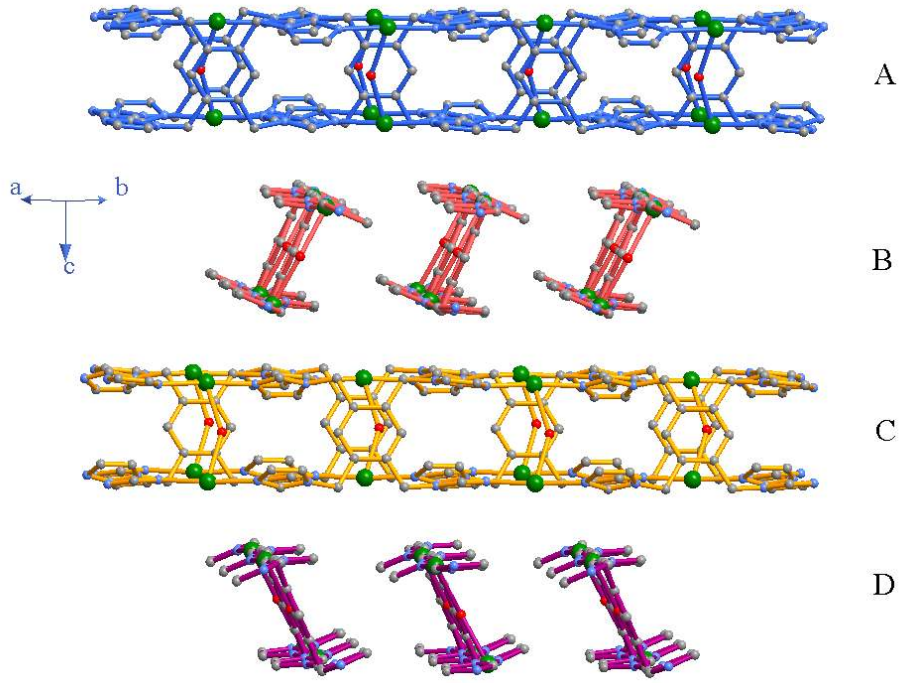
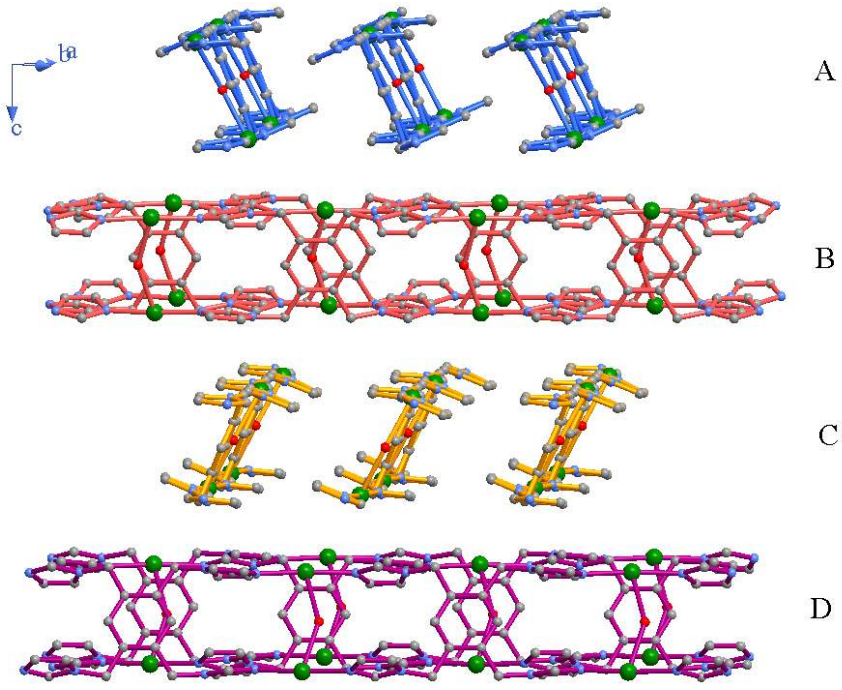


Figure S4. In **5**, if the coordination interactions of Cd(II) atoms with imidazole groups are ignored, the Cd1(II) and Cd(II) atoms are linked together by sulfate anions to give an infinite 1D chain A, the sulfate anions have two different kinds of coordination modes.



(a)



(b)

Figure S5. Different views of the four 1D polymeric chains extended in different directions.

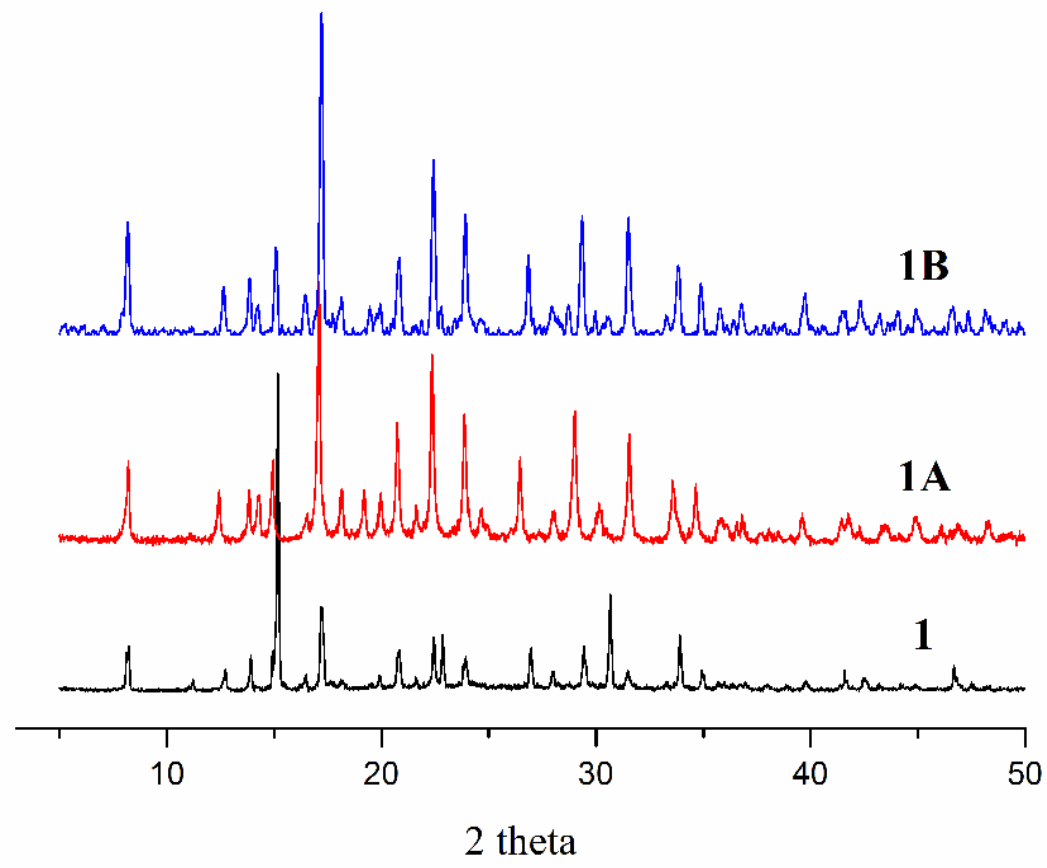


Figure S6. The X-ray powder diffraction patterns of complex **1**, exchanged product **1A** and reversed exchanged product **1B**.

Table S1. Distance (Å) and angles (deg) of hydrogen bonds for the complexes **1-6**

D-H···A	Distance (H···A)	Distance (D···A)	Angle (D-H-A)
Complex **1**			
C4-H4A···O1#1	2.49	3.44(2)	164
C7-H7A···O3#2	2.39	3.19(3)	144
C8-H8A···N1#3	2.55	3.216(9)	126
C11-H11A···O1W#2	2.53	3.31(3)	142
Complex **2**			
C3-H1···O13#4	2.59	3.259(10)	127
C11-H2···O13#5	2.53	3.146(12)	120
C11-H3···N21	2.52	3.214(6)	127
C21-H7···O12#5	2.58	3.510(10)	156
C21-H8···O14#6	2.50	3.411(8)	154
C24-H11···O14#4	2.59	3.518(8)	164
Complex **3**			
C11-H2···F4#7	2.45	3.365(6)	153
C11-H3···F1#2	2.54	3.473(9)	156
C21-H7···N11	2.53	3.213(5)	126
Complex **4**			
O1W-H1WB···Cl1#8	2.32	3.128(10)	160
C9-H9···O1W#9	2.43	3.199(11)	140
Complex **5**			
O1-H1···N122#10	1.88(3)	2.719(3)	174(3)
O1-H2···O13	1.75(3)	2.633(4)	168(3)
O2-H3···N152	1.98(3)	2.779(4)	167(3)
O2-H4···O14	1.93(3)	2.695(3)	172(3)
O3-H5···O22	2.10(4)	2.870(3)	165(3)
O3-H6···O2	2.00(4)	2.851(3)	179(5)

C6-H8···O12	2.51	3.416(3)	158
C11-H10···O2#11	2.49	3.252(3)	133
C12-H11···O2	2.51	3.397(4)	156
C22-H16···O2#11	2.50	3.434(4)	169
C23-H17···O24#12	2.44	3.347(4)	160
C41-H19···O1#13	2.37	3.261(3)	149
C42-H21···O21#14	2.42	3.279(3)	150
C52-H26···O21#13	2.37	3.267(3)	157
C54-H28···O12	2.43	3.151(3)	133
C111-H31···O13#13	2.59	3.506(3)	154
C121-H37···O13#13	2.23	3.168(4)	159
C143-H44···O24#15	2.45	3.362(4)	161
C144-H45···O3#12	2.42	3.312(3)	157
Complex **6**			
O1-H1---O13	1.99(3)	2.753(3)	163(3)
O2-H2---O14#16	2.04(3)	2.837(3)	174(3)
O2-H3---O3#17	2.07(4)	2.790(3)	161(4)
O3-H4---O13	2.02(2)	2.866(3)	175(3)
O3-H5---O11#18	2.02(2)	2.865(3)	170(3)
O4-H6---O14#18	2.07(3)	2.991(4)	171(4)
O4-H7---O3	2.26(4)	3.069(4)	149(3)
C21-H15---O12#14	2.55	3.443(4)	151
C22-H17---O3#14	2.50	3.408(4)	159
C23-H18---O14#19	2.44	3.357(4)	161
C24-H19---O4	2.50	3.225(4)	133

Symmetry transformations used to generate equivalent atoms: #1: -1/3+y, 1/3-x+y, -2/3-z. #2: 1/3-x+y, 2/3-x, -1/3+z. #3: 1/3-x, 2/3-y, -4/3-z. #4: 1/3-x, 2/3-y, 2/3-z. #5: -x+y, -x, z. #6: y, -x+y, 1-z. #7: -1/3+y, 1/3-x+y, 1/3-z. #8: x, 3/2-y, -1/2+z. #9: 1+x, 3/2-y, 1/2+z. #10: 1+x, -1+y, z. #11: 1-x, 1-y, -z. #12: -x, 1-y, -z. #13: -x, 1-y, 1-z. #14: x, 1+y, z. #15: -1+x, 1+y, z. #16: y, x, -z. #17: -1+x, y, z. #18: 1/2+x, 1/2-y, 1/4-z. #19: 1+x, 1+y, z.