Supporting information

Structure diversity and reversible anion exchange properties of cadmium(II) complexes with 1,3,5-tris(imidazol-1-ylmethyl)benzene: counteranion-directed flexible ligand conformational variation

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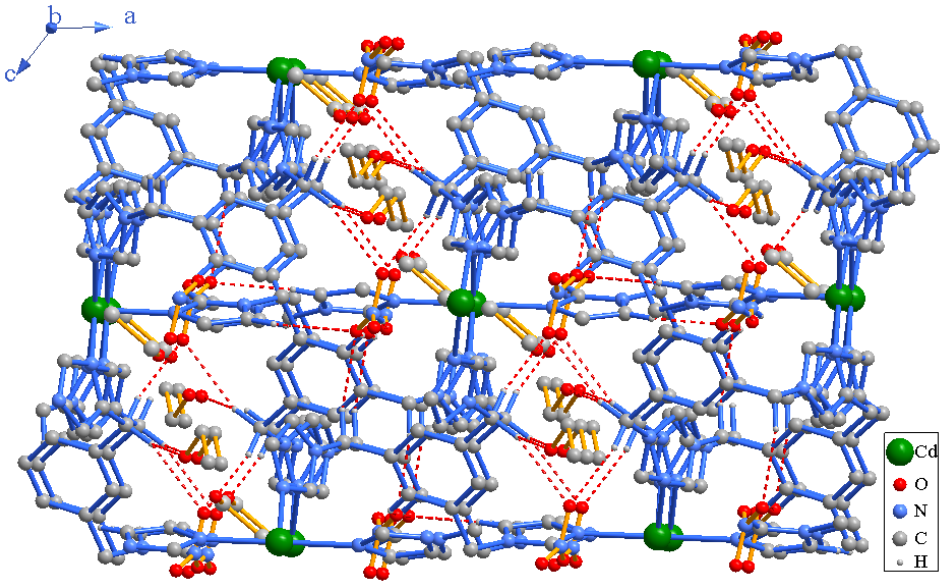

Fig. S1. The ethanol molecules and nitrate anions were filled in channels of the 3D framework of **2**.

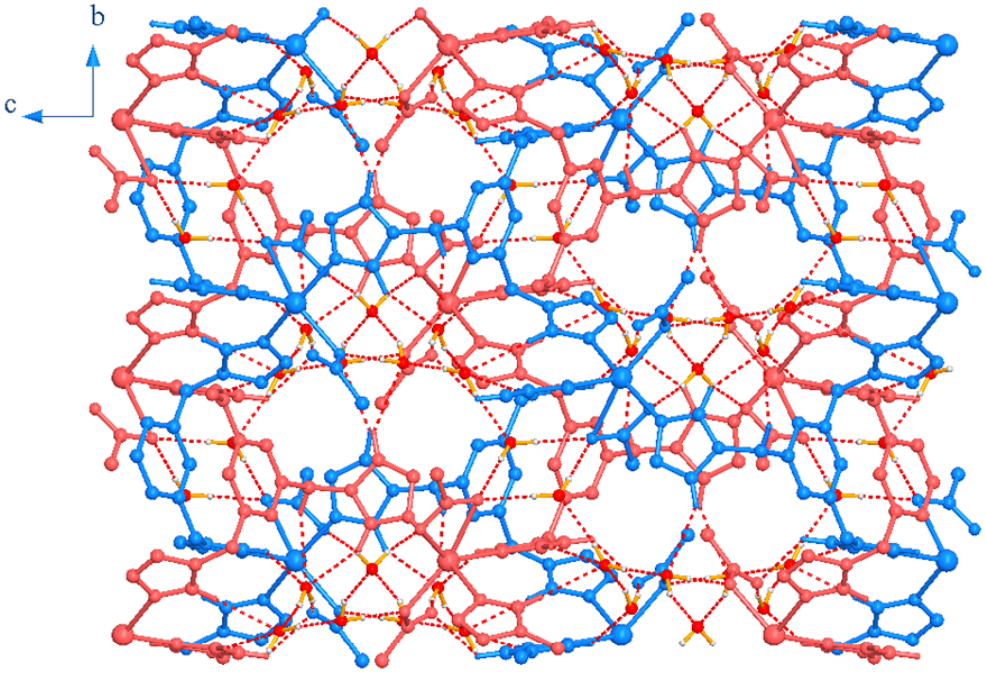

Fig. S2. Crystal packing diagram of **3** with the hydrogen bonds indicated by the dashed lines.

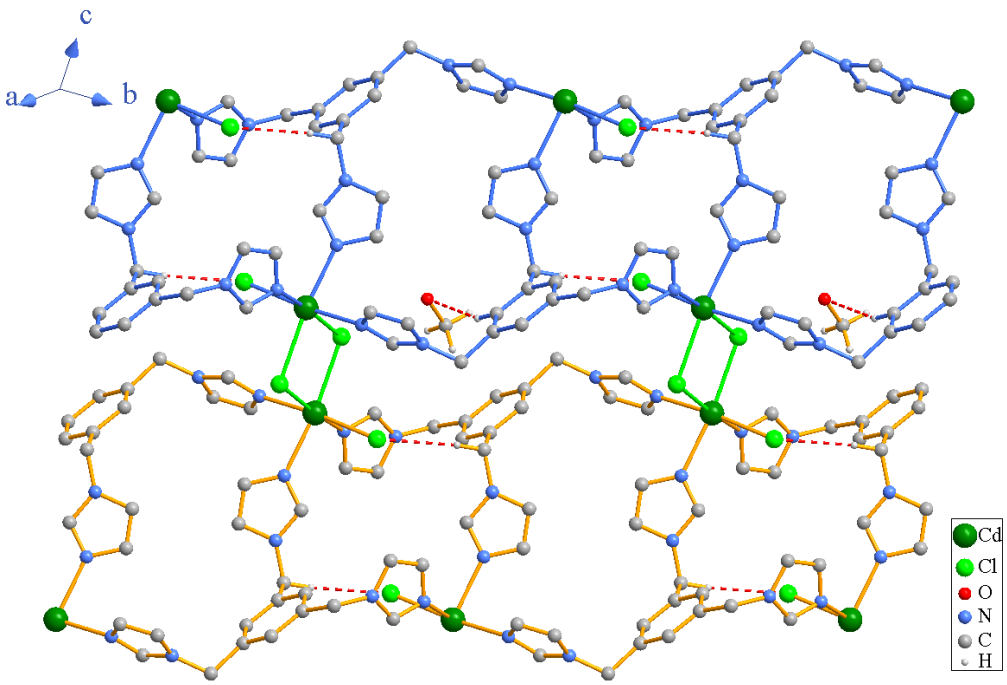

Fig. S3. The intermolecular hydrogen bonds in the 2D network of **4.**

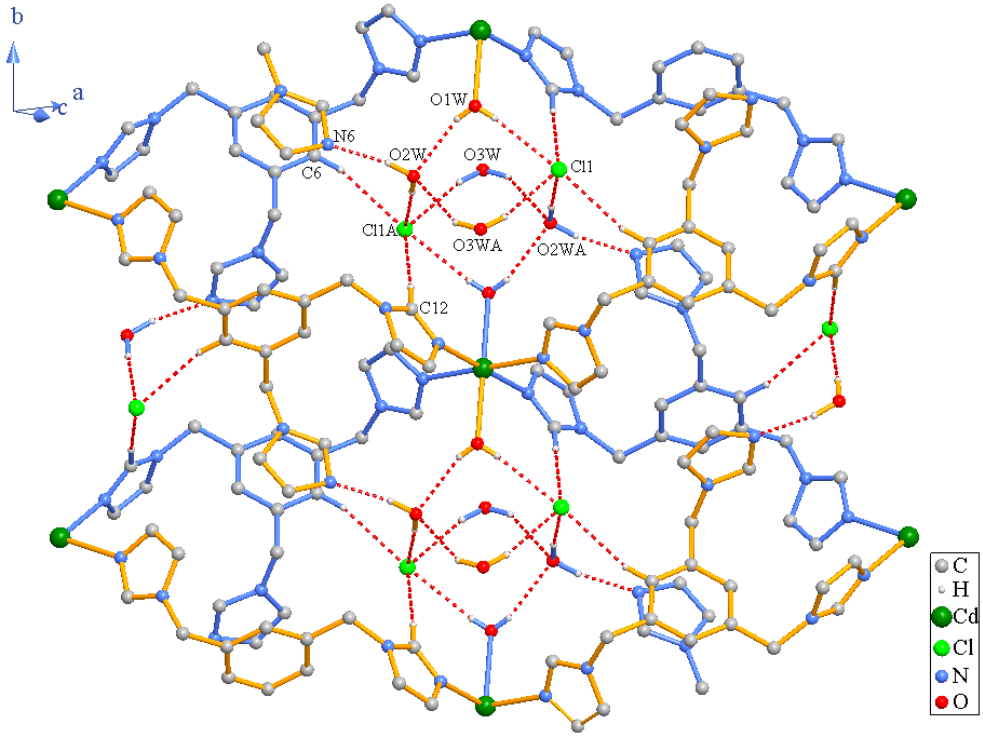

Fig. S4. The hydrogen bonds within the 2D network of **5** indicate in the red dashed lines.

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

D-H---A	Distance (H---A)	Distance (D---A)	Angle (D-H---A)
Complex **1**			
C1-H1---F1#1	2.4900	3.336(4)	152
C4-H4B---F2#2, 3, 4	2.4800	3.275(4)	139
Complex **2**			
C6-H3---O11#5	2.5700	3.242(11)	128
C11-H5---O11#6	2.5200	3.383(10)	146
C31-H9---O13#7	2.2100	3.109(17)	151
C31-H10---O13	2.6000	3.550(18)	161
C31-H10---O22	2.6000	3.31(2)	128
C52-H16---O12	2.2400	3.133(9)	156
C54-H18---O11#5	2.4700	3.325(17)	150
Complex **3**			
O5-H25---O1	1.79(3)	2.690(2)	168(3)
O6-H26---O2	2.01(3)	2.872(3)	175(3)
O6-H27---O2#8	2.12(3)	2.927(3)	175(2)
O7-H28---O9	1.85(4)	2.726(3)	175(3)
O7-H29---O6#9	2.08(3)	2.858(3)	171(4)
O8-H30---O4	2.03(4)	2.866(3)	159(3)
O8-H31---O7#10	2(4)	2.849(3)	163(4)
O9-H32---O5	2.11(4)	2.825(3)	154(4)
O9-H32---O5	2.11(4)	2.825(3)	154(4)
O9-H33---O3	1.76(4)	2.694(3)	175(4)
C12-H6---O8	2.5100	3.365(3)	151
C13-H7---O7#11	2.5600	3.417(3)	151
C14-H8---O4#12	2.4900	3.137(3)	125

C32-H11---O7#13	2.4500	3.282(3)	146
C51-H14---O8#14	2.5700	3.392(3)	141
C52-H16---O8#14	2.4200	3.218(4)	141
C54-H18---O9#12	2.5600	3.371(4)	144
Complex **4**			
C4-H4A---O1#15	2.6000	3.462(9)	155
C11-H11A---Cl2	2.7200	3.664(7)	166
Complex **5**			
O1W-H1WA---Cl1	2.48(4)	3.160(4)	170(4)
O1W-H1WB---O2W#16	2.18(6)	2.812(6)	160(7)
O2W-H2WB---Cl1#17	2.29(6)	3.164(4)	176(5)
O2W-H2WA---N6#18	1.91(4)	2.769(6)	169(5)
O3W-H3WA---Cl1#19	2.32(5)	3.191(6)	167(6)
O3W-H3WB---O2W#20	2.16(5)	2.955(7)	151(6)
C6-H6---Cl1#15	2.6600	3.568(4)	165
C12-H12---Cl1#17	2.6100	3.541(4)	177
C7-H7B---Cl1#21	2.7800	3.668(4)	152
C10-H10---O3W#22	2.5900	3.375(7)	143
Complex **6**			
C34-H13---I2	3.110	3.969	151
C52-H16---I2#23	3.066	3.896	147
C32-H11---I3#23	3.171	3.792	125

Symmetry transformations used to generate equivalent atoms: #1: 1+x, y, z. #2: 2/3-x, 1/3-y, 1/3-z. #3: 2/3+y, 1/3-x+y, 1/3-z. #4: 2/3+x-y, 1/3+x, 1/3-z. #5: 3/2-x, 1/2+y, 3/2-z. #6: -1/2+x, 3/2-y, -1/2+z. #7: 3/2-x, 3/2-y, 1-z. #8: 3/2-x, 1/2-y, 1-z. #9: x, 1-y, 1/2+z. #10: 1-x, y, 3/2-z. #11: x, 1-y, -1/2+z. #12: 1-x, 1-y, 1-z. #13: -1/2+x, 1/2-y, -1/2+z. #14: 1/2-x, 1/2-y, 1-z. #15: x, -1+y, z. #16: -1+x, 3/2-y, -1/2+z. #17: 1-x, -1/2+y, 1/2-z. #18: x, 1+y, z. #19: 1+x, -1+y, z. #20: x, 1/2-y, -1/2+z. #21: -x, -1/2+y, 1/2-z. #22: 1-x, 1/2+y, 1/2-z. #23: -1+x, y, z.