Electronic supplementary information

Cadmium(II) Complexes with 3,5-Di(1H-imidazol-1-yl)benzoate: Topological and Structural Diversity Tuned by Counteranions

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Table S1 Selected Bond Lengths (Å) and Bond Angles (º) for Complexes **1 - 4**

1

Cd(1)-O(2)#1	2.375(4)	Cd(1)-N(3)#2	2.251(5)
Cd(1)-O(3)	2.401(4)	Cd(1)-N(1)	2.266(5)
Cd(1)-O(1)#1	2.406(4)	Cd(1)-O(4)	2.300(4)
N(1)-Cd(1)-O(3)	87.78(17)	N(3)#2-Cd(1)-N(1)	100.96(19)
O(4)-Cd(1)-O(3)	55.44(15)	N(3)#2-Cd(1)-O(4)	134.77(18)
O(2)#1-Cd(1)-O(3)	142.57(14)	N(1)-Cd(1)-O(4)	102.16(17)
N(3)#2-Cd(1)-O(1)#1	87.65(17)	N(3)#2-Cd(1)-O(2)#1	128.20(17)
N(1)-Cd(1)-O(1)#1	145.37(17)	N(1)-Cd(1)-O(2)#1	94.95(17)
O(4)-Cd(1)-O(1)#1	94.63(15)	O(4)-Cd(1)-O(2)#1	87.67(16)
O(2)#1-Cd(1)-O(1)#1	55.36(15)	N(3)#2-Cd(1)-O(3)	87.42(17)
O(3)-Cd(1)-O(1)#1	126.37(16)		

2

Cd(1)-O(1)	2.350(3)	Cd(1)-O(2)	2.1919(15)
Cd(1)-N(1)#3	2.281(4)		
O(2)#4-Cd(1)-O(2)	180.0	N(1)#5-Cd(1)-O(1)	91.02(13)
O(2)-Cd(1)-N(1)#3	91.21(11)	N(1)#3-Cd(1)-N(1)#5	180.0

O(2)-Cd(1)-N(1)#5	88.79(11)	O(2)-Cd(1)-O(1)	95.61(10)
O(2)#4-Cd(1)-O(1)	84.39(10)	O(1)-Cd(1)-O(1)#4	180.0
N(1)#3-Cd(1)-O(1)	88.98(13)		

3

Cd(1)-N(3)#10	2.250(6)	Cd(1)-O(6)	2.266(5)
Cd(1)-O(3)	2.335(6)	Cd(1)-O(10)	2.368(5)
Cd(1)-O(2)	2.397(5)	Cd(1)-O(1)	2.532(5)
Cd(1)-O(4)	2.563(5)	Cd(2)-N(1)#6	2.235(6)
Cd(2)-N(7)#7	2.283(6)	Cd(2)-N(5)#8	2.320(7)
Cd(2)-O(7)#9	2.337(5)	Cd(2)-O(5)	2.390(5)
Cd(2)-O(7)	2.431(5)		
N(3)#10-Cd(1)-O(6)	93.6(2)	N(3)#10-Cd(1)-O(3)	142.7(2)
O(6)-Cd(1)-O(3)	81.1(2)	N(3)#10-Cd(1)-O(10)	92.6(2)
O(6)-Cd(1)-O(10)	168.1(2)	O(3)-Cd(1)-O(10)	87.9(2)
N(3)#10-Cd(1)-O(2)	85.4(2)	O(6)-Cd(1)-O(2)	105.2(2)
O(3)-Cd(1)-O(2)	131.72(19)	O(10)-Cd(1)-O(2)	85.43(18)
N(3)#10-Cd(1)-O(1)	136.9(2)	O(6)-Cd(1)-O(1)	87.79(19)
O(3)-Cd(1)-O(1)	80.06(18)	O(10)-Cd(1)-O(1)	94.58(18)
O(2)-Cd(1)-O(1)	53.04(17)	N(3)#10-Cd(1)-O(4)	89.9(2)
O(6)-Cd(1)-O(4)	86.1(2)	O(3)-Cd(1)-O(4)	53.04(18)
O(10)-Cd(1)-O(4)	83.76(19)	O(2)-Cd(1)-O(4)	168.01(18)
O(1)-Cd(1)-O(4)	133.08(18)	N(1)#6-Cd(2)-N(7)#7	177.8(2)
N(1)#6-Cd(2)-N(5)#8	95.9(2)	N(7)#7-Cd(2)-N(5)#8	82.5(2)
N(1)#6-Cd(2)-O(7)#9	96.8(2)	N(7)#7-Cd(2)-O(7)#9	85.3(2)
N(5)#9-Cd(2)-O(7)#9	120.3(2)	N(1)#6-Cd(2)-O(5)	89.9(2)
N(7)#7-Cd(2)-O(5)	88.4(2)	N(5)#8-Cd(2)-O(5)	81.5(2)
O(7)#9-Cd(2)-O(5)	156.11(19)	N(1)#6-Cd(2)-O(7)	88.6(2)
N(7)#7-Cd(2)-O(7)	92.6(2)	N(5)#8-Cd(2)-O(7)	164.3(2)
O(7)#9-Cd(2)-O(7)	73.81(17)	O(5)-Cd(2)-O(7)	83.51(19)

4

Cd(1)-N(5)	2.283(3)	Cd(1)-N(7)#11	2.289(3)
Cd(1)-N(1)	2.331(3)	Cd(1)-N(3)#12	2.362(3)
Cd(1)-O(1)#13	2.441(3)		

N(5)-Cd(1)-N(7)#11	97.46(11)	N(5)-Cd(1)-N(1)	146.96(11)
N(7)#11-Cd(1)-N(1)	95.94(10)	N(5)-Cd(1)-N(3)#12	85.32(12)
N(7)#11-Cd(1)-N(3)#12	173.18(11)	N(1)-Cd(1)-N(3)#12	84.87(11)
N(5)-Cd(1)-O(1)#13	133.56(10)	N(7)#11-Cd(1)-O(1)#13	81.81(10)
N(1)-Cd(1)-O(1)#13	78.23(10)	N(3)#12-Cd(1)-O(1)#13	91.76(11)

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

Table S2 Hydrogen bonding distances (Å) and angles (º) for complexes **1**-**4**

D – H ··· A / D ··· A	*d*(D-H)	*d*(H ···A)	*d*(D ···A)	∠(D – H ··· A)
		Complex **1**		
C10 - H10 ··· O4#1	0.93	2.52	3.360(8)	150
C8 - H8 ··· O3#2	0.93	2.49	3.272(9)	142
O5 ··· O3#3			2.814	
O5 ··· O1			2.912	
		Complex **2**		
C4 - H4A ··· O3#4	0.93	2.42	3.348(7)	180
C6 - H6A ··· O3#4	0.93	2.37	3.269(5)	161
O2 ··· O3			2.535	
		Complex **3**		
C10 - H10 ··· O7#5	0.93	2.59	3.198(11)	124
C10 - H10 ··· O8#5	0.93	2.44	3.344(12)	166
C17 - H17 ··· O12	0.93	2.47	3.344(11)	157
O4 ··· O12#6			2.941	
O10 ··· O3#7			2.765	
O10 ··· O1#7			2.765	
O10 ··· O14#8			2.784	
O5 ··· O1			2.848	
O5 ··· O13			2.986	
O2 ··· O11			3.002	
O15 ··· O4#9			2.832	
		Complex **4**		
C9 - H9 ··· O5#10	0.93	2.49	3.385(5)	161
C10 - H10 ··· O1#11	0.93	2.41	2.942(4)	117
C15 - H15 ··· O5#12	0.93	2.38	3.296(5)	168
C20 - H20 ··· O5#12	0.93	2.53	3.445(5)	168
C23 - H23 ··· O2#11	0.93	2.58	3.161(5)	121
C25 - H25 ··· O3#13	0.93	2.34	2.982(5)	126
C25 - H25 ··· O4#13	0.93	2.45	3.267(5)	147
O5 ··· O3#14			2.749	
O5 ··· O4#12			2.910	

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

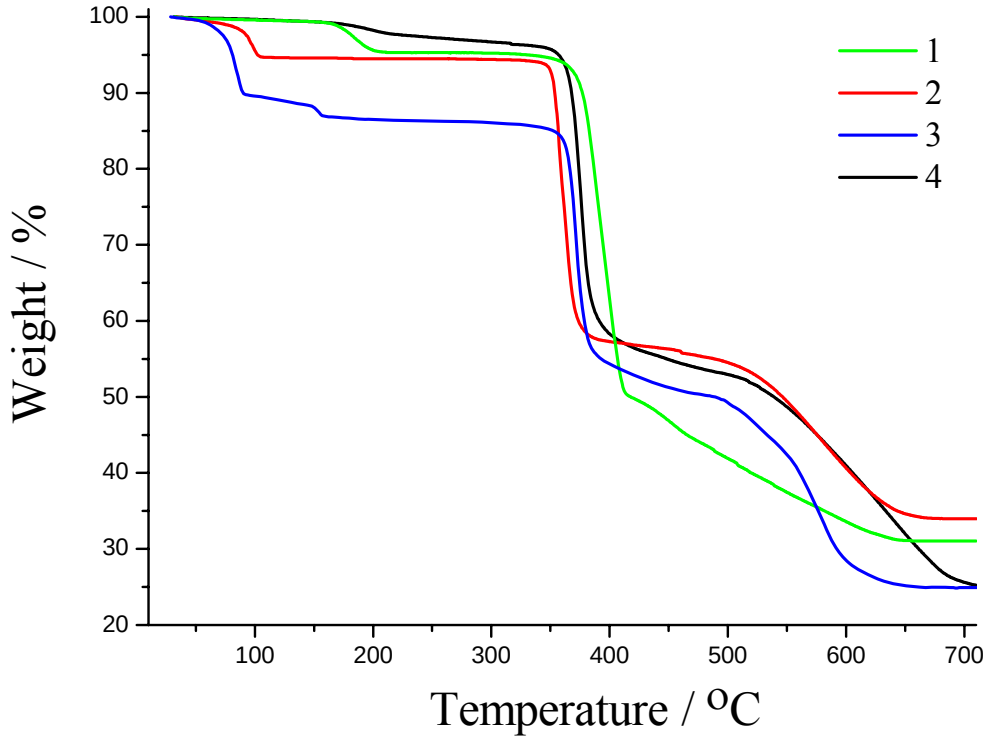

Figure S1. The TG curves of **1-4**.

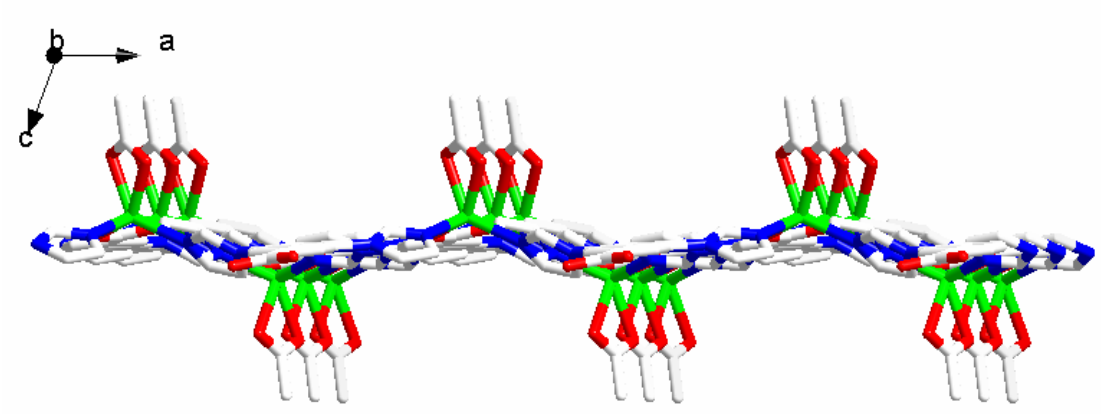

Figure S2. The acetate is alternating above and below the 2D plane in **1**.

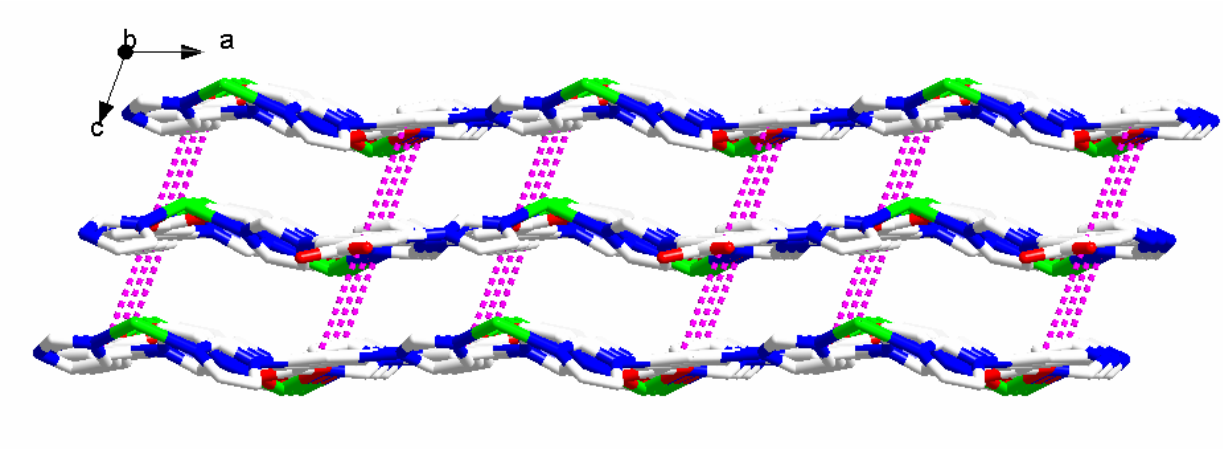

Figure S3. The π-π interactions between the 2D layers in **1**.

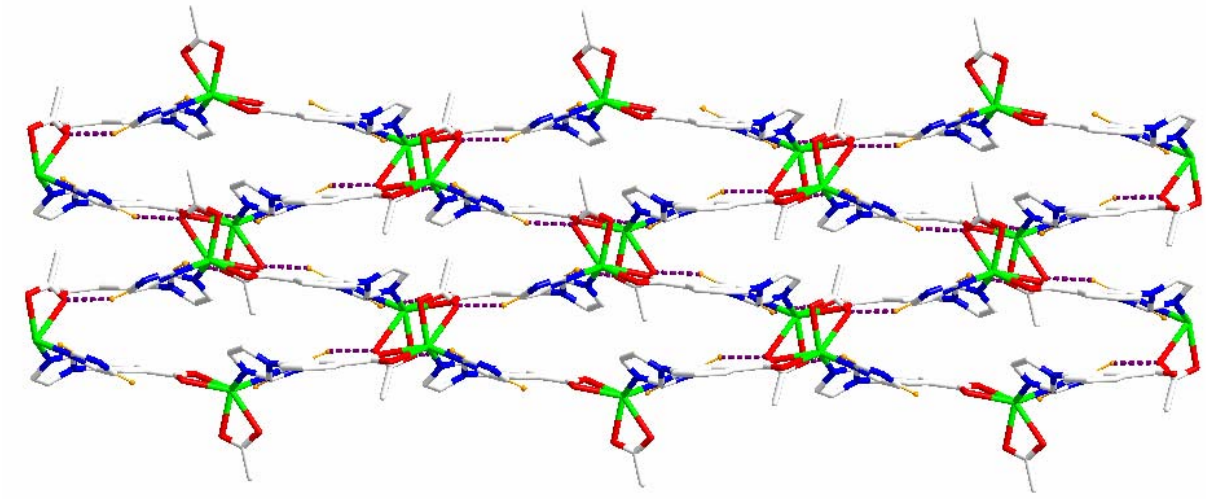

Figure S4. 3D packing diagram of **1**. The dashed lines represent of the hydrogen bonds.

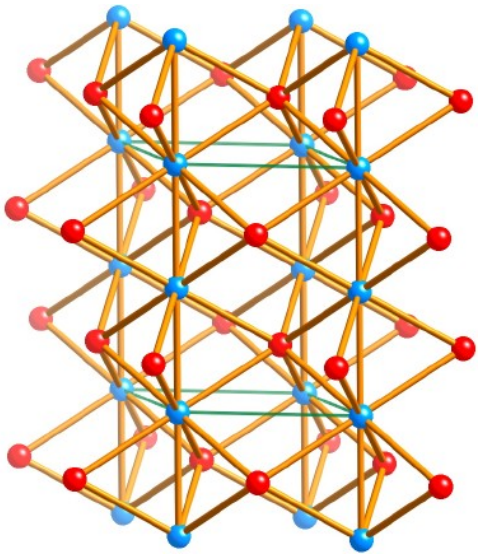

Figure S5. The (6,8)-connected **seh** net.

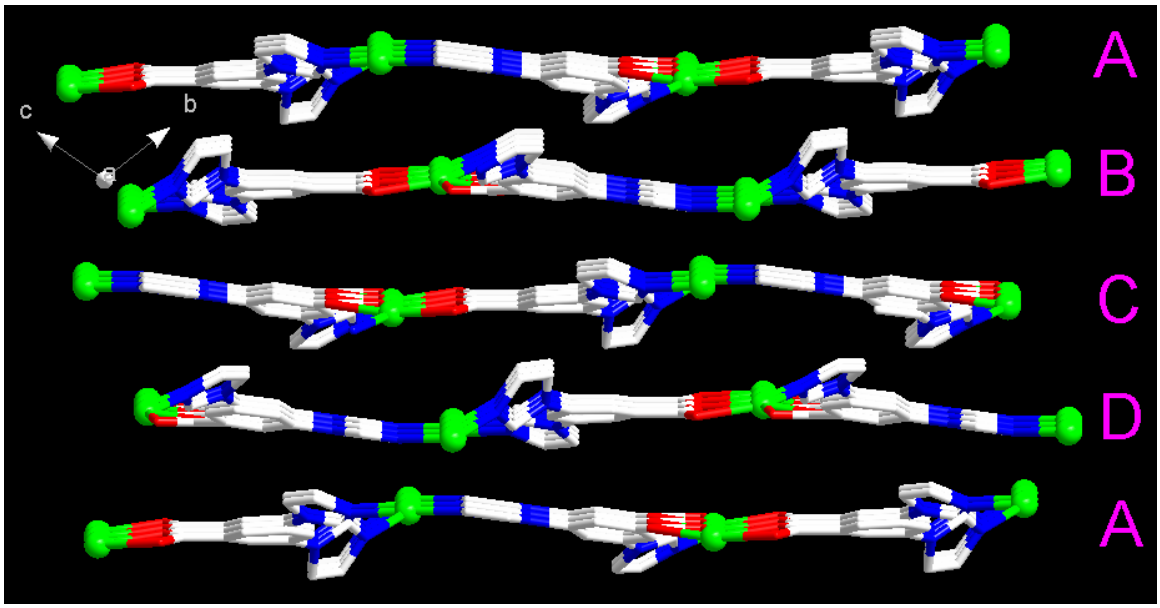

Figure S6. The packing diagram of 2D layers in **3**.

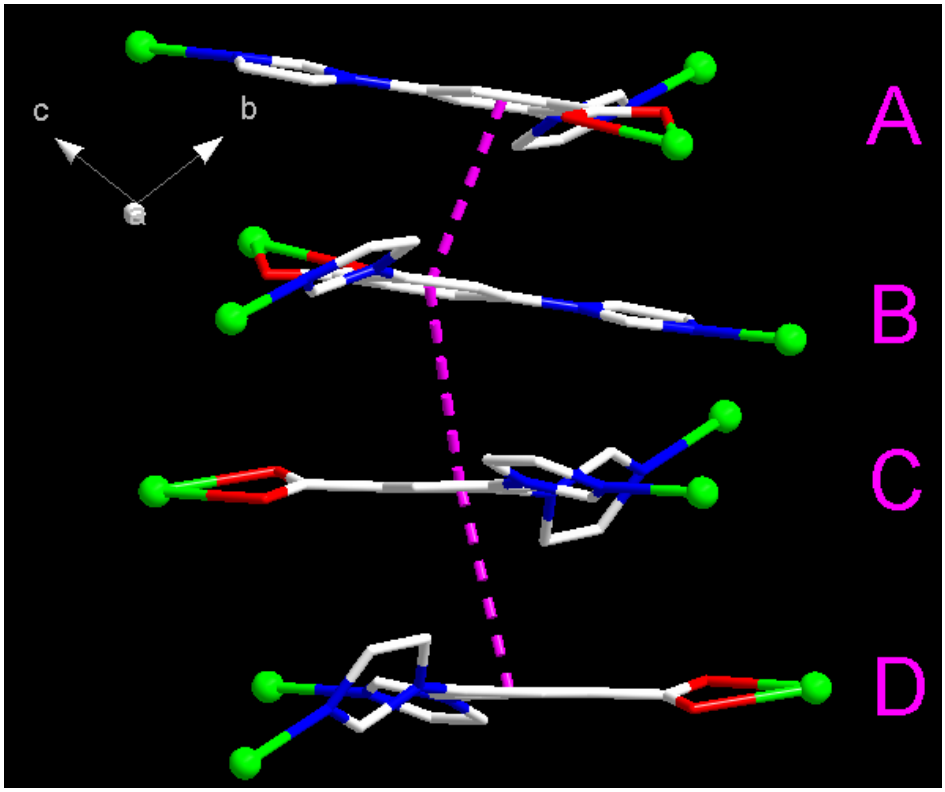

Figure S7. The schematic representation of π-π interactions between the 2D layers in **3**.

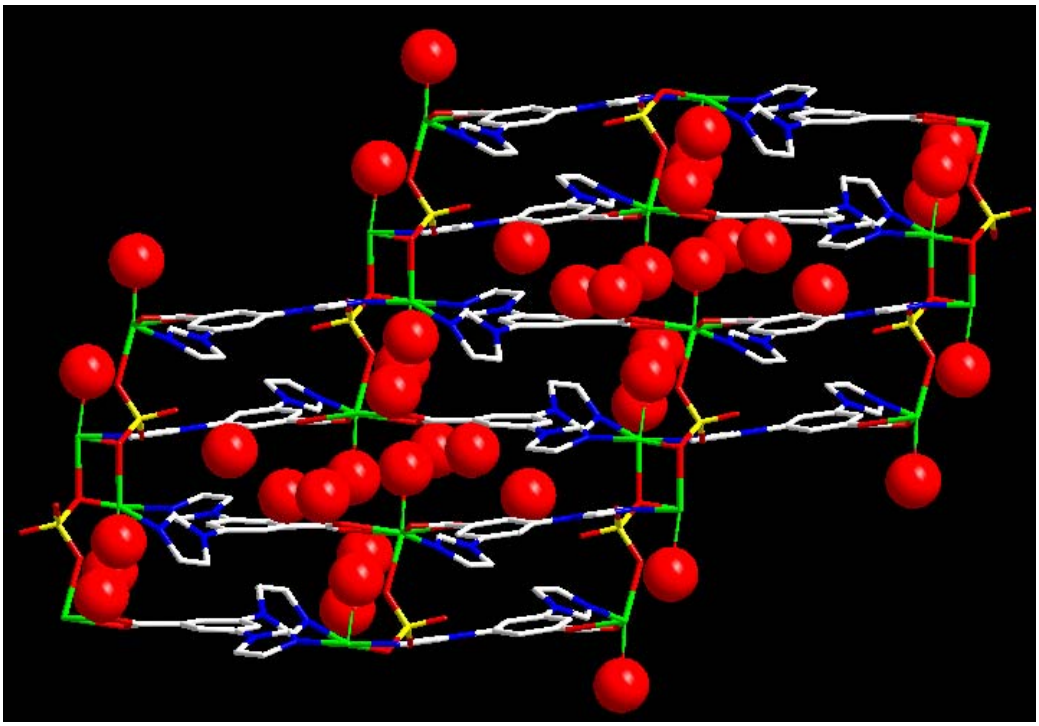

Figure S8. The 3D structure of **3**. Red balls represent of the coordinated and uncoordinated water molecules.

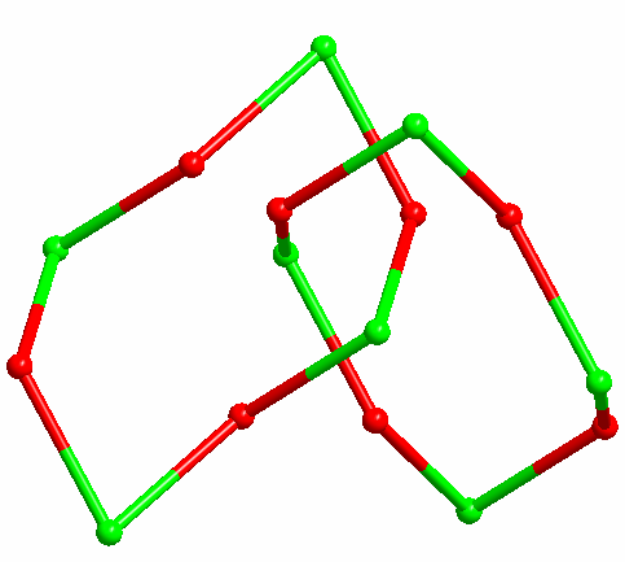

Figure S9. The close-up view of self-penetrated rings in **4**.