Electronic Supplementary Material (ESI) for Dalton Transactions

MOFs Constructed with Newly Designed Imidazole Dicarboxylate Bearing 2-position Aromatic Substituent: Hydro(solvo)thermal Syntheses, Crystal Structures and Properties

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Supporting Information

Table S1. Selected bond distances (Å) and angles (deg) for compounds **1 - 6**

1[a]			
Cd(1)-N(2)#1	2.202(6)	Cd(1)-N(1)	2.254(6)
Cd(1)-O(1)#2	2.265(5)	N(2)-Cd(1)#3	2.202(6)
Cd(1)-O(1)	2.395(6)	Cd(1)-O(4)#1	2.522(7)
Cd(1)-N(2)#3	2.203(10)	O(1)-Cd(1)#2	2.265(5)
O(4)-Cd(1)#3	2.522(7)		
N(2)#1-Cd(1)-N(1)	111.3(2)	N(2)#1-Cd(1)-O(1)#2	100.6(2)
N(1)-Cd(1)-O(1)#2	141.8(2)	N(2)#1-Cd(1)-N(3)	111.0(4)
N(1)-Cd(1)-N(3)	90.0(4)	O(1)#2-Cd(1)-N(3)	97.8(4)
N(2)#1-Cd(1)-O(1)	144.9(2)	N(1)-Cd(1)-O(1)	71.4(2)
O(1)#2-Cd(1)-O(1)	70.4(2)	N(3)-Cd(1)-O(1)	103.9(4)
N(2)#1-Cd(1)-O(4)#1	70.8(2)	N(1)-Cd(1)-O(4)#1	85.8(3)
O(1)#2-Cd(1)-O(4)#1	85.4(3)	N(3)-Cd(1)-O(4)#1	175.8(4)
O(1)-Cd(1)-O(4)#1	74.6(2)		
2[b]			
Sr(1)-O(2)	2.490(3)	Sr(1)-O(3)	2.526(3)
Sr(1)-O(1)#1	2.543(3)	Sr(1)-O(4)#2	2.651(3)

Sr(1)-O(4)#3	2.702(3)	Sr(1)-O(2)#4	2.709(3)
Sr(1)-O(1)#4	2.716(3)	Sr(1)-O(3)#3	2.809(4)
Sr(1)-O(5)	2.803(4)	O(1)-Sr(1)#5	2.716(3)
O(1)-Sr(1)#6	2.543(3)	O(2)-Sr(1)#5	2.709(3)
O(4)-Sr(1)#7	2.651(3)	O(4)-Sr(1)#3	2.809(3)
O(2)-Sr(1)-O(3)	70.55(11)	O(2)-Sr(1)-O(1)#1	155.55(12)
O(3)-Sr(1)-O(1)#1	97.25(10)	O(2)-Sr(1)-O(4)#2	64.66(11)
O(3)-Sr(1)-O(4)#2	115.43(10)	O(1)#1-Sr(1)-O(4)#2	104.84(10)
O(2)-Sr(1)-O(4)#3	134.99(11)	O(3)-Sr(1)-O(4)#3	113.36(10)
O(1)#1-Sr(1)-O(4)#3	69.01(10)	O(4)#2-Sr(1)-O(4)#3	131.21(5)
O(2)-Sr(1)-O(2)#4	118.08(8)	O(3)-Sr(1)-O(2)#4	171.37(10)
O(1)#1-Sr(1)-O(2)#4	74.72(9)	O(4)#2-Sr(1)-O(2)#4	70.44(9)
O(4)#3-Sr(1)-O(2)#4	61.16(9)	O(2)-Sr(1)-O(1)#4	75.42(10)
O(3)-Sr(1)-O(1)#4	138.81(11)	O(1)#1-Sr(1)-O(1)#4	122.57(8)
O(4)#2-Sr(1)-O(1)#4	67.29(10)	O(4)#3-Sr(1)-O(1)#4	76.14(9)
O(2)#4-Sr(1)-O(1)#4	48.44(9)	O(2)-Sr(1)-O(3)#3	111.77(11)
O(3)-Sr(1)-O(3)#3	66.71(12)	O(1)#1-Sr(1)-O(3)#3	80.52(10)
O(4)#2-Sr(1)-O(3)#3	173.58(10)	O(4)#3-Sr(1)-O(3)#3	47.03(8)
O(2)#4-Sr(1)-O(3)#3	108.19(10)	O(1)#4-Sr(1)-O(3)#3	106.94(10)
O(2)-Sr(1)-O(5)	86.81(11)	O(3)-Sr(1)-O(5)	69.56(11)
O(1)#1-Sr(1)-O(5)	68.89(10)	O(4)#2-Sr(1)-O(5)	64.06(10)
O(4)#3-Sr(1)-O(5)	137.80(10)	O(2)#4-Sr(1)-O(5)	109.52(11)
O(1)#4-Sr(1)-O(5)	131.25(10)	O(3)#3-Sr(1)-O(5)	121.80(10)
3[c]			
Zn(1)-O(2)#2	2.106(2)	Zn(1)-O(3)	2.111(2)
Zn(1)-O(5)	2.269(3)	Zn(1)-O(6)	2.206(2)
Zn(1)-N(1)	2.062(2)	Zn(1)-N(2)#2	2.069(2)
Zn(2)-O(1)	1.999(2)	Zn(2)-O(1)#2	1.999(2)
Zn(2)-O(4)#3	2,048(2)	Zn(2)-O(4)	2.048(2)
Zn(2)-O(7)#3	2.167(3)	Zn(2)-O(7)	2.167(3)
O(2)#2-Zn(1)-O(3)	167.93(8)	O(2)#2-Zn(1)-O(5)	85.17(10)
O(2)#2-Zn(1)-O(6)	83.62(9)	O(3)-Zn(1)-O(5)	91.22(10)

O(3)-Zn(1)-O(6)	84.36(9)	N(1)-Zn(1)-O(2)#2	112.13(9)
N(1)-Zn(1)-O(3)	78.77(9)	N(1)-Zn(1)-O(5)	83.24(10)
N(1)-Zn(1)-O(6)	154.29(10)	N(1)-Zn(1)-N(2)#2	111.19(10)
N(2)#2-Zn(1)-O(2)#2	78.66(9)	N(2)#2-Zn(1)-O(3)	102.74(10)
N(2)#2-Zn(1)-O(5)	161.45(10)	N(2)#2-Zn(1)-O(6)	91.29(10)
O(1)-Zn(2)-O(1)#3	180.00	O(1)-Zn(2)-O(4)#3	85.46(9)
O(1)#3-Zn(2)-O(4)#3	94.54(9)	O(1)#3-Zn(2)-O(4)	85.46(9)
O(1)-Zn(2)-O(4)	94.54(9)	O(1)#3-Zn(2)-O(7)#3	91.68(11)
O(1)-Zn(2)-O(7)#3	88.32(11)	O(1)#3-Zn(2)-O(7)	88.32(11)
O(1)-Zn(2)-O(7)	91.68(11)	O(4)#3-Zn(2)-O(4)	180.00
O(4)-Zn(2)-O(7)#3	91.79(11)	O(4)#3-Zn(2)-O(7)#3	88.21(11)
O(4)#3-Zn(2)-O(7)	91.79(11)	O(4)-Zn(2)-O(7)	88.21(11)
O(7)#3-Zn(2)-O(7)	179.998(1)		
4[d]			
Mn(1)-O(3)	2.170(4)	Mn(1)-O(2)#1	2.184(4)
Mn(1)-N(1)	2.196(5)	Mn(1)-N(2)#1	2.192(5)
Mn(1)-O(6)	2.251(5)	Mn(1)-O(5)	2.233(4)
Mn(2)-O(4)#2	2.056(4)	Mn(2)-O(4)	2.056(4)
Mn(2)-O(1)	2.113(4)	Mn(2)-O(1)#2	2.113(4)
Mn(2)-O(7)	2.219(7)	Mn(2)-O(7)#2	2.219(7)
Mn(1)#3-O(2)	2.184(4)	Mn(1)#3-N(2)	2.192(5)
O(3)-Mn(1)-O(2)#1	169.91(17)	O(3)-Mn(1)-N(1)	75.06(17)
O(4)#1-Mn(1)-N(2)	103.42(17)	O(3)-Mn(1)-N(2)#1	115.43(18)
O(2)#1-Mn(1)-N(2)#1	74.64(17)	N(2)#1-Mn(1)-N(1)	106.51(19)
O(3)-Mn(1)-O(5)	86.86(17)	O(2)#1-Mn(1)-O(5)	83.30(17)
N(1)-Mn(1)-O(5)	94.49(18)	N(2)#1-Mn(1)-O(5)	152.38(19)
O(5)-Mn(1)-O(6)	81.77(19)	O(2)#1-Mn(1)-O(6)	98.24(18)
N(1)-Mn(1)-O(6)	157.45(18)	N(2)#1-Mn(1)-O(6)	85.11(19)
O(5)-Mn(1)-O(6)	81.77(19)	O(4)#2-Mn(2)-O(4)	180.00
O(4)#2-Mn(2)-O(1)	89.93(17)	O(4)-Mn(2)-O(1)	90.07(17)
O(4)#2-Mn(2)-O(1)#2	90.08(17)	O(4)-Mn(2)-O(1)#2	89.93(17)
O(1)-Mn(2)-O(1)#2	179.997(1)	O(4)#2-Mn(2)-O(7)	90.1(2)

O(4)-Mn(2)-O(7)	89.9(2)	O(1)-Mn(2)-O(7)	90.6(3)
O(1)#2-Mn(2)-O(7)	89.4(3)	O(4)#2-Mn(2)-O(7)#2	89.9(2)
O(4)-Mn(2)-O(7)#2	90.1(2)	O(1)-Mn(2)-O(7)#2	89.4(3)
O(1)#2-Mn(2)-O(7)#2	90.6(3)	O(7)-Mn(2)-O(7)#2	179.997(1)
5[e]			
Mg(1)-O(1)	2.0174(14)	Mg(1)-O(6)	2.0335(14)
Mg(1)-O(4)	2.0390(14)	Mg(1)-O(3)	2.0446(13)
Mg(1)-O(2)	2.0589(13)	Mg(1)-O(5)	2.1903(15)
O(1)-Mg(1)-O(6)	99.01(6)	O(1)-Mg(1)-O(4)	171.31(6)
O(6)-Mg(1)-O(4)	88.96(6)	O(1)-Mg(1)-O(3)	83.95(5)
O(6)-Mg(1)-O(3)	92.40(6)	O(4)-Mg(1)-O(3)	92.29(5)
O(1)-Mg(1)-O(2)	89.24(5)	O(6)-Mg(1)-O(2)	90.75(5)
O(4)-Mg(1)-O(2)	94.17(5)	O(3)-Mg(1)-O(2)	172.87(6)
O(1)-Mg(1)-O(5)	94.99(6)	O(6)-Mg(1)-O(5)	166.00(6)
O(4)-Mg(1)-O(5)	77.10(5)	O(3)-Mg(1)-O(5)	89.50(6)
O(2)-Mg(1)-O(5)	88.99(5)		
6[f]			
Ca(1)-O(1)	2.3746(18)	Ca(1)-O(2)#2	2.3897(19)
Ca(1)-O(3)	2.3755(18)	Ca(1)-O(3)#3	2.5363(18)
Ca(1)-O(4)#3	2.7384(19)	Ca(1)-O(4)#1	2.3810(18)
Ca(1)-O(5)	2.574(2)	Ca(1)-O(6)	2.375(2)
Ca(1)#5-O(2)	2.3897(19)	O(3)-Ca(1)#4	2.5363(18)
Ca(1)#6-O(4)	2.3810(18)	Ca(1)#4-O(4)	2.7384(19)
O(1)-Ca(1)-O(2)#2	131.51(7)	O(1)-Ca(1)-O(3)#3	145.71(7)
O(1)-Ca(1)-O(3)	76.25(6)	O(1)-Ca(1)-O(4)#1	88.48(7)
O(1)-Ca(1)-O(4)#3	133.60(7)	O(1)-Ca(1)-O(5)	68.52(7)
O(1)-Ca(1)-O(6)	75.06(7)	O(2)#2-Ca(1)-O(3)#3	82.15(7)
O(2)#2-Ca(1)-O(4)#3	76.65(7)	O(2)#4-Ca(1)-O(5)	71.83(7)
O(3)-Ca(1)-O(3)#3	117.98(5)	O(3)-Ca(1)-O(4)#1	163.74(7)
O(3)#3-Ca(1)-O(5)	129.54(7)	O(3)-Ca(1)-O(5)	103.29(7)
O(3)-Ca(1)-O(6)	89.49(7)	O(4)#1-Ca(1)-O(2)#2	107.66(7)
O(4)#1-Ca(1)-O(3)#3	72.22(6)	O(4)#1-Ca(1)-O(4)#3	120.75(5)

O(4)#1-Ca(1)-O(5)	75.60(7)	O(5)-Ca(1)-O(4)#3	147.93(6)
O(6)-Ca(1)-O(2)#2	150.94(8)	O(6)-Ca(1)-O(3)#3	74.14(7)
O(6)-Ca(1)-O(4)#1	81.08(7)	O(6)-Ca(1)-O(4)#1	81.08(7)
O(6)-Ca(1)-O(5)	136.78(7)		

Symmetry transformations used to generate equivalent atoms: [a] #1: -y+5/4, x-1/4, z-1/4. #2: -x+2, -y+1, -z+2. #3: y+1/4, -x+5/4, z+1/4. [b] #1:x, y+1, z. #2: x, -y+1/2, z+1/2. #3: -x, -y+1, -z. #4: -x, y+1/2, -z+1/2. #5: x, y-1, z. #6: -x, y-1/2, -z+1/2. #7: x, -y+1/2, z-1/2. #7: x, -y+5/2, z-1/2. [c] #1: 2/3-y+x, 1/3+x, 1/3-z. #2: -1/3+y, 1/3-y+x, 1/3-z. #3: 1-x, 1-y, 1-z. [d] #1: x-y, x, -z. #2: -x+2/3,-y+1/3,-z-2/3. #3: y, -x+y, -z. [e] #1: x, -y+5/2, z+1/2. #2: x, y+1, z. #3: x, -y+5/2, z-1/2. #4: x, y-1, z. [f] #1: x, y+1, z. #2: x, -y+5/2, z+1/2. #3: -x, y+1/2, -z+3/2. #4: -x, y-1/2, -z+3/2. #5: x, 5/2-y, -1/2+z. #6: x, y-1, z.

Table S2. Hydrogen bonds distances (Å) and angles (deg) for **2, 5** and **6**

2			
D-H...A	d(H...A)	d(D...A)	∠(DHA)
O(5)-H(5A)...O(4)#2	2.05	2.896(5)	179.8
O(5)-H(5B)...O(3)	2.28	3.061(6)	153.2
5			
D-H...A	d(H...A)	d(D...A)	∠(DHA)
N(1)-H(1)...O(5)#3	2.37	3.221(2)	170.1
N(1)-H(1)...O(4)#3	2.57	3.002(19)	112.5
O(5)-H(5A)...N(2)#2	1.967(11)	2.798(2)	162.5(17)
O(6)-H(6A)...O(2)#5	2.120(9)	2.974(18)	177(2)
O(6)-H(6B)...O(4)#6	2.561(15)	3.264(18)	142(2)
6			
D-H...A	d(H...A)	d(D...A)	∠(DHA)
O(5)-H(2W)-N(1)#2	1.98	2.806(3)	164.8
O(6)-H(3W)-O(1)#7	2.59	3.132(3)	122.7
O(6)-H(3W)-O(2)#7	2.01	2.779(3)	150.5
O(6)-H(4W)-O(6)#7	2.53	3.214(4)	138.8
N(2)-H(2)-O(1)#6	2.35	2.958(3)	127.9
N(2)-H(2)-O(5)#6	2.32	3.123(3)	155.2

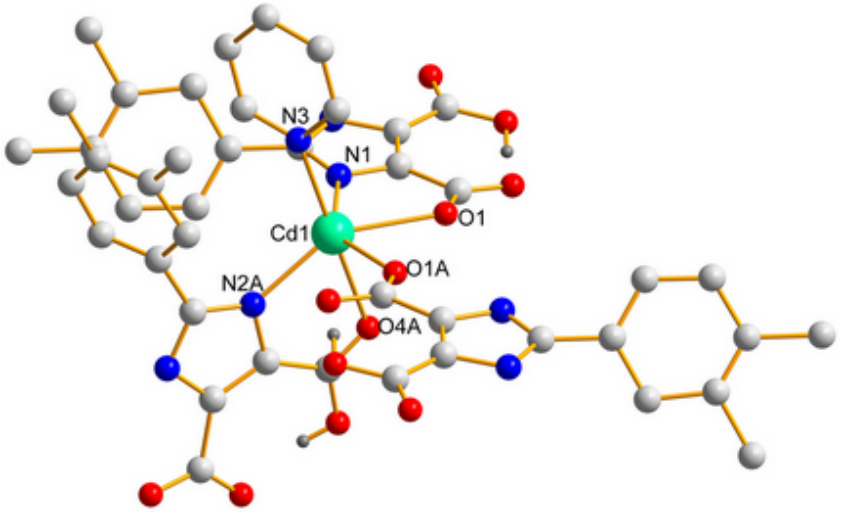


Figure S1. Coordination environment of Cd(II) atom in polymer **1** (Partial H atoms omitted for clarity).

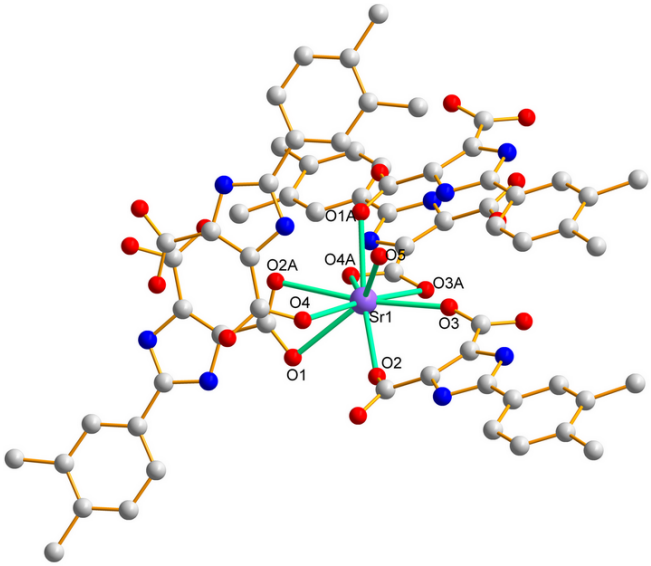
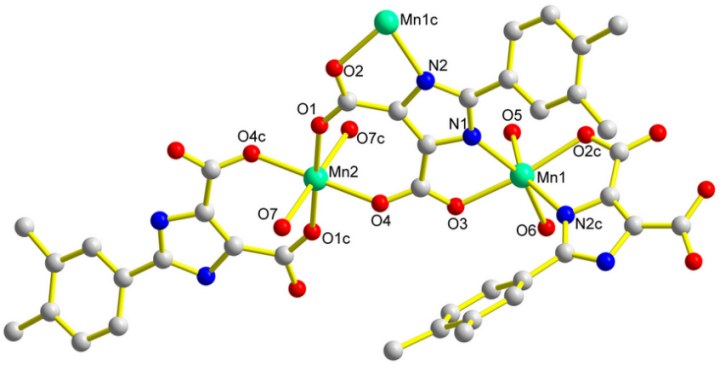
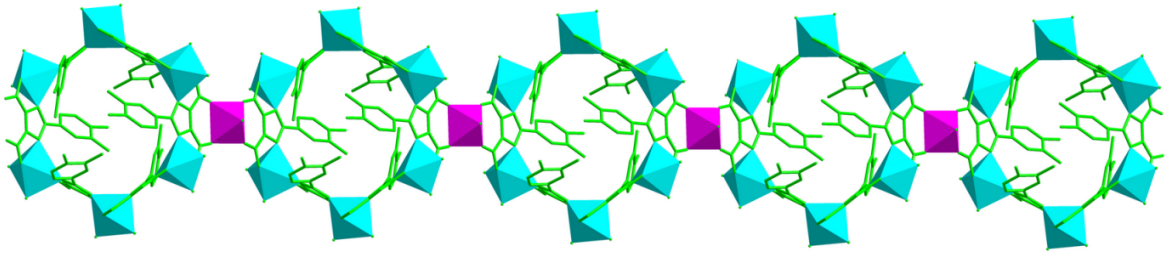


Figure S2. Coordination arrangement of the Sr(II) in polymer **2** (Partial H atoms omitted for clarity).

(a)



(b)



(c)

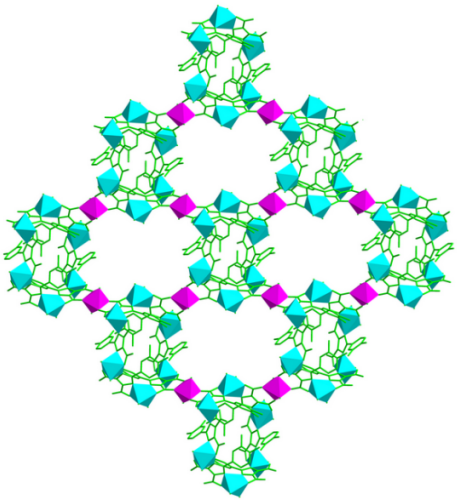


Figure S3. (a) Ball and stick drawing of the coordination environments of Mn atoms and organic ligands in **4**. Hydrogen atoms are omitted for clarity. (b) View the 1D chains of **4** (the Mn1 octahedral coordination polyhedrons are turquoise, the Mn2 octahedral coordination polyhedrons are pink). (c) View of the 2D layer of **4** perpendicular to the *c* axis.

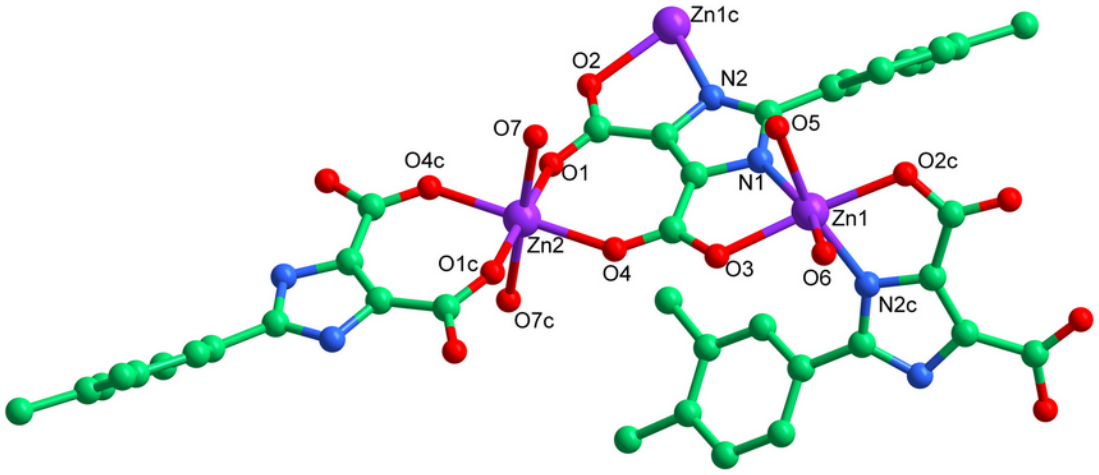


Figure S4. Ball and stick drawing of the coordination environments of Zn atoms and organic ligands in **3**. Hydrogen atoms are omitted for clarity.

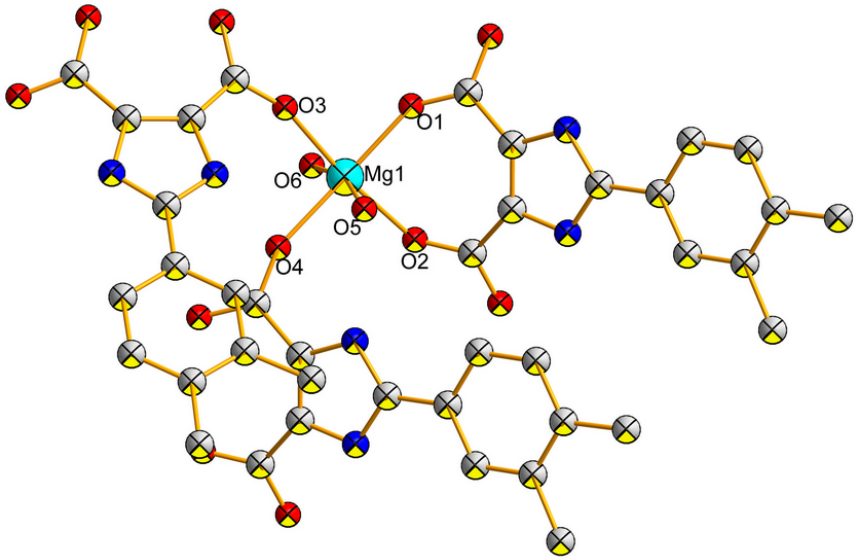


Figure S5. Perspective view of polymer **5** with atom labeling scheme (H atoms omitted for clarity).

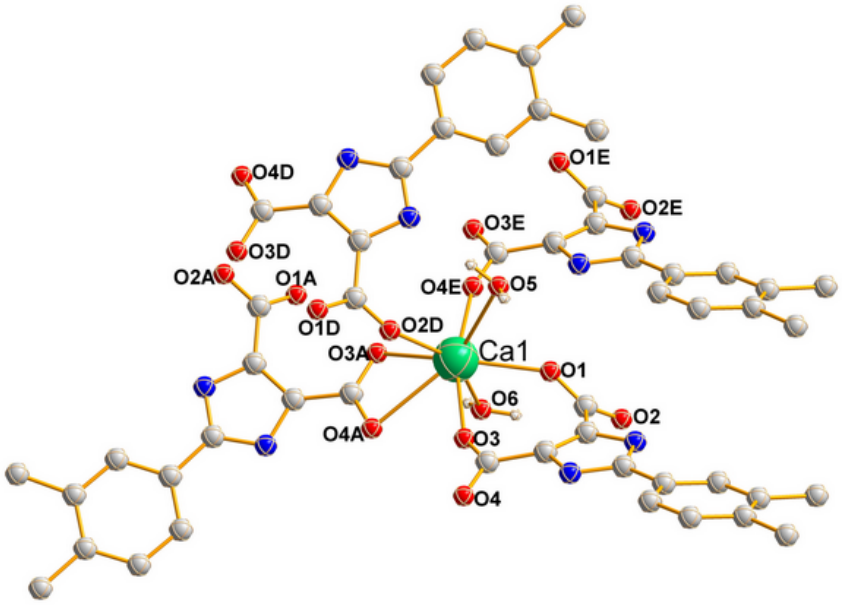
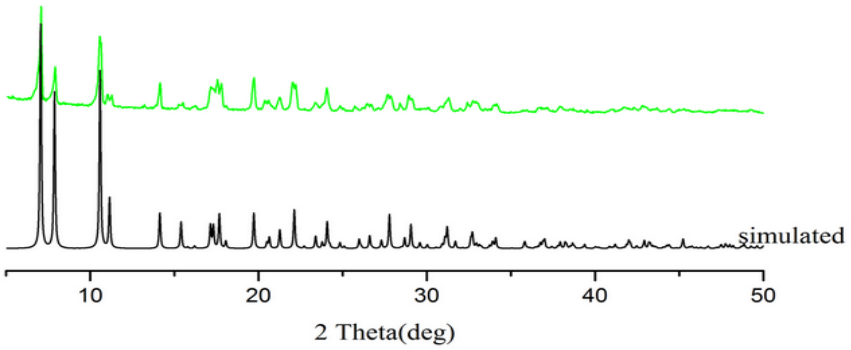
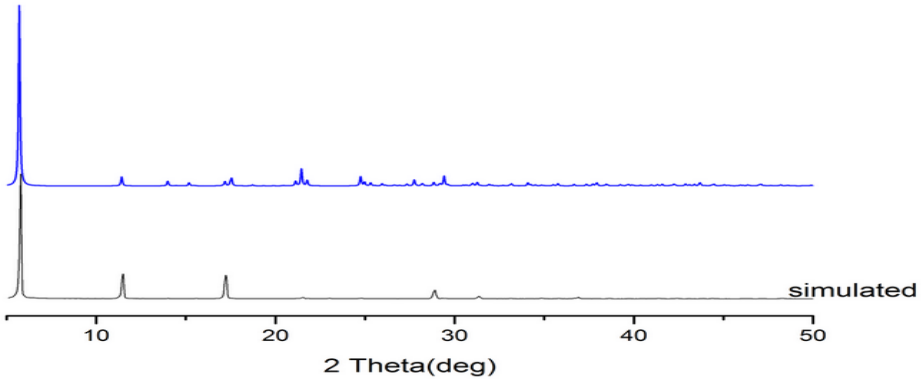


Figure S6. Perspective view of polymer **6** with atom labeling scheme (H atoms omitted for clarity).

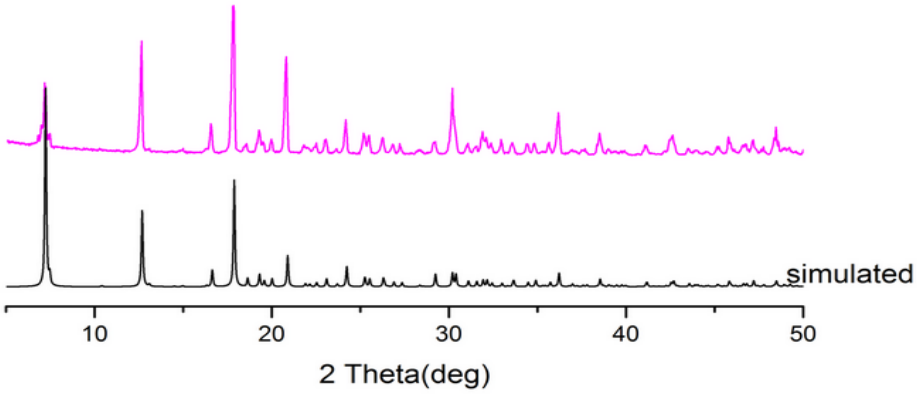
(a)



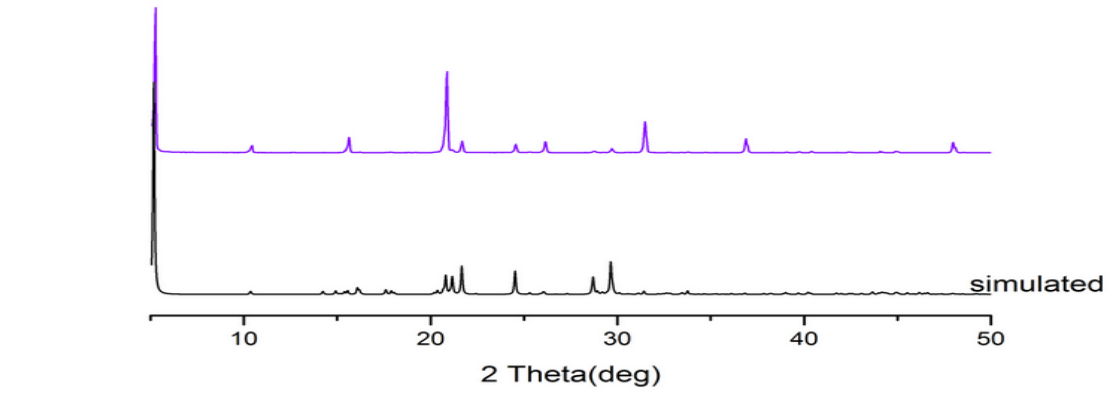
(b)



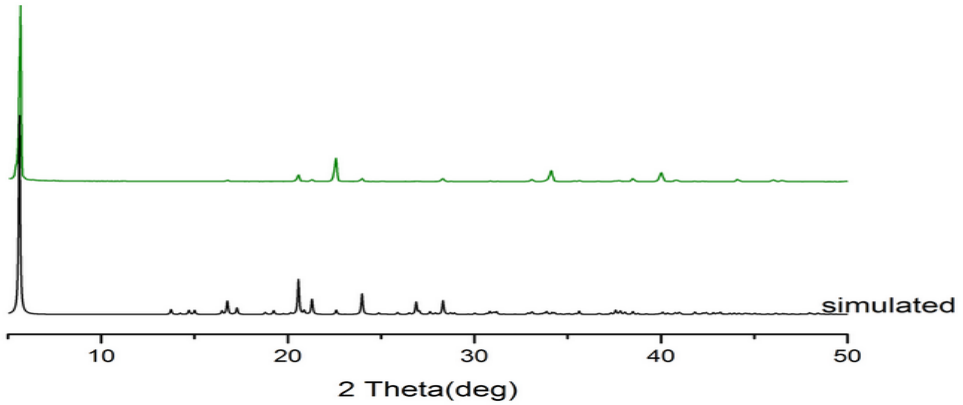
(c)



(d)



(e)



(f)

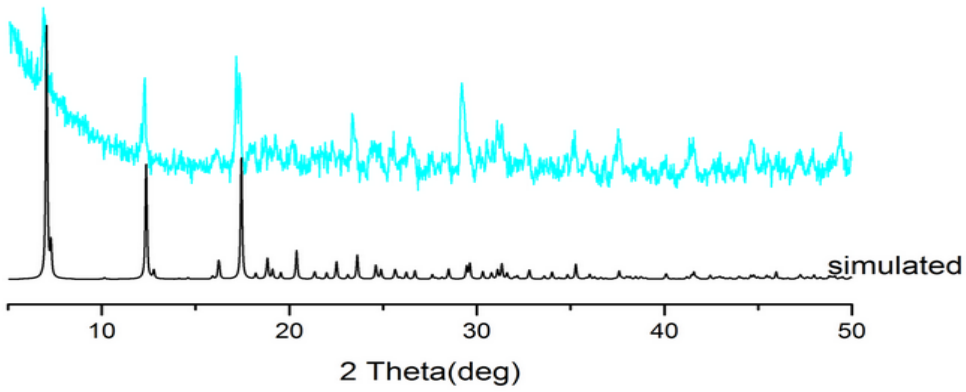


Figure S7. XRPD pattern of polymers **1 - 6** are shown from (a) to (f), respectively.