Assembly of a series of MOFs based on the 2-(*m*-methoxyphenyl)-imidazole dicarboxylate ligand

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Supporting information

Table S1. Selected bond distances (Å) and angles (deg) for compounds **1** –**7**

1[a]			
Sr(1)-O(7)#1	2.4828(18)	Sr(1)-O(5)	2.542(2)
Sr(1)-O(6)#2	2.544(2)	Sr(1)-O(3)#1	2.677(2)
Sr(1)-O(3)	2.701(2)	Sr(1)-O(6)	2.7013(19)
Sr(1)-O(7)	2.719(2)	Sr(1)-O(2)	2.775(3)
O(7)#1-Sr(1)-O(5)	70.70(7)	O(7)#1-Sr(1)-O(6)#2	157.68(6)
O(5)-Sr(1)-O(6)#2	97.23(7)	O(7)#1-Sr(1)-O(3)#1	64.68(6)
O(5)-Sr(1)-O(3)#1	114.68(7)	O(6)#2-Sr(1)-O(3)#1	106.51(6)
O(7)#1-Sr(1)-O(3)	132.62(6)	O(5)-Sr(1)-O(3)	113.63(6)
O(6)#2-Sr(1)-O(3)	69.08(6)	O(3)#1-Sr(1)-O(3)	131.64(3)
O(7)#1-Sr(1)-O(6)	75.37(6)	O(5)-Sr(1)-O(6)	139.59(7)
O(6)#2-Sr(1)-O(6)	121.67(5)	O(3)#1-Sr(1)-O(6)	67.21(6)
O(3)-Sr(1)-O(6)	75.04(6)	O(7)#1-Sr(1)-O(7)	118.33(5)
O(5)-Sr(1)-O(7)	170.96(6)	O(6)#2-Sr(1)-O(7)	74.08(6)
O(3)#1-Sr(1)-O(7)	71.04(6)	O(3)-Sr(1)-O(7)	61.35(6)
O(6)-Sr(1)-O(7)	48.35(6)	O(7)#1-Sr(1)-O(2)	88.87(7)
O(5)-Sr(1)-O(2)	69.69(7)	O(6)#2-Sr(1)-O(2)	69.10(7)
O(3)#1-Sr(1)-O(2)	64.43(7)	O(3)-Sr(1)-O(2)	138.11(7)

O(6)-Sr(1)-O(2)	131.33(7)	O(7)-Sr(1)-O(2)	108.54(7)
O(7)#1-Sr(1)-O(5)#3	109.74(7)	O(5)-Sr(1)-O(5)#3	67.01(8)
O(6)#2-Sr(1)-O(5)#3	80.85(6)	O(3)#1-Sr(1)-O(5)#3	171.81(6)
O(3)-Sr(1)-O(5)#3	47.05(6)	O(6)-Sr(1)-O(5)#3	106.06(6)
O(7)-Sr(1)-O(5)#3	108.40(6)	O(2)-Sr(1)-O(5)#3	122.58(7)

2[b]

Sr(1)-O(2)#2	2.548(3)	Sr(1)-O(4)	2.488(3)
Sr(1)-O(2)#4	2.773(3)	Sr(1)-N(1)	2.737(3)
O(4)#1-Sr(1)-O(4)	97.30(17)	O(2)#2-Sr(1)-O(2)#3	100.00(14)
O(4)-Sr(1)-O(2)#2	152.75(10)	O(4)-Sr(1)-N(1)#1	79.32(10)
O(4)-Sr(1)-O(2)#3	87.72(10)	O(2)#3-Sr(1)-N(1)#1	90.94(10)
N(1)#1-Sr(1)-N(1)	123.69(15)	O(4)-Sr(1)-N(1)	64.01(10)
O(4)#1-Sr(1)-O(2)#4	99.06(10)	O(2)#3-Sr(1)-N(1)	126.17(9)
O(4)-Sr(1)-O(2)#4	141.35(9)	O(2)#2-Sr(1)-O(2)#4	62.84(5)
N(1)-Sr(1)-O(2)#4	153.77(9)	N(1)#1-Sr(1)-O(2)#4	76.89(9)
O(4)-Sr(1)-O(2)#5	99.06(10)	O(2)#2-Sr(1)-O(2)#5	62.84(5)
N(1)-Sr(1)-O(2)#5	76.89(9)	N(1)#1-Sr(1)-O(2)#5	153.77(9)
O(2)#4-Sr(1)-O(2)#5	89.50(12)		

3[c]

N(1)-Cd(2)	2.311(5)	O(6)-Cd(1)	2.387(4)
N(3)-Cd(1)	2.314(5)	O(9)-Cd(2)#2	2.283(4)
N(4)-Cd(2)#1	2.246(5)	O(9)-Cd(2)#1	2.408(4)
O(1)-Cd(1)	2.363(5)	O(11)-Cd(2)	2.318(5)
O(2)-Cd(2)	2.299(4)	Cd(1)-N(3)#3	2.314(5)
Cd(1)-O(1)#3	2.363(5)	Cd(1)-O(6)#3	2.387(4)
Cd(2)-N(4)#1	2.246(5)	Cd(2)-O(9)#4	2.283(4)
N(3)-Cd(1)-N(3)#3	180.00	N(3)#3-Cd(1)-O(1)	91.22(17)
N(3)-Cd(1)-O(1)	88.78(17)	N(3)#3-Cd(1)-O(1)#3	88.78(17)
N(3)-Cd(1)-O(1)#3	91.22(17)	O(1)-Cd(1)-O(1)#3	180.000(1)

N(3)#3-Cd(1)-O(6)#3	72.98(16)	N(3)-Cd(1)-O(6)#3	107.02(16)
O(1)-Cd(1)-O(6)#3	102.37(16)	O(1)#3-Cd(1)-O(6)#3	77.63(16)
N(3)#3-Cd(1)-O(6)	107.02(16)	N(3)-Cd(1)-O(6)	72.98(16)
O(1)-Cd(1)-O(6)	77.63(16)	O(1)#3-Cd(1)-O(6)	102.37(16)
O(6)#3-Cd(1)-O(6)	180.000(1)	N(4)#1-Cd(2)-O(9)#4	142.97(17)
N(4)#1-Cd(2)-O(2)	106.02(17)	O(9)#4-Cd(2)-O(2)	87.16(16)
N(4)#1-Cd(2)-N(1)	111.86(18)	O(9)#4-Cd(2)-N(1)	105.00(17)
O(2)-Cd(2)-N(1)	73.79(17)	N(4)#1-Cd(2)-O(11)	93.15(19)
O(9)#4-Cd(2)-O(11)	83.51(19)	O(2)-Cd(2)-O(11)	158.17(18)
N(1)-Cd(2)-O(11)	89.61(19)	N(4)#1-Cd(2)-O(9)#1	71.43(16)
O(9)#4-Cd(2)-O(9)#1	71.61(17)	O(2)-Cd(2)-O(9)#1	114.12(16)
N(1)-Cd(2)-O(9)#1	170.76(18)	O(11)-Cd(2)-O(9)#1	81.50(18)

4[d]

Cu(1)-N(4)#1	1.987(2)	Cu(1)-O(3)	1.9966(16)
Cu(1)-N(2)	2.0106(18)	Cu(1)-N(3)	2.010(2)
Cu(1)-N(1)	2.2853(18)	N(4)-Cu(1)#2	1.987(2)
N(4)#1-Cu(1)-O(3)	89.16(7)	N(4)#1-Cu(1)-N(2)	91.24(7)
O(3)-Cu(1)-N(2)	177.25(7)	N(4)#1-Cu(1)-N(3)	163.49(8)
O(3)-Cu(1)-N(3)	83.12(6)	N(2)-Cu(1)-N(3)	97.17(7)
N(4)#1-Cu(1)-N(1)	109.89(7)	O(3)-Cu(1)-N(1)	99.61(7)
N(2)-Cu(1)-N(1)	77.69(7)	N(3)-Cu(1)-N(1)	85.86(7)

5[e]

N(1)-Cd(2)	2.248(6)	N(2)-Cd(1)	2.300(6)
N(3)-Cd(1)	2.351(7)	N(4)-Cd(1)	2.332(7)
N(5)-Cd(2)	2.318(7)	N(6)-Cd(2)	2.381(7)
N(7)-Cd(2)	2.276(6)	N(8)-Cd(1)	2.237(6)
O(1)-Cd(2)	2.391(6)	O(4)-Cd(1)	2.379(5)
O(6)-Cd(1)	2.416(6)	O(9)-Cd(2)	2.387(6)
N(8)-Cd(1)-N(2)	114.0(5)	N(8)-Cd(1)-N(3)	98.7(2)

N(2)-Cd(1)-N(3)	94.5(2)	N(8)-Cd(1)-N(4)	105.8(2)
N(2)-Cd(1)-N(4)	139.4(2)	N(3)-Cd(1)-N(4)	71.3(3)
N(8)-Cd(1)-O(4)	146.3(2)	N(2)-Cd(1)-O(4)	73.1(2)
N(3)-Cd(1)-O(4)	113.9(2)	N(4)-Cd(1)-O(4)	78.5(2)
N(8)-Cd(1)-O(6)	71.9(2)	N(2)-Cd(1)-O(6)	89.5(2)
N(3)-Cd(1)-O(6)	170.6(2)	N(4)-Cd(1)-O(6)	110.8(3)
O(4)-Cd(1)-O(6)	75.4(2)	N(1)-Cd(2)-N(7)	150.3(2)
N(1)-Cd(2)-N(5)	103.6(2)	N(7)-Cd(2)-N(5)	100.5(2)
N(1)-Cd(2)-N(6)	119.8(2)	N(7)-Cd(2)-N(6)	73.0(3)
N(5)-Cd(2)-O(9)	158.0(3)	N(6)-Cd(2)-O(9)	84.6(2)
O(1)-Cd(2)-O(9)	109.5(2)	N(7)-Cd(2)-O(1)	89.1(2)
		6[f]	
Cd(1)-N(8)	2.268(3)	Cd(1)-N(2)	2.306(3)
Cd(1)-N(4)	2.337(3)	Cd(1)-O(3)	2.349(3)
Cd(1)-N(3)	2.378(3)	Cd(1)-O(10)	2.4285(19)
Cd(2)-N(10)	2.278(3)	Cd(2)-N(1)	2.292(3)
Cd(2)-N(5)	2.326(3)	Cd(2)-O(5)	2.359(2)
Cd(2)-O(2)	2.360(2)	Cd(2)-N(6)	2.373(3)
N(8)-Cd(1)-N(2)	139.62(9)	N(8)-Cd(1)-N(4)	96.83(9)
N(2)-Cd(1)-N(4)	113.89(9)	N(8)-Cd(1)-O(3)	89.76(9)
N(2)-Cd(1)-O(3)	73.45(8)	N(4)-Cd(1)-O(3)	155.19(8)
N(8)-Cd(1)-N(3)	109.63(9)	N(2)-Cd(1)-N(3)	105.27(9)
N(4)-Cd(1)-N(3)	70.13(9)	O(3)-Cd(1)-N(3)	85.11(8)
N(8)-Cd(1)-O(10)	71.97(8)	N(2)-Cd(1)-O(10)	82.47(8)
N(4)-Cd(1)-O(10)	89.20(8)	O(3)-Cd(1)-O(10)	115.55(7)
N(3)-Cd(1)-O(10)	159.33(8)	N(10)-Cd(2)-N(1)	118.70(9)
N(10)-Cd(2)-N(5)	99.92(9)	N(1)-Cd(2)-N(5)	105.92(9)
N(10)-Cd(2)-O(5)	73.01(8)	N(1)-Cd(2)-O(5)	91.04(8)
N(5)-Cd(2)-O(5)	162.89(8)	N(10)-Cd(2)-O(2)	162.42(8)

N(1)-Cd(2)-O(2)	72.82(8)	N(5)-Cd(2)-O(2)	88.53(8)
O(5)-Cd(2)-O(2)	94.51(8)	N(10)-Cd(2)-N(6)	81.86(9)
N(1)-Cd(2)-N(6)	159.11(9)	N(5)-Cd(2)-N(6)	71.51(9)
O(5)-Cd(2)-N(6)	91.85(8)	O(2)-Cd(2)-N(6)	86.33(8)

7[g]

Co(1)-O(6)#1	2.0789(19)	Co(1)-O(6)	2.0789(19)
Co(1)-O(2)	2.0890(17)	Co(1)-O(2)#1	2.0890(17)
Co(1)-N(2)#1	2.2061(19)	Co(1)-N(2)	2.2061(19)
Co(2)-O(7)	2.0606(18)	Co(2)-O(7)#2	2.0606(18)
Co(2)-N(1)#2	2.1465(19)	Co(2)-N(1)	2.1465(19)
Co(2)-O(5)	2.1514(17)	Co(2)-O(5)#2	2.1514(17)
O(6)#1-Co(1)-O(6)	180.0	O(6)#1-Co(1)-O(2)	89.91(7)
O(6)-Co(1)-O(2)	90.09(7)	O(6)#1-Co(1)-O(2)#1	90.09(7)
O(6)-Co(1)-O(2)#1	89.91(7)	O(2)-Co(1)-O(2)#1	180.0
O(6)#1-Co(1)-N(2)#1	91.13(8)	O(6)-Co(1)-N(2)#1	88.87(8)
O(2)-Co(1)-N(2)#1	100.16(7)	O(2)#1-Co(1)-N(2)#1	79.84(7)
O(6)#1-Co(1)-N(2)	88.87(8)	O(6)-Co(1)-N(2)	91.13(8)
O(2)-Co(1)-N(2)	79.84(7)	O(2)#1-Co(1)-N(2)	100.16(7)
N(2)#1-Co(1)-N(2)	180.0	O(7)-Co(2)-O(7)#2	180.00(10)
O(7)-Co(2)-N(1)#2	88.31(7)	O(7)#2-Co(2)-N(1)#2	91.69(7)
O(7)-Co(2)-N(1)	91.69(7)	O(7)#2-Co(2)-N(1)	88.31(7)
N(1)#2-Co(2)-N(1)	180.00(9)	O(7)-Co(2)-O(5)	92.22(7)
O(7)#2-Co(2)-O(5)	87.78(7)	N(1)#2-Co(2)-O(5)	101.33(7)
N(1)-Co(2)-O(5)	78.67(7)	O(7)-Co(2)-O(5)#2	87.78(7)
O(7)#2-Co(2)-O(5)#2	92.22(7)	N(1)#2-Co(2)-O(5)#2	78.67(7)
N(1)-Co(2)-O(5)#2	101.33(7)	O(5)-Co(2)-O(5)#2	180.00(14)

Symmetry transformations used to generate equivalent atoms: [a] #1: -x+1, y+1/2, -z+3/2. #2: -x+1, y-1/2, -z+3/2. #3: -x+1, -y+1, -z+1. [b] #1: -x+1, -y+1/2, z+0. #2: y-1/4, -x+3/4, z-1/4. #3: -y+5/4, x-1/4, z-1/4. #4: x, y-1/2, -z. #5: -x+1, -y+1, -z. [c] #1: -x+2, -y+2, -z+1 #2: x+1, y, z. #3: -x+2, -y+1, -z+1. #4: x-1, y, z. [d] #1: -x+1/2, y+1/2, z . #2: -x+1/2, y-1/2,

z. [e]#1: -x+1, y-1/2, -z+1/2. #2: -x+1, y+1/2, -z+1/2. [f]#1: -x+2, y-1/2, -z. #2: -x+2, y+1/2, -z. [g]#1: -x+1, -y, -z+1. #2: -x+2, -y, -z

Table S2. Hydrogen bonds distances (Å) and angles (deg) for **1, 3, 4, 6** and and **7.**

1[a]			
D-H...A	d(H...A)	d(D...A)	∠(DHA)
O(2)-H(1W)...N(3)#6	2.10(5)	2.800(4)	166(5)
N(2)-H(2W)...O(2)#1	1.966(18)	2.808(6)	171(9)
3[c]			
O(3)-H(3)...O(1)	1.74	2.556(7)	170.8
O(7)-H(7)...O(8)	1.66	2.476(6)	174.9
N(2)-H(2)...O(5)#5	2.26	3.073(8)	156.8
O(11)-H(11A)...O(6)#6	2.23	2.859(6)	131.3
O(11)-H(11B)...O(7)#6	2.56	3.146(7)	126.6
4[d]			
O(5)-H(5)...O(2)	1.68	2.493(2)	173.1
6[f]			
O(9)-H(9A)...O(1)#3	2.32	3.046(4)	148.6
O(9)-H(9A)...O(7)#3	2.65	3.361(4)	145.6
O(8)-H(8A)...O(9)#1	1.66	2.476(4)	178.8
7[g]			
O(4)-H(4)...O(3)	1.65	2.465(2)	175.8
O(7)-H(7)...O(3)#3	1.87	2.678(2)	170.2
O(6)-H(6)...O(5)#4	1.99	2.781(2)	162.7
O(7)-H(10)...O(1)#5	1.82(4)	2.694(3)	169(4)

[a] #6: -x+1,-y+1,-z+2 [c]#5: -x+1, -y+2, -z+2, #6: x-1, y+1, z. [f]#3: x+1, y, z. [g]#3: -x+1, -y, -z, #4: x, y, z+1. #5: x, y, z-1.

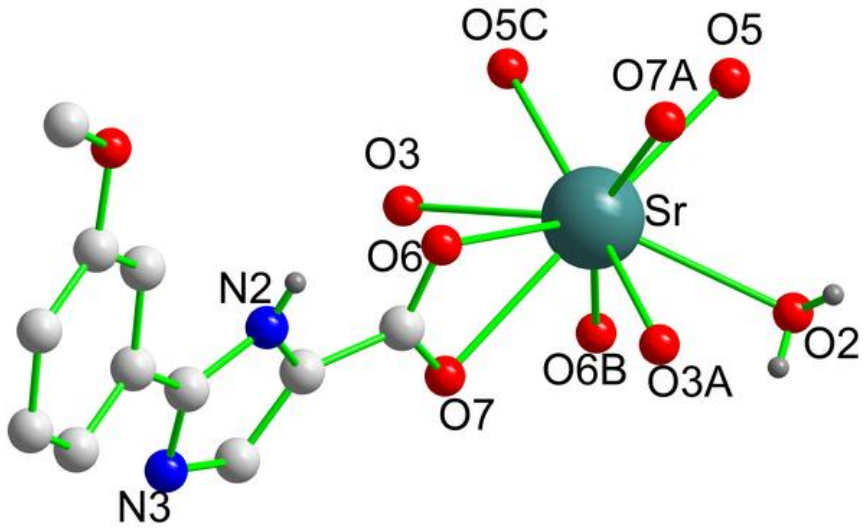

Figure S1. Molecular structure of complex **1** (H atoms omitted for clarity).

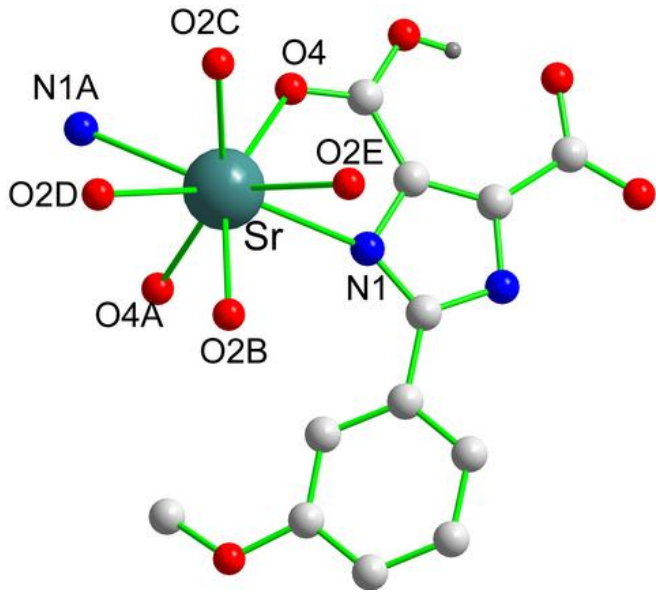

Figure S2. Coordination arrangement of the Sr(II) in complex **2** (H atoms omitted for clarity)

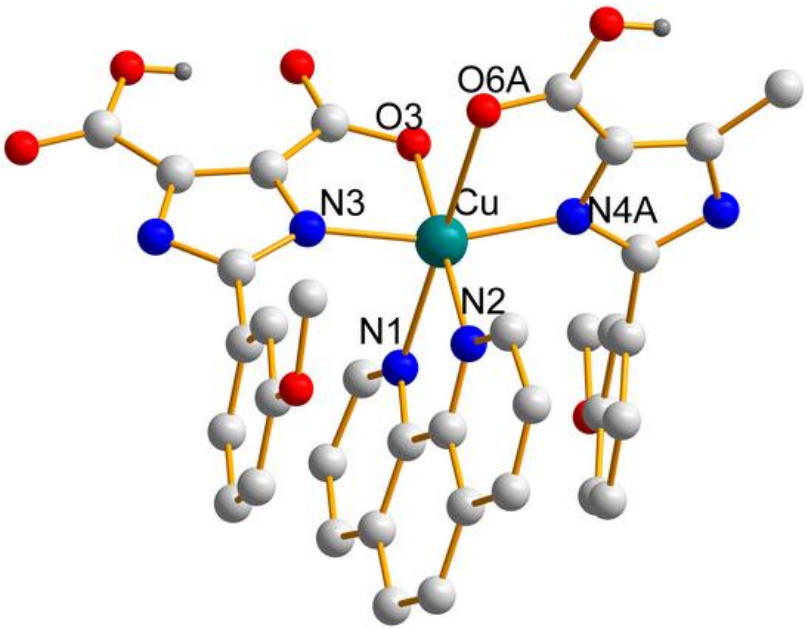

Figure S3. Coordination environment of Cu(II) atom in polymer **4** (H atoms omitted for clarity).

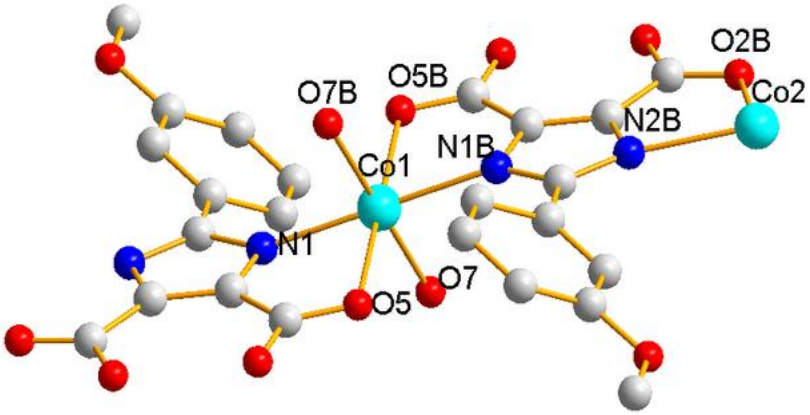

Figure S4. Coordination environment of Co(II) atom in polymer **7** (H atoms omitted for clarity).