Electronic Supplementary Material (ESI) for CrystEngComm

Design and construction of six metal-organic frameworks with 2-*p*-methoxyphenyl-1*H*-imidazole-4,5-dicarboxylate

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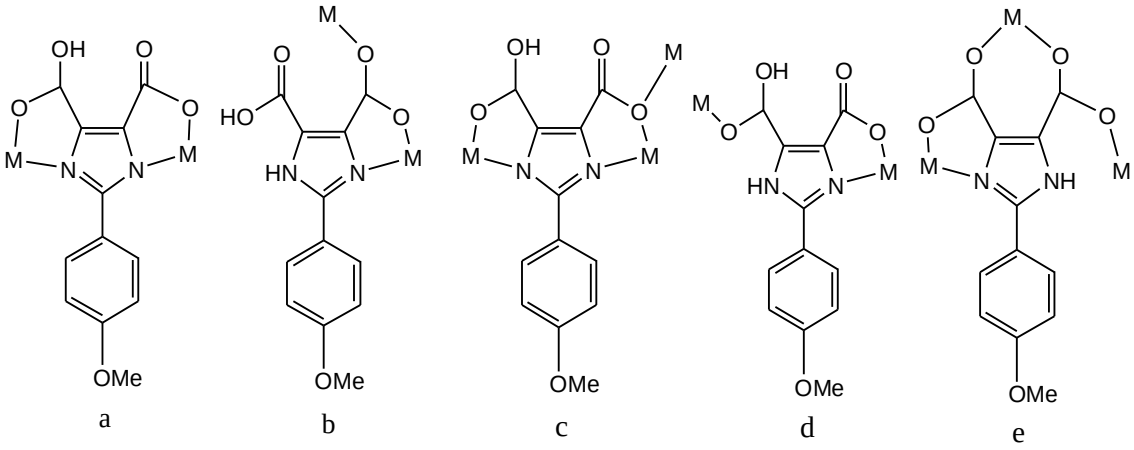
Supporting Information



Scheme S1. Coordination modes of $H_{3-n}MOPhIDC^{n-}$ anions (n = 1 or 2)

Table S1. Selected Bond Angles (deg) for Polymers **1** – **6**

		1[a]	
N(2)#1-Cu(1)-N(1)	172.5(2)	N(2)#1-Cu(1)-O(4)#1	83.96(14)
N(1)-Cu(1)-O(4)#1	89.15(15)	N(2)#1-Cu(1)-O(6)	96.99(16)
N(1)-Cu(1)-O(6)	90.51(17)	O(4)#1-Cu(1)-O(6)	149.73(13)
N(2)#1-Cu(1)-O(1)	100.22(13)	N(1)-Cu(1)-O(1)	79.57(13)
O(4)#1-Cu(1)-O(1)	112.62(12)	O(6)-Cu(1)-O(1)	97.05(13)
		2[b]	
N(2)-Zn(1)-N(4)	98.35(11)	N(2)-Zn(1)-N(3)	103.14(12)
N(4)-Zn(1)-N(3)	76.61(12)	N(2) -Zn(1)-N(1)#1	165.69(12)
N(4)-Zn(1)-N(1)#1	94.07(11)	N(3)-Zn(1)-N(1)#1	86.60(12)
N(2)-Zn(1)-O(1)	79.07(10)	N(4)-Zn(1)-O(1)	100.17(11)
N(3)-Zn(1)-O(1)	176.27(11)	N(1)#1-Zn(1)-O(1)	91.79(11)
N(2)-Zn(1)-O(4)#1	91.22(11)	N(4)-Zn(1)-O(4)#1	166.40(11)
N(3)-Zn(1)-O(4)#1	91.87(12)	N(1)#1-Zn(1)-O(4)#1	77.84(10)
O(1)-Zn(1)-O(4)#1	91.08(11)		
		3[c]	
N(4)-Co(1)-N(2)	95.71(7)	N(4)-Co(1)-N(3)	76.88(7)
N(2)-Co(1)-N(3)	102.66(7)	N(4)-Co(1)-N(1)#1	94.22(7)
N(2)-Co(1)-N(1)#1	168.21(7)	N(3)-Co(1)-N(1)#1	85.78(7)
N(4)-Co(1)-O(1)	100.42(7)	N(2)-Co(1)-O(1)	79.29(6)
N(3)-Co(1)-O(1)	176.76(6)	N(1)#1-Co(1)-O(1)	92.68(7)
N(4)-Co(1)-O(4)#1	168.85(7)	N(2)-Co(1)-O(4)#1	92.01(6)
N(3)-Co(1)-O(4)#1	93.59(7)	N(1)#1-Co(1)-O(4)#1	79.12(6)
O(1)-Co(1)-O(4)#1	88.91(6)		
		4[d]	
N(1)-Co(1)-N(4)	96.64(7)	N(1)-Co(1)-N(2)#1	167.34(6)

N(4)-Co(1)-N(2)#1	95.46(6)	N(1)-Co(1)-O(1)	79.84(6)
N(4)-Co(1)-O(1)	98.12(6)	N(2)#1-Co(1)-O(1)	94.79(6)
N(1)-Co(1)-N(3)	102.71(6)	N(4)-Co(1)-N(3)	77.90(7)
N(2)#1-Co(1)-N(3)	83.45(6)	O(1)-Co(1)-N(3)	175.43(6)
N(1)-Co(1)-O(4)#1	89.50(6)	N(4)-Co(1)-O(4)#1	169.99(6)
N(2)#1-Co(1)-O(4)#1	79.06(6)	O(1)-Co(1)-O(4)#1	90.73(6)
N(3)-Co(1)-O(4)#1	93.06(6)		

5[e]

N(3)-Cd(1)-N(3)#1	180.00	N(3)-Cd(1)-O(6)	73.78(7)
N(3)#1-Cd(1)-O(6)	106.22(7)	N(3)-Cd(1)-O(6)#1	106.22(7)
N(3)#1-Cd(1)-O(6)#1	73.78(7)	O(6)-Cd(1)-O(6)#1	180.00
N(3)-Cd(1)-O(1)#1	89.34(7)	N(3)#1-Cd(1)-O(1)#1	90.66(7)
O(6)-Cd(1)-O(1)#1	98.97(7)	O(6)#1-Cd(1)-O(1)#1	81.03(7)
N(3)-Cd(1)-O(1)	90.66(7)	N(3)#1-Cd(1)-O(1)	89.34(7)
O(6)-Cd(1)-O(1)	81.03(7)	O(6)#1-Cd(1)-O(1)	98.97(7)
O(1)#1-Cd(1)-O(1)	180.00	N(4)#2-Cd(2)-N(1)#3	112.07(8)
N(4)#2-Cd(2)-O(9)	145.39(7)	N(1)#3-Cd(2)-O(9)	102.30(7)
N(4)#2-Cd(2)-O(2)#3	109.00(7)	N(1)#3-Cd(2)-O(2)#3	73.69(7)
O(9)-Cd(2)-O(2)#3	83.95(7)	N(4)#2-Cd(2)-O(11)	93.75(8)
N(1)#3-Cd(2)-O(11)	89.05(8)	O(9)-Cd(2)-O(11)	82.56(9)
O(2)#3-Cd(2)-O(11)	155.25(7)	N(4)#2-Cd(2)-O(9)#2	71.71(7)
N(1)#3-Cd(2)-O(9)#2	168.05(8)	O(9)-Cd(2)-O(9)#2	73.80(7)
O(2)#3-Cd(2)-O(9)#2	116.48(7)	O(11)-Cd(2)-O(9)#2	79.29(8)

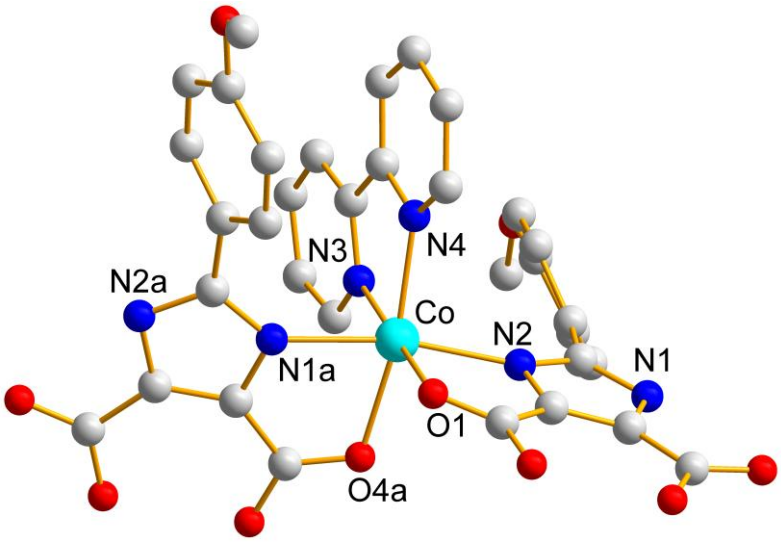
6[f]

O(3)-Co(1)-O(1)	91.60(8)	O(3)-Co(1)-O(4)#1	92.35(8)
O(1)-Co(1)-O(4)#1	85.22(7)	O(3)-Co(1)-N(5)	88.74(9)
O(1)-Co(1)-N(5)	90.89(9)	O(4)#1-Co(1)-N(5)	175.98(8)
O(3)-Co(1)-O(5)	176.49(7)	O(1)-Co(1)-O(5)	90.81(8)
O(4)#1-Co(1)-O(5)	90.40(8)	N(5)-Co(1)-O(5)	88.66(9)

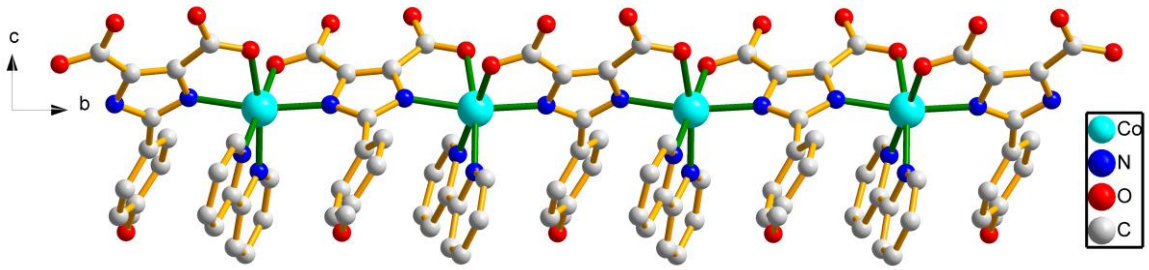
O(3)-Co(1)-N(1)#1	90.27(9)	O(1)-Co(1)-N(1)#1	162.19(8)
O(4)#1-Co(1)-N(1)#1	77.01(8)	N(5)-Co(1)-N(1)#1	106.86(9)
O(5)-Co(1)-N(1)#1	88.22(9)	O(2)-Co(2)-O(2)#2	180.00
O(2)-Co(2)-N(4)#3	90.32(8)	O(2)#2-Co(2)-N(4)#3	89.68(8)
O(2)-Co(2)-N(4)#4	89.68(8)	O(2)#2-Co(2)-N(4)#4	90.32(8)
N(4)#3-Co(2)-N(4)#4	180.00	O(2)-Co(2)-O(8)#3	90.89(8)
O(2)#2-Co(2)-O(8)#3	89.11(8)	N(4)#3-Co(2)-O(8)#3	78.05(8)
N(4)#4-Co(2)-O(8)#3	101.95(8)	O(2)-Co(2)-O(8)#4	89.11(8)
O(2)#2-Co(2)-O(8)#4	90.89(8)	N(4)#3-Co(2)-O(8)#4	101.95(8)
N(4)#4-Co(2)-O(8)#4	78.05(8)	O(8)#3-Co(2)-O(8)#4	180.000

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

(a)



(b)



(c)

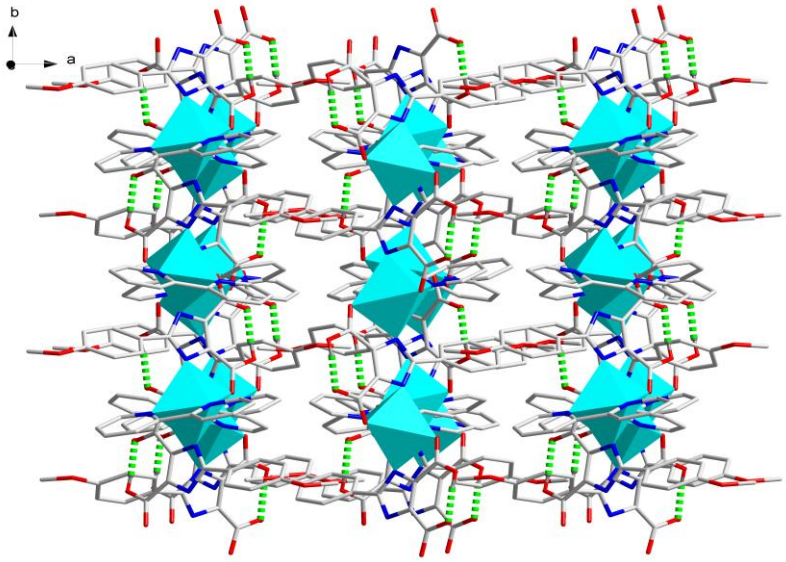


Figure S1. (a) Coordination arrangements of the Co(II) in polymer **3** (H atoms omitted for clarity). (b) View of the 1-D chain supported by Co(II) ions and μ_2-HMOPhIDC^{2-} ligands. (c) View of the 3-D supramolecular framework of polymer **3.**

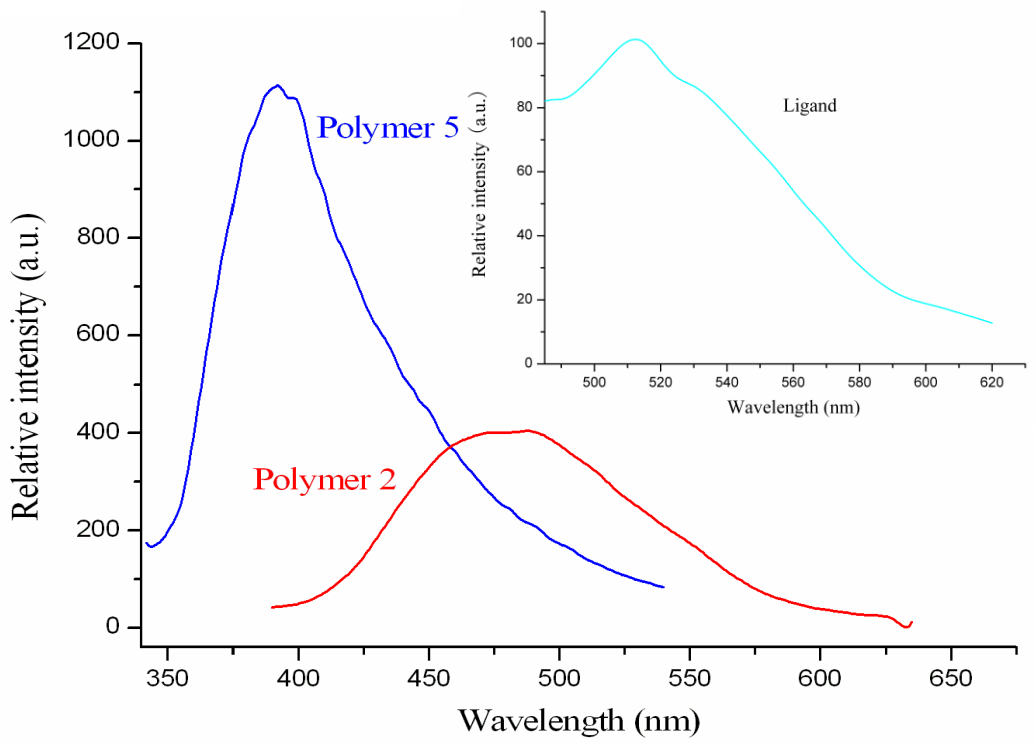


Figure S2. The solid-state photoluminescent spectra of the free H_3MOPhIDC ligand (cyan), polymers **2** (red) and **5** (blue) at room temperature.