Supporting Information

Syntheses, Structures and Photoluminescence of Zinc(II) Coordination Polymers Based on Carboxylates and Flexible Bis-[(pyridyl)-benzimidazole] Ligands

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Table S1. Selected bond lengths [Å] and angles [°] for **1**-**6**[a]

		Compound **1**	
Zn(1)-N(2)	2.008(6)	Zn(1)-O(4)	2.043(5)
Zn(1)-O(3)#1	2.044(4)	Zn(1)-O(2)#2	2.087(4)
Zn(1)-N(3)	2.392(8)	Zn(1)-O(1)#2	2.436(6)
N(2)-Zn(1)-O(4)	115.2(3)	N(2)-Zn(1)-O(3)#1	115.8(2)
O(4)-Zn(1)-O(3)#1	89.81(18)	N(2)-Zn(1)-O(2)#2	131.8(2)
O(4)-Zn(1)-O(2)#2	93.25(18)	O(3)#1-Zn(1)-O(2)#2	101.44(19)
N(2)-Zn(1)-N(3)	71.5(3)	O(4)-Zn(1)-N(3)	167.2(2)
O(3)#1-Zn(1)-N(3)	77.4(2)	O(2)#2-Zn(1)-N(3)	89.2(2)
N(2)-Zn(1)-O(1)#2	84.3(2)	O(4)-Zn(1)-O(1)#2	88.6(2)
O(3)#1-Zn(1)-O(1)#2	158.25(18)	O(2)#2-Zn(1)-O(1)#2	57.03(18)
N(3)-Zn(1)-O(1)#2	103.2(2)		
		Compound **2**	
Zn(1)-O(3)	1.974(5)	Zn(1)-N(1)	2.046(7)
Zn(1)-O(1W)	2.092(7)	Zn(1)-O(1)	2.098(5)
Zn(1)-N(3)	2.315(8)		
O(3)-Zn(1)-N(1)	107.7(3)	O(3)-Zn(1)-O(1W)	129.2(2)
N(1)-Zn(1)-O(1W)	120.5(3)	O(3)-Zn(1)-O(1)	100.0(2)
N(1)-Zn(1)-O(1)	99.0(3)	O(1W)-Zn(1)-O(1)	87.9(2)
O(3)-Zn(1)-N(3)	95.8(2)	N(1)-Zn(1)-N(3)	75.2(3)
O(1W)-Zn(1)-N(3)	82.7(3)	O(1)-Zn(1)-N(3)	164.2(2)
		Compound **3**	
Zn(1)-O(1)	1.959(5)	Zn(1)-O(3)#1	1.977(5)
Zn(1)-N(1)	2.003(6)	Zn(1)-N(2)	2.153(6)
O(1)-Zn(1)-O(3)#1	105.9(2)	O(1)-Zn(1)-N(1)	116.9(3)
O(3)#1-Zn(1)-N(1)	128.5(2)	O(1)-Zn(1)-N(2)	124.6(2)
O(3)#1-Zn(1)-N(2)	100.6(2)	N(1)-Zn(1)-N(2)	78.3(3)
		Compound **4**	
Zn(1)-N(1)	2.053(5)	Zn(1)-O(1)	2.069(4)
Zn(1)-N(3)	2.134(6)	Zn(1)-O(4)#1	2.166(5)
Zn(1)-O(3)#1	2.176(4)	Zn(1)-O(2)	2.246(5)
N(1)-Zn(1)-O(1)	153.54(18)	N(1)-Zn(1)-N(3)	78.5(2)
O(1)-Zn(1)-N(3)	95.04(19)	N(1)-Zn(1)-O(4)#1	97.76(18)
O(1)-Zn(1)-O(4)#1	99.37(18)	N(3)-Zn(1)-O(4)#1	152.17(19)
N(1)-Zn(1)-O(3)#1	104.72(17)	O(1)-Zn(1)-O(3)#1	101.30(18)
N(3)-Zn(1)-O(3)#1	94.1(2)	O(4)#1-Zn(1)-O(3)#1	59.84(19)
N(1)-Zn(1)-O(2)	97.12(19)	O(1)-Zn(1)-O(2)	59.41(18)
N(3)-Zn(1)-O(2)	104.9(2)	O(4)#1-Zn(1)-O(2)	102.9(2)
O(3)#1-Zn(1)-O(2)	153.5(2)		
		Compound **5**	
Zn(1)-O(4)	1.949(3)	Zn(1)-O(1)#1	1.975(3)
Zn(1)-O(2)#2	2.023(3)	Zn(1)-N(2)	2.045(3)

Zn(1)-N(3)	2.284(3)		
O(4)-Zn(1)-O(1)#1	101.8(1)	O(4)-Zn(1)-O(2)#2	96.8(1)
O(1)#1-Zn(1)-O(2)#2	110.8(1)	O(4)-Zn(1)-N(2)	147.4(1)
O(1)#1-Zn(1)-N(2)	104.6(1)	O(2)#2-Zn(1)-N(2)	91.5(1)
O(4)-Zn(1)-N(3)	87.3(1)	O(1)#1-Zn(1)-N(3)	90.2(1)
O(2)#2-Zn(1)-N(3)	157.1(1)	N(2)-Zn(1)-N(3)	73.8(1)
		Compound **6**	
Zn(1)-O(1)	1.985(3)	Zn(1)-O(4)	1.987(3)
Zn(1)-O(3)#1	2.015(2)	Zn(1)-N(1)	2.071(3)
Zn(1)-N(2)	2.278(3)		
O(1)-Zn(1)-O(4)	98.49(13)	O(1)-Zn(1)-O(3)#1	98.29(12)
O(4)-Zn(1)-O(3)#1	112.20(11)	O(1)-Zn(1)-N(1)	150.99(13)
O(4)-Zn(1)-N(1)	104.17(11)	O(3)#1-Zn(1)-N(1)	89.75(11)
O(1)-Zn(1)-N(2)	87.22(12)	O(4)-Zn(1)-N(2)	92.14(12)
O(3)#1-Zn(1)-N(2)	153.73(12)	N(1)-Zn(1)-N(2)	74.20(12)

Symmetry codes For **1:** #1 -x+1,y,-z+1/2; #2 x,-y,z-1/2. For **3**: #1 x+1/2,-y+1/2,z-1/2. For **4**: #1 x,-y+1,z+1/2. For **5**: #1 x+1/2,-y+1/2,z+1/2; #2 -x-1/2,y-1/2,-z+1/2. For **6**: #1 -x+1,-y,-z.

Table S2. Hydrogen-bond geometries for compounds **1**-**6**(Å, ^{o})

D-H···A	D-H [Å]	H···A [Å]	D···A [Å]	<D-H···A [˚]
		Compound **1**		
O(1W)-H(1A)...O(2)	0.83(5)	2.19(3)	2.979(8)	157(7)
O(1W)-H(1B)...O(4)#1	0.83(7)	2.32(4)	3.102(7)	156(8)
		Compound **2**		
O(1W)-H(1A)...O(4)#4	0.85(6)	2.31(9)	2.825(9)	120(9)

Symmetry codes For **1**: #1 -x+1,y,-z+1/2. For **2**: #4 -x+1,-y+1,-z+2.

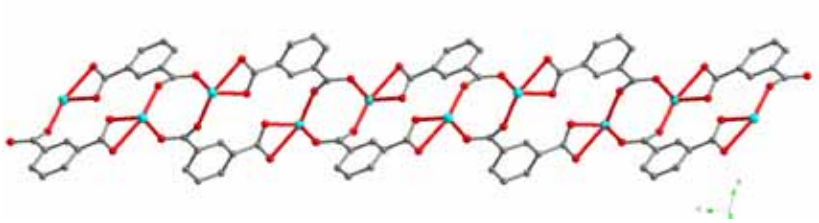
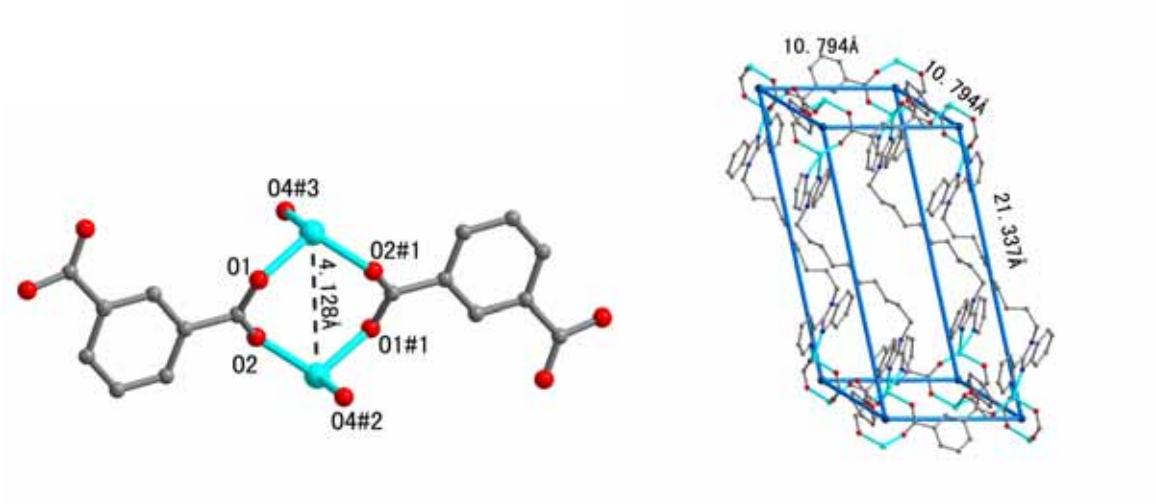
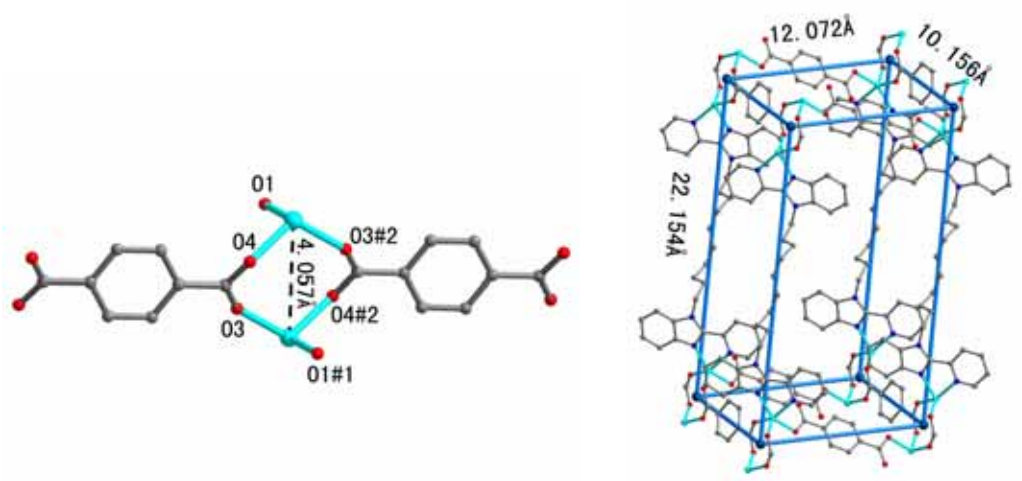


Figure S1. The Zn–*m*-BDC double chain in **1**

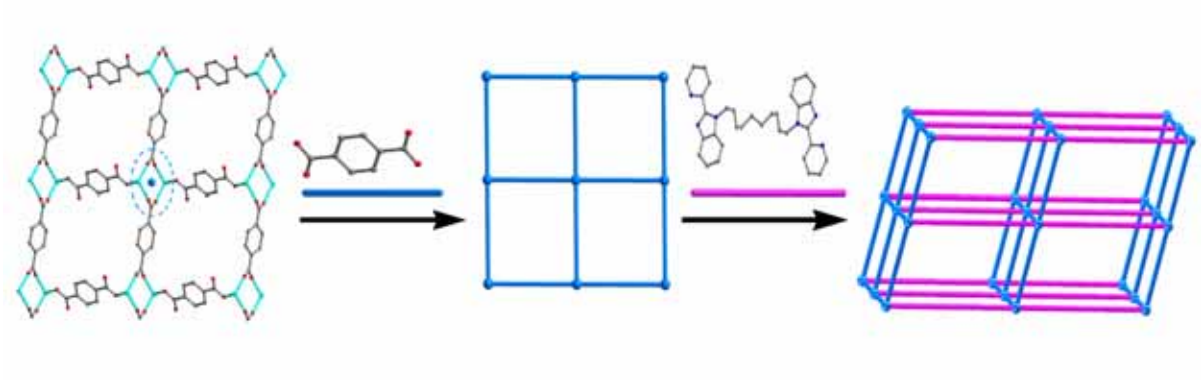


(a) (b)

Figure S2. (a) The bimetallic unit $[Zn_2(CO_2)_2]$ in **5**. (b) The dimensional sizes of the 3D framework of **5**.



(a) (b)



(c)

Figure S3. (a) The bimetallic unit $[Zn_2(CO_2)_2]$ in **6**. (b) The dimensional sizes of the 3D framework of **6**. (c) Schematic view of the α-Po network of **6**.

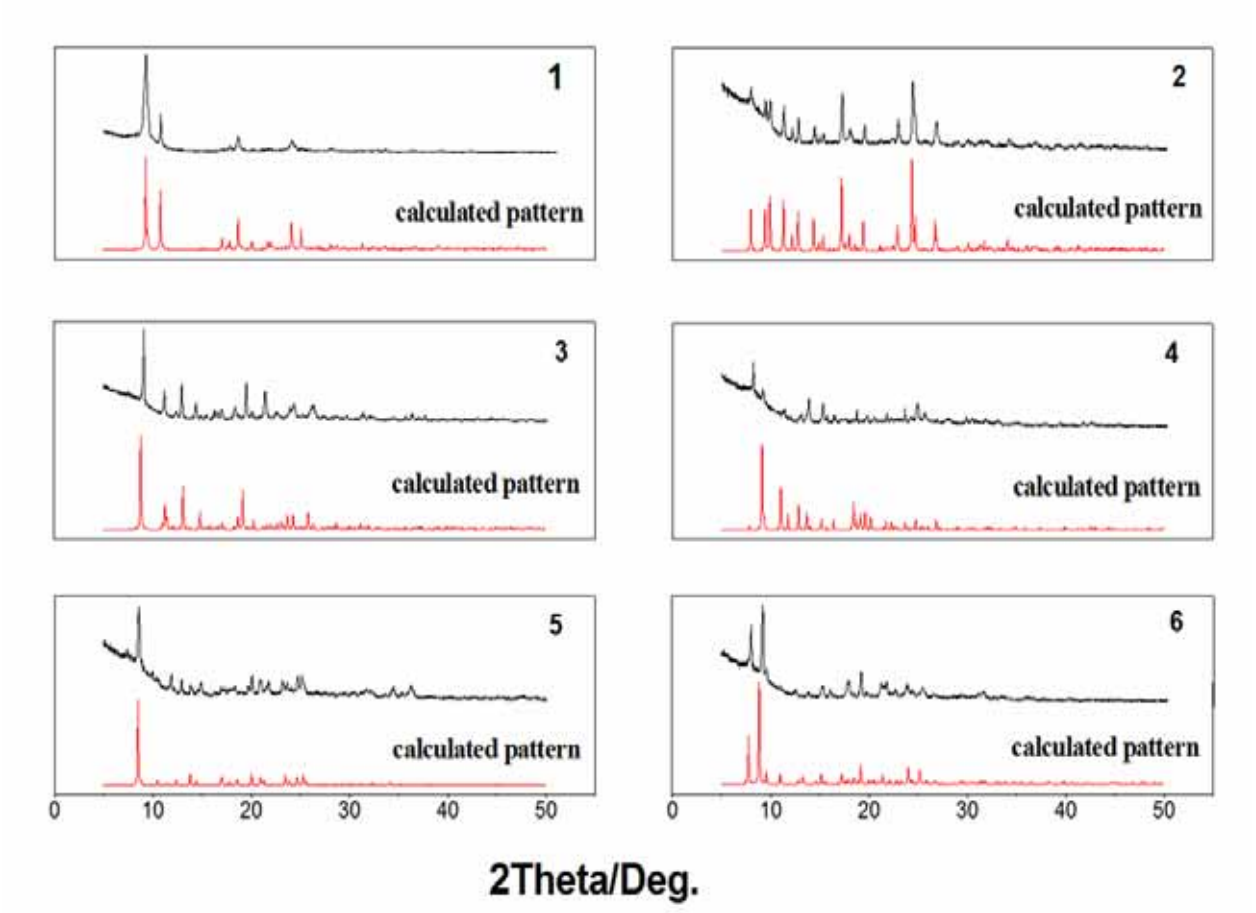


Figure S4. The calculated and experimental PXRD patterns of compounds **1**–**6**.