Electronic Supplementary Material (ESI) for CrystEngComm

Supporting information for

Positional Isomeric and Substitutent Effect on the Assemblies of a Series of d^{10} Coordination Polymers Based Upon Unsymmetric Tricarboxylate Acids and Nitrogen-Containing Ligands

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Table S1. Selected bond lengths (Å) and angles (°) of compounds **1**-**7**.

		1	
Zn(1)-O(6B)	1.948(2)	Zn(1)-O(1)	2.031(3)
Zn(1)-O(4A)	1.956(2)	Zn(1)-O(2C)	1.955(2)
O(4)-Zn(1)-O(6B)	105.45(11)	O(1)-Zn(1)-O(6B)	96.73(11)
O(4A)-Zn(1)-O(2C)	127.57(12)	O(1)-Zn(1)-O(2C)	106.55(12)
O(6B)-Zn(1)-O(2C)	112.07(12)	O(1)-Zn(1)-O(4A)	103.86(10)
		2	
Cd(1)-O(1)	2.301(12)	Cd(1)-O(2C)	2.198(8)
Cd(1)-O(4A)	2.319(8)	Cd(1)-O(5B)	2.355(8)
Cd(1)-O(3A)	2.393(9)	Cd(1)-O(6B)	2.479(9)
O(1)-Cd(1)-O(2C)	101.5(3)	O(1)-Cd(1)-O(3A)	83.8(3)
O(1)-Cd(1)-O(5B)	130.6(3)	O(1)-Cd(1)-O(6B)	80.5(3)
O(1)-Cd(1)-O(4A)	106.4(3)	O(2C)-Cd(1)-O(3A)	115.5(3)
O(2C)-Cd(1)-O(4A)	148.6(3)	O(2C)-Cd(1)-O(5B)	84.2(3)
O(3A)-Cd(1)-O(4A)	55.0(3)	O(3A)-Cd(1)-O(5B)	138.0(3)
O(2C)-Cd(1)-O(6B)	114.3(3)	O(3A)-Cd(1)-O(6B)	129.8(3)
O(4A)-Cd(1)-O(5B)	88.4(3)	O(4A)-Cd(1)-O(6B)	84.6(3)
O(5B)-Cd(1)-O(6B)	53.7(3)		
		3	
Zn(1)-O(1A)	1.937(3)	Zn(1)-O(3)	2.203(3)
Zn(1)-N(1)	2.033(3)	Zn(1)-N(2B)	2.058(3)
Zn(1)-O(4)	2.133(3)	O(1A)-Zn(1)-O(3)	104.56(14)
O(1A)-Zn(1)-O(4)	111.05(13)	O(1A)-Zn(1)-N(1)	108.86(14)
O(3)-Zn(1)-O(4)	60.02(14)	O(3)-Zn(1)-N(1)	142.68(14)
O(1A)-Zn(1)-N(2B)	91.51(13)	O(3)-Zn(1)-N(2B)	90.41(14)
O(4)-Zn(1)-N(1)	92.21(14)	O(4)-Zn(1)-N(2B)	145.90(15)
N(1)-Zn(1)-N(2B)	104.66(14)		
		4	
Zn(1)-O(1)	1.952(4)	Zn(1)-O(7)	2.170(5)
Zn(1)-N(2B)	2.044(6)	Zn(2)-O(3)	2.082(7)
Zn(1)-N(1)	2.184(5)	Zn(2)-O(4)	2.460(11)
Zn(2)-O(3')	1.927(14)	Zn(2)-N(3)	2.044(4)
O(1)-Zn(1)-O(7)	92.84(13)	O(1)-Zn(1)-N(1)	86.17(13)
O(1)-Zn(1)-O(1A)	113.0(2)	O(1)-Zn(1)-N(2B)	123.43(11)
O(7)-Zn(1)-N(1)	178.2(2)	O(7)-Zn(1)-N(2B)	88.5(2)
O(3)-Zn(2)-O(4)	57.5(3)	O(3)-Zn(2)-O(3C)	132.4(5)
N(1)-Zn(1)-N(2B)	93.3(2)	O(3)-Zn(2)-O(4C)	90.3(4)
O(3)-Zn(2)-N(3)	120.5(3)	O(3)-Zn(2)-N(3C)	91.4(2)
O(4)-Zn(2)-O(4C)	97.5(5)	O(4)-Zn(2)-N(3)	91.6(3)
O(4)-Zn(2)-N(3C)	147.4(3)	N(3)-Zn(2)-N(3C)	97.4(2)
		5	
Cd(1)-O(4A)	2.361(8)	Cd(1)-O(8)	2.310(8)
Cd(1)-O(11A)	2.309(7)	Cd(1)-N(2B)	2.324(0)
Cd(1)-O(10)	2.271(7)	Cd(2)-O(3A)	2.304(7)
Cd(2)-N(1)	2.293(0)	Cd(2)-O(5)	2.316(7)
Cd(2)-O(7)	2.387(7)	Cd(2)-O(9)	2.450(7)
Cd(2)-O(6)	2.549(7)	O(4A)-Cd(1)-O(8)	165.6(3)
O(5)-Cd(2)-N(1)	145.8(3)	O(4A)-Cd(1)-O(10)	93.6 (3)
O(5)-Cd(2)-O(9)	87.0(3)	O(4A)-Cd(1)-N(2B)	90.4(3)
O(4A)-Cd(1)-O(11A)	102.3(2)	O(8)-Cd(1)-O(10)	80.9(3)
O(8)-Cd(1)-O(11A)	91.3(3)	O(5)-Cd(2)-O(7)	90.9(3)
O(3A)-Cd(2)-O(5)	88.2(3)	O(3A)-Cd(2)-O(6)	138.6(3)
O(8)-Cd(1)-N(2B)	83.6(3)	O(3A)-Cd(2)-O(7)	88.6(3)
O(3A)-Cd(2)-O(9)	102.2(3)	O(3A)-Cd(2)-N(1)	124.6(3)
O(5)-Cd(2)-O(6)	54.2(3)		
		6	
Cd(1)-O(4A)	2.323(8)	Cd(1)-O(8)	2.315(8)
Cd(1)-O(11A)	2.263(7)	Cd(1)-O(12A)	2.633(7)
Cd(1)-O(10)	2.242(7)	Cd(1)-N(2B)	2.302(9)
Cd(2)-O(3A)	2.286(7)	Cd(2)-O(5)	2.285(7)
Cd(2)-O(7)	2.343(7)	Cd(2)-O(9)	2.430(7)
Cd(2)-O(6)	2.538(7)	Cd(2)-N(1)	2.261(8)
O(4A)-Cd(1)-O(8)	169.5(2)	O(4A)-Cd(1)-O(10)	96.1(3)
O(4A)-Cd(1)-O(12A)	90.5(2)	O(4A)-Cd(1)-N(2B)	89.8(3)

O(4A)-Cd(1)-O(11A)	100.6(2)	O(8)-Cd(1)-O(10)	79.4(3)
O(8)-Cd(1)-O(11A)	89.4(3)	O(8)-Cd(1)-O(12A)	98.2(2)
O(3A)-Cd(2)-O(5)	88.2(3)	O(3A)-Cd(2)-O(6)	138.6(2)
O(8)-Cd(1)-N(2B)	86.0(3)	O(3A)-Cd(2)-O(7)	88.9(3)
O(3A)-Cd(2)-O(9)	103.7(2)	O(3A)-Cd(2)-N(1)	123.9(3)
O(5)-Cd(2)-O(7)	90.3(2)	O(5)-Cd(2)-O(9)	85.7(2)
O(5)-Cd(2)-O(6)	54.3(2)	O(5)-Cd(2)-N(1)	147.1(3)
		7	
Zn(1)-O(1')	1.867(16)	Zn(1)-N(1)	2.043(5)
O(1')-Zn(1)-O(1'A)	76.7(9)	N(1)-Zn(1)-N(1A)	97.9(3)
O(1')-Zn(1)-N(1)	103.9(5)	O(1')-Zn(1)-N(1A)	142.2(5)

[a] Symmetry codes: **1**, A, x, -y+3/2, z-1/2; B, -x, -y+2, -z+1; C, -x+1, -y+2, -z+1; **2**, A, x, -y+1/2, z-1/2; B, -x+1, -y+1, -z; C, -x+2, -y+1, -z; **3**, A, x-1/2, -y+1/2, -z+2; B, x, -y-1/2, z+1/2; **4**, A, x, y, -z+3/2; B, -x+3, y+1/2, z; C, x, -y+3/2, -z+2; **5**, A, x+1, y, z; B, x, -y+1/2, z-1/2; **6**, A, x-1, y, z; B, x, -y+1/2, z+1/2; **7**, A, -x, y, -z+1/2.

Table S2. The bond geometries of the hydrogen bonding interactions in compounds **1**-**7**.

D-H···A	d(D···A)/Å	<DHA/ º
1		
N2-H2A···O7	2.761	150.99
N2-H2B···O3^{i}	2.827	136.32
N2'-H2'B···O3'^{i}	2.726	162.99
O7-H18C···N2'	3.150	143.72
2		
N1-H1A···O6^{i}	2.974	158.91
N1-H1B···O3^{ii}	2.928	142.38
3		
O5-H5···O2^{i}	2.611	132.28
4		
O5-H5A···O3^{i}	2.748	161.21
O5-H5A···O4'^{i}	2.945	146.52
O7-H7B···O2	2.722	169.70
5		
O1-H1···O12^{i}	2.758	159.51
O7-H7A···O3^{ii}	2.826	153.70
O7-H7B···O5^{iii}	2.753	153.21
O8-H8A···O11^{iv}	2.803	177.19
O8-H8B···O16^{v}	2.715	176.95
O13-H13···O15^{vi}	2.587	171.54
O15-H15A···O10^{vii}	2.840	166.96
O15-H15B···O1^{viii}	2.848	166.45
O16-H16A···O9^{ix}	2.968	174.89
O16-H16B···O14^{x}	2.911	174.91
6		
O1-H1A···O12	2.673	158.40
O7-H7A···O3^{ii}	2.753	154.55
O7-H7B···O5^{iii}	2.705	152.86
O8-H8A···O11^{iv}	2.809	174.95
O8-H8B···O16^{v}	2.689	175.20
O13-H13···O15^{vi}	2.546	168.99
O15-H15A···O1^{vii}	2.819	165.89
O15-H15B···O10^{viii}	2.772	166.27
O16-H16A···O9^{ix}	2.874	175.90
O16-H16B···O14^{x}	2.859	176.43
7		
O4-H4···O5	2.567	161.71
O4'-H4'···O5	2.825	149.67
O5-H5C···O2^{i}	2.741	156.45
O5-H5D···O4^{ii}	2.727	141.34

Symmetry codes: For **1**, i, x, -y+3/2, z-1/2; ii, x, -y+3/2, z-1/2. For **2**, i, -x+1, -y+1, -z+1; ii, -x, y+1/2, -z+3/2. For **3**, i, x, -y+1/2, z-1/2. For **4**, i, -x+1, y-1/2, z. For **5**, i, x, -y+1/2, z-1/2; ii, -x+1, -y, -z; iii, -x+2, -y, -z; iv, -x+2, -y+1, -z; v, x+1, y, z; vi, -x+1, y-1/2, -z+1/2; vii, x-1, y, z; viii, x, -y+1/2, z+1/2; ix, -x+1, -y+1, -z; x, -x+1, y+1/2, -z+1/2; For **6**, i, x, -y+1/2, z-1/2; ii, -x+1, -y+1, -z+1; iii, -x, -y+1, -z+1; iv, -x, -y, -z+1; v, x-1, -y+1/2, z-1/2; vi, -x+1, y-1/2, -z+1/2; vii, x, -y+3/2, z-1/2; viii, x+1, y+1, z; xi, -x+1, y+1/2, -z+3/2; x, -x+1, -y+1, -z+1. For **7**, i, -x+1/2, y-1/2, -z+1/2; ii, -x+1/2, -y+1/2, -z.

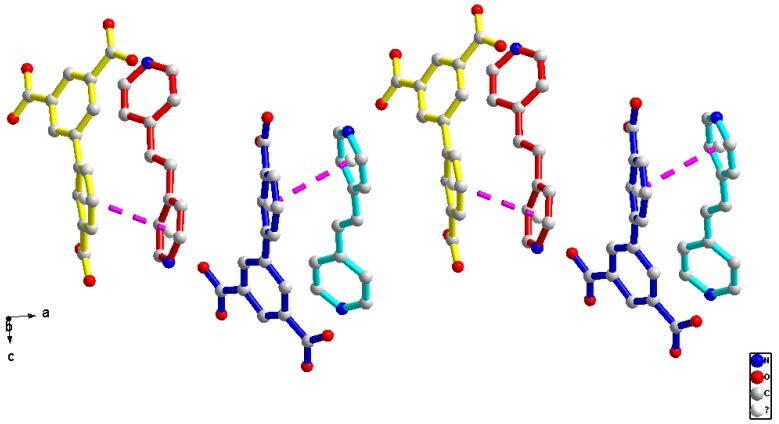
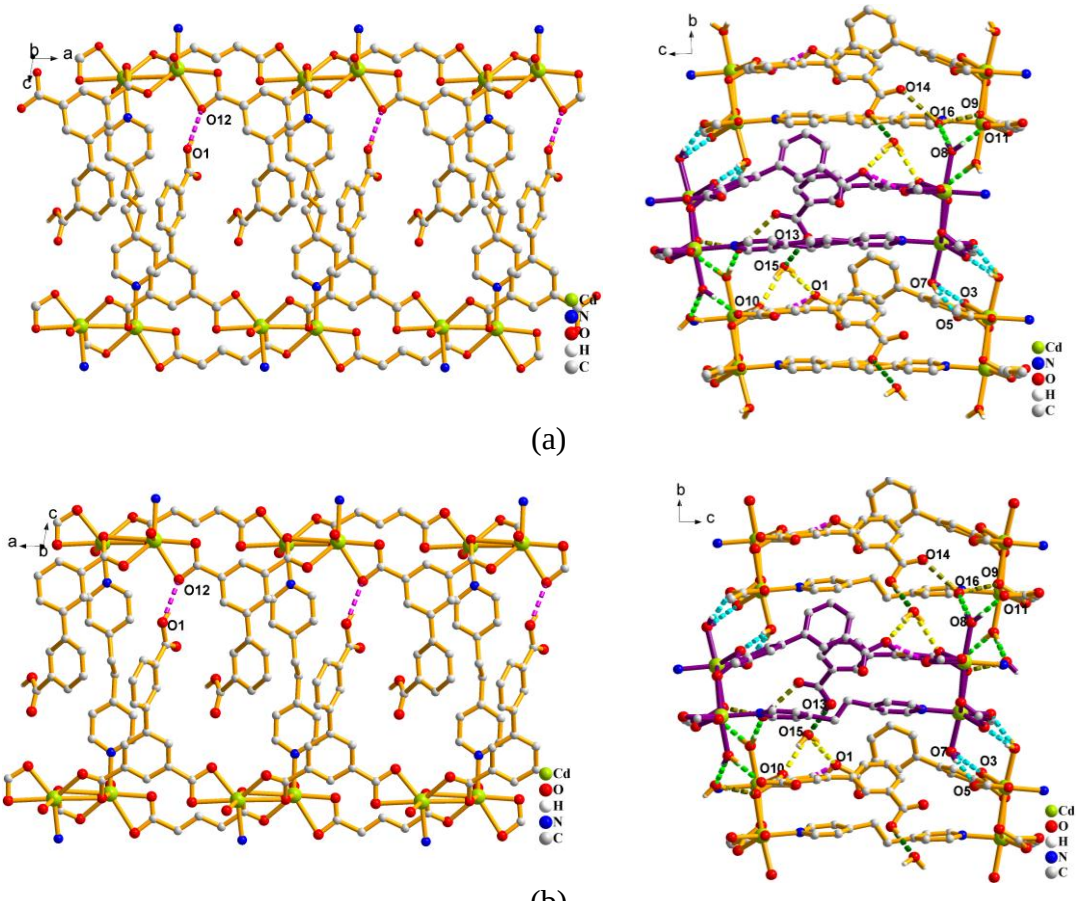


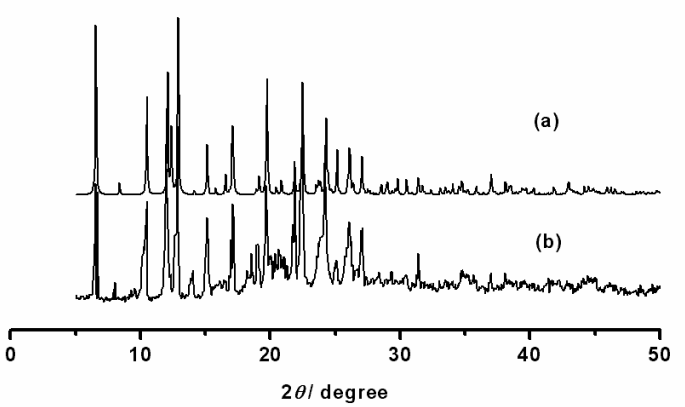
Figure S1. View of π···π interactions within the layer in compound **3**. Different interpenetrating units are illustrated in different colors.



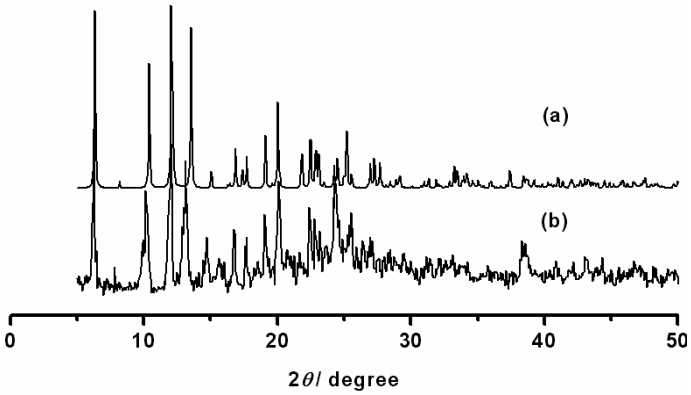
(a)

(b)

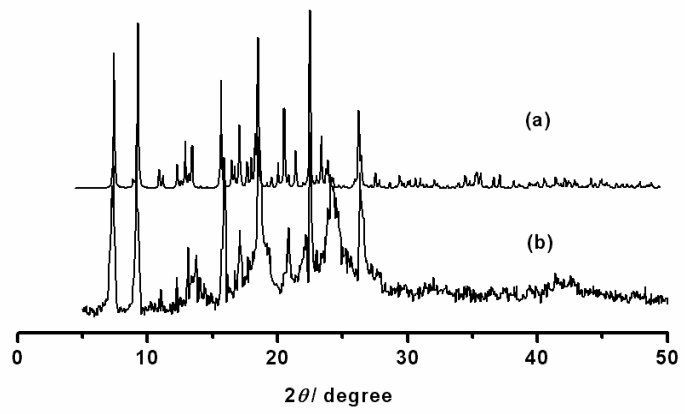
Figure S2. (a) Left: A view of O-H···O interactions within the layer in compound **5**. Right: Perspective view of O-H···O interactions between the neighboring layers in compound **5** (different types of hydrogen bonds are illustrated in five colors). (b) Left: A view of O-H···O interactions within the layer in compound **6**. Right: Perspective view of O-H···O interactions between the neighboring layers in compound **6** (different types of hydrogen bonds are illustrated in five colors).



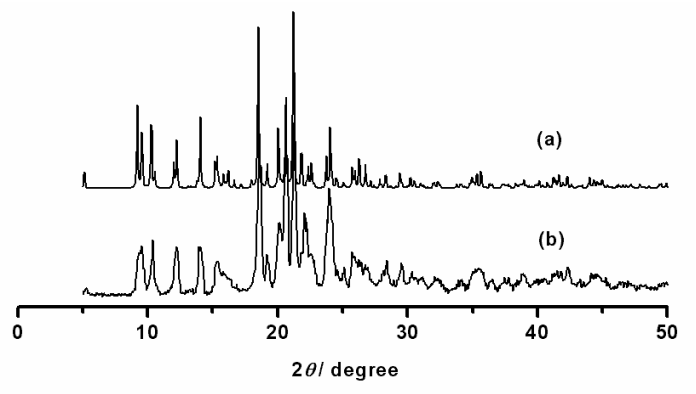
compound **1**



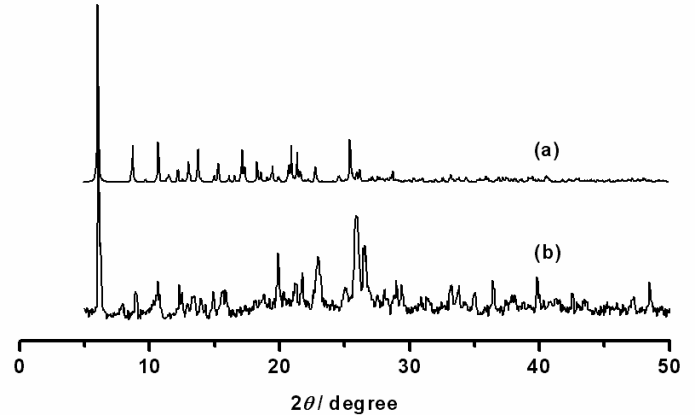
compound **2**



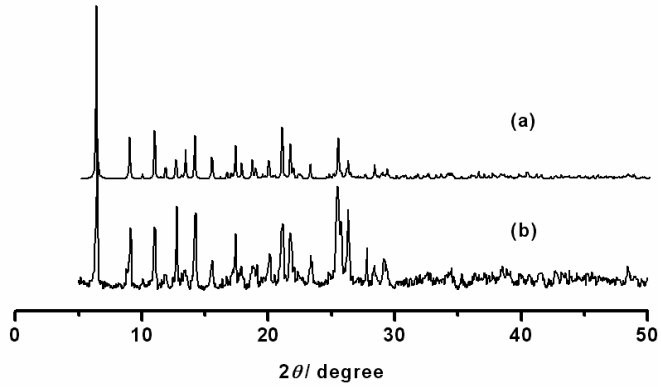
compound **3**



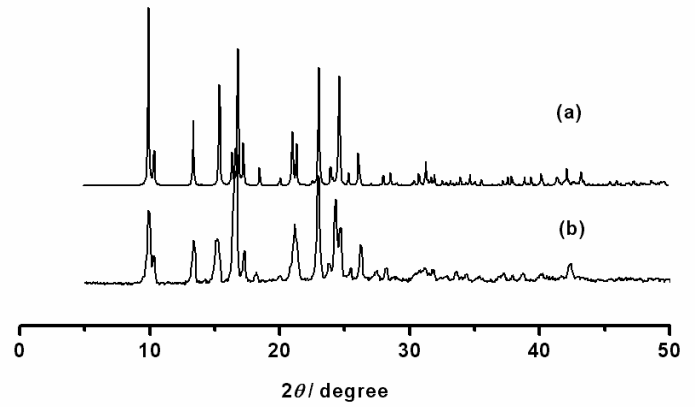
compound **4**



compound **5**



compound **6**



compound **7**

Figure S3. Powder XRD pattern of compounds **1**-**7**. (a) simulated and (b) as-synthesized.

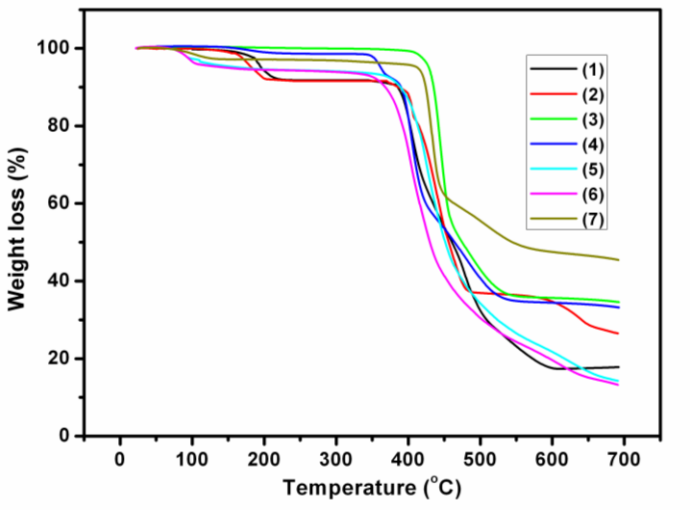
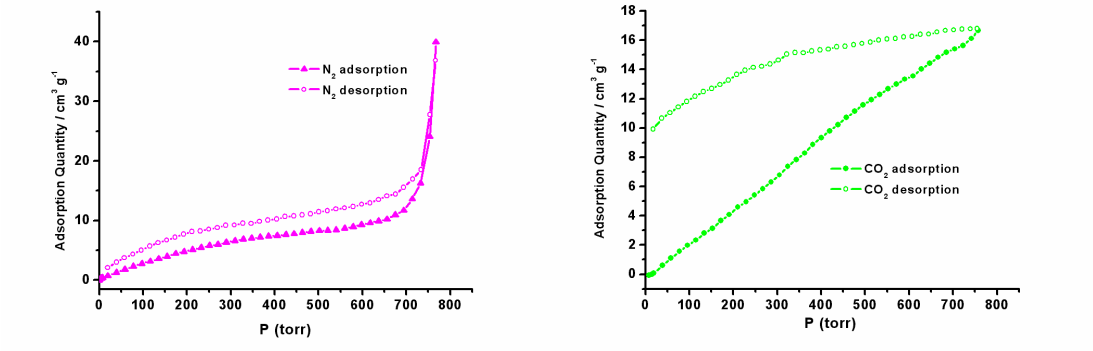
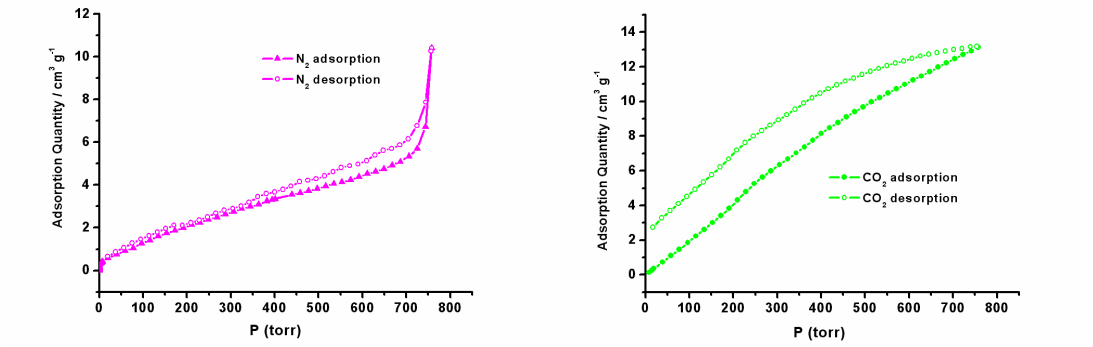


Figure S4. TGA data of compounds **1**-**7**.



(a)



(b)

Figure S5. Gas sorption isotherms of the activated **1** (a) and **2** (b). Sorption and desorption data are show as filled and open symbols, respectively.

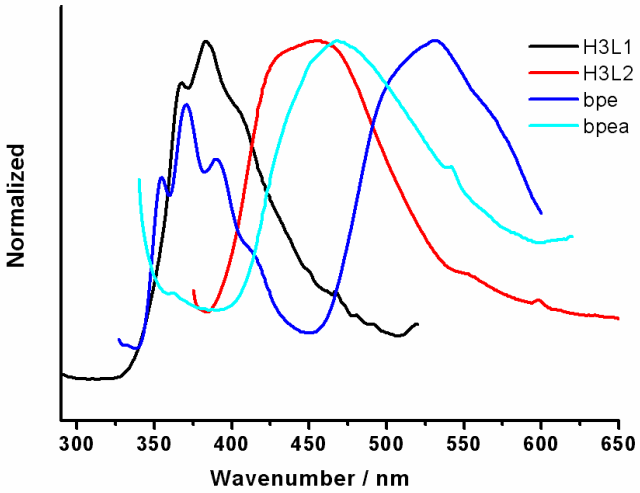


Figure S6. Normalized solid-state photoluminescence spectra of the ligands at room temperature.