Supplementary Information

Syntheses, structures and luminescent properties of six divalent metal terephthalate coordination polymers based on three new flexible bis(imidazole) ligands

Wei-Guan Yuan, Fang Xiong, Hong-Ling Zhang, Wei Tang, Shu-Fang Zhang, Zhan He, Lin-Hai Jing and Da-Bin Qin*

Key Laboratory of Chemical Synthesis and Pollution Control of Sichuan Province, School of Chemistry and Chemical Engineering, China West Normal University, Nanchong 637002, P. R. China. E-mail: qdbkyl@cwnu.edu.cn Fax: (+86)-817-256-8081.

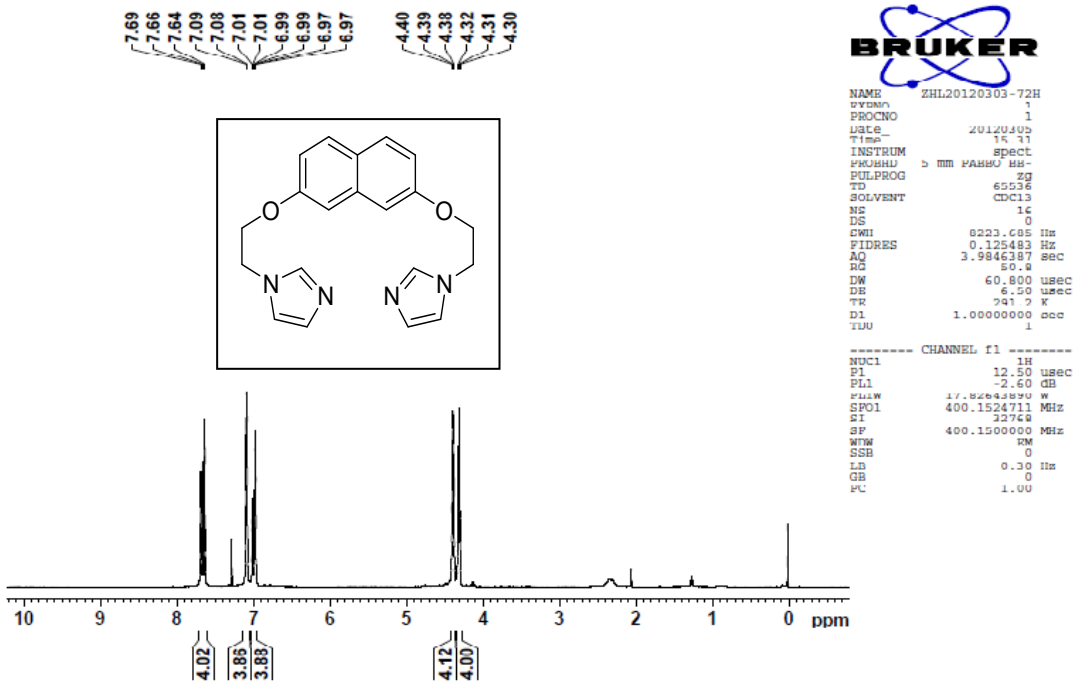

Fig. S1. The ^{1}H NMR spectra of **L1**

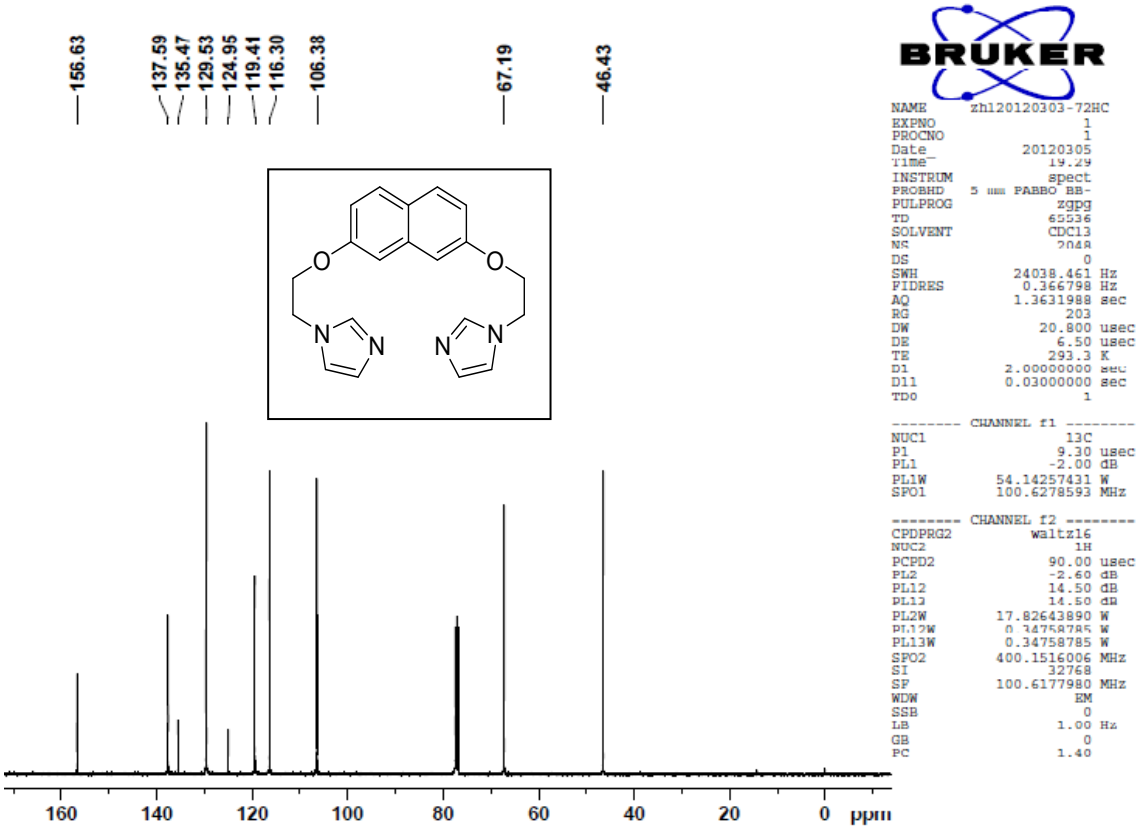

Fig. S2. The ^{13}C NMR spectra of **L1**

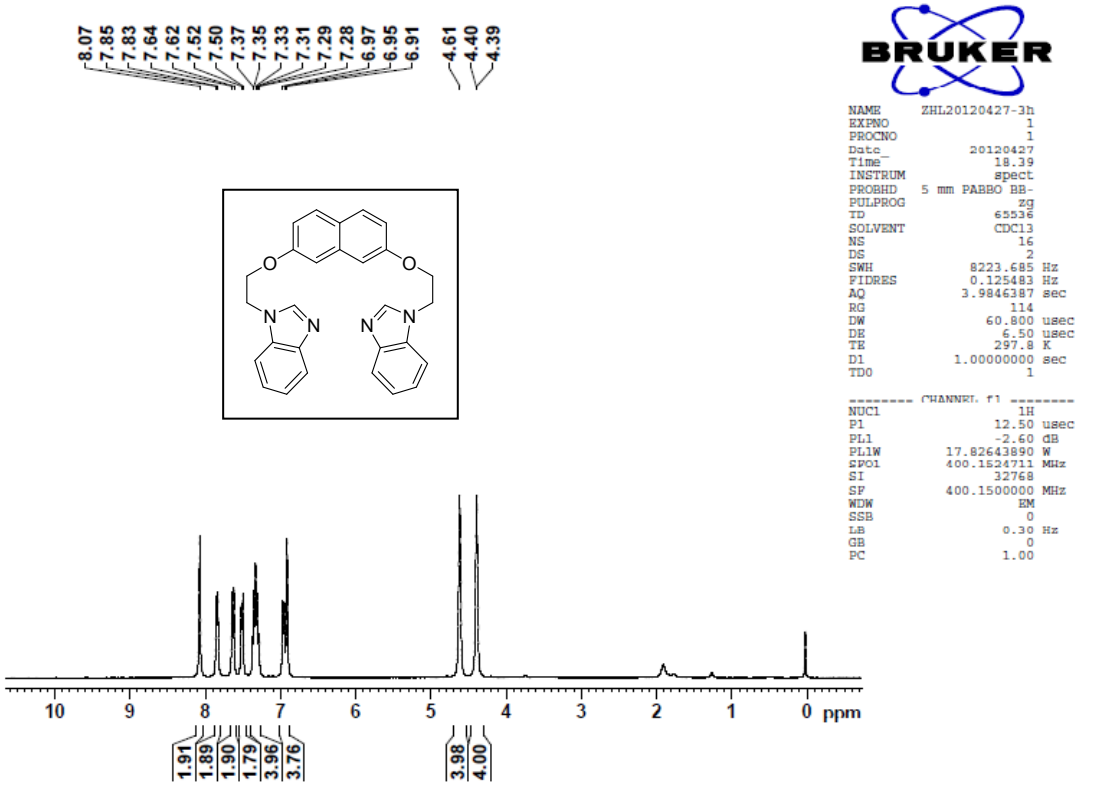

Fig. S3. The ^{1}H NMR spectra of **L2**

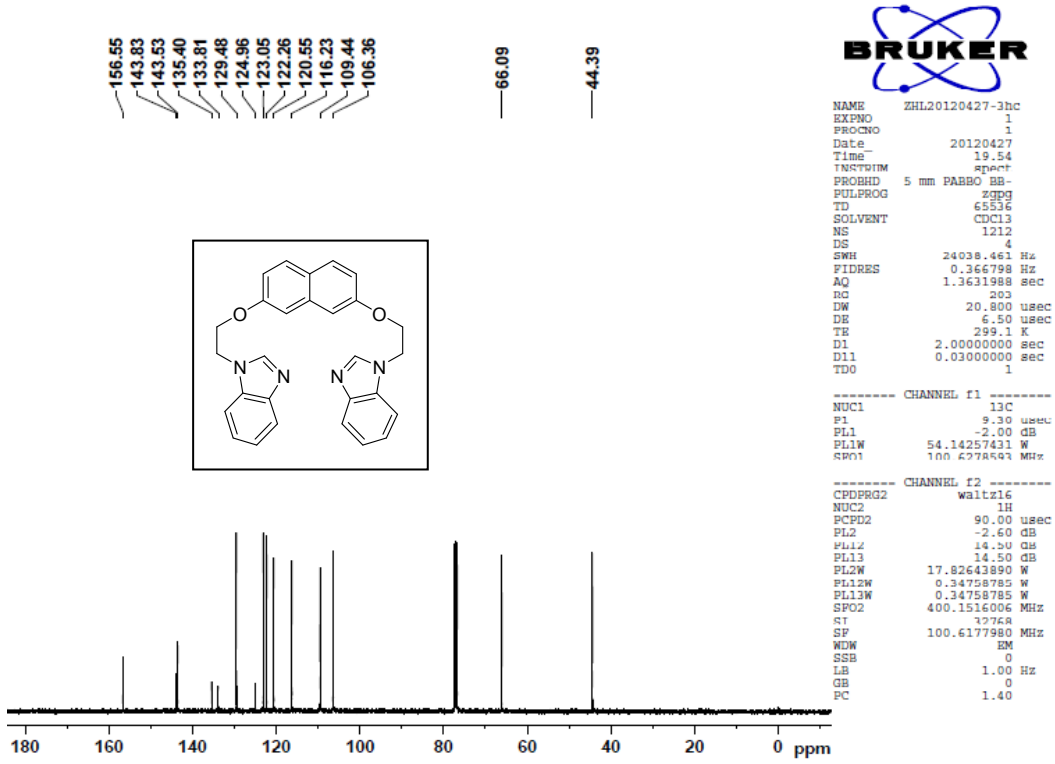

Fig. S4. The ^{13}C NMR spectra of **L2**

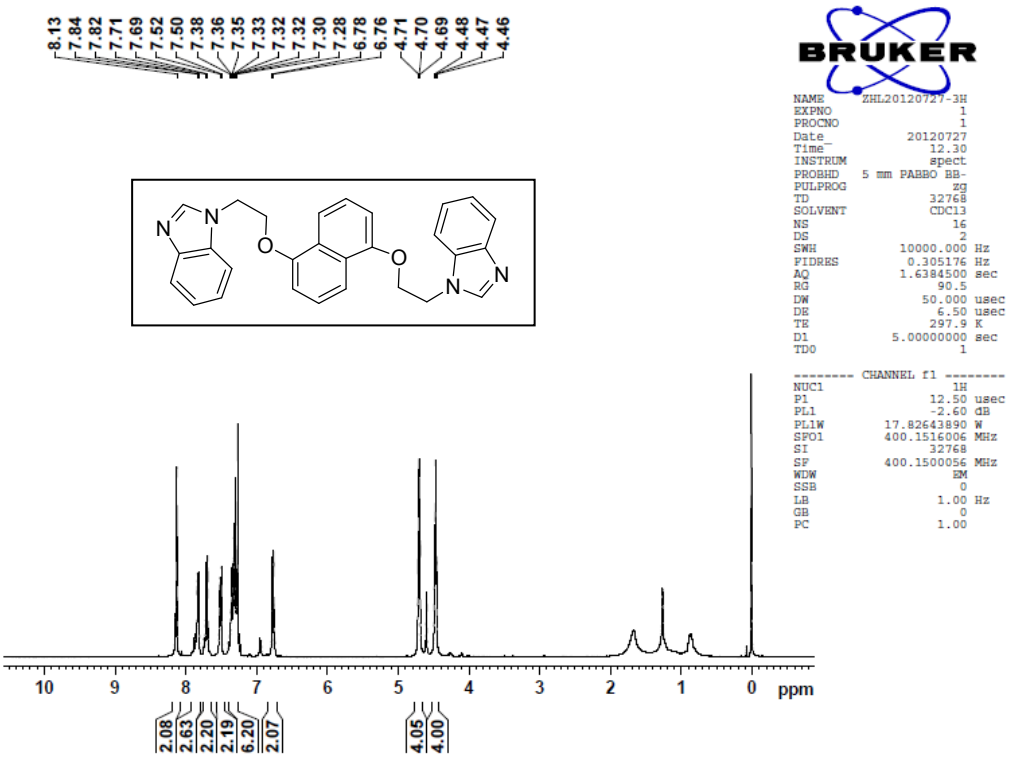

Fig. S5. The ^{1}H NMR spectra of **L3**

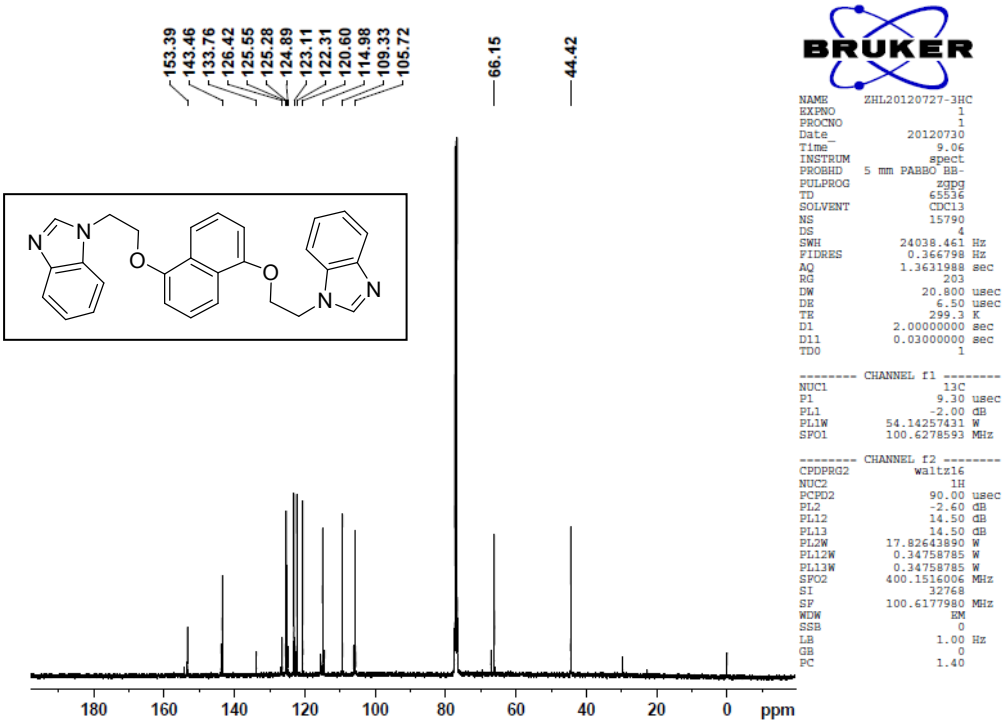

Fig. S6. The ^{13}C NMR spectra of **L3**

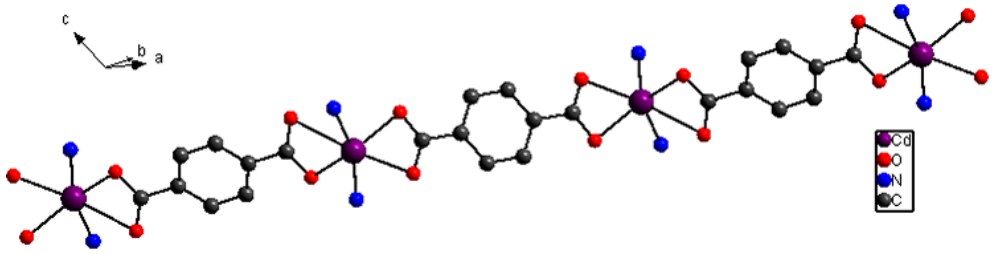

Fig. S7. View of the linear chain constructed by *p*-bdc^{2-}ligands and Cd ions in compound **1**

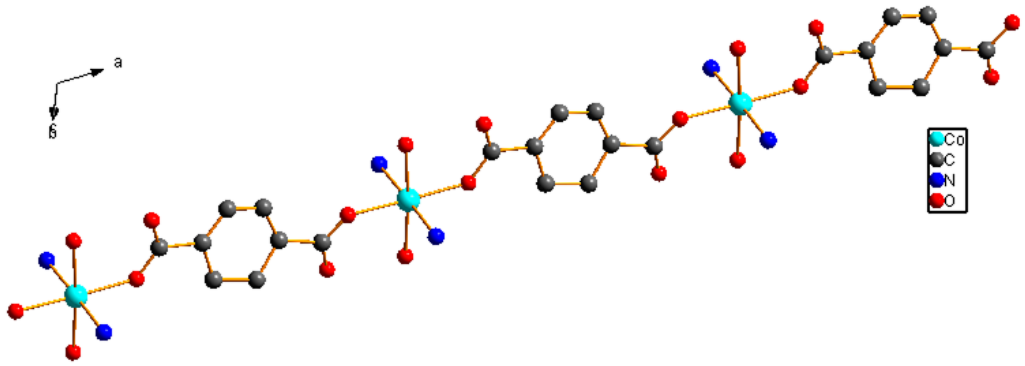

Fig. S8. View of the linear chain constructed by *p*-bdc^{2-}ligands and Co ions in compound **2**

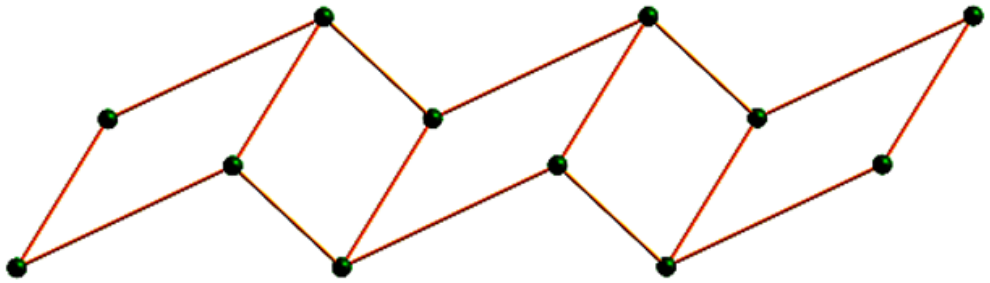

Fig. S9. Topological representation of 1D network of compound **3**

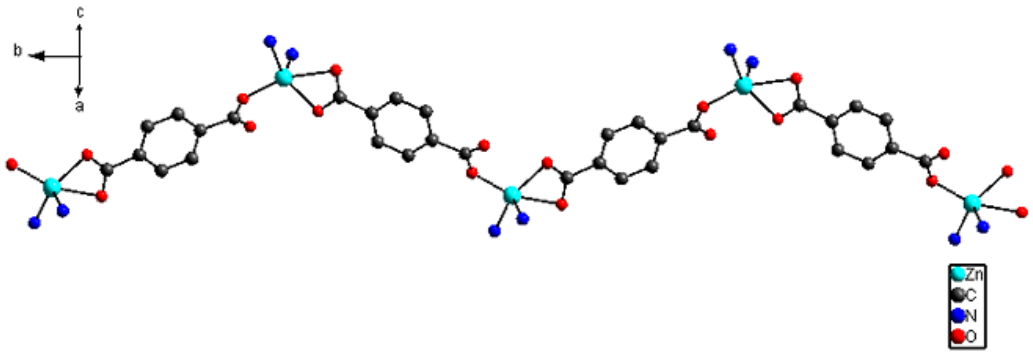

Fig. S10. Schematic view of a wavelike chain constructed by *p*-bdc^{2-} ligands and Zn cations in compound **4**

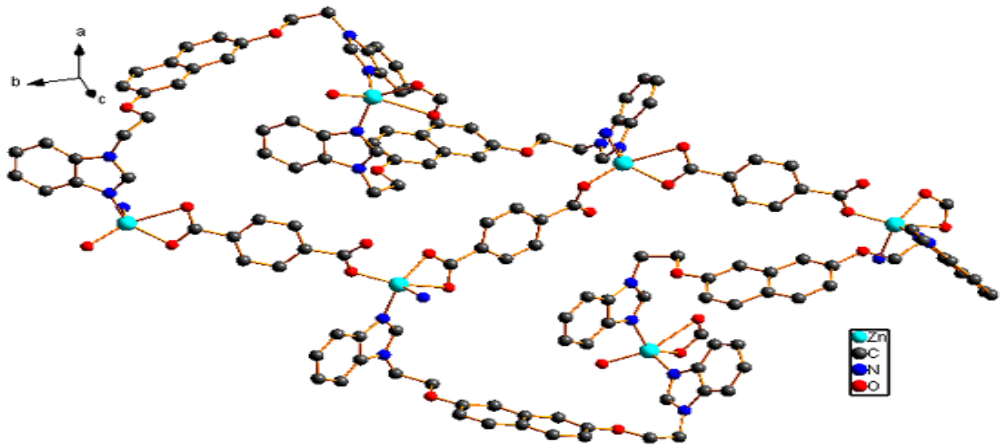

Fig. S11. Schematic representation of the basic building unit of 2D framework in compound **4**

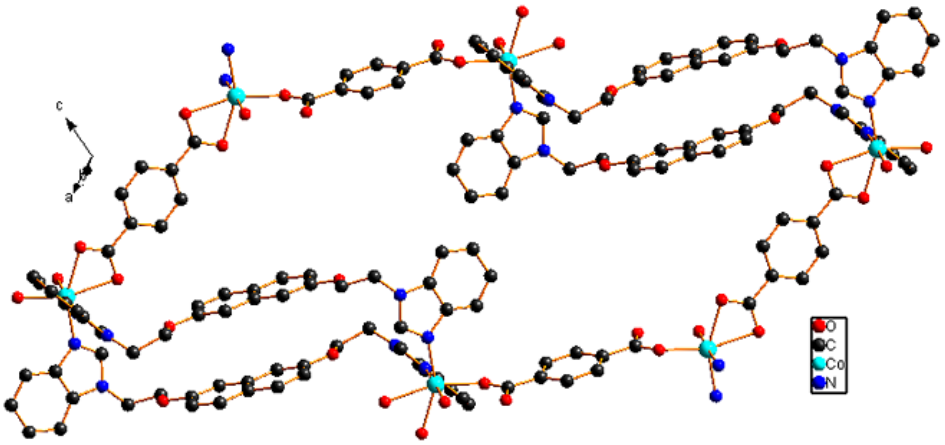

Fig. S12. Schematic representation of the basic building unit of 2D framework in compound **5**

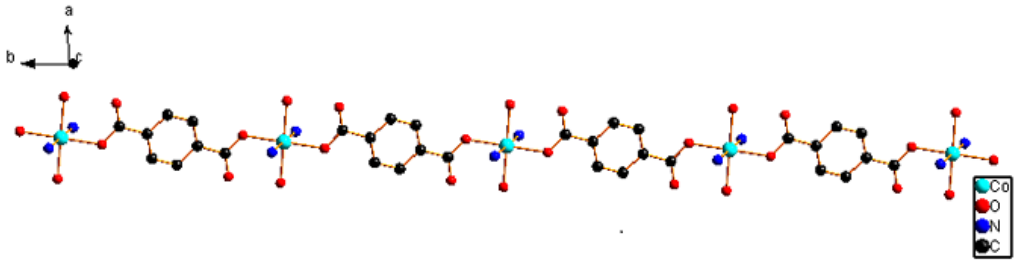

Fig. S13. Schematic view of a linear chain constructed by *p*-bdc^{2-} ligands and Co cations in compound **6**

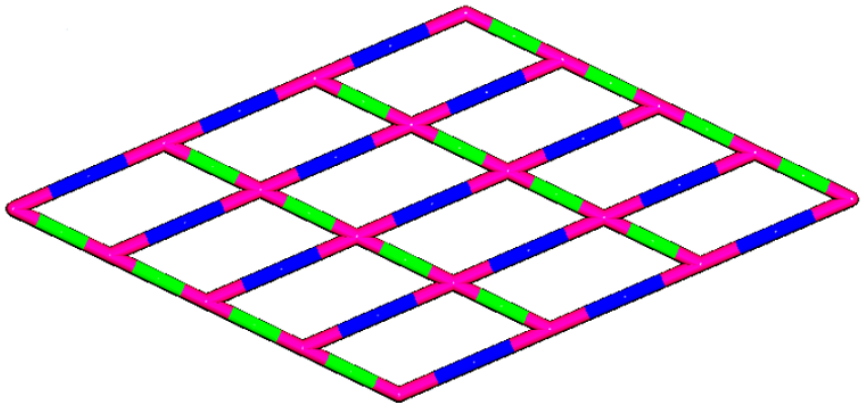

Fig. S14. Schematic representation of 2D topology of **6** (the pink sticks represent the Co center, green sticks represent the L3 ligand and the blue sticks represent *p*-bdc^{2-}).

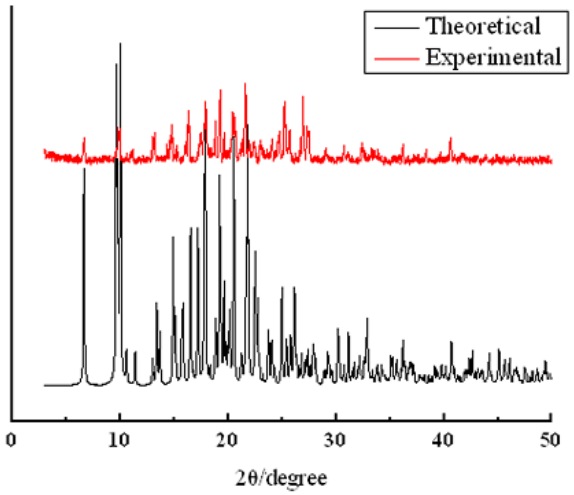

Fig. S15. The theoretical and experimental PXRD pattern of **1**

Fig. S16. The theoretical and experimental PXRD pattern of **2**

Fig. S17. The theoretical and experimental PXRD pattern of **3**

Fig. S18. The theoretical and experimental PXRD pattern of **4**

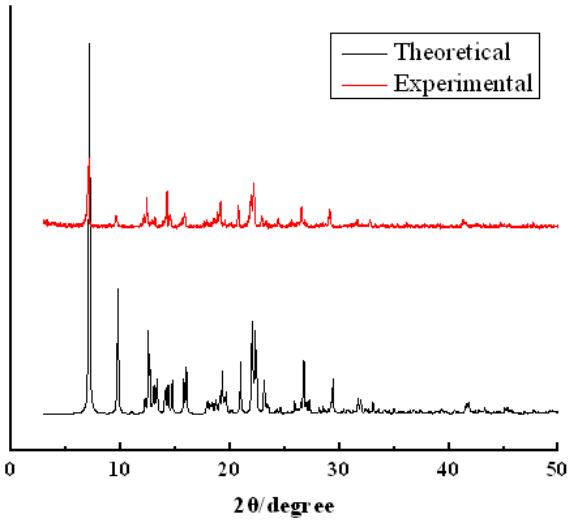

Fig. S19. The theoretical and experimental PXRD pattern of **5**

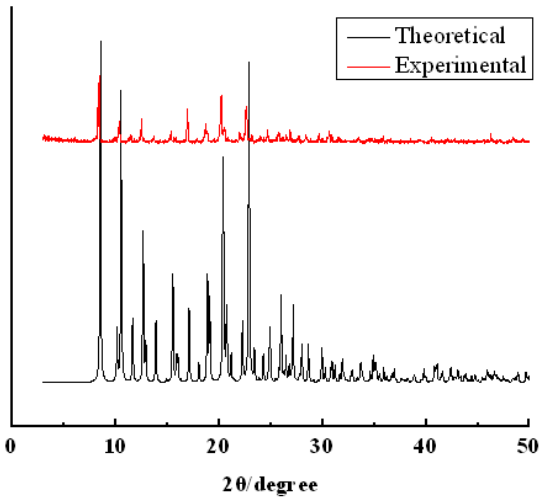

Fig. S20. The theoretical and experimental PXRD pattern of **6**

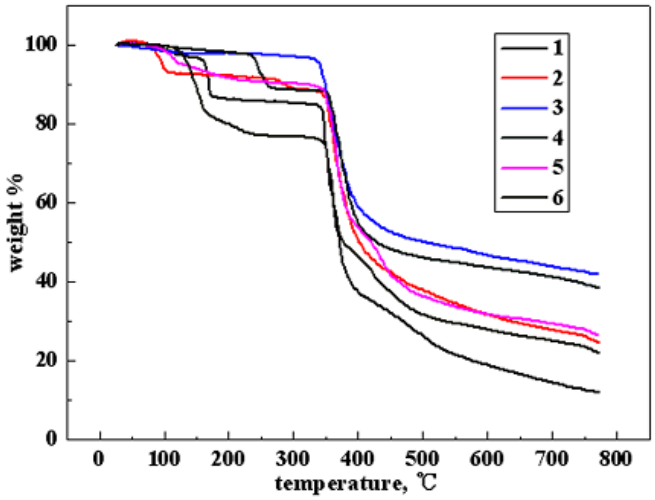

Fig. S21. TGA curves of compounds **1-6**

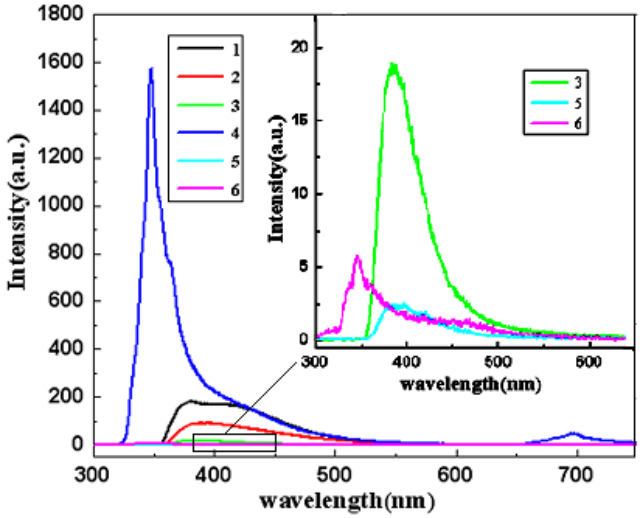

Fig. S22. Solid-state photoluminescence spectra for compounds **1-6**

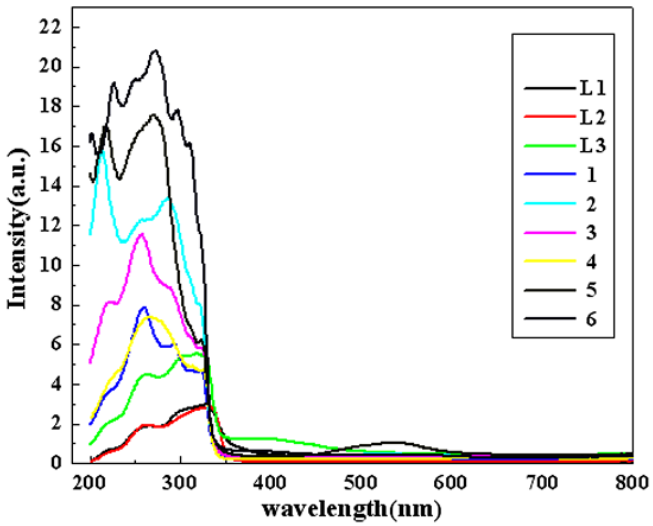

Fig. S23. Solid-state UV-vis diffuse reflectance spectra for compounds **1-6**

Table S1. Selected bond distances (Å) and angles (°) for **1**.

Cd(1)-O(5)	2.230(3)	Cd(1)-N(1)	2.250(3)
Cd(1)-O(3)	2.307(2)	Cd(1)-N(4)	2.264(3)
Cd(1)-O(4)	2.372(2)		
O(5)-Cd(1)-N(1)	120.38(9)	O(5)-Cd(1)-N(4)	98.48(10)
N(1)-Cd(1)-N(4)	92.32(10)	O(5)-Cd(1)-O(3)	116.06(10)
N(1)-Cd(1)-O(3)	96.99(9)	N(4)-Cd(1)-O(3)	132.15(9)
O(5)-Cd(1)-O(4)	103.63(9)	N(1)-Cd(1)-O(4)	135.64(9)
N(4)-Cd(1)-O(4)	86.20(9)	O(3)-Cd(1)-O(4)	55.33(8)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$1+x, y, z; $^{\#2}$x, 1.5-y, 0.5+z.

Table S2. Selected bond distances (Å) and angles (°) for **2**.

Co(1)-O(3)	2.083(6)	Co(1)-N(1)	2.089(8)
Co(1)- N(4)	2.095(8)	Co(1)-O(6)	2.116(6)
Co(1)-O(2W)	2.156(7)	Co(1)- O(1W)	2.158(7)
O(3)-Co(1)-N(1)	90. 8(3)	O(3)-Co(1)-N(4)	90.6(3)
N(1)-Co(1)-N(4)	178.5(3)	O(3)-Co(1)-O(6)	176. 6(3)
N(1)-Co(1)-O(6)	90.7(3)	N(4)-Co(1)-O(6)	88.0(3)

O(3)-Co(1)-O(2W)	92.0(2)	N(1)-Co(1)-O(2W)	89.8(3)
N(4)-Co(1)-O(2W)	90.7(3)	O(6)-Co(1)-O(2W)	84.9(3)
O(3)-Co(1)-O(1W)	92.9(3)	N(1)-Co(1)-O(1W)	89.8(3)
N(4)-Co(1)-O(1W)	89.5(3)	O(6)-Co(1)-O(1W)	90.2(3)
O(2W)-Co(1)-O(1W)	175.1(2)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$x-2, y-1, z; $^{\#2}$1-x, -y, 1-x, 3+z.

Table S3. Selected bond distances (Å) and angles (°) for **3**.

Zn(1)-O5	1.942(3)	Zn(1)-N5	1.978(4)
Zn(1)-N1	1.982(4)	Zn(1)-O3	1.987(3)
Zn(2)-O9$^{\#1}$	1.920(4)	Zn(2)-O8	1.929(4)
Zn(2)-N4$^{\#1}$	1.957(5)	Zn(2)-N8$^{\#3}$	1.968(4)
O(5)- Zn(1)-N(5)	103. 47(16)	O(5)- Zn(1)-N(1)	108.85(16)
N(5)- Zn(1)-N(1)	120.20(17)	O(5)- Zn(1)-O(3)	96. 70(15)
N(5)- Zn(1)-O(3)	109.43(15)	N(1)- Zn(1)-O(3)	114.89(16)
O(9)$^{\#1}$- Zn(2)-O(8)	96.81(16)	O(9)- Zn(2)-N(4)$^{\#1}$	110.20(17)
O(8)- Zn(2)-N(4)$^{\#1}$	107.76(18)	O(9)$^{\#1}$- Zn(2)-N(8)$^{\#3}$	112.77(18)
O(8)- Zn(2)-N(8)$^{\#3}$	116.32(17)	N(4)$^{\#1}$- Zn(2)-N(8)$^{\#3}$	111.95(19)

Symmetry transformations used to generate equivalent atoms: $^{\#1}$3-x, 1-y, 1-z; $^{\#2}$x-2, y-1, z; $^{\#3}$x+2, y+1, z.

Table S4. Selected bond distances (Å) and angles (°) for **4**.

Zn(1)-O4	1.930(3)	Zn(1)-N1	2.005(3)
Zn(1)-O6$^{\#1}$	2.007(4)	Zn(1)- N4$^{\#2}$	2.033(3)
Zn(1)-O5	2.499(6)		
O(4)- Zn(1)-N(1)	115. 58(13)	O(4)- Zn(1)- O(6)	108.50(16)
N(1)- Zn(1)- O(6)$^{\#1}$	104.17(14)	O(4)- Zn(1)- N(4)	95. 35(13)
N(1)- Zn(1)- N(4)	102.83(13)	O(6)$^{\#1}$- Zn(1)- N(4)$^{\#2}$	133.68(18)
O(6)- Zn(1)- N(5)	55.49(17)	O(5)- Zn(1)- N(4)	82.86(16)

O(5)- Zn(1)- N(1)	101.04(16)	O(5)- Zn(1)- O(4)	146.81(16)
O(5)- Zn(1)- O(6)	55.49(17)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$1-x, -0.5+y, 1.5-z; $^{\#2}$1.5-x, -0.5+y, z.

Table S5. Selected bond distances (Å) and angles (°) for **5**.

Co(1)-O5	2.041(6)	Co(1)-N1	2.087(7)
Co(1)- N4$^{\#1}$	2.113(9)	Co(1)-O3	2.169(5)
Co(1)-O4	2.246(6)	Co(1)- O1W	2.136(6)
O(5)-Co(1)-N(1)	101. 6(3)	O(5)-Co(1)- N(4)$^{\#1}$	92.3(3)
N(1)-Co(1)- N(4)$^{\#1}$	89.4(3)	O(5)-Co(1)- O(1W)	89.8(2)
N(1)-Co(1)- O(1W)	91.7(3)	N(4)$^{\#1}$-Co(1)- O(1W)	177.4(3)
O(5)-Co(1)-O(3)	103.6(2)	N(1)-Co(1)-O(3)	154.7(3)
N(4)-Co(1)-O(3)	90.8(3)	O(1W)-Co(1)-O(3)	87.4(2)
O(5)-Co(1)-O(4)	162.2(2)	N(1)-Co(1)-O(4)	95.4(2)
N(4)$^{\#1}$-Co(1)-O(4)	92.9(3)	O(1W)-Co(1)-O(4)	84.6(2)
O(3)-Co(1)-O(4)	59.3(2)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$-x, 1-y, -z.

Table S6. Selected bond distances (Å) and angles (°) for **6**.

Co(1)-O2$^{\#1}$	2.097(3)	Co(1)- O1W$^{\#1}$	2.098(4)
Co(1)- N1$^{\#1}$	2.128(3)		
O(2)$^{\#1}$-Co(1)- O(2)	180. 00(1)	O(2)-Co(1)- O(1W)	88.19(12)
O(2)$^{\#1}$-Co(1)- O(1W)	91.81(12)	O(1W)-Co(1)-O(1W)	180. 00(1)
O(2)$^{\#1}$-Co(1)- N(1)	94.37(11)	O(2)-Co(1)- N(1)$^{\#1}$	85.63(11)
O(1W)$^{\#1}$-Co(1)- N(1)$^{\#1}$	88.63(14)	O(1W)-Co(1)- N(1)$^{\#1}$	91.37(14)
N(1)$^{\#1}$-Co(1)- N(1)	180. 00(2)		

Symmetry transformations used to generate equivalent atoms: $^{\#1}$-x, -2-y, 2+z.