# *Electronic Supplementary Information*

## Two unique (4,5,6)-connected 2D $Cd^{II}$ coordination polymers based on 5-nitro-1,2,3-benzenetricarboxylic acid ligand

*Lu-Fang Ma[a,b], Jian-Hua Qin[a], Li-Ya Wang[a *], Dong-Sheng Li[b*]*

[a]*College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang 471022, China;*

[b]*College of Mechanical & Material Engineering, Functional Materials Research Institute, China Three Gorges University, Yichang 443002, China.*

*To whom correspondence should be addressed.*
*E-mail address: wlya@lynu.edu.cn (L.-Y. Wang), Tel./Fax: +86-379-65511205*
*lidongsheng1@126.com (D.-S. Li), Tel./Fax: +86-717-6397516*

***RSC Advances***

**X-ray crystallography.** Single crystal X-ray diffraction analyses of the two complexes were carried out on a Bruker SMART APEX II CCD diffractometer equipped with a graphite-monochromated Mo Kα radiation (λ = 0.71073Å) by using the φ /ω scan technique at room temperature. The structures were solved by direct methods with SHELXS-97. Empirical absorption corrections were applied with SADABS program. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were assigned with common isotropic displacement factors and included in the final refinement by use of geometrical restrains. A full-matrix least-squares refinement on F2 was carried out using SHELXL-97. In the structure of **2**, the disordered carbon atoms and nitrogen atoms of 1,1′-(1,4-butanediyl)bis(imidaz-ole) groups were restrained in order to obtain reasonable thermal parameters.

**Table S1** Selected bond lengths (Å) and angles (º) for **1** and **2**.

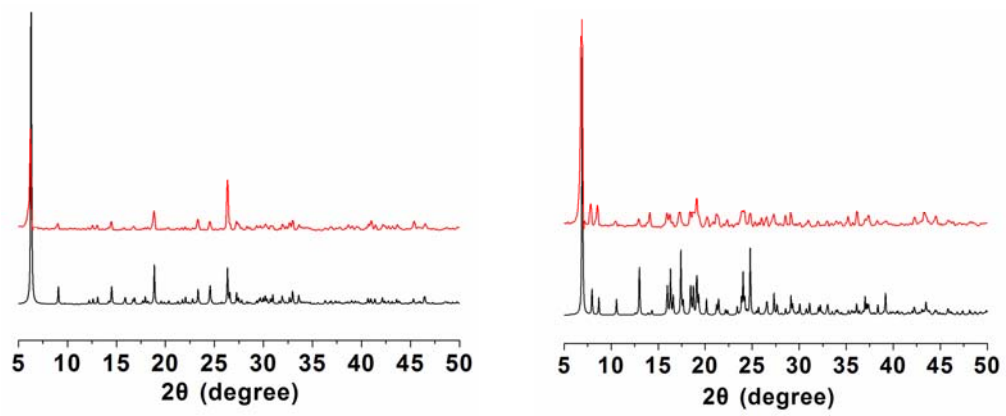
| **1** | | | |
|---|---|---|---|
| Cd(1)-O(5)#1 | 2.2675(16) | O(4)#2-Cd(2)-O(18) | 147.27(6) |
| Cd(1)-O(10) | 2.2724(16) | O(11)-Cd(2)-O(18) | 76.98(5) |
| Cd(1)-O(1) | 2.3044(16) | O(1)-Cd(2)-O(18) | 71.83(5) |
| Cd(1)-O(12)#1 | 2.3356(15) | O(19)-Cd(2)-O(11)#3 | 96.92(6) |
| Cd(1)-O(17) | 2.3919(16) | O(4)#2-Cd(2)-O(11)#3 | 90.86(6) |
| Cd(2)-O(19) | 2.3241(19) | O(11)-Cd(2)-O(11)#3 | 70.70(6) |
| Cd(2)-O(4)#2 | 2.3307(18) | O(1)-Cd(2)-O(11)#3 | 150.61(5) |
| Cd(2)-O(11) | 2.3451(16) | O(18)-Cd(2)-O(11)#3 | 80.35(5) |
| Cd(2)-O(1) | 2.3891(16) | O(19)-Cd(2)-O(3)#2 | 128.22(6) |
| Cd(2)-O(18) | 2.3893(16) | O(4)#2-Cd(2)-O(3)#2 | 53.84(6) |
| Cd(2)-O(11)#3 | 2.4731(16) | O(11)-Cd(2)-O(3)#2 | 77.03(5) |
| Cd(2)-O(3)#2 | 2.5363(17) | O(1)-Cd(2)-O(3)#2 | 119.19(6) |
| Cd(3)-O(20) | 2.2875(18) | O(18)-Cd(2)-O(3)#2 | 152.32(5) |
| Cd(3)-O(2) | 2.3392(16) | O(11)#3-Cd(2)-O(3)#2 | 82.25(5) |
| Cd(3)-O(14)#1 | 2.3816(19) | O(20)-Cd(3)-O(2) | 149.46(6) |
| Cd(3)-O(12) | 2.4121(16) | O(20)-Cd(3)-O(14)#1 | 71.26(6) |
| Cd(3)-O(13)#1 | 2.4175(17) | O(2)-Cd(3)-O(14)#1 | 134.34(6) |
| Cd(3)-O(17)#2 | 2.4300(16) | O(20)-Cd(3)-O(12) | 87.89(6) |

| | | | |
|---|---|---|---|
| Cd(3)-O(6)#4 | 2.5893(19) | O(2)-Cd(3)-O(12) | 86.68(5) |
| O(5)#1-Cd(1)-O(10) | 156.21(7) | O(14)#1-Cd(3)-O(12) | 125.55(6) |
| O(5)#1-Cd(1)-O(1) | 101.38(6) | O(20)-Cd(3)-O(13)#1 | 125.83(6) |
| **2** | | | |
| Cd(1)-O(4)#1 | 2.2172(19) | Cd(1)-O(4) | 2.6237(18) |
| Cd(1)-N(5')#2 | 2.228(2) | Cd(2)-N(2) | 2.280(2) |
| Cd(1)-N(5)#2 | 2.228(2) | Cd(2)-N(2)#4 | 2.280(2) |
| Cd(1)-O(2)#3 | 2.3008(19) | Cd(2)-O(6) | 2.3394(18) |
| Cd(1)-O(5) | 2.334(2) | Cd(2)-O(6)#4 | 2.3394(18) |
| Cd(1)-O(1)#3 | 2.474(2) | Cd(2)-O(9) | 2.367(2) |
| Cd(2)-O(9)#4 | 2.367(2) | O(2)#3-Cd(1)-O(4) | 149.86(7) |
| O(6)-Cd(2)-O(9) | 90.87(7) | O(5)-Cd(1)-O(4) | 73.19(6) |
| O(6)#5-Cd(2)-O(9) | 89.12(7) | O(1)#3-Cd(1)-O(4) | 138.19(7) |
| N(2)-Cd(2)-O(9)#4 | 93.22(8) | N(2)-Cd(2)-N(2)#4 | 179.999(1) |
| N(2)#4-Cd(2)-O(9)#4 | 86.78(8) | N(2)-Cd(2)-O(6) | 88.87(8) |
| O(4)#1-Cd(1)-N(5)#2 | 125.31(8) | N(2)#4-Cd(2)-O(6) | 91.13(8) |
| O(4)#1-Cd(1)-O(2)#3 | 91.87(7) | O(6)-Cd(2)-O(6)#4 | 180.0 |
| N(5)#2-Cd(1)-O(2)#3 | 132.14(8) | N(2)-Cd(2)-O(9) | 86.78(8) |
| O(4)#2-Cd(1)-O(5) | 90.01(7) | N(2)#4-Cd(2)-O(9) | 93.22(8) |

Symmetry transformations used to generate equivalent atoms: #1: x, –y+3/2, z–1/2; #2: x, –y+3/2, z+1/2; #3: –x+2, –y+2, –z+2; #4: –x+2, –y+1, –z+2 for **1**. #1: –x+2, –y+1, –z+3; #2: x+1, y, z+2: #3 x, y, z–1; #4: –x+1, –y+1, –z+2 for **2**.

**Table S2** Dihedral angles (°) between the carboxylic groups and aromatic rings of **nbta**$^{3-}$.

| | Outer carboxyl | Inner carboxyl | Outer carboxyl |
|---|---|---|---|
| $[Cd_3(\mathbf{nbta})_2(H_2O)_4]$ (**1**) | 14.3 | 71.0 | 47.2 |
| | 31.9 | 77.4 | 6.9 |
| $[Cd_3(\mathbf{nbta})_2(bbi)_2(H_2O)_2]$ (**2**) | 9.4 | 98.4 | 131.0 |
| $\{[Cd_3(\mathbf{nbta})_2(bpa)_2]\}_n$[11c] | 44.8 | 87.0 | 29.2 |
| $\{[Cd_3(\mathbf{nbta})_2(bpy)_5(H_2O)_2](H_2O)_6\}_n$[11d] | 44.3 | 83.7 | 37.9 |




(a) (b)

**Fig. S1**. XRPD pattern of **1** (a) and **2** (b)

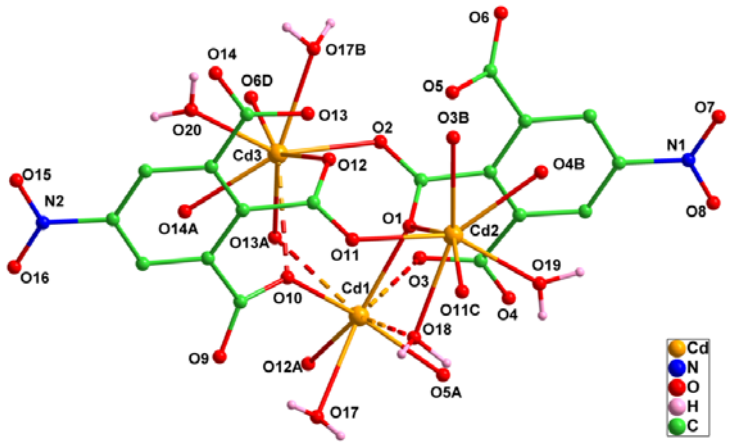



**Fig. S2**. Coordination environments of Cd(II) ions in **1**. Symmetry codes: A, x, –y + 3/2, z – 1/2; B, x, –y + 3/2, z + 1/2; C, –x + 2, – y + 2, –z +2; D, –x + 2, –y + 1, –z + 2 (Only H atoms of the water molecules are shown for clarity).

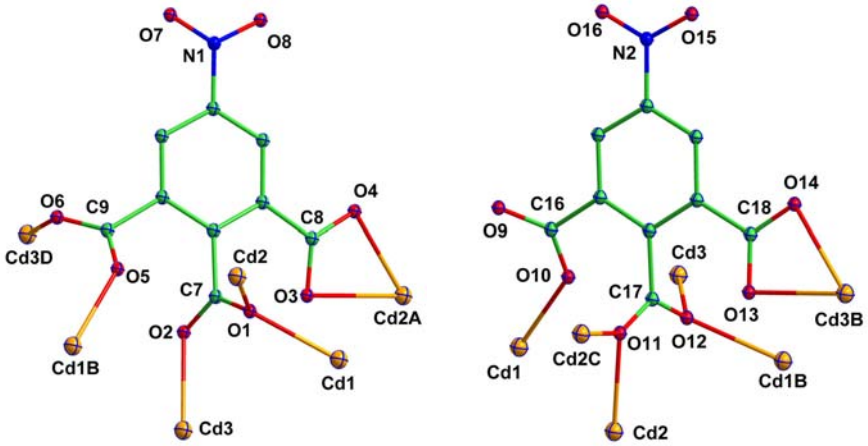



**Fig. S3**. Coordination modes of **nbta** ligand in **1** (symmetry codes: A: *x*, –*y*+3/2, *z*–1/2; B: *x*, –*y*+3/2, *z*+1/2; C: –*x*+2, –*y*+2, –*z*+2; D: –*x*+2, –*y*+1, –*z*+2).

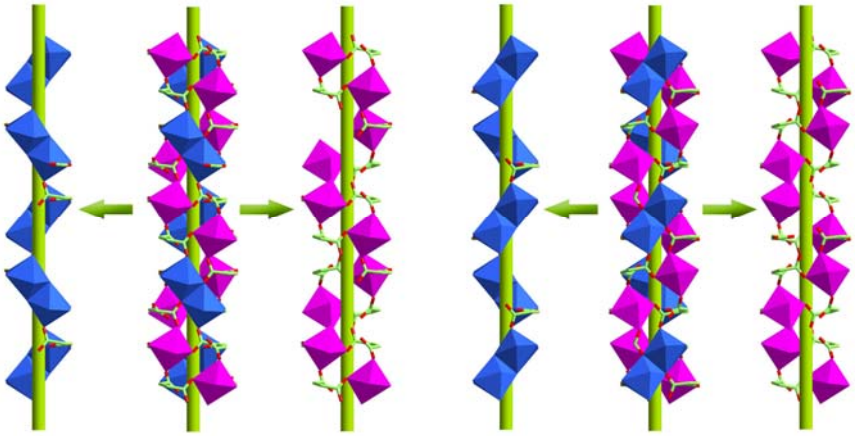


**Fig. S4**. Two intertwined left- and right-handed helices in **1**.

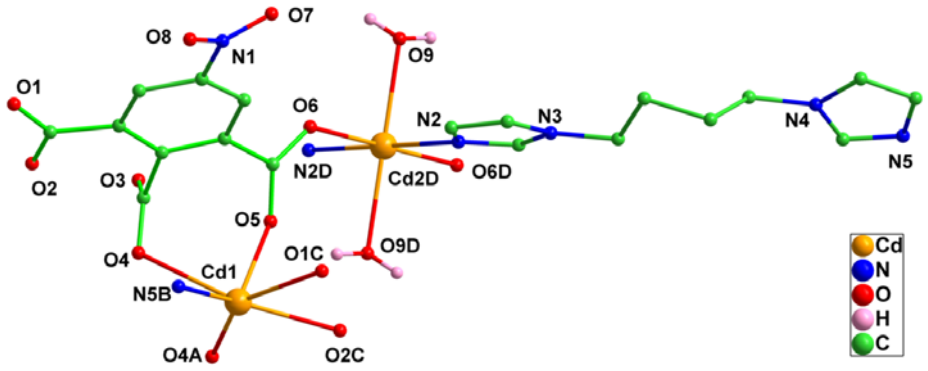



**Fig. S5**. Coordination environments of Cd(II) ions in **2**. Symmetry codes: A, –x + 2, –y + 1, –z + 3; B, x + 1, y, z + 2; C, x, y, –z + 1; D, –x + 1, –y + 1, –z + 2 (Only H atoms of water molecules are shown for clarity). The disordered nitrogen and carbon atoms are omitted for clarity.

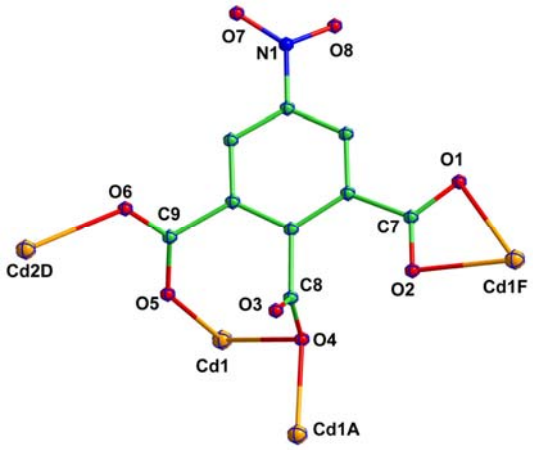
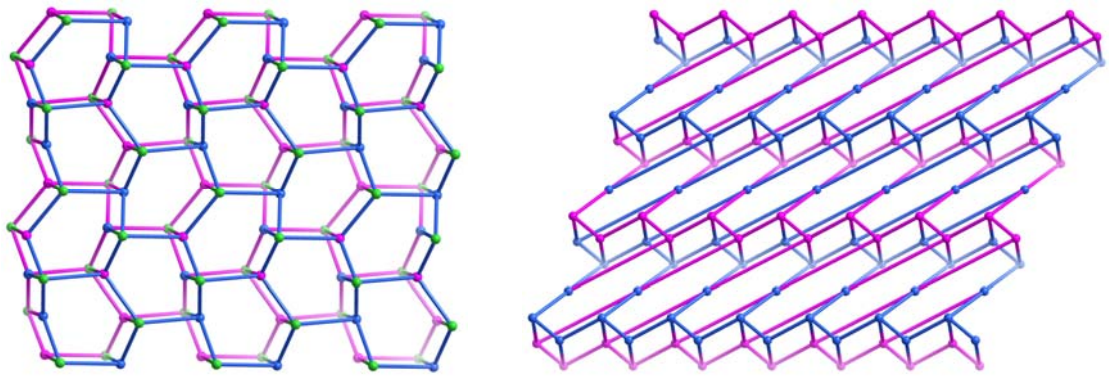
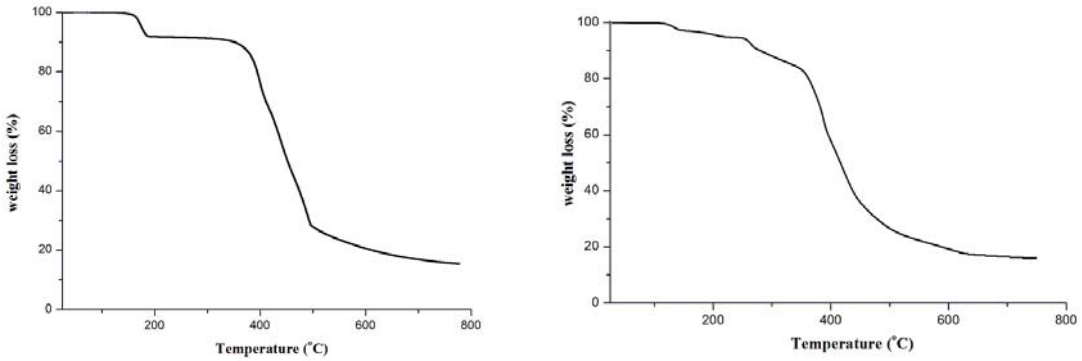



**Fig. S6**. Coordination modes of the **nbta** ligand in **2** (symmetry codes: A: –*x*+2, –*y*+1, –*z*+3; B: *x*+1, *y*, *z*+2; C: *x*, *y*, *z*–1; D: –*x*+1, –*y*+1, –*z*+2; E: *x*–1, *y*, *z*–2; F: *x*, *y*, *z*+1).



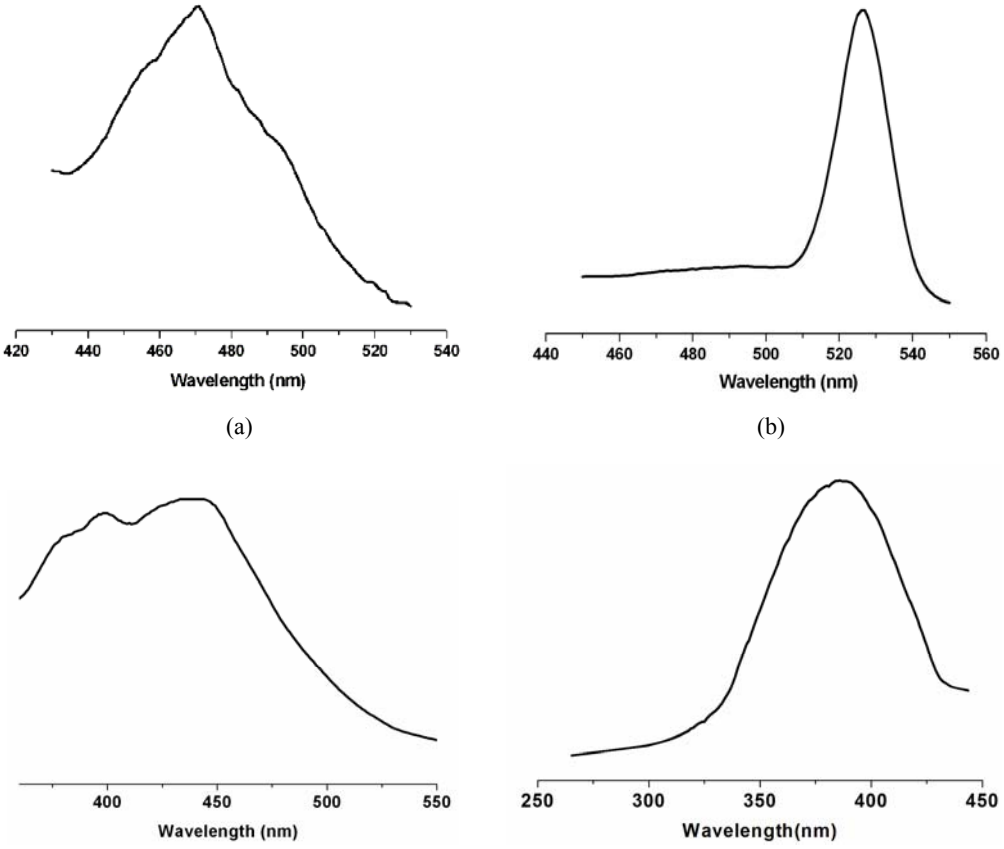
(a) (b)

**Fig. S7**. Two 4-connected 2-D nets in **1** (a) and **2** (b), arising from the different linkages of the adjacent $6^3$ nets (for **1**, the Cd1 nodes are ignored).




(a) (b)

**Fig. S8**. TG curves of **1** (a) and **2** (b).




(a) (b)

(c) (d)

**Fig. S9**. Solid-state emission spectrum of **1** (a), **2** (b), $H_3$**nbta** (c), and bib (d) at room temperature.