

## *Electronic supplementary information (ESI)*

### **Anion- and auxiliary ligand-directed synthesis of cadmium(II) complexes with 3,5-di(1H-imidazol-1-yl)benzoate †‡**

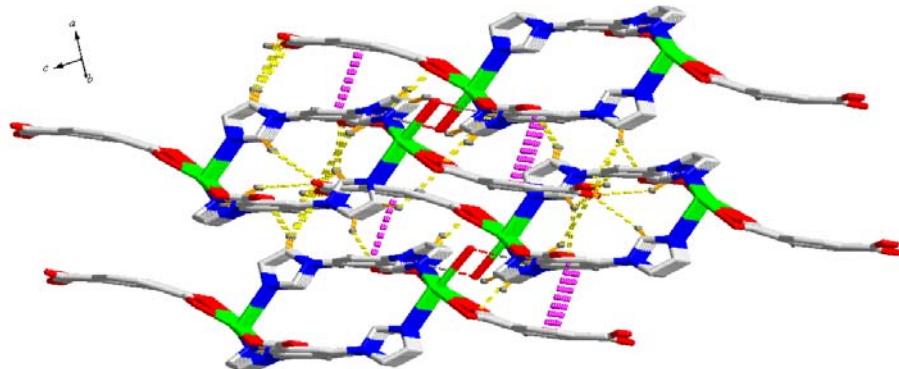
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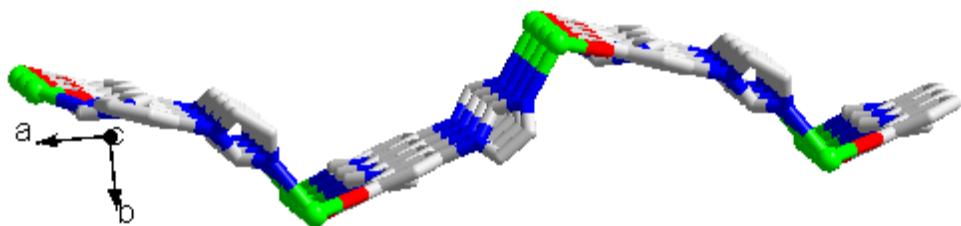
**Table S1.** Hydrogen bonding distances/ Å and angel/ ° for complexes **1** and **5**.

| D-H···A         | <i>d</i> (D···A) | $\angle$ (D-H···A) |
|-----------------|------------------|--------------------|
|                 | <b>1</b>         |                    |
| O5-H2···O1#1    | 2.613(3)         | 164(5)             |
| C19-H4···O4#2   | 3.437(4)         | 152                |
| C2-H15···O5#3   | 3.204(4)         | 160                |
| C11-H20···O4#4  | 3.336(4)         | 174                |
| C12-H21···O7#5  | 3.106(4)         | 117                |
|                 | <b>5</b>         |                    |
| O10-H111···O4#1 | 3.066(5)         | 131(7)             |
| O10-H111···O6#1 | 2.916(5)         | 149(7)             |
| O9-H113···O2#2  | 2.999(5)         | 152(6)             |
| O9-H114···O4#3  | 2.807(4)         | 157(5)             |
| C8-H8···O10     | 3.366(6)         | 148                |
| C10-H10···O8#4  | 3.435(4)         | 165                |
| C13-H13···O5#5  | 3.084(4)         | 121                |
| C13-H13···O9#2  | 3.364(5)         | 147                |
| C17-H17···O10#6 | 3.406(5)         | 149                |

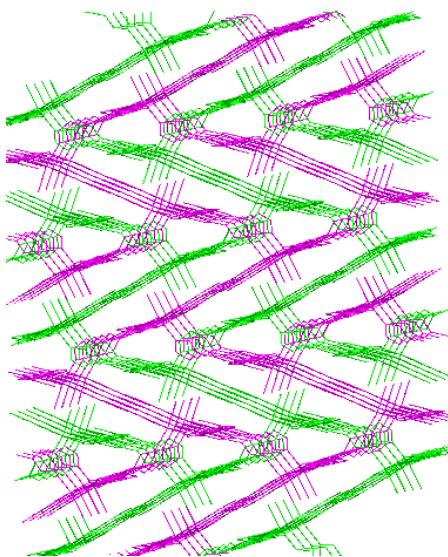
Symmetry transformations used to generate equivalent atoms: For **1**: #1 -1+x, y, -1+z; #2 2-x, 3-y, 1-z; #3 1+x, y, 1+z; #4 2-x, 2-y, 1-z; #5 -1+x, -1+y, z. For **5**: #1 2-x, 1-y, -z; #2 1-x, 1-y, -z; #3 2-x, 2-y, -1-z; #4 1-x, 2-y, -z; #5 -1+x, -1+y, 1+z; #6 x, 1+y, z.



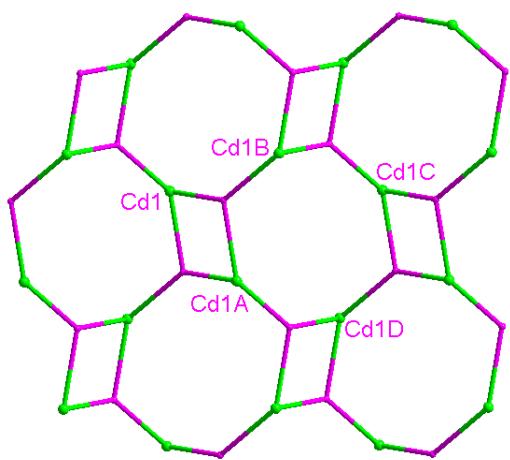
**Figure S1.** The 3D packing diagram of complex **1**, in which the pink dotted lines represent the  $\pi$ --- $\pi$  interactions and the yellow ones represent the hydrogen bonds.



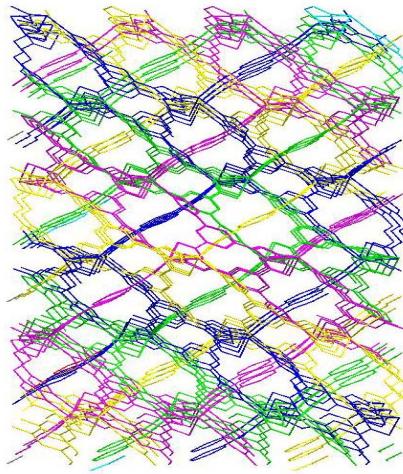
**Figure S2.** The wave-like 2D 6<sup>3</sup>-hcb layer in **2**.



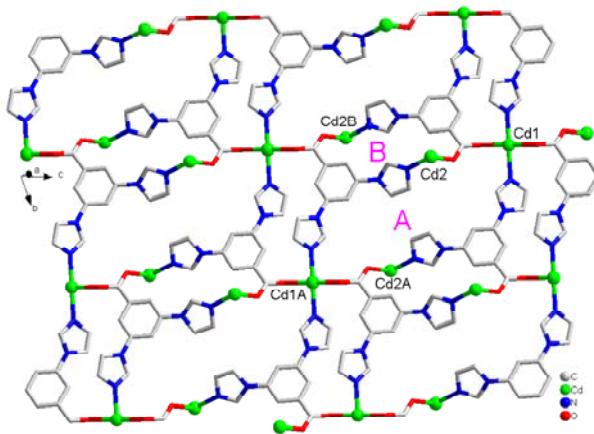
**Figure S3.** Representation of 2-fold interpenetration in complex **2**.



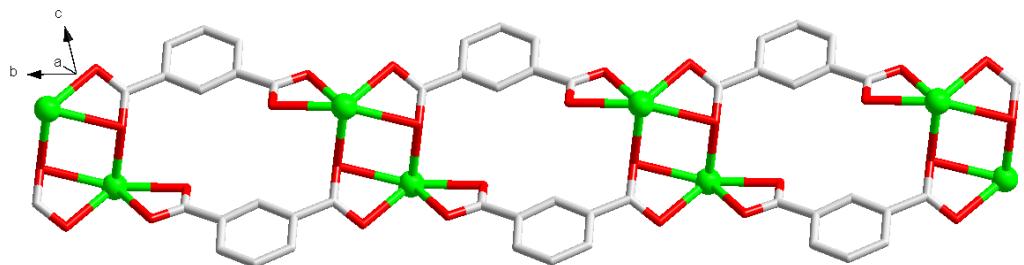
**Figure S4.** The Scheme representation of  $(4,8^2)$  net in **3**.



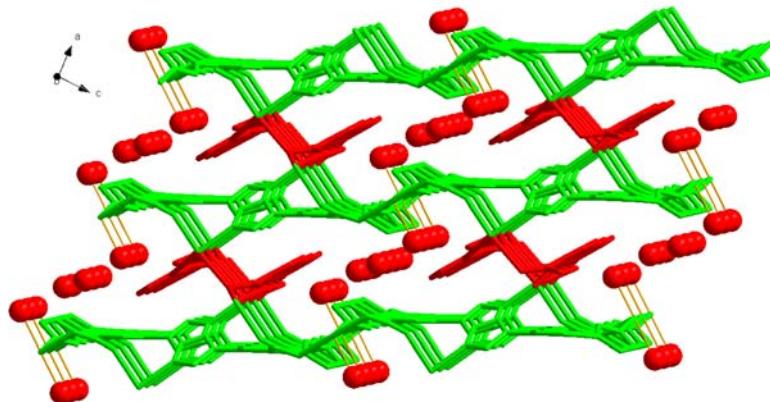
**Figure S5.** Representation of 4-fold interpenetration in complex **3**.



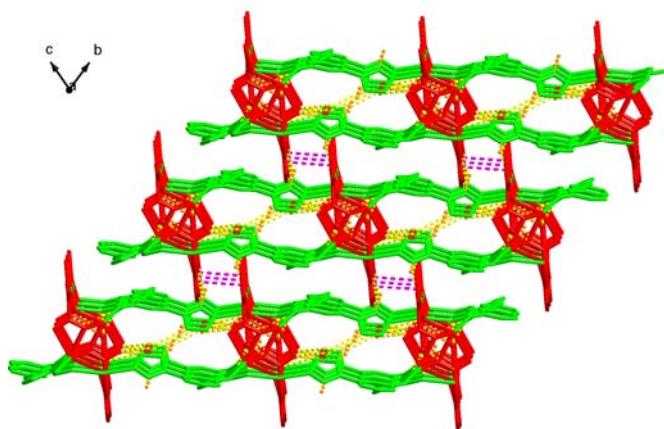
**Figure S6.** The  $\text{L}^-$ -Cd layer in **4**.



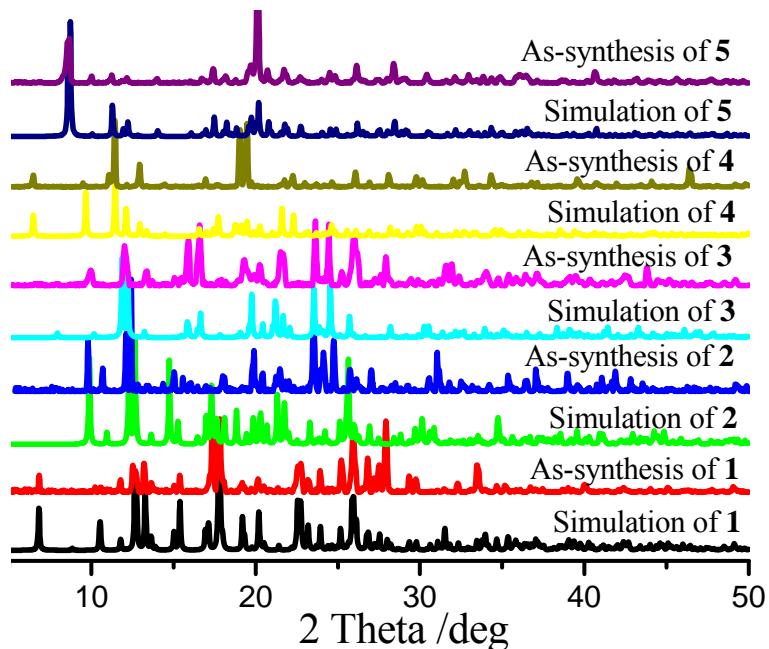
**Figure S7.** The  $\text{MBDA}^{2-}$ -Cd chain in **4**.



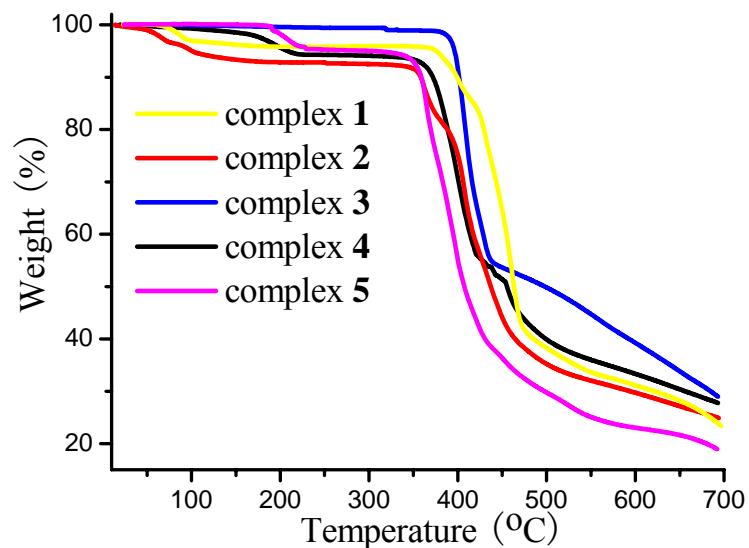
**Figure S8.** The coordinated and uncoordinated water molecules in **4** (Red:  $\text{MBDA}^{2-}$ -Cd chains; Green: the  $\text{L}^-$ -Cd layers). The red balls represented the water molecules.



**Figure S9.** The 3D packing diagram of complex **5**, in which the pink dotted lines represented the  $\pi\cdots\pi$  interaction and the yellow ones represented the hydrogen bonds.



**Figure S10.** The simulated and as-synthesized PXRD of complexes **1**–**5**.



**Figure S11.** The TG curves of complexes **1-5**.