Characterization, adsorption properties, metal ion-exchange and crystal-to-crystal transformation of Cd₃[(Cd₄Cl)₃(BTT)₈(H₂O)₁₂]₂ framework, where BTT³⁻ = 1,3,5-benzenetristetrazolate

Ju-Hsiou Liao*,a, Wan-Ting Chena, Cherng-Shiaw Tsaia, Chih-Chieh Wangb

Department of Chemistry and Biochemistry, National Chung Cheng University
168 University Road, Min-Hsiung, Chia-Yi, Taiwan, and Department of Chemistry, Soochow University, 70 Linhsi Road, Shihlin, Taipei, Taiwan

Supporting Information

Contents

Fig. S1 (a) Simulated powder X-ray diffraction pattern (in red) of 1, based on single-crystal data. (b) Experimental powder X-ray diffraction pattern of the as-synthesized product (in blue).

Fig. S2 Experimental X-ray powder diffraction patterns of (a) 1, (b) 2 and (c) 3.

Fig. S3 Thermogravimetric analysis of 1.

Fig. S4 (a) Experimental powder X-ray diffraction pattern (in black) of as-synthesized 1. (b) Experimental powder X-ray diffraction pattern (in red) of 1 annealed at 150°C.

Fig. S5 (a) Infrared spectrum of as-synthesized 1. (b) Infrared spectrum of 1 annealed at 150°C. DMF solvent molecules are not completely removed.

Table S1 The results of ICP-MS for the ion-exchanged products
Fig. S1

![X-ray diffraction patterns for Figure S1](image)

Fig. S2

![X-ray diffraction patterns for Figure S2](image)
**Fig. S3**

![Graph showing weight percentage vs temperature](image)

- Atmosphere: N$_2$
- Heating rate: 3°C/min
- Flow rate: 30 ml/min

**Fig. S4**

![Graph showing intensity vs 2θ](image)

- (a) Intensity (a.u.)
- (b) Intensity (a.u.)
Fig. S5

![Spectrum Image](image)

Table S1

The results of ICP-MS for the ion-exchanged products

<table>
<thead>
<tr>
<th>Sample\M²⁺</th>
<th>Co²⁺ (ppm)</th>
<th>Ni²⁺ (ppm)</th>
<th>Cd²⁺ (ppm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>364</td>
<td>NA</td>
<td>0.86</td>
</tr>
<tr>
<td>3</td>
<td>NA</td>
<td>314</td>
<td>1.75</td>
</tr>
</tbody>
</table>