**Supporting Information**

Cationic Cd(II) metal−organic framework based on tetrakis(1,2,4-triazol-1-yl)methane

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Figure S1. Powder X-ray diffractions of **1**.



Figure S2. Powder X-ray diffractions of **1** after immersing the crystals in different solvents.



Figure S3. N2 sorption isotherms of **1** at 77 K.



Figure S4. Infrared spectrum of **1**.

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

|  |  |  |  |
| --- | --- | --- | --- |
| Cd1−O1 | 2.363(12) | N(1)−Cd(1)−O(1) | 79.2(7) |
| Cd1−N1 | 2.248(8) | N(1)#3−Cd(1)−O(1) | 87.9(16) |
| Cd1−N1#1 | 2.25(2) | N(1)#3−Cd(1)−N(1)#2 | 89.7(7) |
| Cd1−N1#2 | 2.248(9) | N(1)#1−Cd(1)−N(1)#3 | 172(2) |
| Cd1−N1#3 | 2.25(3) | N(1)#1−Cd(1)−N(1)#2 | 89.7(7) |
| N(1)#1−Cd(1)−O(1) | 84.3(15) | N(1)−Cd(1)−N(1)#1 | 89.7(7) |
| N(1)#2−Cd(1)−O(1) | 92.9(18) | N(1)−Cd(1)−N(1)#3 | 89.7(7) |

#1: -*x*+1/2, *y*, *z*; #2: 1/2-*x*, 1/2-*y*, *z*; #3: *x*, 1/2-*y*, *z*

Table S2. Selected hydrogen bond data for tmmp·H2O.

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Interaction | H…A (Å) | D…A (Å) | **D-H**…A (deg) | Symmetry operation |
| O(1)-H(1B)...O(1) | 1.54 | 2.073(4) | 117.3 | x-1/4, -y+5/4, z-1/4 |
| O(1)-H(1A)...N(3) | 2.37 | 3.023(8) | 133.4 | x-1/4, -y+5/4, z-1/4 |
| C(1)-H(1)...O(1) | 2.36 | 3.286(8) | 171.9 | x-1/4, -y+5/4, z+3/4 |
| C(4)-H(4)...O(1) | 2.42 | 3.344(7) | 176.4 | x-1/4, -y+5/4, z+3/4 |
| C(2)-H(2)...N(2) | 2.60 | 3.431(5) | 148.8 | -x+3/2, -y+1/2, -z+1/2 |
| C(1)-H(1)...O(1) | 2.50 | 3.225(8) | 134.5 | -x+3/2, -y+1, z+1/2 |