Electronic Supplementary Material (ESI) for RSC Advances.


# Supporting Information

## Structures and photocatalytic properties of two new Zn(II) coordination polymers based on semi-rigid V-shaped multicarboxylate ligand

Shan-He Zhou[a], Jun Wang[a]*, Yi-Wei Liu[b], Yuyu Zhong[b], Yan-Chun Sun[a], Bin Xie[a], Aiqing Ma[b]*, Amita Singh,[c] Mohd. Muddassir,[d] Abhinav Kumar[c]*

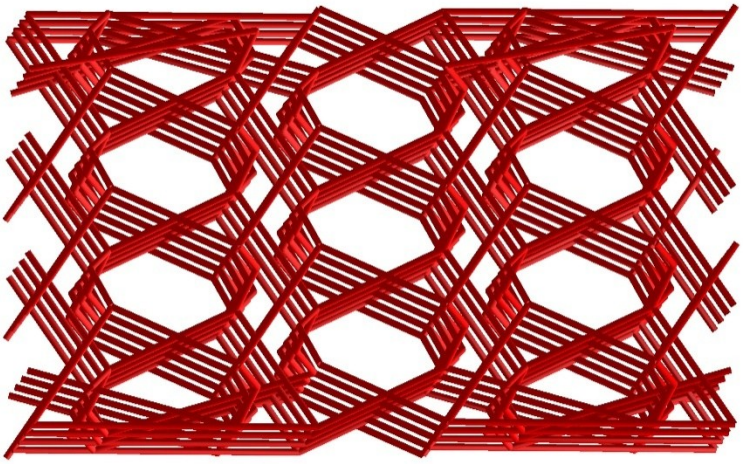

Fig. S1 Topological representation (view along the a axis) of the 4-connected 3D net

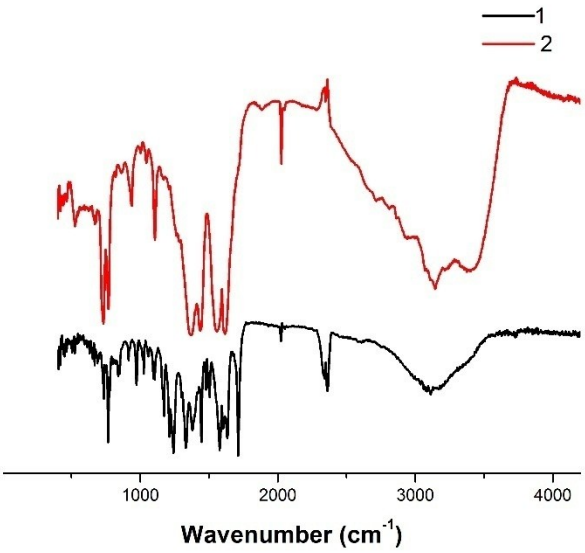


Fig. S2 view of the IR.

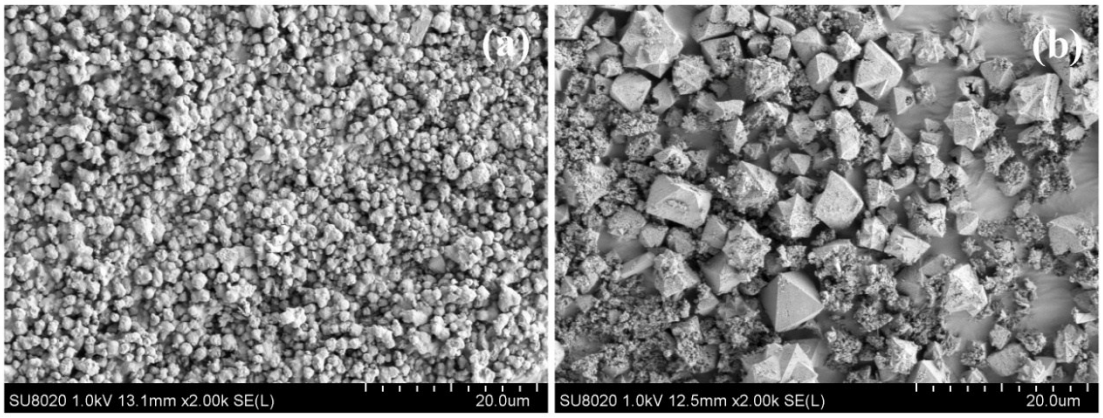


Fig. S3 SEM image of title CP s. The magnifications of picture were 100 thousand.

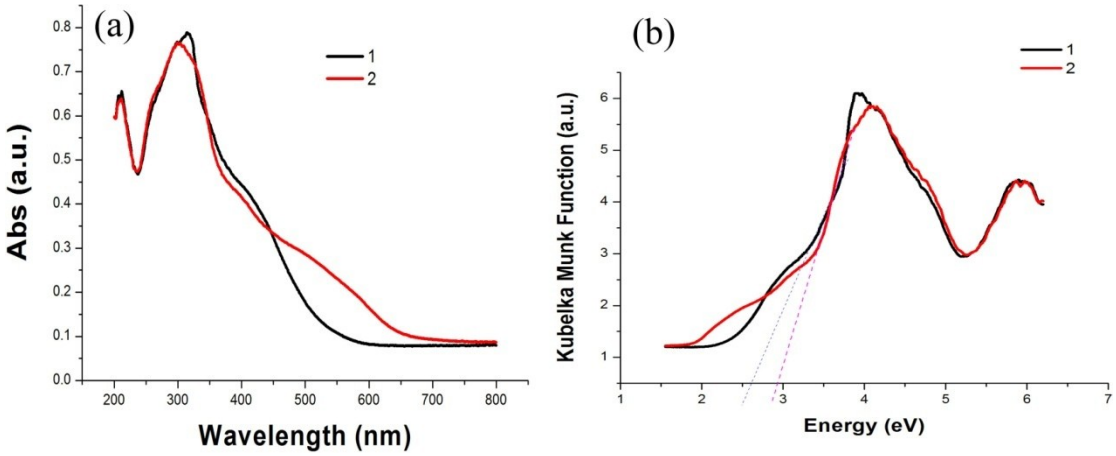


Fig.S4 (a)The UV-visible absorption spectrum of **1** and **2** and (b) Solid-state optical diffuse-reflection spectra of **1** and **2** derived from diffuse reflectance data at ambient temperature.

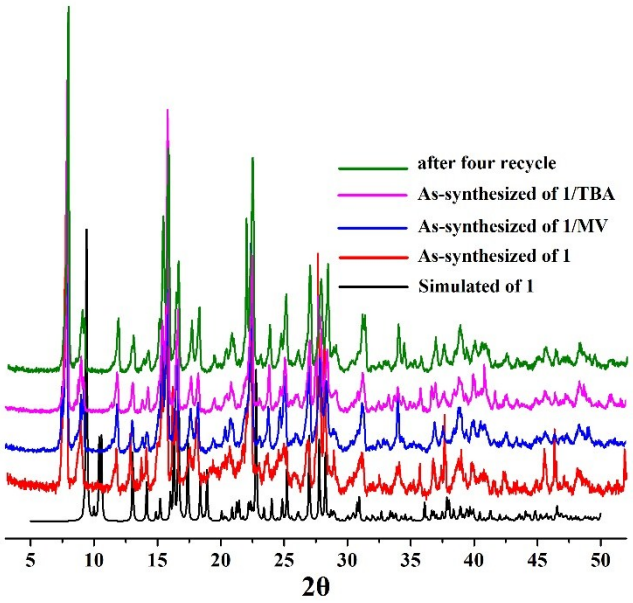


Fig. S5 view of the PXRD patterns of **1** under the different conditions.

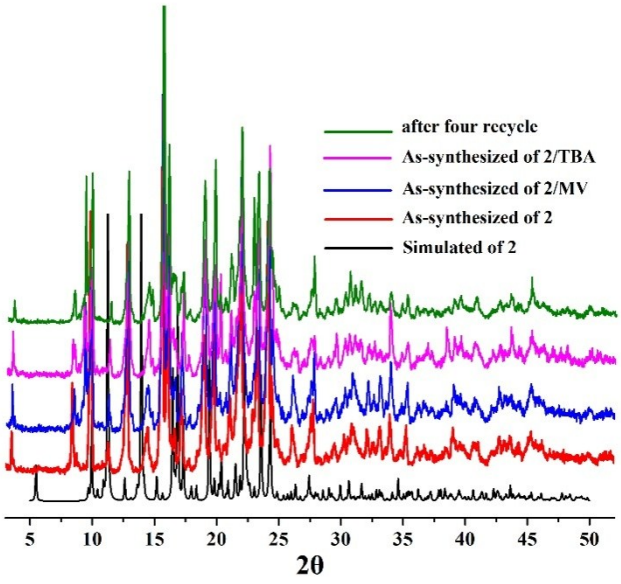


Fig. S6 view of the PXRD patterns of **2** under the different conditions.

**Table 1. Crystallographic data and structure refinement details for CPs 1-2**

| Parameter | **1** | **2** |
|---|---|---|
| Formula weight | 539.80 | 1263.07 |
| Crystal system | Triclinic | Monoclinic |
| Space group | *P-1* | *C2/c* |
| Crystal Color | Colorless | Colorless |
| *a*, Å | 9.9215(14) | 32.621(5) |
| *b*, Å | 11.0863(16) | 9.236(4) |
| *c*, Å | 12.2729(17) | 18.455(5) |
| *α*, ° | 111.943(2) | 90 |
| *β*, ° | 102.760(2) | 98.21(2) |
| *γ*, ° | 106.552(2) | 90 |
| *V*, Å $^3$ | 1116.0(3) | 5503(3) |
| *Z* | 2 | 4 |
| $\rho_{calcd}$, g/cm$^3$ | 1.606 | 1.525 |
| μ, mm$^{-1}$ | 1.157 | 2.150 |
| *F*(000) | 552 | 2568 |

| | | |
|---|---|---|
| θ Range, deg | 2.4-27.7 | 4.8-66.0 |
| Reflection Collected | 5246 | 4727 |
| Independent reflections ($R_{int}$) | 0.016 | 0.043 |
| Reflections with $I > 2\sigma(I)$ | 4233 | 3321 |
| Number of parameters | 332 | 409 |
| $R_1$, $wR_2(I > 2\sigma(I))^*$ | 0.0326, 0.0824 | 0.0993, 0.2785 |
| $R_1$, $wR_2$ (all data)** | 0.0417, 0.0866 | 0.1236, 0.3126 |

* $R = \sum(F_o - F_c)/\sum(F_o)$, ** $wR_2 = \{\sum[w(F_o^2 - F_c^2)^2]/\sum(F_o^2)^2\}^{1/2}$.

**Table 2.** Selected bond distances (Å) and angles (deg) for **1-2**

| | | | |
|---|---|---|---|
| | **1** | | |
| Zn(1)-O(1) | 2.0287(18) | Zn(1)-O(8) | 2.0951(16) |
| Zn(1)-N(1) | 2.1134(18) | Zn(1)-N(2) | 2.109(2) |
| Zn(1)-O(3)#1 | 2.0757(18) | | |
| | **2** | | |
| Zn-O(6) | 2.229(10) | Zn-N(3) | 2.013(12) |
| Zn-O(6)#1 | 2.061(11) | Zn-O(7)#1 | 2.121(7) |
| Zn(01)-O(1) | 1.909(9) | Zn(01)-N(1) | 2.015(6) |
| Zn(01)-N(2) | 2.086(8) | Zn(01)-O(4)#2 | 1.955(6) |
| | **1** | | |
| O(1)-Zn(1)-O(8) | 89.83(7) | O(1)-Zn(1)-N(1) | 93.20(7) |
| O(1)-Zn(1)-N(2) | 132.16(7) | O(1)-Zn(1)-O(3)#1 | 127.92(7) |
| O(8)-Zn(1)-N(1) | 165.01(8) | O(8)-Zn(1)-N(2) | 89.53(7) |
| O(3)#1-Zn(1)-O(8) | 94.21(7) | N(1)-Zn(1)-N(2) | 77.57(8) |
| O(3)#1-Zn(1)-N(1) | 95.49(7) | O(3)#1-Zn(1)-N(2) | 99.82(7) |
| | **2** | | |
| O(6)-Zn-N(3) | 123.9(4) | O(6)-Zn-O(6)#1 | 86.8(4) |
| O(1)-Zn-O(7)#1 | 136.6(6) | O(6)#1-Zn-N(3) | 91.3(5) |
| O(7)#1-Zn-N(3) | 88.6(5) | O(6)#1-Zn-O(7)#1 | 62.3(5) |
| O(1) -Zn(01)-N(1) | 139.6(3) | O(1)-Zn(01)-N(2) | 101.7(3) |
| O(1)-Zn(01)-O(4)#2 | 106.0(3) | N(1)-Zn(01)-N(2) | 100.3(3) |
| O(4)#2-Zn(01)-N(1) | 106.3(2) | O(4)#2-Zn(01)-N(2) | 93.0(3) |

Symmetry Cddes: **For 1**: #1= 1+x, y, z. **For 2**: #1 = 1-x, y, 3/2 -z; #2 = x, 1-y, -1/2+z.