Supplementary Information

Multifaceted Properties of Engineered Three-Dimensional Zn(II)-Metal-Organic Coordination Polymer: Synthesis, Crystal Structure, Efficient Photocatalytic Degradation of Organic Dye and Selective Luminescent Sensing

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Crystals Information:

Crystals of Zn were thin needles, and all were at least twinned (most were heavily intergrown in addition to twinning). I collected data from a needle with only two twin domains. The voids between the MOF nodes and ligands are filled with solvate molecules, but these were too disordered to build a model for. I thus used Squeeze to correct for their contribution to the scattering. I refined the N-heterocycle as disordered. The final result is not too bad.

Here what I added to the cif:

The crystal under investigation was found to be non-merohedrally twinned. The orientation matrices for the two components were identified using the program Cell_Now, with the two components being related by a 180 degree rotation around the real c-axis. The two components were integrated using Saint and corrected for absorption using twinabs, resulting in the following statistics:

13106 data (2845 unique) involve domain 1 only, mean I/sigma 10.0

13069 data (2855 unique) involve domain 2 only, mean I/sigma 5.6

22002 data (5444 unique) involve 2 domains, mean I/sigma 8.6

The exact twin matrix identified by the integration program was found to be:

-0.99999 0.00018 -0.12315

-0.00010 -1.00000 -0.00066

-0.00019 -0.00055 0.99999

The structure was solved using direct methods with only the non-overlapping reflections of component 1. The structure was refined using the hklf 5 routine with all reflections of component 1 (including the overlapping ones), resulting in a BASF value of 0.250(1).

The Rint value given is for all reflections and is based on agreement between observed single and composite intensities and those calculated from refined unique intensities and twin fractions (TWINABS (Sheldrick, 2012)).

One of the nitrogen heterocycles is disordered by a slight tilt. The two disordered moieties were restrained to have similar geometries and both were restrained to be close to planar. Atom N1 was excluded from the disorder. Uij components of ADPs for disordered atoms closer to each other than 2.0 Angstrom were restrained to be similar. Subject to these conditions the occupancy ratio refined to 0.53(2) to 0.47(2).

In addition to twinning, the structure also exhibits large volume sections (ca. 53.4 % oif the unit cell volume) consisting of highly disordered solvate or other small molecules. No satisfactory model for the solvate molecules could be developed, and the contribution of the solvate molecules was instead taken into account by reverse Fourier transform methods. The data were first detwinned (using the LIST 8 function of Shelxl2018) and then the cif and fcf files were subjected to the SQUEEZE routine as implemented in the program Platon. The resultant files were used in the further refinement. (Both the hklf 5 type HKL

file and the detwinned FAB file are appended to this cif file). A volume of 2797 cubic Angstrom per unit cell containing 690 electrons was corrected for.

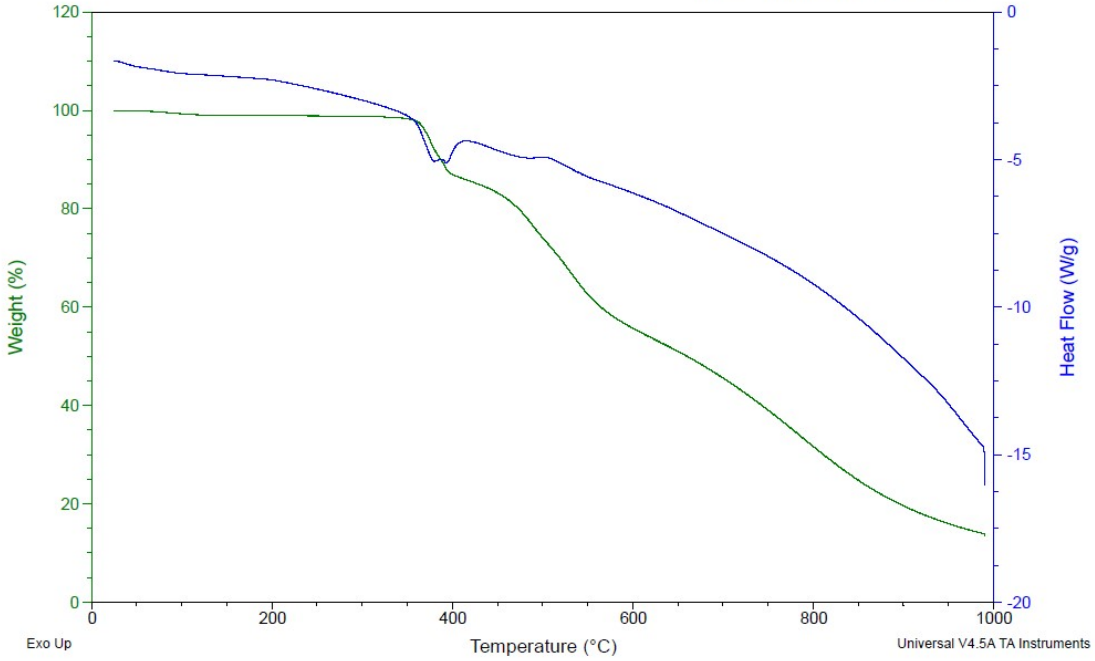

Figure S1. The TGA/DSC spectra for **ZnCP**.

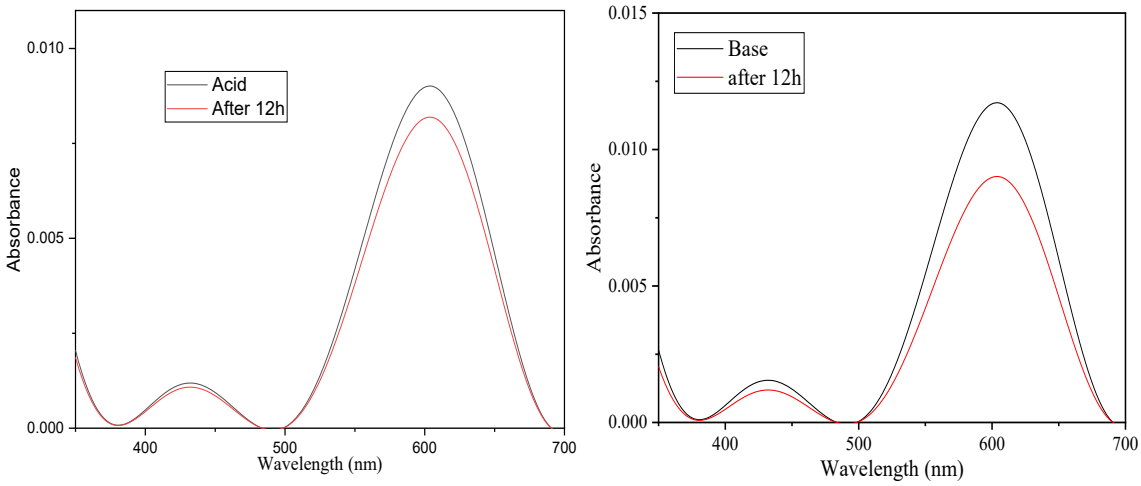

Figure S2. The Absorption spectrum for **ZnCP** a) acidic medium (0.1M H_2SO_4), and b) basic medium (1M KOH)

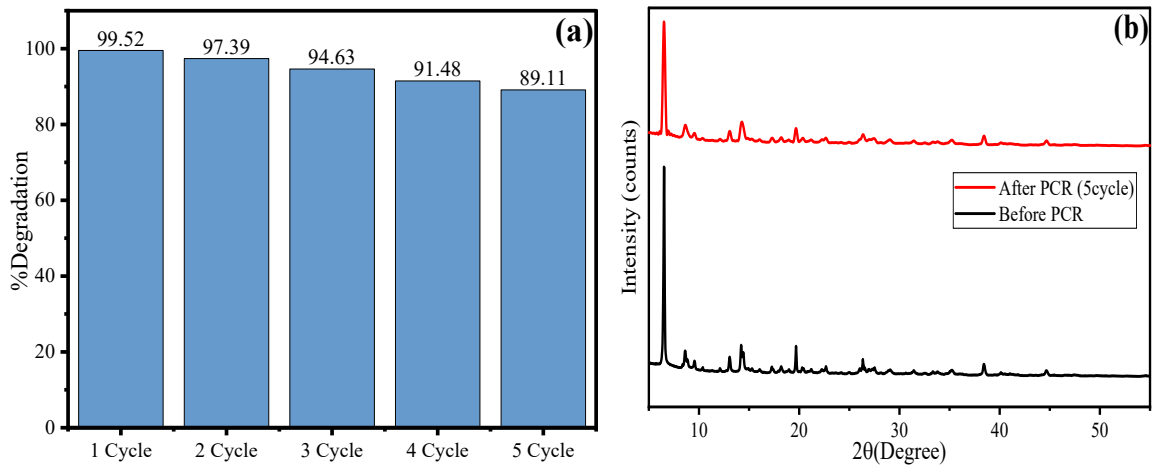

Figure S3. Reusability experiments up to consecutive 5 cycles of photocatalytic degradation of MG dye under optimum conditions (b) PXRD of synthesize **ZnCP** before and after the photocatalytic reaction (PCR)

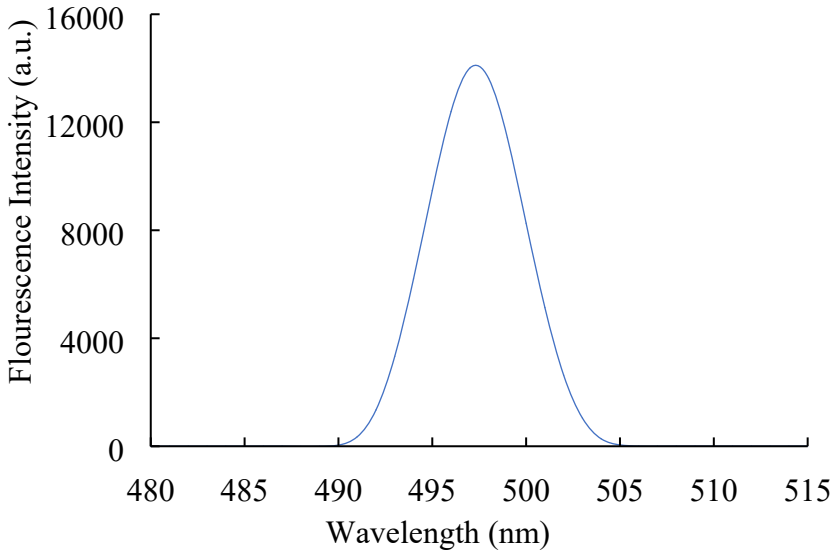

Figure S4. The luminescence spectrum for **ZnCP** in the absence of VOCs.