Supporting Information

Synthesis, Crystal Structure, Photoluminescence Properties and Antibacterial Activity of a Zn(||) Coordination Polymer Based on Paddle-Wheel Cluster

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1 X-ray Powder Diffraction Analyses

Phase purity of complex **1** is sustained by the powder X-ray diffraction pattern, Figure S1. The most peak positions of simulated and experimental patterns are in good agreement with each other, the differences in intensity may be due to the preferred orientation of the powder samples.



Figure S1. The powder XRD patterns and the simulated one from the single-crystal diffraction data for complex **1**.

2 IR Spectra

FT-IR spectrum of complex **1** was also investigated, Figure S2. The sharp bands at about 1650 cm⁻¹ and 1404 cm⁻¹ are attributed to asymmetric and symmetric stretching vibrations of carboxylic group, respectively.[1-2]



Figure S2. FT-IR spectra of complex 1.

3 Thermogravimetric Analyse

To assess the thermal stability and their structural variation with the temperature, thermogravimetric analysis (TGA) of complex **1** was performed under a N₂ atmosphere by using single-phase polycrystalline samples, Figure S3. Complex **1** has two identifiable weight loss steps: the first one is consistent with the removal of two lattice ethanol molecules (obsd 84.21%, calcd 84.27%), which appears between 48 and 157 °C. The second weight loss from 157 °C to 373 °C can be ascribed to the removal of one lattice ethanol molecule (obsd 76.44%, calcd 76.41%). The last one is attributed to the collapse of the framework, which is in the range of 373 °C to 561 °C. It worth pointed out that complex **1** with such high thermal stability are beneficial for their antibacterial application.



Figure S3. TG curve of complex 1.



Figure S4. The solid state photoluminescence spectra of complex 1 and H₂BCPPO at room temperature.

Reference

[1] Sun, D.; Han, L.; Yuan, S.; Deng, Y.; Xu, M.; Sun, D. Four New Cd(II) Coordination Polymers with Mixed Multidentate N-Donors and Biphenyl-Based Polycarboxylate Ligands: Syntheses, Structures, and Photoluminescent Properties. *Cryst. Growth Des.* 2013, 13, 377-385.

[2] Zhang, L.; Guo, J.; Meng, Q.; Wang, R.; Sun, D. Syntheses, structures and characteristics of four metal-organic coordination polymers based on 5-hydroxyisophthalic acid and N-containing auxiliary ligands. *CrystEngComm*, 2013, 15, 9578-9587.