Chunying Xu, Xinhua Lou* and Shimin Wang

Crystal structure of poly-[bis(μ₃-5-hydroxyisophthalato-κ⁢³⁴⁰⁰⁰⁰⁰⁰°')(μ₂-1,4-bis(2-ethylbenzimidazol-1-ylmethyl)benzene-κ²⁴⁰⁰⁰⁰⁰⁰°')dizinc(II)], C₄₀H₃₀N₄O₅Zn₂

Abstract

C₄₀H₃₀N₄O₅Zn₂, triclinic, P̅₁ (No. 2), a = 8.5232(17) Å, b = 9.947(2) Å, c = 11.555(2) Å, α = 72.76(3)°, β = 77.78(3)°, γ = 70.13(3)°, V = 873.2(3) Å³, Z = 1, R₁(F) = 0.0363, wR₂(F²) = 0.0852, T = 293(2) K.

CCDC no.: 1473960

Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

A mixture of 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (73.2 mg, 0.2 mmol), Zn(Ac)₂ - 2H₂O (21.9 mg, 0.1 mmol), 5-hydroxyisophthalic acid (36.4 mg, 0.2 mmol), and H₂O (10 mL) were placed in a Teflon-lined stainless steel vessel, heated to 170 °C for 4 days, and then cooled to room temperature for 24 h. Colorless block crystals of the title complex were obtained.

*Corresponding author: Xinhua Lou, College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China, e-mail: louxinhuancs@163.com

Chunying Xu: College of Chemistry and Chemical Engineering, Luoyang Normal University, Luoyang, Henan 471022, P. R. China

Shimin Wang: Department of Materials and Chemical Engineering, Henan Institute of Engineering, Zhengzhou, Henan 451191, P. R. China

© 2016 Chunying Xu et al., published by De Gruyter.

This work is licensed under the Creative Commons Attribution-NonCommercial-NoDerivatives 3.0 License.
may adjust the structural features and build complicated and fascinating MOFs [8].

Single crystal structure analysis reveals that there is one half 1,4-bis(2-methylbenzimidazol-1-ylmethyl)benzene (bmb), one 5-hydroxyisophthalate (hip) and one Zn(II) ion in the asymmetric unit. As shown in the figure, the Zn(II) is four-coordinated in a tetrahedral geometry, ligated by three oxygen atoms (O1, O2, and O3) from three symmetry-related 5-hydroxyisophthalate, one nitrogen atoms (N1) from bmb. The bond lengths are Zn(1)—O(1) = 1.966(2) Å, Zn(1)—O(2) = 2.005(2) Å, Zn(1)—O(3) = 1.912(2) Å, and Zn(1)—N(1) = 1.990(2) Å, respectively. They are in the normal ranges [9]. The two methylbenzimidazol arms of bmb bend in opposite directions to bridge adjacent Zn(hip) chains to form a 2D layer structure.

Acknowledgements: This work was financially supported by the Science and technology research key project of the Education Department of Henan Province (2014A1500025) and the Provincial cultivation fund of Luoyang normal university (2013-PYJJ-005).

References

5. Xin, L. Y.; Liu, G. Z.; Wang, L. Y.: New coordination polymers from 1D Chain, 2D layer to 3D framework constructed from 1,2-phenylenediacetic acid and 1,3-bis(4-pyridyl)propane flexible ligands. J. Solid State Chem. 184 (2011) 1387–1392.