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NOTE

3-Dimensional 4-Connected Metal-Organic Frameworks of Zinc(II) Built from 5-Aminotetrazole

ZHIQIANG JIANG

Biology and Chemistry Engineering College of Panzhihua University, Sichuan 617000, P.R. China

Corresponding author: E-mail: myjiangzq@163.com

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A novel metal-organic frameworks, [compound **1**, $Zn(ATZ)_2$, ATZ = 5-aminotetrazole], has been synthesized by the solvothermal reaction of zinc nitrate and 5-aminotetrazole. Compound **1** displays a unique three-dimensional four-connected dia topological network.

Key Words: Metal-organic frameworks, Zinc, 5-Aminotetrazole.

Current interest in the synthesis of crystalline 4-connected zeolite-like materials is rapidly expanding owing to their intriguing architectures and potential applications[1-4]. Imidazole and its derivative with various interesting coordination chemistry and a strong networking ability have been extensively used as organic linkers for construction of novel 4-connected zeolitic imidazolate frameworks (ZIF)[5,6]. Because they have highest content of nitrogen among the organic substances and show surprisingly high thermal stabilities, 5-aminotetrazole are prospective materials for the generation of gases, such as blowing agents, solid propellants and other combustible and thermally decomposing systems[7,8]. In this work, we report a novel metal-organic frameworks, [$Zn(ATZ)_2$, ATZ = 5-aminotetrazole].

All reagents and solvents employed were commercially available and used as received without further purification.

Preparation of compound: A mixture of $Zn(NO_3)_2 \cdot 6H_2O$ (0.1499 g, 0.51 mmol), pyrazine (0.0300 g 0.37 mmol), 5-aminotetrazole (ATZ, 0.0935 g, 1.1 mmol), 2,6-naphthalenedicarboxylic acid (2,6-ntd, 0.0512 g 0.24 mmol), tetramethylammonium bromide (0.0300 g 0.20 mmol), 2-imidazolidinone (1.9903 g, 20 mmol), methanol (3.0 mL) and *N,N*-dimethylacetamide (DMA, 3.0 mL) in a 23 mL teflon-lined stainless steel vessel was heated at 120 ºC for 96 h and then cooled to room temperature. The resulting colourless transparent crystals were obtained, washed using acetone and dried at room temperature.

X-crystallography: Suitable single crystals of [$Zn(ATZ)_2$] were carefully selected under an optical microscope and glued to thin glass fibers. Whereafter, single-crystal X-ray diffraction analyses were performed on a computer-controlled XCalibur E CCD diffractometer with graphite-monochromated MoK_α radiation ($\lambda_{MoK\alpha}$ = 0.71073 Å) at T = 293.2 K. Empirical absorption corrections were made using the SADABS program[9]. The structures were solved using the direct method and refined by full-matrix least-squares methods on F^2 by using the SHELX-97 program package[10]. All non-hydrogen atoms were refined anisotropically and hydrogen atoms attached to carbon or nitrogen atoms were fixed at their ideal positions.

Structure description: Single-crystal X-ray analysis revealed that the asymmetric unit of compound **1** contains one Zn^{2+} cation, two independent anionic ATZ^- ligands (Fig. 1a). Each ATZ^- anion serves as μ_2-bridge linking two Zn atoms and each Zn atom is surrounded by four ATZ^- ligands, where the four-coordinated Zn atom adopts a tetrahedral geometry (Fig. 1b). Interestingly, there are a cage comprising twelve ATZ ligands and these cages constructed three-dimensional frameworks (Fig. 1c). A better insight into the nature of this intricate framework can be achieved by the application of a topological approach. As shown in Fig. 1d and 1e, if every Zn atom acts as a nodal point, each nodal point was further linked to result in four-connected frameworks, which can be abstracted as a uninodal 4-connected typical dia topological net. The result of topological analysis indicates this network has extended point symbol of 6(2).6(2).6(2).6(2).6(2).6(2).

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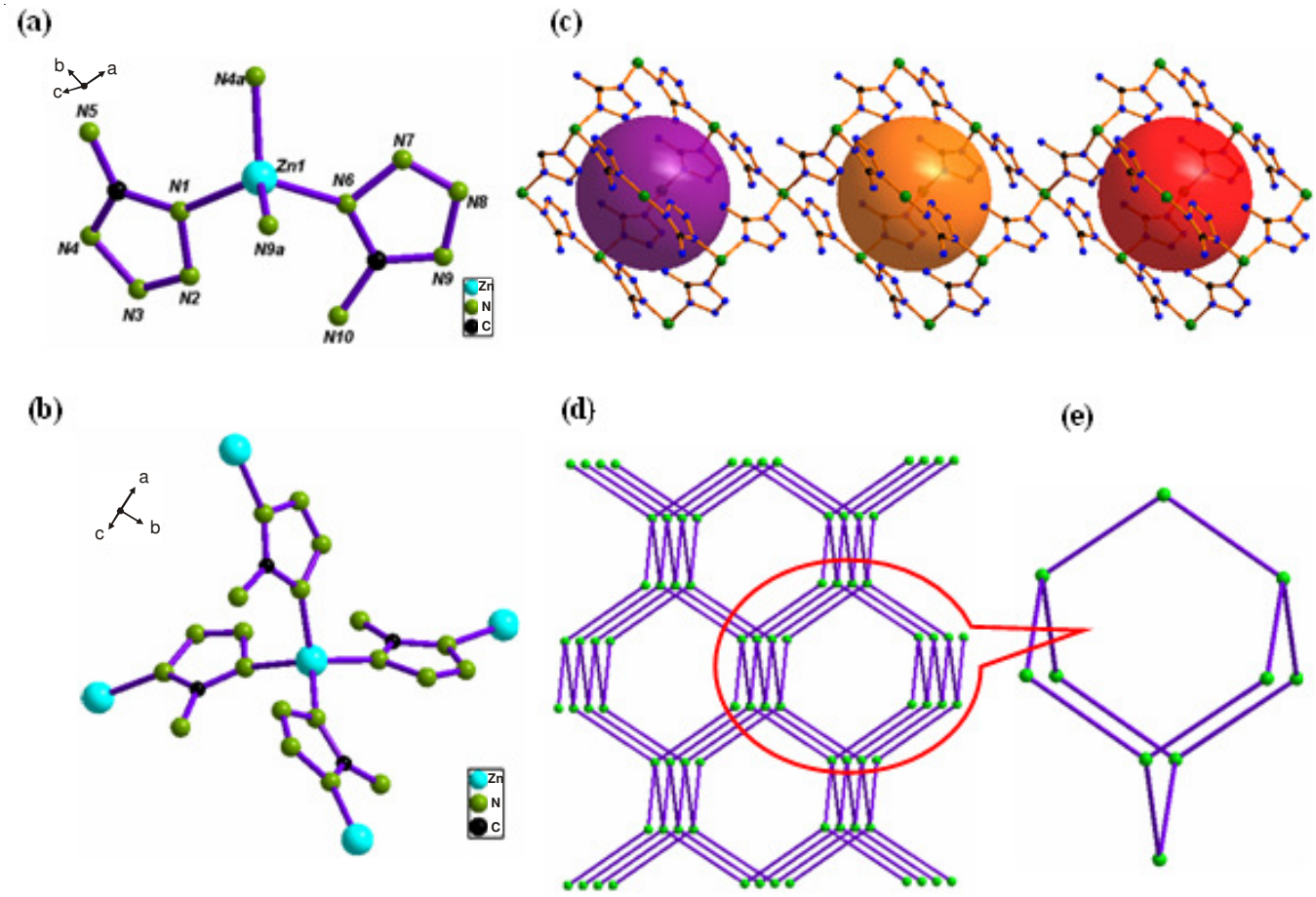

Fig. 1. (a) and (b) Coordination environment around the zinc(II) atoms and ATZ ligands in compound **1**; (c) The units of cage in compound **1**; (d) The topology of compound **1**; (e) The dia topology in the topology of compound **1**

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