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NOTE

An Intriguing Multinuclear Cluster Based on Zinc and Benzotriazole Under Solvothermal Synthesis

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The intriguing multinuclear cluster [compound **1**, $Zn_9(btz)_{12}(CH_3COO)_6$, btz = benzotriazole] was obtained by solvothermal reactions using zinc(II) nitrate and benzotriazole and its crystal structure was solved from conventional single-crystal X-ray data. Crystal data for compound $Zn_9(btz)_{12}(CH_3COO)_6$: triclinic space group P-1, a = 13.0714(4) Å, b = 14.0576(4) Å, c = 16.0683(5) Å, α = 69.265(3)°, β = 78.194(2)°, γ = 65.436(3)°, V = 2505.71(13) $Å^3$ and Z = 1.

Key Words: Zinc, Benzotriazole, Multinuclear cluster, Solvothermal.

It is very important to choose suitable building block while the two-dimensional or three-dimensional frameworks are constructed. Metal-organic replica of inorganic minerals with connectivity equal to ten is rare to date. One promising approach for the creation of highly connected topologies is to use polynuclear metal clusters as nodes[1-5]. So multinuclear clusters built from some triazole homologs have attracted much attention owing to high possibility and their structural diversities of the architectures[6]. In this work, we present an intriguing multinuclear cluster employing benzotriazole.

The chemicals with reagent-grade quality employed were commercially available and used as received without further purification.

Preparation of compound: Compounds **1** was synthesized under solvothermal conditions using a 23 mL capped scintillation vial. In a typical reaction, $Zn(NO_3)_2{\cdot}6H_2O$ (0.1029 g, 0.35 mmol), pyrazine (0.0273 g, 0.33 mmol), benzotriazole (btz, 0.0681 g, 0.57 mmol), were added to *N,N*-dimethylacetamide (DMA, 8 mL). The reactants were stirred to form a clear liquid prior to heating at 120 ºC for 6 days. Colourless transparent single crystals of $Zn_9(btz)_{12}(CH_3COO)_6$ suitable for X-ray diffraction were obtained.

X-crystallography: Suitable single crystals were selected under a polarizing microscope and fixed with epoxy cement on fine glass fibers which were mounted 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. The hydrogen atoms bound to carbon were located by geometrically calculations. All non-hydrogen atoms were refined by full-matrix least-squares techniques. All calculations were performed by the SHELXTL 97 program[7].

Structure description: A single-crystal X-ray diffraction analysis shows that compound **1** crystallizes in P-1 space group. The asymmetric unit of **1** possesses of five unique metal ions and two coordination models of zinc, Both Zn1 and Zn2 are six-coordinated by six N-donors of benzotriazole, while Zn3, Zn4 and Zn5 are surrounded by three benzotriazole nitrogen atoms plus two oxygen atoms of one chelating carboxylate groups of one deprotonated acetic acid ligand from the decomposition of DMA solvent *in situ*. The Z-O/N bond lengths are in the normal range.

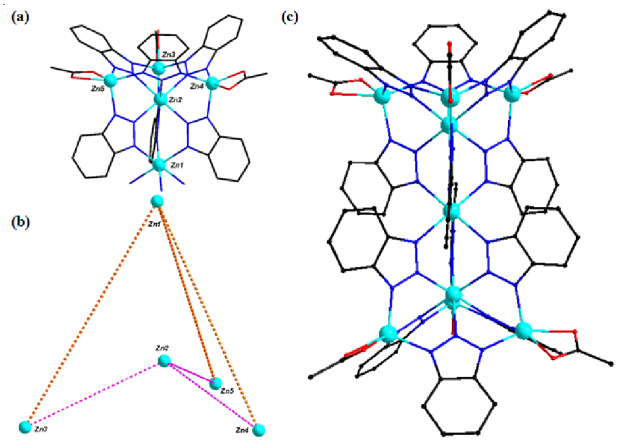

Fig. 1. (a) Coordination environment around the Zn atoms in 1; (b) schematic representation of two tetrahedrons in the asymmetric unit of 1; (c) perspective view of Zn cluster of $Zn_9(btz)_{12}(CH_3COO)_6$. Hydrogen atoms are omitted

An unprecedented structural feature of the asymmetric unit is the presence of two tetrahedrons, comprising Zn1, Zn3, Zn4, Zn5 with Zn--Zn distances of 6.009 Å-6.105 Å and Zn2, Zn3, Zn4, Zn5 with Zn--Zn distances of 3.573 Å-3.610 Å, respectively. The center Zn atoms (Zn1 and Zn2) are located on a special top position of the tetrahedrons. In the structure of $Zn_9(btz)_{12}(CH_3COO)_6$, Zn1 locates at a special site with a symmetry center, so that other tetrahedrons are generated and construct a nine-nuclear Zn cluster (Fig. 1c).

REFERENCES

1. J.G. Haasnoot, *Coord. Chem. Rev.*, **131**, 200 (2000).
2. X.L. Wang, C. Qin, E.B. Wang, Z.M. Su, L. Xu and S.R. Batten, *Chem. Commun.*, 4789 (2005).
3. X.L. Wang, C. Qin, E.B. Wang, Z.-M. Su, Y.G. Li and L. Xu, *Angew. Chem., Int. Ed.*, **45**, 7411 (2006).
4. X.L. Wang, C. Qin, E.B. Wang and Z.M. Su, *Chem.-Eur. J.*, **12**, 2680 (2006).
5. Z.Q. Jiang, *Asian J. Chem.*, **25**, 2353 (2013).
6. X.L. Wang, C. Qin, Y.Q. Lan, K.Z. Shao, Z.M. Su and E.B. Wang, *Chem. Commun.*, 410 (2009).
7. G.M. Sheldrick, SHELXTL97, Program for the Refinement of Crystal Structure, University of Gottingen, Germany (1997).