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Crystallographic report

A three-dimensional zinc trimesate framework: $[(CH_3)_2NH_2][Zn(C_9H_3O_6)]\cdot(C_3H_7NO)$

Xiao-Jun Zhao[1] **and Jun Tao**[2]*

[1]Chemistry Section, College of Pharmaceutical Sciences, Guangzhou University of Traditional Chinese Medicine, Guangzhou 510405, People's Republic of China
[2]Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, People's Republic of China

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The structure features an anionic three-dimensional network built from zinc ions and trimesate ligands. The structure contains parallelogrammic channels in which H_2NMe_2 molecules interact with dimethylformamide guest molecules and the framework through hydrogen bonds. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: solvothermal synthesis; trimesate; metal–organic framework; crystal structure

COMMENT

Metal–organic frameworks have been largely investigated in the past several decades because of their interesting topologies and potential applications in the fields of gas storage, catalysis and ion exchange.[1–3] As a continuation of our work in this field,[4,5] we report a three-dimensional (3-D) framework, $[(CH_3)_2NH_2][Zn(C_9H_3O_6)]\cdot(C_3H_7NO)$ (**1**), which is shown to contain one-dimensional channels. The zinc, Fig. 1, is tetrahedrally surrounded by four oxygen atoms from four different trimesate (L) ligands; one carboxylate group (O1, O2) is bidentate and the other two are monodentate. The connectivity between dinuclear zinc units and L gives rise to a 3-D anionic framework featuring parallelogrammic channels encapsulating hydrogen-bond-supported H_2NMe_2 and dimethylformamide (DMF) molecules (Fig. 2).

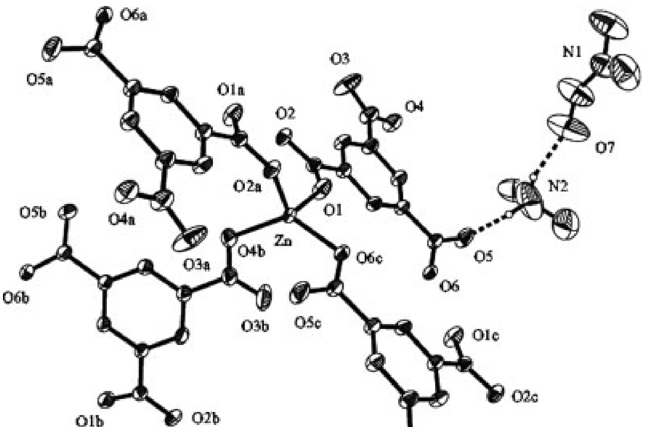

Figure 1. Zinc atom geometry in **1** (35% probability); carbon-bound hydrogen atoms are omitted for clarity. Key geometric parameters: Zn–O1 1.957(2), Zn–O2a 1.963(2), Zn–O4b 1.924(2), Zn–O6c 1.928(2), N2–H···O5 2.680(5), N2–H···O7 2.868(8) Å; O1–Zn–O2a 114.37(8), O1–Zn–O4b 113.53(9), O1–Zn–O6c 94.59(7), O2a–Zn–O4b 99.43(8), O2a–Zn–O6c 109.97(8), O4b–Zn–O6c 125.82(8)°. Symmetry operations: (a) $1-x, -y, 1-z$; (b) $1.5-x, 1+y, 1.5-z$; (c) $2-x, -y, 1-z$.

EXPERIMENTAL

Trimesic acid (0.070 g, 0.30 mmol) and $Zn(NO_3)_2\cdot 6H_2O$ (0.110 g, 0.30 mmol) were dissolved in DMF (10 ml) at room temperature. The solution was transferred into a Parr Teflon-lined stainless steel vessel (23 cm^3), then the vessel was sealed and heated to 110 °C for 10 days,

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*Correspondence to: Jun Tao, Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, People's Republic of China.
E-mail: taojun@jingxian.xmu.edu.cn

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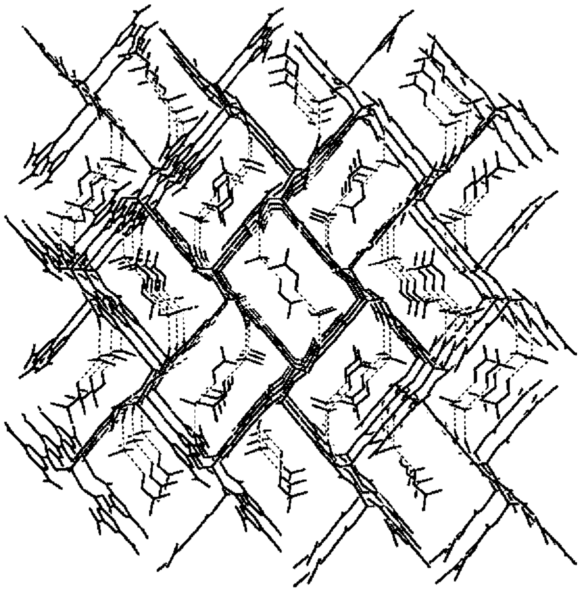

Figure 2. The 3-D structure of **1** viewed along the *a* axis.

and finally cooled at 5 °C h^{-1} to room temperature. Colorless block-like crystals were collected by hand, washed with DMF and distilled water. Intensity data were collected at 298 K on a Bruker Apex CCD diffractometer for a colorless block crystal 0.18 × 0.24 × 0.25 mm^3. $C_{14}H_{18}N_2O_7Zn$, $M = 391.67$, monoclinic, $P2_1/n$, $a = 9.4469(4)$ Å, $b = 16.2456(7)$ Å, $c = 11.5176(8)$ Å, $\beta = 97.027(1)°$, $V = 1754.34(16)$ $Å^3$, $Z = 4$; 4064 unique data ($\theta = 28.4°$), 3372 data with $I \geq 2\sigma(I)$, $R = 0.040$ (obs. data), $wR = 0.119$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 250088.

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REFERENCES

1. Batten SR, Robson R. *Angew. Chem. Int. Ed.* 1998; **37**: 1460.
2. Eddaoudi M, Moler DB, Li H, Chen B, Reineke TM, O'Keeffe M, Yaghi OM. *Acc. Chem. Res.* 2001; **34**: 319.
3. Kitagawa S, Kitaura R, Noro S. *Angew. Chem. Int. Ed.* 2004; **43**: 2334.
4. Tao J, Yin X, Huang RB, Zheng LS. *Inorg. Chem. Commun.* 2002; **5**: 1000.
5. Tao J, Yin X, Jiang YB, Huang RB, Zheng LS. *Inorg. Chem. Commun.* 2003; **6**: 1171.