APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2003; **17**: 877–878
Main Group Metal Compounds
Published online in Wiley InterScience (www.interscience.wiley.com). DOI:10.1002/aoc.546

Crystallographic report

Crystal structure of a two-dimensional coordination polymer: tetraaqua-1,2,4,5-benzenetetracarboxylato-(pyrazine)dizinc(II) dihydrate

Shi-Yao Yang[1]*, La-Sheng Long[1], Rong-Bin Huang[1], Lan-Sun Zheng[1] and Seik Weng Ng[2]**

[1]Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, People's Republic of China
[2]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Received 8 August 2003; Revised 11 August 2003; Accepted 12 August 2003

The structure of $\{[Zn_2(1,2,4,5\text{-btc})(pz)(H_2O)_4]\cdot 2(H_2O)\}_n$ (1,2,4,5-btc = 1, 2, 4, 5-benzenetetracarboxylate, pz = pyrazine) is a two-dimensional coordination network. The zinc(II) center is in a distorted octahedral NO_5 coordination environment that is defined by one nitrogen atom of pyrazine, three oxygen atoms of carboxyl groups from 1,2,4,5-benzenetetracarboxylate tetraanions and two water molecules. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: zinc; 1,2,4,5-benzenetetracarboxylate; pyrazine; coordination polymer

COMMENT

The assembly of coordination polymers is of great current interest, and in this context a number of coordination polymers of zinc benzenepolycarboxylates with *N*-heterocycles have been reported.[1–4] Here, we report the hydrothermal synthesis and crystal structure of a coordination polymer, $\{[Zn_2(1,2,4,5\text{-btc})(pz)(H_2O)_4]\cdot 2(H_2O)\}_n$, (1,2,4,5-btc = 1,2,4,5-benzenetetracarboxylate, pz = pyrazine). Crystallography shows that the zinc(II) center exists in a distorted octahedral NO_5 environment that is defined by the nitrogen atom of pyrazine, the two oxygen atoms of a chelating $-CO_2$ group from a 1,2,4,5-benzenetetracarboxylate anion, the oxygen atom of a unidentate $-CO_2$ belonging to another tetraanion and two water molecules (Fig. 1). The tetracarboxylate anion and the pyrazine molecule are each located

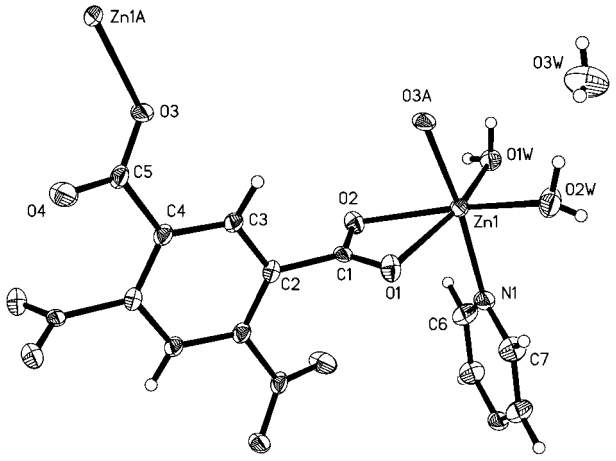

Figure 1. ORTEP plot showing the coordination environment of the zinc atom at the 50% probability level. Key geometry parameters: Zn1–O3A 2.020(3), Zn1–O2W 2.022(4), Zn1–O1W 2.070(3), Zn1–N1 2.134(3), Zn1–O1 2.170(3), Zn1–O2 2.224(3) Å; O3A–Zn1–O2W 90.7(1), O3A–Zn1–O1W 94.7(1), O2W–Zn1–O1W 97.7(2), O3A–Zn1–N1 172.2(1), O2W–Zn1–N1 92.3(2), O1W–Zn1–N1 92.0(1), O3A–Zn1–O1 88.3(1), O2W–Zn1–O1 103.5(1), O1W–Zn1–O1 158.6(1), N1–Zn1–O1 84.1(1), O3A–Zn1–O2 84.2(1), O2W–Zn1–O2 162.1(1), O1W–Zn1–O2 99.8(1), N1–Zn1–O2 90.9(1), O1–Zn1–O2 59.3(1)°. Symmetry operation: A = $1-x$, $1-y$, $2-z$.

*Correspondence to: Shi-Yao Yang, Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, People's Republic of China.
E-mail: syyang@yanan.xmu.edu.cn
**Correspondence to: La-Sheng Long, Department of Chemistry and State Key Laboratory for Physical Chemistry of Solid Surfaces, Xiamen University, Xiamen 361005, People's Republic of China.
E-mail: lslong@jingxian.xmu.edu.cn
Contract/grant sponsor: National Science Foundation of China; Contract/grant numbers: 20271044; 20273052.
Contract/grant sponsor: NSF of Fujian Province; Contract/grant number: E0110001.

Copyright © 2003 John Wiley & Sons, Ltd.

about a center of inversion. Each tetracarboxylate anion connects four zinc atoms and each pyrazine connects two. The bonding pattern leads to the formation of layers (Fig. 2) that are linked into a three-dimensional network by hydrogen bonds involving the water molecules and the oxygen atoms of the carboxyl groups.

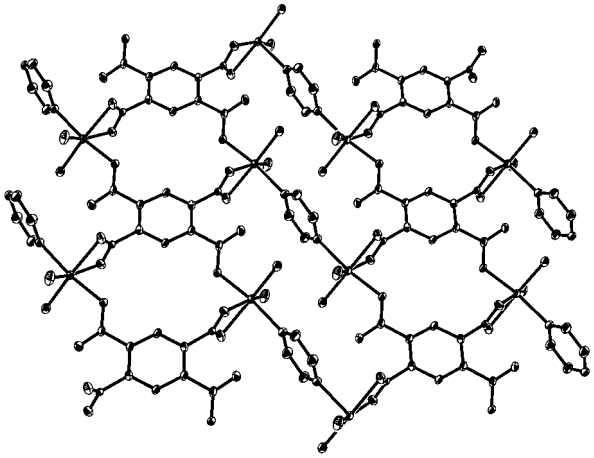

Figure 2. ORTEP plot of the two-dimensional structure at the 50% probability level. Lattice water molecules and hydrogen atoms are omitted.

EXPERIMENTAL

1,2,4,5-Benzenetetracarboxylic acid anhydride (pyromellitic anhydride, 0.22 g, 1 mmol) dissolved in water (15 ml) containing tetramethylammonium hydroxide (0.36 g, 4 mmol). Zinc dinitrate hexahydrate (0.60 g, 2 mmol) and pyrazine (0.16 g, 2 mmol) dissolved in water (3 ml) were added. The mixture was placed in a 20 ml Teflon-lined stainless-steel bomb. The bomb was heated to 180 °C for 100 h. Crystals separated from the solution when the bomb was cooled down at 5 °C h^{-1}. Intensity data were collected at 298 K on a Bruker Smart Apex CCD diffractometer for a crystal 0.44 × 0.10 × 0.06 mm^3. $C_{14}H_{18}N_2O_{14}Zn_2$, $M = 569.04$, triclinic, $P\bar{1}$, $a = 7.2233(6)$, $b = 8.0983(7)$, $c = 9.3433(8)$ Å, $\alpha = 95.932(2)$, $\beta = 102.381(1)$, $\gamma = 116.170(1)°$, $V = 466.74(7)$ $Å^3$, $Z = 1$; 2081 unique data ($\theta = 28.5°$), 1649 data with $I > 2\sigma(I)$. $R_1 = 0.044$, $wR_2 = 0.116$; $\rho_{max} = 0.70$ e $Å^{-3}$. Program used: SHELXL and ORTEP. CCDC deposition number: 216989.

Acknowledgements

We thank the National Science Foundation of China (grant nos 20271044 and 20273052) and NSF of Fujian Province, P.R. China (E0110001).

REFERENCES

1. Tao J, Tong ML, Chen XM. *J. Chem. Soc. Dalton Trans.* 2000; 3669.
2. Tao J, Tong ML, Shi JX, Chen XM, Ng SW. *Chem. Commun.* 2001; 2043.
3. Yang SY, Long LS, Tao J, Huang RB, Zheng LS. *Main Group Met. Chem.* 2002; **25**: 699.
4. Yang SY, Hu JY, Long LS, Huang RB, Zheng LS, Ng SW. *Appl. Organometal Chem.* 2003; **17**: 815.

Copyright © 2003 John Wiley & Sons, Ltd.