APPLIED ORGANOMETALLIC CHEMISTRY
Appl. Organometal. Chem. 2004; **18**: 91–92

Crystallographic report

A three-dimensional coordination polymer: poly-[μ_7-1,2,4,5-benzenetetracarboxylato-bis(*N*,*N*-dimethylformamide)dizinc(II)]

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Received 24 September 2003; Revised 20 October 2003; Accepted 21 October 2003

The structure of the title compound, $[Zn_2(btc)(DMF)_2]_n$ (btc = 1,2,4,5-benzenetetracarboxylate, DMF = *N*,*N*-dimethylformamide), shows that the octahedrally and tetrahedrally coordinated zinc atoms (present in the ratio 1 : 1) are linked by btc ligands to form a three-dimensional network comprising cross-linked channels occupied by coordinated DMF molecules.

KEYWORDS: zinc; 1,2,4,5-benzenetetracarboxylate; DMF; network structure

COMMENT

The assembly of coordination polymers with metal ions and carboxylic ligands in organic solvents is a practical method of preparation.[1–5] In the title compound, $[Zn_2(btc)(DMF)_2]_n$ (btc = 1,2,4,5-benzenetetracarboxylate, DMF = *N*,*N*-dimethylformamide), the two independent zinc atoms in the structure exist in different coordination geometries (Fig. 1). The Zn1 atom is coordinated by four oxygen atoms of carboxyl groups from three symmetry-related btc tetra-anions and two oxygen atoms from DMF molecules, leading to an octahedral geometry. The Zn2 atom exists in a tetrahedral geometry defined by four oxygen atoms derived from four btc tetra-anions. Thus, each btc tetra-anion connects seven zinc atoms and this leads to the formation of a three-dimensional network (Fig. 2) containing cross-linked channels running along the unit cell *c*-axis. The channels are occupied by coordinated DMF molecules attached to Zn1.

EXPERIMENTAL

1,2,4,5-Benzenetetracarboxylic acid anhydride (pyromellitic anhydride, 21.8 g, 0.1 mol) and zinc dinitrate hexahydrate (29.7 g, 0.1 mol) were dissolved in DMF (100 ml). The solution was allowed to stand undisturbed for 2 weeks and colorless crystals were deposited. Intensity data were collected at 298 K on a Bruker Smart Apex CCD diffractometer for a crystal $0.32 \times 0.32 \times 0.42$ mm^3. $C_{16}H_{16}N_2O_{10}Zn_2$, $M = 527.05$, tetragonal, $P4_2bc$, $a = 18.7775(8)$, $c = 11.8105(5)$ Å, $V = 4164.3(3)$ Å^3, $Z = 8$; 5039 unique data ($\theta = 28.3°$), 4508 data with $I > 2\sigma(I)$. $R_1 = 0.033$, $wR_2 = 0.093$; $\rho_{max} = 0.79$ e – Å^{-3}. Program used: SHELXL and ORTEP. CCDC deposition number: 220 249.

Acknowledgements

The National Science Foundation of China is thanked for support. (grant nos 20271044 and 20273052).

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Contract/grant sponsor: National Science Foundation of China; Contract/grant number: 20271044; 20273052.

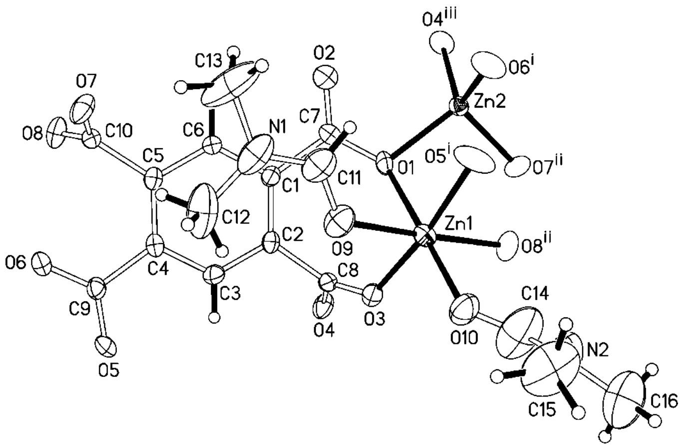

Figure 1. ORTEP plot (50% probability level) of the asymmetric unit in $[Zn_2(btc)(DMF)_2]_n$. Key geometric parameters: Zn1–O1 2.265(3), Zn1–O3 2.035(3), Zn1–O9 2.107(3), Zn1–O10 2.040(3), Zn1–O5^{i} 2.053(3), Zn1–O8^{ii} 2.088(2), Zn2–O1 1.993(2), Zn2–O4^{iii} 1.958(3), Zn2–O6^{i} 1.961(3), Zn2–O7^{ii} 1.977(3) Å; O1–Zn1–O3 80.2(1), O1–Zn1–O9 90.7(1), O1–Zn1–O10 177.5(1), O1–Zn2–O4^{iii} 113.8(1), O1–Zn2–O6^{i} 108.6(1), O1–Zn2–O7^{ii} 100.6(1), O3–Zn1–O9 91.0(1), O3–Zn1–O10 97.7(1), O3–Zn1–O5^{i} 171.4(1), O3–Zn1–O8^{ii} 92.5(1), O9–Zn1–O10 90.6(1), O1^{i}–Zn1–O5 91.3(1), O1^{ii}–Zn1–O8 90.8(1), O4^{iii}–Zn2–O6^{i} 110.7(1), O4^{iii}–Zn2–O7^{ii} 108.3(1), O5^{i}–Zn1–O8^{ii} 88.8(1), O5^{i}–Zn1–O9 87.8(1), O5^{i}–Zn1–O10 90.8(1), O6^{i}–Zn2–O7^{ii} 114.7(1), O8^{ii}–Zn1–O10 88.0(1), O8^{ii}–Zn1–O9 176.3(1)°. Symmetry operations: i, $y+1, -x+1, z+1/2$; ii, $-x+3/2, y+1/2, z$; iii, $y+1/2, x-1/2, z+1/2$.

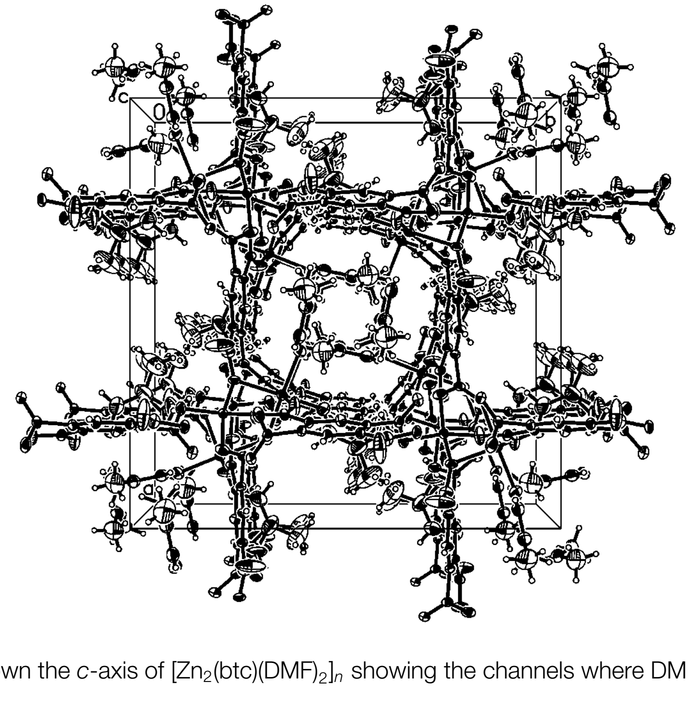

Figure 2. View down the *c*-axis of $[Zn_2(btc)(DMF)_2]_n$ showing the channels where DMF molecules reside.

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