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Main Group Metal Compounds **AOC**

Crystallographic report

A three-dimensional coordination polymer: $[Zn_6(btc)_4(4,4'\text{-bipy})_5]_n$ (btc = 1,2,4-benzenetricarboxylate; 4,4′-bipy = 4,4′-bipyridine)

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The three-dimensional (3D) coordination polymer $[Zn_6(btc)_4(4,4'\text{-bipy})_5]_n$ (1) (btc = 1,2,4-benzenetricarboxylate; 4,4′-bipy = 4,4′-bipyridine) has been prepared hydrothermally. The zinc(II) centers in 1 are bridged by btc ligands to form a trinuclear subunit, which is further linked by 4,4′-bipy and btc ligands to construct the 3D coordination architecture. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: zinc; 1,2,4-benzenetricarboxylate; 4,4′-bipyridine; coordination polymer

COMMENT

Based on our investigation on rational design and preparation of the rigid aromatic carboxylate-based d^{10} metal coordination polymers,[1,2] we now extend our work to systems containing two different organic ligands and report here the synthesis and crystal structure of a novel three-dimensional coordination polymer $[Zn_6(btc)_4(4,4'\text{-bipy})_5]_n$ (**1**) (btc = 1,2,4-benzenetricarboxylate; 4,4′-bipy = 4,4′-bipyridine). In **1**, both Zn1 and Zn2 are tetrahedrally coordinated, whereas Zn3 is hexa-coordinated exhibiting a distorted octahedral geometry, as shown in Fig. 1. The three zinc centers are bridged by the btc ligands to form a trinuclear subunit, which is connected through 4,4′-bipy and btc ligands to construct a three-dimensional architecture.

EXPERIMENTAL

Synthesis

A mixture of $Zn(NO_3)_2 \cdot 6H_2O$, 1,2,4-benzenetricarboxylic acid anhydride, 4,4′-bipy and water in a molar ratio 1.5 : 1 : 1 : 1000 was adjusted to approximately pH 7 with 1 mol l^{-1} NaOH and then was heated to 180 °C for 5 days. The pale-yellow block crystals of **1** were collected upon slow cooling.

Crystallography

Intensity data were collected at 298 K on Smart Apex 2000 diffractometer for a pale-yellow crystal, $0.07 \times 0.12 \times 0.29$ mm^3. $C_{86}H_{52}N_{10}O_{24}Zn_6$, $M = 2001.60$, triclinic, $P\bar{1}$, $a = 11.7737(8)$, $b = 11.7974(8)$, $c = 15.3172(10)$ Å, $\alpha = 106.556(1)°$, $\beta = 106.275(1)°$, $\gamma = 92.983(1)°$, $V = 1937.4(2)$ Å^3, $Z = 1$; 8508 unique data ($\theta_{max} = 28.3°$), 7169 data with $I > 2\sigma(I)$. $R_1 = 0.051$, $wR_2 = 0.126$; $\rho_{max} = 0.94$ eÅ^{-3}. Programs used: SHELXL and ORTEP. CCDC deposition number: 204137.

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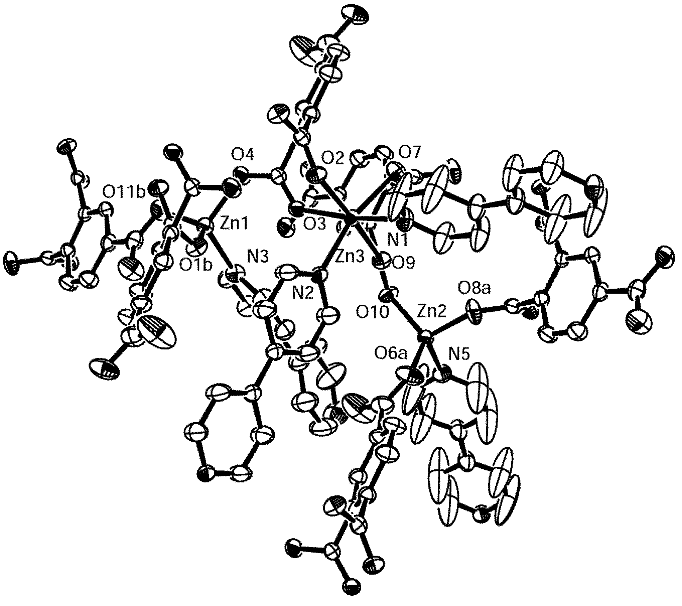

Figure 1. ORTEP plot showing the coordination environment of zinc atoms at the 50% probability level; hydrogen atoms are omitted for clarity. Key geometry parameters: Zn1–O1a 1.931(3), Zn1–O4 1.960(3), Zn1–O11b 1.954(3), Zn1–N3 2.037(4), Zn2–O6c 1.913(3), Zn2–O8d 1.931(3), Zn2–O10 1.948(3), Zn2–N5 2.029(4), Zn3–O2 2.089(3), Zn3–O3 2.131(3), Zn3–O7 2.146(3), Zn3–O9 2.114(3), Zn3–N1 2.192(4), Zn3–N2 2.160(3) Å, O1a–Zn1–O11b 125.38(13), O1a–Zn1–O4 111.51(13), O1a–Zn1–N3 106.11(14), O4–Zn1–N3 108.06(14), O4–Zn1–O11b 101.62(13), O11b–Zn1–N3 103.02(14), O6c–Zn2–O8d 95.69(16), O6c–Zn2–O10 123.58(16), O8d–Zn2–O10 110.51(14), O6c–Zn2–N5 107.65(16), O8d–Zn2–N5 114.13(15), O10–Zn2–N5 105.47(15), O2–Zn3–O3 82.39(11), O2–Zn3–O7 99.12(12), O2–Zn3–O9 174.59(11), O2–Zn3–N1 87.63(13), O2–Zn3–N2 91.28(12), O3–Zn3–O7 100.59(11), O3–Zn3–O9 92.29(11), O3–Zn3–N1 170.02(13), O3–Zn3–N2 88.04(12), O7–Zn3–O9 82.80(11), O7–Zn3–N1 80.93(13), O7–Zn3–N2 167.23(13), O9–Zn3–N1 97.69(13), O9–Zn3–N2 87.51(12), N2–Zn3–N1 92.20(14)°. Symmetry operation: $a = -x + 2, -y, -z$; $b = -x + 2, -y - 1, -z$; $c = x - 1, y, z$; $d = -x + 2, -y, -z + 1$.