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Main Group Metal Compounds **AOC**

Crystallographic report

[Diaqua bis(2,2′-bipyridine)(μ-naphthalene-1,4,5,8-tetracarboxylato)]dizinc(II) tetrahydrate

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The title complex features a two-dimensional polymeric structure owing to the presence of μ_4-bridging naphthalene-1,4,5,8-tetracarboxylate ligands. The trigonal bipyramidal coordination geometry for zinc is completed by a chelating 2,2′-bipyridine and a water molecule. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; naphthalene-1,4,5,8-tetracarboxylate; zinc

COMMENT

Continuing our work in metal–organic framework structures,[1,2] the title complex was investigated and shown to feature a two-dimensional structure whose eight-membered ring-building unit comprises four naphthalene-1,4,5,8-tetracarboxylate (L) ligands (each is disposed about a centre of inversion) and four zinc atoms. Each L ligand is tetradentate, forming a bond to zinc using one oxygen atom of each carboxylate group. The zinc atom coordination geometry (Fig. 1) is trigonal bipyramidal with the N1 and O1w atoms defining the axial positions.

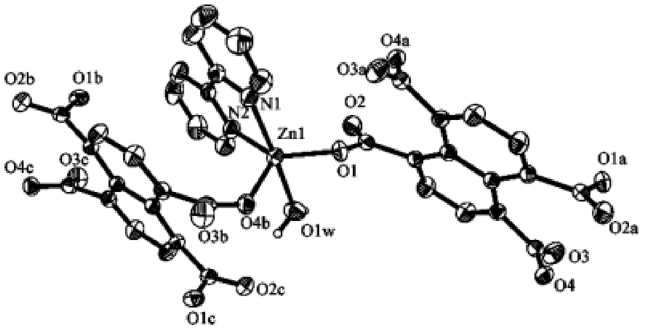

Figure 1. ORTEP plot showing the zinc atom coordination environment; hydrogen atoms and solvent molecules are omitted for clarity. Key geometric parameters: Zn–O1 2.015(2), Zn–O4b 2.015(2), Zn–O1w 2.072(2), Zn–N1 2.111(2), Zn–N2 2.102(2) Å; O1–Zn–O1w 91.34(8), O1–Zn–N1 93.74(8), O1–Zn–N2 143.50(8), O1–Zn–O4b 100.31(8), O1w–Zn–O4b 86.84(8), O1w–Zn–N1 173.94(9), N1–Zn–N2 77.36(9)°. Symmetry operations: (a) $-x,\ 1-y,\ -z$; (b) $\frac{1}{2}-x,\ -y,\ \frac{1}{2}-z$; (c) $\frac{1}{2}+x,\ \frac{1}{2}-y,\ \frac{1}{2}+z$.

EXPERIMENTAL

Naphthalene-1,4,5,8-tetracarboxylic diandydride (0.070 g, 0.25 mmol) was suspended in an aqueous solution (5 ml) and NaOH (1 M) was added dropwise with stirring until complete dissolution. The solution was adjusted to pH 7.0 and transferred into a Parr Teflon-lined stainless steel vessel (23 ml) containing $Zn(NO_3)_2{\cdot}6H_2O$ (0.158 g, 0.50 mmol) and 2,2′-bpy (0.078 g, 0.50 mmol). Additional water (3 ml) was added, the vessel sealed, heated to 180 °C for 5 days, and finally cooled at 5 °C h^{-1} to room temperature. Red plate-like crystals were collected by hand, washed with distilled water, and air dried. Intensity data were collected at 298 K on a Bruker Apex CCD diffractometer for a red plate 0.06 × 0.12 × 0.32 mm^3. $C_{17}H_{16}N_2O_7Zn$, $M = 425.69$, monoclinic, $P2_1/n$, $a = 10.3924(6)$, $b = 15.8057(9)$, $c = 11.3783(6)$, $\beta = 116.229(1)°$, $V = 1676.55(16)$ Å^3, $Z = 4$; 3936 unique data ($\theta = 28.3°$), 3185 data with $I \geq 2\sigma(I)$. $R = 0.042$ (obs. data), $wR = 0.116$ (all data);

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$\rho_{max} = 1.16\ e^-\ Å^{-3}$ (near zinc). Programs used: SHELXL and ORTEP. CCDC deposition number: 23 5956.

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