

Huan-Yu Wang,^a Shan Gao,^a
 Jing-Gui Zhao^a and Seik Weng
 Ng^{b*}

^aCollege of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China, and ^bDepartment of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
 T = 293 K
 Mean $\sigma(\text{C}-\text{C}) = 0.007 \text{ \AA}$
 Disorder in main residue
 R factor = 0.062
 wR factor = 0.194
 Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

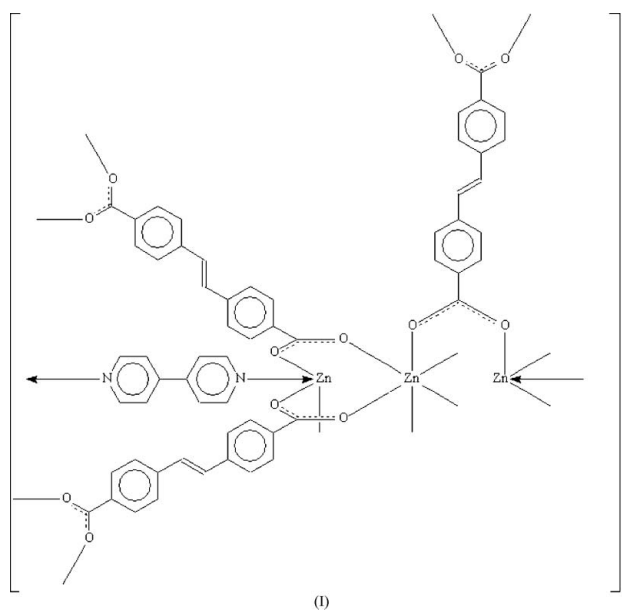
Poly[(μ_2 -4,4'-bipyridine)tris[μ_4 -(*E*)-4,4'-(ethene-1,2-diyl)dibenzoato]zinc(II)]

One of the two independent Zn atoms of the polymeric title compound, $[\text{Zn}_3(\text{C}_{16}\text{H}_{10}\text{O}_4)_3(\text{C}_{10}\text{H}_8\text{N}_2)]_n$, lies on a special position of site symmetry 3 and the other on a special position of site symmetry $\bar{3}$. The carboxylate ends of the 4,4'-(ethene-1,2-diyl)dibenzoate dianion, which lies on a special position of site symmetry $\bar{1}$, each bridge these two independent Zn atoms. The bipyridine-coordinated Zn atom on the threefold axis has a tetrahedral geometry, whereas the other Zn atom is coordinated by the O atoms of six different dianions in an octahedral geometry.

Received 31 October 2006
 Accepted 9 November 2006

Comment

Two studies have detailed the manganese and cadmium derivatives of (*E*)-4,4'-(1,2-ethenediyl)dibenzoic acid. The compounds, which adopt three-dimensional motifs, have the metal atoms in tetrahedral and octahedral geometries (Wang *et al.*, 2006*a,b*). As expected, the isostructural compounds are porous. The hypothetical $\text{Zn}_3(\text{C}_{16}\text{H}_{10}\text{O}_4)_3(\text{H}_2\text{O})_2$ analog would have about 16% of its unit-cell volume empty. The present study extends the study of phenanthroline-chelated zinc (ethene-1,2-diyl)dibenzoate (Wang *et al.*, 2006). The present 4,4'-bipyridine adduct, (I) (Fig. 1), which has the *N*-heterocycle in place of the water of the hypothetical zinc compound, is not porous as *PLATON* (Spek, 2003) does not indicate any voids.



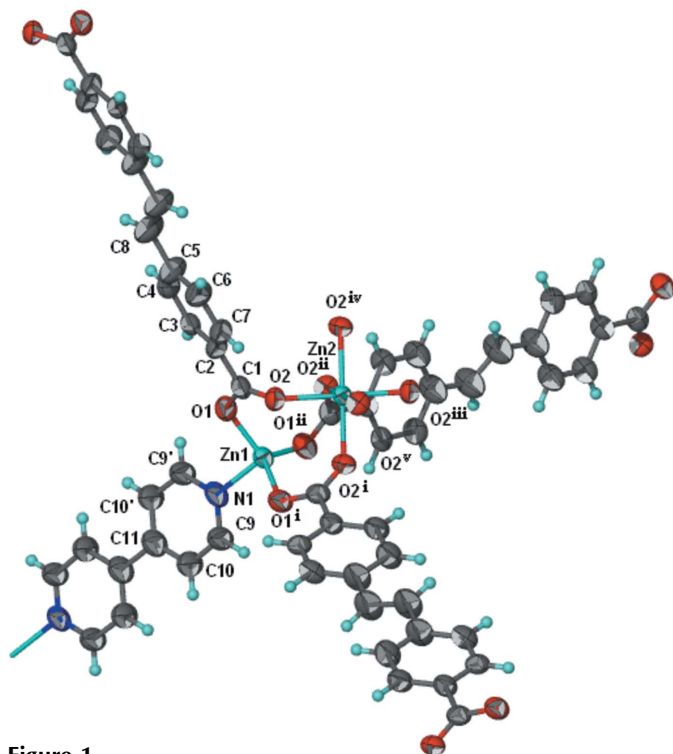


Figure 1
A fragment of the three-dimensional network structure of (I). Displacement ellipsoids are drawn at the 50% probability level, and H atoms are shown as spheres of arbitrary radii. Symmetry codes are given in Table 1. Only one disorder component is shown.

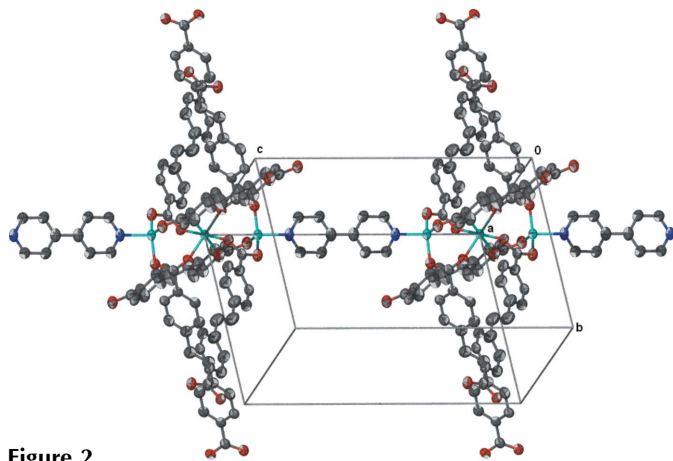


Figure 2
Packing diagram, illustrating the 4,4'-bipyridine bridges along the *c* axis. Only one disorder component is shown. H atoms have been omitted.

threefold axis. This ligand bridges the Zn atoms at $(0, 0, z)$ and $(0, 0, 1 - z)$. The carboxylate O atoms of 4,4'-(ethene-1,2-diyl)dibenzoate dianion bridge the Zn atom on the $\bar{3}$ site at $(0, 0, 0)$ and the Zn atom on the 3 site at $(0, 0, z)$. The Zn atom on the 3 site adopts a four-coordinate ZnO_3N trigonally distorted tetrahedral coordination geometry, with O–Zn–O angles of $117.3(1)^\circ$ and N–Zn–O angles of $99.6(1)^\circ$. The Zn atom on the $\bar{3}$ site is coordinated by O atoms of six different dianions in a six-coordinate ZnO_6 octahedral geometry (Fig. 1) with *cis*-O–Zn–O angles of $89.9(1)$ and $90.1(1)^\circ$. The bipyridine ligand serves as a bridge, linking adjacent formula units into a linear chain along the *c* axis (Fig. 2); these chains are then

linked through covalent zinc–carboxylate bonds into a three-dimensional network.

Experimental

Zinc acetate dihydrate (0.44 g, 2 mmol), (*E*)-4,4'-(ethene-1,2-diyl)dibenzoic acid (0.47 g, 2 mmol), triethylamine (0.3 ml, 2 mmol), 4,4'-bipyridine (0.31 g, 2 mmol) and water (10 ml) were placed in a 23-ml Teflon-lined stainless steel Parr bomb. The bomb was heated to 423 K for 5 d and then cooled to room temperature; colorless crystals separated from the solution and were selected manually.

Crystal data

$[Zn_3(C_{16}H_{10}O_4)(C_{10}H_8N_2)]$
 $M_r = 1151.01$
 Trigonal, $R\bar{3}$
 $a = 16.134(1) \text{ \AA}$
 $c = 18.162(1) \text{ \AA}$
 $V = 4094.1(3) \text{ \AA}^3$
 $Z = 3$

$D_x = 1.401 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 1.37 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
 Prism, colorless
 $0.30 \times 0.24 \times 0.18 \text{ mm}$

Data collection

Rigaku R-Axis RAPID IP
 diffractometer
 ω scans
 Absorption correction: multi-scan
 (ABSCOR; Higashi, 1995)
 $T_{\min} = 0.421$, $T_{\max} = 0.791$

13477 measured reflections
 2086 independent reflections
 1249 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.076$
 $\theta_{\max} = 27.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.062$
 $wR(F^2) = 0.194$
 $S = 1.11$
 2086 reflections
 139 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0927P)^2 + 8.7373P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.62 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.88 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.0013 (4)

Table 1

Selected bond lengths (\AA).

| | | | |
|----------------------|-----------|-----------------------|-----------|
| Zn1–O1 | 1.946 (4) | Zn2–O2 ⁱ | 2.087 (3) |
| Zn1–O1 ⁱ | 1.946 (4) | Zn2–O2 ⁱⁱ | 2.087 (3) |
| Zn1–O1 ⁱⁱ | 1.946 (4) | Zn2–O2 ⁱⁱⁱ | 2.087 (3) |
| Zn1–N1 | 2.071 (7) | Zn2–O2 ^{iv} | 2.087 (3) |
| Zn2–O2 | 2.087 (3) | Zn2–O2 ^v | 2.087 (3) |

Symmetry codes: (i) $-y + 1, x - y - 1, z$; (ii) $-x + y + 2, -x + 1, z$; (iii) $-x + 2, -y, -z + 2$; (iv) $y + 1, -x + y + 1, -z + 2$; (v) $x - y, x - 1, -z + 2$.

The $C_6H_4-CH=CH-C_6H_4$ portion of the dicarboxylate group is disordered in the phenylene ring, along the C2–C5 vector. As it is disordered over an inversion site, the occupancy is exactly 0.5:0.5. The C–C distances were restrained to $1.390(5) \text{ \AA}$. The 1,4-related distances were restrained to $2.78(1) \text{ \AA}$. The four C–C single bonds were restrained to $1.500(5) \text{ \AA}$ and the C=C distance to $1.350(5) \text{ \AA}$. The six-membered ring was restrained to be nearly flat for both the unprimed and primed components. Additionally, the displacement parameters of the primed atoms were set to those of the unprimed atoms. The 4,4'-bipyridine group is disordered about the threefold axis; the independent unit was selected as a six-membered N1/C9/C10/C11/C10'/C9' ring whose N1 and C11 atoms are on the symmetry element. The N–C distance was restrained to $1.350(5) \text{ \AA}$ and the C–C distances to $1.390(5) \text{ \AA}$. The displacement parameters of the

primed atoms were set to those of the unprimed atoms. The vibration of all C atoms was restrained to be nearly isotropic. Somewhat tight restraints were applied to prevent a wide spread of bond distances. Carbon-bound H atoms were positioned geometrically (C–H = 0.93 Å) and were included in the refinement in the riding-model approximation, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2006).

We thank the Heilongjiang Province Natural Science Foundation (No. B200501), the Scientific Fund for Remark-

able Teachers of Heilongjiang Province (No. 1054 G036) and the University of Malaya for supporting this study.

References

- Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Higashi, T. (1995). *ABSCOR*. Rigaku Corporation, Tokyo, Japan.
Rigaku (1998). *RAPID-AUTO*. Rigaku Corporation, Tokyo, Japan.
Rigaku/MSC (2002). *CrystalStructure*. Rigaku/MSC Inc. The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wang, H.-Y., Gao, S., Zhao, J.-G. & Ng, S. W. (2006a). *Acta Cryst. E* **62**, m3127–m3128.
Wang, H.-Y., Gao, S., Zhao, J.-G. & Ng, S. W. (2006b). *Acta Cryst. E* **62**, m3129–m3130.
Wang, X.-L., Qin, C., Wang, E.-B. & Xu, L. (2006). *Cryst. Growth Des.* **6**, 2061–2065.
Westrip, S. P. (2006). *publCIF*. In preparation.