

Wen-Jiang Ao, Zhao-Hui Li,*
Xu-Xu Wang and Xian-Zhi FuInstitute of Photocatalysis, Fuzhou University,
Fuzhou, Fujian, 350002, People's Republic of
ChinaCorrespondence e-mail:
zhaohuili1969@yahoo.com

Key indicators

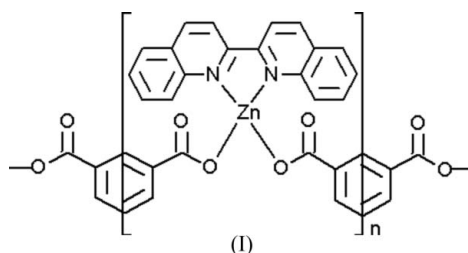
Single-crystal X-ray study
 $T = 173\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
 R factor = 0.036
 wR factor = 0.095
Data-to-parameter ratio = 16.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*catena*-Poly[[*(2,2'*-diquinolyl- $\kappa^2\text{N},\text{N}'$)zinc(II)]- μ -isophthalato- $\kappa^2\text{O}:\text{O}'$]

In the title complex, $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{18}\text{H}_{12}\text{N}_2)]_n$, isophthalate (ipa) acts as a bis-monodentate ligand, forming a one-dimensional helical chain. A significant π - π stacking interaction helps to pack adjacent chains into a molecular zipper. The Zn atom is coordinated by two N and two O atoms in a distorted tetrahedral geometry.

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Comment

Over the past few years, there has been a considerable interest in supramolecular architectures containing non-linear flexible and V-shaped dicarboxylates (Plater *et al.*, 2001; Zheng *et al.*, 2001). The incorporation of ancillary 1,10-phenanthroline (phen) or 2,2'-bipyridine (2,2'-bipy) into the V-shaped metal-dicarboxylate system can lead to one-dimensional chiral chains and may provide potential supramolecular recognition sites to form a supralattice by π - π aromatic stacking (Liu *et al.*, 2002; Chen *et al.*, 2002).



The title compound, (I), consists of one-dimensional chiral helical chains (Fig. 1). The Zn atom has a distorted tetrahedral coordination (Table 1), formed by two N atoms from the 2,2'-diquinolyl (quin) ligand and two O atoms from two different isophthalate (ipa) ligands (Fig. 2). The dicarboxylate ligand functions in a bis-monodentate mode, connecting the tetrahedral metal centres into a chiral helical chain running along the crystallographic 2_1 axis in the b direction, with a pitch of 11.779 (3) Å. Pairs of quin ligands are alternately attached to either side of the chain. A face-to-face distance of 3.542 (9) Å between quin ligands in adjacent chains suggests significant π - π stacking interaction. Adjacent zigzag chains are packed through intercalation of the lateral quin ligands in a zipper-like fashion to form two-dimensional networks parallel to the bc plane (Fig. 3).

Such a molecular zipper was first observed in $[\text{Cu}_2(\text{ipa})_2(\text{phen})_2\cdot\text{H}_2\text{O}]_n$ (Chen *et al.*, 2002). Comparing complex (I) with its bipy $[\text{Zn}_2(\text{ipa})_2(2,2'\text{-bipy})_2]_n$ and phen $[\text{Zn}(\text{ipa})(\text{phen})]_n$ analogues (Zhang *et al.*, 2003), we find that terminal ligands have a substantial effect on the coordination environment of Zn and the formation of the supralattice archi-

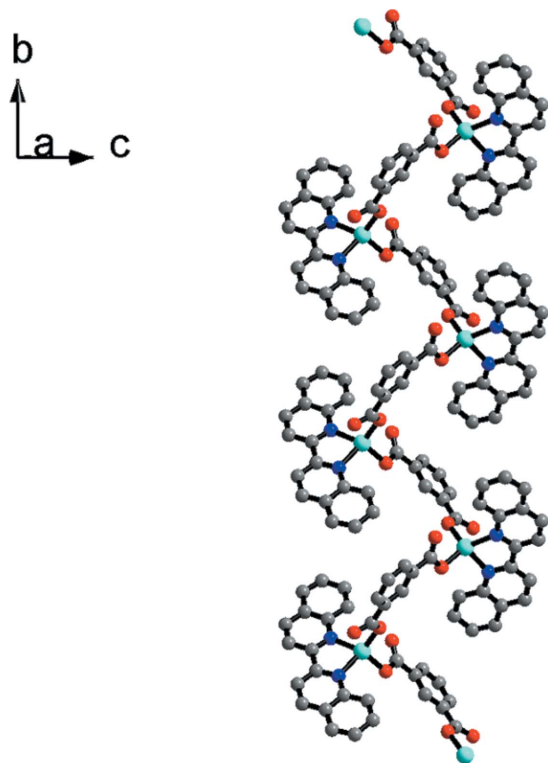


Figure 1
The single-stranded helical chain in (I). H atoms have been omitted.

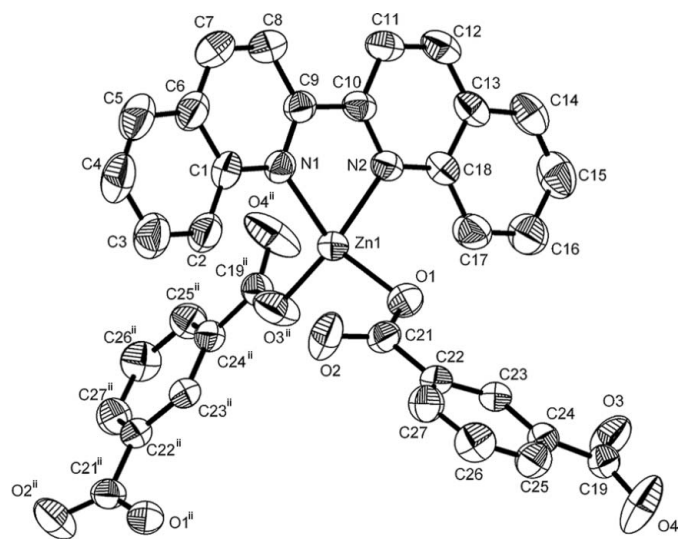


Figure 2
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry code: (ii) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$]

ture. For the relatively small and flexible 2,2'-bipy, Zn has an octahedral coordination environment and the π - π stacking interaction packs the polymeric chain into a three-dimensional network. Although a similar molecular zipper can be obtained for $[\text{Zn}(\text{ipa})(\text{phen})]_n$ and $[\text{Zn}(\text{ipa})(\text{quin})]_n$, different coordination environments around Zn are observed in these two

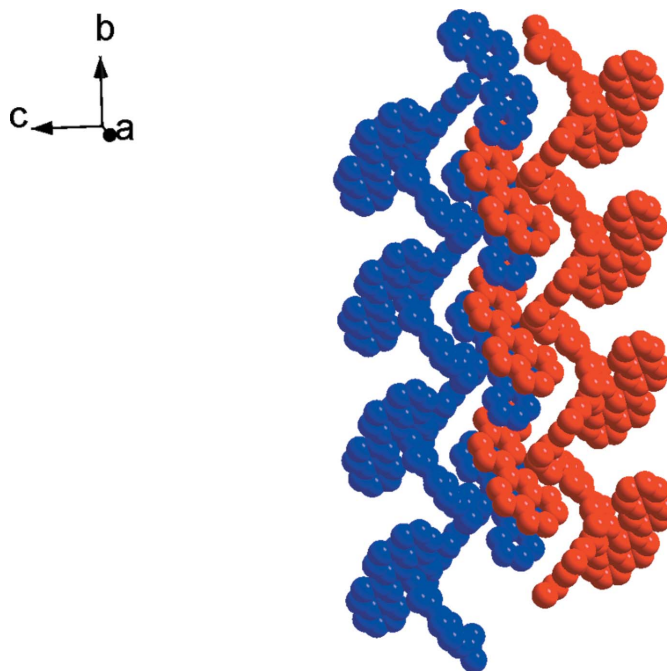


Figure 3
The zipper-like double-stranded helical chains in (I).

complexes, namely five-coordinated distorted trigonal-bipyramidal coordination in the former compound and four-coordinated tetrahedral coordination in the latter.

Experimental

A mixture of zinc acetate (0.11 g, 0.5 mmol), quin (0.128 g, 0.5 mmol) and ipa (0.083 g, 0.5 mmol) was dissolved in 16 ml H_2O -EtOH (1:1) and the pH was adjusted to 6 with aqueous ammonia (25%). The mixture was sealed in a 25 ml stainless steel reactor with a Teflon liner and heated at 443 K for 5 d. Colourless cuboid crystals of (I) were collected by filtration in a yield of ca 60%.

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_{18}\text{H}_{12}\text{N}_2)]$
 $M_r = 485.78$
 Monoclinic, $P2_1/c$
 $a = 8.664$ (4) Å
 $b = 11.779$ (3) Å
 $c = 20.803$ (7) Å
 $\beta = 95.812$ (16)°
 $V = 2112.1$ (13) Å³
 $Z = 4$

$D_x = 1.528$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 15151 reflections
 $\theta = 12$ -18°
 $\mu = 1.20$ mm⁻¹
 $T = 173$ (2) K
 Cuboid, colourless
 0.10 × 0.10 × 0.10 mm

Data collection

Rigaku Weissenberg IP diffractometer
 ω scans
 Absorption correction: multi-scan (TEXSAN; Molecular Structure Corporation, 1999)
 $T_{\min} = 0.831$, $T_{\max} = 0.864$
 20895 measured reflections

4835 independent reflections
 3719 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.035$
 $\theta_{\max} = 27.5^\circ$
 $h = -11 \rightarrow 11$
 $k = -15 \rightarrow 15$
 $l = -27 \rightarrow 25$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.036$
 $wR(F^2) = 0.096$
 $S = 1.00$
 4835 reflections
 298 parameters
 H-atom parameters constrained

$$w = 1/[\sigma^2(F_o^2) + (0.0496P)^2 + 0.6028P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.37 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters (\AA , $^\circ$).

Zn1—O3 ⁱ	1.9183 (18)	O2—C21	1.221 (3)
Zn1—O1	1.9401 (17)	O3—C19	1.255 (3)
Zn1—N1	2.0746 (19)	O3—Zn1 ⁱⁱⁱ	1.9183 (18)
Zn1—N2	2.0763 (18)	O4—C19	1.219 (3)
O1—C21	1.275 (3)		
O3 ⁱ —Zn1—O1	105.53 (8)	C19—O3—Zn1 ⁱⁱⁱ	115.85 (16)
O3 ⁱ —Zn1—N1	113.10 (9)	O4—C19—O3	122.8 (2)
O1—Zn1—N1	129.42 (8)	O4—C19—C24	120.9 (2)
O3 ⁱ —Zn1—N2	126.98 (9)	O3—C19—C24	116.1 (2)
O1—Zn1—N2	101.29 (8)	O2—C21—O1	123.6 (2)
N1—Zn1—N2	80.66 (8)	O2—C21—C22	120.9 (2)
C21—O1—Zn1	111.45 (15)	O1—C21—C22	115.5 (2)

Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (iii) $-x, y - \frac{1}{2}, -z + \frac{1}{2}$.

H atoms were positioned geometrically and refined as riding, with C—H = 0.95 \AA and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$.

Data collection: *TEXSAN* (Molecular Structure Corporation, 1999); cell refinement: *TEXSAN*; data reduction: *TEXSAN*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Sheldrick, 2001); software used to prepare material for publication: *SHELXL97*.

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