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Key indicators

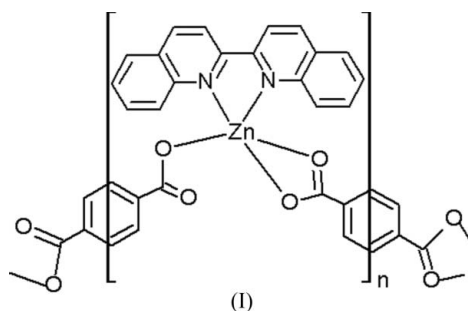
Single-crystal X-ray study
 $T = 298\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.010\text{ \AA}$
 R factor = 0.074
 wR factor = 0.177
Data-to-parameter ratio = 15.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*catena*-Poly[[*(2,2'*-diquinoly)zinc(II)]-
 μ -terephthalato]

The title complex, $[\text{Zn}(\text{C}_{18}\text{H}_{12}\text{N}_2)(\text{C}_8\text{H}_4\text{O}_4)]_n$, consists of a one-dimensional zigzag $[\text{Zn}(\text{tpa})(\text{quin})]_n$ chain (tpa = terephthalate and quin = 2,2'-diquinoly) with a pitch of 17.907 (2) Å. The tpa ligands bridge two Zn atoms in alternately bis(bidentate) and bis(monodentate) coordination modes. Each Zn atom is coordinated by two N atoms from a chelating quin, two O atoms from one bis(bidentate) tpa and one O atom from one bis(monodentate) tpa. The five-coordinate Zn geometry can be best described as distorted trigonal-bipyramidal.

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Comment

Due to its versatile bonding mode, tpa (terephthalate) is one of the most widely used bridging ligands. One-, two- and three-dimensional coordination polymers built from tpa have been reported (Li *et al.*, 1999; Groenman *et al.*, 1998; Zhang *et al.*, 1998; Hong *et al.*, 1998; Franesconi *et al.*, 1981). The introduction of terminal ligands into the metal-terephthalate system can reduce the available metal-ion binding sites and result in the formation of low-dimensional frameworks (Chen *et al.*, 2002; Liu *et al.*, 2003). One-dimensional polymeric chains have been prepared from mixed ligands of tpa and 2,2'-bipyridine or 1,10-phenanthroline (Sun *et al.*, 2001). However, the metal-coordination environment, as well as the superlattice architecture, can be affected by the size and rigidity of the terminal ligands.



In this paper, we report the synthesis of the title complex, (I). X-ray crystallography reveals that complex (I) consists of a one-dimensional zigzag $[\text{Zn}(\text{tpa})(\text{quin})]_n$ chain (quin = 2,2'-diquinoly) with a pitch of 17.907 (2) Å (Fig. 1). Each Zn atom is five-coordinated by two N atoms of a chelating quin ligand, two O atoms from one bis(bidentate) tpa ligand, and one O atom from one bis(monodentate) tpa ligand.

The coordination of Zn1 can be best described as distorted trigonal bipyramidal, with atoms N1 and O3 occupying the

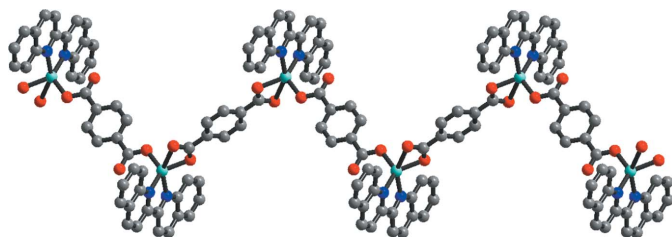


Figure 1
The one-dimensional zigzag polymeric chain in (I). H atoms have been omitted.

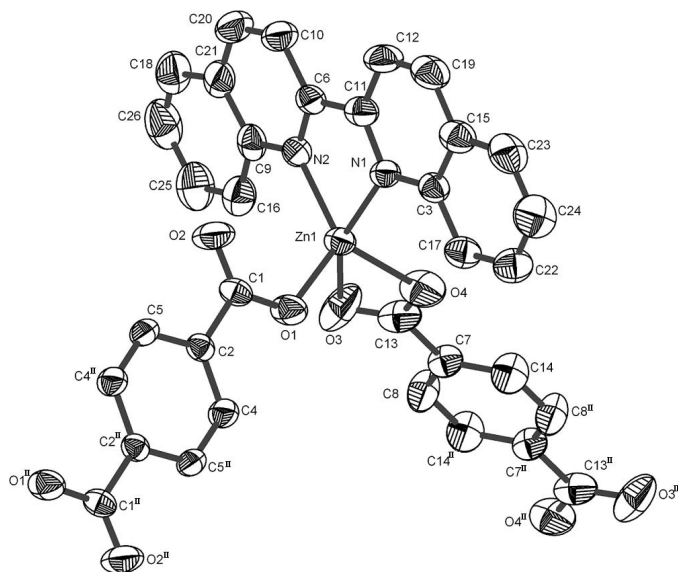


Figure 2
A view of (I), with the atom-numbering scheme and 50% probability displacement ellipsoids. H atoms have been omitted for clarity. [Symmetry code: (ii) $-x, -y, -z$.]

axial positions and N2, O4 and O1 forming the equatorial plane. The Zn atom deviates slightly from the equatorial plane [0.208 (2) Å] (Fig. 2). The Zn1–O3 distance [2.445 (6) Å] is among the longest Zn–O bonds ever observed in the literature (Zhang *et al.*, 2003).

Unlike the previously reported [Zn(tpa)(phen)(H₂O)]_n complex, in which tpa bridges two Zn atoms in a bis(monodentate) coordination mode (Sun *et al.*, 2001), the tpa ligands in complex (I) bridge two Zn atoms in alternately bis(bidentate) and bis(monodentate) coordination modes. Such a coordination mode is rarely observed among one-dimensional polymeric chains linked by tpa ligands. To the best of our knowledge, the only other example with a similar coordination mode is [Zn₂(tpa)₂(pz)(H₂O)₂]_n (Yang *et al.*, 2003).

Adjacent zigzag chains have weak intermolecular π – π interactions between the quin rings in an offset fashion, with a face-to-face distance of 3.529 (9) Å. This extends the zigzag chains into a two-dimensional supramolecular structure (Fig. 3) parallel to the *ac* plane.

Experimental

A mixture of zinc acetate (0.11 g, 0.5 mmol), quin (0.128 g, 0.5 mmol) and tpa (0.083 g, 0.5 mmol) was dissolved in H₂O–EtOH (16 ml, 1:1 *v/v*). The pH was adjusted to 6 with NH₄OH (25%). The mixture was sealed in a 25 ml stainless-steel reactor with a Teflon liner and heated at 453 K for 5 d. After cooling to room temperature at a rate of 5 K h^{–1}, colourless block crystals of (I) were collected by filtration in a yield of *ca* 50%.

Crystal data

[Zn(C₁₈H₁₂N₂)(C₈H₄O₄)]
M_r = 485.78
Triclinic, *P* $\bar{1}$
a = 9.4805 (9) Å
b = 10.0292 (12) Å
c = 13.2442 (6) Å
 α = 69.979 (3)°
 β = 69.134 (6)°
 γ = 68.493 (2)°

V = 1061.78 (17) Å³
Z = 2
D_x = 1.519 Mg m^{–3}
Mo *K* α radiation
 μ = 1.19 mm^{–1}
T = 298 (2) K
Plate, colourless
0.15 × 0.15 × 0.05 mm

Data collection

Rigaku Weissenberg IP
diffractometer
 ω scans
Absorption correction: multi-scan
(*TEXRAY*; Molecular Structure
Corporation, 1999)
T_{min} = 0.79, *T_{max}* = 0.98

9225 measured reflections
4732 independent reflections
3092 reflections with *I* > 2 σ (*I*)
R_{int} = 0.068
 θ_{\max} = 27.5°

Refinement

Refinement on *F*²
R[*F*² > 2 σ (*F*²)] = 0.074
wR(*F*²) = 0.177
S = 1.09
4732 reflections
298 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 2.7152P]$
where $P = (F_o^2 + 2F_c^2)/3$
(Δ/σ)_{max} < 0.001
 $\Delta\rho_{\max}$ = 0.48 e Å^{–3}
 $\Delta\rho_{\min}$ = –0.53 e Å^{–3}

Table 1

Selected geometric parameters (Å, °).

Zn1–O1	1.943 (4)	Zn1–N1	2.105 (4)
Zn1–O4	2.015 (5)	Zn1–O3	2.445 (6)
Zn1–N2	2.088 (5)		
O1–Zn1–O4	104.69 (18)	N1–Zn1–O3	151.73 (18)
O1–Zn1–N2	122.28 (18)	O1–Zn1–C13	98.20 (18)
O4–Zn1–N2	129.77 (19)	O4–Zn1–C13	28.9 (2)
O1–Zn1–N1	112.12 (17)	N2–Zn1–C13	119.4 (2)
O4–Zn1–N1	99.19 (19)	N1–Zn1–C13	126.8 (2)
N2–Zn1–N1	80.03 (18)	O3–Zn1–C13	28.8 (2)
O1–Zn1–O3	91.02 (18)	C1–O1–Zn1	117.9 (3)
O4–Zn1–O3	57.7 (2)	C13–O3–Zn1	80.7 (4)
N2–Zn1–O3	101.76 (18)	C13–O4–Zn1	100.3 (5)

The H atoms were positioned geometrically. They were assigned isotropic displacement parameters and allowed to ride on their respective parent atoms, with C–H = 0.95 Å and *U*_{iso} = 1.2*U*_{eq}(C) before the final cycle of least-squares refinement.

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

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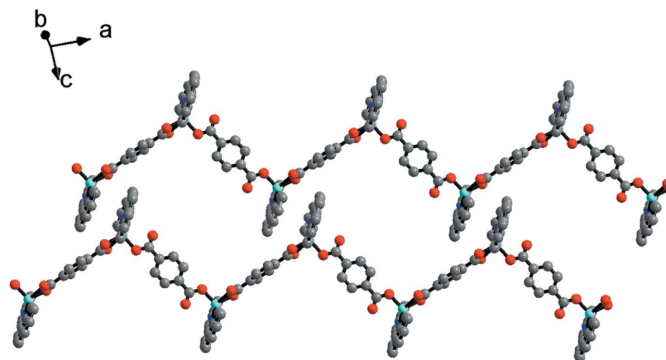


Figure 3

The π - π interactions between two adjacent zigzag chains in (I). H atoms have been omitted.

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