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Key indicators

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma(C-C)$  = 0.007 Å  
 R factor = 0.059  
 wR factor = 0.151  
 Data-to-parameter ratio = 15.6

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

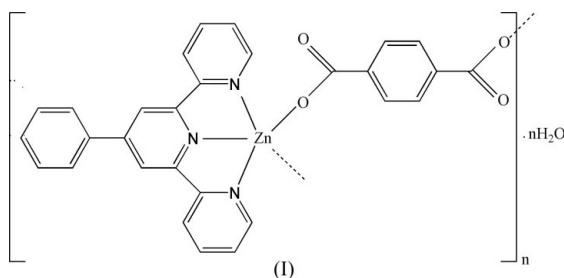
**catena-Poly[[[(4'-phenyl-2,2':6',2''-terpyridine- $\kappa^3N,N',N''$ )zinc(II)]- $\mu$ -terephthalato- $\kappa^2O:O'$ ] monohydrate]**

The title compound,  $\{[Zn(C_8H_4O_4)(C_{21}H_{15}N_3)] \cdot H_2O\}_n$ , is a one-dimensional polymeric complex bridged by centrosymmetric dicarboxylate dianions. Each Zn atom is five-coordinate, bonded to two carboxyl O atoms from the dicarboxylate dianions and to three N atoms from the heterocycle, which chelates to the Zn atom in a  $\kappa^3N,N',N''$  manner.

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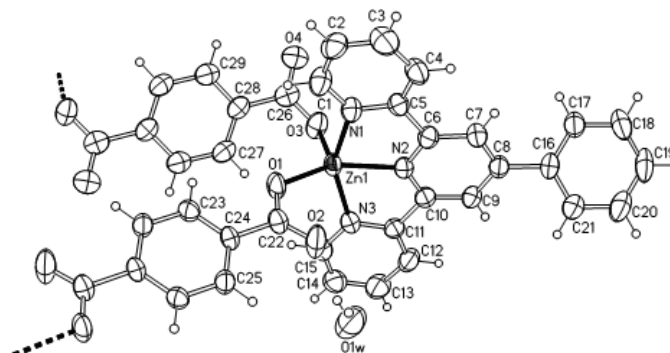
Comment

Terephthalate (TPT) has been widely used as a bridging unit in the synthesis of polymeric complexes (Verdaguer *et al.*, 1984; Bakalbassis *et al.*, 1986). In the present work, instead of a binuclear complex, the title polymeric ribbon complex, (I), was obtained by the hydrothermal reaction of zinc dichloride, terephthalonitrile and terpyridine, as reported by Sun *et al.* (2001). Terephthalonitrile was hydrolysed to form TPT, which was crucial for the synthesis of the polymer (Fun *et al.*, 1999).

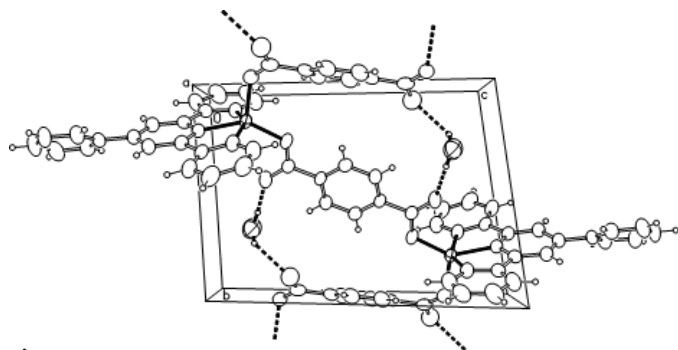


Each Zn atom in (I) is five-coordinate, bonded to two carboxyl O atoms from the dicarboxylate dianions and to three N atoms from the heterocycle (Table 1), which chelates to the Zn in a  $\kappa^3N,N',N''$  manner.

According to the structural index  $\tau$  of 0.1533 (Addison *et al.*, 1984; Atakol *et al.*, 1999), the coordination geometry about Zn is approximately distorted trigonal-square-pyramidal, with



**Figure 1**  
 A view of (I), with the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii.



**Figure 2**

A view of the hydrogen-bonded ribbon structure. Hydrogen bonds are shown as dashed lines.

atom O3 occupying the axial site and atoms N1, N2, N3 and O1 forming the square plane (Fig. 1).

In the crystal packing, each centrosymmetric TPT anion acts as an amphimonodentate bridging ligand and binds with two  $Zn^{2+}$  ions to form a zigzag  $\cdots Zn-TPT-Zn-TPT \cdots$  chain, with alternating O1 and O3 TPT species. Terpyridine is a tridentate ligand, to complete the coordination about each Zn atom (Fig. 2).

A water molecule was found in (I). It acts as a bridge to connect, *via* hydrogen bonds (Table 2), alternate TPT anions through carbonyl atoms, giving rise to a ribbon-like structure (Fig. 2), which is different from the *trans*-zigzag structures observed by Sun *et al.* (2001) and the sheet-like network structure observed by Tu *et al.* (2005).

## Experimental

To an aqueous solution (15 ml) of  $ZnCl_2$  (0.082 g, 0.5 mmol) were added terephthalonitrile (0.068 g, 0.5 mmol) and 4'-phenyl-2,2':6',2''-terpyridine (0.154 g, 0.5 mmol), using the procedure of Constable *et al.* (1990). The mixture was placed in a 25 ml Teflon-lined Parr bomb and heated at 443 K for 72 h. The bomb was then cooled to room temperature at a rate of 5 K  $h^{-1}$ . Needle-shaped colourless crystals of (I) were collected in a yield of ca 30%. Elemental analysis, calculated for  $[Zn(C_8H_4O_4)(C_{21}H_{15}N_3)] \cdot H_2O$ : C 62.49, H 3.77, N 7.54%; found: C 62.61, H 3.62, N 7.68%. IR (KBr,  $cm^{-1}$ ): 3426 (*br, s*), 3065 (*w*), 2360 (*w*), 1591 (*vs*), 1482 (*m*), 1373 (*s*), 1017 (*m*), 752 (*m*).

### Crystal data

$[Zn(C_8H_4O_4)(C_{21}H_{15}N_3)] \cdot H_2O$	$Z = 2$
$M_r = 556.86$	$D_x = 1.507 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 9.3325$ (8) Å	Cell parameters from 2041 reflections
$b = 10.7217$ (9) Å	$\theta = 2.5\text{--}21.8^\circ$
$c = 14.2612$ (12) Å	$\mu = 1.05 \text{ mm}^{-1}$
$\alpha = 77.400$ (1)°	$T = 295$ (2) K
$\beta = 71.961$ (1)°	Needle, colourless
$\gamma = 65.437$ (1)°	$0.29 \times 0.09 \times 0.08 \text{ mm}$
$V = 1227.44$ (18) Å <sup>3</sup>	

### Data collection

Bruker APEX area-detector diffractometer	5482 independent reflections
$\varphi$ and $\omega$ scans	4213 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2002)	$R_{int} = 0.029$
$T_{min} = 0.713$ , $T_{max} = 0.921$	$\theta_{max} = 27.5^\circ$
10 674 measured reflections	$h = -12 \rightarrow 11$
	$k = -13 \rightarrow 13$
	$l = -17 \rightarrow 18$

### Refinement

Refinement on $F^2$	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.059$	$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2]$
$wR(F^2) = 0.151$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.12$	$(\Delta/\sigma)_{max} = 0.001$
5482 reflections	$\Delta\rho_{max} = 0.53 \text{ e \AA}^{-3}$
351 parameters	$\Delta\rho_{min} = -0.40 \text{ e \AA}^{-3}$

**Table 1**

Selected geometric parameters (Å, °).

Zn1—O1	1.934 (2)	Zn1—N2	2.065 (3)
Zn1—O3	1.972 (3)	Zn1—N3	2.153 (3)
Zn1—N1	2.177 (3)		
O1—Zn1—O3	109.8 (1)	O3—Zn1—N2	108.6 (1)
O1—Zn1—N1	96.4 (1)	O3—Zn1—N3	96.1 (1)
O1—Zn1—N2	141.6 (1)	N1—Zn1—N2	75.3 (1)
O1—Zn1—N3	102.3 (1)	N1—Zn1—N3	150.8 (1)
O3—Zn1—N1	98.6 (1)	N2—Zn1—N3	76.0 (1)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O1W—H1W1 $\cdots$ O2	0.85 (1)	1.92 (2)	2.759 (5)	166 (4)
O1W—H1W2 $\cdots$ O4 <sup>i</sup>	0.86 (1)	2.16 (4)	2.793 (6)	130 (5)

Symmetry codes: (i)  $x + 1, y - 1, z$ .

Aromatic H atoms were placed in calculated positions [ $C-H = 0.93$  Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ ], and were included in the refinement in the riding-model approximation. Water H atoms were located in a Fourier difference map and refined with distance restraints of  $O-H = 0.85$  (1) and  $H \cdots H = 1.39$  (1) Å.

Data collection: SMART (Bruker, 2002); cell refinement: SAINT (Bruker, 2002); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPII (Johnson, 1976); software used to prepare material for publication: SHELXL97.

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