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# Poly[$\mu_4$-5-(3-carboxylatophenyl)-1*H*-tetrazolato-zinc(II)]

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**Key indicators**

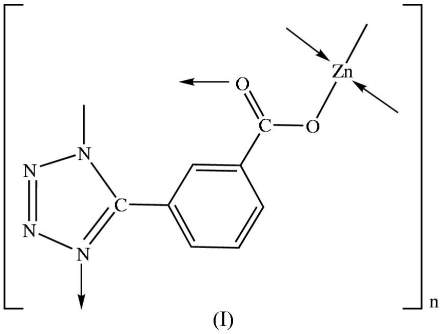
Single-crystal X-ray study
*T* = 296 K
Mean $\sigma$(C–C) = 0.006 Å
*R* factor = 0.051
*wR* factor = 0.118
Data-to-parameter ratio = 14.3

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

The title compound, $[Zn(C_8H_4N_4O_2)]_n$, is a coordination polymer prepared by the hydrothermal reaction of zinc chloride and 3-(1*H*-tetrazol-5-yl)benzoic acid. The zinc cation is tetrahedrally coordinated by two N atoms and two O atoms from four ligands, resulting in a three-dimensional framework encapsulating one-dimensional channels.

## Comment

Coordination frameworks with channels or pores have received much attention over the past decade because of their potential applications in catalysis (Seo *et al.*, 2000), separation (Uemura *et al.*, 2002), ion exchange (Yaghi & Li, 1995) and gas storage (Rosi *et al.*, 2003). Multifunctional organic ligands are necessary for constructing such frameworks. Among a variety of organic ligands used, 5,5′-(1,4-phenylene)bis(1*H*-tetrazole) (PBT) is one of the most important (Xiong *et al.*, 2002; Xue *et al.*, 2002; Tao *et al.*, 2004).



(I)

We report here the synthesis and crystal structure of the title compound, (I), a new coordination polymer of zinc and 3-(1*H*-tetrazol-5-yl)benzoic acid, which is a ligand related to PBT with two different functional groups; *viz*. one carboxylate group and one tetrazolate ring. Compound (I) was obtained by the hydrothermal reaction of zinc chloride and 3-(1*H*-tetrazol-5-yl)benzoic acid.

In the structure of (I), the Zn cation is tetrahedrally coordinated (Table 1) by two N atoms and hydroxyl and carbonyl O atoms from four different ligands (Fig. 1), resulting in a three-dimensional framework with two types of channels propagating along the *a* axis (Fig. 2). These channels are to small to have any content.

## Experimental

Zinc chloride (0.5 mmol, 0.068 g) and 3-(1*H*-tetrazol-5-yl)benzoic acid (0.5 mmol, 0.110 g) were dissolved in water (8 ml) with stirring. The solution was transferred into a Teflon-lined stainless steel autoclave and heated to 433 K for 5 d, then cooled to room temperature. Colorless block-shaped crystals of (I) suitable for diffraction were recovered.

*Crystal data*

$[Zn(C_8H_4N_4O_2)]$
$M_r = 253.52$
Monoclinic, $P2_1/c$
$a = 4.9026\ (5)$ Å
$b = 17.0331\ (16)$ Å
$c = 10.479\ (1)$ Å
$\beta = 97.880\ (2)^\circ$
$V = 866.80\ (15)$ Å$^3$
$Z = 4$
$D_x = 1.943$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 1428 reflections
$\theta = 2.3$–$27.3^\circ$
$\mu = 2.81$ mm$^{-1}$
$T = 296\ (2)$ K
Prism, colorless
$0.14 \times 0.08 \times 0.06$ mm

*Data collection*

Bruker SMART APEX CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{\min} = 0.694$, $T_{\max} = 0.849$
5040 measured reflections
1943 independent reflections
1613 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.036$
$\theta_{\max} = 27.5^\circ$
$h = -6 \rightarrow 6$
$k = -22 \rightarrow 11$
$l = -13 \rightarrow 13$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.118$
$S = 1.12$
1943 reflections
136 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.4756P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 1.13$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.55$ e Å$^{-3}$

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| Zn1—O2$^{\rm i}$ | 1.945 (3) | Zn1—N1$^{\rm ii}$ | 1.974 (3) |
| Zn1—O1 | 1.968 (3) | Zn1—N4$^{\rm iii}$ | 1.992 (3) |
| | | | |
| O2$^{\rm i}$—Zn1—O1 | 108.28 (12) | O2$^{\rm i}$—Zn1—N4$^{\rm iii}$ | 108.02 (13) |
| O2$^{\rm i}$—Zn1—N1$^{\rm ii}$ | 113.96 (14) | O1—Zn1—N4$^{\rm iii}$ | 103.90 (14) |
| O1—Zn1—N1$^{\rm ii}$ | 104.33 (14) | N1$^{\rm ii}$—Zn1—N4$^{\rm iii}$ | 117.46 (15) |

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

All aromatic H atoms were constrained to an ideal geometry, with C—H distances of 0.93 Å, and refined as riding with the constraint $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$ applied. The highest residual peak is located 0.82 Å from atom Zn1.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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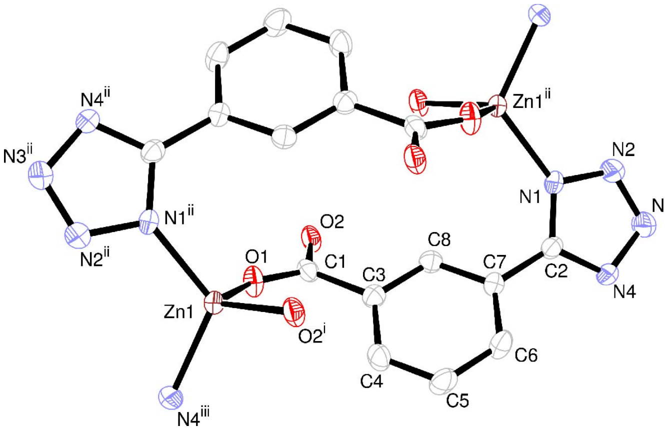

**Figure 1**
A fragment of (I), showing the zinc cation environment, with displacement ellipsoids drawn at the 50% probability level. H atoms have been omitted for clarity. [Symmetry codes: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$; (ii) $-x, -y, -z$; (iii) $x, -y - \frac{1}{2}, z - \frac{1}{2}$.]

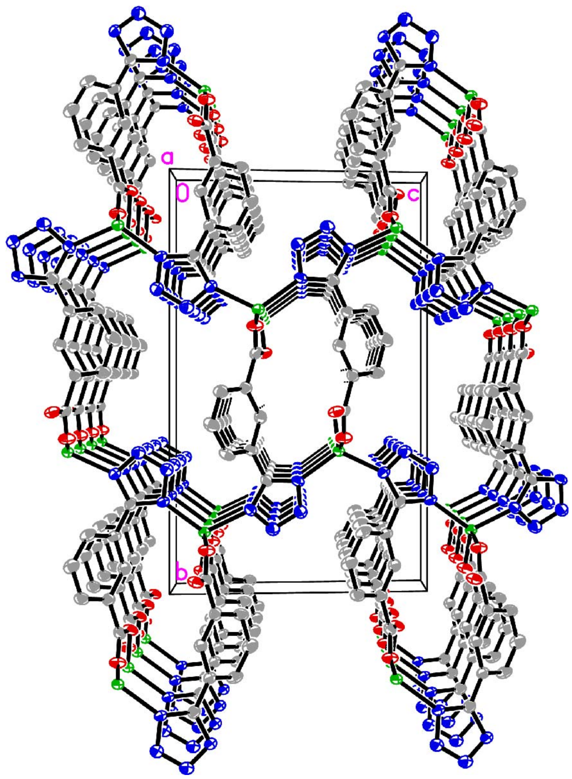

**Figure 2**
Packing digram of (I), showing the channels along the *a* axis.

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