

**catena-Poly[[[bis(1*H*-imidazole- $\kappa$ N<sup>3</sup>)zinc(II)]- $\mu$ -terephthalato- $\kappa^2$ O:O'] trihydrate]**

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**Key indicators**

Single-crystal X-ray study  
 T = 295 K  
 Mean  $\sigma$ (C–C) = 0.003 Å  
 R factor = 0.027  
 wR factor = 0.071  
 Data-to-parameter ratio = 13.1

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

In the title polymeric complex,  $\{[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_3\text{H}_4\text{N}_2)_2] \cdot 3\text{H}_2\text{O}\}_n$ , the  $\text{Zn}^{\text{II}}$  atom is coordinated by two terephthalate dianions and two imidazole ligands in a distorted tetrahedral geometry. The terephthalate dianions are located on inversion centres and bridge neighbouring  $\text{Zn}^{\text{II}}$  atoms to form zigzag polymeric complex chains. The interplanar distance of 3.212 (17) Å between parallel imidazole rings of adjacent polymeric chains suggests the existence of  $\pi$ – $\pi$  stacking.

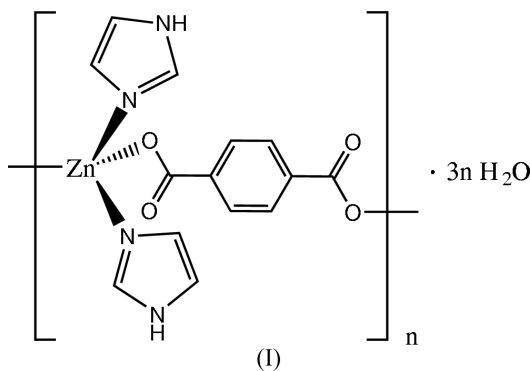
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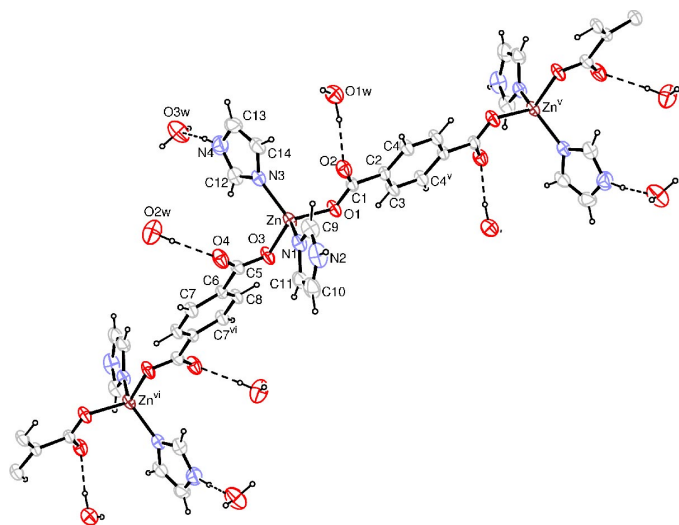
**Comment**

As  $\pi$ – $\pi$  stacking between aromatic rings is correlated with the electron-transfer process in some biological systems (Deisenhofer & Michel, 1989), we are interested in the study of the nature of  $\pi$ – $\pi$  stacking in metal complexes (Liu *et al.*, 2004; Pan & Xu, 2004). As a part of our ongoing investigations, the title polymeric  $\text{Zn}^{\text{II}}$  complex, (I), incorporating imidazole, has recently been prepared, and its X-ray structure shows the existence of  $\pi$ – $\pi$  stacking between imidazole rings.



The structure of a fragment of (I) is shown in Fig. 1. The  $\text{Zn}^{\text{II}}$  atom is coordinated by two imidazole ligands and two terephthalate dianions in a distorted tetrahedral geometry. The bond angles involving the metal centre range from 103.64 (7) to 122.75 (8)° (Table 1). The terephthalate dianions are located on inversion centres and bridge neighbouring  $\text{Zn}^{\text{II}}$  atoms through terminal carboxyl groups to form zigzag polymeric complex chains (Figs. 1 and 2). The carboxyl groups of the terephthalate ions coordinate to the  $\text{Zn}^{\text{II}}$  atom in a monodentate manner. The uncoordinated carboxyl O atoms (O2 and O4) are hydrogen-bonded to the uncoordinated water molecules, resulting in a linkage between adjacent polymeric chains (Fig. 1).

The interplanar distance of 3.212 (17) Å between parallel imidazole rings suggests the existence of  $\pi$ – $\pi$  stacking (Fig. 2).



**Figure 1**  
The structure of a fragment of (I), showing 30% probability displacement ellipsoids [symmetry codes: (v)  $2 - x, -y, -z$ ; (vi)  $1 - x, 2 - y, 2 - z$ ]. Hydrogen bonds are shown as dashed lines.

## Experimental

All reagents were commercially available and of analytical grade. An ethanol solution (5 ml) of imidazole (2 mmol) was mixed with an aqueous solution (5 ml) of  $\text{ZnCl}_2$  (1 mmol), and the mixture was refluxed for 1 h. An aqueous solution (8 ml) containing terephthalic acid (1 mmol) and  $\text{Na}_2\text{CO}_3$  (2 mmol) was then added to this mixture, which was refluxed for a further 1 h. After cooling to room temperature, the solution was filtered. Colourless single crystals of (I) were obtained after 20 d.

### Crystal data

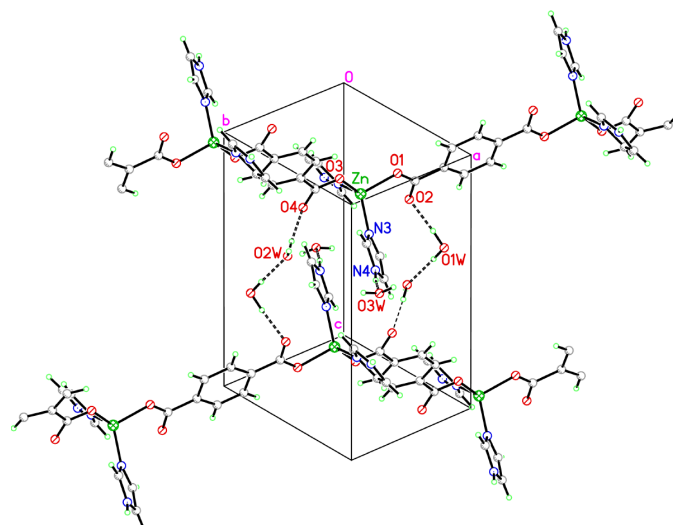
$[\text{Zn}(\text{C}_8\text{H}_4\text{O}_4)(\text{C}_3\text{H}_4\text{N}_2)_2] \cdot 3\text{H}_2\text{O}$	$Z = 2$
$M_r = 419.69$	$D_x = 1.580 \text{ Mg m}^{-3}$
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 8.3046$ (4) Å	Cell parameters from 2893 reflections
$b = 9.5443$ (4) Å	$\theta = 2.8\text{--}24.0^\circ$
$c = 12.0048$ (8) Å	$\mu = 1.44 \text{ mm}^{-1}$
$\alpha = 81.220$ (3)°	$T = 295$ (2) K
$\beta = 70.030$ (2)°	Prism, colourless
$\gamma = 83.678$ (2)°	$0.28 \times 0.22 \times 0.10 \text{ mm}$
$V = 882.10$ (8) Å <sup>3</sup>	

### Data collection

Rigaku R-Axis RAPID diffractometer	3076 independent reflections
$\omega$ scans	2807 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	$R_{\text{int}} = 0.024$
$T_{\text{min}} = 0.665, T_{\text{max}} = 0.860$	$\theta_{\text{max}} = 25.0^\circ$
6595 measured reflections	$h = -9 \rightarrow 9$
	$k = -11 \rightarrow 11$
	$l = -14 \rightarrow 14$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.0328P)^2 + 0.4577P]$
$R[F^2 > 2\sigma(F^2)] = 0.027$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.071$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
3076 reflections	$\Delta\rho_{\text{min}} = -0.35 \text{ e \AA}^{-3}$
235 parameters	Extinction correction: none
H-atom parameters constrained	



**Figure 2**  
The partially overlapped arrangement of imidazole rings, showing  $\pi$ - $\pi$  stacking [symmetry code: (i)  $1 - x, 1 - y, 1 - z$ ]. Hydrogen bonds are shown as dashed lines.

**Table 1**

Selected geometric parameters (Å, °).

Zn—O1	1.9883 (15)	Zn—N1	1.9735 (18)
Zn—O3	1.9660 (15)	Zn—N3	1.9940 (19)
O1—Zn—O3	103.95 (6)	O3—Zn—N1	106.84 (7)
O1—Zn—N1	111.57 (7)	O3—Zn—N3	103.64 (7)
O1—Zn—N3	106.29 (7)	N1—Zn—N3	122.75 (8)

**Table 2**

Hydrogen-bond geometry (Å, °).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
O1W—H13 <sup>i</sup> ···O2	0.95	1.87	2.818 (2)	174
O1W—H14 <sup>i</sup> ···O2W <sup>ii</sup>	0.87	1.91	2.768 (3)	170
O2W—H15 <sup>i</sup> ···O4	0.85	2.03	2.886 (3)	177
O2W—H16 <sup>i</sup> ···O2 <sup>iii</sup>	0.93	1.98	2.893 (3)	168
O3W—H17 <sup>i</sup> ···O1W <sup>iii</sup>	0.88	1.94	2.790 (3)	164
O3W—H18 <sup>i</sup> ···O4 <sup>iii</sup>	0.90	1.95	2.821 (3)	163
N2—H6 <sup>i</sup> ···O1W <sup>iv</sup>	0.86	2.03	2.877 (3)	168
N4—H10 <sup>i</sup> ···O3W	0.86	1.94	2.781 (3)	164

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

H atoms on aromatic rings were placed in calculated positions, with  $\text{C—H} = 0.96$  Å and  $\text{N—H} = 0.86$  Å, and were included in the final cycle of refinement in the riding model, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}$  of the carrier atoms. Water H atoms were located in a difference Fourier map and refined as riding in their as-found positions relative to the O atoms, with fixed isotropic displacement parameters of  $0.05$  Å<sup>2</sup>.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997) and *XP* (Siemens, 1994); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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