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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.057
 wR factor = 0.106
Data-to-parameter ratio = 15.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.**catena-Poly[[triazquazinc(II)]- μ -5-hydroxyisophthalato- $\kappa^2\text{O}:\text{O}'$]**

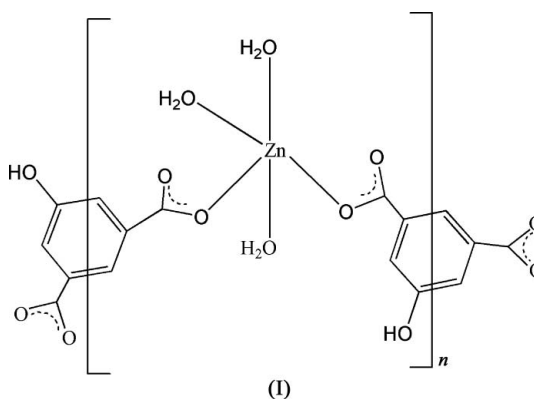
In the title compound, $[\text{Zn}(\text{C}_8\text{H}_4\text{O}_5)(\text{H}_2\text{O})_3]_n$, the Zn^{II} atom is in a five-coordinated environment defined by three aqua O atoms and two carboxylate O atoms from two different 5-hydroxyisophthalate dianions. In the 5-hydroxyisophthalate dianions, two carboxylate groups coordinate two Zn^{II} cations in a bidentate bridging coordination mode, forming a zigzag chain. In addition, $\text{O}-\text{H} \cdots \text{O}$ intermolecular hydrogen bonds link the chains into a three-dimensional network.

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Comment

Benzenedicarboxylic acids such as benzene-1,4-dicarboxylic acid and 5-hydroxyisophthalic acid are versatile ligands and can function as monodentate, bidentate or tridentate ligands; they can also bridge or chelate (Hong & You, 2004; Sun *et al.*, 2001; Xiao & Zhu, 2003). In continuation of our study of the chemistry of benzenedicarboxylate ligands (Xiao, Hu & Li, 2004; Xiao, Li, Ye & Hu, 2004; Xiao *et al.*, 2005; Zhu *et al.*, 2004), we present here the title compound, (I), in which the 5-hydroxyisophthalate dianion functions as a bridge between adjacent Zn^{II} centers.



In (I), the Zn^{II} atom is in a five-coordinate environment defined by three aqua O atoms and two carboxylate O atoms from two different 5-hydroxyisophthalate dianions (Fig. 1). The $\text{Zn}-\text{O}1$ and $\text{Zn}-\text{O}4^i$ [symmetry code: (i) $x + \frac{1}{2}, y - \frac{1}{2}, 1 - z$] bond lengths are in agreement with analogous literature values in complexes containing a bidentate bridging 5-hydroxyisophthalate ligand (Plater *et al.*, 2001; Li *et al.*, 2004). In the 5-hydroxyisophthalate dianions, two carboxylate groups coordinate two Zn^{II} cations in a bidentate bridging coordination mode, forming a zigzag chain (Fig. 2).

The stability of the solid-state structure of (I) is enhanced significantly by hydrogen-bonding interactions (Table 2). These link neighbouring zigzag chains into a three-dimensional network (Fig. 3).

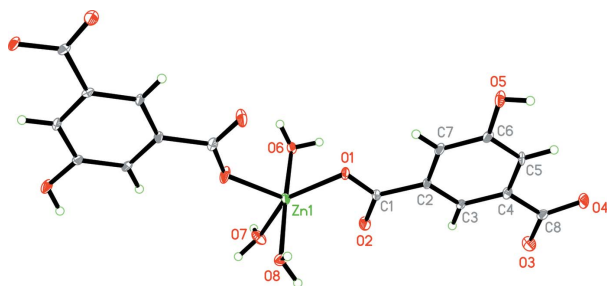


Figure 1
The coordination environment of the Zn atom in (I), showing the atom numbering and displacement ellipsoids drawn at the 30% probability level. [Symmetry code for unlabeled atoms: $x + \frac{1}{2}, y - \frac{1}{2}, 1 - z$.]

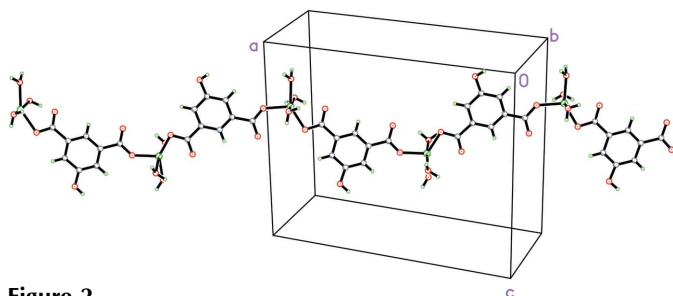


Figure 2
The polymeric zigzag chain structure of (I).

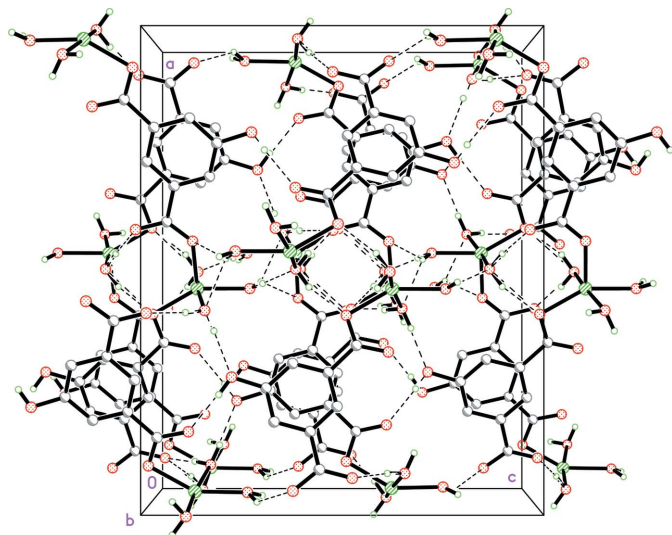


Figure 3
The crystal packing of (I), showing the three-dimensional network structure formed by hydrogen bonding interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted.

This investigation was performed independently of another investigation reporting the same structure, which is presented in the following paper (Wang *et al.*, 2006).

Experimental

A solution (15 ml) of dimethylformamide containing $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ (0.3 mmol, 0.088 g) and 5-hydroxyisophthalic acid (0.3 mmol, 0.052 g) was added slowly to a methanol solution (10 ml) of 1,4-diazabicyclo[2.2.2]octane (0.3 mmol, 0.034 g). Colorless crystals

suitable for X-ray analysis were obtained from the solution after two months at room temperature.

Crystal data

$[\text{Zn}(\text{C}_8\text{H}_4\text{O}_5)(\text{H}_2\text{O})_3]$
 $M_r = 299.53$
Orthorhombic, *Pccn*
 $a = 18.3046$ (17) Å
 $b = 7.3920$ (7) Å
 $c = 15.0771$ (14) Å
 $V = 2040.0$ (3) Å³
 $Z = 8$
 $D_x = 1.950$ Mg m⁻³

Mo $K\alpha$ radiation
Cell parameters from 4149 reflections
 $\theta = 2.2\text{--}28.2^\circ$
 $\mu = 2.44$ mm⁻¹
 $T = 298$ (2) K
Prism, colorless
 $0.25 \times 0.22 \times 0.10$ mm

Data collection

Bruker APEX area-detector diffractometer
 φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2002a)
 $T_{\min} = 0.581, T_{\max} = 0.793$
11667 measured reflections

2327 independent reflections
2179 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.033$
 $\theta_{\max} = 27.5^\circ$
 $h = -23 \rightarrow 21$
 $k = -9 \rightarrow 8$
 $l = -18 \rightarrow 19$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.057$
 $wR(F^2) = 0.106$
 $S = 1.31$
2327 reflections
155 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0207P)^2 + 8.2421P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.60$ e Å⁻³
 $\Delta\rho_{\min} = -0.69$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Zn1—O4 ⁱ	1.983 (3)	Zn1—O8	2.088 (3)
Zn1—O1	2.036 (3)	Zn1—O6	2.142 (3)
Zn1—O7	2.040 (3)		
O4 ⁱ —Zn1—O1	116.59 (12)	O7—Zn1—O8	85.28 (12)
O4 ⁱ —Zn1—O7	96.52 (13)	O4 ⁱ —Zn1—O6	94.90 (13)
O1—Zn1—O7	146.83 (12)	O1—Zn1—O6	88.82 (11)
O4 ⁱ —Zn1—O8	90.99 (13)	O7—Zn1—O6	86.45 (11)
O1—Zn1—O8	95.39 (11)	O8—Zn1—O6	170.34 (11)

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

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{—}H\cdots A$	$D\text{—}H$	$H\cdots A$	$D\cdots A$	$D\text{—}H\cdots A$
O5—H5A ⁱⁱ ···O2 ⁱⁱ	0.82	1.83	2.646 (4)	176
O6—H6A ⁱⁱⁱ ···O1 ⁱⁱⁱ	0.85	1.83	2.642 (4)	158.0
O6—H6B ⁱⁱⁱ ···O3 ^{iv}	0.85	1.83	2.656 (4)	162.3
O7—H7A ^v ···O6 ^v	0.85	1.95	2.794 (4)	174.5
O7—H7B ^v ···O8 ^{vi}	0.85	2.28	2.966 (4)	137.8
O7—H7B ^v ···O4 ^{vii}	0.85	2.49	3.228 (5)	145.4
O8—H8A ^{viii} ···O3 ^{viii}	0.85	1.83	2.677 (4)	172.3
O8—H8B ^{viii} ···O5 ^{ix}	0.85	1.86	2.711 (4)	176.6

Symmetry codes: (ii) $-x + \frac{1}{2}, y, z - \frac{1}{2}$; (iii) $-x + 1, -y + 2, -z + 1$; (iv) $-x + \frac{1}{2}, -y + \frac{3}{2}, z$; (v) $-x + 1, y - \frac{1}{2}, -z + \frac{3}{2}$; (vi) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$; (vii) $-x + \frac{1}{2}, y, z + \frac{1}{2}$; (viii) $-x + \frac{1}{2}, -y + \frac{3}{2}, z$; (ix) $x, -y + \frac{3}{2}, z + \frac{1}{2}$.

Water H atoms were located in a difference map and were refined isotropically, with O—H distances restrained to 0.85 (1) Å and with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$. The hydroxyl H atoms were positioned geometrically (O—H = 0.82 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H})$ values equal to $1.5U_{\text{eq}}(\text{O})$ of the parent atoms.

The remaining H atoms were positioned geometrically (C–H = 0.93 Å) and allowed to ride on their parent atoms, with $U_{\text{iso}}(\text{H})$ values equal to $1.2U_{\text{eq}}(\text{C})$ of the parent atoms.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINTE* (Bruker, 2002); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2002*b*); software used to prepare material for publication: *SHELXL97*.

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