

catena-Poly[[aqua(μ -5-carboxyimidazole-4-carboxylato- $\kappa^4 N^3, O^4: N^1, O^5$)zinc(II)] hemihydrate]

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Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$
Disorder in solvent or counterion
 R factor = 0.039
 wR factor = 0.106
Data-to-parameter ratio = 13.7

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

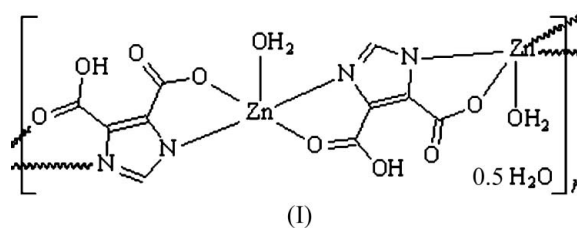
The title compound, $\{[\text{Zn}(\text{HIDC})(\text{H}_2\text{O})]\cdot 0.5\text{H}_2\text{O}\}_n$ (HIDC^{2-} is the imidazole-4,5-dicarboxylate dianion, $\text{C}_5\text{H}_2\text{N}_2\text{O}_4$), exists as a one-dimensional coordination polymer formed by HIDC^{2-} ligands bridging Zn^{II} atoms, with a $\text{Zn}\cdots\text{Zn}$ separation of $6.156(2)\text{ \AA}$. The Zn^{II} ion exists in a distorted square-pyramidal coordination, involving two N and two O atoms from two symmetry-related bidentate HIDC^{2-} groups, and one water molecule.

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Comment

Crystal structures of several metal complexes with the 4,5-imidazoledicarboxylic acid (H_3IDC) ligand have been reported (Fang & Zhang, 2006; Gao, Liu *et al.*, 2004; Gao, Zhang *et al.*, 2004; Liu *et al.*, 2004; Shimizu *et al.*, 2004; Wang *et al.*, 2005; Zhao *et al.*, 2005), in which the ligand is deprotonated to different levels (H_2IDC^- , HIDC^{2-} and IDC^{3-}) and in varying positions, resulting in different coordination modes with different structures and compositions. We report here the crystal structure of the title compound, (I).



In compound (I), the ligand exists as an HIDC^{2-} dianion. Each Zn^{II} ion is five-coordinated by two N atoms and two O atoms (one O each from the carboxylic and carboxylate groups) from two bidentate symmetry-related HIDC^{2-} ligands, and one water molecule, to give a distorted square-pyramidal coordination geometry (Fig. 1 and Table 1). The N and O atoms of the HIDC^{2-} ligands lie in the basal plane and the water molecule occupies the apical position. The HIDC^{2-} ligand is planar, with an r.m.s. deviation of 0.012 \AA . The planarity is facilitated by an intramolecular $\text{O1}-\text{H1}\cdots\text{O4}$ hydrogen bond. The dihedral angle between the two HIDC^{2-} groups around the Zn^{II} center is $11.7(4)^\circ$.

Each HIDC^{2-} group of (I) acts as an *N,O*-chelating bridging ligand linking two Zn^{II} ions, generating a one-dimensional chain running along the *b*-axis direction. Within this chain, the adjacent $\text{Zn}\cdots\text{Zn}$ separation is $6.156(2)\text{ \AA}$. The chains are arranged in layers parallel to the *bc* plane and intermolecular $\text{O}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 2) link them, forming a three-dimensional supramolecular framework.

Experimental

A mixture of 1*H*-imidazole-4,5-dicarbonitrile (24 mg, 0.2 mmol), ZnCl₂ (28 mg, 0.2 mmol) and NaOH (9 mg, 0.2 mmol) in water (15 ml) was placed in a Teflon-lined stainless steel Parr bomb. The bomb was heated at 413 K for 24 h. It was then cooled to room temperature over a period of 24 h. Colourless crystals were isolated in 20% yield.

Crystal data

[Zn(C ₅ H ₂ N ₂ O ₄)(H ₂ O)]·0.5H ₂ O	<i>Z</i> = 8
<i>M_r</i> = 246.48	<i>D_x</i> = 2.152 Mg m ^{−3}
Monoclinic, <i>C</i> 2/ <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 13.735 (3) Å	<i>μ</i> = 3.23 mm ^{−1}
<i>b</i> = 12.088 (2) Å	<i>T</i> = 293 (2) K
<i>c</i> = 9.942 (2) Å	Block, colorless
<i>β</i> = 112.79 (3)°	0.10 × 0.08 × 0.06 mm
<i>V</i> = 1521.8 (5) Å ³	

Data collection

Rigaku R-AXIS RAPID diffractometer	7258 measured reflections
<i>ω</i> scans	1740 independent reflections
Absorption correction: multi-scan (<i>ABSCOR</i> ; Higashi, 1995)	1472 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T</i> _{min} = 0.739, <i>T</i> _{max} = 0.830	<i>R</i> _{int} = 0.049
	<i>θ</i> _{max} = 27.5°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0574P)^2 + 2.183P]$
$R[F^2 > 2\sigma(F^2)] = 0.039$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	(Δ/σ) _{max} = 0.001
<i>S</i> = 1.06	Δρ _{max} = 0.66 e Å ^{−3}
1740 reflections	Δρ _{min} = −0.43 e Å ^{−3}
127 parameters	
H atoms treated by a mixture of independent and constrained refinement	

Table 1

Selected geometric parameters (Å, °).

Zn1—N1	1.985 (2)	Zn1—O3 ⁱ	2.199 (3)
Zn1—N2 ⁱ	1.985 (2)	Zn1—O1W	2.020 (3)
Zn1—O2	2.201 (3)		
N2 ⁱ —Zn1—N1	153.04 (12)	N2 ⁱ —Zn1—O3 ⁱ	79.74 (10)
N1—Zn1—O2	79.20 (10)	N2 ⁱ —Zn1—O1W	100.37 (10)
N1—Zn1—O3 ⁱ	95.19 (10)	O1W—Zn1—O2	96.76 (11)
N1—Zn1—O1W	106.56 (10)	O1W—Zn1—O3 ⁱ	97.74 (10)
N2 ⁱ —Zn1—O2	99.12 (10)	O3 ⁱ —Zn1—O2	165.43 (10)

Symmetry code: (i) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.

Table 2

Hydrogen-bond geometry (Å, °).

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1...O4	0.85 (1)	1.87 (2)	2.700 (3)	165 (5)
O1W—H1WA...O3 ⁱⁱ	0.84	1.89	2.693 (3)	158
O1W—H1WB...O4 ⁱⁱⁱ	0.85	2.15	2.847 (3)	140
O1W—H1WB...O2W	0.85	2.41	2.847 (2)	113

Symmetry codes: (ii) $-x + \frac{3}{2}, -y + \frac{1}{2}, -z + 1$; (iii) $x + \frac{1}{2}, y + \frac{1}{2}, z$.

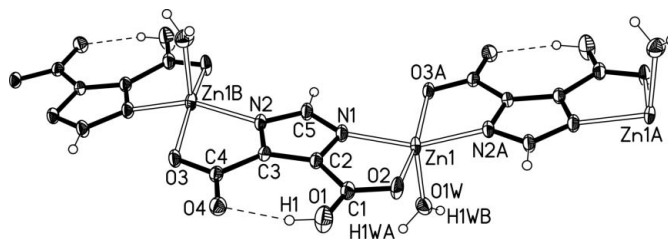


Figure 1

Part of the polymeric chain in (I), showing displacement ellipsoids drawn at the 30% probability level. Intramolecular hydrogen bonds are shown as dashed lines. [Symmetry codes: (A) $\frac{3}{2} - x, \frac{1}{2} + y, \frac{1}{2} - z$; (B) $\frac{3}{2} - x, y - \frac{1}{2}, \frac{1}{2} - z$.]

The H atom of the carboxyl group was located in a difference map, and refined with an O—H distance restraint of 0.85 (1) Å. Water H atoms were located in a difference map and were not refined. H atoms bound to C atoms were placed in calculated positions (C—H = 0.93 Å) and refined using a riding model. The *U*_{iso}(H) values for all H atoms were set at 1.2*U*_{eq}(C,O). The uncoordinated water molecule was disordered about a twofold rotation axis and it was refined with an occupation factor of 0.50. The H atoms of the disordered water molecule were not located.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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