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Poly[[aquazinc(II)]-μ_3-imidazole-4,5-dicarboxylato]

Xian-Fa Zhang, Shan Gao,* Li-Hua Huo and Hui Zhao

Laboratory of Functional Materials, School of Chemistry and Materials Science, Heilongjiang University, Harbin 150080, People's Republic of China

Correspondence e-mail:
shangao67@yahoo.com

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In the title coordination polymer, $[Zn(C_5H_2N_2O_4)(H_2O)]_n$, each Zn^{II} atom is six-coordinated by one N atom [Zn—N = 2.250 (7) Å] and four O atoms [Zn—O = 2.289 (6)–2.435 (6) Å] from three different HIDC ligands (H$_3$IDC = imidazole-4,5-dicarboxylic acid), and one water molecule [Zn—O = 2.311 (6) Å] in a highly distorted octahedral geometry. In the crystal structure, a three-dimensional supramolecular network is constructed *via* hydrogen-bonding interactions involving the water molecules, uncoordinated imidazole N atom and carboxylate O atoms.

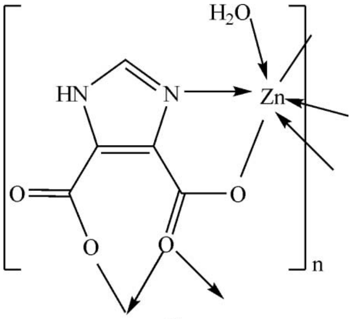
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.011 Å
R factor = 0.056
wR factor = 0.200
Data-to-parameter ratio = 13.0

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

Comment

N-Heterocyclic carboxylic acids, such as imidazole-4,5-dicarboxylic acid (H$_3$IDC), are recognized as efficient N/O donors exhibiting versatile coordination modes and hydrogen bonding. H$_3$IDC acid can be successively deprotonated to furnish H$_2$IDC$^-$, HIDC^{2-} and IDC^{3-} anions, which give rise to a wide range of supramolecular architectures (Zhang *et al.*, 2005, 2006; Lu *et al.*, 2006). Here we report the synthesis and structure of the title two-dimensional Zn^{II} polymer, (I).



(I)

The asymmetric unit of (I) (Fig. 1) comprises one Zn^{II} atom, one HIDC^{2-} anion and one coordinating water molecule. Each Zn^{II} atom is six-coordinated by one N and four O atoms from three HIDC^{2-} ligands and one water molecule in a highly distorted octahedral geometry (Table 1). Each HIDC^{2-} anion serves as a pentadentate bridging ligand to link three Zn^{II} atoms, with the formation of two-dimensional layers (Fig. 2). A short $Cg\cdots Cg^{v}$ distance of 3.3618 (12) Å between the centroids (Cg) of neighbouring imidazole rings (N1/C2/C3/N2/C5) indicates strong π–π stacking interaction within the layer [symmetry code: (v) $-x + 2, -y + 1, -z + 1$]. In the crystal structure, a three-dimensional supramolecular network is constructed *via* hydrogen-bonding interactions involving the water molecules, uncoordinated imidazole N atom and carboxylate O atoms (Table 2).

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Experimental

1*H*-Imidazole-4,5-dicarboxylic acid (1.54 g, 10 mmol), zinc diacetate dihydrate (2.20 g, 10 mmol), and NaOH (0.4 g, 10 mmol) were dissolved in an aqueous solution (25 ml). The mixture was sealed in a 50 ml Teflon-lined stainless steel bomb and held at 403 K for 5 d. The bomb was gradually cooled to room temperature, and colourless crystals were obtained after several days.

Crystal data

$[Zn(C_5H_2N_2O_4)(H_2O)]$
$M_r = 237.49$
Monoclinic, $P2_1/n$
$a = 6.613\ (3)$ Å
$b = 9.979\ (4)$ Å
$c = 10.582\ (5)$ Å
$\beta = 105.748\ (15)^\circ$
$V = 672.2\ (5)$ Å^3

$Z = 4$
$D_x = 2.347$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 3.64$ mm^{-1}
$T = 295\ (2)$ K
Prism, colourless
0.32 × 0.24 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.369$, $T_{max} = 0.520$

5206 measured reflections
1531 independent reflections
1458 reflections with $I > 2\sigma(I)$
$R_{int} = 0.023$
$\theta_{max} = 27.5^\circ$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.200$
$S = 1.09$
1531 reflections
118 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1448P)^2 + 3.7247P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.68$ e Å^{-3}
$\Delta\rho_{min} = -1.11$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.250 (7)	Zn1—O2^{ii}	2.319 (6)
Zn1—O2^{i}	2.289 (6)	Zn1—O4^{ii}	2.375 (6)
Zn1—O1*W*	2.311 (6)	Zn1—O1	2.435 (6)
N1—Zn1—O2^{i}	116.6 (2)	O1*W*—Zn1—O4^{ii}	141.6 (2)
N1—Zn1—O1*W*	111.1 (2)	O2^{ii}—Zn1—O4^{ii}	77.7 (2)
O2^{i}—Zn1—O1*W*	81.2 (3)	N1—Zn1—O1	70.4 (2)
N1—Zn1—O2^{ii}	164.8 (2)	O2^{i}—Zn1—O1	159.0 (2)
O2^{i}—Zn1—O2^{ii}	71.4 (2)	O1*W*—Zn1—O1	77.9 (2)
O1*W*—Zn1—O2^{ii}	82.2 (2)	O2^{ii}—Zn1—O1	106.9 (2)
N1—Zn1—O4^{ii}	87.2 (2)	O4^{ii}—Zn1—O1	77.2 (2)
O2^{i}—Zn1—O4^{ii}	121.5 (2)		

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*1···O3^{iii}	0.82	1.92	2.707 (9)	161
O1*W*—H1*W*2···O4^{iv}	0.82	2.32	2.886 (9)	127
N2—H2···O4^{v}	0.86	1.93	2.782 (9)	169

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

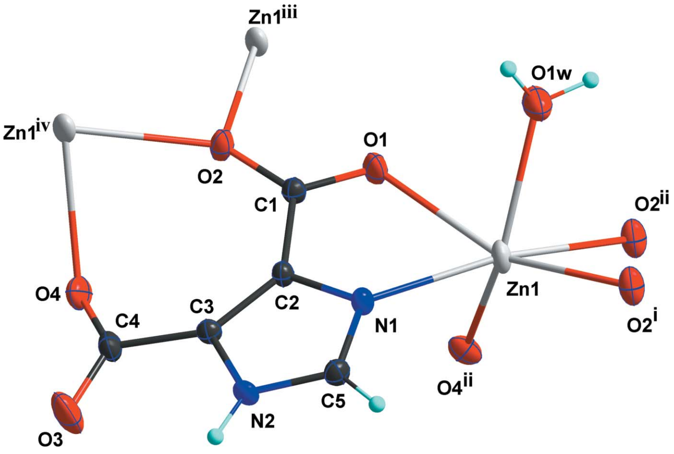

Figure 1
Part of the polymeric structure of the title complex showing the atomic labelling and 30% probability displacement ellipsoids [symmetry codes: (i) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $-x+\frac{2}{3}, y-1/2, -z+\frac{1}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$].

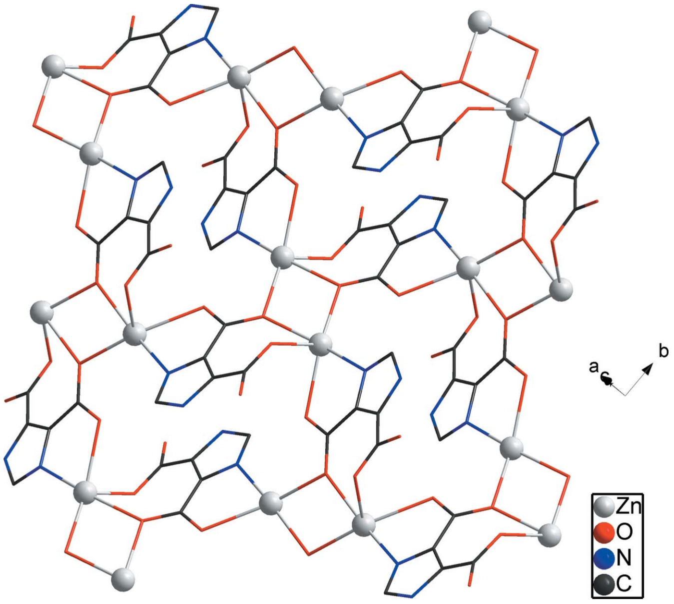

Figure 2
A portion of the crystal packing, showing the two-dimensional layer in (I). H atoms and water molecules have been omitted for clarity.

The C- and N-bound H atoms were placed in calculated positions (C—H = 0.93 Å, N—H = 0.86 Å) and refined in the riding-model approximation with $U_{iso}(H) = 1.2U_{eq}(C,N)$. The H atoms of the water molecule were placed at chemically sensible positions on the basis of hydrogen bonds with O—H = 0.82 Å and $U_{iso}(H) = 1.2U_{eq}(O)$, and not refined. The highest residual peak and deepest hole are situated 0.45 (2) Å from Zn1 and 0.43 (2) Å from O1, respectively.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); 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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