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Diaquabis(5-carboxy-1*H*-imidazole-4-carboxylato-κ^2N^3,O^4)zinc(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.023
wR factor = 0.064
Data-to-parameter ratio = 12.9

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

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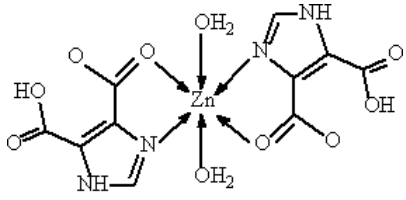
In the title complex, $[Zn(H_2IDC)_2(H_2O)_2]$ (where H_2IDC^- is the 5-carboxy-1*H*-imidazole-4-carboxylate monoanion, $C_5H_3N_2O_4$), the Zn^{II} atom is located on an inversion centre, is *trans*-coordinated by two *N,O*-bidentate H_2IDC^- ligands and two water molecules and shows an approximately octahedral configuration. A three-dimensional supramolecular architecture is formed *via* hydrogen-bond interactions.

Comment

Recently, we are interested in the solid-state coordination chemistry of *N*-heterocyclic carboxylic acids, such as imidazoledicarboxylic acid (H_3IDC), which is recognized as possessing efficient *N/O* donors exhibiting versatile coordination behavior and hydrogen bonding, and which can be successively deprotonated to generate the H_2IDC^-, $HIDC^{2-}$ and IDC^{3-} anions. To date, there have been some reports on mononuclear (Zhang *et al.*, 2004; Xiao *et al.*, 2004; Ma *et al.*, 2003; Sengupta *et al.*, 2001; Sanna *et al.*, 1998) and dinuclear (Rajendiran *et al.*, 2003) complexes based on the H_3IDC ligand. For example, Ma *et al.* (2003) and Zhang *et al.* (2004) have described the structures of the mononuclear complexes $[Cd(H_2IDC)(H_2O)_2]$ and $[Mn(H_2IDC)(H_2O)_2]$, in which both Mn^{II} and Cd^{II} ions exhibit octahedral geometries with the H_2IDC^- ligand. The present Zn^{II} complex, $[Zn(H_2IDC)(H_2O)_2]$, (I), is isomorphous with the Cd^{II} and Mn^{II} analogs. Similar structural descriptions of these analogs apply to the present isomorphous complex.



(I)

The carboxylic acid ligand bears a formal charge of −1, and the free carboxylate atoms O3 and O2 form an intramolecular hydrogen bond (Table 2). The Zn^{II} atom lies on an inversion centre, is *trans*-coordinated by two N,O-bidentate H_2IDC^- ligands [Zn—N = 2.0742 (13) Å and Zn—O = 2.1445 (12) Å] and two water molecules [Zn—O = 2.1565 (14) Å] and has an approximately octahedral geometry. The H_2IDC^- ligand behaves as a chelating unit that binds through the aromatic amino and negatively charged carboxyl atoms, giving a five-membered chelate ring. A three-dimensional supramolecular network is constructed *via* hydrogen-bonding interactions,

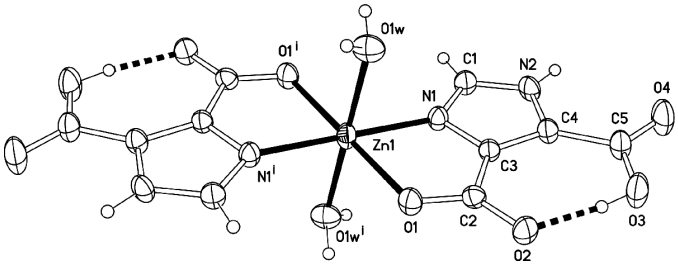


Figure 1
*ORTEP*II (Johnson, 1976) plot of the title complex, with displacement ellipsoids drawn at the 30% probability level. Hydrogen bonds are shown as dashed lines. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

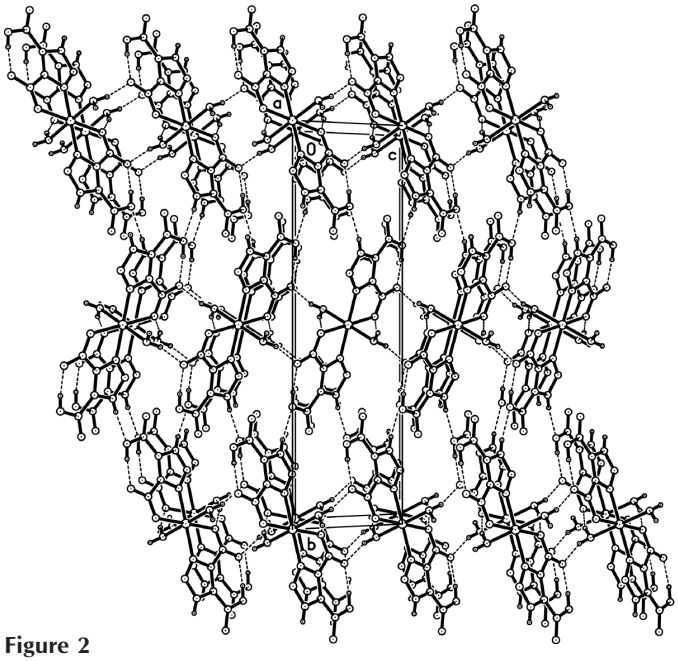


Figure 2
Packing diagram of the title complex. Hydrogen bonds are shown as dashed lines.

involving the water molecules, the uncoordinated imidazole N atom, and carboxylate O atoms of H_2IDC^- ligands (Table 2 and Fig. 2).

Experimental

1*H*-Imidazole-4,5-dicarboxylic acid (4.60 g, 20 mmol) and zinc diacetate dihydrate (4.40 g, 20 mmol) were dissolved in water. The mixture was sealed in a 25 ml Teflon-lined stainless steel bomb and held at 403 K for 3 d. The bomb was cooled naturally to room temperature, and colorless prismatic crystals were obtained after several days. Analysis calculated for $C_{10}H_{10}N_4O_{10}Zn$: C 29.18, H 2.45, N 13.61%; found: C 29.34, H 2.51, N 13.56%.

Crystal data

$[Zn(C_5H_3N_2O_4)_2(H_2O)_2]$
$M_r = 411.61$
Monoclinic, $P2_1/n$
$a = 5.0974$ (10) Å
$b = 22.414$ (5) Å
$c = 6.5617$ (13) Å
$\beta = 111.87$ (3)°
$V = 695.7$ (3) Å^3
$Z = 2$
$D_x = 1.965$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6098 reflections
$\theta = 3.5$–27.5°
$\mu = 1.84$ mm^{-1}
$T = 293$ (2) K
Prism, colorless
0.37 × 0.24 × 0.19 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.595$, $T_{max} = 0.706$
6667 measured reflections
1599 independent reflections
1441 reflections with $I > 2\sigma(I)$
$R_{int} = 0.024$
$\theta_{max} = 27.5°$
$h = -5 \rightarrow 6$
$k = -29 \rightarrow 28$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.023$
$wR(F^2) = 0.064$
$S = 1.05$
1599 reflections
124 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0382P)^2 + 0.2368P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.0742 (13)	O2—C2	1.2611 (18)
Zn1—O1	2.1445 (12)	O3—C5	1.314 (2)
Zn1—O1*W*	2.1565 (14)	O4—C5	1.209 (2)
O1—C2	1.2578 (19)		
N1—Zn1—N1^{i}	180	O1^{i}—Zn1—O1	180
N1^{i}—Zn1—O1	99.98 (5)	O1^{i}—Zn1—O1*W*	91.19 (5)
N1—Zn1—O1	80.02 (5)	O1—Zn1—O1*W*	88.81 (5)
N1—Zn1—O1*W*	86.26 (5)	O1*W*^{i}—Zn1—O1*W*	180
N1^{i}—Zn1—O1*W*	93.74 (5)		

Symmetry code: (i) $1-x, 1-y, 1-z$.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H6···O3^{ii}	0.86	2.02	2.869 (3)	170
N2—H6···O4^{ii}	0.86	2.58	3.155 (3)	125
O3—H7···O2	0.85 (2)	1.67 (2)	2.519 (3)	173 (3)
O1*W*—H1*W*1···O2^{iii}	0.84 (3)	1.96 (3)	2.772 (3)	162 (2)
O1*W*—H1*W*2···O1^{iv}	0.85 (3)	1.92 (3)	2.733 (3)	160 (2)

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

H atoms attached to C and N atoms were placed in calculated positions [C—H = 0.93 Å or N—H = 0.86 Å and U_{iso}(H) = $1.2U_{eq}$(C,N)] using the riding-model approximation. The carboxy and water H atoms were located in a difference map and refined with an O—H distance restraint of 0.85 (1) Å and U_{iso}(H) = $1.5U_{eq}$(O).

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS*97(Sheldrick, 1997); program(s) used to refine structure: *SHELXS*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97..

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