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Diaqua-*trans*-bis(pyridazine-3-carboxylato-κ^2O,N)-zinc(II)

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In the structure of the title compound, $[Zn(C_5H_3N_2O_2)_2(H_2O)_2]$, the Zn^{II} ion is located on a centre of symmetry. The coordination around the Zn^{II} atom is slightly distorted octahedral, with two equatorial pyridazine-3-carboxylate ligands in a *trans* arrangement. A pyridazine-ring N atom [Zn—N = 2.0742 (15) Å] and one carboxylate O atom [Zn1—O2 = 2.0744 (14) Å] from each ligand coordinate to the metal. Two water O atoms [Zn—O = 2.1934 (17) Å] are coordinated in axial positions. The coordinated water molecules act as hydrogen-bond donors to the unbonded carboxylate O atoms in adjacent monomers, forming a three-dimensional network.

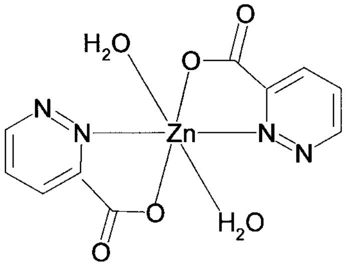
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.041
wR factor = 0.113
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.

Comment

Until now, the structures of only two metal complexes with pyridazine-3-carboxylate and water ligands have been determined. A manganese(II) complex dihydrate (Ardivinata *et al.*, 1989) and a zinc(II) complex dihydrate (Gryz *et al.*, 2003) are triclinic and contain monomeric molecules with slightly distorted octahedral coordination around the metal ion. The title zinc(II) complex, (I), in contrast, is monoclinic. It contains monomeric complex molecules, but does not contain uncoordinated solvent water molecules. The zinc(II) ion is located on a centre of inversion and is coordinated by two equatorial ligand molecules in a *trans* arrangement, both ligands chelating *via* the *N*,*O*-bonding sites. Two water O atoms in the axial positions complete a slightly distorted octahedron around the metal ion. This is illustrated in Fig. 1, which also shows the atom-labelling scheme.



(I)

The metal ion, the pyridazine ring and carboxylate atoms are almost coplanar; the mean deviation from the average ligand molecule plane is 0.011 (1) Å. The Zn—O and Zn—N bond distances and angles within the metal coordination octahedron, as well as within the pyridazine ligand in the title compound are almost the same as those observed in the triclinic form of Zn^{II}–pyridizinate (Gryz *et al.*, 2003). A packing diagram is displayed in Fig. 2 and shows how the monomers connect *via* hydrogen bonds, which link the

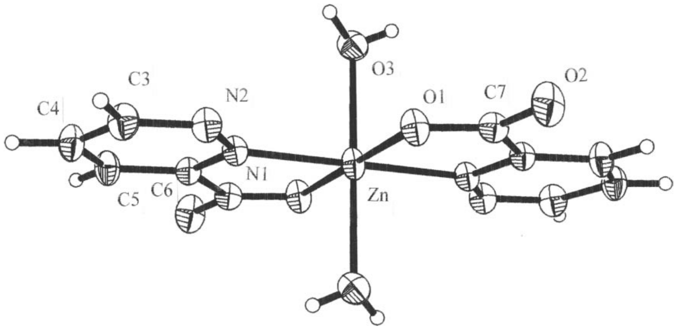


Figure 1
The title molecule with atom-labelling scheme. Unlabelled atoms are related by the symmetry code ($x-1$, $y-1$, $z-1$). Displacement ellipsoids are drawn at the 50% probability level.

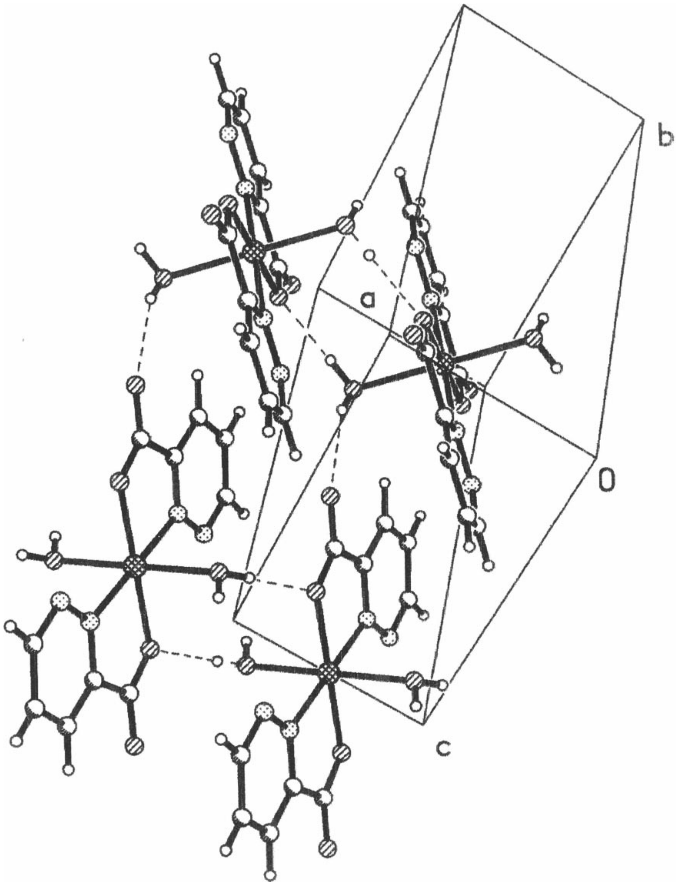


Figure 2
Packing of the title molecules in the crystal structure. Dashed lines indicate hydrogen bonds.

coordinated water molecules with the uncoordinated carboxylate O atoms in adjacent monomers to give a three-dimensional network. The relevant hydrogen-bond details are listed in Table 1.

Experimental

A hot solution containing zinc(II) acetate tetrahydrate (1 mmol) in water (50 ml) and another containing pyridazine-3-carboxylic acid (2 mmol) in water (50 ml) were mixed and boiled with stirring under reflux for 2 h. After cooling to room temperature, single crystals deposited overnight. They were identified by X-ray diffraction as crystals of the triclinic form (Gryz *et al.*, 2003). Part of the sample was dissolved in warm methanol (100 ml), yielding, after evaporation over a period of 2 d, pale-yellow single crystals of the title compound in the form of rectangular plates.

Crystal data

$[Zn(C_5H_3N_2O_2)_2(H_2O)_2]$
$M_r = 347.61$
Monoclinic, $P2_1/c$
$a = 5.227$ (1) Å
$b = 11.709$ (2) Å
$c = 9.799$ (2) Å
$\beta = 101.63$ (3)°
$V = 587.4$ (2) Å^3
$Z = 2$

$D_x = 1.965$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 6$–13°
$\mu = 2.13$ mm^{-1}
$T = 293$ (2) K
Block, pale yellow
0.37 × 0.21 × 0.18 mm

Data collection

Kuma *KM*-4 four-circle diffractometer
$\omega/2\theta$ scans
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2000)
$T_{min} = 0.245$, $T_{max} = 0.357$
1750 measured reflections
1601 independent reflections

1529 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 30.1°$
$h = -7 \rightarrow 0$
$k = 0 \rightarrow 16$
$l = -13 \rightarrow 13$
3 standard reflections every 200 reflections intensity decay: 3.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.114$
$S = 1.08$
1601 reflections
117 parameters
All H-atom parameters refinemed

$w = 1/[\sigma^2(F_o^2) + (0.0855P)^2 + 0.2546P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 1.19$ e Å^{-3}
$\Delta\rho_{min} = -1.88$ e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H31···O2^{i}	0.86 (4)	1.92 (4)	2.784 (2)	178 (4)
O3—H32···O1^{ii}	0.75 (3)	2.20 (5)	2.896 (2)	155 (5)

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

H atoms were refined independently with isotropic displacement parameters. The largest electron-density peak is 0.83 Å from atom Zn1 and the deepest hole is 0.86 Å from the same atom.

Data collection: *KM*-4 *Software* (Kuma, 1996); cell refinement: *KM*-4 *Software*; data reduction: *DATAPROC* (Kuma, 2001); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1992); software used to prepare material for publication: *SHELXL*97.

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