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Key indicators

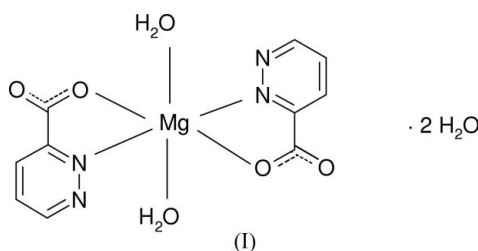
Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.041
 wR factor = 0.137
Data-to-parameter ratio = 15.8For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.*trans*-Diaquabis(pyridazine-3-carboxylato- κ^2N,O)-
magnesium(II) dihydrate

The title compound, $[\text{Mg}(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$, contains centrosymmetric neutral complex molecules. The pyridazine-3-carboxylate ligands bond in an *N,O*-bidentate mode and the octahedral Mg coordination is completed by two *trans* water molecules. There are also two non-coordinated water molecules. $\text{O}-\text{H} \cdots \text{O}$ and $\text{O}-\text{H} \cdots \text{N}$ hydrogen bonds are present, resulting in a three-dimensional network.

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Comment

The title compound, (I), is isostructural with the analogous complexes of manganese (Ardivinata *et al.*, 1989) and zinc (Gryz *et al.*, 2003) with the same ligands.



The structure of (I) is triclinic and its unit cell contains one monomeric $[\text{Mg}(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})_2]$ complex molecule and two non-coordinated water molecules. The Mg^{II} cation is located on an inversion centre and is coordinated by two equatorial bidentate-*N,O* ligand molecules. Two axial water O atoms complete a slightly distorted octahedron around the metal ion (Fig. 1 and Table 1). The pyridazine ring is almost planar (r.m.s. deviation 0.0106 Å) and the carboxylate group is rotated from the mean ring plane by 5.3 (3)°.

Fig. 2 shows a packing diagram for (I) and the hydrogen-bonding scheme. Hydrogen bonds link the water molecules to uncoordinated carboxylate O atoms and uncoordinated hetero-ring N atoms in adjacent monomers, forming a three-dimensional network (Table 2). Monomeric molecules with octahedral coordination around the Mg^{II} cation have been also reported for magnesium(II) picolinate (Deloume *et al.*, 1973) and magnesium aminopyrazinate (Ptasiewicz-Bąk *et al.*, 1997). In both these compounds, the ligand molecules chelate the metal ion *via* an *N,O*-bonding mode. However, the ligand planes are in a *cis* arrangement, with a dihedral angle between the planes of 95° in the former complex and 67.3 (5)° in the latter.

Experimental

A hot aqueous solution (50 ml) containing pyridazine-3-carboxylic acid (2 mmol) was added with constant stirring to a hot aqueous

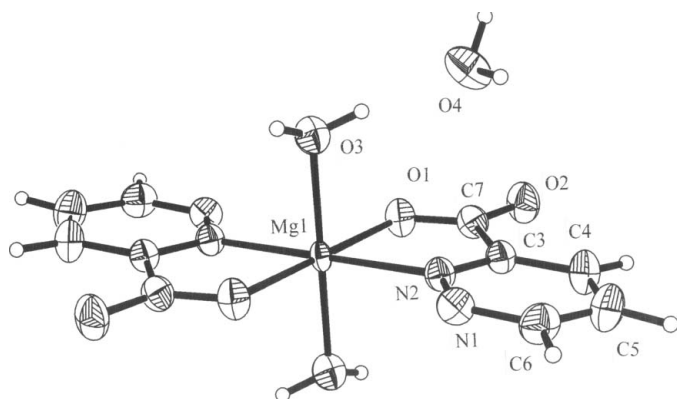


Figure 1
A view of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). Unlabelled atoms are generated by the symmetry operation $(1 - x, 1 - y, 1 - z)$.

solution (50 ml) containing magnesium acetate tetrahydrate (1 mmol). After boiling for 1 h, the solution was left to crystallize at room temperature. After several days, single crystals of (I) in the form of colourless blocks deposited in the mother liquid. These were washed with cold water and ethanol and dried in air.

Crystal data

$[\text{Mg}(\text{C}_5\text{H}_3\text{N}_2\text{O}_2)_2(\text{H}_2\text{O})_2] \cdot 2\text{H}_2\text{O}$ $Z = 1$
 $M_r = 342.56$ $D_x = 1.586 \text{ Mg m}^{-3}$
 Triclinic, $P\bar{1}$ Mo $K\alpha$ radiation
 Cell parameters from 25 reflections
 $a = 5.338 (1) \text{ \AA}$ $\theta = 6\text{--}15^\circ$
 $b = 7.468 (2) \text{ \AA}$ $\mu = 0.18 \text{ mm}^{-1}$
 $c = 9.641 (2) \text{ \AA}$ $T = 293 (2) \text{ K}$
 $\alpha = 79.23 (3)^\circ$ Rod, colourless
 $\beta = 88.91 (3)^\circ$ $0.40 \times 0.09 \times 0.07 \text{ mm}$
 $\gamma = 71.93 (3)^\circ$
 $V = 358.63 (13) \text{ \AA}^3$

Data collection

Kuma KM-4 four-circle diffractometer 1463 reflections with $I > 2\sigma(I)$
 $\omega/2\theta$ scans $R_{\text{int}} = 0.023$
 Absorption correction: analytical $\theta_{\text{max}} = 30.1^\circ$
 (*CrysAlis RED*; Oxford Diffraction, 2000) $h = -7 \rightarrow 0$
 $T_{\text{min}} = 0.978, T_{\text{max}} = 0.986$ $k = -10 \rightarrow 10$
 2327 measured reflections $l = -13 \rightarrow 13$
 2117 independent reflections 3 standard reflections every 200 reflections intensity decay: 2.1%

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.089P)^2 + 0.0392P]$
 $R[F^2 > 2\sigma(F^2)] = 0.041$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.137$ $(\Delta/\sigma)_{\text{max}} < 0.001$
 $S = 1.06$ $\Delta\rho_{\text{max}} = 0.60 \text{ e \AA}^{-3}$
 2117 reflections $\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$
 134 parameters
 All H-atom parameters refined

Table 1
Selected geometric parameters ($\text{\AA}, ^\circ$).

Mg1—O1	2.0406 (13)	Mg1—N2	2.1769 (16)
Mg1—O3	2.0909 (14)		
O1—Mg1—N2	77.39 (5)		

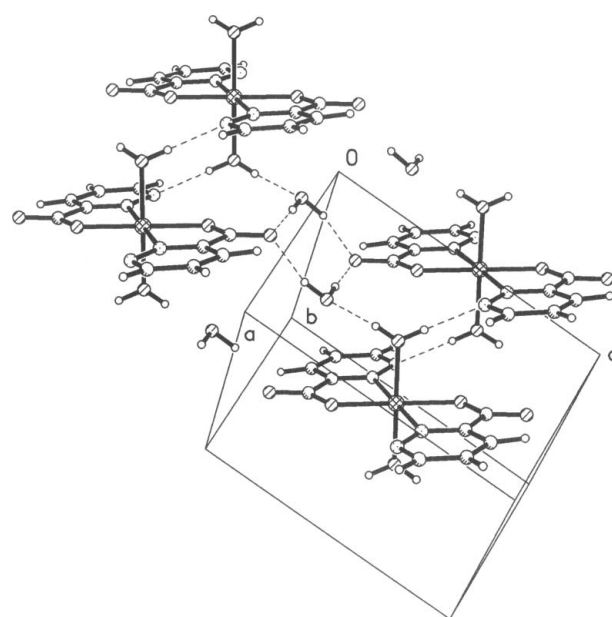


Figure 2
The packing of (I), with dashed lines indicating hydrogen bonds.

Table 2
Hydrogen-bond geometry ($\text{\AA}, ^\circ$).

$D\text{—}H \cdots A$	$D\text{—}H$	$H \cdots A$	$D \cdots A$	$D\text{—}H \cdots A$
O3—H32 \cdots O4	0.88 (3)	1.86 (3)	2.737 (2)	175 (3)
O3—H31 \cdots N1 ⁱ	0.87 (4)	2.04 (4)	2.899 (2)	170 (3)
O4—H41 \cdots O2 ⁱⁱ	1.00 (3)	1.82 (3)	2.822 (2)	173 (3)
O4—H42 \cdots O2 ⁱⁱⁱ	0.99 (3)	1.92 (3)	2.888 (2)	165 (3)

Symmetry codes: (i) $-x, -y + 1, -z + 1$; (ii) $x - 1, y, z$; (iii) $-x + 1, -y + 1, -z$.

H atoms were located in difference maps and freely refined with isotropic displacement parameters. Refined C—H distances are in the range 1.00 (2)–1.02 (3) \AA .

Data collection: *KM-4 Software* (Kuma, 1996); cell refinement: *KM-4 Software*; data reduction: *DATAPROC* (Kuma, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1992); software used to prepare material for publication: *SHELXL97*.

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