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Tetraaquabis[(2-oxo-4*H*-pyridin-1-yl)acetato]-magnesium(II)

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Key indicators

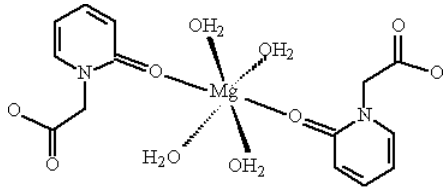
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.043
wR factor = 0.120
Data-to-parameter ratio = 15.1

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

The title complex, tetraaquabis[(2-oxo-1,2-dihydropyridin-1-yl)acetato]magnesium(II), $[Mg(C_7H_6NO_3)_2(H_2O)_4]$, is a neutral mononuclear molecule consisting of an Mg^{II} ion, two (2-oxo-4*H*-pyridin-1-yl)acetate ligands and four coordinated water molecules. The Mg^{II} atom, located on a symmetry center, has octahedral coordination involving two carbonyl O atoms of different (2-oxo-4*H*-pyridin-1-yl)acetate ligands and four water molecules. O—H···O intermolecular hydrogen bonds form a layer structure.

Comment

(4-Oxo-4*H*-pyridin-1-yl)acetic acid, known as an important medical intermediate (Edwards *et al.*, 1977), is a potential multidentate ligand with a versatile binding mode. However, there is little information on the structure of metal complexes of this acid. Recently, we used the 4-oxo-1(4*H*)-(carboxymethyl)pyridinium hydroxide inner salt to prepare metal complexes (Gao *et al.*, 2004; Zhang *et al.*, 2004). In order to explore the structural properties of related complexes, we have synthesized the title magnesium(II) complex, (I), by the reaction of (2-oxo-4*H*-pyridin-1-yl)acetic acid with magnesium(II) nitrate hexahydrate under basic conditions. The crystal structure of (I) is described here.



(I)

As illustrated in Fig. 1, the title complex has a mononuclear structure, in which the (2-oxo-4*H*-pyridin-1-yl)acetate groups are bonded to the Mg^{II} atom through the carbonyl O atoms in a monodentate fashion. The Mg^{II} atom is located on an inversion center and is coordinated by two carbonyl O atoms and four water molecules, forming an octahedral coordination geometry. The $Mg—O_{carbonyl}$ bond distance is 2.027 (1) Å, and the average $Mg—O_{water}$ distance is 2.080 (1) Å. The carboxy group and pyridine ring in the (2-oxo-4*H*-pyridin-1-yl)acetate anion are not coplanar; they form a dihedral angle of 80.8 (3)°. The C2—C3, C4—C5 and C1—O3 bond lengths are 1.360 (3), 1.351 (3) and 1.246 (2) Å, respectively. O—H···O intermolecular hydrogen bonds are formed between water molecules and the uncoordinated O atoms in the carboxylate groups of adjacent molecules, with O···O distances in the range 2.717 (2)–2.933 (2) Å and O—H···O bond angles of

175 (3)–179 (2)°, resulting in a layered structure (Table 2 and Fig. 2).

Experimental

The title complex was prepared by the addition of $Mg(NO_3)_2{\cdot}6H_2O$ (5.13 g, 20 mmol) to an aqueous solution of (2-oxo-4*H*-pyridin-1-yl)acetic acid (5.84 g, 40 mmol). The resulting solution was stirred and the pH was adjusted to 7 with 0.2 *M* NaOH solution. After evaporation at room temperature for a week, colorless single crystals were obtained from the filtered solution. Analysis calculated for $C_{14}H_{20}MgN_2O_{10}$: C 43.12, H 4.63, N 7.01%; found: C 41.97, H 5.03, N 6.99%.

Crystal data

$[Mg(C_7H_6NO_3)_2(H_2O)_4]$	D_x = 1.486 Mg m^{-3}
M_r = 400.63	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 5735 reflections
a = 10.550 (2) Å	θ = 3.3–27.4°
b = 7.099 (1) Å	μ = 0.16 mm^{-1}
c = 13.056 (3) Å	T = 293 (2) K
β = 113.70 (3)°	Prism, colorless
V = 895.3 (4) Å^3	0.38 × 0.24 × 0.20 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	2054 independent reflections
	1839 reflections with $I > 2\sigma(I)$
ω scans	R_{int} = 0.029
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	θ_{max} = 27.5°
	$h = -13 \rightarrow 13$
T_{min} = 0.943, T_{max} = 0.969	$k = -8 \rightarrow 9$
8176 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 0.2876P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.043	
$wR(F^2)$ = 0.120	
S = 1.06	$(\Delta/\sigma)_{max} < 0.001$
2054 reflections	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
136 parameters	$\Delta\rho_{min}$ = −0.27 e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Mg1—O1*W*	2.060 (1)	O3—C1	1.246 (2)
Mg1—O2*W*	2.099 (1)	C2—C3	1.360 (3)
Mg1—O3	2.027 (1)	C4—C5	1.351 (3)
O3—Mg1—O1*W*	90.97 (7)	O1*W*—Mg1—O2*W*	91.08 (5)
O3—Mg1—O1*W*^{i}	89.03 (7)	O1*W*—Mg1—O2*W*^{i}	88.92 (5)
O3—Mg1—O2*W*^{i}	88.51 (5)	N1—C6—C7	111.3 (1)
O3—Mg1—O2*W*	91.49 (5)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*2···O1^{ii}	0.86 (2)	1.88 (1)	2.735 (2)	175 (3)
O1*W*—H1*W*1···O1^{iii}	0.86 (2)	1.93 (1)	2.779 (2)	175 (3)
O2*W*—H2*W*2···O2^{iv}	0.86 (2)	1.86 (1)	2.717 (2)	177 (2)
O2*W*—H2*W*1···O1^{i}	0.86 (2)	2.09 (2)	2.933 (2)	179 (2)

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

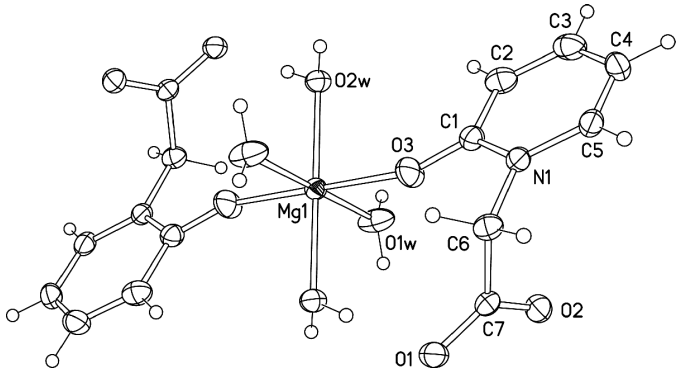


Figure 1
Structure of the title compound, showing 30% probability displacement ellipsoids for the non-H atoms.

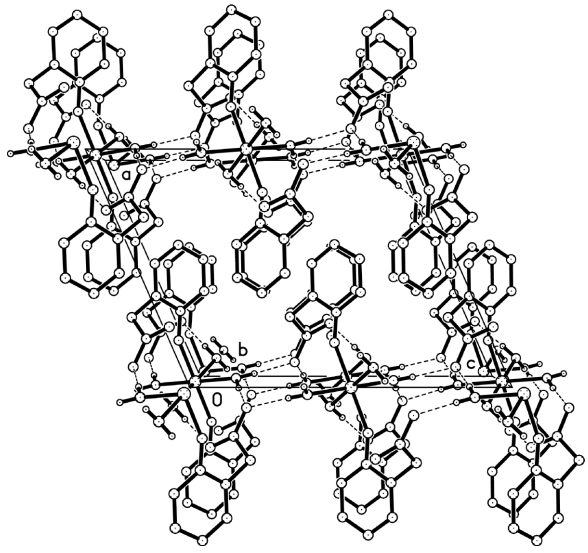


Figure 2
Packing diagram of the complex, viewed along the *b* axis. Hydrogen bonds are shown as dashed lines.

H atoms of the water molecules were located in difference Fourier maps and refined isotropically, with the O—H and H···H distances restrained to 0.85 (1) and 1.39 (1) Å, respectively, and with U_{iso}(H) = 1.5U_{eq}(O). The other H atoms were placed in calculated positions [C—H = 0.93 and 0.97 Å] and were included in the refinement in the riding model approximation, with U_{iso}(H) = 1.2U_{eq}(C).

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

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