Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Hexaaquamagnesium(II) bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.004 Å
R factor = 0.055
wR factor = 0.177
Data-to-parameter ratio = 14.9

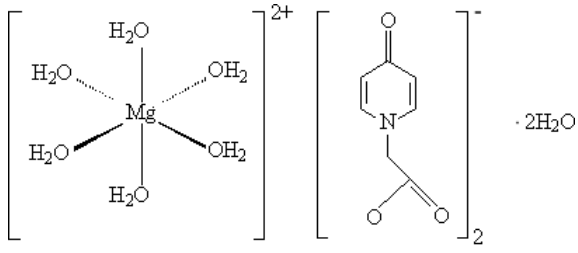
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

In the title compound, $[Mg(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$, the Mg^{II} atom lies on a centre of symmetry and is coordinated by six water molecules in an octahedral geometry. A three-dimensional supramolecular framework is formed *via* O—H···O hydrogen bonds between the anions and cations.

Received 22 November 2004
Accepted 26 November 2004
Online 30 November 2004

Comment

Recently, we have described the complexes $[M(H_2O)_6](4\text{-OPA})_2\cdot 2H_2O$ [4-OPA$^-$ is the (4-oxo-4*H*-pyridin-1-yl)-acetate anion, *M* = Zn, Ni; Gao *et al.*, 2004; Zhang *et al.*, 2004], in which 4-OPA$^-$ exists as an $[O{=}C(CH{=}CH)_2N{-}CH_2{-}CO_2]^-$ counterion having a double-bonded O atom connected to the ring. In order to explore further the coordination behaviour and solid-state structure of metal salts with the 4-HOPA ligand, we used $Mg(NO_3)_2\cdot 6H_2O$ under similar reaction conditions to synthesize the title hexaaquamagnesium(II) complex, (I).



(I)

The title compound is found to be isostructural with the Zn^{II} and Ni^{II} analogues. A similar description applies to the present complex (Fig. 1).

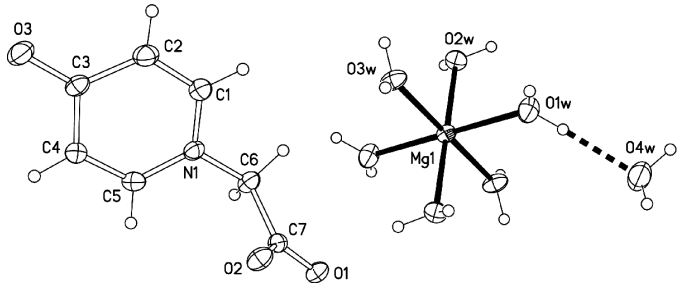


Figure 1
The structural components of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. The hydrogen bond is shown as a dashed line. The symmetry code for the unlabelled aqua ligands is as in Table 1.

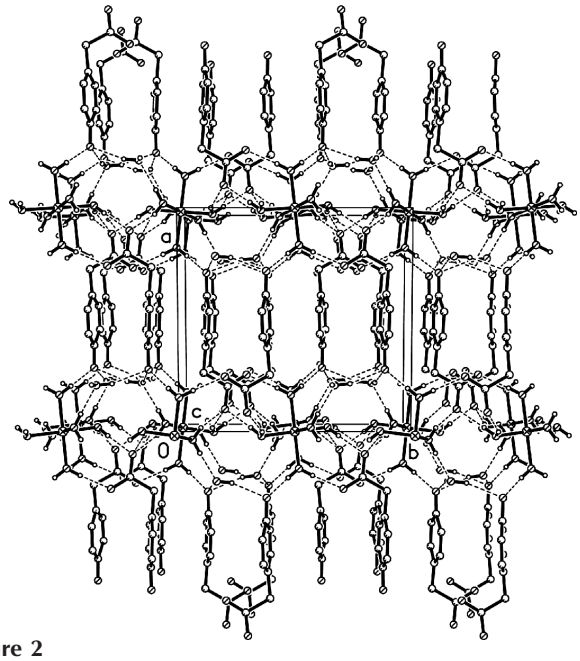


Figure 2
A packing diagram for (I), viewed along the *c* axis. Hydrogen bonds are shown as dashed lines. H atoms bonded to C atoms have been omitted.

Experimental

The title complex was prepared by the addition of $Mg(NO_3)_2{\cdot}6H_2O$ (1.94 g, 10 mmol) to an aqueous solution of (4-oxo-4*H*-pyridin-1-yl)acetic acid (2.92 g, 20 mmol). The pH was adjusted to 7 with 0.2 *M* NaOH solution. Colourless crystals of (I) were obtained from the filtered solution over several days. CHN analysis, calculated for $[Mg(H_2O)_6](C_7H_6NO_3)_2{\cdot}2H_2O$: C 35.57, H 5.97, N 5.93%; found: C 35.77, H 5.84, N 6.06%.

Crystal data

$[Mg(H_2O)_6](C_7H_6NO_3)_2{\cdot}2H_2O$
M_r = 472.69
Monoclinic, $P2_1/c$
a = 12.486 (3) Å
b = 12.904 (3) Å
c = 6.8131 (14) Å
β = 99.21 (3)°
V = 1083.6 (4) Å^3
Z = 2
D_x = 1.449 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9023 reflections
θ = 3.2–27.5°
μ = 0.16 mm^{-1}
T = 296 (2) K
Prism, colourless
0.38 × 0.26 × 0.17 mm

Data collection

Rigaku RAXIS-RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.953, T_{max} = 0.974
9164 measured reflections
2477 independent reflections
2212 reflections with $I > 2\sigma(I)$
R_{int} = 0.022
θ_{max} = 27.5°
$h = -16 \rightarrow 16$
$k = -16 \rightarrow 16$
$l = -8 \rightarrow 8$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.177
S = 1.08
2477 reflections
166 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0802P)^2 + 1.5072P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Mg1—O1*W*	2.0735 (19)	O2—C7	1.245 (3)
Mg1—O2*W*	2.0652 (19)	O3—C3	1.272 (3)
Mg1—O3*W*	2.0490 (18)	C1—C2	1.353 (4)
O1—C7	1.253 (3)	C4—C5	1.356 (4)
O2*W*—Mg1—O1*W*	89.98 (9)	O3*W*—Mg1—O2*W*	89.68 (8)
O2*W*—Mg1—O1*W*^{i}	90.02 (9)	O3*W*—Mg1—O2*W*^{i}	90.32 (8)
O3*W*—Mg1—O1*W*	90.97 (9)	N1—C6—C7	113.9 (2)
O3*W*—Mg1—O1*W*^{i}	89.03 (9)		

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*
O1*W*—H1*W*1···O4*W*	0.85 (3)	1.89 (3)	2.734 (3)	172 (4)
O1*W*—H1*W*2···O1^{ii}	0.85 (3)	2.01 (3)	2.837 (3)	164 (3)
O2*W*—H2*W*2···O1^{iii}	0.85 (3)	1.89 (3)	2.709 (3)	162 (3)
O2*W*—H2*W*1···O1^{i}	0.85 (3)	2.06 (3)	2.847 (3)	153 (3)
O3*W*—H3*W*2···O3^{iv}	0.85 (3)	1.92 (3)	2.754 (3)	170 (4)
O3*W*—H3*W*1···O2^{v}	0.84 (3)	1.88 (3)	2.719 (3)	173 (3)
O4*W*—H4*W*2···O3^{vi}	0.85 (3)	1.98 (3)	2.809 (4)	163 (5)
O4*W*—H4*W*1···O3^{vii}	0.85 (3)	2.17 (2)	2.978 (4)	158 (5)

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

H atoms on C atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å and U_{iso}(H) = 1.2U_{eq} (C), and were included in the refinement in the riding-model approximation. Water H atoms were located in difference Fourier maps and refined with the restraints O—H = 0.85 (1) Å, H···H = 1.39 (1) Å, and with 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: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors thank the National Natural Science Foundation of China (grant No. 20101003), Heilongjiang Province Natural Science Foundation (grant No. B007), the Scientific Fund of Remarkable Teachers of Heilongjiang Province (grant No.1054G036) and Heilongjiang University for supporting this study.

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