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

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.029
wR factor = 0.078
Data-to-parameter ratio = 14.5

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

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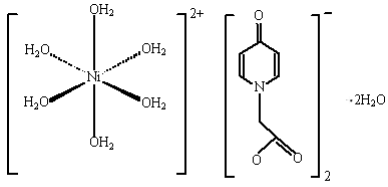
The title complex, $[Ni(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$, was synthesized by the reaction of $Ni(CH_3COO)_2\cdot 4H_2O$ and (4-oxo-4*H*-pyridin-1-yl)acetic acid in an aqueous solution. The nickel^{II} ion, which lies on a center of symmetry, is coordinated by six water molecules to form an octahedron [Ni—O = 2.047 (1)–2.057 (1) Å]. A three-dimensional supramolecular framework is formed *via* hydrogen bonds between the anions and cations.

Comment

A recent study documented the structure of hexaaquazinc(II) bis[(4-oxo-4*H*-pyridin-1-yl)acetate] dihydrate (Gao *et al.*, 2004). The nickel(II) analog, (I), was synthesized under similar reaction conditions in this study. The structure of the Zn complex has been presented in detail; a similar description applies to the present isomorphous complex (Fig. 1).



(I)

The cation lies on a center of symmetry. A three-dimensional supramolecular network is formed by intermolecular hydrogen bonds between water molecules and O atoms of (4-oxo-4*H*-pyridin-1-yl)acetate (Table 1 and Fig. 2).

Experimental

The title complex was prepared by the addition of $Ni(CH_3COO)_2\cdot 4H_2O$ (4.98 g, 20 mmol) to an aqueous solution of (4-oxo-4*H*-pyridin-1-yl)acetic acid (58.40 g, 40 mmol); the pH was adjusted to 7 with 0.2 *M* NaOH solution. Green single crystals were obtained from the filtered solution over several days. CH&N analysis: calculated for

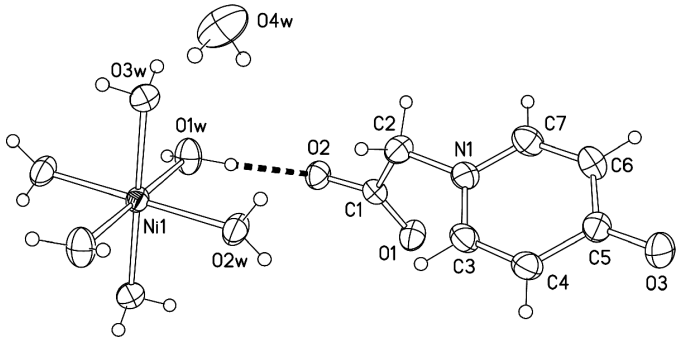


Figure 1
View of the title compound, with 50% probability ellipsoids for the non-H atoms.

$[Ni(H_2O)_6](C_7H_6NO_3)_2.2H_2O$: C 33.16, H 5.57, N 5.52%; found: C 33.02, H 5.68, N 5.35%.

Crystal data

$[Ni(H_2O)_6](C_7H_6NO_3)_2\cdot 2H_2O$	D_x = 1.585 Mg m^{-3}
M_r = 507.07	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 6398 reflections
a = 12.387 (3) Å	θ = 3.6–27.4°
b = 12.816 (3) Å	μ = 0.99 mm^{-1}
c = 6.766 (1) Å	T = 293 (2) K
β = 98.42 (3)°	Prism, green
V = 1062.6 (4) Å^3	0.36 × 0.25 × 0.18 mm
Z = 2	

Data collection

Rigaku R-AXIS RAPID diffractometer	2423 independent reflections
ω scans	2237 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	R_{int} = 0.027
T_{min} = 0.718, T_{max} = 0.842	θ_{max} = 27.5°
10195 measured reflections	$h = -16 \rightarrow 16$
	$k = -16 \rightarrow 16$
	$l = -8 \rightarrow 8$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0539P)^2 + 0.226P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.029	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2)$ = 0.078	$\Delta\rho_{max}$ = 0.35 e Å^{-3}
S = 1.04	$\Delta\rho_{min}$ = −0.77 e Å^{-3}
2423 reflections	Extinction correction: *SHELXL*
167 parameters	Extinction coefficient: 0.37 (1)
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

Ni1—O2*W*	2.047 (1)	O2—C1	1.263 (2)
Ni1—O3*W*	2.050 (1)	O3—C5	1.278 (2)
Ni1—O1*W*	2.057 (1)	C3—C4	1.358 (2)
O1—C1	1.243 (2)	C6—C7	1.362 (2)
O2*W*—Ni1—O3*W*	88.31 (4)	O2*W*—Ni1—O1*W*	92.50 (6)
O2*W*—Ni1—O3*W*^{i}	91.69 (4)	O3*W*—Ni1—O1*W*	88.71 (5)
O2*W*—Ni1—O1*W*^{i}	87.50 (6)	N1—C2—C1	114.0 (1)
O3*W*—Ni1—O1*W*^{i}	91.29 (5)		

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*W*—H1*W*2···O2	0.856 (19)	2.02 (1)	2.839 (2)	162 (2)
O1*W*—H1*W*1···O4*W*^{ii}	0.841 (9)	1.88 (1)	2.722 (2)	174 (2)
O2*W*—H2*W*1···O1^{iii}	0.843 (9)	1.854 (9)	2.694 (2)	174 (2)
O2*W*—H2*W*2···O3^{iv}	0.840 (19)	1.90 (1)	2.739 (2)	170 (2)
O3*W*—H3*W*1···O2^{v}	0.847 (9)	2.08 (1)	2.848 (2)	150 (2)
O3*W*—H3*W*2···O2^{vi}	0.850 (9)	1.86 (1)	2.696 (2)	170 (2)
O4*W*—H4*W*1···O3^{vii}	0.857 (9)	1.98 (1)	2.795 (2)	159 (3)
O4*W*—H4*W*2···O3^{iv}	0.850 (9)	2.16 (1)	2.975 (2)	162 (3)

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

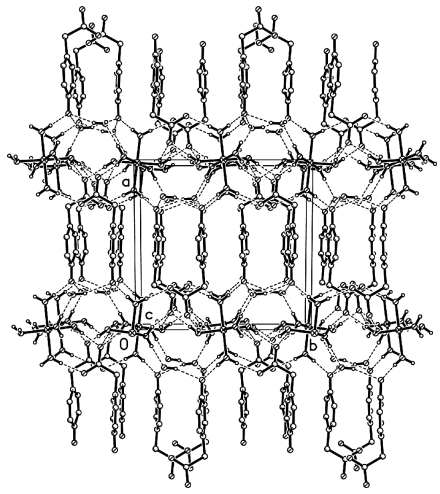


Figure 2
Packing diagram of the complex, viewed along the *c* axis

H atoms bonded to 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. The H atoms of water molecules were located in Fourier difference maps and refined subject to the restraints O—H = 0.85 (1) Å and H···H = 1.39 (1) Å, with U_{iso}(H) = 1.5U_{eq}(O).

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC and Rigaku Corporation, 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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