

A monoclinic polymorph of bis(2-aminoacetato)nickel(II) monohydrate

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Key indicators

Single-crystal X-ray study
 $T = 295$ K
 Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.025
 wR factor = 0.063
 Data-to-parameter ratio = 12.7

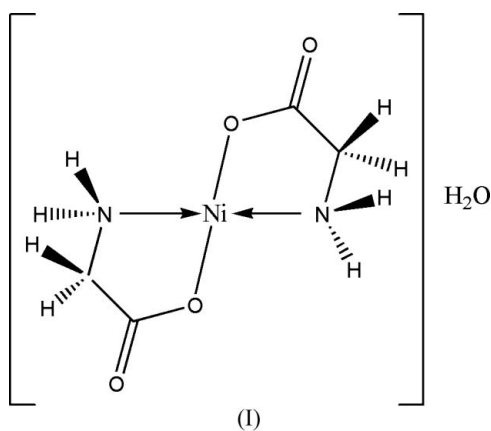
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The Ni atom in the title compound, $[\text{Ni}(\text{C}_2\text{H}_4\text{NO}_2)_2]\cdot\text{H}_2\text{O}$, is chelated by two N atoms and two O atoms of amino acid ligands in a distorted square-planar geometry. The Ni atom lies on a centre of symmetry and the water O atom lies on a twofold rotation axis. In the crystal structure, adjacent molecules are linked by $\text{Ni}\cdots\text{O}$ interactions to form a sheet. O atoms of water molecules and N atoms of the 2-aminoacetates contribute to hydrogen bonds, leading to the formation of a three-dimensional network.

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Comment

Transition metal compounds containing amino acid ligands have been of great interest for many years because of their biological significance. These compounds play an important role in biocatalysis and enzyme reactions and occur in the active sites of several important classes of metalloproteins. As an extension of work on the structural characterization of amino acid complexes (Sun & You, 2004; Ding *et al.*, 2006), the title mononuclear nickel(II) compound, (I), is reported here.



The crystal structure of (I), was first reported in the orthorhombic space group $P2_12_12_1$ (Ding *et al.*, 2006). Here, we report the structure of a second polymorph of (I) in the monoclinic space group $C2/c$.

The four coordinating atoms around the central metal Ni^{II} atom are coplanar. Selected bond distances and angles are given in Table 1. The Ni atom lies on a special position of site symmetry $\bar{1}$. The two *trans* angles at the Ni^{II} centre are 180° and the other angles are close to 90° (Table 1), thus indicating a slightly distorted square-planar geometry. The Ni—O and Ni—N bond lengths are comparable with the corresponding values observed in other similar nickel complexes (Sun & You, 2004; Ding *et al.*, 2006). This is due to the strain created by the

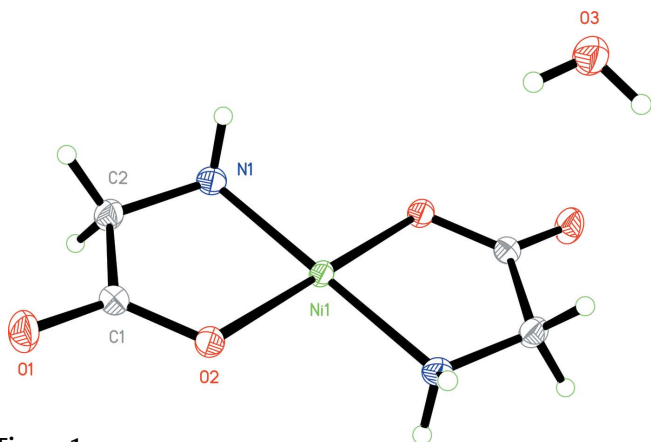


Figure 1
The structure of the title compound, (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Symmetry code for the unlabelled ligand is as in Table 1.

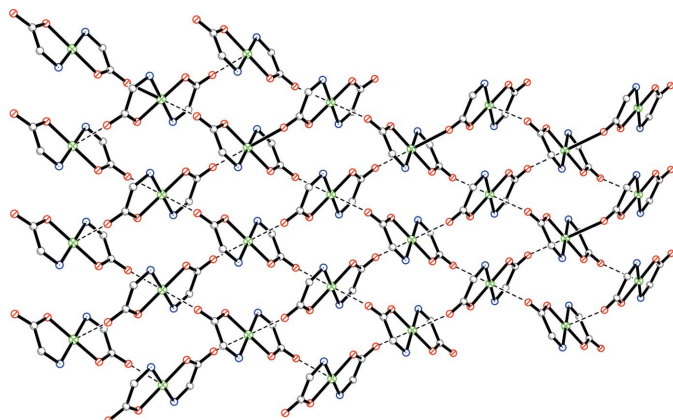


Figure 2
The sheets of adjacent molecules of (I), linked by Ni...O interactions (dashed lines).

five-membered chelate ring. Water atom O3 lies on a twofold rotation axis.

In the crystal structure of (I), adjacent molecules are linked by Ni...O interactions [2.68 (2) Å] between coordinated Ni atoms and O1 atoms of carboxylate groups, to form a two-dimensional sheet structure parallel to the *bc* plane, as shown in Fig. 2. The network is further connected by intermolecular hydrogen bonds, one of the O—H...O type and two of the N—H...O type, leading to the formation of a three-dimensional network (Table 2 and Fig. 3).

Experimental

2-Aminoacetic acid and nickel(II) acetate were commercially available and were used without further purification. A mixture of 2-aminoacetic acid (about 0.2 mmol, 15 mg) and Ni(CH₃COO)₂·2H₂O (0.1 mmol, 21.3 mg) was dissolved in an aqueous solution (50%) of methanol (3 ml). The solution was then heated in a 10 ml stainless-steel Teflon-lined reactor at 413 K for 36 h, followed by cooling to room temperature at 3 K h⁻¹. Green plate-shaped crystals of (I) were collected by filtration, washed with methanol and dried at ambient temperature (yield 56%). Analysis, calculated for [Ni(C₂H₄NO₂)₂](H₂O): C 21.37, H 4.48, N 12.46%; found: C 21.33, H 4.42, N 12.39%.

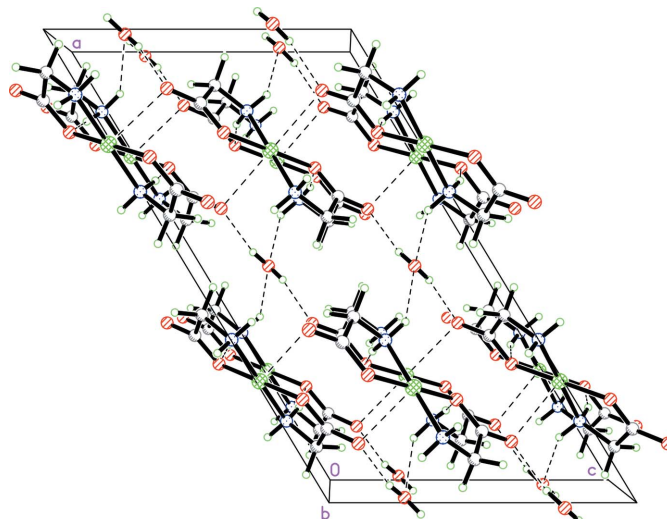


Figure 3
The crystal packing of (I), viewed along the *b* axis. H atoms have been omitted for clarity. Dashed lines indicate hydrogen bonds and Ni...O interactions.

Crystal data

[Ni(C₂H₄NO₂)₂]·H₂O
M_r = 224.85
Monoclinic, *C2/c*
a = 17.328 (2) Å
b = 5.2372 (7) Å
c = 9.6386 (12) Å
β = 121.090 (2)°
V = 749.04 (17) Å³

Z = 4
D_x = 1.994 Mg m⁻³
Mo *Kα* radiation
μ = 2.58 mm⁻¹
T = 295 (2) K
Plate, green
0.15 × 0.09 × 0.01 mm

Data collection

Bruker APEX CCD area-detector diffractometer
φ and *ω* scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.754, *T_{max}* = 0.975

2856 measured reflections
776 independent reflections
703 reflections with *I* > 2σ(*I*)
R_{int} = 0.026
θ_{max} = 26.5°

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.025
wR(*F*²) = 0.063
S = 1.09
776 reflections
61 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0288P)^2 + 0.6273P]$
where $P = (F_o^2 + 2F_c^2)/3$
(Δσ)_{max} < 0.001
Δρ_{max} = 0.33 e Å⁻³
Δρ_{min} = -0.31 e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—O2	1.963 (1)	Ni1—N1	1.976 (2)
O2—Ni1—N1	84.7 (1)	N1 ¹ —Ni1—N1	180
O2—Ni1—N1 ¹	95.3 (1)	O2 ¹ —Ni1—O2	180
O2—Ni1—N1—C2	-9.1 (2)	Ni1—N1—C2—C1	13.4 (2)
N1—Ni1—O2—C1	2.6 (2)	O1—C1—C2—N1	168.7 (2)
Ni1—O2—C1—O1	-176.4 (2)	O2—C1—C2—N1	-12.4 (3)
Ni1—O2—C1—C2	4.8 (3)		

Symmetry code: (i) $-x + \frac{1}{2}, -y + \frac{1}{2}, -z + 1$.

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$O3-H3\cdots O1^{ii}$	0.831 (10)	1.953 (13)	2.767 (2)	166 (4)
$N1-H1B\cdots O3^{iii}$	0.90	2.28	3.045 (2)	143
$N1-H1A\cdots O2^{iv}$	0.90	2.18	3.019 (2)	156

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

Atom H3 was located in a difference Fourier map and refined, with its $U_{iso}(H)$ value fixed at 0.08 \AA^2 . All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C–H and N–H distances of 0.97 Å and 0.90 Å, respectively, and with $U_{iso}(H) = 1.2U_{eq}(C,N)$.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT-Plus* (Bruker, 2002); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics:

SHELXTL (Bruker, 2002); software used to prepare material for publication: *SHELXTL*.

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