metal-organic papers

Bis(2-aminoacetato-κ^2N,O)aquanickel(II)

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The title compound, [Ni($C_2H_5NO_2$)$_2$(H_2O)], is a mononuclear nickel(II) complex. The Ni^{II} atom is five-coordinated by two N atoms and two O atoms from two glycinate ligands in basal plane positions, and by one O atom from a coordinated water molecule in the apical position, forming a slightly distorted square-pyramidal geometry. In the crystal structure, molecules are linked through intermolecular N—H···O and O—H···O hydrogen bonds, forming a three-dimensional network.

Comment

Transition metal compounds containing amino acid ligands are of great interest due to their biological activity and are present in the active sites of several important classes of metalloproteins. As an extension of the work on the structural characterization of amino acid complexes (Sun & You, 2004), a mononuclear nickel(II) compound, (I), is reported here.

(I)
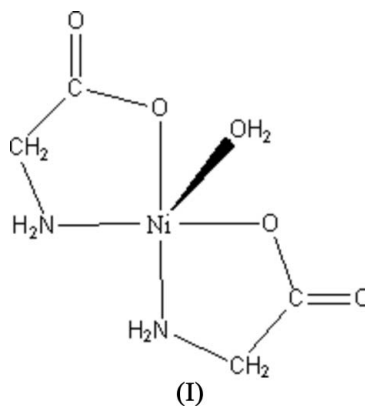
The molecular structure of (I), with the atomic labeling scheme, is illustrated in Fig. 1, and selected bond distances, bond angles and torsion angles are given in Table 1. In (I), the Ni atom is in a square-pyramidal geometry, coordinated by two N atoms and two O atoms from two 2-aminoacetate acid ligands in the basal position, and by one O atom from a coordinated water molecule in the apical position. The slightly distorted square-pyramidal geometry is revealed by the bond angles between the apical and basal donor atoms (Table 1). In the basal positions, the four coordinating atoms around Ni are approximately coplanar, giving a square-planar coordination with an average deviation of 0.032 (4) Å; the Ni atom lies 0.052 (2) Å above this plane; the two *trans* angles O1—Ni1—N2 and O3—Ni–N1 deviate from the ideal angle of 180° by 5.2 (2) and 2.3 (2)°, respectively; the other angles around the central Ni atom deviate from the ideal angle of 90°, ranging from 84.6 (2) to 95.7 (2)°; this indicates a slightly distorted
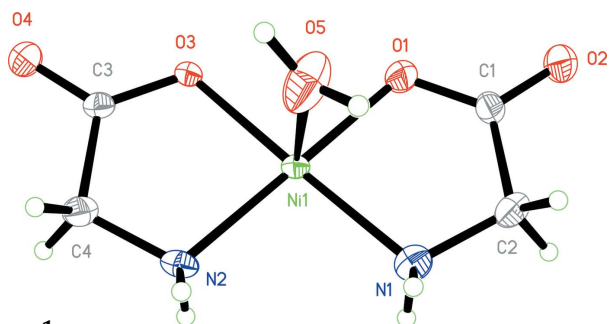
Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

square-pyramidal coordination of the Ni atom. The same character is also revealed by the torsion angles in the structure (Table 1).

In the crystal structure, the molecules are linked *via* three intermolecular N—H···O hydrogen bonds and two O—H···O hydrogen bonds, forming a three-dimensional network (details are given in Table 2 and Fig. 2).

Experimental

All chemicals were obtained from a commercial source and used without further purification. 2-Aminoacetic acid (0.2 mmol, 15.0 mg) and Ni(CH$_3$COO)$_2$·2H$_2$O (0.1 mmol, 21.3 mg) were dissolved in 20% EtOH aqueous solution (15 ml). The mixture was stirred for 30 min at room temperature to give a clear green solution. After allowing the solution to stand in air for 15 d, covered by a piece of filter paper, blue needle-shaped crystals of (I) formed at the bottom of the vessel on slow evaporation of the solvent.

Crystal data

[Ni(C$_2$H$_5$NO$_2$)$_2$(H$_2$O)]	Mo $K\alpha$ radiation
$M_r = 224.85$	Cell parameters from 652
Orthorhombic, $P2_12_12_1$	reflections
$a = 5.2174 (15)$ Å	$\theta = 2.4–16.6°$
$b = 10.823 (3)$ Å	$\mu = 2.53$ mm^{-1}
$c = 13.517 (4)$ Å	$T = 290 (2)$ K
$V = 763.3 (4)$ Å^3	Needle, blue
$Z = 4$	$0.13 \times 0.01 \times 0.01$ mm
$D_x = 1.957$ Mg m^{-3}	

Data collection

Bruker APEX area-detector	1585 independent reflections
diffractometer	1245 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.105$
Absorption correction: multi-scan	$\theta_{max} = 26.5°$
(*SADABS*; Sheldrick, 1996)	$h = -6 \rightarrow 6$
$T_{min} = 0.935$, $T_{max} = 0.975$	$k = -13 \rightarrow 13$
8284 measured reflections	$l = -16 \rightarrow 16$

Refinement

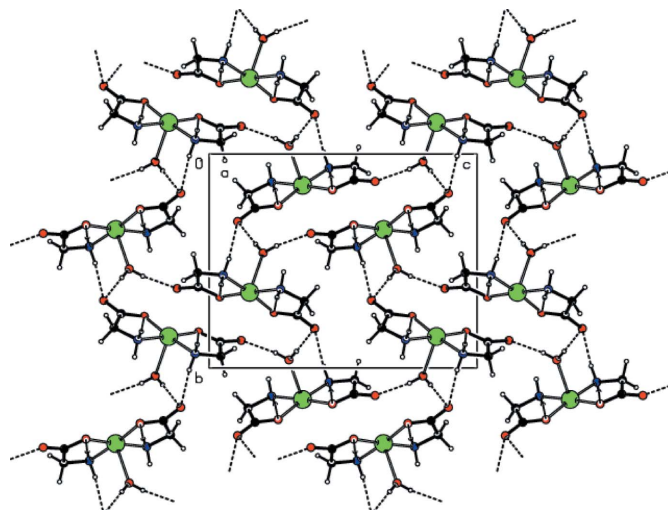|	
Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0242P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.051$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.079$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.01$	$\Delta\rho_{max} = 0.51$ e Å^{-3}
1585 reflections	$\Delta\rho_{min} = -0.39$ e Å^{-3}
115 parameters	Absolute structure: Flack (1983),
H atoms treated by a mixture of	634 Freidel pairs
independent and constrained	Flack parameter: 0.01 (4)
refinement	

Figure 2
The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	1.996 (4)	Ni1—O3	1.960 (3)
Ni1—N2	1.982 (4)	Ni1—O5	2.385 (4)
Ni1—O1	1.955 (4)		
O1—Ni1—N1	84.6 (2)	N2—Ni1—O5	95.7 (2)
O3—Ni1—N2	84.6 (2)	O1—Ni1—O5	89.2 (2)
O1—Ni1—O3	93.4 (2)	O3—Ni1—O5	91.3 (2)
N2—Ni1—N1	97.3 (2)	O1—Ni1—N2	174.8 (2)
N1—Ni1—O5	89.7 (2)	O3—Ni1—N1	177.7 (2)
O3—Ni1—O1—C1	−178.9 (4)	N2—Ni1—N1—C2	179.5 (4)
N1—Ni1—O1—C1	0.0 (4)	O5—Ni1—N1—C2	−84.8 (4)
O5—Ni1—O1—C1	89.8 (4)	O3—Ni1—N2—C4	−4.9 (4)
O1—Ni1—O3—C3	177.6 (4)	N1—Ni1—N2—C4	176.3 (4)
N2—Ni1—O3—C3	2.5 (4)	O5—Ni1—N2—C4	85.9 (4)
O5—Ni1—O3—C3	−93.1 (4)	O1—C1—C2—N1	8.0 (7)
O1—Ni1—N1—C2	4.4 (4)	O3—C3—C4—N2	−4.7 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1B···O1^i	0.90	2.22	3.110 (6)	169
N2—H2A···O3^i	0.90	2.15	3.024 (6)	164
N2—H2B···O2^{ii}	0.90	2.09	2.980 (6)	171
O5—H5A···O4^{iii}	0.821 (10)	1.952 (12)	2.769 (6)	173 (5)
O5—H5B···O2^{iv}	0.823 (10)	1.986 (13)	2.808 (6)	177 (6)

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

The H atoms of the water ligand were located in a difference Fourier map and refined isotropically, with U_{iso}(H) values fixed at 0.08 Å^2, and with O—H and H···H distances restrained to 0.84 (1) and 1.37 (2) Å, respectively. The other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H = 0.97 Å and N—H = 0.90 Å, and with U_{iso}(H) = 1.2U_{eq}(C,N).

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