

catena-Poly[[*(2-amino-3-hydroxypropionato)*-nickel(II)]- μ -*2-amino-3-hydroxypropionato*]Yu-Xi Sun^{a*} and Zhong-Lu You^b^aDepartment of Chemistry, Qufu Normal University, Qufu 273165, People's Republic of China, and ^bDepartment of Chemistry, Lanzhou University, Lanzhou 730000, People's Republic of China

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Key indicators

Single-crystal X-ray study

T = 293 K

Mean $\sigma(\text{C}-\text{C}) = 0.006 \text{ \AA}$

R factor = 0.037

wR factor = 0.067

Data-to-parameter ratio = 13.2

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

In the crystal structure of the title compound, $[\text{Ni}(\text{C}_3\text{H}_6\text{NO}_3)_2]_n$, the Ni^{II} atom has a distorted square-pyramidal coordination geometry. In the basal plane, the Ni atom is coordinated by two N atoms and two O atoms of the amino acid ligands. The apical position is occupied by a propionate O atom of one of the the amino acid ligands, forming chains extending in the **b** direction.

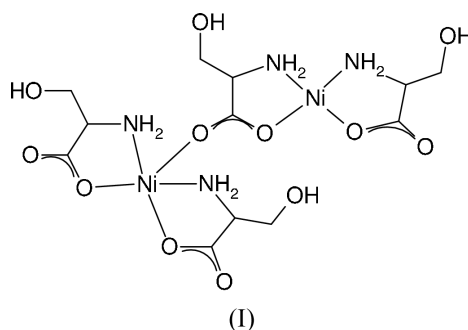
Received 19 July 2004

Accepted 27 July 2004

Online 31 July 2004

Comment

Transition metal compounds containing Schiff base ligands have been of great interest for many years. These compounds play an important role in the development of coordination chemistry related to catalysis and enzymatic reactions, magnetism and molecular architectures. Since nickel compounds have important applications in the design and construction of new magnetic materials, the study of nickel compounds is of great interest in various aspects of chemistry (Zolezzi *et al.*, 2002; Ray *et al.*, 2003; Koner *et al.*, 2003). As an extension of the work on the structural characterization of Schiff base complexes, the crystal structure of a mononuclear nickel(II) compound, (I), is reported here.



Compound (I) is an electronically neutral nickel(II) compound, as shown in Fig. 1. Selected bond distances and angles are given in Table 1. The Ni atom has a square-pyramidal coordination polyhedron, coordinated by two N atoms and three O atoms from two amino acid ligands. The significant distortion of the square pyramid is revealed by the bond angles between the apical and basal donor atoms (Table 1). The bond angles between the donor atoms in the basal positions show less distortion. The apical bond of the square pyramid is much longer than the basal bonds (Table 1).

The bond angles N1–Ni1–O2 and N2–Ni1–O4 deviate from 90° by 5.95 (13) and 7.48 (13)°, respectively. This is due to the strain created by the five-membered chelate rings, *viz.* Ni1/N1/C2/C1/O2 and Ni1/N2/C5/C4/O4. The dihedral angle between the two rings, defined by atoms Ni1/N1/O2 and

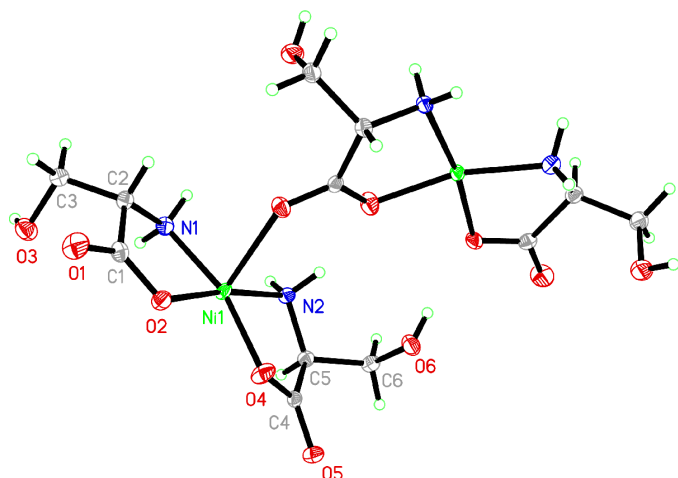


Figure 1
Twice the asymmetric unit of the title compound, (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

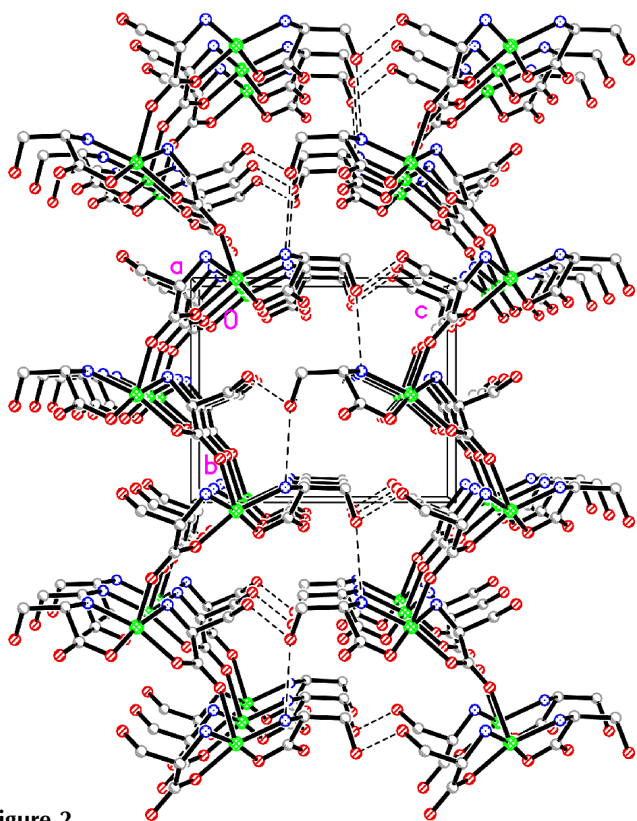


Figure 2
The crystal packing of (I), viewed along the *b* axis. Hydrogen bonds are shown as dashed lines. H atoms have been omitted for clarity.

Ni1/N2/O4, is $166.2(2)^\circ$. Atom Ni1 deviates by $0.510(2) \text{ \AA}$ from the plane defined by atoms N1/C2/C1/O2 and by $0.541(2) \text{ \AA}$ from the plane defined by atoms N2/C5/C4/O4. The torsion angles Ni1–N1–C2–C3 and Ni1–N2–C5–C6 are $-150.9(3)$ and $-145.1(3)^\circ$, respectively.

In the crystal structure, the Ni atoms are connected *via* the carboxylate O anions, forming chains parallel to the *b* axis. The chains are further connected by intermolecular N–H \cdots O and O–H \cdots O hydrogen bonds, forming sheets parallel to the *bc* plane (details are given in Table 2 and Fig. 2).

Experimental

2-Amino-3-hydroxypropionic acid and nickel acetate were available commercially and were used without further purification. 2-Amino-3-hydroxypropionic acid (0.1 mmol, 10.5 mg) and $\text{Ni}(\text{CH}_3\text{COO})_2 \cdot 2\text{H}_2\text{O}$ (0.1 mmol, 21.3 mg) were dissolved in methanol (10 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 12 d, green block-shaped crystals of (I) had formed at the bottom of the vessel on slow evaporation of the solvent (yield 72.3%). Analysis found: C 26.8, H 4.6, N 10.4%; calculated for $\text{C}_{12}\text{H}_{24}\text{NiN}_4\text{O}_{12}$: C 27.0, H 4.5, N 10.5%.

Crystal data

$[\text{Ni}(\text{C}_3\text{H}_6\text{NO}_3)_2]$
 $M_r = 266.89$
 Monoclinic, $P2_1$
 $a = 5.638(2) \text{ \AA}$
 $b = 8.394(2) \text{ \AA}$
 $c = 9.897(2) \text{ \AA}$
 $\beta = 90.61(3)^\circ$
 $V = 468.4(2) \text{ \AA}^3$
 $Z = 2$

$D_x = 1.893 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 Cell parameters from 1038 reflections
 $\theta = 3.2\text{--}26.6^\circ$
 $\mu = 2.08 \text{ mm}^{-1}$
 $T = 293(2) \text{ K}$
 Block, green
 $0.32 \times 0.23 \times 0.18 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.535$, $T_{\max} = 0.684$
 2754 measured reflections

1822 independent reflections
 1677 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 26.5^\circ$
 $h = -7 \rightarrow 6$
 $k = -10 \rightarrow 10$
 $l = -12 \rightarrow 6$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.037$
 $wR(F^2) = 0.067$
 $S = 0.96$
 1822 reflections
 138 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2)]$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.41 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.34 \text{ e \AA}^{-3}$
 Absolute structure: Flack (1983);
 781 Friedel pairs
 Flack parameter = 0.01 (2)

Table 1

Selected geometric parameters (\AA , $^\circ$).

Ni1–O2	1.936 (3)	Ni1–N2	1.988 (3)
Ni1–O4	1.965 (3)	Ni1–O5 ⁱ	2.368 (3)
Ni1–N1	1.979 (3)		
O2–Ni1–O4	88.56 (13)	N1–Ni1–N2	104.47 (14)
O2–Ni1–N1	84.05 (13)	O2–Ni1–O5 ⁱ	90.65 (11)
O4–Ni1–N1	164.35 (15)	O4–Ni1–O5 ⁱ	106.71 (12)
O2–Ni1–N2	171.06 (14)	N1–Ni1–O5 ⁱ	87.21 (13)
O4–Ni1–N2	82.52 (13)	N2–Ni1–O5 ⁱ	92.42 (12)

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

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

<i>D</i> –H \cdots <i>A</i>	<i>D</i> –H	H \cdots <i>A</i>	<i>D</i> \cdots <i>A</i>	<i>D</i> –H \cdots <i>A</i>
N2–H2B \cdots O4 ⁱ	0.90	2.14	2.973 (4)	153
N2–H2A \cdots O5 ⁱⁱ	0.90	2.30	3.005 (4)	135
N1–H1B \cdots O1 ⁱⁱⁱ	0.90	2.16	2.970 (4)	149
N1–H1A \cdots O3 ^{iv}	0.90	2.11	2.935 (5)	153
O6–H6 \cdots O2 ^v	0.82	1.90	2.691 (4)	163
O3–H3 \cdots O6 ^v	0.82	1.93	2.730 (4)	166

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

The H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H, O—H and N—H distances of 0.97–0.98, 0.82 and 0.90 Å, respectively, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C/N})$ and $1.5U_{\text{eq}}(\text{O})$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINTE* (Siemens, 1996); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics: *SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

The authors thank Qufu Normal University for the research grant.

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