Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

The two-dimensional network polymer of (ethanol)(μ_3-*N*-salicyclideneglycinato)nickel(II)

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Received 28 June 2005
Accepted 28 June 2005
Online 6 July 2005

In the title complex, $[\mathrm{Ni}(\mathrm{C_9H_7NO_3})(\mathrm{C_2H_6O})]_n$, each Ni atom is octahedrally coordinated by four O atoms and one N atom from three fully deprotonated N-salicylideneglycinate (salgly) anions and by one O atom from an ethanol molecule. Two inversion-related Ni^{2+} ions are bridged by two O atoms from the phenolate groups of two salgly anions, forming a centrosymmetric dimeric unit which is further linked by carboxylate O atoms to give a two-dimensional network coordination polymer in the *bc* plane.

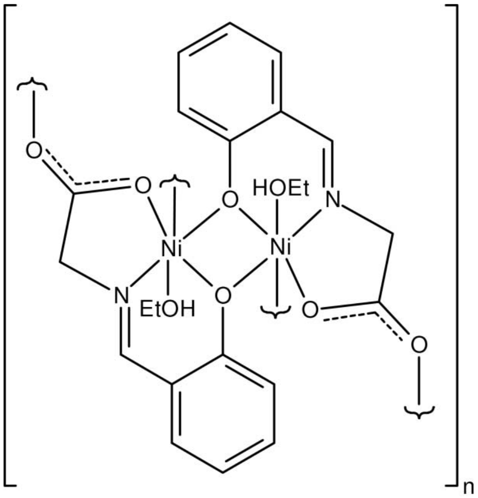
Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.005 Å
R factor = 0.034
wR factor = 0.090
Data-to-parameter ratio = 13.1

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

Comment

Recently, considerable efforts have been devoted to crystal engineering of supramolecular architectures assembled by means of coordination covalent bonding, hydrogen bonding or other weak intermolecular interactions (Moulton & Zaworotko, 2001), because of interesting topological structures and many potential applications in the design of cavity or porous materials (Liang *et al.*, 2001). Metal complexes of Schiff bases synthesized by the condensation of salicylaldehyde with glycine and other α-amino acids (Erxleben & Schumacher, 2001; He *et al.*, 1990; Liu & Gao, 1998; Zhang *et al.*, 2000) have received attention owing to their catalytic properties (Reddy *et al.*, 2000; Wang *et al.*, 2002) and antibacterial activities (Liu *et al.*, 1995). Warda (1997) reported a one-dimensional chain coordination polymer, $[\mathrm{Cu}(\mathrm{C_9H_7NO_3})(\mathrm{C_5H_8N_2})_2]_n$ with the Schiff base ligand derived from salicylaldehyde and glycine. Here a two-dimensional $\mathrm{Ni^{II}}$ polymer, (I), constructed through bridging coordination covalent bonding, is reported (Fig. 1).



(I)

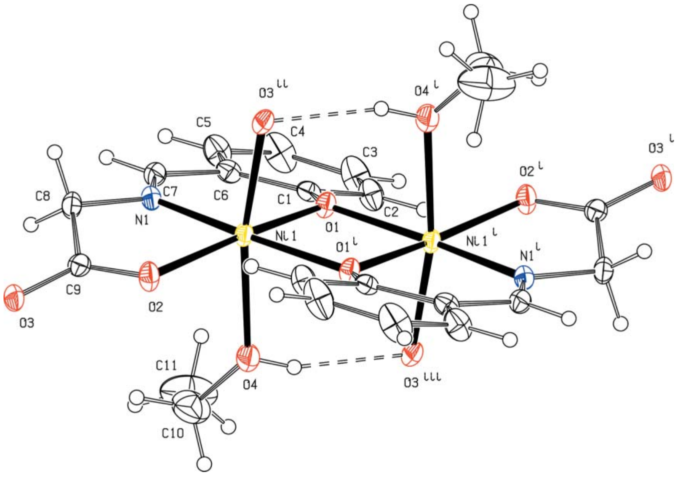


Figure 1
The dimeric unit of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme. Hydrogen bonds are shown dashed. [Symmetry codes: (i) $1 - x, 1 - y, 1 - z$; (ii) $1 - x, \frac{1}{2} - y, \frac{1}{2} + z$; (iii) $x, \frac{1}{2} - y, \frac{1}{2} + z$.]

Each Ni^{II} centre adopts a distorted octahedral configuration defined by one ethanol O atom, and four O atoms and one N atom from three fully deprotonated *N*-salicylideneglycinate (salgly) anions. In the polymer, each Ni^{2+} centre is linked to another inversion-related Ni^{2+} centre by two O atoms of phenolate groups to give a centrosymmetric dimeric unit and a planar four-membered ring [plane 1; $Ni1/O1/Ni1^i/O1^i$; symmetry operation: (i) $1 - x, 1 - y, 1 - z$], and these dimeric units are linked *via* O atoms of the carboxylate groups to form a two-dimensional network in the *bc* plane (Fig. 2).

Chelation of Ni by the salgly anions forms a six-membered ring (plane 2; Ni1/O1/C1/C6/C7/N1) and a five-membered ring (plane 3; Ni1/N1/C8/C9/O2), which contribute to the stability of the complex. The dihedral angle between planes 1 and 2 is 6.44 (10)° and that between planes 1 and 3 is 9.27 (11)°, indicating that these groups are all close to coplanar.

There are considerable distortions of the octahedral coordination of Ni. The *cis* angles are in the range 81.05 (9)–105.82 (8)°, while the *trans* angles are as low as 167.79 (9)° (Table 1). The Ni—O bond lengths are in the range 2.017 (2)–2.153 (3) Å and the Ni—N bond length is 1.982 (3) Å. The two-dimensional network coordination polymer is further stabilized by hydrogen bonding between the ethanol hydroxy group and atom O3 of an adjacent carboxylate group (Table 2).

Experimental

The Schiff base ligand salgly was prepared according to the method described by Liu & Gao (1998). Single crystals of the title complex suitable for X-ray crystallographic analysis were obtained by solvothermal reaction of $Ni(NO_3)_2 \cdot 4H_2O$ (0.4 mmol), salgly (0.4 mmol), ethanol (3 ml), dimethylformamide (0.8 ml) and triethylamine (0.2 ml). The reagents were placed in a thick Pyrex tube (*ca* 20 cm long). The tube was cooled with liquid N_2 and the air was evacuated. The sealed tube was heated at 353 K for 4 d to yield green block-shaped crystals in about 57% yield.

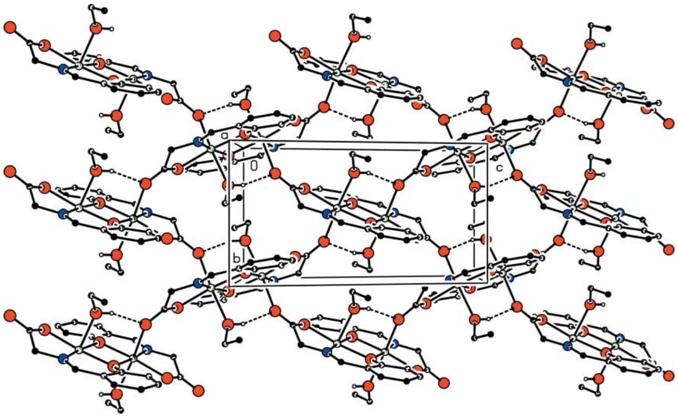


Figure 2
A view of the two-dimensional network structure of (I). Dashed lines represent hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted.

Crystal data

$[Ni(C_9H_7NO_3)(C_2H_6O)]$
$M_r = 281.93$
Monoclinic, $P2_1/c$
$a = 11.656$ (3) Å
$b = 7.326$ (2) Å
$c = 14.012$ (2) Å
$\beta = 109.09$ (1)°
$V = 1130.7$ (4) Å^3
$Z = 4$

$D_x = 1.656$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 29 reflections
$\theta = 3.1$–13.7°
$\mu = 1.72$ mm^{-1}
$T = 296$ (2) K
Block, green
0.40 × 0.32 × 0.18 mm

Data collection

Siemens *P*4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.538$, $T_{max} = 0.734$
2476 measured reflections
2102 independent reflections
1659 reflections with $I > 2\sigma(I)$

$R_{int} = 0.019$
$\theta_{max} = 25.5°$
$h = 0 \rightarrow 14$
$k = 0 \rightarrow 8$
$l = -16 \rightarrow 16$
3 standard reflections every 97 reflections intensity decay: 2.2%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.090$
$S = 1.00$
2102 reflections
160 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0531P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.90$ e Å^{-3}
$\Delta\rho_{min} = -0.42$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0068 (10)

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	1.982 (3)	Ni1—O2	2.057 (2)
Ni1—O1	2.017 (2)	Ni1—O3^{ii}	2.099 (2)
Ni1—O1^{i}	2.057 (2)	Ni1—O4	2.153 (3)
N1—Ni1—O1	91.62 (9)	O1^{i}—Ni1—O3^{ii}	85.13 (8)
N1—Ni1—O1^{i}	172.55 (9)	O2—Ni1—O3^{ii}	98.30 (9)
O1—Ni1—O1^{i}	81.05 (9)	N1—Ni1—O4	95.75 (10)
N1—Ni1—O2	81.23 (9)	O1—Ni1—O4	87.10 (9)
O1—Ni1—O2	168.87 (9)	O1^{i}—Ni1—O4	82.66 (9)
O1^{i}—Ni1—O2	105.82 (8)	O2—Ni1—O4	85.16 (10)
N1—Ni1—O3^{ii}	96.35 (10)	O3^{ii}—Ni1—O4	167.79 (9)
O1—Ni1—O3^{ii}	90.92 (9)		

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

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

D—H···A	D—H	H···A	D···A	D—H···A
O4—H4···O3^{iii}	0.82 (1)	1.98 (2)	2.762 (3)	161 (4)

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

H atoms on C atoms were positioned geometrically and were allowed to ride on their parent atoms, with C—H =0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C). The ethanol hydroxy H atom was located in a difference map and refined, subject to an O—H restraint of 0.815 (10) Å. High displacement parameters suggest some disorder in the ethanol ligand, but this could not be resolved.

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Sheldrick, 1997*b*); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the Youth Science Foundation of Guangxi, the Natural Science Foundation of Guangxi Autonomous Region of the People's Republic of China and the Project of One Hundred Plan of Guangxi Universities for support.

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