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[*N*,*N*′-Bis(3-methylsalicylidene)propane-1,3-diaminato]nickel(II) methanol solvate

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The title compound, $[Ni(C_{19}H_{20}N_2O_2)]\cdot CH_3OH$, is mononuclear. The Ni^{II} ion is four-coordinated in a square-planar configuration by two N atoms and two O atoms of the Schiff base ligand. The Ni^{II} complex and solvent molecule possess crystallographic mirror symmetry. The solvent molecules are linked to the nickel(II) complexes through intermolecular O—H···O hydrogen bonds.

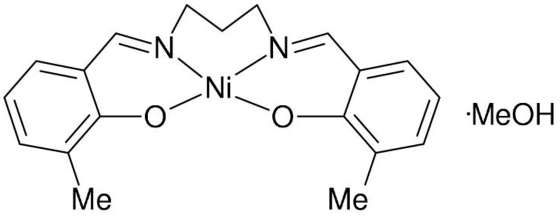
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.006 Å
R factor = 0.055
wR factor = 0.162
Data-to-parameter ratio = 17.5

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

Comment

N,*N*′-Bis(salicylidene)-1,3-diaminopropane (BSDP) is a versatile tetradentate ligand, which forms stable complexes with a large number of transition metal ions (You & Zhu, 2004; You *et al.*, 2004*a*). However, complexes related to the BSDP derivative *N*,*N*′-bis(3-methylsalicylidene)-1,3-diaminopropane have seldom been reported. The prime interest in these complexes is their ability to afford functional solid materials with potentially controllable properties and novel molecular structures (Koner *et al.*, 2003; Palopoli *et al.*, 2000). We have focused our attention on the assembly of transition metal ions with flexible ligands, since they can adopt diverse coordination modes according to the geometric needs of the metal ions (You *et al.*, 2005; You, Xiong & Zhu, 2004). We report here a new nickel(II) complex, the title compound, (I).


(I)

Complex (I) is a mononuclear nickel(II) compound (Fig. 1). The complex contains an [*N*,*N*′-bis(3-methylsalicylidene)-1,3-propanediaminato]nickel(II) complex and an MeOH molecule. The Ni^{II} ion is four-coordinated in a square-planar configuration by two N atoms and two O atoms of the Schiff base ligand. The molecules possess mirror symmetry, with atoms Ni1, C9, H9*A*, H9*B*, C11, H11*A*, O2 and H2 lying on the crystallographic mirror plane. The value of the *trans* angles in the NiO_2N_2 square plane is 171.75 (12)°, indicating a slightly distorted square-planar geometry. The Ni atom is 0.013 (3) Å out of the plane defined by the four donor atoms in the complex. The Ni—O and Ni—N bond lengths (Table 1) are comparable to the corresponding values observed in other Schiff base nickel(II) complexes (Ma *et al.*, 2005; You *et al.*, 2004*b*).

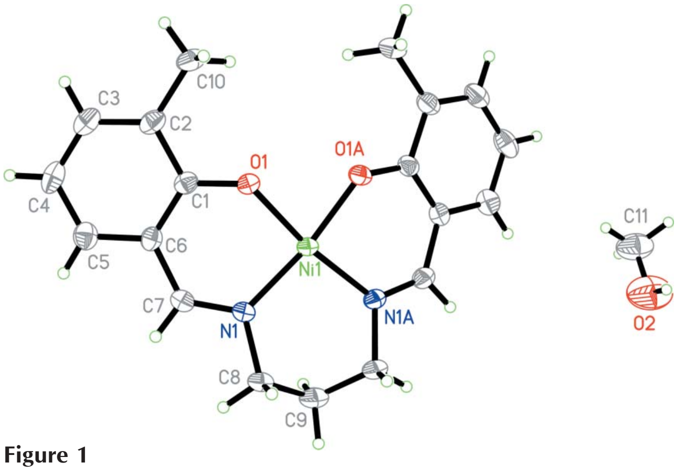


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. The suffix A corresponds to symmetry code (i) in Table 1.

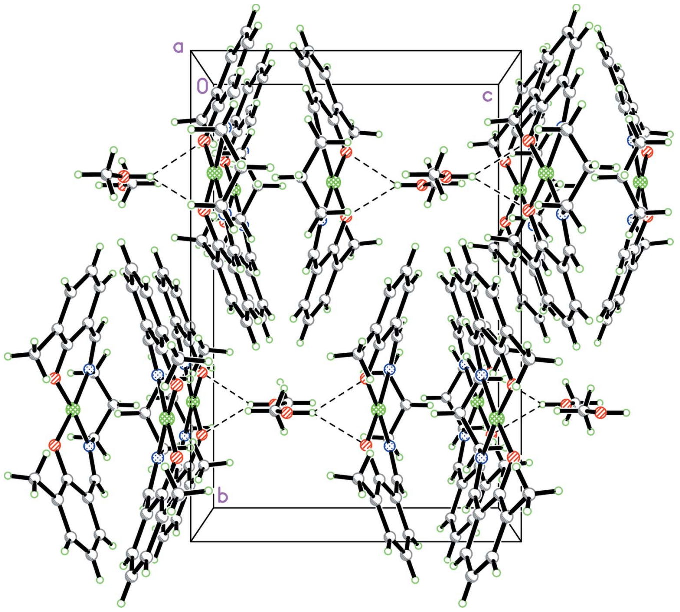


Figure 2
The crystal packing of (I), viewed along the *a* axis. Dashed lines represent the intermolecular hydrogen bonds.

There is an overall butterfly shape to the nickel(II) complex molecule of (I), as evidenced by the dihedral angle [43.3 (2)°] between the two aromatic rings. The dihedral angle between the NiO_2N_2 square plane and the benzene ring is 21.9 (2)°.

The six-membered chelate ring containing the metal, azomethine N atoms and three C atoms of the connecting 1,3-diaminopropane group adopts a chair conformation. The distances of the two *para*-positioned atoms, Ni1 and C9, from the mean plane of the other four atoms are 0.446 (2) and −0.676 (2) Å, respectively.

The methanol molecules are linked to the nickel(II) complexes through intermolecular O—H⋯O hydrogen bonds (Table 2 and Fig. 2).

Experimental

3-Methylsalicylaldehyde (0.2 mmol, 27.2 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a yellow solution. To the solution was added an MeOH solution of $Ni(CH_3COO)_2\cdot 4H_2O$ (0.1 mmol, 24.9 mg), with stirring. The mixture was stirred for another 10 min at room temperature. After the filtrate had been left to stand in air for 7 d, green block-shaped crystals were formed.

Crystal data

$[Ni(C_{19}H_{20}N_2O_2)]\cdot CH_4O$
$M_r = 399.12$
Orthorhombic, *Pnma*
$a = 10.371$ (3) Å
$b = 16.447$ (4) Å
$c = 11.070$ (3) Å
$V = 1888.2$ (9) Å^3
$Z = 4$
$D_x = 1.404$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2668 reflections
$\theta = 2.2$–20.9°
$\mu = 1.05$ mm^{-1}
$T = 298$ (2) K
Block, green
0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.818$, $T_{max} = 0.902$
15295 measured reflections
2237 independent reflections
1724 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 27.5°$
$h = -13 \rightarrow 13$
$k = -21 \rightarrow 21$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.162$
$S = 1.06$
2237 reflections
128 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0805P)^2 + 1.5511P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.82$ e Å^{-3}
$\Delta\rho_{min} = -0.75$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.849 (3)	Ni1—N1	1.897 (3)
O1—Ni1—O1^{i}	79.94 (17)	O1—Ni1—N1	91.85 (13)
O1—Ni1—N1^{i}	171.75 (12)	N1^{i}—Ni1—N1	96.36 (19)

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

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O2—H2⋯O1^{ii}	0.90 (1)	2.31 (2)	3.091 (9)	144 (3)
O2—H2⋯O1^{iii}	0.90 (1)	2.31 (2)	3.091 (9)	144 (3)

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

Atom H2 was located in a difference Fourier map and refined isotropically, with the O—H distance restrained to 0.90 (1) Å, and with U_{iso}(H) fixed at 0.08 Å^2. The other H atoms were placed in idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.97 Å, and with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$. The U^{ij} components of atom O2 were restrained to isotropic behaviour.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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