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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.035
 wR factor = 0.087
Data-to-parameter ratio = 17.3

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

***N,N'*-Bis(3-methylsalicylidene)-1,3-propanediaminato]nickel(II)**

The title compound, $[\text{Ni}(\text{C}_{19}\text{H}_{20}\text{N}_2\text{O}_2)]$, is mononuclear. The Ni^{II} atom is four-coordinated in a square-planar configuration by two N atoms and two O atoms of the Schiff base ligand. The molecule possesses crystallographic mirror symmetry.

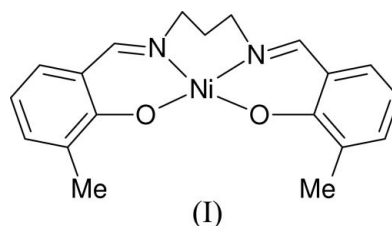
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Comment

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.*, 2004a). However, complexes related to the BSDP derivative *N,N'*-bis(3-methylsalicylidene)-1,3-diaminopropane have seldom been reported (You, 2005). 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, (I).



Complex (I) is a mononuclear nickel(II) compound (Fig. 1). The Ni^{II} atom is four-coordinated in a square-planar coordination configuration by two N atoms and two O atoms of the Schiff base ligand. The molecule possesses mirror symmetry, with atoms Ni1, C10, H10A and H10B lying on the crystallographic mirror plane. The value of the *trans* angles in the NiO_2N_2 square plane is $172.88(10)^\circ$, indicating a slightly distorted square-planar geometry. The Ni atom is $0.050(2)$ 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 *[N,N'*-bis(salicylidene)-1,3-propanediaminato](methanol)(thiocyanato)nickel(II) (You *et al.*, 2004b).

There is an overall butterfly shape to the nickel(II) complex, as evidenced by the dihedral angle $[65.4(1)^\circ]$ between the two aromatic rings. The dihedral angle between the NiO_2N_2 square plane and the benzene ring is $32.8(1)^\circ$.

The six-membered chelate ring containing the metal, azomethine N atoms and three C atoms of the connecting 1,3-

diaminopropane group adopts a boat conformation. The distances of the two *para*-positioned atoms, Ni1 and C10, from the mean plane of the other four atoms are 0.517 (6) and 0.670 (8) Å, respectively. No significant hydrogen bonding interaction is observed in the crystal structure.

Experimental

3-Methylsalicylaldehyde (0.2 mmol, 27.2 mg) and 1,3-diaminopropane (0.1 mmol, 7.4 mg) were dissolved in EtOH (10 ml). The mixture was stirred at room temperature for 10 min to give a yellow solution. To the solution was added an EtOH solution of Ni(CH₃-COO)₂·4H₂O (0.1 mmol, 24.9 mg), with stirring. The mixture was stirred for another 10 min at room temperature. The filtrate was allowed to stand in air for 2 d and yielded green crystals.

Crystal data

[Ni(C ₁₀ H ₂₀ N ₂ O ₂)]	Mo K α radiation
$M_r = 367.08$	Cell parameters from 3072 reflections
Orthorhombic, $A2_1am$	$\theta = 3.4\text{--}23.9^\circ$
$a = 7.529$ (2) Å	$\mu = 1.16$ mm ⁻¹
$b = 10.399$ (2) Å	$T = 298$ (2) K
$c = 21.555$ (3) Å	Lath, green
$V = 1687.6$ (6) Å ³	$0.28 \times 0.16 \times 0.07$ mm
$Z = 4$	
$D_x = 1.445$ Mg m ⁻³	

Data collection

Bruker SMART CCD area-detector diffractometer	1960 independent reflections
ω scans	1821 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$R_{int} = 0.035$
$T_{min} = 0.737$, $T_{max} = 0.923$	$\theta_{max} = 27.5^\circ$
9442 measured reflections	$h = -9 \rightarrow 9$
	$k = -13 \rightarrow 13$
	$l = -27 \rightarrow 27$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0418P)^2 + 0.6633P]$
$R[F^2 > 2\sigma(F^2)] = 0.035$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.087$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.05$	$\Delta\rho_{max} = 0.32$ e Å ⁻³
1960 reflections	$\Delta\rho_{min} = -0.27$ e Å ⁻³
113 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	884 Friedel pairs
	Flack parameter: 0.02 (2)

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	1.847 (2)	Ni1—N1	1.889 (2)
O1 ⁱ —Ni1—O1	82.18 (12)	O1—Ni1—N1	91.31 (10)
O1 ⁱ —Ni1—N1	172.88 (10)	N1—Ni1—N1 ⁱ	95.03 (16)

Symmetry code: (i) $x, y, -z + 1$.

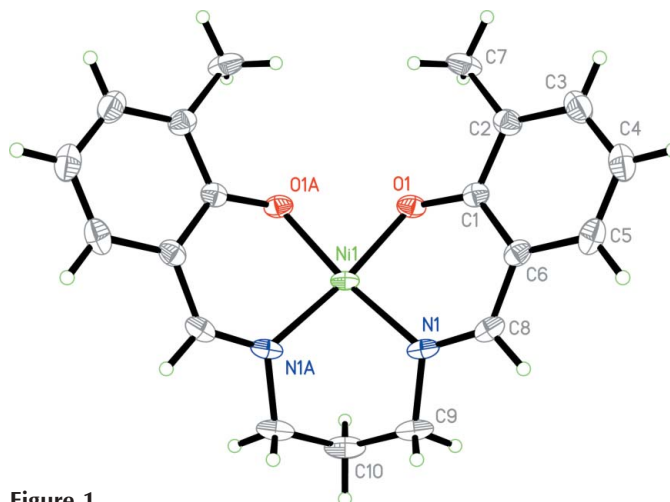


Figure 1

The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. Suffix A denotes symmetry operator ($x, y, 1 - z$).

The 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 unconventional space group $A2_1am$ was used to solve the structure. The structure can not be solved by direct method when the conventional space group $Cmc2_1$ was applied.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; 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.

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