

Zhong-Lu You

Department of Chemistry and Chemical Engineering, Liaoning Normal University, Dalian 116029, People's Republic of China

Correspondence e-mail:
youzhonglu@yahoo.com.cn

Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.005$ Å
 R factor = 0.056
 wR factor = 0.174
Data-to-parameter ratio = 17.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

Bis{1-[3-(dimethylamino)propyliminomethyl]-naphtholato}nickel(II) bis(perchlorate)

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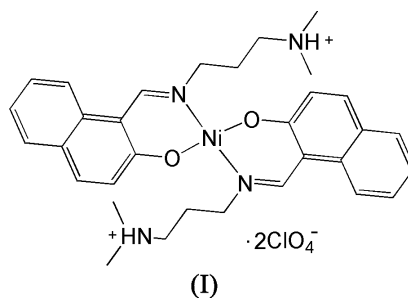
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In the molecular structure of the title complex, $[\text{Ni}(\text{C}_{16}\text{H}_{20}\text{N}_2\text{O})_2](\text{ClO}_4)_2$, the Ni^{II} atom lies on a crystallographic centre of symmetry and is four-coordinated by two phenolate O and two imine N atoms, forming a slightly distorted square-planar coordination. In the crystal structure, cations and anions are linked through intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds forming chains in the $[101]$ direction.

Comment

Recently, we have reported a few transition metal complexes derived from the tridentate Schiff base ligands 2-[3-(cyclohexylamino)propyliminomethyl]phenol (CHPP) and 2-[3-(cyclohexylamino)propyliminomethyl]naphthol (CHPN) (You & Zhu, 2004; You, Lin *et al.*, 2004; You, Xiong *et al.*, 2004). However, structures of complexes of the Schiff base ligand 1-[3-(dimethylaminopropylimino)methyl]naphthol (DMPN), a similar ligand to CHPP and CHPN, have never been reported. The prime interest in these complexes is their ability to afford functional solid materials with potentially controllable properties and novel molecular structures (Polt *et al.*, 2003; Kim *et al.*, 2005; Yamada, 1999).

The title complex, (I), consists of an $[\text{Ni}(\text{C}_{16}\text{H}_{20}\text{N}_2\text{O})_2]^{2+}$ cation and two perchlorate anions (Fig. 1). The Ni^{II} ion in the cation, lying on an inversion centre, is four-coordinated by two phenolate O and two imine N atoms, forming a square-planar coordination. The amine N atoms are protonated and do not coordinate to the Ni^{II} atom. The Ni—O and Ni—N bond lengths (Table 1) are comparable to the corresponding values observed in the Schiff base nickel(II) complexes that we reported earlier (You *et al.*, 2006; You & Niu, 2006; You, 2006). The two *trans* angles at the nickel(II) centre are 180° , by symmetry, and all other angles are close to 90° , *viz.* $88.99(11)^\circ$ and $91.01(11)^\circ$, thus indicating a very slightly distorted square-planar geometry.



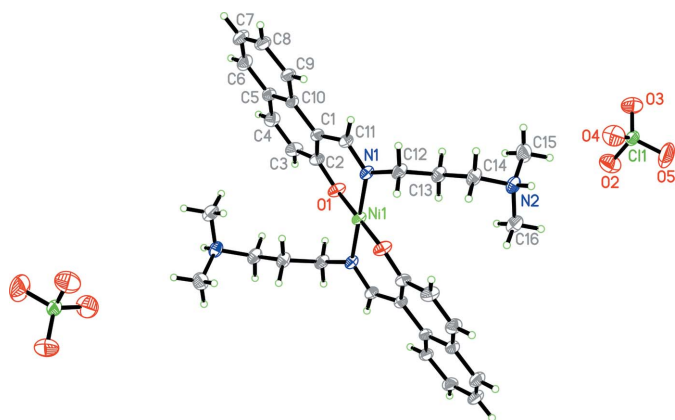


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids. Unlabelled atoms are related by the symmetry operator ($2 - x, 2 - y, 1 - z$).

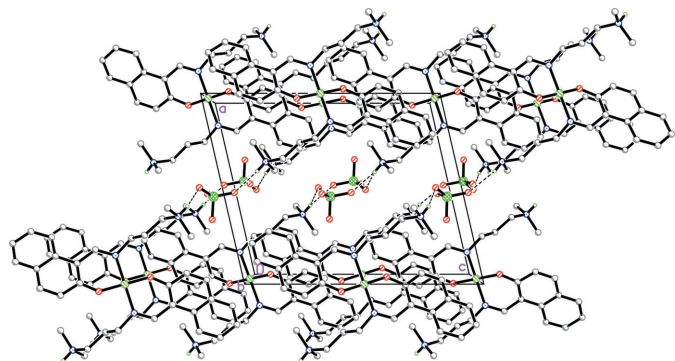


Figure 2
The crystal packing of (I), viewed along the b axis. Intermolecular hydrogen bonds are shown as dashed lines.

hydrogen bonds (Table 2), to form one-dimensional chains along $[101]$ (Fig. 2).

Experimental

All reagents were commercial grade and were used without further purification. 2-Hydroxy-1-naphthaldehyde (0.2 mmol, 34.3 mg) and N,N -dimethylpropane-1,3-diamine (0.2 mmol, 20.4 mg) were dissolved in MeOH (10 ml). The mixture was stirred at room temperature for 10 min to give a clear yellow solution. To this solution was added an aqueous solution (3 ml) of $\text{Ni}(\text{ClO}_4)_2 \cdot 7\text{H}_2\text{O}$ (0.1 mmol, 38.4 mg), with stirring. The mixture was stirred for another 10 min at room temperature. After keeping the filtrate in air for 8 d, green block-shaped crystals were formed. Analysis found: C 49.72, H 5.31, N 7.41%; calculated for $\text{C}_{32}\text{H}_{40}\text{Cl}_2\text{N}_4\text{NiO}_{10}$: C 49.90, H 5.23, N 7.27%.

Crystal data

$[\text{Ni}(\text{C}_{16}\text{H}_{20}\text{N}_2\text{O})_2](\text{ClO}_4)_2$
 $M_r = 770.29$
 Monoclinic, $P2_1/c$
 $a = 12.218$ (2) Å
 $b = 9.648$ (1) Å
 $c = 14.974$ (2) Å
 $\beta = 103.016$ (1)°
 $V = 1719.8$ (4) Å³

$Z = 2$
 $D_x = 1.487$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.78$ mm⁻¹
 $T = 298$ (2) K
 Block, green
 $0.23 \times 0.20 \times 0.18$ mm

Data collection

Bruker SMART 1000 CCD area-detector diffractometer
 ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.841, T_{\max} = 0.872$

14363 measured reflections
 3929 independent reflections
 2996 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.030$
 $\theta_{\text{max}} = 27.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.056$
 $wR(F^2) = 0.174$
 $S = 1.07$
 3929 reflections
 228 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.082P)^2 + 1.7986P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.90 \text{ e \AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.58 \text{ e \AA}^{-3}$

Table 1

Selected geometric parameters (Å, °).

Ni1—O1	1.832 (2)	Ni1—N1	1.903 (3)
O1 ⁱ —Ni1—O1	180	O1—Ni1—N1	91.01 (11)
O1—Ni1—N1 ⁱ	88.99 (11)	N1 ⁱ —Ni1—N1	180

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

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2—H2 ⁱⁱ ···O5 ⁱⁱⁱ	0.90 (4)	2.46 (4)	2.992 (5)	119 (4)
N2—H2 ⁱⁱ ···O3 ⁱⁱⁱ	0.90 (4)	2.14 (2)	2.970 (5)	153 (4)

Symmetry codes: (ii) $-x + 1, -y + 1, -z$; (iii) $x, y + 1, z$.

Atom H2 was located in a difference Fourier map and refined isotropically, with the N—H distance restrained to 0.90 (1) Å, and with $U_{\text{iso}}(\text{H})$ values fixed at 0.08 Å². 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 $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{C})$. The U^{ij} components of atom O5 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, 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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