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trans-Bis{2-[3-(cyclohexylamino)propyliminomethyl]phenolato}nickel(II) dinitrate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.006 Å
R factor = 0.063
wR factor = 0.148
Data-to-parameter ratio = 16.1

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

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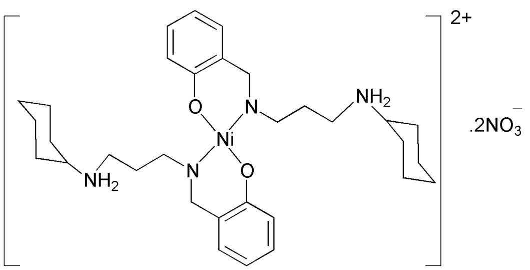
The title compound, $[Ni(C_{16}H_{24}N_2O)_2](NO_3)_2$, is a mononuclear nickel(II) compound. The Ni^{II} atom is coordinated by two N atoms and two O atoms from the Schiff base ligands. The four atoms around the metal are coplanar, constituting a slightly distorted square-planar geometry. The complex is located on an inversion center. All of the nitrate O atoms and all amine N atoms in the Schiff base ligands contribute to hydrogen bonds, leading to the formation of a three-dimensional network.

Comment

Recently, we have reported a few Schiff base complexes (You, Lin *et al.*, 2003; You, Qu *et al.*, 2003; You, Xiong *et al.*, 2004; You, Zhu & Liu, 2004). As an extension of our work on the structural characterization of Schiff base complexes, a mononuclear nickel(II) complex, (I), is reported here.



(I)

The structure of the title compound, (I) (Fig. 1), consists of a mononuclear $[Ni(C_{16}H_{24}N_2O)_2]^{2+}$ cation and two nitrate anions. The Ni atom, on an inversion center, is in a square-planar geometry and is four-coordinated by two N atoms and two O atoms from the Schiff base ligands. The four coordi-

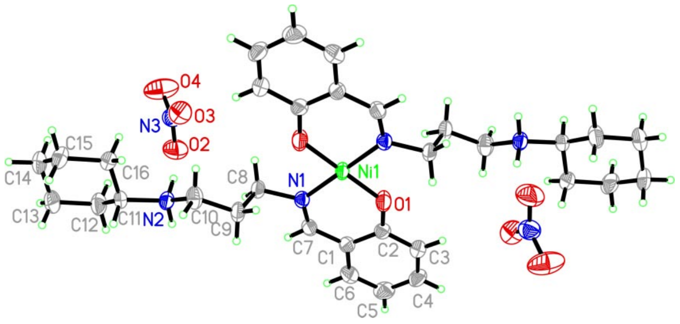


Figure 1
The structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

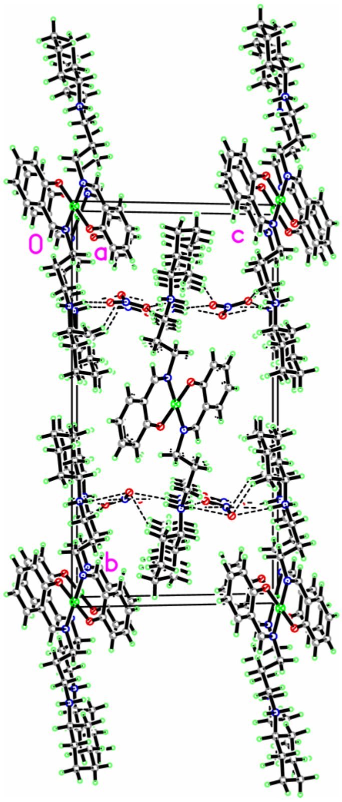


Figure 2
The crystal packing of (I), viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

nating atoms around the central metal are coplanar, forming a square-planar geometry around the Ni atom. The two *trans* angles at the nickel(II) center are 180°, by symmetry (Table 1), and all other angles are close to 90°, *viz.* 87.15 (12) and 92.85 (12)°, thus indicating a slightly distorted square-planar geometry. The Ni1—O1 bond length [1.827 (3) Å] is comparable to that observed in another Schiff base complex [1.833 (3) Å; Zhu *et al.*, 2004]. The Ni1—N1 bond distance [1.919 (3) Å] is a little longer than the value [1.876 (3) Å] observed in the same previously reported complex.

In the crystal structure, all of the nitrate O atoms and all the amine N atoms in the Schiff base ligands contribute to the formation of hydrogen bonds, leading to the formation of a three-dimensional network (Fig. 2 and Table 2). As expected, the cyclohexyl groups in the complex adopt chair conformations to minimize steric effects.

Experimental

N-Cyclohexyl-1,3-diaminopropane and salicylaldehyde were available commercially and were used without further purification. *N*-Cyclohexyl-1,3-diaminopropane (0.2 mmol, 31.2 mg) and salicylaldehyde (0.2 mmol, 24.4 mg) were dissolved in methanol (10 ml). The mixture was stirred for 1 h to obtain a clear orange solution of *L* (0.2 mmol), where *L* is 2-[(3-cyclohexylaminopropylimino)methyl]phenol. To the solution of *L* was added a solution of Ni(NO$_3$)$_2$·6H$_2$O (0.1 mmol, 29.1 mg) in methanol (10 ml), with stirring. After keeping the resulting solution in air for 9 d, green block-shaped crystals were formed at the bottom of the vessel on slow evaporation of the solvents. The crystals were isolated, washed three times with methanol and dried in a vacuum desiccator using anhydrous CaCl$_2$ (yield 70.1%). Analysis found: C 54.6, H 6.9, N 11.9%; calculated for C$_{32}$H$_{48}$N$_6$NiO$_8$: C 54.8, H 7.1, N 11.8%.

Crystal data

[Ni(C$_{16}$H$_{24}$N$_2$O)$_2$](NO$_3$)$_2$
M_r = 703.47
Monoclinic, $P2_1/c$
a = 6.444 (2) Å
b = 22.946 (5) Å
c = 11.961 (2) Å
β = 102.02 (3)°
V = 1729.9 (6) Å^3
Z = 2

D_x = 1.351 Mg m^{-3}
Mo *K*α radiation
Cell parameters from 1144 reflections
θ = 2.5–19.9°
μ = 0.62 mm^{-1}
T = 293 (2) K
Block, green
0.18 × 0.15 × 0.13 mm

Data collection

Siemens SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Blessing, 1995)
$T_{\min}$ = 0.897, $T_{\max}$ = 0.924
7948 measured reflections

3573 independent reflections
1985 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.063
$\theta_{\max}$ = 26.5°
$h = -8 \rightarrow 4$
$k = -28 \rightarrow 27$
$l = -14 \rightarrow 15$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.148
S = 0.95
3573 reflections
222 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0601P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max}$ = 0.48 e Å^{-3}
$\Delta\rho_{\min}$ = −0.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.827 (3)	Ni1—N1	1.919 (3)
O1$^{\rm i}$—Ni1—O1	180	O1—Ni1—N1	92.85 (12)
O1$^{\rm i}$—Ni1—N1	87.15 (12)	N1—Ni1—N1$^{\rm i}$	180

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

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

D—H⋯*A*	*D*—H	H⋯*A*	*D*⋯*A*	*D*—H⋯*A*
N2—H2*B*⋯N3$^{\rm ii}$	0.932 (10)	2.542 (12)	3.458 (6)	168 (3)
N2—H2*B*⋯O3$^{\rm ii}$	0.932 (10)	2.36 (2)	3.125 (5)	139 (3)
N2—H2*B*⋯O4$^{\rm ii}$	0.932 (10)	1.980 (15)	2.887 (5)	164 (3)
N2—H2*A*⋯N3	0.926 (10)	2.558 (15)	3.462 (6)	165 (3)
N2—H2*A*⋯O2	0.926 (10)	2.26 (2)	3.105 (5)	150 (3)
N2—H2*A*⋯O3	0.926 (10)	2.234 (17)	3.076 (5)	151 (3)

Symmetry codes: (ii) $x, \frac{3}{2} - y, \frac{1}{2} + z$.

All H atoms, except H2*A* and H2*B*, were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.93–0.98 Å, and with $U_{\rm iso}$(H) = 1.2 $U_{\rm eq}$(C). Atoms H2*A* and H2*B* were located in a difference Fourier map and were refined isotropically.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1996); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997*a*); molecular graphics:

SHELXTL (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.

Sheldrick, G. M. (1997*a*). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.

Sheldrick, G. M. (1997*b*). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.

Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.

You, Z.-L., Lin, Y.-S., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* E**59**, m1025–m1027.

You, Z.-L., Qu, Y., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2003). *Acta Cryst.* E**59**, m1038–m1040.

You, Z.-L., Xiong, Z.-D., Liu, W.-S., Tan, M.-Y. & Zhu, H.-L. (2004). *Acta Cryst.* E**60**, m79–m81.

You, Z.-L., Zhu, H.-L. & Liu, W.-S. (2004). *Acta Cryst.* E**60**, m560–m562.

Zhu, B., Ruang, W. & Zhu, Z. (2004). *Acta Cryst.* E**60**, m634–m636.