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[*N*,*N*′-Ethylenebis(salicylideneiminato)]nickel(II) chloroform solvate

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.046
wR factor = 0.147
Data-to-parameter ratio = 18.2

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

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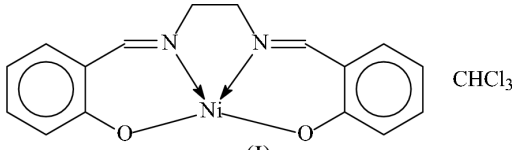
In the crystal structure of the title compound, $[Cu(C_8H_7NO)_2]\cdot CHCl_3$, the nickel complex and the solvent molecule both have crystallographic mirror symmetry. The Ni atom exists in square-planar geometry.

Comment

The crystal structure of [*N*,*N*′-ethylenebis(salicylideneiminato)]nickel(II) was first reported in 1970 (Shkol'nikova *et al.*, 1970) and redetermined to improved precision some 13 years later (Manfredotti & Guastini, 1983). It has since between re-determined twice more (DiMauro & Kozlowski, 2002; Kondo *et al.*, 2003). The same complex has now been isolated as the chloroform solvate, (I) (Fig. 1), and is described here.



(I)

In the title solvate, the square-planar geometry of the Ni atom is almost the same as in the unsolvated structure. Atoms Ni1, C9, and Cl1 occupy special positions on a mirror plane.

The $CHCl_3$ molecule interacts with the nickel complex by way of a bifurcated C—H···(O,O′) bond (Fig.1, Table 2).

Experimental

Nickel nitrate hexahydrate (0.58 g, 2 mmol) and an excess of triethylamine (1 ml) were added to *N*,*N*′-ethylenebis(salicylideneimine) (0.54 g, 2 mmol) dissolved in a small volume of ethanol. The mixture was heated for 1 h. After removal of the solvent, a red solid was collected, and this was purified by recrystallization from chloroform. Red prismatic crystals of (I) were obtained. CHN elemental analysis, calculated for $C_{17}H_{15}N_2O_2Cl_3Ni$: C 45.95, H 3.40, N 6.30%; found: C 45.91, H 3.43, N 6.28%.

Crystal data

$[Cu(C_8H_7NO)_2]\cdot CHCl_3$
M_r = 444.37
Orthorhombic, *Pnnm*
a = 6.997 (1) Å
b = 14.221 (3) Å
c = 18.355 (4) Å
V = 1826.4 (6) Å^3
Z = 4
D_x = 1.616 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 14 841 reflections
θ = 3.1–27.5°
μ = 1.51 mm^{-1}
T = 295 (2) K
Prism, red
0.35 × 0.26 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID diffractometer	2150 independent reflections
ω scans	1766 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)	$R_{int} = 0.023$
$T_{min} = 0.507$, $T_{max} = 0.764$	$\theta_{max} = 27.5^\circ$
16 264 measured reflections	$h = -9 \rightarrow 8$
	$k = -18 \rightarrow 18$
	$l = -22 \rightarrow 23$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0952P)^2 + 0.4858P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.046$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.147$	$\Delta\rho_{max} = 0.73$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.56$ e Å^{-3}
2150 reflections	Extinction correction: none
118 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.844 (2)	Ni1—N1	1.843 (3)
O1—Ni1—O1^{i}	84.6 (1)	O1—Ni1—N1^{i}	178.9 (1)
O1—Ni1—N1	94.8 (1)	N1—Ni1—N1^{i}	85.9 (2)

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

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9···O1	0.98	2.43	3.292 (5)	147
C9—H9···O1^{i}	0.98	2.43	3.292 (5)	147

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

H atoms were placed in calculated positions (C—H = 0.93–0.98 Å) and refined as riding, with the constraint $U_{iso}(H) = 1.2U_{eq}(C)$ applied in all cases.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

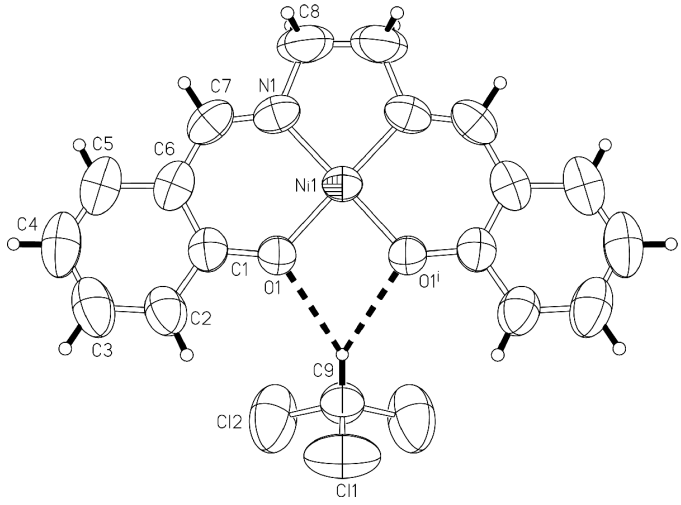


Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as small spheres of arbitrary radii. C—H···O interactions are shown as dashed lines. [Symmetry code (i): $x, y, 1-z$.]

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