Bis(5-bromo-*N*-cyclohexylsalicylideneamin-ato-$\kappa^2 N,O$)nickel(II)

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Key indicators

Single-crystal X-ray study

$T = 295$ K

Mean σ(C–C) = 0.005 Å

R factor = 0.033

wR factor = 0.091

Data-to-parameter ratio = 19.7

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

The Ni atom in the title compound, [Ni(C$_{13}$H$_{15}$BrNO)$_2$], is chelated through the O and N atoms of the ligands in a distorted square-planar geometry. The Ni atom lies on a twofold rotation axis. Adjacent molecules are linked by Br···Br interactions into a chain.

Comment

The Cambridge Structural Database (Version 5.25; Allen, 2002) lists several hundred examples of metal complexes of Schiff bases that are based on the salicylideneaminate system. Among the nickel(II) derivatives is nickel bis(*N*-cyclohexyl-salicylideneaminate), which possesses a bulky cyclohexyl ring; the metal atom shows square-planar coordination [Ni—O = 1.903 (2) Å and Ni—N = 1.995 (2) Å] (Bhatia *et al.*, 1983). The introduction of a Br substituent in the ligand, producing the title compound, (I) (Fig. 1), distorts the geometry significantly from square planar, although the substituent is far from the metal atom. The Ni atom lies on a special position of site symmetry 2; adjacent molecules are linked by Br···Br inter-actions into a chain (Fig. 2).

(I)
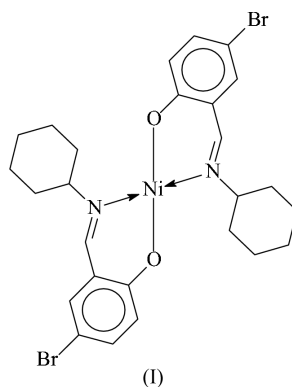
Experimental

Cyclohexylamine (0.2 mmol, 20 mg) and 5-bromosalicylaldehyde (0.2 mmol, 40 mg) were dissolved in methanol (10 ml) to give a yellow solution after several minutes of stirring. A methanol solution (10 ml) of nickel nitrate tetrahydrate (0.2 mmol, 51 mg) was then added. Green crystals separated from the solution after about a week.

Crystal data

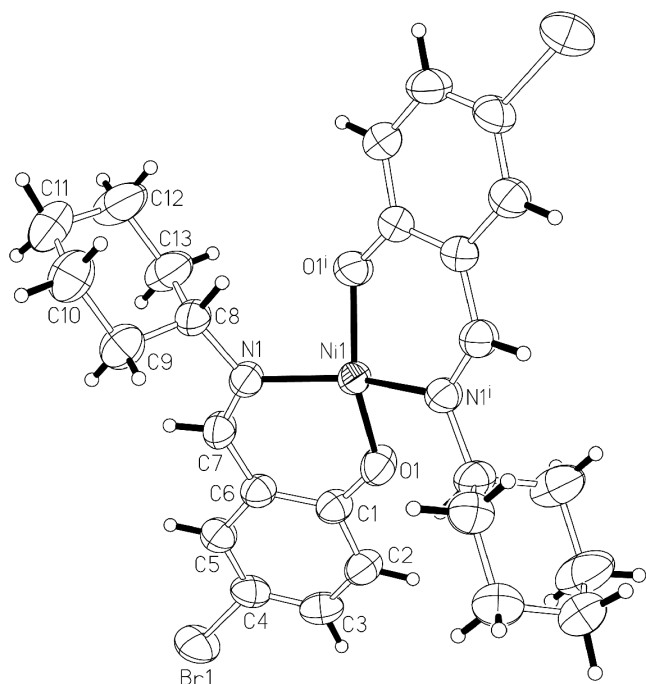|	
[Ni(C$_{13}$H$_{15}$BrNO)$_2$]	$D_x = 1.606$ Mg m^{-3}
$M_r = 621.05$	Mo $K\alpha$ radiation
Monoclinic, $C2/c$	Cell parameters from 4617
$a = 17.2129$ (9) Å	reflections
$b = 13.5010$ (7) Å	$\theta = 2.4$–26.7°
$c = 11.3932$ (6) Å	$\mu = 3.89$ mm^{-1}
$\beta = 103.979$ (1)°	$T = 295$ (2) K
$V = 2569.3$ (2) Å^3	Block, green
$Z = 4$	$0.22 \times 0.12 \times 0.08$ mm

Figure 1
ORTEPII plot (Johnson, 1976), showing the atom-numbering scheme of (I). Displacement ellipsoids are drawn at the 50% probability level and H atoms are shown as spheres of arbitrary radii. Symmetry code as in Table 1.

Data collection

Bruker SMART APEX area-detector diffractometer	2952 independent reflections
	2397 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.028$
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)	$\theta_{max} = 27.5°$
	$h = -22 \rightarrow 22$
$T_{min} = 0.469$, $T_{max} = 0.731$	$k = -17 \rightarrow 17$
14551 measured reflections	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$+ 3.2642P]$
$wR(F^2) = 0.091$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
2952 reflections	$\Delta\rho_{max} = 0.53$ e Å^{-3}
150 parameters	$\Delta\rho_{min} = -0.49$ e Å^{-3}
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.897 (2)	Ni1—N1	1.971 (2)
O1—Ni1—O1^i	152.3 (1)	O1—Ni1—N1^i	92.4 (1)
O1—Ni1—N1	93.7 (1)	N1—Ni1—N1^i	154.4 (1)

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

H atoms were placed in calculated positions [sp^2 and aromatic C—H = 0.93 Å, methine C—H = 0.98 Å and methylene C—H = 0.97 Å; $U_{iso}(H) = 1.2U_{eq}(C)$] and were included in the refinement in the riding-model approximation.
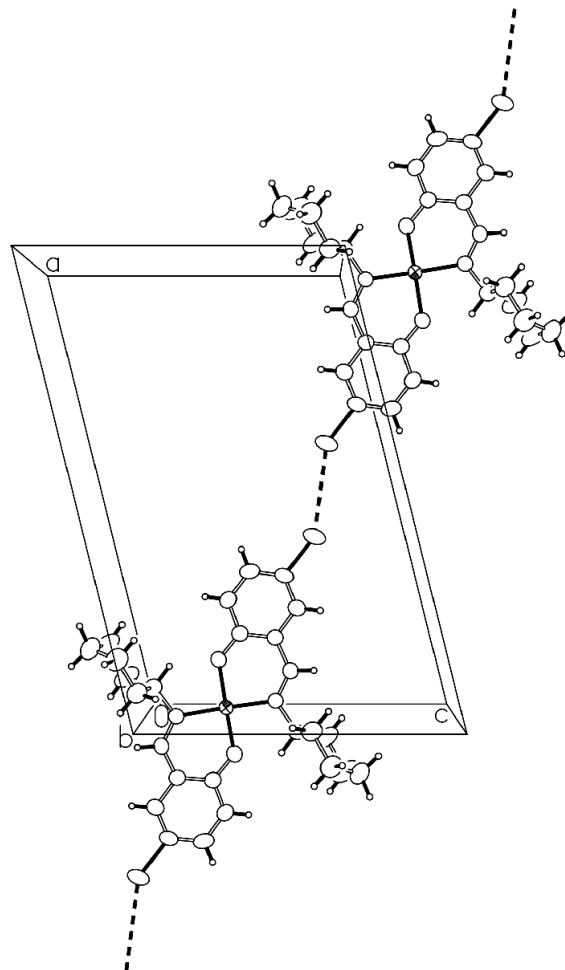

Figure 2
ORTEPII plot (Johnson, 1976), illustrating the intermolecular Br···Br contacts [3.620 (1) Å] that link molecules into a chain.

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; 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*.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bhatia, S. C., Syal, V. K., Kashyap, R. P. & Jain, P. C. (1983). *Acta Cryst.* C**39**, 199–200.
Bruker (2002). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.