metal-organic papers

{2,4-Dibromo-6-[2-(dimethylamino)ethyl-iminomethyl]phenolato}thiocyanatonickel(II)

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The title compound, [Ni($C_{11}H_{13}Br_2N_2O$)(NCS)], is a mononuclear nickel(II) compound. The square-planar geometry of the Ni^{II} atom is provided by one O and two N atoms of the tridentate ligand and one N atom of the thiocyanate anion.

Comment

The reaction of copper acetate, ammonium thiocyanate and the Schiff base ligand DBMP (DBMP = 2,4-dibromo-6-[(2-dimethylaminoethylimino)methyl]phenolate) in MeOH solution yields {2,4-dibromo-6-[(2-dimethylaminoethylimino)methyl]phenolato}(thiocyanato)copper(II), [Cu($C_{11}H_{13}Br_2N_2O$)(NCS)] (Wang *et al.*, 2006). However, when the copper acetate was replaced by nickel nitrate, we obtained the title nickel(II) complex, (I), which is isostructural with the copper(II) complex.

(I)
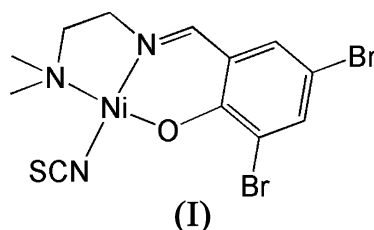
Details of the molecular geometry of (I) are given in Table 1 and the complex is shown in Fig. 1. The Schiff base ligand acts as a tridentate ligand, ligating to the Ni^{II} atom *via* the NNO donor atoms. The Ni^{II} atom is four-coordinated in a square-planar geometry by two N atoms [Ni—N1 = 1.934 (5) Å and Ni—N2 = 2.048 (5) Å], one O atom from the DBMP ligand [Ni—O1 = 1.914 (4) Å] and one N atom from the thiocyanate anion [Ni—N3 = 1.935 (5) Å]. The Ni atom deviates by 0.010 (4) Å from the N1–N3/O1 plane.

Experimental

All chemicals were of reagent grade and commercially available from the Shanghai Chemical Reagents Company of China, and were used without further purification. To an MeOH solution (30 ml) of 3,5-dibromosalicylaldehyde (0.282 g, 1.0 mmol) was added an MeOH solution (20 ml) of *N,N*-dimethylethane-1,2-diamine (0.084 g, 1.0 mmol) with stirring. To this mixture was added an aqueous solution (10 ml) of ammonium thiocyanate (0.076 g, 1.0 mmol) and an aqueous solution (10 ml) of Ni(NO$_3$)$_2$·6H$_2$O (0.291 g, 1.0 mmol) with stirring. The mixture was refluxed for 1 h, affording a clear green solution. This was allowed to stand at room temperature for two weeks and well shaped green single crystals of (I) were obtained by slow evaporation.

Crystal data

[Ni(C₁₁H₁₃Br₂N₂O)(NCS)]

$[Ni(C_{11}H_{13}Br_2N_2O)(NCS)]$
$M_r = 465.84$
Monoclinic, $P2_1/n$
$a = 7.138 (1)$ Å
$b = 19.227 (3)$ Å
$c = 11.229 (2)$ Å
$\beta = 90.995 (2)°$
$V = 1540.9 (4)$ Å³

$Z = 4$
$D_x = 2.008$ Mg m⁻³
Mo $K\alpha$ radiation
$T = 298 (2)$ K
Rhomb, green
$0.33 \times 0.31 \times 0.30$ mm

Data collection

Bruker SMART 1000 CCD area-
detector diffractometer
ω scans
Absorption correction: multi-scan
($SADABS$; Sheldrick, 2000)
$T_{min} = 0.126$, $T_{max} = 0.139$

13292 measured reflections
3667 independent reflections
2073 reflections with $I > 2\sigma(I)$
$R_{int} = 0.073$
$\theta_{max} = 28.3°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.122$
$S = 1.01$
3667 reflections
183 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0315P)^2 + 2.0314P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.70$ e Å⁻³
$\Delta\rho_{min} = -0.53$ e Å⁻³

Table 1
Selected geometric parameters (Å, °).

Ni1—O1	1.914 (4)	Ni1—N3	1.935 (5)
Ni1—N1	1.934 (5)	Ni1—N2	2.048 (5)
O1—Ni1—N1	92.34 (18)	O1—Ni1—N2	174.8 (2)
O1—Ni1—N3	91.2 (2)	N1—Ni1—N2	84.6 (2)
N1—Ni1—N3	173.7 (2)	N3—Ni1—N2	92.3 (2)

All H atoms were placed in geometrically idealized positions, with Csp^2—H = 0.93 Å and Csp^3—H = 0.96–0.97 Å, and constrained to
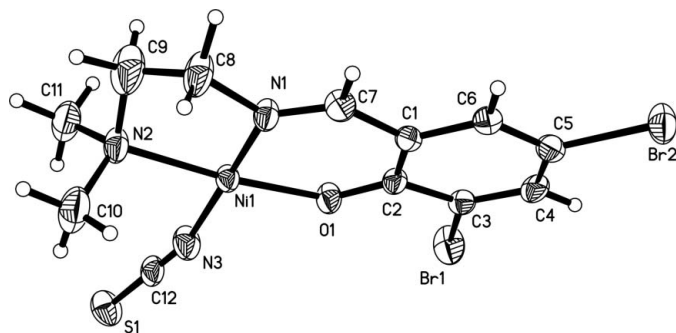

Figure 1
The structure of (I), with displacement ellipsoids drawn at the 30% probability level.

ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms.

Data collection: $SMART$ (Bruker, 2000); cell refinement: $SAINT$ (Bruker, 2000); data reduction: $SAINT$; program(s) used to solve structure: $SHELXS97$ (Sheldrick, 1997); program(s) used to refine structure: $SHELXL97$ (Sheldrick, 1997); molecular graphics: $SHELXTL/PC$ (Sheldrick, 1999); software used to prepare material for publication: $SHELXTL/PC$.

References

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