Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

cis-Bis(*N*,*N*-dimethyl-*N*′-2-chlorobenzoylthioureato)nickel(II)

Fatih Mehmet Emen,[a] Ulrich Flörke,[b]* Nevzat Külcü[a] and Hakan Arslan[a]

[a]Department of Chemistry, Faculty of Arts and Science, Mersin University, Mersin, Turkey, and [b]Department Chemie, Fakultät für Naturwissenschaften, Universität Paderborn, Warburgerstr. 100, D-33098 Paderborn, Germany

Correspondence e-mail: uf@chemie.uni-paderborn.de

Key indicators

Single-crystal X-ray study
T = 203 K
Mean σ(C–C) = 0.008 Å
R factor = 0.056
wR factor = 0.172
Data-to-parameter ratio = 18.4

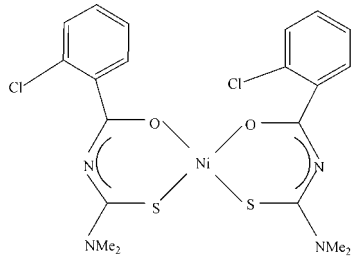
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 3 July 2003
Accepted 4 July 2003
Online 17 July 2003

The Ni atom of the title compound, $[Ni(C_{10}H_{10}ClN_2OS)_2]$, shows square-planar coordination geometry with two thiocarbonyl S and two carbonyl O atoms from two ligand moieties.

Comment

In the course of our investigation on new thiourea derivatives, a series of related metal complexes, including the title compound, (I), was synthesized (Arslan *et al.*, 2003). The molecular structure of (I) is closely related to that of the *N*,*N*-diethyl complex (Bailey *et al.*, 1988). The central Ni atom shows slightly distorted square-planar coordination by two pairs of S and O atoms from two chelating thioureate ligands. The S atoms are in a *cis* configuration. The maximum deviations from the S_2O_2 mean plane are 0.031 (4) Å for oxygen, 0.026 (2) Å for sulfur and 0.003 (1) Å for nickel. Ni—O [average 1.862 (4) Å] and Ni—S [average 2.1443 (15) Å] bond lengths are in the expected ranges. The planes of the two benzoyl rings subtend an angle of 66.2 (2)°; the corresponding torsion angles are O1—C2—C3—C8 = 56.1 (7)° and O2—C12—C13—C18 = 147.9 (6)°. The planes of the molecules are stacked in parallel sheets along [001]. Possible weak intermolecular hydrogen-bond interactions are C16—H16*A*···O1($x+\frac{1}{2}$, $-y+\frac{1}{2}$, $-z$), with H···O = 2.56 Å and C—H···O = 161°, and C4—H4*A*···N1($x-\frac{1}{2}$, y, $-z+\frac{1}{2}$), with H···N = 2.73 Å and C—H···N = 170°. Intramolecular interactions are C9—H9*A*···N1, with H···N = 2.20 Å and C—H···N = 105°, C19—H19*A*···N3, with H···N = 2.17 Å and C—H···N = 106°, C10—H10*A*···S1, with H···S = 2.33 Å and C—H···S = 114°, and C20—H20*A*···S2, with H···S = 2.28 Å and C—H···S = 115°; all these values are normalized for C—H = 1.08 Å.



(I)

Experimental

A solution of $NiCl_2{\cdot}6H_2O$ (2 mmol) in ethanol was added dropwise to a solution of *N*,*N*-dimethyl-*N*′-2-chlorobenzoyl-thioureate (4 mmol) in dichloromethane at room temperature. The solid product was filtered off and recrystallized from ethanol/dichloromethane (1:1).

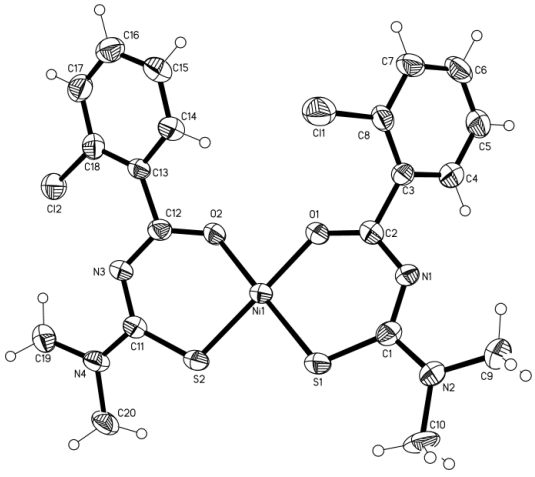


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

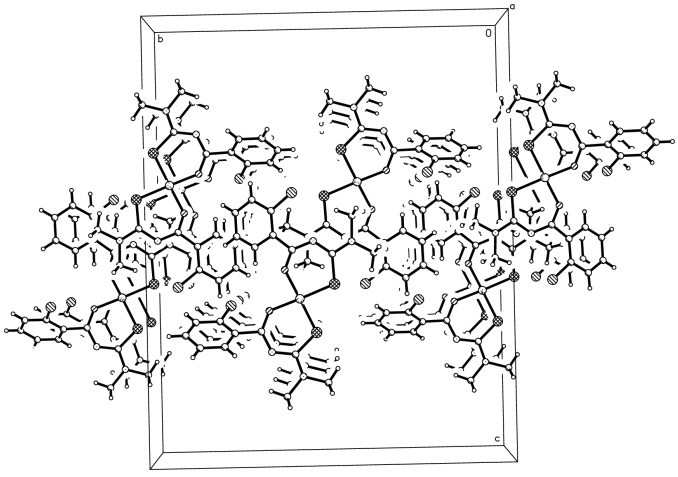


Figure 2
The crystal packing in (I), viewed along [001].

Crystal data

$[Ni(C_{10}H_{10}ClN_2OS)_2]$
M_r = 542.13
Orthorhombic, *Pbca*
a = 7.3679 (14) Å
b = 22.280 (4) Å
c = 27.448 (4) Å
V = 4505.8 (14) Å^3
Z = 8
D_x = 1.598 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 29 reflections
θ = 7.6–15.0°
μ = 1.31 mm^{-1}
T = 203 (2) K
Prism, violet
0.44 × 0.22 × 0.14 mm

Data collection

Bruker *P*4 diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.548, T_{max} = 0.832
6492 measured reflections
5178 independent reflections
2254 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°
$h = -9 \rightarrow 1$
$k = -1 \rightarrow 28$
$l = -35 \rightarrow 1$
3 standard reflections
every 397 reflections
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.172
S = 1.01
5178 reflections
281 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0624P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.54 e Å^{-3}
$\Delta\rho_{min}$ = −0.55 e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00029 (9)

Table 1
Selected geometric parameters (Å, °).

Ni1—O2	1.857 (4)	O1—C2	1.265 (6)
Ni1—O1	1.866 (4)	O2—C12	1.275 (6)
Ni1—S1	2.1430 (15)	N1—C2	1.310 (7)
Ni1—S2	2.1456 (15)	N1—C1	1.345 (7)
S1—C1	1.733 (5)	N3—C12	1.316 (7)
S2—C11	1.731 (6)	N3—C11	1.352 (7)
O2—Ni1—O1	83.85 (15)	O2—Ni1—S2	94.51 (12)
O2—Ni1—S1	178.16 (15)	O1—Ni1—S2	177.54 (14)
O1—Ni1—S1	95.13 (12)	S1—Ni1—S2	86.55 (6)

H atoms were placed at calculated positions, riding on the attached C atoms, with isotropic displacement parameters $U_{iso}(H) = 1.2U_{eq}(C)$, or $1.5U_{eq}(C)$ for methyl groups.

Data collection: *XSCANS* (Bruker, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL* (Bruker, 1998); program(s) used to solve structure: *SHELXTL*; program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

References

Arslan, H., Flörke, U. & Külcü, N. (2003). *Transition Met. Chem.* In the press.
Bailey, R. A., Rothaupt, K. L. & Kullnig, R. K. (1988). *Inorg. Chim. Acta*, **147**, 233–236.
Bruker (1996). *XSCANS*. Version 2.21. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1998). *SHELXTL*. Version 5.1. Bruker AXS Inc., Madison, Wisconsin, USA.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.