

cis-Bis[*N*-(2-chlorobenzoyl)-*N*',*N*'-diphenyl thioureato]nickel(II) dichloromethane solvate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean $\sigma(\text{C}-\text{C})$ = 0.005 Å
R factor = 0.043
wR factor = 0.063
Data-to-parameter ratio = 15.9

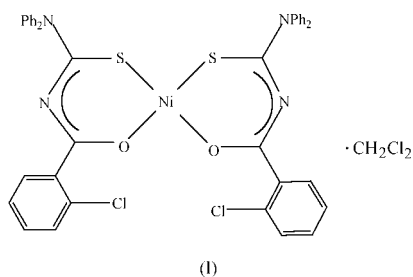
For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The Ni atom of the title compound, $[\text{Ni}(\text{C}_{20}\text{H}_{14}\text{ClN}_2\text{OS})_2]\cdot\text{CH}_2\text{Cl}_2$, shows a square-planar coordination geometry with two thiocarbonyl S and two carbonyl O atoms from two ligand moieties. The complex crystallizes with one solvent CH_2Cl_2 molecule per asymmetric unit.

Received 23 July 2003
Accepted 1 August 2003
Online 8 August 2003

Comment

The title compound, (I), is another example of our newly synthesized thioureato metal complexes (Arslan *et al.*, 2003). Its central Ni atom is almost square-planar, coordinated by two pairs of S and O atoms from the two chelating thioureate ligands, which show *cis* configurations (Fig. 1). Ni—O [mean 1.859 (2) Å] and Ni—S [mean 2.1394 (9) Å] bond lengths are in the expected ranges and compare well with those from the related dimethyl (Emen *et al.*, 2003) or diethyl complex (Bailey *et al.*, 1988). The two benzoyl ring planes subtend an angle of 79.9 (1)°; the corresponding torsion angles are O1—C7—C6—C1 130.9 (3)° and O2—C27—C26—C21 39.1 (4)°



The crystal packing shows the molecules stacked in parallel sheets along [100] (Fig. 2), accompanied by the following intermolecular contacts: C31—H31A···O1ⁱ, with H···O 2.46 Å and C—H···O 152°; C10—H10A···Cl2ⁱⁱ, with H···Cl 2.78 Å and C—H···Cl 157°, and C19—H19A···Cl1ⁱⁱⁱ, with H···Cl 2.87 Å and C—H···Cl 126° [symmetry codes: (i) $-x, 1-y, -z$; (ii) $x+1, y, z$; (iii) $2-x, 2-y, 1-z$]. Possible intramolecular interactions are C5—H5A···O1, with H···O 2.61 Å and C—H···O 90°, and C25—H25A···N3, with H···N 2.52 Å and C—H···N 94°. All these values are normalized for C—H = 1.08 Å. There is one solvent dichloromethane molecule per asymmetric unit.

Experimental

Compound (I) was prepared according to the method of Polat (2002), by converting 2-chlorobenzoyl chloride into 2-chlorobenzoyl isothiocyanate and then condensing with diphenylamine in CH_2Cl_2 solution at 298 K. The compound was recrystallized from ethanol-dichloromethane.

Crystal data

[Ni(C₂₀H₁₄ClN₂OS)₂].CH₂Cl₂
M_r = 875.32
 Triclinic, *P* $\bar{1}$
a = 8.4277 (7) Å
b = 14.2923 (11) Å
c = 17.4582 (13) Å
 α = 103.671 (2)°
 β = 98.230 (2)°
 γ = 103.877 (2)°
V = 1938.6 (3) Å³

Z = 2
D_x = 1.500 Mg m⁻³
 Mo *K*α radiation
 Cell parameters from 1694 reflections
 θ = 2.5–23.3°
 μ = 0.93 mm⁻¹
T = 173 (2) K
 Prism, red
 0.20 × 0.18 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2002)
T_{min} = 0.818, *T_{max}* = 0.912
 11 475 measured reflections

7764 independent reflections
 4564 reflections with *I* > 2σ(*I*)
R_{int} = 0.038
 θ_{max} = 26.4°
h = -10 → 10
k = -14 → 17
l = -21 → 21

Refinement

Refinement on *F*²
R[*F*² > 2σ(*F*²)] = 0.043
wR(*F*²) = 0.063
S = 0.81
 7764 reflections
 487 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0001P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} = 0.001$
 $\Delta\rho_{max} = 0.48 \text{ e \AA}^{-3}$
 $\Delta\rho_{min} = -0.37 \text{ e \AA}^{-3}$

H atoms were placed at calculated positions, riding on their parent C atoms C–H = 0.95 Å, with isotropic displacement parameters *U*_{iso}(H) = 1.2*U*_{eq}(C).

Data collection: SMART (Bruker, 2002); cell refinement: SMART; data reduction: SAINT (Bruker, 2002); program(s) used to solve structure: SHELXTL (Bruker, 2002); program(s) used to refine structure: SHELXTL; molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

This work was supported by Mersin University Research Fund.

References

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 Bruker (2002). SMART (Version 5.62), SAINT (Version 6.02), SHELXTL (Version 6.10) and SADABS (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.

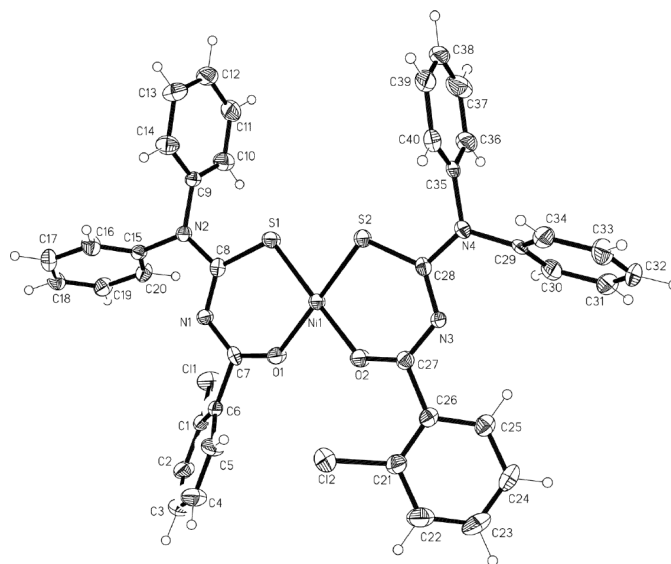


Figure 1 The molecular structure of (I). Displacement ellipsoids are drawn at the 50% probability level. The solvent CH₂Cl₂ molecule has been omitted.

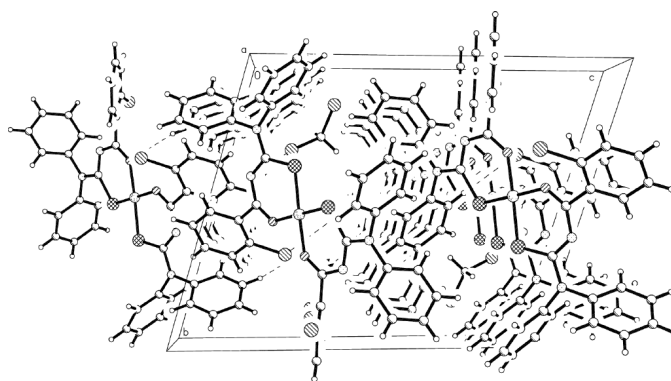


Figure 2 Packing diagram for (I), viewed along [100]. Intermolecular C–H...Cl contacts are indicated by dashed lines.

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