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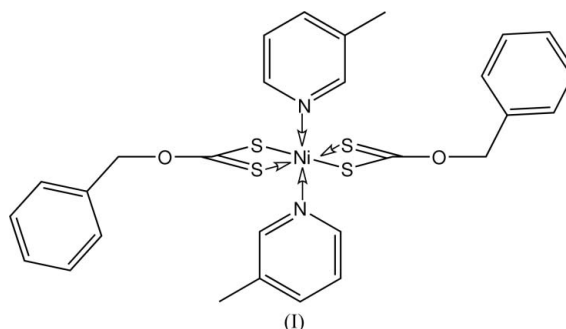
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Key indicators

Single-crystal X-ray study
T = 293 K
Mean $\sigma(\text{C}-\text{C}) = 0.005 \text{ \AA}$
R factor = 0.042
wR factor = 0.091
Data-to-parameter ratio = 17.0For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.Bis(*O*-benzyl dithiocarbonato- κ^2S,S')bis(3-methylpyridine- κN)nickel(II)The Ni atom in the title complex, $[\text{Ni}(\text{S}_2\text{COCH}_2\text{Ph})_2(\text{NC}_5\text{H}_3\text{Me-3})_2]$ or $[\text{Ni}(\text{C}_8\text{H}_7\text{OS}_2)_2(\text{C}_6\text{H}_7\text{N})_2]$, is octahedrally coordinated within a *trans*- N_2S_4 donor set, with the Ni atom located on a centre of inversion.Received 2 November 2006
Accepted 17 November 2006

Comment

Nitrogen-containing adducts of nickel(II) xanthates (xanthate = $^-\text{S}_2\text{COR}$) are known to adopt a variety of supramolecular assemblies (Tiekink & Haiduc, 2005). As a continuation of our interest in this area, the title complex, (I), was investigated. The Ni atom in (I) (Fig. 1) is located on a centre of inversion and exists within a *trans*- N_2S_4 donor set that defines an approximately octahedral coordination geometry. The chelating xanthate ligand forms essentially equivalent Ni–S bond distances; this equivalence is reflected in the parameters defining the xanthate ligand (Table 1). Distortions from an ideal octahedral geometry may be related primarily to the acute chelate angle.Molecules associate into a three-dimensional supramolecular array *via* a variety of $\text{C}-\text{H}\cdots\pi$ interactions. Centrosymmetrically related 3-methylpyridine molecules associate *via* $\text{C14}-\text{H14c}\cdots\text{Cg1}$ [Cg1 is the centroid of ring $\text{N1}/\text{C9}-\text{C13}$ at $(-x, 1 - y, -z)$] contacts of 2.95 \AA , with an angle of 138° at H14c . The other side of the $\text{N1}/\text{C9}-\text{C13}$ ring is also associated with a $\text{C6}-\text{H6}$ group, with a separation of 2.98 \AA and an angle at H6 of 150° (symmetry code: $-1 + x, y, 1 + z$). Finally, there are $\text{C}-\text{H}\cdots\pi$ contacts involving the benzyl residues so that the $\text{C2}-\text{H2a}\cdots\text{Cg2}$ separation is 2.90 \AA [Cg2 is the centroid of ring $\text{C3}-\text{C8}$ at $(-1 - x, -y, 1 - z)$], with an angle at H2a of 129° . A view of the crystal packing is shown in Fig. 2.

Experimental

A dichloromethane solution (10 ml) containing nickel(II) bis(benzylxanthate) (0.212 g) was treated with excess 3-picoline, added

dropwise. The colour changed from brown to green. Crystals were obtained by layering with hexane.

Crystal data

$[\text{Ni}(\text{C}_8\text{H}_7\text{OS}_2)_2(\text{C}_6\text{H}_7\text{N})_2]$	$V = 711.78 (12) \text{ \AA}^3$
$M_r = 611.47$	$Z = 1$
Triclinic, $P\bar{1}$	$D_x = 1.427 \text{ Mg m}^{-3}$
$a = 6.6339 (7) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.7275 (10) \text{ \AA}$	$\mu = 1.00 \text{ mm}^{-1}$
$c = 11.7926 (11) \text{ \AA}$	$T = 293 (2) \text{ K}$
$\alpha = 72.178 (2)^\circ$	Block, green
$\beta = 86.966 (2)^\circ$	$0.25 \times 0.13 \times 0.12 \text{ mm}$
$\gamma = 79.262 (2)^\circ$	

Data collection

Bruker AXS SMART CCD diffractometer	7678 measured reflections
φ and ω scans	2898 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 2000)	2573 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.795$, $T_{\max} = 0.889$	$R_{\text{int}} = 0.036$
	$\theta_{\text{max}} = 26.4^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0263P)^2 + 0.313P]$
$R[F^2 > 2\sigma(F^2)] = 0.042$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.091$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.12$	$\Delta\rho_{\text{max}} = 0.35 \text{ e \AA}^{-3}$
2898 reflections	$\Delta\rho_{\text{min}} = -0.30 \text{ e \AA}^{-3}$
170 parameters	
H-atom parameters constrained	

Table 1

Selected geometric parameters (\AA , $^\circ$).

Ni—S1	2.4466 (6)	S1—C1	1.692 (2)
Ni—S2	2.4641 (7)	S2—C1	1.687 (2)
Ni—N1	2.105 (2)	O1—C1	1.339 (3)
S1—Ni—S2	73.60 (2)	Ni—S1—C1	82.91 (8)
S1 ⁱ —Ni—S2	106.40 (2)	Ni—S2—C1	82.46 (9)
S1—Ni—N1	89.83 (6)	S1—C1—S2	121.02 (15)
S1—Ni—N1 ⁱ	90.17 (6)	S1—C1—O1	115.32 (17)
S2—Ni—N1	90.43 (6)	S2—C1—O1	123.66 (18)

Symmetry code: (i) $-x, -y, -z$.

The H atoms were included in the riding-model approximation, with $\text{C—H} = 0.93\text{--}0.97 \text{ \AA}$ and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{methyl C})$ or $1.2U_{\text{eq}}(\text{other C})$. The C14 methyl group was allowed to rotate about its local threefold axis.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *PATY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

The authors thank the National Council for University Research, Bucharest, for a CEEX grant.

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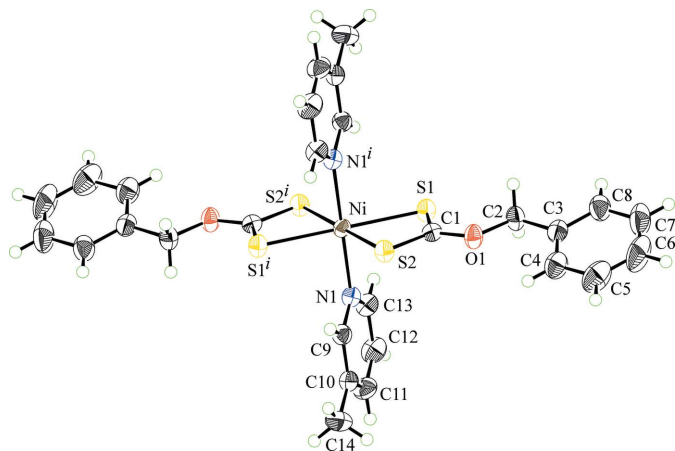


Figure 1

The molecular structure of (I), showing the crystallographic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $-x, -y, -z$.]

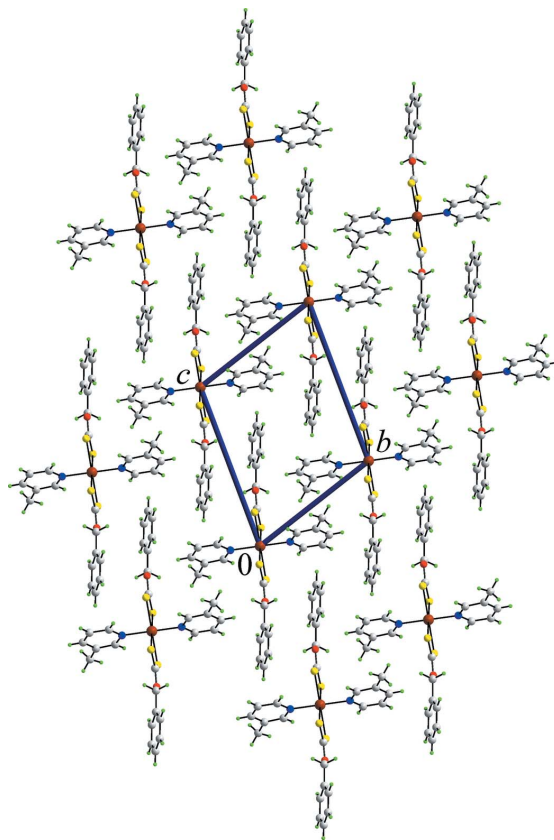


Figure 2

A view of the packing in (I) (Brandenburg, 2006). Colour code: Ni brown, S yellow, O red, N blue, C grey and H green.

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