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Tris(*N*,*N*-diethyldithiocarbamato-$\kappa^2 S,S'$)nickel(II)

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.022
wR factor = 0.060
Data-to-parameter ratio = 28.1

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

The title compound, $[Ni(C_5H_{10}NS_2)_3]$, belongs to the symmetry point group C_2. The Ni atom, one ring C atom and its adjacent N atom are located on a twofold rotation axis. Thus, there is just one half-molecule in the asymmetric unit. The compound is isostructural with the Fe and Co analogues.

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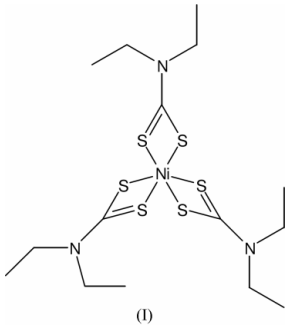
Comment

The title compound, (I), belongs to the symmetry point group C_2. Atoms Ni1, C1 and N1 are located on a twofold rotation axis. Thus, there is just one half-molecule in the asymmetric unit. Compound (I) is isostructural with the Fe (Leipoldt & Coppens, 1973) and Co analogues (Brennan & Bernal, 1969; Merlino, 1968; Healy *et al.*, 1990; Kong *et al.*, 1998).



(I)

Experimental

In an effort to synthesize a macrocyclic transition metal complex, we added nickel nitrate hexahydrate, tris(2-aminoethyl)amine and sodium diethyldithiocarbamate to DMSO as solvent medium. From the product mixture, we isolated suitable single crystals. The resulting structure was totally unexpected.

Crystal data

$[Ni(C_5H_{10}NS_2)_3]$
M_r = 503.49
Monoclinic, *C*2/*c*
a = 14.0208 (9) Å
b = 10.2305 (7) Å
c = 16.9031 (11) Å
β = 109.630 (5)°
V = 2283.7 (3) Å^3
Z = 4
D_x = 1.464 Mg m^{-3}
Mo *Kα* radiation
Cell parameters from 15127 reflections
θ = 3.7–29.9°
μ = 1.40 mm^{-1}
T = 173 (2) K
Block, light violet
0.20 × 0.20 × 0.10 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 1990; Blessing, 1995)
T_{min} = 0.767, T_{max} = 0.872
16440 measured reflections
3232 independent reflections
2635 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 29.7°
h = −19 → 18
k = −14 → 14
l = −23 → 23

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.022$	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.061$	$(\Delta/\sigma)_{max} = 0.002$
$S = 0.96$	$\Delta\rho_{max} = 0.39$ e Å^{-3}
3232 reflections	$\Delta\rho_{min} = -0.80$ e Å^{-3}
115 parameters	

Table 1
Selected geometric parameters (Å).

Ni1—S3	2.2677 (4)	C1—S2	1.7161 (11)
Ni1—S1	2.2709 (4)	C4—S3	1.7166 (13)
Ni1—S2	2.2717 (4)	C4—S1	1.7178 (13)

All H atoms could be located in a difference Fourier synthesis and were refined with fixed individual displacement parameters [U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C_{methyl})], using a riding model with secondary C—H = 0.99 Å or methyl C—H = 0.98 Å.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991).

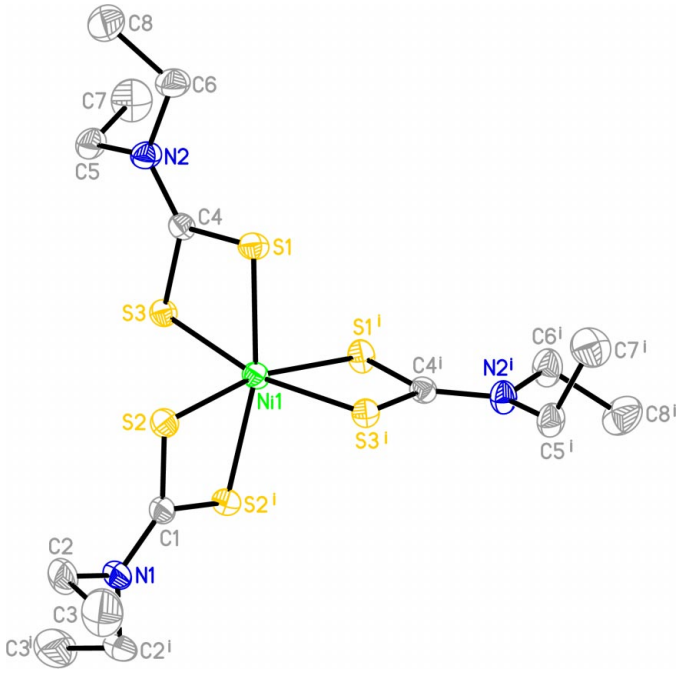


Figure 1
Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level. H atoms have been omitted for clarity. [Symmetry code: (i) $1 - x, y, \frac{3}{2} - z$.]

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