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Bis(*N*-cyclohexyl-*N*-ethyldithiocarbamato-*S*,*S*′)lead(II)

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Key indicators

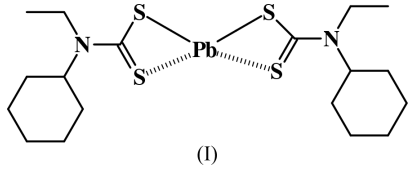
Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.011 Å
R factor = 0.053
wR factor = 0.146
Data-to-parameter ratio = 35.3

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

The Pb atom in the title compound, $[Pb(C_9H_{16}NS_2)_2]$, is chelated in an anisobidentate manner by the dithiocarbamate group [Pb—S = 2.710 (2)/2.883(2) Å and 2.700 (2)/2.841(2) Å]. The four-coordinate geometry is raised to six through the involvement of the double-bonded S atoms of adjacent dithiocarbamato groups; the Pb···S interactions [Pb···S = 3.457 (2) and 3.508 (2) Å] result in a chain structure for the compound.

Comment

Several lead(II) dithiocarbamates have been reported in the literature, *e.g.* bis(dimethyldithiocarbamato)lead (Iwasaki, 1980), bis(diethyldithiocarbamato)lead (Zvonkova *et al.*, 1967), bis(diisopropyldithiocarbamato)lead (Ito & Iwasaki, 1980) and bis(*N*-ethyl-*N*-isopropyldithiocarbamato)lead(II) (Trindade *et al.*, 1997; Ng, 1999). These compounds, as well as the title dithiocarbamate, (I), have the Pb atoms in a distorted tetrahedral geometry, and adjacent molecules are linked by Pb···S interactions into chains. The bond dimensions as well as the interactions in the title compound are similar to those found in other dithiocarbamates, and the size of the cyclohexyl ring does not appear to affect the packing.



(I)

Experimental

An excess quantity of carbon disulfide was added dropwise to a solution of lead(II) chloride and ethylcyclohexylamine (1:2 molar ratio) in ethanol. The dithiocarbamate slowly separated from solution; this was collected and air dried to afford crystals (m.p. 421–422 K). Elemental analysis, found (calculated in parenthesis): C 35.37 (35.36), H 4.75 (5.23), N 4.73 (4.58), S 21.44% (20.96%).

Crystal data

$[Pb(C_9H_{16}NS_2)_2]$
M_r = 611.89
Triclinic, $P\overline{1}$
a = 9.7180 (2) Å
b = 10.1871 (2) Å
c = 11.8751 (3) Å
α = 95.586 (1)°
β = 92.978 (1)°
γ = 99.142 (1)°
V = 1152.45 (4) Å^3
Z = 2
D_x = 1.763 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4596 reflections
θ = 2.6–33.2°
μ = 7.69 mm^{-1}
T = 298 (2) K
Parallelepiped, yellow
0.48 × 0.28 × 0.24 mm

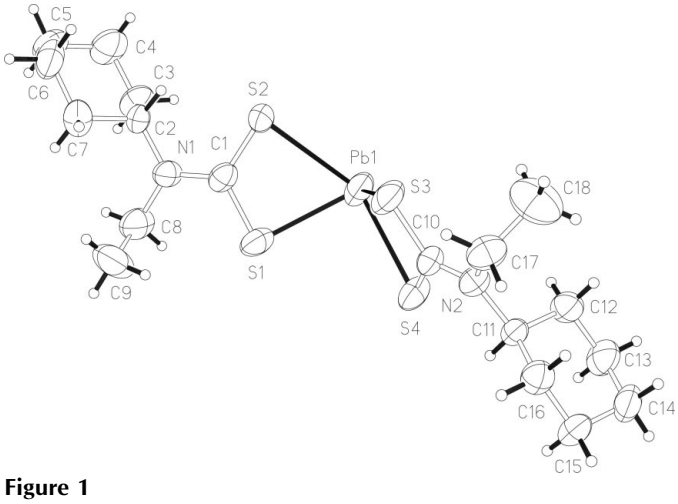


Figure 1
*ORTEP*II (Johnson, 1976) plot of (I) at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

Data collection

Siemens CCD area-detector diffractometer	7977 independent reflections
ω scans	4557 reflections with $(I) > 2\sigma(I)$
Absorption correction: empirical (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.030$
$T_{min} = 0.073$, $T_{max} = 0.158$	$\theta_{max} = 33.18^\circ$
10 652 measured reflections	$h = -11 \rightarrow 14$
	$k = -15 \rightarrow 15$
	$l = -18 \rightarrow 14$

Refinement

Refinement on F^2	H atoms constrained
$R[F^2 > 2\sigma(F^2)] = 0.053$	$w = 1/[\sigma^2(F_o^2) + (0.0650P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.146$	$(\Delta/\sigma)_{max} < 0.001$
$S = 0.99$	$\Delta\rho_{max} = 1.32$ e Å^{-3}
7977 reflections	$\Delta\rho_{min} = -2.09$ e Å^{-3}
226 parameters	

Table 1
Selected geometric parameters (Å, °).

Pb1—S1	2.710 (2)	Pb1—S3	2.700 (2)
Pb1—S2	2.883 (2)	Pb1—S4	2.841 (2)
Pb1—S2^{i}	3.508 (2)	Pb1—S4^{ii}	3.457 (2)
S1—Pb1—S2	64.0 (1)	S2—Pb1—S4^{ii}	141.6 (1)
S1—Pb1—S2^{i}	117.3 (1)	S2^{i}—Pb1—S3	122.1 (1)
S1—Pb1—S3	98.9 (1)	S2^{i}—Pb1—S4	148.0 (1)
S1—Pb1—S4	90.0 (1)	S2^{i}—Pb1—S4^{ii}	80.8 (1)
S1—Pb1—S4^{ii}	111.4 (1)	S3—Pb1—S4	64.6 (1)
S2—Pb1—S2^{i}	70.4 (1)	S3—Pb1—S4^{ii}	127.5 (1)
S2—Pb1—S3	89.9 (1)	S4—Pb1—S4^{ii}	73.3 (1)
S2—Pb1—S4	140.9 (1)		

Symmetry codes: (i) $-x, 1-y, -z$; (ii) $1-x, 1-y, -z$.

The diffraction data are complete to $\theta = 25^\circ$; the overall, slightly low, completeness of the diffraction data is because of the incompleteness in the $25 < \theta < 33^\circ$ range.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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