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N-Benzylmethanaminium *N*-benzyl-*N*-methyldithiocarbamate

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Key indicators

Single-crystal X-ray study
T = 233 K
Mean σ(C–C) = 0.002 Å
R factor = 0.037
wR factor = 0.096
Data-to-parameter ratio = 18.8

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

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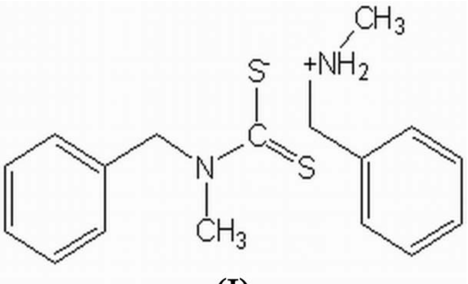
The title compound, $C_8H_{12}N^+\cdot C_9H_{10}NS_2^-$, is salt formed between a dithiocarbamate and an asymmetric secondary amine. The crystal packing is stabilized by N—H···S hydrogen bonds.

Comment

Dithiocarbamates find extensive applications as biocides, as additives for lubricants (Shivram & Vinal, 2003), as tumour-cell inhibitors (Scozzafava *et al.*, 2001), as compounds exhibiting nephrotoxicity, nausea, ototoxicity, neurotoxicity and myelotoxicity (Von Hoff *et al.*, 1979), and as fungicides and insecticides (Leroux, 1996). Dithiocarbamates have been widely reported in the last three years, owing to their anti-oxidant, antiviral and anti-inflammatory properties and metal transport in membranes (Faraglia *et al.*, 2005). Dithiocarbamate complexes are also used as a precursors in chemical vapour deposition processes and as catalysts (Bochmann, 1996). Dithiocarbamates are a versatile class of ligand which also stabilize transition metals in a wide range of oxidation states (Hogarth, 2005). Ammonium pyrrolidinedithiocarbamate (APDTC) has been widely used as a chelating agent for the determination of trace metals, due to its thermodynamically stable metal complexes (Dapaah & Ayame, 1998). In the rubber industry, *N*-ethyl-*N*-phenyldithiocarbamate (EPDTC) is used in the process of vulcanization of rubber compounds to form a group of ultra-accelerators in the curing process. The crystal structure of the title compound, (I), was determined in order to establish the mutual orientation of the anion and cation.



(I)

Compound (I) is a salt of a dithiocarbamate and an asymmetric secondary amine. The C1—S1 and C1—S2 bond distances of 1.714 (2) and 1.716 (2) Å, respectively, show partial double-bond character, due to the delocalization of negative charge on the S atoms.

The crystal packing is stabilized by N—H···S hydrogen bonds (Table 1).

Experimental

The title compound was synthesized by a modification of the method of Garje & Jain (2003). Dropwise addition of carbon disulfide (2.96 ml, 50.0 mmol, Aldrich) in to an *n*-hexane solution (50 ml) of *N*-methylbenzylamine (4.92 ml, 50.0 mmol, Aldrich) with constant stirring at 273 K resulted a solid product, which was filtered off, washed with an excess of *n*-hexane and recrystallized from a solution in dichloromethane–*n*-hexane (9:1). Colourless prismatic crystals of (I) suitable for single-crystal X-ray diffraction analysis were obtained in 80% yield.

Crystal data

$C_8H_{12}N^+\cdot C_9H_{10}NS_2^-$
$M_r = 318.49$
Monoclinic, $P2_1/n$
$a = 10.0903$ (2) Å
$b = 15.3530$ (4) Å
$c = 11.3422$ (3) Å
$\beta = 105.801$ (2)°
$V = 1690.70$ (7) Å^3
$Z = 4$
$D_x = 1.251$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.31$ mm^{-1}
$T = 233$ (2) K
Prism, colourless
0.3 × 0.25 × 0.15 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: none
10817 measured reflections
3742 independent reflections
3213 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\rm max} = 27.2°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.096$
$S = 1.04$
3742 reflections
199 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0391P)^2 + 0.5808P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.37$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.45$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.019 (2)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2NA···S1	0.917 (19)	2.293 (19)	3.1630 (15)	158.3 (17)
N2—H2NB···S2$^{\rm i}$	0.90 (2)	2.38 (2)	3.2131 (15)	153.0 (17)

Symmetry code: (i) $-x, -y+1, -z$.

The H atoms on N2 were located in a difference map and refined isotropically. All H atoms bound to C atoms were refined using a riding model, with C—H = 0.94 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic H, C—H = 0.98 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for CH$_2$, and C—H = 0.97 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for CH$_3$.

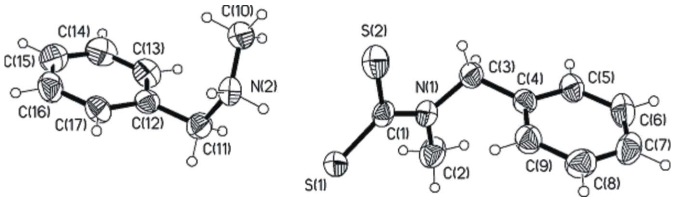


Figure 1
A perspective view of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXL97*.

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