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Crystallographic report

Tris(*N*,*N*-dimethyldithiocarbamato)arsenic(III) dichloromethane solvate

Danlin Chen, Chian Sing Lai and Edward R. T. Tiekink*

Department of Chemistry, National University of Singapore, Singapore 117543, Singapore

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The structure of $As(S_2CNMe_2)_3$ has approximate threefold symmetry and features essentially monodentate dithiocarbamate ligands, so that the geometry is trigonal pyramidal. Copyright © 2003 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; arsenic; dithiocarbamate

COMMENT

The dithiocarbamate ligands in $As(S_2CNMe_2)_3$ essentially coordinate in the monodentate mode forming As–S distances of approximately 2.3 Å; Fig. 1. The thione sulfur atoms are about 2.9 Å from the arsenic atom. An alternate description of the coordination geometry is one based on a distorted octahedron in which the lone pair of electrons projects out of the triangular face defined by the S2, S4 and S6 atoms, thereby elongating these bonds. Binary arsenic(III) dithiocarbamates[1–3] and the more studied xanthates $As(S_2COR)_3$,[4–9] essentially adopt the same structural motif as described for $As(S_2CNMe_2)_3$.

EXPERIMENTAL

Crystals were isolated as a dichloromethane solvate from a dichloromethane/ethanol (1/1) solution containing $As(S_2CNMe_2)_3$ that had been prepared by the standard method;[1] m. p. 211.5–212.4 °C. NMR ($CDCl_3$): ^1H, δ 3.34 (CH_3) ppm; ^{13}C, δ 198.6 (C_{quat}), 43.1 (CH_3) ppm. Intensity data for **I** were collected at 223 K on a Bruker AXS SMART CCD diffractometer for a colourless block 0.21 × 0.23 × 0.31 mm^3. $C_{10}H_{20}AsCl_2N_3S_6$, $M = 520.5$, monoclinic, $P2_1/c$, $a = 13.1676(9)$, $b = 7.2662(5)$, $c = 22.8898(15)$ Å, $\beta = 92.005(2)°$, $V = 2188.7(3)$ Å^3, $Z = 4$, 6387 unique data (θ_{max} 30.0°), $R = 0.053$ (all data), $wR = 0.114$ (all data), $\rho_{max} = 1.17$ e$^-$ Å^{-3} (near arsenic). Programs used: teXsan, DIRDIF, SHELXL, and ORTEP. CCDC deposition number: 210 642.

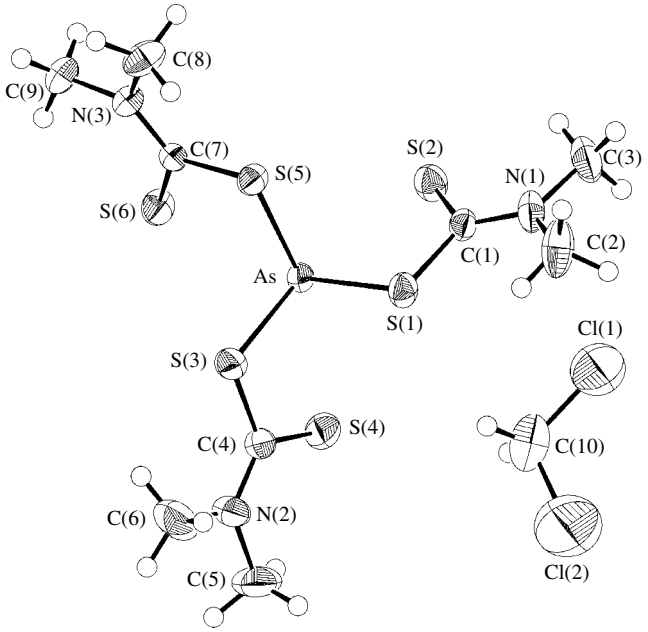

Figure 1. Molecular structure of $As(S_2CNMe_2)_3 \cdot CH_2Cl_2$. Key geometric parameters: As–S(1) 2.3083(7), As–S(3) 2.3089(7), As–S(5) 2.3333(6) Å; S(1)–As–S(3) 89.67(3), S(1)–As–S(5) 88.57(2), S(3)–As–S(5) 87.94(2)°.

*Correspondence to: Edward R. T. Tiekink, Department of Chemistry, National University of Singapore, Singapore 117543, Singapore.
E-mail: chmtert@nus.edu.sg
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