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Crystallographic report

Bis[tris(morpholindithiocarbamato)bismuth(III)]

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The dimeric and centrosymmetric structure of $\{Bi[S_2CN(CH_2CH_2)_2O]_3\}_2$ features chelating dithiocarbamate ligands and intermolecular Bi–S interactions, so that a distorted pentagonal bipyramidal S_7 coordination geometry results. Copyright © 2004 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; bismuth; dithiocarbamate

COMMENT

The structural chemistry of bismuth 1,1-dithiolates is both rich and diverse, with a variety of structural motifs known.[1–4] In the title structure (Fig. 1), a dimeric structure is found with a seven-coordinate distorted S_7 pentagonal bipyramidal geometry for bismuth in accord with related structures.

EXPERIMENTAL

An aqueous solution of $Bi(NO_3)_3{\cdot}5H_2O$ (1.0 mmol) and mannite (1.0 mmol) was added to an aqueous solution of sodium morpholindithiocarbamate (3.0 mmol) and stirred for 0.5 h at 50 °C. The yellow product was recrystallized from acetonitrile solution to give yellow crystals, m.p. 299 °C (dec.). IR (KBr), ν: 1490, 1464, 1382, 1138, 997, 924, 911, 452 cm^{-1}. Intensity data were collected at 293 K on a Bruker Smart 1000 CCD for a block $0.04 \times 0.08 \times 0.20$ mm^3. $C_{15}H_{24}BiN_3O_3S_6$, $M = 695.71$, monoclinic, $P2_1/c$, $a = 12.904(5)$, $b = 20.060(7)$, $c = 9.053(3)$ Å, $\beta = 94.387(7)^o$, $V = 2336.5(14)$ $Å^3$, $Z = 4$, 3982 unique data ($\theta_{max} = 25.0°$), $R = 0.044$ (1955 data with $I > 2\sigma(I)$), $wR = 0.072$ (all data). Programs used: SHELXL and ORTEP. CCDC deposition number: 232523.

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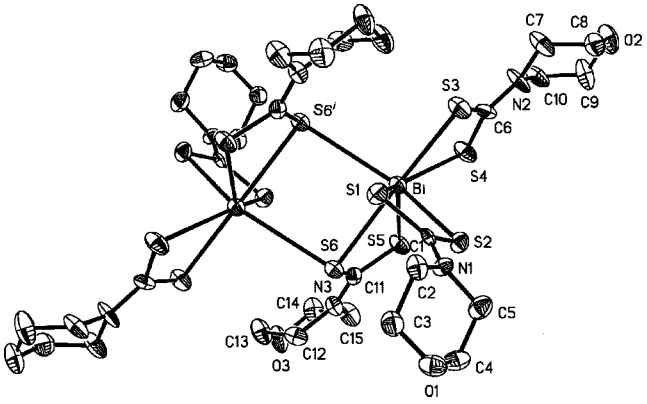

Figure 1. The molecular structure of $\{Bi[S_2CN(CH_2CH_2)_2O]_3\}_2$; hydrogen atoms have been omitted for clarity. Key geometric parameters: Bi–S1 2.864(3), Bi1–S2 2.591(3), Bi–S3 2.839(3), Bi–S4 2.783(3), Bi–S5 2.799(3), Bi–S6 2.943(3), Bi–S(6)^i 3.223(3) Å. Symmetry operation i : $1-x$, $-y$, $2-z$.

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