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Crystallographic report

Bis[(nitro)bis(dithiotetrahydropyrrolocarbamato) bismuth(III)]

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The loosely associated centrosymmetric structure of $[Bi(S_2CNC_4H_8)_2(NO_3)]_2$ features chelating dithiocarbamate and nitrate ligands, as well as weak intermolecular Bi–S interactions, so that a distorted pentagonal bipyramidal S_5O_2 coordination geometry results. Copyright © 2005 John Wiley & Sons, Ltd.

KEYWORDS: crystal structure; bismuth; dithiocarbamate; nitrate

COMMENT

The structural chemistry of bismuth 1,1-dithiolates is both rich and diverse, so that monomeric,[1] dimeric,[2] and linear polymeric species are known.[3] In the title structure (Fig. 1), a mixed-ligand loosely associated dimeric structure containing both dithiocarbamate and nitrate ligands is found. The bismuth atom is in a seven-coordinated, distorted S_5O_2 pentagonal bipyramidal geometry owing to one of the dithiocarbamate ligands chelating one bismuth center and, via the S4 atom, simultaneously bridging a centrosymmetrically related bismuth atom.

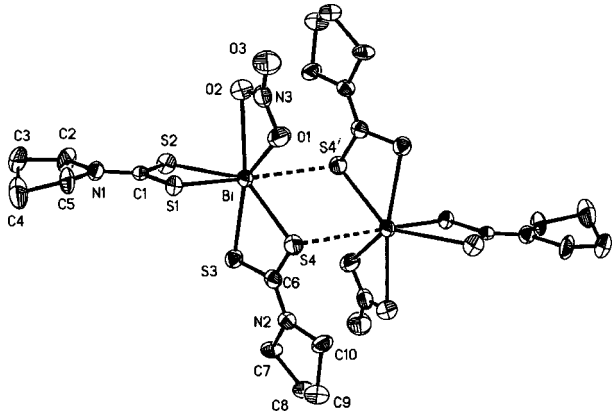

Figure 1. The molecular structure of $[Bi(S_2CNC_4H_8)_2(NO_3)]_2$; hydrogen atoms are omitted for clarity. Key geometric parameters: Bi–S1 2.5727(15), Bi–S2 2.7786(17), Bi–S3 2.6656(16), Bi–S4 2.7727(17), Bi–O1 2.630(5), Bi–O2 2.738(4), Bi–S4^i 3.4320(18) Å. Symmetry operation *i*: $1-x, -y, 1-z$.

EXPERIMENTAL

$[Bi(NO_3)(S_2CNC_4H_8)_2]_2$ was obtained from the 1 : 2 reaction between $Bi(NO_3)_3 \cdot 5H_2O$ and the sodium salt of the ligand as per the literature method.[2] Crystals were isolated from the slow evaporation of a CH_3CN solution of the compound; m.p. 335 °C (dec.). IR (KBr) ν: 1631, 1500, 1443, 1385, 1148, 1021, 993, 693, 553, 450 cm^{-1}. Data were collected at 299 K on a Bruker Smart 1000 CCD for a block $0.10 \times 0.10 \times 0.20$ mm^3. $C_{20}H_{32}Bi_2N_6O_6S_8$, $M = 1126.96$, monoclinic, $P2_1/n$, $a = 6.4718(13)$, $b = 26.738(6)$, $c = 10.423(2)$ Å, $\beta = 106.384(3)°$, $V = 1730.3(6)$ $Å^3$, $Z = 2$, $R = 0.029$ (2040 data with $I \geq 2\sigma(I)$; θ_{max} 25.0°), $wR = 0.045$ (all 3047 data). Programs used: SHELXL and ORTEP. CCDC deposition number: 179 925.

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