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Crystallographic report

Bis[bis(*N*-methyl-*N*-phenyldithiocarbamato)-(methylxanthato)bismuth(III)]

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The centrosymmetric structure of $\{Bi[S_2CN(Me)Ph]_2(S_2COMe)\}_2$ features chelating dithiocarbamate and xanthate ligands, as well as 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; xanthate

COMMENT

The structural chemistry of bismuth dithiocarbamates and bismuth xanthates is both rich and diverse, so that monomeric,[1] dimeric,[2–6] and linear polymeric species are known.[7–9] In the title structure (Fig. 1), a mixed dimeric structure containing both dithiocarbamate and xanthate ligands is found. The bismuth atoms are seven-coordinated distorted S_7 pentagonal bipyramidal geometry owing to one of the dithiocarbamate ligands chelating one bismuth centre and via the S3 atom simultaneously bridging a centrosymmetrically related bismuth atom.

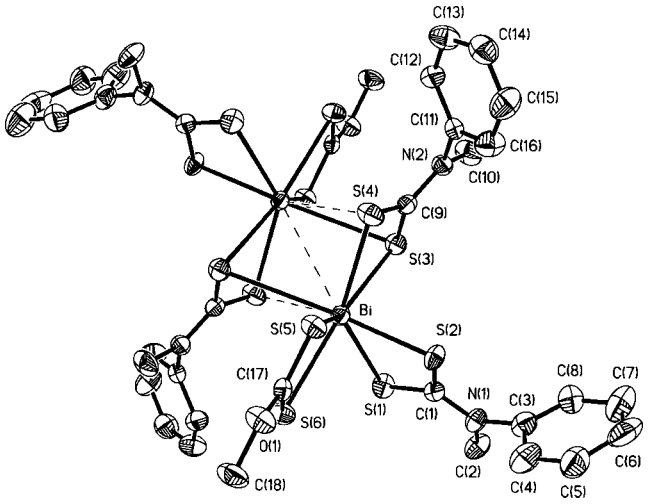

Figure 1. The molecular structure of $\{Bi[S_2CN(Me)Ph]_2(S_2COMe)\}_2$. Key geometric parameters: Bi–S1 2.9193(16), Bi1–S2 2.6122(14), Bi–S3 2.9392(18), Bi–S4 2.7925(17), Bi–S5 2.7470(15), Bi–S6 2.8984(19), Bi–S3^i 3.2490(16) Å; S1–Bi–S2, 64.55(4), S1–Bi–S3 79.49(5), S1–Bi–S4 135.84(5), S1–Bi–S5 132.40(5), S1–Bi–S6 80.44(5), S2–Bi–S3 87.90(5), S2–Bi–S4 91.29(5), S2–Bi–S5 85.50(5), S2–Bi–S6 92.19(5), S3–Bi–S4 62.35(4), S3–Bi–S5 138.29(4), S3–Bi–S6 157.70(4), S4–Bi–S5 76.67(5), S4–Bi–S6 139.91(4), S5–Bi–S6 63.84(5), S1–Bi–S3^i 124.83(4), S2–Bi–S3^i 166.73(4), S3–Bi–S3^i 102.66(4), S4–Bi–S3^i 86.65(5), S5–Bi–S3^i 81.27(4), S6–Bi–S3^i 81.10(5)°. Symmetry code *i*: $-x+1, -y+2, -z+1$.

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 *N*-methyl-*N*-phenyldithiocarbamate (2.0 mmol) and sodium methylxanthate (1.0 mmol) and stirred for 2.0 h at 50 °C. A yellow solid was obtained by filtration. The product was recrystallized from acetonitrile to give yellow crystals, m.p. 274 °C (dec.). IR (KBr) ν: 3045, 2933, 2851, 1468, 1372, 1256, 1153, 1001, 954, 553, 464 cm^{-1}. Intensity data were collected at 298 K on a Bruker Smart 1000 CCD for a block $0.10 \times 0.10 \times 0.30$ mm^3. $C_{18}H_{19}BiN_2OS_6$, $M = 680.69$, triclinic, $P\bar{1}$, $a = 10.272(2)$, $b = 10.523(2)$, $c = 12.700(3)$Å, $\alpha = 99.821(3)$, $\beta = 92.494(3)$, $\gamma = 116.729(3)°$, $V = 1196.8(4)$Å^3, $Z = 2$, 4393 unique data ($\theta_{max} = 26.4°$), $R_1 = 0.035$ (3262 data with $I > 2\sigma(I)$), $wR_2 = 0.052$

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(all data); $\rho_{max} = 1.08\ e^{-}\ Å^{-3}$. Programs used: SHELXL and ORTEP. CCDC deposition number: 179929.

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