Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

trans-Tetrabromobis(dimethylamine)tin

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Received 11 October 2002
Accepted 21 October 2002
Online 31 October 2002

Key indicators

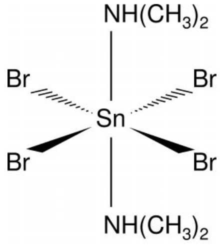
Single-crystal X-ray study
T = 298 K
Mean σ(N–C) = 0.005 Å
R factor = 0.025
wR factor = 0.065
Data-to-parameter ratio = 21.9

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

The title compound, [$SnBr_4(C_2H_7N)_2$], consists of separate centrosymmetric molecules with nearly octahedral geometry, in which the central Sn metal is surrounded by four Br atoms and two dimethylamine ligands. The unique Sn—N bond length is 2.244 (3) Å and the two Sn—Br lengths are 2.5867 (11) and 2.5707 (12) Å. The C—N bond lengths of the amine ligand are 1.482 (6) and 1.492 (6) Å. The unique angle in the $SnBr_4$ plane is 90.82 (3)°, and the axial to equatorial angles are 86.18 (10) and 85.46 (10)°.

Comment

Recently, we have utilized reactions between common germanium hydrides and SnD_4 to grow epitaxic layers of $Ge_{1-x}Sn_x$ semiconductors on Si(100) substrates. The bandgaps of these materials are intermediate between those of Ge (Eg = 0.066 eV) and Sn (Eg = 0.1 eV), and decrease monotonically with increasing Sn concentration in the alloy, indicating that this material will have important application in Si-based devices, such as IR photodetectors. The application of pure SnD_4 is the essential component in the preparation of these metastable and technologically important materials. SnD_4 is synthesized by reduction of $SnBr_4$ with $LiAlD_4$ and it is typically isolated as a volatile liquid, which is unstable at room temperature with respect to Sn and D_2. Nevertheless, mixtures of the compound with high-purity H_2 have the necessary stability at 295 K to be used as viable CVD sources in deposition of $Ge_{1-x}Sn_x$ (Bauer, Taraci *et al.*, 2002). Ongoing efforts to further stabilize SnD_4 by adduct formation with simple Lewis bases, such as dimethylamine, have led to the synthesis of the previously unknown complex $SnBr_4[HN(CH_3)_2]_2$. This compound is currently utilized to prepare the corresponding SnH_4 and SnD_4 derivatives as viable low-temperature CVD precursors of Sn.



(I)

The central Sn metal of the title compound is sixfold coordinated, with four Br atoms arranged in square-planar fashion and the two amine ligands nearly perpendicular to the $SnBr_4$ plane (Fig. 1). The Sn—Br bond distances are

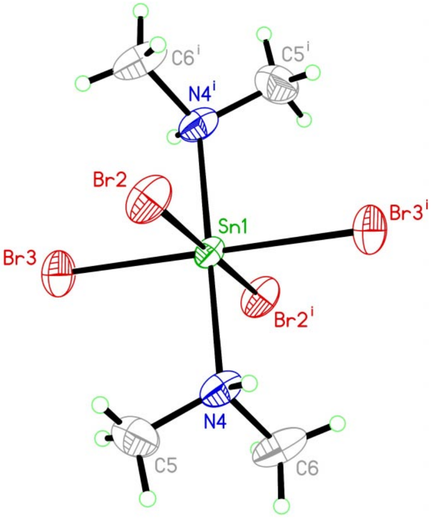


Figure 1
Displacement ellipsoid plot shown at the 50% probability level [symmetry code: (i) $-x$, $-y$, $-z$].

2.5867 (11) (Sn1—Br2) and 2.5707 (12) Å (Sn1—Br3). These values are significantly longer than those reported for a related $SnBr_4$(dioxane) complex (Bauer, Groy & Kouvetakis, 2002), which are in the range 2.5005 (7)–2.5045 (6) Å. The angles within the $SnBr_4$ square plane are nearly 90° [90.82 (3)° for Br2—Sn1—Br3] and the angles between the plane and the axis of the $HN(CH_3)_2$ ligands are 86.18 (10) (N4—Sn1—Br2) and 85.46 (10)° (N4—Sn1—Br3).

All H-atom positions were calculated based on idealized geometry. The H atoms were then allowed to ride on their bonding partners during the final stages of refinement. There is an indication of intermolecular interaction between one amine H atom and the nearest neighbor Br atom, since the Br2···H4*A* distance is 2.63 Å and the N4—H4*A*···Br2 angle is 150°.

Experimental

$SnBr_4[HN(CH_3)_2]_2$ is readily synthesized in toluene by direct combination of $SnBr_4$ with purified $HN(CH_3)_2$. This compound has been characterized by spectroscopic methods and combustion analysis. Single crystals have been grown by slowly cooling concentrated toluene solutions of the compound.

Crystal data

$[SnBr_4(C_2H_7N)_2]$
$M_r = 528.50$
Monoclinic, $P2_1/c$
$a = 6.592$ (4) Å
$b = 12.029$ (7) Å
$c = 8.326$ (5) Å
$\beta = 96.114$ (11)°
$V = 656.5$ (7) Å^3
$Z = 2$

$D_x = 2.674$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3041 reflections
$\theta = 3.0$–25.1°
$\mu = 14.08$ mm^{-1}
$T = 298$ (2) K
Block, colorless
0.28 × 0.21 × 0.14 mm

Data collection

Bruker SMART APEX diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2001)
$T_{min} = 0.034$, $T_{max} = 0.135$
5130 measured reflections

1161 independent reflections
1028 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 25.1°$
$h = -7 \rightarrow 7$
$k = -14 \rightarrow 14$
$l = -9 \rightarrow 9$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.065$
$S = 1.05$
1161 reflections
53 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0306P)^2 + 0.2351P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.71$ e Å^{-3}
$\Delta\rho_{min} = -0.73$ e Å^{-3}
Extinction correction: *SHELXTL*
Extinction coefficient: 0.0021 (5)

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

The authors thank the National Science Foundation for its contribution toward the purchase of the single-crystal diffraction instrument that was used in this study (CHE-9808440). JK acknowledges NSF support (DMR-0221993).

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Acta Cryst. (2002). E**58**, m684–m685 Cole Ritter III *et al.* • $[SnBr_4(C_2H_7N)_2]$ **m685**