Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Hydrogen bonding in dibromo[2-(dimethylaminomethyl)phenyl][2-(dimethylammoniomethyl)phenyl]tin(IV) tetrabromo[2-(dimethylaminomethyl)phenyl]tin(IV)

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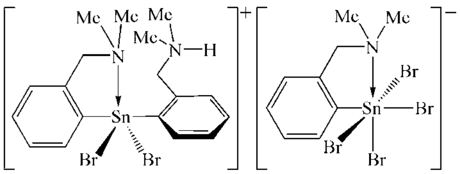
Received 23 October 2006
Accepted 28 November 2006
Online 13 January 2007

The molecular structure of the title compound, $[SnBr_2(C_9H_{12}N)(C_9H_{13}N)][SnBr_4(C_9H_{12}N)]$, consists of a dibromobis[2-(dimethylaminomethyl)phenyl][2-dimethylammoniomethyl)phenyl]tin(IV) cation and a tetrabromo[2-(dimethylaminomethyl)phenyl]tin(IV) anion. As a result of strong intramolecular N→Sn interactions, distorted trigonal–bipyramidal and octahedral coordination geometries are established for the metal centres of the diorganotin(IV) and monoorganotin(IV) fragments, respectively. The cation and anion are linked together by two Br···H contacts, while three additional similar contacts result in a dimeric fragment which repeats in a two-dimensional supramolecular arrangement.

Comment

During our work on organotin(IV) halides containing the $2-(Me_2NCH_2)C_6H_4$ group (Varga, 2003; Varga *et al.*, 2001, 2005, 2006), we isolated the title compound, (I), in which two ionic organotin(IV) fragments are present (Fig. 1). The structure is similar to that of the chloride derivative (Novak *et al.*, 2006), but for the latter no intra- or intermolecular interactions were discussed.



(I)

The cationic fragment of compound (I) contains an Sn atom with a trigonal–bipyramidal coordination geometry due to the strong intramolecular N→Sn interaction established by the N atom of the pendant arm from one organic ligand [Sn2—N2 = 2.421 (8) Å], while the other pendant arm is protonated at the N atom and is twisted away from the Sn centre. The anion has a hexacoordinated Sn atom, with the C atom of the ligand and the N atom from the intramolecularly coordinated NMe_2 group [Sn1—N1 = 2.425 (6) Å] in *cis* positions.

Both the (C,N)CSnBr$_2$ and (C,N)SnBr$_4$ cores are distorted from ideal geometry as a consequence of the small 'bite' of the pendant arm ligand [C10—Sn2—N2 = 75.5 (3)° and C1—Sn1—N1 = 78.4 (3)°]. The deviation of the metal atom (Sn2) from the equatorial plane (C10/C19/Br6) is 0.23 Å towards atom Br5 in the case of the cation, while in the anion, atom C1 is displaced by 0.55 Å from the best plane determined by atoms Sn1/Br3/Br2/Br4, towards the pendant arm.

The intramolecular N→Sn interaction induces planar chirality at the metal centre (Varga *et al.*, 2005, 2006) and the title compound crystallizes as a racemate, *i.e.* a mixture of $S_{N2}R_{N1}$ and $R_{N2}S_{N1}$ isomers.

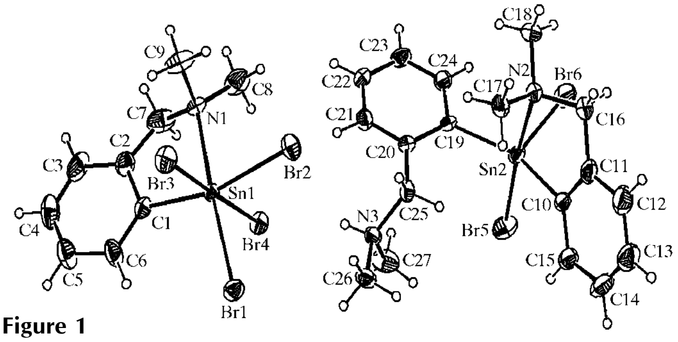


Figure 1
A view of compound (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii.

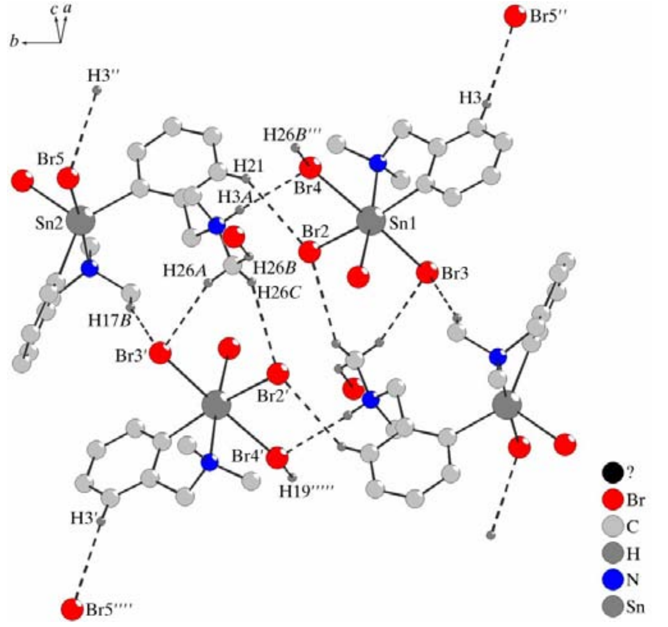


Figure 2
The hydrogen bonding (dashed lines) in the crystal structure of compound (I). [Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$; (iv) $x-1, y, z-1$; (v) $x, y, z-1$.]

DOI: 10.1107/S010827010605150X

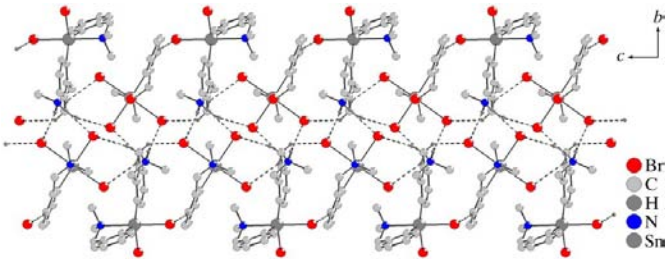


Figure 3
The supramolecular arrangement of (I). Hydrogen bonds are shown as dashed lines.

The anion and cation of (I) are linked together by a hydrogen-bond contact between one Br atom from the $S_{\rm N1}$-[{2-(Me$_2$NCH$_2$)C$_6$H$_4$}SnBr$_4$]$^-$ anion and the H atom from the protonated pendant arm of the $R_{\rm N2}$-[{2-(Me$_2$NCH$_2$)C$_6$H$_4$}{2-(Me$_2$NHCH$_2$)C$_6$H$_4$}SnBr$_2$]$^+$ cation [Br4···H3$A^{\rm i}$ = 2.54 Å; symmetry code: (i) $1 - x, -y, -z$]. Also, another hydrogen-bond type of interaction is formed between the $R_{\rm N2}S_{\rm N1}$ and $S_{\rm N2}R_{\rm N1}$ units (Br4···H26A = 3.116 Å), leading to a dimeric fragment (Fig. 2). This fragment is repeated in a two-dimensional supramolecular arrangement through the weak Br···H contacts (range 2.94–3.11 Å) (Fig. 3).

By contrast, a different supramolecular arrangement based on Cl···H contacts is observed for the chloride analogue (Novak *et al.*, 2006). On the basis of the CIF file kindly provided by the Cambridge Crystallographic Data Centre, we found that in this case the anion and cation are connected through two Cl···H interactions (Cl1···H17B = 2.81 Å and Cl3···H17C = 2.82 Å), while three other interactions [Cl1···H12$^{\rm vi}$ = 2.78 Å, Cl1···H16B = 2.98 Å and Cl4···H1$^{\rm vi}$ = 2.39 Å; symmetry code: (vi) $-x, -y, -z+1$] lead to the formation of a dimeric structure. An interaction between the dimeric units (Cl2···H18C = 2.89 Å) connects them into a polymeric chain.

Experimental

The title compound was obtained by the reaction between [{2-(Me$_2$NCH$_2$)C$_6$H$_4$}{2-(Me$_2$NHCH$_2$)C$_6$H$_4$}SnCl$_2$]$^+$[{2-(Me$_2$NCH$_2$)-C$_6$H$_4$}SnCl$_4$]$^-$ and excess KBr in a CH$_2$Cl$_2$–H$_2$O mixture (1:1). Crystals of (I) suitable for X-ray diffraction were obtained from a solution in a CH$_2$Cl$_2$–*n*-hexane (1:4) mixture.

Crystal data

[SnBr$_2$(C$_9$H$_{12}$N)(C$_9$H$_{13}$N)]-[SnBr$_4$(C$_9$H$_{12}$N)]
M_r = 1120.44
Monoclinic, $P2_1/c$
a = 9.5330 (5) Å
b = 36.635 (2) Å
c = 10.0344 (6) Å
β = 95.4790 (10)°
V = 3488.4 (3) Å^3
Z = 4
D_x = 2.133 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 8.33 mm^{-1}
T = 297 (2) K
Block, colourless
0.24 × 0.21 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{\rm min}$ = 0.141, $T_{\rm max}$ = 0.368
25246 measured reflections
6137 independent reflections
5141 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.048
$\theta_{\rm max}$ = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.122
S = 1.11
6137 reflections
353 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0502P)^2 + 13.0344P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max}$ = 0.001
$\Delta\rho_{\rm max}$ = 1.10 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.98 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Br1—Sn1	2.5847 (10)	C1—Sn1	2.125 (8)
Br2—Sn1	2.5386 (10)	C10—Sn2	2.128 (8)
Br3—Sn1	2.6154 (10)	C19—Sn2	2.123 (8)
Br4—Sn1	2.7274 (10)	N1—Sn1	2.425 (6)
Br5—Sn2	2.6083 (14)	N2—Sn2	2.421 (8)
Br6—Sn2	2.4975 (11)		
C1—Sn1—N1	78.4 (3)	Br1—Sn1—Br4	88.41 (3)
C1—Sn1—Br2	165.1 (2)	Br3—Sn1—Br4	177.93 (4)
N1—Sn1—Br2	87.07 (17)	C19—Sn2—C10	141.6 (3)
C1—Sn1—Br1	102.3 (2)	C19—Sn2—N2	90.0 (3)
N1—Sn1—Br1	174.79 (16)	C10—Sn2—N2	75.5 (3)
Br2—Sn1—Br1	92.42 (4)	C19—Sn2—Br6	105.1 (2)
C1—Sn1—Br3	88.0 (2)	C10—Sn2—Br6	109.6 (2)
N1—Sn1—Br3	94.09 (16)	N2—Sn2—Br6	88.09 (16)
Br2—Sn1—Br3	89.94 (4)	C19—Sn2—Br5	95.3 (2)
Br1—Sn1—Br3	91.10 (3)	C10—Sn2—Br5	97.2 (3)
C1—Sn1—Br4	94.1 (2)	N2—Sn2—Br5	172.63 (17)
N1—Sn1—Br4	86.39 (16)	Br6—Sn2—Br5	95.46 (5)
Br2—Sn1—Br4	88.07 (3)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···Br4	0.86 (5)	2.54 (5)	3.373 (7)	161 (5)
C21—H21···Br2	0.93	2.96	3.714 (7)	139
C26—H26C···Br2$^{\rm i}$	0.96	2.94	3.698 (9)	137
C26—H26A···Br3$^{\rm i}$	0.96	2.94	3.652 (10)	132
C17—H17B···Br3$^{\rm i}$	0.96	3.07	3.999 (10)	162
C3—H3···Br5$^{\rm ii}$	0.93	3.02	3.926 (12)	166
C26—H26B···Br4$^{\rm iii}$	0.96	3.11	3.897 (9)	140

Symmetry codes: (i) $-x+1, -y+1, -z$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+1, -y+1, -z+1$.

All H atoms bonded to C atoms were placed in calculated positions and refined using a riding model, with C—H = 0.93–0.97 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl or 1.2$U_{\rm eq}$(C) for aryl H atoms. The methyl groups were allowed to rotate but not to tip. Atom H3A bonded to atom N3 was refined with an N—H DFIX restraint of 0.87 (5) Å.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SMART*; data reduction: *SAINT-Plus* (Bruker, 2000); program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *publCIF* (Westrip, 2006).

The authors thank the National Centre for X-ray Diffraction, Babes-Bolyai University, Cluj-Napoca, Romania, for performing the single-crystal X-ray diffraction study.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: AV3053). Services for accessing these data are described at the back of the journal.

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