

## Bis(2-bromopyridinium) hexabromido-stannate(IV)

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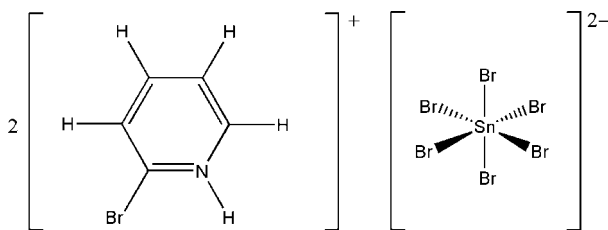
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 Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.020$  Å;  $R$  factor = 0.068;  $wR$  factor = 0.178; data-to-parameter ratio = 27.0.

The asymmetric unit of the title compound,  $(\text{C}_5\text{H}_5\text{BrN})_2\text{[SnBr}_6\text{]}$ , contains one cation and one half-anion. The  $[\text{SnBr}_6]^{2-}$  anion is located on an inversion center and forms a quasi-regular octahedral arrangement. The crystal structure consists of two-dimensional supramolecular layers assembled via hydrogen-bonding interactions of  $\text{N}-\text{H}\cdots\text{Br}-\text{Sn}$  [ $D\cdots A = 3.375$  (13)– $3.562$  (13) Å and  $D-\text{H}\cdots A = 127$ – $142^\circ$ , along with  $\text{C}-\text{Br}\cdots\text{Br}$  synthons [3.667 (2) and 3.778 (3) Å]. These layers are parallel to the  $bc$  plane and built up from anions interacting extensively with the six surrounding cations.

### Related literature

The title salt is isomorphous with the Te analogue (Fernandes *et al.*, 2004). For related literature, see: Al-Far & Ali (2007); Ali, Al-Far & Al-Sou'od (2007); Ali & Al-Far (2007); Ali, Al-Far & Ng (2007); Allen *et al.* (1987); Aruta *et al.* (2005); Hill (1998); Kagan *et al.* (1999); Knutson *et al.* (2005); Raptopoulou *et al.* (2002); Tudela & Khan (1991); Willey *et al.* (1998).



### Experimental

#### Crystal data

 $(\text{C}_5\text{H}_5\text{BrN})_2[\text{SnBr}_6]$   
 $M_r = 916.12$   
 Triclinic,  $P\bar{1}$   
 $a = 7.4037$  (15) Å  
 $b = 8.3393$  (17) Å  
 $c = 9.4302$  (19) Å

 $\alpha = 73.14$  (3)°  
 $\beta = 67.98$  (3)°  
 $\gamma = 82.44$  (3)°  
 $V = 516.4$  (2) Å<sup>3</sup>  
 $Z = 1$   
 Mo  $K\alpha$  radiation

 $\mu = 16.71$  mm<sup>-1</sup>  
 $T = 293$  (2) K

 $0.16 \times 0.13 \times 0.08$  mm

#### Data collection

 Bruker–Siemens SMART APEX diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2007)  
 $T_{\min} = 0.058$ ,  $T_{\max} = 0.261$ 

 2266 measured reflections  
 1807 independent reflections  
 1308 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.091$ 

#### Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.068$   
 $wR(F^2) = 0.178$   
 $S = 1.02$   
 1807 reflections

 67 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\text{max}} = 3.31$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -1.87$  e Å<sup>-3</sup>
**Table 1**

Selected geometric parameters (Å, °).

Sn1—Br3	2.5939 (15)	Sn1—Br4	2.6174 (17)
Sn1—Br1	2.6027 (15)		
Br3—Sn1—Br1	89.06 (5)	Br1—Sn1—Br4 <sup>i</sup>	90.21 (5)
Br3 <sup>i</sup> —Sn1—Br1	90.94 (5)	Br3—Sn1—Br4	90.57 (6)
Br3—Sn1—Br4 <sup>i</sup>	89.43 (6)	Br1—Sn1—Br4	89.79 (5)

 Symmetry code: (i)  $-x + 1, -y + 1, -z$ .

**Table 2**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
N1—H1 <sup>ii</sup> ⋯Br4 <sup>ii</sup>	0.86	2.65	3.375 (13)	142
N1—H1 <sup>iii</sup> ⋯Br1 <sup>iii</sup>	0.86	2.98	3.562 (13)	127

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

Data collection: SMART (Bruker, 2006); cell refinement: SAINT-Plus (Bruker, 2006); data reduction: SAINT-Plus; program(s) used to solve structure: XS in SHELXTL (Sheldrick, 2008); program(s) used to refine structure: XL in SHELXTL; molecular graphics: XP in SHELXTL; software used to prepare material for publication: XCIF in SHELXTL.

Al al-Bayt University and Al-Balqa'a Applied University are thanked for supporting this work

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BX2139).

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## supporting information

*Acta Cryst.* (2008). E64, m749–m750 [doi:10.1107/S1600536808012129]

**Bis(2-bromopyridinium) hexabromidostannate(IV)****Basem Fares Ali, Rawhi H. Al-Far and Salim F. Haddad****S1. Comment**

Noncovalent interactions play an important role in organizing structural units in both natural and artificial systems. Hybrid organic-inorganic compounds are of great interest owing to their ionic, electrical, magnetic and optical properties (Hill, 1998; Kagan *et al.*, 1999; Raptopoulou *et al.*, 2002). Tin metal-halo based hybrids are of particular interest as being materials with interesting optical and magnetic properties (Aruta *et al.*, 2005; Knutson *et al.*, 2005; Kagan *et al.*, 1999). We are currently carrying out studies about lattice including different types of intermolecular interactions (aryl $\cdots$ aryl,  $X\cdots X$ ,  $X\cdots$ aryl and  $X\cdots H$ ). Within our research of hybrid compounds containing tin metal (Al-Far & Ali 2007; Ali, Al-Far & Al-Sou'od, 2007; Ali & Al-Far, 2007; Ali, Al-Far & Ng, 2007), the crystal structure of the title salt, (I), has been investigated.

The asymmetric unit of (I) contains one cation and one-half anion (Fig. 1). The whole  $(2\text{-Br}-\text{C}_5\text{H}_5\text{N})_2[\text{SnBr}_6]$  geometry is generated through an inversion center with tin being lying on the special crystallographic position of  $(1/2, 1/2, 0)$ . The  $(\text{SnBr}_6)^{2-}$  anion forms a quasi-octahedral geometry (Table 1), with the Sn—Br bond lengths are almost invariant. These lengths are in accordance with tin-bromide distances reported for  $(\text{SnBr}_6)^{2-}$  anion containing compounds (Willey *et al.*, 1998; Tudela & Khan 1991; Al-Far & Ali 2007; Ali, Al-Far & Al-Sou'od, 2007; Ali & Al-Far, 2007; Ali, Al-Far & Ng, 2007). Bond lengths and angles within the cation are as expected (Allen *et al.*, 1987).

The packing of the structure (Fig. 2) can be described as layers of alternating anions and cations parallel to  $bc$  plane. In these layers each  $(\text{SnBr}_6)^{2-}$  anion is interacting with six cations *via* two N—H $\cdots$ Br interactions (Table 2) and the symmetry related ones along with two Br $\cdots$ Br interactions and symmetry related ones [Br2 $\cdots$ Br4 and Br2 $\cdots$ Br1 of 3.6666 (23) and 3.7779 (29) Å, respectively; Fig. 2].

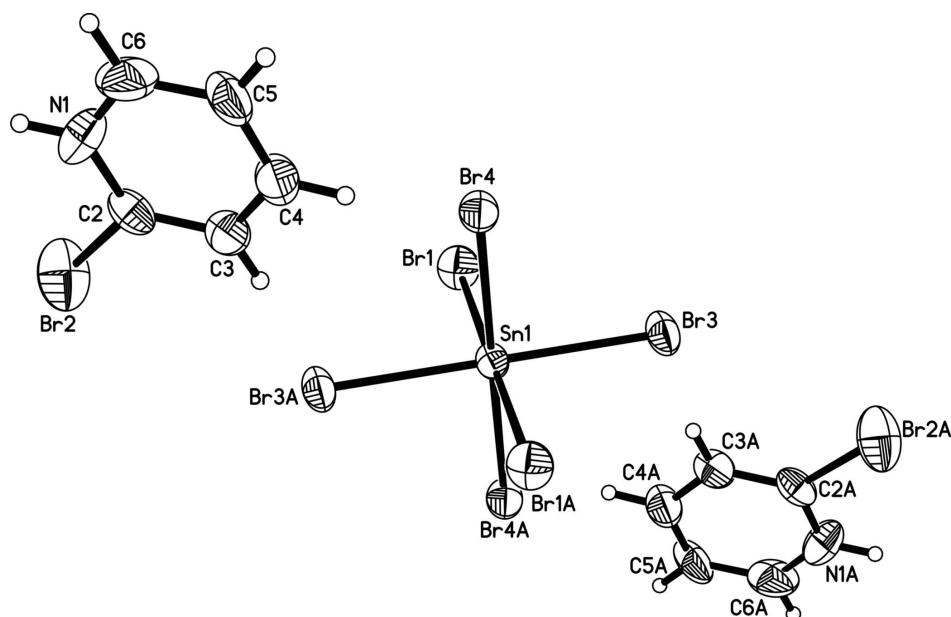
The N—H $\cdots$ N interactions along with C—Br $\cdots$ Br synthons are potential building blocks for this stable supramolecular lattice. The stability of this lattice is evident in the isostructurality with the reported Te analogue (Fernandes *et al.*, 2004).

**S2. Experimental**

Warm solution of Sn metal (1.0 mmol) dissolved in absolute ethanol (10 ml) and HBr (60%, 5 ml), was added dropwise to a stirred hot solution of 2-bromopyridine (2 mmol) dissolved in ethanol (10 ml). The mixture was then treated with liquid Br<sub>2</sub> (2 ml) and refluxed for 3/2 h. The resulting mixture was then filtered off, and allowed to stand undisturbed at room temperature. The salt crystallized over 1 d as nice yellow block crystals (yield: 83%).

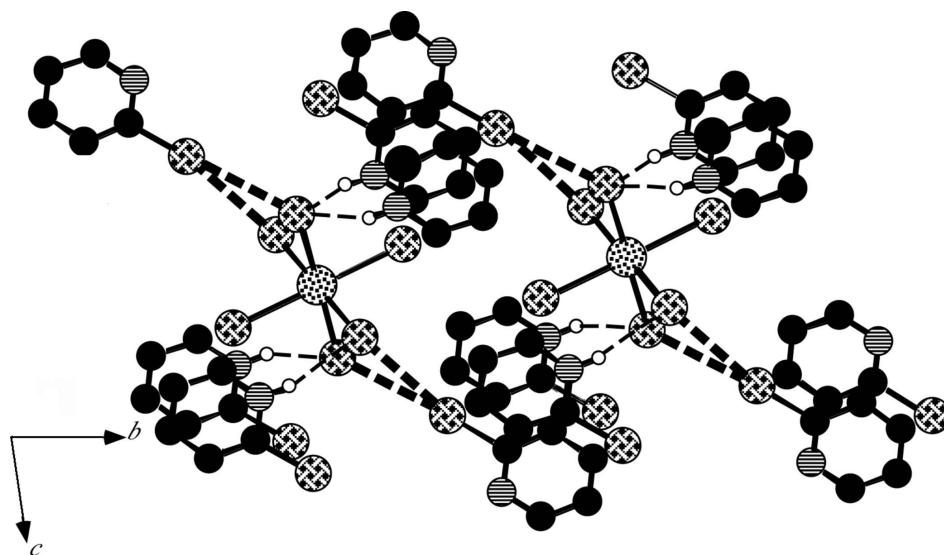
**S3. Refinement**

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93 Å for aromatic H, and constrained to ride on their parent atoms, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$ .



**Figure 1**

A view of the asymmetric unit of (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.



**Figure 2**

A packing diagram of (I). Hydrogen bonds (dashed lines) and Br...Br interactions (thick dashed lines) are shown for  $(\text{SnBr}_6)^{2-}$  anions and six surrounding cations.

### Bis(2-bromopyridinium) hexabromidostannate(IV)

#### Crystal data

$(\text{C}_5\text{H}_5\text{BrN})_2[\text{SnBr}_6]$

$M_r = 916.12$

Triclinic,  $P\bar{1}$

Hall symbol:  $-P\ 1$

$a = 7.4037\ (15)\ \text{\AA}$

$b = 8.3393\ (17)\ \text{\AA}$

$c = 9.4302\ (19)\ \text{\AA}$

$\alpha = 73.14\ (3)^\circ$

$\beta = 67.98 (3)^\circ$   
 $\gamma = 82.44 (3)^\circ$   
 $V = 516.4 (2) \text{ \AA}^3$   
 $Z = 1$   
 $F(000) = 414$   
 $D_x = 2.946 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 255 reflections  
 $\theta = 2.1\text{--}27.7^\circ$   
 $\mu = 16.71 \text{ mm}^{-1}$   
 $T = 293 \text{ K}$   
 Block, yellow  
 $0.16 \times 0.13 \times 0.08 \text{ mm}$

*Data collection*

Bruker–Siemens SMART APEX  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution:  $8.3 \text{ pixels mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2007)  
 $T_{\min} = 0.058, T_{\max} = 0.261$

2266 measured reflections  
 1807 independent reflections  
 1308 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.091$   
 $\theta_{\max} = 25.0^\circ, \theta_{\min} = 2.4^\circ$   
 $h = -1 \rightarrow 8$   
 $k = -9 \rightarrow 9$   
 $l = -10 \rightarrow 11$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.068$   
 $wR(F^2) = 0.178$   
 $S = 1.02$   
 1807 reflections  
 67 parameters  
 0 restraints  
 Primary atom site location: structure-invariant  
 direct methods

Secondary atom site location: difference Fourier  
 map  
 Hydrogen site location: inferred from  
 neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.1076P)^2 + 1.002P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 3.31 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -1.87 \text{ e \AA}^{-3}$

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > \sigma(F^2)$  is used only for calculating  $R$ -factors(gt) etc. and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.5000	0.5000	0.0000	0.0271 (4)
Br4	0.80819 (19)	0.51691 (17)	-0.25738 (17)	0.0365 (4)
Br3	0.5601 (2)	0.17999 (16)	0.09614 (18)	0.0394 (4)
Br1	0.2879 (2)	0.43877 (19)	-0.14375 (19)	0.0426 (4)
Br2	0.6761 (3)	0.2489 (2)	-0.4484 (2)	0.0674 (6)
C2	0.7936 (19)	0.1051 (18)	-0.5793 (18)	0.038 (3)*
N1	0.9316 (17)	0.1687 (17)	-0.7225 (17)	0.049 (3)*
H1	0.9575	0.2732	-0.7499	0.059*
C3	0.751 (2)	-0.0578 (18)	-0.5321 (19)	0.042 (3)*

H3	0.6604	-0.1039	-0.4324	0.051*
C4	0.845 (2)	-0.155 (2)	-0.6371 (19)	0.047 (4)*
H4	0.8119	-0.2665	-0.6094	0.057*
C5	0.990 (2)	-0.090 (2)	-0.784 (2)	0.051 (4)*
H5	1.0572	-0.1560	-0.8526	0.061*
C6	1.028 (3)	0.077 (2)	-0.822 (2)	0.060 (5)*
H6	1.1225	0.1254	-0.9183	0.072*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn1	0.0304 (6)	0.0249 (6)	0.0213 (7)	0.0021 (5)	-0.0058 (5)	-0.0048 (5)
Br4	0.0387 (7)	0.0322 (7)	0.0294 (8)	-0.0003 (5)	-0.0011 (6)	-0.0094 (6)
Br3	0.0462 (8)	0.0258 (7)	0.0340 (9)	0.0066 (6)	-0.0067 (6)	-0.0034 (6)
Br1	0.0491 (8)	0.0446 (8)	0.0391 (9)	-0.0002 (6)	-0.0226 (7)	-0.0094 (7)
Br2	0.1089 (15)	0.0522 (10)	0.0491 (11)	0.0059 (10)	-0.0295 (11)	-0.0268 (9)

*Geometric parameters (Å, °)*

Sn1—Br3	2.5939 (15)	N1—C6	1.32 (2)
Sn1—Br3 <sup>i</sup>	2.5939 (15)	N1—H1	0.8600
Sn1—Br1	2.6027 (15)	C3—C4	1.39 (2)
Sn1—Br1 <sup>i</sup>	2.6027 (15)	C3—H3	0.9300
Sn1—Br4 <sup>i</sup>	2.6174 (17)	C4—C5	1.40 (2)
Sn1—Br4	2.6174 (17)	C4—H4	0.9300
Br2—C2	1.870 (15)	C5—C6	1.37 (2)
C2—C3	1.34 (2)	C5—H5	0.9300
C2—N1	1.357 (19)	C6—H6	0.9300
Br3—Sn1—Br3 <sup>i</sup>	180.0	N1—C2—Br2	117.9 (11)
Br3—Sn1—Br1	89.06 (5)	C6—N1—C2	122.7 (14)
Br3 <sup>i</sup> —Sn1—Br1	90.94 (5)	C6—N1—H1	118.6
Br3—Sn1—Br1 <sup>i</sup>	90.94 (5)	C2—N1—H1	118.6
Br3 <sup>i</sup> —Sn1—Br1 <sup>i</sup>	89.06 (5)	C2—C3—C4	117.8 (15)
Br1—Sn1—Br1 <sup>i</sup>	180.00 (5)	C2—C3—H3	121.1
Br3—Sn1—Br4 <sup>i</sup>	89.43 (6)	C4—C3—H3	121.1
Br3 <sup>i</sup> —Sn1—Br4 <sup>i</sup>	90.57 (6)	C3—C4—C5	121.7 (15)
Br1—Sn1—Br4 <sup>i</sup>	90.21 (5)	C3—C4—H4	119.1
Br1 <sup>i</sup> —Sn1—Br4 <sup>i</sup>	89.79 (5)	C5—C4—H4	119.1
Br3—Sn1—Br4	90.57 (6)	C6—C5—C4	116.8 (17)
Br3 <sup>i</sup> —Sn1—Br4	89.43 (6)	C6—C5—H5	121.6
Br1—Sn1—Br4	89.79 (5)	C4—C5—H5	121.6
Br1 <sup>i</sup> —Sn1—Br4	90.21 (5)	N1—C6—C5	120.6 (17)
Br4 <sup>i</sup> —Sn1—Br4	180.0	N1—C6—H6	119.7
C3—C2—N1	120.3 (15)	C5—C6—H6	119.7
C3—C2—Br2	121.8 (12)		
C3—C2—N1—C6	1 (2)	C2—C3—C4—C5	4 (2)

Br2—C2—N1—C6	177.7 (12)	C3—C4—C5—C6	-3 (2)
N1—C2—C3—C4	-3 (2)	C2—N1—C6—C5	1 (3)
Br2—C2—C3—C4	-179.9 (11)	C4—C5—C6—N1	0 (3)

Symmetry code: (i)  $-x+1, -y+1, -z$ .

*Hydrogen-bond geometry (Å, °)*

<i>D—H...A</i>	<i>D—H</i>	<i>H...A</i>	<i>D...A</i>	<i>D—H...A</i>
N1—H1...Br4 <sup>ii</sup>	0.86	2.65	3.375 (13)	142
N1—H1...Br1 <sup>iii</sup>	0.86	2.98	3.562 (13)	127

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