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Bromoantimonates with bis(pyridinium)-type dications obtained via oxidation by dibromine: Diverse structural types and features of interactions pattern

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1. Introduction

Research focusing on anionic halide complexes of p-block metals and metalloids, such as Bi, Pb, Sn, Te etc., has a long history [1,2]; in the last years, it is additionally encouraged by recent trends in materials science, in particular, by exploitation of iodometalates (especially those of Pb(II)) as solar cells components [3–7]. From the point of view of structural chemistry, these compounds demonstrate fascinating diversity of geometries [8–14] (for example, alone for Bi(III), about 40 structural types of halometalate anions are known [15]), making them very attractive and spectacular study objects.

In comparison with bismuth, halide complexes of antimony have an important feature: while halobismuthates(V) are unknown, Sb(III) can be oxidized into Sb(V) [16,17] by Cl₂ or Br₂, commonly giving mononuclear [SbX₆]⁻ (neutral Sb(V) halides are known for X = Cl, but not for X = Br). Interestingly, in the case of Br₂ diversity of products is significantly more prominent than for Cl₂. The first works examining behavior of "[SbBr₆]³⁻ + CatBr_x + Br₂" systems appeared almost 90 years ago [18] and, even despite the lack of physical methods, it was shown that there can be isolated dark crystalline solids with different, sometimes abnormally high

ABSTRACT

Bromoantimonate(III) species, which can be generated in solution by reaction of Sb_2O_3 and HBr, can be oxidized by Br_2 into mixed-valence complexes or bromoantimonates(V). The outcome of these reactions governs by the nature of cation which salt is used for isolation of solid complexes. Using bromides of three 1,*n*-bis(pyridinium)alkane cations (PyC_n , where X = 2, 3 and 4), we isolated three complexes: (PyC_2){[SbBr₆](Br₃)} (1), (PyC_3)₂[Sb₂Br₉][SbBr₆] (2) and (PyC_4){[SbBr₆](Br₃)} (3), respectively. Their structures were determined by X-ray diffractometry. For 1 and 3, the energies of non-covalent interactions between tribromide units and [SbBr₆]⁻ were estimated using DFT calculations.

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Br content (such as "SbBr₉" or even "SbBr₁₀", as followed from element analysis). Few decades later, the works by Lawton and Jacobson [19–24] shed light on the real nature of these compounds. As followed from XRD data, the outcome of these reactions was strongly affected by certain cations which bromide salt was taken in reaction. Depending on this, there could form compounds containing a) Sb(III) anions and dibromine units connected with each other by specific interactions (which were later defined as halogen bonding [25,26]), b) mixed-valence mononuclear {SbBr₆}, c) [SbBr₆]⁻ alone or d) accompanied by tribromide units etc; overall, about one dozen of structures were described.

Several years ago, we decided to revisit this area, performing a large series of experiments involving bromides of various pyridines (overall, we reported over 20 examples [27]), quinolones and isoquinolines etc [28]. We have shown that diversity of products is indeed great: while $[SbBr_6]^-$ remained the only antimony-containing "building block" we observed, there can be $\{Br_2\}$, $\{Br_3\}$ or even $\{Br_5\}$ units in the structure, creating sophisticated system of noncovalent interactions in solid state (as follows from DFT calculations, the energies can exceed 4.5 kcal/mol).

Continuing our work, we turned to salts of pyridine-based dications (those are readily available by reactions between substituted by and 1, ω -dibromoalkanes). In our most recent report [29], we noted that in one case the use of precursor of this type led to unusual complex with stabilized Z-shaped decabromide in solid state.





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Hereby we present three new bromoantimonates which were isolated in presence of bis(pyridinium)ethane (PyC₂), -propane (PyC₃) and -butane (PyC₄, respectively) salts – (PyC₂){[SbBr₆](Br₃)} (1), (PyC₃)₂[Sb₂Br₉][SbBr₆] (2) and (PyC₄){[SbBr₆](Br₃)} (3); features of non-covalent interactions in their crystal structures, as well as thermal stabilities, are discussed.

2. Experimental part

2.1. General remarks

Bromides of PyC₂, PyC₃ and PyC₄ were obtained by reactions of pyridine and corresponding 1,x-dibromoalkanes (2.05:1) in acetonitrile (reflux, overnight) with nearly quantitative yields; their purity was confirmed by ¹H NMR and element analysis data. All reagents were obtained from commercial sources and used as purchased. In all cases, concentrated HBr was used. **Caution:** for work with Br₂-containing solutions, safety measures must be taken (obligatory use of fume hood, skin and eye protection).

2.2. Synthesis of 1-3

1: 8.4 mg (0.029 mmol) of Sb₂O₃ were dissolved in 7 ml of concentrated HBr, followed by addition of 1 ml of 1 M Br₂ solution in HBr and solution of 20 mg (0.058 mg) of PyC₂Br₂ in 5 ml of HBr. The mixture was kept at 6 °C for 18 h, resulting in dark cherry-red crystals of **1.** Yield 79%. For C₁₂H₁₄Br₉N₂Sb calcd, %: C, 14.2; H, 1.4; N, 2.8; found, %: C, 14.4; H, 1.4; H, 2.8.

2: the procedure was similar to **1**, using 18 mg (0.063 mmol) of Sb₂O₃ in 5 ml of HBr, 1 ml of HBr/Br₂ solution and 15 mg (0.042 mmol) of PyC₃Br₂ in 4 ml of HBr. Crystals of **2** form within wo days. Yield 81%. For $C_{26}H_{32}Br_{15}N_4Sb_3$ calcd, %: C, 16.0; H, 1.7; N, 2.9; found, %: C, 16.1; H, 1.7; N, 3.0.

3: the procedure was similar to **1**, using 10 mg (0.035 mmol) of Sb₂O₃ in 10 ml of HBr, 1 ml of HBr/Br₂ and 26 mg (0.07 mmol) of PyC₄Br₂ in 2 ml of HBr. The crystals of **3** form within 18 h. Yield 70%. For $C_{14}H_{18}Br_9N_2Sb$ calcd, %: C, 16.1; H, 1.7; N, 2.7; found, %: C, 16.3; H, 1.8; N, 2.7.

2.3. X-ray diffractometry

Crystallographic data and refinement details for 1-3 are given in Table 1. Diffraction data were collected on a New Xcalibur (Agilent Technologies) diffractometer with MoKa radiation $(\lambda = 0.71073)$ by doing φ scans of narrow (0.5°) frames at 130 K. Absorption correction was done empirically using SCALE3 Agilent ABSPACK (CrysAlisPro, Technologies, Version 1.171.37.35). Structures were solved with SHELXT [30] method and refined by full-matrix least-squares treatment against |F|2 in anisotropic approximation with SHELX 2014/7 [31] in ShelXle [32] program. Hydrogen atoms were refined in geometrically calculated positions (1 and 3) and some H-atoms were located directly from experiment in the case of 2. The crystallographic data have been deposed in the Cambridge Crystallographic Data Centre under the deposition codes CCDC 2,058,211 (1), 2,058,212 (2) and 2,058,213 (3).

Thermogravimetric analyses (TGA) were carried out on a TG 209 F1 Iris thermobalance (NETZSCH, Germany). The measurements were made in a helium flow using the heating rate of 10 $^{\circ}$ -C min⁻¹, the gas flow rate of 60 ml min⁻¹ and open Al crucibles.

Details of DFT calculations and PXRD are given in SI.

3. Results and discussion

Complexes 1 and 3 belong to the same structural type (one of the most common among the products of reactions between bromoantimonates(III) and Br₂). In both crystal structures, there are mononuclear [Sb^VBr₆]⁻ anions (the Sb-Br bond lengths are similar to those found [27] in other related compounds (2.544-2.565 and 2.546-2.566 Å, respectively)) accompanied by symmetric tribromides (Br-Br = 2.539 and 2.547 Å, respectively). These units build infinite linear supramolecular chains (Fig. 1) due to the presence of Br...Br non-covalent interactions (3.467 and 3.394 Å, respectively, which are less than the sum of Bondi's van der Waals radii for two Br atoms (3.66 Å, [33,34] viz. 95% and 93% from the vdW_{sum}). These short $Br \cdots Br$ contacts between $[Sb^{V}Br_{6}]^{-}$ and tribromides units are particularly interesting as they are anion-anion contacts and should be destabilized by repulsion between samesign ions, but crystal-packing effects and σ -hole-like non-covalent interactions (Fig. 2) are strong enough for stabilization of such supramolecular associates in the solid state.

The Sb-Br_{term}-Br_{Br3} and Br_{term}-Br_{br3}-Br_{Br3} angles are 158.5 and 164.1° in **1** and 158.6 and 150.0° in **3**, respectively. Applying the classification of halogen \cdots halogen contacts which was proposed by Desiraju et al. [36] and is widely exploited now [37], those must be regarded as Type I interactions. Interestingly, the contacts between bromide ligands of neighboring [SbBr₆]⁻ are absent in **1** and **3**, despite those were encountered in other Sb(V) bromide complexes [27]. In both these structures, there are numerous short H \cdots Br contacts which are common for halometalates with organic cations.

Complex 2 represents a very rare case of mixed-valence bromoantimonate (among the whole palette of products of "[Sb^{III}Br₆]³⁻ $^{-}$ + Br₂ + CatBr_x" reactions, only one such case was described yet; under such conditions Sb(III) is typically oxidized to Sb(V)). There are two types of anions in the crystal structure. First, there are binuclear [Sb₂Br₉]³⁻ anions built of two face-sharing {SbBr₆} octahedra (this is a very common structural type for group 15 halometalates [38-40]); the Sb-Br distances match well with the ranges found in other relevant structures (Sb-Br_{term} = 2.643-2.681 Å, Sb- μ_2 -Br = 2.935–3.045 Å). Second, there are mononuclear [Sb^VBr₆]⁻ which show prominent disordering. Only two trans-Br positions are ordered (Sb-Br = 2.547 Å), while each of four bromide ligands is disordered over four positions with different occupancies (Figs. 3a and b). The system of non-covalent interactions in this structure is more sophisticated then in 1 and 3. It is very likely that there are contacts between Br_{term} in neighboring [SbBr₆]⁻, but their lengths cannot be estimated in a straightforward manner. Additionally, there are interactions between non-disordered Br_{term} of $[SbBr_6]^-$ and μ_2 -Br of $[Sb_2Br_9]^{3-}$ (3.353 Å).

In order to estimate the energies of Br \cdots Br energies in the crystals of **1** and **3**, we followed the protocol which was used by us for investigation of supramolecular features in structures of other related halometalates [27], as well as in other complexes [41–45] (DFT calculations for non-optimized structures and QTAIM analysis [46] of electronic density distribution). Results are shown in Table 2 and presented on Figs. 3a and b. The energy values (2.1–2.5 kcal/mol) agree well with those found in other polybromide-bromoantimonate(V) associates [27]. Applying relevant criteria, we can state that these interactions are: a) attractive [47] and b) purely supramolecular (covalent contribution is absent [48]). Unfortunately, we had to exclude structure **2** from consideration due to disordering which makes application of abovementioned approach impossible.

According to PXRD (SI), **1–3** can be isolated as single phases, allowing their further characterization. The TGA curves for **1** and **3** are shown on Fig. 4. It can be seen that those are very similar;

Ta	ble	1
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XRD details for 1-3.

	1	2	3
Chemical formula	$C_{12}H_{14}Br_9N_2Sb$	C ₂₆ H ₃₂ Br ₁₅ N ₄ Sb ₃	$C_{14}H_{18}Br_9N_2Sb$
Mr	1027.19	1964.45	1055.24
Crystal system, space group	Triclinic, P1	Orthorhombic, Pmmn	Triclinic, P1
a, b, c (Å)	7.3269 (4), 9.1941 (6), 9.7994 (6)	20.3785 (8), 15.5018 (5), 7.4618 (3)	7.8627 (3), 9.1285 (4), 10.1514 (5)
α, β, γ (°)	64.474 (6), 80.207 (5), 86.244 (5)	90, 90, 90	68.392 (4), 89.669 (4), 72.048 (4)
V (Å ³ )	586.99 (7)	2357.21 (15)	639.63 (5)
Z	1	2	1
μ (mm ⁻¹ )	16.49	14.45	15.14
Crystal size (mm)	$0.32\times0.15\times0.15$	$0.32 \times 0.10 \times 0.10$	$0.15\times0.15\times0.10$
T _{min} , T _{max}	0.110, 1.000	0.270, 1.000	0.415, 1.000
No. of measured, independent and observed $[I > 2\sigma(I)]$ reflections	4408, 2564, 2191	7835, 2788, 2443	5389, 2803, 2305
R _{int}	0.036	0.032	0.032
$\theta$ values (°)	$\theta_{max}$ = 29.0, $\theta_{min}$ = 3.4	$\theta_{max} = 29.0, \ \theta_{min} = 3.3$	$\theta_{max} = 28.9, \ \theta_{min} = 3.4$
$(\sin \theta / \lambda)_{max} (Å^{-1})$	0.683	0.683	0.680
Range of h, k, l	$-7 \leq h \leq 9$ ,	$-18 \leq h \leq 27$ ,	$-10 \leq h \leq 7$ ,
	$-12 \leq k \leq 11$ ,	$-19 \leq k \leq 11$ ,	$-12 \leq k \leq 10$ ,
	$-12 \leq l \leq 12$	$-9 \le l \le 6$	$-13 \leq l \leq 12$
$R[F^2 > 2\sigma(F^2)], wR(F^2), S$	0.045, 0.107, 1.03	0.031, 0.071, 1.07	0.036, 0.073, 1.06
No. of reflections, parameters, restraints	2564, 112, 0	2788, 149, 1	2803, 121, 0
H-atom treatment	H-atom parameters constrained	H atoms treated by a mixture of independent and constrained refinement	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0314P)^2 + 2.7599P]$ where $P = (F_o^2 + 2F_c^2)/3$	$w = 1/[\sigma^2(F_o^2) + (0.0245P)^2 + 0.1266P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta  ho_{max}$ , $\Delta  ho_{min}$ (e Å ⁻³ )	1.65, -2.73	1.89, -2.06	0.97, -0.90



**Fig. 1.** Supramolecular chains built of  $[Sb^VBr_6]^-$  and  $Br_3^-$  units in the structures of **1** and **3.** Here and below: Sb black, Br olive-green, non-covalent interactions dashed.

in both cases, the first stage of mass loss approximately corresponds to elimination of three Br (for **1**, that is 23.3%) – probably, due to the loss of Br₂ by tribromide and partial reduction of  $[Sb^v-Br_6]^-$ . The endo-effect at  $\approx 125$  °C is, most likely, related to this process. For **2** (Fig. 5), pattern of thermal decomposition is more sophisticated and cannot be interpreted in a straightforward manner (it must be noted, however, that the such problems with TGA



Fig. 3a. Anionic part in the structure of 2. All positions of bromide ligands in  $[{\rm SbBr}_6]^-$  are shown.



Fig. 2. The shape of lowest unoccupied molecular orbital and electrostatic surface potential distribution in the  $[Sb^VBr_6]^-$  anion reveal the presence of nominal  $\sigma$ -holes  $(V_{s,max} = -66 \text{ kcal/mol})$  on bromide ligands. Note that very similar situation was recently observed by us for  $[Sb^{IIB}r_5]^{2-}$  anion [35].

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**Fig. 3b.** Contour line diagram of the Laplacian of electron density distribution  $\nabla^2 \rho$ (**r**), bond paths, and selected zero-flux surfaces (top), visualization of electron localization function (ELF, center) and reduced density gradient (RDG, bottom) analyses for intermolecular interactions Br $\cdots$ Br in **1**. Bond critical points (3, -1) are shown in blue, nuclear critical points (3, -3) – in pale brown, bond paths are shown as pale brown lines, length units – Å, and the color scale for the ELF and RDG maps are presented in a.u.



Fig. 5. TG (black), DTG (red) and DTA (blue) curves for 2.

#### Table 2

Values of the density of all electrons  $-\rho(\mathbf{r})$ , Laplacian of electron density  $-\nabla^2 \rho(\mathbf{r})$  and appropriate  $\lambda_2$  eigenvalues, energy density  $-H_b$ , potential energy density  $-V(\mathbf{r})$ , and Lagrangian kinetic energy  $-G(\mathbf{r})$  (a.u.) at the bond critical points (3, -1), corresponding to intermolecular interactions  $B\mathbf{r}\cdots B\mathbf{r}$  in the X-ray structures **1** and **3**, and estimated strength for these interactions  $E_{int}$  (kcal/mol).

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	Contact	$\rho(\mathbf{r})$	$ abla^2  ho(\mathbf{r})$	$\lambda_2$	H _b	V( <b>r</b> )	G( <b>r</b> )	E _{int} ^a	Eint ^b
	1 Br…Br 3.466 Å 3	0.010	0.026	-0.010	0.000	-0.006	0.006	2.2	2.1
	BrBr 3.394 Å	0.012	0.031	-0.012	0.000	-0.007	0.007	2.5	2.5
	$A = -0.58(-V(\pi))[40]$								

^b  $E_{int} = 0.58(-V(\mathbf{r}))[49]$ 

were reported for other Sb(V) bromide complexes [27] (excluding the most trivial case –  $Cat[Sb^vBr_6]$ ).

## 4. Conclusions

Most commonly, Sb(III) bromide complexes undergo complete oxidation by Br₂ giving [SbBr₆]⁻. Yet, only two exceptions were reported: dibromine-containing  $(Me_4N)_3\{[Sb_2Br_9](Br_2)\}$  [24] and the complex containing  $[Sb^{III}Br_6]^{3-}$  and  $[Sb^VBr_6]^-$ ; the latter forms in presence of pyridinium cations [50]. Our results described above clearly indicate that, although formation of mixed-valence bro-

moantimonates is rare, the latter can be structurally diverse, featuring unprecedented patterns of halogen—halogen interactions. Considering that the latter can be responsible for electronic transport within halometalates [51], we believe that further research aiming expansion of experimental data on compounds of this class are justified; corresponding studies are underway in our group.

# **CRediT authorship contribution statement**

Mikhail A. Bondarenko: Investigation. Pavel A. Abramov: Investigation, Formal analysis, Validation, Writing - original draft. Pavel E. Plyusnin: Investigation. Alexander S. Novikov: Data curation, Conceptualization, Visualization, Writing - original draft. Maxim N. Sokolov: Supervision, Methodology, Writing - review & editing. Sergey A. Adonin: Funding acquisition, Conceptualization, Formal analysis, Project administration, Writing - original draft, Writing - review & editing.

### **Declaration of Competing Interest**

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.poly.2021.115217.

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