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Short Communications

On the Crystal Structure of $NH_4SnBr_3.H_2O$

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From a solution of tin(II) bromide and ammonium bromide in water a compound with the stoichiometric composition $NH_4SnBr_3.H_2O$ can be crystallized. The translucent needle-like crystals rapidly become opaque in air. All "single crystals" investigated consisted of two crystals grown together along the *a* axis.

An X-ray investigation using Weissenberg techniques showed the crystals to have monoclinic symmetry. Possible space groups are No. 4, $P2_1$ and No. 11, $P2_1/m$.[1] The cell dimensions, as refined from Guinier powder diffraction data, are (21 °C):

$a = 9.4476 \pm 0.0008$ Å, $b = 4.4637 \pm 0.0005$ Å,
$c = 9.6242 \pm 0.0007$ Å, $\beta = 100.714 \pm 0.007°$,
$V = 398.79 \pm 0.06$ Å^3

There are two formula units of $NH_4SnBr_3.H_2O$ in the unit cell.

A comparison between a three-dimensional Patterson synthesis and theoretical vectors calculated from the point position $P2_1/m$:2(e) *i.e.* $\pm(x,\frac{1}{4},z)$ yielded the tin and bromine positions. Difference Fourier calculations showed possible ammonium and water positions. Both positions are remote from tin; water cannot therefore be a ligand. Least squares refinement of *h0l* and *h1l* data yielded an *R*-value of 15.3 %. The structure investigation is to be continued.

Table 1. Approximate atomic parameters for $NH_4SnBr_3.H_2O$.

Atom	*x*	*y*	*z*
Sn	0.146	0.250	0.131
Br(1)	0.359	0.250	0.349
Br(2)	0.990	0.250	0.725
Br(3)	0.699	0.250	0.996
NH_4	0.382	0.250	0.731
H_2O	0.765	0.250	0.394

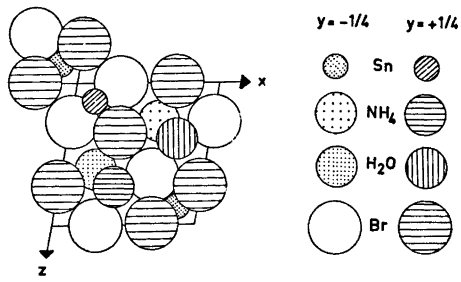

Fig. 1. A projection of the structure of $NH_4SnBr_3.H_2O$ on the *xz* plane.

Fig. 1 shows a projection of the structure on the *xz* plane. Tin has five bromine atoms as nearest neighbours, four of which form a somewhat distorted square with Sn—Br distances of 3.04—3.05 Å. These four bromine atoms are in the same plane. The tin atom is only slightly displaced from this plane. The fifth bromine atom is on the other side of the plane, 2.62 Å from tin. This distance is the shortest found in the five tin(II)-bromine compounds hitherto investigated.[2]

Tin is thus surrounded by a tetragonal pyramide of bromide ions. The crystal structure can be visualized as chains, parallel to the *b* axis, of such tetragonal pyramids sharing edges. Between these chains water molecules and ammonium ions form rows in the *y*-direction.

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1. *International Tables for X-Ray Crystallography*, 2nd Ed., Kynoch Press, Birmingham 1952, Vol. I.
2. Andersson, J. *Acta Chem. Scand. A 29* (1975) 956.

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