Short Communications

On the Crystal Structure of NH₄SnBr₃·H₂O

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From a solution of tin(II) bromide and ammonium bromide in water a compound with the stoichiometric composition NH₄SnBr₃·H₂O 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, P2₁, and No. 11, P2₁/m.¹ The cell dimensions, as refined from Guinier powder diffraction data, are (21 °C):

\[ a = 9.4476 \pm 0.0008 \text{ Å}, \quad b = 4.4637 \pm 0.0005 \text{ Å}, \]
\[ c = 9.6242 \pm 0.0007 \text{ Å}, \quad \beta = 100.714 \pm 0.007°, \]
\[ V = 398.79 \pm 0.06 \text{ Å}³ \]

There are two formula units of NH₄SnBr₃·H₂O in the unit cell.

A comparison between a three-dimensional Patterson synthesis and theoretical vectors calculated from the point position \( P2₁/m; 2(e) \) i.e. \( ±(x,±x,±z) \) 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 \( hhl \) data yielded an R-value of 15.3 %. The structure investigation is to be continued.

Fig. 1 shows a projection of the structure on the \( zz \) 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 pyramid 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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Table 1. Approximate atomic parameters for NH₄SnBr₃·H₂O.

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<thead>
<tr>
<th>Atom</th>
<th>( x )</th>
<th>( y )</th>
<th>( z )</th>
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<tr>
<td>Sn</td>
<td>0.146</td>
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<td>Br(1)</td>
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<td>Br(2)</td>
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<td>Br(3)</td>
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<td>H₂O</td>
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<td>0.394</td>
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