On the Crystal Structure of a Tin(II) Bromide Hydrate, $3SnBr_2.H_2O$

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The crystal structure of $3SnBr_2.H_2O$ has been determined from X-ray diffraction data collected by Weissenberg techniques.

The unit cell dimensions are: $a = 12.26$ Å, $b = 4.31$ Å, $c = 24.42$ Å, $\beta = 110.5°$, $V = 1207$ Å^3.

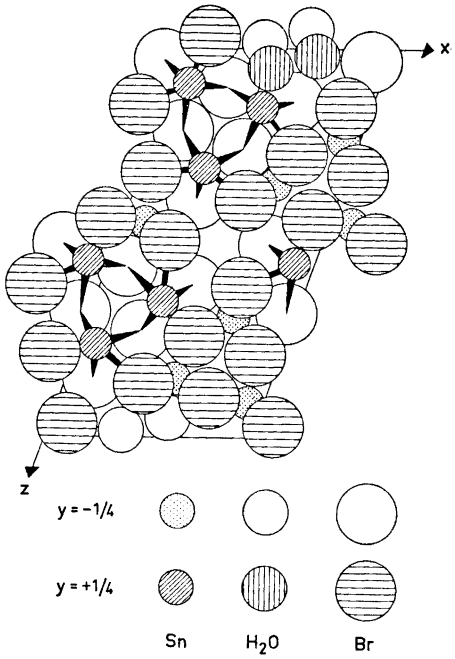

Fig. 1. Projection of the structure of $3SnBr_2.H_2O$ on the xz plane.

Possible space groups are No. 4, $P2_1$ and No. 11, $P2_1/m$,[1] and there are four formula units in the unit cell.

Preliminary information concerning the structure was obtained from a comparison between bromine-bromine vectors in $2SnBr_2.H_2O$ [2] and peaks on $P(u0w)$ in the three-dimensional Patterson synthesis based on data from $3SnBr_2.H_2O$. The remaining bromine positions and the tin positions were determined by comparing vectors in trial structures with the peaks on $P(u0w)$. A difference electron density map gave the positions of the oxygen atoms.

With all atoms occupying the point position $P2_1/m$: 2(e),[1] a least squares refinement of the $h0l$ and $h1l$ data yielded an R-value of 15.4 %. Further refinement of the structure is in progress.

Fig. 1 shows a projection of the structure of $3SnBr_2.H_2O$ on the xz plane. The configuration of ligands around tin is basically the same as in $2SnBr_2.H_2O$,[2] $6SnBr_2.5H_2O$,[3] and $3PbBr_2.2H_2O$,[4] *i.e.* a trigonal prism of bromine atoms with bromine and water capping prism faces.

The Sn – Br distances range from 2.77 Å to 3.68 Å and the Sn – O bond distance is 2.35 Å.

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