

## On the Crystal Structure of a Tn(II) Bromide Hydrate, $6\text{SnBr}_2 \cdot 5\text{H}_2\text{O}$

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The crystal structure of  $6\text{SnBr}_2 \cdot 5\text{H}_2\text{O}$  has been determined by single crystal X-ray methods. Crystals of this compound have monoclinic symmetry, and the following cell dimensions have been determined from Guinier powder diffraction data:

$$a = 12.280 \text{ \AA}, b = 4.317 \text{ \AA}, c = 26.069 \text{ \AA}, \beta = 94.27^\circ, \text{ and } V = 1378.2 \text{ \AA}^3$$

There are two formula units in the unit cell. Possible space groups are No. 4,  $P2_1$  and No. 11,  $P2_1/m$ .<sup>1</sup>

The tin and bromine positions were determined from a three-dimensional Patterson synthesis, the structure determination being facilitated by comparison with the structure of  $2\text{SnBr}_2 \cdot \text{H}_2\text{O}$ .<sup>2</sup> Difference electron density maps revealed the oxygen positions. Assuming all atoms to be situated in the point position  $P2_1/m: 2(e)$ ,<sup>1</sup> a least squares refinement of the  $h0l$  and  $h1l$  reflexions yielded an  $R$ -value of 15.1%. The structure is to be refined further.

Fig. 1 shows a projection of the structure on the  $xz$  plane. All tin atoms have basically the same coordination polyhedron – a trigonal prism of bromine atoms. In addition there are bromine or water molecules capping prism faces so that the tin coordination is sevenfold or eightfold.

Besides being related to the structure of  $2\text{SnBr}_2 \cdot \text{H}_2\text{O}$ , the structure investigated also shows similarities to a lead(II) bromide hydrate  $3\text{PbBr}_2 \cdot 2\text{H}_2\text{O}$ .<sup>3</sup>

The Sn–Br distances range from 2.78 Å to 3.79 Å and the Sn–O bond distances are 2.18 Å and 2.33 Å.

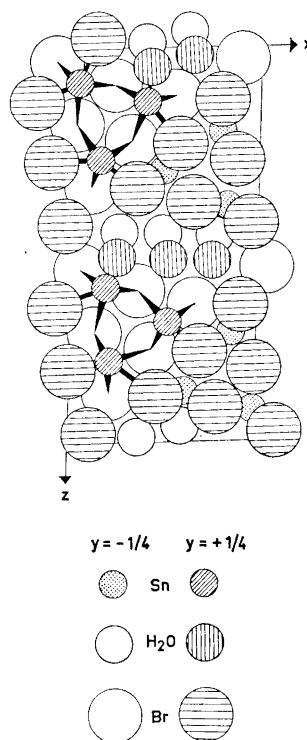


Fig. 1. A projection of the structure of  $6\text{SnBr}_2 \cdot 5\text{H}_2\text{O}$  on the  $xz$  plane.

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