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The absolute configuration of natural strychnine.

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In order to illustrate that the X-ray method of determining absolute configuration may be applied to compounds of arbitrary complexity we proposed the determination on strychnine hydrobromide 2 aq., the atomic coordinates of which have been given by Robertson & Beevers (1951). These authors give a comparison of observed and calculated values of about 80 structure factors. Recalculating these, we found the agreement better than the authors' comparison shows. We may thus expect the coordinates to be well within the range given.

After the experience of Peterson (1955) showing that Cu $K\alpha$ rays have a sufficiently large anomalous effect with Br atoms, we dispensed with the U $L\alpha$ rays which have previously been used for exciting Br (Trommel & Bijvoet, 1954). The values of $\Delta f'_{Br}$ and $\Delta f''_{Br}$ for copper rays amount to $-0{\cdot}9$ and $1{\cdot}5$ respectively (Dauben & Templeton, 1955).

The crystal used in the determination was obtained from a solution of strychnine hydrobromide in water with a slight excess of HBr. As described by Robertson & Beevers, it had the form of a lath parallel to the a axis with a rectangular cross-section of about $0{\cdot}03 \times 0{\cdot}12$ mm. Because of this rectangular cross-section no spurious intensity differences by absorption effects between hkl and $\bar{h}\bar{k}\bar{l}$ reflexions were to be feared, and consequently cylindrical grinding could be omitted.

An equi-inclination Weissenberg diagram was made of the first layer line around the a axis with the aid of an integrating Weissenberg camera.

Previous calculation had shown that the series of reflexions 111, 112, 113 and 114 were most suitable for our determination. The differences between reflexion and counter-reflexion were clearly observable in this series and could be measured with a photometer. The calculated and observed values of the intensities—expressed in different units—are given in Table 1.

Table 1. *Calculated and observed intensities of reflexions* hkl *and* $\bar{h}\bar{k}\bar{l}$ *from strychnine* $HBr.2H_2O$ (Cu $K\alpha$ *rays*)

	Calculated		Observed	
hkl	I_{hkl}	$I_{\bar{h}\bar{k}\bar{l}}$	I_{hkl}	$I_{\bar{h}\bar{k}\bar{l}}$
111	295	> 264	40·8	< 45·5
112	513	< 567	82·5	> 75·0
113	200	< 259	37·1	> 31·6
114	372	~ 378	56·6	= 56·6

The former are based on the model corresponding to the coordinates of Robertson & Beevers in a right-handed coordinate system.

The comparison of the observed and calculated differences shows that the model used in the calculations is the mirror image of the actual molecule.

Natural strychnine, therefore, has the configuration of Fig. 1. It may be remarked that in the 111 reflexion the contribution to the structure factor coming from the normally scattering atoms is such that a shift of 3° in all atomic positions cannot change the sign of the resulting component normal to the bromine contribution, even when all changes in this component accumulate. As the coordinates are accurate within this limit the reliability of the calculated difference for the 111 and $\bar{1}\bar{1}\bar{1}$ reflexions is beyond doubt.

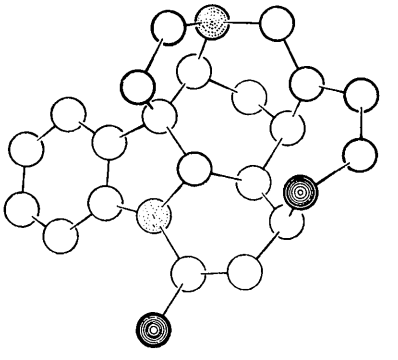

Fig. 1. Absolute configuration of the natural strychnine molecule.

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Crystallographic properties of 9-aminoacridine hemihydrate.

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The compound 9-aminoacridine is interesting as it belongs to the space group D_{2h}^{24}–*Fddd*. This assignment is based on *b*-axis and *c*-axis single-crystal rotation patterns and *b*-axis and *c*-axis zero-layer Weissenberg patterns. According to Donnay & Nowacki (1954) there is no other strictly organic compound, that is, group 7 aside from