Molecular Structure of Xylerythrin — a Fungus Pigment SIXTEN ABRAHAMSSON and MAUREEN INNES

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Xylerythrin is a pigment from the fungus Peniophora sanguinea Bres. It has been isolated and studied chemically by Gripenberg.¹ He suggested that we determine the molecular structure by X-ray methods of the bisbromoacetate of the pigment. The crystals are triclinic with

$$a = 11.36 \text{ Å}$$
 $b = 9.24 \text{ Å}$ $c = 13.36 \text{ Å}$
 $\alpha = 78.1^{\circ}$ $\beta = 89.2^{\circ}$ $\gamma = 81.0^{\circ}$

The space-group was assumed to be $P\overline{1}$ and this was not contradicted during the structure refinement. There are two molecules per unit cell. The structure was solved by the usual heavy-atom technique and refined by anisotropic least-squares treat-

ment. The present R-value for the 1745 independent reflections is 10.4 %. By this investigation the molecular structure of the pigment has been determined in all details to be (I) without using any chemical information. Gripenberg describes the chemical implications in an accompanying paper. A spacial drawing of the bisbromo-acetate derivative is shown in Fig. 1. A full account of the structure analysis will be published later.

 Gripenberg, J. Acta Chem. Scand. 19 (1965) 2242.

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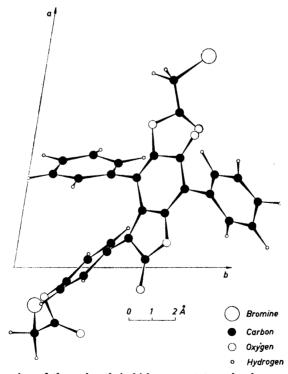


Fig. 1. Spacial drawing of the xylerythrin bisbromoacetate molecule as seen along the c-axis.

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