Tetrahedron Letters No.47, pp. 4859–4860, 1968. Pergamon Press. Printed in Great Britain.

CRYSTAL STRUCTURE OF IODOPHYLLANTHIN

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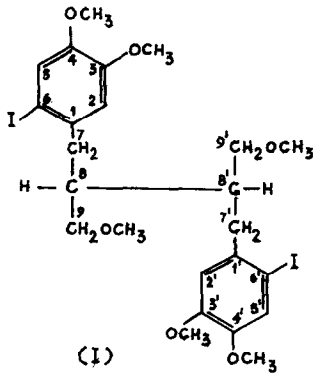
(Received in UK 16 July 1968; accepted for publication 21 August 1968)

In the course of X-ray investigation of some physiologically active compounds[1-4], the authors have taken up the study of iodophyllanthin ($I_2C_{24}O_6H_{32}$, m.p.112°) derived from phyllanthin which is the major crystalline compound obtained from the leaves of phyllanthus niruri Linn[5-7]. Recently, Row et al.[8-9] made a detailed chemical and N M R study of the compound and concluded that its structure is (+) 3, 3', 4,4',9,9'-hexamethoxy-8:8'-butyrolignan (I).



(I)

The configuration of iodophyllanthin is shown to be 8S,8'S[10]. An interesting feature of this molecule is that the orientation of the groups around 8C, 8'C produces a symmetry in the molecule which the authors propose to study by the structural analysis of iodophyllanthin. The present communication gives results regarding its space group and unit cell dimensions.

The unit cell dimensions have been determined from the rotation and zero layer photographs about the three crystallographic axes using CuKα radiation. The crystal is found to belong to the orthorhombic system with the following cell dimensions: a = 7.357 Å ; b = 21.855 Å ; c = 16.328 Å.

The density of the crystal is determined by the flotation method using calcium bromide solution. The observed value 1.63 gm/cc. is found to be in agreement with the value 1.68 gm/cc. calculated for four molecules per unit cell.

Examination of the 0kl, h0l, hk0 and hkl Weissenberg photographs showed the following systemmatic absences:

hkl : h + k = 0dd 0kl : (k = 0dd) h0l : (h = 0dd)

hk0 : h + k = 0dd l = 0dd l = 0dd

This uniquely determines the space group of the crystal as $C222_1$.

There are eight equivalent positions for this space group, whereas the number of molecules in the unit cell is fonly four. Hence the four molecules should occupy one of the two sets of four special positions with two fold symmetry[11] Thus the X-ray study shows that the molecule of iodophyllanthin should possess a two-fold rotation axis, a conclusion which agrees with the structure obtained by the N M R and chemical studies.

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