# The Molecular Structure of *Cedrela odorata* Substance B

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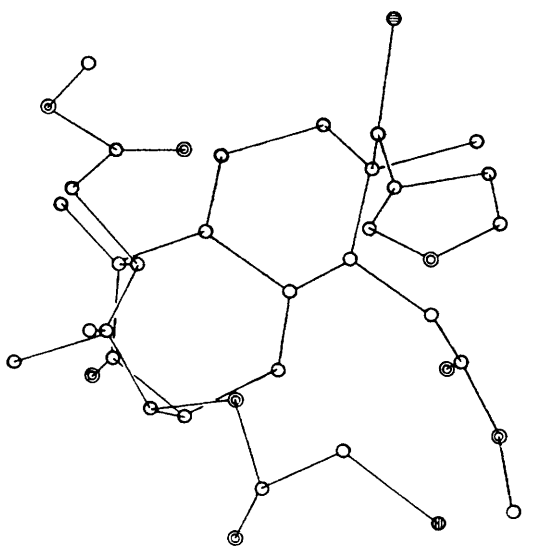
BEVAN *et al.*[1] have described the isolation of two substances A and B from the timber of *Cedrela odorata*. Substance A was shown[1] to be 7-deacetoxy-7-oxogedunin(I). Substance B has been shown to have the structure(II) based on chemical[2] and crystallographic evidence. Crystallographic evidence was provided by the analysis of the crystal structure of an iodoacetate, obtained from substance B by the following conversions:[3] Treatment of substance B(II) with methanol and sulphuric acid gave a methylation product(III). This was reduced with sodium borohydride to an alcohol(IV) which reacted with chloroacetyl chloride to give a chloroacetate. The chloroacetate was converted by sodium iodide into the iodoacetate.

The reaction of the alcohol(IV) with chloroacetyl chloride was presumed only to have formed a chloroacetate, but the results of the crystallographic analysis showed that the methoxy-group at C–17 of the alcohol was replaced by a chlorine atom, evidently during the same reaction. The presence of the chlorine atom was later confirmed by chemical analysis.

The colourless crystals of the iodoacetate are orthorhombic, with cell dimensions $a = 10{\cdot}8$, $b = 16{\cdot}0$, $c = 18{\cdot}6$ Å. The space group is $P2_12_12_1$. With the assumption that the unit cell contained four molecules, the measured density, 1·432g. cm.$^{-3}$, gave a molecular weight of $693 \pm 7$. Equi-inclination Weissenberg photographs were taken with copper $K\alpha$ radiation, and 991 independent reflections of measurable intensity were visually estimated; 312 other reflections were too weak to be measured. The position of the iodine atom was determined from a three-dimensional Patterson synthesis, and those of the light atoms from a series of $F_0$ and $F_0 - F_c$ syntheses. The $R$ factor is now 18·3%. Further refinement is in progress.

The molecule of the iodoacetate is shown in perspective in Figure 1, and more conventionally in Figure 2. The position of the double bond



○ ≡ CARBON, ◎ ≡ OXYGEN, ⊜ ≡ CHLORINE, ⊕ ≡ IODINE.

FIGURE 1

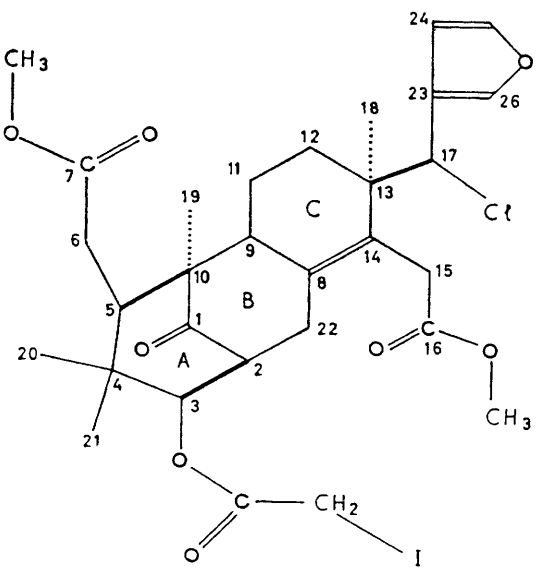
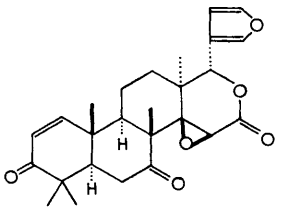


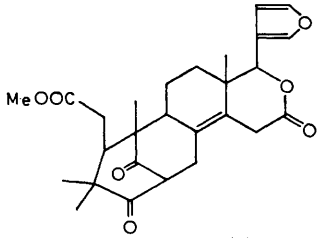

FIGURE 2

[1] C. W. L. Bevan, J. W. Powell, and D. A. H. Taylor, *J. Chem. Soc.*, 1963, 980.
[2] C. W. L. Bevan, J. W. Powell, and D. A. H. Taylor, *Chem. Comm.*, 1965, 281.
[3] J. W. Powell *et al.* Unpublished.

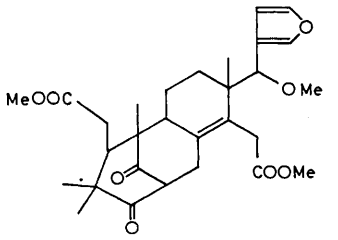
between C–8 and C–14 was established by the planarity of the atoms 8, 9, 22, 14, 13, and 15. The carbonyl group at position-1 was distinguished from a C–$CH_3$ group by the planarity of the oxygen atom and the carbon atoms 10, 1, and 2.



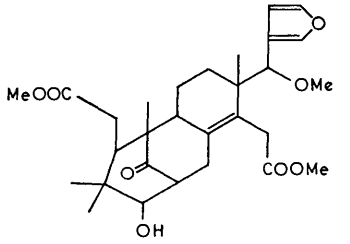

(I)




(II)




(III)




(IV)

The mean plane through the atoms of ring A is almost perpendicular to that through the atoms of rings B and C.

The molecular formula is $C_{30}H_{38}O_8ClI$, corresponding to a molecular weight of 688·4, which agrees with the value stated above.

The structure of the alcohol (IV) and the methylation product (III) can be deduced immediately from that of the iodoacetate (Figure 2). These structures give strong support to that proposed[3] for Substance B (II). Substance B therefore appears to be identical with mexicanolide,[4] which was isolated from *Cedrela mexicana*.

We are grateful to Professor C. W. L. Bevan for presenting us with the problem, to Professor Dorothy Hodgkin, Professor D. A. H. Taylor, and Dr. J. W. Powell for some useful suggestions, and further to Dr. J. W. Powell who did the preliminary work on the preparation of the iodoacetate.

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[4] J. D. Connolly, R. McCrindle, and K. H. Overton, *Chem. Comm.*, 1965, 162.