Methyl Ivorensate, an A-Seco-limonoid from *Khaya ivorensis*

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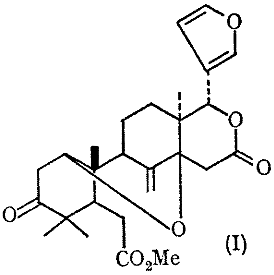
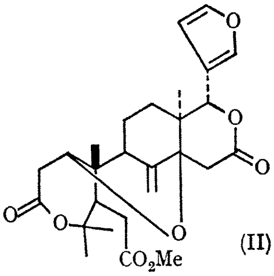
Summary A new compound from *Khaya ivorensis* is shown to be the A-seco-limonoid (II).

THE limonoids are a group of oxidised triterpenes found in plants of the families Rutaceae and Meliaceae. Limonoids from the Rutaceae, *e.g.* obacunone, are characterised by having A opened, whereas no compounds from the Meliaceae have yet been shown to have this feature.[1]

The timber of *Khaya ivorensis* contains about 0·1% of khivorin; the mother-liquors contain a large number of other limonoids, of which methyl angolensate (I) is the next most plentiful.[2] In a detailed investigation of these mother-liquors we have now isolated a new compound, methyl ivorensate, $C_{27}H_{34}O_8$, m.p. 279—281°, $[\alpha]_D$ $-97{\cdot}5°$. This has one oxygen atom more than methyl angolensate. The n.m.r. spectrum was very similar to that of methyl angolensate, showing the same structural features, in particular the exocyclic methylene group and the 1-H oxide proton were readily recognised. The only major differences were that the resonance frequencies of two methyl groups had shifted strongly downfield, from 64, 73 c./s. (at 60 Mc./s.) in methyl angolensate to 82, 95 c./s. in methyl ivorensate; and that the 5-H, 6-H_2 system, which in methyl angolensate gives a complex absorption pattern, showing hindrance to free rotation, in methyl ivorensate appears as a triplet and a two-proton doublet, showing free rotation of the side-chain. In the i.r. spectrum, a band at 1720 cm.$^{-1}$ appears to have moved to 1740 cm.$^{-1}$. There is no hydroxy-group, no extra carbonyl group, and the n.m.r. spectrum shows no additional bands in the region characteristic of protons vicinal to ether rings. It appeared that the only likely structure was (II), in which the 3-ketone was oxidised to a ring-A lactone; this would account for the strong downfield shift of two methyl groups, as occurs in dihydro-obacunone relative to 7-oxo-7-deacetoxygedunin. In agreement with this, the saponification equivalent of methyl ivorensate was found to be 163. It is known that the vinyl group in methyl angolensate is unusually resistant to oxidation,[3] so it seemed probable that perbenzoic acid oxidation of methyl angolensate would yield the corresponding lactone (II). In fact, the reaction produced a moderate yield of a compound identical with methyl ivorensate, which confirms the structure (II) assigned to the latter compound. This is the first A-seco-limonoid to be obtained from plants of the family Meliaceae.



(I)



(II)

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