Extractives from *Fagara zanthoxyloides* (Lam.)

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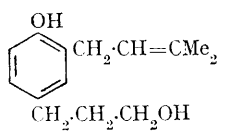
EXTRACTION of the timber of *Fagara zanthoxyloides* (Lam.) (Rutaceae) gave an oil. This was separated into phenolic and neutral fractions; chromatography of the phenolic fraction gave as main product a substance $C_{14}H_{20}O_2$, which we name zanthoxylol. The n.m.r. spectrum of this showed that it was a trisubstituted benzene derivative containing two hydroxyl groups.

The following bands appeared in the spectrum. δ 3·3 (2H doublet, Ar·C*H*$_2$·CH=), 5·27 (1H triplet, =C*H*–CH$_2$), 1·7 6 proton singlet, [(C*H*$_3$)$_2$·C=], and 2·5 (2H complex, Ar·C*H*$_2$·CH$_2$); 1·85 (2H, complex, CH$_2$·C*H*$_2$·CH$_2$), 3·6 (2H triplet, CH$_2$·C*H*$_2$OH). This suggested that the compound was an isomer of 2-dimethylallyl-4-(3′-hydroxypropyl)phenol (I).

Acetylation esterified the aliphatic hydroxyl group; hydrogenation gave a dihydro-compound, of which the methyl ether was a crystalline solid, m.p. 49—50°. The spectral properties of these derivatives agreed with the above structure.

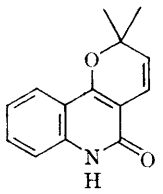
Treatment of zanothoxylol with acid gave a new compound in which the spectral signals due to the two methyl groups on a double bond and to the double-bond proton itself were missing, and two tertiary methyl groups absorbing at δ 1·3 appeared instead. This compound appeared to be a 2,2-dimethylchroman; showing that in zanthoxylol the dimethylallyl group is *ortho* to the phenolic OH. The infrared spectrum of the natural product and its derivatives showed two aromatic bands at 820, 790 cm.$^{-1}$, suggesting a 1,2,4-trisubstituted compound, so it seemed probable that the propyl alcohol residue was *para* to the phenolic hydroxyl; as in (I).



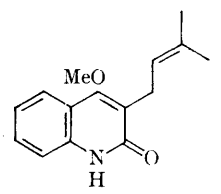
(I)

This has been confirmed by synthesis of a degradation product. The alcoholic hydroxyl group in dihydrozanthoxylol was removed by treatment with hydriodic acid and then zinc and acetic acid, to give 2-(3′-methylbutyl)-4-propylphenol. This was synthesised from 2-(3′-methylbutyl)phenyl propionate by Fries rearrangement followed by Clemmensen reduction; the natural and the synthetic material were identical in all respects. 2-(3′-Methylbutyl)-6-propylphenol, which was synthesised from the allyl ether of 2-(3′-methylbutyl)-phenol by Claisen rearrangement followed by hydrogenation, had different spectral properties.

A small amount of a crystalline solid $C_{15}H_{17}O_2N$,



(II)



(III)

m.p. 133° was also obtained. The n.m.r. spectrum of this showed four aromatic protons, an *O*-methyl group, and the group $Ar{\cdot}CH_2{\cdot}CH{=}CMe_2$. The infrared spectrum was similar to that of a 2-quinolone (ν_{max} 1660 cm.$^{-1}$). Insufficient of the material has been obtained for further investigation; but in view of the close similarity to flindersine (II) an alkaloid also isolated from the timber of Rutaceae, we consider our substance to be 3-dimethylallyl-4-methoxy-2-quinolone (III).

(*Received, May 23rd,* 1966; *Com.* 349.)