INVESTIGATION OF THE RESIN OF THE ROOTS OF Ferula iaeschkeana

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UDC 547.913.5:668.5:547.587.52

In an investigation of the resin of the roots of Ferula iaeschkeana Vatke, collected in the Turkmen SSSR we obtained a substance with the composition $C_{22}H_{30}O_4$ (I) which could not be crystallized. On chromatography in a thin layer of alumina, it gave a single spot with R_f 0.5 [solvent: chloroform−ethanol (99:1); Al_2O_3, activity grade III]. The UV spectrum had a maximum at 263 nm, log ε 4.20. The IR spectrum of the substance had strong bands at (cm^{-1}) 3350 (OH), 1690 (ester CO), 1610, 1590, and 1520 (aromatic ring). A band at 1285 cm^{-1}, together with the maxima at 1690, 1610, 1590, and 1520 cm^{-1}, is extremely characteristic for aromatic esters and may serve as a reliable proof that the compound under consideration belongs to this class.

The acetylation of (I) led to a monoacetyl derivative (II), $C_{24}H_{32}O_5$, with R_f 0.31 (solvent: $CHCl_3$ + five drops of C_2H_5OH, Al_2O_3, activity grade II) in the IR spectrum of which there were bands at (cm^{-1}) 3530 (OH), 1780 (acetyl CO), 1710 (ester CO), and 1615 and 1520 (aromatic ring). The presence in the IR spectrum of (II) of maxima at 3530 and 1780 cm^{-1} shows that (I) contains two OH groups, one of them being phenolic and the other tertiary.

In the NMR spectrum of (II) (here and below, 100 MHz, δ scale, solution in CCl_4) there is the singlet of the methyl of an acetyl group at 2.35 ppm ($CH_3-\underset{|}{C}=O$). However, there is no signal of a proton at an acetyl group in the weak-field region of the spectrum. In the spectrum of (I) there are a one-proton multiplet at 5.3 ppm and an unresolved triplet at 5.61 ppm (1H). In the NMR spectrum of (II), the protons of the aromatic ring appear in the form of two-proton doublets with centers at 7.19 and 8.03 ppm, J = 9 Hz, showing the para substitution of the benzene ring. Doublets of CH_3 groups at 0.96 and 1.05 ppm, J = 7 Hz, belong to an isopropyl group, a singlet at 1.20 ppm to an angular methyl, and a singlet at 1.93 ppm to a vinyl methyl.

The saponification of (I) gave a sesquiterpene alcohol with the composition $C_{15}H_{26}O_2$, mp 88-89°C, and an acid $C_7H_6O_3$ with mp 211-212.5°C. From its IR and NMR spectra and the absence of a depression of the melting point of a mixture with an authentic sample, the acid was identified as p-hydroxybenzoic acid.

The NMR spectrum of the alcohol showed the signals of the CH_3 residues of an isopropyl group (doublets at 0.89 and 0.92 ppm, J = 7 Hz), of an angular methyl group (singlet at 0.98 ppm), and of a vinyl methyl group (singlet at 1.78 ppm). The olefinic proton appeared in the NMR spectrum of the alcohol in the form of an unresolved multiplet at 5.38 ppm (1H). The proton in the geminal position to the OH group also appeared in the form of a multiplet, at 3.83 ppm (1H).

The results of a direct comparison of the IR spectra of the alcohol obtained, of ferutinol [1, 2] and of chimgandiol [3] have shown that they are identical.

Thus, the substance that we have isolated is feringin [2] or its stereoisomer.

LITERATURE CITED

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V. L. Komarov Institute of Botany, Academy of Sciences of the Azerbaidzhan SSR. Translated from Khimiya Prirodnykh Soedinenii, No. 5, p. 664, September-October, 1973. Original article submitted February 21, 1973.