AN AROMATIC COMPOUND FROM Ferula karatavica

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The resin (30 g) from the roots of Ferula karatavica Rgl. et Schmalh. was chromatographed on alumina (1000 g, activity grade III) and eluted with chloroform–petroleum ether (1:4). A crystalline substance (I) with the composition $C_{11}H_{12}O_4$, mp 85-86°C (70% ethanol), was isolated. This compound is a new one and has not previously been found in the resin of this plant.

The IR spectrum of (I) (mull in paraffin oil) has characteristic absorption bands at (cm^{-1}) 1680 (CO of a conjugated ketone), 1630, 1605, 1530 (C=C of an aromatic system).

The NMR spectrum of (I) (100 MHz, CCl_4, δ scale) has the triplet signal of the protons of a primary methyl group (1.10 ppm, 3H, J=7 Hz), the quartet signal of the protons of a methylene group in an ethyl grouping (2.96 ppm, 2H, J=7 Hz), the singlet signal of the protons of a methyl group in a methoxy grouping (3.86 ppm, 3H), and the singlet signal of the protons of a dioxymethylene group (5.94 ppm, 2H).

In the weak-field region of the spectrum there are the signals of two protons of an aromatic ring (6.97 ppm, 1H, J=2 Hz, and 7.10 ppm, 1H, J=2 Hz). The magnitude of the coupling constants of the aromatic protons shows their meta position [1]. On the basis of the facts given, for compound (I) we propose the structure of 3,4-dioxymethylene-5-methoxy-1-(1-oxopropyl)benzene. The mass spectrum of (I) (MKh-1303, at 250°C, ionizing voltage 30 V) included the peak of the molecular ion with m/e 208 (38%), corresponding to the suggested empirical formula.

α-Cleavage with respect to the carbonyl oxygen atom leads to the formation of an ion with m/e 179 (100%). Then from the maximum ion (m/e 179) are successively ejected molecules of carbon monoxide (fragment with m/e 151), formaldehyde (fragment with m/e 121), and acetylene (fragment with m/e 95).

The transitions $208^+ \rightarrow 179^+$ and $179^+ \rightarrow 151^+$ are confirmed by the presence in the mass spectrum of (I) of metastable peaks with m/e 154.2 (calculated 154) and with m/e 127.4 (calculated 127.3), respectively.

Thus, the results of mass spectroscopy also agree well with the structure proposed for this compound.

LITERATURE CITED

1. N. Bhacca and D. Williams, Applications of NMR Spectroscopy in Organic Chemistry, Holden-Day, San Francisco (1964).

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