A CHEMICAL STUDY OF THE ESSENTIAL OIL

OF Libanotis intermedia

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The present paper gives the results of a study of the sesquiterpenes of the essential oil of the fruit of Libanotis intermedia.

By chromatography on silica using as eluents petroleum ether and ethyl acetate, we separated the essential oil into a hydrocarbon fraction and an oxygen-containing fraction. After the terpene hydrocarbons had been distilled off, the sesquiterpenes were fractionated under vacuum, and then each fraction was chromatographed repeatedly on alkaline alumina (activity grade II). This separation gave three compounds which we have provisionally named A, B, and C, their properties being given in Table 1.

A 10% solution of bromine in chloroform colored all three substances an intense violet, and the Ehrlich-Miller reagent gave an emerald green color, which shows the azulene nature of the sesquiterpenes under investigation [1, 2].

Substance A, $C_{15}H_{24}$; IR spectrum, cm⁻¹: 1694 w, 1638 s, 1493 s, 1142 w, 892 s. In the IR spectrum of the hydrogenated compound, the bands with frequencies characteristic for double bonds (1638 and 892 cm⁻¹) have disappeared. Substance A is a bicyclic sesquiterpene hydrocarbon of the azulene series with two nonconjugated double bonds (exaltation of the molecular refraction 0.43).

Substance B, $C_{15}H_{24}$: IR spectrum, cm⁻¹: 1730 s, 1648 s, 1452 s, 1379 s, 1170 w, 892 s. This shows that it is cicyclic sesquiterpene hydrocarbon of the azulene series with nonconjugated double bonds (exaltation of the molecular diffraction 0.41).

Substance C, $C_{15}H_{24}$; IR spectrum, cm⁻¹: 1730 s, 1640 s, 1459 s, 1383 s, 1230 w, 1178 w, 892 s. The substance may be a bicyclic sesquiterpene hydrocarbon of the azulene series with two double bonds (depression of the molecular refraction 0.40).

The dehydration of the sesquiterpene hydrocarbons [3, 4] gave a blue-violet azulene forming a trinitrobenzene derivative melting at 87-88°C and a trinitrotoluene derivative melting at 70-71°C. IR spectrum of the azulene, cm⁻¹: 1666, 728 (double bonds), 1258, 1367, 1457 (methyl groups). The properties of this azulene differ from those of known natural azulenes.

The sesquiterpenes that we are studying are possibly isomers of the libanotenes of the oil of the Libanotis transcaucasica [5].

In the department of microbiology, O. V. Chuiko has found that the sesquiterpenes of Libanotis intermedia are bactericidal to the hemolytic streptococcus but are less active towards yeasts; bacilli, including

B. coli; Pseudomonas pyocyanea; and Staphylococcus hemolyticus. Azulene has a better anti-in-flammatory action.

TABLE 1

Sub-	bр , °С (3 mm)	20 d 4	20 n _D ,	[d] 20 deg	MR	
stance					found	calculated
A B C	130—131,5 134—136,0 138—140,5	0,8938 0,9035 0,9190	1,4990 1,4995 1,5055	-5,80 -8,40 -7,90	66,57 66,55 65,74	66,14 66,14 66,14

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