BRIEF COMMUNICATIONS

2-METHYLHEXA-2,4-DIENE — A COMPONENT OF THE ESSENTIAL OIL OF *Achillea filipendulina*

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From the essential oil of *Achillea filipendulina* Lam. (fernleaf yarrow), by fractional distillation and preparative gas–liquid chromatography (GLC) we have isolated a substance with bp 107°C/698 mm, n_D^{20} 1,4682, d_{20}^{20} 0.7440, $[\alpha]_D^{20}$ 0°, the identification of which could not be performed previously because of its polymerization [1].

The substance has the composition C_7H_{12}, and on hydrogenation over platinum oxide (according to Adams) it added two moles of hydrogen. The UV spectrum of the hydrocarbon has an absorption band at λ_{max} 236 nm (log ε 3.25, hexane). This characterizes it as a diene with conjugated double bonds. The presence in its IR spectrum of a strong absorption band at 968 cm^{-1} permits the assumption that one of the multiple bonds belongs to a trans-disubstituted —CH=CH— group [2]. The other multiple bond apparently forms a —CH=C$(CH_3)_2$ group (absorption band at 1376 cm^{-1}).

The PMR spectrum of the hydrocarbon shows the signals of three olefinic protons at 5-6.4 ppm, and at 1.6-1.8 ppm there is a distorted 9-proton doublet due to the superposition of the poorly resolved signal of the protons of the methyls of an isopropylidene group and a signal in the form of a doublet from the protons of a methyl group.

The results obtained permit the conclusion that the substance isolated is trans-2-methylhexyl-2,4-diene.

The constants of the hydrogenation product of the hydrocarbon (bp 87°C/690 mm, n_D^{20} 1.3857, d_{20}^{20} 0.6793) and its mass spectrum are identical with the constants and mass spectrum of 2-methylhexane [3-6]. Furthermore, when the substance isolated was oxidized by Délépine's method [7], acetone and acetic and oxalic acids were identified among the reaction products.

The essential oil also contains the cis isomer of 2-methylhexa-2,4-diene. This conclusion is based on the fact that the hydrogenation of the fraction containing the two isomers in equal amounts yielded a product giving a single peak on GLC analysis. The amount of cis-isomer is 5-6 times less than the amount of trans isomer.

It must be mentioned that the octylene identified previously in the essential oil of the fernleaf yarrow [8] obviously consists of a mixture of 2-methylhexa-2,4-diene and achillene (2,5-dimethyl-4-vinyl-hexa-2,5-diene) [1].

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