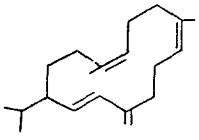
NEW DITERPENES, ISOCEMBRENE AND ISOCEMBROL, IN THE OLEORESIN OF PINUS SIBIRICA

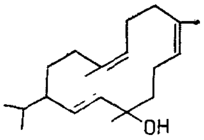
N. K. Kashtanova, A. I. Lisina, and V. A. Pentegova

Khimiya Prirodnykh Soedinenii, Vol. 4, No. 1, pp. 52–53, 1968

From the neutral part of the oleoresin of Pinus sibirica (R) Mayr. we have isolated two new diterpene compounds with 14-membered rings: a hydrocarbon $C_{20}H_{34}O$, which we have called isocembrene (I) and isocembrol (II).



I



II

Isocembrene with c $[\alpha]^{20}_D$ +60.3° (c 2, 60; chloroform), n^{20}_D 1.5230 contains two double bonds. In the IR spectrum of the compound bands at 890, 1655, and 3085 cm^{-1} correspond to an exomethylene double bond, whose presence is confirmed by ozonization, and the band at 970 cm^{-1} to a trans-disubstituted and that at 815 cm^{-1} to a trisubstituted double bond. The UV spectrum has a maximum at 238 mμ (log ε 4.3).

The isomerization of I on alumina containing silver nitrate gave cembrene. The exhaustive hydrogenation of I over platinum oxide gave octahydrocembrene, and exhaustive hydrogenation over $Pd/CaCO_3$ gave a hydrocarbon with c$[\alpha]^{20}_D$ +43.0° (c 0.86; chloroform), n^{20}_D 1.4990, mol. wt. 275 (mass spectrometry) identical with that described by Dauben et al. [1].

The dehydrogenation of isocembrene with selenium gave 2, 9-dimethyl-7-isopropylphenanthrene.

Isocembrol $C_{20}H_{34}O$ with $[\alpha]^{20}_D + 80.1°$ (c 3.20; chloroform), n^{20}_D 1.5035 is an isomer of cembrol, which we have described previously [2]. We have ascribed bands at 815 and 1665 cm^{-1} in the IR spectrum of isocembrol to a trisubstituted double bond, a band at 970 cm^{-1} to a trans-disubstituted double bond, and one at 3615 cm^{-1} to a tertiary hydroxyl.

Isocembrol contains three double bonds. The UV spectrum shows the absence of conjugation in this compound (in the 220–400 mμ region).

Under the action of acid chlorides, thionyl chloride, and acetic acid, isocembrol readily dehydrates to cembrane, and on the sorbent (SiO_2 + $AgNO_3$) to isocembrene (I).

The NMR spectra of the compound do not contradict the structures proposed.

REFERENCES

1. W. G. Dauben, W. E. Thessen, and P. R. Resnick, J. Org. Chem., 30, 1693, 1965.
2. A. I. Lisina, A. I. Rezvukhin, and V. A. Pentegova, KhPS [Chemistry of Natural Compounds], 250, 1965.

8 September 1967

Novosibirsk Institute of Organic Chemistry,
Siberian Division, AS USSR