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Essential oils and their constituents

Part XLI. Identification of sesquiterpene hydrocarbons in oil of opoponax*

In a paper from this laboratory the occurrence of isomeric bisabolenes in oil of opoponax has been reported². A personal communication, received since, claiming the presence of only α -santalene and α -bisabolene in this oil³ prompted us to re-examine our samples following column and gas chromatographic purification.

Fig. 1 shows the gas chromatogram of the sesquiterpene fraction as originally recorded employing the silicone nitrile XE-60 column². Four fractions corresponding

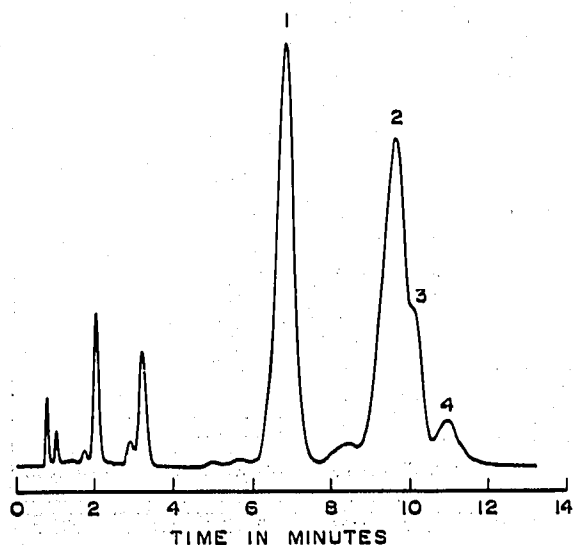


Fig. 1. Gas chromatogram of the sesquiterpene fraction of oil of opoponax.

* For the previous paper, see ref. 1.

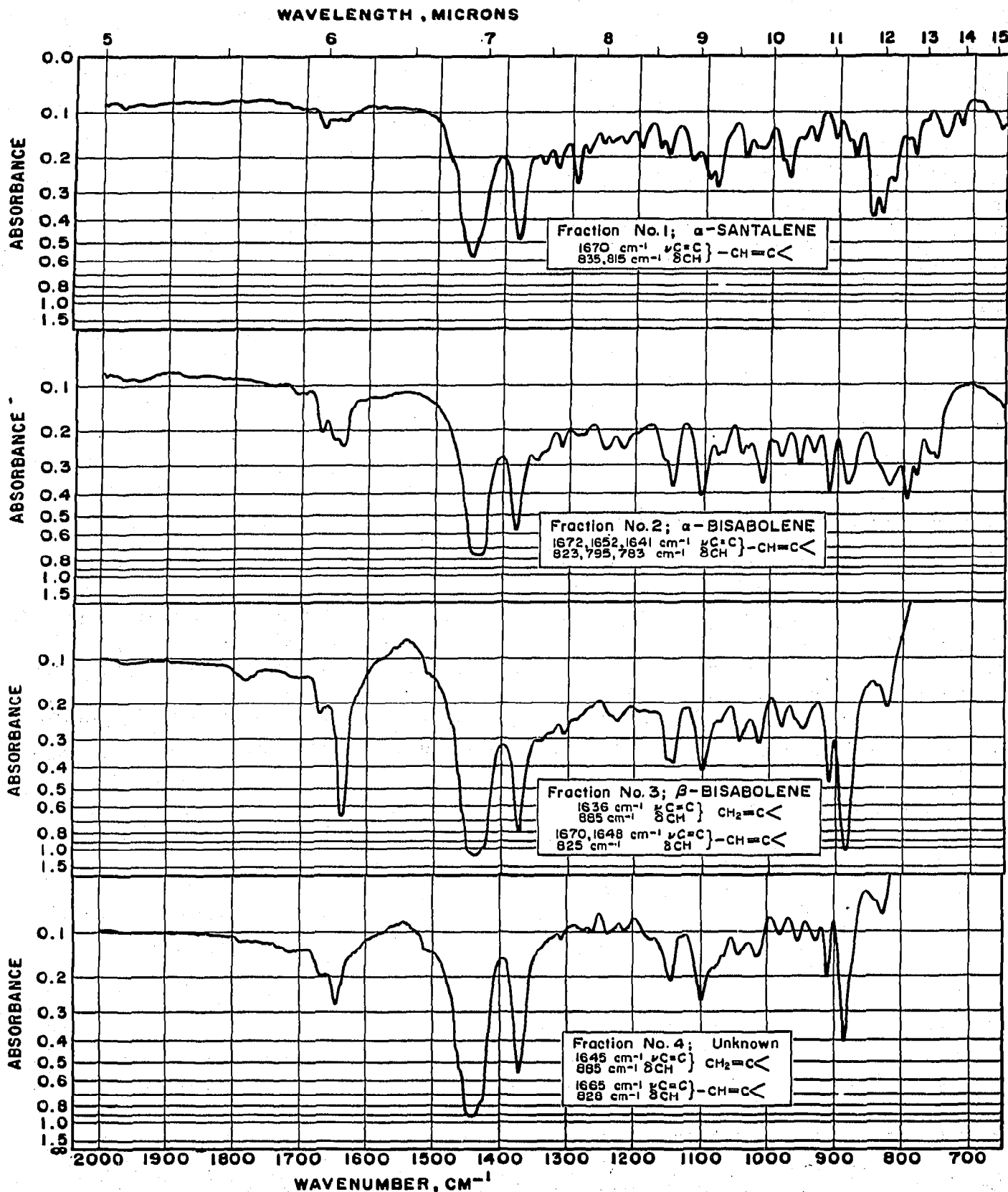
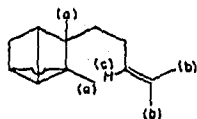
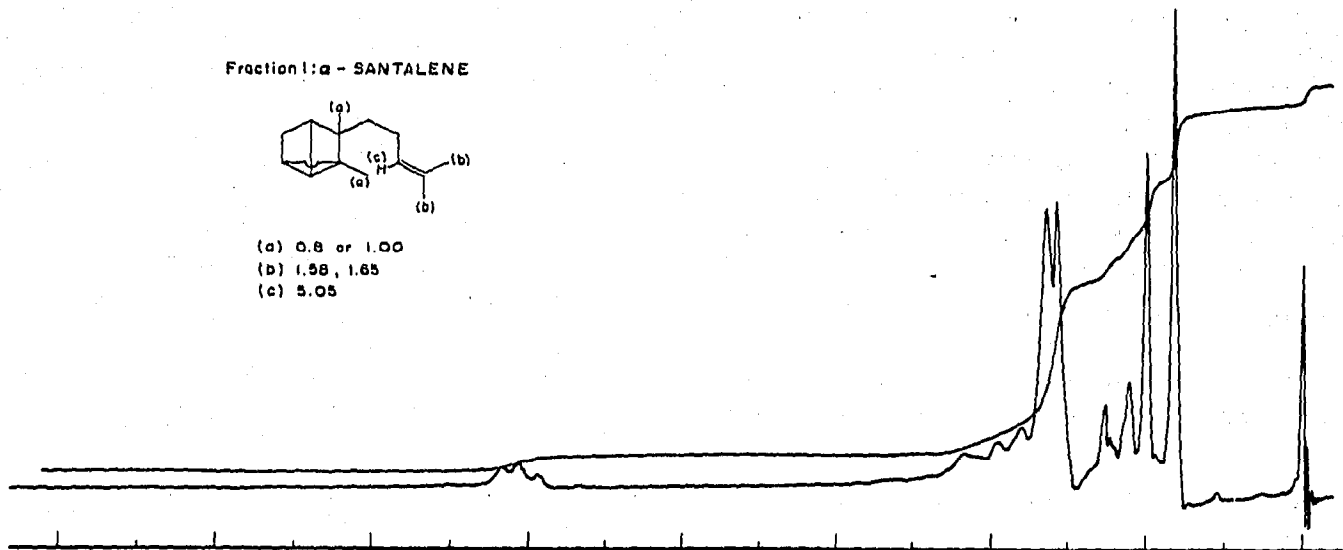


Fig. 2. Infrared spectra of the gas chromatographic fractions. Instrument: Perkin-Elmer 221. Phase: fraction Nos. 1 and 2, liquid film; fraction Nos. 3 and 4, CCl₄ solution.

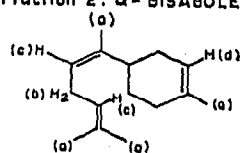
Fraction 1: α -SANTALENE



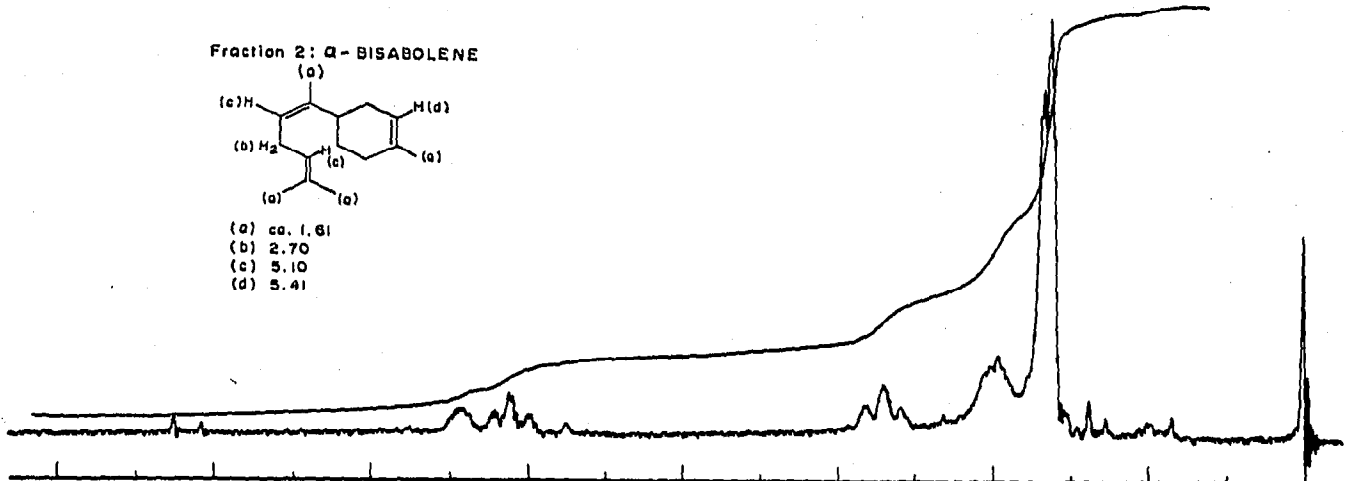
- (a) 0.8 or 1.00
- (b) 1.98, 1.65
- (c) 5.05



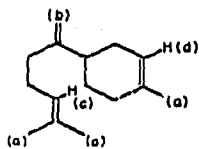
Fraction 2: α -BISABOLENE



- (a) ca. 1.61
- (b) 2.70
- (c) 5.10
- (d) 5.41



Fraction 3: β -BISABOLENE



- (a) 1.60, 1.65
- (b) 4.70
- (c) 5.05
- (d) 5.35
- CHCl₃ 6.95

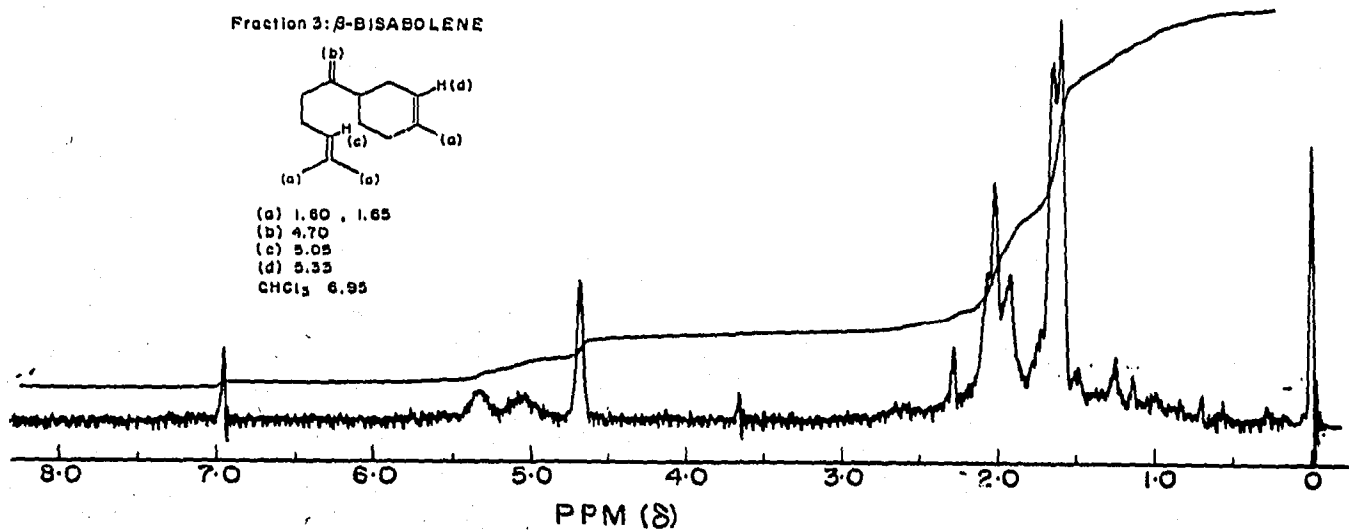


Fig. 3. NMR spectra of the gas chromatographic fractions. Instrument: Varian A-60A. Solvent: CDCl₃. Internal Reference: TMS.

to the peaks so numbered were collected. The infrared and NMR spectra of fractions 1 and 2 (Figs. 2 and 3) agreed with those of α -santalene and α -bisabolene. The infrared spectrum of fraction 3 was identical to that reported for β -bisabolene⁴. The NMR spectrum of the fraction was consistent with the structure of β -bisabolene and also agreed with that measured for this sesquiterpene by BATES⁵. Fraction 4 could not be re-examined due to polymerisation during storage. Its infrared spectrum as originally obtained (Fig. 2) was found to be identical with that of regenerated bisabolene⁴.

We, therefore, conclude that oil of opoponax contains α -santalene, α -bisabolene and β -bisabolene, as well as some other isomeric bisabolene.

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