

Natural Occurrence of α -Cadinene

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The sesquiterpene hydrocarbon, α -cadinene (I) has been isolated from Japanese hop (*Humulus lupulus* L.) for the first time.

The hydrocarbon (I) is a colorless oil, $C_{15}H_{24}$, $[\alpha]_D^{25} -62.4^\circ$ (c 0.868, $CHCl_3$). Its NMR (CCl_4) spectrum shows two vinyl protons at δ (ppm) 5.32 (1H), and 5.52 (1H). Besides the signals of isopropyl group at δ 0.78 (3H, d, $J=7$ cps), and 0.91 (3H, d, $J=7$ cps), the spectrum shows six protons at 1.65 (broad s.) corresponding to two vinyl methyl groups. The MS spectrum exhibits the molecular ion peak at m/e 204 and the base peak, at m/e 105 together with a considerably abundant peak at m/e 161 ($M-43$).

On partial hydrogenation with platinum oxide in a mixture of methanol and ether, a single product was provided. The IR spectrum of the product was identical with that of the dihydrocadinene prepared from γ -cadinene. The hydrocarbon (I) yielded crystalline dihydrochloride, $[\alpha]_D^{25} -38.1^\circ$ (c 1.608, $CHCl_3$), mp 115–116°C, by treating with dry hydrogen chloride in ether solution. The product showed no depression of the mixed melting point with an authentic sample of (–)-cadinene dihydrochloride^{1–3} of known absolute configuration. In addition, the IR spectrum of I is different from that of β -cadinene^{4,5} as shown in Fig. 1.

The above evidence leads to α -cadinene structure (I) for this hydrocarbon.

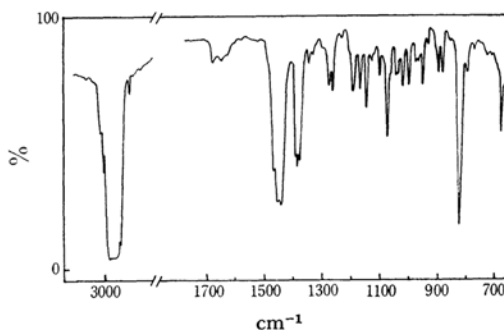


Fig. 1. IR spectrum of I.



(I)

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