(*E*)-9-Isopropyl-6-methyldeca-5,9-dien-2-one, a Terpenoid C_{14}-Ketone with a Novel Skeleton

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Summary The isolation and synthesis of (*E*)-9-isopropyl-6-methyldeca-5,9-dien-2-one, a terpenoid C_{14}-ketone with a novel skeleton from costus root oil (*Saussurea lappa* Clarke) are reported.

IN the course of analysis of the oil of costus root (*Saussurea lappa* Clarke) we isolated† a compound having the empirical formula $C_{14}H_{24}O$ (confirmed by mass spectrum and n.m.r. integration curve) with ν_{max} (neat) 3110, 1715, 1660, 1640, and 885 cm^{-1}; δ (90 MHz, $CDCl_3$) 1·01 (6H, d, *J* 6·5 Hz), 1·62 (3H, br s), 2·09 (4H, br s), 2·13 (3H, s), 2·16—2·62 (5H, m), 4·67 (1H, br s), 4·73 (1H, br s), and 5·09 (1H, br t, *J* 6 Hz); *m/e* 208 (M^+, $<1\%$) and 43 (100%). These data suggested the presence of a non-conjugated –CO–Me group, $>C{=}CH_2$ and –CH=C–Me olefinic systems, and an isopropyl group. The biogenetically satisfying, hypothetical structure

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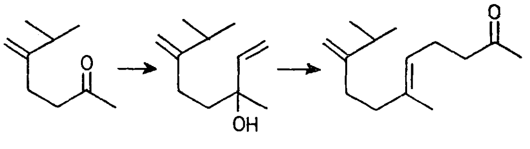
† Isolation involved extraction of the carbonyl compounds with Girard reagent P, column chromatography on SiO_2, and g.l.c. The concentration of the title compound in the commercial oil is *ca.* 0·03%.

(**1**)‡ accounts for all of these units and is in good agreement with the n.m.r. spectrum observed. Structure (**1**) (including the geometry of the double bond) was confirmed by synthesis.



(2) (3) (1)

Addition of vinyl magnesium bromide (in tetrahydrofuran) to thuja ketone (**2**)[1] gave the known alcohol (**3**) which, on Carroll reaction[2] with ethyl acetoacetate in the presence of sodium acetate, gave a mixture (70% yield) of the two possible geometric isomers of (**1**) (2:1 ratio) which was separated by preparative g.l.c. The more abundant isomer (with longer retention time on both polar and apolar columns) proved identical in all respects with the natural product. It was unambiguously assigned the (*E*)-configuration by a comparison of the n.m.r. spectra of both isomers of (**1**) with those of authentic samples of (*E*)- and (*Z*)-geranylacetone.

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‡ Considering the close structural similarity between the ketone (**1**) and the irones, one might speculate that these compounds are also biogenetically related.

[1] H. Grütter, R. Helg, and H. Schinz, *Helv. Chim. Acta*, 1952, **35**, 771.

[2] M. F. Carroll, *J. Chem. Soc.*, 1940, **704**, 1266; 1941, **507**.