

with a 50% xylene solution of chloroprene in a sealed glass tube for 5 hours at 150°. The contents of the tube gradually blackened and only a viscous mass was obtained. Extraction of this material with ether, acetone and benzene failed to give any material corresponding to an adduct. Hydroquinone, du Pont "terpene B" and *t*-butylcatechol did not appear to inhibit the formation of the viscous material.

A 1.8-g. sample of anthracene, 8.4 g. of chloroprene in 50% xylene solution using "terpene B" polymerization inhibitor was heated for 24 hours at 130° in a sealed glass tube. At the end of this time the anthracene was recovered unchanged.

Acknowledgment.—The carbon hydrogen analyses were performed by the Galbraith Laboratories and the nitrogen analyses by Mrs. Patricia Ramey.

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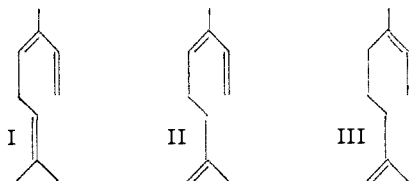
RECEIVED OCTOBER 1, 1951

The Structure of Ocimene

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RECEIVED OCTOBER 9, 1951

The hydrocarbon which has been named ocimene was first isolated by van Romburgh¹ from the essential oil of *Ocimum basilicum* and has since been identified in many other essential oils. Formula II although generally accepted² appears to be incorrect and should be replaced by I.



Jones and Smith³ isolated from the oil of flowering *Tagetes glandulifera* a substance closely similar in various physical and chemical properties to van Romburgh's ocimene and regarded these two substances as identical. The ocimene from this source has now been submitted to quantitative ozonolysis and found to yield 95–96% of the acetone expected on Formula I. This may be compared with acetone yields (96–97%) obtained from pure β -citronellol phenylazophenylurethan⁴ prepared from β -citronellol, the infrared spectrum⁵ of which indicated the presence of less than 1% of α -citronellol. As acetone in this case can result only from the isopropylidene group, the ocimene examined must be I, although the presence of a few per cent. of II is not excluded. In possessing the isopropylidene structure this sample of ocimene resembles the samples of myrcene, citronellol, geraniol, linalol and other acyclic terpenoids so far examined.⁶

(1) P. van Romburgh, *Proc. K. Acad. Wetensch. Amsterdam*, **3**, 454 (1900).

(2) (a) J. L. Simonsen and L. N. Owen, "The Terpenes," Vol. I, University Press, Cambridge, 1947, p. 19. (b) Maria Lipp in "Richer's Chemistry of the Carbon Compounds," Vol. II, edited by R. Anschutz, T. W. J. Taylor and A. F. Millidge, Elsevier, Amsterdam, 1938, p. 200. (c) L. F. Fieser and M. Fieser, "Organic Chemistry," D. C. Heath and Co., Boston, Mass., 2nd Ed., 1950, p. 1013.

(3) T. G. H. Jones and F. B. Smith, *J. Chem. Soc.*, **127**, 2530 (1925).

(4) M. D. Sutherland, *This Journal*, **73**, 2385 (1951).

(5) R. Werner and M. D. Sutherland, accompanying paper.

(6) (a) Y. R. Naves, G. Brus and J. Allard, *Compt. rend.*, **200**, 1112 (1935); (b) J. Doeuivre, *Bull. soc. chim.*, [5] **3**, 613 (1936); (c) M. F. Carroll, *Perfumery and Essential Oil Record*, **38**, 226 (1947); (d) D. Barnard, *et al.*, *J. Chem. Soc.*, 915 (1950); (e) M. F. Carroll, R. G.

The structure II for ocimene from *O. basilicum* is due to Enklaar who worked almost alone on the problem for about twenty years. Enklaar⁷ at first suggested I in accordance with the 27% yield of acetone obtained from ocimene ozonide but later preferred II although the strongest evidence for this was a color reaction indicating a γ -dicarbonyl compound amongst the ozonolysis products. In 1938 Dupont and Desreux⁸ after examining Raman spectra concluded that a sample of van Romburgh's ocimene was rich in I and that the dihydro ocimene obtained by sodium and alcohol reduction was free from III.

These results of Enklaar and of Dupont and Desreux show that ocimene from *O. basilicum* contains at least a substantial proportion of I. On the other hand, there is no very satisfactory evidence that II is present in any proportion and the results of Dupont and Desreux speak strongly for the absence of II. The close correspondence in physical properties between the ocimene of Enklaar and that of Jones and Smith also favors an identity in structure and an absence of II. Thus no acceptable evidence for the existence of II in essential oils has yet been put forward and the name ocimene should be reserved for the hydrocarbon of structure I first isolated from *Ocimum basilicum*.

Experimental

A sample of crude ocimene from *Tagetes glandulifera* (kindly provided by Professor T. G. H. Jones) was redistilled at 10 mm. pressure and a fraction of b.p. 63° (10 mm.), d_{25}^{25} 0.7947, n_{25}^{25} 1.4836 and $[\alpha]_D +0.12^\circ$ selected. The ozonolysis procedure of Kuhn and Roth⁹ was modified principally by the use of 15–20 mg. samples, an ozonation period of 15 minutes at an oxygen flow rate of 20 ml. per minute, (ozone concentration 8% by weight) and a sufficient excess of $M/5$ $KMnO_4$ (20 ml.) to ensure that some remained unreacted at the end of the distillation. Under these conditions samples of ocimene yielded 94.9, 95.4 and 96.0% of the acetone calculated on formula I. Levulinic and pyruvic acids (10 mg.) processed separately resulted in iodine consumption equivalent to less than 1% of the acetone resulting from 15 mg. of ocimene.

Mason, H. W. Thompson and R. C. S. Wood, *ibid.*, 3457 (1950); (f) Y. R. Naves, *Bull. soc. chim.*, [5] **18**, 506 (1951).

(7) C. J. Enklaar, *Rec. trav. chim.*, **26**, 157 (1907); **27**, 422 (1908); **36**, 215 (1917); **45**, 337 (1926).

(8) G. Dupont and V. Desreux, *Bull. soc. chim.*, [5] **6**, 337 (1938).

(9) R. Kuhn and H. Roth, *Ber.*, **65**, 1285 (1932).

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The Infrared Spectrum of α -Citronellol

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RECEIVED NOVEMBER 1, 1951

In the published reports^{1,2} of the infrared spectrum of various samples of citronellol, the absence of the bands characteristic of the isopropenyl group has been taken as proof of the virtual absence of α -citronellol, which itself has not been available for infrared examination.

The infrared spectrum of the previously de-

(1) D. Barnard, L. Bateman, A. J. Harding, H. P. Koch, N. Shepard and G. B. M. Sutherland, *J. Chem. Soc.*, 915 (1950).

(2) M. F. Carroll, R. G. Mason, H. W. Thompson and R. C. S. Wood, *ibid.*, 3457 (1950).