

PHYTOCHEMICAL REPORTS

β -SPATHULENE: A NEW SESQUITERPENE IN *SCHINUS MOLLE* OIL*

STUART J. TERHUNE, JAMES W. HOGG and BRIAN M. LAWRENCE
Stange Canada Ltd., 3340 Orlando Drive, Mississauga, Ontario, Canada, L4V 1C7

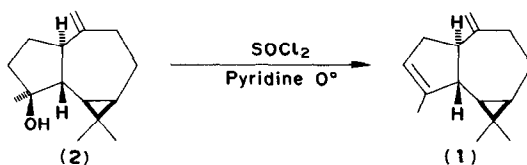
(Received 24 September 1973. Accepted 16 October 1973)

Key Word Index—*Schinus molle*; Anacardiaceae; essential oil; sesquiterpene; β -spathulene.

The chemical composition of *Schinus molle* L., commonly known as the Brazil or California pepper tree, has been the subject of a few investigations. For example, the following compounds have been isolated from the essential oil: β -phellandrene,^{1,2,3,5} α -pinene,^{2,3,5} carvacrol,² *o*-ethyl phenol,⁴ β -pinene,⁵ camphene,⁵ myrcene,⁵ α -phellandrene,⁵ limonene,⁵ and *p*-cymene.⁵ It is the purpose of this note to report on the isolation and structural elucidation of a new sesquiterpene hydrocarbon, named β -spathulene (**1**). To our knowledge this is the first time that β -spathulene has been found naturally occurring.

RESULTS

The data obtained from IR, NMR (22 protons) and MS ($M^+ = 202$) (see Table 1) shows that the compound has a molecular formula of $C_{15}H_{22}$ and that it was consistent with the gross structure **1**. The stereochemistry of **1** was confirmed by dehydrating spathulenol⁶ **2** to give β -spathulene **1**. As the optical rotation of β -spathulene was not determined because of insufficient sample, the specific optical isomer of β -spathulene isolated from *Schinus molle* is not known.



EXPERIMENTAL

Plant material and oil removal. The fruit from *S. molle* was collected from the outskirts of Mexico City, Mexico. The essential oil was obtained by steam distillation of the dried fruit.

* Part XV in the series "Essential Oils and Their Constituents". For Part XIV see (1974) *Phytochemistry* **13**, to be published.

¹ ANON (1909) *Semi-Ann. Rept. Schimmel & Co.* (April) 83.

² GONZALEZ, A. (1937) *Chem. Abstr.* **31**, 5105.

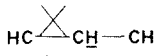
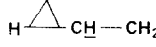
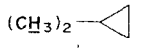
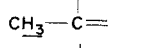
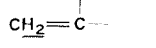
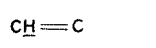
³ CREMONINI, A. (1928) *Ann. Chim Applicata* **18**, 361.

⁴ MONTES, A. L., BANDINELLI, C. O. and DAVIDSON, E. (1961) *Ann. Soc. Ciec. (Argentina)* **172**, 3.

⁵ BERNHARD, R. A. and WROLSTAD, R. (1963) *J. Food Sci.* **28**, 59.

⁶ BOYER, R. C. and JEFFERIES, P. R. (1963) *Chem. Ind.* 1245.

TABLE 1. NMR AND MS DATA FOR β -SPATHULENE

δ	No. of protons	Type	Hz	Inference
0.423*	1	$d \times d$	≈ 10.09	
0.755*	1	m	—	
1.02*	3	s	—	—
1.05*	3	s	—	
1.59	3	s	—	
4.49*	2	bs	—	
5.15	1	bs	—	

$m/e = 159, 131, 105, 91$ and 202 m.u.

* These peaks are also found in NMR of spathulenol.

Isolation of β -spathulene. After $\text{AgNO}_3\text{-Al}_2\text{O}_3$ column chromatography on the sesquiterpene hydrocarbon fraction,^{7,8} β -spathulene was isolated from the appropriate fraction by preparative GC over Carbowax 6000.

Dehydration of spathulenol to β -spathulene was done with pyridine- SOCl_2 using a procedure described previously.⁹

Spectroscopy. IR spectrum was run as a thin film (0.05 mm spacer), $\mu = 3.25, 3.30, 6.13, 7.29, 8.49, 9.67, 9.90, 10.32, 11.30, 12.55, 13.02$ and 15.70μ . The NMR was run as a 1% soln in CDCl_3 on a Varian Aerograph 220 MHz spectrometer.

⁷ LAWRENCE, B. M., TERHUNE, S. J. and HOGG, J. W. (1971) *Flavour Industry* 2, 173.

⁸ LAWRENCE, B. M. (1971) *Can. Inst. Food Technol. J.* 4, A44.

⁹ HOGG, J. W., TERHUNE, S. J. and LAWRENCE, B. M. (1971) *Am. Perfum. Cosmet.* 86, 33.

Phytochemistry, 1974, Vol. 13, pp. 866 to 867. Pergamon Press. Printed in England.

N-METHYLTYRAMINE FROM *OPUNTIA CLAVATA**

RANDALL L. VANDERVEEN, LESLIE G. WEST and JERRY L. McLAUGHLIN

Department of Medicinal Chemistry and Pharmacognosy, School of Pharmacy and Pharmacal Sciences,
Purdue University, West Lafayette, IN 47907, U.S.A.

(Received 12 September 1973. Accepted 26 October 1973)

Key Word Index—*Opuntia clavata*; Cactaceae; cactus alkaloids; *N*-methyltyramine; hordenine; tyramine.

Plant. Whole plants of *Opuntia clavata* Eng. Living specimens are being maintained in our greenhouse. *Source.* Collected near Albuquerque, New Mexico; identification confirmed by Dr. Harold A. Mackay†. *Previous work.* Unidentified alkaloids detected in

* Part XXIV in the series "Cactus Alkaloids". For Part XXIII see WEST, L. G., VANDERVEEN, R. L. and McLAUGHLIN, J. L. (1974) *Phytochemistry* 13, 666.

† Department of Biology, University of New Mexico, Albuquerque.