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SHORT COMMUNICATION

ESDRAGOLE, THE MAIN COMPOUND IN THE VOLATILE OIL OF *TAGETES FILIFOLIA* (COMPOSITAE)

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Abstract—The volatile oil of *Tagetes filifolia* Lag. contains more than 95% of a compound, which by TLC and i.r. spectral comparison and by conversion to anethole, has been identified as esdragole.

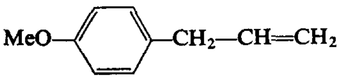
INTRODUCTION

Tagetes filifolia Lag. (Compositae), growing wild in Yucatan, Mexico, is known under the confusing name of "Irish Lace" as an ornamental plant, and is grown in house gardens. A plant with the same scientific name, described as native to Argentina, has been previously investigated.[1,2] The essence, prepared from the Argentina plant, is described as "resembling citrus essences", and the odor of the fresh plant as "like esterified geraniol". D-Limonene and citral have been isolated from this Argentina plant.

However, *Tagetes filifolia* Lag. of Mexico has a strong odor similar to *Pimpinella anisum* L. and *Artemisia dracunculus* L. Therefore the following investigation was made to determine the chemical composition of its volatile oil.

RESULTS AND DISCUSSION

The fresh, whole plant yields 0·3% of a yellowish volatile oil. TLC of a 5% solution in CH_2Cl_2 shows a single spot, after development with hexane–ether (85:15) on Silica gel GF_{254}. The R_f value is 85 (chamber saturation); detection was by short wave u.v. light. Also, spraying with a reagent[3] sufficiently sensitive to detect compounds in other volatile oils, gave only one spot at 85, and showed a little residue at the origin. The i.r. spectrum of the pure volatile oil showed the characteristic peaks for an allylic group at 1632, 994 and 914 cm.$^{-1}$ The odor and the R_f value were similar to esdragole (I). Comparison with the i.r. spectrum of synthetic esdragole (Fig. 1) and with a chart published by Naves[4] showed it to be identical.



(I) Esdragole

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[1] G. A. FESTER, *Ciencia Invest.* (*Buenos Aires*) **3**, 237 (1947).
[2] G. A. FESTER, M. A. GARGALLO and E. A. MARTINUZZI, *Anales Soc. Cienti. Arg.* **144**, 457 (1947).
[3] H. BOHRMANN, E. STAHL and H. MITSUHASHI, *Chem. Pharm. Bull.* (*Japan*) **15**, 1606 (1967).
[4] Y. R. NAVES, *Bull. Soc. Chim. Fr.* 566 (1958).

Final confirmation was obtained by heating the oil with methanolic KOH and converting it, by allyl-propenyl rearrangement, to anethole (m.p. 20·5–21·5°).

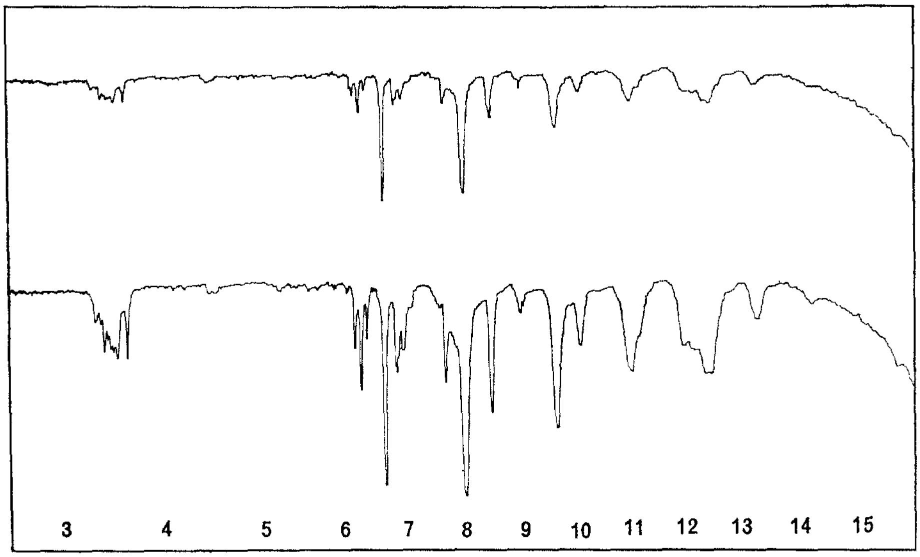

FIG. 1. i.r. ABSORPTION SPECTRA OF PURE VOLATILE OIL OF *Tagetes Filifolia* Lag. (UPPER), AND OF SYNTHETIC ESDRAGOLE (LOWER). WAVELENGTH IN μ.

As esdragole has been shown to possess a strong bactericidal action,[5] a volatile oil with such a high content of it is of medicinal interest. The identity of the investigated plant was established by carefully checking it with original specimens in the Harvard University Herbarium, Cambridge, Massachusetts. Therefore it is possible that the Argentina plant with the same scientific name is either a chemical race of *Tagetes filifolia* Lag. or another species.

EXPERIMENTAL

Freshly harvested plants (350 g) were cut in pieces and instantly distilled with water steam for 2 hr. The oil was taken into ether, dried over Na_2SO_4, filtered off, and freed of the solvent (yield 1·17 g). TLC plates were prepared according to the standard procedures,[6] using Silica gel GF_{254} Merck, and were developed with hexane–ether (85:15) to a distance of 10 cm. The spraying reagent was prepared from: (A) 4·5 g anisaldehyde dissolved in 90 ml glacial acetic acid, to which 860 ml methanol and then 45 ml conc. H_2SO_4 had been added (the latter dropwise with stirring); and (B) 10% solution of phosphomolybdic acid. For spraying, 10% of B is added to A, the mixture being stable for several days. I.r. spectra were taken as films on a Beckman IR-8* spectrophotometer. The allyl-propenyl-rearrangement was carried out as follows. 0·2 g of the oil was refluxed with 20% methanolic KOH, then placed on a column of silica gel and eluted with CH_2Cl_2. After evaporation of the solvent, 0·19 g of pure anethole was obtained (m.p. 20·5–21 5°).

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* Beckman Instruments, Palo Alto, California.

[5] W. RITZERFELD, *Arzneimittelforsch.* **9**, 521 (1959).

[6] E. STAHL, *Duennschicht-Chromatographie, ein Laboratoriumshandbuch*, 2. Auflage, Berlin, Springer Verlag (1967).