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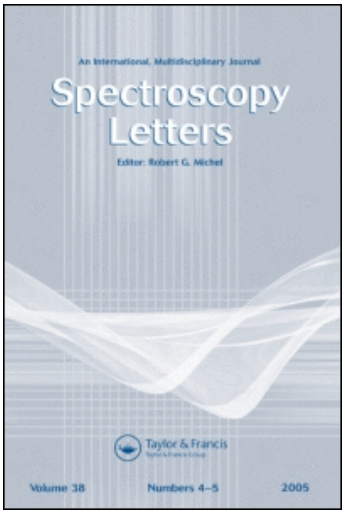

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Physico-Chemical Characteristics and Spectroscopy of Ducrosia isamaelis Oil

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PHYSICO-CHEMICAL CHARACTERISTICS AND SPECTROSCOPY OF DUCROSIA ISAMAELIS OIL

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Key Word Index - Physical constants, Ducrosia ismaelis oil, GLC-Mass spectrometry-analysis, Ducrosia ismaelis oil, skin infections, folk medicine. Ducrosia ismaelis oil, IR and NMR analysis. Ducrosia ismaelis, GLC/MS, Ducrosia isamaelis, TLC, Ducrosia isamaelis, physico-chemical properties.

Abstract - The essential oil of Ducrosia ismaelis, Asch. was prepared and its physical (specific gravity, refractive index, and optical rotation) and chemical standards (ester percentage) were determined. The constituents of the oil were identified using TLC, IR, PMR and GLC/Mass spectrometry techniques. Myrecene, N-undecane, α-pinene, n-butylbenzene, γ-cadinene, 3,5-dimethylstyrene, 5-methylindan, P-menthadiene, cymene, γ-terpinene, sabinene, decanol, and fenchone are the major constituents.

INTRODUCTION

The genus Ducrosia, Boiss. of the family Umbelliferae is distributed from Egypt to Pakistan [1]. Of the five species of this genus D. ismaelis, Aschers. occurs in Saudi Arabia [2].

It is a herb indigenous to the central province of Saudi Arabia [2]. The plant has a characteristic aromatic odour. In

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folk medicine the leaves and flowering tops are applied externally to cure skin infections and are also used as insect and reptile repellents [3].

Apart from a single work carried out by Woe et al. (1977) [4] reporting extract of D. ismaelis, literature review revealed that the oil constituents have not been investigated.

In the present work we report the chemical composition of the volatile oil of D. ismaelis based on physico-chemical characteristics and spectroscopic studies.

EXPERIMENTAL

Material

The plant examined in this work was collected in March, at the flowering stage from Dirriah Road, northern Riyadh (central zone). Its identity as Ducrosia ismaelis, Aschers, was confirmed[1]. It was dried in shade and powdered.

Successive quantities (250 g each) were subjected to steam distillation which produced a volatile oil (average yield 4%).

The physico-chemical characteristics of the isolated oil are presented in Table I.

TLC was done on silica gel G plates 0.25 mm thick, developed in chloroform-benzene (1:1) and (4:1) solvent systems [5]. After development, the spots were visualized by spraying with anisaldehyde reagent [5].

[1]The plant material was identified as Ducrosia ismaelis Asch. (Umbelliferae) by Dr. A.M. Migahid, Department of Botany, College of Science, King Saud University, Riyadh, Saudi Arabia. A voucher specimen is available in the herbarium of the College of of Pharmacy, King Saud University, Riyadh, Saudi Arabia.

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Table I - Physico-Chemical Characteristics of Isolated Oil.

Property	Description	Property	Description
Colour	Light yellow	Ester percentage	5.91
Odour	Aromatic, characteristic. Fragrant on dilution.	IR[e]	3450 (broad band), 2950, 2860, 2720 (weak band), 1728 (strong band), 1700 (shoulder), 1600 (very weak band), 1465, 1385, 1140, 1030, 720 cm^{-1}.
Sp. gr.[a]	D_4^{20} 0.9573		
Refractive index[b]	nD^{24} 1.04570		
Optical rotation[c].	$[\alpha]_D^{24}$ -4.5 (10% in ethanol)	PMR[f]	7(m), 5.17(m), 4.43(s), 2.33 (broad s), 2.17(s), 2.03(s). 1.72(q), 1.48(s), 1.30(s), 0.95(s) and 0.78(s) ppm.

a. Pycnometer, 2 ml capacity.

b. Zeiss Abbe refractometer.

c. Perkin Elmer 241 MC Polarimeter, ordinary cell 1 mm, 0.25 ml.

d. According to E:P. 1973 method.

e. .580 B IR Spectrophotometer-Perking Elmer.

f. Varian T 60A - 60 MHz using tetramethylsilane as internal standard.

GLC - Mass Spectrometry

Mass spectra of the volatile oil constituents were recorded using a gas chromatograph-mass spectrophotometer. The chromatographic glass capillary column (20-25 m X 0.25 mm) already packed with Carbowax was conditioned isothermally at 100°C for 10 minutes, and then the temperature was programmed at 2°C/min. up to 250°C. Helium pressure was adjusted to 0.2 bar and Ros injection was used. The

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Table II. Constituents of the Oil by GLC-Mass Spectrometry.

Compound	Retention Time, min.	Molecular Weight.	M^+
1. n-Undecane.	2 : 33	156	156
2. β-Pinene	2 : 47	136.23	136
3. n-Butylbenzene.	2 : 57	134.21	134
4. Myrecene.	3 : 30	136.23	136
5. Sabinene.	4 : 50	136.23	136
6. γ-Terpinene.	4 : 46	136.23	136
7. Cymene.	5 : 18	134.21	134
8. 2:4(8)-p-menthadiene.	5 : 34	136.23	136
9. 5-Methylindan.	5 : 52	131.19	131
10. Fenchone.	9 : 16	152.23	152
11. 3,5-Dimethylstyrene.	11 : 16	130.18	130
12. δ-Cadinene.	14 : 38	204.34	204
13. 1-Decanol.	28 : 37	158	158

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injector port temperature was 245°C. Mass spectra were determined by electron impact with an electron energy of 70 eV. The mass range was scanned from 20 up to 1810 a.m.u. in 60 MS.

RESULTS AND DISCUSSION

The IR and PMR data revealed the presence of free alcohols (3450 cm^{-1}), alkenes and highly conjugated alkenes (1600-1700 cm^{-1};

4.43-5.17 ppm), aromatic functions [1465-1600 cm^{-1}; 6-7.33 ppm, (multiplet centered at 7 ppm)], alicyclic structures (singlets at 0.78, 0.95, 1.3, 1.48, 2.03, 2.17 and 2.33 ppm and quartet at 1.72 ppm) and cyclic ketones 1718 cm^{-1} which nearly identical with Fenchone [6].

GLC-mass spectrometry studies indicated the presence of several compounds (Table II). The major components on the GLC trace are identified by sequence numbers that correspond to mass spectral sequence numbers. The mass spectra so obtained were compared with those of authentic compounds, and demonstrated identical fragmentation characteristics [7]. The mass fragmentation pattern of most components showed molecular ion peaks at atomic mass units equivalent to their molecular weights.

From the data obtained, the volatile oil was considered to be one of the alcohol and ester poor volatile oils, since 1-decanol was the sole alcohol identified.

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