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STUDIES ON THE ESSENTIAL OILS OF THE PAKISTANI SPECIES OF THE FAMILY UMELLIFERAE

Part XXXIX. *Aegopodium burtii* E. Nasir (Sholkonar) Oil of the Whole Plant

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The percentage yield, physicochemical characteristics and chemical composition of the essential oil of *Aegopodium burtii* have been determined. The oil, with a yield of 0.1% contains α-pinene (14.4%), camphene (6.3%), limonene (7.6%), β-caryophyllene (4.5%) geranyl acetate (10.9%), geranyl and bornyl acetate (5.4%), bornyl acetate (3.9%), thymol (10.0%) ethyl hexyl phthalate (21.1%), an unknown alcohol (5.1%), lauric acid (9.7%) and tarry material (2.1%). The persence of ethyl hexyl phthalate in the Umbelliferae species is an interesting finding. The species is used against stomach disorders by the local inhabitants.

INTRODUCTION

Aegopodium is a genus of 7–8 European and Asian species. The plants are annual or perennial herbs. Only two species namely *Aegopodium burtii* and *Aegopodium alpestre* have been reported to grow wild in Pakistan. Besides its use against stomach disorders the seed of the species are used as a substitute of caraway.

Even though a large quantity of *Aegopodium burtii* grows in Pakistan yet no investigations have so far been carried out on the physicochemical characteristics and chemical composition of this species. The present work has, therefore, been pursued with a view to filling this gap in our knowledge of the essential oil of the species.

MATERIAL AND METHODS

The plant at seedling stage was collected from Kalam (Swat) for these studies. The essential oil from the species was recovered by dry steam-distillation [1]. The water-soluble fraction of the oil was extracted from the aqueous distillate with diethyl ether. The water-cohobation oil thus obtained was combined with the essential oil, because the two oils were identical by TLC and IR and the resultant oil studies. The general methods employed for the determination of the physicochemical properties of the oil have been reported earlier [1, 2].

The oil was separated into hydrocarbons and oxygenated components by column chromatography using activated silica gel as an adsorbent. The hydrocarbon fraction of the oil was eluted with n-hexane and the oxygenated fractions with progressively increasing proportions of diethyl ether (1–20%) in n-hexane. The hydrocarbon fraction was further resolved into individual components by GLC using a copper column (3 m x 3 mm) packed with SE-30, nitrogen as the carrier gas and flame ionisation detector. The column temperature was maintained at 110° and 170° for the resolution and identification of monoterpenes and sesquiterpenes respectively. The oxygenated components as separated by column chromatography were identified by TLC, GLC and IR comparison and also by converting into their known derivatives.

RESULTS

The percentage yield, physicochemical properties and chemical composition of the essential oil of *Aegopodium burtii* are reported in Table 1–2.

DISCUSSION

The essential oil distilled from the whole plant of

Table 1. Percentage yield and physicochemical values of the essential oil of *Aegopdium burtii* whole plant.

Distillation time (hr)	14
Yield of oil (%)	0.1
Specific gravity	0.8212^{30}
Refractive index	1.3370^{30}
Optical rotation	$+14^{\circ}\ 15'^{30}$
Acid value	21.30
Ester value	1.67

The superscripts indicate the temperature at which these parameters were determined.

Table 2. Percentage composition of the essential oil of *Aegopodium burtii* whole plant.

Eluent	Component	Percentage
n-Hexane	Hydrocarbons*	32.8
	α-Pinene	14.4
	Camphene	6.3
	Limonene	7.6
	β-Caryophyllene	4.5
1% diethyl ether in n-hexane	Geranyl acetate	10.9
2% diethyl ether in n-hexane	Geranyl and bornyl acetate	54
2% diethyl ether in n-hexane	Bornyl acetate	3.9
4% diethyl ether in n-hexane	Thymol	10.0
6% diethyl ether in n-hexane	Ethylhexyl phthalate	21.1
10% diethyl ether in n-hexane	Unknown alcohol	5.1
20% diethyl ether in n-hexane	Lauric acid	9.7
50% diethyl ether in n-hexane	Tarry material	2.1

*Resolved and estimated by GLC.

Aegopodium burtii is good to smell. The hydrocarbon fraction of the oil is composed of monoterpenes and sesquiterpenes. The fraction was resolved by GLC and the various constituents identified against their standard samples.

The ester fraction of the oil was rechromatographed on silica gel columns and the two esters namely geranyl acetate and bornyl acetate thus obtained were identified by TLC, GLC and IR comparison with their standard samples. Thymol was identified by its m.p., 52° and IR comparison with the standard sample extracted from the seed of *Trachyspermum ammi* [1].

The major oxygenated component of the oil is ethyl hexyl phathalate, m.p. 40°. The presence of this compound in Umbelliferae species is an interesting and new finding. The compound was identified by IR (3.5, 5.9, 6.2, 6.3, 6.9, 7.3, 8.0, 9.0, 9.6, 10.5, 13.6, 14.3 nm) comparison with its standard spectrum. The molecular weight of the compound is 390 by mass spectrometry. From proton NMR spectrum, the formula which fits is $C_{24}H_{38}O_4$ and this is confirmed by elemental analysis. However, the authors like to do some more chemical work on this novel compound and a detailed studies on this phthalate will be communicated later on.

Elution of the column with 20% diethyl ether in n-hexane gave an acidic component. It was semisolid at room temperature. The compound was recrystallised from n-hexane and identified as lauric acid from its m.p. 43° and IR comparison with the standard spectrum.

The presence of ethyl hexyl phthalate and lauric acid in the essential oil of *Aegopodium burtii* is quite interesting. Pharmacological studies on the species may prove valuable.

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