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CONSTITUENTS OF THE ESSENTIAL OIL OF *CYMBOPOGON JAWARANCUSA*

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Key Word Index—*Cymbopogon jawarancusa*; Gramineae; Cymbopogoneae; Khavi grass; piperitone; essential oil; GC–MS analysis.

Abstract—The composition of the essential oil of Khavi grass, *Cymbopogon jawarancusa*, was investigated by glass capillary gas chromatography in combination with mass spectrometry. Sixty-four compounds were identified, 55 of which are reported for the first time. The oil contains a high percentage of piperitone (60–70%), which is mainly responsible for the smell of Khavi grass.

Cymbopogon jawarancusa is a perfumed grass which is widely distributed in India and Pakistan. Chemically it has not been extensively studied but in 1921 Simonsen [1] investigated the physico-chemical properties of the essential oil and later [2] reported an oil composition of up to 24% carene, 80% piperitone, 2% of an unidentified alcohol and small quantities of octanoic, decanoic and hexadecanoic acids (free or esterified). In 1973, Grag and Nigam [3] obtained the oil in 0.6% yield and their chromatographic analysis showed 20% Δ^4-carene, 2% Δ^3-carene, 1.5% β-caryophyllene, 1% *p*-cymene, 44% piperitone, 18% piperitol, 10% perillyl alcohol, 1% farnesol and 2% hexadecanoic acid.

In the present investigation, the essential oil from the grass was obtained by three procedures: vacuum steam distillation, steam distillation and solvent extraction, and the yield and quality of the oils compared. The essential oils were analysed by glass capillary gas chromatography (GC)[2] [4] (on polar and apolar stationary phases) in combination with mass spectrometry (electron impact and chemical ionization). To simplify identification, the hydrocarbons were separated from the oxygen fraction by column chromatography on Si gel. By this technique some artifacts were introduced. Free fatty acids were isolated as methyl esters and analysed on a FFAP capillary column. The results of the GC–MS analysis of the essential oil of the Khavi grass are given in Table 1. Four classes of terpenoids are represented: Peaks 1–13 (A) monoterpene hydrocarbons; peaks 14–42 (B) oxygenated monoterpenoids; peaks 43–69 (C) sesquiterpene hydrocarbons and peaks 70–81 (D) oxygenated sesquiterpenoids. The volatile monoterpenes (A) are present in high concentration (3% of total oil) in the vacuum steam distillate due to the low temperature separation technique. However, the concentration of (A) was not as high in the steam distilled oil and still less in solvent extracted oil. The oxygenated monoterpenoids (B) especially piperitone (present up to 70%) constitute the bulk of the oil. The concentration of the oxygenated sesquiterpenoids (D) in the vacuum steam distilled oil is not high. However, the solvent extracted oil contains up to 10% of oxygenated sesquiterpenoids. Identifications were confirmed by analysis of the separated hydrocarbon and oxygen fraction on Carbowax 20 M and PMPE capillary columns. Although the Si gel was purified by a pretreatment, some artifacts were observed. Germacrene D clearly present in the total oil was absent in the hydrocarbon fraction and copa-camphene and ε-muurolene were only identified in the hydrocarbon fraction. This is not surprising as some terpenes are known to isomerize on Si gel [5].

The free fatty acids consist of the normal plant fatty acids from C_{10} to $C_{18:2}$ but there is also some pentadecanoic acid in the mixture.

EXPERIMENTAL

Preparation of the essential oil. Cymbopogon jawarancusa from the Peshawar region, Pakistan, was identified by A. R. Baig of the Pakistan Forest Institute, Peshawar.

Vacuum steam distillation (VSD). Vacuum steam distillation was carried out on 200 g of cut grass (whole plant) in an all glass assembly. Distillation was stopped after 6 hr and the oil extr. with 200 ml CH_2Cl_2. The soln was dried and solvent removed through a fractionation column with a cold finger, at normal pres. with a reflux ratio of 6:1. The yield of the oil was 3 g (1.5%). *Steam distillation (SD).* Steam dist. was carried out in the normal way in an all glass assembly on 200 g of cut grass for 8 hr. The dist. oil was extr. with CH_2Cl_2, dried and the solvent removed as described above. The yield was 3.6 g (1.8%). *Solvent extraction (SE).* 250 g of cut grass was extracted overnight in 3 l. CH_2Cl_2 and then refluxed for 8 hr with stirring. The evap. extract was dist. between 50 and 180° under vacuum in N_2. The yield of the oil was 5.5 g (2.2%).

Separation of the essential oil into hydrocarbon and oxygen containing fractions. 0.5 g of VSD oil was chromat. on Si gel (80 g). The hydrocarbon fraction (10%) was eluted with *n*-pentane (1 l.) and the oxygen fraction (90%) with MeOH (1 l.). Solvents were removed as above.

Extraction of acids. 0.3 g of the oxygen fraction was dissolved in 10 ml of Et_2O and extracted twice with 5% aq. KOH. The extract was acidified with 5% HCl, extracted with Et_2O and the Et_2O extract dried over Na_2SO_4 and conc. The acids made up *ca* 1% of the total oil.

Gas chromatographic analysis. The (GC)[2] analyses were carried

Table 1. Constituents of the essential oil of *Cymbopogon jawarancusa*

Peak No.	Compound	% of total oil	Peak No.	Compound	% of total oil
1	Monoterpene	0·02	34	Piperitone	65.40
2	α-Pinene	0·05	35	Myrtenal	0.08
3	Camphene	0.10	36	Isoborneol	trace
4	*p*-Cymene	0.60	37	Methylthymyl ether	trace
5	Myrcene	0.02	38	Contamination	0.10
6	Δ^4-Carene	I.I	39	Oxygenated monoterpenoid	trace
7	*cis*-Allo-ocimene*	trace	40	Oxygenated monoterpenoid	trace
8	*o*-Cymene	0.05	41	1,8-Cineol*	trace
9a	Limonene	0.08	43	α-Copaene	0.10
9b	Δ^3-Carene		44a	α-Ylangene	0.60
10	Δ^2-Carene	0.10	44b	β-Santalene	
11	*trans*-Allo-ocimene*	0.04	45	α-Cubebene	0.40
12	Fenchone	0·03	46	β-Elemene	0.40
13	Terpinolene	0.03	47	Sesquiterpene	trace
14	Linalol	0.20	48	Sesquiterpene	0.10
15	Oxygenated monoterpenoid	0.01	49	Sesquiterpene	0.20
16	Oxygenated monoterpenoid	0·01	50	β-Caryophyllene	1.20
17	*trans*-*p*-Menth-2-ene-1-ol*	0.50	51	β-Ylangene	0.10
18	Oxygenated monoterpenoid	0.01	52	α-Chamigrene	trace
19a	Camphor	0.25	53	Sesquiterpene	0.10
19b	*cis*-*p*-Menth-2-ene-1-ol*		54	Alloaromadendrene	0.05
20	Terpene alcohol	0.04	55	α-Humulene	0.10
21	5,6-Dimethyl-5-nor-bornen-2-ol*	0.06	56	Longifolene	0.10
22	Borneol	0.10	57	Sesquiterpene	0.20
23	*trans*-Thuj-2-ene-4-ol	0.10	58	Germacrene-D	0.60
24	Terpinen-4-ol	0.05	61	α-Muurolene	0.40
26	α-Terpineol	1.20	62	Cuparene	0.25
27	*cis*-Piperitol	0.80	63	δ-Elemene	0.10
28	Eucarvone	0.10	64	Calamene	0.40
29	*trans*-Piperitol	0.07	65	δ-Cadinene	1.00
30	Oxygenated monoterpenoid	0.02	66	Bazzanene	0.10
31	Verbenone	0.08	67	α-Farnesene	0.25
32	Lavandulol	0.09	68	Kasuralcohol*	0.10
33	Geraniol	0.04	69	Elemol	0.10
				TOTAL	94.00%

The rest are traces and unidentified oxygenated sesquiterpenoids

* Incomplete identification.

out on a GC with FID. Wide bore capillary columns were coated according to the procedures developed in this laboratory [4, 6]. The most complete chromatograms were obtained on a 100 m–0.5 mm i.d. SE-30 capillary column (WCOT), H_2 flow 5 ml/min, temp. 70–200° at 2°/min. The column was connected to the GC instrument with capillary inserts [7].

Gas chromatography–mass spectrometry. GC–MS analysis were obtained on a quadrupole instrument equipped with an all glass chromatographic inlet system and a data system.

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