

UV and IR Spectral Studies of Essential Oil of *A. indica*, *M. hortensis* and *E. triplinerve* Leaves

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In the present communication the quantitative estimation of the constituents of the essential oils of *A. indica*, *M. hortensis* and *E. triplinerve* plants has been carried out by UV and IR spectral analysis.

INTRODUCTION

In our earlier communications¹⁻³, we have reported the presence of some terpenoidal components in the essential oils of leaves of *Anisomeles indica*, *Majorana hortensis* and *Eupatorium triplinerve* plant. During the course of further investigations, it has been found that essential oil of *A. indica* (0.7%), *M. hortensis* (0.5%) and *E. triplinerve* (0.6%) possess antimicrobial activities of good reputation^{4,5}.

The plants *A. indica* and *M. hortensis* (N.O. Labiatae)⁶ and *E. triplinerve* (N.O. Compositae)⁶ grow in the Indian gardens. The plant materials were supplied by M/s United Chemical & Allied Products, Calcutta and authenticated by the Department of Botany.

Essential oils of these plants were reported to possess important medicinal values^{7,8}, i.e. *A. indica* is used as astringent, carminative, while the oil of *M. hortensis* is used for curing acute diarrhoea, paralytic limbs and the oil of *E. triplinerve* is used as a stimulant and diaphoretic; in addition to it fresh leaves are used as a haemostatic agent.⁹

Earlier workers¹⁰⁻¹⁴ have reported the presence of stigmasterol, β -sitosterol, phytosterols, tetraacosane, tetracorunel, β -amyrin, friedelin, betulonic acid, macrocyclic diterpenes in addition to apananin, ayapin, glucoside (apigenin), in which they have reported their cytotoxic activities and antimicrobial activities.

EXPERIMENTAL

Essential oils have been obtained from the leaves of *A. indica*, *M. hortensis* and *E. triplinerve* by steam distillation method using Clevenger's apparatus. The physico-chemical constants of essential oils of above plants are shown in Table 1. The UV spectra were obtained from cells of 1 cm path length and having concentrations 10^{-3} to 10^{-5} molar range using Beckman DK-2A spectrophotometer. The spectrometric estimation methods described below:

Estimation of Methyl Chavicol: 0.210 Gm of the essential oil of *M. hortensis*, 0.200 gm. of the essential oil of *E. triplinerve* and 0.320 grams of the essential

TABLE 1
 PHYSICO-CHEMICAL PROPERTIES OF ESSENTIAL OIL

S. No.	Constants	Essential oils of plant		
		<i>A. indica</i>	<i>M. hortensis</i>	<i>E. triplinerve</i>
1.	Sp. gravity	0.911 at 35°C	0.845 at 33°C	0.786 at 36°C
2.	Refractive index at 14.5°C	1.5070	1.5060	1.5101
3.	Phenol content	47.50	48.00	41.50
4.	Optical rotation	-4 to +8°	+40.30°	+39.10°
5.	Acid value	5.4	5.6	5.0
6.	Ester Value	37.00	38.00	36.00
7.	Ester value after acetylation	44.27	44.26	43.86

oil of *A. indica* were dissolved separately in 5.0 ml of A.R. grade ethanol. These solutions were diluted separately to the concentration of 45.4×10^{-4} , 50.2×10^{-4} and 40×10^{-4} gm/5 ml respectively and their UV spectra were recorded. The optical densities at maximum absorption ($\lambda_{\max} = 233 \text{ m}\mu$) were noted separately and result are compiled in Table 2.

TABLE 2

S. No.	Plants (leaf)	Constituents*					
		Methyl Chavicol		Caryophyllene		Limonene	
		O.D.	%	O.D.	%	O.D.	%
1.	<i>A. indica</i>	0.47	9.76	0.49	15.8	0.05	3.4
2.	<i>M. hortensis</i>	0.20	3.6	0.30	8.1	0.04	3.0
3.	<i>E. triplinerve</i>	0.26	4.3	0.36	11.83	—	—

O.D. = Optical density

*Constituents from E. Oil of plant leaves.

Estimation of Caryophyllene: 0.45 Gm of essential oil of *A. indica*, 0.50 gm of essential oil of *M. hortensis* and 0.640 gm of essential oil of *E. triplinerve* were dissolved separately in 5 ml A.R. grade EtOH and the solutions use diluted to give concentrations 58.3×10^{-3} , 69.1×10^{-3} and 57.3×10^{-3} gms./5 ml respectively and their UV spectrum recorded. Their optical densities at the maximum absorption ($\lambda_{\max} = 284 \text{ m}\mu$) were noted separately.

Estimation of Limonene: 0.35 Gm of the essential oil of *A. indica*, 0.47 gms of essential oil of *M. hortensis* were dissolved separately in 5.0 ml of A.R. EtOH and the solutions diluted to give concentration of 98.3×10^{-4} and 90×10^{-4} gm/5 ml respectively and their UV spectrum recorded and noted their optical densities at maximal absorption ($\lambda_{\max} = 252 \text{ m}\mu$) respectively. The results of spectrophotometric estimation are compiled in Table 2.

The following volatile constituents obtained from the essential oil of *A. indica*, *M. hortensis* and *E. triplinerve* leaves by column chromatography were studied by IR analysis. The IR spectrum were obtained from liquid film of 0.1 mm using Perkin-Elmer IR spectrograph No. 397.

The spectra assignments of all the components are compiled below:

α -Terpineol: The IR spectrum of α -terpineol showed various bands at 3340 (–OH), 2885 ($-\overset{\text{H}}{\underset{|}{\text{C}}}=\text{CH}$), 1456 ($-\text{CH}_2$), 1405 ($-\text{C}-\text{CH}_3$), 1185 (CH-bonding), 1150 ($=\text{CH}_2$ group), 915–840, 800 cm^{-1} ($-\text{CH}$ bonding), indicated the presence of $-\text{C}=\text{CH}$ group, $=\text{CH}$ group, primary alcohol, alkane and alkene groups.

α -Limonene: The IR spectra of α -limonene showed the bands at 2900 (C-H stretch, $-\text{CH}_3$ group), 1620 (C–C multiple bond, $-\text{C}=\text{CH}_2$ group), 1460 (C–H bonding, $-\text{CH}_3$ group), 1400 (C–H bonding, $-\text{CH}_3$ group), 1295 (C–H bonding, alkene disubstitution), 1015 (C–C multiple bond stretch, alkene), 960 (C–H bonding alkene, $\text{CH}_2=\text{C}-\text{CH}_3$), 910, 895 (C–H bonding, alkene, mono and disubstitution) and 800, 780 cm^{-1} (C–H bonding, alkene) their characteristic confirms the presence of cyclo-hexane ring, $-\text{CH}_3$ and $\text{H}_3\text{C}-\overset{\text{H}}{\underset{|}{\text{C}}}=\text{CH}_2$ groups.

Eugenol: The IR spectra of eugenol showed the characteristic bands at 3500 (alco. group, O–H), 2956 (C–H–stretch, C–H group), 2250 (C–C multiple bond stretch, $-\text{C}=\text{C}-$ group), 2330 (C–C multiple bond stretch, $-\text{C}=\text{C}-$ group), 1900 (C–C, $-\text{C}=\text{C}-$ group), 1670 ($-\text{C}-\text{O}-$ stretch, $-\text{OCH}_3$), 1650 (C–C multiple bonding, alkene mono substituted), 1515, 1450 and 1430 cm^{-1} (C–C multiple bonding aromatic), 1385 (C–H bonding, $-\text{CH}_3$ group), 1295 (C–H bonding, $=\text{CH}_2$), 995 (C–H bonding, alkene mono substituted) and 800 cm^{-1} (C–H bonding).

Methyl Chavicol: In IR spectra the various characteristic bands at 1673 m $\nu(\text{C}=\text{C})$, 1645s, 1540s and 1610 w cm^{-1} $\nu(\text{C}-\text{C})$, 1265s and 1025s $\nu(\text{C}-\text{O}-\text{C})$, 1000, 930 w (π , C–H) and 835 m cm^{-1} (C–H), indicated the presence of terminal vinyl group.

α -Pinene: In IR spectra, we obtained the various characteristic bands at 3000 ($-\text{C}-\text{H}-$), 1680 (C–C), 1490 (C–H, bonding $-\text{CH}_2$), 1455 (C–H, $-\text{CH}_2$ group), 1410 ($-\text{CH}=\overset{\text{H}}{\underset{|}{\text{C}}}-$) C–H bonding, 1400 (C–C bonding), ($-\overset{\text{H}}{\underset{|}{\text{C}}}-$ tertiary group), 1290 (C–H-, alkane substituted) and 890 cm^{-1} (C–H), trisubstitution.

α -Borneol: In the IR spectra various characteristic band at 3500 (O–H stretch, $-\overset{\text{H}}{\underset{|}{\text{C}}}-\text{OH}$ group), 2900 ($-\text{CH}$, $-\text{CH}_3$ group), 1740 (C–O stretch, $-\text{C}-\text{O}$ group), 1480 (C–H bonding, $-\text{CH}_2$ group), 1430 (C–H bonding, $-\text{CH}_2$ group), 995 (C–H bonding $=\text{CH}$ group) and 915 cm^{-1} (C–H bonding, $=\text{CH}_2$ group) confirms the presence of $-\text{C}-\text{O}$ group.

1.8 Cineole: In IR spectra, various bands at 2965 (C–H stretch, CH_3 group), 1450 (C–H bonding, alkane $-\text{CH}_3$), 1400 (C–H bonding, $\text{CH}_3-\overset{\text{H}}{\underset{|}{\text{C}}}-\text{CH}_3$), 1280 (C–O stretch, C–O bond), 1100 (C–O stretch), 1060 (C–O banding, C–O group) 965 (C–H bonding, C–H group), 940 (C–H group) and 840 cm^{-1} (C-bonding, C–H group), indicated the presence of $-\text{CH}_3$ group, methylene group, and $-\text{CH}_2-\text{C}-\text{O}$ group.

Citral: The IR spectra of citral showed characteristic bands at 3465 ($-\overset{\text{H}}{\underset{|}{\text{C}}}-\text{O}$, C–O

stretch) 2900 (C–H stretch, –CH₃ group), 1740 (>C=O group), 1440, 1400 (C–H bonding, –CH₂ group), 1200 (C–O stretch, –C–O group), 985 and 845 cm⁻¹ (C–H bonding, =CH₂ group) indicated the presence of –CH₃, C=O, –CH₂ and =CH group.

p-Cymene: In IR spectra of various bands at 2920 (C–H stretch, –CH₃ group), 1940 (C–C multiple bond, alkene group, –CH=CH group), 1700 (C–C multiple bonding, –C$\begin{matrix} \text{CH}_3 \\ \text{CH}_3 \end{matrix}$ group) 1600 (C–C multiple bond, aromatic), 1470 (C–H bonding, –CH₃ group), 1440 (C–H bonding, –CH₂ group), 1390 (C–H bonding, tert. butyl group), 1160 and 1070 (C–C multiple stretch, –CH=CH-group), 1050 (C–multiple stretch, –CH=CH– group), 820 (C–H bonding two adjacent H–atoms) and 700 cm⁻¹ (C–H bonding), alkane disubstituted were indicated, the presence of *p*-cymene.

Caryophyllene: In the IR spectra, the various characteristic bands at 2985–2900 (C–H), 1810 w (>:CH₂), 1680 w ν(C : C), 1640 m ν(C : C), 1400, 1390 m (δ C–H), 895 s (π C–H), 850, 830 w (π C–H) indicated the presence of cyclobutane ring, geminal dimethyl group, nature of ethylenic substitution etc.

All the above assignments of components confirmed their identity. The results of spectral analysis are in good agreement with the results of chromatographic analysis.

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