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A STUDY OF REFRACTIVE INDICES OF 3-(4-FLUOROPHENYL)-1-PHENYLPROP-2-EN-1-ONE IN METHANOL AND BENZENE MIXTURES 298K

S. K. CHAVAN* and B. A. GOP

P.G. Department of Chemistry, D.B.F Dayanand College of Arts and Science,
SOLAPUR – 413002 (M.S.) INDIA

ABSTRACT

3-(4-Fluorophenyl)-1-phenylprop-2-en-1-one has been synthesized and characterized by M.P, Infrared spectroscopy, thin layer chromatography, ^{1}H NMR and gas chromatography mass data. The refractive indices of 3-(4-fluorophenyl)-1-phenylprop-2-en-1-one in methanol and benzene mixtures (0-100%) by weight been measured at 298 K. The data obtained was utilized to calculate various parameters such as molar refraction (R_m), polarisability constant (α), molar volume (V_m), free volume (V_f) internal pressure (π_i), Rao's molar sound velocity (Rm) and specific refraction (r), which was used to estimate the nature of dipole and solute-solvent, solvent-solvent interactions.

Key words: Refractive index, Mole fraction, Polarisability, Molar refraction, Molar volume, Free volume.

INTRODUCTION

Essential biological molecule varieties are made from aromatic ketone called Chalcone. Chalcones are also known as phenyl styryl ketone and benzalacetophenone. They have anti-bacterial activity, anti-fungal activity, anti-tumor activity and antiinflammatory activities.

An aldol condense reaction between acetophenone and benzaldehyde in presence of base makes chalcones, which calls Claisen-Schmidt condensation. In this reaction, carbonyl group makes new carbon-carbon bond. By the presence of reactive α, β unsaturated keto function in chalcone is seen to be responsible for their antimicrobial activity[1]. In recent times, chalcones are reviewing for their different activities. Chalcone is key compound for synthesis of more biologic importance heterocyclic compounds so medicinal chemists have

*Author for correspondence; E-mail: dr_skchavan@yahoo.co.in, gop.balaji@yahoo.com;
Ph.: +91-9423588618

vast interest to make chalcones general methods are used for making 3-(4-fluorophenyl)-1-phenylprop-2-en-1-one by the use strong base like potassium hydroxide.

Various chalcones were synthesized by many researchers[2-6]. They are known to exhibit various biological properties viz antimalarial, antifungal, antibacterial anti-inflammatory antituberculosis activity. Now a day the knowledge of the thermodynamic and acoustical properties of liquid mixtures with chalcones is of immense importance for understanding the molecular interactions between the components.

The study of refractive index is an important property to understand the structural arrangement of atoms in molecule and many researchers Wagh[7] has been studied molar refraction and polarisability constants of substituted chalcones and ketones. The study of refractive indices of mixed solvents is done by many co-workers.[8-11]

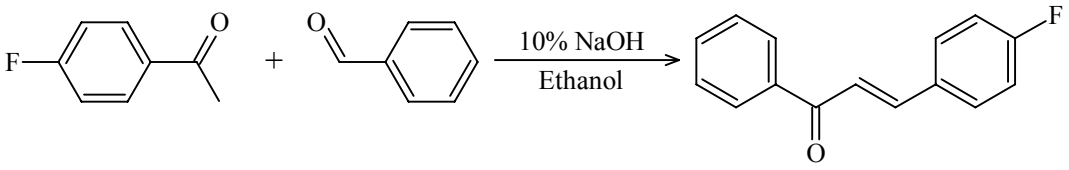
The present work deals with the study of measurement of refractive index of 3-(4-fluorophenyl)-1-phenylprop-2-en-1-one in methanol and benzene media was done by refractive index measurement different parameters such as molar refraction, polarisability and specific refraction have been calculated at 298 K.

EXPERIMENTAL

All chemicals used were of analytical reagent (AR) grade (Rankem). Binary liquid mixtures of methanol and benzene (0-100% by weight) were prepared in airtight stoppard volumetric flasks to minimize leakage of volatile liquids. The weighing was done by using electronic balance with a Precision ± 0.001 mg. The double walled capillary pycnometer was used for the measurement of densities of mixtures with an accuracy 0.1 Kg/m^3. Cannon Ubbelohde viscometer was used for the measurement of viscosity with an accuracy of 0.05%. The flow of time solutions (ts) were measured with a digital stop clock with an accuracy of ± 0.01s (Model RACER) Abbe's refractometer having accuracy with (± 0.01 units) is used for the measurement of refractive index. The temperature of prism box was maintained constant by circulating water from thermostat at 298 K.

Synthesis

A mixture of 4'-fluoroacetophenone (10 mmol) and benzaldehyde (10 mmol) was stirred for 24 hrs in presence of KOH as a catalyst the product was isolated and recrystallized from ethanol. The purity of compound was checked by thin layer chromatography, melting point, the characterization of synthesized compound was done by IR, ^1H NMR and gas chromatography mass spectroscopy data.



p Flouroacetophenone Benzaldehyde 4-fluorochalcone

Fig. 1: Structure of synthesized compound along with its IUPAC name

Spectra of synthesized compounds

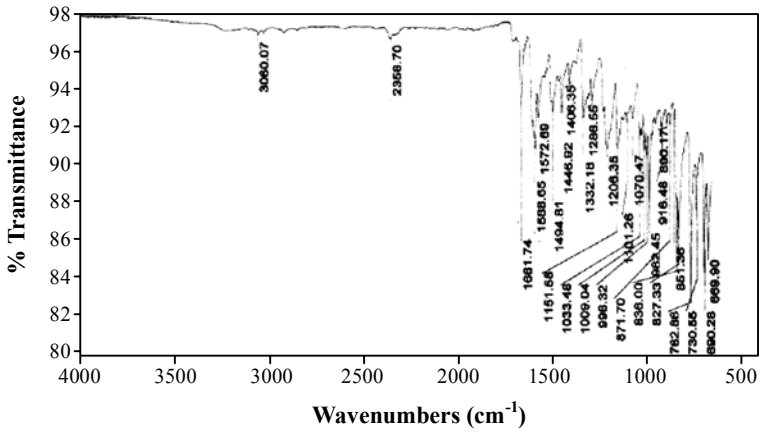


Fig. 2: IR Spectra of synthesized compound

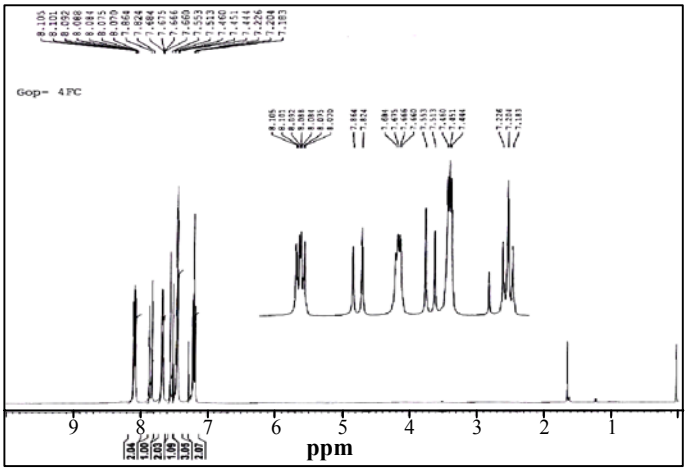


Fig. 3: ^{1}H NMR Spectra of synthesized compound

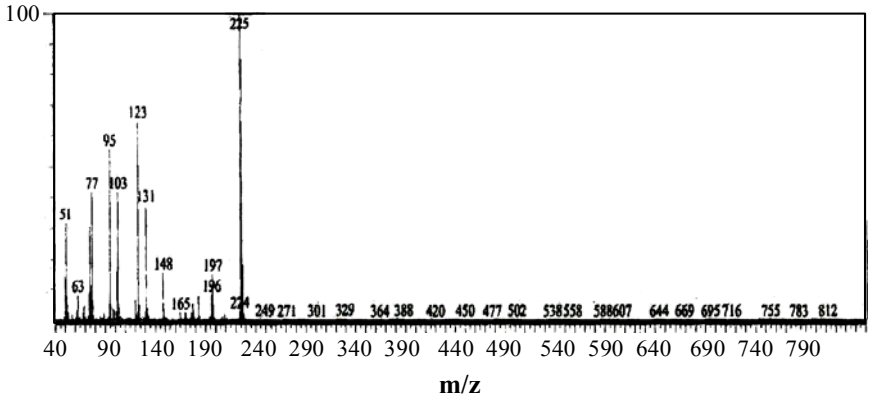


Fig. 4: Mass spectra of synthesized compound

RESULTS AND DISCUSSION

In the present work, the preparation of different solutions by varying the percentage of methanol (0-100% by weight) with addition of chalcones this solution are used for investigation of refractive index measurement. The results obtained for varying in % of methanol are listed in Table 1. The refractive index values decreases[12-13] with increase in % of methanol and decrease in benzene this may be due to dispersion force which is the molecular force, results in decrease in molar refraction and polarizability. The linear decrease in Rao's molar sound function (Rm) and molar compressibility (W) suggests the absence of complex and aggregates formation takes place in both methanol and benzene.

The decrease in free volume[14] (V_f) indicate the increase of cohesive forces and vice versa in the solution of methanol and benzene. The decrease in free volume (Vm) causes increase in internal pressure and vice versa the increase in internal pressure[15] (π_i) is the resultant forces of attraction between the molecules in solution suggests the solute-solvent interactions as shown in Table 2.

Thus, it may predicted that for binary liquid mixtures on addition of 3-(4-fluorophenyl)-1-phenylprop-2-en-1-one there is decrease in molar refraction as well as polarizability this decrease is due to the fact that the solute-solvent interaction may be more strong than solvent-solvent interactions.

The molar refraction of solvent and solution mixtures[16-17] were determined from,

$$R_{M\text{-}B} = \frac{n^2 - 1}{n^2 - 2} \times \{(x_1 m_1 + x_2 m_2)|d\}$$

Where, R_m = Molar refraction

X_1 = Mole fraction of solvent

N = R.I of Solution

X_2 = Mole fraction of solution

M_1, M_2 = Molecular weights of solvent

D = Density of solution and solution

The polarisability constant [18](α) of solution was calculated using equation,

$$\alpha = \frac{3 R_m}{4 \pi No}$$

Where, α = Molar polarisability

N_O = Avogadro's number = 6.023×10^{23}

Effective molecular mass[19] can be calculated (M_{eff}) the relation

$$M_{eff} = \sum X_i M_i$$

Where, Xi = Mole fraction[20] and Mi = molecular weight of i^{th} component.

The molar volume (V_m) can be calculated by the Equation,

$$V_m = \frac{M_{eff}}{\rho_0}$$

Free volume[21] was calculated by,

$$V_f = \frac{(M_{eff} \times U)^{3/2}}{K\eta}$$

Where, $K = 4.028 \times 10^9$ for all liquids, which is a temperature independent constant.

The Rao's molar sound function[22] (R_m) was calculated by equation,

$$R_m = \frac{M_{eff} \times U}{K \times \eta}$$

The results obtained are listed in Table 1 and 2.

Table 1: Density, refractive index, molar refraction, specific refraction and polarizability constant of 3-(4-fluorophenyl)-1-phenylprop-2-en-1-one in Benzene + Methanol mixture at 298 K

Physical parameters					
% of Methanol (by weight)	**Density (g/cm^3)**	**Refractive index (n)**	**Specific refraction (r)**	**Molar refraction (R_m)**	**Polarizability constant (α) x 10^{-23}**
0	0.8690	1.504	0.3316	25.870	1.0250
10	0.8535	1.467	0.3248	22.381	0.8871
20	0.8456	1.450	0.3179	19.577	0.7759
30	0.8406	1.434	0.3109	17.280	0.6849
40	0.8337	1.421	0.3036	15.347	0.6083
50	0.8245	1.404	0.2962	13.712	0.5435
60	0.8183	1.390	0.2887	12.306	0.4878
70	0.8109	1.375	0.2811	11.087	0.4394
80	0.8047	1.360	0.2733	10.018	0.3971
90	0.7988	1.349	0.2653	09.073	0.3596
100	0.7830	1.320	0.2572	08.232	0.3263

Table 2: Mole fraction, effective molecular weight, molar volume, free volume, internal pressure and molar sound velocity of 3-(4-fluorophenyl)-1-phenylprop-2-en-1-one in Benzene + Methanol mixture at 298 K

% Methanol (by weight)	**Mole fraction**		**Effective molecular weight (M_{eff})**	**Molar volume (V_m) m^3mol^{-1}**	**Free volume (V_f) × 10^{-7} m^3mol^{-1}**	**Internal pressure (π_i) × 10^3 atm**	**Rao's molar sound velocity (Rm) m/s**
	X_1	**X_2**					
0	0.0000	1.0000	78.000	89.760	2.2250	40.790	980.52
10	0.1977	0.8022	68.900	80.110	0.8011	61.853	862.94
20	0.3568	0.6432	61.587	72.210	0.6399	71.439	774.64
30	0.4874	0.5128	55.578	65.657	0.5407	80.516	701.13
40	0.5966	0.4034	50.555	60.125	0.4580	90.239	638.59

Cont…

% Methanol (by weight)	Mole fraction		Effective molecular weight (M_{eff})	Molar volume (V_m) m^3mol^{-1}	Free volume (V_f) × 10^{-7} m^3mol^{-1}	Internal pressure (π_i) × 10^3 atm	Rao's molar sound velocity (Rm) m/s
	X_1	X_2					
50	0.6893	0.3107	46.293	55.566	0.3992	99.568	588.64
60	0.7689	0.2310	42.628	51.587	0.3498	109.33	545.75
70	0.8381	0.1619	39.447	48.133	0.3120	118.95	506.23
80	0.8987	0.1013	36.660	45.085	0.2813	128.62	472.93
90	0.9523	0.0477	34.194	42.445	0.2617	137.16	443.11
100	1.0000	0.0000	32.000	40.562	0.2473	144.07	420.17

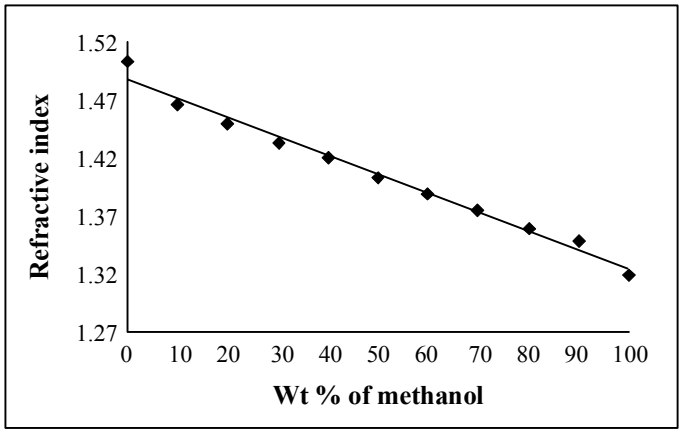


Fig 5: Relation between refractive index and % composition of methanol

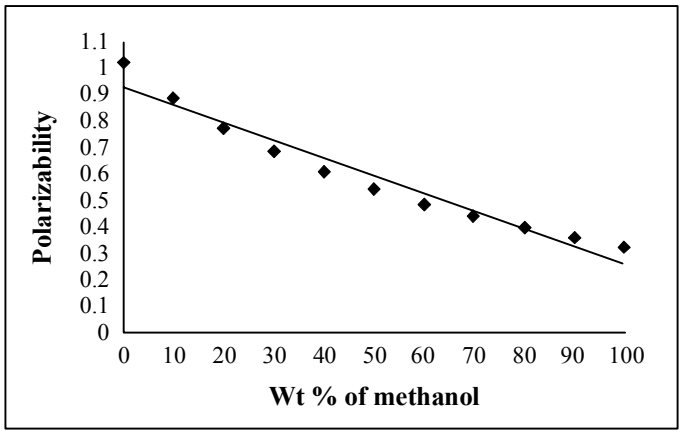


Fig 6: Relation between polarizability and % composition of methanol

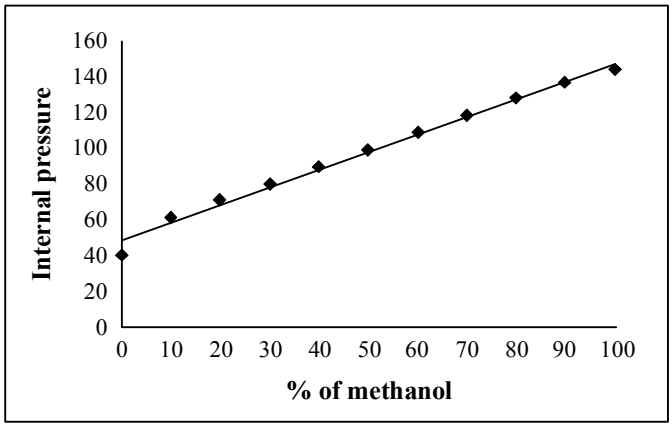


Fig 7: Relation between internal pressure and % composition of methanol

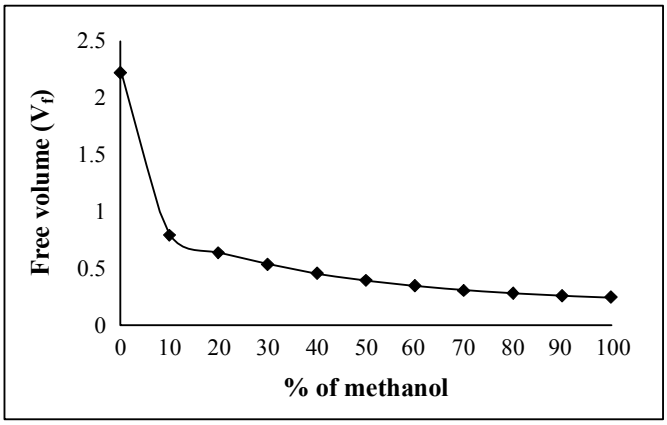


Fig 8: Relation between free volume and % composition of methanol

CONCLUSION

For binary liquid mixtures, on addition of 3-(4-fluorophenyl)-1-phenylprop-2-en-1- there was a decrease in molar refraction as well as polarizability. This decrease is due to the fact that the solute-solvent interaction may be more strong than solvent-solvent interactions.

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