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Refractometry Study of Some Substituted Isoxazoline in 70 % Ethanol-Water Medium at Different Temperature

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ABSTRACT: The present study deals with the study of molar refraction & polarizability constant of some substituted isoxazoline in 70% ethanol-water at different temperatures. The data and result obtained have been used to compute intermolecular interaction.

Key words: Substituted isoxazoline

70% ethanol-water

Refractometry study

L_1:3-(2-Hydroxy-5-methylphenyl)-5-(4-methoxyphenyl) isoxazoline

L_2 :3-(2-Hydroxy-3-chloro-5-methylphenyl)-5-(4-methoxyphenyl)isoxazoline

L_3:3-(2-Hydroxy-3-bromo-5-methylphenyl)-5-(4-methoxyphenyl) isoxazoline

L_4:3-(2-Hydroxy-3-bromo-5-methylphenyl)-5-(3,4-dioxymethylenephenyl)isoxazoline

INTRODUCTION

A refractometer is a laboratory or field device for the measurement of an index of refraction. Ernst Abbe was the first to develop a laboratory refractometer. The knowledge of refractive index property at different temperatures of liquid mixture is an important step for their structure and characterization. Along with other thermodynamic data, refractive index values are useful for practical purpose in engineering calculation. Refractive index is useful to assess purity of substance, to calculate molecular electronic polarizability[1].

Refractive index has many applications and it is directly related to interactions in the solution[2]. It is applied to identify a substance, confirm purity or measure its concentration. Thermodynamic methods based on density and the refractive index is used for investigated intermolecular interaction in solution[3,4]. Valuable information on electronic polarizability of individual ions in solution can be collected from refractive index and makes refractive data[5]. Refractive index studied are being increasingly used as a tool for understanding molecular interaction in solution[6,7]. Pharmacokinetics and pharmacodynamics of drug is governed by different interactions in solution such as drug-solvent, drug-drug and drug-co-solute interaction.

Refractivity index and molar refractivity of binary liquid mixture at 298.15, 303.15, 308.15 and 313.15 K has been determined by Shukla et al[8]. Rajesh et al[9] had supplied rating of sweetness by molar refractivity and ionization potential. Study of molar refraction and polarisability constant of aqueous solution of KCl and $KBrO_3$ at different temperature has been done by Nikumb & Rathi[10].Shrivastav et al[11] have been studied molar refractivity based SAR IQSPR study of benzoic acid derivation against price in terms of median lethal dose. Deosarkas et al[12] studied effect of solvent on molar refraction and polarizability of 4-amino-5-chloro-N-2-(diethylamino ethyl)-2-methoxy benzamide hydrochloride hydrate solution at 30°C.

Effect of change in concentration of solute and solvent or molar refraction and polarizability constant of some thiopyrimidine derivatives have been studied by Wadekar et al[13].Quantifying the charge transfer phenomenon by molar refractivity in binding of L_1-quinoinyl derivatives as antimalarials have been studied by Neelima et al[14]. Verification of specific refraction and molar refraction for homologous alcohol series at 30°C by suggested formula has done by Patel & Patel[15]. Refractivity index, molar refraction & polarisability constant of various compounds were studied by many workers[16-19].

APPARATUS AND PROCEDURE:

The refractive indices of different solution were measured by Abbe's refractometer (±0.001). The temperature of the prism is maintained constant at required temperature by circulating water from thermostat. The refractometric readings were taken as described in literature. Initially the refractometer was calibrated with glass piece (n=1.5220) provided with instrument.

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Weighing was carried out on single pan electronic balance (±0.001g).Density were measured by bicapillary pyknometer. For evaluation the molar refraction and polarizability constant of the compounds, we prepared solution in 70% ethanol-water at 20°C, 25°C and 30°C. The temperature was maintained by using the thermostat. The data obtained was used to compute intermolecular interaction.

OBSERVATION AND CALCULATION:

Molar refractivity is a measure of total polarizability of a mole of substance and is dependant on the temperature, the index of refraction and the pressure.

$$R_m = \frac{4}{3}\pi N_A \alpha \qquad \text{..... (1)}$$

Where, N_A – 6.022 x 10^{23} an Avogadro's constant

α - is the mean polarizability of a molecule

Molar refractivity is calculated by the Lorentz formula.

$$Rm = \frac{n^2-1}{n^2+1}\times\frac{M}{\rho} \qquad \text{..... (2)}$$

Where, M is mol wt

n is refractive index

ρ is density

R_m – Molar refraction

Molecular polarizability of solution was calculated using equation

$$\alpha = \frac{3}{4}\frac{R_m}{\pi N_A} \qquad \text{..... (3)}$$

Table - 1Measurement of Molar refraction (Rm) and polarizability constant at different temperature for L_1

Temp. K	Density g cm^{-3}	Refractive index n	Molar refraction R_m cm^3mol^{-1}	Polarizability constant α x 10^{-23} cm^3mol^{-1}
303.15	0.7928	1.413	89.0062	3.5297
298.15	0.7939	1.415	89.2656	3.5405
293.15	0.7951	1.416	89.3195	3.5427

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Table – 2 Measurement of Molar refraction (Rm) and polarizability constant at different temperature for L_2

Temp. K	Density g cm^{-3}	Refractive index n	Molar refraction R_m cm^3mol^{-1}	Polarizability constant $\alpha \times 10^{-23}$ cm^3mol^{-1}
303.15	0.7894	1.414	100.4738	3.9851
298.15	0.7897	1.415	100.6487	3.9920
293.15	0.7899	1.417	101.8223	4.0386

Table – 3 Measurement of Molar refraction (Rm) and polarizability constant at different temperature for L_3

Temp. K	Density g cm^{-3}	Refractive index n	Molar refraction R_m cm^3mol^{-1}	Polarizability constant $\alpha \times 10^{-23}$ cm^3mol^{-1}
303.15	0.7915	1.416	114.7411	4.5502
298.15	0.7927	1.417	114.8090	4.5537
293.15	0.7939	1.418	114.8760	4.5564

Table – 4 Measurement of Molar refraction (Rm) and polarizability constant at different temperature for L_4

Temp. K	Density g cm^{-3}	Refractive index n	Molar refraction R_m cm^3mol^{-1}	Polarizability constant $\alpha \times 10^{-23}$ cm^3mol^{-1}
303.15	0.7862	1.415	119.7300	4.7481
298.15	0.7874	1.416	119.8000	4.7517
293.15	0.7885	1.417	119.8857	4.7551

RESULT & DISCUSSION

The present investigation includes the measurement of density and refractive index of substituted isoxazoline at different temperatures.

The values of density and refractive index are shown in Table (1-4). These values increases with decrease in temperature. The increase in density with decrease in temperature is due to decrease in molar volume of solvent. However the increase in refractive index is due to the fact that the solute-solute and solute-solvent interaction stronger with decrease in temperature.

The value of molar refraction of ligands (L_1 to L_4) are presented in Table 1-4 at different temperatures 303.15 K, 298.15 K and 293.15 K. From the data, it can be predicted that, when the temperature decreases, the molar refractivity increases.

At the same time, polarizability constant (α) also increases. This may be attributed to the fact that with decrease in temperature, there is increase in dielectric constant and also considerable dipole association take place which would be accomplished by polarizability.

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CONCLUSION

Refractometer was an acceptable, rapid & convenient method for determining refractive index & polarizability constant.Polarizability depends on solute-solute interaction, solute-solvent interaction as well as molecular interaction.

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