



**STUDY OF REFRACTIVE INDEX, DENSITY, MOLAR REFRACTION AND
POLARIZABILITY CONSTANT OF SUBSTITUTED HETEROCYCLIC COMPOUNDS
IN DIFFERENT MIXTURE BY REFRACTOMETRIC TECHNIQUE AT 305K**

Dr. Vijay S. Jagtap*

Department of Chemistry, S.P.M.Science and Gilani Arts Commerce College Ghatanji, Dist. Yavatmal (MS) 445301.

***Corresponding Author: Dr. Vijay S. Jagtap**

Department of Chemistry, S.P.M.Science and Gilani Arts Commerce College Ghatanji, Dist. Yavatmal (MS) 445301.

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ABSTRACT

Refractive index of substituted Pyrazole Carboxylic Acid derivatives are determined by using Abbe's refractometer. From the data refractive index, density, molar refraction (R_m) and polarizability constant (α) are calculated. The calculated data is used to study the solute-solute, solute-solvent and solvent-solvent interaction in the system.

KEYWORDS: Pyrazole Carboxylic Acid derivatives, Abbe's refractometer, Molar refraction (R_m), Polarizability constant (α).

INTRODUCTION

Refractive index is one of the most important properties of liquid. Refractive index of liquid solutions can be easily and rapidly achieved by using Abbe's refractometer. Polarizability constant and molar polarization for heterocyclic antiemetic and anti-inflammatory drugs in binary solvent mixture ethanol-water, methanol-water and DMSO-water determined by measurement of refractive index^[1] Refractive indices of binary liquid mixtures and 1, 3 diaryl carbamides in different percentage of binary liquid mixture such as acetone-water, dioxane-water & DMSO-water at 27 °C were determined. To explain solute-solvent, solvent-solvent interactions data obtained is used to calculate molar refraction & polarizability constant.^[2] A rapid refractometric method for the estimation of the iodine value of freshly prepared linseed oil is described. For this purpose the oil at laboratory temperature from finely ground flax seed, is used which determining the refractive index at 25 °C.^[3] Refractive index, molar refractivities and molar polarizability constant of heterocyclic compounds such as 2-Thiazol-4-yl-1H benzimidazole, 5-nitro-2-Thiazol-4-yl-1H benzimidazole and 2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid have been studied in Ethanol, Methanol, Acetone, DMF, and THF media at 303 K $\pm$ 0.10°C temperature and different concentrations (0.625x10⁻³ to 10.0x 10⁻³M).^[4] The apparent molar volumes and viscosities of three alkali metal chlorides, namely, lithium chloride, sodium chloride, and potassium chloride, have been determined in a 40 mass % tetrahydrofuran + water mixture at 303, 308, 313, and 318 K.^[5] It has been estimated that due

to Vitamin A deficiency approximately 250 000 to 500 000 malnourished children go blind each year approximately half of whom die within a year of becoming blind. The most recent survey data obtained from 8 state surveys in 2003 suggest that 62% of preschoolers in India are vitamin A deficient, having serum retinol concentrations lower than 20 μ g/dL. Against this background of rural deficiency, researcher conducted this study to assess the prevalence of symptoms of vitamin A deficiency in schoolchildren in India.^[6]

The interaction of metal ions with pyrazoles and diketones as antidiabetic drugs in 70% DMSO-Water, refractive index and polarizability constant and molar refraction in different concentration at 300K have been reported.^[7] studies of blends of epoxy with unsaturated polyester resin in chloroform were carried out by viscosity, ultrasonic velocity, and refractive methods at 297K using viscosity data^[8] Electrical conductances of tetrabutylammonium bromide, sodium tetraphenylborate, and sodium bromide in methanol - water mixtures at 298.15K, and 308.15K, and 318.15K have been reported.^[9] Study of volumetric, refractometric, of glycylglycine in aqueous FeCl₂ solution at temperatures 288.15K to 318.15 K is studied^[10] Densities and refractive indices have been measured for glycylglycine in aqueous FeCl₂ solution as a function of concentration at T=(288.15 to 318.15) K. Acoustic and refractometric study of binary mixtures of 1- Propanol + Benzonitrile at 313 K is reported.^[11] Relative and specific viscosities of Aceclofenacin 70% Dioxane water mixture at different

temperature is studied.^[12] Refractive properties and internal pressures of binary mixtures of octan-1-ol with chloroform, 2-dichloroethane and 1, 1, 2, 2-tetrachloroethane at 298.15 and 308.15 K have been reported.^[13] Refractive indices of binary liquid mixture at different temperatures is investigated.^[14]

The present work deals with the study of molar refraction and polarizability constant refractive index and density of following substituted carboxylic acid derivatives in DMSO and ethanol with different percentage is reported.

- 1) **Ligand A (L_A)**= 1- phenyl-3-(4'-methyl) phenyl-1H-pyrazol-4-carboxylic acid
- 2) **Ligand B (L_B)**= 1- phenyl-3-(4'-bromo) phenyl-1H-pyrazol-4-carboxylic acid
- 3) **Ligand C (L_C)**= 1- phenyl-3-(4'-ethyl) phenyl-1H-pyrazol-4-carboxylic acid
- 4) **Ligand D (L_D)**= 1,3-diphenyl-1H-pyrazol-4-carboxylic acid

MATERIALS AND METHODS

The refractive indices of solution and solvent mixture under investigation are determined using Abbe's refractometer and density of solution is measured using 10ml specific gravity bottle. The accuracy of Abbe's refractometer is within ± 0.001 units. Initially, the refractometer is calibrated with glass piece ($n=1.5220$) provided with instrument. The constant temperature of the prism box is maintained by circulating water from thermostat at $32 \pm 0.1^\circ\text{C}$. All weighings are made on one pan digital balance with an accuracy of ± 0.001 gm. The ligands of which physical parameters are to be explored are synthesized by using reported protocol. The solutions of compounds under study are prepared in DMSO and ethanol by keeping constant ligand concentration system (0.01M). All chemical used are of A.R. grade.

RESULTS AND DISCUSSION

It is often desirable to know the refractive index of a solute. This index can be derived from the refractive indices of solution and solvent on using a suitable mixture rule. The molar refraction of solvent, solution can be determined by following equation.

$$R_{\text{SOL-W}} = X_1 R_1 + X_2 R_2 \quad (1)$$

Where,

R_1 and R_2 are molar refractions of solvent and water respectively.

The molar refraction of solutions of ligand in solvent - water mixtures are determined from-

$$R_{\text{Mix}} = \frac{(n^2-1)}{(n^2+2)} + \left\{ \frac{[X_1 M_1 + X_2 M_2 + X_3 M_3]}{d} \right\} \quad (2)$$

Where,

n is the refractive index of solution, d is the density of solution, X_1 is mole fraction of solvent, X_2 is mole fraction of water and X_3 is mole fraction of solute, M_1 , M_2 and M_3 are molecular weights of solvent, water and

solute respectively.

The molar refraction of ligand can be calculated as –
 $R_{\text{lig}} = R_{\text{Mix}} - R_{\text{SOL-W}} \quad (3)$

The polarizability constant (α) of ligand can be calculated from following relation-

$$R_{\text{lig}} = \frac{4}{3} \pi N_0 \alpha \quad (4)$$

Where,

N_0 is Avogadro's number.

In the present study, the value of molar refraction and polarizability constant of substituted 1- phenyl-3-aryl-1H-pyrazol-4-carboxylic acid in various percentage of different solvent mixture at temperature 300K are reported. The experimental data shows that there is increased in refractive index with increase in percentage composition of solvent. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution.

Table 1: Values of molar refraction of different % of solvent mixture.

% of solvent mixture	Molar refraction[R]	
	Ethanol	DMSO
20	12.5481	19.1245
40	11.6471	18.7410
60	10.1213	17.2420
80	7.9540	13.8321
100	4.2145	4.4654

Table 2: Values of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) at 300K.

Conc. In %	Constant ligand concentration system (0.01M) with change in DMSO percentage			
	Refractive index (n)	Density (d) g/cm ³	Rm x 10 ³ cm ³ /mol	α x 10 ⁻²³ cm ³
Ligand L_A				
20	1.355	1.0232	64.468	2.5566
40	1.340	1.0036	70.754	2.8058
60	1.347	0.9835	76.613	3.0300
80	1.361	0.9843	80.2823	3.1830
100	1.377	0.9866	84.032	3.3324
Ligand L_B				
20	1.361	1.0261	71.280	2.8267
40	1.345	1.0046	78.267	3.1030
60	1.363	0.9830	87.170	3.4570
80	1.380	0.9804	92.234	3.6577
100	1.394	0.9808	96.325	3.8199
Ligand L_C				
20	1.364	1.0285	71.642	2.8410
40	1.348	1.0099	78.612	3.117
60	1.365	0.9856	87.346	3.460
80	1.383	0.9184	92.629	3.673
100	1.396	0.9818	96.435	3.824
Ligand L_D				
20	1.367	1.0512	79.799	3.1646
40	1.352	1.0210	87.895	3.4850
60	1.369	0.9880	97.677	3.8736
80	1.385	0.9423	103.170	4.0914
100	1.399	0.9858	107.328	4.2563

Table 3: Values of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) at 305K.

Conc. In %	Constant ligand concentration system (0.01M) with change in Ethanol percentage			
	Refractive index (n)	Density (d) g/cm ³	Rm x 10 ³ cm ³ /mol	α x 10 ⁻²³ cm ³
Ligand L_A				
20	1.363	0.9110	73.3500	2.90
40	1.372	0.938	81.3961	3.22
60	1.407	0.9686	88.9328	3.52
80	1.435	1.0024	92.1871	3.65
100	1.454	1.029	94.0129	3.72
Ligand L_B				
20	1.356	0.9044	79.2924	3.14
40	1.369	0.9315	88.9440	3.52
60	1.411	0.9609	98.8309	3.91
80	1.442	0.9934	103.0900	4.08
100	1.467	1.0204	106.485	4.22
Ligand L_C				
20	1.358	0.9060	79.4811	3.15
40	1.35	0.9343	84.5635	3.35
60	1.366	0.9635	88.9154	3.52
80	1.388	0.9970	91.6173	3.63
100	1.404	1.0241	93.5165	3.70
Ligand L_D				
20	1.355	0.9113	87.0388	3.45
40	1.351	0.9388	93.6236	3.71

60	1.371	0.9689	99.3289	3.93
80	1.392	1.0019	102.099	4.04
100	1.411	1.0296	104.5470	4.14

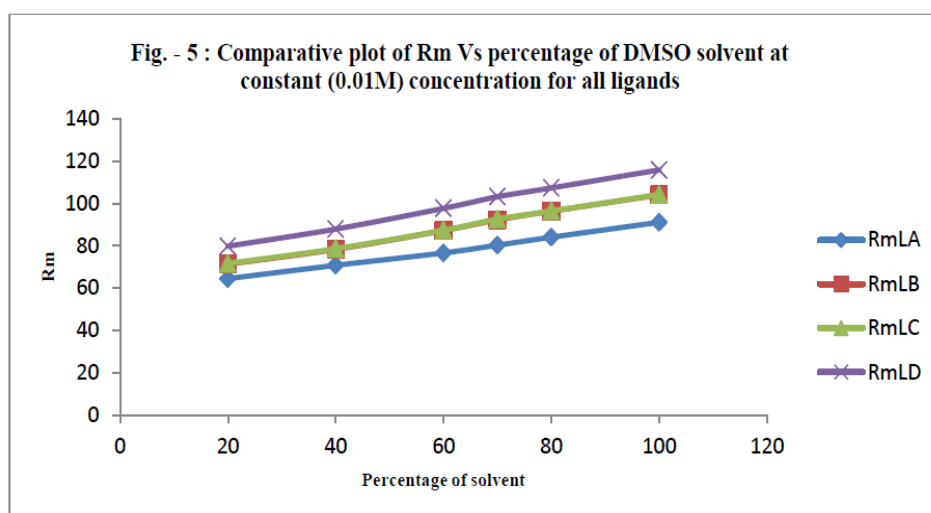
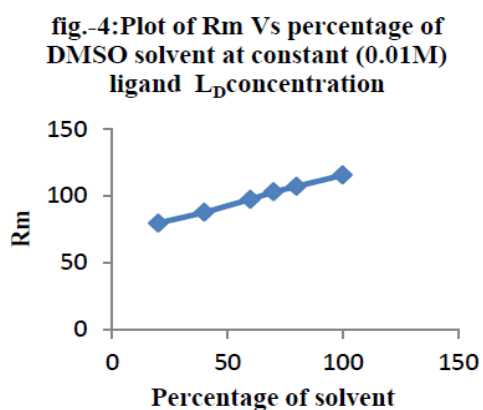
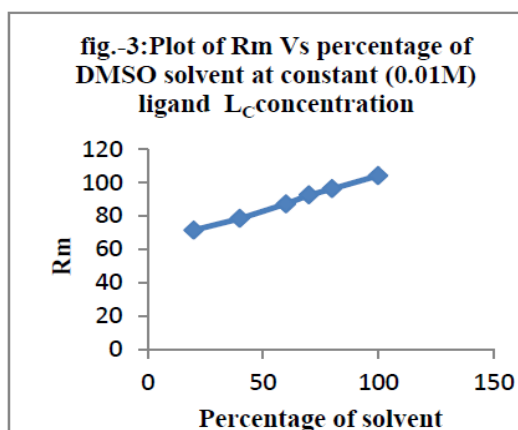
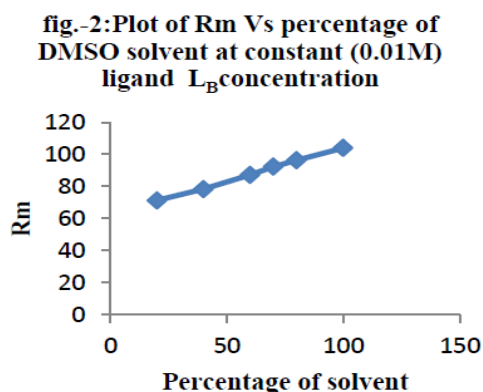
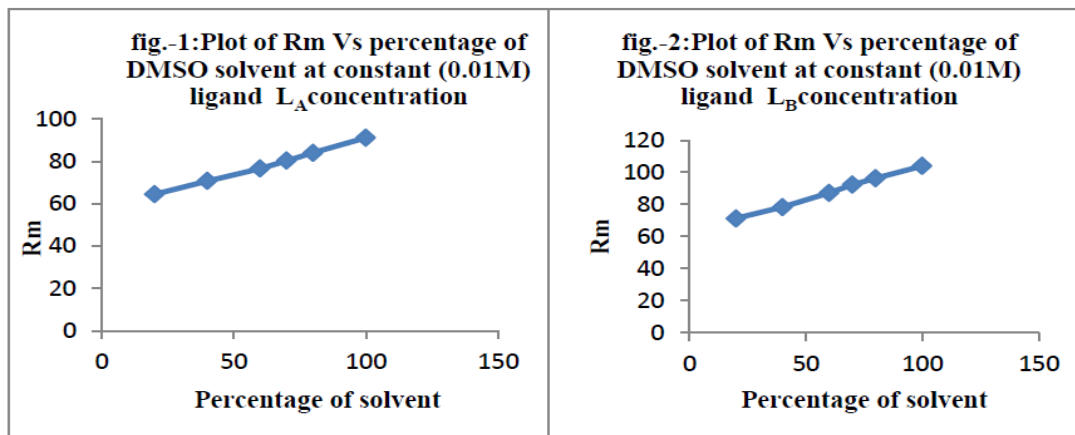


Fig. 1 to 5: Graphical representation of molar refractivity (Rm) versus change in DMSO solvent percentage at constant (0.01M) ligand concentration.

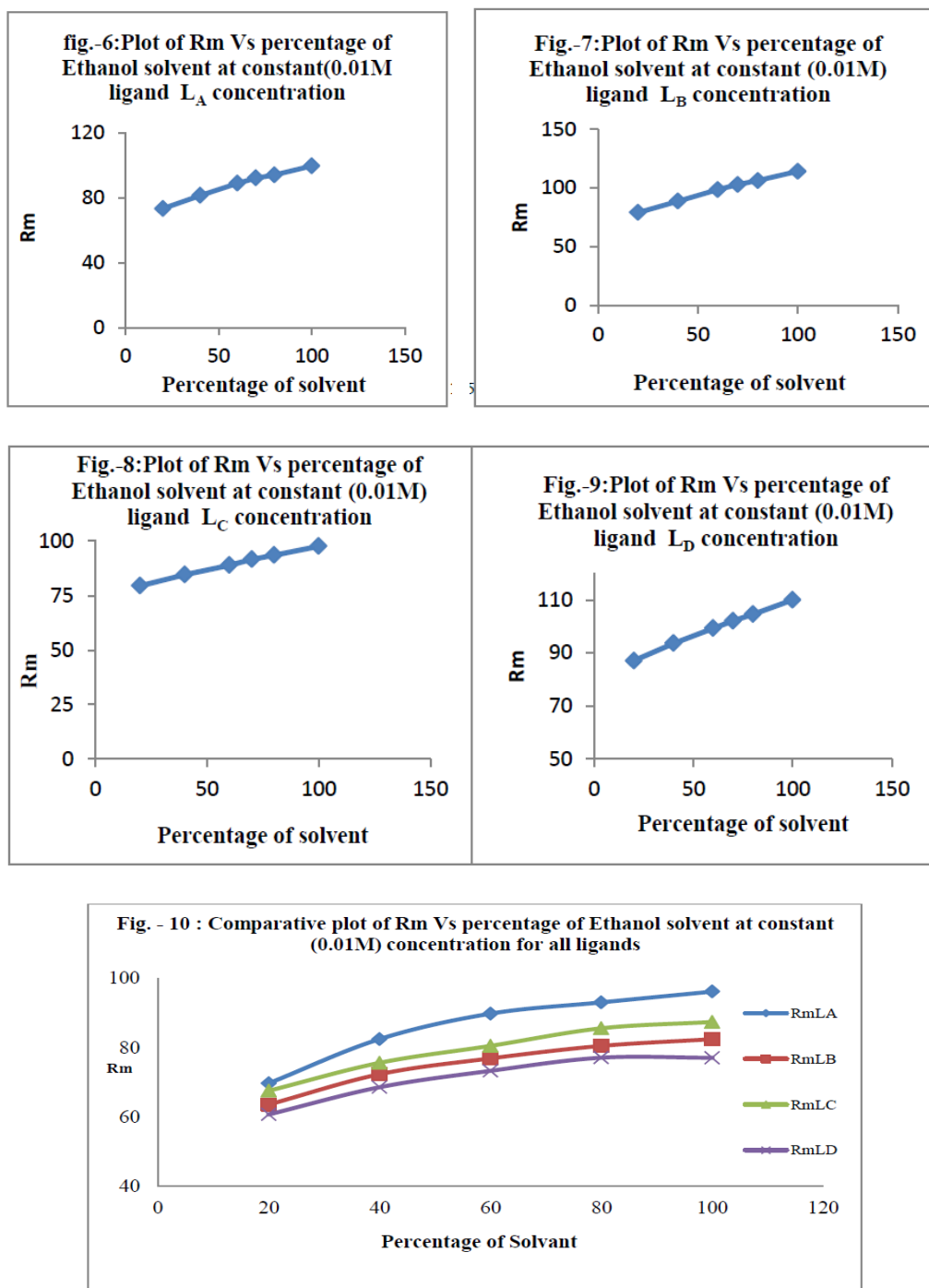


Fig. 6 to 10: Graphical representation of molar refraction (R_m) versus change in Ethanol solvent percentage at constant (0.01M) ligand concentration.

The refractive index (n), density (d), molar refraction (R_m) and polarizability constant (α) of substituted pyrazole carboxylic acid derivatives in different percentage of solvent are presented in table no. 2 and 3. It is observed that the values of molar refraction and polarizability constant increase with increase in percentage of organic solvent. The graphs of molar refraction (R_m) versus different percentage compositions of organic solvent are plotted. These are shown in fig. no. 1 to 10. From this it is observed that there is a linear relationship between molar refraction and concentration.

It is observed that molar refraction increases linearly as the percentage composition of organic solvent increases. This is attributed to the dispersion force and it is the molecular force which arises from temporary dipole moment. The cumulative dipole-dipole interaction creates a weak dispersion force resulting in an increase in molar refraction and polarizability constant.

CONCLUSION

Refractometric study of substituted pyrazole carboxylic acid derivatives in different percentage of binary mixture

is done. It seen that refractive index increases as the percentage composition of binary mixture increases. It observed that molar refraction and polarizability constant of substituted pyrazole carboxylic acid derivatives increases as the percentage composition of organic solvent binary mixture increases. From this study, it is clear that when the percentage of solvent increases the solute solvent interaction increases. The increase in the value of molar refraction as well as polarizability constant with increase in percent composition of organic solvent part can be attributed to dispersion force.

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REFERENCES

1. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
2. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
3. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
4. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
5. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
6. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
7. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
8. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
9. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
10. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
11. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
12. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
13. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.
14. Belokar GU, Burghate AS, Physical parameter study of heterocyclic antiemetic and anti-inflammatory drugs by refractometry. *Rasayan Journal Chem*, 2014; 7(4): 317–319.