Refractive index, density, molar refraction and polarizability constant of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in different binary mixture

V. S. Jagtap

S. P. M. Science And Gilani Arts Commerce College Ghatanji Dist Yavatmal.

ABSTRACT

Refractive index is useful for qualitative analysis of substances because each substance has constant and unique refractive index that can be determined with great accuracy**.** Refractive index of Substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives are determined by using Abbe's refractometer. Refractive index and density, molar refraction (Rm) and polarizability constant (a) are calculated from data. To study the solute-solute, solute-solvent and solvent-solvent interaction in the system, calculated data is used

Keywords: Substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives, , Molar refraction , Polarizability constant , Abbe's refractometer.

INTRODUCTION

Refractive index is one of the important properties of liquid.The refractive index is defined as the ratio of the speed of light in vacuum.The definition above is sometimes referred to as the absolute refractive index to distinguish it from definitions where the speed of light in other reference media than vacuum is used . Densities and refractive indices have been measured for glycylglycine in aqueous FeCl2 solution.[i] . Oswal etal[ii] have studied dielectric constants and refractive indices of binary mixtures. Bhatia etal[iii]. molar refraction and molar refraction of 1,3-diarylcarbamides in different percentage of binary liquid mixturewas done[iv]. Refractive index of substituted benzofurones in different solvents have reported.[v]Refractometric study of azomethine drugs in different composition was reported[vi] Molecule and macromolecule solutions by surface plasmon resonance was determined by refractive index increment. [vii] Refractive indices and refractive index increment of a synthetic polymethyl-methacrylate (PMMA) solutions at 488 nm were Measured .[viii] Density and refractive index was reported for substituted-2,3-dihydroquinazolin- 4(1H)-ones have been measured in binary mixtures with different composition , percentage, and at constant ligand concentration of 0.01M.[ix] Refractive indices and refractive index of Substituted Thiopyrimidines in Different Binary Mixture was studied.[x]

Refractometric study of some substituted oxoimidazoline drugs in different concentration of solute and solvents are reported [xi] . Refractive index and densities have studied for substituted N, N'-bis(salicyliden)-arylmethanediamine[xii]. Molar refraction and polarisability constant of 2-hydroxyl-5-methyl-4-methoxy chalcone in different percentage of water have studied[xiii].. Densities and refractive index of different substituted hydrazone have investigated and from this data molar refraction (Rm) and polarizability constant (α) was reported.[xiv].

Refractometric study of six binary mixtures of N-butyl bromide with aniline, carbon tetrachloride, benzene, xylene, toluene and n-heptane for the entire concentration range have done at 303.15 K[xv]. Refractive index, density, molar refraction and polarizability constant of substituted 2-oxo-2Hchromene-3-carbohydrazide derivatives in different binary mixturewas done [16]

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The present work deals with the study of molar refraction and polarizability constant of following substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acidderivatives and ethanol with different percentage is done.

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 ± 0.1°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[25]. The solutions of compounds under study are prepared in 1, 4-dioxane 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.[xxii] The molar refraction of solvent, solution can be determined by following equation.[xxiii]

$$R_{DMF\text{-}W} = X_1R_1 + X_2R_2 \quad (1)$$

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

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

$$R_{Mix} = \frac{(n^2-1)}{(n^2+2)} + \left\{\frac{[X_1M_1+X_2M_2+X_3M_3]}{d}\right\} \qquad (2)$$

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 –

$$R_{lig} = R_{Mix} - R_{DMF\text{-}W} \qquad (3)$$

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

$$R_{lig} = 4/3\ \pi N o \alpha \qquad (4)$$

Where, No 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 (20%, 40%, 60%, 80%, 100%) 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	7.954	13.8321
100	4.2145	4.4654

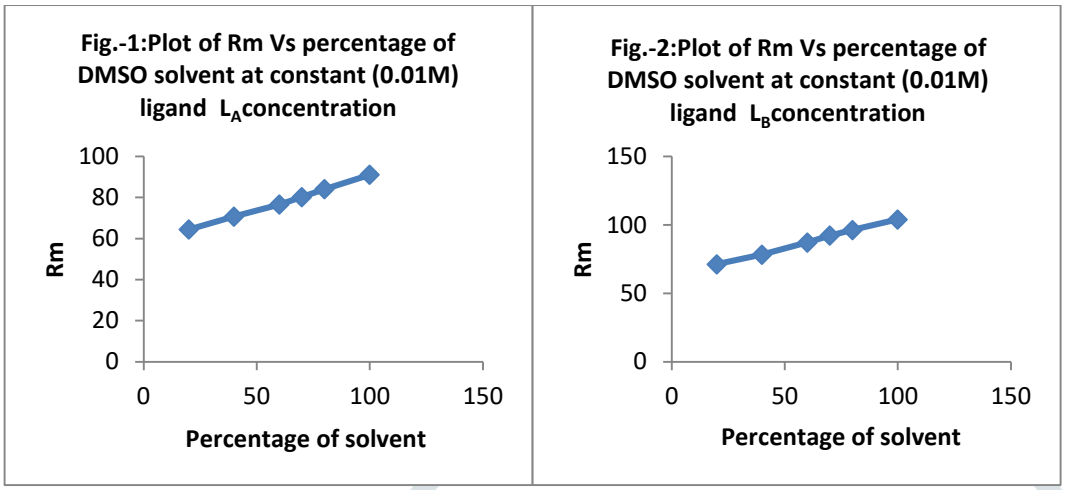
Table- 2: Values of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) at 300K

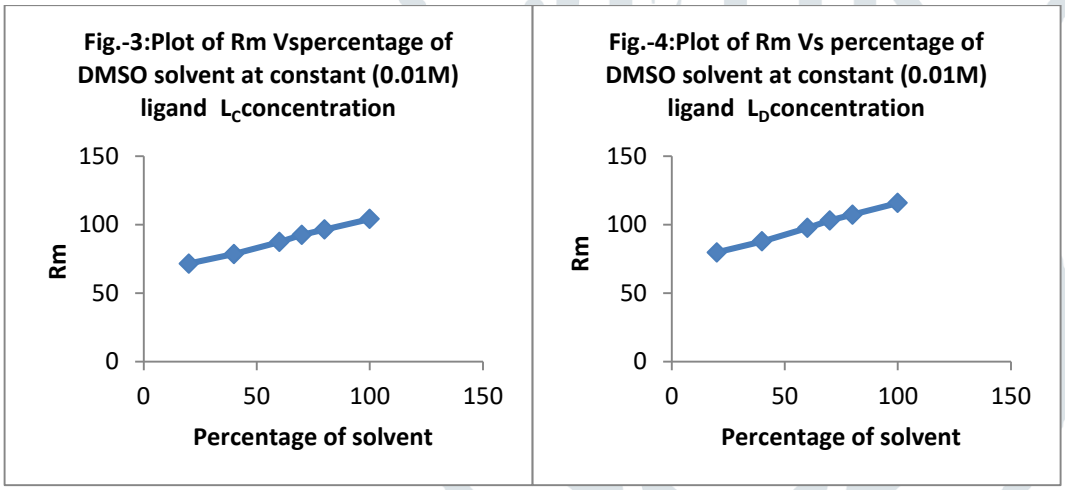
Conc. In %	Constant ligand concentration system (0.01M) with change in DMSO percentage			
	Refractive index (n)	**Density (d) g/cm^3**	**Rm x 10^3 cm^3/mol**	**α x 10^{-23} cm^3**
Ligand L_A				
20	1.355	1.0232	64.4684	2.5566
40	1.34	1.0036	70.754	2.8058
60	1.347	0.9835	76.613	3.03
80	1.361	0.9843	80.28232	3.183
100	1.377	0.9866	84.0325	3.3324
Ligand L_B				
20	1.361	1.0261	71.280	2.8267
40	1.345	1.0046	78.267	3.103
60	1.363	0.983	87.17	3.457
80	1.38	0.9804	92.234	3.6577
100	1.394	0.9808	96.3250	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	87.3465	3.46
80	1.383	0.9184	92.6298	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	1.021	87.895	3.485
60	1.369	0.988	97.677	3.8736
80	1.385	0.9423	103.17	4.0914
100	1.399	0.9858	107.3281	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	73.350	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	88.944	3.52
60	1.411	0.9609	98.8309	3.91
80	1.442	0.9934	103.09	4.08
100	1.467	1.0204	106.485	4.22
Ligand L_C				
20	1.358	0.906	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	104.547	4.14

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





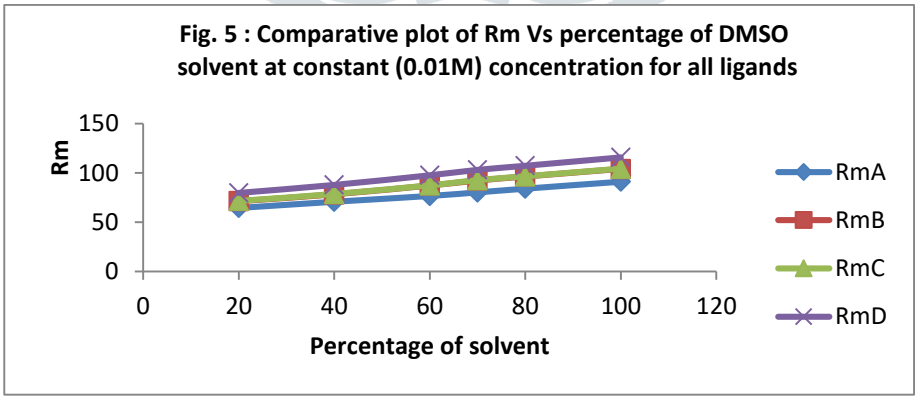
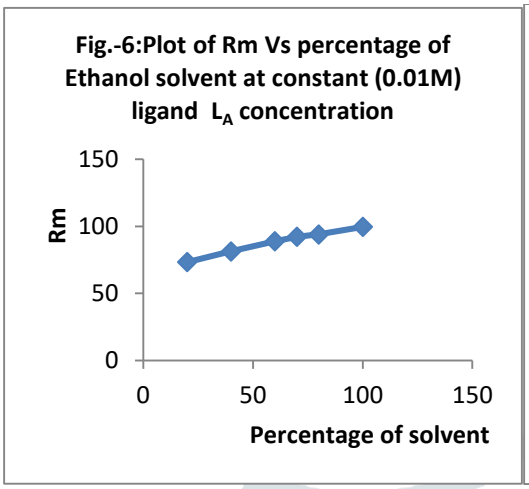
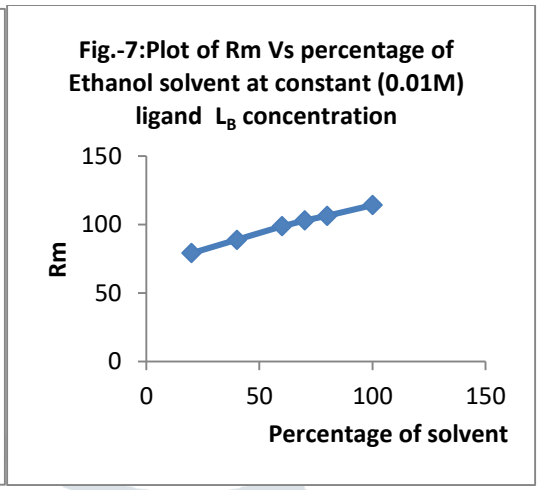
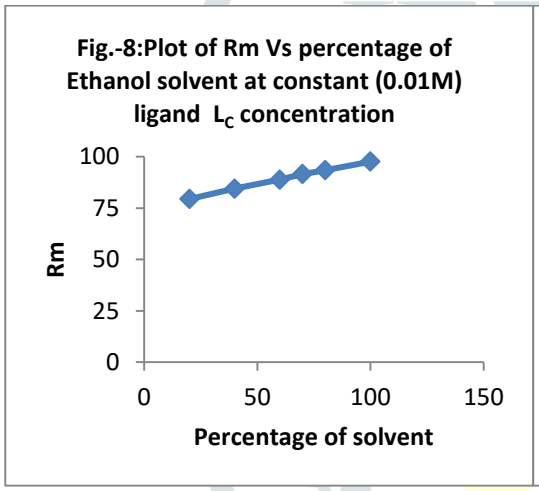
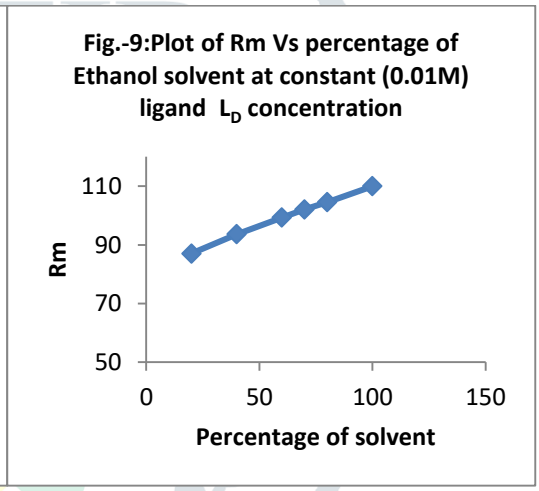


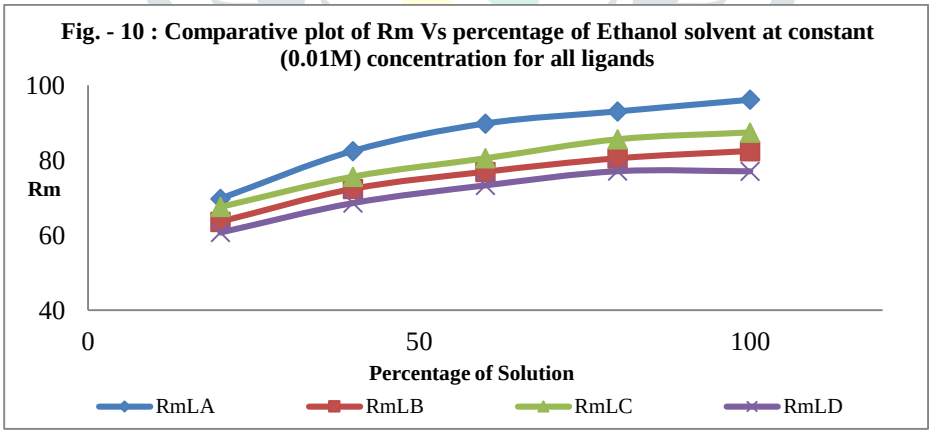
Fig. 6 to 10: Graphical representation of molar refraction (Rm) versus change in Ethanol solvent percentage at constant (0.01M) ligand concentration











The refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) of substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives in different percentage of solvent are presented in table no. 2 and 3. It observed that the values of molar refraction and polarizability constant increases with increase in percentage of organic solvent. The graphs of molar refraction (Rm) versus different percentage compositions of organic solvent are plotted. These are shown in fig. no. 1 to 10. From this it is observe that there is 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 weak dispersion force resulting in increase in molar refraction and polarizability constant.

CONCLUSION

Refractometric study of substituted 1-phenyl-3-aryl-1H-pyrazol-4-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 2-oxo-2-H-chromene-3-carbohydrazide 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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REFERENCE

[i]. Santosh M S, Bhat D K, Bhatt A S, *J. Chem. Eng. Data*, 55,**(2010)**, 4048.

[ii] Oswal S L and Rathman M V, *Indian J Chem*, 26 **(1987)** 29.

[iii]. Bhatia S C, Tripathi N and Dubey G P, *Indian J Chem*, 41A (2) **(2002)** 266.

[iv] S. S. Ubarhande, A. S. Burghate, B. N. Berad, and J. D. Turak RASAYAN JournalofChemistry,vol.4,no.3,pp.585–587,2011.

[v]] V. S. Jamode, J. C. Dadhichi, D. D. Malkhede, M. L. Narwade, J. Ind. Coun. Chemist, 2005, 22(2), 35.

[vi] A. V. Kawalkar, D. S. Hedaoo and M. P. Wadekar*Journal of Chemical and Pharmaceutical Research, 2015 7(8):600-606

[vii]] T. Tumolo, Lankness, M.S. Baptista, Anal. Biochem., 2004, 333(2), 273

[viii] R. Ghazy, B. El-Baradie, A. El-Shaer, F. Elmekawey, Opt. Laser Technol., 1999, 31(5), 33

[ix] D.S.Hedaoo, M.M.Kalaskar, M.P.Wadekar, Der Chemica Sinica, 2015, 6(6), 7

[x] M. P. Wadekar*, A. S. Shrirao, R. R. Tayade Journal of Chemical, Biological and Physical Sciences ; Nov. 2014 – Jan. 2015, Vol. 5, No. 1; 81-90.

[xi]. Tayade R R, Kalaskar M M, Wadekar M P, *Der Chemica Sinica*, 5(5), **(2014)**, 12.

[xii]. Li Y, Yang Z S, Wang F D, *Bioorg. Med. Chem.*, 11, **(2003)**, 4363.

[xiii]. Burghate A S, Agrawal P B, Quazi S W, Narawade M L, *Asian. J. Chem.*, 13 (4), **(2001)**, 1652.

[xiv]. Khadse P, Chamdani A S, Wadekar M P. *Int. J. Chem. Phys. Sci*., 4, **(2015)**, 136.

[xv]. Ansari N H, Trivedi A, Sharma D, Chandra P, *Open J. Phys. Chem.*, 4, **(2014)**, 1.

[xvi]. Tayade R R, Kalaskar M M, Wadekar M P, *Der Chemica Sinica*, 5(5), **(2014)**, 12.

[xvii]. Li Y, Yang Z S, Wang F D, *Bioorg. Med. Chem*., 11, **(2003)**, 4363.

[xviii]. Burghate A S, Agrawal P B, Quazi S W, Narawade M L, *Asian. J. Chem.*, 13 (4), **(2001)**, 1652.

[xix]. Khadse P, Chamdani A S, Wadekar M P. *Int. J. Chem. Phys. Sci*., 4, **(2015)**, 136.

[xx]. Ansari N H, Trivedi A, Sharma D, Chandra P, *Open J. Phys. Chem.*, 4, **(2014)**, 1.

[xxi] P. P. Choudhari1, D. S. Hedaoo2, M. P. Wadekar1* Journal of Chemical, Biological and Physical Science November 2016 – January 2017, Vol. 7, No. 1; 028-038.

[xxii]. Heller W, *J. Phys. Chem.* 69(4), **(1965)**, 1123.

[xxiii]. Wadekar M P, Shrirao A S, Tayade R R, *Der Pharma Chemica*, 6(6), **(2014)**, 90.

[xxiv]. a) Karanth V R, Bhat D K, *J. Chem. Eng. Data*, 58, **(2013)**, 271;

b) Dhondge S S, *J. Chem. Eng. Data*, 55, **(2010)**,3962;

c) Solomonov B N, Varfolomeev M A, Nagrimanov R N, Novikov V B, Ziganshin M A, Gerasimov A V, Verevkin S P, *J. Chem. Eng. Data*, *60*(3), (**2015)**, 748.

[xxv]. a) Wang J, Xie X Q, Hou T, Xu X, *J. Phys. Chem. A*,111(20), **(2007)**, 4443;

b) Burghate A S, Agrawal P B, Quazi S W, Narwade M L, *Asian J. Chem.*, 13(4), **(2001)**, 1652.