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Refractive Index, Density, Molar Refraction and Polarizability Constant of substituted1-phenyl-3-aryl-1H-pyrazol-4-carboxylic Acid Derivativesin Different Binary Mixture

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ABSTRACT

Refractive index of Substituted1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives are determined by using Abbe's refractometer. Refractive index, density, molar refraction and polarizability constant are calculated from data. Calculated data is used to study the solute-solute, solute-solvent and solvent-solvent interaction in the system.

Keywords : Substituted1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives, Molar refraction (Rm), Polarizability constant (α), Abbe's refractometer.

I. INTRODUCTION

Refractive index is useful for qualitative analysis of substances that can be determined with great accuracy. Refractive index of liquid which gives idea about geometry and structure of molecule. Measurement of refractive index shows applications in pharmaceutical, chemical, agriculture, food, oil and beverage industries.

The refractometric study of substituted aminopyrimidine in both polar[1] and non-polar solvent is reported.[2] Refractrometry study of some substituted isoxazoline in 70% ethanol water medium at different temperature is done. [3]Study molecular interaction of substituted azomethine drugs is done by refractometrically.[4] The refractometric technique is use to studied the molecular interactions of an electrolyte in binary mixture of liquids.[5,6,7] Some homologous series such as n-ethanoate, methyl alkanoates and ethyl alkanoates are studied by refractometry technique.[8] The density and refractive index of binary systems ester + n-methyl-2-hydroxyethyl ammonium hexanoate is studied.[9] Refractive index and density is studied for substituted N,N'-bis(salicyliden)-arylmethanediamine.[10] Density and refractive index for substituted 2,3-dihydroquinazolin-4(1H)-ones is reported.[11] Molar refraction and polarisability constant of 2-hydroxyl-5-methyl-4-methoxy chalcone is studied in different percentage of water.[12] Densities and refractive index of different substituted hydrazone have investigated and from this data, molar refraction (Rm) and polarizability constant (α) was reported.[13] Refractometry technique is used to determined the serum protein concentrations in ring-necked pheasants.[14] Refractometry technique is used to measure the dissolved solids content of both pure and impure sucrose solutions in the sugar industry.[15] The refractometer offers an alternative method of determining soluble solids in citrus juice.[16] Refractometric technique is considered as an important tool for the measurement of glucose concentrations in body fluids such as blood and the intercellular fluid.[17] Refractometric study of substituted heterocyclic compounds such as 5-ethoxycarbonyl-4-(4-bromo-phenyl)-6-methyl-3, 4-dihydropyrimidine-2-(1H)one, 5-ethoxy carbonyl-4-(4-nitro-phenyl)-6-methyl-3, 4-dihydropyrimidine-2-(1H)one have done in dioxane, ethanol, THF and DMF at 303K.[18] Molar refractions for aqueous solution KCl and KBrO3 have studied.[19] Molar refraction and polarizability constant have studied for 2-hydroxy-5-ethyl-benzene and 2-amino-5-chloro-benzene sulphonic acid in dioxane and DMF-water medium respectively.[20] The dielectric constant and refractive index is reported for phenols in mixture of benzene acetone and carbon tetrachloride.[21] Molar polarizability constant for allopurinal, acenocoumarol, warfarin and amoxicillin in different solvents are done.[22] Refractometric study of some substituted oxoimidazoline drugs in different concentration of solute and solvents are reported.[23]

Density and refractive index of binary liquid mixture have studied for eucalyptol with hydrocarbon at different temperature.[24] Refractive index, molar polarizability constant and molar refractivity of lisinopril in acetone, DMF, methanol, ethanol, THF and dioxane media in different concentrations have studied.[25] 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.[26] Refractive index, density, molar refraction and polarizability constant of substituted 2-oxo-2Hchromene-3-carbohydrazide derivatives in different binary mixtureare done.[27] Comparison of refractive index of aqueous mixture of zinc and lead acetate with different temperature at different concentration is done.[28]

The present work deals with the study of molar refraction and polarizability constant of following compounds in nonaqueous solvent such as acetone, methanol and DMF (with different percentage)

1) Ligand A (LA)= 1- phenyl-3-(4'- methyl) phenyl-1H-pyrazol-4-carboxylic acid
2) Ligand B (LB)= 1- phenyl-3-(4'- bromo) phenyl-1H-pyrazol-4-carboxylic acid
3) Ligand C (LC)= 1- phenyl-3-(4'- ethyl) phenyl-1H-pyrazol-4-carboxylic acid
4) Ligand D (LD)= 1,3-diphenyl-1H- pyrazol-4-carboxylic acid

II. EXPERIMENTAL

The refractive indices of solution and solvent mixture under study are determined using Abbe's refractometer. Density of solutions is measured using 10 ml specific gravity bottle. Initially the refractometer is calibrated with glass piece (n=1.5220) provided with instrument. All weighings are done on one pan digital balance with an accuracy of 0.001 gm. The accuracy of Abbe's refractometer is within ±0.001 units. The constant temperature of the prism box is maintained by circulating water from thermostat at 32 □ 0.1□C. The ligands of which physical parameters are to be explored are synthesized by using reported protocol.[29] The solutions of compounds under study are prepared in different solvents acetone, ,methanol and DMF by keeping constant ligand concentration system (0.01M). All chemical usedare of A.R. grade.

III. 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.[30] The molar refraction of solvent, solution can be determined by following equation.[31]

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

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

The molar refraction[32,33,34] of solutions of ligand in solvent -water mixtures are determined from-

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

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

$$R_{lig} = R_{Mix} - R_{SOL\text{-}W} \quad (3)$$

The polarizability constant (α)[35,36]of ligand can be calculated from following relation

$$R_{lig} = 4/3\ \pi No\alpha \quad (4)$$

Where, No is Avogadro's number.

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

% of solvent mixture	Molar refraction [R]		
	Acetone	Methanol	DMF
20	11.6541	7.8365	17.1769
40	10.9249	6.9123	16.4054
60	9.8437	5.7142	15.1130
80	7.9125	4.1451	11.2451
100	4.20143	7.8214	4.5215

Table- 2: The data ofrefractive index (n), density (d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of acetone solvent at 300K.

Conc. In %	Constant ligand concentration system (0.01M) with change in Acetone percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x10^3 cm^3/mol	α x10-23 cm^3
Ligand L_A				
20	1.350	1.0104	64.2307	2.54
40	1.344	1.0329	69.1980	2.74
60	1.375	1.0740	74.8700	2.96
80	1.397	1.0980	77.9559	3.09
100	1.414	1.1033	81.2921	3.22
Ligand L_B				
20	1.352	1.0110	70.4089	2.79
40	1.345	1.0339	75.7414	3.00
60	1.377	1.0755	82.1400	3.25
80	1.398	1.0980	85.4065	3.38
100	1.410	1.1046	88.2109	3.49
Ligand L_C				
20	1.355	1.0139	70.8081	2.80
40	1.350	1.0359	76.5864	3.03
60	1.381	1.0775	82.7677	3.28
80	1.402	1.1005	86.0180	3.41
100	1.456	1.2041	88.7874	3.52
Ligand L_D				
20	1.358	1.1055	72.5540	2.87
40	1.353	1.1295	78.5364	3.11
60	1.384	1.1740	84.8524	3.36
80	1.406	1.1993	88.3675	3.50
100	1.420	1.2046	91.4747	3.62

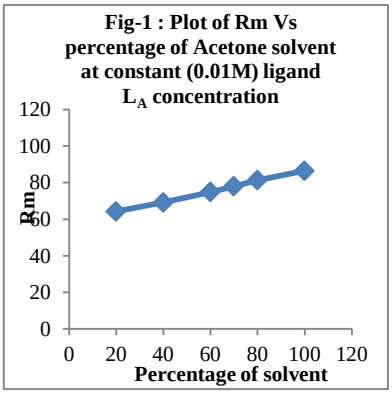
Table-3 : The data ofrefractive index (n), density (d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of DMSO solvent at 300K.

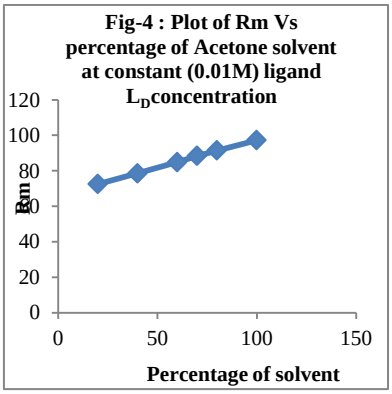
Conc. In %	Constant ligand concentration system (0.01M) with change in methanol percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x10^3 cm^3/mol	α x10^{-23} cm^3
Ligand L_A				
20	1.342	0.8986	69.9365	2.77
40	1.337	0.9280	74.6476	2.96
60	1.357	0.9563	79.4426	3.15
80	1.382	0.9894	82.5437	3.22
100	1.398	1.0053	85.0147	3.37
Ligand L_B				
20	1.347	0.9101	76.3953	3.02
40	1.342	0.9395	81.6583	3.23
60	1.368	0.9673	88.2880	3.45
80	1.388	0.9989	90.5071	3.59
100	1.404	1.0152	93.4167	3.70
Ligand L_C				
20	1.351	0.9122	77.0315	3.05
40	1.345	0.9416	82.1037	3.25
60	1.363	0.9697	86.9247	3.44
80	1.385	1.0037	89.6710	3.55
100	1.398	1.0195	91.8935	3.64
Ligand L_D				
20	1.363	0.9142	87.8472	3.48
40	1.354	0.9438	93.0433	3.68
60	1.372	0.9719	98.3732	3.90
80	1.394	1.0049	101.3344	4.01
100	1.410	1.0215	104.2224	4.13

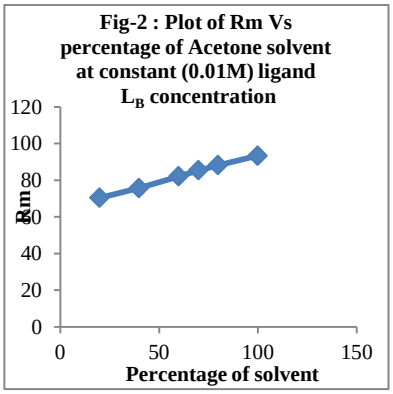
Table- 4 The data ofrefractive index (n), density (d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of DMF solvent at 300K.

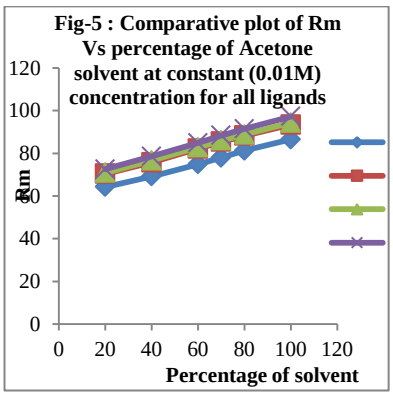
Conc. In %	Constant ligand concentration system (0.01M) with change in DMF percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x10^3 cm^3/mol	α x10^{-23} cm^3
Ligand L_A				
20	1.361	1.0939	61.1766	2.42
40	1.356	1.1097	66.6449	2.64
60	1.378	1.1160	72.7905	2.88
80	1.404	1.1390	77.2921	3.06
100	1.441	1.1661	82.6214	3.27
Ligand L_B				
20	1.364	1.1902	61.8640	2.45
40	1.358	1.2061	67.3457	2.67
60	1.381	1.2122	73.8155	2.92
80	1.408	1.2342	78.6839	3.12
100	1.445	1.2612	84.1643	3.33
Ligand L_C				
20	1.367	1.1898	62.3612	2.47
40	1.362	1.2055	68.0552	2.69
60	1.386	1.2114	74.7301	2.96
80	1.413	1.2311	79.6007	3.15
100	1.450	1.2602	85.0490	3.37
Ligand L_D				
20	1.373	1.2100	68.4446	2.71
40	1.365	1.2271	74.7295	2.96
60	1.387	1.2334	81.6373	3.23
80	1.415	1.2586	86.9299	3.44
100	1.453	1.2887	92.8455	3.68

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









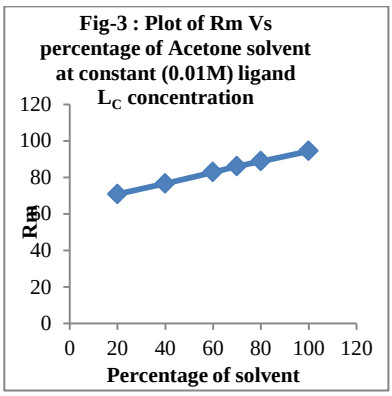
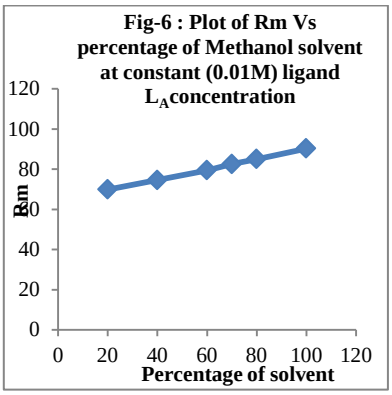
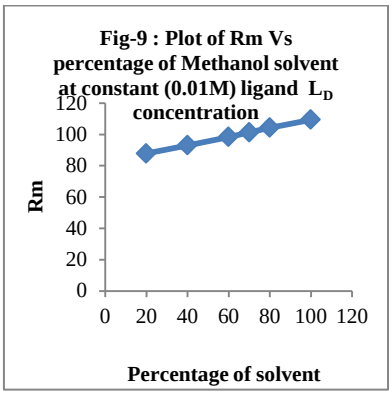
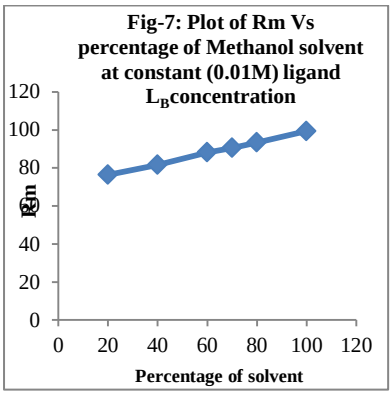
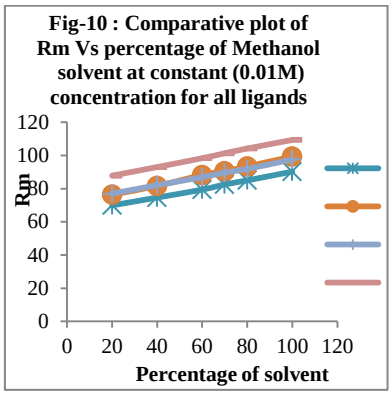


Fig. 6 to 10: Graphical representation of molar refraction (Rm) versus change in methanol solvent percentage at constant (0.01M) ligand concentration









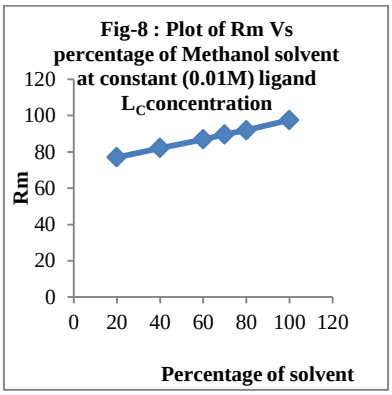
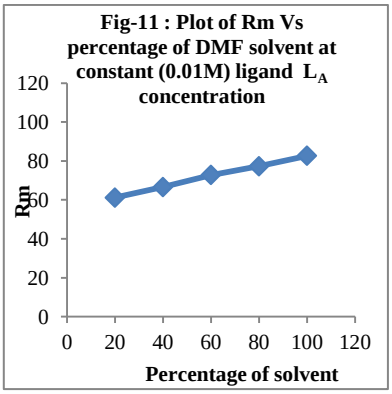
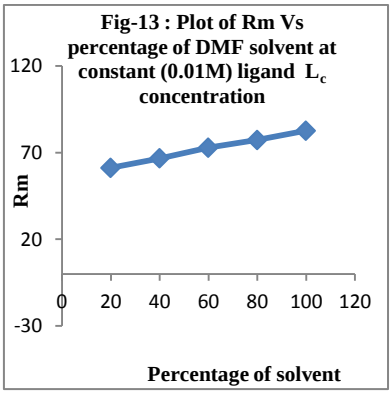
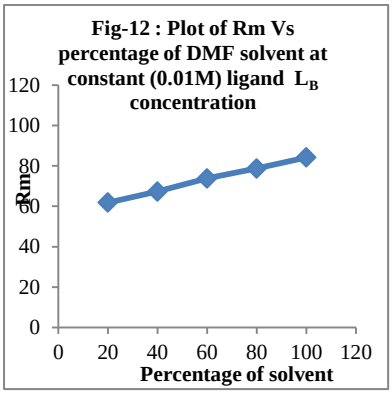
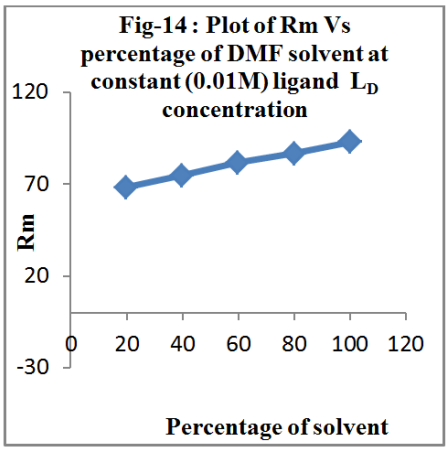


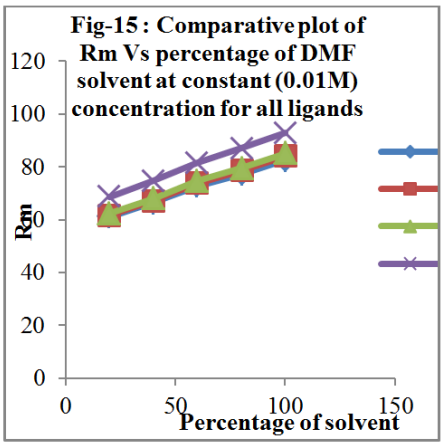
Fig. 11 to 15 : Graphical representation of molar refraction (Rm) versus change in DMF solvent percentage at constant (0.01M) ligand concentration











IV. CONCLUSION

In the present investigation the value of molar refraction and polarizability constant of Substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in various percentage of different solvent mixture at temperature 300K are reported. The experimental data shows that there is decrease in refractive index with decrease in percentage composition of solvent. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution under study. The data of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) of Substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in different percentage of solvent is presented in table no. 1 to 4. It is observed that increase in percentage of organic solvent, the values of molar refraction and polarizability constant increases.The graphs of molar refraction (Rm) versus different percentage compositions of organic solvent are plotted. These are shown in fig. no. 1 to 15. From this it is observe that there is linear relationship between molar refraction and concentration. It shows 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.

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