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Refractometric Study of some substituted pyrazole carboxylic acid Derivatives in different binary mixtures at 300 K

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Abstract:
Refractometric study of substituted pyrazole carboxylic acid derivatives were carried out in different binary mixture at 300K. Abbe's refractometer used to measure refractive index. molarrefractions and polarizability constants values in different binary mixtures are determined . The solute-solute, solute-solvent and solvent-solvent interaction in the system are predicted by using relative data.

Keywords: substituted pyrazole carboxylic acid derivatives, refractive index. molar refraction, polarizability constant.

Introduction:

Measurement of refractive index shows applications in pharmaceutical, chemical, agriculture, food, oil and beverage industries. The refractometric study of substituted aminopyrimidine in polar solvent is reported. [1] Study molecular interaction of substituted azomethine drugs is done by refractometrically.[2] Some homologous series such as n-ethanoate, methyl alkanoates and ethyl alkanoates are studied by refractometry technique. [3] Refractive index and density is studied for substituted N,N'-bis(salicyliden)-arylmethanediamine.
[4] Density and refractive index for substituted 2,3-dihydroquinazolin-4(1H)-ones is reported. [5] Molar refractions for aqueous solution KCl and KBrO3 have studied. [6] Densities and refractive index of different substituted hydrazone have investigated and from this data, molar refraction (Rm) and polarizability constant (α) was reported. [7] Refractometry technique is used to measure the dissolved solids content of both pure and impure sucrose solutions in the sugar industry.[8] Refractometric technique is considered as an important tool for the measurement of glucose concentrations in body fluids such as blood and the intercellular fluid. [9] 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. [10] The dielectric constant and refractive index is reported for phenols in mixture of benzene acetone and carbon tetrachloride.[11] Refractometric study of some substituted oxoimidazoline drugs in different concentration of solute and solvents are reported. [12] 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. [13] Refractive index, density, molar refraction and polarizability constant of substituted 2-oxo-2Hchromene-3-carbohydrazide derivatives in different binary mixtureare done. [14] Comparison of refractive index of aqueous mixture of zinc

and lead acetate with different temperature at different concentration is done. [15]

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

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. [16] 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.

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. [17] The molar refraction of solvent, solution can be determined by following equation. [18]

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

Where, R1 and R2 are molar refractions of solvent and water respectively.

The molar refraction [19,20,21] of solutions of ligand in solvent -water mixtures are determined from-

(2)

Where,

n is the refractive index of solution, d is the density of solution, X1 is mole fraction of solvent, X2 is mole fraction of water and X3 is mole fraction of solute, M1, M2 and M3 are molecular weights of solvent, water and solute respectively.

The molar refraction of ligand can be calculated as –

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

The polarizability constant (□) [22,23] of ligand can be calculated from following relation-

$$R_{lig} = 4/3 \square N_o \square \quad (4)$$

Where, No is Avogadro's number

In the present study, at various percentage of different solvent mixture at temperature 300K, molar refraction and polarizability constant value of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid are reported. The experimental data gives idea 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: Molar refraction values for different % of solvent mixture

solvent mixture %	Molar refraction [R]	
	Acetone	DMSO
20	12.6076	17.0523
40	11.9057	16.2511
60	10.7286	11.7181
80	8.8921	9.1420
100	5.1917	7.8523

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

Conc. In %	ligand concentration (0.01M) with change in Acetone 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: Refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α)values at 300K

Conc. In %	ligand concentration (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	1.363	0.9110	73.3500	2.90
40	1.372	0.9380	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	1.0290	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	106.4850	4.22
Ligand L_C				
20	1.358	0.9060	79.4811	3.15
40	1.350	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	102.0990	4.04
100	1.411	1.0296	104.5470	4.14

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 DMSO solvent percentage at constant (0.01M) ligand concentration

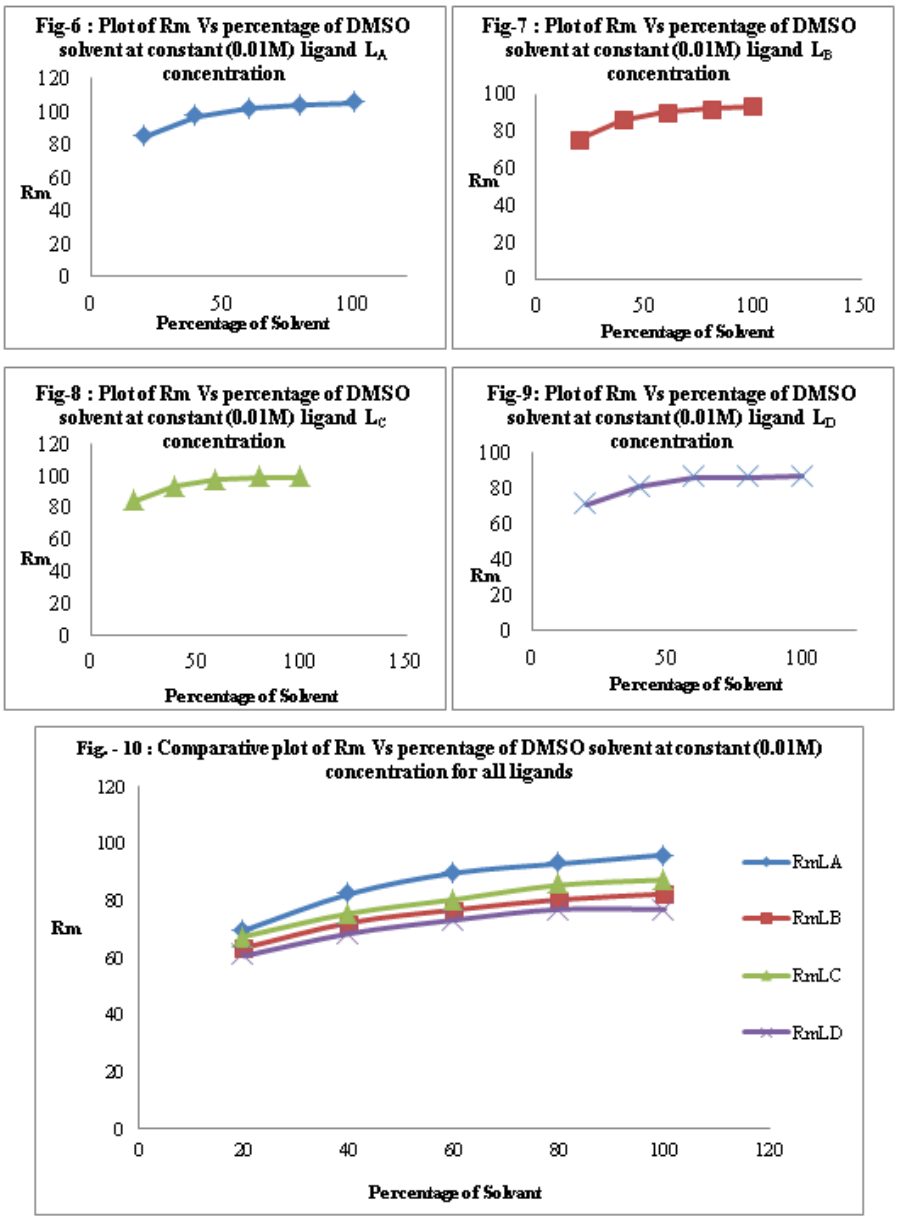

Table no. 2 and 3 indicates the refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in different percentage of solvents.From data it is observed that molar refraction and polarizability constant values increases with increase in organic solvent percentage. molar refraction (Rm)graphs versus compositions of different percentage of organic solvent are plotted. These are shown in fig. no. 1 to 10. From this it is clear that linear relationship observed between molar refraction and concentration. It is observed that as the percentage composition of organic solvent increases, molar refraction values increases. Due to temporary dipole moment 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:

Substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in different percentage of binary mixture is studied by refractometric technique. If the percentage composition of binary mixture increases refractive index increases. It observed that as the percentage composition of organic solvent binary mixture increases molar refraction and polarizability constant of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid increases. From this study, it is clear that when solute solvent interaction increases. the percentage of solvent increases. dispersion force play an important role to increase in the value of molar refraction and polarizability constant with increase in percent composition of organic solvent.

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