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Research Article

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Refractometric study of substituted aminopyrimidine in non-polar solvent

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ABSTRACT

Refractive indices of 2-Amino [4-(3-nitro phenyl)-6-phenyl-1,6-dihydro]-1,3- pyrimidine, 2-Amino [4,6-diphenyl-1,6-dihydro]-1,3- pyrimidine, 2-Amino [4-(4-hydroxy phenyl)- 6-phenyl-1,6-dihydro]-1,3-pyrimidine, and 2-Amino [4-(2-hydroxy phenyl)- 6-phenyl-1,6-dihydro]-1,3-pyrimidine have been studied in (DMF) and (1,4-dioxane) media at 27±0.1 ^{0}C. The data obtained is utilized to determine the molar refraction and polarizability constant.

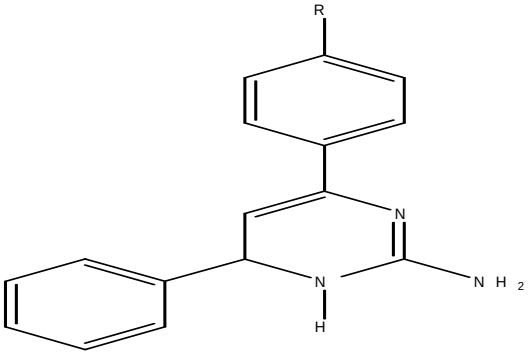
Keywords: Refractive indices, molar refraction, polarizability constant.

INTRODUCTION

The refractive index is the useful physical characteristic of liquid by means of which pure compounds are identified and with which industrial processes are monitored and controlled. The refractive index of a liquid can be easily determined to a high degree of accuracy. It is one of the important additives properties of liquid. It varies with temperature and wavelength of light used. Generally, the D-line of sodium is used for standard measurement. Instruments used for measuring refractive indices are known as refractometers. The refractive index and the dipole polarizability are fundamental electrooptical properties of matter.

Dadhichi et al[1] have investigated viscosity, refractivity index and metal ligand stability constant of substituted benzofurones in different solvents. Zhi Zhou have studied novel fiber optic refractometric method for liquid and gaseous media[2]. Kshirsagar et al have studied effect of dioxane on *N*-(4-hydroxy-6-methyl-1,3,5-triazin-2-yl)-*N*'-phenylthiocarbamide at 25°C in 60% dioxane-water system at various concentrations[3]. The refractometric study of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in different binary mixture is reported[4-5]. The refractive index of various solutions shows a linear relationship with concentration of potassium salts[6]. In the optical polymer films refractometric properties were studied[7-8]. Refractive indices of binary, ternary liquid solutions and solutions of biologically important compounds have been studied[9-10]. Refractometric measurement have been studied in of 2-chloro-4-aminophenol in ethanol-water system[11-12]. Refractive indices and molar refraction of 1, 3-diarylcarbamides in different percentage of binary liquid mixture were studied by Ubarhande et al [13]. Oswal et al[14] have studied refractivity properties of some homologues series such as nethanoate, methyl alkanoats and ethyl alkanoatesete. Sonar[15] and N.S. Pawar have studied the molar refraction and polarizability constant of substituted heterocyclic compounds in different media from refractive indices. Burghate et al[16] have studied the molar refraction and polarizabitity constant of substituted chalcones in different percentage of acetone-water mixture. Pandey et al[17] have done refractometric and dielectric study of binary liquid mixtures at different temperature. The present work deals with the study of molar refraction and polarizability constants of some substituted

aminopyrimidine drugs in same concentration of ligand in different percentages of solvent concentration. Substituted aminopyrimidine used for present work are-



Ligand A (L_A) - *2-Amino [4-(3-nitro phenyl)-6-phenyl-1,6-dihydro]-1,3- pyrimidine*
Ligand B (L_B) - *2-Amino [4,6-diphenyl-1,6-dihydro]-1,3- pyrimidine*
Ligand C (L_C) - *2-Amino [4-(4-hydroxy phenyl)- 6-phenyl-1,6-dihydro]-1,3-pyrimidine and*
Ligand D (L_D) - *2-Amino [4-(2-hydroxy phenyl)- 6-phenyl-1,6-dihydro]-1,3-pyrimidine*

EXPERIMENTAL SECTION

The refractive indices of solvent mixture and solutions were measured by Abbe's refractometer (±0.001). Initially, the refractometer was calibrated with glass piece (n=1.5220) provided with the instrument. For evaluating the molar refraction and polarizability constant of the compounds, solution of 0.01M concentration were prepared in different percentage (20%, 40%, 60%, 80%, 100%) by adding accurately weighed substituted aminopyrimidine in DMF-Water, Dioxane-Water solvent mixture at 300K. The temperature was maintained by using the thermostat. The data obtained was used to compute intermolecular interactions. The refractometric readings were taken as described in literature[18]. Carbon dioxide free double distilled water was used. The entire chemicals used are of A.R. grade. All weighing were made on one pan digital balance (petit balance AD_50B) with an accuracy of + 0.001 gm. The density of solutions were determined by a bicapillary Pyknometer (±0.2%) having a bulb volume of about 10 cm^3 and capillary having an internal diameter of 1mm and calibrated with deionised doubly distilled water. The accuracy of density measurements were within ±0.1kgm^{-3}.

RESULTS AND DISCUSSION

The molar refraction of solvent and solution are determined using Lorentz-Lorentz equation.

The molar refraction of solvent - water mixtures are determined from-

$R_{S\text{-}W} = X_1R_1 + X_2R_2$ …….(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-

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

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 is calculated as –

$R_{lig} = R_{mix} - R_{s-w}$ ……. (3)

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

$R_{lig} = 4/3\ \pi No\alpha$ ……. (4)

where, No is Avogadro's number.

Table 1: Values of molar refraction of different % of DMF- Water mixture

% of solvent mixture	Molar Refraction
20	17.0959
40	16.4094
60	15.1196
80	11.7214
100	4.5214

Table 2: The values of refractive index (n), density (gm/cm^{-3}), molar refraction (Rm) and polarizability constant (α) at 300K

Conc. in %	Constant Ligand concentration system(0.01M) with change in DMF percentage			
	Refractive index (n)	Density (d) gm/cm^3	Rmx10^3 cm^3/mole	α x10^{-23} cm^3
Ligand L_A				
20	1.357	0.9875	53.4815	2.1209
40	1.367	0.9985	60.5734	2.4021
60	1.385	1.0027	65.5396	2.5991
80	1.414	1.0137	70.5870	2.7992
100	1.424	1.0206	72.5089	2.8754
Ligand L_B				
20	1.352	0.9839	44.9957	1.7843
40	1.375	1.0042	52.0522	2.0642
60	1.391	0.9997	56.4691	2.2393
80	1.416	1.0183	59.7758	2.3705
100	1.423	1.0210	61.2622	2.4294
Ligand L_C				
20	1.356	0.9879	48.1345	1.9088
40	1.372	0.9980	55.3230	2.1939
60	1.390	0.9992	59.9828	2.3787
80	1.413	1.0258	62.7433	2.4882
100	1.422	1.0231	64.9266	2.5747
Ligand L_D				
20	1.358	0.9925	48.1532	1.9096
40	1.370	1.0061	54.6134	2.1658
60	1.395	1.0086	60.0970	2.3832
80	1.412	1.0029	64.0439	2.5397
100	1.427	1.0051	66.7783	2.6482

Table 3: Values of molar refraction of different % of Dioxane- Water mixture

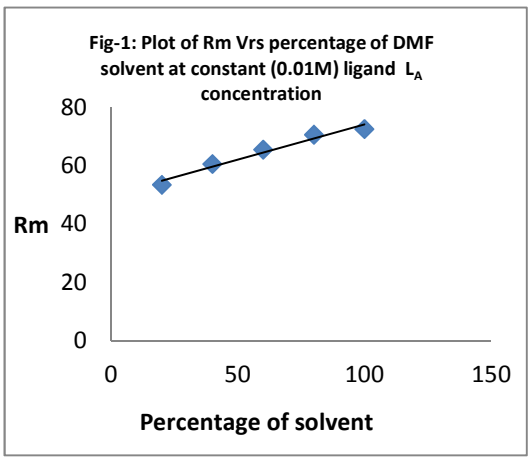
% of solvent mixture	Molar Refraction
20	19.5510
40	18.7919
60	17.1890
80	13.6509
100	4.4548

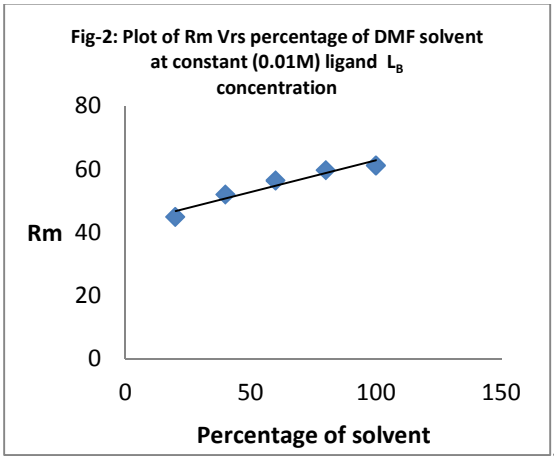
Table 4: The values of refractive index (n), density (gm/cm^{-3}), molar refraction (Rm) and polarizability constant (α) at 300K

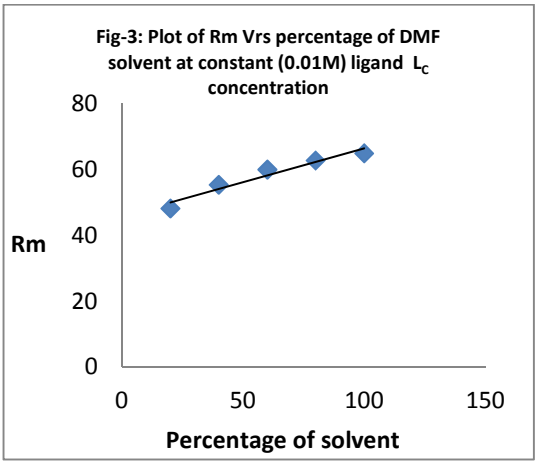
Conc. in %	Constant Ligand concentration system(0.01M) with change in Dioxane percentage			
	Refractive index (n)	Density (d) gm/cm^3	Rmx10^3 cm^3/mole	α x10^{-23} cm^3
Ligand L_A				
20	1.368	1.0605	51.2733	2.0333
40	1.371	1.0415	58.7646	2.3304
60	1.372	0.9980	64.0067	2.5383
80	1.398	0.9993	69.3133	2.7487
100	1.417	1.0011	73.0175	2.8956
Ligand L_B				
20	1.353	1.0652	41.7468	1.6555
40	1.365	1.0841	47.1634	1.8703
60	1.371	1.0022	53.8717	2.1363
80	1.377	0.9945	56.2230	2.2296
100	1.416	1.0015	61.6917	2.4465
Ligand L_C				
20	1.353	1.0600	44.6073	1.7689
40	1.355	0.9983	53.1460	2.1076
60	1.371	0.9990	57.5096	2.2806
80	1.389	0.9969	61.3783	2.4340
100	1.414	1.0007	65.4250	2.5945
Ligand L_D				
20	1.363	1.0622	45.6465	1.8102
40	1.365	0.9963	54.5973	2.1651
60	1.376	0.9977	58.2797	2.3112
80	1.390	1.0018	61.2184	2.4277
100	1.410	0.9995	64.9510	2.5757

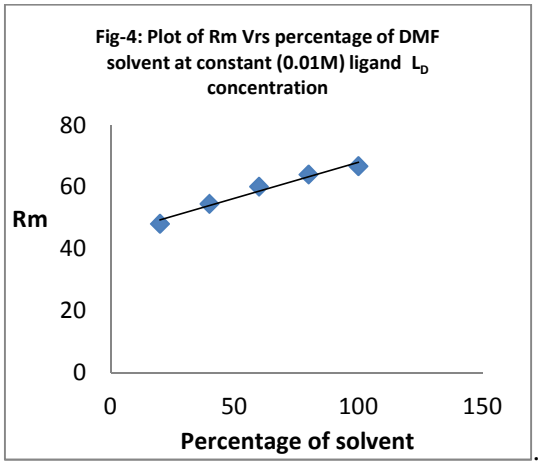
The value of molar refraction of different percent of (DMF-water) and (Dioxane -water) solvent shown in table-1and 3 respectively. From the data it is observed that value of molar refraction goes on decreasing with the decrease in amount of water in percent mixture. Molar refraction is greater in polar protic solvent(water) than polar aprotic solvent (DMF). This is due to the ability of formation hydrogen bonding of protic solvent(water).

Fig 1-5: Graphical representation of molar refraction (Rm) verses change in DMF solvent percentage at constant (0.01M) ligand concentration









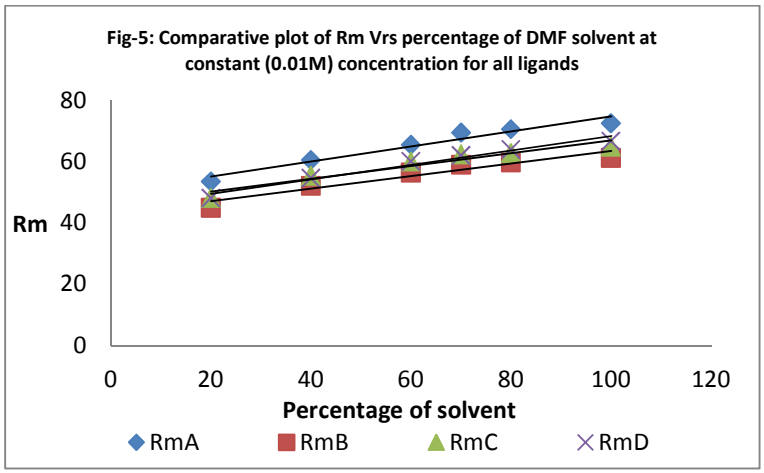
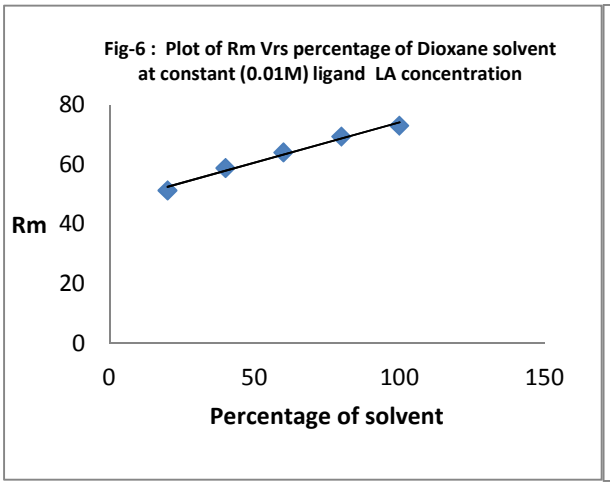
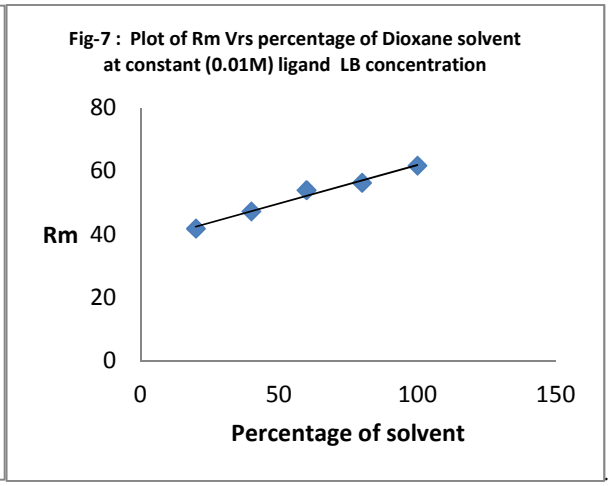
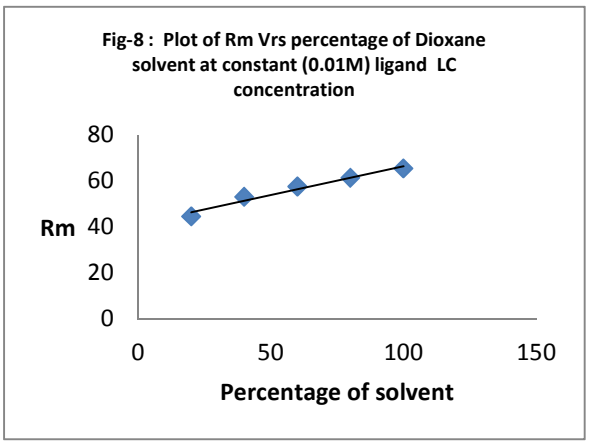
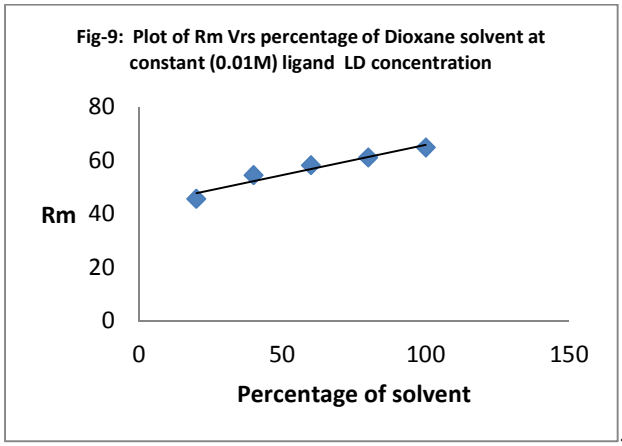


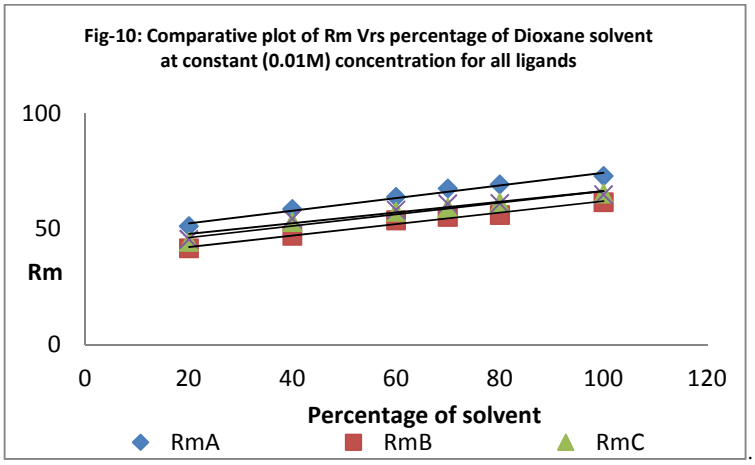
Fig 6-10: Graphical representation of molar refraction (Rm) versus change in Dioxane solvent percentage at constant (0.01M) ligand concentration.











The data of molar refraction and polarizability constant of substituted aminopyrimidine drugs having same concentration in different percentage of (DMF-water) and (Dioxane-water) solvent presented in table-2 and 4 respectively. It shows that the values of molar refraction and polarizability constant of substituted aminopyrimidine drugs increases with increase in percentage of organic solvents. This is due to fact that the dipole in substituted aminopyrimidine drugs lies perpendicular to the longer axis of molecule and with increase in percentage of solvents causing decrease in dielectric constant of medium, considerable dipole association takes place. The graph Rm verses concentration are plotted and shown in fig. 1 to 10. It is seen that there is linear relationship between molar refraction and concentration.

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