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# Refractometric study of substituted aminopyrimidine in polar solvent

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**ABSTRACT**

*Measurement of refractive index has done by Abbe's refractometer for four* substituted aminopyrimidine drugs. *From the data of refractive index and density, molar refraction ($R_m$) and polarizability constant ($\alpha$) are calculated. The values of these parameters and their variations are used to explain interactions taking place in the solution.*

**Keywords:** Refractive index, molar refraction, polarizability constant.

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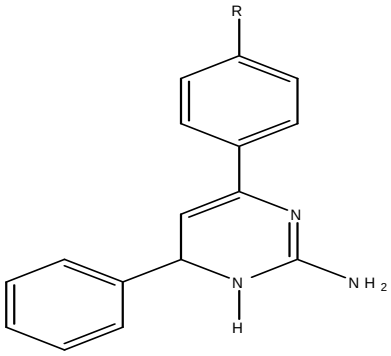
## INTRODUCTION

The refractive index is the characteristics of a given material. It is defined as the ratio of speed of light in vacuum to its speed in given material. The refractive index of a material is the most important property of any optical system that uses refraction. Refractometry is a well-established technique for the analysis of gases, liquids and solids. Recently, refractometric analysis is applied for the study of biomolecular interactions. The information regarding the transport property of the ion-solvent interactions can obtained from refractrometric measurements. These measurements provide useful information about solute-solute and solute-solvent interactions.

One of the unique and important properties of liquid is refractive index. When a ray of light passes from less dense to denser medium then there is a change in the direction of ray and angle of refraction changes and ultimately the refractive index is changed. The result obtained during this investigation directly through light on the dipole association of ligand, intermolecular attraction between solute and solvent, dielectric constant of medium, polarizability and mutual compensation of dipoles. These interactions have been studied in aqueous and non aqueous solutions by many workers[1-3]. Oswal et al[4] have studied dielectric constants and refractive indices of binary mixtures. Dadhichi et al[5] have investigated the measurement of viscosity, refractive index of substituted benzofurones in different solvents. The properties of liquid such as viscosity, refractive index and ultrasonic velocity of binary mixtures are studied by many workers[6-10]. Sengwa[11] have studied dielectric constants and refractive indices of binary mixtures. Devsarkar[12], Dhondge[13] and Pethe[14] have studied the refractive indices in mixed solvents. Wagh[15] has studied molar refraction and polarizability of 2-amino-5-chloro-benzene sulphonic acid and 2-hydroxy ethyl benzene in dioxane water and DMF-water medium respectively. The refractometric study of azomethine drugs is done[16]. The refractometric study of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in different binary mixture is reported[17-18].

The present work deals with the study of molar refraction and polarizability constants of some different substituted aminopyrimidine drugs in same concentration of ligand in different percentages of solvent concentration. Substituted aminopyrimidene 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*

## MATERIALS AND METHODS

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, the solution of 0.01M concentration were prepared in different percentage (20%, 40%, 60%, 80%, 100%) by adding accurately weighed substituted aminopyrimidine in Ethanol-Water, Methanol -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[19]. 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 ±0.1$kgm^{-3}$.

## 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-

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

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 –

$$R_{lig} = R_{mix} - R_{s-w} \quad \text{.....(3)}$$

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

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

where, No is Avogadro's number.

**Table 1: Values of molar refraction of different % of ethanol- water mixture**

| % of solvent mixture | Molar Refraction |
|---|---|
| 20 | 12.4983 |
| 40 | 11.5390 |
| 60 | 10.1181 |
| 80 | 7.8878 |
| 100 | 4.2067 |

**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 ethanol percentage | | | |
|---|---|---|---|---|
| | Refractive index (n) | Density (d) $gm/cm^3$ | Rm $x10^3$ $cm^3$/mole | α $x10^{-23}$ $cm^3$ |
| **Ligand $L_A$** | | | | |
| 20 | 1.352 | 1.0047 | 51.5675 | 2.0450 |
| 40 | 1.354 | 1.0022 | 58.0015 | 2.3001 |
| 60 | 1.356 | 1.0106 | 60.1691 | 2.3861 |
| 80 | 1.364 | 1.0096 | 62.7263 | 2.4875 |
| 100 | 1.400 | 1.1002 | 63.4006 | 2.5142 |
| **Ligand $L_B$** | | | | |
| 20 | 1.344 | 1.0040 | 42.9099 | 1.7016 |
| 40 | 1.345 | 1.0027 | 48.0154 | 1.9041 |
| 60 | 1.354 | 1.0171 | 50.3986 | 1.9986 |
| 80 | 1.416 | 1.0728 | 56.2933 | 2.2324 |
| 100 | 1.420 | 1.0070 | 61.2397 | 2.4285 |
| **Ligand $L_C$** | | | | |
| 20 | 1.352 | 1.0024 | 46.6533 | 1.8501 |
| 40 | 1.353 | 1.0033 | 52.1185 | 2.0668 |
| 60 | 1.357 | 1.0134 | 54.2338 | 2.1507 |
| 80 | 1.362 | 1.0136 | 56.0441 | 2.2225 |
| 100 | 1.364 | 1.0042 | 57.5685 | 2.2829 |
| **Ligand $L_D$** | | | | |
| 20 | 1.347 | 0.9939 | 46.4518 | 1.8421 |
| 40 | 1.349 | 1.0120 | 51.1423 | 2.0281 |
| 60 | 1.351 | 1.0107 | 53.5563 | 2.1238 |
| 80 | 1.363 | 1.0091 | 56.4308 | 2.2378 |
| 100 | 1.365 | 0.9984 | 58.0445 | 2.3018 |

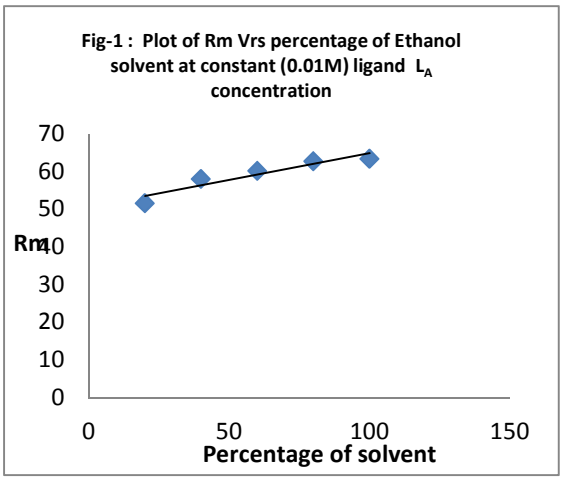
**Table 3: Values of molar refraction of different % of methanol- water mixture**

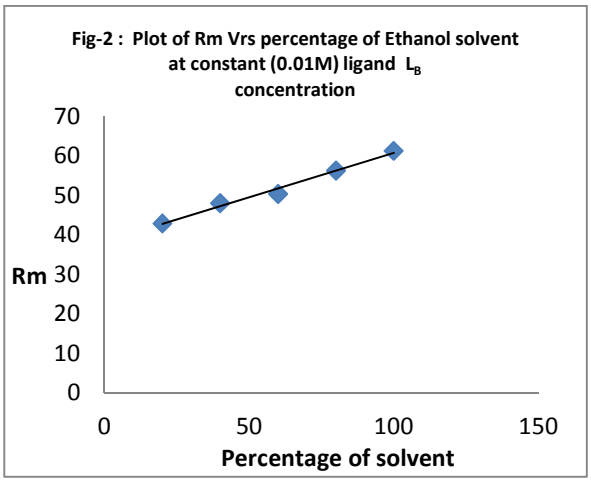
| % of solvent mixture | Molar Refraction |
|---|---|
| 20 | 8.5567 |
| 40 | 7.8236 |
| 60 | 6.8605 |
| 80 | 5.6834 |
| 100 | 4.0666 |

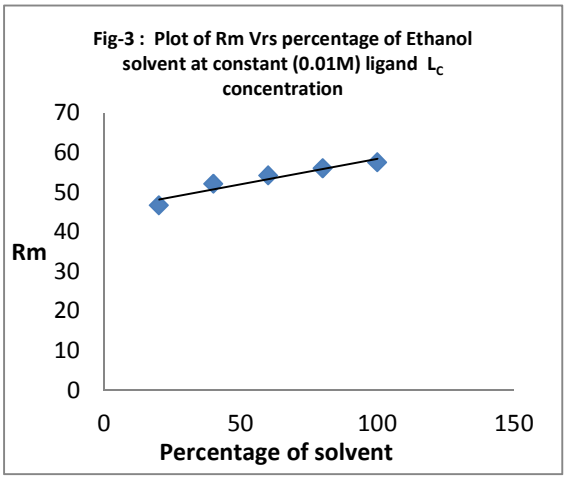
**Table 4: The values of refractive index (n), density (gm/cm$^{-3}$), molar refraction (Rm) and polarizability constant(α) at 300K**

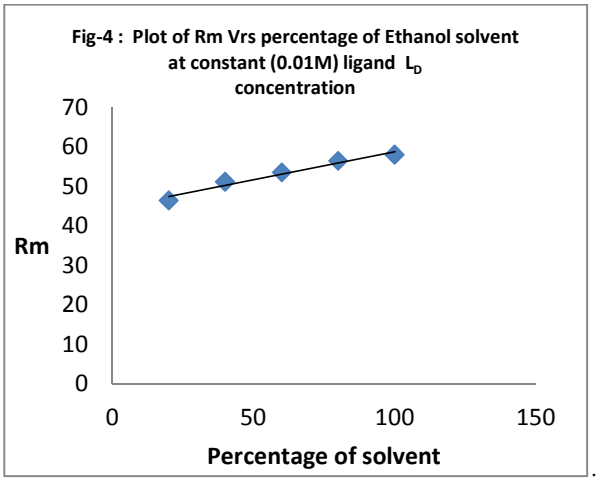
| Conc. in % | Constant ligand concentration system(0.01M) with change in methanol percentage | | | |
|---|---|---|---|---|
| | Refractive index (n) | Density(d) gm/cm$^3$ | Rm x10$^3$ cm$^3$/mole | α x10$^{-23}$ cm$^3$ |
| **Ligand $L_A$** | | | | |
| 20 | 1.311 | 0.9164 | 50.1351 | 1.9882 |
| 40 | 1.330 | 1.0058 | 53.7739 | 2.1325 |
| 60 | 1.357 | 1.0371 | 58.2540 | 2.3101 |
| 80 | 1.360 | 0.9476 | 65.5709 | 2.6003 |
| 100 | 1.410 | 1.0080 | 70.0700 | 2.7787 |
| **Ligand $L_B$** | | | | |
| 20 | 1.338 | 1.0006 | 42.0544 | 1.6677 |
| 40 | 1.341 | 1.0045 | 47.0210 | 1.8647 |
| 60 | 1.342 | 1.0428 | 47.2236 | 1.8727 |
| 80 | 1.351 | 0.9921 | 51.8562 | 2.0564 |
| 100 | 1.369 | 1.0078 | 54.0567 | 2.1437 |
| **Ligand $L_C$** | | | | |
| 20 | 1.332 | 1.0037 | 43.8588 | 1.7393 |
| 40 | 1.334 | 1.0097 | 48.8383 | 1.9367 |
| 60 | 1.338 | 1.0385 | 49.9247 | 1.9798 |
| 80 | 1.341 | 0.9758 | 54.6601 | 2.1676 |
| 100 | 1.357 | 1.0058 | 55.9608 | 2.2192 |
| **Ligand $L_D$** | | | | |
| 20 | 1.380 | 1.0104 | 49.1941 | 1.9508 |
| 40 | 1.383 | 1.0152 | 54.9356 | 2.1785 |
| 60 | 1.394 | 1.0182 | 58.4200 | 2.3167 |
| 80 | 1.410 | 1.0248 | 61.3575 | 2.4332 |
| 100 | 1.430 | 1.0289 | 64.5144 | 2.5584 |

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





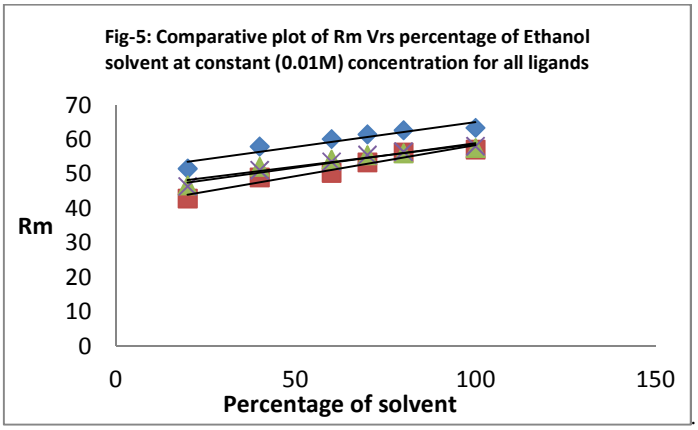
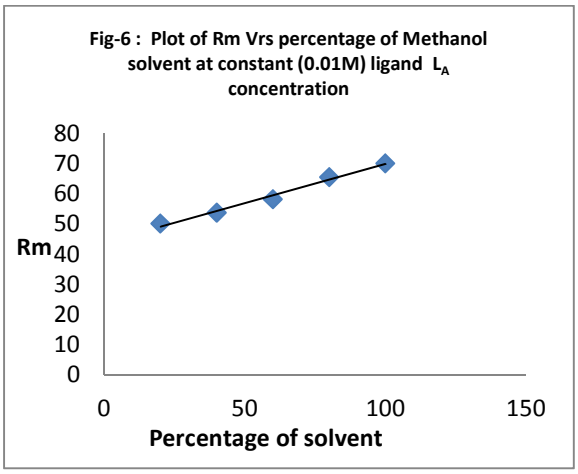
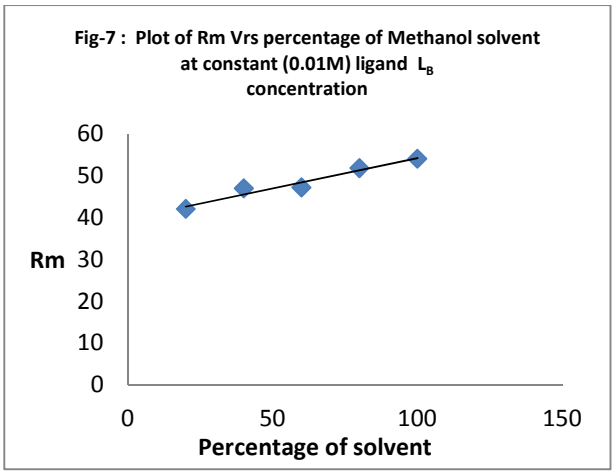
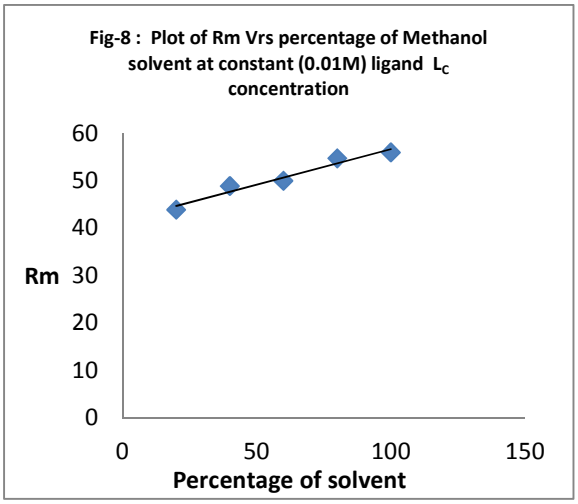
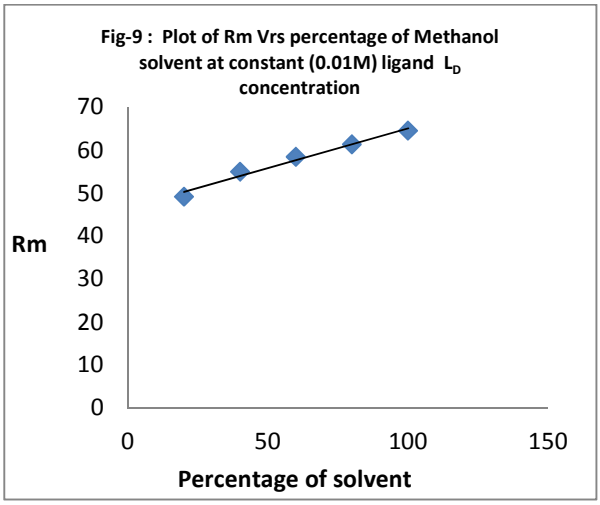



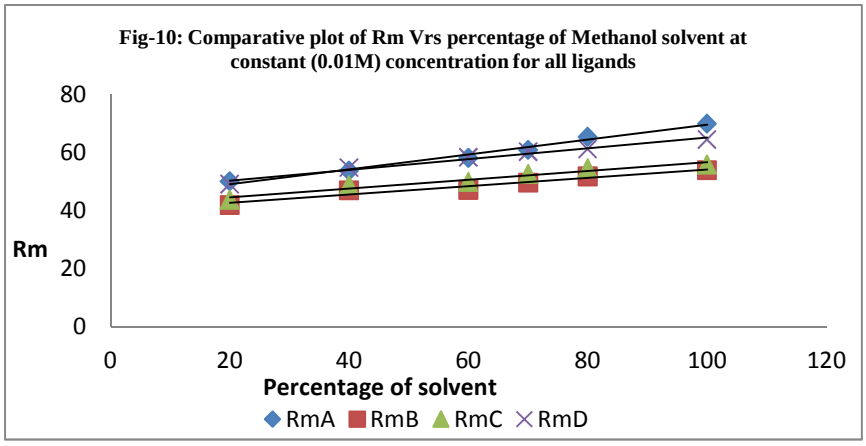

**Fig 6-10: Graphical representation of molar refraction (Rm) versus change in Methanol solvent percentage at constant (0.01M) ligand concentration**






The values of molar refraction of different percent of (Ethanol-Water) and (Methanol-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 than polar aprotic solvent. This is due to the ability of formation hydrogen bonding of protic solvent.

The data of molar refraction and polarizability constant of substituted aminopyrimidine drugs having same concentration in different percentage of (Ethanol- Water) and (Methanol -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 take place. The graphs of Rm versus concentration are plotted. These are shown in fig. 1 to 10. It is seen that there is linear relationship between molar refraction and concentration.

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