Studies of molar refraction and polarizability constant of 6-(4-chlorophenyl)-1,2,3,4-tetrahydro-2,4-dioxopyrimidine-5-carbonitrile in 60% DMSO in the temperature range 298 to 313 K

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Abstract

Objectives: The main purpose of this study is to investigate the impact of 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile in binary solution at different concentrations and valuable information on electronic polarizability and molecular interactions in the solution. Methods: 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile was synthesized and purified by recrystallization technique in laboratory. DMSO used is of analytical reagent grade (AR) of minimum assay of 99.9%. Stock solutions of 0.02 (mol L\(^{-1}\)) of compound were prepared by dissolving calculated amounts in 60% dimethyl sulphoxide solution. Solutions in various concentration ranges from 0.002 to 0.010(mol L\(^{-1}\)). The pycknometer was calibrated by measuring the densities of triple distilled water. The densities of distilled organic liquids like acetone, toluene and carbon tetrachloride were evaluated with respect to density of water. Refractive index were measured by Abbe’s Refractometer (AR-56, COSLAB) having range 1.3000 to 1.7100. The desired temperature was maintained by circulating water through refractometer. Findings: In the present work we found that density, refractive index, molar refraction and polarizability constant increases the increase in concentration due to decrease in angle of refraction or increase in angle of incidence. The decrease in density with increase in temperature is due to increase in molar volume of solvent. However, the decrease in refractive index is due to the fact that the solute-solute and solute-solvent interactions weaken with increase in temperature. This can be correlated that change in these properties changes the intermolecular attraction between solute and solvent. With increase in temperature the interaction between solute and solvent weakens and hence molar refraction and polarizability decreases. Novelty: The work incorporated with the study of molar refraction and molar polarizability of 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile...
has been not studied until now. So we wish to present the systematic measurement of refractive index of 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile in 60% DMSO in the temperature range 298 to 313 K at different concentration. From refractive index we have calculated molar refraction and molar polarizability which has provided important information regarding interactions between solute and solvent.

**Keywords:** 6-(4-chlorophenyl)-1; 2; 3; 4-tetrahydro-2; 4-dioxopyrimidine-5-carbonitrile; refractive index; molar refraction; molar polarizability

## 1 Introduction

Pyrimidines are heterocyclic compounds having various biological significance and biological activities [2-4]. The interaction of organic compounds with polar aprotic solvent is important to study physiological action, pharmacodynamics, pharmakinetic in living organism. The intermolecular interaction between solute and solvent can be studies by properties like density, viscosity, conductivity, refractive index [5-7]. Refractive index is an important additive property of molecular structure of liquid and can be measured easily with high degree of accuracy. Refractive index is property which passing of light beam through rarer to denser medium which causes bending of light toward normal in such away that ratio of Sin angle of incidence to Sin angle of refraction is constant (Snell’s Law). The extent of refraction depends on relative concentration of atom or molecules and the structure of molecule. It also gives an idea about geometry, structure of molecule. It is additive property and depends on on structural arrangement of atom in molecule. This structural arrangement in responsible for interactions in solvent medium. To understand different interactions, refractive index, molar refraction and polarizability constant of various mixtures are studied by various researchers [8-14].

## 2 Result and Discussion

The present investigation considers the density and refractive measurement of 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile in 60% binary mixtures of DMSO-water in different concentration at temperature 298 to 313 K. Use of molar refraction ($R_m$) and Polarizability constant ($\alpha$) plays an important role in studying drug interaction. They are related with intermolecular forces also. Hence, they are applicable to study drug design, QSRR and QSAR studies [15] and plays important role in modeling many molecular properties and biological activities. The results obtained are reported in the tables and respective graphical representations are shown in graphs. The molar refraction and polarizability constant for solvent and solution are determined by using Lorentz-Lorentz equation as

$$R_m = \frac{n^2 - 1}{n^2 + 2} \times \frac{M}{d} = \frac{4}{3} \pi N \alpha \tag{1}$$

Where, $n$ is the refractive index of solution, $M$ is the molecular weight of solution, $N$ is the Avogadro's constant and $\alpha$ is the polarizability constant.

The calculated values of molar refraction and polarizability constant are presented in Tables 1, 2, 3 and 4. Variation of refractive index with concentration is shown in Figure 1 by plotting graph of refractive index ($n$) verses concentration ($C$). Concentration dependence of refractive index is studied by equation

$$n = K \times C + n^0 \tag{2}$$

Where, $n$ is the refractive index of solution $K$ is the slope and $n^0$ is the intercept.
It is seen that both $R_m$ and $\alpha$ increases with increase in concentration and decreases with temperature. This shows that as temperature increases there is decrease in the polarizability which results in decrease in interaction between solute and solvent. The values of $R_m$ and $\alpha$ are higher at low concentration and low temperature. The variation of molar refraction and polarizability constant for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile with concentration at different temperature is shown in Figures 2 and 3.

It is also clearly seen that the refractive index of various solutions shows a linear relationship with concentrations. Temperature dependent quantity, specific refraction characterizes electronic polarizability of a substance. The increase value of molar refraction ($R_m$) indicates strong solute-solvent interactions. On the basis of the results of Fajan's and co-workers (16) it can be concluded that

1. The refractivity of compound is lowered by neighboring solvent molecules. It is lowered more in the presence of polar solvent molecules.
2. The combination of compound in aqueous DMSO is then accompanied by a net increase in the refractivity.
3. The close perusal of present investigation shows that there is increase in polarizability as well as molar refraction with increase in concentration. This may be due to dispersion force. It is the molecular force which arises from temporary dipole moment.

**Table 1.** Density, refractive index, molar refraction and polarizability constant for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile for different concentration at 298 K

| Conc molL$^{-1}$ | Density (d) g cm$^{-3}$ | Refractive Index (n) | Molar Refraction (R$_m$) cm$^3$ mol$^{-1}$ | Polarizability constant $\alpha \times 10^{-23}$ | n$_0$ | K (L mol$^{-1}$) |
|------------------|-----------------------|---------------------|--------------------------------|---------------------------------|------|----------------|
| 0.002            | 1.08657               | 1.4281              | 58.6145                      | 2.32330                        |      |                |
| 0.004            | 1.08697               | 1.4283              | 58.6168                      | 2.32338                        |      |                |
| 0.006            | 1.08734               | 1.4285              | 58.6208                      | 2.32354                        |      | 1.4280 0.0750  |
| 0.008            | 1.0874                | 1.4286              | 58.6295                      | 2.32388                        |      |                |
| 0.010            | 1.08755               | 1.4287              | 58.6334                      | 2.32404                        |      |                |

**Table 2.** Density, refractive index, molar refraction and polarizability constant for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile for different concentration at 303 K

| Conc molL$^{-1}$ | Density (d) g cm$^{-3}$ | Refractive Index (n) | Molar Refraction (R$_m$) cm$^3$ mol$^{-1}$ | Polarizability constant $\alpha \times 10^{-23}$ | n$_0$ | K (L mol$^{-1}$) |
|------------------|-----------------------|---------------------|--------------------------------|---------------------------------|------|----------------|
| 0.002            | 1.08473               | 1.427               | 58.5821                      | 2.32200                        |      |                |
| 0.004            | 1.0848                | 1.4271              | 58.5903                      | 2.32233                        |      |                |
| 0.006            | 1.08512               | 1.4273              | 58.5970                      | 2.32260                        |      | 1.4269 0.0656  |
| 0.008            | 1.08525               | 1.4274              | 58.6019                      | 2.32279                        |      |                |
| 0.010            | 1.08532               | 1.4275              | 58.6101                      | 2.32312                        |      |                |

**Table 3.** Density, refractive index, molar refraction and polarizability constant for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile for different concentration at 308 K

| Conc molL$^{-1}$ | Density (d) g cm$^{-3}$ | Refractive Index (n) | Molar Refraction (R$_m$) cm$^3$ mol$^{-1}$ | Polarizability constant $\alpha \times 10^{-23}$ | n$_0$ | K (L mol$^{-1}$) |
|------------------|-----------------------|---------------------|--------------------------------|---------------------------------|------|----------------|
| 0.002            | 1.08356               | 1.4262              | 58.5493                      | 2.32071                        |      |                |
| 0.004            | 1.08376               | 1.4263              | 58.5505                      | 2.32075                        |      |                |
| 0.006            | 1.08383               | 1.4265              | 58.5707                      | 2.32155                        |      | 1.4261 0.0653  |
| 0.008            | 1.08395               | 1.4266              | 58.5762                      | 2.32177                        |      |                |
| 0.010            | 1.08412               | 1.4267              | 58.5790                      | 2.32188                        |      |                |
Table 4. Density, refractive index, molar refraction and polarizability constant for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile for different concentration at 313 K

| Conc molL\(^{-1}\) | Density (d) cm\(^{-3}\) | Refractive Index (n) | Molar Refraction \((R_m)\) cm\(^3\)mol\(^{-1}\) | Polarizability constant \((\alpha) \times 10^{\text{-23}}\) | n\(_0\) | K (L mol\(^{-1}\)) |
|---------------------|-------------------------|----------------------|-----------------------------------------------|----------------------------------|-------|-----------------|
| 0.002               | 1.08156                 | 1.4252               | 58.5372                                       | 2.32023                          |
| 0.004               | 1.08175                 | 1.4253               | 58.5390                                       | 2.32030                          |
| 0.006               | 1.08193                 | 1.4254               | 58.5412                                       | 2.32038                          |
| 0.008               | 1.08205                 | 1.4256               | 58.5588                                       | 2.32108                          |
| 0.010               | 1.08223                 | 1.4257               | 58.5611                                       | 2.32117                          |

Fig 1. Variation of refractive index (n) with concentration (C) of 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile at different temperature

Fig 2. Variation of molar \((R_m)\) for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile with concentration
Fig 3. Variation of polarizability constant ($\alpha$) for 6-(4-chlorophenyl)-1, 2, 3, 4-tetrahydro-2, 4-dioxopyrimidine-5-carbonitrile with concentration

3 Conclusion

It is concluded that density and refractive measurement are strongly dependent on concentration and temperature. The increase in densities with concentration may be due to strengthening of solute-solvent interactions. Density and refractive index shows linear relationship with concentration. The increase in polarizability as well as molar refraction with increase in concentration is due to dispersion force. Increase in concentration causes enhancement in polarizability to solution due to interaction between solute and solvent. But these interactions are found to decreases with increase in temperature. This decreasing magnitude indicates weak solute-solvent interactions.

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