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Effect of change in concentration of solute and solvent on molar refraction and polarizability constant of some thiopyrimidine derivatives

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ABSTRACT

The study of substituted thiopyrimidine drugs have been investigated by measuring the densities and refractive index of different concentration solution in 70% (DMF+water) binary mixture. Also extension with this all above parameters are investigated in different composition of solvent having same concentration of ligand. It could be seen that molar refraction and polarizability constant of substituted thiopyrimidine drugs decreases with decrease in concentration of ligand in 70%(DMF+ water) solvent and increases with increase in percentage composition of solvent when ligand concentration is constant. This data have been used to determine solute-solute, solute-solvent and solvent-solvent interaction in the system.

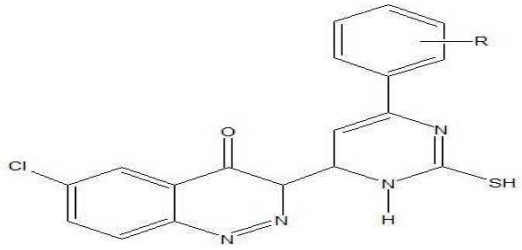
Key words: substituted thiopyrimidine drugs, molar refraction (Rm), polarizability constant (α), refractometry.

INTRODUCTION

In medicinal chemistry pyrimidine derivatives have been very well known for their therapeutic applications. Many pyrimidine derivatives have been developed as chemotherapeutic agents and are widely used. A survey of literature has shown that compounds having a pyrimidine nucleus possess a broad range of biological activities such as anticancer antiviral[1], antibacterial[2], antimalarial3], antihypertensive[4] and anti-inflammmatory activities[5-6]. So physic-chemical study of substituted thiopyrimidine has an importance.

The refractive index is an important additive property of liquid. It also depends on the structural arrangement of atom in molecule and ionic strength of solution[7]. The value of refractive index depends upon the temperature as well as the wavelength of light used. The properties of liquid such as viscosity, refractive index and ultrasonic velocity of binary mixtures are studied by many workers[8-12]. The study the refractive indices in mixed solvent has much importance[13-16]. The researcher gives more value to study additive properties such as molar refractivity and molar polarizability constant of different drugs[17-20].

The present work deals with the study of molar refraction and polarizability constant of some different substituted thiopyrimidine drugs of different concentration in 70% (DMF+water) solvent and with same concentration of ligand in different percent composition of solvent. Substituted thiopyrimidines used for present work are-



L_1: R = -H

L_2: R = -2-Choro

L_3: R = -3-Chloro

L_4: R = -3-Bromo

L_1: 6-chloro-3-(2-mercapto-6-phenyl-3,4-dihydropyrimidin-4-yl)cinnolin-4(3H)one
L_2: 6-chloro-3-(6-(2-chlorophenyl)-2-mercapto-3,4-dihydropyrimidi-4-yl) cinnolin-4(3H) one
L_3: 6-chloro-3-(6-(3-chlorophenyl)-2-mercapto-3,4-dihydropyrimidin-4-yl) cinnolin-4(3H) one
L_4: 3-(6-(3-bromophenyl)-2-mercapto-3,4-dihydropyrimidin-4-yl)-6-chlorocinnolin- 4(3H)one

MATERIALS AND METHODS

All chemicals of AR grade were used and purified by standard procedure. The ligands of which physical parameters is to be explore are synthesized by using reported protocol[21]. In the present investigation, refractive indices of liquid mixture were measured with the help of Abbe's refractometer, specially designed to measure the refractive indices of the small quantities of the transparent liquid solution ranging from 1.300 to 1.700 rapidly by direct reading. The solution of ligand in different percent composition of (DMF-water) mixture as well as in different concentration ($0.625x10^{-3}$to $10x10^{-3}$) in 70% (DMF+water) mixture were prepared by weight. All the weighing were made on one pan digital balance (petit balance AD_50B) with an accuracy of (±0.001) gm. The densities of solutions were determined by precalibrated pyknometer (± 0.1%). The constant temperature of the prism box is maintained by circulating water from thermostat at (300 ± 0.1)K.

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

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

where , R_1 and R_2 are molar refractions of DMF and water respectively.

The molar refraction of solution of ligand in DMF-water mixture are determined from-

$$RMix = \frac{(n2-1)}{(n2+2)} + \left\{\frac{[X1M1 + X2M2 + X3M3]}{d}\right\} \quad \text{.... (2)}$$

where,
n is the refractive index of solution, d is the density of solution.
X_1, X_2 and X_3 iare mole fraction of DMF, water and solute respectively.

M_1, M_2 and M_3 are molecular weights of DMF, Water and Solute respectively.

The molar refraction of ligand is calculated as –

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

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

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

where, No is Avogadro's number.

RESULTS AND DISCUSSION

Table 1: Values of Molar Refraction of Different % of DMF- Water Mixture

Percentage of DMF	[R]
20	4.9724
40	6.2842
60	8.2282
80	11.5872
100	19.0610
70	9.7189

Table 2: The values of refractive index (n) and density(d), molar refraction (Rm), polarizability constant (α) of different molar solution of ligand in 70% (DMF -Water) solvent at 300K

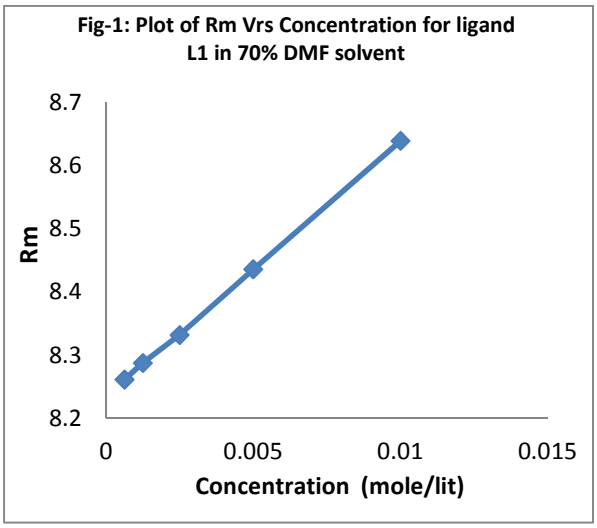
Conc in Mol/Lit	70% (DMF+ Water) system			
	Refractive index (n)	Density(d) gm/cm^3	$Rmx10^3$ cm^3/mole	$\alpha \times 10^{-24}$ cm^3
L1				
0.01	1.409	1.1263	8.6395	3.4261
0.005	1.405	1.1253	8.4361	3.3455
0.0025	1.403	1.1252	8.3319	3.3042
0.00125	1.402	1.1241	8.2876	3.2866
0.000625	1.401	1.1229	8.2610	3.2760
L2				
0.01	1.413	1.2253	8.0360	3.1868
0.005	1.409	1.2243	7.8343	3.1068
0.0025	1.407	1.2242	7.7313	3.0660
0.00125	1.406	1.2231	7.6866	3.0482
0.000625	1.405	1.2231	7.6530	3.0349
L3				
0.01	1.411	1.2246	8.0065	3.1751
0.005	1.408	1.2224	7.8296	3.1049
0.0025	1.406	1.2192	7.7467	3.0721
0.00125	1.405	1.2185	7.6989	3.0531
0.000625	1.404	1.2179	7.6687	3.0412
L4				
0.01	1.413	1.2532	7.8908	3.1292
0.005	1.410	1.2502	7.7053	3.0556
0.0025	1.406	1.2433	7.6050	3.0159
0.00125	1.404	1.2402	7.5523	2.9950
0.000625	1.403	1.2396	7.5199	2.9821

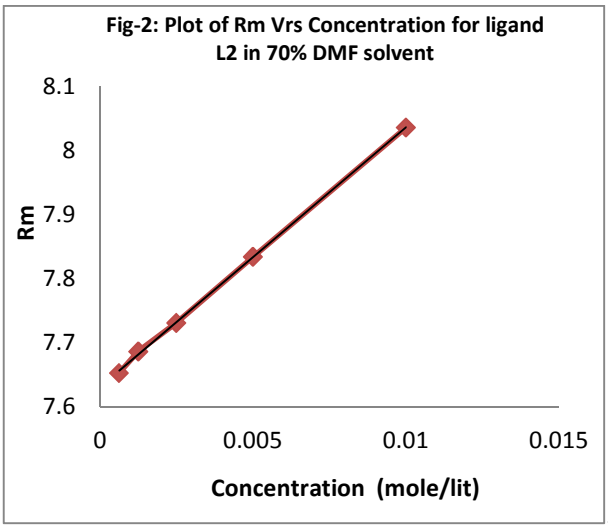
Table-1 represent values of molar refraction of pure solvent in different percent composition. It is observe that the values of molar refractivity and polarizability constant decreases with decreasing concentration of substituted thiopyrimidine drugs in 70% (DMF+ Water) solvent. The calculated value of molar refraction and molar polarizability constant for different concentration of substituted thiopyrimidine drugs in 70% (DMF+ Water) solvent shown in table-2. It could be seen that from table-2, the values of refractive index decreases with decrease in concentration of solution. As the concentration of solute decreases, distance between the molecules of solute increases. Hence refractive index, molar refraction and polarizability constant of ligand dercreses. The substituent which has less effect of polarization has greater value of molar refraction and polarizability constant than other substituent. Graphical representation are shown in fig (1 to 5).

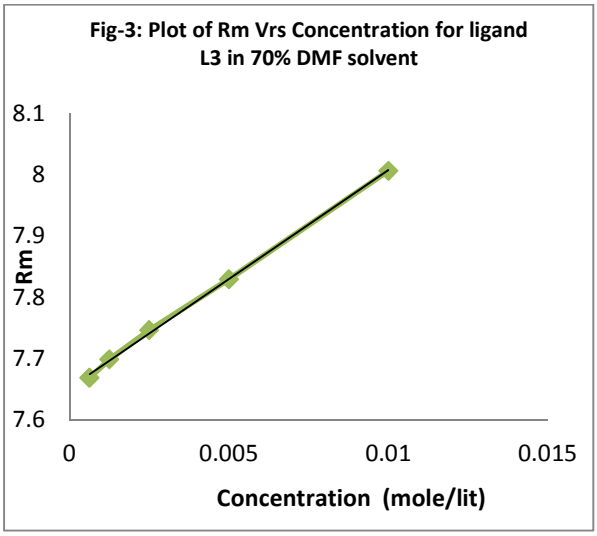
Table 3: The values of refractive index (n) and density(d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand in different percent of (DMF -Water) solvent at 300K.

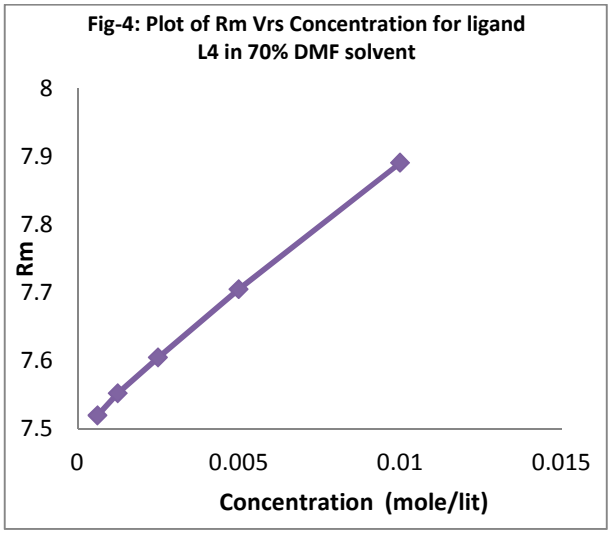
Conc in Mol/Lit	0.01M ligand system			
	Refractive index (n)	Density(d) gm/cm^3	$Rmx10^3$ cm^3/mole	α $x10^{-23}$ cm^3
L1				
20	1.361	1.0939	61.1766	2.4260
40	1.356	1.1097	66.6449	2.6429
60	1.378	1.1168	72.7905	2.8866
80	1.404	1.1396	77.2921	3.0651
100	1.441	1.1661	82.6214	3.2765
L2				
20	1.364	1.1902	61.8643	2.4533
40	1.358	1.2061	67.3457	2.6707
60	1.381	1.2122	73.8154	2.9272
80	1.408	1.2343	78.6839	3.1203
100	1.445	1.2612	84.1643	3.3377
L3				
20	1.367	1.1895	62.3612	2.4730
40	1.362	1.2055	68.0552	2.6988
60	1.386	1.2114	74.7301	2.9635
80	1.413	1.2332	79.6007	3.1567
100	1.450	1.2602	85.0497	3.3728
L4				
20	1.370	1.2105	68.4446	2.7143
40	1.365	1.2271	74.7295	2.9635
60	1.387	1.2334	81.6373	3.2374
80	1.415	1.2586	86.9299	3.4473
100	1.453	1.2887	92.8455	3.6819

Fig- 1 to 5: Graphical representation of molar refraction (Rm) verses concentration in 70% (DMF+water) solvent









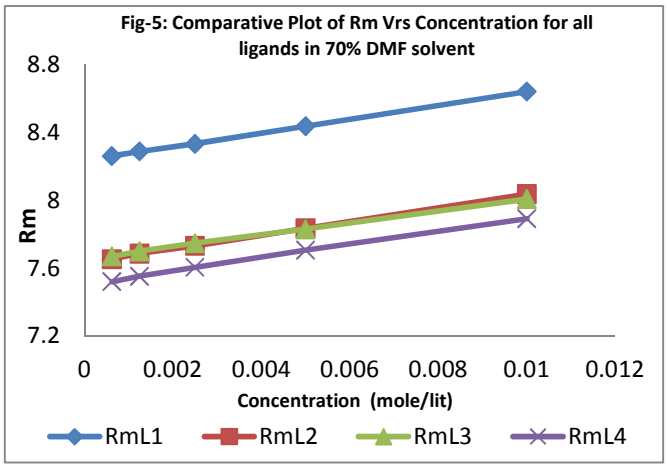
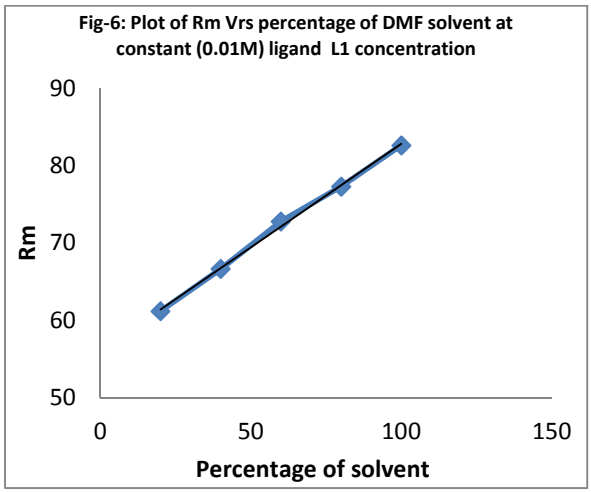
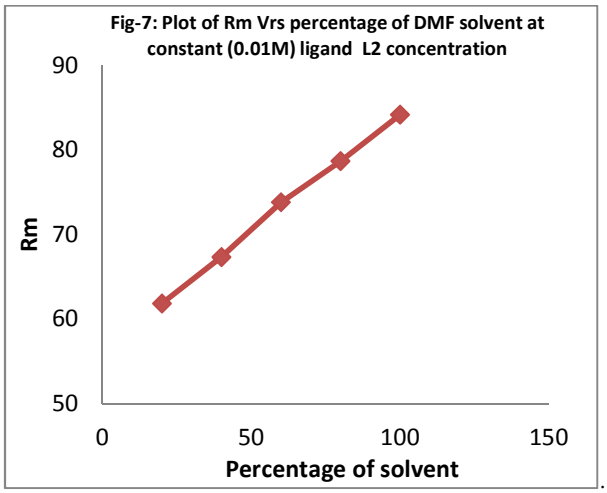
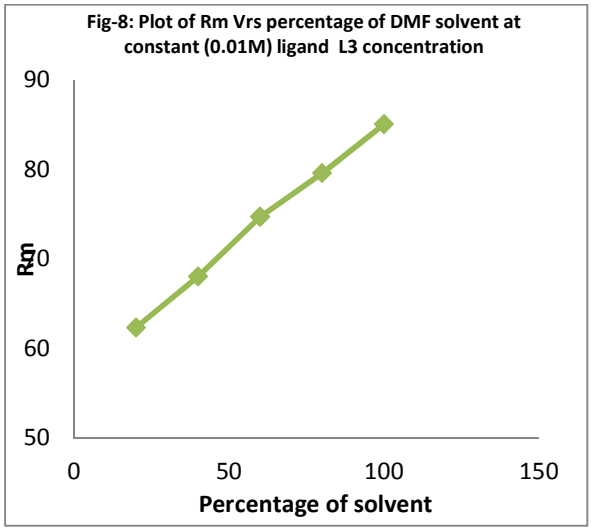
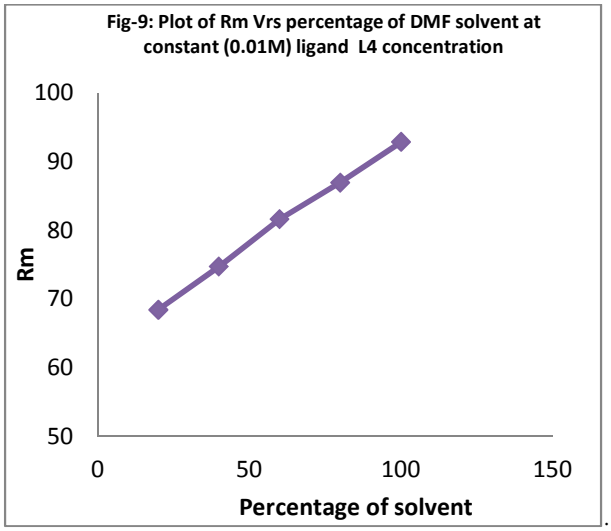


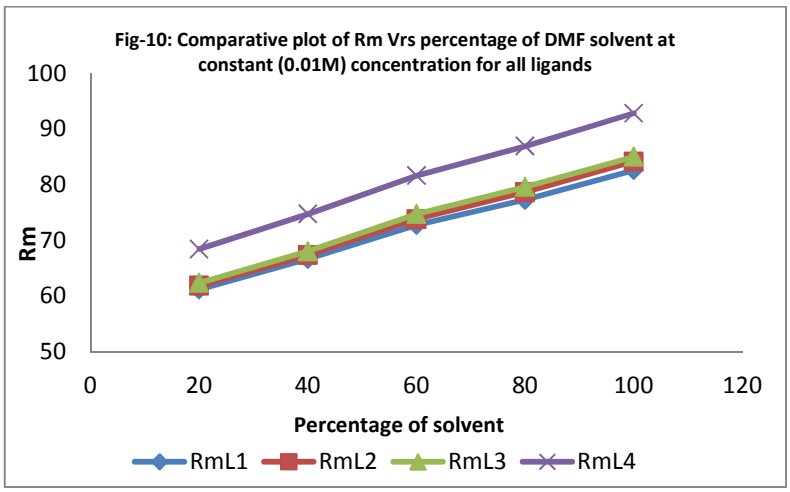
Fig- 6 to 10: Graphical representation of molar refraction (Rm) verses in different percentage of (DMF+water) solvent for constant ligand concentration (0.01M)











The values of molar refraction and polarizability constant of substituted thiopyrimidine drugs having same concentration in different percent composition of (DMF+ Water) solvent presented in table-3. It is observed that the value of molar refraction and polarizability constant of substituted thiopyrimidine drugs increases with increase in percentage of organic solvent. Mostly it depends on polarity of substituent and distance of attachment. This is due to fact that the dipole in substituted thiopyrimidine drugs lies perpendicular to the longer axis of molecule and with increase in percentage of solvent causing decrease in dielectric constant of medium and considerable dipole association take place. The graph Rm verses concentration are plotted and shown in fig. (6 to 10).

CONCLUSION

It could be seen that there is linear relationship between molar refraction and concentration. By comparing the values of refractive index of solution to that of standard curves, the concentration of solute can be determined with good accuracy. In this case we get a same trends of molar refraction and polarizability constant which depends upon polar and bulky nature of substituent. It is observed that the substance containing more polar groups normally have higher refractive index than substance containing less polar groups.

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