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Der Pharmacia Sinica, 2015, 6(8):25-30

Der Pharmacia Sinica
ISSN: 0976-8688
CODEN (USA): PSHIBD

Molecular interaction study of substituted azomethine drugs refractometrically

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ABSTRACT

The densities and refractive index of substituted azomethine drugs of different concentration in 70% (DMF+water) binary mixture has been studied. The experimental data shows that the molar refraction and polarizability constant of substituted azomethine drugs decreases with decrease in concentration of ligand in 70%(DMF+ water) solvent and increases with increase in percent of organic solvent, over a constant ligand concentration. The data helps to predict the solute-solute, solute-solvent and solvent-solvent interaction in the system.

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

INTRODUCTION

The nature and extent of molecular interactions occurring between solute and solvent molecules are best illustrated with the help of Volumetric and acoustic investigations of aqueous solutions of nonelectrolytes. Refractive index is one of the important properties of liquid. Measurement of refractive index shows very interesting applications in pharmaceutical, chemical, agriculture, food, oil and beverage industries. The most useful application of refractive index is that,it helps for the detection of an aromatic contents of liquid in pure hydrocarbons.

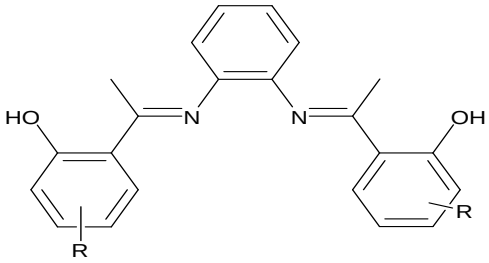
Determination of density, refractive indices of (thiamine hydrochloride + water) and (pyridoxine hydrochloride + water) at different temperatures and concentration was reported[1].

Literature survey also reveals the densities, speeds of sound, refractive indices and different derived parameters for aqueous binary mixtures of different glycol ethers at 298.15 K and one atmospheric pressure[2].The properties of liquid such as viscosity, refractive index and ultrasonic velocity of binary mixtures are studied by many workers[3]. Many researcher carried out the measurement of refractive indices in mixed solvents[4]. Determination of molar refraction and polarizability constant provide valuable information to understand molecular interaction. The properties of liquid such as refractive index in binary mixture were studied by many workers[5]. Determination of molar refraction and polarizability constant of some substituted sulphonic acid have been studied by many people[6]. Mehrotra[7], Das[8] and Kapadi[9] collectively studied the molecular interaction of an electrolyte in binary mixture of liquids. Effect of change in concentration of solute and solvent on molar refraction and polarizability constant of some thiopyrimidine derivatives was also reported[10]. Oswal[11] have studied dielectric constants and refractive indices of binary mixtures.

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. 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. Following drugs used for the present work.

L_1 *=2,2'-(benzene-1,2diylbis[nitrilo(1E)eth-1-yl-1-ylidene]-dibenzene-1,4-diol*
L_2 *= 2,2'-(benzene-1,2diylbis[nitrilo(1E)eth-1-ylidene)bis(4-nitrophenol)*
L_3=*4'4-(benzene-1,2diylbis[nitrilo(1E)eth-1-yl-1-ylidene]bis(2,-chloro phenol)*
L_4=*4'4-(benzene-1,2diylbis[nitrilo(1E)eth-1-yl-1-ylidene]bis(2,6dichloro phenol)*



Calculation

The molar refraction of solvent and solution are determined by using Lorentz-Lorentz equation. The molar refraction of different solvent, mixtures are determined from-

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

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

The molar refraction of solutions of ligand in DMF-water mixtures 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, X_1 is mole fraction of DMF, X_2 is mole fraction of water, X_3 is mole fraction of solute, M_1, M_2 and M_3 are molecular weights of DMF, water and solute respectively. d is the density of solution.

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	16.5232
40	15.3105
60	14.2711
80	11.0945
100	6.2351
70	12.0595

Table 2: Densities, refractive indices, Molar polarization (Rm) and polarizability constant(α) in 70% (DMF + Water) solvent at 303K

Conc in Mol/Lit	70% DMF+ Water system			
	Refractive index (n)	Density(d) gm/cm^3	Rm x10^3 cm^3/mole	α x10^{-24} cm^3
L1				
0.01	1.419	1.0392	9.5712	3.7956
0.005	1.412	1.0373	9.2944	3.6858
0.0025	1.405	1.033	9.1171	3.6155
0.00125	1.401	1.0302	9.0223	3.5786
0.000625	1.397	1.0281	8.9441	3.5469
L2				
0.01	1.431	1.0464	9.7976	3.8854
0.005	1.421	1.0439	9.4393	3.7433
0.0025	1.412	1.0408	9.1996	3.6483
0.00125	1.407	1.0374	9.0864	3.6034
0.000625	1.401	1.033	8.9841	3.5628
L3				
0.01	1.421	1.0523	9.5255	3.7775
0.005	1.415	1.0498	9.2593	3.6719
0.0025	1.409	1.0475	9.0775	3.5998
0.00125	1.405	1.0457	8.9729	3.5583
0.000625	1.402	1.0431	8.9156	3.5356
L4				
0.01	1.423	1.0655	9.5479	3.7864
0.005	1.413	1.0548	9.1579	3.6317
0.0025	1.406	1.0527	9.9437	3.5468
0.00125	1.399	1.0501	9.9807	3.4821
0.000625	1.393	1.0478	9.6892	3.4458

Table-1 represents the 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 decrease in concentration of water in volatile solvent DMF.

From table 2, it is observed that, molar refraction(Rm) and polarizability constant(α) of substituted azomethine drugs(0.01M) in 70% (DMF+ Water) solvent decreases with increase in percentage of DMF mixture. The decreasing order of molar refraction for different ligands are $L_2 > L_1 > L_4 > L_3$.

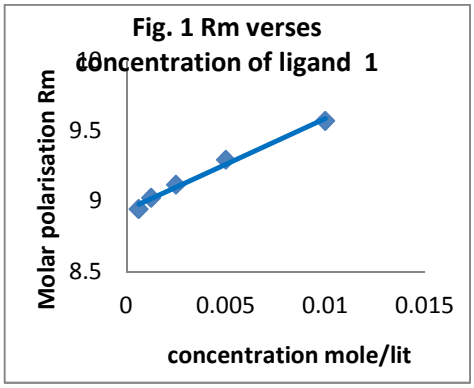
It could be seen from table-3 that, the values of refractive index, densities, molar refraction and polarizability constant increases with increase in amount of pure volatile solvent. The decreasing order of molar refraction for different ligand are $L_4 > L_2 > L_3 > L_1$.

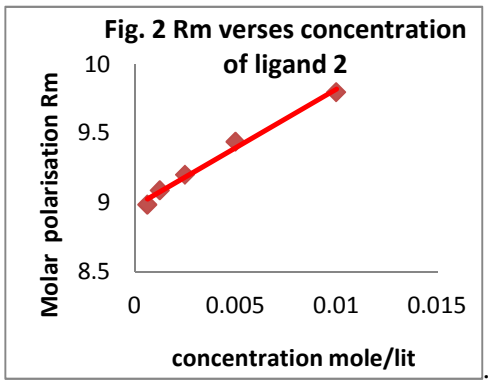
Graphical representation of molar refraction Vs change in concentration of drug are shown in fig (1 to 5). The values of molar refraction and polarizability constant of substituted azomethine drugs increases with increase in change in concentration of drugs. Fig (6 to 10) represent plot of percent composition Vs molar refraction.

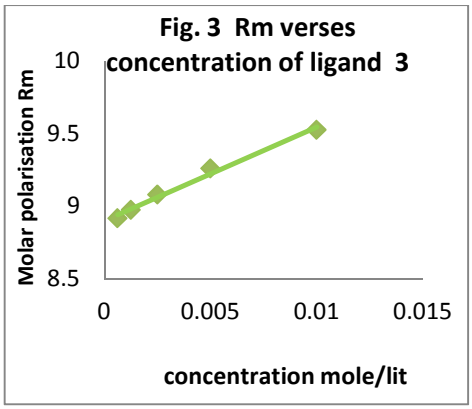
Table 3: Densities, refractive indices, Molar polarization (Rm) and polarizability constant(α) of 0.01M ligands in different DMF at 303K

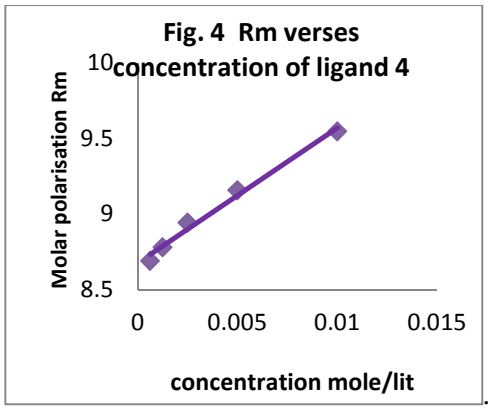
Conc in %	DMF+ Water system			
	Refractive index (n)	Density (d) gm/cm^3	Rm x10^3 cm^3/mole	α x10^{-23} cm^3
L1				
20	1.365	1.0241	68.4143	2.7131
40	1.375	1.0277	76.8523	3.0477
60	1.387	1.0310	82.0755	3.2548
80	1.399	1.0339	85.8895	3.4061
100	1.423	1.0362	91.3938	3.6244
L2				
20	1.372	1.0072	80.1483	3.1784
40	1.381	1.0176	89.7146	3.5578
60	1.389	1.0237	95.7871	3.7986
80	1.413	1.0278	102.7618	4.0752
100	1.436	1.0313	108.7893	4.3142
L3				
20	1.383	1.0093	78.165	3.0997
40	1.385	1.0130	87.6158	4.0364
60	1.392	1.0231	91.8471	4.2786
80	1.416	1.0267	98.5262	4575
100	1.432	1.0310	101.9107	4.7239
L4				
20	1.387	10109	89.8924	3.5648
40	1.391	1.0195	101.78	4.0364
60	1.395	1.0232	107.89	4.2786
80	1.418	1.0276	115.36	4.575
100	1.437	1.035	119.12	4.7239

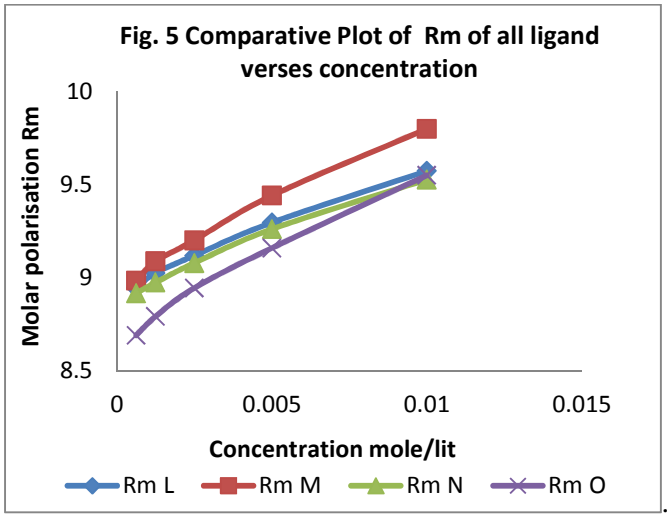
Graphical representation of molar polarization (Rm) of all ligand verses change in concentration in 70% DMF solvent



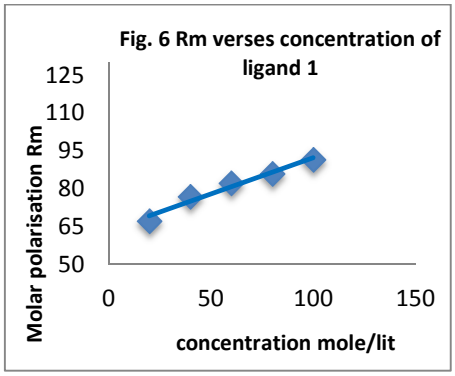


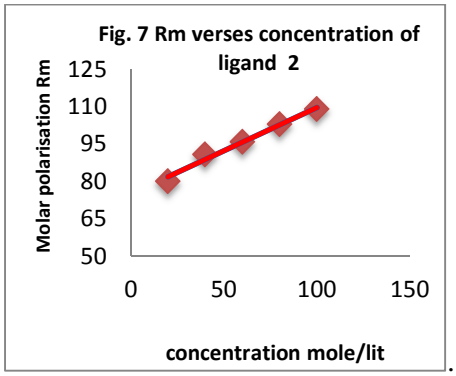


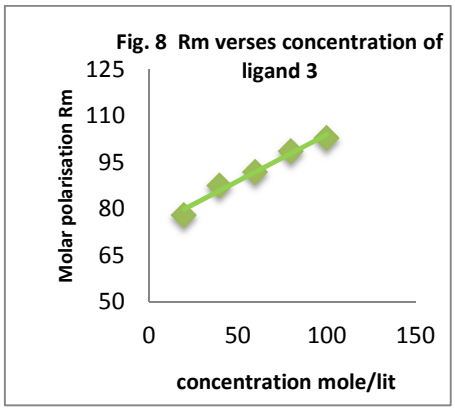


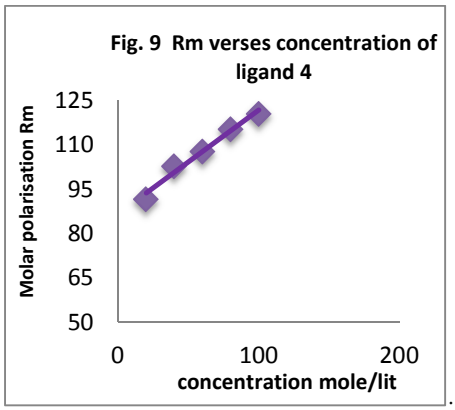


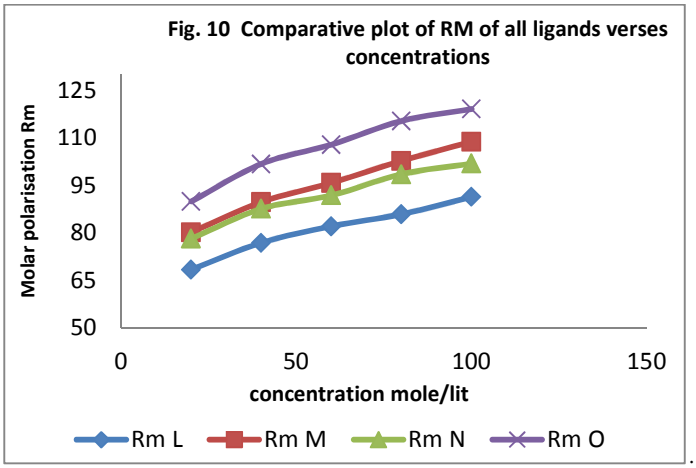
Graphical representation of molar polarization (Rm) of all ligand at 0.01M verses concentration in different percentage of DMF solvent











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