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Der Pharmacia Lettre, 2016, 8 (15):16-21
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ISSN 0975-5071
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Refractometric study of substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives in different binary mixtures

P. P. Choudhari[1], H. S. Chandak[2] and M. P. Wadekar[1*]

[1]Applied Chemistry Division, Govt. Vidarbha Institute of Science and Humanities, Amravati, (MS), India
[2]Dept. of Chemistry, G. S. Science, Arts and Commerce College, Khamgaon(M.S.)

ABSTRACT

Refractometric study of substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives is done in different binary mixture. Measurement of refractive index is done using Abbe's refractometer. Molar refractions and polarizability constants are determined by using experimental data. The parameters obtained are used to determine molecular interaction between solutes and solvents.

Keywords: Substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives, molar refraction (Rm) and polarizability constant (α).

INTRODUCTION

Refractive index is useful for qualitative analysis of substances because each substance has constant and unique refractive index that can be determined with great accuracy. Density and refraction index are two physical properties easy to measure and can be used to characterize an ionic liquid mixture[1].Refractometric technique is considered as an important tool for the measurement of glucose concentrations in body fluids such as blood and the intercellular fluid[2]. Density and refractive index of compound is one of the important additives properties[3]. The refractometric method widely used as field methods to assess antimalarial drug quality[4]. Refractometric study is reported for the S-trizinothiocarbamides in dioxane-water[5]. The refractometric properties have very important role in medicinal and drug chemistry[6]. Many researchers have reported the refractive indices in mixed solvents[7-8]. Dielectric constants and refractive indices of binary mixtures are studied[9]. Refractometric measurement of N-(4-hydroxy-6-methyl-1, 3, 5-triazin-2-yl)-N'-phenylthiocarbamide at 298K in 60% dioxane-water system at various concentration have reported[10]. Density and refractive index are studied for n-ethanoate, methyl alkanoates and ethyl alkanoates[11]. Refractometric study of binary liquid mixture of eucalyptol with hydrocarbon at different temperature is done[12]. Refractometric measurement has done for binary mixture of bromoalkane and non polar hydrocarbons[13]. Molar refraction and polarizability constant of some substituted sulphonic acid at different concentration and different percentage of organic solvent-water mixtures have studied[14-16]. Refractometric study of substituted aminopyrimidine in non-polar solvent is reported[17]. Molar refraction and polarizability constant are studied for substituted heterocyclic compounds in different media[18]. Refractive index, molar polarizability constant and molar refractivity of lisinopril have studied in acetone, DMF, methanol, ethanol, THF and dioxane media in different concentrations[19]. The refractometric study of substituted aminopyrimidine in polar solvents is performed[20].

Refractometric study of substituted N, N'-bis(salicyliden) arylmethanediamine in different binary mixture is reported[21]. Refractive index and densities of oxalate salts have studied at 298.15K[22]. Molar refractions have studied for aqueous solution of KCl and $KBrO_3$ at different temperature[23]. Refractometric study of some substituted oxoimidazoline drugs in different concentration of solute and solvents is reported[24].

The present work deals with the study of molar refraction and polarizability constant of following substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives in 1, 4-dioxane and ethanol (with different percentage) is done.
Ligand(L_A) = N-[(E)-1-(5-bromo-2-hydroxy-phenyl)ethylideneamino]-2-oxo chromene-3-carboxamide
Ligand (L_B) = N-[(E)-1-(5-chloro-2-hydroxy-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide
Ligand(L_C) = N-[(E)-1-(3,5-dichloro-2-hydroxy-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide
Ligand (L_D) = N-[(E)-1-(2-hydroxy-5-methyl-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide

MATERIALS AND METHODS

The refractive indices of solution and solvent mixture under investigation are determined using Abbe's refractometer and density of solution is measured using 10ml specific gravity bottle. The accuracy of Abbe's refractometer is within ± 0.001 units. Initially, the refractometer is calibrated with glass piece (n=1.5220) provided with instrument. The constant temperature of the prism box is maintained by circulating water from thermostat at 32 ± 0.1°C. All weighings are made on one pan digital balance with an accuracy of ± 0.001 gm. The ligands of which physical parameters are to be explored are synthesized by using reported protocol[25]. The solutions of compounds under study are prepared in 1, 4-dioxane and ethanol by keeping constant ligand concentration system (0.01M). All chemical used are of A.R. grade.

RESULTS AND DISCUSSION

It is important to know the refractive index of a solute. This index can be derived from the refractive indices of solution and solvent on using a suitable mixture rule[26]. The molar refraction of solvent, solution can be determined by following equation[27].

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

Where, R_1 and R_2 are molar refractions of solvent and water respectively.

The molar refraction[28-30] of solutions of ligand in solvent-water mixtures are determined from-

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

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 can be calculated as –
$$R_{lig} = R_{Mix} - R_{SOL\text{-}W} \quad (3)$$

The polarizability constant (α)[31-32] of ligand can be calculated from following relation-
$$R_{lig} = 4/3\ \pi N o \alpha \quad (4)$$

Where, No is Avogadro's number.

In the present study the value of molar refraction and polarizability constant of substituted 2-oxo-2-H-chromene-3-carbohydrazide in various percentage (20%, 40%, 60%, 80%, 100%) of different solvent mixture at temperature 305K are reported. The experimental data shows that there is increased in refractive index with increase in percentage composition of solvent. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution.

Table-1: Values of molar refraction of different % of solvent mixture

% of solvent mixture	Molar refraction [R]	
	Ethanol	Dioxane
20	12.4928	19.7541
40	11.5217	18.2147
60	10.0924	17.8347
80	7.8247	13.0578
100	4.3458	4.4937

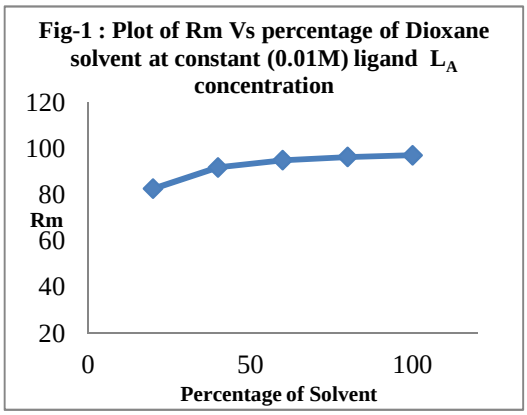
Table- 2: Values of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) at 305K

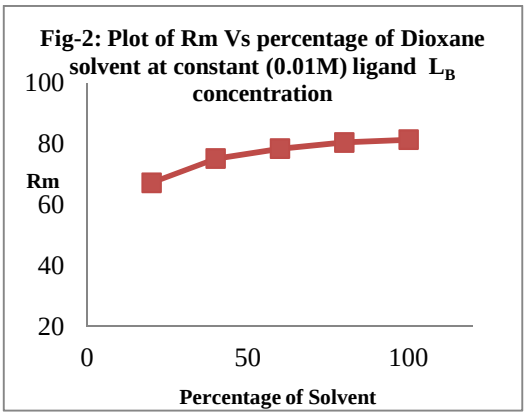
Conc. In %	Constant ligand concentration system (0.01M) with change in Dioxane percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x 10^3 cm^3/mol	α x 10^{-23} cm^3
Ligand L_A				
20	1.415	1.0037	81.9109	3.2483
40	1.417	1.0091	91.6260	3.6336
60	1.418	1.0147	95.1488	3.7733
80	1.420	1.0196	97.1368	3.8521
100	1.421	1.0225	98.3331	3.8995
Ligand L_B				
20	1.410	1.0751	67.2530	2.6670
40	1.414	1.0853	75.1901	2.9818
60	1.417	1.0909	78.4190	3.1098
80	1.420	1.0929	80.4572	3.1906
100	1.421	1.0967	81.3890	3.2276
Ligand L_C				
20	1.412	1.0737	73.8263	2.9277
40	1.415	1.0865	82.2157	3.2604
60	1.417	1.0870	85.9819	3.4097
80	1.418	1.0900	87.7742	3.4808
100	1.419	1.0936	88.8198	3.5223
Ligand L_D				
20	1.412	1.0417	66.0243	2.6183
40	1.418	1.0574	73.6892	2.9222
60	1.423	1.0592	77.4297	3.0706
80	1.425	1.0685	78.7177	3.1217
100	1.426	1.0722	79.6250	3.1576

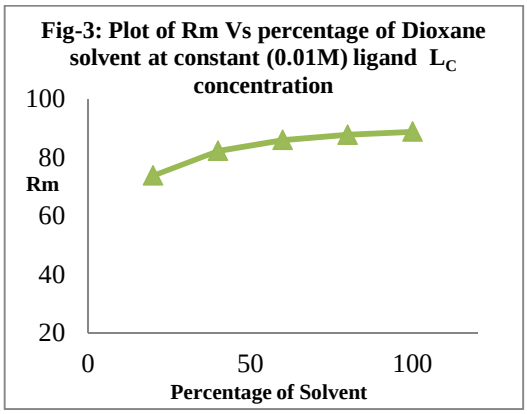
Table-3: Values of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) at 305K

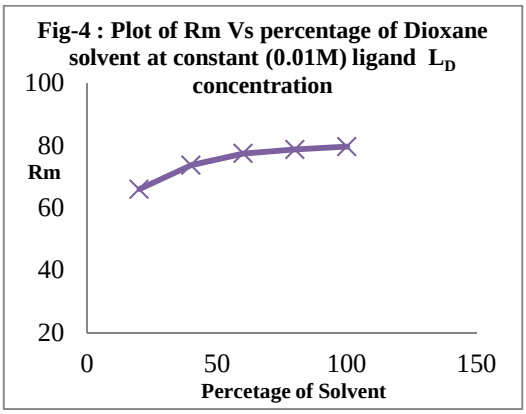
Conc. In %	Constant ligand concentration system (0.01M) with change in Ethanol percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x 10^3 cm^3/mol	α x 10^{-23} cm^3
Ligand L_A				
20	1.349	1.0018	69.7461	2.7659
40	1.373	1.0060	82.4831	3.2710
60	1.393	1.0080	89.8184	3.5619
80	1.401	1.0115	93.0655	3.6907
100	1.411	1.0133	96.1714	3.8139
Ligand L_B				
20	1.362	1.0090	63.6147	2.5228
40	1.371	1.0136	72.3642	2.8697
60	1.384	1.0240	76.9155	3.0502
80	1.398	1.0311	80.5151	3.1930
100	1.408	1.0424	82.4605	3.2701
Ligand L_C				
20	1.368	1.0522	67.5842	2.6802
40	1.371	1.0592	75.6441	2.9998
60	1.386	1.0735	80.5270	3.1935
80	1.405	1.0762	85.5982	3.3946
100	1.412	1.0836	87.4220	3.4669
Ligand L_D				
20	1.367	1.0131	60.7555	2.4098
40	1.373	1.0171	68.6115	2.7209
60	1.388	1.0262	73.3302	2.9080
80	1.402	1.0282	77.1145	3.0581
100	1.406	1.0499	77.1662	3.0602

Fig. 1 to 5: Graphical representation of molar refraction (Rm) versus change in Dioxane solvent percentage at constant (0.01M) ligand concentration









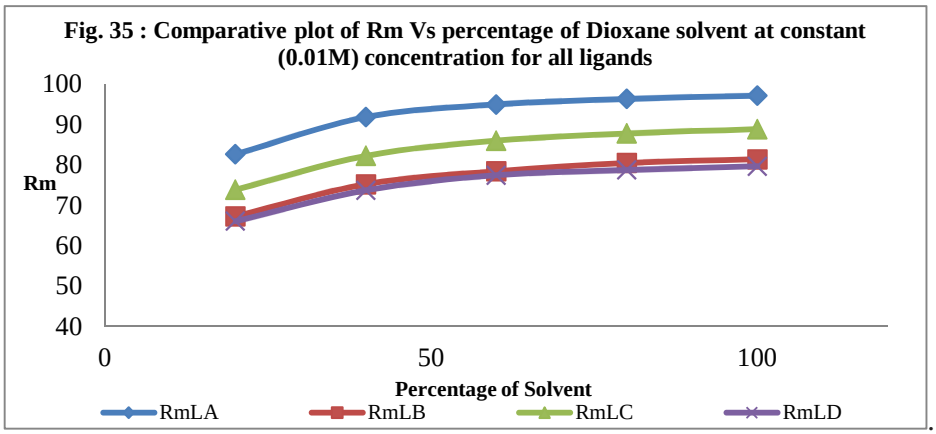
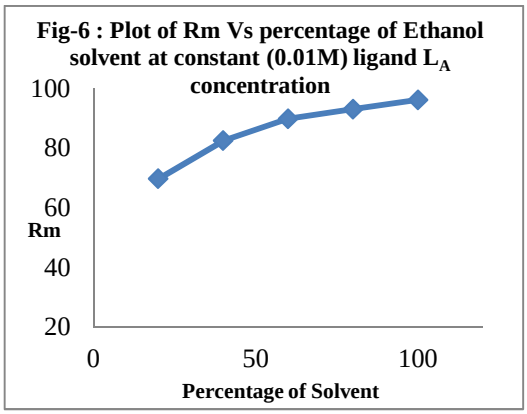
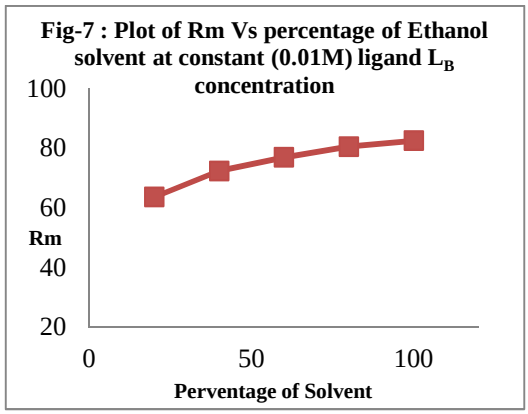
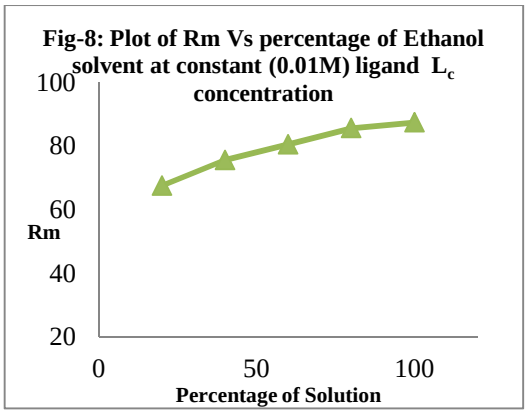
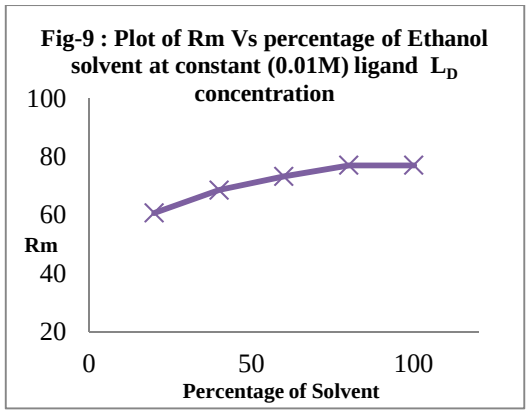


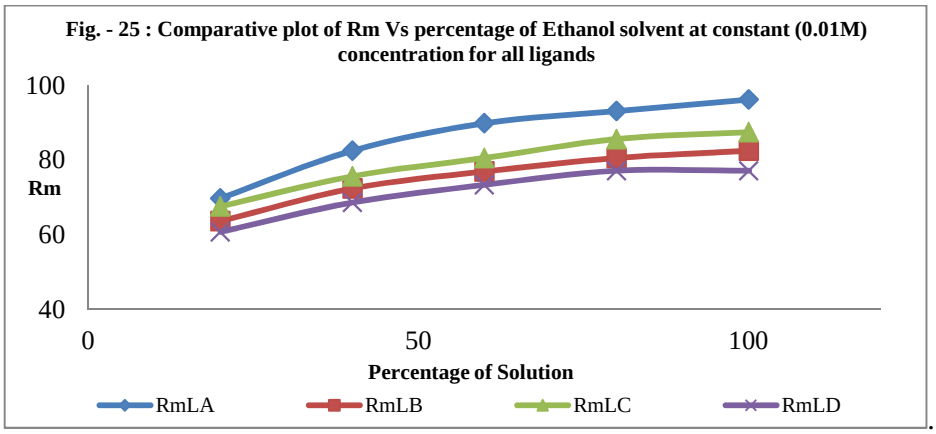
Fig. 6 to 10: Graphical representation of molar refraction (Rm) versus change in Ethanol solvent percentage at constant (0.01M) ligand concentration











The refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) of substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives in different percentage of solvent are presented in table no. 2 and 3. It observed that the values of molar refraction and polarizability constant increases with increase in percentage of organic solvent. The graphs of molar refraction (Rm) versus different percentage compositions of organic solvent are plotted. These are shown in fig. no. 1 to 10. From this it is observe that there is linear relationship between molar refraction and concentration. It is observed that molar refraction increases linearly as the percentage composition of organic solvent increases. This is attributed to the dispersion force and it is the molecular force which arises from temporary dipole moment. The cumulative dipole-dipole interaction creates weak dispersion force resulting in increase in molar refraction and polarizability constant.

Acknowledgement
The authors gratefully acknowledge The Director; Head, Department of Chemistry, Govt. Vidarbha Institute of Science and Humanities, Amravati for providing necessary facilities and help when needed for the work.

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