Journal of Chemical, Biological and Physical Sciences

An International Peer Review E-3 Journal of Sciences

*Available online at*www.jcbsc.org

Section C: Physical Sciences

CODEN (USA): JCBPAT Research Article

Refractive index, density, molar refraction and polarizability constant of substituted 2-oxo-2*H*-chromene-3-carbohydrazide derivatives in different binary mixture

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Received: 25 October 2016; **Revised:** 04 November 2016**; Accepted:** 08 November 2016

Abstract: Refractive index of substituted 2-oxo-2H-chromene-3-carbohydrazide derivatives are determined by using Abbe's refractometer. From the data of refractive index and density, molar refraction (Rm) and polarizability constant (a) are calculated. The calculated data is used to study the solute-solute, solute-solvent and solvent-solvent interaction in the system

Keywords: 2-oxo-2H-chromene-3-carbohydrazide derivatives, Abbe's refractometer, Molar refraction (Rm), Polarizability constant (α).

INTRODUCTION

Measurement of refractive index shows various applications in chemical, food, pharmaceutical, agriculture, oil and beverage industries. Refractive index of substituted benzofurones in different solvents have investigated[1].The measurement of refractive indices in mixed solvent are helpful to understand the molecular interaction in the components of mixture[2-4].Refractometric study gives useful information about solute solvent interaction in binary liquid mixtures at different temperatures[5].Determination of molar refraction and polarizability constant provide valuable information to understand molecular interactions in binary mixtures[6-9].

Polarizability constant and molar refraction of some substituted sulphonic acid have reported[10-11].Refractometric study of substituted heterocyclic compounds such as 5-ethoxycarbonyl-4-(4-bromo-phenyl)-6-methyl-3, 4-dihydropyrimidine-2-(1H)one, 5-ethoxy carbonyl-4-(4-nitro-phenyl)-6-methyl-3, 4-dihydropyrimidine-2-(1H)one have done in dioxane, ethanol, THF and DMF at 303K and different concentration[12]. Molar refraction and polarizability constant have studied for 2-hydroxy-5-ethyl-benzene and 2-amino-5-chloro-benzene sulphonic acid in dioxane-water and DMF-water medium respectively[13]. Determination of molar refraction and polarizability constant is done for some substituted azomethine drugs[14].The refractive index is studied for phenols in carbon tetrachloride, benzene and acetone[15]. Density and refraction index measurements have done for 2-chloro-4-amino phenol in ethanol-water system[16]. Molecular interactions in different media of substituted thiazolylschiff's bases have reported[17].

Additive properties such as molar refractivity and molar polarizability constant have studied for allopurinal, acenocoumarol, warfarin and amoxicillin in different solvents[18].The molecular interaction of an electrolyte in binary mixture of liquids are studied by refractometric technique[19-21]. Densities and refractive indices of binary, ternary liquid solutions of biologically important compounds have studied[22]. Refractive index measurement for the solutions of four derivatives of substituted 2, 3-dihydroquinazolin-4(1*H*)-ones are reported[23].The refratometric study of some schiff base complexes with metals Co, Cu and Ni is reported[24]. Molar refraction (Rm) and polarizability constant (α) have studied for substituted N, N'-bis (salicyliden)-arylmethanediamine[25]. Solute solvent interaction for 2-hydroxyl-5-methyl-4-methoxy chalcone is reported[26]. Refractometric measurement is reported for1, 3-diaryl carbamides in different percentage of binary liquid mixture[27]. Molar refraction (Rm) and polarizability constant (α) of different substituted hydrazone are determined[28]. Interaction between N-butyl bromide and six binary mixtures of aniline, carbon tetrachloride, benzene, xylene, toluene and n-heptane for the entire concentration range is studied at 303.15 K[29].

The present work deals with the study of molar refraction and polarizability constant of following 2-oxo-2*H*-chromene-3-carbohydrazide derivatives in non-aqueous solvent such as acetone, DMSO and DMF (with different percentage).

1. ***Ligand(L_A)=N-[(E)-1-(5-bromo-2-hydroxy-phenyl) ethylideneamino]-2-oxo-chromene-3-carboxamide***
2. ***Ligand(L_B)=N-[(E)-1-(5-chloro-2-hydroxy-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide***
3. ***Ligand (L_C) = N-[(E)-1-(3, 5-dichloro-2-hydroxy-phenyl) ethylideneamino]-2-oxo-chromene-3-carboxamide.***
4. ***Ligand(L_D)=N-[(E)-1-(2-hydroxy-5-methyl-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide***

EXPERIMENTAL

The refractive indices of solution and solvent mixture under study are determined using Abbe's refractometer. Density of solutions is measured using 10mlspecific gravity bottle. Initially the refractometer is calibrated with glass piece (n=1.5220) provided with instrument. All weighing are done on one pan digital balance with an accuracy of ± 0.001 gm. The accuracy of Abbe's refractometer is within ± 0.001 units. The constant temperature of the prism box is maintained by circulating water from thermostat at 32 ± 0.1°C. The ligands of which physical parameters are to

be explored are synthesized by using reported protocol[30]. The solutions of compounds under study are prepared in different solvents acetone, DMSO and DMF by keeping constant ligand concentration system (0.01M). All chemical used are of A.R. grade.

RESULTS AND DISCUSSION

It is important to know refractive index of the solute. This index can be derived from the refractive indices of solution and solvent by using a suitable mixture rule[31]. The molar refraction of solvent, solution can be determined by following equation[32].

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

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

The molar refraction[33-35] 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)[36-37] of ligand can be calculated from following relation-

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

Where, No is Avogadro's number.

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

% of solvent mixture	Molar refraction [R]		
	Acetone	DMSO	DMF
20	11.6076	16.0523	17.1127
40	10.9057	15.2511	16.4094
60	9.7286	12.7181	14.8109
80	7.8921	10.1420	11.7934
100	4.1917	7.8523	4.4403

In the present investigation the value of molar refraction and polarizability constant of substituted 2-oxo-2*H*-chromene-3-carbohydrazide in various percentage of different solvent mixture at temperature 305K are reported. The experimental data shows that there is decrease in refractive index with decrease in percentage composition of solvent. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution under study.

The data of refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) of substituted 2-oxo-2*H*-chromene-3-carbohydrazide in different percentage of solvent is presented in

table no. 1 to 4. It is 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 15. From this it is observe that there is linear relationship between molar refraction and concentration. It shows 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.

Table- 2: The data of refractive index (n), density (d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of acetone solvent at 305K.

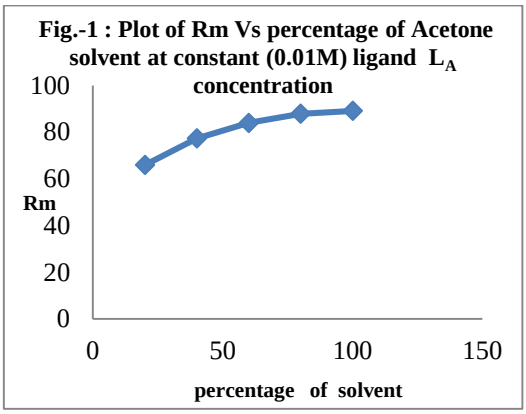
Conc. In %	Constant ligand concentration system (0.01M) with change in Acetone percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x10^3 cm^3/mol	α x10-23 cm^3
Ligand L_A				
20	1.351	1.0681	65.9968	2.6172
40	1.373	1.0776	77.3192	3.0662
60	1.393	1.0827	83.9842	3.3306
80	1.405	1.0851	87.8968	3.4857
100	1.407	1.0885	89.1472	3.5353
Ligand L_B				
20	1.351	1.0781	58.1159	2.3047
40	1.378	1.0900	68.7048	2.7240
60	1.393	1.0914	73.9760	2.9337
80	1.398	1.0933	76.2710	3.0247
100	1.410	1.0968	79.0561	3.1351
Ligand L_C				
20	1.353	1.0768	63.8470	2.5320
40	1.376	1.0847	75.0580	2.9766
60	1.397	1.0850	82.0341	3.2532
80	1.401	1.0918	84.0033	3.3313
100	1.413	1.0964	86.9679	3.4489
Ligand L_D				
20	1.391	1.0662	61.3065	2.4312
40	1.402	1.0696	70.0185	2.7767
60	1.405	1.0759	72.9595	2.8933
80	1.418	1.0816	76.2015	3.0219
100	1.423	1.0860	77.6787	3.0805

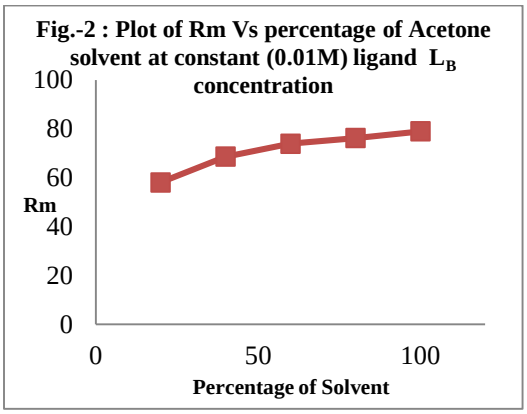
Table-3 : The data of refractive index (n), density (d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of DMSO solvent at 305K.

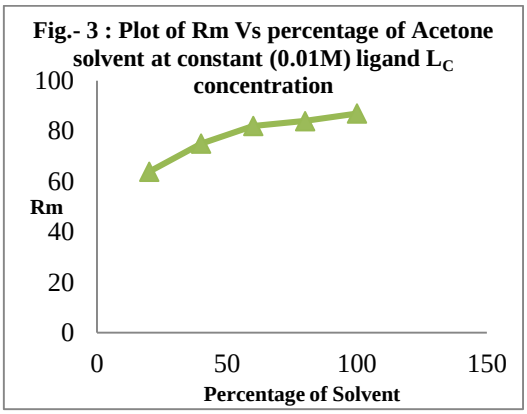
Conc. In %	Constant ligand concentration system (0.01M) with change in DMSO percentage			
	Refractive index (n)	**Density (d) g/cm^3**	**Rm x10^3 cm^3/mol**	**α x10^{-23} cm^3**
Ligand L_A				
20	1.430	1.0014	84.5924	3.3547
40	1.438	1.0022	96.1778	3.8141
60	1.447	1.0084	101.372	4.0201
80	1.456	1.0254	103.601	4.1085
100	1.462	1.0426	104.396	4.1400
Ligand L_B				
20	1.433	1.0001	75.7460	3.0039
40	1.439	1.0014	85.6604	3.3970
60	1.447	1.0059	90.2366	3.5785
80	1.456	1.0245	92.0632	3.6509
100	1.461	1.0366	93.0390	3.6896
Ligand L_C				
20	1.443	1.0112	83.4266	3.3084
40	1.445	1.0168	93.2415	3.6977
60	1.447	1.0213	97.1029	3.8508
80	1.448	1.0321	98.3227	3.8996
100	1.449	1.0440	98.6730	3.9131
Ligand L_D				
20	1.432	1.0132	70.6822	2.8030
40	1.439	1.0173	79.8457	3.1664
60	1.449	1.0219	84.4212	3.3479
80	1.455	1.0347	86.1347	3.4158
100	1.461	1.0500	86.9570	3.4484

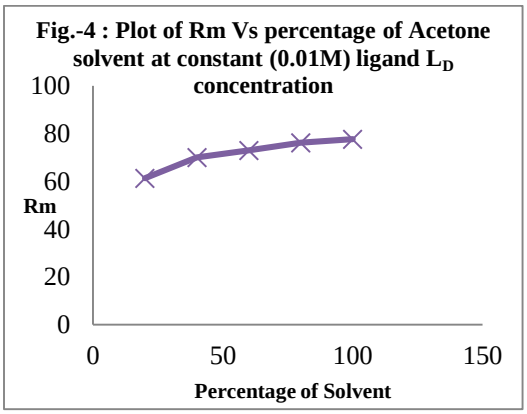
Table- 4 The data of refractive index (n), density (d), molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of DMF solvent at 305K.

Conc. In %	Constant ligand concentration system (0.01M) with change in DMF percentage			
	Refractive index (n)	Density (d) g/cm^3	Rm x10^3 cm^3/mol	α x10^{-23} cm^3
Ligand L_A				
20	1.420	1.0083	82.2407	3.2614
40	1.422	1.0334	90.2193	3.5778
60	1.423	1.0597	91.8542	3.6427
80	1.424	1.0798	92.2769	3.6594
100	1.438	1.1170	92.9621	3.6866
Ligand L_B				
20	1.419	1.0007	73.5027	2.9149
40	1.420	1.0256	80.4035	3.1886
60	1.421	1.0396	82.7960	3.2834
80	1.422	1.0583	82.8672	3.3404
100	1.423	1.1040	88.5032	3.5098
Ligand L_C				
20	1.420	1.0040	80.1425	3.1782
40	1.422	1.0260	88.1616	3.4962
60	1.424	1.0553	89.6667	3.5559
80	1.426	1.0704	90.6682	3.5956
100	1.431	1.0872	91.3637	3.6232
Ligand L_D				
20	1.419	1.0006	69.6297	2.7613
40	1.421	1.0289	76.0460	3.0157
60	1.424	1.0555	77.6876	3.0809
80	1.428	1.0814	78.0780	3.0963
100	1.435	1.1049	78.5132	3.1136









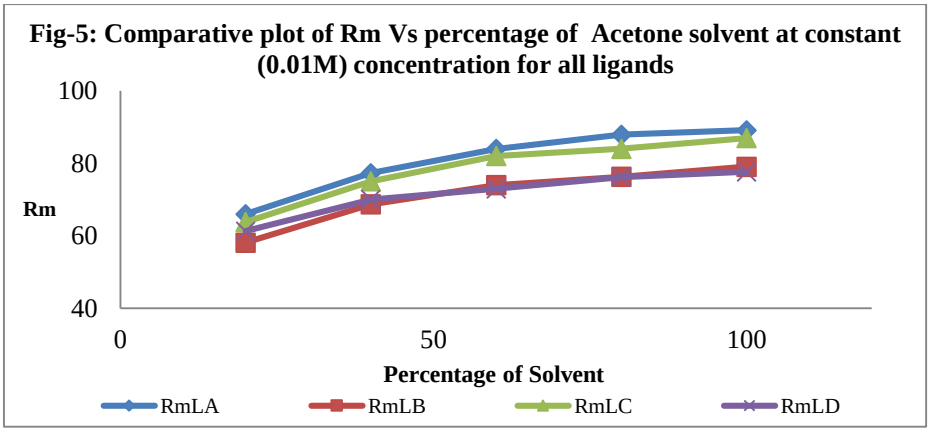
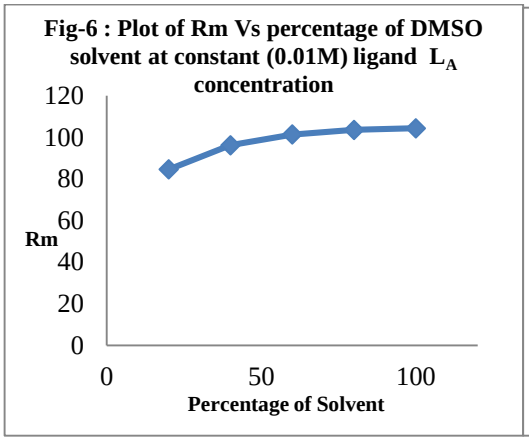
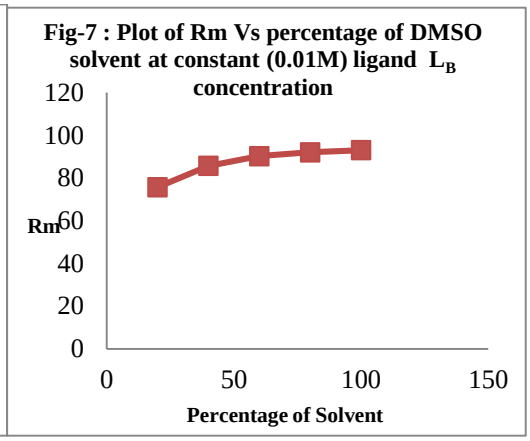
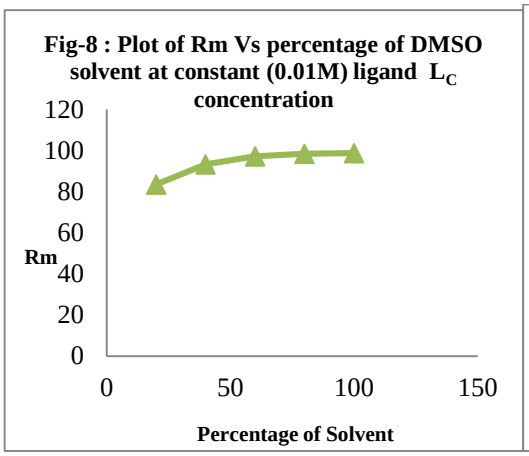
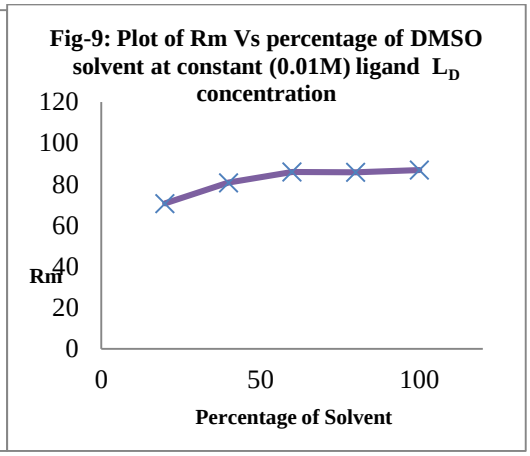


Fig.1 to 5: Graphical representation of molar refraction (Rm) versus change in Acetone solvent percentage at constant (0.01M) ligand concentration









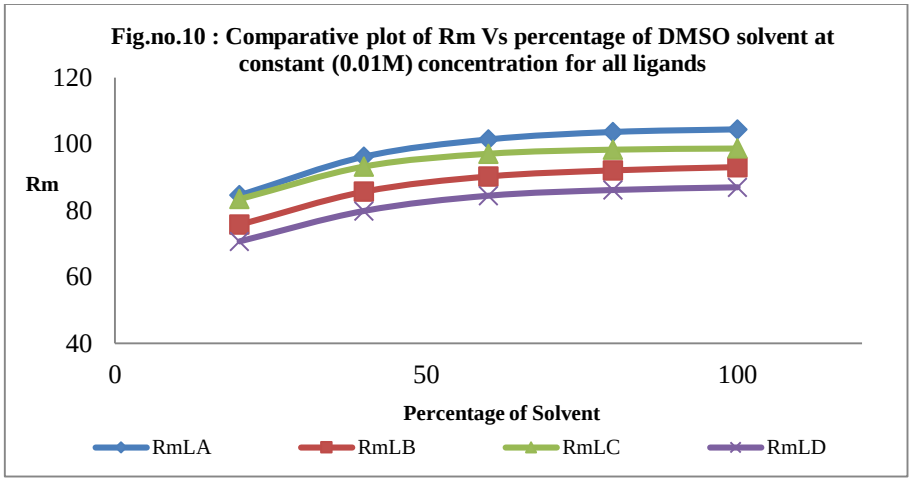
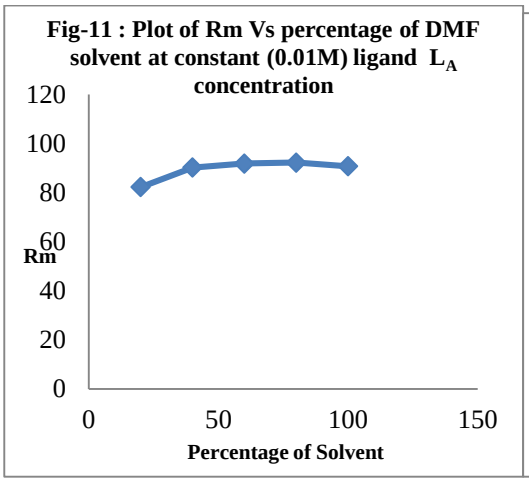
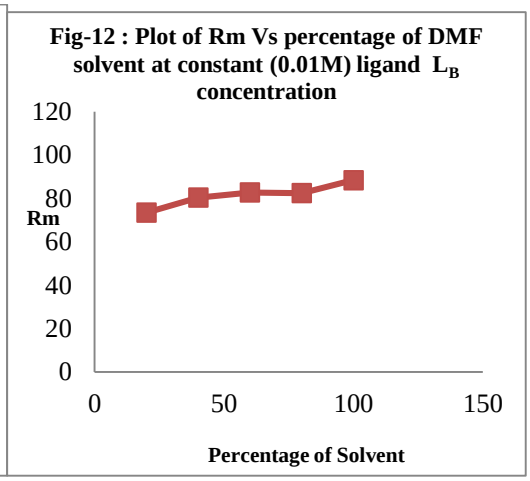
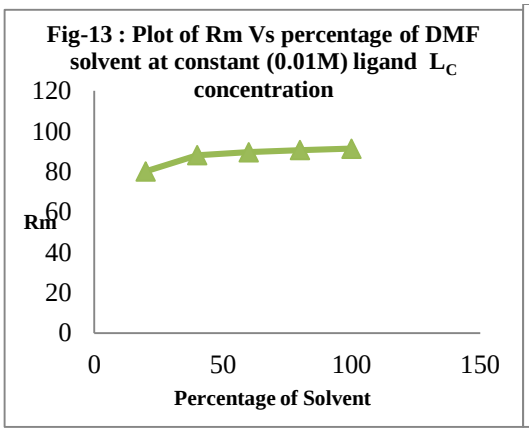
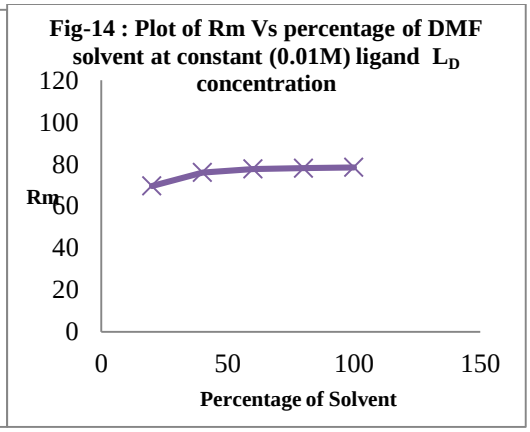


Fig. 5 to 10: Graphical representation of molar refraction (Rm) versus change in DMSO solvent percentage at constant (0.01M) ligand concentration









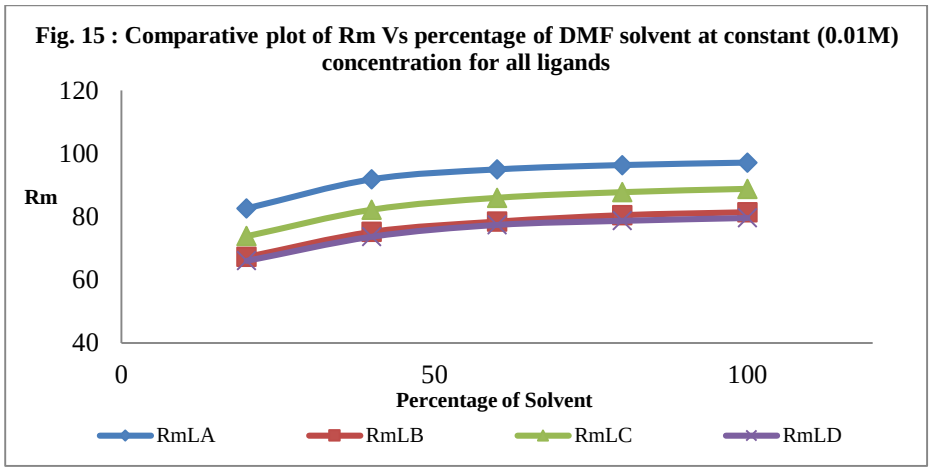


Fig. 10 to 15: Graphical representation of molar refraction (Rm) versus change in DMF solvent percentage at constant (0.01M) ligand concentration

CONCLUSIONS

Refractometric study of substituted 2-oxo-2*H*-chromene-3-carbohydrazide derivatives in different percentage of binary mixture is done The values of molar refraction (R_m) and polarizability constant (α) have calculated from the data of density and refractive index. It is seen that refractive index increases as the percentage composition of organic solvent component in the binary mixture increase. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution under study. It observed that molar refraction and polarizability constant of substituted 2-oxo-2*H*-chromene-3-carbohydrazide derivatives increases as the percentage composition of organic solvent in binary mixture increases. The increase in the value of polarizability constant as well as molar refraction with increase in percent composition of organic solvent part can be attributed to dispersion force.

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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