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Refractometric Study of Quinoline Pyrimidines in Different Binary Mixture

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Abstract: Molar refraction (Rm) and polarizability constant (α) of some different substituted drugs have been investigated by measuring the densities and refractive index of solution of different percent composition in binary mixture. It could be seen that molar refraction and polarizability constant of substituted Quinoline Pyrimidines drugs increases with increase in percent composition of organic solvents. This data have been used to determine solute-solute, solute-solvent and solvent-solvent interactions in the system.

Keyword: substituted Quinoline Pyrimidines, molar refraction (Rm), polarizability constant (α), refractometry.

INTRODUCTION

Pyrimidine moiety is an important class of nitrogen containing heterocycles[1] and is widely used as a key building block for pharmaceutical agents. Its derivatives exhibit antibacterial, antifungal[2], analgesic[3], calcium antagonist[4], anti-inflammatory[5] and anti-tumor[6] activity. In addition, several marine natural products with interesting biological activities containing pyrimidine core have recently been isolated.[7]

Solvent plays an important role in the molecular interaction. Each solvent has different behavior with solute molecule. So the study of interaction between different solvent with solute becomes important. The

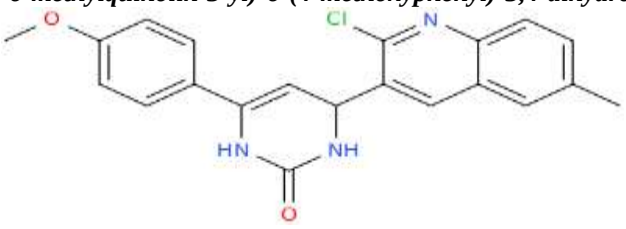
present work deals with the study of molar refraction and polarizability constant of different substituted Quinoline Pyrimidines[8] drugs in different percent composition of DMSO, methanol and acetone solvent.

The refractive index is an important additive property of liquid. It also depends on the structural arrangement of atom in molecule. The value of refractive index depends upon the temperature as well as associative and dissociative phenomena takes place in solution. When a light of beam passes from one substance to another, the beam bends so that it travels in different direction. If it is passed from less dense to high denser medium, it is refracted toward normal to form angle of refraction which is less than angle of incident. The refractive index is the ratio of angle of incident to the angle of refraction.

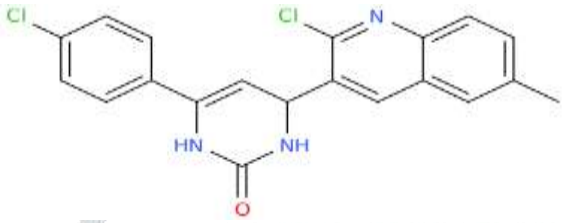
The properties of liquid such as viscosity, refractive index and ultrasonic velocity of binary mixtures are studied by many workers[9-11]. Many researcher carried out the measurement of refractive indices in mixed solvents[12-15]. Determination of molar refraction and polarizability constant provide valuable information to understand molecular interaction. The properties of liquid such as refractive index in binary mixture were studied by many workers[16-18]. Determination of molar refraction and polarizability constant of some substituted sulphonic acid have been studied by many people[18-21].

Substituted Quinoline Pyrimidines used for present work are-

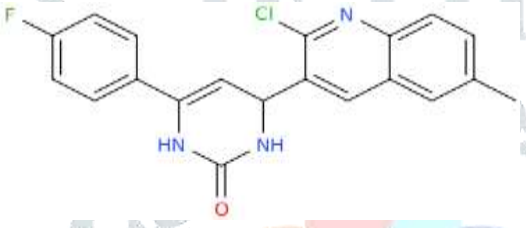
L_1: *4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-methoxyphenyl)-3,4-dihydropyrimidin-2(1H)-one*



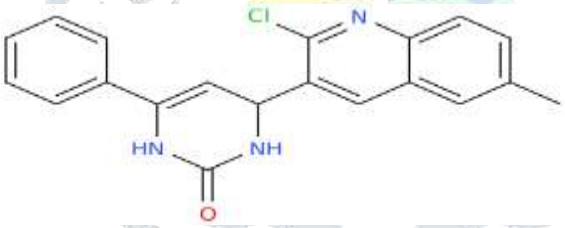
L_2: *4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-chlorophenyl)-3,4-dihydropyrimidin-2(1H)-one*



L_3: *4-(2-Chloro-6-methylquinolin-3-yl)-6-(4-fluorophenyl)-3,4-dihydropyrimidin-2(1H)-one*



L_4- *4-(2-Chloro-6-methylquinolin-3-yl)-6-phenyl-3,4-dihydropyrimidin-2(1H)-one*



MATERIAL AND METHOD

The ligands of which physical parameters is to be explore are synthesized by using reported protocol. In the present investigation, refractive indices of liquid mixtures were measured with the help of Abbe's refractometer, specially designed to measure the refractive indices of the small quantities of the transparent liquid ranging from 1.300 to 1.700 rapidly by direct reading. The solutions of ligand in different percent composition of binary mixtures were prepared by weight. All the weighings 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 a precalibrated bicapillary pyknometer (± 0.1%). The constant temperature of the prism box is maintained by circulating water from thermostat at (27± 0.1)^{0}C.

CALCULATION

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

$R_{solvent\text{-}water} = X_1R_1 + X_2R_2$ .....(1)

Where, R_1 and R_2 are molar refractions of pure solvent and water respectively.
The molar refraction of solutions of ligand in solvent-water mixtures are determined from-

$$R_{Mix} = \frac{(n_2-1)}{(n_2+1)} + \frac{X_1M_1+X_2M_2+X_3M_3}{d} \quad \ldots. (2)$$

Where,
n is the refractive index of solution, d is the density of solution.

X_1, X_2 and X_3 are mole fraction of solvent, water and solute respectively.

M_1, M_2 and M_3 are molecular weights of solvent, water and solute respectively.

The molar refraction of ligand is calculated as –

$R_{lig} = R_{mix} - R_{solvent-water}$ .....(3)

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

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

Where, No is Avogadro's number.

RESULT AND DISCUSSION

Table 1: Values of Molar Refraction of different composition of solvents.

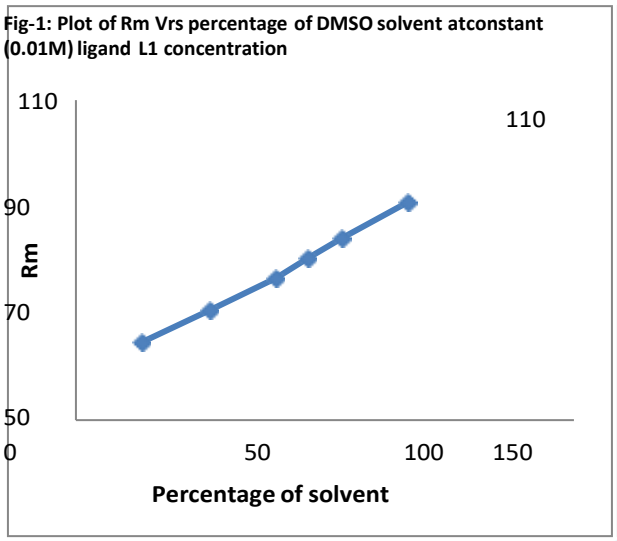
of solventmixture	Molar Refraction [R]		
	DMSO	Methanol	Acetone
20	4.9610	4.6384	4.8789
40	6.3419	5.3725	6.1633
60	8.4739	6.2148	7.5919
80	11.8704	7.1835	9.2701
100	17.3754	9.3556	14.1466
70	8.9532	7.6225	7.8813

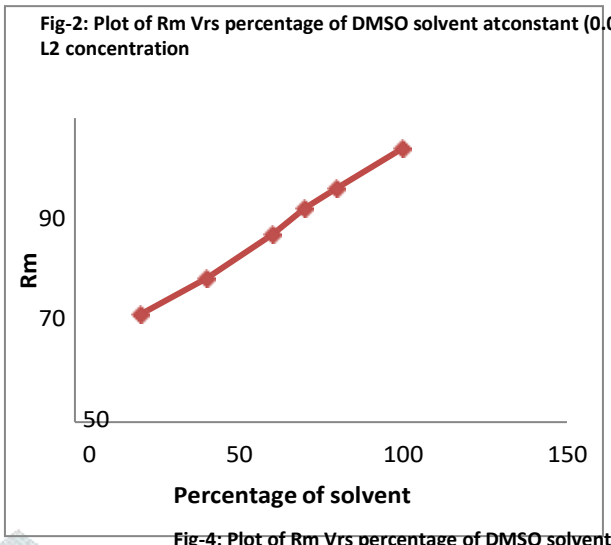
Table 2: The values of refractive index (n) and density(d) of 0.01M solution of ligand in differentcomposition of DMSO, Methanol and Acetone solvent at 300K.

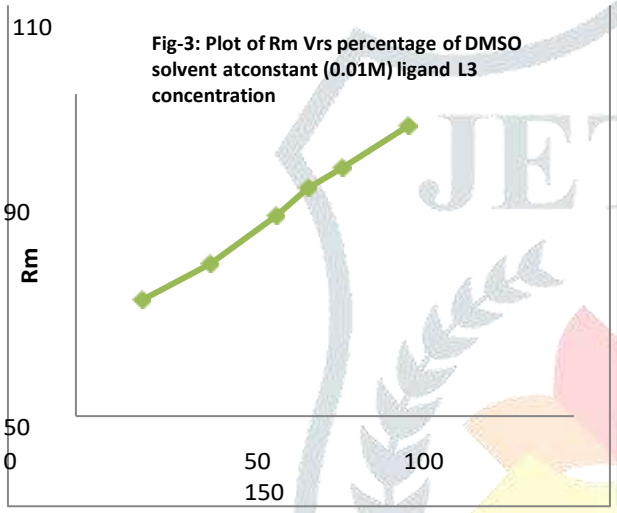
npositionin %	Refractive index (n)			Density (d) gm/cm^3		
	DMSO	Methanol	Acetone	DMSO	Methanol	Acetone
Ligand L_1						
20	1.435	1.432	1.250	1.1232	0.7986	1.1104
40	1.240	1.237	1.244	1.0136	0.7280	1.1329
60	1.247	1.257	1.275	0.7835	0.7563	1.1745
70	1.261	1.282	1.297	0.8843	0.8894	1.1987
80	1.277	1.298	1.314	0.8866	1.1053	1.0033
100	1.308	1.356	1.408	0.8889	1.1798	1.1526
Ligand L_2						
20	1.261	1.247	1.252	1.1261	0.8103	1.1118
40	1.245	1.242	1.245	1.0146	0.8395	1.1339
60	1.263	1.268	1.277	0.8838	0.8671	1.1755
70	1.280	1.288	1.298	0.8804	0.8998	1.1986
80	1.294	1.304	1.310	0.8808	1.0058	1.0046
100	1.322	1.362	1.397	0.8802	1.0800	1.1515
Ligand L_3						
20	1.264	1.251	1.255	1.0185	0.8122	1.0039
40	1.248	1.245	1.250	1.0090	0.8418	1.0259
60	1.265	1.263	1.281	0.9767	0.9696	1.0775
70	1.383	1.385	1.402	0.9831	1.0125	1.1105
80	1.296	1.298	1.356	0.7841	1.1190	1.1041
100	1.325	1.353	1.457	0.8840	1.0715	1.2629
Ligand L_4						
20	1.267	1.263	1.258	1.0215	0.7142	1.0055
40	1.252	1.254	1.253	1.1107	0.8438	1.1195
60	1.269	1.272	1.284	0.9788	0.8719	1.0745
70	1.285	1.294	1.306	0.9742	1.0149	1.993
80	1.299	1.310	1.320	0.8855	1.0112	1.1046
100	1.229	1.363	1.414	0.9760	1.1958	1.2656

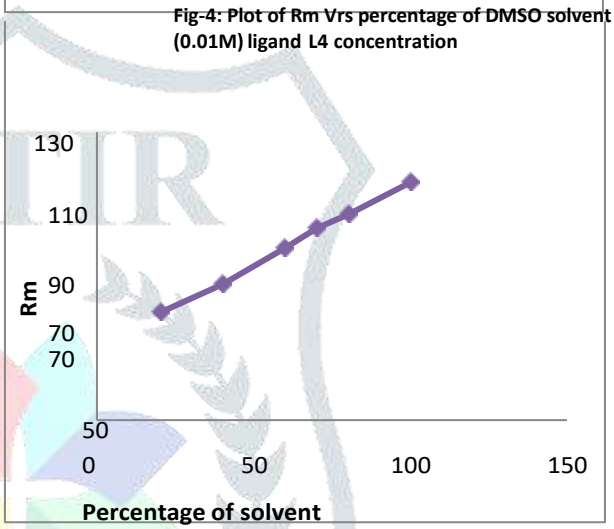
Table 3: The values of Molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand in different composition of DMSO, Methanol and Acetone solvent at 300K.

npositionin %	ar refraction (Rm)x10^3 cm^3/mole			polarizability constant (α) x10^{-23} cm^3		
	DMSO	Methanol	Acetone	DMSO	Methanol	Acetone
Ligand L_1						
20	67.4684	68.9365	65.2307	2.4566	2.5734	2.4471
40	69.7540	73.6476	66.1984	2.7058	2.8602	2.6442
60	77.6137	78.4426	73.8707	3.1382	3.0504	2.8691
70	81.2823	82.8433	76.9559	3.0837	3.1734	3.0814
80	83.0322	84.0147	80.2921	3.2324	3.2714	3.1238
100	92.0956	91.2799	87.5203	3.5125	3.4802	3.3311
Ligand L_2						
20	72.2800	75.3995	71.4089	2.7267	3.1297	2.2471
40	77.2674	80.6584	74.7414	3.0038	3.1383	2.6442
60	86.1776	87.2288	81.1403	3.1571	3.1988	2.8691
70	93.2359	91.5370	84.4065	3.3577	3.2904	3.1914
80	95.3250	92.4167	87.2108	3.6199	3.4046	3.1238
100	101.991	98.3704	94.3863	4.0239	3.2407	3.41311
Ligand L_3						
20	72.6404	76.0315	709082	2.3410	3.0148	2.4080
40	77.6101	81.1037	75.5864	3.0174	3.1559	3.0171
60	87.1476	86.4246	82.4677	3.1639	3.2471	3.1823
70	91.6298	88.6709	85.0180	3.5734	3.3560	3.2112
80	94.4352	90.8993	84.7874	3.4243	3.2444	3.2210
100	102.234	99.5572	95.3360	4.0336	3.2688	3.5410
Ligand L_4						
20	77.7995	83.8472	74.5540	3.0646	3.2837	2.7772
40	86.8959	92.0433	77.5364	3.3856	3.5898	3.0145
60	96.6777	97.3732	83.8524	3.7736	3.8011	3.2649
70	101.171	100.334	87.3675	4.0114	4.0086	3.1043
80	104.328	103.222	92.4747	4.1563	4.0331	3.2276
100	110.844	105.375	93.2486	4.0940	4.1375	3.2565









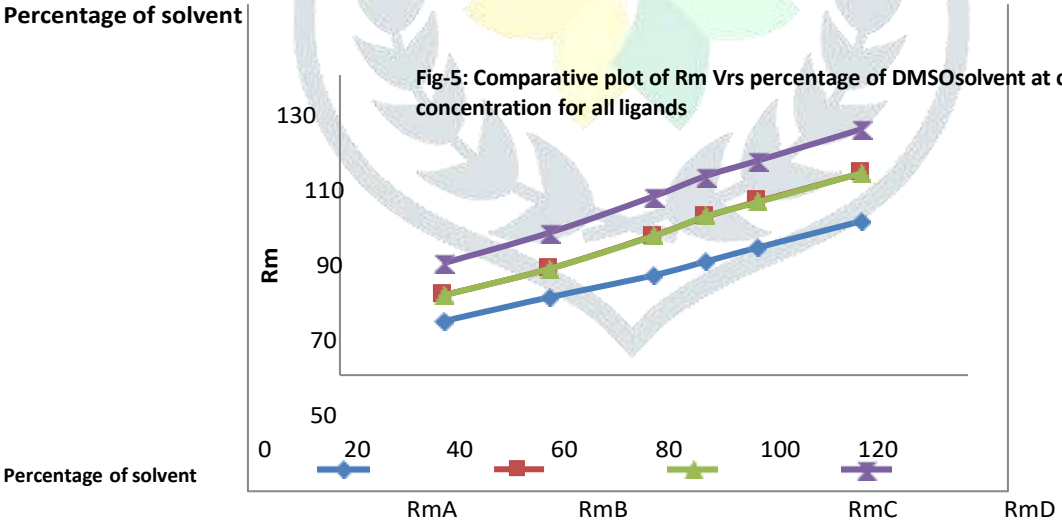


Fig- 1 to 5: Graphical representation of Molar refraction (Rm) Vs percent Composition of DMSO solventat 0.01M concentration of ligands.

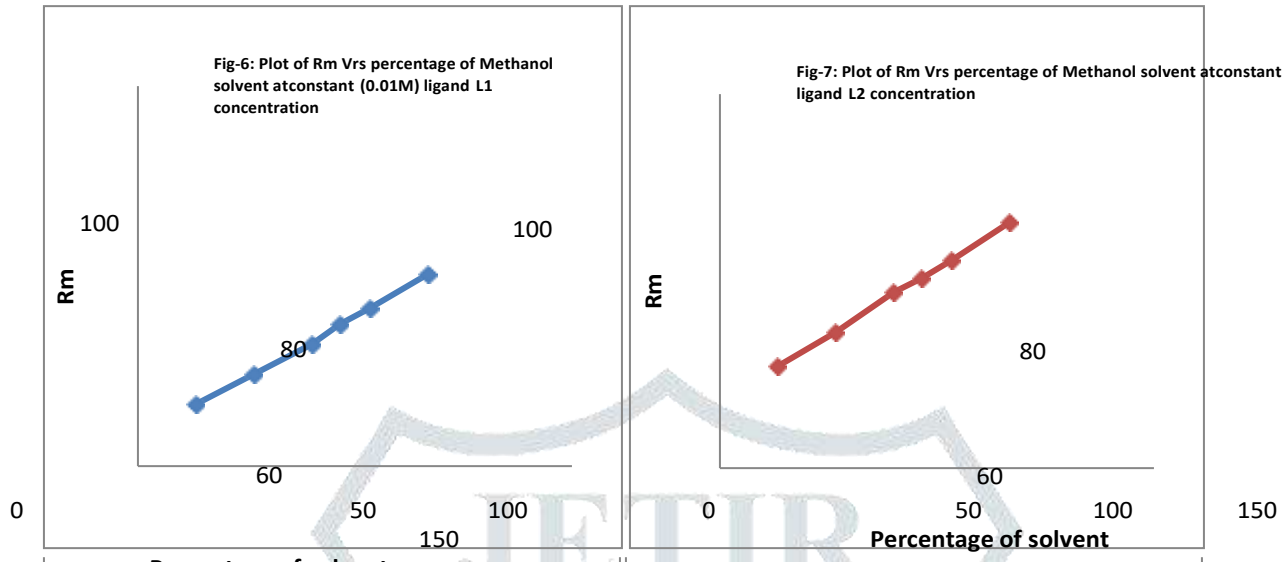


Fig-6: Plot of Rm Vrs percentage of Methanol solvent atconstant (0.01M) ligand L1 concentration

Fig-7: Plot of Rm Vrs percentage of Methanol solvent atconstant (0.01M) ligand L2 concentration

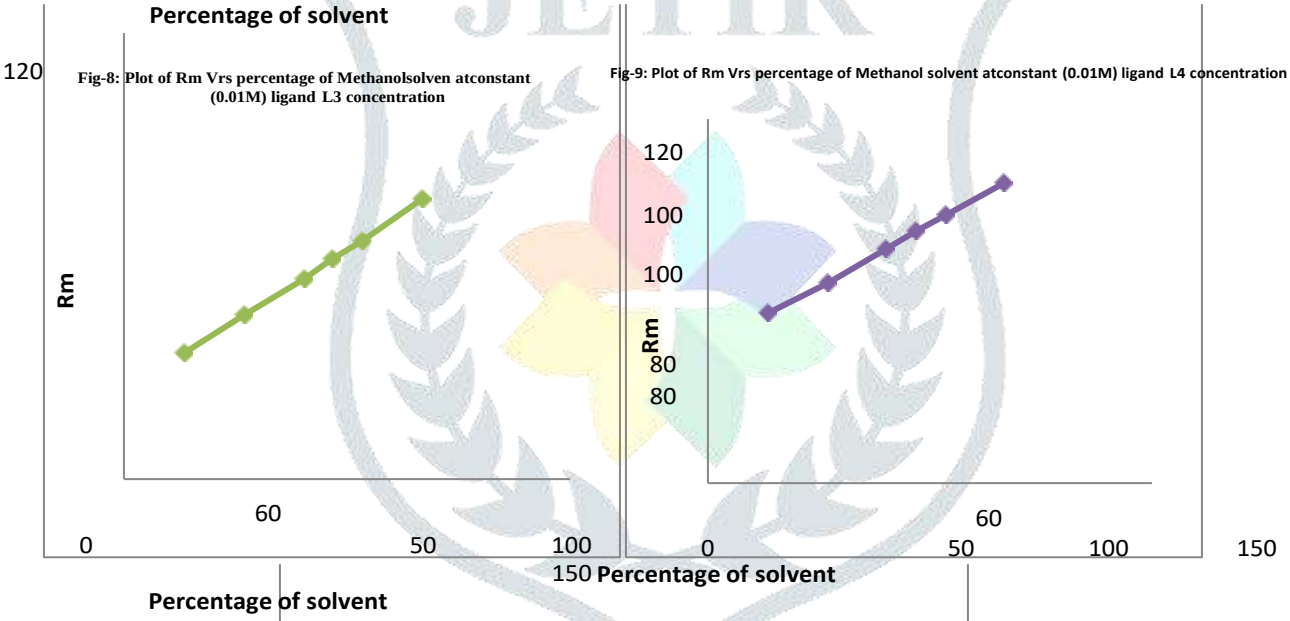


Fig-8: Plot of Rm Vrs percentage of Methanolsolven atconstant (0.01M) ligand L3 concentration

Fig-9: Plot of Rm Vrs percentage of Methanol solvent atconstant (0.01M) ligand L4 concentration

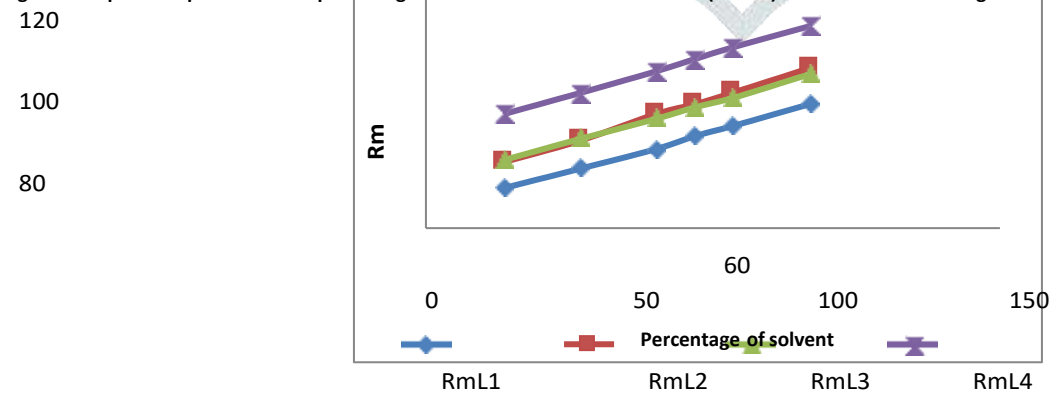
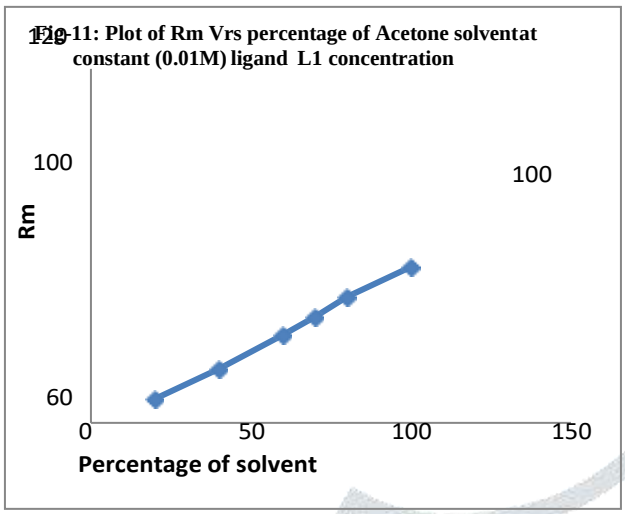
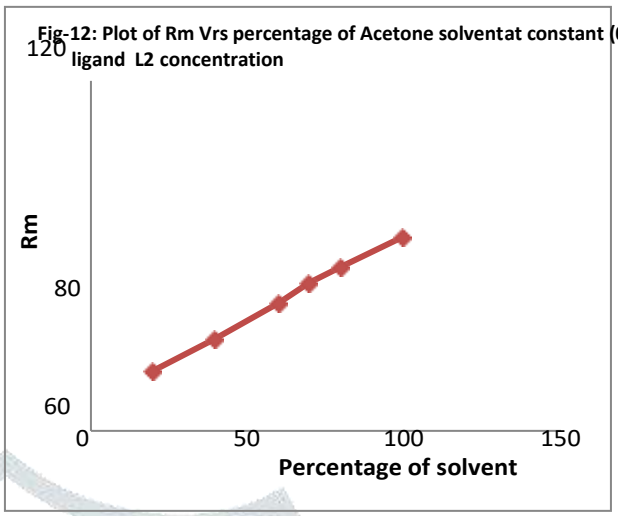
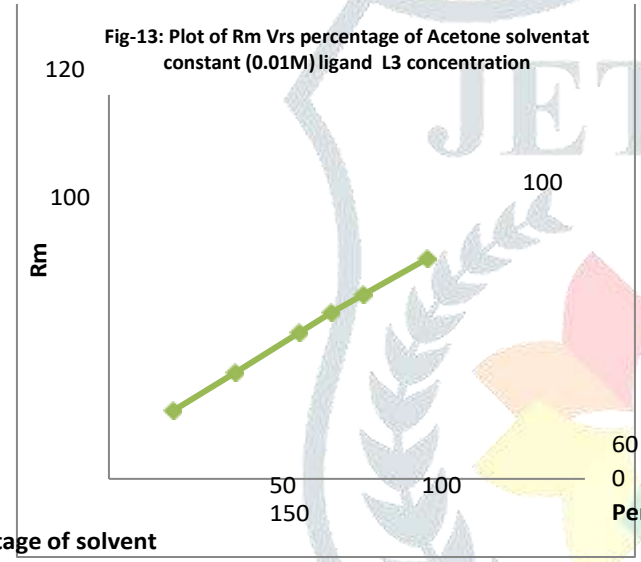


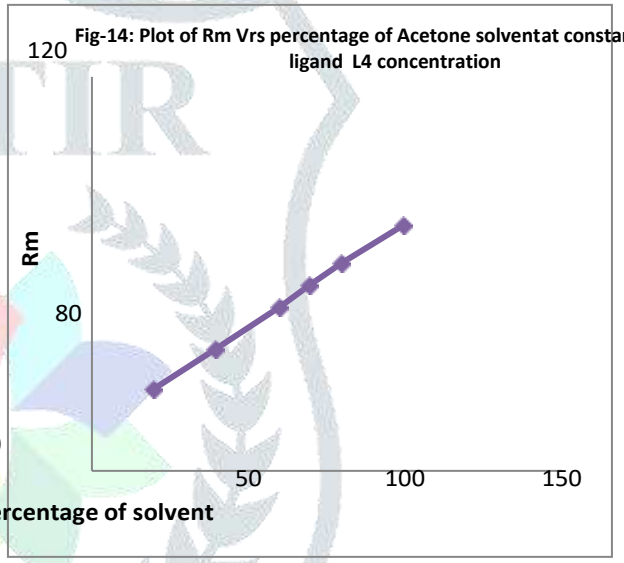
Fig-10: Comparative plot of Rm Vrs percentage of Methanolsolvent at constant (0.01M) concentration for all ligands

Fig- 6 to 10: Graphical representation of Molar refraction (Rm) Vs percent Composition of Methanolsolvent at 0.01M concentration of ligands.









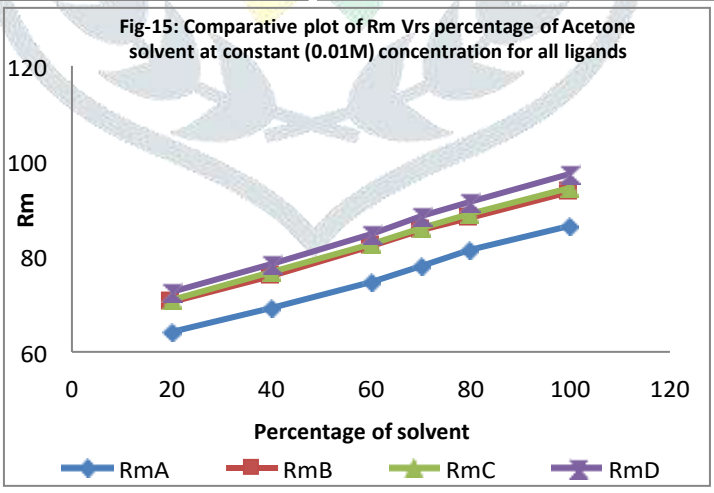


Fig- 11 to 15: Graphical representation of Molar refraction (Rm) Vs percent Composition of Acetonesolvent at 0.01M concentration of ligands.

The value of molar refraction of different percent composition in binary mixture are shown in table-1. From the data it is observed that value of molar refraction goes on increasing with the decrease in amount of water in percent composition. Comparatively molar refraction of DMSO is greater than acetone and methanol this is due to more value of dipole moment of DMSO.

Table-2 shows the comparative data of refractive indices and densities of DMSO, acetone and methanolin different percent composition with water. From this, it is observe that, refractive index and density increases with the increase in percent composition of organic solvent. Graphical representation between molar refraction and percent composition of DMSO, methanol and acetone shows linear relationship. (Fig.1-5 DMSO, fig.6-10 methanol, fig.11-15 acetone) Those solvent having more value of dipole moment shows greater refractive index and density, also there is same trend in case of ligand used. Ligand having more dipole moment shows greater value of refractive index and less value of density.

Table-3 shows the comparative data of molar refraction and polarizability constant. These parameter provide important information about structural orientation of ligand in solution. From this it is observed that, molar refraction and polarizability constant in methanol is higher than DMSO and acetone. The trend regarding increasing value of molar refraction and polarizability constant is methanol > DMSO > acetone. From this observation it is concluded that, methanol has strong hydrogen bonding, which make solution more viscous which is responsible for more bending of light towords normal. In case of DMSO, it has more value of molar refraction and polarizability constant than acetone because it has more dipole moment.

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