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Refractometric study of substituted-2,3-dihydroquinazolin-4(1*H*)-ones in different binary mixture

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ABSTRACT

Density and refractive index for substituted-2,3-dihydroquinazolin- 4(1H)-ones have been measured in binary mixtures with different composition as per percentage, maintaining constant ligand concentration (0.01M). Measurement of refractive index is done using Abbe's refractometer. The values of molar refraction (R_m) and polarizability constant (α) have been calculated from the data. Molar refraction and polarizability constant of the investigated systems are increases with increase in percent composition of organic solvents. These parameters and their variation tendencies have been expounded in terms of the interactions between solutes and solvents.

Keywords: Substituted-2,3-Dihydroquinazolin-4(1H)-ones, molar refraction and polarizability constant.

INTRODUCTION

The refractive index and the dipole polarizability are fundamental electrooptical properties of matter[1]. The refractive index of a liquid can be easily determined to a high degree of accuracy. It is a characteristic property of a liquid. It is one of the important additives properties of liquid[2]. It varies with temperature and wavelength of light used. Generally, the D-line of sodium is used for standard measurement. Instruments used for measuring refractive indices are known as refractometers[3].

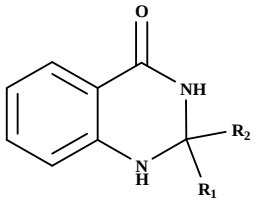
Refractive index is the useful physical characteristic of liquid by means of which pure compounds are identified and with which industrial processes are monitored and controlled[4]. The use of measurements of index of refraction as a quick, convenient, and accurate way to estimate densities of liquid mixtures has been reported[5-7]. The refractive index of liquids is a physical property so easily determined with accuracy that it has become a standard for their characterization[8]. Density and refractive index measurements are expected to shed some light on both solute-solute and solute-solvent interactions[9-11]. The refractometric technique is used to study the miscibility of polymer blend[12]. The use of molar refraction is proposed for the estimation of vapor pressure of pure hydrocarbons from C_1 to C_{100}[13]. Specific refractive index increments have been measured for solutions of neutral water-soluble polymer in binary solvents of formamide/water over the whole range of solvent composition[14]. Density and refraction index are two physical properties easy to measure and can be used to characterize an ionic liquid mixture[15]. Refractometric study is done by many workers on differtent compounds[16-20].

2,3-Dihydroquinazolin-4(1*H*)-one derivatives are playing crucial role in the context of drug intermediates, biological and pharmaceutical applications[21-25]. They have drawn much more attention because of their activities such as

antibacterial[26], diuretic[27], anticancer[28], antihyperlipidemic[29], antiparkinsonism[30], antimicrobial[31], anti-inflammatory[32], bronchodilator[33], antihypertensive[34], antiproliferative[35] and antimitotic[36] activities.

Absorption, distribution, metabolism, and excretion (ADME) and chemical reactivity-related toxicity are the important factors of drugs[37-39]. Most of the drugs are hydrophobic. This property of hydrophobicity would render drugs difficult to eliminate, since in the absence of metabolism, they would accumulate in fat and cellular phospholipid bilayers[40] in cells. These modern days there is an upsurge in topical formulations such that it can be prepared by varying physico-chemical properties and providing better localized action[41].

The present work deals with the study of molar refraction and polarizability constant of following compounds in non aqueous solvent such as DMF, acetone and1,4-dioxane (with different percentage).



L_A : R_1= 4-hydroxy-3-methoxyphenyl
L_B : R_1= 2-hydroxyphenyl
L_C : R_1= 3-hydroxyphenyl
L_D : R_1= 4-hydroxyphenyl
R_2 = H for all

Ligand A (L_A)= *2-(4-hydroxy-3-methoxyphenyl)-2,3-dihydroquinazolin-4(1H)-one*
Ligand B (L_B)= *2-(2-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*
Ligand C (L_C)= *2-(3-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*
Ligand D (L_D)= *2-(4-hydroxyphenyl) -2,3-dihydroquinazolin-4(1H)-one*

MATERIALS AND METHODS

The ligands of which physical parameters are to be explored are synthesized by using reported protocol[42]. The analytical grade solvents and freshly prepared doubly distilled water are used. The solutions of compounds under study are prepared in different solvent like DMF, acetone and 1,4-dioxane by keeping constant ligand concentration system (0.01M). The density measurement is done using a specific gravity bottle. All the weights are taken on one pan digital balance (petit balance AD-50B) with an accuracy of ± 0.001 gm. The refractive indices are measured by Abbe's refractometer at 27 ± 0.1°C. 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 27C ± 0.1^0C. Refractometer is calibrated by using glass test piece of known refractive index supplied with the instrument.

RESULTS AND DISCUSSION

It is often desirable 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[43]. The molar refraction of solvent, solution can be determined by following equation[44].

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

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

The molar refraction[45-47] 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 –

$$R_{lig} = R_{Mix} - R_{DMF-W} \quad (3)$$

The polarizability constant (α)[48-49] of ligand can be calculated from following relation-

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

Where, No is Avogadro's number.

The data of density and refractive index measurement is presented in table no 02. Using equation no 01 to 04 calculations are made to determine the values of molar refraction and polarizability constant. The experimental data of refractive index at the temperature *T*=300K is presented here. The experimental data shows that generally 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.

Table 1: Values of molar refraction of different composition of solvents

% of solvent mixture	Molar Refraction [R]		
	DMF	Acetone	Dioxane
20	17.1569	11.6287	19.6676
40	16.4094	10.9571	18.7919
60	14.9730	9.8437	17.2276
80	11.9243	7.9248	13.8024
100	4.5403	4.2067	4.4692

Table 2: The values of refractive index (n) and density(d) of 0.01M solution of ligand in different composition of DMF, Acetone and Dioxane solvent at 300K

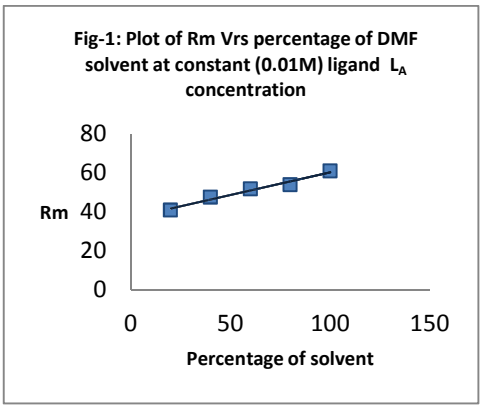
Composition in %	Refractive index (n)			Dens ity (d) gm/cm^3		
	DMF	Acetone	Dioxane	DMF	Acetone	Dioxane
Ligand (L_A)						
20	1.359	1.347	1.359	1.0655	0.8780	0.9948
40	1.380	1.357	1.372	1.0757	0.8655	1.0050
60	1.403	1.364	1.389	1.0834	0.8404	1.0047
80	1.421	1.367	1.402	1.1025	0.8161	1.0164
100	1.431	1.362	1.416	1.0080	0.7956	1.0580
Ligand (L_B)						
20	1.362	1.346	1.354	1.0706	1.0351	0.9687
40	1.386	1.357	1.367	1.0844	1.0194	0.9832
60	1.404	1.854	1.385	1.0850	1.6335	0.9949
80	1.418	1.367	1.401	1.0913	0.7549	1.0108
100	1.431	1.365	1.416	1.0780	0.6858	1.0157
Ligand (L_C)						
20	1.371	1.346	1.353	1.0717	1.0350	0.9692
40	1.382	1.356	1.371	1.0851	0.9875	0.9862
60	1.397	1.359	1.388	1.0919	1.0021	0.9973
80	1.410	1.367	1.398	1.1064	0.9395	0.9932
100	1.430	1.363	1.419	1.0669	0.8774	1.0592
Ligand (L_D)						
20	1.355	1.345	1.353	1.0686	1.0155	0.9810
40	1.377	1.356	1.370	1.0882	1.0082	0.9932
60	1.401	1.364	1.385	1.0886	0.9606	0.9991
80	1.420	1.367	1.399	1.0926	0.9440	1.0082
100	1.430	1.364	1.417	1.0885	0.8779	1.0574

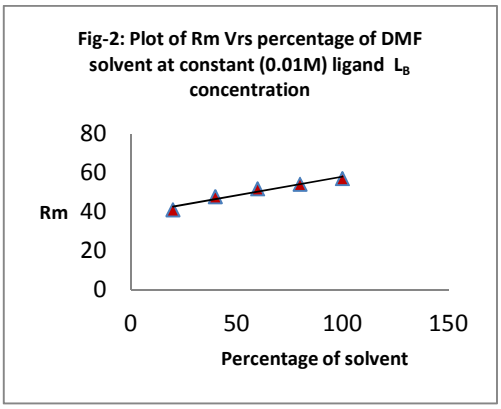
The graphs are plotted using percentage of solvent versus molar refraction (R_m). In all the graphs, it is found that molar refraction increases linearly with the increasing percentage composition of organic solvent component in the binary mixture. Molar refraction is related to the internal forces among the constituents of a liquid mixture. Similarly, polarizability constant increases in the same manner as that of molar refraction suggesting the validity of equation no 04. The polarizability of a molecule can be obtained by summing up the contributions of a variety of atoms and/or functional groups in the molecule. Here is the reasoning: molar refraction (R_m) is found to be an additive property, polarizability is related to molar refraction by the Lorentz-Lorenz equation and therefore polarizability should be an additive property.

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. It is the molecular force which arises from the temporary dipole moment.

Table 3: The values of molar refraction (Rm), polarizability constant (α) of 0.01M solution of ligand indifferent composition of DMF, Acetone and Dioxane solvent at 300K

Composition in %	Molar refraction (Rm) x10^3 (cm^3/mol)			Polarizability cons tant (α) x10^{-23} (cm^3)		
	DMF	Acetone	Dioxane	DMF	Acetone	Dioxane
Ligand (L_A)						
20	40.9573	48.0670	43.9492	1.6242	1.9061	1.7428
40	47.5968	55.7647	50.0946	1.8875	2.2114	1.9866
60	51.8062	60.7921	54.2607	2.0544	2.4108	2.1518
80	54.0004	64.3748	56.3684	2.1414	2.5529	2.2354
100	61.0491	66.0421	56.5206	2.4210	2.6190	2.2414
Ligand (L_B)						
20	41.0667	40.6634	44.5673	1.6285	1.6125	1.7674
40	47.8811	47.3429	50.5906	1.8988	1.8774	2.0062
60	51.8395	62.9030	54.2917	2.0558	2.4945	2.1530
80	54.2132	69.5937	56.5563	2.1499	2.7598	2.2428
100	57.0876	77.1882	58.8748	2.2639	3.0610	2.3347
Ligand (L_C)						
20	41.9371	40.6670	44.4308	1.6631	1.6127	1.7619
40	47.4070	48.7495	50.9267	1.8800	1.9332	2.0196
60	50.7230	50.3565	54.5373	2.0115	1.9969	2.1627
80	52.5738	55.9152	57.1764	2.0849	2.2174	2.2674
100	57.5625	60.0356	56.8098	2.2827	2.3808	2.2529
Ligand (L_D)						
20	45.5439	46.5712	49.4513	1.8061	1.8468	1.9610
40	52.6945	53.8534	56.8948	2.0897	2.1356	2.2562
60	57.9168	60.0120	61.0012	2.2968	2.3798	2.4191
80	61.3614	62.8022	63.7082	2.4334	2.4905	2.5264
100	63.6756	67.8879	63.9584	2.5251	2.6922	2.5363





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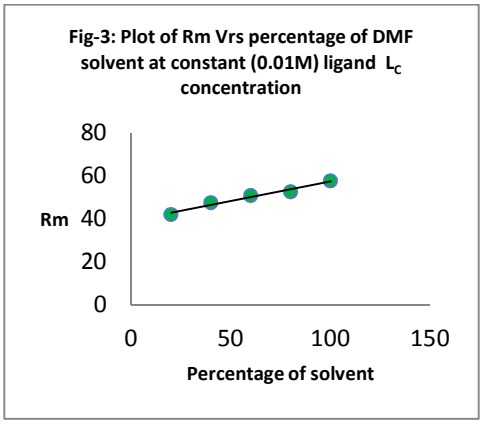
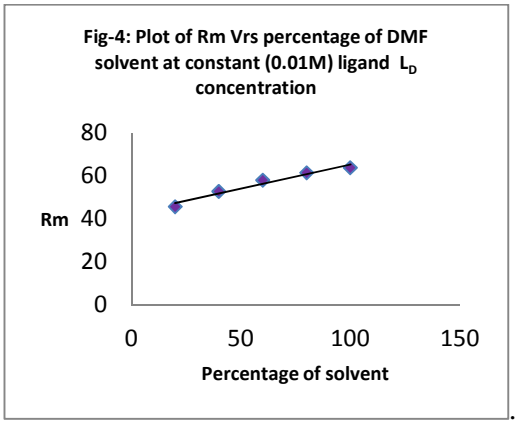




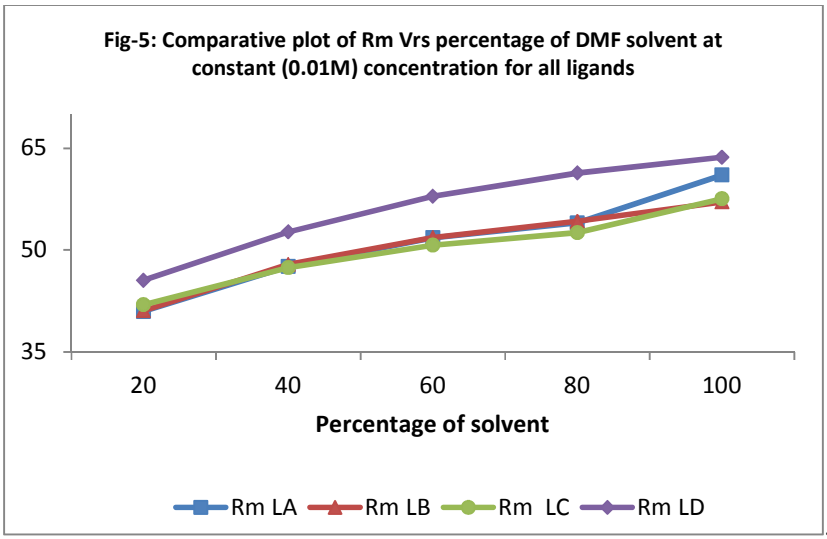
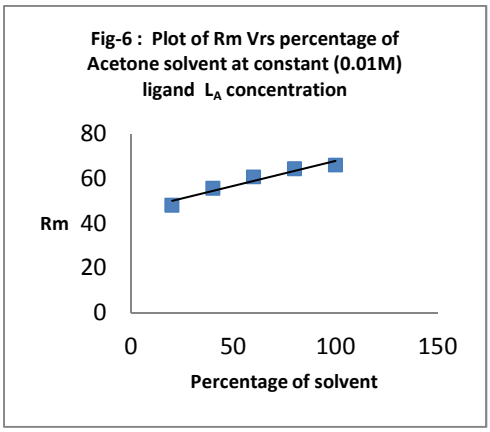
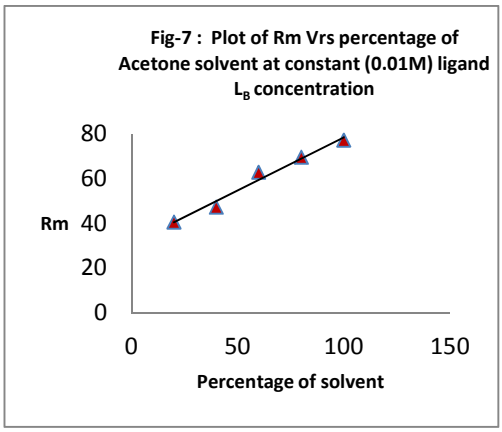
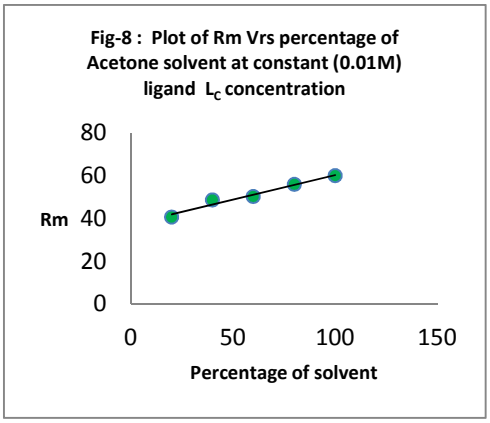
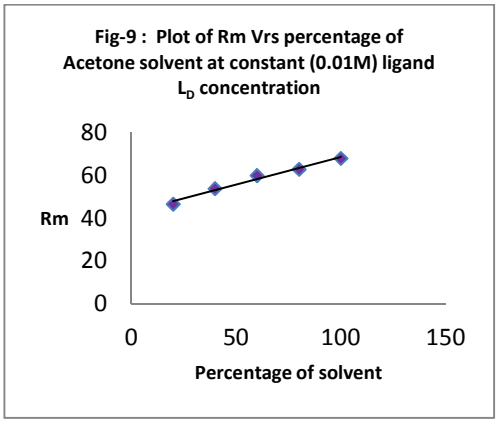


Fig. 1 to 5: Graphical representation of molar refraction (Rm) versus change in DMF solvent percentage at constant (0.01M) ligand concentration









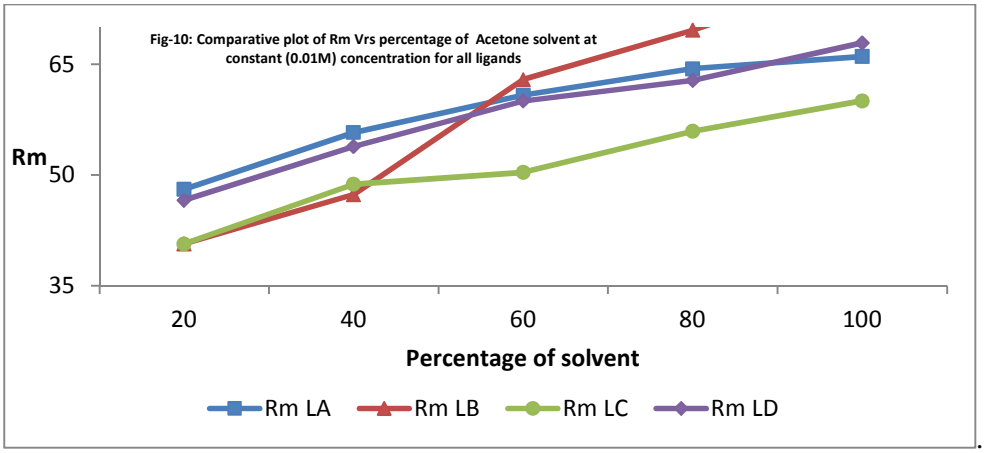
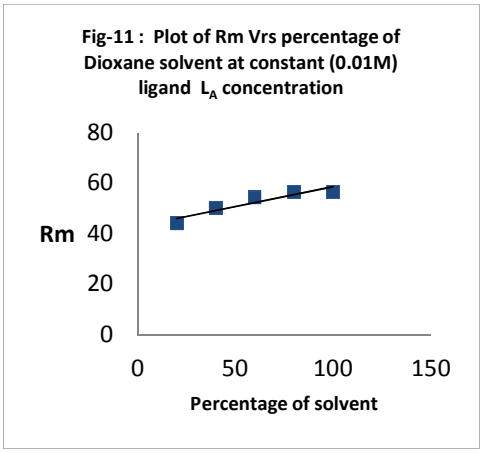
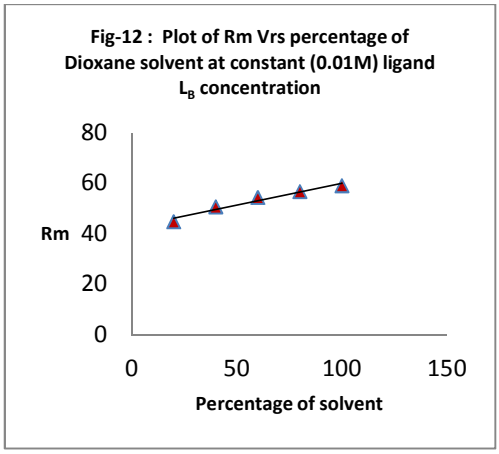
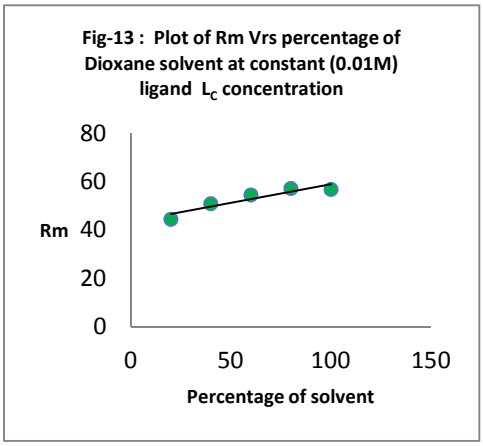
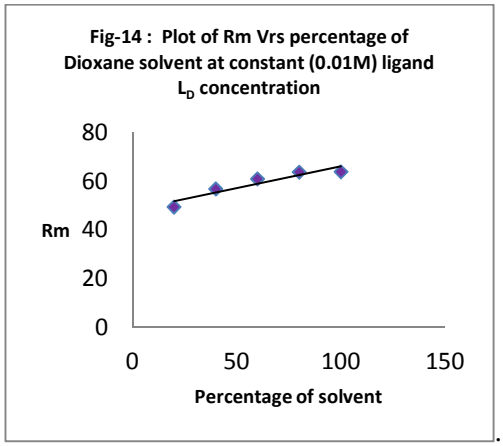


Fig. 6 to 10: Graphical representation of molar refraction (Rm) versus change in Acetone solvent percentage at constant (0.01M) ligand concentration









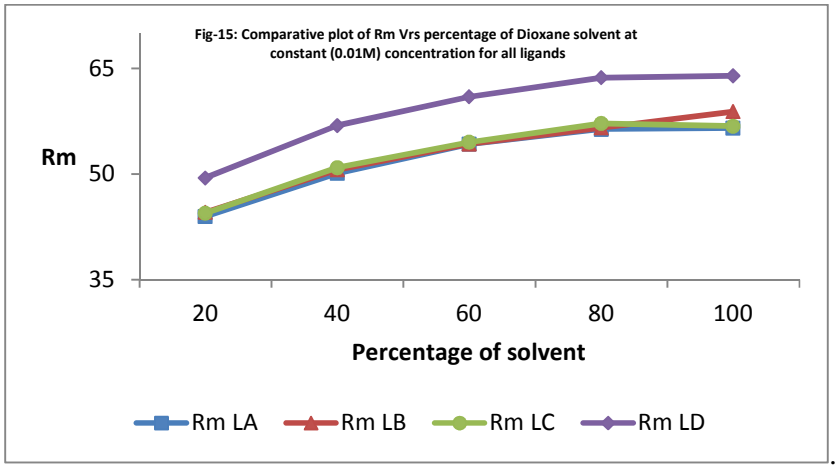


Fig. 11 to 15: Graphical representation of molar refraction (Rm) versus change in Dioxane solvent percentage at constant (0.01M) ligand concentration

CONCLUSION

In the present investigation, refractometric study of substituted-2,3-Dihydroquinazolin-4(1*H*)-ones in different binary mixture is done. The values of molar refraction (R_m) and polarizability constant (α) have been calculated from the data of density and refractive index. The experimental data shows that generally 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. 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.

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