Journal of Advanced Scientific Research

Available online through http://www.sciensage.info

ISSN
0976-9595
Research Article

INVESTIGATIONS IN THE REFRACTROMETRIC STUDY OF SUBSTITUTED-DIHYDROPYRIMIDIN-2(1H) ONE IN DIFFERENT SOLVENTS

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ABSTRACT

Refractive index, molar refraction and molar polarizability constant of Substituted-dihydropyrimidin-2(1H) One had been studied in different percentage of binary liquid mixture such as DMF-Water, THF-Water, Dioxane-Water, and Ethanol-Water at 27°C. There values were measured by Abbe's refractrometer. The details acquire from Refractrometric investigations was utilized to calculate molar refraction & polarizability constant which describe solute-solvent, solvent-solvent interactions.

Keywords: 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) one (Ligand 1), 5-ethoxy carbonyl-4-(4-nitro phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne (Ligand 2), Solvent-Water different percentage composition, Refractive index, molar polarization, polarizability constants..

1. INTRODUCTION

Refractive index is an important and exceptional property of liquid. Abbe's refractometer is used to evaluate refractive index of liquid solution. In various industries and in chemical analysis measurements of refractive index in combination with density, boiling point, melting point and other analytical data have wide applicability. The composition of binary liquid mixture is determined by prediction of refractive indices of binary liquid mixture. The basic practical implementation of refractrometry, mainly requires the mensuration of concentration of one substance dissolved in another. Using refractive index anyone can clear its idea of aromatic content of liquid for pure hydrocarbon.

The refraction occurs when a shaft of light travel from one medium to another that is, the shaft of light gets bend so it moves in different direction. The angle of refraction (r) is slighter than angle of incident (i), if the light is allowed to pass from less concentrated to high concentrated medium. The refractive index (n) of the medium is the ratio of the velocity of light in vacuum to medium. The value of refractive index depends upon the wavelength of light used and its temperature. With high degree of accuracy, the measurement of refractive indices is possible. For Standard measurement of refractive index, the D-light of sodium is used. The symbol $^{20}n_D$ represents that refractive index has been find out at 20°C using D-line of sodium as the light source.

In the current investigation, with the help of Abbe's refractrometer, refractive indices of liquid mixtures are used to measure. Abbe's refractrometer is specially designed to measure the refractive indices of the small quantities of the solutions, transparent liquids, and it gives the range from 1.300 to 1.700 swiftly by straight reading.

In literature survey, relation between refractive index and density, dielectric permittivity and Surface tension occurs and it make use of refractive index so one can calculate the molecular composition of hydrogen bond complex.

2. LITERATURE REVIEW

The properties of refractivity of methyl alkanoates, n-ethanoate, ethyl alkanoates (homologous series) have been studied by Oswal SL, and co-workers [1], additive properties of molar polarizability constant and refractivity of Lincomycine, Pyridoxin in different solvent or media is Studied by Meshram YK and Ingle SR [2]. Nagargose DR [3] highlighted their studies on polarizability of 3 - acetyl –methyl -(2H)-pyran-2, 4,-(3H)-dione derivative and viscosity in different phase systems and polarizability constant, molar refraction, viscosity is affected by nature of solute. Polarizability constant and molar refraction of various heterocyclic compound have been revealed by Arbad BR, and co-workers [4]. Number of analyst are interested in interaction of solute-solvent of binary mixture [5-6]. The Properties of electrolytic and non-electrolytic solvent such as, molar refraction, polarizability constant, viscosity interact with various solute and give rise to numerous physical parameter of solvent mixture was studied by Raikar SK and Aminabhavi TM [7]. Many researcher and their co-workers show light on properties of solutions i.e., refractive index, ultrasonic velocity and viscosity of liquid mixture of binary solution [8-15]. Rathnaan MV and Oswal SL [16] show some light on refractive index, indices and dielectric constant of binary mixture. Pandey JD, and co-workers [17] has thrown light on refractivity of binary solutions and ternary solutions.

Refractive index of liquid mixture is assessing and applied extensively by various theoretical methods. During recent past years, experimental work of dielectric constant and refractive index of solutions and solution mixture gives valuable and reliable knowledge of specific interactions between the components.

Additive properties such as molar polarizability constant and molar refraction or refractivity of amoxicillin, acenocoumarol, allopurinol, warfarin indifferent media was highlighted by Sonune KM, and co-workers [18]. The calculations of two quantities of more than one, two or three i.e. multi component mixture was gain by finding out relationship of refractive index with mass density and consistency of the mixing rule has been studied by Yangang Liu, Daum, Peter H. [19].

The study of heterocyclic compound under feasible environments has done by Syal VK., and co-workers [20]. and they shed light on the velocity and ultrasonic velocity of PEG-study of acoustical properties, PEG-8000, viscosity coefficient. Yadava SS, and co-workers [21] revealed that the binary mixture such as bromo-alkane and nonpolar hydrocarbon and molecular interaction between the component of binary mixture are also find out by refractive indices and molar refraction.

3. EXPERIMENTAL

3.1. Material and methods

The compound such as 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) one, 5-ethoxy carbonyl-4-(4-nitro phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) one, were synthesized by an appropriate method in the laboratory and their purity was checked by TLC, IR and M.P. The compound was dissolved by appropriate amount of weight in different solvents like Ethanol, THF, DMF and Dioxane. The instrument used for weighing was Mechaniki Zaktady Precyzying Gdansk Balance made in Poland with accuracy (+0.001gm). The bi-capillary pycnometer (+0.2%) having a bulb volume of about 10 cm^3 was used to measure densities of solution and in bi-capillary the internal diameter of capillary was 1mm. Abbe's refractometer was used to measure the refractive indices of solvent mixtures and solutions at 27°C. Abbe's refractometer had an accuracy within (+0.001) unit at different concentrations (0.63 x 10-3 to 10.0 x 10-3M). Abbe's refractometer was calibrated with glass piece (n=1.5220) provided with the instrument and by circulating water from thermostat, the temperature of the prism box was maintained constant.

3.2. General equations used for calculation

Molar refraction at different molarity and polarizability constants and refractive indices were calculated from equation.

$$Rm = \frac{n^2 - 1}{n^2 + 2} \times \frac{m}{d}$$

Where,

m = Mass of ligand in grams.
d = Density of solution of ligand.
n = Refractive index.
Rm = Molar refraction

Similarly, Rm was calculated by using equation:

$$Rm = \frac{4}{3} \pi N_o \propto$$

$$\propto = \frac{3\,Rm}{4\,\pi\,N_o}$$

Where,

N_o = Avogadro's number having value 6.023×10^{23} mole.

$\propto$ = Polarizability constant.

Lorentz-Lorentz equation is used to determine the molar refraction of solvent and solution.

One can estimate molar refraction of solution by:

$$Rm\,(sol^n) = X_1Rm_1 + X_2Rm_2$$

Where,

Rm = Molar refraction
X_1 and X_2 = Mole fraction of solvent and solute in solution.
Rm_1 and Rm_2 = Molar refraction of solvent and solute.

The actual or true volume of molecule in mole is represented by molar refraction.

The calculation of molar refraction of solute is done by given formula as:

$$Rm_{(solute)} = R_{(mixture)} - R_{(solvent)}$$

4. RESULTS AND DISCUSSION

By using Abbe's refractometer, we calculated refractive index of solvent and solution at different concentrations and the values of molar refraction, polarizability constant and refractive index were estimated and shown in table 1 to 4 for different systems.

4.1. Observation tables

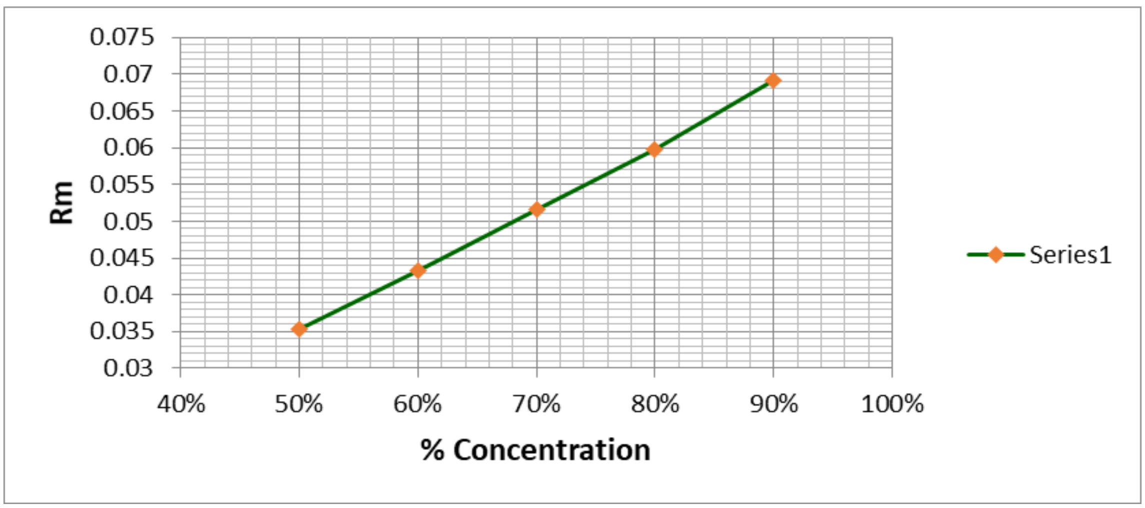
Ligand-1: 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) one.

Molecular formula: $C_{15}H_{18}O_4N_2$

4.1.1. 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DMF

Table 1:

Sr. NO	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_\infty = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant $\propto$
1	90 %	1.4320	2.0506	0.2791	0.0692	2.7447×10^{-26}
2	80 %	1.4260	2.0335	0.2718	0.0598	2.3711×10^{-26}
3	70 %	1.4240	2.0278	0.2673	0.0516	2.0455×10^{-26}
4	60 %	1.4170	2.0079	0.2618	0.0432	1.7130×10^{-26}
5	50 %	1.4090	1.9852	0.2557	0.0353	1.3991×10^{-26}

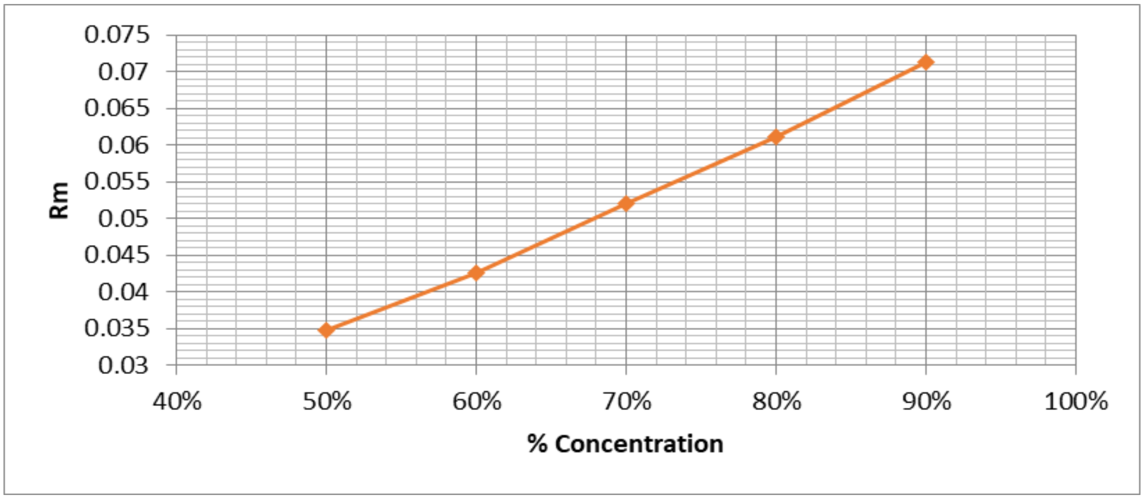


Graph 1:

4.1.2. 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in THF

Table 2:

Sr. NO	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_\infty = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant $\propto$
1	90 %	1.4210	2.0192	0.2873	0.0713	2.8256×10^{-26}
2	80 %	1.4140	1.9994	0.2780	0.0612	2.4254×10^{-26}
3	70 %	1.4060	1.9768	0.2697	0.0520	2.0641×10^{-26}
4	60 %	1.3940	1.9432	0.2585	0.0426	1.6894×10^{-26}
5	50 %	1.3900	1.9321	0.2519	0.0348	1.3788×10^{-26}

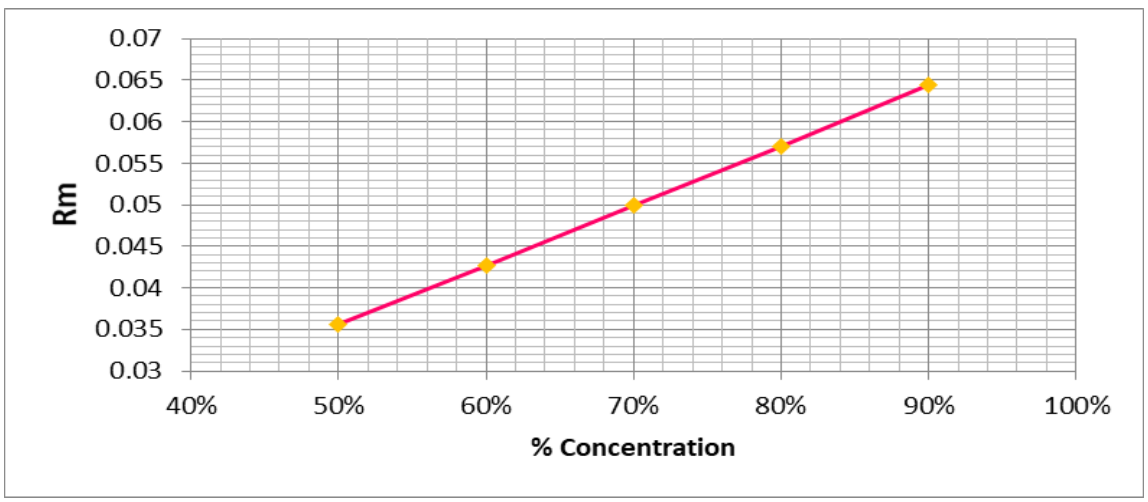


Graph 2:

4.1.3. 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in THF

Table 3:

Sr. NO	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_{\infty} = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant $\propto$
1	90 %	1.4230	2.0249	0.2597	0.0644	2.5543×10^{-26}
2	80 %	1.4160	2.0050	0.2595	0.0571	2.2643×10^{-26}
3	70 %	1.4080	1.9825	0.2587	0.0499	1.9803×10^{-26}
4	60 %	1.3990	1.9572	0.2585	0.0427	1.6933×10^{-26}
5	50 %	1.3870	1.9238	0.2583	0.0356	1.4135×10^{-26}



Graph 3:

4.1.4. 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in Ethanol

Ligand-2: 5-ethoxy carbonyl-4-(4-nitro phenyl)-6-methyl-3, 4 dihydropyrimidine-2(1H) 0ne.

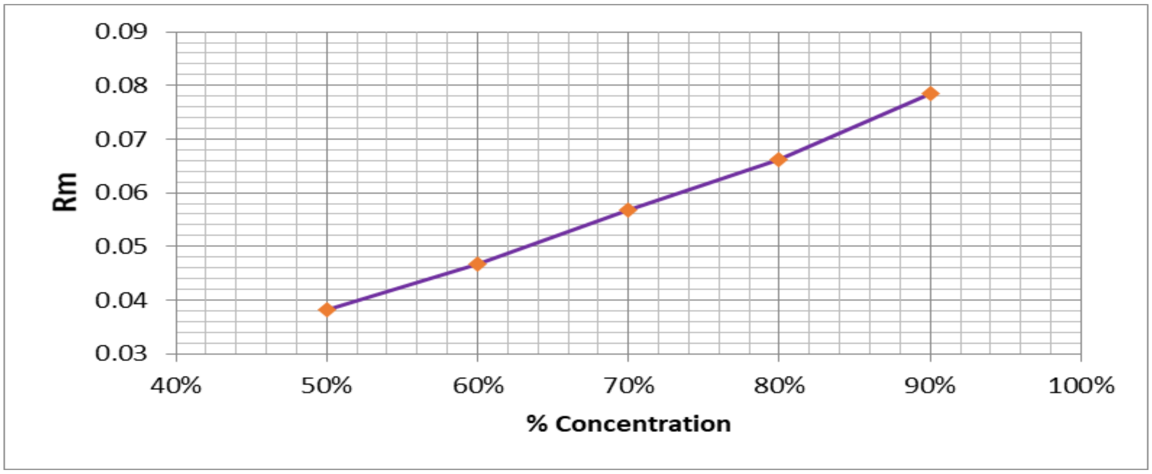
Molecular formula: $C_{14}H_{15}O_5N_3$.

4.1.5. 5-ethoxy carbonyl-4-(4-nitro phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DMF

4.1.6. 5-ethoxy carbonyl-4-(4-nitrophenyl)-6 methyl -3,4 dihydropyrimidine-2(1H) 0ne in THF

Table 4:

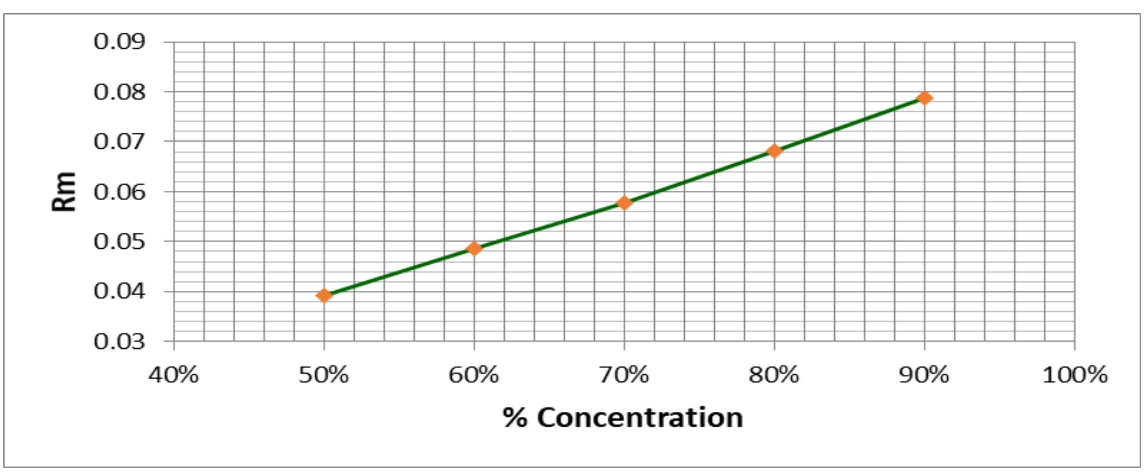
Sr. NO	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_{\infty} = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant $\propto$
1	90 %	1.4150	2.0022	0.3160	0.0784	3.1078×10^{-26}
2	80 %	1.4120	1.9937	0.3010	0.0662	2.6260×10^{-26}
3	70 %	1.4090	1.9852	0.2941	0.0568	2.2508×10^{-26}
4	60 %	1.4020	1.9656	0.2834	0.0468	1.8542×10^{-26}
5	50 %	1.3980	1.9544	0.2762	0.0381	1.5114×10^{-26}



Graph 4:

Table 5:

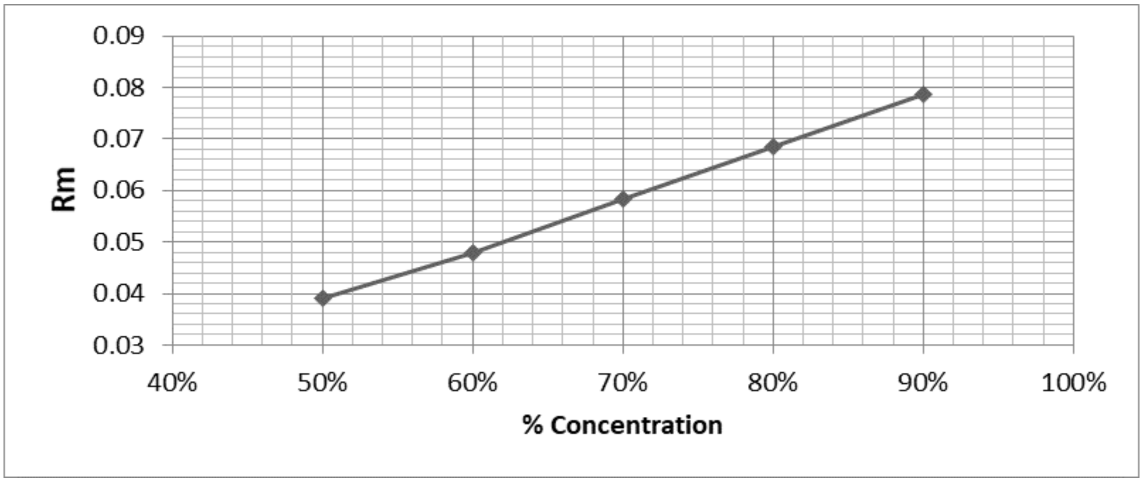
Sr. NO	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_{\infty} = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant $\propto$
1	90 %	1.4430	2.0822	0.2877	0.0788	3.1266×10^{-26}
2	80 %	1.4360	2.0621	0.2793	0.0681	2.7022×10^{-26}
3	70 %	1.4250	2.0306	0.2712	0.0578	2.2909×10^{-26}
4	60 %	1.4220	2.0221	0.2661	0.0487	1.9310×10^{-26}
5	50 %	1.4120	1.9937	0.2584	0.0393	1.5578×10^{-26}



Graph 5:

Table 6:

Sr. No.	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_{\infty} = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant ∝
1	90 %	1.4150	2.0022	0.2870	0.0786	3.1181×10^{-26}
2	80 %	1.4130	1.9965	0.2812	0.0686	2.7213×10^{-26}
3	70 %	1.4080	1.9825	0.2743	0.0584	2.3169×10^{-26}
4	60 %	1.3950	1.9460	0.2622	0.0480	1.9028×10^{-26}
5	50 %	1.3890	1.9293	0.2568	0.0390	1.5480×10^{-26}

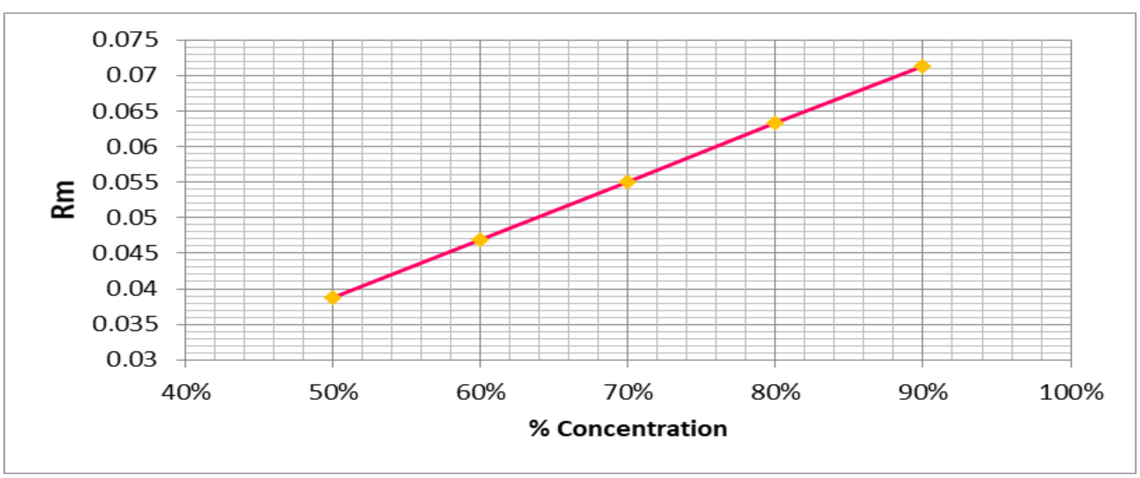


Graph 6:

4.1.7. 5-ethoxy carbonyl-4-(4-nitro phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in Dioxane

Table 7:

Sr. No.	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_{\infty} = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant ∝
1	90 %	1.4280	2.0392	0.2602	0.0713	2.8275×10^{-26}
2	80 %	1.4220	2.0220	0.2594	0.0633	2.5102×10^{-26}
3	70 %	1.4150	2.0022	0.2588	0.0551	2.1861×10^{-26}
4	60 %	1.4020	1.9656	0.2563	0.0469	1.8601×10^{-26}
5	50 %	1.3910	1.9349	0.2545	0.0387	1.5341×10^{-26}

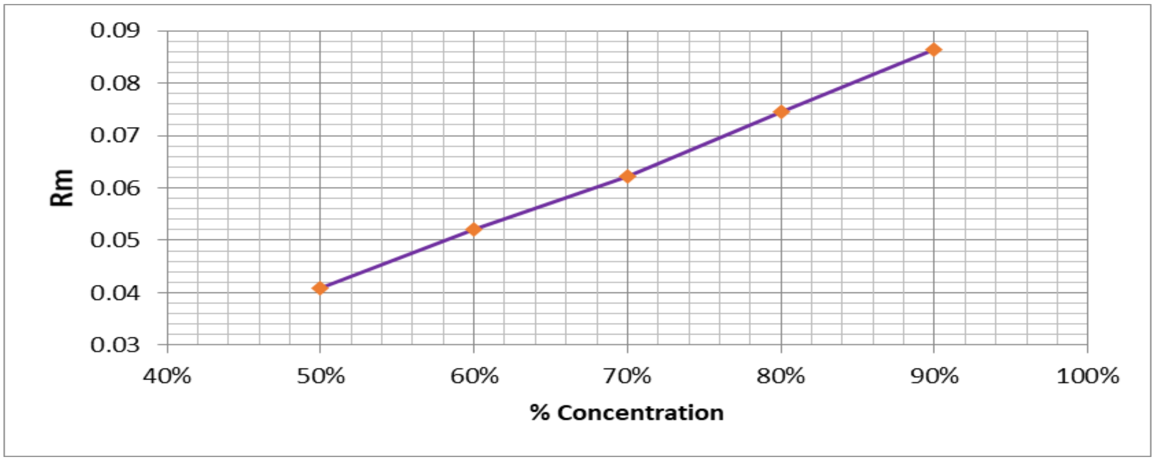


Graph 7:

4.1.8. 5-ethoxy carbonyl-4-(4-nitro phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in Ethanol.

Table 8:

Sr. No.	Conc. %	Refractive Index (n)	High Frequency dielectric constant $\varepsilon_\infty = n^2$	Specific Refraction R	Molar Refraction Rm	Polarizability Constant ∝
1	90 %	1.4150	2.0022	0.3152	0.0864	3.4255×10^{-26}
2	80 %	1.4120	1.9937	0.3058	0.0746	2.9590×10^{-26}
3	70 %	1.4080	1.9825	0.2925	0.0623	2.4708×10^{-26}
4	60 %	1.4040	1.9712	0.2845	0.0521	2.0648×10^{-26}
5	50 %	1.3990	1.9238	0.2690	0.0409	1.6213×10^{-26}



Graph 8:

5. CONCLUSION

Molar Refraction, Polarizability Constant (∝), Refractive index are important physical parameter of liquids. The potential of refractrometry depends on sensitivity and time of measuring.

The value of Molar Refraction (Rm), Polarizability Constant (∝), Refractive Index (n), Specific Refraction (R), High Frequency dielectric constant of Ligand - 1 and Ligand-2 in DMF-Water, THF-Water, Dioxane-Water, and Ethanol-Water are shown in Table 4.1.1 to 4.2.4 and the graphs between specific refraction verses concentration are plotted for each table and shown in graphs 4.1.1 to 4.2.4. From graph we noticed that Molar refraction and Concentration has linear relationship and from this we can calculate the concentration of unknown ligand.

From table 4.1.1 to 4.2.4 for ligand 1 and 2 we found that the values of Molar refraction and Polarizability constant for ethanol-water are found to be greater than DMF-water, THF-water, and Dioxane-water because ethanol is polar solvent while DMF, THF and Dioxane are non-polar solvent, and polar solvent contains Hydrogen-bonding and so they form complex with solute but non-polar solvent has lack of H-bonding so they do not form complex with solute. Generally, it is noticed that the substances which carry more polarizability (soft) group will normally have higher refractive indices than substances which carry less polarizability (hard) groups.

6. ACKNOWLEDGEMENT

I am grateful to Miss. Suchita T.Peddiwar, Miss. Kavita Khobragade, Dr. Dipti K. Ingole and Mr. S.V. Pusala who has honestly helped me and gave inspirational support which was the most precious contribution for the completion of this work.

Conflict of interest

The author hereby declares that there is no conflict of interest.

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