ORIGINAL RESEARCH PAPER | Science | Volume : 6 | Issue : 7 | July 2016 | ISSN - 2249-555X | IF : 3.919 | IC Value : 74.50

Refractrometry Study of Some Substituted Heterocyclic Compound in Different Solvent

KEYWORDS: Molar refractivities , molar polarizability constant and Viscosity coefficient, Behaviour, histology

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ABSTRACT *Refractive index, molar refractivity and molar polarizability constant of substituted heterocyclic compound such as 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne, 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne, have been studied in DMF, THF, Dioxan, Ethanol media at 303 K ± 0.1°C temperature and different concentration (0.625x 10-3to 10.0x 10-3M). The values of molar refraction (Rm) and molar polarizability (α) constant are found to be decreasedwith decreasing concentration of solute in solvent. Viscosity coefficient (A, B) evaluate by using jone-dole equation. These parameters throw the light on the solute – solvent interaction and solute – solute interaction.*

INTRODUCTION

The refractive index is an important additive property of liquid. In regular practice, the major use of refractrometry is in chemical, food, agriculture, pharmaceutical, oil and beverage industries. The practical application of refractrometry, mainly involves the measurement of concentration of one substance dissolved in another. For pure hydrocarbon, one can get an idea of aromatic content of liquid using refractive index.

When a beam of light passes from one medium to another, it suffers refraction that is, the beam of light bending so that it travels indifferent direction. If the light is passes from less dense to high denser medium then it is refracted toward normal so that the angle of refraction (r) is less than angle of incident (i). The ratio of the velocity of light in vacuum to that in the medium is the refractive index (n) of the medium.Refractive indices can be measured easily with a high degree of accuracy. The value depends upon the temperature as well as the wavelength of light used. Generally, the D-light of sodium is used for standard measurements. The symbol 20nD indicates that refractive index has been determined at 20°C using D- line of sodium as the light source.

The extent of Refraction depends on :-

1) The relative concentration of atom or molecule.

2) the structure of atom or molecule.

So refractive index gives idea about geometry and structure of molecule. Refraction of light is additive property; it also depends on the structural arrangement of atom in molecule. Sometimes, this can be used to determine the structure of an unknown compound whose molecular formula is known.

In the present investigation, refractive indices of liquid mixtures were measured with the help of Abbe's refractrometer, specially designed to measure the refractive indices of the small quantities of the transparent liquids, solutions ranging from 1.300 to 1.700 rapidly by direct reading. From literature it was found that much work have been done over many of the substitutedheterocyclic drugs, chalcones, pyrazolines is oxazapine and various ketones by

spectrophotometrically and Refractometrically.

Thermo-physical properties of a solution provide complementary information about the mixing process and interactions between their components. In literature several correlation have been found between refractive index and density, Surface tension dielectric permittivity and use of refractive index to calculate the molecular composition of hydrogen bonded complex. Oswal et.a[1]l have been studied refractivity properties of some homologous series such as n-ethanoate, methyl alkanoates, ethyl alkanoates etc. were measured in the temperature range from298.15 to 333.150K. Meshram YK and et.al[2] has been studied additive properties such as molar refractivity and molar polarizability constant of Pyridoxin, Lincomycine in different media. Arbad BR and et al[3] have studied the molar refraction and polarizability constant. Nagargioje et al[4] have studied to viscosity and polarizability of 3 – acetyl -methyl– (2H) – pyran – 2, 4, - (3H) – dione derivative in different phase systems and nature of solute affects viscosity, molar refraction and polarizability constants. Various researchers are interested to find out binary liquid mixture interaction along with Soult[55 -66] viscosity, molar refraction and polarizability constant of electrolytic and non-electrolytic solvent with solute give various new physical parameters of solvent mixture[77]. The property of liquid such as viscosity refractive index and ultrasonic velocity of binary mixture are studied by many workers[88- 915] Oswal et[1016] al have studied dielectric constant and refractive index indices of binary mixture. Theoretical study of refractivity of binary and ternary solutions has been done by J.D. Pandey and et al[1117]

Experimental measurement of refractive index and dielec-

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tric constant of liquid and liquid mixture have gained much importance during recent past since these data given reliable information regarding the specific interactions between the components.

The measurement of dielectric constant have been mostly in binary mixtures and for ternary system dielectric data are available. Different theoretical methods have been extensively applied to evaluate refractive index of liquid mixture.

Sonune et.al[1218]. has been studied additive properties such as molar refractivity and molar polarizability constant of allopurinal, acenocoumarol, warfarin and amoxicillin indifferent media. Yangang Liu[1319] has studied relationship of refractive index to massdensityand consistencyof the mixing rule use to calculate these two quantities of multicomponent mixture like ambient aerosols with the index-densityrelationship.

Syal and et.al.[1420] has been studied the ultrasonic velocityand viscosity of PEG-8000, PEG- studyofacoustical properties, viscositycoefficient of substituted heterocyclic compounds under suitable condition. Anand Yadava S.S.[1521] has studied refractive indices of binary mixture of bromoalkane and nonpolar hydrocarbons, also studied molecular interaction between the components of binary mixtures.

However study of molar refractivity, molar polarizability constant and viscosity coefficents of substituted heterocyclic compounds such as 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne, 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne, have been studied in DMF, THF, Dioxan, Ethanol media under identical set of experimental condition. This could cover minifold aspect of solute-solvent interactions scanty. Therefore the present work is undertaken to make the systematic study of abovesubstituted heterocyclic compoundsrefractometricallyat 303 K.

Experimental

The solution of 5-ethoxy carbonyl-4-phenyl-6-methyl-3, 4 dihydropyrimidine-2(1H) 0ne, 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne, are prepared in different solvent like DMF, THF, Dioxan, Ethanol by dissolving an appropriate amount by weight. The compound is synthesized in the laboratory by standard method and purity is checked by M.P, TLC, IR, and NMR. All the weighing were made on mechaniki Zaktady Precyzying Gdansk Balance made inPoland (+0.001gm). The densities of solutions were determined by a bi-capillary pynometer (+0.2%) having a bulb volume of about 10 cm3and capillary having an internal diameter of 1mm. The refractive indices of solvent mixture and solutions were measure by Abbe's refractometer at 27 0C. The accuracy of Abbe's refractometer was within (+0.001) unit at different concentrations (0.63 x 10-3 to 10.0 x 10-3M). The temperature of the prism box is maintained constant by circulating water from thermostat calibrated with glass piece (n=1.5220) provided with the instrument.

T… refraction at different mo… s can be calculated from

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

Where, m = Mass of ligand in grams.

d = Density of solution of ligand.

n = Refractive index.

Rm= Molar refraction

Simillarly, Rm can be calculated by using equation :

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

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

Where,

No= Avogadro's number having value mole.

$\propto$ = Polarizablity constant.

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

The molar refraction of solution are determine from :

Rm (soln) = X1Rm1 + X2Rm2

Where,

Rm= Molar refraction

X1 and X2 = Mole fraction of solvent and solute in solution.

Rm1 and Rm2 = Molar refraction of solvent and solute.

The molar refraction represents actual or true volume of substance molecule in mole.

The molar refraction of solute can be calculated as :-

Rm(solute) = R(mixture) – R(solvent)

The refractive index of solvent and solution at different concentration are measured from Abbe's refractometer and the values of refractive index, molar refraction, and polarizablity constant are evaluated and present in table no 1.1 to 2.4 for different system.

Ligand-1:

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

Molecular formula: C14H16O3N2

Observation Table 1.1 :- 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in THF

Sr. No	Molarity	R.I. (n)	€∞=n2 High frequency dielectric constant	Specific Refraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4020	1.9656	0.2671	0.0177	7.0192×10^{-27}
2	0.005 M	1.3930	1.9404	0.2671	0.0085	3.3806×10^{-27}
3	0.0025 M	1.3900	1.9321	0.2608	0.0042	1.6755×10^{-27}
4	0.00125 M	1.3890	1.9293	0.2608	0.0021	0.8379×10^{-27}
5	0.00063 M	1.3830	1.9127	0.2582	0.0010	0.4096×10^{-27}

Table : 1.1

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1.2 :- 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DMF

Observation Table 1.2 :- 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DMF

Sr.No	Molarity	R.I. (n)	€∞=n2 High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4110	1.9909	0.2770	0.0180	7.1402×10^{-27}
2	0.005 M	1.4100	1.9881	0.2767	0.0090	3.5668×10^{-27}
3	0.0025 M	1.4090	1.9852	0.2764	0.0045	1.7757×10^{-27}
4	0.00125 M	1.3920	1.9377	0.2665	0.0022	0.8559×10^{-27}
5	0.00063 M	1.3900	1.9321	0.2656	0.0011	0.4213×10^{-27}

Table : 1.2

Observation Table 1.3 :- 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DIOXAN

Sr.No	Molarity	R.I. (n)	€∞=n2High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4070	1.9797	0.2529	0.0164	6.5197×10^{-27}
2	0.005 M	1.4000	1.9600	0.2497	0.0081	3.2180×10^{-27}
3	0.0025 M	1.3920	1.9377	0.2454	0.0040	1.5768×10^{-27}
4	0.00125 M	1.3820	1.9099	0.2399	0.0019	0.7706×10^{-27}
5	0.00063 M	1.3760	1.8934	0.2368	0.0009	0.3757×10^{-27}

Table : 1.3

Observation Table 1.4 :- 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in ETHANOL.

Sr.No	Molarity	R.I. (n)	€∞=n2High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4120	1.9937	0.3257	0.0212	8.4073×10^{-27}
2	0.005 M	1.4090	1.9852	0.3240	0.0105	4.1759×10^{-27}
3	0.0025 M	1.3800	1.9044	0.3043	0.0049	1.9549×10^{-27}
4	0.00125 M	1.3720	1.8824	0.2990	0.0024	0.9605×10^{-27}
5	0.00063 M	1.3700	1.8769	0.2981	0.0012	0.4729×10^{-27}

Table : 1.4

Ligand-2 :-

2.1 :- 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in THF.

Molecular formula: C15H18O4N2

Observation Table

Sr.No	Molarity	R.I. (n)	€∞=n2High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4040	1.9712	0.2931	0.0202	8.0210×10^{-27}
2	0.005 M	1.4010	1.9628	0.2916	0.0101	4.0053×10^{-27}
3	0.0025 M	1.3920	1.9377	0.2860	0.0049	1.9565×10^{-27}
4	0.00125 M	1.3810	1.9072	0.2790	0.0024	0.9543×10^{-27}
5	0.00063 M	1.3790	1.9016	0.2780	0.0012	0.4793×10^{-27}

Table : 2.1

2.2 :- 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DMF.

Observation Table :-

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Sr.No	Molarity	R.I. (n)	€∞=n2High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4050	1.9740	0.2745	0.0189	7.5099×10^{-27}
2	0.005 M	1.3940	1.9432	0.2679	0.0092	3.6484×10^{-27}
3	0.0025 M	1.3840	1.9210	0.2633	0.0046	1.8242×10^{-27}
4	0.00125 M	1.3730	1.8989	0.2587	0.0022	0.8850×10^{-27}
5	0.00063 M	1.3700	1.8769	0.2540	0.0011	0.4379×10^{-27}

Table : 2.2

2.3 :- 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DIOXAN .

Observation Table :-

Sr.No	Molarity	R.I. (n)	€∞=n2High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4210	2.0192	0.2597	0.0179	7.1068×10^{-27}
2	0.005 M	1.4180	2.0107	0.2589	0.0089	3.5422×10^{-27}
3	0.0025 M	1.4060	1.9768	0.2529	0.0044	1.7449×10^{-27}
4	0.00125 M	1.4020	1.9656	0.2513	0.0022	0.8725×10^{-27}
5	0.00063 M	1.3920	1.9377	0.2464	0.0011	0.4362×10^{-27}

Table : 2.3

2.4 :- 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in ETHANOL.

Observation Table :-

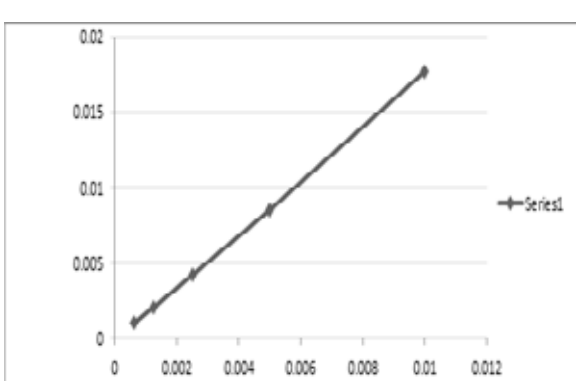
Sr.No	Molarity	R.I. (n)	€∞=n2High frequency dielectric constant	SpecificRefraction (R)	Molr Refraction Rm	Polarizability Constant
1	0.01 M	1.4140	1.9994	0.3262	0.0225	8.9271×10^{-27}
2	0.005 M	1.4020	1.9656	0.3184	0.0110	4.3623×10^{-27}
3	0.0025 M	1.4000	1.9600	0.3177	0.0055	2.1811×10^{-27}
4	0.00125 M	1.3910	1.9349	0.3122	0.0027	1.0679×10^{-27}
5	0.00063 M	1.3860	1.9210	0.3100	0.0013	0.5345×10^{-27}

Table : 2.4

Ligand-1: Graph

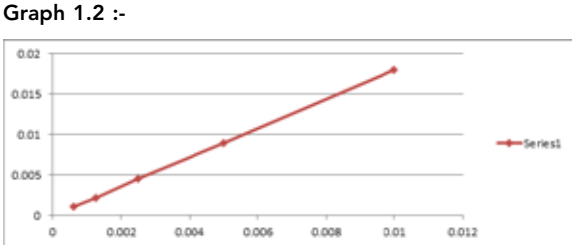
5-ethoxy carbonyl-4-phenyl-6-methyl-3,4-dihydropyrimidine-2(1H) 0ne.

Graph1.1:-



Graph 1.1 :-Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in THF.

Graph 1.2 :-



Graph 1.2 :-Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-phenyl-6-methyl-3, 4 dihydropyrimidine-2(1H) 0ne in DMF.

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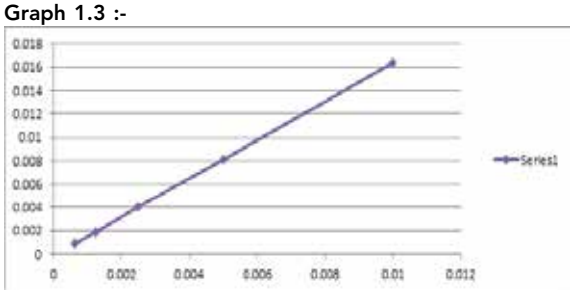
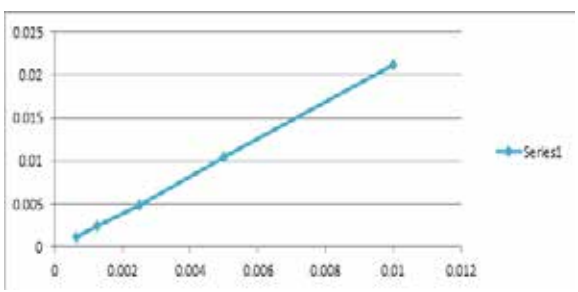
Graph 1.3 :-



Graph 1.3 :-Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in Dioxan.

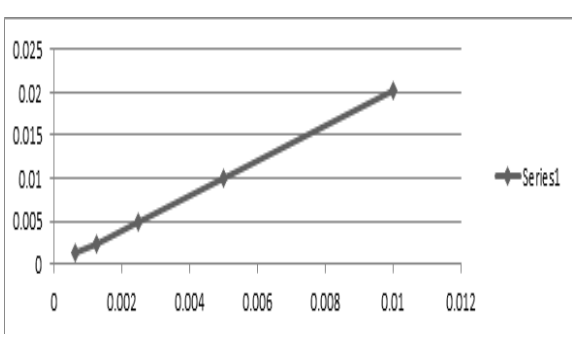
Graph 1.4 :-



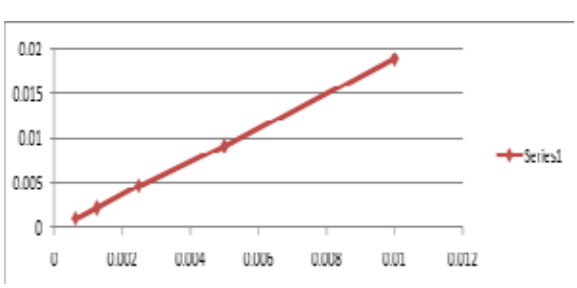
Graph 1.4 :-Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-phenyl-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in Ethanol.

Ligand-2: Graph

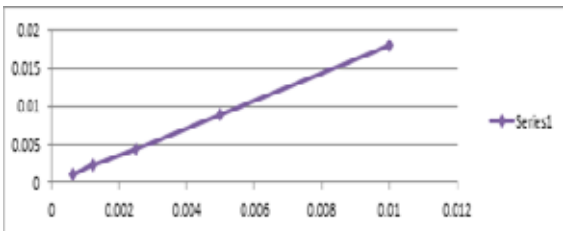
5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne.



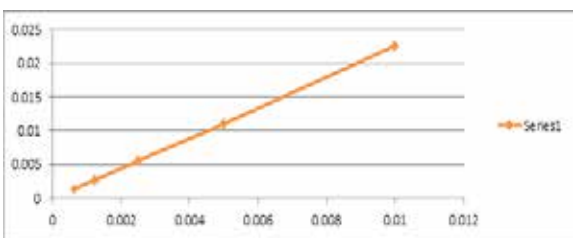
Graph 2.1 :- Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in THF.



Graph 2.2 :- Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in DMF.



Graph 2.3 :- Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne in Dioxan.:-



Graph 2.4 :- Specific Refraction (R) Vs Concentration (C) for 5-ethoxy carbonyl-4-(4-methoxy phenyl)-6-methyl-3,4 dihydropyrimidine-2(1H) 0ne inEthanol.

RESULTS AND DISCUSSION

The value of molar refraction (Rm) and molar polarizability constant (α) of polar solvents, like Ethanol, is found to be greater than non polar solvents like DMF. Because polar solvent contains H- bonding, may form complex with solute, but non polar solvent does not contains H-bonding and does not form complex with solute.

This may be characteristics to the fact that the dipole in the compound lies perpendicular to the longer axis of the molecule shows intermolecular attraction take place which will be accompanied by increase the value of molar refraction and molar polarizability constant with increasing concentration of solution because of mutual compensation of dipoles.

The values of molar refraction and polarizability constant of different ligands are presented in table 1.1 to1.4. The graphs between specific refraction verses concentration are plotted and show in figure 1.1to 1.4 it could be seen that there is linear relationship between molar refraction and concentration from this. The concentration of unknown solution of the ligand calculated.

It is also observed that the refractive index is linearly related to percentage of dissolved solids in a solution in deferent solvent. By related to percentage the value of the refractive index of a solution to that of a stander curves the concentration of solute can be determined with good accuracy. It is observed that the substances containing more polarizability (soft) group will normally have higher refractive indexes than substances containing less polarizability (hard) groups.

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