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# Study of Some Physical Properties of Substituted Pyrazole Carboxylic Acid by Refractometric Technique at 300k in Different Binary Mixtures

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***ABSTRACT: Refractometric study of substituted pyrazole carboxylic acid derivatives were carried out in different binary mixture at 300K. Abbe's refractometer used to measure refractive index. molar refractions and polarizability constants values in different binary mixtures are determined . The solute-solute, solute-solvent and solvent-solvent interaction in the system are predicted by using relative data***

***Keywords: substituted pyrazole carboxylic acid derivatives, refractive index. molar refraction, polarizability constant.***

## I. INTRODUCTION

Measurement of refractive index shows applications in pharmaceutical, chemical, agriculture, food, oil and beverage industries. The refractometric study of substituted aminopyrimidine in polar solvent is reported. [1] Study molecular interaction of substituted azomethine drugs is done by refractometrically.[2] Some homologous series such as n-ethanoate, methyl alkanoates and ethyl alkanoates are studied by refractometry technique. [3] Refractive index and density is studied for substituted N,N'-bis(salicyliden)-arylmethanediamine. [4] Density and refractive index for substituted 2,3-dihydroquinazolin-4(1H)-ones is reported. [5] Molar refractions for aqueous solution KCl and $KBrO_3$ have studied. [6] Densities and refractive index of different substituted hydrazone have investigated and from this data, molar refraction (Rm) and polarizability constant (α) was reported. [7] Refractometry technique is used to measure the dissolved solids content of both pure and impure sucrose solutions in the sugar industry.[8] Refractometric technique is considered as an important tool for the measurement of glucose concentrations in body fluids such as blood and the intercellular fluid. [9]Molar refraction and polarizability constant have studied for 2-hydroxy-5-ethyl-benzene and 2-amino-5-chloro-benzene sulphonic acid in dioxane and DMF-water medium respectively. [10] The dielectric constant and refractive index is reported for phenols in mixture of benzene acetone and carbon tetrachloride.[11]Refractometric study of some substituted oxoimidazoline drugs in different concentration of solute and solvents are reported. [12] Refractometric study of six binary mixtures of N-butyl bromide with aniline, carbon tetrachloride, benzene, xylene, toluene and n-heptane for the entire concentration range have done at 303.15 K. [13] Refractive index, density, molar refraction and polarizability constant of substituted 2-oxo-2Hchromene-3-carbohydrazide derivatives in different binary mixture are done. [14] Comparison of refractive index of aqueous mixture of zinc and lead acetate with different temperature at different concentration is done. [15]

The present work deals with the study of molar refraction and polarizability constant of following compounds in nonaqueous solvent such as acetone, methanol and DMF (with different percentage)

1) Ligand A ($L_A$)= 1- phenyl-3-(4'- methyl) phenyl-1H- pyrazol-4-carboxylic acid
2) Ligand B ($L_B$)= 1- phenyl-3-(4'- bromo) phenyl-1H- pyrazol-4-carboxylic acid
3) Ligand C ($L_C$)= 1- phenyl-3-(4'- ethyl) phenyl-1H- pyrazol-4-carboxylic acid
4) Ligand D ($L_D$)= 1,3-diphenyl-1H- pyrazol-4-carboxylic acid

## II. EXPERIMENTAL

The refractive indices of solution and solvent mixture under study are determined using Abbe's refractometer. Density of solutions is measured using 10 ml specific gravity bottle. Initially the refractometer is calibrated with glass piece (n=1.5220) provided with instrument. All weightings 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. [16] The solutions of compounds under study are prepared in different solvents acetone, ,methanol and DMF by keeping constant ligand concentration system (0.01M). All chemical used are of A.R. grade.

## III. 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. [17]The molar refraction of solvent, solution can be determined by following equation. [18]

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

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

The molar refraction [19,20,21] of solutions of ligand in solvent -water mixtures are determined from-

$$R_{Mix} = \frac{(n^2-1)}{(n^2+2)} + \left\{\frac{[X_1M_1+X_2M_2+X_3M_3]}{d}\right\} \qquad (2)$$

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 –

$$R_{lig} = R_{Mix} - R_{SOL-W} \qquad (3)$$

The polarizability constant (α) [22,23]of ligand can be calculated from following relation-

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

Where, No is Avogadro's numbe

In the present study, at various percentage of different solvent mixture at temperature 300K, molar refraction and polarizability constant value of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid are reported. The experimental data gives idea that there is increased in refractive index with increase in percentage composition of solvent. This is an indication of the fact that refractive index is correlated with the interactions occurring in the solution.

Table-1: Molar refraction values for different % of solvent mixture

| Solvent mixture % | Molar refraction [R] | |
|---|---|---|
| | Ethanol | DMSO |
| 20 | 12.5481 | 19.1245 |
| 40 | 11.6471 | 18.7410 |
| 60 | 10.1213 | 17.2420 |
| 80 | 7.9540 | 13.8321 |
| 100 | 4.2145 | 4.4654 |

Table- 2: Refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) values at 300K

| Conc. In % | ligand concentration (0.01M) with change in DMSO percentage | | | |
|---|---|---|---|---|
| | Refractive index (n) | Density (d) $g/cm^3$ | Rm x $10^3$ $cm^3/mol$ | α x $10^{-23}$ $cm^3$ |
| Ligand $L_A$ | | | | |
| 20 | 1.355 | 1.0232 | 64.468 | 2.5566 |
| 40 | 1.340 | 1.0036 | 70.754 | 2.8058 |
| 60 | 1.347 | 0.9835 | 76.613 | 3.0300 |
| 80 | 1.361 | 0.9843 | 80.2823 | 3.1830 |
| 100 | 1.377 | 0.9866 | 84.032 | 3.3324 |

| | | | | |
|---|---|---|---|---|
| Ligand $L_B$ | | | | |
| 20 | 1.361 | 1.0261 | 71.280 | 2.8267 |
| 40 | 1.345 | 1.0046 | 78.267 | 3.1030 |
| 60 | 1.363 | 0.9830 | 87.170 | 3.4570 |
| 80 | 1.380 | 0.9804 | 92.234 | 3.6577 |
| 100 | 1.394 | 0.9808 | 96.325 | 3.8199 |
| Ligand $L_C$ | | | | |
| 20 | 1.364 | 1.0285 | 71.642 | 2.8410 |
| 40 | 1.348 | 1.0099 | 78.612 | 3.117 |
| 60 | 1.365 | 0.9856 | 87.346 | 3.460 |
| 80 | 1.383 | 0.9184 | 92.629 | 3.673 |
| 100 | 1.396 | 0.9818 | 96.435 | 3.824 |
| Ligand $L_D$ | | | | |
| 20 | 1.367 | 1.0512 | 79.799 | 3.1646 |
| 40 | 1.352 | 1.0210 | 87.895 | 3.4850 |
| 60 | 1.369 | 0.9880 | 97.677 | 3.8736 |
| 80 | 1.385 | 0.9423 | 103.170 | 4.0914 |
| 100 | 1.399 | 0.9858 | 107.328 | 4.2563 |

Table-3: Refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α)values at 300K

| Conc. In % | ligand concentration (0.01M) with change in Ethanol percentage | | | |
|---|---|---|---|---|
| | Refractive index (n) | Density (d) $g/cm^3$ | Rm x $10^3$ $cm^3/mol$ | α x $10^{-23}$ $cm^3$ |
| Ligand $L_A$ | | | | |
| 20 | 1.363 | 0.9110 | 73.3500 | 2.90 |
| 40 | 1.372 | 0.9380 | 81.3961 | 3.22 |
| 60 | 1.407 | 0.9686 | 88.9328 | 3.52 |
| 80 | 1.435 | 1.0024 | 92.1871 | 3.65 |
| 100 | 1.454 | 1.0290 | 94.0129 | 3.72 |
| Ligand $L_B$ | | | | |
| 20 | 1.356 | 0.9044 | 79.2924 | 3.14 |
| 40 | 1.369 | 0.9315 | 88.9440 | 3.52 |
| 60 | 1.411 | 0.9609 | 98.8309 | 3.91 |
| 80 | 1.442 | 0.9934 | 103.0900 | 4.08 |
| 100 | 1.467 | 1.0204 | 106.4850 | 4.22 |
| Ligand $L_C$ | | | | |
| 20 | 1.358 | 0.9060 | 79.4811 | 3.15 |
| 40 | 1.350 | 0.9343 | 84.5635 | 3.35 |
| 60 | 1.366 | 0.9635 | 88.9154 | 3.52 |
| 80 | 1.388 | 0.9970 | 91.6173 | 3.63 |

| | | | | |
|---|---|---|---|---|
| 100 | 1.404 | 1.0241 | 93.5165 | 3.70 |
| Ligand $L_D$ | | | | |
| 20 | 1.355 | 0.9113 | 87.0388 | 3.45 |
| 40 | 1.351 | 0.9388 | 93.6236 | 3.71 |
| 60 | 1.371 | 0.9689 | 99.3289 | 3.93 |
| 80 | 1.392 | 1.0019 | 102.0990 | 4.04 |
| 100 | 1.411 | 1.0296 | 104.5470 | 4.14 |

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

**Fig.-1:Plot of Rm Vs percentage of DMSO solvent at constant (0.01M) ligand $L_A$concentration**

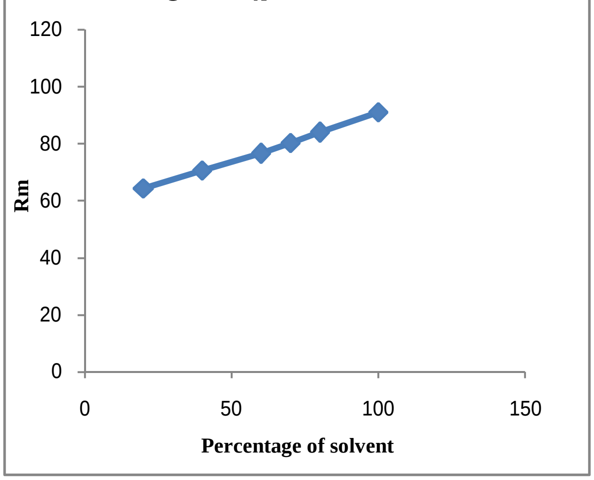



**Fig.-2:Plot of Rm Vs percentage of DMSO solvent at constant (0.01M) ligand $L_B$concentration**

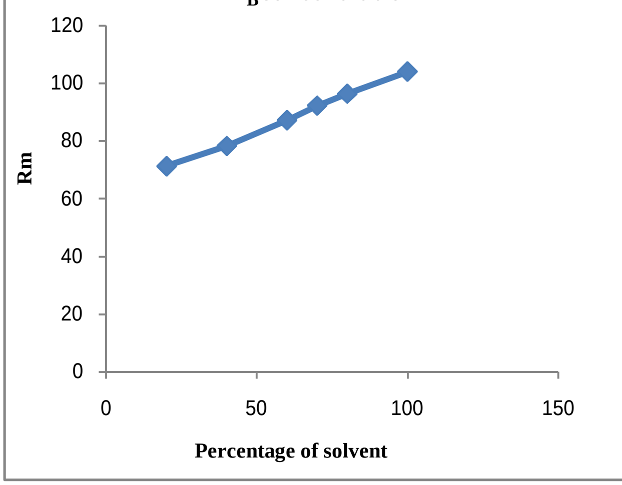



**Fig.-3:Plot of Rm Vs percentage of DMSO solvent at constant (0.01M) ligand $L_C$concentration**

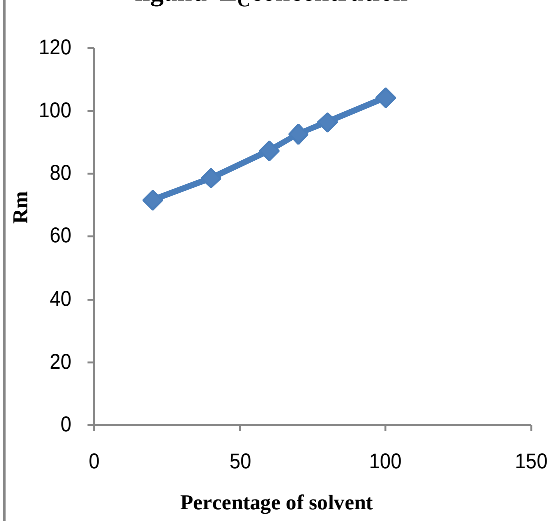
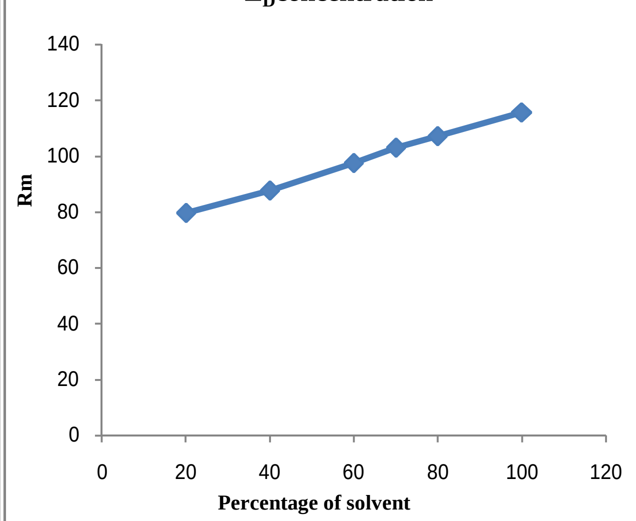



**Fig.-4:Plot of Rm Vs percentage of DMSO solvent at constant (0.01M) ligand $L_D$concentration**



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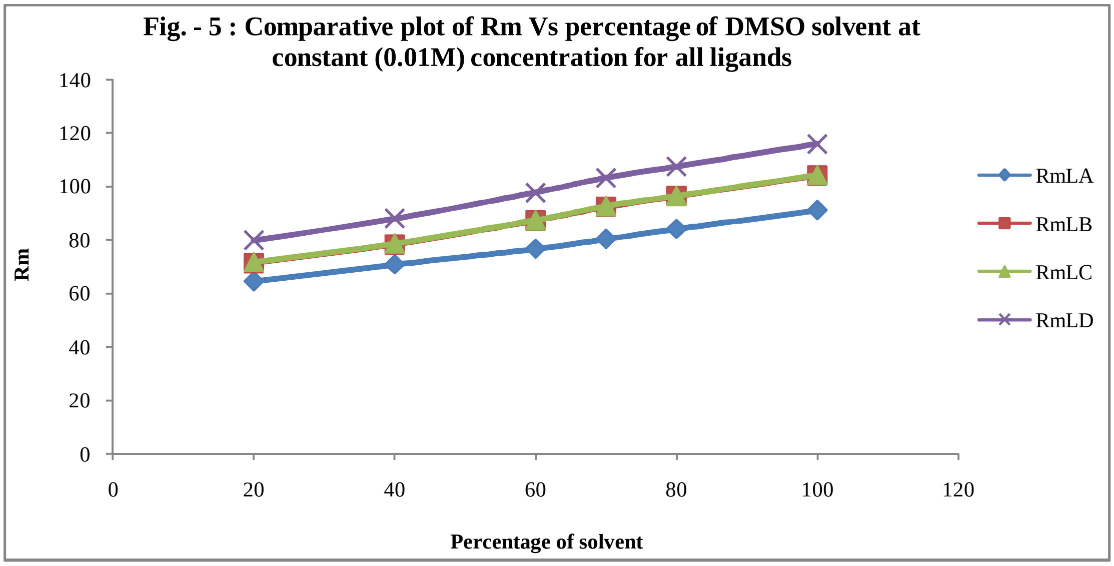


**Fig. - 5 : Comparative plot of Rm Vs percentage of DMSO solvent at constant (0.01M) concentration for all ligands**

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

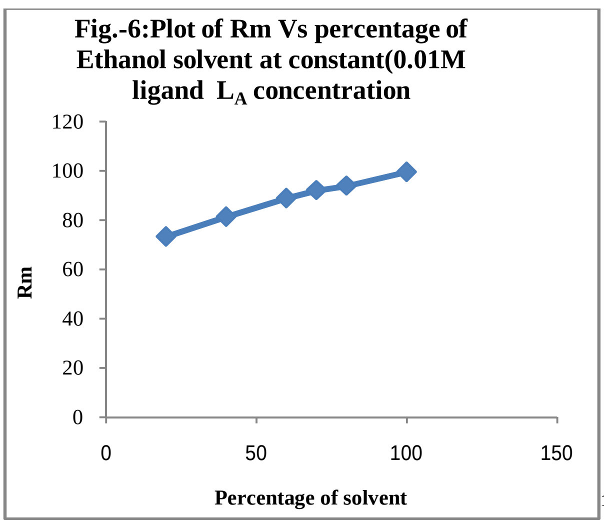


**Fig.-6:Plot of Rm Vs percentage of Ethanol solvent at constant(0.01M ligand $L_A$ concentration**

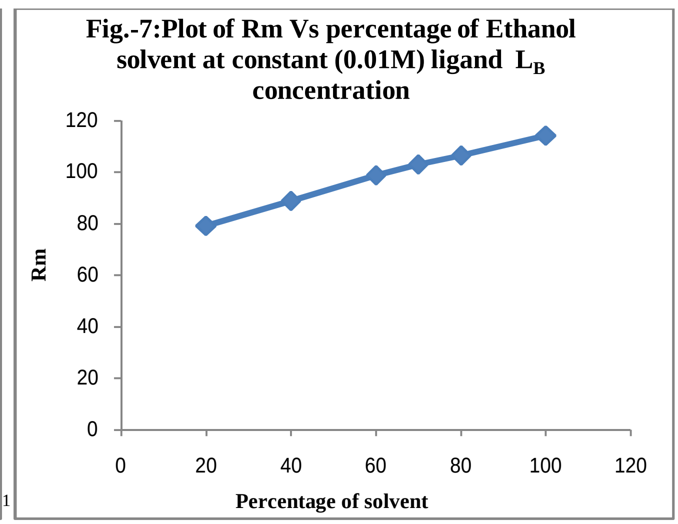


**Fig.-7:Plot of Rm Vs percentage of Ethanol solvent at constant (0.01M) ligand $L_B$ concentration**

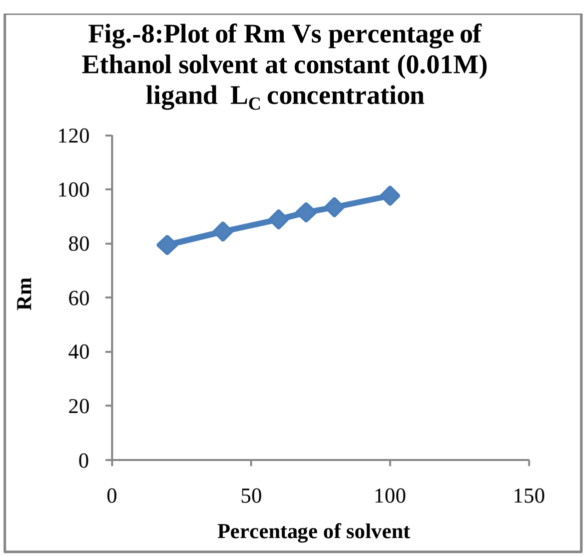


**Fig.-8:Plot of Rm Vs percentage of Ethanol solvent at constant (0.01M) ligand $L_C$ concentration**

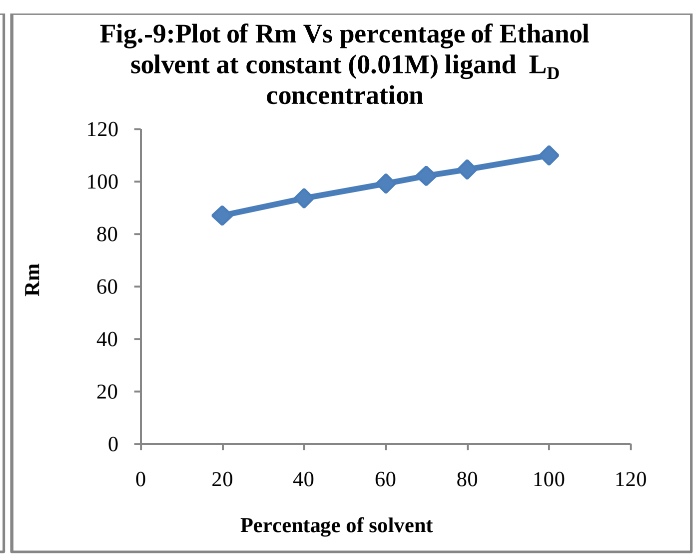


**Fig.-9:Plot of Rm Vs percentage of Ethanol solvent at constant (0.01M) ligand $L_D$ concentration**

**Fig. - 10 : Comparative plot of Rm Vs percentage of Ethanol solvent at constant (0.01M) concentration for all ligands**

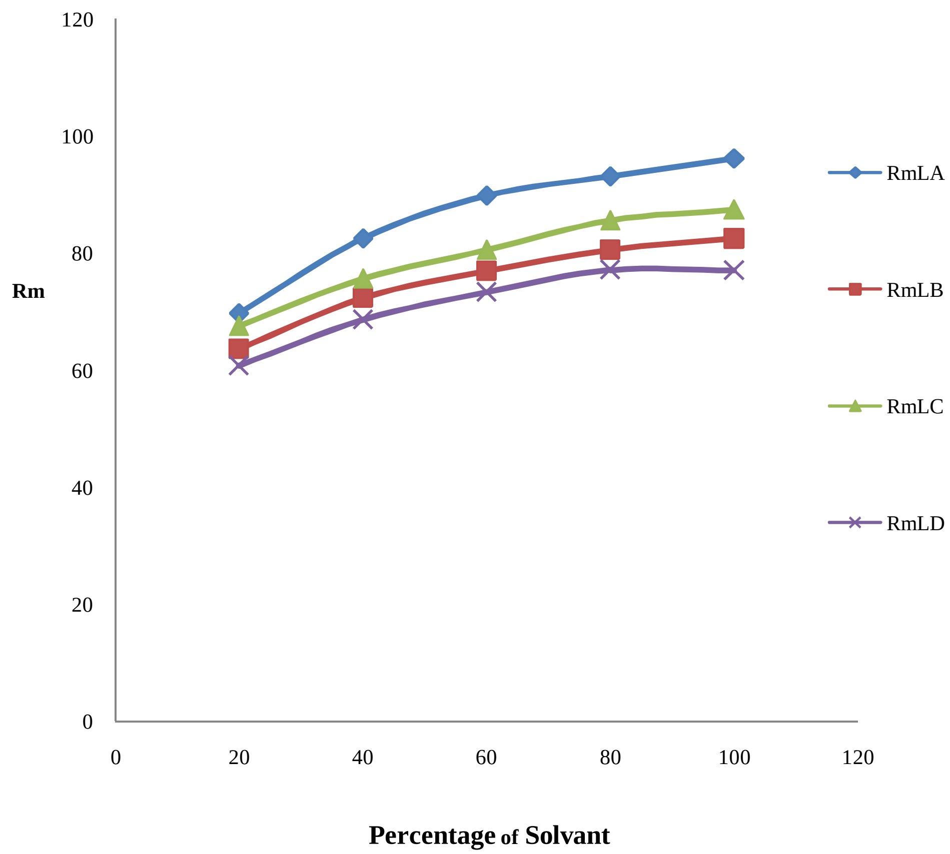


Table no. 2 and 3 indicates the refractive index (n), density (d), molar refraction (Rm) and polarizability constant (α) of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in different percentage of solvents. From data it is observed that molar refraction and polarizability constant values increases with increase in organic solvent percentage. molar refraction (Rm)graphs versus compositions of different percentage of organic solvent are plotted. These are shown in fig. no. 1 to 10. From this it is clear that linear relationship observed between molar refraction and concentration. It is observed that as the percentage composition of organic solvent increases, molar refraction values increases. Due to temporary dipole moment 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.

## IV. CONCLUSION

Substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid derivatives in different percentage of binary mixture is studied by refractometric technique. If the percentage composition of binary mixture increases refractive index increases. It observed that as the percentage composition of organic solvent binary mixture increases molar refraction and polarizability constant of substituted 1-phenyl-3-aryl-1H-pyrazol-4-carboxylic acid increases. From this study, it is clear that when solute solvent interaction increases. the percentage of solvent increases. dispersion force play an important role to increase in the value of molar refraction and polarizability constant with increase in percent composition of organic solvent.

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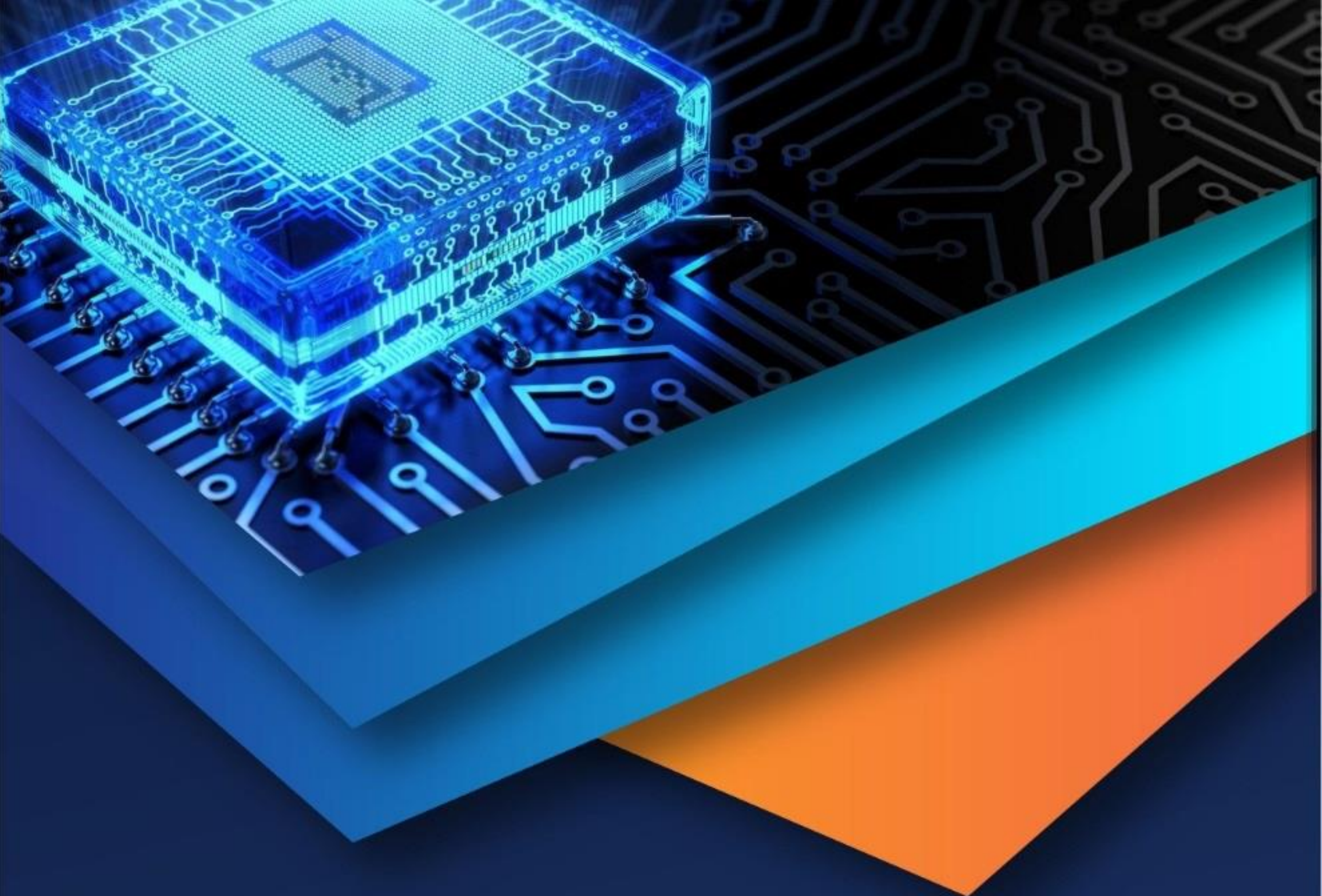


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