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Studies of additive properties of some simple heterocyclic drugs in different solvent by refractometrically

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Abstract
Refractive index, molar refractivity and molar polarizability constant of heterocyclic compound such as Pyridoxine, Lincomycine have been studied in Ethanol, DMF, DMSO, and THF media at 303 K ± 0.1^0 C temperature and different concentration (0.625x 10^{-3} to 10.0x 10^{-3} M). The values of molar refraction (Rm) and molar polarizability (α) constant are found to be decreased with 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.

Keywords: ZnO NP, XRD, Behaviour, histology, brain, ovary

Introduction

An important additive property of molecular structure of liquid is Refractive index. For pure hydrocarbon, one can get an idea of aromatic content of liquid using refractive index. The refractive index is the ratio of angle of incident to the angle of refraction and it depends on the temperature and wave length of light. When a light of beam passes from one substance to another, the beam is bent so that it travels in different direction. If it is passed from less dense to denser medium it is refracted toward normal to form angle of refraction which is less than angle of incident.

The extent of refraction depends on –i) the relative concentration of atom or molecule ii). Structure of an atom or a molecule. So refractive index gives idea about geometry and structure of molecule. Refraction of light is additive property, but also depends on the structural arrangement of atom in molecule. This can sometime be used to determine the structure of an unknown compound whose molecular formula is known.

From literature it was found that much work have been done over many of the substituted heterocyclic 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.

D.R. Nagargioje *et al* [1] have studied to viscosity and polarizability of 3 – acetyl -6 methyl – (2H) – pyran – 2, 4, - (3H) – dione derivative in different phase systems and nature of solute affects viscosity, molar refraction and polarizability constants. Agrawal *et al* [2] have studied the molar refraction and polarizability constant. Various researchers are interested to find out binary liquid mixture interaction along with soult [3-4] viscosity, molar refraction and polarizability constant of electrolytic and non-electrolytic solvent with solute give various new physical parameters of solvent mixture [5-6]. The property of liquid such as viscosity refractive index and ultrasonic velocity of binary mixture are studied by many workers [7 – 14] Oswal *et al* [15] 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* [16].

Experimental measurement of refractive index and dielectric 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* [17]. has been studied additive properties such as molar refractivity and molar polarizability constant of allopurinol, acenocoumarol, warfarin and amoxicillin in different media. Yangang Liu [18] has studied relationship of refractive index to mass density and consistency of the mixing rule use to calculate these two quantities of multicomponent mixture like ambient aerosols with the index-density relationship.
Sangita Sharma *et al*. has been studied density and refractive index of binary liquid mixture Eucalyptol with Hydrocarbon at different temperature. Anand Yadava S.S. has studied refractive indices of binary mixture of bromoalkane and non-polar hydrocarbons, also studied molecular interaction between the components of binary mixtures. This could cover manifold aspect of solute – solvent interaction scanty. Therefore the present work is undertaken to make the systematic study of above substituted studied the ultrasonic velocity and viscosity of PEG-8000, PEG- study of acoustical properties, viscosity coefficient of substituted heterocyclic compounds under suitable condition.
However study of molar refractivity, molar polarizability constant and viscosity coefficients of substituted heterocyclic compound such as salicylic acid in non-aqueous solvent such as ethanol, DMF, THF, DMSO under identical set of experimental condition.

Experimental
The solution of Pyridoxine, Lincomycine are prepared in different solvent like ethanol, DMF, DMSO and THF 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 in Poland (±0.001gm).
The densities of solutions were determined by a bi-capillary pynometer (+0.2%) having a bulb volume of about 10 cm^3 and capillary having an internal diameter of 1mm. The refractive indices of solvent mixture and solutions were measure by Abbe's refractometer at 27 ^{0}C. 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.
The molar refraction of solvents and solution mixtures are determined from the equation

$$R_m = \frac{(n^2 - 1)}{(n^2 + 2)} \times \frac{M}{d} \quad ------- \quad (1)$$

Where:-
M – is the mass of ligand in gram,
d – is the density of solution of ligand,
n – is refractive index and R_m – is the molar refraction.

Similarly Rm can be calculated by using the equation.

$$R_m = \frac{4}{3}\ \pi k N c \alpha. \text{ ------------------- } (2)$$

$$\alpha = \frac{3}{4} \cdot \frac{R_m}{\pi N_C} \text{ --------------------- } (3)$$

Where Nc is the avogadro's number having value 6.023 x 1023 per mole, α − is the polarizability constant.

$$R_m(soln) = X_1 R_{M1} + X_2 R_{m2} \text{ ---------------------- } (4)$$

Where:-
R_m – Molar refraction.
α_1 and α_2 – mole fraction of solvent and solute in solution.
Rm_1 and Rm_2 be the molar refractivity of solvent and solute.
The molar refraction represents actual or true volume of the substance molecules in mole.
The molar refraction of solute can be calculated as.

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

The refractive index of solvent and solution at different concentration are measured from Abbe's refractometer and the values of index molar refraction and polarizability constant are evaluated presented in 1to 6 different system.

Ligand 1. Pyridoxine: Molecular formula $C_8H_{11}NO_3$
Molecular weight: 169.1778

1. Pyridoxine in DMF:
1) Wt. of empty density bottle = 7.180gm
2) Wt. of density bottle + water =17.840gm
3) Wt. of water =10.66gm
4) Density of water (M/V)=10.66/10=1.066gm/cc
5) Wt. of substance dissolved for 0.01 M solution = 0.169gm
6) Wt. of substance dissolved in 0.005M Solution = 0.084gm
7) Wt. of substance dissolved for 0.0025M solution=0.042 gm
8) Wt. of substance dissolved for 0.00125M solution = 0.0211 gm
9) Wt. of substance dissolved for 0.00063 M Solution=0.010 gm
10) Wt. of 0.01M solution in density bottle =16.980gm
11) Wt. of 0.01M solution =16.980-7.180 =9.800 gm
12) Density of 0.01 M solution=9.800/10=0.98 gm/cc
13) Wt. of density bottle + 0.005 M solution=16.950gm
14) Wt. of 0.005M solution= 9.770 gm
15) Density of 0.005M solution =9.770/10 = 0.977 gm/cc
16) Wt. of density bottle + 0.0025M solution = 16.905 gm
17) Wt. of 0.0025 M solution = 9.705 gm
18) Density of 0.0025M solution = 0.972 gm/cc
19) Wt. of density bottle + 0.00125 M solution = 16.885 gm
20) Wt. of 0.00125 M solution = 9.705gm
21) Density of 0.00125 M solution =0.9705gm/cc
22) Wt. of density bottle + 0.00063 M solution = 16.855 gm
23) Wt. of 0.00063M solution = 9.675gm
24) Density of 0.00063 M solution = 0.9675 gm/cc

Table 1: Refractometry data, system – Pyridoxine, Solvent – DMF

Sr. No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.416	0.2560	2.0050	0.04332	0.001717x10^{-23}
2	0.005M	1.401	0.2485	1.9620	0.02103	0.000834x10^{-23}
3	0.0025M	1.388	0.2426	1.9260	0.01026	0.000407x10^{-23}
4	0.00125M	1.376	0.2364	1.8930	0.00499	0.000198x10^{-23}
5	0.00625M	1.362	0.2355	1.8550	0.00242	0.000096x10^{-23}

2. Pyridoxine in THF :

1. Wt. of empty density bottle = 7.180gm
   Wt. of density bottle + water =17.840gm
2. Wt. of water =10.66gm
3. Density of water (M/V)=10.66/10=1.066gm/cc
4. Wt. of substance dissolved for 0.01 M solution = 0.169gm
5. Wt. of substance dissolved in 0.005M Solution = 0.084gm
6. Wt. of substance dissolved for 0.0025M solution=0.042 gm
7. Wt. of substance dissolved for 0.00125M solution = 0.0211 gm
8. Wt. of substance dissolved for 0.00063 M Solution=0.010 gm
9. Wt. of 0.01M solution in density bottle =16.956gm
10. Wt. of 0.01M solution =16.956-7.180 =9.776gm
11. Density of 0.01 M solution=9.776/10=0.9776 gm/cc
12. Wt. of density bottle + 0.005 M solution=16.934gm
13. Wt. of 0.005M solution= 9.750 gm
14. Density of 0.005M solution =9.750/10 = 0.975 gm/cc
15. Wt. of density bottle + 0.0025M solution = 16.908 gm
16. Wt. of 0.0025 M solution = 9.728 gm
17. Density of 0.0025M solution = 0.972 gm/cc
18. Wt. of density bottle + 0.00125 M solution = 16.880 gm
19. Wt. of 0.00125 M solution = 9.700gm
20. Density of 0.00125 M solution =0.970gm/cc
21. Wt. of density bottle + 0.00063 M solution = 16.865 gm
22. Wt. of 0.00063M solution = 9.9685gm
23. Density of 0.00063 M solution = 0.9968 gm/cc

Table 2: Refractometry data, system – Pyridoxine, Solvent – THF

Sr. No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.447	0.2676	2.0920	0.04023	0.0018336x10^{-23}
2	0.005M	1.435	0.2675	2.0590	0.02263	0.0008477x10^{-23}
3	0.0025M	1.421	0.2608	2.0190	0.0111003	0.0004375x10^{-23}
4	0.00125M	1.405	0.2548	1.9850	0.00534	0.0002119x10^{-23}
5	0.00625M	1.401	0.2547	1.9820	0.00257	0.0001022x10^{-23}

3. Pyridoxine in Ethanol

1. Wt. of empty density bottle = 7.180gm
2. Wt. of density bottle + water =17.840gm
3. Wt. of water =10.66gm
4. Density of water (M/V)=10.66/10=1.066gm/cc
5. Wt. of substance dissolved for 0.01 M solution = 0.169gm
6. Wt. of substance dissolved in 0.005M Solution = 0.084gm
7. Wt. of substance dissolved for 0.0025M solution=0.042 gm
8. Wt. of substance dissolved for 0.00125M solution = 0.0211 gm
9. Wt. of substance dissolved for 0.00063 M Solution=0.010 gm
10. Wt. of 0.01M solution in density bottle =17.185gm
11. Wt. of 0.01M solution =17.185-7.180 =10.003gm
12. Density of 0.01 M solution=10.003/10=1.003 gm/cc
13. Wt. of density bottle + 0.005 M solution=17.170gm
14. Wt. of 0.005M solution= 9.990 gm
15. Density of 0.005M solution =9.990/10 = 0.9990 gm/cc
16. Wt. of density bottle + 0.0025M solution = 17.160 gm
17. Wt. of 0.0025 M solution = 9.800 gm
18. Density of 0.0025M solution = 0.980 gm/cc
19. Wt. of density bottle + 0.00125 M solution = 17.140 gm
20. Wt. of 0.00125 M solution = 9.960gm
21. Density of 0.00125 M solution =0.9960gm/cc
22. Wt. of density bottle + 0.00063 M solution = 17.128 gm
23. Wt. of 0.00063M solution = 9.948gm
24. Density of 0.00063 M solution = 0.9948 gm/cc

Table 3: Refractometry data, system – Pyridoxine, Solvent – Ethanol

Sr. No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.356	0.2184	1.8387	0.0368	0.0014615x10^{-23}
2	0.005M	1.341	0.2103	1.7982	0.0177	0.0003462x10^{-23}
3	0.0025M	1.327	0.2027	1.7601	0.0087	0.0003462x10^{-23}
4	0.00125M	1.317	0.1974	1.7344	0.0042	0.0001656x10^{-23}
5	0.0063M	1.305	0.1909	1.7030	0.0020	0.0000801x10^{-23}

4. Pyridoxine in DMSO :

1. Wt. of empty density bottle = 7.180gm
2. Wt. of density bottle + water =17.840gm
3. Wt. of water =10.66gm
4. Density of water (M/V)=10.66/10=1.066gm/cc
5. Wt. of substance dissolved for 0.01 M solution = 0.169gm
6. Wt. of substance dissolved in 0.005M Solution = 0.084gm
7. Wt. of substance dissolved for 0.0025M solution=0.042 gm
8. Wt. of substance dissolved for 0.00125M solution = 0.0211 gm
9. Wt. of substance dissolved for 0.00063 M Solution=0.010 gm
10. Wt. of 0.01M solution in density bottle =17.050gm
11. Wt. of 0.01M solution =17.050-7.180 =9.870gm
12. Density of 0.01 M solution=9.870/10=0.987gm/cc
13. Wt. of density bottle + 0.005 M solution=17.020gm
14. Wt. of 0.005M solution= 9.840 gm
15. Density of 0.005M solution =9.840/10 = 0.9840 gm/cc
16. Wt. of density bottle + 0.0025M solution = 17.010 gm
17. Wt. of 0.0025 M solution = 9.830 gm
18. Density of 0.0025M solution = 0.983 gm/cc
19. Wt. of density bottle + 0.00125 M solution = 16.950 gm
20. Wt. of 0.00125 M solution = 9.800gm
21. Density of 0.00125 M solution =0.980gm/cc
22. Wt. of density bottle + 0.00063 M solution = 16.950 gm
23. Wt. of 0.00063M solution = 9.77gm
24. Density of 0.00063 M solution = 0.977 gm/cc

Table 4: Refractometry data, system – Pyridoxine, Solvent – DMSO

Sr.No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.327	0.2049	1.7606	0.03467	$0.0013752x10^{-23}$
2	0.005M	1.315	0.1987	1.7292	0.01680	$0.0006666x10^{-23}$
3	0.0025M	1.305	0.1931	1.7030	0.00816	$0.0003239x10^{-23}$
4	0.00125M	1.293	0.1866	1.6718	0.00394	$0.0001665x10^{-23}$
5	0.0063M	1.281	0.1801	1.6409	0.00190	$0.0000755x10^{-23}$

Table 5: Lincomycin in DMF

Sr.No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.335	0.2633	1.782	0.10430	$0.004136x10^{-23}$
2	0.005M	1.321	0.2484	1.721	0.04918	$0.001950x10^{-23}$
3	0.0025M	1.308	0.2534	1.710	0.02509	$0.000995x10^{-23}$
4	0.00125M	1.297	0.2508	1.684	0.01241	$0.000492x10^{-23}$
5	0.0063M	1.284	0.2472	1.651	0.00612	$0.0002427x10^{-23}$

Table 6: Lincomycin in THF

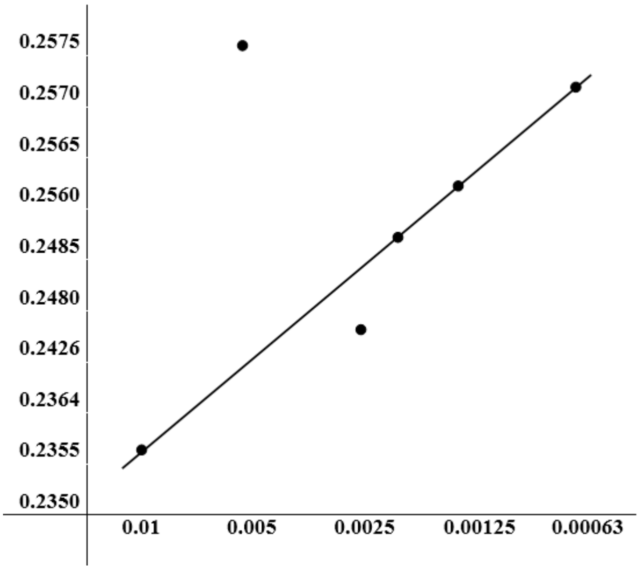
Sr.No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.427	0.010123	2.036	0.004007	$0.0001589x10^{-23}$
2	0.005M	1.412	0.2835	1.992	0.05014	$0.002226x10^{-23}$
3	0.0025M	1.400	0.2793	1.961	0.02765	$0.001096x10^{-23}$
4	0.00125M	1.387	0.2790	1.926	0.013815	$0.0005479x10^{-23}$
5	0.0063M	1.375	0.2766	1.892	0.006847	$0.0002715x10^{-23}$

Table 7: Lincomycin in Ethanol

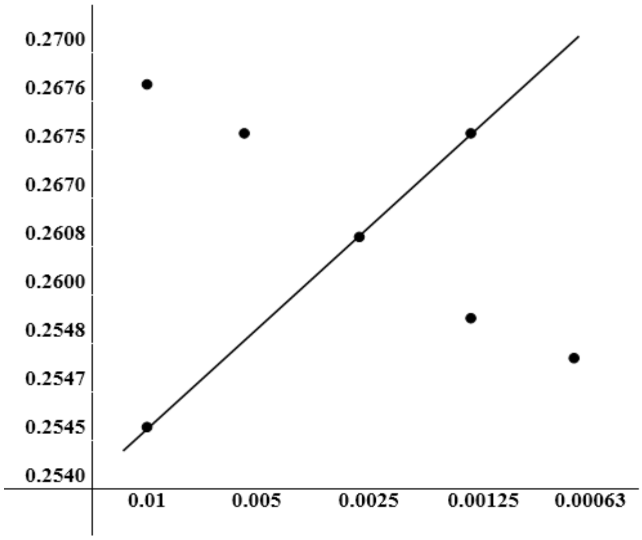
Sr.No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.348	0.2709	1.817	0.1072	$0.004254x10^{-23}$
2	0.005M	1.336	0.2669	1.784	0.0528	$0.002096x10^{-23}$
3	0.0025M	1.322	0.2606	1.747	0.02585	$0.001025x10^{-23}$
4	0.00125M	1.309	0.2540	1.713	0.01259	$0.0004966x10^{-23}$
5	0.0063M	1.298	0.2495	1.684	0.006189	$0.0002454x10^{-23}$

Table 8: Lincomycin in DMSO

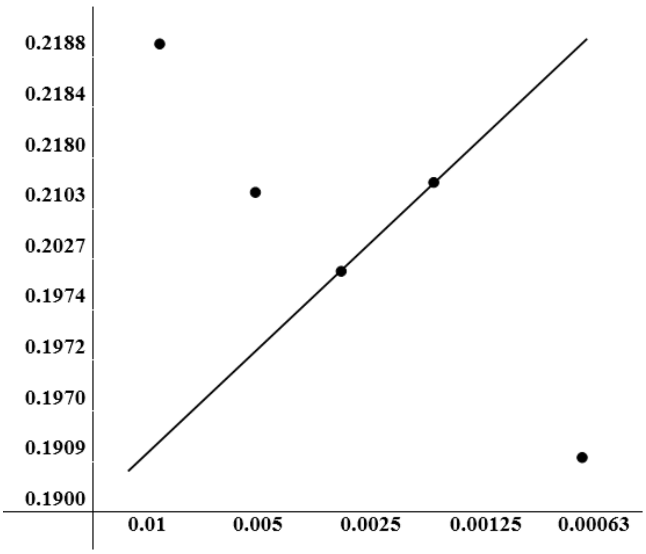
Sr.No	Molarity	R.I. (n)	Specific Refraction (R)	€∞=n² High frequency dielectric constant	Molr Refraction Rm	Polarizability Constant (α)
1	0.01 M	1.319	0.2508	1.739	0.09932	$0.003938x10^{-23}$
2	0.005M	1.305	0.2462	1.703	0.04875	$0.001931x10^{-23}$
3	0.0025M	1.292	0.2434	1.669	0.02410	$0.0009556x10^{-23}$
4	0.00125M	1.279	0.2289	1.597	0.011331	$0.0004439x10^{-23}$
5	0.0063M	1.266	0.2330	1.602	0.005769	$0.0002287x10^{-23}$



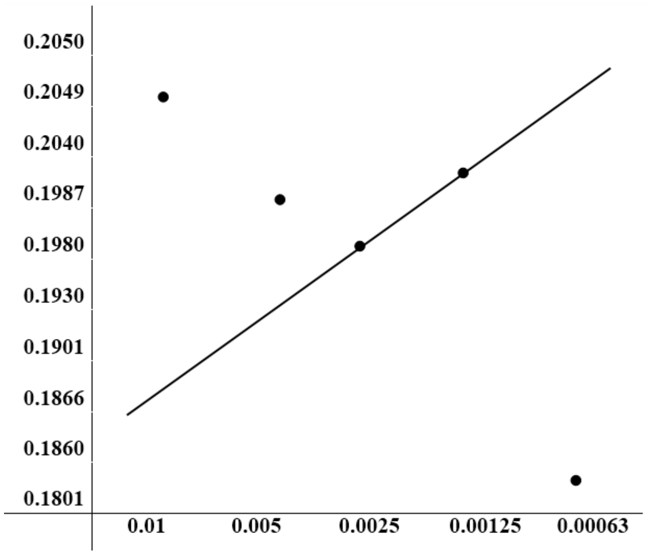
Graph 1: Specific Refraction [R] Vs Concentration [C] For – Pyridoxine Solvent - DMF



Graph 2: Specific Refraction [R] Vs Concentration [C] For – Pyridoxine Solvent - THF



Graph 3: Specific Refraction [R] Vs Concentration [C] For – Pyridoxine Solvent - Ethanol



Graph 4: Specific Refraction [R] Vs Concentration [C] For – Pyridoxine Solvent - DMSO

Results and Discussion

The value of molar refraction (R_m) 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 to 8.

The graphs between specific refraction verses concentration are plotted and show in figure 1 to 8 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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