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Studies on Viscosity, Density and Refractive Index of Substituted Heterocyclic Compounds in Different Media

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ABSTRACT

The molar refractivity, molar polarizability and viscosity coefficients of two heterocyclic compounds, Oxymetazoline (6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)-2,4-dimethylphenol) and Amikacin ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide), were examined in a variety of solvents, including ethanol, methanol, acetone, dimethylformamide (DMF), and tetrahydrofuran (THF). The study was conducted at 3030 K ± 0.1°C and covered a concentration range from 0.625 × 10^{-3} M to 10.0 × 10^{-3} M. The results show a decrease in both molar refractivity and molar polarizability with lower solute concentrations. Additionally, viscosity coefficients were determined using the Jones-Dole equation, which helped elucidate the interactions between the solute-solvent and the solute-solute interactions. These findings provide valuable insights into the molecular behaviour of the compounds in different solvents.

Keywords: Molar refractivity, molar polarizability, viscosity coefficients, solute-solvent interactions, heterocyclic compounds.

Introduction

The refractive index is a fundamental physical property that provides crucial insights into the molecular structure of liquids. For pure hydrocarbons, the refractive index can be handy in estimating the aromatic content of a liquid. When light transitions from one medium to another, it refracts, altering its direction. If the light moves from a less dense medium to a denser one, it refracts toward the normal, causing the angle of refraction to be smaller than the angle of incidence. The refractive index is defined as the ratio of the angle of incidence to the angle of refraction and is influenced by the temperature and wavelength of light.

The degree of refraction depends on several factors, including the concentration of atoms or molecules in the medium and their structural arrangement. Consequently, the refractive index offers critical insights into the geometry and structure of a molecule. While refraction is an additive property, it is also influenced by the molecular structure, which can sometimes be used to deduce the structure of an unknown compound when the molecular formula is known.

In a seminal study, R. Shukla. et. al.[1,2] examined the refractive index and density of binary liquid mixtures, including Eucalyptol and hydrocarbons, at varying temperatures, shedding light on how molecular interactions affect optical properties in such mixtures.

A. Hagahni. et. al.[3] expanded this investigation by studying the refractivity of various homologous series, such as methyl alkanoates and ethyl alkanoates, across a broad temperature range (298.15–333.15 K), highlighting the temperature dependence of the refractive index.

Y. Liu. et. al.[4] explored the relationship between refractive index and mass density in multicomponent mixtures like ambient aerosols, using an index-density relationship to predict the refractive properties of complex mixtures. This approach helped better to understand aerosol formation and behavior in the atmosphere. Similarly, M. Teodorescu. et. Al [5] studied the refractive indices of binary mixtures of bromoalkane and non-polar hydrocarbons, emphasising how molecular interactions affect the refractive index in these systems.

Y. K. Meshram. et. al.[6] contributed to the understanding of the refractive index by exploring additive properties like molar refractivity and molar polarizability constants in pharmaceutical compounds, such as allopurinol, acenocoumarol, warfarin, and amoxicillin, in different solvent media. Their findings revealed the impact of solvent choice on the optical properties of these compounds, important for drug formulation. Other studies have further deepened the understanding of refractive properties in binary mixtures.

S. Pradhan et. al.[7] investigated the refractive indices and viscosities of new binary solvent mixtures, providing detailed insights into how molecular interactions influence the optical and transport properties of these mixtures. Hema et al.[8] provided further clarity on how solvent polarity influences refractive indices in binary and ternary mixtures, showing how optical behaviors can be tailored by manipulating solvent composition recent years, more research has focused on understanding the impact of heterocyclic compounds in non-aqueous solutions.

J. George. et al.[9] examined the temperature dependence of the refractive index in ionic liquid mixtures, providing a deeper understanding of refractive index behaviour in extreme conditions. A. N. Sonar. et.al.[10] investigated how the size and structure of heterocyclic compounds influence their refractive index and optical properties when mixed with solvents.

Alongside G. R. Nibrate[11] has been studied the ultrasonic velocity, viscosity, and acoustic properties of PEG-8000 and various substituted heterocyclic compounds, focusing on the relationship between refractive index and other transport properties. Despite these advances, the study of molar refractivity, molar polarizability constants, and viscosity coefficients of substituted heterocyclic compounds remains underexplored. For instance, compounds such as Oxymetazoline and Amikacin, in non-aqueous solvents such as ethanol, methanol, acetone, DMF, and THF could provide a deeper understanding of solute-solvent interactions and their impact on the refractive index.

Experimental:

The substituted heterocyclic compounds discussed above are of significant importance. Solutions of these compounds were prepared by dissolving the appropriate amount of each compound in different solvents, including ethanol, methanol, acetone, DMF, dioxane, and THF.

For density measurements, the weight of each compound was determined using a Contech balance with an accuracy of 0.001 g. The refractive index of both the solvents and the solutions was measured over a range of 0.625×10^{-3} to 10×10^{-3} using an Abbe refractometer, which has an accuracy of ± 0.01 unit. The temperature of the refractometer's prism box was kept constant at 303 K by circulating water from a thermostat. The refractometer was calibrated using a glass test piece with a known refractive index, which was provided with the instrument.

The molar refraction of the solvent and the solution was calculated using the Lorentz-Lorentz equation. (1)

$$R_m = \frac{(n^2-1)}{(n^2+2)} X \frac{M}{d} = \frac{4}{3} \pi N\alpha$$

The entire viscosity data was analyzed using the Jones-dole equation. (2)

$$\eta_{sp}/\sqrt{c} = A + B\sqrt{c}$$

Where:

η- Refractive index

M- Molecular weight

d- Density of solution

R Molar refraction

N- Avogadro's number

α- Molar polarizability constant.

X_1, and X_2, Mole fraction of solvent and solute in solution.

Viscosity measurements were performed using an Ostwald viscometer (10 mL), and the flow time was measured with a digital clock with an accuracy of 0.01 seconds.

The refractive index of the solvent and solution at various temperatures was measured using an Abbe refractometer. The calculated values of molar refraction and the molar polarizability constant are presented in Tables 1-3 for different systems.

Table 1: Molar refraction and polarizability constant values for different systems at 303 K.

System: **Oxymetazoline** (6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)- 2,4-dimethylphenol).

Solvents: Ethanol, Methanol, Acetone, DMF, THF Concentrations (mol/L): 10%, 5%, 2.5%, 1.25%, 0.625%

Concⁿ inn moles/lit.	Medium									
	Ethanol		Methanol		Acetone		DMF		THE	
	R_m	α x 10^{-26}	R_m	α x 10^{-26}	R_m	α x 10^{-26}	R_m	α x 10^{-26}	R_m	α x 10^{-26}
10 x 10^{-3}	0.05807	2.30	0.05583	2.21	0.05907	2.34	0.05625	7.11	0.05736	2.27

5 x 10^{-3}	0.05786	2.29	0.05525	2.19	0.05889	2.33	0.05307	6.83	0.05703	2.25
2.5 x 10^{-3}	0.05752	2.28	0.05502	2.18	0.05866	2.33	0.05282	6.32	0.05665	2.23
1.25x 10^{-3}	0.05712	2.26	0.05474	2.17	0.05827	2.31	0.05253	6.19	0.05599	2.22
0.625 x 10^{-3}	0.05659	2.24	0.05460	2.15	0.05758	2.28	0.05231	6.14	0.05547	2.20

Table 2: Molar refraction and polarizability constant values for different systems at 303 K.

System: **Amikacin** ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide).
Solvents: Ethanol, Methanol, Acetone, DMF, THF Concentrations (mol/L): 10%, 5%, 2.5%, 1.25%, 0.625%

Conc^{n} inn moles/lit.	Medium									
	Ethanol		Methanol		Acetone		DMF		THE	
	R_m	α x 10^{-26}	R_m	α x 10^{-26}	R_m	α x 10^{-26}	R_m	α x 10^{-26}	R_m	α x 10^{-26}
10 x 10^{-3}	0.07023	2.78	0.06853	2.72	0.07195	2.85	0.06388	2.53	0.07137	2.83
5 x 10^{-3}	0.06983	2.76	0.06829	2.71	0.07172	2.83	0.06358	2.52	0.07096	2.81
2.5 x 10^{-3}	0.06956	2.75	0.06783	2.18	0.07127	2.82	0.06326	2.50	0.07042	2.79
1.25x 10^{-3}	0.06923	2.74	0.06751	2.67	0.07096	2.81	0.06298	2.51	0.07001	2.77
0.625 x 10^{-3}	0.06894	2.72	0.06701	2.65	0.07064	2.80	0.06287	2.48	0.06955	2.75

Table 3: η_r, $\eta_{sp}/\sqrt{c}$, Falkenhagen coefficient (A), Jones-Dole Coefficient (B) of heterocyclic compounds in a different solvent.

Con^{n} mole lit $^{-1}$	Density in kg m^{-3}	Flow time (T) sec	η_r	$\eta_{sp}/\sqrt{c}$	A	B
Oxymetazoline(6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)-2,4-dimethylphenol) + Ethyl alcohol						
0.01	0.82289	434	1.1662	1.66078	25595	-9.0720
0.005	0.82200	422	1.1352	1.91322		
0.0025	0.82154	413	1.1053	2.10321		
0.00125	0.82131	403	1.0782	2.20736		
0.00625	0.82118	393	1.0591	2.36388		
Amikacin ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide) + Ethyl alcohol						
0.01	0.82334	535	1.4355	4.35539	75871	-32.889
0.005	0.82232	507	1.3639	5.14667		
0.0025	0.82166	484	1.2985	5.96959		
0.00125	0.82139	458	1.2281	6.45761		
0.00625	0.82122	436	1.1693	6.76395		
Oxymetazoline (6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl) - 2,4-dimethylphenol) + Methyl alcohol						
0.01	0.79997	349	1.2798	2.9932	55513	-28.640
0.005	0.79711	337	1.2350	3.32518		
0.0025	0.79661	329	1.2051	4.14578		
0.00125	0.79636	318	1.1645	4.33364		
0.00625	0.79620	302	1.1205	4.61903		
Amikacin ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide) + Methyl alcohol						
0.01	0.79856	382	1.3985	3.98470	53861	-14.245
0.005	0.79733	359	1.3124	4.41556		
0.0025	0.79671	335	1.2270	4.54470		
0.00125	0.79642	320	1.1725	4.86501		
0.00625	0.79622	307	1.1279	4.11686		
Oxymetazoline(6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl) - 2,4-dimethylphenol) + Acetone						
0.01	0.80522	155	1.6890	6.88998	11.932	-50.96
0.005	0.80420	146	1.5781	8.17465		
0.0025	0.80370	135	1.4682	9.36620		
0.00125	0.80342	125	1.3732	10.4649		
0.00625	0.80332	116	1.2611	10.4422		
Amikacin ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide) + Acetone						
0.01	0.80567	267	2.9220	19.2196	32.225	-127.78
0.005	0.80444	241	2.6346	23.1146		
0.0025	0.80382	215	2.3388	26.7752		
0.00125	0.80352	181	2.9683	27.3833		

Oxymetazoline(6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)-2,4-dimethylphenol) + DMF						
0.01	1.01362	489	1.5604	5.60418	10.176	-49.158
0.005	1.01310	452	1.4385	6.20051		
0.0025	1.01212	435	1.3827	7.65698		
0.00125	1.01185	405	1.2932	8.29615		
0.00625	1.01170	386	1.2325	9.30471		
Amikacin ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide) + DMF						
0.01	1.011406	453	1.4429	4.41991	8.609	-42.159
0.005	1.01127	432	1.3786	5.35349		
0.0025	1.01221	420	1.3416	6.83175		
0.00125	1.01192	392	1.2520	7.39556		
0.00625	1.01175	371	1.1849	7.12695		
Oxymetazoline(6-tert-butyl-3-(4,5-dihydro-1H-imidazol-2-ylmethyl)-2,4-dimethylphenol) + THF						
0.01	0.88775	125	1.2644	2.64402	5.6488	-30.150
0.005	0.88714	123	1.2432	3.44101		
0.0025	0.88683	123	1.2124	4.25146		
0.00125	0.55668	116	1.1719	4.86352		
0.00625	0.88660	112	1.1312	5.25768		
Amikacin ((2S)-4-amino-N-[(1R,2S,3S,4R,5S)-5-amino-2-[(2S,3R,4S,5S,6R)-4-amino-3,5-dihydroxy-6-(hydroxymethyl)oxan-2-yl]oxy-4-[(2R,3R,4S,5S,6R)-6-(aminomethyl)-3,4,5-trihydroxyoxan-2-yl]oxy-3-hydroxycyclohexyl]-2-hydroxybutanamide) + THF						
0.01	0.88830	126	1.2753	2.75294	4.8386	-21.471
0.005	0.88728	121	1.2335	3.30061		
0.0025	0.88690	117	1.1825	3.64697		
0.00125	0.88671	112	1.1416	4.00782		
0.00625	0.88660	109	1.1113	4.45029		

Table 3: η_r, $\eta_{sp}/\sqrt{c}$, Falkenhagen coefficient (A), Jones-Dole Coefficient (B) of heterocyclic compounds in a different solvent above.

Result and Discussion:

The molar refraction (Rm) and molar polarizability constant (a) values are higher in polar solvents such as ethanol, methanol, and acetone than in non-polar solvents like DMF. This is because polar solvents, which contain hydrogen bonding, can form complexes with the solute, whereas non-polar solvents lack hydrogen bonding and do not form such complexes.

This behaviour may be attributed to the fact that the dipole in the compound is oriented perpendicular to the longer axis of the molecule, leading to intermolecular attraction. As a result, molar refraction and molar polarizability constants increase with higher concentrations of the solution due to the mutual alignment of dipoles.

Tables 1-2 show that molar refractivity and molar polarizability constants decrease with decreasing solution concentration.

Table 3, that the 'A' (Falkenhagen coefficient) values are positive for all systems studied. The positive 'A' values indicate strong solute-solute interactions among the molecules. Conversely, the 'B' (Jones-Dole coefficient) values are negative for all drugs studied. A negative 'B' coefficient characterizes the solute as a "surface breaker," indicating weak solute-solvent interactions.

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