

STUDIES ON VISCOSITY, DENSITY AND REFRACTIVE INDEX OF SUBSTITUTED HETEROCYCLIC COMPOUNDS IN DIFFERENT MEDIA

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ABSTRACT

Refractive index, molar refractivities and molar polarizability constant of heterocyclic compounds such as 2-Thiazol-4-yl-1H benzimidazole, 5-nitro-2-Thiazol-4-yl-1H benzimidazole and 2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid have been studied in Ethanol, Methanol, Acetone, DMF, and THF media at 303 K \pm 0.1^oC temperature and different concentrations (0.625x10⁻³ to 10.0x 10⁻³M). The values of molar refraction (R_m) and molar polarizability (α) constant are found to be decreased with decreasing concentration of solute in solvent. Viscosity coefficient (A, B) evaluate by using John–Dole equation. These parameters throw the light on the solute-solvent interaction and solute-solute interaction.

Key words: Molar refractivities, molar polarizability constant and Viscosity coefficient.

INTRODUCTION

The refractive index is an important additive property of molecular structure of liquid. For pure hydrocarbon, one can get an idea of aromatic content of liquid using refractive index. 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 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. The extent of refraction depends on –i) the relative concentration of atom or molecule ii) The structure of atom or 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 some time be used to determine the structure of an unknown compound whose molecular formula is known.

Sangita Sharma et. al.¹ has been studied density and refractive index of binary liquid mixture Eucalyptol with Hydrocarbon at different temperature. Oswal et.al.² have been studied refractivity properties of some homologous series such as n-ethanoate, methyl alkanoates, ethyl alkanoates etc. were measured in the temperature range from 298.15 to 333.15^oK. The properties of liquid such as refractive index, ultrasonic velocity and viscosity of binary mixture are studied by many workers³⁻⁴. Yangang Liu⁵ 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. Anand Yadava S.S.⁶ has studied refractive indices of binary mixture of bromoalkane and non polar hydrocarbons, also studied molecular interaction between the components of binary mixtures. Sonune et. al.⁷ has been studied additive properties such as molar refractivity and molar polarizability constant of allopurinol, acenocoumarol, warfarin and amoxicillin in different media. Syal⁸ et.al. has been 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 compounds such as 2-Thiazol-4-yl-1H benzimidazole, 5-nitro-2-Thiazol-4-yl-1H benzimidazole and 2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid in non aqueous solvent such as ethanol, methanol, acetone, DMF, and THF under identical set of experimental condition. This could cover manifold aspect of solute-solvent interactions scanty. Therefore the present work is undertaken to make the systematic study of above substituted heterocyclic compounds refractometrically at 303 K. Syal⁸ et.al. has been studied the ultrasonic velocity and viscosity of PEG-8000, PEG- study of acoustical properties, viscosity coefficient of substituted heterocyclic compounds under suitable condition.

EXPERIMENTAL

Above all substituted heterocyclic compounds have most important. The solution of above compound is prepared in different solvent like ethanol, methanol, and acetone, DMF, Dioxane and THF by dissolving an appropriate amount by weight.

For density measurement all the weight took on contech balance (0.001gm). The refractive index of solvent and solutions are measured at different (0.625x10⁻³ to 10x10⁻³) by Abbe's refractometer having accuracy with ± 0.01 unit. The constant temperature of the prism box is maintained by circulating water from thermostat at 303 K. Refractometer was calibrated using glass test piece of known refractive index supplied with the instrument.

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

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

The entire viscosity data have been analyzed by using Jones-dole equation.

$$\eta_{sp} / \sqrt{c} = A + B \sqrt{c} \quad (2)$$

n- Refractive index M- Molecular weight d- Density of solution R_m- Molar refraction N- Avogadro's number α- Molar polarizability constant X₁ and X₂ Mole fraction of solvent and solute in solution.

The refractive index of solvent and solution at different are measured by Abbe refractometer. The calculated value of molar refraction and molar polarizability constant shown in Tables 1 - 5 for different system.

For viscosity measurement Ostwald viscometer (10 ml) was used. The flow time measure by using digital clock (0.01 sec).

Table-1: The values of molar refraction and polarizability constant at 303 K
System: 2-Thiazol-4-yl-1H benzimidazole

Conc ⁿ mole/lit.	Medium									
	Ethanol		Methanol		Acetone		DMF		THF	
	R _m	α x 10 ⁻²⁶								
10 x10 ⁻³	0.05808	2.30	0.05583	2.21	0.05908	2.34	0.05625	7.11	0.05736	2.27
5 x10 ⁻³	0.05788	2.29	0.05526	2.19	0.05889	2.33	0.05307	6.85	0.05704	2.26
2.5 x10 ⁻³	0.05751	2.28	0.05501	2.18	0.05865	2.32	0.05282	6.34	0.05645	2.24
1.25 x10 ⁻³	0.05713	2.26	0.05475	2.17	0.05825	2.31	0.05252	6.21	0.05598	2.22
0.625 x10 ⁻³	0.05660	2.24	0.05461	2.16	0.05759	2.28	0.05232	6.13	0.05549	2.20

RESULTS AND DISCUSSION

The value of molar refraction (R_m) and molar polarizability constant (α) of polar solvents, like Ethanol, Methanol, and Acetone are 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.

From above tables (1-3), it could be seen that molar refractivity and molar polarizability constants decreases with decreasing the concentration of solution.

From Table-4 it is observed that the value of 'A' (Falkenhagen coefficient) are positive in all system studied. 'A' is measure of ionic interaction. It indicates that there is a strong solute-solute interaction in solute molecules. 'B' is Jones–Dole coefficient measures solute –solvent interaction. The value of "B" coefficient is negative in all drugs. Solute with negative 'B' coefficient is characterized as "Surface breaker" indicating weak solute-solvent interactions.

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Table-2: The values of molar refraction and polarizability constant at 303 K
System: 5-nitro-2-Thiazol-4-yl-1H benzimidazole

Conc ⁿ mole/lit.	in Medium									
	Ethanol		Methanol		Acetone		DMF		THF	
	R _m	α x 10 ⁻²⁶								
10 x10 ⁻³	0.07023	2.78	0.06853	2.72	0.07194	2.85	0.06388	2.53	0.07137	2.83
5 x10 ⁻³	0.06983	2.77	0.06829	2.71	0.7172	2.84	0.06358	2.52	0.07097	2.81
2.5 x10 ⁻³	0.06956	2.76	0.06783	2.69	0.07127	2.82	0.06325	2.51	0.07041	2.79
1.25 x10 ⁻³	0.06923	2.74	0.06752	2.68	0.07097	2.81	0.06299	2.50	0.06999	2.77
0.625 x10 ⁻³	0.06894	2.73	0.06702	2.66	0.07065	2.80	0.06288	2.49	0.06955	2.76

Table-3: The values of molar refraction and polarizability constant at 303 K
System: 2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid

Conc ⁿ mole/lit.	in Medium									
	Ethanol		Methanol		Acetone		DMF		THF	
	R _m	α x 10 ⁻²⁶								
10 x10 ⁻³	0.07411	2.94	0.07250	2.87	0.07608	3.01	0.06858	2.72	0.07515	2.98
5 x10 ⁻³	0.07377	2.92	0.07208	2.86	0.07585	3.01	0.06827	2.70	0.07456	2.95
2.5 x10 ⁻³	0.07324	2.90	0.07178	2.84	0.07556	2.99	0.06805	2.70	0.07398	2.93
1.25 x10 ⁻³	0.07292	2.89	0.07126	2.82	0.07507	2.97	0.06794	2.69	0.07337	2.91
0.625 x10 ⁻³	0.07259	2.88	0.07091	2.81	0.07473	2.96	0.06767	2.68	0.07292	2.89

Table-4: η_r , η_{sp} / \sqrt{c} , Falkenhagen coefficient (A), Jones–Dole coefficient (B) of heterocyclic compounds in different solvents

Concentration mole lit ⁻¹	Density kg m ⁻³	Flow time(T) Sec.	η_r	$\frac{\eta_{sp}}{\sqrt{c}}$	A	B
2-Thiazol-4-yl-1H benzimidazole + Ethyl Alcohol						
0.01	0.82289	434	1.1661	1.66077	2.5596	-9.0719
0.005	0.82200	423	1.1353	1.91322		
0.0025	0.82155	412	1.1052	2.10320		
0.00125	0.82132	402	1.0780	2.20735		
0.000625	0.82119	395	1.0591	2.36387		
5-nitro-2-Thiazol-4-yl-1H benzimidazole + Ethyl Alcohol						
0.01	0.82234	534	1.4355	4.35538	7.5873	-32.887
0.005	0.82230	508	1.3639	5.14666		
0.0025	0.82166	484	1.2985	5.96957		
0.00125	0.82139	458	1.2283	6.45760		
0.000625	0.82124	436	1.1691	6.76393		
2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid + Ethyl Alcohol						
0.01	0.82335	497	1.3361	3.3609	4.9658	-16.386
0.005	0.82333	471	1.2662	3.76421		
0.0025	0.82168	450	1.2073	4.14579		
0.00125	0.82139	430	1.1532	4.33364		
0.000625	0.82124	416	1.1155	4.61903		
2-Thiazol-4-yl-1H benzimidazole + Methyl Alcohol						
0.01	0.79998	349	1.2799	2.79932	5.5514	-28.640
0.005	0.79710	338	1.2351	3.32519		
0.0025	0.79660	330	1.2051	4.10272		
0.00125	0.79635	319	1.1646	4.65561		
0.000625	0.79622	303	1.1206	4.82427		
5-nitro-2-Thiazol-4-yl-1H benzimidazole + Methyl Alcohol						
0.01	0.79856	382	1.3985	3.98469	5.3861	-14.245
0.005	0.79732	359	1.3122	4.41555		
0.0025	0.79672	336	1.2272	4.54465		
0.00125	0.79642	321	1.1720	4.8650		
0.000625	0.79623	309	1.1279	5.11686		
2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid + Methyl Alcohol						
0.01	0.79870	322	1.1790	1.79021	4.9658	-16.386
0.005	0.79732	310	1.1331	1.88261		
0.0025	0.79671	301	1.0994	1.98764		
0.00125	0.79640	294	1.0734	2.07598		
0.000625	0.79630	289	1.0550	2.20038		
2-Thiazol-4-yl-1H benzimidazole + Acetone						
0.01	0.80521	155	1.68901	5.781	11.932	-50.96
0.005	0.80420	145	1.4683	8.17485		
0.0025	0.80370	135	1.3700	9.36610		
0.00125	0.80345	126	1.2611	10.4649		
0.000625	0.80332	116		10.4423		
5-nitro-2-Thiazol-4-yl-1H benzimidazole + Acetone						
0.01	0.80566	268	2.9220	19.2197	32.224	-127.79
0.005	0.80443	242	2.6345	23.1147		
0.0025	0.80382	215	2.3388	26.7752		
0.00125	0.80351	181	1.9682	27.3834		

2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid + Acetone						
0.01	0.80579	199	2.1700	11.7002		
0.005	0.80450	183	1.9924	14.0339		
0.0025	0.80385	170	1.8493	16.9864	25.435	-147.29
0.00125	0.80352	157	1.7072	20.0027		
0.000625	0.80335	145	1.5764	23.0553		
2-Thiazol-4-yl-1H benzimidazole + DMF						
0.01	1.01361	489	1.5604	5.60419		
0.005	1.01311	451	1.4384	6.20051		
0.0025	1.01210	434	1.3828	7.65699	10.176	-49.159
0.00125	1.01185	406	1.2933	8.29615		
0.000625	1.01171	387	1.2326	9.30472		
5-nitro-2-Thiazol-4-yl-1H benzimidazole + DMF						
0.01	1.01406	452	1.4429	4.41991		
0.005	1.01128	433	1.3785	5.35349		
0.0025	1.01222	421	1.3416	6.83172	8.609	-42.158
0.00125	1.01191	393	1.2520	7.12695		
0.000625	1.01175	372	1.1849	7.39556		
2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid + DMF						
0.01	1.01419	446	1.4240	4.24019		
0.005	1.01290	437	1.3935	5.56505		
0.0025	1.01225	429	1.3671	7.34240	12.984	-94.79
0.00125	1.01192	421	1.3412	9.65027		
0.000625	1.01191	404	1.2870	11.4807		
2-Thiazol-4-yl-1H benzimidazole + THF						
0.01	0.88775	125	1.2644	2.64403		
0.005	0.88714	123	1.2433	3.44101		
0.0025	0.88683	120	1.2126	4.25146	5.6489	-30.150
0.00125	0.88668	116	1.1719	4.86353		
0.000625	0.88660	112	1.1314	5.25769		
5-nitro-2-Thiazol-4-yl-1H benzimidazole + THF						
0.01	0.88829	126	1.2753	2.75294		
0.005	0.88727	122	1.2334	3.30060		
0.0025	0.88690	117	1.1824	3.64697	4.8387	-21.471
0.00125	0.88672	113	1.1417	4.00782		
0.000625	0.88662	110	1.1113	4.45029		
2-(2-Thiazol-4-yl)-1H benzimidazole-1-yl-acetic acid + THF						
0.01	0.88771	127	1.2846	2.84580		
0.005	0.88732	124	1.2537	3.58762		
0.0025	0.88690	120	1.2127	4.25347	5.595	-28.295
0.00125	0.88671	115	1.1629	4.57914		
0.000625	0.88662	111	1.1214	4.85469		

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