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STUDY OF MOLECULAR INTERACTIONS OF SUBSTITUTED 2-OXO-2-H-CHROMENE-3-CARBOHYDRAZIDE DERIVATIVES IN BINARY SOLVENTS USING ULTRASONIC INTERFEROMETER

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ABSTRACT

At 32°C, the apparent molal volume (v), apparent molal compressibility (k), relative association (RA), and solvation number (Sn) of substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives in 60% DMF-water were measured. The data is used to determine the interaction that is taking place in the solution. The ultrasonic technique is used to determine the interaction of a solute and a solvent. The variation of factors in binary mixtures with different concentrations indicates a significant interaction between solute and solvent molecules, associative molecular interaction, and ion-solvent interaction.

Keywords: Substituted 2-oxo-2-H-chromene-3-carbohydrazide derivatives, acoustic parameters ϕ_v,ϕ_k, R_A, S_n.

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INTRODUCTION

The ultrasonic technique is effective in recent years for the study of various compounds. The nature and strength of the molecules in ultrasonic research have numerous applications in pharmaceutical, agricultural, industrial, biological, and material science.[1] The effect of ultrasonication on the fluid flow of heavy crude oil was investigated.[2] The ultrasonic pulse velocity measurement determines the structure and strength of the compounds in the liquid mixture.[3] At three separate temperatures, an ultrasonic study of 1-alkanol in a binary mixture of tetrahydrofuran and 1-chlorobutane,[4] had been executed, as well as the molecular interaction of organic liquid in CCl_4 at each temperature.[5] The ultrasonic technique is unique in food processing because it improves mass transfer and food preservation while also assisting with thermal treatment and food analysis.[6] The ultrasonic technique is used to determine the thickness of biological tissue and the thickness of the skin.[7] The ultrasonic technique was used to investigate the antimicrobial activity and anti-inflammatory properties of phenylalanine analogues of the Schiff base.[8] The chemical interaction within these ternary systems has been analyzed using sonication statistics for numerous alcohols at 303K in varying concentrations.[9] This same ultrasonic strategy was used to examine the current flow behaviour in the Al-Al_2O_3-p-CdTe-Me structure at 30ºC.[10] Ultrasonic studies of binary digits cluster centres of Trichloroethylene with 1-pentanol and 1-heptanol were accomplished.[11] Determination of ultrasonic parameter of 3-phenyl-1- (2',4'-difluorophenyl) prop-2-en-1-one in binary mixture.[12] The ultrasonic technique is used to investigate the interaction of hyaluronic and the cationic surfactant septonex.[13] Ultrasonic study was conducted on an aqueous solution of L-Methionine.[14] Ultrasound is unique in the study of the interaction of diethylene glycol, ethylene glycol, and triethylene glycol in an aqueous glycerol solution.[15] Ultrasonic flow speed intensity determination for binary liquid mixtures of 2, 2, and 4-trimethylpentane (TMP) with benzene, toluene, o-xylene, m-xylene, and p-xylene have down.[16] At 30°C, the ultrasonic technique was used to investigate aromatic ketones and N-methylaniline (NMANI).[17] Through the use of acoustic wave methodologies in solution theory as well as molecular dynamics.[18]

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EXPERIMENTAL

Material and Methods

In this regard, authors examined the ultra-sonic properties of the mentioned coumarin derivatives in a binary mixture of 60% (DMF+Water) at multiple ligand concentrations at 32°C.
2-oxo-2H-chromene-3-carbohydrazide derivations have been constructed.
Ligand (C_A) = N-[(E)-1-(5-bromo-2-hydroxy-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide
Ligand (C_B) = N-[(E)-1-(5-chloro-2-hydroxy-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide
Ligand(C_C)=N-[(E)-1-(3,5-dichloro-2-hydroxy-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide
Ligand (C_D) = N-[(E)-1-(2-hydroxy-5-methyl-phenyl)ethylideneamino]-2-oxo-chromene-3-carboxamide

The ligands noted previous paragraph are being synthesized[19] and used.[20] Chemicals of analytical grades were used. Density measurements have been performed using the specific gravity bottle.

Detection Method

The following formula is used to determine the wavelength of the acoustic waves.[21]

$$2D = \lambda \quad (1)$$

Where λ is called wavelength and D is the distance in mm

By knowing, the wavelength, the ultrasonic velocity is calculated by the following equation;

$$\text{Ultrasonic velocity (U)} = \lambda \text{ x Frequency x } 103 \quad (2)$$

The following equations are used for the calculation of the apparent molal volume[22] (ϕ_v) and apparent molal compressibility (ϕ_k).[23]

$$\text{For calculation the Apparent molal volume } (\phi_v) = \frac{M}{d_s} + \frac{(d_o - d_s)\times 10^3}{(m d_s d_0)} \quad (3)$$

Apparent molal compressibility is calculated by using this equation

$$(\phi_k) = \frac{1000(\beta_s d_o - \beta_o d_s)}{m d_s d_o} + \frac{\beta_s M}{d_s} \quad (4)$$

For this do- densities of the pure solvent, d_s - density of the solution,
m – molality, M - molecular weight of solute.

The relative association (R_A)[24] is calculated by the equation:

$$\text{Relative association } (R_A) = \left(\frac{d_s}{d_o}\right) \times \left(\frac{U_o}{U_s}\right)^{1/3} \quad (5)$$

Where Uo and Us are ultrasonic velocity in solvent and ultrasonic velocity of solution respectively. The density of a pure solvent is denoted by d_0, while the density of a solution is denoted by ds. The molality of the solute is m and the Molecular weight of the solute is M, adiabatic compressibility of pure solvent is βo. The following equation is used for the Solvation number (Sn).[25]

$$\text{Solvation number (Sn)} = \phi_k / \beta 0 \text{ x } (M/ d0) \quad (6)$$

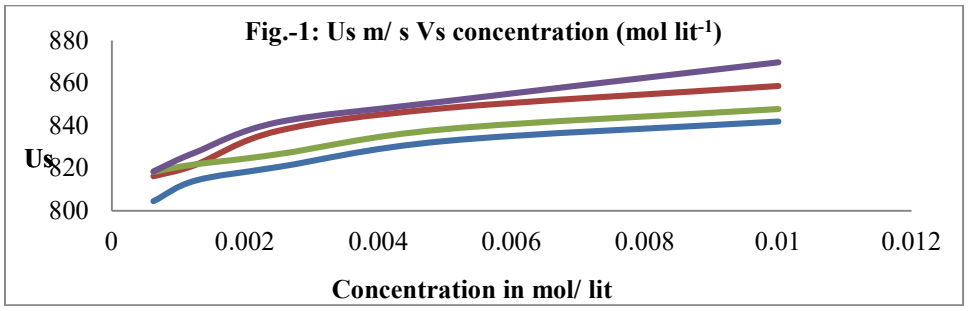
RESULTS AND DISCUSSION

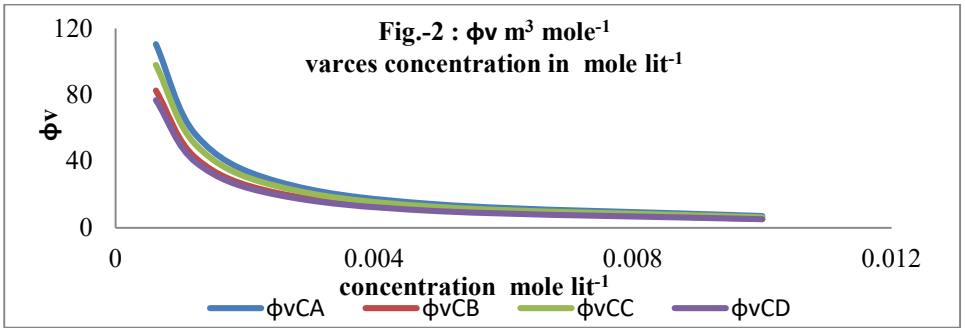
The apparent molal volume (ϕ_v) of ion-solvent interactions is utilized to identify them. Even as the concentration of the system declines, the apparent molal volume (ϕv) increases. As a result, the system exhibits strong ion-solvent interaction. As concentration decreases, apparent molal compressibility (ϕ_k) increases. The graph we created depicts the same type of variation. The graph which we plot shows the same type of variation. The relative association (R_A) increases as the concentrations decrease. Figure 4 illustrated the variety throughout relative association to concentrations. In the given system, relative association (R_A) increases as concentration decreases. The property of relative association (R_A) is useful for understanding the interaction between solute and solvent. The weak solute-solvent interaction is observed. The solvation number (Sn) tends to decrease as concentration increases. The differences in salvation and concentration are evident. The variation in salvation and concentration shows that it has a closely packed structure.

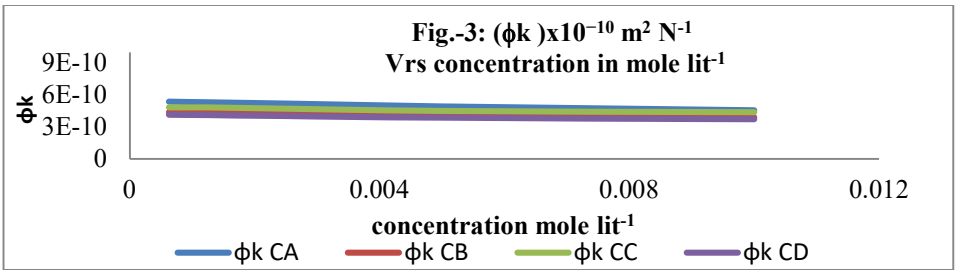
Table-1: Concentration (m), Apparent Molal Volume (ϕ_v), Apparent Molal Compressibility (ϕ_k), Relative Association (R_A) and Solvation Number (S_n) in 60% (DMF+Water) Solvent at 305K

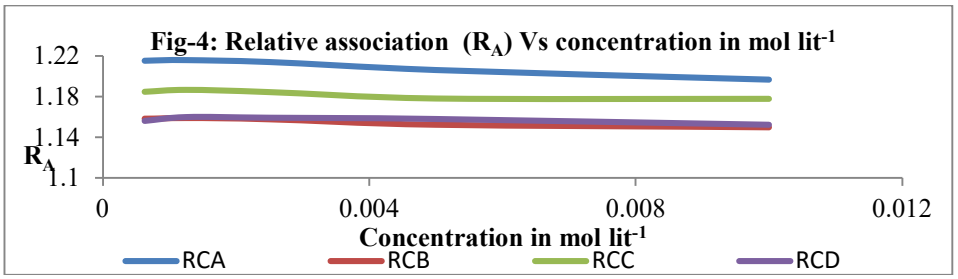
Conc. (m) (mol lit^{-1})	Apparent molal volume (ϕ_v) (m^3mol^{-1})	Apparent molal compressibility (ϕ_k) x 10^{-10} (m^2N^{-1})	Relative association (R_A)	Solvation number (S_n)
		Ligand C_A		
0.01	7.13	4.56	1.19	0.60
0.005	14.07	4.93	1.20	0.65
0.0025	27.96	5.20	1.204	0.69
0.00125	55.56	5.32	1.21	0.71
0.000625	110.63	5.37	1.23	0.71
		Ligand C_B		
0.01	5.40	3.92	1.1442	0.58
0.005	10.70	4.03	1.15	0.60
0.0025	21.01	4.26	1.1522	0.63
0.00125	41.62	4.35	1.1524	0.65
0.000625	82.68	4.38	1.1551	0.66
		Ligand C_C		
0.01	6.36	4.38	1.171	0.59
0.005	12.55	4.50	1.173	0.6145
0.0025	24.91	4.72	1.180	0.6452
0.00125	49.52	4.83	1.182	0.6596
0.000625	98.17	4.85	1.1845	0.6632
		Ligand C_D		
0.01	5.06	3.72	1.14	0.5876
0.005	10.05	3.87	1.239	0.6125
0.0025	19.7973	4.01	1.244	0.6368
0.00125	39.0797	4.12	1.245	0.6509
0.000625	76.8870	4.135	1.251	0.6538

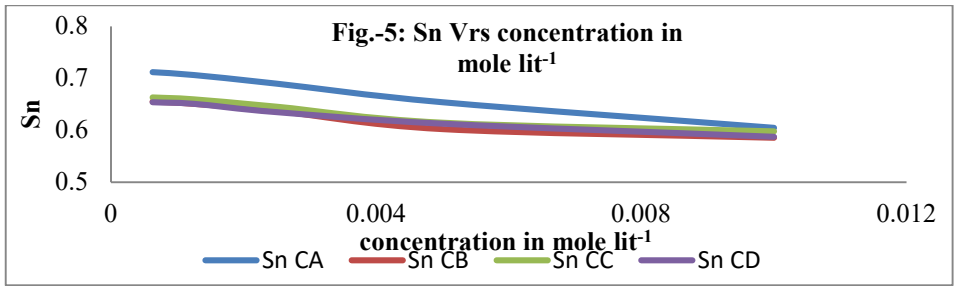
Graphical Presentations of Acoustic Parameter Us apparent molal volume (ϕ_v), Apparent molal compressibility (ϕ_k), relative association (R_A) and solvation number (S_n).











CONCLUSION

The ultrasonic method is used to identify the acoustic parameter which is used to evaluate the ion-solvent interaction in the solution. Though since hydrogen bonding seems to be more prevalent in concentrated solutions, it is compacted in structure as ultrasonic speed increases. Raise in apparent molal volume(ϕ_V), indicate a significant ion-solvent interaction. The apparent molal compressibility (ϕ_K) rises as concentration decreases, causing a weak electrostatic attraction force in the vicinity of ions. Whenever the solute-solvent interaction is weak, the roughly comparable association (R_A) increases. As the concentration in the system increases, the Solvation number(S_N) reduces, implying weak solute-solvent interaction.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interests regarding the publication of this manuscript.

AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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