Magna Scientia Advanced Research and Reviews

eISSN: 2582-9394

Cross Ref DOI: 10.30574/msarr

Journal homepage: https://magnascientiapub.com/journals/msarr/

Magna Scientia
Open access publication

(Research Article)

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Analysis of thermo-acoustic parameters in view to obtain the interaction between acetamide in some salt solutions at different temperature

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Magna Scientia Advanced Research and Reviews, 2024, 10(02), 165–172

Publication history: Received on 22 February 2024; revised on 28 March 2024; accepted on 31 March 2024

Article DOI: https://doi.org/10.30574/msarr.2024.10.2.0054

Abstract

The ultrasonic velocity and density have been calculated for acetamide in the solution NaCl and KCl at different temperatures (viz. 283, 288,293,298K) for various concentrations from 0.02-0.2mol/kg thermodynamic and sound parameters such as adiabatic compressibility, acoustic impedance, relative association, internal pressure, available volume, specific heat ration, relaxation strength, isothermal compressibility, molecular radius, surface tension, enthalpy, Rao's constant, Wada's constant, free length, have been gained from research examination for the (Acetamide +H_2O/NaCl/KCl). To investigate exactly the type of molecular interactions that exist with NaCl and KCl with acetamide. Among them, KCl with Acetamide interacts most strongly, at a higher concentration as compared to NaCl and H_2O solvent. They give stronger solute-solvent interaction with higher mass fractions at higher temperatures.

Keywords*:* Enthalpy; Density; Acetamide; Salts; Intermolecular Interaction.

1. Introduction

At present ultrasonic techniques are used to study, and recognize the particular interaction (such as ion-ion, ion-solvent, and solvent-solvent interaction) in liquid mixtures. Utilizing details from the combination and their interaction with further solutes and solvents that have assembled and evaluated different types of interaction [1]. The ultrasonic method is generally used in the fields of medical, pharmaceutical, engineering, agriculture, and industrial area [2]. The complex configuration affects the structure of proteins and also the direct studies of proteins are very difficult, therefore investigation of the behavior of some compounds of proteins like amino acids, peptides as well as amides is important [3]. Besides amides are used in an efficacious change in proteins denaturation increases with an increasing number of carbon atoms in amides this is believed due to hydrophobic interactions. Besides, there are studies regarding the amide/salt/water in a manner [3]. Previous researchers have done a lot of research on drugs like acetamide with cell cancer (Necla Kulabas, 2016) [4], acetamide and chloroform (Tarun Pant, 2019) [5], acetamide with electrolyte (Nagaraj Pavithra, 2015) [6], acetamide with Ketone, etc. Now we study the interaction between acetamide and saline salt solution influenced by differences in solute concentration and temperature, there are many types of drugs, and among them, we will study only acetamide. In the examination of acetamide in aqueous solution, acetamide is the one type of drug that is also acetic acid amide or ethionamide. It is derived from acetic acid and is the simplest amide with molecular formula CH_3CONH_2.Acetamide mainly consists of a carboxylic acid amide functional group it is a crystalline solid in nature and colorless [7]. Acetamide is used in the preparation of medicine, e.g. Penicillin, Acetamide-250, etc. also used in cancer cells, manufacturing plasticizers, lacquers, and polymeric products.

In present study gives the interaction between the mixture of acetamide with electrolyte salt solution (NaCl and KCl), the human body wants lots of minerals known as necessary minerals like (Na, K, Fe, Si, etc.). A human requires potassium minerals for the actual work of the kidneys, nerves, muscles, heart, and digestive system i.e. two of the cellular

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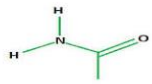
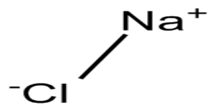
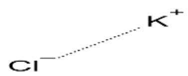
and electrical functions and KCl is an important blood mineral called an electrolyte [8]. NaCl helps restore the human body due to certain conditions and controls blood pressure. This investigation involves the determination of volumetric and acoustical properties for interaction between acetamide and two different electrolyte salt solutions NaCl, and KCl at various concentrations and temperatures [9]. From this data, we calculate some allied parameters and from this, we can find the intermolecular interaction between them. As the concentration and temperature increase the modification of these volumetric and thermoacoustic properties strongly gives the molecular bond present in all three systems, among them, KCl with Acetamide interact most strongly, at higher concentrations as compared to NaCl and H_2O solvent solution. An increase in solute-solvent interaction with higher mass fraction at higher temperatures.

2. Material and Method

2.1. Material

The compounds used in these experiments are all AR-grade compounds with 99% purity of mass fraction. They are all purchased from Hi Media Pvt. Ltd. Mumbai shown in Table 1.

Table 1 Chemical Information

Sr. No.	Compound Name	Molecular Formula	Molecular Weight	CAS No.	Molecular Structure
1	Acetamide	CH_3CONH_2	59.07 g/mol	60-35-5	
2	Water	H_2O	18.0152 g/mol	----------	
3	Sodium Chloride	NaCl	58.44 g/mol	7647-14-5	
4	Potassium Chloride	KCl	74.55 g/mol	7447-40-7	

2.2. Method

The combination of various concentrations in distilled water was prepared and the weight of the substance was calculated by using the digital weighing machine. A digital ultrasonic interferometer is used to calculate the ultrasonic velocity purchase from Vi Microsystem Pvt. Ltd. Chennai, operating at2 MHz frequency. Quartz crystal is used as a source of ultrasonic waves the digital thermostat was used for keeping temperature constant overall experiment the density of the solution was correctly determined with the assistance of a 10 ml specific gravity density bottle.

2.2.1. Defining Relations:

Adiabatic Compressibility (β): Adiabatic compressibility is a consequence of the ultrasonic velocity and the density and it is a friction charge in volume per unit increase of pressure.

$\beta = \frac{1}{\rho \times U^2}$ -------- (m^2N^{-1})

Acoustic Impedance (Z): An acoustic impedance is useful in discussing the relation between density and velocity and it is derived from a given equation.

$Z = U\rho$ ------- ($Kg\text{-}\ m^2s^{-1}$)

Relative Association (R_A): The relative association is derived from the given equation.

$R_A = \{\frac{\rho}{\rho_0}\}\{\frac{U_0}{U}\}^{1/3}$

Internal Pressure (π_i): Internal Pressure depends on temperature concentration and external pressure in the case of the solution.

$\pi_i= \frac{\alpha\times T}{K_T}$……………………………….{N/m^2}

Available Volume (V_a): Available volume is used to calculate the compactness and strength of molecular attraction among solute and solvent.

$V_a=\left\{V_m\left[1-\frac{U}{U_\infty}\right]\right\}$………………………($m^3mol^{-1}$)

Specific Heat Ratio(γ): The specific heat ratio is the specified relation between isothermal compressibility and adiabatic compressibility.

$\gamma\frac{17.1}{T^{\frac{4}{9}}\times\rho^{1/3}}$ …………….. $\{K^{4/9}\}^{-1}\{Kg^{1/3}/m\}^{-1}$

Relaxation strength (r): Relaxation strength is straightly connected with adiabatic compressibility the relation is as follows.

$r= 1- (\frac{U}{U_\infty})^2$

Isothermal Compressibility (K_T): The isothermal compressibility value has been evaluating it has been evaluated from McGowan's equation and this is dependent on velocity and density.

$K_T = \frac{1.33\times10^{-8}}{(6.4\times10^{-4}U^{3/2}\rho)^{3/2}}$……{m^2/N}

Molecular Radius (R_m): The physiochemical properties of matter depend on the size of the molecules. The intermolecular forces of attraction will be stronger if the molecular radius is greater.

$R_m = \{\frac{3b}{16\pi N_A}\}^{1/3}$------ (m)

Surface Tension(σ): The well-known Auerbach connection has been applied to estimate the surface tension of a combination using Flory theory.

$\sigma = (6.3\times10^{-4})\rho U^{3/2}$------ (Nm^{-1})

Relative change in adiabatic compressibility $(\Delta\beta/\beta)=\frac{\Delta\beta}{\beta_0}$

Where, $\Delta\beta = the$ change in adiabatic compressibility

β_0= adiabatic compressibility of solute

Enthalpy (H): Enthalpy is one of the thermo-dynamical properties it dependent on constant pressure.

$H = V_m\times\pi_i$……………{J/Kg}

Solubility parameter (δ): Solubility parameter depends on the internal pressure of the system.

$\delta = \sqrt{\pi_i}$…………. $(Nm^{-2})^{1/2}$

Free Length (L_f): The spacing between two neighboring molecules of the solution is known as intermolecular free length.

$L_f = K(\beta a)^{1/2}$-------------(m)

3. Result and Discussion

The variation in the investigation value of ultrasonic and density and the various thermo-acoustical parameters of acetamide in an aqueous solution of NaCl and KCl gives the information of all systems mentioned.

The graph between ultrasonic velocity and concertation at various temperatures shows that the ultrasonic velocity rises along with the rise in concertation as represented in Fig 1. Acetamide in aqueous solution of NaCl and KCl indicates the presence of association in molecules of the solution. The association of the constituent's molecules may be involved due to dipole interaction and due to the hydrogen bonding between the constituent's molecules. The peak at molar concentration is because of containing the strong bond [10]. The density is known as the measurement of closely packed material together. The variation of the density with concentration is shown in Fig 2. From the graph, it is observed that density rises along with rising concentration indicating that the presence of solute-solvent forces is present because of hydrogen bonding between them [11].

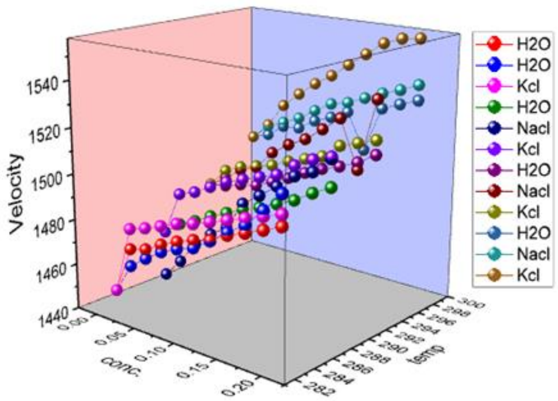


Figure 1 Velocity v/s Concentration at different temperature

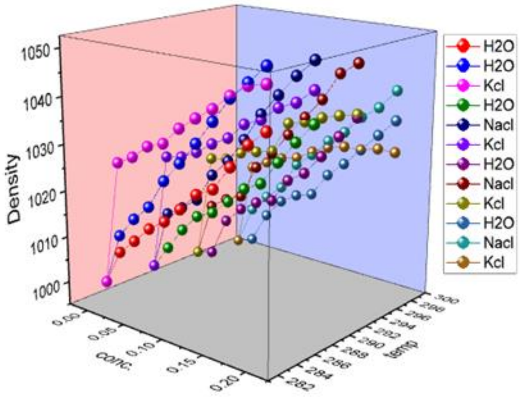


Figure 2 Density v/s Concentration at different temperature

The variation of adiabatic compressibility with concentration and temperature is shown in Fig.3This indicates that there is the presence of solute-solvent forces of the solution. The adiabatic compressibility falls with a rise in the concentration and temperature of the solution. Ion is largely ionized and these ions are near by a layer of solute molecules that are densely packed and oriented along the ions. Decrease an adiabatic compressibility creation of bulky amount of strongly bound the system. [12] The acoustic impedance is depending on velocity and density. The acoustic impendence value along with increasing concentration is shown in Fig 4. This confirms the presence of intermolecular forces between the solute and solvent molecules. which is because of hydrogen bonding present in the solution.[13]

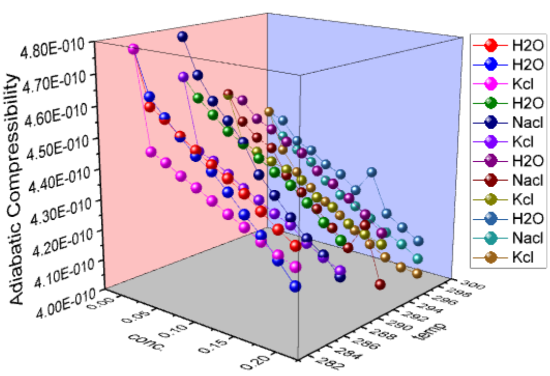


Figure 3 Adiabatic Compressibility v/s Concentration at different temperature

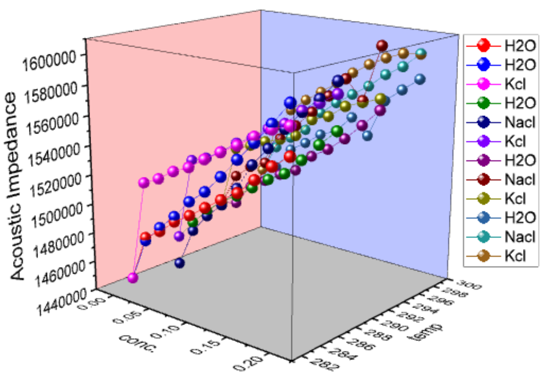


Figure 4 Acoustic Impedance v/s Concentration at different temperature

The variation of relative association values with concentration and temperature is shown in Fig. 5 and it observed that relative association rises along with rising concentration and temperature which indicates there is a close relation between a compound of the molecule and intermolecular interaction [14]. The rate at which the internal energy changes with volume. The variation of internal pressure with various concentrations and temperatures is seen in Fig 6. It is suggested that internal pressure rises along with rising concentration and temperature the association takes place through the hydrogen bonding in the molecules and those are attentively packed inner side of the shielding region [15].

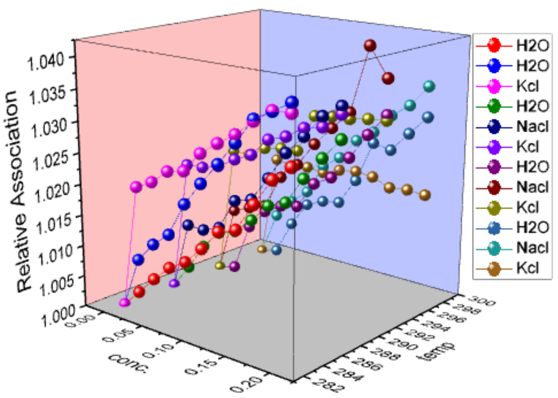


Figure 5 Relative Association v/s Concentration at different temperature

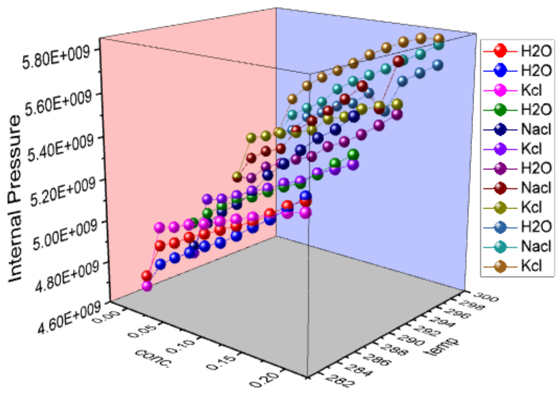


Figure 6 Internal Pressure v/s Concentration at different temperature

The available volume varies inversely with the speed of sound. In the current work it is clear that available volume falling with the rise in concentration is observed as shown in Fig.7 This shows the increase in molecular association through intermolecular hydrogen bonding in the middle of constituents of the solution. This indicates that there is presence of intermolecular forces in the solution [16] The specific heat ratio is the calculable relation between the specific heat at constant volume. The value of the specific heat ratio falls with rising in both molar concentration and temperature as depicted in Fig8. It is revealed that the actuality of specific heat is decreasing constantly with an increase in concentration indicates the presence of intermolecular forces in the solution.[17] It is one of the main properties to explain the molecular interaction present in the system.

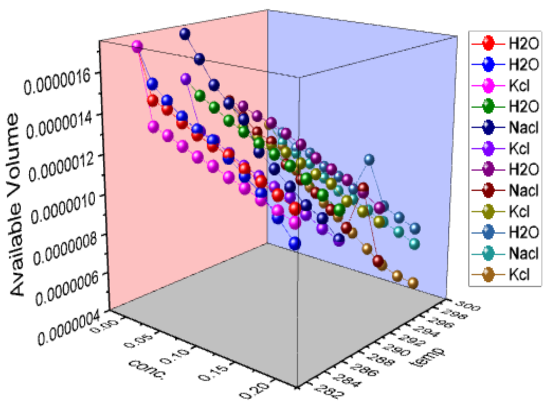


Figure 7 Available Volume v/s Concentration at different temperature

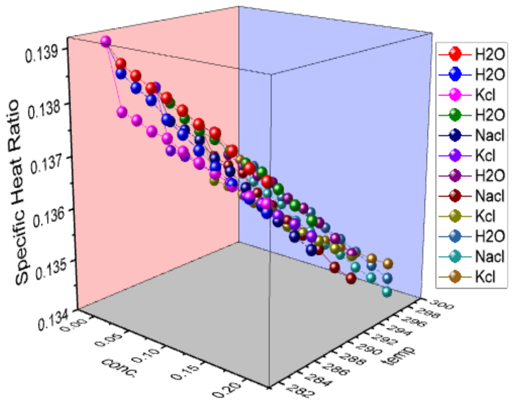


Figure 8 Specific Heat Ratio v/s Concentration at different temperature

When we add solute to solvent the value of relaxation strength decreases in concentration and temperature as shown in Fig 9. This is because of the presence of complex structures in the solution. Lower relaxation strength values indicate higher affinity of the mixture components. The strength at rest is directly related to the adiabatic compressibility [18]. After measuring and computing a graph of isothermal compressibility as opposed to concentration and temperature represented in Fig10. The value of isothermal compressibility falls with rising concentration and temperature. This indicates the presence of strong intermolecular forces in the solution. This trend becomes visible in the outcome of corresponding falling in free volume which conforms to the clustering of molecules and hence suggests the increase in interaction among the constituents[19].

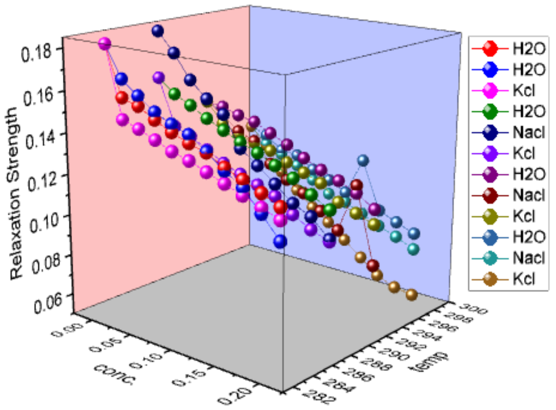


Figure 9 Relaxation Strength v/s Concentration at different temperature

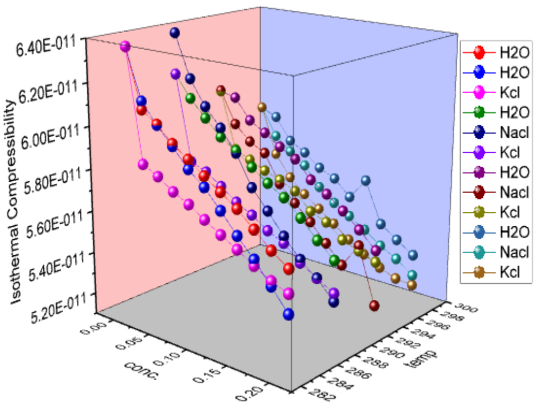


Figure 10 Isothermal Compressibility v/s Concentration at different temperature

The physical and chemical properties of matter depend on the size of the molecule. The variation of molecular radius in different concentrations and temperatures is depicted in Fig 11. It is suggested that molecular radius rises with a rise in both concentration and temperature. It indicates that rising molecular radius gives stronger intermolecular force of attraction further increase in molecular radius confirms the association between solute and solvent [20]. surface tension normally known as interfacial tension is the main property of liquid to reduce its surface area and is called as surface tension. To study the surface composition of an aqueous solution of the mixture this parameter is used as shown in Fig 12. The value of surface tension rises with a rise in temperature and concentration. It indicates the presence of a molecular association between solute-solvent interactions [21].

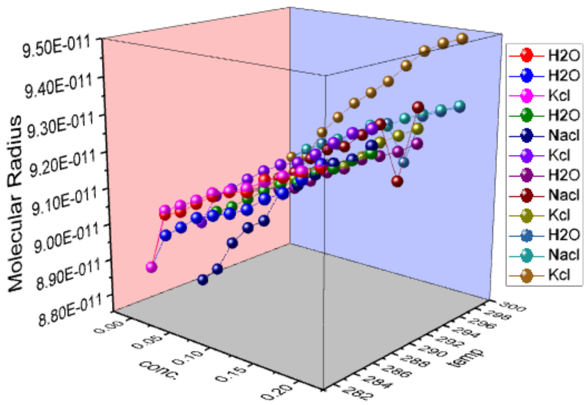


Figure 11 Molecular Radius v/s Concentration at different temperature

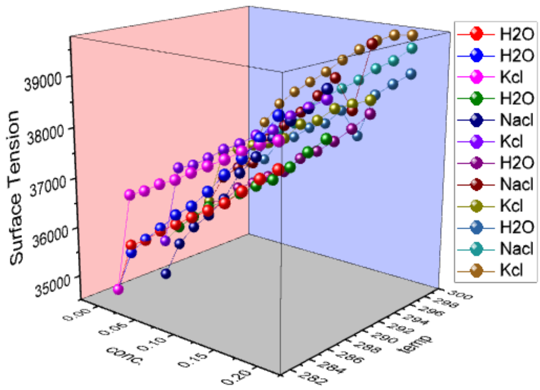


Figure 12 Surface Tension v/s Concentration at different temperature

After determining and calculating a graph of relative change in adiabatic compressibility as opposed to concentration as seen in Fig 13. Negative values of relative change in adiabatic compressibility is occurred and this is because of the solute-solvent interaction. Values of relative change in an adiabatic compressibility rises with concentration rising concentration perhaps assigned to an overall rise in cohesive forces. It shows the presence of hydrogen bonding in the solution [22]. Enthalpy is the sum of the internal energy of any thermodynamic system and the product of its volume and pressure. When we add solute to solvent the value of enthalpy increased with increasing concentration and temperature as depicted in Fig 14. From this, it reveals that the solute and solvent interaction happened in the system. It is concluded that with an increase in concentration and temperature, the enthalpy goes on increasing [23].

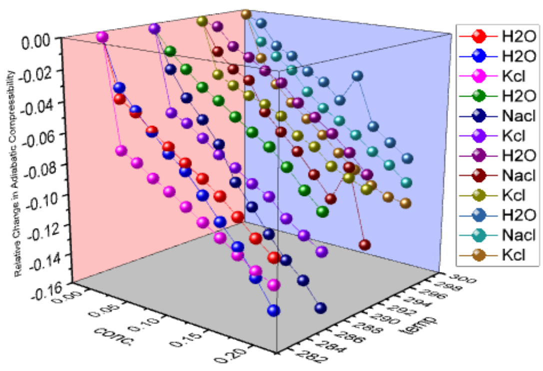


Figure 13 Relative Change in Adiabatic Compressibility v/s Concentration at different temperature

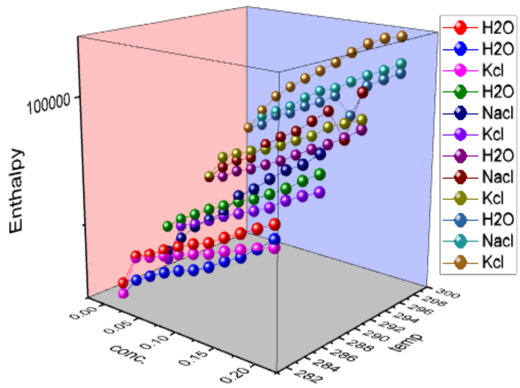


Figure 14 Enthalpy v/s Concentration at different temperature

The free length is the spacing between the middle of the surface of the near molecules. The value of intermolecular free length rises with rising concentration and temperature as shown in fig 17. From this figure it is observed that the presence of intermolecular forces in the solution. The decreasing nature of free length shows that the compactness of the structure is increasing and it is less compressible [24,25]. The solubility parameters depend on the internal pressure of the solution and are calculated with the help of internal pressure data represented in Fig 16. It is seen that the solubility parameters value increases with the concentration and temperature of the solution. This is because the solute mixture has strong hydrogen bonding and strong interaction forces are present in it [26].

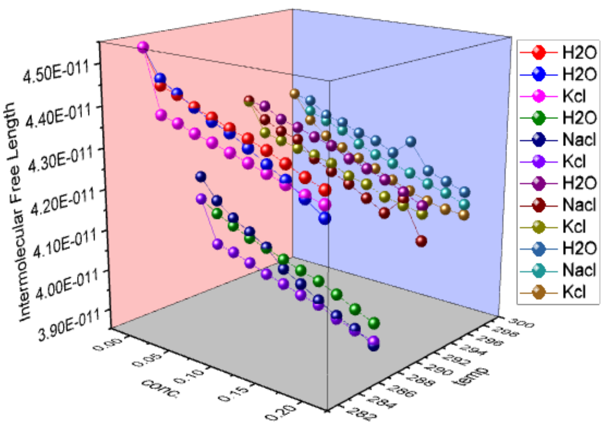


Figure 17 Intermolecular Free Length v/s Concentration at different temperature

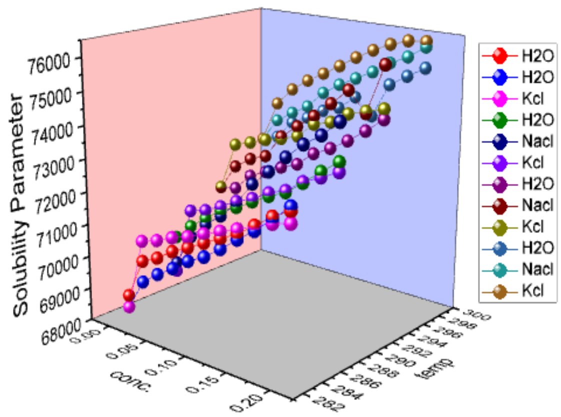


Figure 16 Solubility Parameter v/s Concentration at different temperature

4. Conclusion

In this research we observed ultrasonic velocity and density of the acetamide and aqueous salt solution (NaCl and KCl) at various concentrations of 0.02-0.2M and a temperature range from 283-298 K. Associate to velocity and density we derived some other parameters such as internal pressure, adiabatic compressibility, relative association, acoustic impedance, etc. All this parameter shows the presence of molecular forces between solute and solvent. In the current study we that the concentration and temperature increase the modification of these volumetric and thermoacoustic properties strongly gives the molecular bond present in all the three systems.

- System 1: Acetamide +H_2O
- System 2: Acetamide +NaCl +H_2O
- System 3: Acetamide + KCl + H_2O

Among them, KCl with Acetamide interacts most strongly, at higher concentrations as compared to NaCl and H_2O solvent. They give stronger solute-solvent interaction with higher mass fractions at higher temperatures. The order of interaction found to be as:

Acetamide + KCl + H_2O > Acetamide +NaCl+ H_2O > Acetamide + H_2O

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

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