## RESEARCH



# Studies on solute–solute and solute– solvent interactions of quercetin and 7-hydroxy flavone with nicotinamide in hydro-ethanolic mixed solvents: bioflavonoid-HBD interactions by volumetric and acoustic analysis

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## Abstract

The interaction between quercetin (QUE)/7-hydroxy flavone (7-HF) and nicotinamide (NAM) in drug formulations is an intriguing area of research due to their complementary biological effects. When used together, their combined actions can potentially offer synergistic therapeutic benefits. The objective of the present study is to analyze and interpret the types of interactions among various polar, non-polar, hydrophilic and hydrophobic parts of quaternary systems (QUE + water +ethanol+ NAM) and (7-HF + water + ethanol+ NAM) by volumetric and acoustic approach. The positive values of  $V_{\phi}^{0}$  exhibit an increasing trend with temperature, indicating that there is a significant solute–solvent interaction in the investigated solutions. Positive partial molar expansibilities demonstrate that QUE/7-HF promotes solute–solvent interactions in the system and functions as a structure former in aqueous solutions. The partial isentropic compressibility,  $K_{s}^{0}$  values are higher in 7-HF than in QUE showing greater extent of molecular interactions in 7-HF. From the derived data, the types of solute–solvent and solute–solute interactions and the structural modifications of water molecules were interpreted as a result of the inclusion of QUE/7-HF (solute) and NAM (co-solute) in the solvation shells. This study may provide a better understanding regarding the stronger solute–solvent interactions and structure-building ability of QUE/7-HF + NAM in a hydro-ethanolic medium, which may further help develop a pharmaceutical formulation of their mixture.

## Highlights

- Density and ultrasonic velocity of QUE/7-HF + NAM solutions were studied in hydroethanolic medium.
- The interactions of the solution's polar, nonpolar, and ionic segments were evaluated.
- The predominance of solute-solvent interactions is established.
- QUE/7-HF acts as a structure former in aqueous solutions.
- Pairwise interaction is predominant over triplet interaction.

Keywords Bioflavonoids, Nicotinamide, Volumetric properties, Acoustic parameters, Compressibility

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## Introduction

Flavonoids are commonly found in plant-based foods and beverages (i.e., red wine, tea, apples and onions) and are a broadly distributed class of polyphenolic chemicals. These widely used natural compounds have a variety of biological functions and significant medicinal uses (e.g. inflammation, cardiac problems, AIDS, allergies, tumours, cancers, etc.). The presence of phenolic hydroxyl groups in the flavonoid structure is what is thought to be responsible for bioflavonoids' antioxidant activity [1, 2]. Quercetin (QUE) and 7-hydroxy flavone (7-HF) are natural plant-based pigments and are the most abundant bioflavonoids. The common sources of QUE and 7-HF are fruits, leaves, vegetables, nuts and red wine. The biological properties of quercetin (3,3',4',5,7-pentahydroxyflavone) and 7-hydroxy flavone (7-hydroxy-2-phenylchromen-4-one) make them active ingredients in pharmaceutical and cosmetic industries [3–6]. For their practical applications in nutrition, health, food science, and agriculture, influencing their efficacy, stability, and overall impact, their physicochemical characteristics are very much crucial. The guality and compatibility of these therapeutic molecules that will be used in formulations can also be determined using the information from the physicochemical properties of their solutions. In the last couple of years, the investigations on thermodynamic, physicochemical, and acoustical properties of liquid mixtures with the help of volumetric and ultrasonic techniques have exponential and substantiated advancement [7-9]. Such approaches have become the extensive origin of information on the solute-solvent interactions occurring in a solution and are widely accepted techniques over other methods since these are non-destructive tools (i.e., these do not cause any deformity to the geometry and structure of the compounds) [10]. Thus, without causing any distortion, the analysis of several properties of multi-segment fluid blends is possible through the study of physicochemical properties through volumetric and ultrasonic methods.

The study of volumetric and ultrasonic properties is essential for advancing our understanding of chemical and biological processes, optimizing formulations, and ensuring quality across various applications. Inclusive of the nonspecific dielectric interactions among solvent and solute, another significant kind of solvent–solute interaction is the side-specific intermolecular hydrogen bonding interactions among hydrogen acceptor and donor molecules, which is basic and pivotal to understanding the microscopic function and structure in numerous molecular environments. From the vigorous studies, it has been monitored that abundant photochemical processes are influenced by hydrogen bonding. In view of this, the present work has been made to the molecular level interaction using volumetric and ultra-acoustic techniques for solutions of QUE and 7-HF with the co-solute molecule, NAM (nicotinic acid amide), which is a hydrogen bond donor (HBD) as well as a hydrotropic agent. The hydrogen-bonding interactions between apigenin and water/ethanol (H<sub>2</sub>O/EtOH) were investigated by Zheng et al. with the help of quantum chemical calculations. They found that -OH groups of apigenin molecules are favoured sites for hydrogen bonding [11]. The presence of HBD can sufficiently and directly mix with the target molecules to generate deep eutectic solvent systems, according to the research by Liu et al. [12]. The usage of HBDs also contributes to a strategy for successfully extracting natural products from plants.

Nicotinamide is frequently used to treat Pellagra as well as other skin conditions such as rosacea, acne, and autoimmune bullous [13]. Frequent investigations have presented that nicotinamide is possessive against diseases like Alzheimer's, Huntington's, hypertension, nonmelanoma skin cancer and Parkinson's diseases [14]. Additionally, NAM is known to possess some hydrotropic qualities. The term 'hydrotropy' refers to a solubilization process in which a sparingly soluble solute becomes more soluble in water upon the addition of substantial volumes of a second solute. Though there has been a lot of research on the physico-chemical characteristics of different electrolytes and nonelectrolytes in aqueous solutions, few researchers, it has been noted, have concentrated their research on the physico-chemical characteristics of bioflavonoids in aqueous solutions [15]. The study of the interaction between bioflavonoids and NAM holds significant potential for advancing knowledge in nutrition, health, skincare, and agriculture, with implications for enhancing human well-being and plant resilience. In line with our continuing research on the interactions of pharmacological compounds with hydrotropic agents in the solute-solute, solutesolvent, and ion-solvent regimes [16-21] and nonessential amino acids with food preservatives and saccharides [7, 22-28] vitamins with residual fertilizers [29], bioflavonoids with NAM in water-ethanol mixed solvent [30], a study of the molecular interactions of heterocyclic scaffolds has been attempted in this paper. The goal of this work is to discuss interactions between (solute+solute) and (solute+solvent) in the systems involving (QUE/7-HF+NAM)in hydro-ethanolic medium (ethanol+water) of different compositions.

Abbot et al. have studied different thermodynamic and acoustic properties of QUE in hydro-ethanolic solvent media of sodium dodecyl sulphate [4]. They found the dominance of hydrophobic interactions in the presence of surfactant in the solvent of ethanol+water

 $(EtOH + H_2O)$ . The volumetric and acoustic studies on the mixtures of OUE/7-HF and HBDs in the  $EtOH + H_2O$  mixed solvent have been made to analyze and interpret different kinds of interactions inside the solution. By employing the density data at T = 293.15-313.15 K with a 5 K interval, solute-solvent and solute-solute interactions are predicted and analysed in terms apparent molar volume (V $_{\phi}$ ), partial molar volume  $(V^0_{\varphi})$  and partial molar expansibility  $(E^0_{\varphi})$ . The velocity of ultrasound (U) has been measured in the aqueous mixed solutions (QUE/7-HF+NAM in hydroethanolic medium) of varying concentrations. Various acoustic parameters, such as isentropic compressibility  $(K_s)$ , apparent molar isentropic compressibility  $(K_{s,\phi})$ , isothermal compressibility (K<sub>T</sub>) and acoustic impedance (Z) have been derived at 293.15-303.15 K. The impact (solute-solvent interactions) of these physiologically significant bioflavonoids on the highly structured solvent (NAM+EtOH +  $H_2O$ ) at different temperatures would, therefore, be an attractive area of research. The present study formulated the hypothesis that QUE/7-HF forms specific molecular interactions with NAM in aqueous solution, and that the strength or extent of these interactions varies with temperature, influencing the overall behaviour and stability of the solution. The present study is unique because it combines volumetric and acoustic analysis to explore the interactions of quercetin and 7-hydroxy flavone with nicotinamide in hydro-ethanolic mixed solvents, which is relatively underexplored. This could reveal differential solvation behavior or specific synergistic effects in complex formulations. The choice of hydro-ethanolic mixtures is more reflective of real-world formulations (like pharmaceuticals or nutraceuticals) rather than simple solvent systems, making the study more relevant for practical applications. The previously reported studies have touched on molecular interactions, the detailed analysis focused on hydrogen bonding between flavonoids and NAM using volumetric and acoustic data is a novel approach. The data generated from the current study is valuable because it provides deep insights into the intermolecular interactions that affect solubility and stability, which are essential for developing effective pharmaceutical and nutraceutical formulations. The study of interactions at the molecular level can influence our understanding of how flavonoids like quercetin and 7-hydroxy flavone work in the body, helping predict their pharmacokinetics, bioavailability, and overall effectiveness as therapeutic agents.

## Experimental

## Materials

7-hydroxy flavone Quercetin, and nicotinamide were acquired from Sigma Chemical Co. (Bangalore, India) with percentage purity of 99% or above for the experimental purpose. Specifications of all these compounds are given in Table 1. Using an anhydrous CaCl<sub>2</sub> desiccator, all of these compounds were dried over the course of around 24 h. With the aid of a drying agent, the EtOH was removed over the course of 24 h in a molecular sieve [6]. In order to prepare solutions,  $EtOH + H_2O$  were used as the solvent, and conductivity water (specific conductance  $(2.89 - 3.26 \times 10^{-6})$  Scm<sup>-1</sup>) was collected through a triple distillation and deionization method.

## **Preparation of solutions**

Firstly, 30 v/v and 40 v/v aqueous EtOH solution were prepared. Secondly, 0.5 molal and 1.0 molal aqueous nicotinamide (NAM) solutions were prepared by the addition of NAM in 1 kg of water+EtOH solvent (30 v/v and 40 v/v). Now, the prepared homogeneous mixture of 30 v/v and 40 v/v EtOH with 0.5 mol kg<sup>-1</sup> and 1.0 mol kg<sup>-1</sup> NAM (m<sub>B</sub>) were used as four different solvents in order to prepare desired solutions of QUE and 7-HF with six different concentrations of  $(m_A)$ = 0.0040, 0.0035, 0.0030, 0.0025, 0.0020 and 0.0015 mol  $kg^{-1}$ ). The range captures both low-concentration and high-concentration behavior, providing insight into solubility, aggregation, and stability. It allows for systematic study of concentration-dependent effects on molecular interactions and thermodynamic properties. The concentrations are practical and relevant to drug formulation contexts, offering data that can be translated to real-world applications. By carefully choosing this concentration range, the full spectrum of physicochemical behaviors that QUE and 7-HF exhibit in solution are explored, providing important insights for formulation, stability, and therapeutic potential. Thus, the freshly prepared aqueous QUE and 7-HF solutions are all set for experimental work at laboratory room temperature and pressure (298.15 K, 101 kPa). It was found that the molal uncertainty of the solutions was  $\pm 1 \times 10^{-3}$  mol kg<sup>-1</sup>.

## Methods

## Density measurement

The density data of all the experimental solutions were measured by using a density analyser (Anton Paar DMA<sup>TM</sup> 5000M). In our recently published articles the way of calibration is rationalized [25, 26]. Prior to measuring the density of the solution, the density meter was calibrated using dry air and ultrapure water. First, the

Name <sup>a</sup> and CAS No. of chemicals <sup>b</sup>	Molecular formula and molar mass <sup>c</sup>	Molecular structure	Manufacturers	Mass fraction purity <sup>d</sup>	Purification method <sup>e</sup>
Quercetin <sup>a</sup> (117-39-5) <sup>b</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>7</sub> (0.3022)	НО ОН ОН	Sigma Chemical Co. (Bangalore, India)	·99	Drying over anhydrous CaCl <sub>2</sub>
7-Hydroxy flavone <sup>a</sup> (6665- 86-7) <sup>b</sup>	C <sub>15</sub> H <sub>10</sub> O <sub>3</sub> (0.2382)		Sigma Chemical Co. (Bangalore, India)	·99	Drying over anhydrous CaCl <sub>2</sub>
Nicotinamide <sup>a</sup> (98-92-0) <sup>b</sup>	C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O (0.1221)		Sigma Chemical Co. (Bangalore, India)	99	Drying over anhydrous CaCl <sub>2</sub>
Water <sup>a</sup> (7732-18-5) <sup>b</sup>	<i>H<sub>2</sub>O</i> (0.018)		Loba Chemie Pvt Ltd, Mumbai, India	<i>&gt;</i> 99	None
Ethanol <sup>a</sup> (64-17-5) <sup>b</sup>	C <sub>2</sub> H <sub>5</sub> OH (0.046)		Sigma Chemical Co. (Bangalore, India)	»99	Drying in molecular sieve (3A) for 24 h
	4-				

<sup>a</sup> All reagents were of A. R grade

<sup>b</sup> Chemical Abstract Service registry number

<sup>c</sup> Molar mass of chemical, (kg mol<sup>-1</sup>)

<sup>d</sup> Percentage purity (as manufacturer declared)

<sup>e</sup> All reagents were dried over CaCl<sub>2</sub> until a constant mass was reached

density of deionized water was determined in order to test the instrument's functionality. The instrument (DMA<sup>TM</sup> 5000M) has been able to maintain a consistent temperature with the aid of an internal Peltier thermostat. A microcontroller is used in the construction of the thermostat's control unit. Through 16-bit AD and DA converters, the microprocessor controls the Peltier thermoelectric elements and measures the temperature that has been reached. The values of density were calculated at T=293.15-313.15 K, having an uncertainty of  $\pm 0.45 \times 10^{-3}$ g cm<sup>-3</sup>. The temperature and pressure have the uncertainty of  $\pm 0.01$  K and  $\pm 1.0$  kPa, respectively.

### Ultrasonic velocity

Ultrasonic velocity in a liquid medium can be determined with the help of a simple yet reliable and accurate instrument, known as an ultrasonic interferometer [27]. The wavelength of sound ( $\lambda$ /ms<sup>-1</sup>) for the experimental solution was measured in a single frequency variable path ultrasonic interferometer (Model: F-05 by Mittal Enterprises, New Delhi, India). The instrument is constructed with an ultrasonic measuring cell (10 ml capacity), having a double-walled high-grade steel fabric with a quartz crystal base and a chromium-plated inner surface. The ultrasonic vibration is generated at the quartz crystal when an anodic current reaches it, which is created

by a piezoelectric generator. The pre-established frequency (f) of 2 MHz is set in the device. The tested solution is kept in the sample cell, and a micrometre is fixed with the vertical steel plate. The deflection by the pointer (which is connected to the base of the device) with this steel plate reflects the reading of  $\lambda/2$  in the micrometer. In this way, the wavelength of sound for the experimental liquid solutions were calculated at three different temperature, as stated earlier. The temperature was maintained with the help of an electrostatically heated water bath. Calibration of sound velocity data of the present with respect to a 3 MHz frequency was performed in order to ensure the accuracy and consistency of data.

The ultrasonic velocity, U (speed of the sound) was evaluated by the following equation:

$$U = f \times \lambda. \tag{1}$$

Uncertainty in ultrasonic velocity was found to be  $\pm\,0.5~ms^{-1}$  and for temperature it is  $\pm\,0.01$  K.

## **Results and discussion** Analysis of volumetric properties *Apparent molar volume*

Under atmospheric pressure and a temperature range of (293.15–313.15) K, the experimental densities for the examined solutions (QUE/7 HF in (a)  $EtOH + H_2O$ , and (b)  $EtOH + H_2O + 0.05/1.0 \text{ mol kg}^{-1}$  of NAM) were determined as a function of molality, m of QUE/7 HF [31]. As illustrated in Fig. 1, the examined solutions' density with molality variations at various temperatures (293.15, 298.15, 303.15, 308.15 and 313.15) K under atmospheric pressure are depicted. Inevitably, it



**Fig. 1** Plots of density, ρ vs molality, m for QUE [in **A** 30 v/v EtOH in 0.5 m NAM, **B** 40 v/v EtOH in 1.0 m NAM] and 7-HF [in **C** 30 v/v EtOH in 0.5 m NAM, **D** 40 v/v EtOH in 1.0 m NAM] at different temperatures



Scheme 1 A schematic presentation of possible molecular interactions among different components in the solution

is inaccessible to compare our current results because there isn't enough literature-based data. However, as expected, the examined density values are influenced by solution temperature and concentration [4, 32]. A perusal of table S1 (supplementary material) shows that the density increases with a decrease in the concentration of QUE/7-HF, and this might be attributed to the fact that the volume decreases because of the filling of the interstellar spaces within the large solute molecules, thereby increasing the mass of the molecules [33-35]. The increase in density with decreasing solute concentration is often related to the structural and intermolecular interactions between the solute and solvent molecules. Dilution allows solvent molecules to become more tightly packed, and if volume contraction occurs upon dilution or if the dissolution process is non-ideal, the density of the solution may increase as the concentration of solute decreases. The behavior depends on the specific system and the solute-solvent interactions involved. For the present study the resulting effect is that density decreases because, although the solute's mass is increasing, the volume of the solution does not increase proportionally, causing a net decrease in density.

Figure 1 shows the increase in density with decrease in concentration of solute, i.e. upon dilution density of QUE/7HF solution decreased. This can be explained in terms of the fact that ethanol has a lower density than water, so addition of more solvent can lower the density of the mixture. It can be noticed from table S1 that at certain temperatures and for similar concentrations, the density values are higher for QUE than 7-HF. This may be due to a higher molar mass of QUE than 7-HF. It can also be observed that for a fixed composition of EtOH +  $H_2O$  mixture the density values are higher for higher concentrations of NAM, both in the case of QUE as well as 7-HF. This can also be interpreted in terms of higher number of moles of NAM in the concerned composition of EtOH +  $H_2O$ .

Several kinds of intermolecular interactions can be predicted between solute molecules, hydrophilic, hydrophobic and electron-rich centres of QUE/7-HF with that of NAM (hydrogen donor cum accepter molecules) and EtOH (Scheme 1). The predominance of solute–solute, solutehydrophilic and hydrophilic–hydrophilic interactions among QUE/7-HF molecules over hydrophobic–hydrophobic interactions with the hydrocarbon backbone of the solute and solvent molecule leads to shrinkage in volume resulting from the stronger interactions among solute molecules of QUE/7-HF and that of solvent (hydro-ethanolic solution of NAM), and hence density gets increased. The measured experimental density values are found to decline with a rise in temperature, which may be due to the thermal expansion of the studied solutions.

Utilizing experimental density data, the apparent molar volume,  $V_{\varphi}$  of QUE/7-HF in hydro-ethanolic solvent mixtures of NAM was evaluated (Eq. 2) for different concentration ranges and the various NAM compositions (0.5 mol kg<sup>-1</sup> and 1.0 mol kg<sup>-1</sup>).

$$V_{\phi} = (\rho_0 - \rho)(m\rho\rho_0)^{-1} + M\rho^{-1}, \qquad (2)$$

where M is the molar mass of QUE/7 HF (g mol<sup>-1</sup>),  $\rho_0$  and  $\rho$  are the solvent and solution densities, m is the molality of QUE/7 HF in EtOH + H<sub>2</sub>O, and 0.05 and 1.0 mol kg<sup>-1</sup> of NAM are present in the hydro-ethanolic medium.

The following expression can be used to evaluate the approximation of uncertainty in apparent molar volumes [36].

$$\partial V_{\phi} = -\left(M + 1/m\right)(\partial \rho/\rho^2).$$
 (3)

When calculating the uncertainty of  $V_{\phi}$ , molality uncertainty is less significant than density uncertainty [37, 38]. In low molality ranges, the uncertainty in apparent molar volume can be simply calculated as  $\pm 0.02 \times 10^{-5} m^3 mol^{-1}$  by only taking the uncertainty in solution density  $(\partial \rho)$  into account.

Figure 2 shows a graphical illustration of the relationship between the apparent molar volume ( $V_{\varphi}$ ), molality (m) of QUE/7 HF in EtOH + H<sub>2</sub>O as well as various compositions of NAM, as a function of temperature. In quaternary systems, the computed apparent molar volumes of QUE/7 HF are provided in Table S1.

It is evident from the graphs (Fig. 2) and the data (Table S1) that all the results of  $V_{\varphi}$  are positive, and the values decline with increasing QUE/7 HF content in all the used solvents [27]. The positive values show that QUE/7 HF solutions have strong solute–solvent interactions between their polar groups with the polar part of NAM+EtOH + H<sub>2</sub>O. The decline in the values of



**Fig. 2** Plot of apparent molar volume ( $V_{\phi}$ ) vs square root of molality ( $\sqrt{m}$ ) for (**A**) QUE in 30 v/v EtOH + 0.5 mol kg<sup>-1</sup>NAM, (**B**) QUE in 40 v/v EtOH + 0.5 mol kg<sup>-1</sup>NAM, (**C**) 7-HF in 30 v/v EtOH + 0.5 mol kg<sup>-1</sup>NAM and (**D**) 7-HF in 40 wt % EtOH + 0.5 mol kg<sup>-1</sup>NAM at T = 293.15, 298.15 and 303.15 KR<sup>2</sup> values vary from 0.997 to 0.999

 $V_{\varphi}$  suggests the weakening of solute-solvent interactions in the solution with the increase in concentration. As the concentration of QUE/7-HF increases, the solute molecules are more likely to compete for interactions with solvent molecules and with each other. Several factors, such as saturation of solvent-solute binding sites, solute-solute interactions, disruption of solvent structure, decreasing solvent-solute hydrogen bonding, effect of NAM, etc. can contribute to this weakening of solute-solvent interactions. NAM might promote the formation of more solute-solute interactions rather than solute-solvent interactions. This can further weaken solute-solvent interactions and contribute to the decrease in  $V_{\phi}$ . Hence, as the concentration increases, the solvent molecules become saturated with the solute, leading to stronger solute-solute interactions and less efficient solvation, which decreases the volume expansion and results in a decrease in the apparent molar volume. It is also observed that there is an increase in  $V_{\phi}$  values with temperature, which may be as the water particles going away from the solvation sphere surrounding the solute particles (QUE/7 HF); the increase in temperature promotes electrostriction in the solution and, hence an increase in  $V_{\phi}$  values [25, 32]. It can be noticed from table S1 that there is a downturn in  $V_{\boldsymbol{\varphi}}$  values with the rise in the concentration of QUE/7- HF at all temperatures and compositions of the solvent mixtures. This can be explained by the fact that the interstellar spaces within the big solute molecules are filled, increasing the mass of the molecules, and hence, the volume decreases.

## Partial molar volume

The apparent molar volume at infinite dilution, also known as the partial molar volume, is where the solute molecules are at an infinite distance from one another and surrounded by lone solvent molecules. It solely provides pertinent data regarding solute–solvent interactions, which are unaffected by solute–solute interactions. Since the solute's intrinsic volume is nearly temperature-independent, its temperature dependency aids in describing the structural hydration effect at various temperatures. Following Masson's Eqn (Eq. 4), the partial molar volume of the solutions under study was determined.

$$V_{\phi} = V_{\phi}^0 + S_v \sqrt{m}. \tag{4}$$

The experimental slope, partial molar volume, molality and apparent molar volume are indicated by  $S_v$ ,  $V_{\varphi}^0$ , m and  $V_{\varphi}$ , respectively. Regression analysis is used to calculate the fitting accuracy of Eq. (4), and it is discovered to be above 80% for all solutions under examination at all temperatures. Solute–solvent

interactions are interpreted by  $V_{\varphi}^0$  data, whereas solute–solute interactions by  $S_{\nu}$  data. Table 2 lists the derived results for  $V_{\varphi}^0$ ,  $S_{\nu}$  with their standard errors for QUE/7 HF inEtOH + H<sub>2</sub>O, and in 0.5 mol kg<sup>-1</sup> and 1.0 mol kg<sup>-1</sup> of NAM at various temperatures. The standard deviations for partial molar volume are listed in Table 2.

The process of shell formation (referred to as solvation) around the solutes/ions is established by the interaction of the solvent with that of the dissociated solute. It is clear from Table 2 that there is a substantial solutesolvent interaction present in the examined solutions because the values of  $V^0_{\varphi}$  show an increasing trend with temperature. An increase in temperature causes thermal expansion, which causes some water molecules to get dislodged from the primary solvation layer enclosing QUE/7 HF and go into the bulk, increasing the  $V_{\phi}^{0}$  values. A graphical presentation is given in Fig. 3, which shows the variation of  $V^0_\varphi$  values with temperature for different compositions of solvent mixtures. The alteration of the partial molar volume is influenced by the creation of hydrogen bonds during solution and by hydrophobic hydration. Hydrophobic hydration interaction has a positive influence over volume, while the hydrogen bond interaction has a negative control.

The slope parameter of the linear regression (the volumetric co-efficient,  $S_v$ ) in the Masson equation is a key parameter that reflects the behavior of the solution as the concentration increases. The slope S<sub>v</sub> indicates unfavorable solute-solvent interactions. It provides insight into the interactions between the solute and the solvent. Two hydrophobic co-spheres overlapping is justified by its negative sign [39]. When two polar centers contact in solution, like carbonyl group (C=O), amide nitrogen (N-H) and pyridine nitrogen (N), the solvent cospheres overlap, causing some electrostricted water to return to the bulk solvent and causing a positive volume change. However, when two hydrophobic hydration cospheres (-CH<sub>2</sub> sites of aromatic ring of NAM) overlap and polar groups interact, the volume changes negatively, resulting in a negative  $S_v$ . A negative slope suggests that as the concentration increases, the solute is less effectively solvated, leading to a decrease in the apparent molar volume, possibly due to the formation of solute-solute interactions that reduce the need for solvent accommodation. For the present study, the negative values of S<sub>v</sub> suggest that strong solute-solute interactions should prevail over solute-solvent interactions. The values of S<sub>v</sub> show that there is no such clear trend, which suggests that other important factors have a significant impact on the solute-solute interactions [40].

OII         7+H         OII         7+H         OII         7+H         OII         7+H         OII         7+H         OII           30/V.EOCH+0.5/M.MAM         30/V.EOCH+0.5/M.MAM         31388.205         130.64114         -46.882.64174         -30.4775±112         -2.44         -2.88         86.62         14.39         1985           30.815         31388.205         140.06.4147         -46.882.64.173         -30.4775±112         -2.44         -2.88         36.62         14.39         1985           30.815         3168.82.02         1396.64.123         -51.04.34.134         155.7         1137         23.44         24.43           30.815         3168.82.02         1356.44.123         -51.04.34.132         -2.144.44.134         99.0         23.38         21.44           30.915         3567.41.00         138.94.123         -2.145.84.123         -2.146.84.123         2.74         2.43         2.43           30.915         2564.84.112         168.64.41.13         -36.93.314.102         -1.28         2.44         2.443           30.915         2564.41.12         168.64.121         2.77         -0.22         2.34         2.443         2.443           30.915         2564.41.12         148.84         2.430 </th <th>т/К</th> <th><math>V_{\phi}^{0} \times 10^{5} / m^{3} mol^{-1}</math></th> <th></th> <th><math>S_v \times 10^5/m^3 mol^{-2} kg</math></th> <th></th> <th><math>\sigma \times 10^3</math></th> <th></th> <th><math>E_{\Phi}^{0}/\mathrm{m}^{3}\mathrm{mol}^{-1}\mathrm{K}^{-1}</math></th> <th>7</th> <th><math>\Delta_{tr}V_{\phi}^{0} \times 10^{-10}</math></th> <th>2/m<sup>3</sup>mol<sup>-1</sup></th>	т/К	$V_{\phi}^{0} \times 10^{5} / m^{3} mol^{-1}$		$S_v \times 10^5/m^3 mol^{-2} kg$		$\sigma \times 10^3$		$E_{\Phi}^{0}/\mathrm{m}^{3}\mathrm{mol}^{-1}\mathrm{K}^{-1}$	7	$\Delta_{tr}V_{\phi}^{0} \times 10^{-10}$	2/m <sup>3</sup> mol <sup>-1</sup>
30W/EGCH 4.5/m/MM           20315         29490±107         13266±114         -468826±174         -204775±112         -214         -298         38.62         14.29         1985           20315         29490±107         13266±114         -468826±174         -204775±112         -214         -298         37.09         1328         21.47           20315         33584±202         15394±76         -51,8294±76         -51,8294±712         -407216±347         -407215±395         -11.23         23.39           20815         34618±202         15334±156         -51,8294±72         -51,8294±72         -51,473±129         2.49         900         23.88           30315         25645±166         -22,444±121         21,473±129         2.49         2.40         900         23.88           30315         25645±166         -22,4455±181         1553±123         -90,903±171         -413         24.43         24.45         2.44         2.44         2.44         2.44           30315         25645±166         -22,4456±166         -22,441211         2.145         2.24         2.44         2.44         2.44         2.44           30315         26655±181         15551±123         -90,903±1214         -2.74         2.26		QUE	7-HF	QUE	7-HF	QUE	7-HF	QUE	7-HF	QUE	7-HF
29315 $2940\pm107$ $1326\pm114$ $-468826\pm174$ $-204775\pm112$ $-244$ $-298$ $3662$ $1429$ $1938$ $2147$ 20315 $31388\pm205$ $14016\pm147$ $-97216\pm395$ $-71236\pm123$ $-97216\pm395$ $-71236\pm123$ $-97216\pm395$ $1238$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2139$ $2143$ $2143$ $2143$ $2143$ $2143$ $2143$ $2143$ $2139$ $2139$ $2139$ $2149$ $2149$ $2143$ <td< td=""><td>30 v/v EtOh</td><td>I + 0.5 m NAM</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></td<>	30 v/v EtOh	I + 0.5 m NAM									
29815         31588±205         14016±147 $-497216\pm395$ $-212362\pm125$ 4.20         8.82         37.09         12.83         21.47           30815         3332.2±213         14396±123 $-518364\pm423$ $-21243\pm104$ 150 $3557$ 1137         223           30815 $3332.2\pm213$ 14366±123 $-518364\pm423$ $-21433\pm108$ $-556$ $2.94$ $3.04$ $9.90$ $2.333$ $30767\pm207$ 18392±156 $-536345\pm166$ $-224353\pm172$ $-21443\pm120$ $9.90$ $2.333$ $20015$ 23601±132         14368±166 $-22656\pm121$ $2.77$ $-0.22$ $3.331$ $2.47$ $2.443$ $20015$ $23601\pm132$ 14366±166 $-225654\pm121$ $2.77$ $-0.22$ $3.331$ $1.001$ $1336$ $20015$ $23641\pm112$ $1633\pm1410$ $-40203\pm1166$ $-223738\pm177$ $-4126$ $-126$ $2.43$ $1.46$ $20015$ $2364\pm1411$ $1630$ $4303\pm166$ $-234315\pm166$ $-234315\pm166$ $1.265$ $1.126$ $1.276$ <td< td=""><td>293.15</td><td>2949.0±10.7</td><td>1326.6±11.4</td><td>— 46,882.6 ± 17.4</td><td><math>-20,477.5 \pm 11.2</math></td><td>- 2.44</td><td>- 2.98</td><td>38.62</td><td>14.29</td><td>19.85</td><td>7.83</td></td<>	293.15	2949.0±10.7	1326.6±11.4	— 46,882.6 ± 17.4	$-20,477.5 \pm 11.2$	- 2.44	- 2.98	38.62	14.29	19.85	7.83
3332.2±13         1430.6±123 $-512264.402$ $-21244.4\pm194$ 1.50 $-880$ $3557$ 1137 $2239$ 30815 $34018\pm202$ $15334\pm156$ $-55345\pm423$ $-21433\pm108$ $-556$ $2.94$ $3404$ $990$ $2333$ $30515$ $35631\pm274$ $13689\pm172$ $-5618888\pm527$ $-17473\pm129$ $2.476$ $2.99$ $3404$ $990$ $2333$ $30315$ $2504\pm132$ $14887\pm166$ $-354567\pm166$ $-272654\pm171$ $-475$ $-1.26$ $2940$ $1138$ $1489$ $2915$ $2504\pm131$ $16887\pm166$ $-273654\pm171$ $-475$ $-1.26$ $1236$ $1236$ $1236$ $30315$ $26658\pm181$ $15551\pm123$ $-391931\pm166$ $-223633\pm117$ $-475$ $1236$ $1236$ $1236$ $30315$ $26658\pm181$ $15551\pm123$ $-391931\pm166$ $-2236334\pm124$ $1236$ $1236$ $1236$ $30315$ $26658\pm181$ $15551\pm123$ $-33031\pm107$ $-1438$ $1266$ $1236$	298.15	$3158.8 \pm 20.5$	$1401.6 \pm 14.7$	$-49,721.6 \pm 39.5$	- 21,236.2±12.5	4.20	8.82	37.09	12.83	21.47	7.88
30815 $34018\pm202$ $15234\pm156$ $-356345\pm423$ $-221435\pm108$ $-556$ $294$ $3404$ $990$ $2338$ $300VEC0H+100MMM$ $30057\pm207$ $15899\pm172$ $-561858\pm527$ $-21/473\pm129$ $249$ $-2581$ $32331$ $1001$ $1398$ $29015$ $2362.1\pm274$ $14868\pm180$ $-564567\pm166$ $-225654\pm121$ $277$ $-022$ $3331$ $1001$ $1398$ $29815$ $2362.1\pm274$ $14882\pm166$ $-359333\pm192$ $-225654\pm121$ $277$ $-022$ $3331$ $1001$ $1389$ $29815$ $256304\pm131$ $148754166$ $-23933\pm192$ $-228738\pm177$ $-475$ $1267$ $1276$ $1553$ $31315$ $28576\pm110$ $16334\pm140$ $-402033\pm175$ $-233152\pm124$ $-274$ $066$ $1767$ $1571$ $1640$ $31315$ $28576\pm110$ $14317\pm138$ $-420615\pm164$ $-223650\pm151$ $-223932555$ $2134$ $2137$ $20054$ $277567$ $273555610$ $43136\pm152$ <td>303.15</td> <td>3332.2±21.3</td> <td>1439.6±12.3</td> <td><math>-51,829.6 \pm 40.2</math></td> <td>- 21,244.4±19.4</td> <td>1.50</td> <td>- 8.60</td> <td>35.57</td> <td>11.37</td> <td>22.39</td> <td>7.55</td>	303.15	3332.2±21.3	1439.6±12.3	$-51,829.6 \pm 40.2$	- 21,244.4±19.4	1.50	- 8.60	35.57	11.37	22.39	7.55
31315 $36767\pm 207$ $1589\pm 172$ $-56185\pm 527$ $-217473\pm 129$ $249$ $-2581$ $3251$ $3241$ $2443$ $2443$ $300VeEOH+10mMMM$ $3667\pm 123$ $48857\pm 156$ $-36554\pm 121$ $277$ $-0.22$ $3331$ $1001$ $1398$ $20315$ $25604\pm 132$ $14887\pm 156$ $-37333\pm 192$ $-228738\pm 177$ $-475$ $-1.26$ $2940$ $1138$ $1439$ $20315$ $2504\pm 1121$ $15551\pm 123$ $-391933\pm 166$ $-228733\pm 177$ $-126$ $2940$ $1137$ $1553$ $20315$ $2564\pm 1121$ $15551\pm 123$ $-391933\pm 166$ $-228733\pm 172$ $1137$ $1634$ $1433$ $1654$ $1433$ $30315$ $28576\pm 110$ $16934\pm 131$ $-40303\pm 2114$ $-224331\pm 102$ $1267$ $1237$ $1553$ $31315$ $28576\pm 110$ $16934\pm 131$ $-40303\pm 2114$ $-224331\pm 1192$ $1266$ $1202$ $1202$ $1202$ $1202$ $1202$ $1202$ $1202$ $1202$ $120$	308.15	3481.8±20.2	1523.4±15.6	$-53,634.5 \pm 42.3$	- 22,143.5±10.8	- 5.56	2.94	34.04	9.90	23.38	7.50
	313.15	3676.7±20.7	$1589.9 \pm 17.2$	$-56,185.8\pm52.7$	- 21,747.3±12.9	2.49	- 25.81	32.51	8.44	24.43	6.86
29315 $2362.1\pm274$ $1436.8\pm180$ $-36456.7\pm166$ $-22556.4\pm121$ $2.77$ $-0.22$ $33.31$ $1001$ $13.98$ 29815 $2500.4\pm132$ $1488.7\pm156$ $-37933.3\pm192$ $-22,553.4\pm177$ $-4.75$ $-1.26$ $29.40$ $11.38$ $4489$ 20815 $2564.8\pm181$ $15551.1\pm12.3$ $-39,193.1\pm166$ $-2.2,873.8\pm177$ $-4.75$ $-1.26$ $29.40$ $11.38$ $4489$ $30315$ $2574.1\pm112$ $1633.4\pm14.0$ $-40,270.3\pm175$ $-2.2,873.8\pm177$ $-1.26$ $25.49$ $12.76$ $15.53$ $30315$ $2784.1\pm112$ $1633.4\pm14.0$ $-40,270.3\pm175$ $-2.3,315.5\pm10.2$ $-2.3,303.3\pm21.1$ $2.43,105.7$ $12.67$ $12.76$ $15.51$ $40\sqrt{FOH+405} MAM$ $1431.7\pm13.8$ $-40,2061.5\pm16.4$ $-2.28650.\pm151$ $-2.44$ $0.65$ $17.67$ $15.51$ $16.24$ $20315$ $20752\pm19.3$ $1431.7\pm13.8$ $-40,2061.5\pm16.4$ $-2.28650.\pm151$ $-2.74$ $0.65$ $2.241$ $2.023$ $20315$ $20752\pm19.3$ $1431.7\pm13.8$ $-42,261.5\pm16.4$ $-2.28554.\pm11.9$ $16.67$ $12.67$ $2.141$ $20315$ $2094.0\pm12.8$ $1437.7\pm13.8$ $-2.24,595.1\pm10.9$ $16.64$ $2.143$ $2.023$ $20315$ $2034.0\pm12.8$ $17290.0\pm13.7$ $-43,575.2\pm23.2$ $-2.5554.\pm10.9$ $12.66$ $2.141$ $2.023$ $20315$ $2034.0\pm12.8$ $17290.0\pm13.7$ $-45,565.2\pm12.9$ $1.56$ $-1.26$ $2.241$ $2.143$ $20315$ $2034.2\pm14.7$ $-24,565.7\pm2.87$ <td>30 v/v EtOh</td> <td>l + 1.0 m NAM</td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td> <td></td>	30 v/v EtOh	l + 1.0 m NAM									
298.15 $25004\pm13.2$ $14887\pm15.6$ $-37933\pm19.2$ $-228738\pm17.7$ $-475$ $-1.26$ $29.40$ $11.38$ $14.89$ 303.15 $26458\pm18.1$ $15551\pm12.3$ $-391931\pm16.6$ $-234031\pm10.7$ $-1.43$ $2.65$ $25.49$ $12.76$ $15.53$ 308.15 $2784.1\pm11.2$ $16134\pm14.0$ $-402.703\pm175$ $-23,4031\pm10.7$ $-1.43$ $2.66$ $-2.99$ $215.8$ $14.13$ $16.40$ $313.15$ $2887.6\pm11.0$ $16934\pm13.1$ $-402.03\pm17.5$ $-23,4031\pm10.7$ $-2.24$ $0.65$ $17.67$ $15.51$ $16.24$ $40V$ $60T$ $6334\pm13.1$ $-402.03\pm17.5$ $-23,715.2\pm13.5$ $6.06$ $-2.99$ $21.63$ $12.76$ $15.51$ $16.24$ $40V$ $60T$ $605$ $17.67$ $1637$ $16.24$ $0.2355\pm17.0$ $-431386\pm15.3$ $2.2413$ $10.27$ $16.24$ $20315$ $20752\pm19.3$ $1637\pm12.8$ $-22,8650\pm15.1$ $-2.28650\pm15.1$ $-2.28650\pm15.1$ $-2.267$ $2.241$ $2023$ $20315$ $20732\pm10.3$ $1637\pm12.8$ $-2.28650\pm15.1$ $-2.28650\pm15.1$ $-2.267$ $2.241$ $2023$ $20315$ $20732\pm10.3$ $1637\pm12.8$ $-2.28650\pm15.1$ $-2.28650\pm15.1$ $-2.26651\pm1.1$ $2.210$ $2.241$ $20315$ $20740\pm12.8$ $1777$ $1772$ $2013$ $2023$ $2049$ $2143$ $20315$ $20940\pm12.8$ $1767$ $1767$ $116.2$ $2114$ $2143$ $20315$ $20040\pm12.8$ $17767$ $245657\pm2.877$	293.15	2362.1±27.4	$1436.8 \pm 18.0$	- 36,456.7 ± 16.6	- 22,565.4±12.1	2.77	- 0.22	33.31	10.01	13.98	8.93
303.15 $26458\pm181$ $15551\pm123$ $-39,193.1\pm166$ $-23403.1\pm107$ $-143$ $2.65$ $2.549$ $12.76$ $1553$ 308.15 $27841\pm112$ $16134\pm140$ $-40,2703\pm175$ $-23,152\pm135$ $6.06$ $-2.99$ $2158$ $14,13$ $1640$ $313.15$ $28576\pm110$ $16934\pm13.1$ $-40,203\pm17.5$ $-23,155\pm12.4$ $-2.74$ $0.65$ $1767$ $1551$ $1624$ $40VVECOH+05mVAM$ $14317\pm13.8$ $-40,3093\pm13.1$ $-24,3105\pm12.4$ $-2.24,3105\pm12.4$ $-2.24,305\pm10$ $14317\pm13.8$ $-42,0615\pm16.4$ $-2.24650\pm15.1$ $-4.58$ $1.20$ $1803$ $22241$ $2023$ $293.15$ $23795\pm170$ $14317\pm13.8$ $-42,0615\pm16.4$ $-2.28650\pm15.1$ $-4.58$ $1.20$ $1803$ $2241$ $2023$ $293.15$ $23795\pm170$ $14317\pm13.8$ $-42,0615\pm16.4$ $-2.28650\pm15.1$ $-4.58$ $1.20$ $1803$ $2241$ $2023$ $293.15$ $20272\pm19.9$ $14317\pm13.8$ $-42,0615\pm16.4$ $-2.28650\pm15.1$ $-1.65$ $21.00$ $21.09$ $203.15$ $2037\pm12.10$ $-43,1336\pm15.3$ $-23974\pm13.3$ $817$ $-1.12$ $2007$ $2049$ $21.09$ $303.15$ $30940\pm12.8$ $17290\pm13.7$ $-43,5157\pm2.222-25,857,1\pm11.14.8-1.2221.61.4321.6303.1530940\pm12.817991\pm19.6-45,4567\pm2.87-25,857,1\pm11.14.8-1.2221.61.4321.6303.1530364\pm12.810071\pm1.13-46,1075$	298.15	2500.4±13.2	$1488.7 \pm 15.6$	$-37,933.3 \pm 19.2$	- 22,873.8±17.7	- 4.75	- 1.26	29.40	11.38	14.89	8.75
308.15 $27841\pm11.2$ $16134\pm14.0$ $-40,2703\pm17.5$ $-23,7152\pm13.5$ $6.06$ $-2.99$ $21.58$ $14.13$ $16.40$ $313.15$ $28576\pm11.0$ $16934\pm13.1$ $-40,3093\pm21.1$ $-24,3105\pm12.4$ $-2.74$ $0.65$ $17.67$ $15.51$ $16.24$ $40VVEGOH+0.5MNAM$ $1431.7\pm13.8$ $-42,0615\pm16.4$ $-2.28650\pm15.1$ $-4.58$ $11.20$ $18.03$ $22.41$ $2023$ $293.15$ $27953\pm17.0$ $1431.7\pm13.8$ $-42,0615\pm16.4$ $-2.28650\pm15.1$ $-4.58$ $1.20$ $18.03$ $22.41$ $2023$ $293.15$ $27953\pm17.0$ $1431.7\pm13.8$ $-42,0615\pm16.4$ $-2.28650\pm15.1$ $-4.58$ $1.20$ $18.03$ $22.41$ $2023$ $293.15$ $2375\pm100$ $-43,1386\pm15.3$ $-23,974.\pm13.3$ $8.17$ $-1.12$ $2007$ $2049$ $21.09$ $203.15$ $30340\pm12.8$ $1729.0\pm19.7$ $-43,5796\pm19.7$ $-24,931\pm11.9$ $1.56$ $-1.65$ $22.10$ $18.76$ $21.43$ $303.15$ $30940\pm12.8$ $1729.0\pm13.7$ $-43,575\pm2.32$ $-25,543\pm10.5$ $-24,13$ $16.64$ $21.43$ $303.15$ $30940\pm12.8$ $1799.1\pm19.6$ $-45,4567\pm2.87$ $-25,5543\pm10.5$ $24.13$ $16.64$ $21.43$ $303.15$ $30940\pm12.8$ $1799.1\pm10.6$ $-45,4567\pm2.87$ $-25,5543\pm10.5$ $24.13$ $16.72$ $26.16$ $14.72$ $40VVECOH+10MNAM$ $1709.1\pm10.6$ $-45,4567\pm2.87$ $-16,67,421.5$ $26.16$ $14.72$ $21.61$ $40VVECOH+10MNAM$ $1047.0\pm11.3$	303.15	2645.8±18.1	$1555.1 \pm 12.3$	$-39,193.1 \pm 16.6$	$-23,403.1 \pm 10.7$	- 1.43	2.65	25.49	12.76	15.53	8.70
313.15 $2857.6\pm110$ $1693.4\pm13.1$ $-40,309.3\pm21.1$ $-24,310.5\pm12.4$ $-2.74$ $0.65$ $17.67$ $15.51$ $16.24$ $40VVEC0H+0.5MMM$ $40VVEC0H+0.5MMM$ $1331.7\pm13.8$ $-42,061.5\pm16.4$ $-2.2,865.0\pm15.1$ $-4.58$ $1.20$ $180.3$ $22.41$ $2023$ $293.15$ $2927.2\pm19.3$ $1335.5\pm10.0$ $-43,386\pm15.3$ $-22,3974.7\pm13.3$ $8.17$ $-1.12$ $2007$ $20.49$ $2109$ $203.15$ $2027.2\pm19.3$ $1535.5\pm10.0$ $-43,386\pm15.3$ $-23,974.7\pm13.3$ $8.17$ $-1.12$ $2007$ $20.49$ $2109$ $203.15$ $3013.4\pm10.3$ $1632.2\pm19.9$ $-43,579.6\pm197$ $-24,793.1\pm11.9$ $1.56$ $-1.12$ $2007$ $20.49$ $21.03$ $303.15$ $3013.4\pm10.3$ $1632.2\pm19.9$ $-43,575.7\pm23.2$ $-25,554.3\pm10.5$ $-28,65.9\pm11.1$ $4.32$ $21.21$ $20.49$ $21.03$ $303.15$ $3094.0\pm12.8$ $1729.0\pm13.7$ $-43,515.7\pm23.2$ $-25,554.3\pm10.5$ $-24,63$ $31.66$ $21.41$ $20.76$ $303.15$ $304.0\pm12.8$ $1729.0\pm13.7$ $-43,555.7\pm23.7$ $-25,554.3\pm10.5$ $22.13$ $22.13$ $16.7$ $21.43$ $21.43$ $303.15$ $3264.3\pm14.7$ $1779.9\pm14.9$ $-45,1075\pm27.7$ $-16,14.67\pm1.9$ $0.26$ $892$ $29.71$ $21.91$ $22.13$ $203.15$ $3286.9\pm14.2$ $1047.0\pm11.3$ $-46,1075\pm27.7$ $-16,14.67\pm1.95$ $0.26$ $892$ $29.71$ $21.91$ $22.12$ $203.15$ $3032.5\pm12.6$ $1047.0\pm11.3$	308.15	2784.1±11.2	1613.4±14.0	$-40,270.3 \pm 17.5$	$-23,715.2\pm13.5$	6.06	- 2.99	21.58	14.13	16.40	8.40
	313.15	$2857.6 \pm 11.0$	$1693.4 \pm 13.1$	$-40,309.3 \pm 21.1$	$-24,310.5\pm12.4$	- 2.74	0.65	17.67	15.51	16.24	8.30
293.15 $2795.3\pm170$ $1431.7\pm13.8$ $-42.061.5\pm16.4$ $-2.2865.0\pm15.1$ $-45.8$ $1.20$ $180.3$ $2241$ $2023$ 298.15 $2927.2\pm19.3$ $1535.5\pm10.0$ $-43,138.6\pm15.3$ $-23,974.7\pm13.3$ $8.17$ $-1.12$ $2007$ $20.49$ $21.09$ $203.15$ $3013.4\pm10.3$ $1632.2\pm19.9$ $-43,579.6\pm19.7$ $-23,974.7\pm13.3$ $8.17$ $-1.12$ $2007$ $20.49$ $21.09$ $303.15$ $301.4\pm10.3$ $1632.2\pm19.9$ $-43,57.5\pm23.2$ $-23,93.1\pm11.9$ $1.56$ $21.21$ $20.73$ $20.49$ $21.43$ $308.15$ $3094.0\pm12.8$ $1729.0\pm13.7$ $-43,515.7\pm23.2$ $-25,857.1\pm11.1$ $4.38$ $-1.22$ $26.16$ $14.72$ $21.43$ $313.15$ $3264.3\pm14.7$ $1799.1\pm19.6$ $-45,456.7\pm28.7$ $-25,857.1\pm11.1$ $4.38$ $-1.22$ $26.16$ $14.72$ $21.13$ $40VVEOH+1.0mMAM$ $1779.0\pm11.3$ $-46,107.5\pm27.7$ $-16,146.7\pm19.6$ $0.48$ $-2.34$ $28.96$ $19.30$ $21.25$ $298.15$ $3032.5\pm12.6$ $116.2.9\pm14.9$ $-47,544.9\pm2.44$ $-17,434.1\pm15.9$ $0.26$ $8.92$ $29.51$ $21.93$ $22.15$ $208.15$ $3168.2\pm10.9$ $1253.8\pm17.6$ $-48,698.0\pm196$ $-18,285.3\pm17.2$ $-332.2$ $29.51$ $21.93$ $23.76$ $308.15$ $3168.2\pm10.9$ $1253.8\pm17.6$ $-48,698.0\pm196$ $-16,744.9\pm12.1$ $4.22,72$ $2.329$ $231.3$ $231.3$ $231.34.74\pm15.8$ $140.78\pm12.4$ $-50,019.1\pm14.5$ $-167$ $-1.44$ <t< td=""><td>40 v/v EtOh</td><td>l + 0.5 m NAM</td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td><td></td></t<>	40 v/v EtOh	l + 0.5 m NAM									
29815         2977.±19.3         1535.5±10.0         -43,1386±15.3         -23,974.7±13.3         8.17         -1.12         2007         20,49         2109           303.15         3013.4±10.3         1632.2±19.9         -43,5796±19.7         -24,793.1±11.9         1.56         -1.65         22.10         18.56         21.41           303.15         3013.4±10.3         1632.2±19.9         -43,575/±23.2         -24,793.1±11.9         1.56         -1.65         22.10         18.56         21.41           308.15         3094.0±12.8         1729.0±13.7         -43,575/±23.2         -25,554.3±10.5         -9.80         3.56         24.13         16.64         21.43           313.15         3264.3±14.7         17799.1±19.6         -45,565/±28.7         -25,554.3±10.5         -9.80         3.56         24.13         16.64         21.43           40V/rE(P(H+1.0m NAM         17799.1±19.6         -45,555/±28.7         -25,5557.1±11.1         4.38         -1.22         26.16         19.30         21.25           293.15         2886.9±14.2         1047.0±11.3         -46,107.5±27.7         -16,146.7±15.9         0.26         8.92         29.51         21.91         22.15           293.15         2886.9±14.2         1162.9±14.9         0.26	293.15	$2795.3 \pm 17.0$	1431.7±13.8	- 42,061.5 ± 16.4	- 22,865.0±15.1	- 4.58	1.20	18.03	22.41	20.23	9.03
303.15       3013.4±10.3       1632.2±19.9       -43,5796±19.7       -24,793.1±11.9       1.56       -1.65       22.10       18.56       2141         308.15       30940±12.8       1729.0±13.7       -43,515.7±23.2       -25,554.3±10.5       -9.80       3.56       24.13       16.64       2143         313.15       3264.3±14.7       1799.1±19.6       -43,515.7±23.2       -25,554.3±10.5       -9.80       3.56       24.13       16.64       21.43         313.15       3264.3±14.7       1799.1±19.6       -45,565.4±28.7       -25,554.3±10.1       4.38       -1.22       26.16       14.72       21.13         40\/\/\/\/\/\/\/\/\       1799.1±19.6       -45,4567.4±28.7       -16,146.7±19.6       0.48       -1.22       26.16       19.30       21.25         293.15       2886.9±14.2       1047.0±11.3       -46,1075.4±27.7       -16,146.7±19.6       0.48       -2.34       28.96       19.30       21.25       21.91       22.15         293.15       2886.9±14.2       1162.9±14.9       -47,544.9±24.4       -17,434.1±15.9       0.26       8.92       29.51       21.91       22.15         303.15       3168.2±10.9       1253.8±17.6       -18,48.0±16.5       -11.84       30.05       27.45       29.6 <td>298.15</td> <td>2927.2±19.3</td> <td><math>1535.5 \pm 10.0</math></td> <td><math>-43,138.6\pm15.3</math></td> <td>- 23,974.7±13.3</td> <td>8.17</td> <td>- 1.12</td> <td>20.07</td> <td>20.49</td> <td>21.09</td> <td>9.15</td>	298.15	2927.2±19.3	$1535.5 \pm 10.0$	$-43,138.6\pm15.3$	- 23,974.7±13.3	8.17	- 1.12	20.07	20.49	21.09	9.15
308.15       3094.0±12.8       1729.0±13.7       -43,515.7±23.2       -25,554.3±10.5       -9.80       3.56       24.13       16.64       21.43         313.15       3264.3±14.7       1799.1±19.6       -45,456.7±28.7       -25,857.1±11.1       4.38       -1.22       26.16       14.72       21.13         40.VVEICH+1.0m NAM       233.15       2886.9±14.2       1047.0±11.3       -46,107.5±27.7       -16,146.7±19.6       0.48       -2.34       28.96       19.30       21.25         293.15       2886.9±14.2       1047.0±11.3       -46,107.5±27.7       -16,146.7±19.6       0.48       -2.34       28.96       19.30       21.25         293.15       2886.9±14.2       1047.0±11.3       -46,107.5±27.7       -16,146.7±19.6       0.48       -2.34       28.96       19.30       21.25         293.15       2886.9±14.2       1162.9±14.9       -47,544.9±24.4       -17,434.1±15.9       0.26       8.92       2951       21.91       22.15         303.15       3168.2±10.9       1253.8±17.6       -48,698.0±19.6       -18,285.3±17.2       -3.92       -11.84       30.05       27.95       23.96         303.15       3347.4±15.8       1407.8±14.4       -50,0191±14.5       -20,114.6±12.1       4.52       7.09	303.15	3013.4±10.3	$1632.2 \pm 19.9$	— 43,579.6 ± 19.7	$-24,793.1 \pm 11.9$	1.56	- 1.65	22.10	18.56	21.41	8.48
313.15 3264.3±14.7 1799.1±19.6 -45,456.7±28.7 -25,857.1±11.1 4.38 -1.22 26.16 14.72 21.13 40.\low ErOH+1.0m NAM 293.15 2886.9±14.2 1047.0±11.3 -46,107.5±27.7 -16,146.7±19.6 0.48 -2.34 28.96 19.30 21.25 298.15 3032.5±12.6 1162.9±14.9 -47,544.9±24.4 -17,434.1±15.9 0.26 8.92 2951 21.91 22.15 303.15 3168.2±10.9 1253.8±17.6 -48,6980.±19.6 -18,285.3±17.2 -3.92 -11.84 30.05 24.53 22.96 308.15 3347.4±15.8 1407.8±14.4 -50,019,1±14.5 -20,114.6±12.1 4.52 7.09 30.60 27.15 23.96 313.15 3480.7±10.5 1537.8±21.4 -50,524.2±19.7 -21,548.0±16.5 -1.67 -1.44 31.14 29.76 23.29	308.15	3094.0±12.8	$1729.0 \pm 13.7$	$-43,515.7 \pm 23.2$	$-25,554.3 \pm 10.5$	- 9.80	3.56	24.13	16.64	21.43	8.09
<i>40.\low Etch + 1.0 m NAM</i> 293.15 2886.9 ±14.2 1047.0 ±11.3 - 46,107.5 ±27.7 - 16,146.7 ±19.6 0.48 - 2.34 28.96 19.30 21.25 298.15 303.2.5 ±12.6 1162.9 ±14.9 - 47,544.9 ±24.4 - 17,434.1 ±15.9 0.26 8.92 29.51 21.91 22.15 303.15 3168.2 ±10.9 1253.8 ±17.6 - 48,6980.±19.6 - 18,285.3 ±17.2 - 3.92 - 11.84 30.05 24.53 22.96 308.15 3347.4 ±15.8 1407.8 ±14.4 - 50,0191.±14.5 - 20,114.6 ±12.1 4.52 7.09 30.60 27.15 23.96 313.15 3480.7 ±10.5 1537.8 ±21.4 - 50,524.2 ±19.7 - 21,548.0 ±16.5 - 1.67 - 1.44 31.14 29.76 23.29	313.15	3264.3±14.7	$1799.1 \pm 19.6$	$-45,456.7 \pm 28.7$	$-25,857.1 \pm 11.1$	4.38	- 1.22	26.16	14.72	21.13	8.47
293.15       288.69±14.2       1047.0±11.3       -46,107.5±27.7       -16,146.7±19.6       0.48       -2.34       28.96       19.30       21.25         298.15       303.25±12.6       1162.9±14.9       -47,544.9±24.4       -17,434.1±15.9       0.26       8.92       29.51       21.91       22.15         303.15       3168.2±10.9       1253.8±17.6       -48,698.0±19.6       -18,285.3±17.2       -3.92       -11.84       30.05       24.53       22.96         308.15       3347.4±15.8       1407.8±14.4       -50,0191.±14.5       -20,114.6±12.1       4.52       7.09       30.60       27.15       23.96         313.15       3480.7±10.5       1537.8±21.4       -50,524.2±19.7       -21,548.0±16.5       -1.67       -1.44       31.14       29.76       23.29	40 v/v EtOh	+ + 1.0 m NAM									
29815       3032.5±1.26       1162.9±14.9       -47,544.9±24.4       -17,434.1±15.9       0.26       8.92       29.51       21.91       22.15         303.15       3168.2±10.9       1253.8±17.6       -48,698.0±19.6       -18,285.3±17.2       -3.92       -11.84       30.05       24,53       22.96         308.15       3347.4±15.8       1407.8±14.4       -50,0191.±14.5       -20,114.6±12.1       4.52       7.09       30.60       27.15       23.96         313.15       3480.7±10.5       1537.8±21.4       -50,524.2±19.7       -21,548.0±16.5       -1.67       -1.44       31.14       29.76       23.29	293.15	2886.9±14.2	$1047.0 \pm 11.3$	$-46,107.5 \pm 27.7$	— 16,146.7 ± 19.6	0.48	- 2.34	28.96	19.30	21.25	5.18
303.15       3168.2±10.9       1253.8±17.6       -48,698.0±19.6       -18,285.3±17.2       -3.92       -11.84       30.05       24,53       22.96         308.15       3347.4±15.8       1407.8±14.4       -50,019.1±14.5       -20,114.6±12.1       4.52       7.09       30.60       27.15       23.96         313.15       3480.7±10.5       1537.8±21.4       -50,524.2±19.7       -21,548.0±16.5       -1.67       -1.44       31.14       29.76       23.29	298.15	3032.5±12.6	1162.9±14.9	$-47,544.9\pm24.4$	— 17,434.1 ± 15.9	0.26	8.92	29.51	21.91	22.15	5.42
308.15     3347.4±15.8     1407.8±14.4     -50,019.1±14.5     -20,114.6±12.1     4.52     7.09     30.60     27.15     23.96       313.15     3480.7±10.5     1537.8±21.4     -50,524.2±19.7     -21,548.0±16.5     -1.67     -1.44     31.14     29.76     23.29	303.15	$3168.2 \pm 10.9$	$1253.8 \pm 17.6$	$-48,698.0\pm19.6$	- 18,285.3 ± 17.2	- 3.92	- 11.84	30.05	24.53	22.96	4.70
313.15 34807±10.5 1537.8±21.4 -50,524.2±19.7 -21,548.0±16.5 -1.67 -1.44 31.14 29.76 23.29	308.15	3347.4±15.8	1407.8±14.4	− 50,019.1 ± 14.5	$-20,114.6\pm12.1$	4.52	7.09	30.60	27.15	23.96	4.88
	313.15	$3480.7 \pm 10.5$	$1537.8 \pm 21.4$	$-50,524.2 \pm 19.7$	$-21,548.0\pm16.5$	- 1.67	- 1.44	31.14	29.76	23.29	5.86

$r_{\Phi}^{-0}$ ) and partial molar volume of	al pressure P = 101 kPa



**Fig. 3** Plot of limiting apparent molar volume ( $V_{\Phi}^0$ ) vs temperature (T) for (**A**) QUE and (**B**) 7-HF in 30 v/v EtOH, 30 v/v EtOH + 0.5 mol kg<sup>-1</sup>NAM, 30 v/v EtOH + 1.0 mol kg<sup>-1</sup>NAM at T = 293.15, 298.15 and 303.15 K

## Partial molar expansibility

Volumetric properties are often sensitive to the rise in temperature. The second-order polynomial equation (Eq. 5) can be used to calculate the partial molar volume that is temperature sensitive (also known as partial molar expansibility).

$$V_{\phi}^0 = a + bT + cT^2 \tag{5}$$

T is the temperature in Kelvin in Eq. (5), and the variables a, b, and c recite the empirical parameters whose values for QUE/7 HF in EtOH +  $H_2O$ , and 0.5/1.0 mol kg<sup>-1</sup> of NAM at various temperatures are presented in Table 3. The values of a, b, and c are utilized to compute the

theoretical values of  $V^0_\varphi$  at all experimental temperatures. The following relation can be used to analyze the difference between theoretically predicted and experimentally discovered values of  $V^0_\varphi$ .

$$\sigma = (1/n) \sum \left[ (V^{0}_{\phi(experimental)} - V^{0}_{\phi(calculated)}) / V^{0}_{\phi(experimental)} \right],$$
(6)

where  $\sigma$  (ARD: average relative deviation).  $V_{\varphi}^{0}$  represents apparent molar volume at infinite dilution. The following Eq. (7) can be used to calculate partial molar expansibility, which is the variation of partial molar volume with temperature (single derivative).

**Table 3** Empirical parameters a, b and c of Eq. (5) for QUE and 7-HF with NAM of different concentrations in hydro-ethanolic medium and experimental pressure P = 101 kPa

Solvent system	QUE			7HF		
	$a \times 10^{-2} / \text{m}^3 \text{mol}^-$	$^{1}b \times 10^{-2}/\text{m}^{3}\text{mol}^{-1}\text{K}^{-1}$	$^{-1} c/m^{3}mol^{-1}K^{-2}$	$a \ge 10^{-2} / \text{m}^3 \text{mol}^{-1}$	$b \times 10^{-2} / \text{m}^3 \text{mol}^{-1} \text{K}^{-1}$	$^{-1} c/m^{3}mol^{-1}K^{-2}$
30 v/v EtOH	114.5±1.0	$-0.8 \pm 0.0$	0.1±0.0	110.8±0.2	$-0.8\pm0.0$	0.1±0.0
30 v/v -EtOH + 0.5 NAM	$-214.8 \pm 1.2$	$1.3 \pm 0.0$	$-0.1 \pm 0.0$	$50.6 \pm 0.1$	$-0.3 \pm 0.0$	$0.1 \pm 0.0$
30 v/v -EtOH + 1.0 NAM	$-410.1 \pm 1.0$	$2.6 \pm 0.0$	$-0.3 \pm 0.1$	103.1±0.4	$-0.7 \pm 0.0$	$0.1 \pm 0.0$
40 v/v EtOH	$776.1 \pm 2.0$	$-5.2 \pm 0.0$	$0.8 \pm 0.3$	$-452.0\pm0.3$	$2.8 \pm 0.0$	$-0.4 \pm 0.0$
40 v/v -EtOH + 0.5 NAM	149.7±3.0	$-1.0 \pm 0.0$	$0.2 \pm 0.3$	$-216.7\pm0.5$	1.3±0.0	$-0.1 \pm 0.0$
40 v/v -EtOH+ 1.0 NAM	$-9.15 \pm 0.4$	$-0.9 \pm 0.0$	$0.0 \pm 0.1$	178.6±0.1	$-1.3\pm0.0$	$0.2 \pm 0.0$

The standard errors are given in parenthesis. The standard uncertainties (with 0.68 level of confidence) of experimental temperature and experimental pressure are u(T) = 0.01 K and u(P) = 1.0 kPa, respectively. The standard uncertainties of solvent, (v/v EtOH + 0.5 m/1.0 NAM),  $u(v/v) = \pm 0.01$  v/v), (with 0.68 level of confidence) are  $u(m_B) = \pm 0.01$  v/v

$$\mathbf{E}^{0}_{\phi} = (\partial \mathbf{V}^{0}_{\phi} / \partial \mathbf{T})_{\mathbf{P}} = \mathbf{b} + 2\mathbf{c}\mathbf{T}.$$
(7)

$$(\partial E_{\phi}^{0}/\partial T) = (\partial^{2} V_{\phi}^{0}/\partial T^{2})_{p} = 2c.$$
(8)

Due to the general susceptibility of volumetric properties to temperature change, the investigation of temperature dependency of  $E_{\varphi}^0$  is important. Since all of the analyzed solutions have positive  $E_{\varphi}^0$  values (Table 2) across the entire range of experimental temperatures, it may be assumed that there are robust solute-solvent interactions between the solute and solvent molecules. It can be noticed from Table 2 that the values of  $E^0_{\varphi}$  decrease with increase in temperature in case of QUÉ in 30 v/v EtOH+NAM, which is due to the weakening of solute-solvent interactions. QUE in 40 v/v EtOH+NAM shows a rise in expansibility with temperature, suggesting that the system is more disordered or flexible at higher ethanol concentrations. For the solutions of 7-HF, the  $E_\varphi^0$  values decline in lower concentration of NAM with both 30 v/v and 40 v/v EtOH. This suggests that at lower concentrations of NAM, the solution might become more ordered at higher temperatures. At lower concentrations of NAM in the 7-HF solution, there is less competition between the solute molecules. This means that solutesolvent interactions can become more pronounced as temperature increases. These interactions can lead to a more ordered arrangement of molecules. The NAM molecule, being an amino acid derivative, may be forming hydrogen bonds with the ethanol solvent or with other NAM molecules. These interactions can help structure the solution more effectively at higher temperatures, which reduces the overall energy of the system, thus lowering the  $E_{\phi}^{0}$  values. As the temperature increases, molecular motion becomes more energetic. While this usually causes disorder, in certain conditions (like the present case), the increased motion can lead to a more ordered structure if the temperature helps facilitate stronger intermolecular interactions (e.g., hydrogen bonding). For lower concentrations of NAM, there may be more room for the molecules to interact freely and form these stable structures, whereas at higher concentrations, the molecules might be more in a disordered state due to overcrowding and less room for efficient interactions. Ethanol's own properties (like polarity and hydrogen bonding potential) might support the formation of these more structured arrangements at higher temperatures, leading to lower  $E^0_\varphi$  values. The  $E^0_{\Phi}$  values increase in higher concentration of NAM in both 30 v/v and 40 v/v EtOH considered. This could be due to a more complex interplay between solutesolute and solute-solvent interactions at higher NAM concentrations. Higher NAM concentrations might cause disruption of the solvent structure, especially in systems with ethanol. At higher temperatures, this disruption may result in greater molecular mobility and an overall expansion of the solution, which would lead to an increase in the partial molar expansibility. An increase in  $E^0_{\phi}$  with temperature is also a result of the packing or caging action of the solvent [26]. Positive partial molar expansibilities show QUE/7-HF acts as a structure former in aqueous solutions and promote solute-solvent interactions in the system. These trends are driven by the combined effects of solutesolvent interactions, solvent composition, and solute concentration. The temperature and concentration dependencies reflect how the structural dynamics of the solution change under varying conditions.

## Partial molar volume of transfer

The measurement of limiting molar quantities of transfer offers both quantitative and qualitative information on solute–solvent interactions, since the interactions between solute particles are undetectable at infinite dilution.

The following formula is used to determine the transfer values of the partial molar volume of QUE/7-HF from water to aqueous to ethanolic NAM solutions at infinite dilution:

$$\Delta_{\rm tr} V^0_{\phi\,(water\,\rightarrow\,hydroethanolic\,NAM\,)} = V^0_{\phi(hydroethanolic\,NAM)} - V^0_{\phi(water)}$$
(9)

QUE/7-HF with NAM in hydroethanolic solution is the system under study, and it includes both hydrocarbon and polar moities. To fully understand the guaternary as well as ternary systems under analysys, polar parts and hydrocarbon components may interact in a variety of ways with each other and with the polar water molecules. It is well known that when the hydration strength of the interacting particles increases, the interaction's effectiveness decreases. The deduced values of  $\Delta_{tr} V^0_{\phi}$ are listed in Table 2 from where it can be noticed that  $\Delta_{\rm tr} V^0_{\phi}$  values are positive for QUE/7-HF in all the solvent systems suggesting a strong solute-solvent interactions in the studied system. Furthermore, it can also be seen that there is no regular trend in its values with respect to temperature. That means the hydration behavior of QUE/7-HF in the hydro-ethanolic medium is strongly affected by the solute-solvent interactions. From Table 2 it can be noticed that the values of  $\Delta_{tr} V^0_{\Phi}$  are significantly less for 7-HF as compared to QUE in all the solvents. The smaller size and more compact structure of 7-HF likely result in fewer steric interactions with the surrounding solvent and solute molecules, leading to a lower partial

molar volume of transfer. In contrast, the larger QUE molecule might cause more disruption in the solvent structure and lead to a higher  $\Delta_{tr}V^0_{\varphi}$  value. The number of hydrogen bonds 7-HF can form might be limited due to its smaller size and structure. Therefore, the solvation of 7-HF could be more tight or less expansive compared to QUE, leading to a lower  $\Delta_{tr} V_{\phi}^{0}$ . 7-HF is hydrophilic due to its hydroxyl group, it is less hydrophilic than QUE due to its relatively simpler structure. As a result, 7-HF may be less "hydrated" in the solvent compared to QUE, leading to a smaller volume change when transferred into the solution. Its smaller volume and less extensive solvation result in a lower  $\Delta_{tr} V_{\phi}^{0}$ . The insensitivity towards solvent composition (30 v/v vs. 40 v/v ethanol) for QUE/7-HF suggests that the solute-solvent interactions for both molecules reach a saturation point where changes in solvent composition do not significantly alter the solvation behavior. The role of NAM as a stabilizing agent further contributes to the consistency in the solvation environment, making both solutes less sensitive to the ethanol content in the solvent.

## Analysis of acoustic properties

It has been proven in recent times that indirect determination of solute–solvent, ion–solvent and ion-ion interactions for micro to macromolecular compounds like proteins, saccharides, bio-surfactants, bioflavonoids, etc., in mixed solution media is possible through ultrasonic velocity measurements [4, 5, 41]. Because of the low amplitude and low frequency (2 MHz) of ultrasound, this technique is now a favoured method in the analysis of intermolecular interactions in solutions. Since the configuration of the molecules and their reciprocal interactions influence many structural properties of solvents and solutes, the ultrasonic tool is very significant.

Density data of the experimental solutions of QUE/7-HF in all the four chosen solvents (30 v/v EtOH+0.5 mol kg<sup>-1</sup> NAM, 30 v/v EtOH+1.0 mol kg<sup>-1</sup> NAM, 40 v/v EtOH+0.5 mol kg<sup>-1</sup> NAM, 40 wt % EtOH + 1.0 mol kg<sup>-1</sup> NAM) at temperature T = 293.15 K, 298.15 K and 303.15 K were used to calculate the compressibility parameters. The knowledge of the acoustic parameters sheds light on the kind and extent of solute-solute, solute-solvent, hydrophilic-hydrophilic or hydrophobic-hydrophobic interactions furnished by solute and co-solute in the solution because of structural modifications in the solvation shells. The measured data of ultrasonic velocity (U) for all the solutions at all experimental temperatures are presented in Table 4. Unfortunately, because of a lack of literature data, it is not possible to compare our present results. However,

the investigated density and sound velocity data are dependent on the temperature and concentration of the solutions as expected.

A thorough observation of Table 4 affirms that the ultrasonic velocity U values of the solution follow the same trend as that of density,  $\rho$  i.e. U decreases with a rise in solute concentrations [42, 43]. As explained, the density gets reduced with an increase in solute concentration as well as an increase in water content in the solvent; the compactness of the hydration shells declines the ultrasonic velocity of the solution. Density is an important factor affecting the sound velocity in a medium. In case of a denser medium, the molecules are packed closely. Closer the molecules, the faster is the travelling of sound and vice versa. In our study, the density of the solution gets reduced with concentration, thereby decreasing the sound velocity as well. Furthermore, the decrease in ultrasonic velocity with increasing solute concentration in the studied system is mainly due to the combined effects of the disruption of the solvent structure by the solutes and changes in the compressibility of the medium caused by the interactions between QUE/7-HF, ethanol and water. The presence of NAM further influences these effects by contributing to slower propagation of sound waves, and promoting hydrogen bonding, which can also lead to decreased ultrasonic velocity.

Zhong et al. [44] studied the intra-molecular proton transfer mechanism of flavonoids in regard to hydrogen bond facilitation and found that between flavonoid and water molecules, the intermolecular hydrogen bond C = O + H - O is remarkably reinforced in the hydrogen-bonded flavonoid-(H2O)2 complexes. Henceforth, in the present investigation, the velocity of sound is decreased with an increase in the concentration of QUE/7-HF (solute) and co-solute (NAM) in a hydroethanolic medium because of the formation an active QUE/7-HF –  $(H_2O)_2$  complexes. It can be said that flavonoid- $(H_2O)_2$  complexes are not moving themselves; even though they are forming complexes, they can still vibrate and pass the vibration faster than the low concentration solutions. So, the ultrasonic velocity values decrease with a decrease in the density of the solution. The experimentally calculated values of density, as well as ultrasonic velocity were taken to evaluate the values of isentropic compressibility (K<sub>s</sub>), lowering in compressibility ( $\Delta K_s$ ), specific acoustic impedance (Z), apparent molar compressibility ( $K_{S,\phi}$ ), relative lowering in isentropic compressibility  $(\Delta K_r)$  using the equations given below,

$$K_s = 1/\rho U^2$$
 (Newton – Laplace's equation) (10)

ound velocity (U), isentropic compressibility (K <sub>s</sub> ), apparent molar isentropic compressibility (K <sub>s,<math>\phi</math></sub> ) and isothermal compressibility (K <sub>7</sub> ) for QUE and 7-HF	incentrations in hydro-ethanolic medium at experimental temperatures and experimental pressure P = 101 kPa
und velocit	centration
'alues of sou	fferent cond
Table 4 🗸	NAM of di

with

TEMP (K)	m <sub>A</sub> /mol kg <sup>-1</sup>	U/(ms <sup>-1</sup> )	$K_{s} \times 10^{10} / (m^2 N^{-1})$	K <sub>s,4</sub> ×10 <sup>12</sup> / (m <sup>5</sup> mol <sup>-1</sup> N <sup>-1</sup> )	$K_{T} \times 10^{15} / (m^2 N^{-1})$	U /(m s <sup>-1</sup> )	$K_{s} \times 10^{10} / (m^2 N^{-1})$	$K_{s,\Phi} \times 10^{12} / (m^5 mol^{-1} N^{-1})$	$K_T \times 10^{15} / (m^2 N^{-1})$
		QUE				7-HF			
30 v/v EtOH +	- 0.5 m NAM								
293.15	0.0000	1532.0				1532.0			
	0.0015	1600.0	4.06	- 29.18	5.63	1608.0	4.05	- 27.20	5.64
	0.0020	1596.0	4.08	- 20.13	5.67	1600.0	4.10	- 18.10	5.70
	0.0025	1592.0	4.12	- 13.97	5.72	1596.0	4.12	- 13.17	5.74
	0.0030	1588.0	4.15	- 9.90	5.78	1592.0	4.15	- 9.79	5.78
	0.0035	1584.0	4.19	- 6.96	5.83	1588.0	4.18	- 7.38	5.82
	0.0040	1580.0	4.23	- 4.75	5.89	1584.0	4.20	- 5.48	5.86
298.15	0.0000	1540.0				1540.0			
	0.0015	1604.0	4.05	- 28.47	5.57	1612.0	4.04	- 26.15	5.59
	0.0020	1600.0	4.07	- 19.70	5.61	1604.0	4.09	- 17.30	5.65
	0.0025	1596.0	4.11	- 13.56	5.67	1600.0	4.11	- 12.61	5.69
	0.0030	1592.0	4.14	- 9.54	5.72	1596.0	4.14	- 9.34	5.72
	0.0035	1588.0	4.18	- 6.68	5.78	1592.0	4.17	- 7.03	5.76
	0.0040	1584.0	4.21	- 4.47	5.83	1588.0	4.19	- 5.17	5.81
303.15	0.0000	1552.0				1552.0			
	0.0015	1608.0	4.03	- 26.37	5.52	1616.0	4.03	- 23.62	5.55
	0.0020	1604.0	4.06	- 18.16	5.56	1608.0	4.08	- 15.47	5.60
	0.0025	1600.0	4.10	- 12.39	5.61	1604.0	4.10	- 11.29	5.63
	0.0030	1596.0	4.13	- 8.58	5.67	1600.0	4.13	- 8.32	5.67
	0.0035	1592.0	4.17	- 5.84	5.72	1596.0	4.16	- 6.10	5.71
	0.0040	1588.0	4.20	- 3.76	5.78	1592.0	4.18	- 4.39	5.75
30 v/v EtOH +	- 1.0 m NAM								
293.15	0.0000	1556.0				1556.0			
	0.0015	1592.0	4.01	- 15.96	5.53	1592.0	4.04	- 13.45	5.57
	0.0020	1588.0	4.04	- 10.68	5.56	1588.0	4.06	- 8.82	5.60
	0.0025	1584.0	4.06	- 7.10	5.60	1584.0	4.08	- 5.87	5.64
	0.0030	1580.0	4.10	- 4.42	5.65	1580.0	4.11	- 3.65	5.68
	0.0035	1576.0	4.13	- 2.44	5.70	1576.0	4.14	- 1.95	5.73
	0.0040	1568.0	4.19	- 0.29	5.79	1572.0	4.18	- 0.60	5.78
298.15	0.0000	1560.0				1560.0			
	0.0015	1596.0	4.00	- 16.59	5.47	1600.0	4.01	- 14.60	5.49
	0.0020	1592.0	4.02	- 11.23	5.50	1596.0	4.03	- 9.79	5.52

Table 4 🤅	continued)								
TEMP (K)	m <sub>A</sub> /mol kg <sup>-1</sup>	U/(ms <sup>-1</sup> )	$K_{s} \times 10^{10}/(m^{2}N^{-1})$	$K_{s,\Phi} \times 10^{12}/$ (m <sup>5</sup> mol <sup>-1</sup> N <sup>-1</sup> )	$K_{T} \times 10^{15} / (m^2 N^{-1})$	U/(m s <sup>-1</sup> )	$K_{s} \times 10^{10} / (m^2 N^{-1})$	$K_{5,\Phi} \times 10^{12} / (m^5 mol^{-1} N^{-1})$	$\frac{1}{1} \frac{K_T \times 10^{15}}{(m^2 N^{-1})}$
		QUE				7-HF			
	0.0025	1588.0	4.05	- 7.54	5.54	1588.0	4.07	- 5.83	5.58
	0.0030	1584.0	4.08	- 4.83	5.59	1584.0	4.10	- 3.71	5.62
	0.0035	1580.0	4.11	- 2.83	5.64	1580.0	4.13	- 2.01	5.67
	0.0040	1572.0	4.17	- 0.66	5.72	1576.0	4.16	- 0.67	5.71
303.15	0.0000	1564.0				1564.0			
	0.0015	1600.0	3.99	- 17.40	5.43	1608.0	3.98	- 16.58	5.43
	0.0020	1596.0	4.02	- 11.91	5.46	1604.0	4.00	- 11.31	5.45
	0.0025	1592.0	4.04	- 8.28	5.49	1600.0	4.03	- 7.93	5.49
	0:0030	1588.0	4.07	- 5.59	5.54	1596.0	4.05	- 5.52	5.53
	0.0035	1584.0	4.10	- 3.42	5.59	1592.0	4.08	- 3.61	5.57
	0.0040	1576.0	4.16	- 1.21	5.67	1588.0	4.11	- 2.11	5.61
40 v/v EtOH	+ 0.5 m NAM								
293.15	0.0000	1532.0				1532.0			
	0.0015	1580.0	4.21	- 22.30	5.87	1548.0	4.43	- 7.90	6.19
	0.0020	1576.0	4.24	- 15.42	5.90	1544.0	4.45	- 4.38	6.22
	0.0025	1568.0	4.29	- 10.01	5.97	1540.0	4.48	- 1.89	6.27
	0:0030	1560.0	4.34	- 5.94	6.05	1536.0	4.52	- 0.06	6.32
	0.0035	1552.0	4.40	- 2.81	6.15	1532.0	4.55	1.24	6.37
	0.0040	1548.0	4.44	- 1.00	6.21	1528.0	4.58	2.09	6.41
298.15	0.0000	1536.0				1536.0			
	0.0015	1584.0	4.21	- 23.08	5.82	1564.0	4.35	- 11.99	6.04
	0.0020	1580.0	4.23	- 16.12	5.85	1556.0	4.40	- 6.38	6.11
	0.0025	1572.0	4.27	- 10.69	5.92	1548.0	4.45	- 2.66	6.18
	0:0030	1564.0	4.33	- 6.64	6.00	1544.0	4.48	- 0.73	6.23
	0.0035	1556.0	4.39	- 3.48	6.08	1540.0	4.52	0.68	6.28
	0.0040	1552.0	4.43	- 1.50	6.15	1536.0	4.55	1.67	6.33
303.15	0.0000	1540.0				1540.0			
	0.0015	1588.0	4.19	- 23.77	5.76	1580.0	4.28	- 15.46	5.90
	0.0020	1584.0	4.22	- 16.65	5.79	1576.0	4.30	- 10.26	5.93
	0.0025	1576.0	4.26	- 11.21	5.86	1568.0	4.35	- 5.93	6.00
	0:0030	1568.0	4.31	- 7.15	5.93	1556.0	4.42	- 2.02	6.10
	0.0035	1560.0	4.37	- 4.01	6.02	1552.0	4.48	0.26	6.18

Table 4 (c	ontinued)								
TEMP (K)	m <sub>A</sub> /mol kg <sup>-1</sup>	U/(ms <sup>-1</sup> )	$K_{s} \times 10^{10}/(m^2 N^{-1})$	K <sub>s,Φ</sub> ×10 <sup>12</sup> / (m <sup>5</sup> mol <sup>-1</sup> N <sup>-1</sup> )	$K_{T} \times 10^{15} / (m^2 N^{-1})$	U/(m s <sup>-1</sup> )	$K_5 \times 10^{10} / (m^2 N^{-1})$	K <sub>s,                                    </sub>	$^{1}$ K <sub>T</sub> ×10 <sup>15</sup> / - (m <sup>2</sup> N <sup>-1</sup> )
		QUE				7-HF			
	0.0040	1556.0	4.41	- 2.11	6.08	1544.0	4.51	1.35	6.23
40 v/v EtOH +	+ 1.0 m NAM								
293.15	0.0000	1532.0				1532.0			
	0.0015	1580.0	4.11	- 21.01	5.68	1556.0	4.28	- 9.34	5.93
	0.0020	1572.0	4.16	- 13.05	5.74	1552.0	4.30	- 5.76	5.97
	0.0025	1564.0	4.21	- 7.58	5.83	1548.0	4.33	- 3.35	6.00
	0:0030	1560.0	4.25	- 4.42	5.89	1544.0	4.36	- 1.65	6.04
	0.0035	1552.0	4.31	- 1.45	5.98	1540.0	4.39	- 0.29	6.09
	0.0040	1548.0	4.35	0.22	6.04	1536.0	4.42	0.69	6.13
298.15	0.0000	1540.0				1540.0			
	0.0015	1588.0	4.08	- 21.52	5.60	1560.0	4.27	- 8.51	5.88
	0.0020	1580.0	4.13	- 13.56	5.66	1556.0	4.30	- 5.19	5.91
	0.0025	1572.0	4.18	- 8.17	5.74	1552.0	4.32	- 2.95	5.95
	0:0030	1564.0	4.24	- 4.24	5.83	1548.0	4.35	- 1.31	5.99
	0.0035	1560.0	4.28	- 1.98	5.89	1544.0	4.38	- 0.08	6.03
	0.0040	1556.0	4.32	- 0.13	5.95	1540.0	4.41	0.91	6.08
303.15	0.0000	1544.0				1544.0			
	0.0015	1592.0	4.07	- 22.15	5.54	1564.0	4.26	- 9.03	5.83
	0.0020	1584.0	4.11	- 14.26	5.60	1560.0	4.28	- 5.58	5.86
	0.0025	1576.0	4.16	- 8.90	5.68	1556.0	4.31	- 3.39	5.89
	0:0030	1568.0	4.22	- 4.92	5.76	1552.0	4.33	- 1.71	5.93
	0.0035	1564.0	4.26	- 2.56	5.82	1548.0	4.36	- 0.44	5.97
	0.0040	1560.0	4.30	- 0.58	5.89	1544.0	4.39	0.58	6.02

m signifies the molality of QUE and 7-HF per kg of the solvent (v/v EtOH + 0.5 m/1.0 NAM). The standard uncertainties (with 0.68 level of confidence) are u(m<sub>A</sub>) = 1 × 10<sup>-3</sup> mol kg<sup>-1</sup>, The standard uncertainty in composition of solvent (v/v EtOH + 0.5 m/1.0 NAM) is u(v/v) =  $\pm$  0.01 K, u(P) = 1.0 kPa, and the combined expanded uncertainties (with 0.95 level of confidence) are u<sub>c</sub>(U) =  $\pm$  0.5 kp m<sup>-3</sup>

$$\Delta K_{\rm s} = (K_{\rm s}^0 - K_{\rm s}) \tag{11}$$

 $K_s^0$  is the isentropic compressibility at infinite dilution of solution.

$$\Delta K_{\rm r} = (K_{\rm s}^0 - K_{\rm s})/K_{\rm s}^0$$
(12)

$$K_{s,\phi} = (K_s \rho_0 - K_s^0 \rho) / m_{\rho \rho_0} + M K_s / \rho$$
(13)

The molar mass of the solute and the molal concentration of the solution are represented by M and m, respectively

$$Z = \rho \times U \tag{14}$$

 $K_T$  is the isothermal compressibility and has been obtained by Eq. (15).

$$K_{\rm T} = (17.1 \times 10^{-4}) / (T^{4/9} \rho^{4/3} U^2)$$
(15)

## Isentropic compressibility and isothermal compressibility

In different concentration environments of an aqueous solution system, a wide variety of interacting forces exist, including electrostatic interaction, van der Waals forces, ion-ion, ion-dipole forces, etc. Thus, several equilibria prevail in the said surroundings. These enforce the generation of different moieties like ion pairs (contact, solvent-shared or solvent-separated), solvated ions, hydrated complexes, etc. by virtue of the inherent complexity of solvent molecules surrounding the ions, the evaluation of ultrasonic velocity of sound is a very crucial technique, which considers many important corollaries of ion solvation like compressibility and reduced volume of solvent molecules. In the present study, a considerable electrostatic effect on neighbouring hydro-ethanolic NAM the solvent molecules by the electric field of the existing QUE/7-HF molecules is comparatively less because of the formation of  $QUE/7-HF - (H_2O)_2$  complexes (the result of intermolecular hydrogen bonding of QUE/7-HF). Consequently, the compressibility of the hydro-ethanolic solvent molecules of NAM gets increased. The fusion of isentropic compression of hydration shells of solutes  $(K_{s(solute\ intrinsic)})$  and isentropic compression of solvent molecules  $(K_{s(solvent intrinsic)})$  is framed as isentropic  $compression(K_s)$ . In thermodynamics, the coefficient of compressibility or compressibility of a medium can be understood as the relative change in its volume that counter to change in pressure. Mathematically, isentropic compressibility,  $K_s$  and isothermal compressibility( $K_T$ ) for a system can be presented as,

$$K_{S} = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_{S} \quad (i.e \text{ compressibility at constant entropy}) \quad \textbf{(16)}$$

$$K_{T} = -\frac{1}{V} \left( \frac{\partial V}{\partial P} \right)_{T} \quad (i.e \text{ compressibility at constant temperature})$$
(17)

where T, P and V represent the temperature, pressure and volume, respectively.

Isentropic compression  $(K_s)$  is regarded as a second pressure derivative of the Gibbs free energy that can absolutely be attained from the density ( $\rho$ ) and ultrasonic velocity (U) in solutions by the established familiar Newton-Laplace equation (Eq. 10). The calculated values of K<sub>s</sub> are listed in Table 4, and a graphical presentation is shown in Fig. 4 for QUE/7-HF in 30 v/v EtOH+0.5  $mol kg^{-1}/1.0 mol kg^{-1} NAM$  for more perception. From these figures, an increasing tendency of K<sub>s</sub> is observed for all the experimental solutions as the amount of QUE/7-HF increases. The compressible hydrocarbon core, hydrophilic head group contacts, and counter ion binding existing in the mixed solution have an impact on the system's very compact environment, which is measured by the isentropic compressibility parameter K<sub>s</sub>. It can also be depicted that there is a continuous decline in K<sub>s</sub> values with a rise in temperature because the elevation in thermal agitation reinforces the rate of release of molecules of solvent to the bulk state of the solution from the hydration co-sphere of solute/ hydrophilic entities. An increase in temperature also causes the water structures surrounding the hydrophilic moieties of QUE/7-HF and NAM to be thermally disrupted, strengthening solutesolute interactions. Similarly, the temperature affects the QUE/7-HF solution's conductivity and viscosity in opposite ways because it increases particle mobility through higher thermal and translational energy [30].

Another two significant parameters,  $K_s^0$  and  $S_k$ , the knowledge of what gives more understanding on interactions between solute and solvent particles with each other in the solution can be obtained from the intercept and slope, respectively, from the plot of  $K_s$  vs.  $m^{1/2}$  as per the following relation,

$$K_{\rm s} = K_{\rm s}^0 + S_{\rm k} m^{1/2},$$
 (18)

 $K_s^0$  is the limiting isentropic compressibility or partial isentropic compressibility, i.e., the compressibility of solution at infinite dilution where a negligible amount of solute remains in the solution. In such a state, a large volume of solvent comes in between solute particles, hindering close interaction among solutes. Hence, it is assumed that only the solute–solvent interactions can be perceived in the solution at infinite dilution.



**Fig. 4** Plot of isentropic compressibility,  $K_s$  vs square root of molality m<sup>1/2</sup> for (**A**) QUE in 30 v/v EtOH + 0.5 mol kg<sup>-1</sup>NAM, (**B**) QUE in 30 v/v EtOH + 1.0 mol kg<sup>-1</sup>NAM, (**C**) 7-HF in 30 v/v EtOH + 0.5 mol kg<sup>-1</sup>NAM and (**D**) 7-HF in 30 v/v EtOH + 1.0 mol kg<sup>-1</sup>NAM at T = 293.15, 298.15 and 303.15 K

An interpretation can be induced from the positive values of  $K_s^0$  for all the solutions in the whole range of hydro-ethanolic NAM solvents that strong solute–solvent interactions prevail in the tested solutions. Comparing the values of  $K_s^0$  for QUE and 7-HF in hydro-ethanolic medium from Table 5 it is found that  $K_s^0$  values are higher in 7-HF than in QUE. It can be explained in terms of the formation of more strengthened QUE– $(H_2O)_2$  complexes than 7-HF– $(H_2O)_2$  complexes. The presence of five–OH groups and one C=O group in QUE makes it more available even at infinite dilution for a stronger intermolecular hydrogen bonding with—H atom of–NH<sub>2</sub> from NAM in hydro-ethanolic media. The QUE molecules are thus more hydrated because of the presence of hydrophilic (–OH and C=O groups. The

intra-molecular hydrogen bonding is also greatly exhibited by such flavonoids. Thus, the extent of such intermolecular hydrogen bonding does not exceed in 7-HF to that in QUE. Due to this potent intermolecular hydrogen bonding by QUE, it is hindered from interacting with solvent molecules (NAM), hence less solute (QUE)-solvent (NAM) interaction in the case of QUE. Because of only one –OH group and one C = O group in 7-HF, there is comparatively less intermolecular hydrogen bonding by it with the—H atom of –NH<sub>2</sub> of NAM in hydro-ethanolic media, hence more solute (7-HF)-solvent (aq NAM) interactions.

The slope  $S_k$  indicates solute–solute pairwise interaction, and the values are listed in Table 5. The negative values of  $S_k$  suggest the dominance of hydrophobic–hydrophobic repulsive interactions over **Table 5** Values of  $K_{s}^{0}S_{K}$ ,  $K_{s,\phi}^{0}$ ,  $S_{k,\phi}$  and  $\Delta_{trK_{s,\phi}}^{0}$  for QUE and 7-HF with NAM of different concentrations in hydro-ethanolic medium at experimental temperatures and experimental pressure P = 101 kPa

T/K	$K_{s}^{0} \times 10^{10} / m$	<sup>2</sup> N <sup>-1</sup>	$S_{K} \times 10^{10}/m$	n <sup>2</sup> N <sup>-1</sup> mol <sup>-1/2</sup> kg <sup>1/2</sup>	$K_{s,\phi}^{0} \times 10^{11}/n$	n <sup>5</sup> mol <sup>-1</sup> N <sup>-1</sup>	$S_{k,\phi} \times 10^{10}$ /m <sup>5</sup> N <sup>-1</sup> mol	<sup>-3/2</sup> kg <sup>1/2</sup>	Δ <sup>0</sup> <sub>trKs,φ</sub> /m <sup>5</sup> mo	x 10 <sup>11</sup> pl <sup>-1</sup> N <sup>-1</sup>
	QUE	7-HF	QUE	7-HF	QUE	7-HF	QUE	7-HF	QUE	7-HF
30 v/v-Et	OH + 0.5 m NAN	1								
293.15	$3.78 \pm 0.01$	$3.82 \pm 0.08$	$6.97 \pm 0.03$	$5.97 \pm 0.01$	$-6.51 \pm 0.04$	$-5.80 \pm 0.05$	$59.84 \pm 0.08$	$8.58 \pm 0.04$	1.47	2.18
298.15	$3.77 \pm 0.02$	$3.82 \pm 0.08$	$6.96 \pm 0.03$	$5.87 \pm 0.01$	$-6.39 \pm 0.04$	$-5.58\pm0.04$	19.69±0.07	$8.28 \pm 0.05$	1.38	2.19
303.15	$3.76 \pm 0.02$	$3.82 \pm 0.08$	$6.88 \pm 0.03$	$5.71 \pm 0.01$	$-5.98 \pm 0.04$	$-5.07 \pm 0.04$	19.13±0.04	$7.57 \pm 0.03$	1.66	2.56
30 v/v-Et	OH + 1.0 m NAN	1								
293.15	$3.74 \pm 0.04$	$3.81\pm0.02$	$6.75 \pm 0.07$	$5.59 \pm 0.03$	$-3.92 \pm 0.02$	$-3.24\pm0.02$	$26.25 \pm 0.04$	$5.16 \pm 0.04$	4.06	4.73
298.15	$3.73\pm0.04$	$3.75\pm0.01$	$6.63 \pm 0.07$	$6.41 \pm 0.03$	$-4.02 \pm 0.02$	$-3.53\pm0.02$	$26.36 \pm 0.04$	$5.64\pm0.04$	3.74	4.23
303.15	$3.73\pm0.04$	$3.77 \pm 0.01$	$6.39 \pm 0.07$	$5.24 \pm 0.03$	$-4.14 \pm 0.02$	$-3.79\pm0.02$	$26.45 \pm 0.04$	$5.80\pm0.03$	3.51	3.85
40 v/v-Et	OH <b>+</b> 0.5 m NAN	1								
293.15	$3.82\pm0.04$	$4.18 \pm 0.01$	$9.74 \pm 0.08$	$6.28 \pm 0.03$	$-5.50 \pm 0.03$	$-2.29\pm0.0^{\circ}$	8.78±0.04	$4.07\pm0.03$	1.28	4.49
298.15	$3.82\pm0.04$	$4.05\pm0.01$	$9.50\pm0.07$	$7.94 \pm 0.01$	$-5.62 \pm 0.03$	$-3.15\pm0.02$	$28.87 \pm 0.04$	$5.45\pm0.03$	1.03	3.49
303.15	$3.82\pm0.04$	$3.86\pm0.04$	$9.21 \pm 0.07$	$10.30 \pm 0.05$	$-5.69 \pm 0.03$	$-4.20\pm0.02$	28.89±0.05	$7.07\pm0.04$	0.85	2.37
40 v/v-Et	OH + 1.0 m NAN	1								
293.15	$3.72 \pm 0.02$	$4.06\pm0.01$	$9.98 \pm 0.04$	$5.56 \pm 0.03$	$-5.23 \pm 0.04$	$-2.42\pm0.0^{\circ}$	8.58±0.03	$4.05\pm0.03$	1.55	4.35
298.15	$3.69\pm0.01$	$4.05\pm0.01$	$9.89\pm0.03$	$5.45 \pm 0.03$	$-5.30 \pm 0.04$	$-2.25\pm0.0^{\circ}$	8.64±0.04	$3.80\pm0.02$	1.33	4.38
303.15	$3.69 \pm 0.01$	$4.05\pm0.01$	$9.68 \pm 0.03$	$5.31 \pm 0.03$	$-5.41 \pm 0.04$	$-2.32\pm0.0^{-1}$	8.73±0.04	$3.86\pm0.02$	1.16	4.24

The standard uncertainty in composition of solvent (v/v EtOH + 0.5 m/1.0 NAM) is  $u(v/v) = \pm 0.01 v/v$ . u(T) = 0.01 K, u(P) = 1.0 kPa

hydrophobic–hydrophilic attractive interactions. In the present work, hydrophobic–hydrophobic repulsive interactions are among the nonpolar alkyl backbones of QUE/7-HF and aromatic cyclic pyridine site, and carbon atom of carbonyl (C = O) group of NAM. One more relevant parameter,  $K_T$ (compressibility in isothermal condition) supports gathering more knowledge on reciprocal action occurring among various hydrophobic and hydrophilic sites of the components that prevail in the solution. With the help of the relation given below,  $K_T$  is calculated [45].



Fig. 5 The plots of isothermal compressibility,  $K_T$  vs molaity, m for (A) QUE and (B) 7-HF in 40 v/v EtOH + 1.0 mol kg<sup>-1</sup> NAM at T = 293.15, 298.15 and 303.15 K

**Table 6** Values of acoustic impedance (*Z*), owering in isentropic compressibility ( $\Delta K_s$ ) and and relative lowering of isentropic compressibility ( $\Delta K_s$ ) for QUE and 7-HF with NAM of different concentrations in hydro-ethanolic medium at different temperatures

Temp/K	m/mol kg <sup>-1</sup>	Zkg m <sup>-2</sup> s <sup>-</sup>	-1	$\Delta K_s \times 10^{11}/$	m <sup>2</sup> N <sup>-1</sup>	$\Delta K_r \times 10^2$	
		QUE	7-HF	QUE	7-HF	QUE	7-HF
30 v/v EtOH + 0.5	m						
NAM	0.0015	15.40	15.22	2.40	2.57	7.00	0.00
293.15	0.0015	15.40	15.33	3.48	3.57	7.90	8.09
	0.0020	15.34	15.25	3.21	3.15	7.30	/.14
	0.0025	15.24	15.20	2.86	2.89	6.49	6.56
	0.0030	15.15	15.13	2.51	2.62	5.69	5.95
	0.0035	15.06	15.07	2.15	2.35	4.88	5.33
	0.0040	14.97	15.01	1.79	2.07	4.07	4.68
298.15	0.0015	15.41	15.33	3.31	3.38	7.57	7.71
	0.0020	15.35	15.25	3.06	2.96	6.99	6.76
	0.0025	15.25	15.19	2.69	2.72	6.16	6.20
	0.0030	15.16	15.13	2.34	2.45	5.35	5.59
	0.0035	15.07	15.08	1.99	2.18	4.55	4.98
	0.0040	14.98	15.01	1.63	1.90	3.72	4.33
303.15	0.0015	15.41	15.32	2.95	2.99	6.82	6.90
	0.0020	15.35	15.24	2.70	2.58	6.23	5.95
	0.0025	15.26	15.19	2.35	2.35	5.42	5.43
	0.0030	15.17	15.14	2.00	2.10	4.61	4.84
	0.0035	15.08	15.08	1.65	1.83	3.80	4.21
	0.0040	14.99	15.01	1.29	1.55	2.97	3.57
30 v/v EtOH + 1.0	m NAM						
293.15	0.0015	15.64	15.55	1.78	1.64	4.25	3.91
	0.0020	15.59	15.50	1.56	1.42	3.71	3.38
	0.0025	15.53	15.45	1.28	1.17	3.05	2.80
	0.0030	15.45	15.38	9.60	0.89	2.29	2.12
	0.0035	15.36	15.31	6.28	0.59	1.50	1.40
	0.0040	15.23	15.23	6.16	0.27	0.15	0.65
298.15	0.0015	15.66	15.60	1.82	1.79	4.35	4.27
	0.0020	15.62	15.56	1.60	1.57	3.84	3.76
	0.0025	15 55	15.46	1 3 3	113	3 18	2 70
	0.0030	15.47	15.40	1.02	0.86	2.43	2.06
	0.0035	15 39	15 33	6.91	0.56	1.65	1 34
	0.0040	15.26	15.25	1 31	0.25	0.31	0.60
303 15	0.0015	15.20	15.61	1.97	2.04	4.48	4.86
505.15	0.0070	15.60	15.57	1.67	1.83	3.08	1.00
	0.0020	15.50	15.57	1.00	1.60	3.38	2.91
	0.0023	15.54	15.52	1.41	1.00	2.50	2.00
	0.0030	15.47	15.40	7.00	1.54	2.09	3.20
	0.0035	15.56	15.50	7.90	1.05	1.69	2.31
40	0.0040	15.20	15.31	2.39	0.75	0.57	1.79
40 V/V ELUH + 0.5 I		15.00	14 50	2 45	0.70	E CO	1 7 7
293.13	0.0015	13.02	14.58	2.45	U./8	5.50	1./3
	0.0020	14.97	14.54	2.22	0.52	4.99	1.16
	0.0025	14.88	14.4/	1./4	0.22	3.89	0.49
	0.0030	14./6	14.41	1.18	- 0.11	2.64	- 0.24
	0.0035	14.64	14.34	5./9	- 0.43	1.30	- 0.96
	0.0040	14.55	14.28	1.93	- 0.74	0.43	- 1.64
298.15	0.0015	15.01	14.68	2.50	1.32	5.61	2.95

Temp/K	m/mol kg <sup>-1</sup>	Zkg m <sup>-2</sup> s <sup>-</sup>	-1	$\Delta K_s \times 10^{11}/$	$m^2 N^{-1}$	$\Delta K_r \times 10^2$	
		QUE	7-HF	QUE	7-HF	QUE	7-HF
	0.0020	14.97	14.60	2.28	0.85	5.13	1.91
	0.0025	14.88	14.50	1.81	0.34	4.06	0.76
	0.0030	14.77	14.44	1.27	0.02	2.86	0.05
	0.0035	14.64	14.37	6.88	- 0.31	1.54	- 0.68
	0.0040	14.55	14.31	2.89	- 0.62	0.65	- 1.38
303.15	0.0015	15.01	14.79	2.54	1.77	5.72	3.97
	0.0020	14.97	14.75	2.33	1.54	5.24	3.45
	0.0025	14.89	14.66	1.87	1.05	4.20	2.36
	0.0030	14.78	14.53	1.34	0.31	3.02	0.69
	0.0035	14.66	14.42	7.76	- 0.24	1.74	- 0.55
	0.0040	14.58	14.36	4.05	- 0.57	0.91	- 1.27
40 v/v EtOH + 1.0	m NAM						
293.15	0.0015	15.40	15.00	2.38	1.11	5.46	2.52
	0.0020	15.30	14.96	1.90	0.88	4.38	2.00
	0.0025	15.17	14.91	1.35	0.62	3.10	1.41
	0.0030	15.08	14.86	9.67	0.34	2.22	0.78
	0.0035	14.94	14.79	3.55	0.04	0.82	0.10
	0.0040	14.84	14.73	- 4.00	- 0.25	- 0.09	- 0.57
298.15	0.0015	15.43	15.01	2.39	0.94	5.54	2.16
	0.0020	15.34	14.96	1.94	0.72	4.49	1.65
	0.0025	15.22	14.91	1.41	0.47	3.26	1.07
	0.0030	15.09	14.85	8.23	0.19	1.91	0.44
	0.0035	14.99	14.79	4.38	- 0.09	1.01	- 0.21
	0.0040	14.88	14.73	2.42	- 0.39	0.06	- 0.89
303.15	0.0015	15.44	15.00	2.43	0.98	5.64	2.24
	0.0020	15.35	14.96	2.00	0.76	4.64	1.73
	0.0025	15.24	14.92	1.49	0.52	3.46	1.19
	0.0030	15.11	14.86	9.18	0.25	2.13	0.57
	0.0035	15.01	14.80	5.35	- 0.03	1.24	- 0.07
	0.0040	14.90	14.74	1.10	- 0.33	0.25	- 0.75

## Table 6 (continued)

*m* signifies the molality of QUE and 7-HF per kg of the solvent (v/v EtOH + 0.5 m/1.0 NAM). The standard uncertainties (with 0.68 level of confidence) are  $u(m) = 1 \times 10^{-3}$  mol kg<sup>-1</sup>. The standard uncertainty in composition of solvent (v/v EtOH + 0.5 m/1.0 NAM) is  $u(v/v) = \pm 0.01$  v/v. u(T) = 0.01 K, u(P) = 1.0 kP

$$K_{T} = \left(17.1x\,10^{-4})/(T^{4/9}\rho^{4/3}U^{2}\right) \tag{19}$$

The isothermal compressibility,  $K_T$  data are given in Table 4 and Fig. 5. It is apparent that change in  $K_T$  with the amount of QUE/7-HF and NAM follows a similar trend as in variations of  $K_S$ . These two compressibility factors assist the compressibility loss because of the electrostriction of hydration shells and presence of strong solute–solvent association.

The values of  $\Delta K_s$ , l owering in isentropic compressibility and  $\Delta K_r$ , relative lowering of isentropic compressibility of QUE/7-HF solutions are calculated using Eqs. (11) and (12), and documented in Table 6 with respect to the solutions concentration. It can be noticed that both the values show a reduced trend with the concentration of QUE/7-HF as more NAM (co-solute) molecules are getting engaged by hydrogen bond formation with QUE/7-HF (solute) so that some molecules of water driven out from the secondary solvation shell of solute particles.

## Apparent and partial molar isentropic compressibility

Analogous to that of isothermal compressibilities and isothermal compressions, the isentropic properties of aqueous solutions can be characterized. The compressibility of water molecules surrounding the solute ions in regard to the molecules of water in the bulk is



**Fig. 6** Plot of apparent molar isentropic compressibility,  $K_{s,\phi}$  vs square root of molality m<sup>1/2</sup> for QUE/7-HF in (**A**–**C**) – 30 v/v EtOH at T = 293.15, 298.15 and 303.15 K, respectively and (**D**–**F**) – 40 v/v EtOH at T = 293.15, 298.15 and 303.15 K, respectively.

known as apparent molar isentropic compressibility  $(K_{s,\varphi})$ , which can be denoted in terms of a mathematical relation, i.e.,

$$K_{s,\phi} = -\left(\frac{\partial V_{\phi}}{\partial P}\right)_{T} \tag{20}$$

where the change in molar volume of the solvent on the addition of 1 mol of solute is the apparent molar volume, i.e.,  $V_{\varphi}$ . The parameter can be enumerated by the following equation,

$$K_{s,\phi} = \frac{K_{s}\rho_{0} - K_{s}^{0}\rho}{m\rho\rho_{0}} + MK_{s}/\rho$$
(21)

ρ and  $ρ_0$  are densities of solute and solvent, and m and M are molality and molecular mass of solute. The molecules of water at the periphery of solute particles are greatly electrosricted by the solute molecules, while the bulk water molecules are capable of being compressed to a higher degree. Thus, the apparent molar compressibility,  $K_{s,\phi}$  of the solution is mostly because of the distortion in water molecules' compressibility in the bulk. Using the experimentally obtained ultrasonic velocity, U values for the mixtures of QUE/7-HF in hydro-ethanolic solutions of NAM of different compositions (0.5 mol kg<sup>-1</sup> and 1.0 mol kg<sup>-1</sup>),  $K_{s,\phi}$  values were evaluated under atmospheric pressure at different temperatures (293.15 K, 298.15 K)

and 303.15 K) according to Eq. (21) and are listed in Table 4. The plots of  $K_{s,\phi}$  as a function of the square root of molality, m<sup>1/2</sup> of OUE/7-HF for all the investigated mixed solvents of NAM under atmospheric pressure and at the above-mentioned temperatures are shown in Fig. 6. It can be revealed from Table 4 and representative plots (Fig. 6) that all  $K_{s,\phi}$  for QUE/7-HF in mixed solvents are found to be negative at all the studied temperatures. It is observed that the  $K_{s,\phi}$  values alter to less negative with the increase in QUE/7-HF concentrations. As a result of the association of solute molecules, the bulk part of the solution escapes more water molecules, making the solvation shell formation more feasible. Hence, the intrinsic compression of solute originating from electrostriction of the hydration shells causes lower compressibility of the system. Higher values of  $K_{s,\phi}$  for solutions, QUE/7-HF anticipate that molecules of water surrounding the anion of QUE/7-HF and NAM are less compressible in comparison to the solution in bulk because of the presence of polar and hydrophilic groups of QUE/7-HF and NAM that specify the strong solute-solvent interactions in the solution.

Utilising the following relation, the approximation uncertainty values for the apparent molar isentropic compression,  $K_{s,\phi}$ , have been calculated.

$$\partial K_{s,\phi} = \left\{ \left[ (MK_s/\rho) - K_{s,\phi})(\partial m/m) \right]^2 + \left[ (K_{s,\phi} + K_s^0/m\rho_0)(\partial \rho/\rho) \right]^2 + \left[ K_{s,\phi} + K_s^0/m\rho_0)(\partial K_s/K_s) \right]^2 \right\}^{1/2}$$
(22)

Estimated uncertainty in  $K_{s,\phi}$  is found to be ± 0.014 ×  $10^{-12}$  m<sup>5</sup>mol<sup>-1</sup>N<sup>-1</sup>, which is determined by taking into consideration the effects of U,  $\delta U$ ,  $\rho$  and  $\delta \rho$ .

The partial molar compressibility, or the apparent molar isentropic compressibility at infinite dilution,  $K^0_{s,\phi}$  of solution, is represented by the incorporation of two factors,

$$K_{s,\phi}^{0} = K_{s,\phi(intrinsic)}^{0} + K_{s,\phi(electrostrictive)}^{0}$$
(23)

where,  $K_{s,\phi(intrinsic)} = -(\partial V_{\phi(intrinsic)}/\partial P)_T$  and

 $K_{s,\varphi(electrostrictive)} = -(\partial V_{\varphi(electrostrictive)}/\partial P)_{T}$ 

Since the influence of pressure on crystal volume is minimal,  $K_{s,\phi(intrinsic)}$  is envisaged to be positive or near to zero [46]. Hence,  $K^0_{s,\phi}$  is merely regulated by the electrostriction of water molecules by ions. The negative data of  $K_{s,\phi}$  and  $K^0_{s,\phi}$  indicate that the polar moieties of NAM combine with the molecules of water at the periphery by dipole–dipole interactions. Thus, it is presumed that the polar environment developed by co-solute (in the present study, a hydrogen donor NAM) with water and EtOH makes the hydrophobic interactions accessible among QUE/7-HF.

With the help of the equation given below, apparent molar isentropic compressibility at infinite dilution was evaluated.

$$K_{s,\phi} = K_{s,\phi}^0 + S_{k,\phi}\sqrt{m}$$
(24)

 $S_{k,\varphi}$  and  $K^0_{s,\varphi}$  represent the slope and intercept of the straight line. $K^0_s,\;S_{k,},K^0_{s,\varphi}$  and  $S_{k,\varphi}$  values as well as the respective standard errors, and  $\Delta^0_{trK_{s,\varphi}}$  are illustrated in Table 5. The lowering in negative values of  $K_{s,\phi}^0$  illustrates solute-hydrophilic and solute-solute interactions among the polar groups of co-solute and solute molecules and, thus, consequent removal of the solvation shells. The ejection of water molecules may also be due to the repellent interactions among the hydrophobic parts of QUE/7-HF and NAM molecules. The values of  $K^0_{s,\phi}$  when compared in QUE solutions with that of 7-HF solutions, it is evident (Table 5) that the data are of higher negative magnitude in QUE solutions suggesting stronger solutehydrophilic and hydrophilic-hydrophilic interactions among different parts of QUE and NAM than 7-HF with NAM in hydro-ethanolic media.

## Transfer parameter of limiting apparent molar isentropic compressibility and interaction coefficients

Transfer parameter of limiting apparent molar isentropic compression,  $\Delta^0_{trK_{s,\phi}}$  is another important property which is figured out in the present study in order to explain the

molecular interactions in the investigated systems. As the apparent molar isentropic compressibility is considered at infinite dilution,  $\Delta^0_{trK_{s,\varphi}}$  data are not influenced by solute–solute interactions [47]. Thus, the values of  $\Delta^0_{trK_{s,\varphi}}$  administer knowledge about solute–solvent interactions exist in the solution. The values of  $\Delta^0_{trK_{s,\varphi}}$  are evaluated by the use of the following equation and listed in Table 5.

$$\Delta_{trK_{s,\phi}}^{0} = K_{s,\phi}^{0} \left( \text{in aqueous} \frac{\text{PS}}{\text{SB}} \right) - K_{s,\phi}^{0} (\text{in water})$$
(25)

It is distinct from Table 5 that  $\Delta^0_{trK_{s,\varphi}}$  values for all the compositions of hydro-ethanolic NAM solutions are found to be positive and show a regular upward orientation upon rise in molality of NAM in hydro-ethanolic media. The positive  $\Delta^0_{trK_{s,\varphi}}$  values demonstrate the structure-building nature of QUE/7-HF in the studied solutions.

## Pair-wise and triplet interaction parameters

In complex mixtures, especially those with more than two components (like ternary or multicomponent systems), both pair-wise and triplet interaction parameters are necessary to describe the full complexity of molecular interactions. In mixtures, the pair-wise interaction parameters are often used to describe the activity coefficients and excess thermodynamic properties (enthalpy, entropy, etc.). Pair-wise interactions are crucial in understanding the binding affinity between solute molecules or between solute and solvent. They determine the strength and range of interactions like hydrogen bonding, van der Waals forces, and electrostatic interactions. Triplet interactions are more complex than pair-wise interactions because they describe the behavior of a group of three particles interacting in a non-linear fashion. In thermodynamic models, these interactions account for the influence of higher-order correlations or multi-body interactions beyond just simple pair-wise contacts. Pairwise and triplet parameters are critical in predicting phase diagrams. In industries such as pharmaceuticals, chemical engineering, and materials science, these interaction parameters help design optimal mixtures (e.g., solvents and solutes) for desired properties, including solubility, stability, and efficiency.

To assess the pair (K<sub>AB</sub>) and triplet (K<sub>ABB</sub>) interactions between the solute and cosolute, transfer values can be utilized [48]. Equation (26) can be used to estimate the intercept K<sub>AB</sub> and slope K<sub>ABB</sub> by substituting the terms  $\Delta^0_{trK_{s,\phi}}$  and m<sub>B</sub> with their respective numerical values.

$$\Delta_{\mathrm{tr}K_{\mathrm{s},\phi}}^{0} = 2K_{\mathrm{AB}}m_{\mathrm{B}} + 3K_{\mathrm{ABB}}m_{\mathrm{B}}^{2} + \dots$$
(26)

Symbols A and B are assigned to the solute (QUE/7-HF) and co-solute (hydro-ethanolic NAM), respectively. The obtained values  $K_{AB}$  and triplet  $K_{ABB}$  are documented in table S2. The positive values of  $K_{AB}$  and the negative values of  $K_{ABB}$  for QUE and 7-HF, indicate the presence of dominant pairwise interactions over triplet interactions. As analyzed, the pairwise interactions (positive  $K_{AB}$ ) are higher in 30 v/v-EtOH+NAM than 40 v/v-EtOH+NAM in case of QUE, whereas for 7-HF the pairwise interactions are higher in 40 v/v-EtOH+NAM than 30 v/v-EtOH+NAM.

## Acoustic impedance

The ratio of acoustic pressure to flow is known as acoustic impedance (Z). It is an intensive property of a medium or particular geometry. It delineates how much resistance an ultrasound wave experiences when it passes through a medium. When an ultrasound travels in a solution, its longitudinal sound waves encounter resistance by the particles. Such an obstruction against the sound wave propagation is the acoustic impedance of that medium that depends on the molecular packing of the medium, structure-making/breaking properties of the solute, the caging effect of the solvent and solvation process. With the increase in the concentration of QUE/7-HF, the values of Z decrease (Table 6), which suggests that due to the formation of  $QUE/7HF - (H_2O)_2$  complexes, some of the molecules of water and NAM become free from the secondary solvation shell and make easy for the flow of ultrasound without any such resistance. The hydrogen bond donor (NAM) can also form some intermolecular hydrogen bonds with free water molecules. As a result, the impedance decreases. As can be observed from the Table 6 the values of Z increase with increase in composition of NAM when the hydro-ethanolic volume concentration is made constant. Such a variation can be interpreted in terms of the presence of strong interactions among QUE/7-HF and NAM molecules in the mixed solvent system. The impedance exhibited by the components of the solution to sound waves has a counter effect on the compressibility parameters K<sub>s</sub> and K<sub>T</sub> (indicating increasing variation with a concentration of cosolute (NAM) and solute (QUE/7-HF).

Based on the investigation of volumetric and acoustic properties, this study challenges the notion that solute solvent interactions are readily observed and efficient among QUE/7-HF and NAM molecules in the mixed solvent system. The results are also supported by the conductometric properties of the studied system that was recently published [30]. In light of this, the system under study and the methods chosen offer a novel perspective and anticipate novel interaction patterns or complexes that could be challenging to observe through experimentation.

## Conclusions

In this work, the density and ultrasonic velocity data for solutions for QUE and 7-HF in different compositions of hydro-ethanolic solution of NAM were measured and utilized to evaluate different volumetric and acoustic parameters under atmospheric pressure at different temperatures. As concentration rises, the solute-solvent interactions in the solution appear to be decreasing, as indicated by the decrease in  $V_{\phi}$  values. It is because the presence of NAM encourages more solute-solute interactions than The positive values solute-solvent interactions. of  $(E^0_{\phi})$  clearly demonstrate that the caging effect of the solvent and the solute's capacity to form structures in the systems under study are mutually complemented. There is a continuous decline in Ks values with a rise in temperature. The elevation in thermal agitation reinforces the rate of release of molecules of solvent to the bulk state of the solution from the hydration co-sphere of ionic/hydrophilic The hydrophobic-hydrophobic repulsive entities. interactions are more prevalent than the hydrophobichydrophilic attractive interactions, as indicated by the negative values of Sk. Negative values of apparent molar isentropic compressibility  $(K_{s,\phi})$  and partial molar isentropic compressibility  $(K_{s,\phi}^{0})$  reveal that the compressibility of the bulk water molecules is higher than those in the hydration shells. An illustration of solute-hydrophilic and solute-solute interactions between the polar groups of co-solute and solute molecules is the decrease in negative values of  $K_{s,\phi}^{0}$ , which leads to the elimination of the solvation shells. Pairwise interaction is predominant over triplet interaction as manifested by positive  $K_{AB}$  and negative *K*<sub>ABB</sub> in all solutions. Further, an increase in the acoustic parameter viz. impedance (Z) values with a rise in concentration signifies the existence of strong solutesolvent interactions. This study on physicochemical properties of QUE/7-HF + NAM in the hydro-ethanolic medium may help the researchers to adopt and outline more experimental work on molecular interactions to step forward in the area of biocompatible actives' solubilization and delivery.

## **Supplementary Information**

The online version contains supplementary material available at https://doi. org/10.1186/s13065-025-01463-9.

Supplementary Material 1.

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## Author contributions

LS: Experimentation, conception and design of the data; RKP: prepared all figures; MM: drafting the article or revising it critically for important intellectual content; SS: analysis and interpretation of the data, guided to wrote the main manuscript text, approval of the final version.

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## Declarations

**Ethics approval and consent to participate** Not Applicable.

## **Consent for publication**

Not Applicable.

### Competing Interests

The authors declare no competing interests.

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