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# Ultrasonic Investigation Of The Thermo-Acoustical Properties Of Sorbic Acid In Aqueous Solutions Of Propylene Glycol And Hexylene Glycol

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## Abstract

*This study investigates the thermodynamic and acoustic properties of sorbic acid in aqueous solutions containing propylene glycol (PG) and hexylene glycol (HG) as co-solvents. Measurements were performed across a temperature range of 293.15 K to 308.15 K at a fixed pressure of 0.1 MPa. The prepared solutions contained sorbic acid at concentrations of 0.01, 0.03, and 0.05* $mol.kg^{-1}$. *Using the Anton Paar DSA 5000 M, density and sound velocity were recorded to evaluate key parameters such as thermal expansion coefficients, expansibilities, transfer volumes, and partial molar volumes. Additionally, the study examines the effects of sound velocity on isentropic compressibility, including apparent molar isentropic compression, partial molar isentropic compression, and second-order compressibility factors, providing insights into solute-solvent interactions. By determining pair and triplet interaction coefficients along with empirical constants, the extent of molecular interactions within the solution was assessed. The findings indicate that hexylene glycol exhibits stronger solute-solvent interactions than propylene glycol, as reflected in the derived thermophysical properties. These insights contribute to a better understanding of co-solvent behaviour in aqueous environments, with potential applications in pharmaceutical formulations and food sciences.*

***Keywords:*** *Sorbic acid, Hexylene glycol (HG), Propylene glycol (PG), Volumetric properties, Acoustical properties.*

## 1. INTRODUCTION

Ternary solution (Sorbic acid + water + (PG/HG)] has been examined in the present study at atmospheric pressure and varying temperatures ranging from (293.15 K) to (308.15 K) with concentrations 0.01, 0.03, 0.05 $\mathrm{mol.kg^{-1}}$. The Anton Paar DSA 5000 M can be employed to measure sound speed and density. "Different thermo-acoustic characteristics are determined using the information that was gathered. and partial molar volumes, thermal expansion coefficients, expansibilities, and volumes of transfer were among the properties experimentally measured. All three types of apparent dimensional compression—particular, partial, and transfer—were affected by the speed of sound. To measure crucial solute-solvent interactions, empirical constants, pair and triplet coefficients have been found. According to the properties, propylene glycol has a weaker solute-solvent interaction than hexylene glycol. Numerous investigations have harnessed ultrasonic methods to explore molecular interactions within diverse liquids and mixtures. These studies have been instrumental in unraveling the physicochemical properties of various liquids and their combinations. The versatility of ultrasonic technology extends its reach into a multitude of industries, including pharmaceuticals, clinical applications, cosmetics, food production, leather processing, textiles, and transportation. In these fields, ultrasonic methods are very helpful for studying the effects and a variety of thermophysical properties of liquid mixtures [1-3]. An important step towards better comprehending the molecular forces at work is the extraction of several acoustical and thermodynamic characteristics [4,5]. Knowledge of the nature and intensity of the molecular interactions in the mixture is crucial to this non-destructive method, which is an effective investigative tool. It is possible to gain a better understanding of the complex interactions in liquid mixtures, including hydrogen bonding, dipole-dipole interactions, and induced dipole-dipole interactions, by analysing the density and sound speed [6–9]. A fascinating new field for studying the acoustical properties of binary, ternary, or pure liquid systems has emerged with the advent of ultrasonic technology in recent years. The world of possibilities is huge and inviting, even if there is a lot of research that has used this method previously. This genre of study yields a wealth of information on interactions, flaw detection, structural nuances, and molecular arrangements within liquid systems. The journey to uncover the secrets held within these liquid mixtures is far from complete, and the potential for new discoveries continues to captivate researchers. [10-13] Examining the characteristics and functions of liquid combinations, such as sorbic acid, in aqueous solutions of propylene glycol (PG) and hexylene glycol (HG) at various temperatures and concentrations of 0.01, 0.3 and 0.05 $\mathrm{mol.kg^{-1}}$ is the aim of this work. The study will carefully examine the volumetric and acoustical characteristics of these combinations in order to get a deeper understanding of their characteristics in different contexts. Propylene glycol (PG), an organic chemical, is characterized by its transparent appearance, thick consistency, and no scent, while also exhibiting a mild, sugary flavor. The diol classification of the compound is attributed to the existence of two hydroxyl groups within its molecular configuration. Along with its low toxicity and volatility, PG's flexibility is highlighted by its ability to combine with a varied spectrum of solvents. Propylene glycol (PG) is an essential ingredient in many products due to its many useful properties, including those of pharmaceuticals and personal care items. Use of PG in the production of coffee-based drinks, sodas, ice cream, whipped dairy products, unsaturated polyester resins, and liquid sweeteners is common in these sectors. [14-20] Hexylene glycol (HG) exhibits similar colorless and viscous properties to propylene glycol (PG) and is notable for its distinctively sweet fragrance. This chemical has compatibility with a wide range of organic solvents, hence enhancing its overall usefulness. (HG) has established its presence in various industries, playing a significant role in areas such as food preservation, varnishing, printing ink formulations, lacquers, pesticide manufacture, vehicle manufacturing, textiles, and the chemical and pharmaceutical sectors. [21,22] On the other hand, sorbic acid, which is an organic substance in its regard, assumes a crucial function as a food preservative. The extensive utilization of this substance spans a broad range of food items, including but not limited to dairy products, meat, vegetables, fruits, baked goods, fish, emulsions, and other related categories. The inclusion of sorbic acid in these products plays a crucial role in extending their duration of storage, guaranteeing their standard, and maintaining their state of being fresh [23-25]. In conclusion, this study aims to elucidate the complex characteristics of liquid mixtures, focusing on the dynamic interactions among sorbic acid, propylene glycol, and hexylene glycol. By obtaining accurate measurements of density and sound speed, these studies have the potential to shed light on these materials. Consequently, they can provide useful insights that may contribute to the improvement of various processes and products in a wide range of industries.[26]

Studying the volumetric and acoustic properties of glutaraldehyde, water, and glycol solutions (specifically hexylene and propylene), P. Kaur et al. By combining information on density and sound velocity, thermoacoustic parameters such as volume, isentropic compressibility, excess molar volume, and variations in the speed of sound were calculated. The (PG/HG) solution's molecular interaction with the glutaraldehyde solution is seen clearly in the experimental data graph. It is further demonstrated that the effect of this interaction grows as the molar mass of the solution increases. [27] Thermodynamic and acoustic properties of a material were studied by M. Lamba et al. by manipulating the temperature and concentration of aqueous PG/HG in combination with disodium EDTA. The experimental findings demonstrated a substantial correlation between density and speed of sound throughout the redemption process. [28] in Nabaparna et al. evaluated the electrical conductivity and volumetric properties of a water-based disodium solution at different temperatures and molalities. An extensive review of the current literature revealed a dearth of studies investigating the acoustic volumetric analysis of solutions including (PG/HG) and sorbic acid, a widely used food preservative. As a result, the present work aims to fill this gap by conducting a thorough investigation into the ultrasonic properties of such solutions. Experimental density and velocity measurements were performed at various temperatures to explore the molecular interactions and physicochemical characteristics inside the sorbic acid and PG/HG combination. These measurements were utilized to determine the volumetric and acoustical characteristics of the mixture. [29]

## 2. EXPERIMENTAL PROCEDURES

### 2.1. Materials used

Loba Chemie Pvt. Ltd., an Indian firm, supplied the propylene glycol and hexylene glycol, which have molar masses of 76.09 $\mathrm{g.mol^{-1}}$, and 118.176 $\mathrm{g.mol^{-1}}$, respectively. Additionally, they supplied the sorbic acid part of this experiment, which has a molar mass of 112.13 $\mathrm{g.mol^{-1}}$. The compounds exhibited a consistent purity of

0.99. The compounds were first dried using a vacuum and then dried in a desiccator for more than 48 hours. The goal was to reduce the chemicals' absorption of moisture prior to usage. That whole time, distilled water was utilised nonstop. The water used to generate the trinary solution was double-distilled and deionized using a Millipore Milli-Q Academic water purification system. **Table 1** gives a detailed and easily digestible rundown of all the materials used in this study, including a list of the individual compounds of interest.

### 2.1.1 Analysis of Water content

The water content in the sorbic acid and water solutions was evaluated at varying concentrations (0.01, 0.03, and 0.05 $mol{\cdot}kg^{-1}$) to understand the solution's composition and to ensure accuracy in subsequent measurements. At 0.01 $mol{\cdot}kg^{-1}$ concentration, the water content was found to be 99.887%, while it slightly decreased to 99.664% and 99.443% for concentrations of 0.03 and 0.05 $mol{\cdot}kg^{-1}$, respectively. This reduction in water content with increasing solute concentration aligns with the theoretical expectation that the solute mass fraction increases in the total solution. The high-water content, even at the maximum concentration, underscores the dilute nature of the solutions used in this study. Accurate determination of water content is crucial for experiments involving density and sound velocity measurements, as water contributes significantly to these physical properties. Furthermore, these calculations validate the precision of the preparation protocol, ensuring minimal deviation from the intended molar concentrations and consistent experimental conditions. Water played a crucial role in the preparation of the sorbic acid solutions, and its content was carefully monitored throughout the experiment. The water used in this study was sourced from a Millipore Milli-Q Academic water purification system, ensuring it was of high purity. The water was double-distilled and deionized, followed by degassing to remove any dissolved gases, which could potentially affect the measurements of density and sound velocity. To further ensure the accuracy and consistency of the experimental conditions, the water was placed in a desiccator for 48 hours to reduce its moisture absorption and prevent contamination during storage. The water content in the ternary solutions was determined at various concentrations of sorbic acid, ranging from 0.01 $mol{\cdot}kg^{-1}$ to 0.05 $mol{\cdot}kg^{-1}$. At each concentration, water remained the dominant component of the solution, with its content consistently exceeding 99%. This highwater content is essential as the solvent properties of water significantly influence the physical measurements, such as density and sound velocity. The purity of the water, coupled with the careful control of its storage and preparation, ensured that the water content in each solution remained stable and did not introduce variability into the experimental results. The calculated water content percentages further validate the accuracy of the solution preparation and the precision of the experimental methodology. [1-15]

### 2.2. Apparatus and Methods Used

Two solutions were tested using an Anton Paar DSA 500 M. One solution contained sorbic acid, while the other contained propylene glycol or hexylene glycol. The density and sound velocity of each solution were then calculated. Various solutions were subjected to varying temperatures (293.15 K, 298.25 K, 303.15 K, and 308.15 K), concentrations ranging from 0.01 to 0.05 $\mathrm{mol.kg^{-1}}$, a constant pressure of 0.1 MPa, and a frequency of 3 MHz to control the temperature of the DSA, a Peltier thermostat is employed. Peltier devices contain both cold and hot junctions. The device works by absorbing heat at the cold junction and releasing it at the hot junction as current runs through it. Because of this, a temperature gradient is generated all across the gadget. The density and velocity of the sound can be experimentally evaluated by injecting the solution using a syringe. To determine the density and speed of sound in two separate cells, the Anton Paar DSA 5000 M and the Anton Paar oscillating U-tube technique were utilised. The line begins to oscillate at a specific frequency the second the sample enters the tube. Next, an ultrasonic transducer and receiver are used to measure the thickness of the specimen on both sides of the sound speed measurement cell. The transducer and receiver transmit sound waves at a certain frequency through the specimen. The tube's resonance frequency changes as the density of the sample changes. Each side of the sound-speed measuring cell has its sample thickness determined by this frequency shift. You can figure out how fast sound is travelling by combining the air-to-sound transit time with the distance between the source and the receiver. For its measurements of air or water density at 293.15 K and atmospheric pressure, the Anton Paar DSA 5000 uses triple-distilled degassed water as its calibration. Calibration of the device is set in this way. The density and speed of sound of the sorbic acid solution were measured using a sample of clean distilled water. After purifying it by distillation and deionization, the water was sourced from a trustworthy source. The substance was degassed and triple distilled to guarantee its purity. Following distillation, the water was desiccated for 48 hours to reduce moisture absorption. This approach ensured the water's steady and uncontaminated qualities were maintained throughout the studies. Regular use of an acknowledged density reference standard is necessary to provide accurate results. [30-39].

The standard uncertainties for the temperature, molality, density, and sound speed are $u(T) = 0.01\ K, u(\rho) = 0.5(\ kg.m^{-3})$and $u(c) = 1.0(m.s^{-1})$, respectively. On the other hand, the equivalent sensitivities of the Sartorius CPA 225D weighing balance, speed of sound, and density are $\pm 0.00001\ g, \pm 0.001\ (\ kg.m^{-3})$ and $0.01\ (m.s^{-1})$, respectively. A typical relative error in molality of 1% is included with the given purities for these compounds. Sorbic acid weighing (0.11212, 0.33635, and 0.56065) $g$ was extracted from the aqueous mixture in 100 $g$ of water at concentration ranges of [(0.01, 0.03, and 0.05) $mol.kg^{-1}$ ]. Sorbic acid dissolves in five different molalities in this water-based solution containing glycols: [(0.01, 0.02, 0.03, 0.04, and 0.05) $mol.kg^{-1}$].

## 3. RESULTS AND DISCUSSION

### 3.1. Volumetric properties

A crucial and essential aspect of scientific study is the examination of volumetric properties inside solution systems. The use of specialized tools and procedures allows for the precise measurement of characteristics like density under varied scenarios. These measures provide vital information. Researchers can use thorough regression analysis to develop detailed mathematical correlations between solutes and solvents. The measuring of density is an essential part of this inquiry. The volume and mass of a solution are determined in a comprehensive manner via density measurement. Tools like densitometers and density meters are often used for this purpose. A solution's density is expressed in grammes per milliliter, or $g.ml^{-1}$. The volumetric features of the solution can be thoroughly understood by researchers due to the wealth of information that this measurement technique offers regarding its behaviour.

### 3.1.1. Density

The density values of PG and HG in sorbic acid solutions in water at 0.1 MPa of pressure are shown in **Table 2**. A temperature range of 298.15 K to 308.15 K is used for the experiment, and concentrations ranging (0.01, 0.03, and 0.05 $(mol.kg^{-1})$) are used. The densities of the mixture of distilled water and PG and the mixture of distilled water and HG are compared to the values obtained from existing literature [29,30]. The results indicate a positive correlation between the density values and the concentrations of PG/HG and sorbic acid. When the concentration of solute particles in a solution increases, the solute molecule interacts with other molecules more often. Because of these interactions, the molecules in the solution pack closer together, increasing density for molality. On the other hand, the density values with respect to temperature decrease. As the temperature increases, the average kinetic energy of the molecules in a ternary solution increase. A decrease in cohesive connections and an increase in kinetic energy allow molecules to separate more easily. As the temperature rises, the molecules in the solution enlarge and the density decreases. The behaviour of thermal expansion in liquids is consistent with this trend. The density of a solution decreases as its temperature rises. [40–45] Density of aqueous glycol mixes at various temperatures was determined using experimental measures. The values in the literature [29,30] were compared to these measurements, and the results are shown in **Figure 1**. Shows good arrangement with literature. Scheme 1 illustrates how the solution's molecular and solute-solvent interactions gradually become better as it transitions from PG to HG. There is a strong agreement on several points between the numbers of glycols discovered in the literature and the experiments.

### 3.1.2 Apparent molar volume

The apparent molar volume $(V_\phi)$ readings from the density measurement may be computed using the equation.

$$V_\phi = \frac{M}{\rho} - \frac{(\rho-\rho_0)}{m_A}\rho\rho_0 \qquad (1)$$

This shows the solute's molar mass (M), its molality ($m_A$) per kilogram of the solvent (distilled water + sorbic acid), the density of the solution (ρ), and the density of the solvent ($\rho_0$). The influence of interactions like solute-solvent and solute-solute was investigated using the apparent molar volume. The change in geometric volume of the solvent and the solute molecule as a consequence of their interaction may be added together to get $V_\phi$. In **Table 2**, you can see the apparent molar volume values for two different mixtures one with (water + sorbic acid +PG) and the second one is (water + sorbic acid +HG). For a given concentration of sorbic acid, the values of $V_\phi$. stay consistently positive as temperatures and glycol molality climb. This leads to an acceleration of $V_\phi^0$ values, as depicted in **Figure 2**. The positive values of $V_\phi$which exhibit a strong linear relationship with rising temperature and glycol amount, indicate the possibility of solute-solvent interaction. The high affinity of the insolvent and solvation events characterizes each kind of molecular interaction in the complex. This indicates that the solute and solvent in the solution have a strong connection. **Scheme 1** shows that the solute-solvent interaction changes from PG to HG as the molar mass of the glycol increases. The increase in the values seen with temperature serves as proof of this. Water is more soluble in the glycols due to strong intermolecular hydrogen bonding, dipole-dipole, and dipole-induced dipole interactions. Additionally, water contributes to the ternary mixture's hydrophobic effect and hydration. [46-51]

### 3.1.3 Partial molar volume

The partial molar volume ( $V_\phi^0$) is a critical thermodynamic characteristic that reveals molecule size and interactions in solutions. The formula below calculates the partial molar volume values in a combination containing sorbic acid, water and glycol (PG/HG).

$$V_\phi = V_\phi^0 + S_V^* m_A \qquad (2)$$

We obtained the values of $V_\phi^0$ and the experimental slope $S_V^* m_A$. by using the least square fitting approach. In addition, standard errors were computed. The values of $V_\phi^0$ and $S_V^* m_A$. for the mixture of distilled water and glycols (PG/HG) are shown in **Table 3**. The values of $V_\phi^0$. strongly correlate with rising temperatures and sorbic acid concentrations, as **Figure 3** shows. Strong solute-solvent interactions may be present in the sample since this pattern intensifies with increasing temperature and sorbic acid content. Determine the sample size's significance by computing the standard error and drawing trustworthy conclusions. [46] The increase in $V_\phi^0$ values while transitioning from PG to HG is caused by hydrogen bonding between the OH group in (PG/HG) glycols and the hydrogen atom in water. This demonstrates the exact link that exists between the molar mass of glycols and $V_\phi^0$. The volume increases when two ionic species come into contact with hydrated co-spheres, according to the co-sphere overlap theory. The volume, however, decreases when ion-hydrophobic and hydrophobic-hydrophobic co-spheres come together. Interaction patterns between solutes are indicated by the uneven distribution of $S_V^*$values. Considering that the, $V_\phi^0$ values are larger than the solute-solute interactions, the solute-solvent interactions' positive values imply that the solvent-solute interactions are more significant. [11-15]

### 3.1.4 Partial molar volume of transfer

The formula may be used to determine the partial molar volume of transfer for glycols from water in sorbic acid solutions that are infinitely diminished.

$$\Delta V_\phi^0 = V_\phi^0\,(\text{in aqueous sorbic acid solution}) - V_\phi^0(\text{in water}) \qquad (3)$$

analyzing the partial molar volume of transfer values, $V_\phi^0$. In a liquid system, the solute-solvent interaction may be determined at infinite dilution, but not the solute-solute interaction. The calculated $\Delta V_\phi^0$values are found to be positive, as shown in **Table 4.**

Mixtures of hydrophilic and hydrophobic species can form when the electrostriction of water molecules close to glycols is reduced, releasing fewer water molecules into a larger volume. At a constant temperature, **Table 4** shows the increasing $\Delta V_\phi^0$values for each glycol (PG and HG), together with the different sorbic acid concentrations. Hydrogen bonds are formed between the -OH group of sorbic acid and the hydrophilic glycol groups, according to study findings [47–49]. This interaction results in a reduction of the solute-water hydrophilic connections and the formation of new contacts between hydrophiles, ions, and hydrophobes in the ternary mixture. The co-sphere overlap model describes several interactions. [43, 44]. Hydrophilic groups interact with sorbic acid, while zwitterionic groups in polyethylene glycol do the same for hydrophobic groups. While the hydrophilic groups of polyethylene glycol and sorbic acid interact in a hydrophilic manner, the interactions between the alkyl groups are hydrophobic. [44,45]

### 3.1.5 Temperature dependent partial molar volume

The following polynomial equation can be used to express the influence of the partial molar volume at infinite dilution, $V_{\phi}^{0}$, on absolute temperature.

$$V_{\phi}^{0} = a + b(T - T_{ref}) + c(T - T_{ref})^2 \quad (4)$$

**Table 5** displays the values of the empirical constants a, b, and c as well as the temperature T and reference temperature $T_{ref}$ on the Kelvin scale. This paragraph details the equation used in **Table 5**, which is used to examine the discrepancies between the experimental and estimated values of $V_{\phi}^{0}$.[42]

$$\sigma = \left(\frac{1}{n}\right) \Sigma \left[\mathrm{abs}((X_{EXPTI.} - X_{CALC.})/X_{EXPTI.})\right] \quad (5)$$

$X = V_{\phi}^{0}$ (the apparent molar volume at infinite dilution) in this instance. If the $R^2$ value is large, the deviation values are consistent with the polynomial equation. This is demonstrated by the results of the investigation on $R^2$. As shown in **Table 5**, the empirical constant c accounts for the variation in the$V_{\phi}^{0}$ value. To determine the partial molar expansibilities, the main goal throughout the study of the $V_{\phi}^{0}$ values was to use the following equation. [43 ,45]

$$E_{\phi}^{0} = \left(\frac{\partial E_{\phi}^{0}}{\partial T}\right)_P = b + 2c\,(T - T_{ref}) \quad (6)$$

The ability of the co-solute medium to form and destroy structures is reflected in the sign of the partial derivative of the electrostatic potential with respect to temperature under constant pressure and co-solute concentration conditions. i.e. $\left(\frac{\partial E_{\phi}^{0}}{\partial T}\right)_P$. The solute forms a structure when $\left(\frac{\partial E_{\phi}^{0}}{\partial T}\right)_P$, has positive values. Conversely, the solute disrupts a structure when $\left(\frac{\partial E_{\phi}^{0}}{\partial T}\right)_P$ has negative values [36]. The limited apparent molar expansibilities $E_{\phi}^{0}$ and $\left(\frac{\partial E_{\phi}^{0}}{\partial T}\right)_P$ are displayed in **Table 6**.

All concentrations (0.01, 0.03, 0.05) $\mathrm{mol.kg^{-1}}$ and temperatures (293.15, 298.15, 303.15, 308.15 K) in the study clearly show that the $E_{\phi}^{0}$ values are positive. Glycols possess a positive partial molar expansibility due to their capacity to disrupt hydrogen bonding in water. The molecular motion becomes greater as the temperature rises, which makes glycols a more formidable interference with the structure of water. Greater concentrations result in a higher number of glycol molecules, which leads to a greater disruption of hydrogen bonding in water. This disruption causes a decrease in the ability of water to expand. This trend represents the laws of thermodynamics that govern the interactions between a solute and a solvent. [28, 13, 66]

### 3.2. Ultrasonic properties

Ultrasonic and acoustic methods are used to study sound waves in liquid mixtures, revealing molecular interactions, structure changes, and reaction to temperature and pressure changes. In these investigations, transducers are used in an acoustic or ultrasonic interferometer to produce ultrasonic waves that then travel through the solution under study. The sound velocity in the solution may provide crucial information about the liquid mixture's acoustics. Computed acoustic characteristics that provide insight on the interactions between the components of the solution include acoustic impedance, apparent molar volume, excess properties, and partial molar properties. In order to comprehend complicated solutions with widespread applications, this study is crucial since it promotes scientific and industrial domains while also improving thermodynamic understanding. [50-64]

### 3.2.1. Ultrasonic speed

Sorbic acid, distilled water, and glycols (PG/HG) solutions were used to test the sound speed at different temperatures (293.15 K, 298.15 K, 303.15 K, and 308.15 K) and concentrations (0.01, 0.03, and 0.05 ($\mathrm{mol.kg^{-1}}$). Throughout the experiment, the pressure was kept constant at 0.1 MPa using an Anton Paar DSA 5000 M. The outcomes are shown in **Table 7**. The results were contrasted with those of earlier research that measured sound speed using combinations of water, sorbic acid, propylene glycol (PG), and hexylene glycol (HG). [29,30]. **Figure 4** illustrates data. The chart shows that published and experimental sound speed measurements at various temperatures and glycol molalities are very consistent. For a given concentration of sorbic acid, the speed of sound rises depending on the temperature and molality of the glycol. These values similarly grow as the sorbic acid content rises. Through intramolecular hydration bonds and intermolecular hydrogen bonds inside the glycol molecules, the solute molecules interact with the solvent molecules as well as with one other. The exponential rise in sound speed and the ease of mixing are both explained by this connection. The formation of more monomeric water molecules and a decrease in hydrogen bonding cause the concentration of pure water to rise as the temperature rises. Power water molecules fill in gaps and group together inside the cage-like structure to improve the cage's density. Because the structure of water molecules varies with temperature, ultrasonic vibrations may pass through them. This might be explained by the fact that pure water has a temperature-dependent sound speed, or by the presence of glycols in sorbic acid solutions. In the meanwhile, solvent molecules gain kinetic energy. The average molecular velocity and the interactions between molecules in a solution influence the speed of sound. Intermolecular contacts grow as a result of the more robust molecular motion brought on by rising temperatures. The molarity ratio, which is expressed as moles of solute to kilograms of solvent, may be used to determine the solute concentration in a solution. The interactions between the solute and solvent molecules become more significant as the solute dissolves. These changes may have an impact on the compressibility, density, and other properties of the solution. Consequently, these changes change how acoustic waves are transmitted. Sound velocity is increased by high molality because it promotes solution interactions and structural alterations. [35-50]

### 3.2.2. Apparent Molar Isentropic Compression

An equation for the apparent molar isentropic compression of glycols in aqueous sorbic acid.

$$\mathrm{K_{\phi,S}} = \left(\frac{\mathrm{Mk_S}}{\rho}\right) - \left\{\frac{(\mathrm{k_{S,0}}\rho - \mathrm{k_{S,0}}\rho_0)}{\mathrm{m_A}\rho\rho_0}\right\} \qquad (7)$$

$\mathrm{M}$, $\mathrm{m_A}$, $\rho$, $\rho_0$, $\mathrm{k_{S,0}}$, and $\mathrm{k_{S,}}$, respectively, stand for the solute molar mass, molarity, density of the solvent and the solution, and isentropic compressibility of the pure solvent and the solution. The Laplace-Newton formula is used to determine the isentropic compressibility. [42-45].

$$\mathrm{k_S} = \frac{1}{\mathrm{c^2}\rho} \qquad (8)$$

The letter c stands for the solution's ultrasonic velocity, while the sign for $\rho$ denotes its density. Sound velocity is denoted by the symbol "c." The apparent molar isentropic compressibility ($\mathrm{K_{\phi,S}}$) of sorbic acid for propylene glycol (PG) and hexylene glycol (HG) is determined at various temperatures and concentrations (0.01, 0.03, and 0.05 $\mathrm{mol.kg^{-1}}$). **Figure 5** provides a visual view, and **Table 7** contains the computed findings. Studies show that when temperature rises, the proportion of propylene to hexylene glycol in sorbic acid solution increases. The computed, $\mathrm{K_{\phi,S}}$values clearly demonstrate that all values are negative at all temperatures and concentrations. As the temperature rises, the $\mathrm{K_{\phi,S}}$ values fall, but as the glycol concentration rises, they rise again, according to the obtained values. The presence of sorbic acid and glycol zwitter ions in water forms a water-soluble cluster. This cluster can break apart when exposed to high temperatures, resulting in negative ($\mathrm{K_{\phi,S}}$)values. This fact establishes that the compressibility of liquids is lower when they include ionic charge groups in solutes as opposed to when the liquid contains dissolved solids throughout. The combination decreases water's structural compressibility because the negative values of, $K_{\phi,S}$enhance the alignment impact between the solute and solvent. [11-35]

### 3.2.3. Partial molar isentropic compression

The apparent molar isentropic compression as a function of molality may be used to get the equation for the partial molar isentropic compression.

$$k_{\phi,s} = K^0_{\phi,S} + S^*_K m_A \qquad (9)$$

Where, $K^0_{\phi,S}$, $m_A$, $S^*_K$ results of the least square fitting approach are shown in Table 8 together with the standard errors for the limiting isentropic compression, molality, experimental slope, and interactions of the solute in solutions of aqueous sorbic acid + distilled water + (PG/HG). The values of $K^0_{\phi,S}$ are all negative, as seen in **Table 8**. Additionally, the model presented by Kirkwood [58, 60] indicates that there have been substantial interactions between the molecules of propylene/hexylene glycol and water, which have resulted in the bulk burning of water molecules. **Figure 6** illustrates this visually, showing that as temperature rises, sorbic acid concentration rises and negativity diminishes. According to this hypothesis, electrostriction water has a more closed structure than bulk water, which makes it more compressible. This is because the connection between the water molecules in the system and the glycols (PG/HG) molecules dampens the electrostriction interaction, increasing the molality of the interaction between sorbic acid and glycols (PG/HG). When electrostriction water seeps into the bulk from the solvation layer, the solute's compressibility changes. [14] The (solute-solvent) interactions seem to be the most significant in the mixture, whereas the (solute-solute) interactions are not as significant, as shown by the low $S_K$*values in **Table 8** in comparison to the high, $K^0_{\phi,S}$ values. [51–55].

### 3.2.4. Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer for PG and HG from water to aqueous sorbic acid solutions may be found using the following formula, applied at infinite dilution.

$$\Delta K^0_{\phi,S} = K^0_{\phi,S} \text{ (in aqueous sorbic acid solution)- } K^0_{\phi,S} \text{(in water)} \qquad (10)$$

**Table 9** presents the results of calculations performed on the $\Delta K^0_{\phi,S}$. According to the information in **Table 9**, it can be shown that for all sorbic acid concentrations in PG and HG, the values of $\Delta K^0_{\phi,S}$ indicate a positive trend, with the exception of temperature 303.15 K with a concentration of (0.03) $\mathrm{mol.kg^{-1}}$. in propylene glycol (PG). The sorbic acid aqueous ternary solution's compressibility is increased when propylene and hexylene glycol are added, based on a positive partial molar isentropic compression of transfer values for PG/HG. This information might be valuable in understanding the thermodynamic behavior of the solution and can have implications for various processes, such as chemical reactions or phase transitions, occurring in the system. [14-26, 60-65]

### 3.3. Pair and triplet coefficients

The partial molar isentropic compression of transfer and the partial molar volume of transfer may be computed using this relation.

$$\Delta V^0_{\phi} \text{(water to aqueous sorbic acid solution)} = 2V_{AB}m_B + 3V_{ABB}{m_B}^2$$
$$\Delta K^0_{\phi} \text{(water to aqueous sorbic acid solution)} = 2K_{AB}m_B + 3K_{ABB}{m_B}^2 \qquad (11)$$

The symbol $m_B$ represents the molality of sorbic acid solutions in water. Glycols and sorbic acid are represented by the letters A and B in this context, respectively. Volume and isentropic compression pair and triplet coefficients ($V_{AB}$; $V_{ABB}$ and $K_{AB}$; $K_{ABB}$) respectively are cited in **Table 10**. In order to arrive at the presented results, the researchers used the McMillian and Mayer hypothesis [58]. In order to carry out the required calculations, it is vital to use isentropic compression and partial molar values for volumes ($\Delta V^0_{\phi}$ ; $\Delta K^0_{\phi}$). This theory aims to explain the segregating effects in liquid mixtures, which are the result of molecular interactions between pairs and triplets. The concept in question was investigated further by Franks et al. (39-45), Friedman, and Krishnan. For both glycols (HG and PG) at various concentrations and temperatures, the pair interaction coefficients ($V_{AB}$) are positive. Conversely, three-way $V_{ABB}$ contact is seen negatively. For all (PG/HG) temperatures other than

303.15 K and propylene glycol concentrations of 0.03 $\mathrm{mol.kg^{-1}}$., a positive pair interaction coefficient $K_{AB}$ is seen (PG). With the exception of 303.15 K and 0.03 $\mathrm{mol.kg^{-1}}$., all triplet interaction coefficients $K_{ABB}$ have a negative value for propylene glycol. [12-30, 61-65]

## 4. CONCLUSION

A solution including sorbic acid, water, and PG/HG was investigated for its volumetric and acoustic characteristics at temperatures of 288.15, 298.15, 308.15, and 318.15 K and constant pressure of 0.1 MPa. The measured doses varied between 0.01 and 0.05 $\mathrm{mol.kg^{-1}}$. Specifically, the research reveals the unique structural characteristics of the ternary system. The properties that have been observed suggest that there are substantial interactions between the molecules of the solute and solvent in a solution. The apparent molar volume, the partial molar volume at infinity of dilution, the apparent molar isentropic compression, and the transfer molar volumes has all been examined. Based on the apparent molar properties, a substantial degree of solute-solvent interaction seems to exist. From PG to HG, the $V_{\phi}^{0}$ values have grown substantially due to the larger molar mass and intrinsic volume of HG, which is intensified by a rise in temperature. The numbers exhibit a positive and increasing trend with temperature and larger concentrations of sorbic acid, indicating a greater likelihood of interaction and solvation between glycols (PG/HG) and sorbic acid. The validity of our volumetric findings is corroborated by the values of $K_{\phi,S}$ and $K_{\phi}^{0}$. The experiment's volumetric and aural results are complementary to one another". As the concentration of sorbic acid and glycol (PG/HG) increases, the findings indicate a corresponding rise in molecular interactions. The solute-solvent interactions improve with both hexylene glycol and propylene glycol. The study further reveals that an increase in $\Delta V_{\phi}^{0}$ values is associated with the formation of hydrogen bonds between the hydroxyl (-OH) group of sorbic acid and the hydrophilic groups of glycols. This interaction weakens hydrophilic connections in water, leading to the formation of new contacts among hydrophilic groups, ions, and hydrophobic components within the ternary mixture. The presence of solute-solvent interactions is also supported by the positive values of $E_{\phi}^{0}$ at infinite dilution, which correlates with the observed trends in molar expansibility. Additionally, the second-order temperature derivative highlights structural formations and solute-solvent interactions contributing to the solution's behavior. Spectroscopic analysis further provides insights into chemical interactions and molecular structural modifications. The presence of propylene and hexylene glycol enhances the compressibility ($\Delta K_{\phi,S}^{0}$) of the sorbic acid aqueous ternary solution due to its positive value. The volume of activation ($V_{AB}$) remains positive across all PG/HG samples, whereas $V_{ABB}$ exhibits negative values. A positive pair interaction coefficient ($K_{AB}$) is observed in all PG/HG solutions, except at temperatures exceeding 303.15 K and in propylene glycol solutions with a concentration of 0.03 $\mathrm{mol\cdot kg^{-1}}$. Additionally, triplet interaction coefficients ($K_{ABB}$) generally display negative values, except in the case of propylene glycol at 303.15 K with a concentration of 0.03 $\mathrm{mol.kg^{-1}}$. The combination of sorbic acid with PG/HG has promising applications in various fields, including the development of biodegradable materials, drug delivery systems, wound care products, and food preservation. Experimental findings indicate that molecular interactions between propylene glycol and hexylene glycol in the ternary solution become more pronounced as concentration and temperature conditions vary.

## CREDIT AUTHORSHIP CONTRIBUTION STATEMENT

Ansari Ammara Firdaus was responsible for developing the research concept, methodology, formal analysis, and drafting the initial manuscript. K.C. Juglan played a significant role in the writing, reviewing, and editing process throughout the study. Additionally, Jaza Anwar Sayyed contributed to data visualization and provided guidance during the research. Nabaparna Chakraborty made substantial contributions by conducting an in-depth review, revising the manuscript, generating visual representations, overseeing the project, and offering valuable feedback throughout the process.

## DECLARATION OF COMPETING INTEREST

The authors confirm that there are no financial or personal conflicts of interest that could have influenced the conclusions of this research article.

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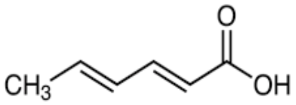
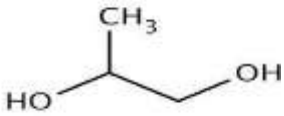
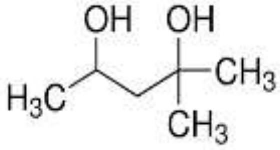
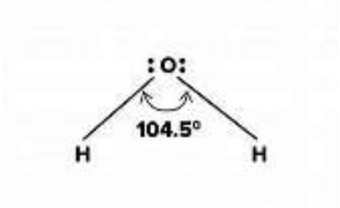
**Table 1:** Specification of chemicals

| Chemical | CAS no. | Molecular weight $\mathbf{g.mol^{-1}}$ | Source | Purification method | Mass fraction purity (supplier) | Structure |
|---|---|---|---|---|---|---|
| Sorbic acid | 110-44-1 | 112.13 | Indian company (Loba Chemie Pvt. Ltd.) | Vacuum dried | 0.99 |  |
| Propylene glycol:(PG) | 57-55-6 | 76.09 | Indian company (Loba Chemie Pvt. Ltd.) | Vacuum dried | 0.99 |  |
| Hexylene glycol:(HG) | 107-41-5 | 118.17 | Indian company (Loba Chemie Pvt. Ltd.) | Vacuum dried | 0.99 |  |
| Distilled Water | **7732-18-5** | **18.02** | **Millipore's Milli-Q** | - | **0.99** |  |

As per the supplier.

**Table 2** Glycols (PG and HG) in aqueous Sorbic acid solutions: values of densities (ρ), apparent molar volume ($V_{\emptyset}$). Under temperature variations and experimental pressure = 0.1 MPa.

| $^{a}m_{A}\,(\mathrm{mol.kg^{-1}})$ | $\rho \times 10^{-3}/(kg.m^{-3})$ | | | | $V_{\emptyset} \times 10^{6}/\,(m^{3}\,mole^{-1})$ | | | |
|---|---|---|---|---|---|---|---|---|
| | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K |
| 0.00 $\mathrm{mol.kg^{-1}}$ | Sorbic acid + PG + Water | | | | | | | |
| 0.00000 | 0.998210 | 0.997040 | 0.995650 | 0.994030 | | | | |
| 0.09957 | 0.998468 | 0.997302 | 0.995917 | 0.994304 | 73.607 | 73.679 | 73.743 | 73.806 |
| 0.19901 | 0.998711 | 0.997550 | 0.996170 | 0.994564 | 73.663 | 73.728 | 73.791 | 73.853 |
| 0.30106 | 0.998948 | 0.997794 | 0.996419 | 0.994817 | 73.712 | 73.767 | 73.829 | 73.901 |
| 0.39926 | 0.999166 | 0.998015 | 0.996645 | 0.995050 | 73.753 | 73.811 | 73.873 | 73.942 |
| 0.50059 | 0.999373 | 0.998230 | 0.996869 | 0.995280 | 73.809 | 73.859 | 73.912 | 73.980 |
| 0.01 $\mathrm{mol.kg^{-1}}$ | Sorbic acid + Water + PG | | | | | | | |
| 0.00000 | 0.998860 | 0.997670 | 0.996290 | 0.994670 | | | | |
| 0.09994 | 0.999110 | 0.997923 | 0.996547 | 0.994927 | 73.651 | 73.728 | 73.800 | 73.879 |
| 0.20011 | 0.999347 | 0.998163 | 0.996789 | 0.995170 | 73.702 | 73.777 | 73.859 | 73.935 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 0.29996 | 0.999569 | 0.998387 | 0.997018 | 0.995398 | 73.755 | 73.832 | 73.907 | 73.991 |
| 0.39998 | 0.999779 | 0.998600 | 0.997235 | 0.995614 | 73.806 | 73.880 | 73.954 | 74.042 |
| 0.49994 | 0.999973 | 0.998800 | 0.997435 | 0.995815 | 73.863 | 73.929 | 74.010 | 74.098 |
| 0.03 $\text{mol.kg}^{-1}$ Sorbic acid + Water + PG | | | | | | | | |
| 0.00000 | 0.999540 | 0.998340 | 0.996970 | 0.995330 | | | | |
| 0.10004 | 0.999781 | 0.998583 | 0.997214 | 0.995578 | 73.699 | 73.776 | 73.849 | 73.926 |
| 0.19997 | 1.000008 | 0.998812 | 0.997444 | 0.995812 | 73.750 | 73.827 | 73.901 | 73.978 |
| 0.29996 | 1.000222 | 0.999028 | 0.997661 | 0.996032 | 73.800 | 73.876 | 73.952 | 74.032 |
| 0.40012 | 1.000423 | 0.999232 | 0.997866 | 0.996239 | 73.851 | 73.926 | 74.002 | 74.086 |
| 0.50013 | 1.000611 | 0.999422 | 0.998060 | 0.996435 | 73.902 | 73.975 | 74.048 | 74.136 |
| 0.05 $\text{mol.kg}^{-1}$ Sorbic acid + Water + PG | | | | | | | | |
| 0.00000 | 1.000290 | 0.999110 | 0.997780 | 0.996120 | | | | |
| 0.09991 | 1.000520 | 0.999341 | 0.998014 | 0.996359 | 73.750 | 73.820 | 73.889 | 73.958 |
| 0.20112 | 1.000739 | 0.999562 | 0.998237 | 0.996589 | 73.804 | 73.871 | 73.943 | 74.001 |
| 0.29999 | 1.000941 | 0.999766 | 0.998443 | 0.996799 | 73.851 | 73.920 | 73.990 | 74.055 |
| 0.39995 | 1.001132 | 0.999958 | 0.998640 | 0.996999 | 73.902 | 73.971 | 74.036 | 74.107 |
| 0.50010 | 1.001311 | 1.000138 | 0.998825 | 0.997188 | 73.952 | 74.022 | 74.083 | 74.155 |
| 0.00 $\text{mol.kg}^{-1}$ Sorbic acid +Water + HG | | | | | | | | |
| 0.00000 | 0.998250 | 0.997080 | 0.995675 | 0.994050 | | | | |
| 0.09993 | 0.998445 | 0.997285 | 0.995918 | 0.994298 | 116.401 | 116.430 | 116.460 | 116.492 |
| 0.19989 | 0.998629 | 0.997479 | 0.996124 | 0.994525 | 116.430 | 116.462 | 116.491 | 116.521 |
| 0.29993 | 0.998804 | 0.997663 | 0.996321 | 0.994741 | 116.461 | 116.492 | 116.521 | 116.550 |
| 0.39895 | 0.998969 | 0.997836 | 0.996505 | 0.994943 | 116.486 | 116.521 | 116.551 | 116.582 |
| 0.49938 | 0.999129 | 0.998006 | 0.996683 | 0.995138 | 116.509 | 116.544 | 116.581 | 116.612 |
| 0.01 $\text{mol.kg}^{-1}$ Sorbic acid + Water + HG | | | | | | | | |
| 0.00000 | 0.998860 | 0.997670 | 0.996290 | 0.994670 | | | | |
| 0.09895 | 0.999046 | 0.997866 | 0.996499 | 0.994899 | 116.423 | 116.452 | 116.484 | 116.512 |
| 0.19989 | 0.999222 | 0.998052 | 0.996697 | 0.995116 | 116.450 | 116.482 | 116.512 | 116.543 |
| 0.30018 | 0.999387 | 0.998228 | 0.996885 | 0.995322 | 116.483 | 116.511 | 116.543 | 116.573 |
| 0.39998 | 0.999544 | 0.998394 | 0.997063 | 0.995518 | 116.511 | 116.542 | 116.573 | 116.603 |
| 0.49899 | 0.999691 | 0.998552 | 0.997231 | 0.995703 | 116.542 | 116.572 | 116.604 | 116.634 |
| 0.03 $\text{mol.kg}^{-1}$ Sorbic acid + Water + HG | | | | | | | | |
| 0.00000 | 0.999790 | 0.998490 | 0.997120 | 0.995480 | | | | |
| 0.10011 | 0.999963 | 0.998674 | 0.997316 | 0.995693 | 116.451 | 116.480 | 116.510 | 116.540 |
| 0.19997 | 1.000125 | 0.998848 | 0.997500 | 0.995894 | 116.482 | 116.510 | 116.540 | 116.570 |
| 0.29995 | 1.000278 | 0.999012 | 0.997676 | 0.996085 | 116.511 | 116.543 | 116.569 | 116.602 |
| 0.39983 | 1.000419 | 0.999165 | 0.997839 | 0.996262 | 116.548 | 116.577 | 116.606 | 116.641 |
| 0.49991 | 1.000552 | 0.999311 | 0.997995 | 0.996433 | 116.581 | 116.606 | 116.635 | 116.671 |
| 0.05 $\text{mol.kg}^{-1}$ Sorbic acid + Water + HG | | | | | | | | |
| 0.00000 | 1.000750 | 0.999420 | 0.997950 | 0.996380 | | | | |
| 0.09994 | 1.000909 | 0.999591 | 0.998134 | 0.996579 | 116.474 | 116.506 | 116.539 | 116.572 |
| 0.20014 | 1.001059 | 0.999752 | 0.998309 | 0.996768 | 116.505 | 116.539 | 116.572 | 116.601 |
| 0.29996 | 1.001197 | 0.999902 | 0.998472 | 0.996944 | 116.541 | 116.574 | 116.606 | 116.640 |
| 0.39992 | 1.001328 | 1.000044 | 0.998626 | 0.997112 | 116.571 | 116.604 | 116.636 | 116.670 |
| 0.49999 | 1.001449 | 1.000178 | 0.998771 | 0.997271 | 116.604 | 116.632 | 116.668 | 116.700 |

[a] $m_A$ is the molality of (PG/HG) in the aqueous solution sorbic acid. Standard uncertainties u are $u(T) = 0.01\text{K}, u(m) = 1\%, u(\rho) = 0.5(\text{ kg.m}^{-3}), u\ (V_{\emptyset}\ ) = \pm\ (0.05 - 0.07)\ \times\ 10^{-6}(\text{m}^3.\text{mol}^{-1})$

**Table 3** Under varying temperatures and experimental pressure = 0.1 MPa, partial molar volumes, $(V_{\emptyset}^{\circ})$ and experimental slopes, $(S_V^*)$ of glycols (PG and HG) in aqueous Sorbic acid solutions, are investigated.

| $^a m_B (\mathrm{mol.kg^{-1}})$ | $V_\emptyset^\circ \times 10^6/(m^3\ mole^{-1})$ | | | | $S_v^* \times 10^6/\ (m^3\ Kg\ mole^{-2})$ | | | |
|---|---|---|---|---|---|---|---|---|
| | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K |
| Propylene glycol (PG) | | | | | | | | |
| 0.00 | 73.56<br>(±0.004) | 73.64<br>(±0.003) | 73.70<br>(±0.003) | 73.77<br>(±0.004) | 0.49<br>(±0.013) | 0.44<br>(±0.009) | 0.42<br>(±0.010) | 0.44<br>(±0.012) |
| 0.01 | 73.60<br>(±0.002) | 73.68<br>(±0.002) | 73.75<br>(±0.002) | 73.83<br>(±0.006) | 0.53<br>(±0.006) | 0.53<br>(±0.006) | 0.51<br>(±0.007) | 0.54<br>(±0.004) |
| 0.03 | 73.65<br>(±0.000) | 73.73<br>(±0.000) | 73.80<br>(±0.002) | 73.87<br>(±0.001) | 0.51<br>(±0.001) | 0.50<br>(±0.001) | 0.50<br>(±0.007) | 0.53<br>(±0.004) |
| 0.05 | 73.70<br>(±0.001) | 73.77<br>(±0.001) | 73.84<br>(±0.003) | 73.91<br>(±0.004) | 0.50<br>(±0.002) | 0.50<br>(±0.002) | 0.48<br>(±0.008) | 0.50<br>(±0.010) |
| Hexylene glycol (HG) | | | | | | | | |
| 0.00 | 116.38<br>(±0.003) | 116.40<br>(±0.003) | 116.43<br>(±0.000) | 116.46<br>(±0.001) | 0.29<br>(±0.009) | 0.30<br>(±0.010) | 0.30<br>(±0.001) | 0.27<br>(±0.004) |
| 0.01 | 116.39<br>(±0.001) | 116.42<br>(±0.001) | 116.45<br>(±0.001) | 116.48<br>(±0.000) | 0.30<br>(±0.004) | 0.30<br>(±0.001) | 0.30<br>(±0.003) | 0.30<br>(±0.001) |
| 0.03 | 116.42<br>(±0.002) | 116.45<br>(±0.001) | 116.48<br>(±0.002) | 116.50<br>(±0.003) | 0.33<br>(±0.007) | 0.32<br>(±0.005) | 0.32<br>(±0.007) | 0.33<br>(±0.009) |
| 0.05 | 116.44<br>(±0.002) | 116.48<br>(±0.002) | 116.51<br>(±0.001) | 116.54<br>(±0.003) | 0.33<br>(±0.005) | 0.32<br>(±0.007) | 0.32<br>(±0.004) | 0.33<br>(±0.010) |

$^a m_B$ is the molality of aqueous sorbic acid solution. Standard uncertainties u are $\mathrm{u(T) = 0.01K, u(m)1\%, u(\rho) = 0.5(\ kg.m^{-3}), u\ (\ V_\emptyset\ ) = \pm\ 0.01\ \times\ 10^6(m^3\ .\ mol^{-1})\ , u(S_v^*) =\ \pm\ 0.03\ \times\ 10^6(m^3.kg.\ mol^{-2})}$

**Table 4** Under different temperature conditions and experimental pressure = 0.1 MPa, the partial molar volumes of transfer (($\Delta V_\emptyset^\circ$) for glycols (PG and HG) in aqueous Sorbic acid solutions are obtained.

| $^a m_B$ $(\mathrm{mol.kg^{-1}})$ | $\Delta V_\emptyset^\circ \times 10^6/(m^3\ mole^{-1})$ | | | | $\Delta V_\emptyset^\circ \times 10^6/(m^3\ mole^{-1})$ | | | |
|---|---|---|---|---|---|---|---|---|
| | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=293.15 K |
| | Propylene glycol (PG) | | | | Hexylene glycol (HG) | | | |
| 0.01 | 0.036 | 0.040 | 0.048 | 0.060 | 0.016 | 0.019 | 0.023 | 0.022 |
| 0.03 | 0.088 | 0.091 | 0.098 | 0.108 | 0.041 | 0.040 | 0.047 | 0.044 |
| 0.05 | 0.140 | 0.133 | 0.140 | 0.140 | 0.066 | 0.072 | 0.078 | 0.078 |

$^a m_B$ is the molality of aqueous sorbic acid solution. Standard uncertainties u are $\mathrm{u(T) = 0.01K, u(m)1\%, u(\rho) = 0.5(\ kg.m^{-3})}$.

**Table 5** The empirical parameters values in Equation (4) for glycols (PG and HG) in aqueous Sorbic acid solutions, under varying temperature conditions and experimental pressure = 0.1 MPa.

| $^a m_B$ $(\ \mathrm{mol.kg^{-1}})$ | $a \times 10^6$ $/(\ m^3\ mole^{-1})$ | $b \times 10^6$ $/(\ m^3\ mole^{-1})$ | $c \times 10^6$ $/(\ m^3\ mole^{-1})$ | $R^2$ | $ARD$ |
|---|---|---|---|---|---|
| Propylene glycol (PG) | | | | | |
| 0.01 | 73.677 | 0.016 | 0.000 | 0.999 | 0.00057 |
| 0.03 | 73.727 | 0.015 | 0.000 | 0.999 | 0.00030 |
| 0.05 | 73.773 | 0.014 | 0.000 | 0.999 | 0.00010 |
| Hexylene glycol (HG) | | | | | |
| 0.01 | 116.422 | 0.006 | 0.000 | 0.999 | 0.00031 |
| 0.03 | 116.448 | 0.006 | 0.000 | 0.999 | 0.00020 |
| 0.05 | 116.475 | 0.007 | 0.000 | 0.999 | 0.00018 |

[a]$m_B$ is the molality of aqueous sorbic acid solution. Standard uncertainties u are $u(T) = 0.01K, u(m)1\%, u(\rho) = 0.5(kg.m^{-3}), u(c) = 1.0(m.s^{-1})$.

**Table 6** Partial molar expansibilities, $(E^\circ_\emptyset)$ for glycols (PG and HG) in aqueous Sorbic acid solution, under varying temperature conditions and experimental pressure = 0.1 MPa.

| | $E^\circ_\emptyset \times 10^6/(m^3\ mole^{-1}.K^{-1})$ | | | | $(\partial E^\circ_\emptyset/\partial T)_P \times 10^6/(m^3.mol^{-1}.K^{-2})$ |
|---|---|---|---|---|---|
| [a]$m_B$ $(mol.kg^{-1})$ | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | |
| Propylene glycol (PG) | | | | | |
| 0.01 | 0.0162 | 0.0155 | 0.0149 | 0.0143 | -0.00012 |
| 0.03 | 0.0159 | 0.0153 | 0.0147 | 0.0141 | -0.00012 |
| 0.05 | 0.0149 | 0.0141 | 0.0133 | 0.0125 | -0.00014 |
| Hexylene glycol (HG) | | | | | |
| 0.01 | 0.0061 | 0.0061 | 0.0060 | 0.0059 | -0.00001 |
| 0.03 | 0.0066 | 0.0600 | 0.0054 | 0.0048 | -0.00006 |
| 0.05 | 0.0070 | 0.0066 | 0.0062 | 0.0058 | -0.00004 |

[a]$m_B$ is the molality of aqueous sorbic acid solution. Standard uncertainties u are $u(T) = 0.01K, u(m)1\%$, $u(\rho) = 0.5(kg.m^{-3}), u(c) = 1.0(m.s^{-1})$.

**Table 7** For glycols (PG and HG) in aqueous Sorbic acid solutions under different temperature settings and experimental pressure = 0.1 MPa, the values of the speed of sound, denoted as (c), and the apparent molar isentropic compression, represented as $(K_{\emptyset,S})$ are calculated.

| [a]$m_A$ $(mol.kg^{-1})$ | $c/(m.\ s^{-1})$ | | | | $K_{\emptyset,S} \times 10^6/m^3\ mole^{-1}.GPa^{-1}$ | | | |
|---|---|---|---|---|---|---|---|---|
| | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=293.15 K |
| 0.00 $mol.kg^{-1}$ | Sorbic acid +PG + Water | | | | | | | |
| 0.00000 | 1481.3 | 1495.5 | 1509.0 | 1519.2 | | | | |
| 0.09957 | 1486.2 | 1500.3 | 1513.5 | 1523.6 | -45.129 | -44.276 | -43.486 | -42.903 |
| 0.19901 | 1490.5 | 1504.4 | 1516.6 | 1526.5 | -45.370 | -44.512 | -43.719 | -43.133 |
| 0.30106 | 1493.9 | 1507.8 | 1520.1 | 1529.5 | -45.458 | -44.599 | -43.805 | -43.219 |
| 0.39926 | 1496.9 | 1510.6 | 1523.0 | 1532.7 | -45.505 | -44.646 | -43.851 | -43.265 |
| 0.50059 | 1499.5 | 1513.5 | 1525.2 | 1534.4 | -45.538 | -44.678 | -43.883 | -43.297 |
| 0.01 $mol.kg^{-1}$ | Sorbic acid + Water + PG | | | | | | | |
| 0.00000 | 1482.8 | 1497.0 | 1510.9 | 1520.7 | | | | |
| 0.09994 | 1487.7 | 1501.8 | 1515.0 | 1525.1 | -45.040 | -44.189 | -43.378 | -42.819 |
| 0.20011 | 1492.0 | 1506.2 | 1518.1 | 1528.0 | -45.279 | -44.424 | -43.610 | -43.048 |
| 0.29996 | 1495.8 | 1509.3 | 1521.5 | 1531.0 | -45.365 | -44.508 | -43.693 | -43.131 |
| 0.39998 | 1498.9 | 1512.1 | 1524.5 | 1534.2 | -45.412 | -44.555 | -43.739 | -43.177 |
| 0.49994 | 1501.7 | 1515.0 | 1526.7 | 1536.2 | -45.443 | -44.586 | -43.770 | -43.207 |
| 0.03 $mol.kg^{-1}$ | Sorbic acid + Water + PG | | | | | | | |
| 0 | 1484.6 | 1498.8 | 1512.7 | 1522.5 | | | | |
| 0.00000 | 1489.5 | 1503.6 | 1516.8 | 1526.9 | -44.932 | -44.083 | -43.275 | -42.719 |
| 0.10004 | 1493.8 | 1507.9 | 1519.9 | 1529.8 | -45.168 | -44.316 | -43.504 | -42.946 |
| 0.19997 | 1497.6 | 1511.1 | 1523.3 | 1532.8 | -45.254 | -44.400 | -43.587 | -43.028 |
| 0.29996 | 1500.7 | 1514.3 | 1526.3 | 1536.0 | -45.301 | -44.446 | -43.633 | -43.073 |
| 0.40012 | 1503.8 | 1517.4 | 1528.9 | 1538.5 | -45.332 | -44.477 | -43.663 | -43.103 |
| 0.05 $mol.kg^{-1}$ | Sorbic acid + Water + PG | | | | | | | |
| 0.00000 | 1486.7 | 1501.0 | 1514.8 | 1524.6 | | | | |
| 0.09991 | 1491.6 | 1505.7 | 1518.7 | 1528.7 | -44.804 | -43.953 | -43.155 | -42.601 |
| 0.20112 | 1495.9 | 1509.8 | 1522.0 | 1531.9 | -45.042 | -44.187 | -43.385 | -42.829 |
| 0.29999 | 1499.7 | 1513.2 | 1525.4 | 1534.9 | -45.125 | -44.269 | -43.465 | -42.909 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| 0.39995 | 1502.8 | 1516.4 | 1528.4 | 1538.1 | -45.171 | -44.314 | -43.510 | -42.953 |
| 0.50010 | 1505.9 | 1519.5 | 1531.0 | 1540.6 | -45.201 | -44.344 | -43.540 | -42.983 |
| 0.00 $mol.kg^{-1}$ | Sorbic acid +HG + Water | | | | | | | |
| 0.00000 | 1482.1 | 1495.5 | 1508.6 | 1519.8 | | | | |
| 0.09993 | 1490.3 | 1504.7 | 1515.5 | 1525.6 | -45.081 | -44.277 | -43.511 | -42.870 |
| 0.19989 | 1500.8 | 1512.4 | 1523.7 | 1533.4 | -45.319 | -44.510 | -43.742 | -43.100 |
| 0.29993 | 1508.5 | 1520.8 | 1531.3 | 1539.7 | -45.403 | -44.594 | -43.824 | -43.182 |
| 0.39895 | 1517.4 | 1528.5 | 1537.6 | 1545.8 | -45.448 | -44.639 | -43.869 | -43.227 |
| 0.49938 | 1523.6 | 1535.7 | 1543.4 | 1551.5 | -45.478 | -44.669 | -43.899 | -43.257 |
| 0.01 $mol.kg^{-1}$ | Sorbic acid + Water + HG | | | | | | | |
| 0.00000 | 1484.1 | 1497.5 | 1510.6 | 1521.8 | | | | |
| 0.09895 | 1492.3 | 1506.7 | 1517.5 | 1527.6 | -44.956 | -44.155 | -43.390 | -42.753 |
| 0.19989 | 1502.8 | 1514.4 | 1525.7 | 1535.4 | -45.196 | -44.391 | -43.624 | -42.985 |
| 0.30018 | 1510.5 | 1522.8 | 1533.3 | 1541.7 | -45.280 | -44.474 | -43.706 | -43.067 |
| 0.39998 | 1519.4 | 1530.5 | 1539.6 | 1547.8 | -45.325 | -44.518 | -43.751 | -43.112 |
| 0.49899 | 1525.6 | 1537.7 | 1545.4 | 1553.5 | -45.353 | -44.547 | -43.780 | -43.141 |
| 0.03 $mol.kg^{-1}$ | Sorbic acid + Water + HG | | | | | | | |
| 0.00000 | 1486.3 | 1499.7 | 1512.8 | 1524.0 | | | | |
| 0.10011 | 1494.5 | 1508.9 | 1519.7 | 1529.8 | -44.828 | -44.031 | -43.270 | -42.634 |
| 0.19997 | 1505.0 | 1516.6 | 1527.9 | 1537.6 | -45.062 | -44.260 | -43.497 | -42.860 |
| 0.29995 | 1512.7 | 1525.0 | 1535.5 | 1543.9 | -45.144 | -44.342 | -43.578 | -42.941 |
| 0.39983 | 1521.6 | 1532.7 | 1541.8 | 1550.0 | -45.188 | -44.386 | -43.622 | -42.985 |
| 0.49991 | 1527.8 | 1539.9 | 1547.6 | 1555.7 | -45.216 | -44.414 | -43.650 | -43.014 |
| 0.05 $mol.kg^{-1}$ | Sorbic acid + Water + HG | | | | | | | |
| 0.00000 | 1488.6 | 1502.0 | 1515.1 | 1526.3 | | | | |
| 0.09994 | 1496.8 | 1511.2 | 1522.0 | 1532.5 | -44.689 | -43.895 | -43.137 | -42.506 |
| 0.20014 | 1507.3 | 1518.9 | 1530.2 | 1540.0 | -44.922 | -44.124 | -43.364 | -42.731 |
| 0.29996 | 1515.5 | 1527.3 | 1537.8 | 1547.2 | -45.003 | -44.205 | -43.444 | -42.810 |
| 0.39992 | 1524.5 | 1535.5 | 1545.1 | 1553.3 | -45.047 | -44.248 | -43.487 | -42.853 |
| 0.49999 | 1530.5 | 1542.2 | 1550.9 | 1560.0 | -45.074 | -44.276 | -43.515 | -42.882 |

[a] $m_A$ is the molality of (PG/HG) in the aqueous solution sorbic acid. Standard uncertainties u are $u(T) = 0.01K, u(m)1\%,\ u(\rho) = 0.5(\,kg.m^{-3}), u(c) = 1.0(m.s^{-1}), u(K_{\emptyset,S}) = \pm 0.25\ \times 10^6(m^3\ mole^{-1}.GPa^{-1})$

**Table 8** The partial molar isentropic compression ($\overset{\circ}{K}_{\emptyset,S}$) for glycols (PG and HG) in aqueous Sorbic acid solutions under varying temperature conditions and experimental pressure = 0.1 MPa.

| [a]$m_B$ ($mol.kg^{-1}$) | $K^{\circ}_{\emptyset,S} \times 10^6/\ (m^3\ mole^{-1}.GPa^{-1})$ | | | | $S_K^* \times 10^6/\ (m^3\ Kg\ mole^{-2}GPa^{-1})$ | | | |
|---|---|---|---|---|---|---|---|---|
| | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K |
| Propylene glycol (PG) | | | | | | | | |
| 0.00 | -45.12<br>(±0.08) | -44.26<br>(±0.08) | -43.47<br>(±0.08) | -42.89<br>(±0.08) | -0.95<br>(±0.24) | -0.94<br>(±0.23) | -0.93<br>(±0.23) | -0.92<br>(±0.23) |
| 0.01 | -45.03<br>(±0.08) | -44.17<br>(±0.08) | -43.36<br>(±0.08) | -42.81<br>(±0.07) | -0.93<br>(±0.23) | -0.92<br>(±0.23) | -0.90<br>(±0.23) | -0.90<br>(±0.22) |
| 0.03 | -44.92<br>(±0.08) | -44.07<br>(±0.08) | -43.26<br>(±0.08) | -42.70<br>(±0.07) | -0.93<br>(±0.23) | -0.91<br>(±0.23) | -0.90<br>(±0.23) | -0.89<br>(±0.22) |
| 0.05 | -44.79<br>(±0.08) | -43.94<br>(±0.08) | -43.14<br>(±0.08) | -42.59<br>(±0.07) | -0.95<br>(±0.24) | -0.94<br>(±0.23) | -0.93<br>(±0.23) | -0.92<br>(±0.23) |
| Hexylene glycol (HG) | | | | | | | | |
| 0.00 | -45.07<br>(±0.08) | -44.26<br>(±0.08) | -43.50<br>(±0.08) | -42.86<br>(±0.08) | -0.92<br>(±0.24) | -0.91<br>(±0.23) | -0.91<br>(±0.23) | -0.90<br>(±0.23) |
| 0.01 | -44.94<br>(±0.08) | -44.14<br>(±0.08) | -43.38<br>(±0.08) | -42.74<br>(±0.07) | -0.93<br>(±0.24) | -0.91<br>(±0.23) | -0.91<br>(±0.23) | -0.91<br>(±0.23) |
| 0.03 | -44.82 | -44.02 | -43.26 | -42.62 | -0.90 | -0.89 | -0.89 | -0.88 |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| | (±0.08) | (±0.08) | (±0.08) | (±0.07) | (±0.23) | (±0.23) | (±0.23) | (±0.22) |
| 0.05 | -44.68<br>(±0.08) | -43.88<br>(±0.08) | -43.13<br>(±0.08) | -42.49<br>(±0.08) | -0.89<br>(±0.23) | -0.88<br>(±0.23) | -0.88<br>(±0.23) | -0.88<br>(±0.22) |

$^{a}m_B$ is the molality of aqueous sorbic acid solution Standard uncertainties u are $u(T) = 0.01K, u(m)1\%$, $u(\rho) = 0.5(\text{ kg.m}^{-3}), u(c) = 1.0(\text{m.s}^{-1}), u(K^{\circ}_{\emptyset,S}) = \pm 0.01 \times 10^{6}(\text{m}^{3}\text{ mole}^{-1}.\text{GPa}^{-1})$, u $(S^{*}_{K}) \times 10^{6}$ $(\text{m}^{3}\text{ Kg mole}^{-2}\text{GPa}^{-1})$

**Table 9** Partial molar isentropic compression transfer, $\Delta K^{\circ}_{\emptyset,S}$ , for glycols (PG and HG) in aqueous Sorbic acid solutions, under varying temperature conditions and experimental pressure = 0.1 MPa.

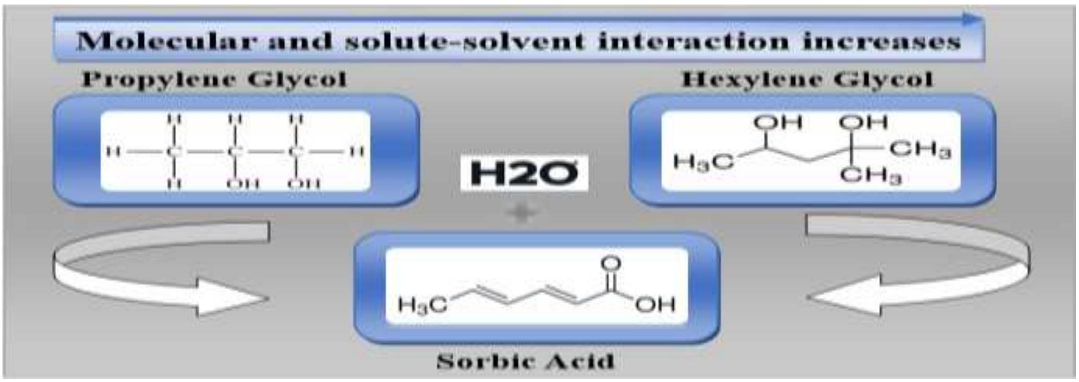
| $^{a}m_B$ $(\text{mol.kg}^{-1})$ | $\Delta K^{\circ}_{\emptyset,S} \times 10^{6}/\ m^{3}\ mole^{-1}.GPa^{-1}s$ | | | | $\Delta K^{\circ}_{\emptyset,S} \times 10^{6}/\ m^{3}\ mole^{-1}.GPa^{-1}$ | | | |
|---|---|---|---|---|---|---|---|---|
| | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K | T=293.15 K | T=298.15 K | T=303.15 K | T=308.15 K |
| | Propylene glycol (PG) | | | | Hexylene glycol (HG) | | | |
| 0.01 | 0.089 | 0.087 | 0.107 | 0.083 | 0.124 | 0.121 | 0.119 | 0.116 |
| 0.03 | 0.198 | 0.192 | -0.469 | 0.183 | 0.252 | 0.246 | 0.400 | 0.234 |
| 0.05 | 0.324 | 0.321 | 0.330 | 0.301 | 0.390 | 0.380 | 0.372 | 0.362 |

$^{a}m_B$ is the molality of aqueous sorbic acid solution. Standard uncertainties u are $u(T) = 0.01K, u(m)1\%$, $u(\rho) = 0.5(\text{ kg.m}^{-3})$

**Table 10** Pair ($V_{AB}$, $K_{AB}$) and triplet ($V_{ABB}$, $K_{ABB}$), for glycols (PG and HG) in aqueous Sorbic acid solutions, under varying temperature conditions and experimental pressure = 0.1 MPa.

| T/K | $V_{AB} \times 10^{6}$ $/\text{m}^{3}\text{mole}^{-2}.\text{Kg}$ | $V_{ABB} \times 10^{6}$ $/\text{m}^{3}\text{mole}^{-1}.\text{Kg}^{2}$ | $K_{AB} \times 10^{6}$ $/\text{m}^{3}\text{mole}^{-2}.\text{Kg}.\text{GPa}^{-1}$ | $K_{ABB} \times 10^{6}$ $/\text{m}^{3}\text{mole}^{-1}.\text{Kg}^{2}.\text{ GPa}^{-1}$ |
|---|---|---|---|---|
| Propylene glycol (PG) | | | | |
| 293.15 | 1.609 | -2.745 | 3.962 | -10.529 |
| 298.15 | 1.924 | -8.433 | 3.683 | -6.936 |
| 303.15 | 2.302 | -12.266 | -14.388 | 227.046 |
| 308.15 | 2.787 | -18.762 | 3.456 | -6.477 |
| Hexylene glycol (HG) | | | | |
| 293.15 | 0.670 | -0.848 | 6.689 | -55.131 |
| 298.15 | 0.769 | -1.048 | 7.496 | -79.714 |
| 303.15 | 0.939 | -1.896 | 11.582 | -133.254 |
| 308.15 | 0.880 | -2.490 | 6.126 | -50.119 |

T/K is the temperatures.



**Scheme 1.** Propylene, hexylene glycol and sorbic acid interaction

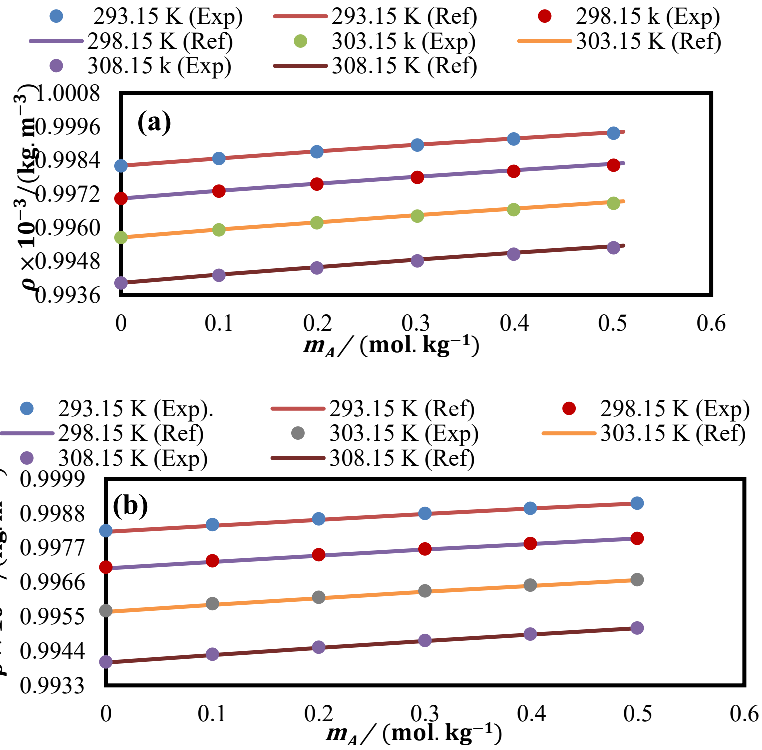
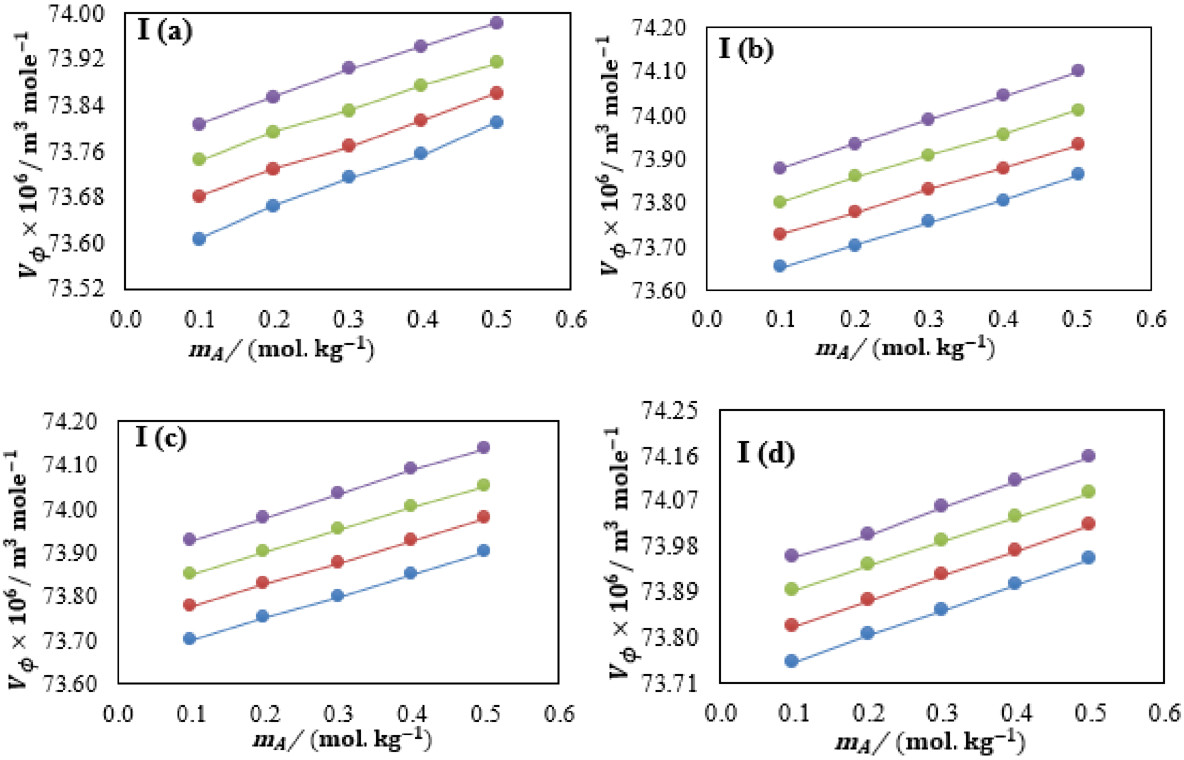


**Fig. 1.** Variations in the experimental densities with the comparison of literature value of (a) (Water + PG) and (b) (Water + HG) based on the molality ($m_A$) of glycols at different temperatures (T) [ 293.15 K, 298.15 K, 303.15 K, and 308.15 K] dots indicate the experimental value, and straight line indicates the reference value [29,30]



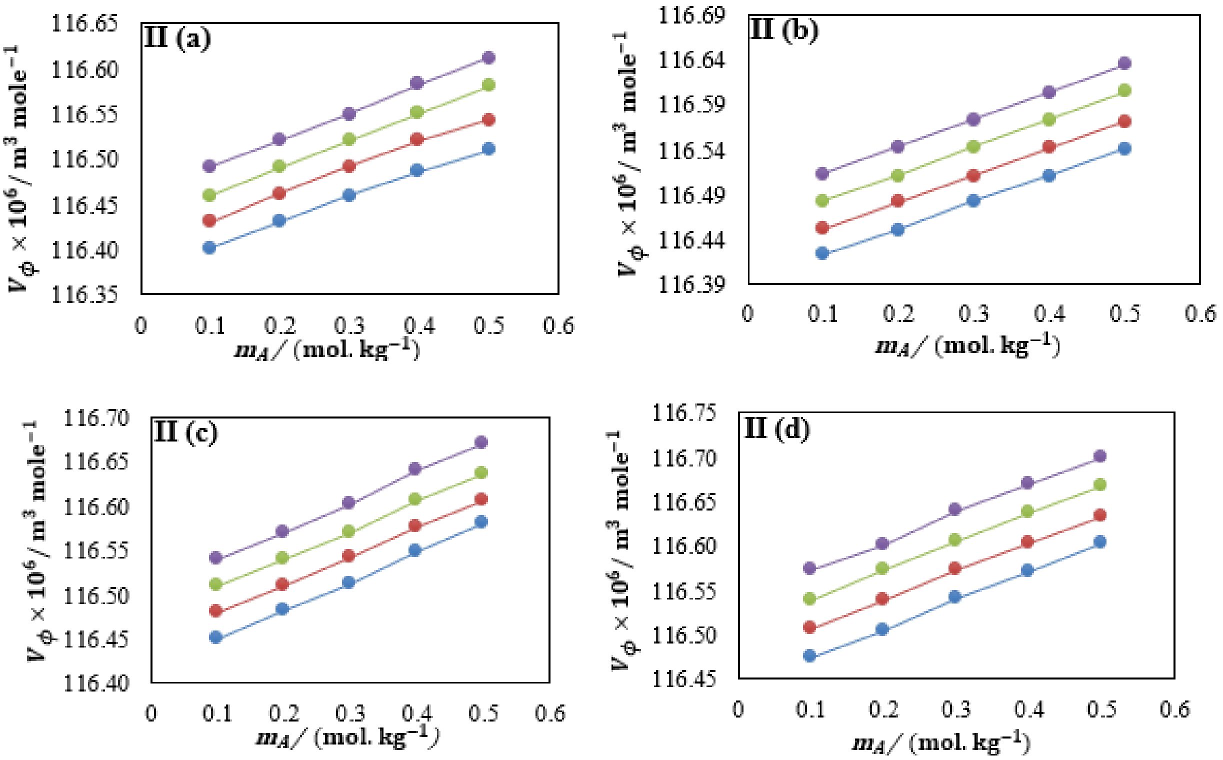


**Fig. 2.** Variation of apparent molar volume, $V_\phi$ of PG (I), and HG (II) (a) 0.0000 sorbic acid, (b) 0.01 sorbic acid, (c) 0.03 sorbic acid, (d) 0.05 sorbic acid, against molality at different temperatures [blue, 293.15 K; red, 298.15 K; green, 303.15 K; violet, 308.15 K]

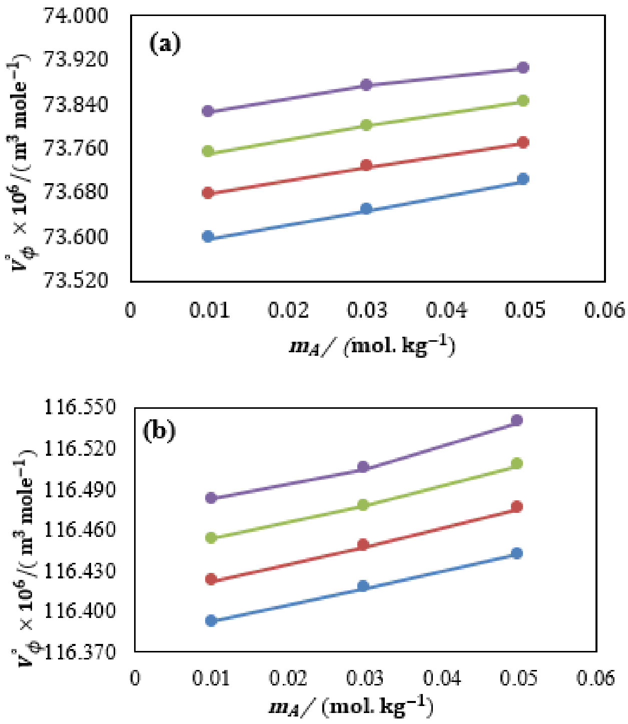


**Fig. 3.** Variation in partial molar volumes, denoted as $V_\phi^\circ$ for two different glycols compounds, specifically (a) PG and (b) HG in aqueous solutions containing sorbic acid at various concentrations and temperatures. The temperatures considered for this analysis were [blue, 293.15 K; red, 298.15 K; green, 303.15 K; violet, 308.15 K]

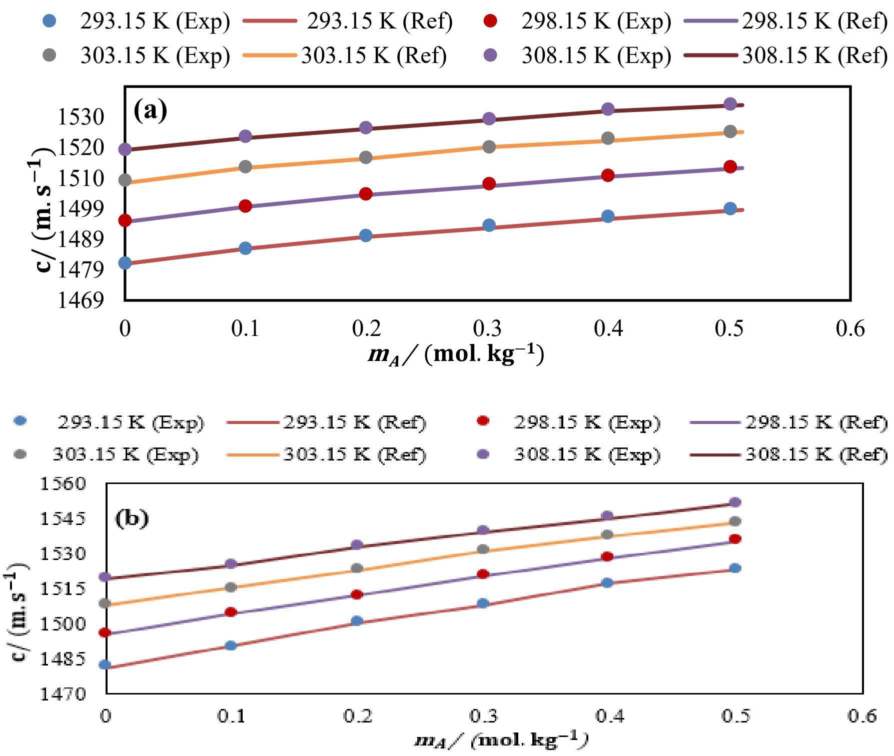
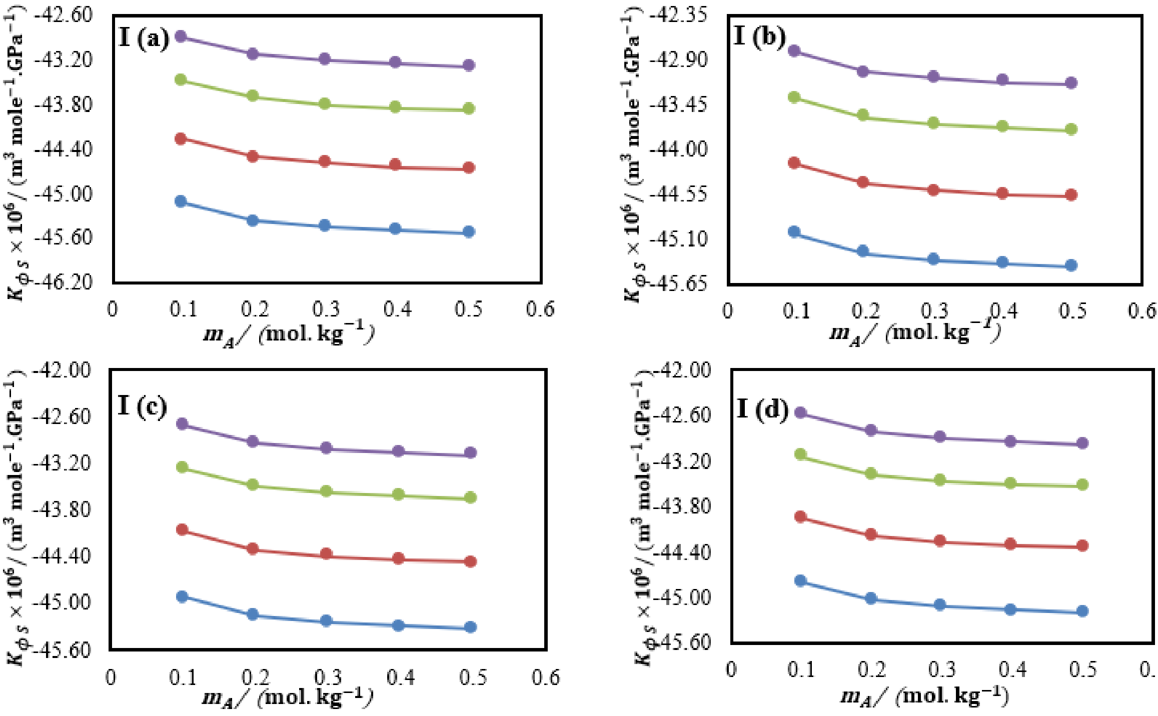


**Fig. 4.** Variations in the experimental sound velocities with the comparison of literature value of (a) (Water + PG) and (b) (Water + HG) based on the molality ($m_A$) of glycols at different temperatures (T) [ 293.15 K, 298.15 K, 303.15 K, and 308.15 K] dots indicate the experimental value, and straight line indicates the reference value [29, 30]



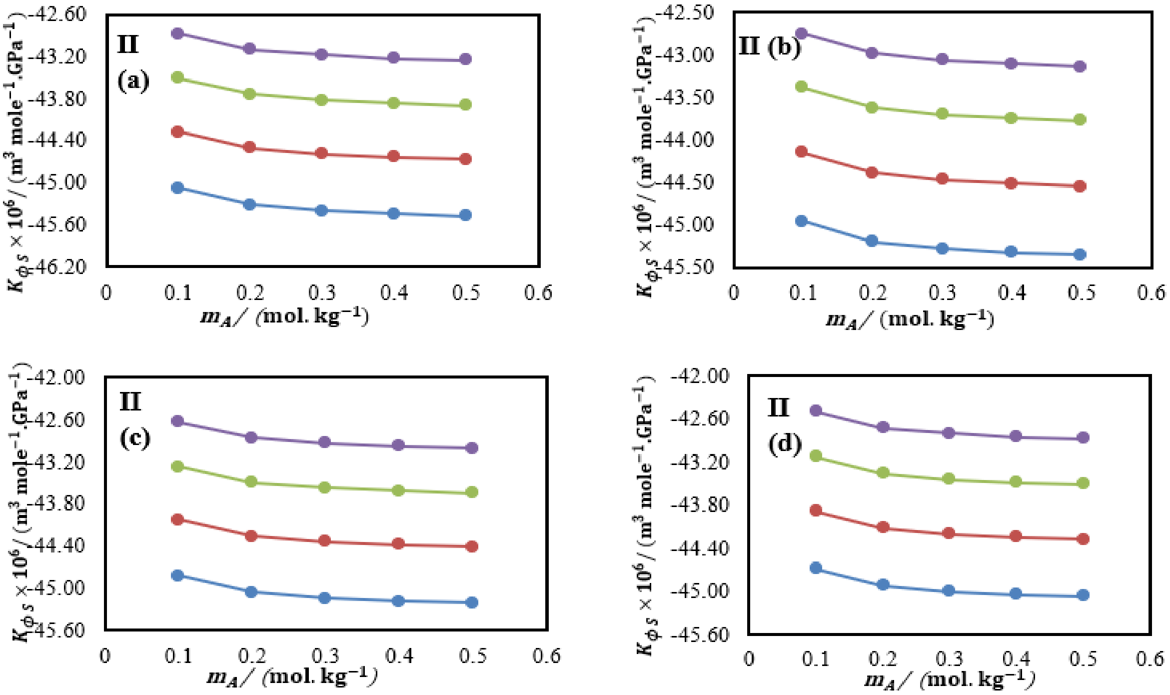


**Fig. 5**. Variation of apparent molar isentropic compression ($K_{\phi,S}$) of PG (I), and HG (II) (a) 0.0000 sorbic acid, (b) 0.01 sorbic acid, (c) 0.03 sorbic acid, (d) 0.05 sorbic acid, against molality at different temperatures [blue, 293.15 K; red, 298.15 K; green, 303.15 K; violet, 308.15 K]

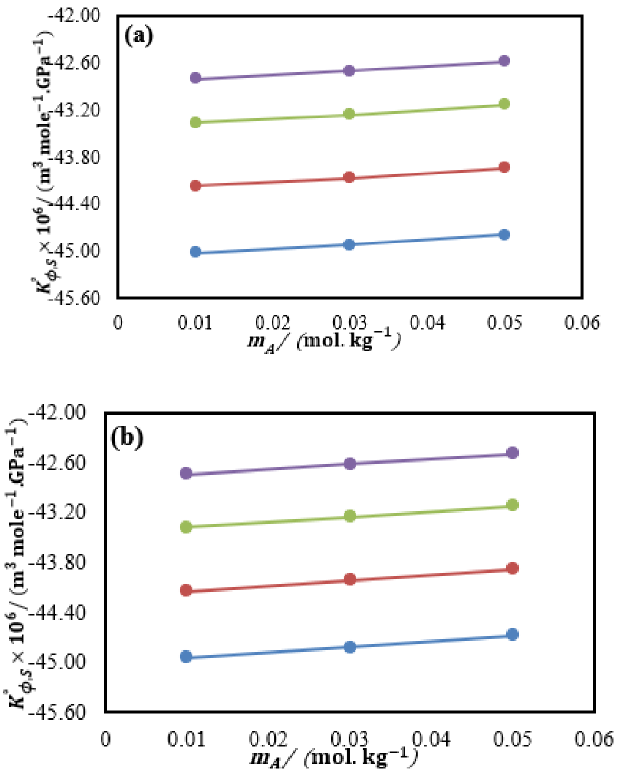


**Fig. 6.** Variation in partial molar isentropic compression, denoted as ($K^{\circ}_{\phi,S}$) two different glycols compounds, specifically (a) PG and (b) HG in aqueous solutions containing sorbic acid at various concentrations and temperatures. The temperatures considered for this analysis were [blue, 293.15 K; red, 298.15 K; green, 303.15 K; violet, 308.15 K]