ACOUSTIC AND THERMODYNAMIC PARAMETER INVESTIGATIONS IN THE MIXTURE CONTAINING VITAMIN B WITH GLYCOLS USING ULTRASONIC TECHNIQUE

Thesis
Submitted in partial fulfillment of the requirements for the
award of the degree of

DOCTOR OF PHILOSOPHY

in

(Physics)

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PUNJAB

2021

DECLARATION

I hereby declare that thesis entitled, "**ACOUSTIC AND THERMODYNAMIC PARAMETER INVESTIGATIONS IN THE MIXTURE CONTAINING VITAMIN B WITH GLYCOLS USING ULTRASONIC TECHNIQUE**" has been submitted by me for the degree of Doctor of Philosophy in Physics to the Lovely Professional University Phagwara is the result of my original and independent work under the guidance of Dr. Kailash Chandra Juglan. This work has not previously formed the basis for the award of any degree, fellowship, in this or any other University or Institute.

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CERTIFICATE

This is to certify that Nabaparna Chakraborty has completed Ph.D. Thesis titled "**Acoustic and thermodynamic parameter investigations in the mixture containing vitamin B with glycols using ultrasonic technique**" under my Guidance and supervision. To the best of my knowledge, the present work is the result of her original investigation and study. No part of the project has ever been submitted for any other Degree or Diploma at any University.The Project is fit for the submission and the partial fulfillment of the conditions for the award of Doctor of Philosophy in Physics.

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ABSTRACT

The ultrasonic technique has been employed in various fields of science for research which provided a riveting approach to explore the acoustic and thermodynamic parameters for different binary and ternary liquid systems. These parameters reveal the various molecular interactions between the different components of the mixtures and administer valuable details regarding the microscopic packing and structure of the constituent molecules in the liquid medium. The ultrasonic wave propagating in the medium predicts the physicochemical behavior of the components of the molecules in the medium. Ultrasonic technique is found to be a very reliable and precise method of investigating the acoustic and volumetric properties of various liquid mixtures such as organic solvents, polymers, electrolyte solutions etc. Due to their non-destructive nature, this method is rapidly used for characterizing fluids by exposing the binding forces among the atoms and molecules in the liquid mixtures which are widely used for different chemical processes in various industries such as pharmaceutical, cosmetic, food, etc. The acoustic and volumetric properties are obtained for the combination of Vitamin B (niacin, Vitamin B_3; d-Panthenol, Vitamin B_5; biotin, Vitamin B_7) with glycols at different temperatures using Anton Paar DSA 5000 M as the function composition range of solvent. In the section I, problem 1, at the temperature range of (293.15, 298.15, 303.15 and 308.15) K, the speed of sound and density values for ternary solution (Niacin+ water + Ethylene glycol (EG) /Diethylene glycol (DEG) / Triethylene glycol (TEG)) are measured at atmospheric pressure and (0.00, 0.02, 0.04 and 0.06) $\text{mol}\cdot\text{kg}^{-1}$ niacin concentrations. The acoustic and volumetric properties of the mixture are analyzed through the calculated parameters i.e Apparent Molar Volume (V_ϕ), Partial Molar Volume (V_ϕ^0) and Partial Molar Volume of transfer (ΔV_ϕ^0), which are determined from the experimental density values and Apparent Molar Isentropic compression ($K_{\phi,S}$), Partial Molar Isentropic compression ($K_{\phi,S}^0$) and Partial Molar Isentropic compression of transfer (ΔK_ϕ^0) are calculated using the speed of sound. The pair and triplet coefficients ($V_{AB}, V_{ABB}, K_{AB}, K_{ABB}$) are calculated, using which the significant details regarding the ternary mixture from these thermodynamical parameters are reviewed in terms of (solute-

solvent) and (solute-solute) interactions. The problem 2 includes the measurement of the densities and speed of sound for liquid mixtures containing vitamin B_3 (niacin) at (0.00, 0.01, 0.03, and 0.05) $mol \cdot kg^{-1}$ concentration in aqueous propylene glycol (PG) and hexylene glycol (HG) at the variation of temperatures from (293.15 to 308.15) K using Anton Paar DSA 5000 M. From the volumetric experimental data, Apparent molar volume (V_{ϕ}), Partial Molar Volume (V_{ϕ}^{0}) and Partial Molar Volume of transfer (ΔV_{ϕ}^{0}) are calculated along with the Apparent Molar Isentropic compression ($K_{\phi,S}$), Partial Molar Isentropic compression ($K_{\phi,S}^{0}$) and Partial Molar Isentropic compression of transfer (ΔK_{ϕ}^{0}) using experimental acoustic data. The positive volumetric data (i.e apparent molar volume and partial molar volume) indicates strong solute-solvent interactions inside the mixture. Along with these values, the empirical constants a, b, and c with the pair and triplet coefficients ($V_{AB}, V_{ABB}, K_{AB}, K_{ABB}$) are also calculated. Significant information regarding the molecular interactions in the ternary solution consisting of Vitamin B_3 (Niacin), water and polyethylene glycols (PEG 200/PEG 600) are attained from the calculated volumetric and acoustic parameters in problem 3. Initially, the density (ρ) and speed of sound (c) for polyethylene glycols (0.1 to 0.5) $mol \cdot kg^{-1}$ in aqueous niacin (0.01, 0.02, and 0.03) $mol \cdot kg^{-1}$ are measured under 0.1 *MPa* pressure as a function of temperature at (293.15-308.15) *K*. Utilizing the experimental density values, the apparent Molar Volume (V_{ϕ}), Partial Molar Volume (V_{ϕ}^{0}) and Partial Molar Volume of transfer (ΔV_{ϕ}^{0}) are calculated and the apparent Molar Isentropic compression ($K_{\phi,S}$), Partial Molar Isentropic compression ($K_{\phi,S}^{0}$) and Partial Molar Isentropic compression of transfer (ΔK_{ϕ}^{0}) are estimated using the speed of sound. The empirical constants *a*, *b*, and *c* along with the pair and triplet coefficients ($V_{AB}, V_{ABB}, K_{AB}, K_{ABB}$) are calculated. Further, in problem 4, at multiple temperatures (288.15-318.15) K the density and speed of sound values for PEGs of molecular weight 400 and 4000 in aqueous niacin solutions were measured in concentrations of (0.00, 0.07, 0.08, and 0.09) $mol \cdot kg^{-1}$. Utilizing these experimental data, the apparent molar properties and partial molar properties were determined to analyze the interactions in aqueous niacin solutions with polyethylene glycols (400/4000). The volumetric parameters such as apparent molar volume, V_ϕ; partial molar volume, V_ϕ^0 and partial molar volume of transfer, ΔV_ϕ^0 which are obtained using experimental density values, while the acoustic parameters i.e. apparent molar isentropic compression, $K_{\phi,S}$; partial molar isentropic compression, $K_{\phi,S}^0$ and partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^0$ are determined with the speed of sound data. These positive volumetric apparent and partial molar properties suggest the presence of strong solute-solvent interactions. The partial molar expansibilities(E_ϕ^0) along with its first derivative $\left(\partial \mathrm{E}_\Phi^0/\partial \mathrm{T}\right)_P$ were calculated. Further, the pair and triplet coefficients are obtained using partial molar isentropic compression of transfer and partial molar volume of the transfer. The problem 5 consists, the interaction of EG, DEG and TEG with biologically active D-Panthenol, as the function of temperature by the combination of acoustic and volumetric methods. Speeds of sound and densities of EG, DEG and TEG in (0.00, 0.05, 0.10 and 0.15) mol·kg^{-1} in aqueous solutions of d-Panthenol have been measured at T=(293.15, 298.15, 303.15 and 308.15) K. From the density data, the apparent molar volume and partial molar volume of transfer for these solutions have been determined. From the speed of sound data, the partial molar isentropic compression and the partial molar isentropic compression of transfer have been determined. The pair and triplet interaction coefficient have also been estimated. These experimental data is further used to calculate the other basic thermodynamic properties i.e. intermolecular free length, acoustic impedance, adiabatic compressibility, Wada's constant, Rao's Constant and Vander Waal's constant, for the ternary mixture of aqueous vitamin B_5 with glycols that is incorporated in problem 6, which gave the insight of the intermolecular reactions inside the mixture. The densities and speed of sound for the binary mixture (propylene glycol/hexylene glycol + water) and ternary mixture (propylene glycol/hexylene glycol + d-Panthenol + water) are obtained at atmospheric pressure and (0.04, 0.08, and 0.12) mol·kg^{-1} concentration of d-Panthenol over the variation of temperature which are explained in problem 7. The apparent molar volume, V_ϕ; partial molar volume, V_ϕ^0 and partial molar volume of transfer, ΔV_ϕ^0 are obtained using experimental density values.

These volumetric data suggests the nature of intermolecular interactions among solute and solvent molecules inside the liquid system. Further, using the speed of sound data apparent molar isentropic compression, $K_{\phi,S}$; partial molar isentropic compression, $K_{\phi,S}^{0}$ and partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^{0}$ are determined. The pair and triplet coefficients along with the partial molar expansibilities(E_{ϕ}^{0}) and its first derivative $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ were calculated using both the volumetric and acoustic data. From the compressibility data, the hydration number (n_h) for glycols in aqueous d-Panthenol solutions are estimated using Passynski's equation and the obtained results are described in terms of cooperative hydration effects and hydrophobic interactions. In problem 8, the interaction in binary solution of polyethylene glycol 200 (PEG 200) and polyethylene glycol 400 (PEG 400) with d-Panthenol at variation of temperatures has been surveyed by merging acoustic and volumetric process. The density and speed of sound of PEG 200 and PEG 400 in the concentrations of (0.00, 0.03, 0.06 and 0.09) mol.kg^{-1} in aqueous solution of d-Panthenol at temperature, T= (288.15, 298.15, 308.15 and 318.15) K and experimental pressure 0.1 MPa is measured. From the data of density, the apparent molar volume (V_{ϕ}), partial molar volume (V_{ϕ}^{0}) and partial molar volume of transfer (ΔV_{ϕ}^{0}), for PEG 200 and PEG 400 in the aqueous solution of d-Panthenol is calculated along with the apparent molar isentropic compression (K_{ϕ}), partial molar isentropic compression (K_{ϕ}^{0}) and the partial molar isentropic compression of transfer, (ΔK_{ϕ}^{0}), from the of speed of sound data. Using the partial molar volume of transfer and partial molar isentropic compression of transfer the pair and triplet coefficients as the functions of temperatures are calculated as well as the partial molar expansibilities (E_{ϕ}^{0}) with its first order derivative $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$are obtained. Further, these calculated parameters are used to describe the results in terms of (solute-solute); (solute-solvent) interactions including the structure making/breaking ability of polyethylene glycols in aqueous solution of d-Panthenol. In problem 9, the density and ultrasonic speed of sound measurement via Anton Paar DSA 5000 M for the binary mixture of (water + polyethylene glycol 600/ polyethylene glycol 6000) and ternary mixture of (water + d-Panthenol + polyethylene glycol 600/ polyethylene glycol 6000) covering the whole range of compositions (0.00, 0.02, 0.07, and 0.12) mol·Kg^{-1}, at 0.01 MPa pressure from (288.15 to 318.15) K. The volumetric properties (apparent molar volume, partial molar volume, and partial molar volume of transfer) are evaluated from the data of density and meanwhile, the speed of sound data is utilized to determine the acoustic properties (apparent molar isentropic compression, partial molar isentropic compression, and partial molar isentropic compression of transfer). This investigation is further extended by calculating the partial molar expansibility with its first derivative and pair-triplet interaction coefficients from these derived thermodynamic parameters. The obtained results from these calculated parameters are expressed as (solute-solvent), (ion-hydrophilic), (hydrophilic-hydrophilic) and (dipole-dipole) interactions prevailing in the liquid sample. Acoustic and volumetric parameters for the liquid mixture (water + Biotin + ethylene glycol/diethylene glycol/triethylene glycol) are evaluated at different temperatures (288.15 K, 298.15 K, 308.15 K, and 318.15 K) and constant pressure of 0.1MPa over the range of biotin concentrations (0.0000, 0.0015, 0.0025, and 0.0035) mol·Kg^{-1} which is comprised in problem 10. The experimental work was carried out by Anton Paar DSA 5000 M, where the density (ρ) and the speed of sound (c) are measured, which are later used to determine the various derived thermodynamic properties, such as, apparent molar properties (apparent molar volume, V_{ϕ}; apparent molar isentropic compression, $K_{\phi,S}$), the partial molar properties (partial molar volume, V_{ϕ}^{0}; partial molar isentropic compression, $K_{\phi,S}^{0}$), the partial molar transfer properties (partial molar volume of transfer, ΔV_{ϕ}^{0}; partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^{0}$) and the partial molar expansibility (E_{ϕ}^{0}) along with its first derivative $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$. The obtained results are explained in terms of the kind of intermolecular interactions developed in the mixture using the co-sphere overlap model. Further, with the partial molar properties the pair and triplet interaction coefficients (V_{AB}, K_{AB}; V_{ABB}, K_{ABB}) are calculated. In problem 11, the analysis of the molecular interactions among the glycols (propylene glycol, PG and hexylene glycol, HG) molecules in (0.000, 0.001, 0.002 and 0.003) mol·Kg^{-1} aqueous solutions of biotin at constant experimental pressure 0.1 MPa and temperature range (288.15 K, 298.15 K, 308.15 K and 318.15 K) have been done. The speed of sound and the density for the liquid mixtures is measured with Anton Paar DSA 5000 M. Various thermodynamic and acoustic parameters are determined using these experimental data. The apparent molar volume (V_{ϕ}), partial molar volume (V_{ϕ}^{0}), partial molar volume of transfer (ΔV_{ϕ}^{0}), apparent molar isentropic compression ($K_{\phi,S}$), partial molar isentropic compression ($K_{\phi,S}^{0}$), partial molar isentropic compression of transfer ($\Delta K_{\phi,S}^{0}$) were estimated using the experimentally obtained density and speed of sound respectively along with the partial molar expansibility(E_{ϕ}^{0}), its first-order derivative $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ and pair-triplet interaction coefficients ($V_{AB},\ K_{AB},\ V_{ABB};\ K_{ABB}$). The apparent molar properties recommend the existence of strong (solute and solvent) interactions in the ternary mixture which is also justified by the positive partial molar expansibility values, while the partial molar properties suggest the formation of the hydrogen bond in the mixture. With Passynski's equation the hydration number (n_h) for PG/HG in aqueous solutions of biotin is calculated utilizing the compressibility data and the obtained results are explained in terms of combined hydration effects and hydrophobic effect. The last problem 12 contains the Knowledge of the thermodynamic properties of polyethylene glycols (polyethylene glycol 200, PEG 200; polyethylene glycol 400, PEG 400) in aqueous biotin solutions provide significant information regarding the intermolecular interactions occurring in the liquid system. The assessments are made through analyzing the volumetric and acoustic properties of the solutions that are determined using the values of density and speed of sounds which are reported in the current study. These experimental values for polyethylene glycols (PEG 200/PEG 400) in (0.0000, 0.0024, 0.0032, and 0.0040) mol·Kg^{-1} biotin solutions are obtained at atmospheric pressure 0.1 MPa and different temperatures (288.15 K, 298.15 K, 308.15 K, and 318.15 K). The apparent molar properties (apparent molar volume, V_{ϕ}; apparent molar isentropic compression, $K_{\phi,S}$), the partial molar properties (partial molar volume, V_{ϕ}^{0}; partial molar isentropic compression, $K_{\phi,S}^{0}$), the partial molar transfer properties (partial molar volume of transfer, ΔV_{ϕ}^{0}; partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^{0}$) and the partial molar expansibility (E_{ϕ}^{0}) are calculated along with its first derivative $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$, from the experimental density and speed of sound values. With these derived parameters the results are discussed which are interpreted as the nature of interactions occurring inside the mixture as per the co-sphere overlap model. The pair and triplet interaction coefficients (V_{AB}, K_{AB}; V_{ABB}, K_{ABB}) are also evaluated in the present investigation using the partial molar properties.

ACKNOWLEDGEMENT

It gives me an immense debt of gratitude to express my sincere thanks to my supervisor, Dr. Kailash Chandra Juglan, Professor, Department of Physics, Lovely Professional University, Phagwara, for providing me the opportunity to carry out research under his excellent guidance. His vision, dynamism, motivation and sincerity have deeply inspired me. I am very grateful for his persistent encouragement, whole-hearted co-operation, care and patience throughout the course of Ph.D. I feel very fortunate to get a chance to work under his patient supervision. I am highly obliged to Dr. Harsh Kumar, Associate Professor, Department of Chemistry, National Institute of Technology, Jalandhar, for not only allowing me to carry out the experimental work in his lab but also for his exceptional guidelines, critical comments and providing an excellent atmosphere for action. His deep insights and expertise helped me throughout the various stages of my research. I am extremely grateful to Mrs. Kirandeep Kaur, Senior Research Fellow, Lovely Professional University, Phagwara, for her obligated support, continuous incitement and valuable suggestions during my Ph.D. I remain indebted for her kind sustenance during my personal difficult times. Finally, I would like to acknowledge the most important persons of my life – my parents, Mrs. Nibedita Chakraborty and Late. Mr. Mridul Ranjan Chakraborty who has been the pillar to my strength, the encouragement to my goals, the root to which I have based my life on. I am indebted to her for always showing me the light at the end of the tunnel. They have taught me to value myself, filled me with courage and confidence at every stage of life.

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LIST OF ABBREVIATIONS

c	Ultrasonic speed
ρ	Density of material
K	Kelvin (Temperature in absolute)
Z	Acoustic impedance
β	Adiabatic compressibility
L_f	Intermolecular free length
R	Rao's constant
W	Wada's constant
b	Vander Waal's Constant
n_1	number of moles of solvent
n_2	Number of moles of solute
V_ϕ	Apparent molar volume
m_A	Molality of the solute
m_B	Molal concentration of cosolute
p	Pressure
Pa	Pascal
T	Temperature
V_ϕ^0	Partial molar volume
ΔV_ϕ^0	Partial molar volume of transfer
a, b, c	Constants of least square fitting of equation 4.4
E_ϕ^0	Partial molar expansibility
$K_{\phi,s}$	Apparent molar isentropic compression
k_s	Isentropic compressibility
$K_{\phi,s}^o$	Partial molar isentropic compression
$\Delta K_{\phi,s}^o$	Partial molar isentropic compression of transfer
S_V^*, S_K^*	Experimental Slopes

V_{AB}	Pair interaction coefficient for volume
V_{ABB}	Pair interaction coefficient for isentropic compression
K_{AB}	Triplet interaction coefficient for volume
K_{ABB}	Triplet interaction coefficient for isentropic compression
EG	Ethylene Glycol
DEG	Diethylene Glycol
TEG	Triethylene Glycol
PG	Propylene Glycol
HG	Hexylene Glycol
PEG-200	Polyethylene Glycol-200
PEG-400	Polyethylene Glycol-400
PEG-600	Polyethylene Glycol-600
PEG-4000	Polyethylene Glycol-4000
PEG-6000	Polyethylene Glycol-6000

CHAPTER 1

INTRODUCTION

1.1 Ultrasonic Investigation

Ultrasonic technique is found to be a very reliable and precise method of investigating the acoustic and volumetric properties of various liquid mixtures such as organic solvents, polymers, electrolyte solutions etc. This kind of technique provides an interesting approach to study the inter-molecular interactions occurring in the sample since the speed of sound is directly related to the binding forces existing in the sample constituents and in a medium the speed of sound for small amplitude of ultrasonic waves is the physical property of that medium which expresses the significant information regarding the packing of fundamental molecules and their microscopic structure in the medium. Thus the speed of sound become very sensitive to the interactions and structure of the sample and as a consequence of this behavior, the information about the arrangement of molecules, their structure, and nature of inter-molecular interactions along with their strength are determined from this method. The ultrasonic waves propagating in a medium provides the valuable knowledge about the hydrogen bonding, dipole interactions, complex formation, dispersive forces etc. occurring in the system. The physical and chemical properties of different fluids are important since in various industries the materials are handled in liquid form, which makes it necessary for the characterization of their physicochemical behavior under different conditions such as multiple temperatures, pressure, solvent concentrations etc. to analyze and enhance their properties. Thus, ultrasonic technique serves as an adaptable non-destructive technique to explore the thermodynamic and physicochemical properties of many liquid-liquid systems which are vigorously used in many industries, for example- chemical, biological, automobile, textile, pharmaceutical, cosmetics, clinical, etc. and there exist a high scope of this study including numerous liquid combinations [1-12]. These techniques are a huge source of information about the structural and molecular changes in liquid mixtures. Within the framework of the theory of physical acoustics, these kind of techniques could also provide useful information about the mixing solution and its temperature dependence. It is an interesting and effective technique to analyze the physicochemical properties of liquid - liquid mixtures, electrolytic mixtures and polymeric solutions. These solutions find wide applications in the medical, pharmaceutical, leather, textile, chemical and solvent solutions industries and the study, understanding and analyzation of the thermodynamic properties of mixtures and different solutions were most significant for their applications in these industries. The spread of ultrasound waves into a substance has become a major test to study its properties. Such studies, such as changes in temperature and concentration, are useful to obtain the insight into the structure and the various linkages of the bound molecular complexes and other related molecular processes. The velocity and the associated acoustic parameters help us to characterize the thermodynamic, physical and chemical aspects of liquid mixtures like association and dissociation of the molecules. To do so, this is one of the most powerful tool to investigate the physiochemical behavior, molecular interactions and their direct applications in diverse fields [13-22]. The thermodynamic properties of various liquid systems such as polymers, organic solvents, solutions of electrolyte etc. are obtained from this method which measures the density and ultrasonic speed of sound of the sample, as they are very much sensitive to the interactions and structure of the fundamental molecules due to its dependability on the existing binding forces and the small amplitude of the propagating ultrasonic waves. Significant information about the packing of molecules, their microscopic structures in medium, hydrogen bond, dipole interactions, complex formations, dispersive forces, molecular interactions along with their strength and nature, structural arrangements of molecules with their shape, etc. are revealed from this non-destructive technique. The ultrasonic technique has been employed in various fields of science for research which provided a riveting approach to explore the acoustic and thermodynamic parameters for different binary and ternary liquid systems [23, 27]. These parameters reveal the various molecular interactions between the different components of the mixtures and administer valuable details regarding the microscopic packing and structure of the constituent molecules in the liquid medium. The ultrasonic wave propagating in the medium predicts the physicochemical behavior of the components of the molecules in the medium. Due to their non-destructive nature, this method is rapidly used for characterizing fluids by exposing the binding forces among the atoms and molecules in the liquid mixtures which are widely used for different chemical processes in various industries such as pharmaceutical, cosmetic, food, etc. Ultrasonic testing is based on the acquisition and quantification of either reflected or transmitted waves (pulse-echo) (through-transmission). Both techniques have their merits, but pulse-echo systems are more beneficial since they only require one-sided access to the thing being studied and can tell you a lot more about concrete than a basic transmission [28-32].

1.2. Ultrasonic Techniques

1.2.1 Magnetostriction Method

A slight change in length occurs when a ferromagnetic rod is put in a magnetic field parallel to its length. Small contractions of the material occur as a result of the magnetic field, and the change in length causes vibrations and relaxations. The contraction is affected by the strength of the magnetic field, the temperature, and the composition of the material. There will be hysteresis and eddy current losses, but it is really simple and inexpensive.

1.2.2. Piezo-Electric Method

When an electric field is applied to one face of a crystal, the crystal's dimension changes on the other faces. Ultrasonic waves are created by the contraction and relaxation of the crystal faces. The benefit of this approach is that it is unaffected by environmental factors like as humidity or temperature, but crystal structuring requires accuracy. The converse of this effect is also true.

1.3. Density and Sound Velocity Analyzer

The Anton Paar DSA 5000M (Density and Speed Analyzer) meter is the most extensively used ultrasonic testing equipment in the world, and it is widely considered as the most exact device for estimating density and sound velocity. In one cycle of sample examination, it determines the sound velocity and density. Its one-of-a-kind measurement method decreases the margin of error for calculating concentration in binary mixes. Other uses for this device include quality control in the manufacturing process, solution preparation, and ternary solution concentration measurements.

DSA has the following features:

- It measures the density and velocity of sound in binary and ternary samples automatically.
- Automatic filling and cleaning of measurement cells at the same time.
- Small sample volume allows for quick and precise measurement.
- Display of sound density and velocity, as well as estimated characteristics, on a continuous basis.
- Automatic viscosity correction throughout the whole viscosity range of the sample
- Generates a sample warning after detecting filling mistakes and gas bubbles in the sample.
- Displays and saves live photos of the oscillating U-tube sensor and the whole filled-in sample for later examination, ensuring entirely transparent measurement operations.

1.4. Glycols

Glycol is an organic compound that has two (-OH) groups that are tied to different atoms of carbon. It is an alcohol that is mainly used in manufacturing plastics, man-made fibers, polyester fibers, and saturated-unsaturated plasticizers. They are employed in numerous industries such as manufacturing, plastic, leather, chemical, cosmetic and pharmaceutical. They, like all other low-molecular-mass alcohols, are soluble in large volumes of water. Various insoluble-water compounds can be rendered clear solutions by coupling action of glycols. Aromatic compounds in glycols have a very high solubility. Aromatic hydroxy compounds and alcohols such as phenols can be mixed in their entirety. They draw moisture from the air and absorb it. Moisture will be caught up and held by the molecules if they are placed in an environment with water vapor. They are used in a variety of applications, such as humectants and dehydrating agents, because of their property. The majority of these applications rely on glycol-water solutions. With the addition of water to a glycol, its properties change. Its humectant value was altered by changes in temperature and humidity. The viscosities of glycols fluctuate inversely with temperature. Their molecules move readily at high temperatures, and as the molecules cool, their viscosity increases, resulting in eventual settling and molecule movement failure. Most plasticizers and solvents with high boiling temperatures are substantially more fluid than these. They are commonly cast off, either alone or in combination with other fluids, with this goal of lowering the viscosities of liquid compositions [33-35].

Ethylene Glycol (EG), Diethylene Glycol (DEG), Triethylene Glycol (TEG), Propylene Glycol (PG), Hexylene Glycol (HG), Polyethylene Glycol-200 (PEG-200), Polyethylene Glycol-400 (PEG-400), Polyethylene Glycol-600 (PEG-600), Polyethylene Glycol-4000 (PEG-4000) and Polyethylene Glycol-6000 (PEG-6000), are only a few of the glycols that are often utilized homologous series diols. These liquids' hygroscopicity makes them ideal for use in printing inks, cellophane, fiber treatment, glue, paper, and leather.

1.4.1 Ethylene Glycol

Ethylene glycol (EG), with the chemical formula ($C_2H_6O_2$), is a liquid compound that consists hydrogen bond network that forms an inter-intramolecular hydrogen bond. It is used in dyes, vaccines, inks, and as coolant. EGs are liquids that are miscible in water across their entire composition range and are highly soluble in polar solvents with H-bonding due to their hygroscopic nature. These glycols are widely employed in the plastics business, where they are utilised to manufacture polyethylene terephthalate, which is then utilised to create pharmaceutical and food-related plastic bottles. They are solvents that include both hydroxyl and oxy groups in the same molecule, resulting in the formation of inter- and intramolecular hydrogen bonds between the -O- and -OH groups. The coolant and anti-freeze industries both use ethylene glycol. It serves as a coolant for automobile engines. Ethylene glycol is also utilised in the fibre sector, such as in the production of fibre glass, which is used in the production of bowling balls and bathtubs, as well as in the production of polyester fibre apparel and the production of packaging bottles and films. Ethylene glycol products are often recyclable, cost-effective, and energy-efficient [33-35].

1.4.2 Diethylene Glycol

Diethylene glycol (DEG) is having the chemical formula ($C_4H_{10}O_3$), which is an odorless and colorless hygroscopic liquid that is miscible in alcohol, water, acetone, and ether. It is mainly found in lotions, skincare products, and deodorants as it is humectant in nature. Diethylene glycol is used in a variety of industries, including the fuel business, agriculture, paints and emulsions business, fabric industry, automotive industry, and de-icing and anti-freeze business. It’s used as a chemical intermediary in unsaturated polyester resin, polyurethane polyols, and thermoplastic polyurethanes, among other things. It's also used as a dehydration agent in natural gas processing [36-38].

1.4.3 Triethylene Glycol

While, triethylene glycol (TEG), is a viscous, colorless, and odorless fluid with the chemical formula ($C_6H_{14}O_4$), which is used in disinfectants and lubricant due to its antimicrobial properties [24-33]. Triethylene glycol is used in a variety of industries, including the cleaning solvents business, functional fluids industry, absorbent and adsorbent business, building material industry, rubber and plastic business, as well as the fabric and automotive industries. Safety glass, separation membranes, and moulded ceramics all employ it as a plasticizer [39-42].

1.4.4 Propylene Glycol

Propylene glycol (PG) is a hygroscopic substance that functions as a common humectant, allowing it to save moisture throughout a wide range of moisture levels. Propylene glycol is a typical carrier for topical applications in cosmetics and cosmetics. Inter and intra hydrogen bonding are self-associated in PG. On combining propylene glycol with methanol and ethanol, the disruption of related particles is detected, and some connection occurs between dissimilar molecules via intra hydrogen association. It consists of two alcohol groups, due to which it is characterized as a diol, is an odorless, colorless, viscous organic compound with less toxicity which is miscible in the number of solvents [43, 44].

1.4.5 Hexylene Glycol

With a typical sweet odor, hexylene glycol (HG) is also miscible in various organic solvents. Being a colorless and viscous compound it is mainly used in pesticide formulation, varnishing, lacquers, printing inks, textiles, pharmaceutical, chemical, and automobile industries. Because of its broad use in a variety of applications, It is regarded as a particularly fascinating fluid. It behaves as a solvent because it breaks down into water and natural solvents, which aids in the delivery of fat and water-soluble compounds. It may also be used to crystallise organic biomolecules11. It is, also known as 2-methyl-2,4-pentanediol, is a chiral diol with two enantiomers: (4R) – () and (4S) – (+). In terms of money, it's referred as MPD. It is stabilized by the formation of intramolecular hydrogen bonds and the constructive arrangement of substituents on nearby carbons [45, 46].

1.4.6 Polyethylene Glycol 200, Polyethylene Glycol 400, Polyethylene Glycol 600, Polyethylene Glycol 4000, and Polyethylene Glycol 6000

Poly (ethylene) glycols (PEG) of various molar masses are employed in a variety of research and technological domains. Due to their low toxicity, they are widely used as laxatives and skin creams. The most important and commonly utilized nonionic polymer in industry is PEG. They are extensively utilized as reaction process regulators of biological macromolecules, and their bioavailability is employed to improve the biochemical activity of proteins. In macromolecules, PEG also acts as a crowding agent. They belong to the polymer family, are polyether compounds with a wide range of uses in industries ranging from manufacturing to pharmaceuticals. They have important therapeutic applications due to their low toxicity. They're used to make a variety of laxatives and skin creams. It is a castoff in polymer cells as an electrolyte solvent and separator. It is also used as a dispersion in toothpastes, as a polar stationary phase in gas chromatography, and in the creation of non-ionic surfactants by combining with hydrophobic compounds. They are also used as plasticizers in the production of edible films, which is a very exciting application [47-54].

1.5 Niacin

Niacin, which is also known as nicotinic acid, is the form of vitamin B_3, used for cholesterol treatment, gastrointestinal problems, liver treatment, DNA repair and so on. They naturally occur in food and are required for production of red blood cells, energy, different enzymes etc. It is a very important compound associated with the several biological functions in human body [55-65].

1.6 D-Panthenol

The solvent compound d-Panthenol is a pro-vitamin B_5 which belongs to the alcohol group, is used in the biosynthesis of coenzyme A due to its biologically active nature. This leads to cell growth inside the body because of enzymatic actions and thus it is used in many cosmetics and pharmaceutical products to enhance their wound healing capacity due to non-mutagenic and non-allergic properties. It is highly viscous, colorless, odorless and water/alcohol soluble at room temperature [66].

1.7 Biotin

Biotin, also known as vitamin H, is associated with the number of metabolic processes in living organisms which is mainly associated with the utilization of carbohydrates, amino acids, glucose, and fats. The deficiency of biotin in the human body can cause hair loss, cell proliferation, skin rashes, abnormal fetal development, brittle nails, and defective immune function. Biotin cannot be synthesized inside the body but depends upon the dietary intake from food. It is primarily present in the liver, egg yolk, some vegetables, and whole cereals [43-46].

1.8 Structure of water

Each hydrogen atoms electron forms a covalent hydrogen connection with one of the six outer shell oxygen electrons in the water (H2O) molecule. The four oxygen electrons are grouped into two non-bonding pairs. As a result, the oxygen atom in H2O is surrounded by four electron pairs that tend to arrange themselves as much as possible, resulting in minimal electrostatic repulsions between pairs of electrons. This produces a tetrahedral shape with an angle of 1090 between electron pairs. Nonbonding pairs of oxygen electrons, on the other hand, are closer to the oxygen atom and, as a result, have a stronger repulsive effect than two covalent-bonding pairs. As a result, two hydrogen atoms are forced together. The tetrahedral geometry is disrupted as a result, and the H-O-H bond angle drops to 104.5^0. Oxygen has a large electronegative charge. This means that the charge distribution resulting from electron pairs involved in the covalent interaction between hydrogen and oxygen atoms is not symmetrical. The density of negative charge is higher near oxygen atoms and lower near hydrogen atoms. With the positive end on the hydrogen atom and the negative end on the oxygen atom, this charge displacement forms an electrical dipole.As a result of the electro-negativity difference between hydrogen and oxygen atoms, partial electric charges are formed in the water molecule.

1.8.1 Hydrogen bonding

A "hydrogen bond exists when a hydrogen atom is joined to two or more other atoms," according to Pimental et al. [67]. The hydrogen bond, in general, refers to a group of three or more atoms that are involved in the X-H-Y configuration, where X and Y might be similar or unlike atoms (F, O, N, Cl etc.,). One of the two bonds, X-H or H-Y, may be stronger than the other (covalent bond) (hydrogen bond). A strong electrostatic dipole-dipole interaction is typically used to characterize the hydrogen bond. Strong electronegative elements like F, O, N, Cl, and others form hydrogen bonds. An atom's ability to make hydrogen bonds is increased by increasing its electro negativity. In virtually all hydrogen bonds, one of the two neighbouring electronegative atoms is closer to the hydrogen atom than the other. Wherever such a possibility exists, the shift in ultrasonic speeds in solid liquid solutions or liquid mixes provides evidence of intermolecular communication through hydrogen bonding. The partial positive charge on a hydrogen atom in one of the water molecules is electrostatically captivated by the partial negative charge on an oxygen atom in an adjacent water molecule. Hydrogen bonding is the term for this process. The hydrogen bond is longer than the O-H covalent link. The length of a hydrogen bond is 117pm, whereas the length of an O-H covalent bond is 99pm. This suggests that the hydrogen bond is much weaker than the covalent link. The hydrogen bond is too weak, resulting in a time fraction of 10-9 seconds for the supplied hydrogen bond.

1.8.2 Hydration of ions

Ions generated by dissolving electrolytes in water interact strongly with water molecules. The molecules of H_2O closest to dissolved ions are sturdily bonded to it due to the strong dipole moment of water, forming an inner or primary hydration sheath.

The negative ends of H_2O molecules are attracted to cations. Bockris [68] proposed a critical viewpoint on the nature of the state of ions and water dipoles in a solution. He proposed that during Brownian motion, the term primary hydration be used to identify solvent molecules closer to the ion that have lost translational degrees of freedom and transfer as a single entity with the ion. The phrase "secondary hydration" refers to solvent molecules that are not included in the primary hydration shell yet have a substantial electrostatic interaction with it. Hydrogen bonding creates a well-organized structure in the primary shell, as well as a well-ordered area with the surrounding water.

1.9 Thermodynamic molecular interactions

The qualities of a material alter when it is dissolved in another substance. The interaction research looks at how the chemical composition of both compounds affects their solubility (the solvent and the solute). When one solute/solvent interacts with another, the result is often a non-ideal solution behavior. A variety of thermodynamic parameters can be used to indicate this departure from ideal behavior. As a result, studying the thermodynamic characteristics of liquid mixes can yield a lot of information on molecular interactions between distinct components. The ultrasonic speed, in combination with viscosity and density, may reveal a lot about the type and intensity of molecular interactions. Numerous acoustical parameters such as acoustic impedance, intermolecular free length, adiabatic compressibility, internal pressure, Gibb's free energy, relaxation time, ultrasonic attenuation, available volume, molar volume, free volume, and enthalpy are computed using density, ultrasonic speed, and viscosity data, providing evidence about the type of interactions present in the liquid mixture. Ion-solvation, which encompasses numerous ion-solvent interactions, is one of the most essential aspects useful in understanding the structural changes of solutes in solutions. The type of the solvent, as well as the size and structure of the ion, influence these interactions. Many thermodynamic properties, such as apparent molar volume, partial molar volume, apparent molar isentropic compressibility, and partial molar isentropic compressibility, are temperature, pressure, and composition dependent, and thus play a critical role in determining the extent and nature of ion-solvation. At infinite dilution, the partial molar volume offers information regarding solute-solvent interactions. At infinite dilution, interactions between solute molecules are negligible, and these features convey information about interactions between solute molecules and the mixed solvent. Because the intrinsic volume of any solute is virtually independent of temperature, the temperature dependence of V_{ϕ}^{0} can be more useful in understanding structural hydration effects. Similarly, the molality dependency of this parameter will aid in the comprehension of solute-solute interactions.

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CHAPTER 2

REVIEW OF LITERATURE

Burton (1948) [1] had measured the sound velocity and density in the mixtures of water with alcohols glycols. In the mixtures the ultrasonic absorption peaks at intermediate concentrations have been found in the solution which contain acetone, ethanol, propanol, isopropanol, d tertiary butanol and in the monoethyl and monobutyl glycol ethers. The magnitude of the peaks increases as one progresses from the ethyl to the butyl derivative, and there is a continous shift of the peak toward higher water concentration in both the series In mixtures containing methanol, glycol, monomethyl glycol ether, or dioxane no absorption peaks were found. In all of the mixtures listed the velocity peaks at intermediate concentrations have been found. Mixtures of tertiary butanol and methanol show neither absorption nor velocity peaks.

Hammes and Lewis (1966) [2] had measured the sound velocity and absorption in the solutions of polyethylene glycol. Over the frequency, temperature, and concentration range. On the polymer solutions the measurement of viscosity uses the Zimm theory, which shows that the viscous relaxation is absent.

Hammes and Schimme1 (1967) [3] had measured the ultrasonic attenuation in both the absence and presence of a synthetic polymer, over the molecular weight range of polyethylene glycol solutions. The relaxation time does not dependent on the concentration over the complete range of molecular weights and molecular weight, as it increases with molecular weight.

Kessler et al. (1970)[4] had studied the ultrasonic absorption spectra for polyethylene glycol at aqueous solution. A multiple relaxation processes has been observed in the broad frequency range. The observed ultrasonic absorption was not taken into account by shear visco-elasticity and the presence of bulk viscosity was considered.

Bagchi et al. (1986) [5] had measured density, absolute viscosities and ultrasonic velocity, for solutions of ISRO polyol, used in the Indian Space Research Organization. It has been studied for various solvents. In highly hydrogen-bonded solvents, the solvation number is found to be higher.

Mehrotra and Upadhayaya (1989) [6] had measured the dissociation constant, degree of dissociation, thermodynamic parameters and critical micelle concentration, for calcium myristate in a mixture of propylene glycol and chloroform at different composition. The results showed in dilute solutions behave like weak electrolytes and with increasing temperature, CMC increases. The results showed that with increasing soap concentrations, the acoustic impedance, ultrasound velocity, molar compressibility, and molar velocity were increased, whereas free intramolecular length and adiabatic compression decreases.

Rao et al. (1990) [7] had measured refractive index, viscosity, speed of sound, and density for N,N-dimethyl formamide (DMF) containing polyvinyl pyrrolidone at different temperatures and concentrations. The acoustic and thermodynamic parameters from the experimental data were calculated. The variations of these parameters with concentration at several temperatures have been studied.

Rajulu and Sab (1995) [8] had measured the sound velocity and density for polyethylene glycol and mixture of water at the temperature of 30°C. The van der Waals constant (b), Rao number (R), specific acoustic impedance (Z), molar compressibility (β), and adiabatic compressibility (β_{ad}). The variations of these parametrs with mole ratio have been analyzed.

Aminabhavi and Gopalkrishna (1995) [9] had measured the molar refractive index, viscosity and density for the binary mixture (water + N,N-dimethylformamide, dimethyl sulfoxide, N,N-dimethylacetamide, acetonitrile, ethylene glycol,diethylene glycol, 1,Cdioxane,tetrahydrofuran, 2-

methoxyethanol,and 2-ethoxyethano) at constant temperature 298.15 K to calculate the excess molar volume, deviation in (molar refractivity, speed ofsound, isentropic compressibility and viscosity).

Mei et al. (1995) [10] had measured the viscosity and density of the binary mixture of (polyethylene glycol+ K_3PO_4/$(NH_4)SO_4$) at constant temperature of 273.15 K.

Moattar and Salabat (1995) [11] had measured the densities of the ternary solutions of (water+polyethylene glycol+ K_2HPO_4/ KH_2PO_4/ Na_2SO_4, Na_2CO_3/$(NH_4)_2SO_4$) at different temperatures and calculates the various thermodynamic parameters.

Magazu et al. (1997) [12] had measured the density and ultrasonic velocity of α-α-trehalose in aqueous solutions, by means of ultrasonic techniques. The data showed no ideal mixing process was present in these aqueous solutions. The behavior of the excess of compressibility with the concentration was interpreted considering that the α-α-trehalose molecules make intramolecular hydrogen bonds at high concentrations.

Eliassi and Modarres (1998)[13] had measured the densities of the binary mixture of (water + polyethylene glycol 400/ 4000/ 6000) at different temperatures to calculate various thermodynamic parameters.

Ali et al. (1999)[14] had measured the viscosities, densities and velocity of sound for pure 1-octanol, ethanol, acetonitrile, N,N-dimethylformamide and 1-hexanol at constant temperature. The excess- adiabatic compressibility, volume, intermolecular fee length, viscosity and acoustic impedance the association molecule have been obtained.

Moattar and Mehrdad (2000)[15] had measured the densities of mixture (water + polymer + salt) to calculate the apparent moral volume.

Baluja and Oza (2001)[16] had measured Gibb's free energy, specific impedance, excess molar volume, isentropic compressibility, excess viscosity, van der Waals constant, molar compressibility, molar sound velocity, intermolecular free length, excess adiabatic compressibility, for methanol, anisole + dimethyl foramide and anisole + chloroform.

Ebner et al. (2002)[17] had studied the properties of D-Panthenol and its applications in the cosmetic, Pharmaceutical field etc. Its beneficial effects had also been reported.

Graber et al. (2002)[18] had measured the viscosity, density and refractive index of the ternary mixture of (water + polyethylene glycol + sodium nitrate) at different temperatures aand excess molar volumes are calculated.

Sisakht et al. (2003)[19] had measured the viscosity and density of the binary mixtures of (polyethylene glycol+water/ethanol) and (polypropylene glycol+ethanol) at different temperatures to calculate various thermodynamic parameters.

Schmelzer et al. (2004)[20] had measured sound velocity and the density for mixtures of water and polyethylene glycols. From the experimental data different acoustical property was obtained, i.e, the adiabatic compressibility using Laplace's equation.

Syal et al. (2005) [21] had investigated and analyzed the viscosity, sound velocity and density of solutions of PEG's in water and with Acetonitrile at constant temperature. From the experiment, the data obtained of density, velocity and viscosity were used to calculate the different acoustical parameters.

Zwirbla et al. (2005) [22] had measured the sound velocities and densities in the temperature variation from 291.15 to 303.15 K, for the mixtures containing water with ethylene glycol and polyethylene glycol 200, 400 and from Laplace's equation the Adiabatic compressibility were calculated .

Moattar and Hamzehzadah (2005)[23] had measured the velocities and densities of the binary mixture of (polyethylene glycol 6000 + disodium succinate/ sodium formate) at different temperatures and calculated the adiabatic compressibility and apparent molar volume.

Kumar and Rao (2007) **[24]** had investigated and analyzed the sound velocity, viscocity and density for the mixture of methanol and ethanol with aqueous propylene glycol. Various thermodynamical and acoustical parameters were obtained, namely excess adiabatic compressibility, excess viscosity, excess free volume, viscous relaxation time, excess free length and excess molar volume. With the experimental values, various relations were campared, i.e Rao's sound velocity relation, Jacobson's equation and impedence relation.

Ayranci and Sahin (2008)[25] had measured density and velocity of polyethylene glycol and ethylene glycols. Various parameters were evaluated and graphically represented.

Palani and Geetha (2008) [26] had measured the density, viscosity and ultrasonic velocity for water+propylene, glycol+tetrahydrofuran, water+propylene, glycol+dimethylformamide, water+propylene, glycol+dimethylsulphoxide and water+propylene glycolþ1,4-dioxane, as a function of the composition at different temperature. Experimental data was used to calculate thermodynamic parameters namely, excess volumet (V_f^E), excess viscosity (η^E), excess Gibb free energy and interaction parameter (d).

JianBan et al. (2008) [27] had measured the density of the binary mixture (water + ethylene glycol) to calculate the excess molar volume and obtained the FTIR spectral data o OH- stretching vibration of water alcohol and bending vibration of water.

Romero et al. (2008) [28] had measured the density of the binary mixture (water + 1-propanol, 1,2-propanediol, 1,3-propanediol, and 1,2,3-propanetrio) at different temperatures and calculate the partial molar volume and excess molar volume of the binary mixture.

Tsierkezos and Palaiologou (2009) [29] had measured the densities and velocity to calculate the isentropic compressibility, excess molar volume, sound deviations and isentropic compressibility deviation for the ternary mixture (water + dimethylsulfoxide + ethylene glycol/ diethylene glycol/ triethylene glycol/tetraethylene glycol/ propylene glycol/ butylene glycol) at constant temperature 298.15 K.

Kinart et al. (2009) [30] had measured the relative permittivity and density of the binary mixture (2-ethoxyethal+ethylene glycol/diethylene glycol/triethylene glycol/ tetraethylene glycol) at different temperatures and calculate the deviations in the relative permittivity and excess molar volume.

Sadeghi and Jamehbozorg (2009) [31] had measured the velocity and density at different temperatures of the ternary mixture (water + polypropylene glycol + sodium di-hydrogen phosphate / di-sodium hydrogen phosphate/ tri-sodium hydrogen phosphate) and constant pressure. With these experimental data various thermodynamics parameters i.e. isentropic compressibility, apparent specific volume, isentropic compressibility deviation and excess specific volume.

Zarei et al. (2009) [32] had calculated the density, viscosity, velocity, and refractive index of the ternary mixture of (methanol+ ethanol+propandiol) and the binary mixture of (methanol/ ethanol +1-2, propandiol) at different temperatures and constant pressure of 81.5 KPa. Various thermodynamic parameters such as excess molar volume, excess partial volume, excess partial molar volume at infinite dilution and thermal expansion coefficient.

Shanmuga et al. (2010)[33] had measured the viscosity, density and ultrasonic velocity for mixtures having Methylmethacrylate+2- Ethoxy ethanol, Methylmethacrylate +2- Methoxy ethanol, Methyl methacrylate+2 Butoxy ethanol at constant temperature. Adiabatic compression, internal pressure, free energy values of Gibbs, and free volume, are calculated from experimental data.

Hosahalli (2010)[34] had studied the oxidation of D-panthenol by MnO4- in the presence and absence of ruthenium(III) catalyst at constant temperature and ionic strength in alkaline medium.

Anbarsu (2010)[35] had studied the interactions among liquid mixtures of Ethyl acetate + 2-Butanone with interferometer method. A drastic change has been observed for Ethyl acetate at 0.6 mole fraction of and of 2-Butanon at 0.4 mole fraction in the in the frequency of FTIR spectrum.

Patil (2010)[36] had measured the viscosity, ultrasonic velocities and density for binary mixtures of 1-Hexanol and 1-Heptanol with Nitrobenzene at at various temperature, atmospheric pressure and over whole range of mole fraction and. By R-K equation the different parameters were calculated.

Egorov et al. (2010)[37] had measured the density of the binary mixture (water + ethylene glycol) at different temperatures to calculate the excess molar volume, partial molar volume and thermal expansion coefficient.

Raman et al. (2010)[38] had experimentally obtained the velocity, viscosity and density of the binary mixture of (water + d-arabinose) at different temperatures and calculated the thermodynamic parameters i.e. shear relaxation time, classical sound absorption, intermolecular free length, hydration number and isentropic compressibility.

Zorebski et al. (2010)[39] had measured the velocities and densities of binary mixture of (2-ethyl-1-hexanol + 1-pentanol / 1-heptanol / 1-nonanol) at constant temperature of 298.15 K with the help of pulse-echo-overlap technique and vibrating tube densitometer. Different thermodynamic parameters such as excess molar volumes, excess molar isentropic compressibility and deviations of speed of sound are evaluated with the experimental data.

Pan (2010)[40] had measured the electric conductance, viscosity and density of the ternary mixture of (water + nicotinic acid + polyethanol) to calculate the partial molar volume, degree of dissociation and viscosity coefficient.

Thiruman and Rajeshwari (2011)[41] had measured the density, sound velocity and viscosity for the mixtures of aromatic hydrocarbons and chlorobenzene with DMSO. The acoustical parameters were calculated using the experimental-data.

Pal and Chauhan (2011)[42] had measured the density and velocity of the ternary mixture (water+2- aminopropanoic acid/ 2-amino-3-methylbutanoic acid/ 2- amino-4-methylpentanoic acid / 2-amino-3-phenylpropanoic acid + fructose/ D- cellobiose / D-melezitose) at different temperatures and calculates the thermodynamic parameters (apparent molar properties, partial molar properties, partial molar transfer properties) to investigate the interactions occurring inside the mixture.

Sadeghi and Azizpour (2011)[43] had measured the density and velocity of the binary mixture (polyvinylpyrrolidone +water/methanol/ ethanol/acetonitrille/1- propanol/ 2-propanol/ 1-butanol) aat different temperatures and atmospheric pressure. With these experimental data various thermodynamic parameters are evaluated such as apparent specific volume, isentropic compressibility, partial specific volume and partial isentropic compressibility.

Yang et al. (2011)[44] had measured the electrical conductance, viscosity and density of the ternary mixture of (water + dextran + nicotinic acid) at different temperatures and calculate the linear coefficients, partial molar volume, linear molar conductance, dielectric coefficients and viscosity (A and B) coefficients.

Sadeghi and Shahabi (2011)[45] had measured conductivity, velocity and density of the ternary mixture (water + sodium dodecylsulfate/ sodidum dodecyl sulfonate + polyethylene glycol) at different temperatures and calculate the thermodynamic parameters as apparent molar volume and isentropic compressibities.

Sahin et al. (2011)[46] had measured the density and the velocity of the ternary mixture of (water + glycine+ polyethylene glycol 400) at different temperatures. With these experimental data various thermodynamic parameters are evaluated such as apparent molar volume, partial molar volume, apparent molar isentropic compression and partial molar isentropic compression.

Zhang et al. (2011)[47] had measured the viscosity and density of the binary mixture of (water + polyethylene glycol 400/ 600/ dimethyl sulfoxide) at different temperatures and calculates the various thermodynamic parameters such as viscosity deviation and excess molar volumes,

Ramteke (2012)[48] had measured the density, viscosity and sound velocity, of the liquid solutions of α-picolin in Ethanol at different temperature. From these data some of acoustical parameters namely, internal pressure, free volume, free length, and adiabatic compressibility, was computed. The variation of ultrasonic velocity and excess adiabatic compressibility implied the existence of molecular interaction between solvent and the solute and the excess adiabatic compressibility was positive over whole concentration range and it became minimum at a concentration (0.5) of α-picoline in ethanol at observed temperatures.

Godhani et al. (2012) [49] had measured the viscosity, ultrasonic velocity and density of chloroform, N-N dimethyle formide and solutions of 2-((4-acetyl-5-(2-hydroxyphenyl)-5-methyl-4,5-dihydro-1,3,4-oxadiazol-2-yl)methylthio)-3-o-tolyquinazolin-4(3H)-1 ($PD_{1\text{-}C}$) in CF and DMF are analyzed at atmospheric pressure and different temperature. Various thermodynamic parameters were determined by using these experimental data.

Parveen et al. (2012) [50] had measured the ultrasonic velocity, density, refractive index and viscosity of mixtures of aniline containing propionic acid and acetic acid at different temperature and molality. In addition, specific heat ratio, the thermal capacity, pseudo-Gruensisen parameter and Debye effective temperature and non-linearity were evaluated by ultrasonic absorption data. From the test data, detours of centripetal excess molar volume, compressibility, excess intramolecular length, relaxation time, deviation in molar refraction, enthalpy, viscosity deviation, entropy, and energy of Gibbs activation from the Redlich-Kister polymerization equation were calculated.

Pathak et al. (2012) [**51**] had measured the density, viscosity and speed velocity of various solvents i.e THF, chloroform and 1,4-dioxane, with epoxy resin solutions at constant temperature. Various thermodynamic parameters were determined.

Katrinak et al. (2012) [**52**] had measured the velocity and density in the binary mixture (water + propane-1,2-diol/ propane-1,3-diol/ propane-1,2, 3-diol) at different temperatures and constant pressure. Various thermodynamic parameters-partial molar volumes and partial molar isentropic compression are calculated with these experimental data**.**

Kaur and Juglan (2013)[53] had measured the density, ultrasonic speed and viscosity of liquid mixtures of polyvinyl acetate in acetic acid using gravity bottle, ultrasonic interferometer, and viscometer respectively at frequency 2MHz and at constant temperature of 295K. The obtained experimental values were used to determine different parameters i.e adiabatic compressibility, intermolecular length, relaxation time, acoustic impedance and ultrasonic attenuation. The variations in the parameters show the possible existance of the molecular interaction among the mixture. As concentration increases the velocity increases.

Pal and Kundu (2013) [54] had measured the attenuation constant (α) and velocity (v) for ultrasonic waves at frequencies 1MHz and 2MHz travelling through the aqueous sodium chloride solution over the concentration region at room temperature (25^0 C). With the increase of concentration the velocity (v) and attenuation constant increases indicating relatively stronger bond among the ions and water molecules solution.

Das et al. (2013) [55] had measured the sound velocity and density of sodium nitroprusside in solutions containing ethylene glycol, CH_3OH, n-propanol, DMSO, and solvents at a fixed temperature. From the experiment parameters and their constants were obtained.

Pal et al. (2013)[56] had measured the density and sound velocity of binary mixture of 1,4-dioxane with 1-propanol,2 propanol,1-butanol and 2-butanol at atmospheric pressure at different temperatures and concentration using DSA. Excess molar concentration, KES and Excess molar volume, are computed from the experimental data. From the experimental density measurements, different parameters and their infinite dilution limits were calculated.

Sannaningannavar et al. (2013) [57] had measured the density and sound velocity at various temperatures for polyethylene glycol having average molecular mass of 400 g mol^{-1} Of these, free intramolecular length (Lf), molar sound rate (Ra), isotropic compressibility (b), molar volume (Vm), acoustic impedance (Z), Schaff Va (s) volume, and molar compressibility. The variations in these parameters at different temperatures were investigated. The data thus obtained is used to determine various other thermodynamic parameters.

Pal et al. (2013) [58] had measured the ultrasonic speeds and densities using an DSA for the liquid mixtures containing dipropylene glycol dimethyl ether, with methyl acetate, n-butyl acetate, and ethyl acetate at different temperature, over the entire composition range and at atmospheric pressure.

Bhavani (2013) [59] had measured the ultrasonic velocities from different relations such as Rao's specific velocity relation, Van dael mixing relation Nomoto's relation, impedence relation and Jungie's theory. The experiental data were compared with the theoretical values.

Begum et al. (2013) [60] had measured the viscosity and density of the (water + triethylene glycol/ tetraethylene glycol/ tetraethylene glycol dimethyl ether) at different temperatures to calculate the excess molar volume and excess viscosities.

Jiang et al. (2013) [61] had measured the viscosities and densities of the mixture (water + L-Ascorbic acid + erythritol / xylitol / mannitol) and (water+ erythritol / xylitol / mannitol) at different temperatures (293.15 to 323.15) K and atmospheric pressure. Utilizing these experimental values the apparent molar volume, partial molar volume and partial molar volume of transfer are evaluated and Jones-Dole equation and Guimaraes were used to correlate the experimental values.

Egorov et al. (2013) [62] had measured the densities of the binary mixtures (water + glycerol) at different temperatures using vibrational densitometer. Thermodynamics parameters such as partial molar isobaric expansions, partial molar volume, partial molar volume, partial molar volume, apparent molar volume and excess molar volumes are calculated.

Banipal et al. (2013) [63] had measured the density, velocity and viscosity of the binary mixture of (water + L-acobaric acid/nicotinic acid/ thiamine hydrochloride/ pyridoxine hydrochloride) at different temperatures and constant atmospheric pressure. With these experimental data various thermodynamic parameters such as apparent molar volume, apparent molar isentropic compression, partial molar volume, partial molar isentropic compression, solvation number and viscosity B coefficients.

Moattar and Tohidifar (2013) [64] had measured the viscosity, velocity and density of the ternary mixture of (water + polyethylene glycol dimethyl ether 2000 + polyethylene glycol 400) at different temperatures. With these experimental values various thermodynamic parameters such as deviation in viscosity, excess Gibb's free energy of activation of viscous flow and excess molar volumes are calculated.

Dixit et al. (2014)[65] had measured the viscosity, ultrasonic velocity and density of liquid mixtures of water n-butanol, and acetic acid ($C_4H_9OH + H_2O + CH_3COOH$) at different concentrations using ultrasonic technique at a constant temperature 289K. The obtained values were used to calculate different acoustic parameters namely Vander Waal constant, , adiabatic compressibility, relaxation time, adiabatic impedance, free intermolecular length ultrasound attenuation, volume present, effective molecular weight, Wada constant, molar volume, free energy, Rao constant, Gibbs enthalpy and internal pressure.

Kumari et al. (2014) [66] had measured the viscosity, density and ultrasonic velocity of tyrosine derivative with non-aqueous dimethyl sulpho oxide (DMSO) at constant temperature of 290 K using ultrasonic interferometer. Using these fundamental parameters were calculated. From these parameters the nonlinear variations were obtained which indicated that a weak interaction among solute and solvent molecules is present.

Naveem and Rao (2014)[67] had measured the velocity of sound and density of the mixture containing Benzyl Benzoate, *n*-butanol, *sec*butanol, *tert*-butanol at temperatures of 308.15K and 313.15K respectively and at different mole fraction. From the experimental data the acoustic parameters namely deviation in excess acoustic impedance, isentropic compressibility, and deviation in ultrasonic velocity was determined for the systems at these temperatures.

Kumar et al. (2014) [68] had measured velocity of sound and Densities of amino acids in binary solutions of sodium dihydrogen phosphate at various temperature and at atmospheric pressure and studies the interactions of L-valine and L-alanine, amino acids glycine, containing sodium dihydrogen phosphate by the combination of acoustic and volumetric measurements as the function of temperature.

Chauhan and Kumar (2014) [69] had measured the densities and velocities for saccharides in aqueous solution of glycine at different temperatures to obtain the partial molar properties, partial molar transfer properties and partial molar expansibilities along with its first and second derivative.

Kondaiah et al. (2014) [70] had measured the density and velocity of the binary mixture (water + ethylene glycol / propylene glycol) at constant temperature to calculate the deviation in isentropic compressibility, excess intermolecular free length, excess acoustic impedance and excess molar volume.

Hagade et al. (2014) [71] had measured the density and velocity of the mixture of (amino acid+ glycine/ L-alanine/ V-valine/ L-leucine/ L-isoleucine +1-butyl-3-methylimidazolium). With these experimental values different thermodynamic parameters such as apparent molar volume, partial molar volume, partial molar volume of transfer, apparent molar isentropic compression, partial molar isentropic compression, partial molar isentropic compression of transfer and hydration number.

Dhondge et al. (2014) [72] had experimentally obtained the viscosity and density values of the binary mixture of (water + nicotinic acid/ nicotinamide) at different temperatures. Various thermodynamic parameters such as apparent molar volume, partial molar volume, partial molar expansibility, thermal expansion coefficient, viscosity (A, B and D) coefficients and hydration number.

Raman et al. (2015) [73] had measured the velocity, viscosity and density of the binary mixture (water + diethylene glycol) at different temperatures to calculate the isentropic compressibility, acoustic impedance, hydration number, intermolecular free length, classical sound absorption and shear relaxation time.

Kaur and Juglan (2015)[74] measured the viscosity, ultrasonic velocity and density and of the liquid mixture of chloroform and methanol by an ultrasonic interfering device, a 30 ml bottle of viscometer and a Oswald viscometer at 2MHz at constant temperature is 295K respectively. The experimental values obtained were then used to determine the various thermal parameters namely mole mass, free intermolecular length, adiabatic compression, acoustic impedance, relaxation time, , molecular weight volume, , constant Wada, ultrasonic attenuation, intrinsic pressure constant, free energy, and Gibbs enthalpy.

Wananjea et al. (2015)[75] had measured ultrasonic velocity and other acoustical parameters namely acoustical impedance, free length, viscous relaxation time and adiabatic compressibility, for aqueous polypropylene glycols, at room temperature. Ultrasonic velocity, free length, acoustic impedance, relaxation time and adiabatic compressibility, has been calculated and discussed in terms of concentration and structural dynamics for the given system. The variance in acoustic parameters has been found to be more complex with the higher concentration of the region for water PPG-425.

Kaur and Juglan (2015)[76] had measured the viscosity, density and sound velocity and of binary liquid mixtures of ethyl acetate and hexane at constant temperature of 292K and at frequency 2MHz using ultrasonic interferometer. The experimental values obtained are then used to determine different acoustic parameters such as acoustic impedance adiabatic compressibility, viscosity, free volume, free intermolecular length, internal pressure, free energy of Gibb, ultrasonic attenuation and enthalpy.

Banipal et al. (2015)[77] had measured the viscosity and density of the mixture (water + NH_4Br + polyhydroxy solute) to evaluate the partial molar properties, Jones-Dole B coefficient, interaction coefficient, first derivative of B coefficients along with the isobaric expansion coefficients and its second order derivative.

Klimaszewski et al. (2015)[78] had calculated the density and velocity of the binary mixture (water + triethylene glycol) at different temperatures to calculate the apparent molar volume, adiabatic compressibility coefficient, thermal coefficients, excess compressibility coefficient, excess molar volume and its derivative.

Krishna et al. (2015)[79] had measured the velocities and densities of the binary mixture of (ionic liquid+alkanediol) to calculate the excess molar isentropic compressibility and excess molar volumes at different temperatures.

Banik and Roy (2015)[80] had measured the viscosity and density of the ternary mixture of (water + nicotinic acid + d-glucose/d-mannitol/ d-sucrose) at different temperatures. With these experimental data various thermodynamic parameters are determined such as apparent molar volume, partial molar volume, partial molar volume of transfer, molar fraction and viscosity B coefficient.

Ebrahimi and Sadeghi (2015)[81] had measured the viscosity, velocity and density of the binary mixture of (water + polyethylene glycol 600/1000/polypropylene glycol 400/ polyethylene glycol dimethyl ether 250/ polyvinyl pyrrolidone 1000) at different temperatures and calculated different thermodynamic parameters such as excess specific volume, apparent specific volume, isentropic compressibility, increment in isentropic compressibility, partial specific volume, partial specific expansibility, partial molar isentropic compressibility and apparent molar isentropic compressibility.

Venkataramanan et al. (2015)[82] had measured the viscosity, velocity and density of the binary mixture of (water+{polyethylene glycol 2000/ 3000/ 6000) at different temperatures to calculate the different thermodynamic parameters such as internal pressure, intermolecular free length, intermolecular free volume, viscous relaxation time and adiabatic compression.

Ebrahimi and Sadeghi (2015)[83] had measured the velocity and density of the ternary mixture of (water+ polypropylene glycol + alanine/ glycine/ serini/proline) at different temperatures. With these experimental val;ues various thermodynamic parameters are evaluated such as apparent molar volume, apparent molar isentropic compression, apparent molar transfer properties, partial molar expansibilities and hydration number.

Thakare and Naik (2016) [84] had measured the density and ultrasonic velocity of solution containing 2-amino-5-nitrothiazole and $NiCl_2$ at various concentrations and temperatures. The experimental values obtained are then used to determine different acoustic parameters namely free intermolecular length, specific acoustic impedance, isentropic compressibility and relative association.

Kumar et al. (2016)[85] had measured the ultrasonic speed, u and densities, ρ of aqueous solutions containing mono methyl ether, ethylene glycol, in the solutions of sodium dodecyl sulphate at various temperatures. Various parameters namely transfer volume, partial molar stretch ability, limiting visible molar volume and apparent molar volume are calculated from density data. For all the alkoxyalkanols with the increase in sodium dodecyl sulfate concentration, the molar volume value decreases, whereas for which there is the increase in these values with the increase in sodium dodecyl sulfate concentration.

Kumar and Behal (2016) [86] had measured the density and ultrasonic speed of the chloramphenicol with L-leucine and the dipeptide glycyl-L-leucine, in aqueous medium at different temperature and at the pressure of 0.1 MPa. For L-leucine and the dipeptide. From the density data the acoustic parameters havebeen obtained.

Ren et al. (2016) [87] had calculated the apparent molar volume, partial molar volume and partial molar volume of transfer for (glycine, L-alanine, L-valine, L-theonine and L-arginine) in aqueous solution of sorbitol as the function of temperature from the experimental viscosities and densities. Further, the interaction coefficients with the correlation of equation of Jones-Dole to retrieve the free energies of activation, partial molar volume of transfer and viscosity B coefficients along with the hydration number are determined.

Romero et al. (2016) [88] had measure the viscosities and densities of the binary mixture (water + ethylene glycol/ glycerol/ meso-erythritol/ xylitol/ d-sorbitol/ myo-inositol) at different temperatures and 75 KPa pressure. From these experimental data the viscosity coefficients B and D, the apparent molar volumes and partial molar expansibilities are evaluated.

Pandit et al. (2016) [89] had measured the viscosities and densities of the ternary mixture of (water + nicotinic acid + sodium malonate) at different temperatures and constant pressure of 101KPa. With the experimental values various thermodynamic parameter such as apparent molar volume, partial molar volume, experimental slope, partial molar expansibility, its first derivative, solvation number and viscosity B coefficient.

Zhu et al. (2017) [90] had measured the viscosities and densities of (glycine/ L-alanine/ L-valine/ L- threonine/ L-arginine) in the aqueous solution of xylitol at multiple temperatures and constant pressure. These experimental values were utilized to determine the apparent molar volume, partial molar volume, partial molar volume of transfer, interaction coefficients, free energy of activation, viscosity B coefficients and hydration number.

Rani et al. (2017) [91] had measured the density, viscosity and velocity at different temperatures to calculate the apparent molar properties, viscosity B coefficients, partial molar properties, partial molar transfer properties, partial molar expansibility, Hepler's constant, thermal expansion coefficient, solvation number and pair-triplet interaction coefficients.

Negadi et al. (2017) [92] had measured the velocities and densities of the binary mixture (water + glycerol/ methanol/ ethanol) at different temperatures using Anton Paar DSA 5000 M. With these experimental values deviation in isentropic compressibility, isentropic compressibility and excess molar volumes.

Mishra et al. (2017) [93] had measured the densities and viscosities of the ternary mixture of (water + nicotinic acid+ sodium gluconate) to calculate the apparent molar volume, partial molar volume, apparent specific volume, solvation number and viscosity B coefficient.

Hoga et al. (2018) [94] had measured the density, velocity and viscosity of the ternary mixture (water + glycerol + ethanol/ ethylene glycol/ diethylene glycol/ triethylene glycol/ polyethylene glycol 200/ polyethylene glycol 300/ polyethylene glycol 400/ polyethylene glycol 600) at different temperatures and pressure and determine the **(**excess molar volume, deviation in isentropic compressibility, deviation in viscosity and excess Gibbs energy of activation for viscous flow).

Moradian et al. (2018) [95] had measured the velocity and density of the ternary mixture of (water + L-valine + polyethylene glycol 400/ 2000/ 6000) at different temperatures and various thermodynamic properties such as apparent molar volume, ap[parent molar isentropic compressibility and isentropic compressibility are calculated.

Rani et al. (2019) [96] had measured the densities, velocities and viscosities of (L- serine and L-arginine) in aqueous thiamine solutions at multiple temperatures to investigate the viscometric, acoustic and volumetric properties of the mixture by calculating the apparent molar and partial molar properties along with the partial molar transfer properties and the coefficient B with its first derivative / are determined with the experimental the viscosity values.

Sharma et al. (2020) [97] had measured the velocity and density of (water + nicotinic acid + d-glactose/ d-glucose/ d-xylose/ maltose monohydrate/ cellobiose) at different temperatures and constant pressure to calculate the apparent and partial molar volumes, apparent and partial isentropic compressibility, partial molar expansibility, pair-triplet interaction coefficients and hydration numbers.

Ijardar (2020) [98] had measured the velocity, density and viscosity of the mixture (deep eutectic solvent + tetrabutylammoniumbromide+ polyethylene glycol) at different temperatures and atmospheric pressure to calculate the thermal expansion, isentropic compressibility, intermolecular free length and activation energy.

Asghar et al. (2021) [99] had measured the viscosities, velocities and densities of binary mixture of (phenol + acetaldehyde) at the constant temperature of 303 K and calculate various thermodynamic properties such as excess molar volume, excess molar isentropic compressibility, coefficients standard deviation and excess properties.

Vankar and Rana (2021) [100] had measured the velocity, viscosity and density of the binary mixture of (methanol + 3-bromoanisole) at different temperatures and calculates the excess molar properties of the mixtures.

Sharma et al. (2021) [101] had measured the viscosity, velocity and density of the binary mixture of (n-hexane +2-chlorotoloune / 4-chlorotolouene / 1,3-dichlorobenzene) at different temperatures and constant atmospheric pressure. From these experimental values various thermodynamic properties such as intermolecular free length, available volume, excess isentropic compressibility, deviation in viscosity, excess ultrasonic speed and excess molar volumes.

Dhivya et al. (2021) [102] had measured the refractive indices, velocity, viscosity and density of the binary mixture of (water + polyethylene glycol 200) at constant temperature of 303 K.

Dubey and Dhingra (2021) [103] had measured the viscosity, velocity and density of the binary mixture of (2-butoxy ethanol + dipropylamine / dimethylamine/ trimethylamine) at different temperatures. From these values the partial molar volume, apparent molar volume, excess Gibb's free energy of activation, deviation in viscosity, excess speed of sound and excess molar volume is calculated.

Diaz and Navaza (2021) [104] had measured the surface tension, viscosity, velocity and density for the ternary mixture of (water + ethanol + hexamethylenetetramine) at different temperatures,

Masilo et al. (2021) [105] had measured the surface tension, refractive indices, sound velocity and density of the binary mixture of (acetic acid + 1-butyl-3-methylimidazolium tetrafluorobarate / 1-butyl-3-methylimidazolium hexafluorophosphate) and (propionic acid + 1-butyl-3-methylimidazolium tetrafluorobarate / 1-butyl-3-methylimidazolium hexafluorophosphate) at different temperatures and constant 0.1 MPa pressure. The FTIR spectrum for the binary mixture is also obtained.

Kumari and Maken (2021) [106] had measured the velocity and density of the binary mixture of (binary DIPA + isomeric butanol) at different temperatures. From these experimental data various thermodynamic parameters such as excess isentropic compressibility, deviation in speed of sound and excess molar volume are calculated.

Darolia et al. (2021) [107] had measured the velocity and density of the binary mixture of (1-methylpiperidine + 2-pyrrolidinone / pyridine) (1-methylpiperidine + 2-pyrrolidinone + pyridine) at different temperatures. Form these experimental measurement excess heat capacities,excess isentropic compressibilities and excess molar volumes are calculated.

Kumari and Maken (2021) [108] had measured the viscosity, velocity and density of the binary mixture of (di-butylamin + 1-butanol / 2-butanol / 2- methylpropan-1,2-ol) at different temperatures. From these experimental data various thermodynamic parameters such as deviation in viscosity, excess isentropic compressibility and excess molar volume are calculated.

Darolia et al. (2021) [109] had measured the molar heat capacity, speed of sound and density of the binary mixture of (piperidine + 2-/3-/4-picolines) at different temperatures. With these experimental values various thermodynamic parameters such as heat capacities, excess isentropic compressibility and excess molar volumes are calculated.

Satheesh et al. (2021) [110] had measured the velocity, viscosity and density of the binary mixture of (isoamyl alcohol + ethanol / 1,2-ethanediol / 1,3- propanediol / 1,4-butanediol / glycerol) at different temperatures and constant atmospheric pressure. Utilizing these values various thermodynamic parameters such as deviation in isentropic compressibility, deviation in viscosity and excess molar volume are calculated.

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CHAPTER 3

OBJECTIVES AND EXPERIMENTAL PROCEDURES

3.1. Objectives of the research

To identify different kinds of chemicals which find its applications in different products used by the people and which are having beneficial properties to the masses so that their properties could be enhanced more for desirable purposes. Most of the research will be done to know the different characteristics of the combinations of liquids which will have its applications in different pharmaceutical, leather, chemical, cosmetics etc industries. In order to do that the following steps will be followed-

i. To obtain experimental data in various physicochemical properties such as density and speed of sound for the water-soluble vitamin B i.e Niacin (B_3), D-Panthenol (B_5) and Biotin (B_7) in aqueous solutions of glycols at different temperature and concentrations.
ii. To calculate the various acoustic and thermodynamic parameters like Apparent molar volume, Partial molar volume, Partial molar volume of transfer, Temperature dependent partial molar volume, Apparent molar isentropic compression, Partial molar isentropic compression, Pair and triplet interaction coefficient, etc from the experimental data.
iii. To examine and to understand various types of inter-molecular interactions occurring in the aqueous solutions of the chemicals at different compositions at different temperatures.

3.2. Experimental procedure

The ternary liquid mixture of an aqueous solutions of water soluble vitamin B and glycols of varying concentrations in the range of molar fractions will be investigated by ultrasonic velocity and density measurement by ultrasound technique using Anton-Paar DSA 5000 M.

Chemicals

In the present investigation chemicals used will be ethylene glycol, diethylene glycol, triethylene glycol, hexylene glycol, propylene glycol polyethylene glycols, niacin, D-Panthenol and biotin having molecular weights of 62.07 g/mol, 106.12 g/mol, 150.18 g/mol, 118.172 g/mol, 79.09 g/mol,18.02 + 44.05n g/mol, 123.11 g/mol, 205.251 g/mol and 244.31 g/mol respectively. The biologically active vitamin B will be used to prepare the solvent mixtures with degassed and triple distilled water. Without further purifications the chemicals will be kept in desiccators over P_2O_5 after vacuum dried.

Measurements

The velocity and density measurement will be done using Anton-Paar DSA 5000 M at different temperatures. The sample is manually inserted in the equipment by the means of a syringe. The two physically independent properties of a single specimen are being defined, as the multipurpose tool is having a density cell and another cell where the velocity of sound is determined separately. In both cells the temperature is governed by built in Peltier-thermostat. The speed of sound and density obtained are used as inputs for different concentration computation models that are integrated into the DSA. For the preparation of the solutions, the degassed and triple distilled water of specific conductance less than 10^{-6} $S{\cdot}cm^{-1}$, have been used and the weighing of solutions were done on the balance having precision of ± 0.00001g. The solutions were having uncertainties in the molalities within $\pm$ 2×10^{-5} $mol{\cdot}kg^{-1}$. The precision in the sound speed and the density measurements were $\pm$ 1×10^{-2} ms^{-1} and $\pm$ 1×10^{-3} $mol{\cdot}kg^{-1}$ respectively and the corresponding standard uncertainty in them approximately was found to be within $\pm$ 5×10^{-2} mS^{-1} and $\pm$ 5×10^{-3} $mol{\cdot}kg^{-1}$ respectively.

The acoustical parameters are obtained experimentally and some parameters are obtained by using these calculated parameters.

Section I		
Problem 1		
Volumetric and ultrasonic studies of molecular interactions of glycols in aqueous Niacin (vitamin B_3) at different temperatures		
		Ethylene Glycol
Water	+ Niacin +	Diethylene Glycol
		Triethylene Glycol
Problem 2		
Study of thermodynamic and acoustic properties of niacin in aqueous hexylene glycol and propylene glycol at different temperatures		
Water	+ Niacin +	Propylene Glycol
		Hexylene Glycol
Problem 3		
Volumetric and Ultrasonic study of polyethylene glycols in aqueous solutions of Niacin at different temperatures		
Water	+ Niacin +	Polyethylene Glycol 200
		Polyethylene Glycol 600
Problem 4		
Volumetric and Ultrasonic Studies of Molecular Interactions of PEG 400 and PEG 4000 in aqueous niacin solutions at Different Temperatures		
Water	+ Niacin +	Polyethylene Glycol 400
		Polyethylene Glycol 4000
Section II		
Problem 5		
Acoustic and thermodynamic study of D-Panthenol in aqueous solutions of glycol at different temperatures		
		Ethylene Glycol
Water	+ D-Panthenol +	Diethylene Glycol

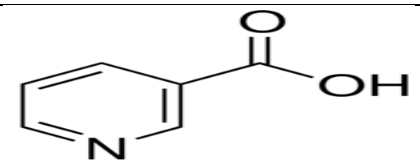
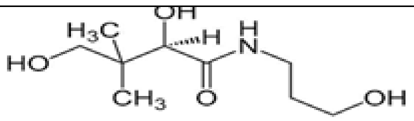
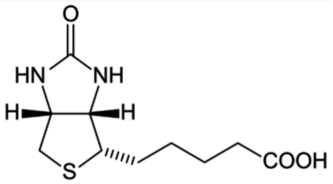
		Triethylene Glycol
Problem 6		
Investigation on temperature-dependent volumetric and acoustical properties of homologous series of glycols containing d-panthenol		
		Ethylene Glycol
Water	+ D-Panthenol +	Diethylene Glycol
		Triethylene Glycol
Problem 7		
Volumetric and ultrasonic studies of molecular interactions propylene glycol and hexylene glycol in aqueous D-Panthenol solutions at various temperatures		
Water	+ D-Panthenol +	Propylene Glycol
		Hexylene Glycol
Problem 8		
Thermodynamics of various interactions in homologous series of polyethylene glycols in aqueous medium of d-panthenol at t= (288.15, 298.15, 308.15 and 318.15) k: a volumetric and acoustic approach		
Water	+ D-Panthenol +	Polyethylene Glycol 200
		Polyethylene Glycol 400
Problem 9		
Measurement of density and ultrasonic speed of sound of polyethylene glycols (600 and 6000) in aqueous vitamin B_5 solutions at different temperatures		
Water	+ D-Panthenol +	Polyethylene Glycol 600
		Polyethylene Glycol 6000
Section III		
Problem 10		
Effect of ethylene glycol/diethylene glycol/triethylene glycol on the thermodynamics of the aqueous biotin solutions at various temperatures		
		Ethylene Glycol

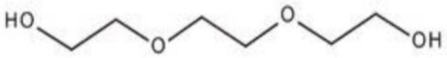
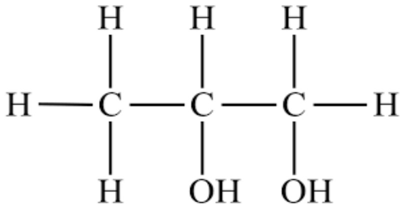
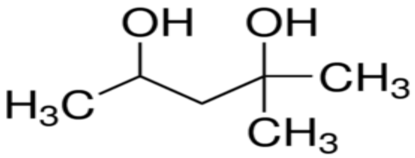
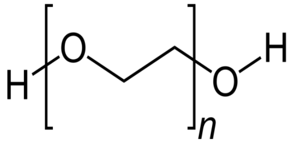
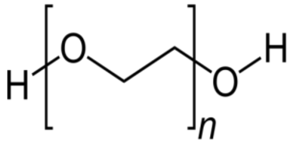
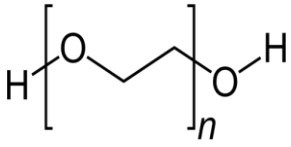
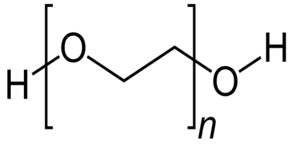
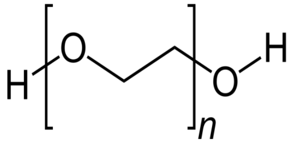
Water	+ Biotin +	Diethylene Glycol
		Triethylene Glycol
Problem 11		
Temperature-dependent thermodynamic and physicochemical studies of glycols in aqueous biotin solutions		
Water	+ Biotin +	Propylene Glycol
		Hexylene Glycol
Problem 12		
Densities and speed of sounds of (biotin + water + polyethylene glycols) solutions at different temperatures and atmospheric pressure		
Water	+ Biotin +	Polyethylene Glycol 200
		Polyethylene Glycol 400

3.3. Chemical structures

The structures of the chemicals used throughout the work are mentioned in following **Table 3.1**.

Table 3.1 List of chemicals structures used.

Name	Chemical structure
Niacin	
D-Panthenol	
Biotin	

Ethylene Glycol	
Diethylene Glycol	
Triethylene Glycol	
Propylene Glycol	
Hexylene Glycol	
Polyethylene Glycol 200	
Polyethylene Glycol 400	
Polyethylene Glycol 600	
Polyethylene Glycol 4000	
Polyethylene Glycol 6000	

3.4 Specifications of the Chemicals used

The specifications of the chemicals used throughout the work are mentioned in following **Table 3.2**.

Table 3.2 List of chemicals used and their specifications.

Sr. No.	Chemical	CAS No.	Molar Mass ($g \cdot mol^{-1}$)	Source	Purification method	Mass fraction purity(supplier)
1.	Niacin	59-67-6	123.11	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
2.	D-Panthenol	81-13-0	205.25	Sigma	Vacuum dried	≥0.98
3.	Biotin	58-85-5	244.31	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
4.	Ethylene Glycol	107-21-1	62.07	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
5.	Diethylene Glycol	111-46-6	106.12	SD. Fine Chem. Ltd., India	Vacuum dried	≥0.99
6.	Triethylene Glycol	112-27-6	150.18	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
7.	Propylene Glycol	57-55-6	76.09	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
8.	Hexylene Glycol	107-41-5	118.176	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99

9.	Polyethylene Glycol 200	25322-68-3	200	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
10.	Polyethylene Glycol 400	25322-68-3	400	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
11.	Polyethylene Glycol 600	25322-68-3	600	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
12.	Polyethylene Glycol 4000	25322-68-3	4000	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99
13.	Polyethylene Glycol 6000	25322-68-3	6000	Loba Chemie Pvt. Ltd. India	Vacuum dried	≥0.99

3.5 Methods and preparations

In **Table 3.1** the structures of the chemicals used throughout the study are provided along with their specifications in **Table 3.2**, which are achieved in their greatest purity. All of the solutions used in the tests were produced using freshly prepared triple distilled and degassed water with a specific conductance of 10-6 Scm^{-1}. All of the liquid samples were weighed on a Sartorius CPA 225D balance with a ±0.00001g precision. Measurements of newly produced samples were taken on the same day to avoid any ageing effects.

3.6 Experimental Techniques

3.6.1 Anton paar DSA 5000M

Within the temperature range of T = (288.15 to 318.15) K and 0.1 MPa pressure, the Anton Paar DSA 5000M densitimeter was used to measure densities and ultrasonic speeds of sound of aqueous solutions of Vitamin B [Vitamin B_3 (Niacin), Vitamin B_5 (D-Panthenol) and Vitamin B_7 (Biotin)] and their mixes with glycols [Ethylene Glycol (EG), Diethylene Glycol (DEG), Triethylene Glycol (TEG), Propylene Glycol (PG), Hexylene Glycol (HG), Polyethylene Glycol 200 (PEG 200), Polyethylene Glycol 400 (PEG 400), Polyethylene Glycol 600 (PEG 600), Polyethylene Glycol 4000 (PEG 4000) and Polyethylene Glycol 6000(PEG 6000)] as additions.

Figure 3.1 Anton Paar DSA 5000 M

Inside this apparatus are density and pulse-echo speed of sound cells, which determine two physically independent variables, density and sound speed, concurrently with a single sample (Figure 3.3 and 3.4). The temperature is regulated by a built-in thermostat in both measurement cells, which are constructed of stainless steel. Two embedded Pt 100 platinum thermometers, in combination with Peltier components, give temperature control accuracy of 0.001 K. The oscillating U-tube concept is used in this gadget. The characteristic frequency fluctuates depending on the density of the sample when around 3.5 mL of the bubble-free sample is placed into a U-shaped glass tube that is being driven to vibrate at its characteristic frequency electronically. The density of the sample may be assessed using a precise determination of the characteristic and a mathematical conversion. When the sample reaches the sound velocity measurement cell, which is surrounded on one side by an ultrasonic transmitter and on the other by a receiver, the transmitter emits sound waves with a defined period through the sample. The speed of sound may then be estimated by calculating the time of received sound waves and taking the distance between the transmitter and receiver into account.

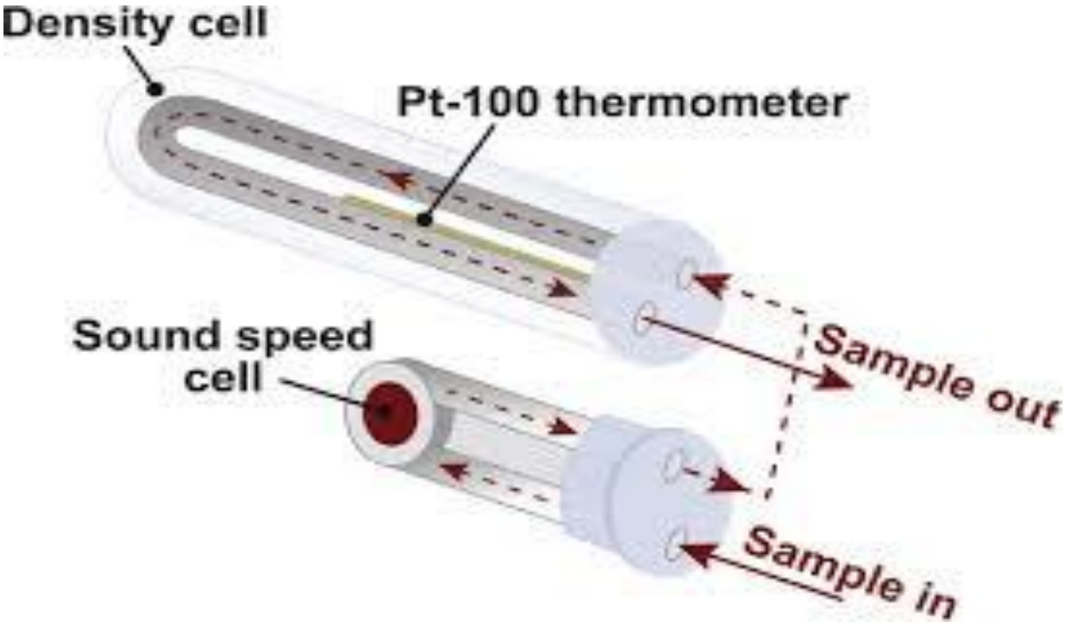


Figure 3.2 Density and sound speed cell of DSA 5000 M

After each usage, the measuring cells were rinsed with water and alcohol. Before each set of measurements, the device was calibrated using double distilled and degassed water and air at various temperatures. The sound densities and speeds were found to be in good accord with previous research. It can detect densities ranging from 0 to 3 g·cm^{-3} and sound speeds between 1000 and 2000 ms^{-1}.

3.6.1.1 Density measurements

Anton Paar DSA 5000 M is used for measuring the density of the ternary mixture.

3.6.1. 2 Ultrasonic speed measurements

Anton Paar DSA 5000 M is used for measuring the density of the ternary mixture.

3.7 Various acoustic parameters

3.7.1 Acoustic impedance

It is the resistance which is offered to the propagation of ultrasonic wave in a material, and is defined by the product of acoustic velocity (U) and density (ρ).

$$Z = \rho \times c \qquad (1)$$

This impedance is used for determining the acoustic reflection and transmission at the boundary of two materials having different acoustics impedances.

3.7.2 Adiabatic compressibility

It can be defined as fractional decrease in volume per unit increase of pressure , when there is no transfer of heat. These changes can be related to compressibility of medium but thermodynamic relations. This can be determined by density of medium and speed of sound using equations of Newton’s which were:

$$\beta = {}^{1}/_{[\rho(c^2)]} \qquad (2)$$

3.7.3 Intermolecular free length

Jacobson proposed an empirical relationship for determining liquid intermolecular free length. It is calculated as

$$L_f = K_T\,(\beta)^{1/2} \qquad (3)$$

The intermolecular free length may alternatively be written in terms of ultrasonic velocity and density as

$$L_f = K\left(c \times \rho^{1/2}\right) \tag{4}$$

3.7.4 Rao's constant

It is the simple relation between velocity of ultrasound and density of mixture and can be given as,

$$R = \left[(c^{\frac{1}{3}})M\right]\Big/\rho \tag{5}$$

3.7.5 Wada's constant

It is the relation between adiabatic compressibility, effective mass and density of the mixture. Relation is as follow as follows,

$$W = (\beta)^{-\frac{1}{7}}\left(\frac{M}{\rho}\right) \tag{6}$$

3.7.6 Vander Waal's Constant

It is determined by using the relation

$$b = \left(\frac{M}{\rho}\right)\left[1 - (RT/Mc^2)\sqrt{1 + (Mc^2/3RT)}-1\right] \tag{7}$$

Where,

Z= Acoustic impedance, β=Adiabatc compressibility, L_f= Intermolecular free length, W= Wada's constant (independent of temperature), R=Rao's constant, b= Vander Waal constant, M=Effective molecular weight, K_T= Temperature of dependent Jacobson's constant, ρ=Density of mixture and c = Ultrasonic velocity in the medium.

3.8 Apparent molar and Partial molar properties

3.8.1 Apparent molar volume

The difference in the volume of the solution and of the pure solvent per mole of solute is defined as the apparent molar volume.

It is the property of the solution which shows the variation in corresponding solution property when that entire component is added to this solution, per mole of component added.

$$V_{\phi} = M/\rho - (\rho - \rho_0)/m_A\, \rho\rho_0 \tag{8}$$

3.8.2 Partial molar volume

The difference of volume of solution when the mole of solute is added to a huge amount of the solution, where no appreciable change in the total concentration of the solution at constant temperature, pressure and number of molecules is observed, it is defined as the partial molar volume of a component.

It is the difference in the volume per mole of the substance added to the mixture.

$$V_{\phi} = V_{\phi}^{0} + S_V^{*} m_A \tag{9}$$

3.8.3 Partial molar volume of transfer

The transfer volume of glycols from water to the aqueous D-Panthenol solutions at infinite dilutions was computed with the following formula

$$\Delta V_{\phi}^{0} = V_{\phi}^{0}(\text{in aqueous Vitamin B solution}) - V_{\phi}^{0}(\text{water}) \tag{10}$$

3.8.4 Temperature dependent partial molar volume

The change in the apparent molar volume, V_{ϕ}^{0} along with temperature at finite dilution is given by the following equation

$$V_{\phi}^{0} = a + b\left(T - T_{ref}\right) + c\left(T - T_{ref}\right)^2 \tag{11}$$

in which T represent the temperature, T_{ref}=298.15 K, a, b and c represent the empirical constants.

3.8.5 Apparent molar isentropic compression

By using the following equation, apparent molar isentropic compression of EG, DEG and TEG in the aqueous solution of D-Panthenol is calculated

$$K_{\phi,S} = (Mk_S/\rho) - \{(k_{S,0}\rho - k_{S,0}\rho_0)/m_A\rho\rho_0\} \quad (12)$$

Where m_A, M, ρ, ρ_0, $k_{s.0}$ and k_s are the molality of solute, the molar mass of the solute, density of the solvent and the solution, isentropic compressibility of the pure solvent and the solution accordingly. The isentropic compressibility is determined by the following expression-

$$k_s = 1/c^2\rho \quad (13)$$

Where ρ and c are the density and ultrasonic velocity of the solution respectively.

3.8.6 Partial molar isentropic compression

By the following equation, the change in apparent molar isentropic compression $K_{\phi,s}$ with the molar concentration is given as

$$K_{\phi,s} = K^o_{\phi,s} + S^*_K m_A \quad (14)$$

Where, S^*_K is an experimental slope suggestive of solute-solute interaction.

3.8.7 Partial molar isentropic compression of transfer

At infinite dilution, the partial molar isentropic compressions $\Delta K^0_{\phi,S}$ of glycols in aqueous solution of chemical sample is calculated with the following equation

$$\Delta K^o_{\phi,s} = K^o_{\phi,s} \text{ (in aqueous Vitamin B solution)} - K^o_{\phi,s} \text{ (in water)} \quad (15)$$

3.8.8 Pair and triplet interaction coefficients

From the following relation, the partial molar volume of transfer and the partial molar isentropic compression of transfer can be obtained

$$\Delta V^0_{\phi}\text{(water to aqueous Vitamin B solution)} = 2V_{AB}m_B + 3V_{ABB}{m_B}^2 \quad (16)$$

$$\Delta K^0_{\phi}\text{(water to aqueous Vitamin B solution)} = 2K_{AB}m_B + 3K_{ABB}{m_B}^2 \quad (17)$$

Where A represent glycols and B represent Vitamin B and m_B denotes the molality of the aqueous Vitamin B solutions. The pair and triplet interaction coefficient are represented by the parameters V_{AB} and V_{ABB} for volume, and K_{AB}, K_{ABB} for isentropic compression.

3.9 Hydration Number

The hydration number for the liquid mixtures is calculated using the undermentioned equation which was developed by Passynsky

$$n_h = \frac{n_1}{n_2}\left(1 - \frac{k_s}{k_s^0}\right) \tag{18}$$

Here, n_1 is the number of moles of solvent, n_2 is the number moles of solute, k_s is the isentropic compressibility of the solution, and k_s^0 is the isentropic compressibility of solvent. It is considered that ions contain two hydration spheres: primary hydration spheres and secondary hydration spheres. The primary hydration sphere consists of water molecules that strongly combine with the ion through an electrostatic ion-dipole attraction. The secondary hydration sphere is made up of water molecules that interact partially with the primary hydration sphere ion and partially with the water structure in the surroundings which merge into the bulk after extending an undefined length from the ion. The calculated hydration numbers using various techniques can be classified into two groups where low values indicate the primary hydration number and larger values implies the primary hydration along with the overall or fractional part of the secondary hydration sphere. These hydration numbers are further used to determine the solvation property of ions with some other properties of solvent in the mixture. The decrement of the hydration numbers with the corresponding molality of glycols shows the ion-association and implies that the calculated hydration numbers from the compressibility data are due to both electrostriction and secondary hydration shell which contributes to hydrophobic hydration. Also, the high hydration numbers are attributed due to the presence of co-operative hydrogen bonding and a decrease in the solvating molecules due to the replacement of water molecules by glycol molecules in the coordination sphere of ions inside the mixture.

CHAPTER 4

RESULTS AND DISCUSSION

Section I

Problem 1

Volumetric and ultrasonic studies of molecular interactions of glycols in aqueous Niacin (vitamin B_3) at different temperatures

In this section, we have reported the densities, ρ and speed of sound c of ethylene glycol (EG), diethylene glycol (DEG) and triethylene glycol (TEG) in (0.00, 0.02, 0.04, 0.06) $mol \cdot kg^{-1}$ aqueous solutions of niacin at temperatures T = (293.15, 298.15, 303.15, 308.15) K.

4.1 Density

The experimentally obtained densities values are indexed in **Table 4.1** for (Niacin+water) and (Niacin+ water+ glycols) for concentrations (0.02, 0.04 and 0.06) $mol \cdot kg^{-1}$ and variation of temperature of (293.15, 298.15, 303.15 and 308.15) K. The (Glycols+ water) density values are taken directly from our previous paper with reference no. [1] from which it is evident from the data that the density values decrease with the temperature but increases with the Niacin concentration and Glycol molality**.** Using **Figure 4.2** the comparison of the literature density values [2] of (Niacin+ water) for temperature 298.15 K and 308.15 K with the experimental values as shown and it is observed that the experimental density values are in the inclination with the literature values.

4.2 Apparent molar volume

The Apparent molar volume is obtained using the following formula using the densities and molalities values

$$V_{\phi} = M/\rho - (\rho - \rho_0)/m_A \, \rho\rho_0 \tag{4.1}$$

Here, M, m_A, ρ, and ρ_0 are representing the molar mass of the solute, the molality of the solute per one kilogram of the solvent (Niacin+ water), the densities of the solution and the solvent respectively. The calculated apparent molar volume values are provided in **Table 4.1** and plotted in **Figure 4.3.** It is observed that the current ternary system of glycols in aqueous vitamin suggest strong solute and solvent interaction due to the positive V_{ϕ} values which increases with the upsurge in niacin concentration and glycol molar mass thus resulting in the increase of interaction from EG to DEG to TED, as shown in **Figure 4.1.** Niacin is very weak acid and glycols can show strong inter and intra molecular hydrogen bonding in presence of water [3, 4]. The existence of (dipole and dipole) interactions and (dipole-induced-dipole) are proven due to the upsurge in the V_{ϕ} values along with the temperatures. Also, this indicates the presence of hydrophilic effect and hydrophobic hydration [5, 6].

4.3 Partial molar volume

The following equation is used to obtain the partial molar volume of the liquid mixtures containing Niacin and glycol-

$$V_{\phi} = V_{\phi}^{0} + S_V^{*} m_A \tag{4.2}$$

Here m_A is the molality of the solute. The partial value of the apparent molar volume is obtained using the least square fitting of V_{ϕ} values and in **Table 4.2** the values of intercept V_{ϕ}^{0} are attributed along with the standard errors which are calculated from least square fitting. The V_{ϕ}^{0} values escalate upon the molar mass of glycols, from EG to DEG to TEG, as graphically described in **Figure 4.4**, thus suggesting the strong bond of hydrogen interaction between the hydrogen atom of water and oxygen atoms of glycols [7, 8]. The existence of solute-solvent interaction among the glycol and niacin molecules is observed which is implied by the V_{ϕ}^{0} values. In two ionic species the co-spheres overlap on each other, hence the volume increases, and due to the overlapping of (hydrophobic and hydrophobic) and (ion and hydrophobic) group the volume decreases as given by the overlap model of co-sphere [9-12]. Also, the V_{ϕ}^{0} data indicate that hydrophobic-hydrophobic interaction is dominated by ion-hydrophilic interaction. The experimental slope S_{V}^{*} with their standard error is reported in the same table. It shows the nature of (solute and solute) interactions as there is an irregular pattern in values of S_{V}^{*}. It consists of both positive and negative values, which are smaller than the V_{ϕ}^{0} values, therefore, implying the domination of (solute and solvent) interactions over (solute and solute) interactions [13].

4.4 Partial molar volume of transfer

Transfer of partial molar volume of glycols from water to niacin aqueous solutions at infinite dilution is computed employing the following formula

$$\Delta V_{\phi}^{0} = V_{\phi}^{0}(\text{in aqueous Niacin}) - V_{\phi}^{0}(\text{water}) \qquad (4.3)$$

The ΔV_{ϕ}^{0} values are listed in **Table 4.3** which are both positive and negative in magnitude with no regular pattern corresponding to the temperatures and concentrations of niacin. The model for pure water structure given by Pauling [14, 15] states the presence of empty areas in the water structures, termed as clathrates. In these spaces, the molecules of various organic solvents penetrate easily thus a very small portion of glycols molecules get situated in the cages of water structure such that the cage network is not eradicated. Perhaps higher content of glycols destroys the cage arrangement of water due to the formation of the new structure and hydrogen bond formation among water and organic molecules [16]. The presence of several interactions such as ion−hydrophobic, ion−hydrophilic, hydrophobic−hydrophobic and hydrophilic−hydrophilic interactions are possible in niacin and glycol (EG / DEG / TEG) molecules which are justified by the co-sphere overlap model regarding ΔV_{ϕ}^{0} values. Also, this provides the information of weak solute-solute interactions in the mixture [9-12].

4.5 Temperature-dependent partial molar volume

With temperatures, the variation in the apparent molar volume at infinite dilution is determined utilizing the following formula

$$V_{\phi}^{0}=a+b\left(T-T_{ref}\right)+c\left(T-T_{ref}\right)^{2} \quad (4.4)$$

Here, $a, b, c,$ are empirical constants listed in **Table 4.4**, T_{ref}=298.15 K, and the temperature in Kelvin is represented as T. The empirical constants are utilized to calculate the V_{ϕ}^{0} values and the aberrations obtained from the experimental data are also maintained in the same table. The coefficient c values are all positive for EG but negative for DEG and TEG. These positive c values define the deviation in the V_{ϕ}^{0} values and the values of R^{2} are found to be the best fit of data. The main purpose of V_{ϕ}^{0} was to obtain partial molar expansibilities values, which are computed using the undermentioned equation

$$E_{\phi}^{0}=\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}=b+2c\left(T-T_{ref}\right) \quad (4.5)$$

At infinite dilution, E_{ϕ}^{0} is the partial molar expansibility. This parameter is the valuable extent of solute-solvent interactions in the liquid mixtures and the following thermodynamic formula is established to evaluate this structure making or structure breaking capability of the liquid system.

$$\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}=\left(\partial^{2}\mathrm{V}_{\phi}/\partial \mathrm{T}^{2}\right)_{p}=2c \quad (4.6)$$

The sign of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ gives insight into the structure making/breaking ability of solution [17, 18]. The minute negative and positive values of this parameter, along with the values of E_{ϕ}^{0} are ascribed in **Table 4.5**, indicating the structure making ability. The E_{ϕ}^{0} values are both positive and negative, showing an irregular trend with temperatures, suggesting the existence of interactions among solute-solvent as previously analyzed from the V_{ϕ}^{0} values. These positive values of E_{ϕ}^{0} infer the interaction among the glycols and niacin molecules due to caging or packing effect [19-21].

4.6 Ultrasonic speed

Experimentally obtained speed of sound values at (293.15, 298.15, 303.15 and 308.15) K for (Niacin+ water) as well as (Niacin+water+ glycols) for (0.02, 0.04 and 0.06) mol·kg^{-1} concentrations are reported in **Table 4.6** and from our previous paper the speed of sound values for (Glycols+ water) is taken directly with reference no. [1]. In **Figure 4.5** the experimental speed of sound values are compared with the literature values [2] for temperature 298.15 K and 308.15 K and are graphically represented**,** which is increasing along with the temperatures and the concentrations of Niacin from (0.02 to 0.04 to 0.06) $\text{mol}\cdot\text{kg}^{-1}$, thus showing the same trend as the literature values. This phenomenon occurs due to the structure of water which consists of 3-dimensional networks of hydrogen bonds [22, 23]. This escalation of the speed of sound values for the glycol and vitamin mixture is by the virtue of the intermolecular hydrogen bonding in solute-solvent molecules and intramolecular hydrogen bonding in solute molecules hence indicates the higher combination rate of the molecules inside the solutions [24]. Also from the table, it is visible that the increment in the values of speed of sound with the molality of glycols refers to the hydrogen bond network insolvent with aqueous Niacin molecule. Furthermore, with the rise in the molar mass of the glycol, the hydrogen bond among the water and niacin molecules get depleted and eventually are abolished but concurrently fresh H-bonds are created amidst Niacin and glycol molecules [25].

4.7. Apparent molar isentropic compression

The Apparent molar isentropic compression for glycols in niacin aqueous solution is obtained using the mentioned formula

$$K_{\phi,S} = (Mk_S/\rho) - \{(k_{S,0}\rho - k_{S,0}\rho_0)/m_A\rho\rho_0\} \tag{4.7}$$

here, the molar mass of solute, densities of the solvent, the molality of solute, and densities of the solution, isentropic compressibility of the pure solvent, and the solution are represented as M, ρ, $m_{A,}$ $\rho_{0,}$ $k_{S.0}$ and k_S respectively. Using the following formula the isentropic compressibility is calculated

$$k_S = 1/c^2\rho \tag{4.8}$$

here, ρ represents the density of the solution and c denotes the values of speed of sound. The calculated $K_{\phi,S}$ values are all negative in magnitude and are listed in **Table 4.6.** The water molecule is more compressible inside bulk solution rather than the water molecules over solute due to negative values of $K_{\phi,S}$ which is decreasing with the thermal reading and upon the increment of the niacin concentration, the $K_{\phi,S}$ values increases as graphically represented in **Figure 4.6** for glycols at all temperatures [26, 27]. Therefore, the water molecules contract as a result of hydrophobic-hydrophobic interactions concerning the non-polar group, and the variation of $K_{\phi,S}$ values indicates the less compressibility of water molecules over the ionic charge group of solute and presents the arrangement of molecules of water in a specific pattern throughout the solute. Further, more loss of structural compressibility of water is observed by greater aligning effect created by solute and solvent due to negative values of $K_{\phi,S}$ [28, 29].

4.8 Partial molar isentropic compression

Using the following equation the partial molar isentropic compression is computed by contemplating the divergence of apparent molar isentropic compression along with the molality

$$k_{\phi,s} = K_{\phi,S}^{0} + S_{k}^{*} m_{A} \qquad (4.9)$$

Where, $K_{\phi,S}^{0}$, S_{K}^{*}, and m_A are the partial molar isentropic compression, the experimental slope of solute and the solute interactions, and the molality of the solute in the aqueous niacin and the $K_{\phi,S}^{0}$ values are reported in **Table 4.7** with the graphical depiction in **Figure 4.7**. The values of intercept $K_{\phi,S}^{0}$, and experimental slope S_{K}^{*} are attributed along with the partial errors which are calculated from least square fitting. The $K_{\phi,S}^{0}$ values are found to be less negative with the niacin concentration and increases with the temperature, thus implying the interactions are strong and attractive among the molecules of water and molecules of glycols [30]. This also suggests the abatement of electrostriction and ejection of molecules of water to bulk. Moreover, at high concentrations, water molecules around glycols are more compressible than at lower concentrations which results due to dehydration of glycols between niacin molecules [31]. The negative values of S_{K}^{*} confirms the existence of solute-solvent interactions at infinite dilution in the liquid mixture [32].

4. 9 Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer for glycol from water to aqueous niacin solutions at infinite dilution is determined using the following formula

$\Delta K_{\phi,s}^{0}$=$K_{\phi,s}^{0}$(in aqueous Niacin)- $K_{\phi,s}^{0}$(in water) (4.10)

The values of $\Delta K_{\phi,s}^{0}$ are listed in **Table 4.8,** which are all positive in nature. It is evident from the table that there exists structure making capability of solute due to the positive $\Delta K_{\phi,s}^{0}$ values and shows the interaction dominance between the zwitterionic center of glycol and niacin. With the glycol molality, the $\Delta K_{\phi,s}^{0}$ values increases, thus the extent of structure making ability increases along with the solute-solvent interactions in the ternary system [33].

4.10 Pair and triplet coefficients

Utilizing the following relation the partial molar volume of transfer and the partial molar isentropic compression of transfer can be obtained from:

ΔV_{ϕ}^{0}(water to aqueous Niacin solution)= $2V_{AB}m_B + 3V_{ABB}{m_B}^2$ (4.11)

ΔK_{ϕ}^{0}(water to aqueous Niacin solution)= $2K_{AB}m_B + 3K_{ABB}{m_B}^2$ (4.12)

Where A, B, and m_B denotes the glycols, niacin, and molality of the aqueous niacin solutions. In **Table 4.9** the pair and triplet interaction coefficients are mentioned for all temperatures which are represented as V_{AB}; V_{ABB} for volume and K_{AB}; K_{ABB} for isentropic compression. **.** In consonance with McMillan-Mayer [34] theory, the pair and triplet interaction are formulated for the liquid mixtures to analyze the parting of effects. This was later discussed by Friedman and Krishnan [35] and Franks et al [36]. The values of pair interaction coefficient V_{AB} are positive except for three values and triplet interaction coefficient V_{ABB} is all negative throughout all the temperatures for all glycols apart for two values which are positive in magnitude. While on the other hand, the pair interaction coefficient K_{AB} is positive for every temperature all over the glycol concentrations. In the case of triplet coefficient K_{ABB} all the values are partially positive and negative. Due to positive values of pair interaction coefficients and large triplet coefficients, it suggests the subjugation of pairwise interaction in (Niacin+ water) and (Niacin+ water +glycols) mixtures for compressibility and volumetric measurements [37].

4.11 Hydration number

Passynsky [38] developed an equation to calculate the hydration number for the liquid mixtures, which is given as follows-

$$n_h = \frac{n_1}{n_2}\left(1 - \frac{k_s}{k_s^0}\right) \tag{4.13}$$

Here, n_1 is the number moles of solvent,
n_2 is the number moles of solute,
k_s is the isentropic compressibility of solution, and
k_s^0 is the isentropic compressibility of solvent.

In **Table 4.10,** the calculated hydration number (n_h) for glycols in aqueous solutions of niacin are presented. It can be seen that the n_h values are very large which indicate the formation of hydrogen bonding in the liquid system and also, the hydration number decreases with the enhancement in the glycol molalities which can be attributed to the hydrophobic hydration for glycols in aqueous niacin solutions [39]. Further, the glycol molecules replaces the water molecules in the co-sphere of the ions and thus decreases the solvating molecules, as the water structure is considerably promoted by glycols which justifies the significant decrease in n_h values with glycol molalities [1, 38]. The hydration number lies between 111 and 555 over entire range of temperatures and concentrations, and it can be noted that the values does not show much of a difference for (EG, DEG and TEG) in all aqueous solution of niacin. This behavior implies the association of predominant out-sphere of hydration water molecules without any loss [1, 40].

Table 4.1

Values of densities, ρ, apparent molar volumes, V_ϕ of glycols in aqueous solutions of niacin at different temperatures and at the experimental pressure=0.1 MPa

$^a m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^6$/ (m^3·mol^{-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
EG+0.00 mol·kg^{-1} niacin								
0.0000	0.99925	0.99704	0.99403	0.99035^b				
0.0989	1.00011	0.99787	0.99484	0.99113	53.36	53.77	54.20	54.61^b
0.1989	1.00096	0.99868	0.99561	0.99188	53.45	53.87	54.35	54.78
0.2997	1.00178	0.99947	0.99636	0.99260	53.53	53.98	54.47	54.89
0.3948	1.00252	1.00018	0.99703	0.99326	53.64	54.09	54.59	55.01
0.5015	1.00334	1.00096	0.99776	0.99397	53.73	54.19	54.72	55.12
EG+0.02 mol·kg^{-1} niacin								
0.0000	0.99901	0.99781	0.99637	0.99479				
0.1107	0.99996	0.99872	0.99724	0.99562	53.47	53.86	54.28	54.73

0.1893	1.00061	0.99935	0.99784	0.99619	53.55	53.94	54.38	54.82
0.3166	1.00164	1.00034	0.99877	0.99708	53.66	54.05	54.51	54.96
0.4187	1.00243	1.00110	0.99949	0.99777	53.75	54.14	54.61	55.04
0.5025	1.00307	1.00169	1.00006	0.99830	53.82	54.23	54.69	55.14
EG+0.04 mol·kg^{-1} niacin								
0.0000	1.00000	0.99871	0.99724	0.99568				
0.1022	1.00087	0.99954	0.99803	0.99643	53.54	53.96	54.39	54.84
0.1926	1.00162	1.00026	0.99872	0.99708	53.61	54.01	54.45	54.91
0.2853	1.00237	1.00097	0.99940	0.99772	53.65	54.07	54.52	54.98
0.3957	1.00324	1.00180	1.00019	0.99847	53.71	54.14	54.58	55.07
0.5359	1.00431	1.00282	1.00115	0.99938	53.79	54.24	54.69	55.16
EG+0.06 mol·kg^{-1} niacin								
0.0000	1.00092	0.99951	0.99804	0.99648				
0.1148	1.00187	1.00042	0.99892	0.99731	53.65	54.07	54.46	54.91
0.1748	1.00236	1.00089	0.99936	0.99774	53.70	54.13	54.52	54.95
0.3093	1.00342	1.00190	1.00034	0.99866	53.80	54.22	54.61	55.05
0.4115	1.00420	1.00265	1.00105	0.99935	53.88	54.30	54.68	55.11

0.4915	1.00479	1.00321	1.00159	0.99986	53.94	54.35	54.74	55.17
DEG+0.00 mol·kg^{-1} niacin								
0.0000	0.99925	0.99704	0.99403	0.99035[b]				
0.0985	1.00068	0.99845	0.99544	0.99175	91.51	91.89	92.23	92.51[b]
0.1974	1.00206	0.99978	0.99677	0.99310	91.72	92.25	92.46	92.71
0.2950	1.00335	1.00102	0.99804	0.99436	91.90	92.50	92.64	92.92
0.4101	1.00483	1.00249	0.99947	0.99578	92.06	92.58	92.85	93.14
0.5006	1.00596	1.00358	1.00053	0.99685	92.17	92.69	93.03	93.31
DEG+0.02 mol·kg^{-1} niacin								
0.0000	0.99901	0.99781	0.99637	0.99479				
0.0979	1.00042	0.99918	0.99771	0.99611	91.61	92.17	92.58	92.89
0.1896	1.00170	1.00041	0.99891	0.99730	91.77	92.33	92.73	93.07
0.2993	1.00316	1.00182	1.00029	0.99865	91.96	92.53	92.92	93.27
0.3731	1.00410	1.00272	1.00118	0.99953	92.08	92.66	93.06	93.39
0.5358	1.00607	1.00462	1.00303	1.00134	92.37	92.95	93.35	93.70

DEG+0.04 mol·kg^{-1} niacin								
0.0000	1.00000	0.99871	0.99724	0.99568				
0.1064	1.00152	1.00018	0.99867	0.99708	91.72	92.23	92.79	93.17
0.1906	1.00267	1.00130	0.99975	0.99814	91.88	92.39	92.93	93.29
0.2888	1.00396	1.00255	1.00097	0.99934	92.05	92.56	93.08	93.44
0.3994	1.00534	1.00389	1.00228	1.00063	92.25	92.76	93.26	93.60
0.4957	1.00649	1.00500	1.00335	1.00169	92.44	92.94	93.44	93.78
DEG+0.06 mol·kg^{-1} niacin								
0.0000	1.00092	0.99951	0.99804	0.99648				
0.1098	1.00244	1.00100	0.99949	0.99789	92.02	92.49	92.97	93.36
0.2041	1.00370	1.00222	1.00068	0.99906	92.14	92.60	93.10	93.48
0.2594	1.00442	1.00292	1.00136	0.99973	92.21	92.68	93.17	93.54
0.3688	1.00580	1.00427	1.00267	1.00102	92.35	92.81	93.30	93.67
0.4976	1.00736	1.00578	1.00413	1.00246	92.51	92.97	93.46	93.81
TEG+0.00 mol·kg^{-1} niacin								
0.0000	0.99925	0.99704	0.99403	0.99035[b]				

0.0965	1.00136	0.99912	0.99609	0.99240	128.13	128.69	129.25	129.73[b]
0.2002	1.00355	1.00127	0.99821	0.99452	128.26	128.85	129.42	129.89
0.2920	1.00541	1.00310	1.00001	0.99632	128.38	128.97	129.60	130.03
0.3986	1.00749	1.00514	1.00202	0.99833	128.53	129.15	129.76	130.19
0.4988	1.00936	1.00699	1.00385	1.00014	128.69	129.28	129.89	130.34
TEG+0.02 $\mathrm{mol\cdot kg^{-1}}$ niacin								
0.0000	0.99901	0.99781	0.99637	0.99479				
0.1018	1.00122	0.99998	0.99850	0.99689	128.24	128.84	129.34	129.85
0.2273	1.00385	1.00254	1.00101	0.99937	128.38	128.99	129.53	130.02
0.3071	1.00545	1.00410	1.00254	1.00088	128.47	129.10	129.65	130.13
0.4162	1.00757	1.00616	1.00456	1.00286	128.61	129.25	129.82	130.30
0.5103	1.00932	1.00788	1.00624	1.00451	128.74	129.37	129.94	130.44
TEG+0.04 $\mathrm{mol\cdot kg^{-1}}$ niacin								
0.0000	1.00000	0.99871	0.99724	0.99568				
0.1072	1.00231	1.00097	0.99946	0.99786	128.35	128.97	129.45	129.96

0.2161	1.00456	1.00317	1.00163	0.99999	128.49	129.11	129.60	130.10
0.2976	1.00619	1.00475	1.00319	1.00153	128.59	129.22	129.72	130.21
0.3993	1.00814	1.00666	1.00506	1.00337	128.73	129.37	129.87	130.38
0.4943	1.00991	1.00839	1.00674	1.00503	128.85	129.48	130.02	130.52
TEG+0.06 mol·kg^{-1} niacin								
0.0000	1.00092	0.99951	0.99804	0.99648				
0.1019	1.00309	1.00163	1.00013	0.99854	128.46	129.10	129.56	130.05
0.2024	1.00516	1.00365	1.00212	1.00050	128.57	129.22	129.68	130.18
0.3091	1.00727	1.00572	1.00415	1.00249	128.69	129.34	129.82	130.31
0.3826	1.00868	1.00709	1.00550	1.00382	128.77	129.43	129.91	130.41
0.5067	1.01098	1.00933	1.00770	1.00598	128.92	129.58	130.07	130.57

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[a] m_A is the molality of glycols in the aqueous solution niacin; standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1},[b]Values of densities for (EG + water, DEG + water and TEG + water) at temperature 298.15 to 308.15 K have been taken from our previous paper [1]

Table 4.2

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_{V}^{*}, of glycols in the aqueous solution of niacin at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$V_{\phi}^{0}\times 10^{6}$/(m^{3}·mol^{-1})				$S_{V}^{*}\times 10^{6}$/(m^{3}·kg·mol^{-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
EG								
0.00	53.26(±0.00)	53.67(±0.00)	54.13(±0.02)	54.54(±0.02)^{b}	0.95(±0.01)	1.03(±0.00)	1.11(±0.04)	1.13(±0.04)^{b}
0.02	53.38(±0.00)	53.76(±0.00)	54.17(±0.00)	54.62(±0.00)	0.89(±0.01)	0.94(±0.01)	1.03(±0.01)	1.02(±0.01)
0.04	53.49(±0.00)	53.89(±0.00)	54.32(±0.00)	54.77(±0.00)	0.57(±0.01)	0.64(±0.00)	0.68(±0.01)	0.74(±0.01)
0.06	53.57(±0.00)	53.99(±0.00)	54.38(±0.00)	54.83(±0.00)	0.76(±0.01)	0.74(±0.01)	0.74(±0.01)	0.69(±0.01)
DEG								
0.00	91.42(±0.02)	91.88(±0.06)	92.11(±0.02)	92.36(±0.02)^{b}	1.48(±0.11)	1.62(±0.13)	1.73(±0.05)	1.85(±0.04)^{b}
0.02	91.44(±0.00)	91.99(±0.00)	92.40(±0.00)	92.72(±0.00)	1.73(±0.01)	1.79(±0.01)	1.76(±0.01)	1.83(±0.01)
0.04	91.52(±0.00)	92.04(±0.00)	92.61(±0.00)	92.99(±0.01)	1.83(±0.01)	1.83(±0.01)	1.65(±0.02)	1.57(±0.04)
0.06	91.88(±0.00)	92.35(±0.00)	92.84(±0.00)	93.24(±0.00)	1.27(±0.00)	1.26(±0.00)	1.25(±0.02)	1.16(±0.01)

TEG								
0.00	127.97(±0.01)	128.55(±0.00)	129.14(±0.02)	129.61(±0.01)[b]	1.44(±0.02)	1.49(±0.01)	1.48(±0.03)	1.41(±0.02)[b]
0.02	128.10(±0.01)	128.70(±0.00)	129.20(±0.00)	129.69(±0.00)	1.22(±0.04)	1.31(±0.02)	1.46(±0.02)	1.46(±0.02)
0.04	128.20(±0.00)	128.82(±0.00)	129.29(±0.00)	129.79(±0.01)	1.31(±0.01)	1.34(±0.01)	1.46(±0.02)	1.45(±0.03)
0.06	128.35(±0.00)	128.98(±0.00)	129.43(±0.00)	129.92(±0.00)	1.12(±0.00)	1.19(±0.00)	1.27(±0.00)	1.29(±0.01)

[a] m_B is the molality of aqueous niacin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}, $u(V_\phi^0)$= ±0.01 × 10^6/(m^3·mol^{-1}) and $u(S_V^*)$=±0.03 × 10^6/(m^3·kg·mol^{-2}), [b] Values of Partial molar volumes (V_ϕ^0) and experimental slopes (S_V^*) for (EG + water, DEG + water and TEG + water) at temperature 298.15 to 308.15 K have been taken from our previous paper [1]

Table 4.3

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in the aqueous solution of niacin at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
EG				
0.02	0.04	0.10	0.29	0.54
0.04	0.07	0.23	0.44	0.69
0.06	0.15	0.33	0.50	0.75
DEG				
0.02	-0.08	0.18	0.58	0.66
0.04	0.00	0.23	0.79	0.93
0.06	0.36	0.54	1.02	1.18
TEG				
0.02	-0.16	0.15	0.42	0.59
0.04	-0.06	0.27	0.51	0.69
0.06	0.09	0.43	0.65	0.82

$^{a}m_{B}$ is the molality of aqueous niacin, standard uncertainties *u* are *u(m) = 1%, u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}.

Table 4.4

Values of empirical parameters of Eq. 4, of glycols in the aqueous solution of niacin at different temperatures.

$^a m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/ (m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
EG					
0.02	53.758	0.080	0.001	0.9999	0.000
0.04	53.892	0.083	0.000	0.9999	0.000
0.06	53.978	0.083	0.000	0.9999	0.004
DEG					
0.02	91.985	0.097	-0.002	0.9999	0.000
0.04	92.074	0.106	-0.001	0.9999	0.000
0.06	92.366	0.095	-0.001	0.9999	0.003
TEG					
0.02	128.687	0.110	-0.001	0.9999	0.000

0.04	128.795	0.110	-0.001	0.9999	0.000
0.06	128.943	0.110	-0.001	0.9999	0.002

[a] m_B is the molality aqueous of niacin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}

Table 4.5

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in aqueous solution of niacin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	E_{ϕ}^{0} ×10^{6}/ (m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K	
EG					
0.02	0.073	0.080	0.087	0.094	0.001
0.04	0.078	0.083	0.088	0.092	0.001
0.06	0.080	0.083	0.085	0.087	0.000
DEG					
0.02	0.120	0.097	0.073	0.049	-0.005
0.04	0.119	0.106	0.093	0.080	-0.003
0.06	0.101	0.095	0.088	0.081	-0.001
TEG					
0.02	0.121	0.110	0.100	0.090	-0.002
0.04	0.122	0.110	0.099	0.087	-0.002
0.06	0.122	0.110	0.099	0.087	-0.002

$^{a}m_B$ is the molality aqueous of niacin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}.

Table 4.6

Values of the speed of sound, c, apparent molar isentropic compression, $K_{\phi,S}$ of glycols in aqueous solutions of niacin at different temperatures and at the experimental pressure=0.1 MPa

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,S} \times 10^6$/ (m^3·mol^{-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
EG+0.00 mol·kg^{-1} niacin								
0.0000	1466.6	1495.9	1519.1	1536.0^{b}				
0.0989	1469.6	1498.9	1521.8	1539.2	-46.06	-44.27	-42.93	-45.43^{b}
0.1989	1472.7	1501.7	1524.0	1542.2	-46.34	-44.54	-43.18	-45.69
0.2997	1475.4	1504.8	1526.2	1544.9	-46.46	-44.65	-43.29	-45.80
0.3948	1478.6	1507.4	1528.3	1547.9	-46.53	-44.71	-43.35	-45.86
0.5015	1481.2	1510.1	1530.3	1550.6	-46.59	-44.77	-43.41	-45.92
EG+0.02 mol·kg^{-1} niacin								
0.0000	1484.8	1498.1	1510.2	1520.5				
0.1107	1487.8	1501.3	1513.1	1523.4	-45.00	-44.20	-43.49	-42.90

0.1893	1490.0	1503.6	1515.0	1525.2	-45.20	-44.39	-43.68	-43.09
0.3166	1493.6	1507.3	1518.3	1527.9	-45.34	-44.53	-43.81	-43.22
0.4187	1496.5	1510.1	1520.9	1530.1	-45.41	-44.60	-43.88	-43.28
0.5025	1498.8	1512.3	1523.0	1531.7	-45.46	-44.64	-43.92	-43.32
EG+0.04 mol·kg^{-1} niacin								
0.0000	1486.6	1499.7	1511.9	1522.3				
0.1022	1489.4	1502.8	1514.6	1525.0	-44.85	-44.07	-43.35	-42.76
0.1926	1491.9	1505.4	1517.0	1527.0	-45.09	-44.30	-43.59	-42.99
0.2853	1494.5	1508.2	1519.3	1528.9	-45.20	-44.41	-43.69	-43.09
0.3957	1497.6	1511.4	1522.1	1531.3	-45.28	-44.49	-43.77	-43.17
0.5359	1501.6	1515.3	1525.5	1534.5	-45.36	-44.56	-43.84	-43.23
EG+0.06 mol·kg^{-1} niacin								
0.0000	1488.0	1501.4	1513.4	1524.3				
0.1148	1491.0	1504.8	1516.5	1527.3	-44.82	-44.02	-43.32	-42.70
0.1748	1492.8	1506.7	1518.1	1528.6	-44.97	-44.17	-43.47	-42.84
0.3093	1496.5	1510.7	1521.5	1531.5	-45.13	-44.33	-43.62	-42.99
0.4115	1499.5	1513.6	1524.2	1533.8	-45.20	-44.39	-43.69	-43.06

0.4915	1501.8	1515.7	1526.2	1535.7	-45.25	-44.44	-43.73	-43.10
DEG+0.00 mol·kg^{-1} niacin								
0.0000	1466.6	1495.8	1519.1	1536.0[b]				
0.0985	1472.1	1501.2	1523.5	1541.6	-46.09	-44.30	-42.95	-42.01[b]
0.1974	1478.0	1506.0	1527.5	1547.2	-46.39	-44.59	-43.23	-42.28
0.2950	1483.8	1510.8	1531.5	1552.7	-46.53	-44.72	-43.36	-42.41
0.4101	1489.4	1516.1	1536.1	1558.1	-46.64	-44.83	-43.46	-42.51
0.5006	1494.7	1520.3	1539.6	1563.2	-46.72	-44.90	-43.53	-42.58
DEG+0.02 mol·kg^{-1} niacin								
0.0000	1484.8	1498.1	1510.2	1520.5				
0.0979	1491.4	1503.2	1514.6	1525.2	-44.97	-44.17	-43.46	-42.87
0.1896	1496.5	1508.0	1519.0	1529.0	-45.25	-44.44	-43.73	-43.14
0.2993	1502.3	1513.4	1523.9	1533.6	-45.40	-44.59	-43.87	-43.28
0.3731	1506.2	1516.8	1526.9	1536.7	-45.47	-44.66	-43.94	-43.35
0.5358	1513.9	1524.5	1534.0	1543.0	-45.60	-44.78	-44.06	-43.46

DEG+0.04 mol·kg^{-1} niacin								
0.0000	1486.6	1499.7	1511.9	1522.3				
0.1064	1493.9	1505.3	1516.9	1527.6	-44.90	-44.11	-43.40	-42.81
0.1906	1498.6	1509.9	1520.9	1531.2	-45.14	-44.35	-43.63	-43.04
0.2888	1504.0	1514.6	1525.5	1535.3	-45.28	-44.48	-43.76	-43.16
0.3994	1509.6	1520.0	1530.3	1540.0	-45.38	-44.59	-43.86	-43.26
0.4957	1514.0	1524.8	1534.6	1543.9	-45.46	-44.66	-43.93	-43.33
DEG+0.06 mol·kg^{-1} niacin								
0.0000	1488.0	1501.4	1513.4	1524.3				
0.1098	1495.6	1507.0	1518.6	1529.7	-44.83	-44.03	-43.33	-42.71
0.2041	1501.0	1512.2	1523.2	1533.8	-45.07	-44.27	-43.56	-42.94
0.2594	1503.8	1514.9	1525.8	1536.0	-45.15	-44.34	-43.64	-43.01
0.3688	1509.8	1520.4	1531.0	1540.7	-45.27	-44.45	-43.75	-43.12
0.4976	1515.9	1526.8	1536.5	1546.1	-45.37	-44.55	-43.84	-43.21
TEG+0.00 mol·kg^{-1} niacin								
0.0000	1466.6	1495.8	1519.1	1536.0^{b}				

0.0965	1474.7	1503.5	1525.1	1544.0	-46.12	-44.33	-42.97	-42.04[b]
0.2002	1483.3	1511.0	1531.3	1552.2	-46.47	-44.66	-43.30	-42.36
0.2920	1491.7	1517.6	1536.9	1560.6	-46.63	-44.82	-43.45	-42.50
0.3986	1499.2	1525.4	1543.3	1567.8	-46.77	-44.95	-43.57	-42.62
0.4988	1508.5	1532.2	1549.4	1576.9	-46.88	-45.05	-43.68	-42.72
TEG+0.02 $\text{mol}\cdot\text{kg}^{-1}$ niacin								
0.0000	1484.8	1498.1	1510.2	1520.5				
0.1018	1493.8	1505.9	1516.7	1526.8	-45.02	-44.22	-43.51	-42.92
0.2273	1503.2	1514.8	1525.0	1534.6	-45.39	-44.58	-43.86	-43.27
0.3071	1509.5	1520.7	1530.5	1539.3	-45.51	-44.70	-43.98	-43.38
0.4162	1518.0	1528.6	1537.7	1546.1	-45.65	-44.83	-44.11	-43.51
0.5102	1524.6	1535.1	1543.9	1551.8	-45.75	-44.93	-44.20	-43.60
TEG+0.04 $\text{mol}\cdot\text{kg}^{-1}$ niacin								
0.0000	1486.6	1499.7	1511.9	1522.3				
0.1072	1495.8	1507.9	1518.8	1529.0	-44.94	-44.15	-43.44	-42.85

0.2161	1505.1	1515.8	1526.4	1535.9	-45.25	-44.46	-43.74	-43.14
0.2976	1510.6	1522.0	1531.9	1540.7	-45.38	-44.59	-43.87	-43.27
0.3993	1519.6	1529.3	1538.7	1547.1	-45.51	-44.71	-43.99	-43.38
0.4943	1526.6	1536.4	1544.6	1553.0	-45.61	-44.81	-44.08	-43.48
TEG+0.06 mol·kg^{-1} niacin								
0.0000	1488.0	1501.4	1513.4	1524.3				
0.1019	1497.5	1509.3	1520.1	1530.9	-44.83	-44.02	-43.33	-42.71
0.2024	1505.6	1516.9	1527.1	1537.3	-45.14	-44.33	-43.63	-43.00
0.3091	1513.3	1524.9	1534.4	1543.9	-45.31	-44.50	-43.79	-43.16
0.3826	1520.1	1530.1	1539.4	1548.5	-45.40	-44.59	-43.88	-43.25
0.5067	1530.1	1539.4	1547.1	1556.3	-45.54	-44.71	-44.00	-43.37

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[a] m_A is the molality of glycols in the aqueous solution niacin; standard uncertainties *u* are *u(m)* = 1%, *u(T)*=0.001 K, *u(ρ)*=0.15(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1},[b]Values of speed of sound for (EG + water, DEG + water and TEG + water) at temperature 298.15 and 308.15 K have been taken from our previous paper [1]

Table 4.7

Partial molar isentropic compression, $K^0_{\phi,s}$, and experimental slopes, S^*_k, of glycols in the aqueous solution of niacin at different temperatures.

[a]m_B/ (mol·kg^{-1})	$K^0_{\phi,s}\times10^6$/(m^3·mol^{-1}· GPa^{-1})				$S^*_k\times10^6$/(kg·m^3·mol^{-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
EG								
0.00	-46.13(±0.06)	-44.34(±0.06)	-42.99(±0.06)	-42.05(±0.06)[b]	-0.83(±0.13)	-0.78(±0.12)	-0.75(±0.12)	-0.73(±0.12)[b]
0.02	-44.94(±0.06)	-44.14(±0.06)	-43.43(±0.06)	-42.85(±0.06)	-1.12(±0.18)	-1.09(±0.18)	-1.05(±0.17)	-1.03(±0.17)
0.04	-44.82(±0.07)	-44.04(±0.07)	-43.33(±0.07)	-42.74(±0.07)	-1.11(±0.22)	-1.07(±0.22)	-1.04(±0.22)	-1.02(±0.21)
0.06	-44.75(±0.05)	-43.95(±0.05)	-43.25(±0.05)	-42.63(±0.05)	-1.10(±0.16)	-1.07(±0.16)	-1.04(±0.15)	-1.01(±0.15)
DEG								
0.00	-46.14(±0.08)	-44.35(±0.06)	-43.00(±0.06)	-42.06(±0.06)[b]	-1.06(±0.13)	-1.00(±0.13)	-0.98(±0.12)	-0.96(±0.12)[b]
0.02	-44.93(±0.08)	-44.13(±0.08)	-43.42(±0.08)	-42.84(±0.08)	-1.38(±0.25)	-1.34(±0.24)	-1.31(±0.24)	-1.28(±0.24)
0.04	-44.83(±0.07)	-44.04(±0.06)	-43.33(±0.06)	-42.74(±0.06)	-1.36(±0.21)	-1.33(±0.21)	-1.29(±0.20)	-1.27(±0.20)

0.06	-44.76(±0.07)	-43.96(±0.06)	-43.26(±0.06)	-42.64(±0.06)	-1.32(±0.22)	-1.29(±0.21)	-1.25(±0.21)	-1.23(±0.21)
TEG								
0.00	-46.15(±0.07)	-44.36(±0.07)	-43.00(±0.06)	-42.06(±0.06)[b]	-1.36(±0.14)	-1.29(±0.14)	-1.25(±0.13)	-1.23(±0.13)[b]
0.02	-44.93(±0.08)	-44.13(±0.08)	-43.42(±0.08)	-42.84(±0.08)	-1.71(±0.24)	-1.67(±0.23)	-1.63(±0.23)	-1.60(±0.23)
0.04	-44.83(±0.07)	-44.05(±0.07)	-43.34(±0.07)	-42.75(±0.07)	-1.68(±0.22)	-1.64(±0.22)	-1.60(±0.21)	-1.57(±0.21)
0.06	-44.73(±0.07)	-43.94(±0.07)	-43.24(±0.07)	-42.62(±0.07)	-1.70(±0.23)	-1.65(±0.23)	-1.61(±0.23)	-1.58(±0.23)

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[a] m_B is the molality of aqueous niacin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}, $u(K_{\phi,s}^{0})$= ±0.01 ×10^{6}/(m^{3}·mol^{-1}·GPa^{-1}) and $u(S_k^*)$= ±0.24×10^{6}/(kg·m^{3}·mol^{-2}· GPa^{-1}), [b]Values of Partial molar isentropic compression, ($K_{\phi,s}^{0}$) and experimental slopes (S_k^*) for (EG + water, DEG + water and TEG + water) at temperature 298.15 to 308.15 K have been taken from our previous paper [1]

Table 4.8

Partial molar isentropic compression transfer, $\Delta K^0_{\phi,s}$, of glycols in aqueous solution of niacin at different temperatures.

${}^a m_B$/ (mol·kg^{-1})	$\Delta K^0_{\phi,s}$, × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
EG				
0.02	0.19	0.09	0.05	0.03
0.04	0.31	0.19	0.15	0.14
0.06	0.38	0.28	0.23	0.25
DEG				
0.02	0.20	0.12	0.07	0.06
0.04	0.30	0.21	0.16	0.16
0.06	0.37	0.29	0.23	0.26
TEG				
0.02	0.20	0.12	0.06	0.06
0.04	0.30	0.20	0.14	0.15
0.06	0.40	0.31	0.24	0.28

${}^a m_B$ is the molality of aqueous niacin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}.

Table 4.9

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of niacin at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
EG				
288.15	-1.08	26.46	5.44	-25.02
298.15	2.64	1.71	2.28	0.84
308.15	8.56	-48.94	1.24	7.66
318.15	15.43	-103.53	0.62	16.26
DEG				
288.15	-5.10	89.74	5.67	-28.86
298.15	2.25	22.82	3.10	-7.60
308.15	15.31	-77.42	1.80	1.20
318.15	17.68	-88.92	1.45	7.72
TEG				
288.15	-5.00	64.68	5.36	-23.31

298.15	3.54	-0.26	2.78	-2.10
308.15	10.88	-62.77	1.20	8.96
318.15	15.85	-102.83	1.14	13.07

T/K is the temperatures, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}.

Table 4.10

Hydration number for glycols in aqueous solutions of niacin at different temperatures

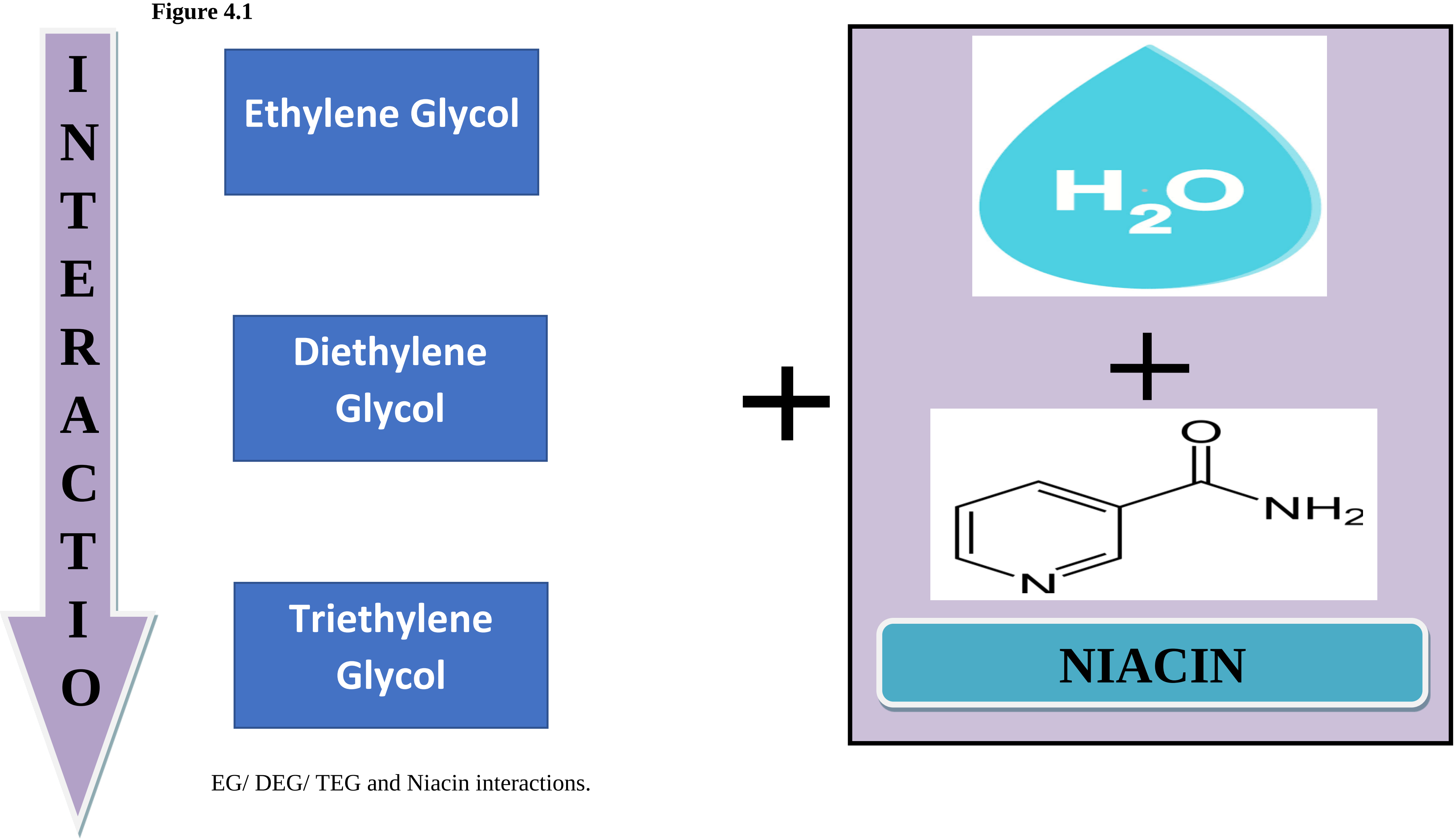
$^{a}m_A$/(mol·kg^{-1})	n_h			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
EG+0.00 mol·kg^{-1} niacin				
0.0989	554.997	555.036	554.997	554.997^{b}
0.1989	277.500	277.519	277.499	277.500
0.2997	185.001	185.014	185.000	185.001
0.3948	138.751	138.761	138.751	138.751
0.5016	111.002	111.009	111.001	111.001
EG+0.02 mol·kg^{-1} niacin				
0.1107	555.022	555.022	555.022	555.022
0.1893	277.512	277.512	277.512	277.512
0.3166	185.009	185.009	185.009	185.009
0.4187	138.757	138.758	138.757	138.757
0.5025	111.006	111.006	111.006	111.006
EG+0.04 mol·kg^{-1} niacin				
0.1022	555.042	555.042	555.042	555.042
0.1926	277.522	277.522	277.522	277.522
0.2853	185.016	185.016	185.015	185.015
0.3957	138.762	138.762	138.762	138.762
0.5359	111.011	111.011	111.010	111.010
EG+0.06 mol·kg^{-1} niacin				
0.1148	555.062	555.062	555.062	555.062
0.1748	277.532	277.532	277.532	277.532
0.3093	185.022	185.023	185.022	185.022
0.4115	138.767	138.768	138.767	138.767
0.4915	111.014	111.014	111.014	111.014
DEG+0.00 mol·kg^{-1} niacin				

0.0985	554.999	555.038	554.998	554.999[b]
0.1974	277.502	277.521	277.501	277.502
0.2951	185.003	185.015	185.002	185.003
0.4101	138.754	138.763	138.752	138.753
0.5006	111.004	111.011	111.003	111.003
DEG+0.02 mol·kg^{-1} niacin				
0.0979	555.025	555.024	555.023	555.024
0.1896	277.515	277.514	277.514	277.513
0.2993	185.012	185.011	185.011	185.010
0.3731	138.759	138.759	138.759	138.758
0.5358	111.009	111.008	111.008	111.008
DEG+0.04 mol·kg^{-1} niacin				
0.1064	555.046	555.044	555.044	555.044
0.1906	277.525	277.524	277.524	277.524
0.2888	185.018	185.017	185.017	185.017
0.3994	138.765	138.764	138.764	138.764
0.4957	111.013	111.012	111.012	111.012
DEG+0.06 mol·kg^{-1} niacin				
0.1098	555.066	555.064	555.064	555.064
0.2041	277.535	277.534	277.534	277.534
0.2594	185.024	185.024	185.023	185.023
0.3688	138.769	138.769	138.769	138.768
0.4976	111.017	111.016	111.016	111.016
TEG+0.00 mol·kg^{-1} niacin				
0.0965	555.002	555.040	555.000	555.001[b]
0.2002	277.505	277.523	277.503	277.504
0.2921	185.005	185.017	185.003	185.005
0.3986	138.756	138.764	138.754	138.755
0.4988	111.006	111.013	111.004	111.006

TEG+0.02 mol·kg^{-1} niacin				
0.1018	555.027	555.026	555.025	555.025
0.2273	277.518	277.517	277.516	277.516
0.3071	185.014	185.013	185.012	185.012
0.4162	138.762	138.761	138.761	138.760
0.5103	111.011	111.010	111.010	111.009
TEG+0.04 mol·kg^{-1} niacin				
0.1072	555.048	555.047	555.046	555.045
0.2161	277.528	277.527	277.526	277.526
0.2976	185.020	185.020	185.019	185.019
0.3993	138.767	138.766	138.766	138.765
0.4943	111.015	111.014	111.014	111.013
TEG+0.06 mol·kg^{-1} niacin				
0.1019	555.068	555.066	555.065	555.065
0.2024	277.537	277.536	277.536	277.535
0.3091	185.027	185.027	185.026	185.026
0.3826	138.772	138.771	138.770	138.770
0.5067	111.019	111.018	111.018	111.017

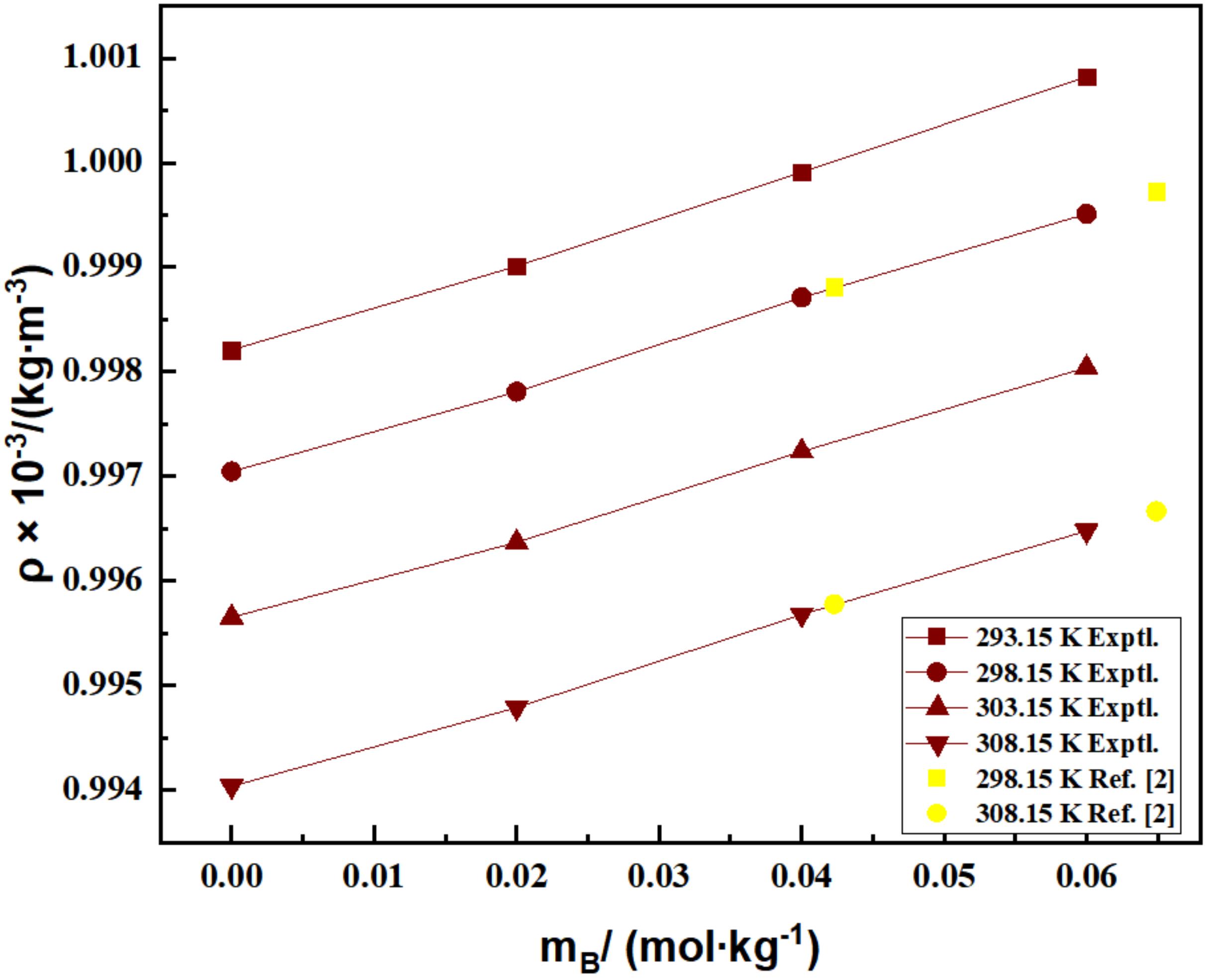
$^{a}m_A$ is the molality of glycols in the aqueous solution niacin, ^{b}Values of hydration number for (EG + water, DEG + water and TEG + water) at temperature 298.15 and 308.15 K have been taken from our previous paper [1]

Figure 4.1



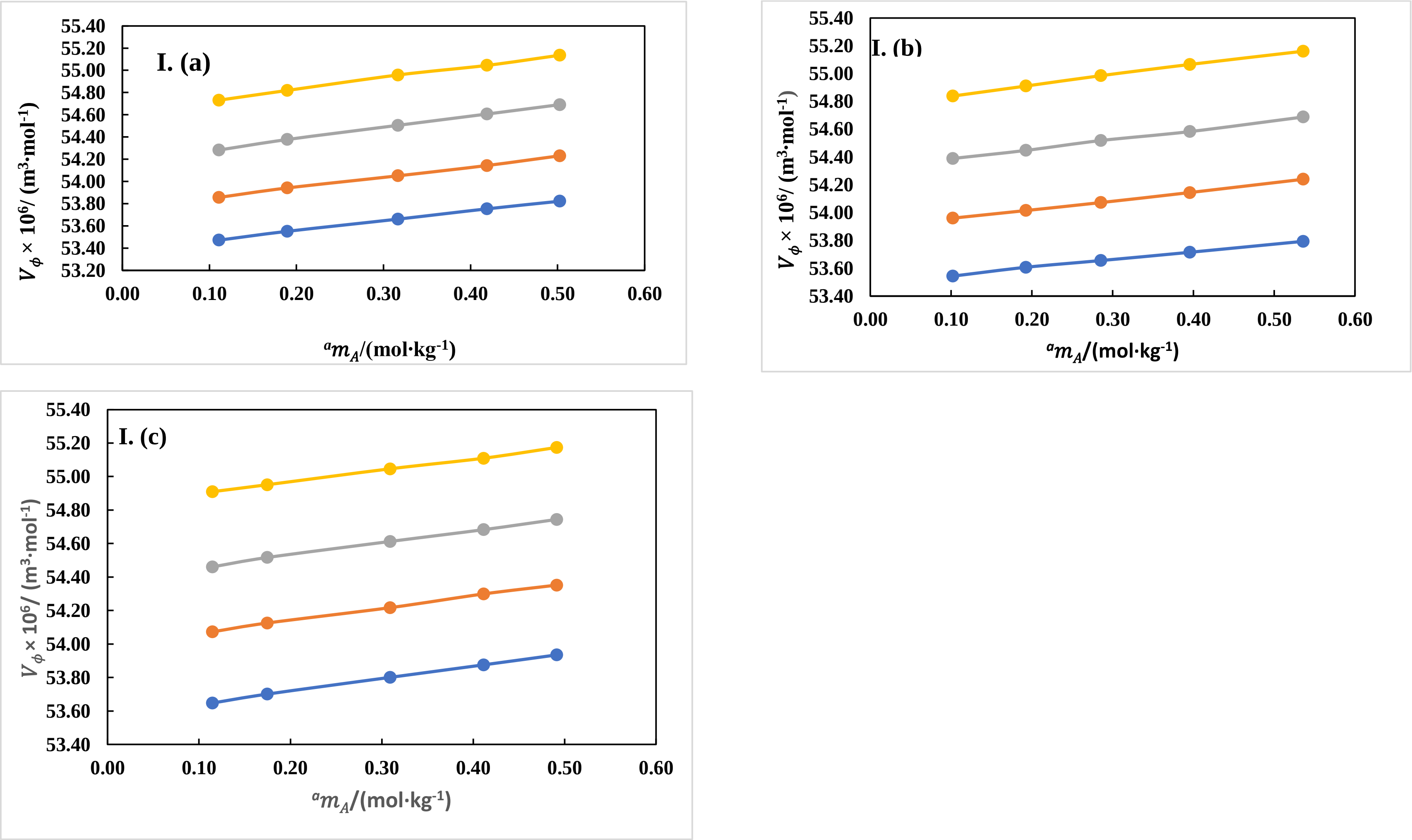
EG/ DEG/ TEG and Niacin interactions.

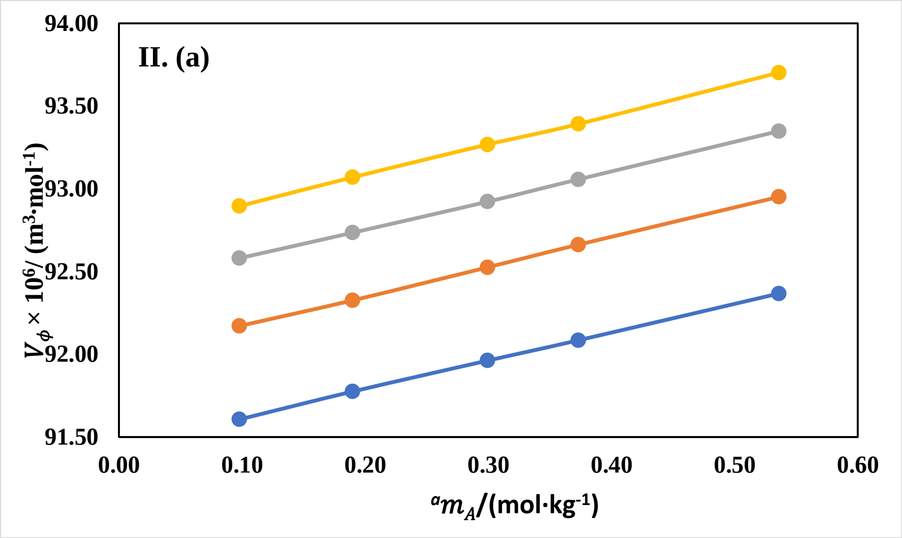
Figure 4.2

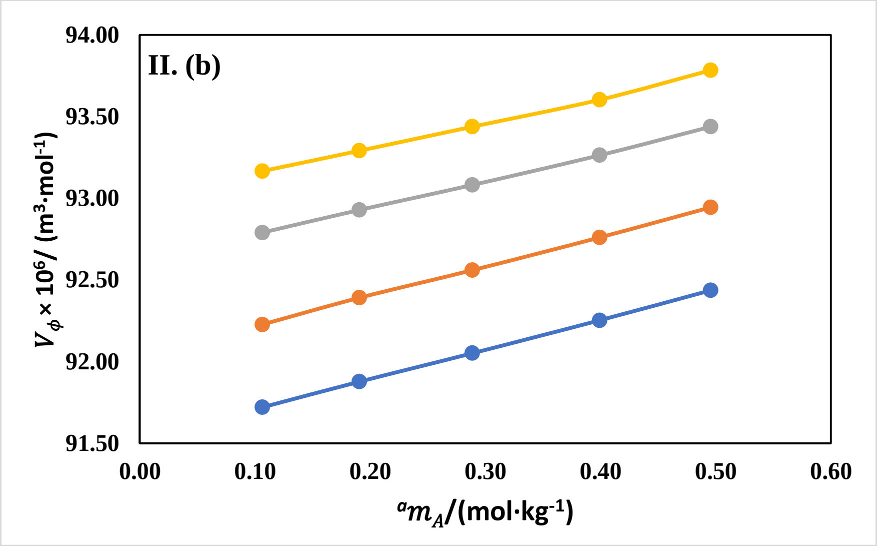


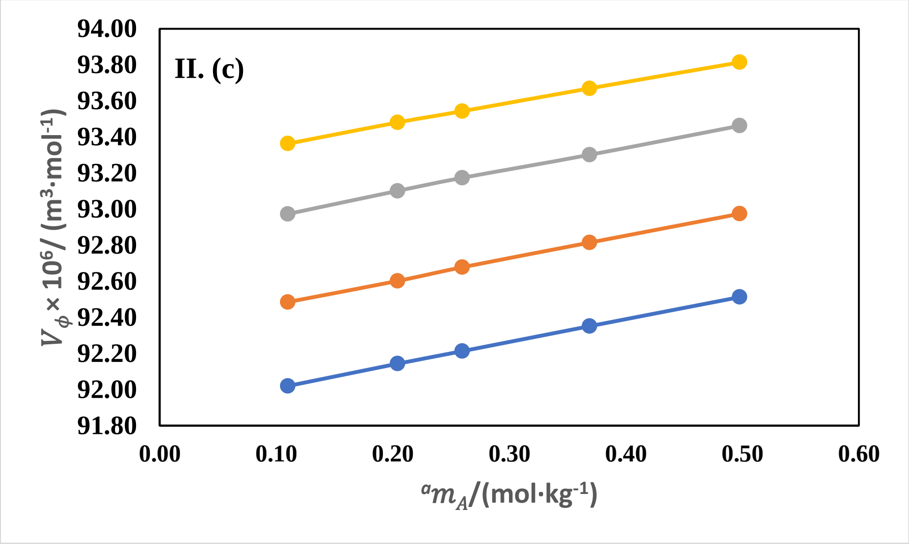
Variation of density for experimental and literature values [2] for (Niacin +Water) at T= 298.15K and T= 308.15 K.

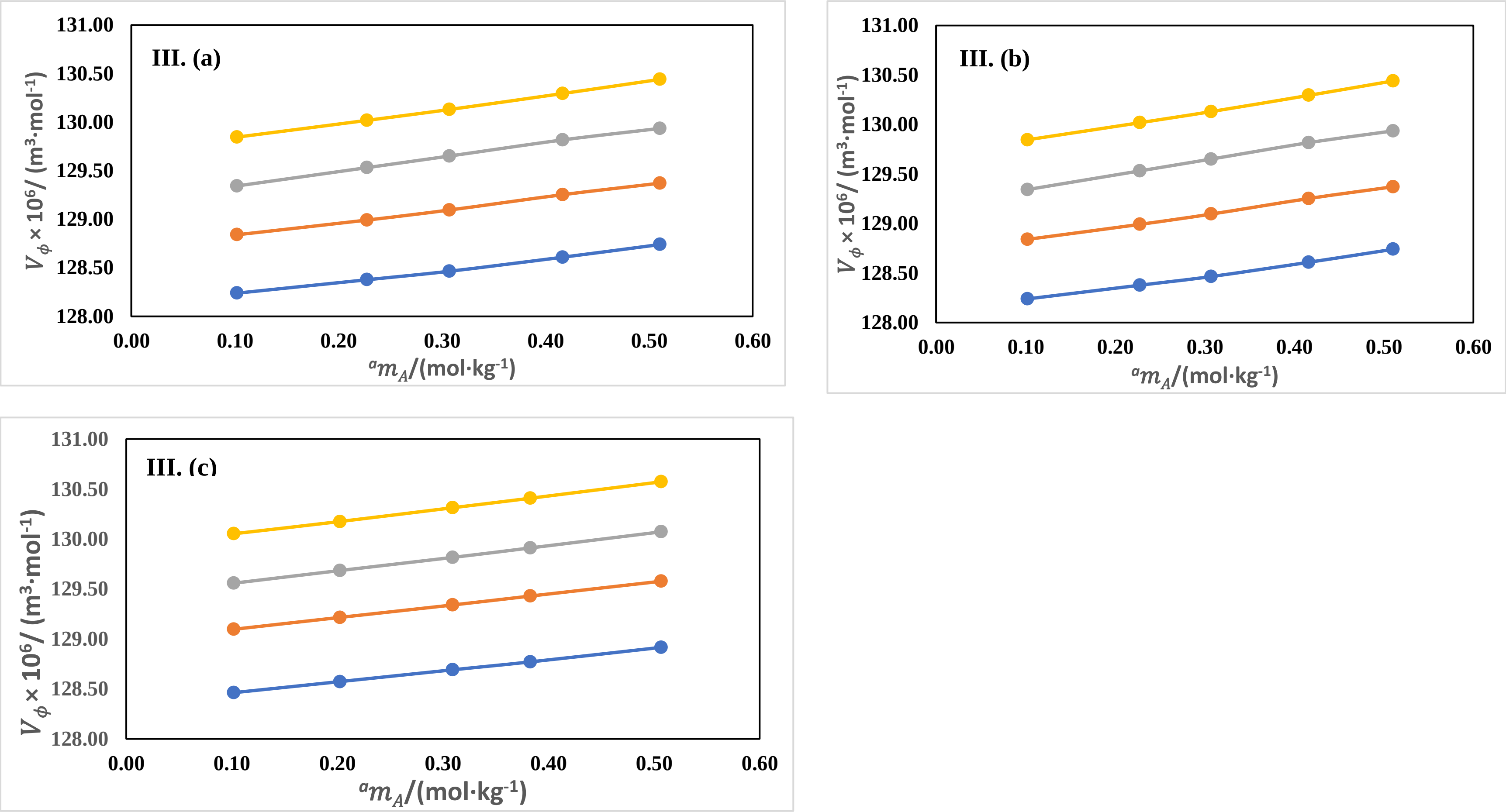
Figure 4.3


I. (a)
I. (b)
I. (c)
$V_\phi \times 10^6$/ (m^3·mol^{-1})
$^a m_A$/(mol·kg^{-1})
55.40
55.20
55.00
54.80
54.60
54.40
54.20
54.00
53.80
53.60
53.40
53.20
0.00
0.10
0.20
0.30
0.40
0.50
0.60


II. (a)
94.00
93.50
93.00
92.50
92.00
91.50
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ (m^3·mol^{-1})
$^a m_A$/(mol·kg^{-1})

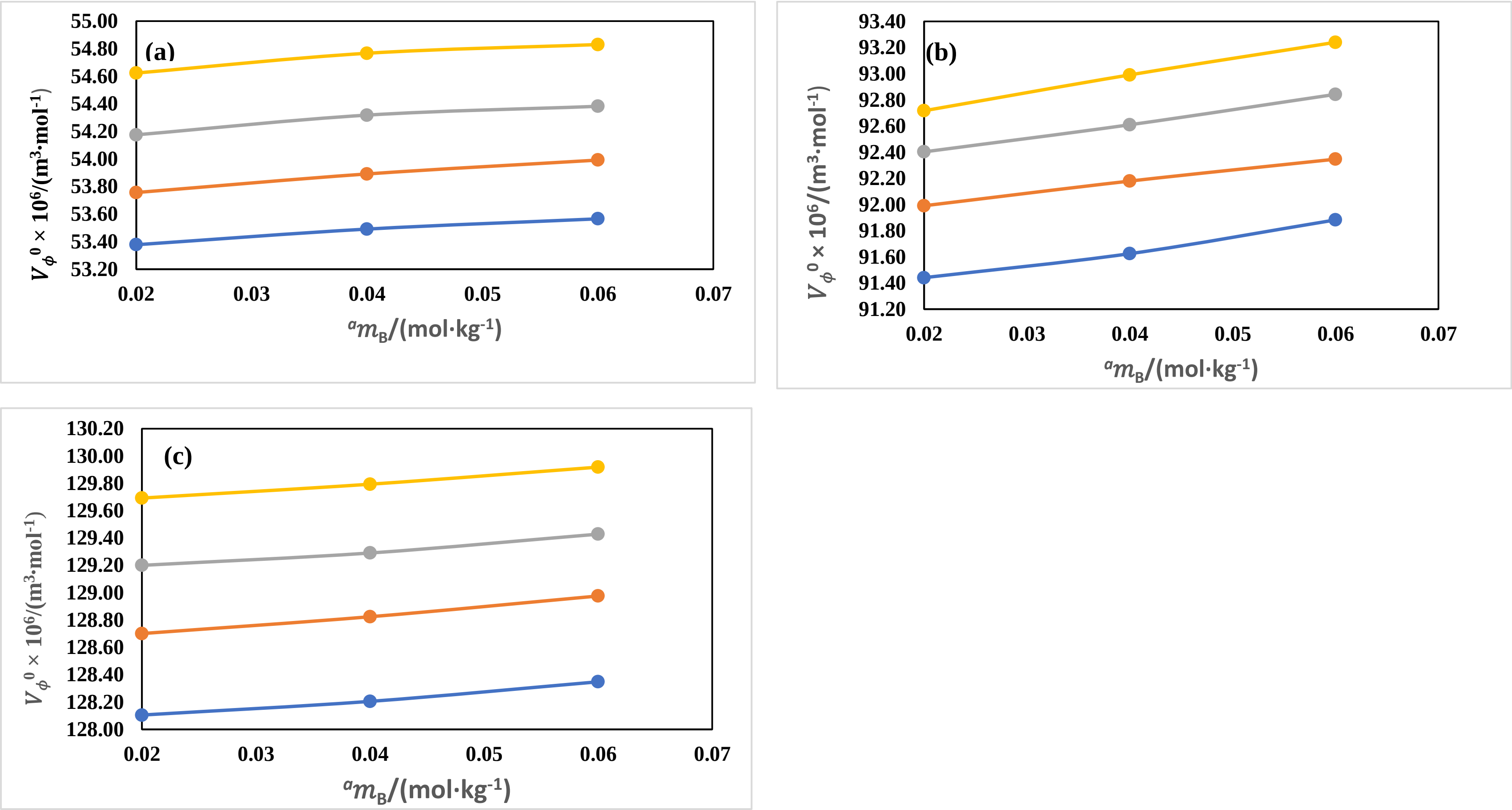

II. (b)
94.00
93.50
93.00
92.50
92.00
91.50
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ (m^3·mol^{-1})
$^a m_A$/(mol·kg^{-1})


II. (c)
94.00
93.80
93.60
93.40
93.20
93.00
92.80
92.60
92.40
92.20
92.00
91.80
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ (m^3·mol^{-1})
$^a m_A$/(mol·kg^{-1})



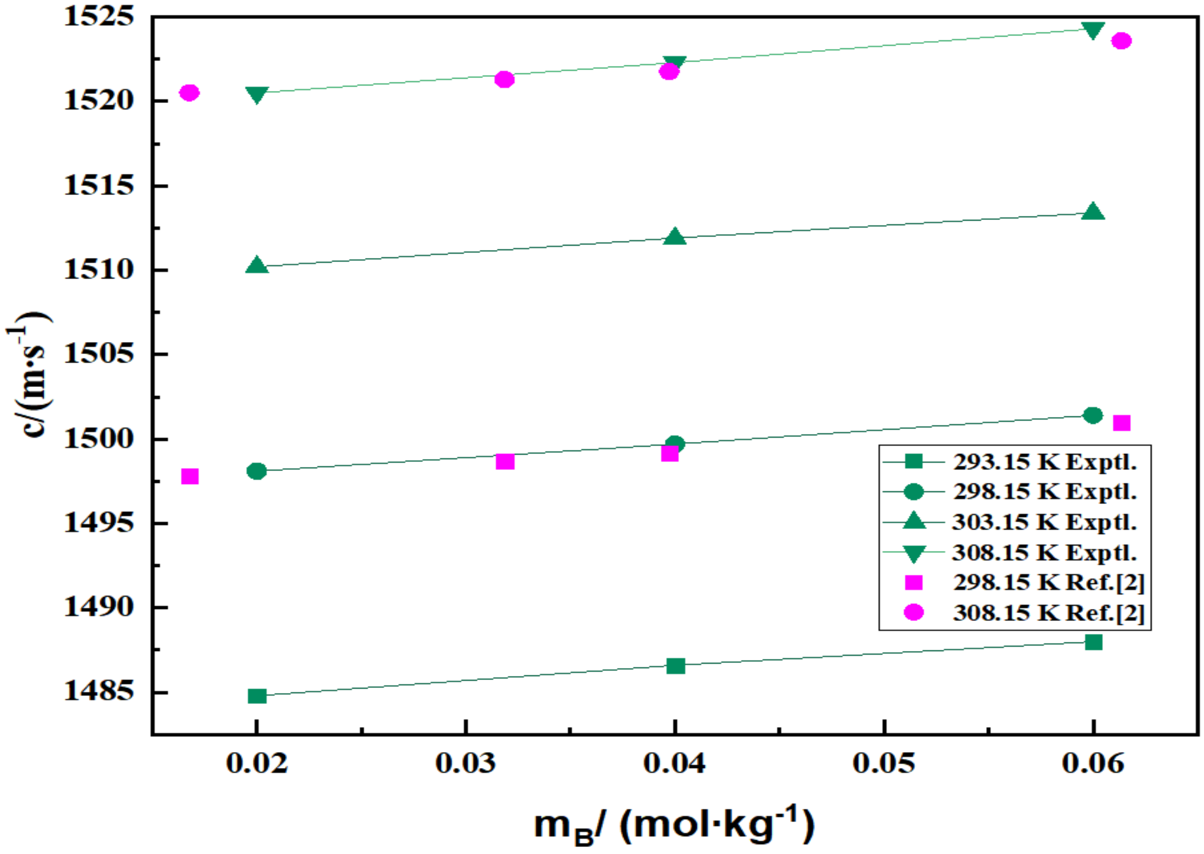
Variation of apparent molar volume, V_ϕ of Ethylene glycol (I), diethylene glycol (II) and triethylene glycol (III) in (a) 0.02 Niacin, (b) 0.04 Niacin, (c) 0.06 Niacin, against molality at different temperatures [blue, 293.15 K; red, 298.15 K; green, 303.15 K; purple 308.15 K]

Figure 4.4



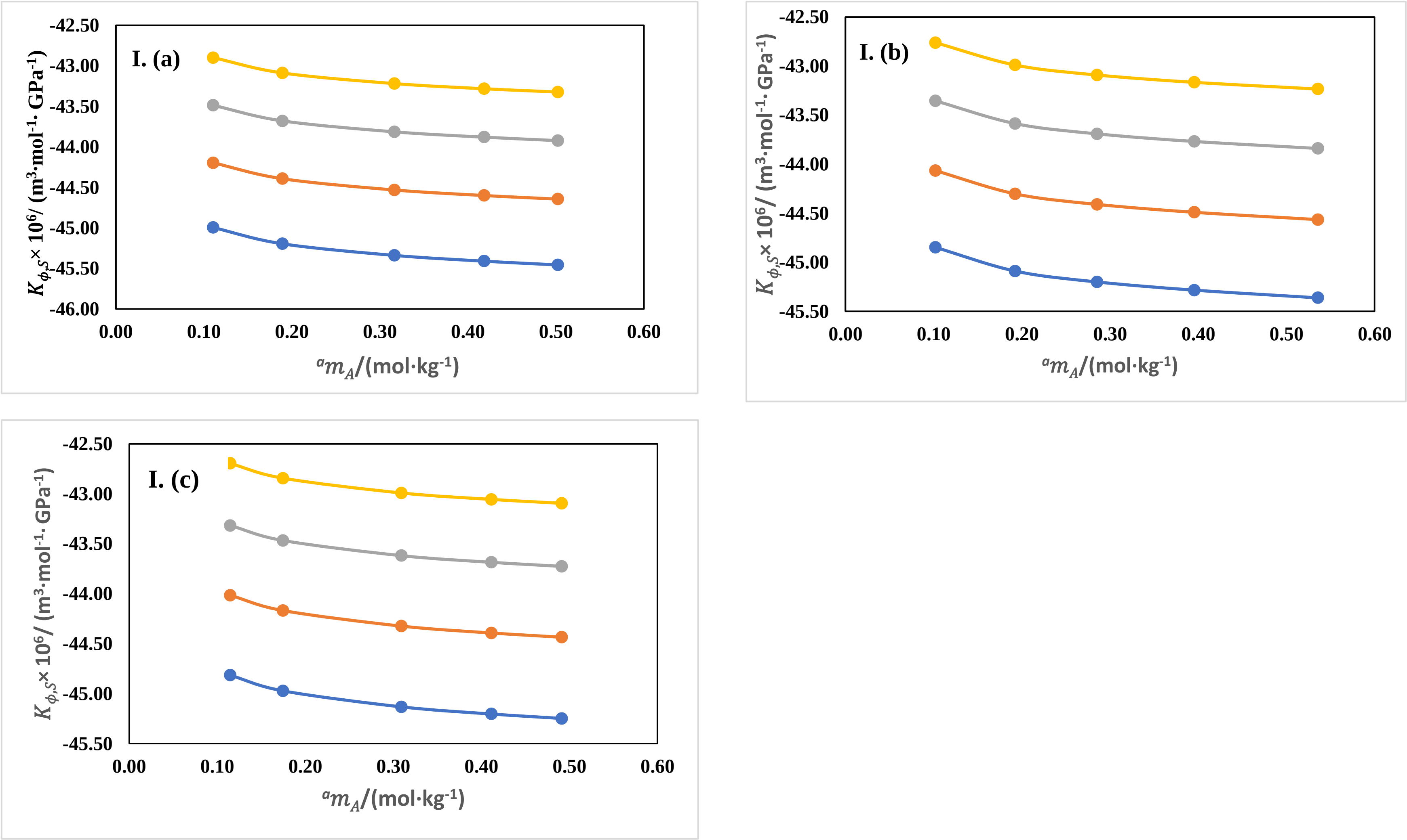
Variation of apparent molar volume, V_ϕ of Ethylene glycol (I), diethylene glycol (II) and triethylene glycol (III) in (a) 0.02 Niacin, (b) 0.04 Niacin, (c) 0.06 Niacin, against molality at different temperatures [blue, 293.15 K; red, 298.15 K; green, 303.15 K; purple 308.15 K]

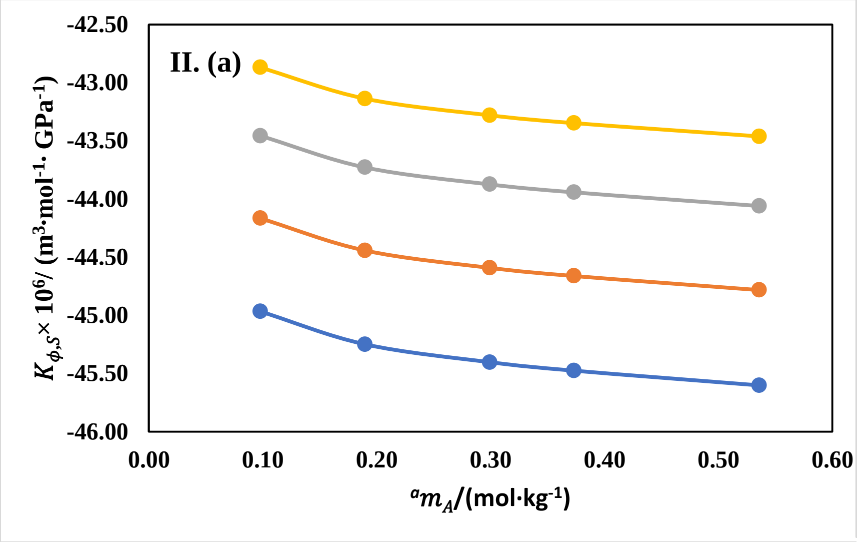
Figure 4.5

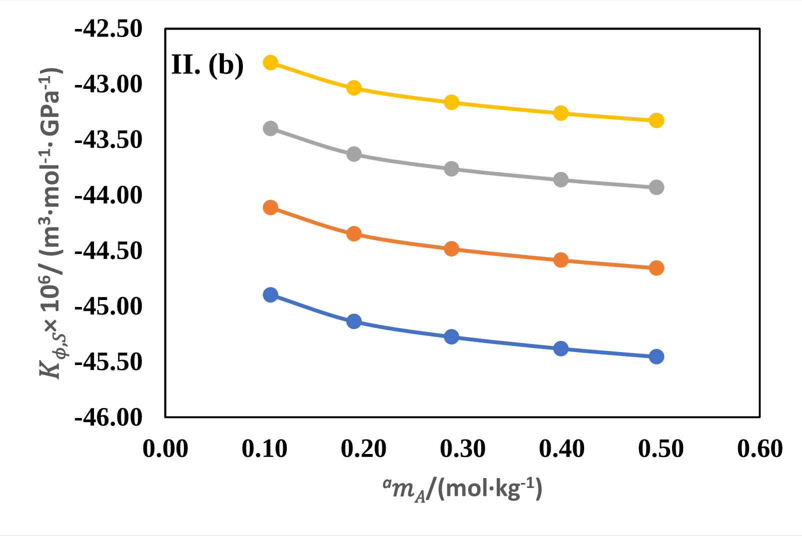


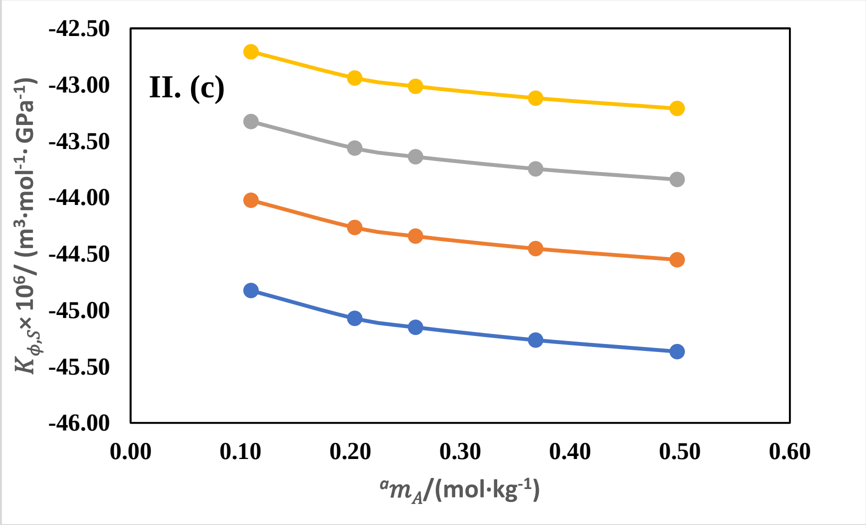
Variation of the speed of sounds for experimental and literature values [2] for (Niacin +Water) at T= 298.15K and T= 308.15

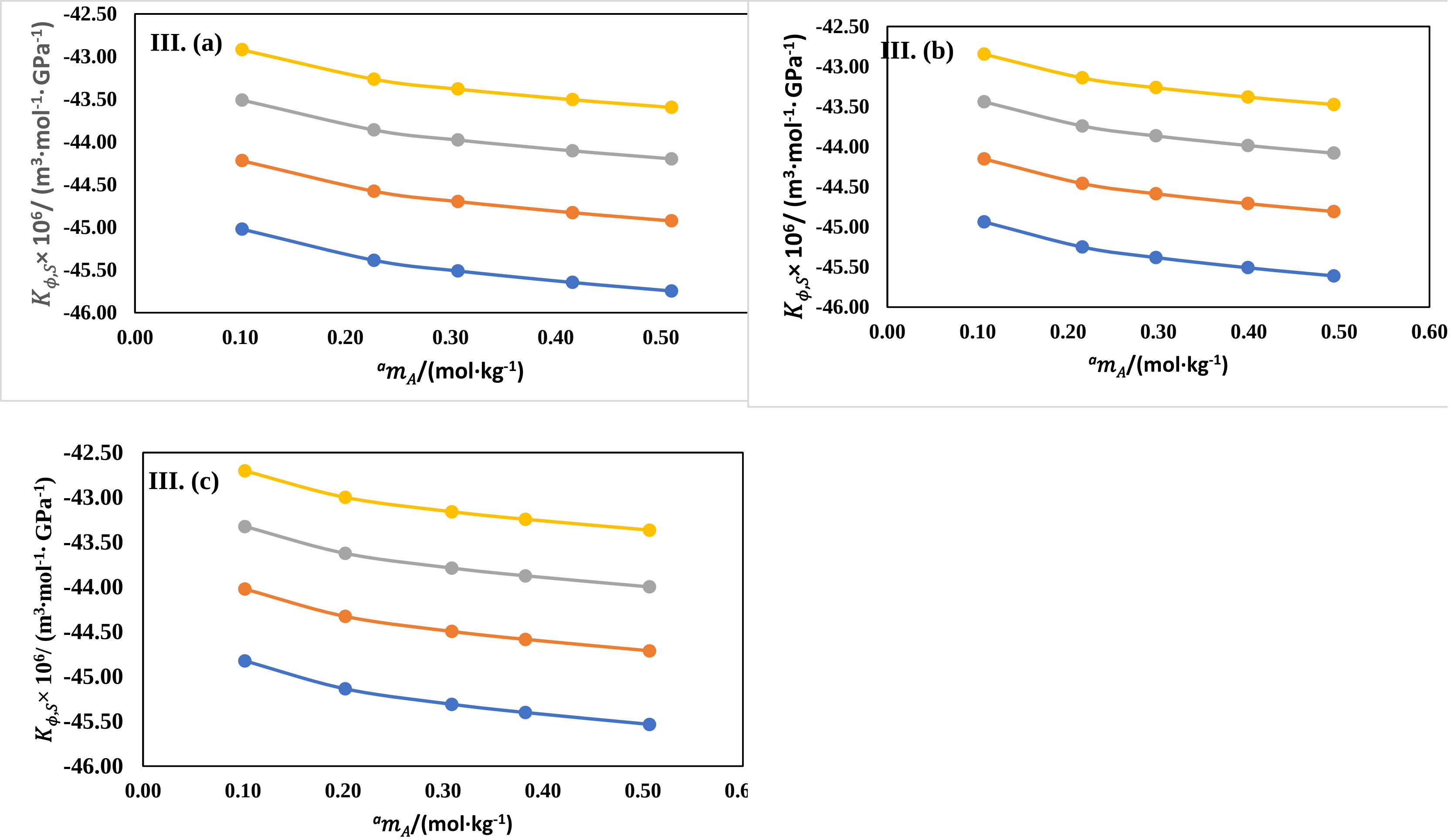
Figure 4.6


I. (a)
-42.50
-43.00
-43.50
-44.00
-44.50
-45.00
-45.50
-46.00
$K_{\phi,S} \times 10^6$/ (m^3·mol^{-1}· GPa^{-1})
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$^a m_A$/(mol·kg^{-1})
I. (b)
-42.50
-43.00
-43.50
-44.00
-44.50
-45.00
-45.50
$K_{\phi,S} \times 10^6$/ (m^3·mol^{-1}· GPa^{-1})
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$^a m_A$/(mol·kg^{-1})
I. (c)
-42.50
-43.00
-43.50
-44.00
-44.50
-45.00
-45.50
$K_{\phi,S} \times 10^6$/ (m^3·mol^{-1}· GPa^{-1})
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$^a m_A$/(mol·kg^{-1})


II. (a)
-42.50
-43.00
-43.50
-44.00
-44.50
-45.00
-45.50
-46.00
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$K_{\phi,S}\times 10^6$/ ($m^3\cdot mol^{-1}\cdot GPa^{-1}$)
$^a m_A$/($mol\cdot kg^{-1}$)

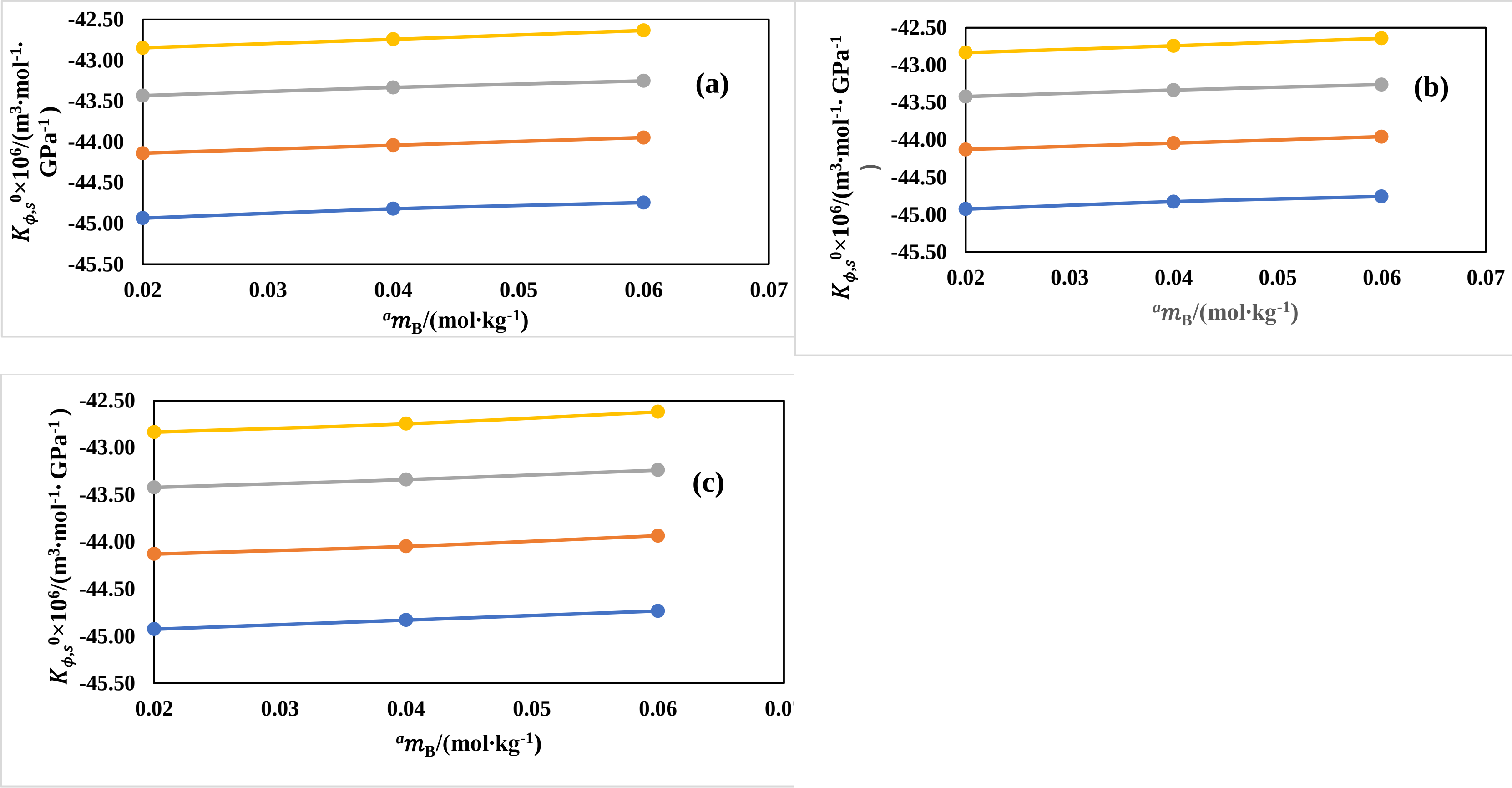

II. (b)
-42.50
-43.00
-43.50
-44.00
-44.50
-45.00
-45.50
-46.00
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$K_{\phi,S}\times 10^6$/ ($m^3\cdot mol^{-1}\cdot GPa^{-1}$)
$^a m_A$/($mol\cdot kg^{-1}$)


II. (c)
-42.50
-43.00
-43.50
-44.00
-44.50
-45.00
-45.50
-46.00
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$K_{\phi,S}\times 10^6$/ ($m^3\cdot mol^{-1}\cdot GPa^{-1}$)
$^a m_A$/($mol\cdot kg^{-1}$)



Variation of apparent molar isentropic compression, $K_{\phi,s,}$ of Ethylene glycol (I), diethylene glycol (II) and triethylene glycol (III) in (a) 0.02 Niacin, (b) 0.04 Niacin, (c) 0.06 Niacin, against molality at different temperatures [blue, 293.15 K; red, 298.15 K; green, 303.15 K; purple 308.15 K]

Figure 4.7



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, of (a) ethylene glycol (b) diethylene glycol (c) triethylene glycol in aqueous Niacin solutions at different temperatures [blue, 293.15 K; red, 298.15 K; green, 303.15 K; purple 308.15 K]

Problem 2

Study of thermodynamic and acoustic properties of niacin in aqueous hexylene glycol and propylene glycol at different temperatures

In this section, we have reported the densities, ρ and speed of sound c of propylene glycol (PG), and hexylene glycol (HG) in (0.00, 0.01, 0.03, 0.05) mol·kg^{-1} aqueous solutions of niacin at temperatures T = (293.15, 298.15, 303.15, 308.15) K.

4.12 Density

In **Table 4.12**, the experimental density values for (niacin +distilled Water+ glycols) at different temperatures ranging from (293.15 to 308.15) K with concentrations (0.01, 0.03 and 0.05) mol·kg^{-1} are mentioned. The density value for (glycols + distilled. water) has been taken from our previous paper [41]. It can be seen in the data that all the density values are decreasing along with the temperatures and increases with more concentration. The decrement of the density values with the temperatures indicates the low hydrogen bonding. Scheme 1 shows the increment of molecular and solute-solvent interactions inside the solution from PG to HG. The comparison between the experimental and literature [2] density values at temperature 298.15 K and 308.15 K for the mixture (niacin+ distilled water) has been displayed in **Figure 4.9**. It is visible that both the experimental and literature values are showing the same trend and thus are in good agreement with each other [42].

4.13 Apparent molar volume

The values apparent molar volume have been described in **Table 4.12** and is graphically represented in **Figure 4.10**, were calculated using the molar mass (M) of the solute, molality (m_A) of the solute per one kg of solvent (niacin +distilled Water), the density of solvent (ρ_0) and solution (ρ) in the equation **4.1**. The calculated V_ϕ values are all positive which is because of the broad intrinsic volume of solute that suggests the existence of strong solute-solvent interactions inside the ternary mixture [43]. With niacin concentration the values of apparent molar volumes tend to increase, which is due to the association of the water molecules in the hydration shell with the OH groups of niacin. This leads to strengthening the hydrogen bond in the solvent due to the constructive interaction of niacin with water [44, 45]. Also, it is observed that with the increase in the molar mass of the glycols from PG to HG, the V_ϕ also increases to all the concentration of niacin and all temperatures. This increase is responsible for the factors hydrophilic effect, hydrophobic hydration in water-rich region physical forces such as dipole-dipole and dipole-induced dipole interactions [42, 46]. The extent of the molecular interaction from PG to HG is displayed in **Figure 4.8**.

4.14 Partial Molar volume

Using the equation **4.2**, the partial molar volume at infinite dilution has been calculated. Here, V_ϕ^0 is partial molar volume, S_V^* is the experimental slope and m_A is the molality of solute per solvent. By utilizing the method of least square fitting the values of partial molar volume and their experimental slope are calculated from apparent molar volume. In **Table 4.13,** the V_ϕ^0 and S_V^* values are provided along with their standard errors. It can be seen that all the V_ϕ^0 values are all positive and rise with the concentration of niacin as shown in **Figure 4.11**. These positive values indicate the presence of strong solute-solvent interaction as well as the existence of ion-hydrophobic and hydrophobic-hydrophobic interaction in the mixture which is preponderated by the ion-hydrophilic interactions. As per the co-sphere overlap model [13, 20], the hydration co-spheres of two ionic spices super-impose on each other and results in an increase in the volume but when ion-hydrophobic groups overlap on hydrophobic-hydrophobic groups, a decrease in the volume is observed. It is noticed that V_ϕ^0 values increase with the molar mass of glycols due to two additional $–CH_3–$ groups and HG as compared to PG, thus implying the influence of hydrocarbon chain in the molecular interaction. The calculated S_V^* values are positive and few are negative in magnitude which proves the presence of weak solute-solute interaction in the liquid system, also the irregular pattern suggests the impact of additional parameters on the solute-solute interaction [41, 47].

4.15 Partial molar volume of transfer

The volumes of transfer for glycols from water to aqueous niacin solutions have been calculated at infinite dilution using the equation no. **4.3**. In **Table 4.14** the calculated ΔV_{ϕ}^{0} values are indexed and they are all having negative values except for few values i.e. for PG at 308.15 K throughout all the concentrations of niacin and HG at 303.15 K only for 0.01 mol·kg^{-1} concentration of niacin. This numerical behaviour implies that the molecular interaction of niacin with (PG/HG) is stronger than the interactions of water with (PG/HG) [48]. Also, ΔV_{ϕ}^{0} values suggest that the contribution of solute-solute interaction is negligible in the liquid system. From co-sphere overlap model [21, 49] it is found that numerous interactions are taking place inside the mixture which are ion-hydrophilic, hydrophilic-hydrophilic, ion-hydrophobic, and hydrophobic-hydrophobic interactions. Regarding this model, the negative ΔV_{ϕ}^{0} values are contributed by ion-hydrophobic and hydrophobic- hydrophobic interactions, and the positive values are accounted for ion-hydrophilic and hydrophilic- hydrophilic interactions [17, 46].

4.16 Temperature-dependent partial molar volume

At infinite dilution, the difference in apparent molar volumes as the function of temperature can be evaluated using the equation **4.4**.The empirical constants are represented by *a*, *b* and *c*, the experimental temperature is represented by T and reference temperature by T_{ref} as T_{ref}= 298.15 K. In **Table 4.15** the evaluated empirical constant values are displayed. The coefficient c values are hardly crucial, are all positive except for two values of HG at (0.03 and 0.05) mol·kg^{-1} concentration of niacin. By the means of these empirical constants, the theoretical values of V_{ϕ}^{0} are calculated and are compared with their experimental values [50, 51]. From these comparisons, the deviations of the experimental values from theoretical values are obtained and is termed as ARD (σ) and listed in the same table. This parameter is determined using the following formula

$$\sigma = (1/\mathrm{n}) \sum \left[\mathrm{abs}\left(\left(\mathrm{Y}_{\mathrm{Exptl.}} - \mathrm{Y}_{\mathrm{Calc.}} \right) / \mathrm{Y}_{\mathrm{Exptl.}} \right) \right] \qquad (4.14)$$

The partial molar volume (V_{ϕ}^{0}) is represented by Y. After all very less deviations are attained, it can be considered that these variations fit properly in the polynomial equation evident from R^2 values. V_{ϕ}^{0} aimed to attain the partial molar expansibilities values using the undermentioned equation **4.5**. At infinite dilution, the partial molar expansibilities i.e. E_{ϕ}^{0}=$\left(\partial^2 \mathrm{V}_{\phi}/\partial \mathrm{T}^2\right)_p$ are treated as a significant parameter to measure the solute-solvent interactions taking place inside the system. A general thermodynamic equation is established by Hepler [52] which estimates the extent of solute as structure breaker and structure maker in any mixture with a solvent is given by equation **4.6**. In **Table 4.16**, the values of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_P$ are presented and its sign determines whether the dissolved solute has structure making or structure breaking tendency. $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_P$ values are all positive, which implies the structure making capacity of solutes [52, 53]. In the same table, E_{ϕ}^{0} values are also mentioned which are partially positive and partially negative at all temperatures and concentration if niacin. The positive E_{ϕ}^{0} values imply the contribution of solute-solvent interaction in the mixture [54]. Also, this can be attributed due to the packing or caging effect [55] between the molecules of niacin and glycols, which describes the interactions among them.

4.17 Ultrasonic Speed

The experimentally obtained speed of sound data at (293.15, 298.15, 303.15, and 308.15) K for (niacin+ water) as well as (niacin+ water+ PG/HG) for (0.01, 0.03, and 0.05) mol·kg^{-1} concentrations are described in **Table 4.17**. The speed of sound values for (PG/HG + water) is taken directly from our previous paper [41]. The experimental speed of sound values are compared with the literature values [2] for temperature 298.15 K and 308.15 K and is graphically presented in **Figure 4.12.** The experimental values are in the same trend as the literature values, i.e. increasing along with the temperatures and the concentrations of niacin from (0.01 to 0.03 to 0.05) mol·kg^{-1}. This is due to the 3-dimensional network water structure in which there exist 3-dimensional networks of hydrogen bonds and the acceleration of the speed of sound values for the glycol and vitamin mixture is due to the intermolecular hydrogen bonding in solute-solvent molecules and intramolecular hydrogen bonding in solute molecules, therefore implies the high combination rate of the molecules inside the solutions. The increment in the values of speed of sound along with the molality of (PG/HG) is due to the hydrogen bond network insolvent with aqueous niacin molecule. The hydrogen bond formed between the water and niacin molecules get reduced corresponding to the increase in the molar mass of the glycol from PG to HG and finally this bond abolish but concurrently fresh H-bonds are created amid of niacin and glycol molecules [1, 23, 44, 56].

4.18 Apparent molar isentropic compression

By the means of following mathematical equation **4.7**, the apparent molar isentropic compression of (PG/HG) in the aqueous and mixed aqueous solution of niacin at different temperatures has been calculated. Utilizing the values of experimental densities of solution (ρ), densities of solvent (ρ_0), molality (m_A) values of (PG/HG) in niacin, and the molar mass of the solute (M) in the equation. The calculated $K_{\phi,S}$ values are presented in **Table 4.17** and are graphically represented in **Figure 4.13**. Using the Laplace-Newton's equation **4.8**, the isentropic compressibility is expressed. The $K_{\phi,S}$ values are all negative and with the increase in the temperature, the values become less negative but with the molality of glycols, the negativity of $K_{\phi,S}$ values increases. It is also observed from the table that with the upsurge of niacin concentration in the mixture, the negativity of the apparent molar isentropic compression decreases. This trend of $K_{\phi,S}$ values indicates that the water molecules are less compressible around ionic charge groups of solute as compared to the bulk solution. This reveals the arrangement of water in a specific pattern throughout the solute [31, 32, 47]. Also, the negative values show more aligning effect due to solute on solvent resulting in a larger loss of structural compressibility of water.

4.19 Partial molar isentropic compression

Using the undermentioned equation **4.9**, the partial molar isentropic compression at infinite dilution has been calculated. Here, $K^0_{\phi,S}$ is partial molar isentropic compression, S^*_k is the experimental slope and m_A is the molality of solute per solvent. By utilizing the method of least square fitting the values of partial molar isentropic compression and their experimental slope are calculated from apparent molar isentropic compression. In **Table 4.18,** the $K^0_{\phi,S}$, and S^*_k values are provided along with their standard errors. It can be seen that all the $K^0_{\phi,S}$ values are all negative and the negativity reduces with the concentration of niacin as shown in **Figure 4.14**. This trend refers to the presence of attractive interactions between water and glycols [29]. With the increase in the temperature, the values become less negative but with the molality of glycols, the negativity of $K^0_{\phi,S}$ values increases thus suggesting the discharge of water molecules to bulk. Moreover, the desiccation of glycol molecules occurs due to the attractive interactions between niacin and water. As the consequence, with the increase in the niacin concentration, the water molecules around glycols become more compressible. The S^*_k values in the table are all negative and refers to the presence of weak solute-solute interaction in the solution [42, 57, 58].

4.20 Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer ($K^0_{\phi,S}$) for all glycols in aqueous niacin solution from water at infinite dilution were evaluated using the equation **4.10**. In **Table 4.19** the $\Delta K^0_{\phi,S}$ values are listed and it can be seen that the values are all positive throughout the temperature as well as over the entire range of niacin concentrations. These positive $\Delta K^0_{\phi,S}$ values refers to the interactions among the molecules of niacin and glycols which dominates the structure making capability of solute. This tendency of structure making of solute increases with the upsurge in the concentration of niacin. This makes the solution molecules less compressible as compared to the pure solvent molecules. This results in the decrement of the compressibility with niacin concentrations. Therefore for negative $K_{\phi,S}^{0}$ values for glycols over multiple concentrations, positive $\Delta K_{\phi,S}^{0}$ values are obtained [59, 60, 61].

4. 21 Pair and triplet interaction coefficients

From the equation **4.11** and **4.12** the partial molar volume of transfer (ΔV_{ϕ}^{0}) and partial molar isentropic compression of transfer (ΔK_{ϕ}^{0}) from water to aqueous niacin solution are calculated. A represent glycols and B represent niacin and m_B denotes the molality of the aqueous niacin solutions. The pair and triplet interaction coefficient are represented by the parameters V_{AB} and V_{ABB} for volume and K_{AB}, K_{ABB} for isentropic compression, and are reported in **Table 4.20** for all the temperatures**.** The pair and triplet coefficients were calculated upon the theory depicted by McMillan and Mayer [34]. This theory states that due to the interaction between pair or more solute molecules, the separation of effects is observed and thus gives rise to the interaction coefficient. Later it was furthermore discussed by Friedman and Krishnan [35] and Franks et al [36]. They added up the consideration of solute-solute interactions in the solvation regions. The values of pair interaction coefficient V_{AB} are negative except for PG it is positive at 308.15 K and for HG it is positive at 303.15 K. Triplet interaction coefficient V_{ABB} is all positive throughout all the temperatures for all glycols apart for three values which are mol in magnitude. While on the other hand, the pair interaction coefficient K_{AB} are all positive for every temperature all over the glycol concentrations. In the case of the triplet coefficient, K_{ABB} all the values are all positive except for three values. Due to positive values of pair interaction coefficients; it suggests the dominance of pairwise interaction in (niacin+ water) and (niacin+ water +glycols) mixtures for compressibility and volumetric measurements [4, 33]. Following the sphere overlapping theory, the water molecules are released from the hydration co-spheres to the bulk when the occurred interaction doesn't favour bonding [9].

Table 4.12

Values of densities, ρ, apparent molar volumes, V_{ϕ} of glycols in aqueous solutions of niacin at different temperatures

${}^{a}m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_{\phi} \times 10^{6}$/(m^{3}·mol^{-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 mol·kg^{-1} niacin + PG				
0.00000	0.99821	0.99704	0.99565	0.99403^{b}				
0.09917	0.99847	0.99731	0.99593	0.99432	73.54	73.55	73.57	73.62^{b}
0.19801	0.99872	0.99757	0.99619	0.99459	73.59	73.61	73.63	73.66
0.30136	0.99896	0.99782	0.99645	0.99486	73.65	73.66	73.68	73.72
0.39826	0.99918	0.99805	0.99668	0.99510	73.69	73.71	73.73	73.77
0.51059	0.99942	0.99830	0.99694	0.99536	73.74	73.75	73.77	73.81
				0.01 mol·kg^{-1} niacin + PG				
0.00000	0.99861	0.99740	0.99600	0.99440				
0.09995	0.99890	0.99769	0.99631	0.99467	73.30	73.41	73.24	73.84
0.20005	0.99915	0.99797	0.99657	0.99495	73.44	73.41	73.48	73.72
0.30106	0.99941	0.99820	0.99684	0.99520	73.49	73.57	73.52	73.77
0.39996	0.99961	0.99844	0.99708	0.99545	73.61	73.61	73.59	73.80
0.50512	0.99984	0.99869	0.99732	0.99570	73.66	73.62	73.65	73.83
				0.03 mol·kg^{-1} niacin + PG				
0.00000	0.99951	0.99821	0.99683	0.99519				
0.10024	0.99979	0.99849	0.99714	0.99545	73.31	73.34	73.29	73.83
0.19987	1.00004	0.99876	0.99741	0.99570	73.44	73.40	73.41	73.88

0.29998	1.00030	0.99901	0.99766	0.99599	73.45	73.47	73.52	73.74
0.40018	1.00056	0.99928	0.99795	0.99626	73.42	73.47	73.46	73.69
0.50113	1.00081	0.99955	0.99822	0.99650	73.43	73.43	73.46	73.74
0.05 mol·kg^{-1} niacin + PG								
0.00000	1.00044	0.99911	0.99763	0.99607				
0.09981	1.00070	0.99940	0.99792	0.99631	73.40	73.15	73.38	73.96
0.20212	1.00097	0.99968	0.99819	0.99655	73.39	73.27	73.47	73.95
0.29999	1.00125	0.99994	0.99846	0.99684	73.29	73.30	73.45	73.77
0.40004	1.00152	1.00021	0.99875	0.99709	73.27	73.32	73.39	73.74
0.50220	1.00179	1.00048	0.99904	0.99738	73.26	73.32	73.36	73.67
0.00 mol·kg^{-1} niacin + HG								
0.00000	0.99821	0.99704	0.99565	0.99403^{b}				
0.09903	0.99840	0.99725	0.99587	0.99427	116.37	116.40	116.42	116.46^{b}
0.20184	0.99860	0.99745	0.99609	0.99450	116.39	116.42	116.45	116.48
0.29963	0.99878	0.99764	0.99629	0.99472	116.41	116.45	116.47	116.50
0.39805	0.99895	0.99782	0.99648	0.99492	116.44	116.48	116.49	116.52
0.49538	0.99911	0.99799	0.99666	0.99512	116.46	116.50	116.51	116.55
0.01 mol·kg^{-1} niacin + HG								
0.00000	0.99861	0.99740	0.99600	0.99440				
0.09899	0.99881	0.99762	0.99621	0.99466	116.33	116.16	116.43	116.21
0.20067	0.99901	0.99784	0.99641	0.99490	116.27	116.18	116.53	116.29
0.30008	0.99918	0.99801	0.99663	0.99511	116.35	116.37	116.44	116.38

0.40023	0.99936	0.99822	0.99684	0.99532	116.35	116.30	116.42	116.40
0.50001	0.99954	0.99840	0.99701	0.99552	116.36	116.34	116.48	116.44
0.03 mol·kg^{-1} niacin + HG								
0.00000	0.99951	0.99821	0.99684	0.99520				
0.10055	0.99971	0.99848	0.99708	0.99548	116.17	115.62	116.10	115.89
0.19998	0.99990	0.99871	0.99731	0.99571	116.20	115.81	116.11	116.09
0.30034	1.00009	0.99890	0.99755	0.99593	116.20	115.98	116.09	116.19
0.40009	1.00030	0.99910	0.99778	0.99615	116.14	116.04	116.06	116.23
0.50210	1.00051	0.99931	0.99798	0.99642	116.10	116.04	116.11	116.13
0.05 mol·kg^{-1} niacin + HG								
0.00000	1.00044	0.99911	0.99764	0.99607				
0.09995	1.00065	0.99939	0.99792	0.99637	115.97	115.43	115.60	115.60
0.20002	1.00087	0.99961	0.99815	0.99662	115.90	115.71	115.82	115.83
0.30172	1.00105	0.99982	0.99842	0.99686	116.02	115.81	115.75	115.91
0.40059	1.00127	1.00001	0.99866	0.99714	115.94	115.93	115.77	115.84
0.50009	1.00150	1.00021	0.99892	0.99742	115.87	115.95	115.73	115.77

[a] m_A is the molality of glycols in the aqueous solution niacin; standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1} and $u(V_\phi)$ =±(0.05-0.07) × 10^6/ (m^3·mol^{-1}), [b]Values of densities for (PG + water and HG + water) at temperature 293.15 and 308.15 K have been taken from our previous paper [41].

Table 4.13

Partial molar volumes, V_ϕ^0, and experimental slopes, S_V^*, of glycols in the aqueous solution of niacin at different temperatures.

[a]m_B/ (mol·kg^{-1})	$V_\phi^0 \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-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
				PG				
0.00000	73.49(±0.005)	73.51(±0.010)	73.53(±0.008)	73.57(±0.005)[b]	0.51(±0.014)	0.49(±0.030)	0.49(±0.025)	0.48(±0.016)[b]
0.01000	73.23(±0.032)	73.34(±0.047)	73.22(±0.068)	73.77(±0.057)	0.89(±0.098)	0.61(±0.142)	0.92(±0.206)	0.08(±0.172)
0.03000	73.35(±0.056)	73.35(±0.045)	73.31(±0.074)	73.89(±0.062)	0.22(±0.169)	0.25(±0.137)	0.38(±0.223)	-0.37(±0.187)
0.05000	73.44(±0.028)	73.15(±0.045)	73.44(±0.051)	74.05(±0.045)	-0.40(±0.086)	0.40(±0.137)	-0.12(±0.155)	-0.77(±0.137)
				HG				
0.00000	116.35(±0.001)	116.37(±0.001)	116.40(±0.001)	116.43(±0.001)[b]	0.22(±0.005)	0.25(±0.005)	0.22(±0.002)	0.24(±0.005)[b]
0.01000	116.29(±0.031)	116.12(±0.066)	116.46(±0.054)	116.17(±0.024)	0.14(±0.094)	0.49(±0.200)	-0.01(±0.164)	0.58(±0.074)
0.03000	116.22(±0.023)	115.57(±0.081)	116.11(±0.028)	115.91(±0.106)	-0.20(±0.099)	1.08(±0.245)	-0.04(±0.084)	0.63(±0.319)
0.05000	115.99(±0.062)	115.38(±0.085)	115.67(±0.091)	115.68(±0.127)	-0.17(±0.188)	1.27(±0.257)	0.21(±0.274)	0.36(±0.382)

[a]m_B is the molality of aqueous niacin, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}, *u*(V_ϕ^0) =±0.01 × 10^6/ (m^3·mol^{-1}) and *u*(S_V^*) =±0.03 × 10^6/ (m^3·mol^{-2})

Table 4.14

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in the aqueous solution of niacin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
		PG		
0.01000	-0.26	-0.17	-0.31	0.20
0.03000	-0.14	-0.16	-0.22	0.32
0.05000	-0.05	-0.36	-0.09	0.48
		HG		
0.01000	-0.06	-0.25	0.06	-0.26
0.03000	-0.13	-0.80	-0.29	-0.52
0.05000	-0.36	-0.99	-0.73	-0.75

$^{a}m_B$ is the molality of aqueous niacin.

Table 4.15

Values of empirical parameters of Eq. 4.4, of glycols in aqueous solution of niacin at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	ARD
			PG		
0.01000	73.20	0.008	0.004	0.9999	0.00109
0.03000	73.25	0.003	0.006	0.9999	0.00078
0.05000	73.19	-0.003	0.009	0.9999	0.00185
			HG		
0.01000	116.29	0.006	-0.001	0.9999	0.00086
0.03000	115.86	-0.031	0.005	0.9999	0.00144
0.05000	115.56	-0.044	0.006	0.9999	0.00156

${}^{a}m_B$ is the molality aqueous of niacin.

Table 4.16

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in the aqueous solution of niacin at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	E_{ϕ}^{0} ×10^{6}/(m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K	
			PG		
0.01000	-0.04	0.01	0.05	0.10	0.01
0.03000	-0.05	0.00	0.06	0.12	0.01
0.05000	-0.09	0.00	0.09	0.18	0.02
			HG		
0.01000	0.02	0.01	-0.01	-0.02	0.00
0.03000	-0.08	-0.03	0.02	0.06	0.01
0.05000	-0.11	-0.04	0.02	0.08	0.01

${}^{a}m_B$ is the molality aqueous of niacin.

Table 4.17

Values of the speed of sound, c, apparent molar isentropic compression, $K_{\phi,s}$ of glycols in aqueous solutions of niacin at different temperatures

$^{a}m_{A}$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s}\times 10^{15}$/(m^{3}·mol^{-1}· Pa^{-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 mol·kg^{-1} niacin + PG								
0.00000	1481.0	1495.0	1508.0	1519.0^{b}				
0.09917	1486.0	1500.0	1513.0	1523.0	-42.62	-44.25	-43.49	-42.90^{b}
0.19801	1490.0	1504.0	1516.0	1526.0	-42.86	-44.49	-43.72	-43.13
0.30136	1493.0	1507.0	1520.0	1529.0	-42.95	-44.58	-43.81	-43.22
0.39826	1496.0	1510.0	1522.0	1532.0	-42.99	-44.62	-43.86	-43.27
0.51059	1499.0	1513.0	1525.0	1534.0	-43.03	-44.66	-43.89	-43.30
0.01 mol·kg^{-1} niacin + PG								
0.00000	1483.6	1497.2	1509.4	1519.9				
0.09995	1488.2	1502.1	1514.4	1524.2	-44.99	-44.18	-43.47	-42.86
0.20005	1492.2	1506.1	1517.6	1527.4	-45.23	-44.41	-43.70	-43.09
0.30106	1495.3	1509.5	1521.7	1530.3	-45.32	-44.50	-43.78	-43.18
0.39996	1498.4	1512.8	1523.9	1533.4	-45.36	-44.55	-43.83	-43.22
0.50512	1501.5	1515.6	1526.7	1535.1	-45.40	-44.58	-43.86	-43.26
0.03 mol·kg^{-1} niacin + PG								
0.00000	1485.6	1498.8	1511.1	1521.5				
0.10024	1490.4	1503.7	1515.9	1525.8	-44.87	-44.09	-43.37	-42.78

0.19987	1494.4	1507.8	1519.1	1528.8	-45.11	-44.32	-43.60	-43.00
0.29998	1497.5	1511.4	1523.1	1531.9	-45.19	-44.41	-43.68	-43.09
0.40018	1500.7	1514.9	1525.9	1535.1	-45.24	-44.45	-43.73	-43.14
0.50113	1503.8	1517.6	1528.5	1536.9	-45.28	-44.49	-43.77	-43.17
0.05 mol·kg^{-1} niacin + PG								
0.00000	1487.3	1500.6	1512.8	1523.2				
0.09981	1492.0	1505.5	1517.6	1527.6	-44.77	-43.98	-43.27	-42.68
0.20212	1496.3	1509.8	1520.9	1530.8	-45.01	-44.22	-43.51	-42.91
0.29999	1499.4	1513.4	1524.8	1533.9	-45.10	-44.30	-43.59	-42.99
0.40004	1502.7	1517.0	1527.7	1536.8	-45.15	-44.35	-43.64	-43.04
0.50220	1506.1	1519.6	1530.4	1538.7	-45.18	-44.38	-43.67	-43.07
0.00 mol·kg^{-1} niacin + HG								
0.00000	1481.0	1495.0	1508.0	1519.0^{b}				
0.09903	1490.0	1504.0	1515.0	1525.0	-45.13	-44.25	-43.49	-42.90^{b}
0.20184	1500.0	1512.0	1523.0	1533.0	-45.38	-44.49	-43.72	-43.13
0.29963	1508.0	1520.0	1531.0	1539.0	-45.46	-44.57	-43.80	-43.21
0.39805	1517.0	1528.0	1537.0	1545.0	-45.50	-44.61	-43.85	-43.26
0.49538	1523.0	1535.0	1543.0	1551.0	-45.53	-44.64	-43.88	-43.29
0.01 mol·kg^{-1} niacin + HG								
0.00000	1483.6	1497.2	1509.4	1519.9				
0.09899	1492.5	1505.9	1517.0	1526.1	-44.98	-44.17	-43.46	-42.86
0.20067	1502.4	1514.1	1525.0	1534.2	-45.23	-44.41	-43.69	-43.09

0.30008	1511.1	1522.2	1533.2	1540.1	-45.31	-44.49	-43.78	-43.17
0.40023	1519.9	1530.3	1539.1	1546.2	-45.36	-44.54	-43.82	-43.22
0.50001	1525.6	1537.4	1545.1	1552.4	-45.39	-44.57	-43.85	-43.25
0.03 mol·kg^{-1} niacin + HG								
0.00000	1485.6	1498.8	1511.1	1521.5				
0.10055	1494.7	1507.2	1519.1	1527.5	-44.87	-44.09	-43.37	-42.78
0.19998	1504.7	1515.2	1526.5	1535.4	-45.10	-44.32	-43.60	-43.01
0.30034	1513.6	1523.4	1534.8	1541.5	-45.19	-44.40	-43.68	-43.09
0.40009	1522.6	1531.3	1540.5	1547.8	-45.24	-44.45	-43.73	-43.14
0.50210	1528.9	1539.3	1547.3	1553.9	-45.27	-44.48	-43.76	-43.17
0.05 mol·kg^{-1} niacin + HG								
0.00000	1487.3	1500.6	1512.8	1523.2				
0.09995	1496.4	1508.5	1520.7	1529.4	-44.77	-43.98	-43.27	-42.68
0.20002	1505.9	1516.7	1528.3	1537.6	-45.01	-44.21	-43.50	-42.91
0.30172	1515.2	1524.9	1536.9	1543.6	-45.09	-44.30	-43.59	-42.99
0.40059	1523.9	1532.5	1542.7	1549.9	-45.14	-44.34	-43.64	-43.04
0.50009	1530.4	1540.4	1549.4	1555.7	-45.17	-44.37	-43.67	-43.08

$^{a}m_A$ is the molality of glycols in the aqueous solution niacin; standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, , *u(T)*=0.05K, *u(ρ)=0.06*(kg·m^{-3}),, *u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}, $u(K_{\phi,S})$ =$\pm 0.25 \times 10^{6}$/ (m^{3}·mol^{-1}· GPa^{-1}), ^{b}Values of speed of sound for (PG + water and HG + water) at temperature 293.15 and 308.15 K have been taken from our previous paper [41].

Table 4.18

Partial molar isentropic compression, $K_{\phi,s}^{0}$, and experimental slopes, S_K^*, of glycols in the aqueous solution of Glycerol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$K_{\phi,s}^{0}$ ×10^{15}/(m^3·mol^{-1}· Pa^{-1})				S_K^* ×10^{15}/(kg·m^3·mol^{-2}· Pa^{-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
				PG				
0.00000	-44.98(±0.08)	-44.24(±0.08)	-43.48(±0.08)	-42.89(±0.08)	-0.93(±0.23)	-0.93(±0.22)	-0.92(±0.22)	-0.91(±0.23)
0.01000	-44.98(±0.07)	-44.16(±0.07)	-43.45(±0.07)	-42.85(±0.07)	-0.94(±0.23)	-0.93(±0.23)	-0.92(±0.22)	-0.91(±0.22)
0.03000	-44.85(±0.07)	-44.07(±0.07)	-43.35(±0.07)	-42.76(±0.07)	-0.95(±0.23)	-0.94(±0.23)	-0.93(±0.22)	-0.92(±0.22)
0.05000	-44.75(±0.07)	-43.97(±0.07)	-43.26(±0.07)	-42.66(±0.07)	-0.96(±0.23)	-0.94(±0.23)	-0.93(±0.22)	-0.92(±0.22)
				HG				
0.00000	-45.12(±0.08)	-44.23(±0.08)	-43.47(±0.08)	-42.88(±0.08)	-0.94(±0.24)	-0.93(±0.24)	-0.93(±0.23)	-0.92(±0.23)
0.01000	-44.97(±0.07)	-44.16(±0.07)	-43.45(±0.07)	-42.84(±0.07)	-0.93(±0.23)	-0.92(±0.23)	-0.92(±0.23)	-0.91(±0.23)
0.03000	-44.86(±0.07)	-44.08(±0.07)	-43.35(±0.07)	-42.77(±0.07)	-0.92(±0.22)	-0.91(±0.22)	-0.91(±0.22)	-0.90(±0.22)
0.05000	-44.76(±0.07)	-43.97(±0.07)	-43.26(±0.07)	-42.67(±0.07)	-0.93(±0.23)	-0.91(±0.22)	-0.92(±0.22)	-0.92(±0.22)

$^{a}m_B$ is the molality of aqueous niacin, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}, *u*($K_{\phi,s}^{0}$) =±0.01 × 10^6/(m^3·mol^{-1}· GPa^{-1})and *u*(S_k^*) =±0.24 × 10^6/(m^3·mol^{-2}· GPa^{-1})

Table 4.19

Partial molar isentropic compression transfer, $\Delta K^0_{\phi,s}$, of glycols in the aqueous solution of niacin at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$\Delta K^0_{\phi,s}$ × 10^{15}/(m^3·mol^{-1}· Pa^{-1})			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
		PG		
0.01000	0.00	0.08	0.03	0.04
0.03000	0.13	0.17	0.13	0.13
0.05000	0.23	0.27	0.22	0.23
		HG		
0.01000	0.15	0.07	0.02	0.04
0.03000	0.26	0.15	0.12	0.11
0.05000	0.36	0.26	0.21	0.21

$^a m_B$ is the molality of aqueous niacin.

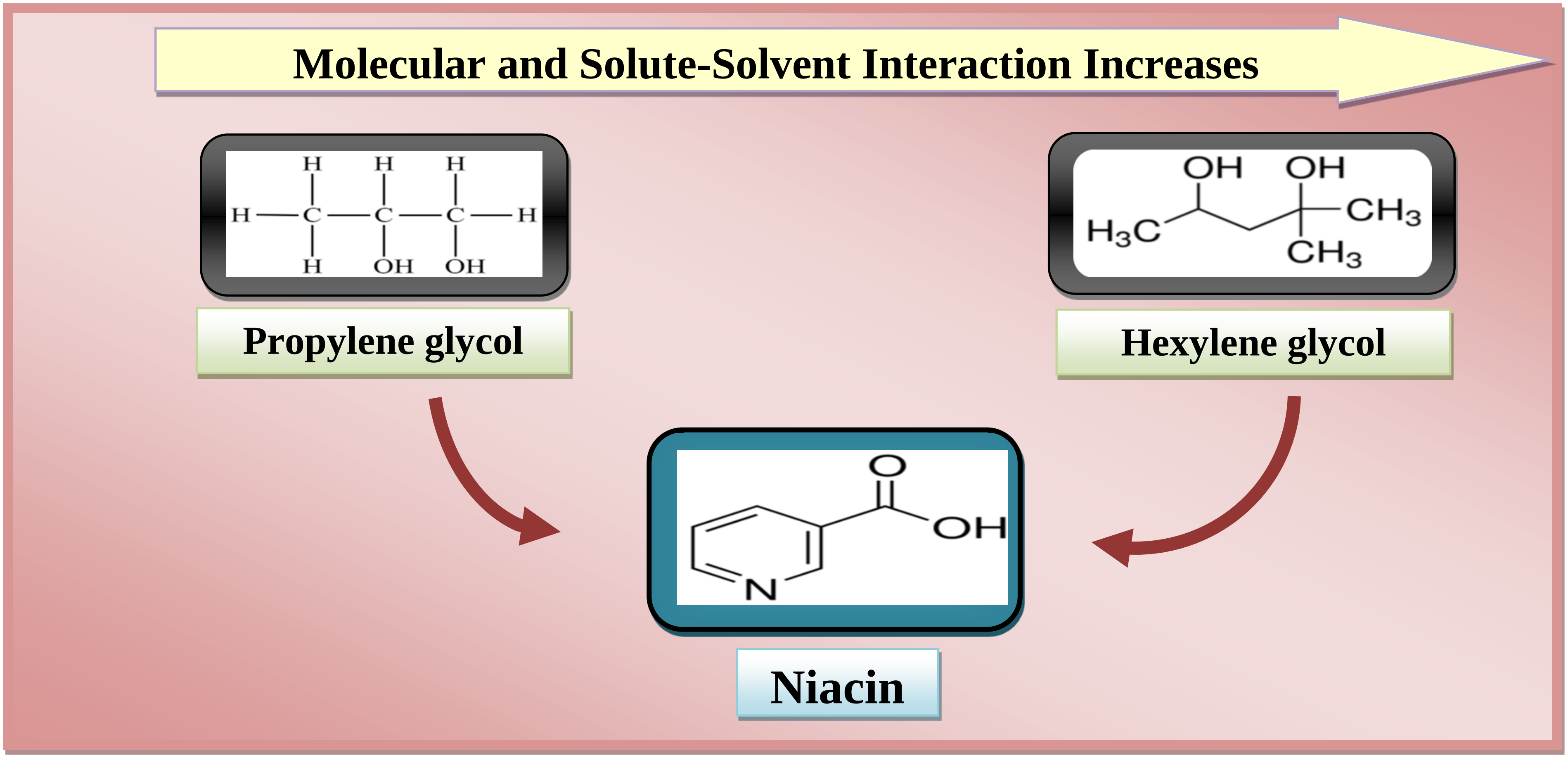
Table 4.20

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of niacin at different temperatures.

T/K	V_{AB} ×10^6/(m^3·mol^{-2}·kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		PG		
293.15	-8.87	114.99	1.10	16.07
298.15	-4.05	8.54	3.35	-8.27
303.15	-11.63	147.09	1.75	6.78
308.15	7.72	-40.53	2.00	3.61
		HG		
293.15	-0.90	-34.79	6.42	-37.95
298.15	-16.64	88.87	2.91	-4.32
303.15	1.03	-112.69	1.44	9.29
308.15	-11.59	55.86	1.58	7.48

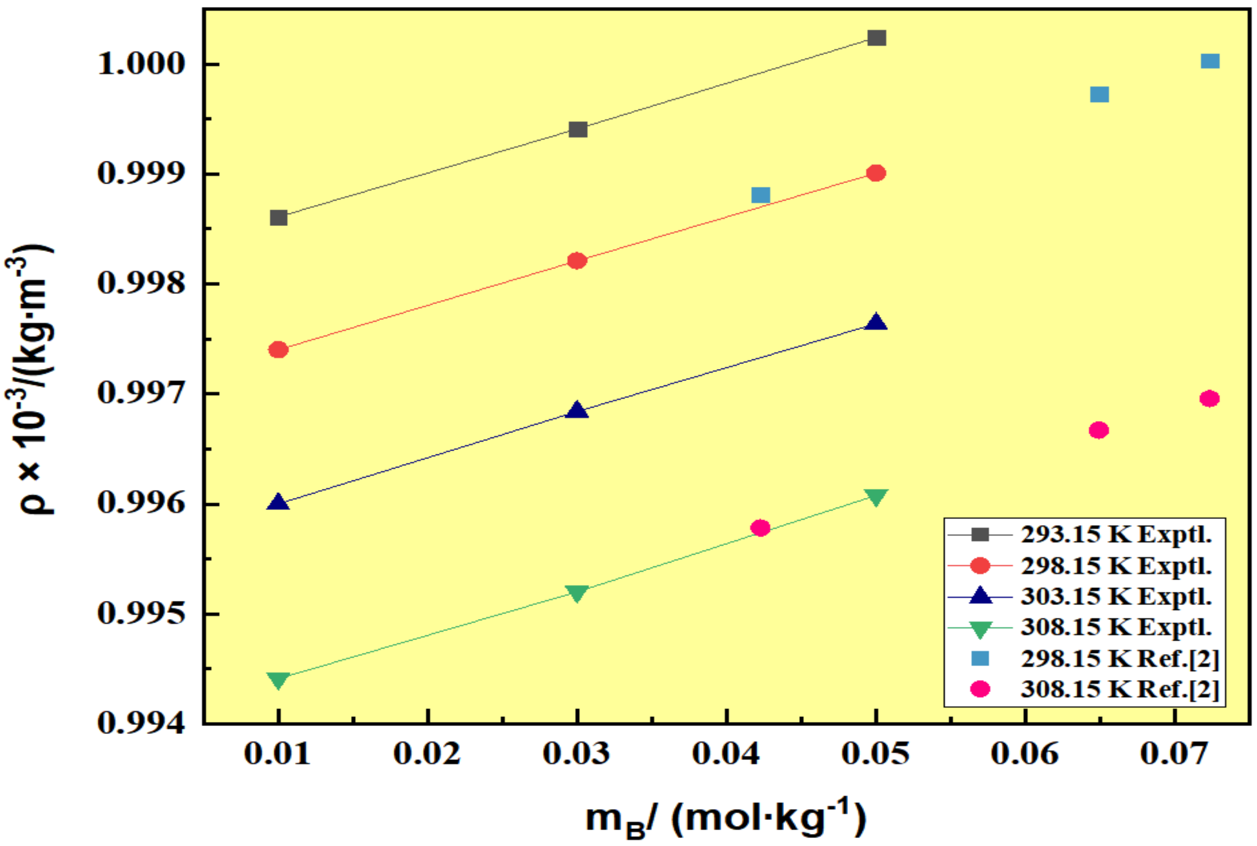
T/K is the temperatures.

Figure 4.8



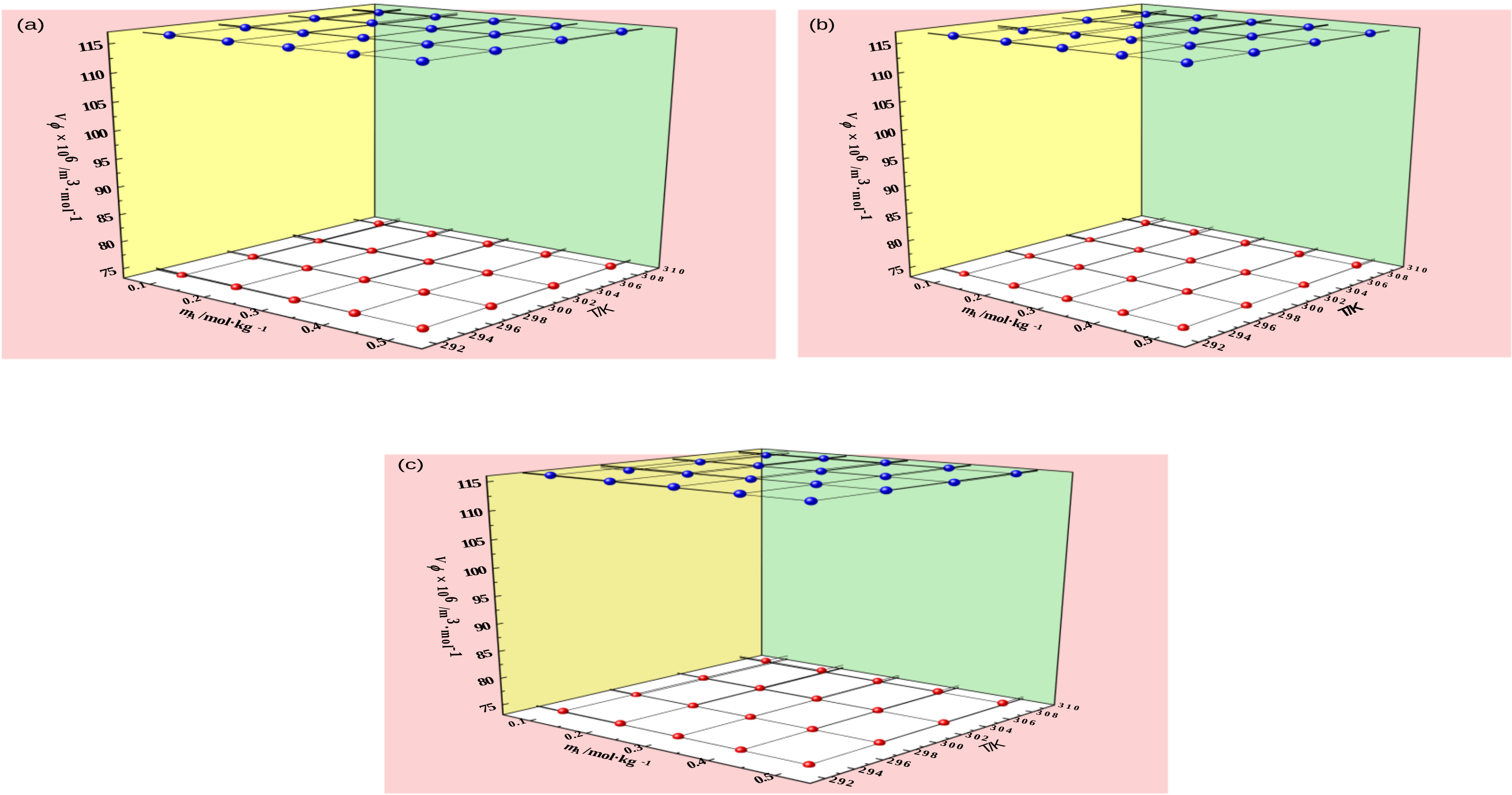
PG/ HG and niacin interactions.

Figure 4.9



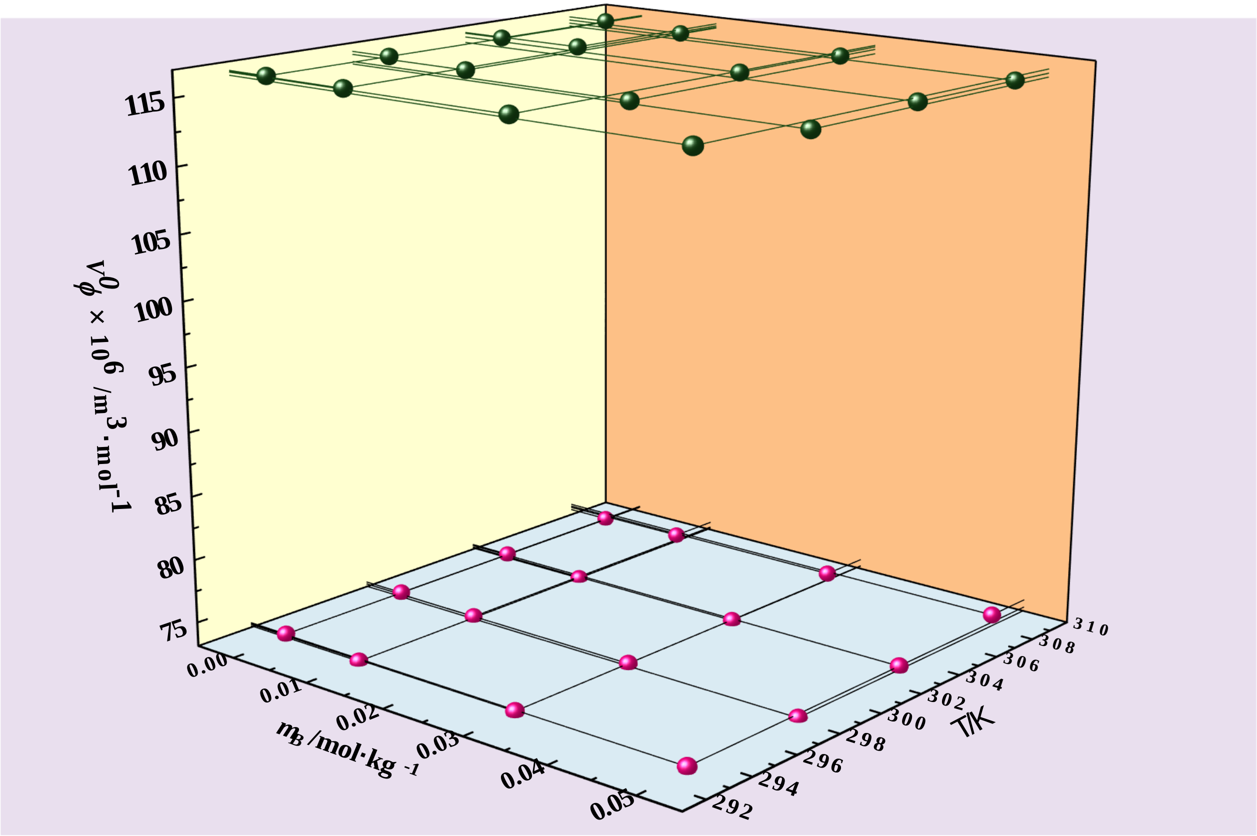
Variation of experimental and literature density values [2] of (niacin +Water) corresponding to the molality (m_B) of aqueous niacin at T= (298.15 and 308.15) K.

Figure 4.10



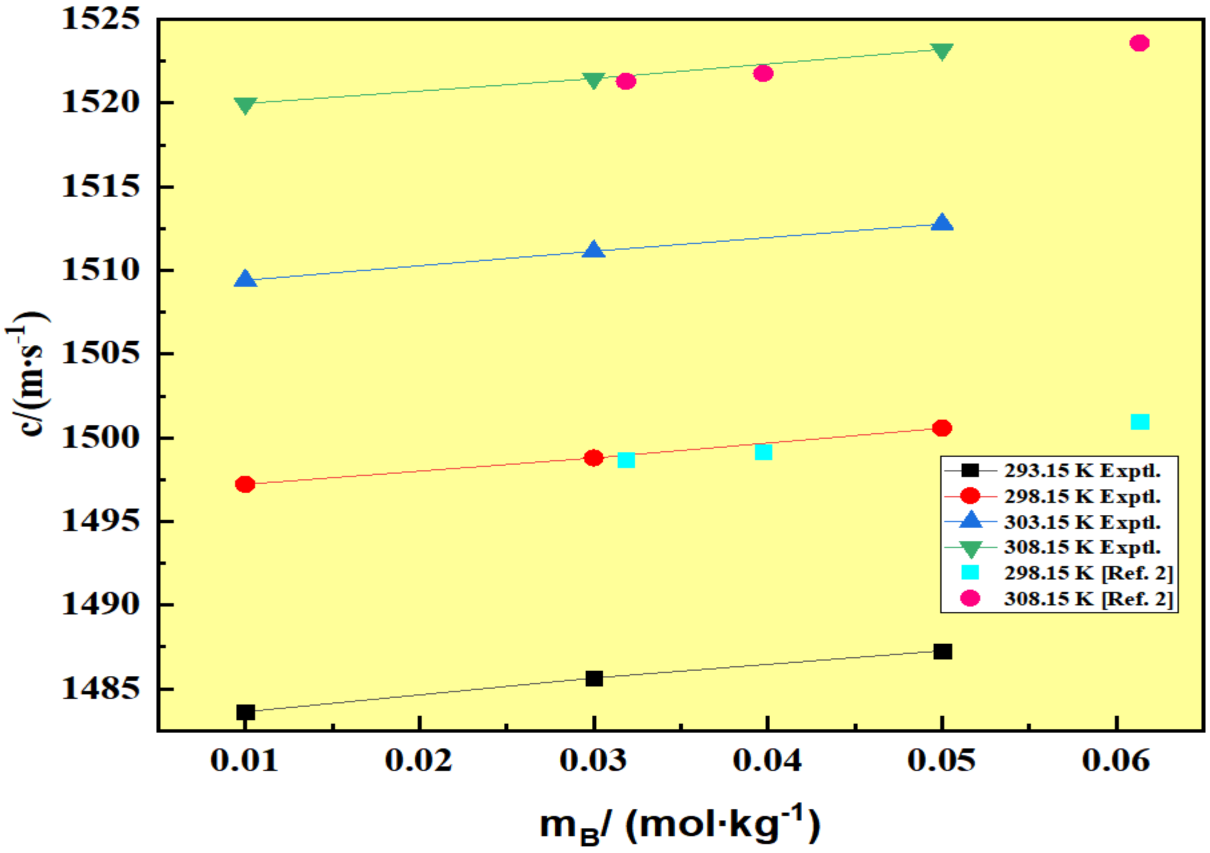
Variation of apparent molar volume, V_{ϕ}, corresponding to the molality (m_A) of glycols in niacin. (a) 0.01 niacin, (b) 0.03 niacin, (c) 0.05 niacin, against molality at a different temperature [red, Propylene glycol and blue, hexylene glycol]

Figure 4.11



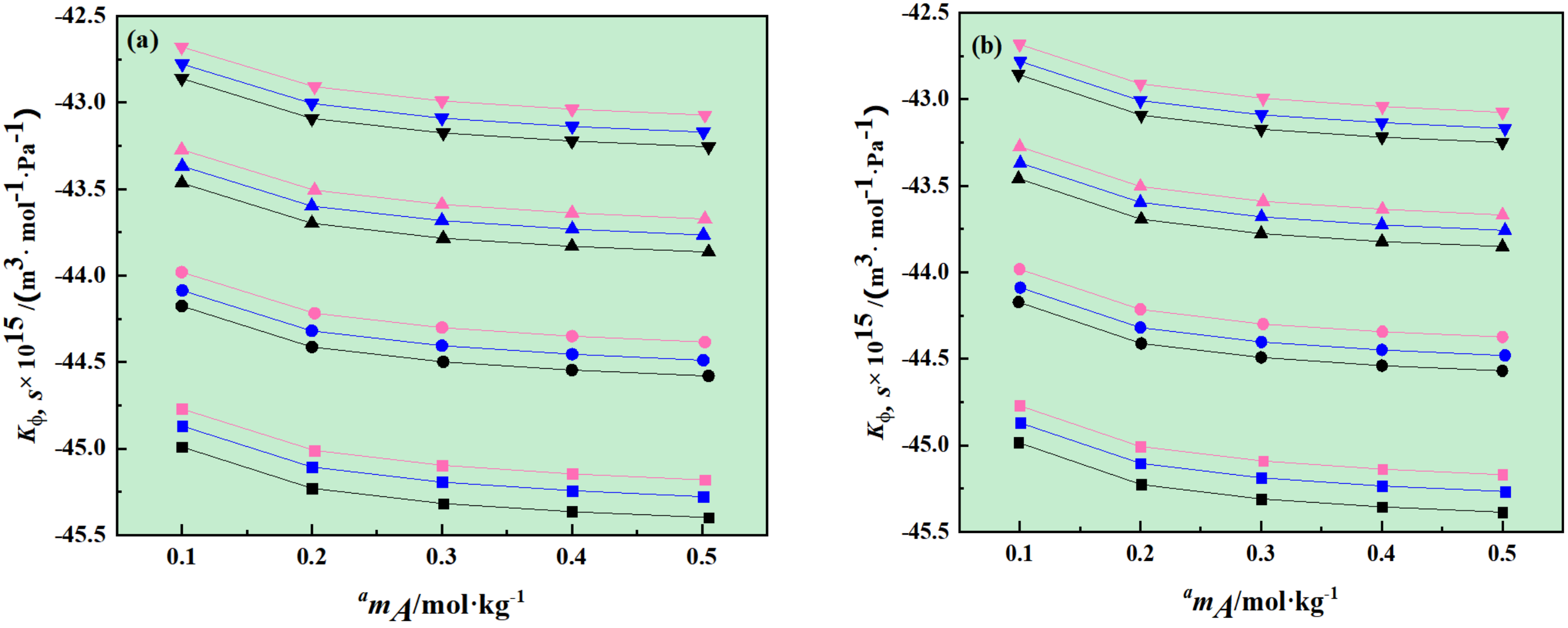
Variation of partial molar volumes, V_ϕ^0, corresponding to the molality (m_B) of niacin. Propylene glycol (color pink) and hexylene glycol (color olive) in different concentrations of aqueous niacin solutions at different temperature.

Figure 4.12



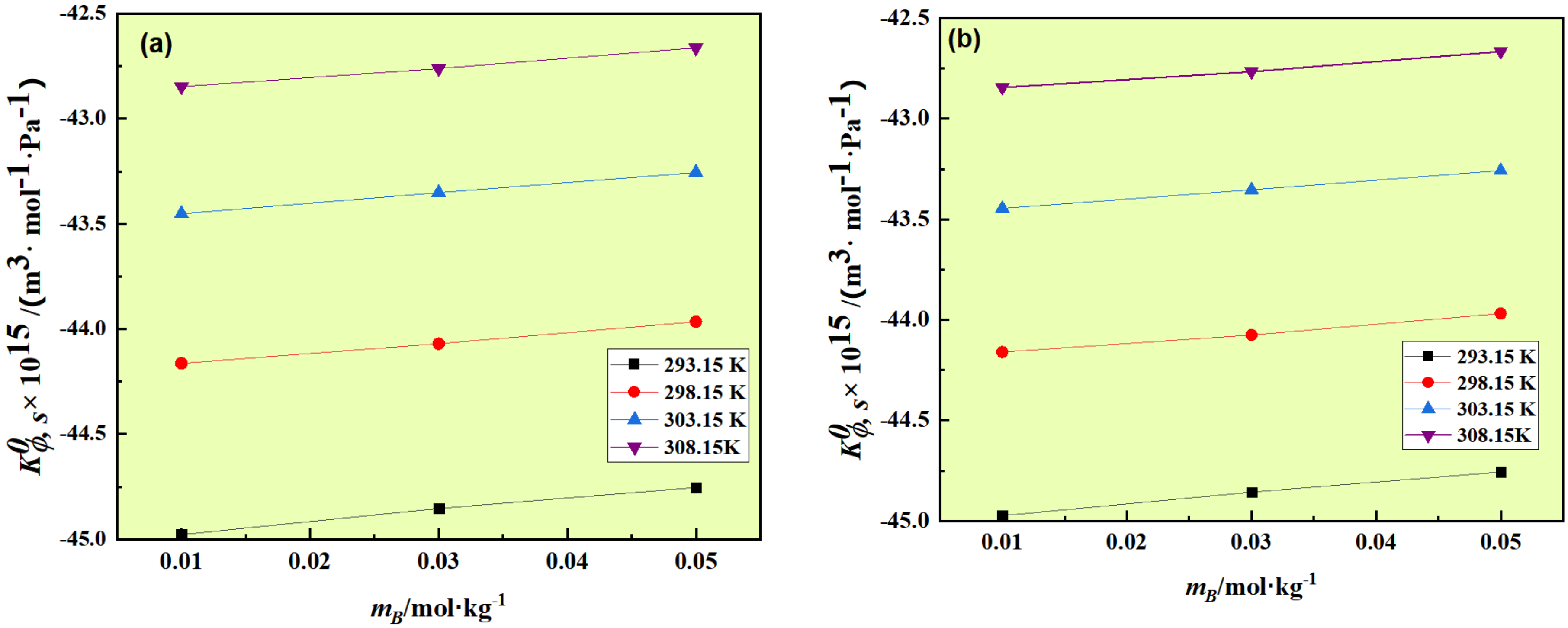
Variation of experimental and literature speed of sound values [2] of (niacin +Water) corresponding to the molality (m_B) of aqueous niacin at T= (298.15 and 308.15) K.

Figure 4.13



Variation of apparent molar isentropic compression, $K_{\phi,s}$, corresponding to the molality (m_A) of glycols in niacin. (a) Propylene glycol and (b) Hexylene glycol in aqueous solutions of **(**pink, 0.01 niacin; blue, 0.03 niacin; black**,** 0.05 niacin**)** against molality at a different temperature [inverted triangle, 308.15 K; triangle, 303.15 K, circle 298.15 K; square, 293.15 K]

Figure 4.14



Variation of partial molar isentropic compression,$K^0_{\phi,s}$, corresponding to the molality (m_A) of glycols in niacin. (a) Propylene glycol, and (b) Hexylene glycol in aqueous niacin solutions at different temperatures.

<u>Problem 3</u>

Volumetric and Ultrasonic study of polyethylene glycols in aqueous solutions of Niacin at different temperatures

In this section, we have reported the densities, ρ and speed of sound c of polyethylene glycol 200 (PEG 200), and polyethylene glycol 600 (PEG 600) in (0.00, 0.01, 0.02, 0.03) mol·kg^{-1} aqueous solutions of niacin at temperatures T = (293.15, 298.15, 303.15, 308.15) K.

4.22 Density

For the liquid combinations of (Niacin+ water) and (Niacin+ water+ polyethylene glycols), the experimentally obtained densities values for temperature variation of (293.15, 298.15, 303.15, and 308.15) *K* and concentrations (0.01, 0.02, and 0.03) *mol·kg^{-1}* are listed in **Table 4.21**. From our previous paper with reference no. [62], the (Polyethylene glycols+ water) density values are taken directly, from which it is clear that the density values decrease with the temperature but increases with the Niacin concentration and polyethylene glycol molality. The solute-solvent interaction increases from PEG 200 to PEG 600, which is presented in **Figure 4.15.** The comparison of the literature density values [2, 57, 63-68] of (Niacin+ water) for with the experimental values at various temperatures are shown using **Figure 4.16** and it is perceived that the experimental density values are in the propensity with the literature values.

4.23 Apparent molar volume

The Apparent molar volume is obtained utilizing the experimental densities of solution (ρ), densities of solvent (ρ_0), and molalities (m_A) values of PEGs in niacin, with the equation **4.1**. The interaction of the solute molecules with solvent results in the change of geometrical volume of solvent and solute molecules. This is termed as apparent molar volumes [69]. In **Table 4.21** the V_ϕ values are indexed and it is observed that the values are all positive thus involves the solute-solvent interaction among the mixture and the interaction increases with the molar mass of PEGs as elucidated in **Figure 4.15**. The augmentation of apparent molar volume with temperature from (293.15 to 308.15) K is described with the simultaneous degeneration with the molality of PEGs in the solution is illustrated in **Figure 4.17,** revealing the existence of a strong hydrogen bond between the PEGs molecules and the vitamin. Moreover, this increment of the V_ϕ values implies the inhabitation of the hydrophilic effect, hydrophobic hydration, (dipole and dipole) interactions, and (dipole-induced-dipole) in the ternary mixture [8, 9, 17, 51].

4.24 Partial molar volume

Equation **4.2** is used to obtain the partial molar volume of the liquid mixtures containing Niacin and polyethylene glycol by employing the V_ϕ values with polyethylene glycol molality (m_A). The partial molar volume gives information regarding the interactions in solute and solvent molecules present in the liquid mixture along with the data concerning the solute-solute interactions. The existence of hydrophilic-hydrophilic interactions, hydrophilic-hydrophobic interactions, through H-bond and hydrophobic-hydrophobic interactions are confirmed by the co-sphere overlap model [33, 70] as a consequence of positive V_ϕ^0 values which are reported in **Table 4.22** along with the standard errors. It is detected from the table that the values of V_ϕ^0 are increasing with the molar mass of PEGs, as evident from **Figure 4.18,** while the values show deduction with the concentration of niacin, which is due to the strong H-bond formed between polyethylene glycols and niacin than in the aqueous polyethylene glycols. As the hydrophilic- hydrophilic interaction among the molecules of niacin and polyethylene glycols increases the interaction, the depression in the V_ϕ^0 values with niacin concentration is observed. The experimental slope S_V^*, using the least square fitting of V_ϕ is determined and is attributed in the same table along with their standard errors. These values show no regular pattern concerning temperature as well as niacin concentration but since all the observed values are negative in magnitude, it establishes the supremacy of solute-solvent interaction over solute-solute interaction [4, 28, 32].

4.25 Partial molar volume of transfer

Transfer of partial molar volume of glycols from water to niacin aqueous solutions at infinite dilution is computed employing the equation **4.3** and reported in **Table 4.23.** Partial molar volume of transfer employs the qualitative and quantitative study of the solute-solvent interaction inside the mixture without considering the interactions due to solute-solute molecules [71]. The values of ΔV_ϕ^0 are all negative in magnitude except for the values of PEG 200 in (0.01 and 0.02) $mol{\cdot}kg^{-1}$ at 293.15 K, (0.02 and 0.03) $mol{\cdot}kg^{-1}$ at 303.15 K and for PEG 600 in 0.02 $mol{\cdot}kg^{-1}$ at 303.15 K. The ΔV_ϕ^0 values are decreasing with the rise in the molar mass of the polyethylene glycols but no steady pattern is observed with the upsurge of temperature. Thus the obtained negative values declare that the interaction among niacin and polyethylene glycols dominates the interactions between the polyethylene glycols and water. Following Pauling [14, 15], the model concerning the pure water organizational grid, clathrates, which are the devoid spaces present in the structure of water, gets easily infiltrated by the diverse molecules. To sustain the cage network of water, a small portion of polyethylene glycols gets positioned in the cages of water. Although the generation of H-bond between the organic and water molecules eradicates the water cage structure with more content of polyethylene glycols [3,72].

4.26 Temperature-dependent partial molar volume

With temperatures, the variation in the apparent molar volume at infinite dilution is determined utilizing equation **4.4.** Here, $a, b, c,$ are empirical constants listed in **Table 4.24**, T_{ref}=298.15 K, and the temperature in Kelvin is represented as T. In the same table the empirical constants, which are utilized to calculate the V_ϕ^0 values and the errors obtained from the experimental data are also maintained. The coefficient c values, which are scarcely significant, are all negative. With the help of these empirical constants, the theoretical values of V_ϕ^0 are calculated and are compared with the experimental values [42]. From these comparisons, the deviations of the experimental values from theoretical values are obtained and are termed as ARD (σ) and listed in the same table. This parameter is determined using the equation **4.14**. Here, Y is the partial molar volume (V_ϕ^0). Since very fewer variations are achieved, it can be anticipated that these variations fit properly in the polynomial equation evident from R^2 values [17]. V_ϕ^0 aimed to attain the partial molar expansibilities values and its first derivative using equation **4.5** and **4.6**. Calculated E_ϕ^0 values along with $\left(\partial \mathrm{E}_\phi^0/\partial \mathrm{T}\right)_P$ values are reported in **Table 4.25.** It is seen that the values of E_ϕ^0which are few negative and the rest are positive in magnitude, implying the presence of solute-solvent interactions, also prevailed by apparent molar volume values $\left(V_\phi\right)$. This parameter is the valuable extent of solute-solvent interactions in the liquid mixtures and the following thermodynamic formula is established to evaluate this structure making or structure breaking capability of the liquid system. $\left(\partial \mathrm{E}_\phi^0/\partial \mathrm{T}\right)_P$ values provide the knowledge about the structure making/breaking ability in the liquid system. The negative sign of the $\left(\partial \mathrm{E}_\phi^0/\partial \mathrm{T}\right)_P$ values establishes the presence of structure breaking capability in the mixture [24, 58, 73].

4.27 Ultrasonic speed

In **Table 4.26,** the experimentally obtained speed of sound values at (293.15, 298.15, 303.15 and 308.15) K for (Niacin+ water) as well as (Niacin+ water+ polyethylene glycols) for (0.02, 0.04 and 0.06) $mol \cdot kg^{-1}$ concentrations are described. For (polyethylene glycols+ water) the speed of sound values is taken directly from our previous paper with reference no. [62]. the experimental speed of sound values are compared with the literature values [2] for different temperatures and In **Figure 4.19** are graphically presented**.** The experimental values are showing the same trend as the literature values, i.e. increasing along with the temperatures and the concentrations of Niacin from (0.01 to 0.02 to 0.03) $mol \cdot kg^{-1}$. This is because of the water structure, having 3-dimensional networks of hydrogen bonds and the acceleration of the speed of sound values for the polyethylene glycol and vitamin mixture is due to the intermolecular hydrogen bonding in solute-solvent molecules and intramolecular hydrogen bonding in solute molecules, therefore suggests the high combination rate of the molecules inside the solutions.

Moreover, the upsurge in the values of speed of sound along with the molality of glycols attributes the hydrogen bond network insolvent with aqueous Niacin molecule. Also, with the increment in the molar mass of the polyethylene glycol, the hydrogen bond between the water and niacin molecules gets reduced and finally are abrogate but concurrently fresh H-bonds are created amidst of Niacin and glycol molecules [17, 23].

4.28 Apparent molar isentropic compression

The Apparent molar isentropic compression for glycols in niacin aqueous solution is obtained using the equation **4.7** utilizing the experimental densities of solution (ρ), densities of solvent (ρ_0), molalities (m_A) values of PEGs in niacin and reported in **Table 4.26**. Here, M is the molar mass of the solute. Using Laplace-Newton's equation **4.8**, the isentropic compressibility is expressed [74]. Here, ρ represents the density of the solution and c denotes the values of speed of sound. The isentropic compressibility (k_s) consist of two terms-

i. Solvent intrinsic compressibility
ii. Solute intrinsic compressibility

The first one arises due to compression of the solvent molecules and the second one emerges because of the hydration crust of polyethylene glycols compression. The existence of a more compressed water molecule innards the bulk solution despite the solute which occurs due to negative values of apparent molar isentropic compression ($K_{\phi,S}$) as evident from table. The negative $K_{\phi,S}$ values are decreasing with the temperature and concentration of niacin while the negativity increases along the molality of the polyethylene glycols which is presented in **Figure 4.20**. Hence due to hydrophobic interactions of polar groups, the water molecule contract and become less compressible over the ionic charge group of solute showing the arrangement of water molecules throughout the solute [21, 22, 75].

4.29 Partial molar isentropic compression

Using the equation **4.9** the partial molar isentropic compression is computed by contemplating the divergence of apparent molar isentropic compression along with the molality. Where, $K_{\phi,S}^{0}$, S_{K}^{*}, and m_A are the limiting isentropic compression, the experimental slope of solute and the solute interactions, and the molality of the solute in the aqueous niacin. Using the least square method, the experimental intercept $K_{\phi,S}^{0}$, and slope S_{k}^{*} with their standard errors are reported in **Table 4.27**. The $K_{\phi,S}^{0}$ values are all negative. Further, the negativity decreases with the rise in the temperature, and niacin concentration, which is graphically represented in **Figure 4.21**, suggests the substantial interactions within the water and polyethylene glycol molecules with the emission of water molecules to bulk. At infinite dilution, the negative values of S_{k}^{*} are observed, which shows increment with the rise in temperature of the ternary mixture but decreases with the niacin concentration, consequently theorize the solute-solvent interactions [29, 30].

4.30 Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer for glycol from water to aqueous niacin solutions at infinite dilution is determined using the equation **4.10**. The $\Delta K_{\phi,s}^{0}$ values which are positive except for PEGs in (0.01 and 0.02) $mol \cdot kg^{-1}$ at 308.15 K, are mentioned in **Table 4.28,** which reveals the structure making ability of solute. The values of $\Delta K_{\phi,s}^{0}$ is increasing with the niacin concentration, thus suggesting the increment of structure making capacity with the concentration of niacin and predominance of the zwitterionic center of polyethylene glycol and niacin [31].

4.31 Pair and triplet coefficients

Utilizing the equation **4.11** and **4.12** the partial molar volume of transfer and the partial molar isentropic compression of transfer can be obtained from. Where A represents glycols and B represents niacin and m_B denotes the molality of the aqueous niacin solutions. The pair and triplet interaction coefficient are represented by the parameters

V_{AB}, V_{ABB} for volume and K_{AB}, K_{ABB} for isentropic compression, and are reported in **Table 4.29** for all the temperatures**.** McMillan-Mayer [34] theory of solutions has been used to calculate the pair and triplet interaction of the liquid mixtures to analyze the parting of effects which was later discussed by Friedman and Krishnan [35] and Franks et al [36]. The values of pair interaction coefficient V_{AB} are negative except for PEG 200 at 293.15 *K* and PEG 600 at 303.15 *K* and triplet interaction coefficient V_{ABB} is all negative except for PEG 200 at (303.15 and 308.15) *K* and PEG 600 at 303.15 *K* throughout all the temperatures for all polyethylene glycols. Whereas the pair interaction coefficient K_{AB} is positive for every temperature all over the glycol concentrations except for PEG 200 at 308.15 *K*. For of triplet coefficient K_{ABB} is negative except for PEG 200 at 303.15 *K* and PEG 600 at (303.15 and 308.15) *K*. Due to positive values of pair interaction coefficients, it suggests the dominance of pairwise interaction in (Niacin+ water) and (Niacin+ water +polyethylene glycols) mixtures for compressibility and volumetric measurements and owing to the overlay of hydration sphere co-solute-solute fragments [42, 44].

Table 4.21

Values of densities, ρ, apparent molar volumes, V_{ϕ} of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

$^{a}m_A/(\text{mol}\cdot\text{kg}^{-1})$	$\rho \times 10^{-3}/(\text{kg}\cdot\text{m}^{-3})$				$V_{\phi} \times 10^{6}/(\text{m}^{3}\cdot\text{mol}^{-1})$			
	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 mol·kg^{-1} Niacin + PEG 200								
0.00000	0.998211	0.997047	0.995656	0.994039^{b}				
0.10649	1.001086	0.999925	0.998514	0.996894	172.77	172.91	173.30	173.57^{b}
0.20264	1.003682	1.002521	1.001091	0.999471	172.32	172.47	172.87	173.12
0.30183	1.006360	1.005199	1.003749	1.002129	171.86	172.02	172.42	172.67
0.40099	1.009038	1.007877	1.006407	1.004787	171.40	171.56	171.97	172.21
0.50154	1.011753	1.010592	1.009101	1.007481	170.94	171.10	171.51	171.75
0.01 mol·kg^{-1} Niacin + PEG 200								
0.00000	0.998610	0.997400	0.996000	0.994410				
0.10009	1.001250	1.000128	0.998698	0.997148	173.37	172.65	173.16	172.99
0.20057	1.004012	1.002812	1.001412	0.999845	172.34	172.46	172.66	172.78
0.29997	1.006655	1.005485	1.004085	1.002535	172.00	172.03	172.24	172.32
0.40054	1.009399	1.008199	1.006779	1.005199	171.42	171.56	171.82	172.02

0.50090	1.012111	1.010911	1.009471	1.007911	170.94	171.09	171.38	171.54
0.02 mol·kg^{-1} Niacin + PEG 200								
0.00000	0.999010	0.997810	0.996440	0.994790				
0.10001	1.001687	1.000590	0.999087	0.997587	172.91	172.04	173.60	172.30
0.20056	1.004393	1.003193	1.001793	1.000303	172.38	172.55	172.90	172.32
0.29991	1.007063	1.005863	1.004503	1.003023	171.91	172.08	172.24	171.89
0.40071	1.009799	1.008579	1.007199	1.005699	171.37	171.59	171.82	171.66
0.49994	1.012445	1.011250	1.009895	1.008395	170.97	171.13	171.30	171.21
0.03 mol·kg^{-1} Niacin + PEG 200								
0.00000	0.999410	0.998210	0.996840	0.995200				
0.09743	1.002078	1.000918	0.999399	0.997938	172.24	172.00	173.76	172.12
0.21003	1.005096	1.003906	1.002506	1.001006	172.04	172.16	172.51	172.05
0.31962	1.008094	1.006884	1.005484	1.003984	171.43	171.63	171.93	171.70
0.40405	1.010390	1.009180	1.007780	1.006280	171.03	171.23	171.50	171.37
0.49999	1.012970	1.011690	1.010370	1.008890	170.65	170.99	171.08	170.97
0.00 mol·kg^{-1} Niacin + PEG 600								
0.00000	0.998211	0.997047	0.995656	0.994039[b]				
0.10411	1.007362	1.005952	1.004385	1.002661	508.21	511.26	513.54	513.33[b]
0.19978	1.015771	1.014132	1.012402	1.010582	504.00	507.08	509.50	511.29

0.30099	1.024667	1.022784	1.020883	1.018962	499.62	502.79	505.27	507.09
0.40249	1.033589	1.031463	1.029388	1.027366	495.31	498.56	501.10	502.94
0.50775	1.042841	1.040463	1.03821	1.036082	490.91	494.25	496.84	498.71
0.01 mol·kg^{-1} Niacin + PEG 600								
0.00000	0.998610	0.997400	0.996000	0.994410				
0.10515	1.007937	1.006370	1.004788	1.003199	507.15	511.21	513.63	514.30
0.19524	1.015944	1.014286	1.012411	1.010782	503.07	506.06	509.29	510.17
0.30210	1.025232	1.023325	1.021326	1.019657	499.16	502.25	505.06	506.01
0.40600	1.034460	1.032177	1.030090	1.028295	494.54	498.09	500.63	501.87
0.49904	1.042842	1.040470	1.038318	1.035926	490.24	493.50	495.86	498.43
0.02 mol·kg^{-1} Niacin + PEG 600								
0.00000	0.999010	0.997810	0.996440	0.994790				
0.10384	1.008310	1.006850	1.005300	1.003740	506.14	509.26	511.66	511.44
0.20696	1.017463	1.015807	1.014096	1.012308	501.98	504.87	507.23	508.65
0.30368	1.025969	1.024140	1.022103	1.020330	498.20	501.01	504.05	505.19
0.39971	1.033993	1.031983	1.030179	1.028388	495.55	498.38	500.20	501.27
0.50857	1.043053	1.041060	1.039259	1.037312	492.13	494.47	496.03	497.39
0.03 mol·kg^{-1} Niacin + PEG 600								
0.00000	0.999410	0.998210	0.996840	0.995200				

0.10409	1.008896	1.007407	1.005937	1.004240	504.33	507.72	509.30	510.57
0.20554	1.017907	1.016409	1.014790	1.012840	500.98	503.04	504.92	507.25
0.29967	1.026129	1.024555	1.022573	1.020676	497.78	499.66	502.51	504.15
0.40272	1.035250	1.033470	1.031370	1.029348	493.55	495.70	498.35	500.12
0.50316	1.044402	1.042201	1.039840	1.037509	488.82	491.67	494.57	496.87

$^{a}m_A$ is the molality of polyethylene glycols in the aqueous solution of Niacin; standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.01K, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)$=0.01 MPa, ^{b}Values of densities and V_ϕ for (PEG 200 + water and PEG 600 + water) at temperature 298.15 and 308.15 K have been taken from our previous paper [62].

Table 4.22

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_{V}^{*}, of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

[a]m_B / (mol·kg^{-1})	$V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})				$S_{V}^{*} \times 10^{6}$/(m^{3}·kg·mol^{-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
PEG 200								
0.00	173.25(±0.003)	173.39(±0.002)	173.79(±0.004)	174.06(±0.001)[b]	-4.61(±0.008)	-4.57(±0.007)	-4.53(±0.011)	-4.60(±0.004)[b]
0.01	173.75(±0.202)	173.17(±0.108)	173.58(±0.026)	173.42(±0.083)	-5.78(±0.608)	-4.02(±0.327)	-4.42(±0.679)	-3.65(±0.251)
0.02	173.38(±0.042)	172.71(±0.378)	174.08(±0.103)	172.73(±0.148)	-4.89(±0.128)	-2.77(±1.139)	-5.69(±0.311)	-2.85(±0.446)
0.03	172.75(±0.119)	172.49(±0.227)	174.12(±0.267)	172.54(±0.145)	-4.17(±0.354)	-2.90(±0.674)	-6.42(±0.791)	-2.94(±0.431)
PEG 600								
0.00	512.60(±0.086)	515.51(±0.081)	517.79(±0.072)	519.55(±0.077)[b]	-42.85(±0.257)	-42.01(±0.241)	-41.38(±0.216)	-41.18(±0.230)[b]
0.01	511.61(±0.310)	515.30(±0.612)	518.22(±0.361)	518.24(±0.268)	-42.39(±0.931)	-43.37(±1.839)	-44.21(±1.084)	-40.07(±0.806)
0.02	509.27(±0.529)	512.56(±0.519)	515.47(±0.248)	515.57(±0.456)	-34.38(±1.565)	-36.00(±1.547)	-38.22(±0.739)	-35.39(±1.357)
0.03	508.80(±0.586)	511.57(±0.295)	512.91(±0.451)	514.31(±0.218)	-38.64(±1.754)	-39.66(±0.883)	-36.24(±1.350)	-34.69(±0.653)

[a] m_B is the molality of Niacin; standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.01K, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)$=0.01 *MPa* [b] Values of V_{ϕ}^{0} and S_{V}^{*} for (PEG 200 + water and PEG 600 + water) at temperature 298.15 and 308.15 K have been taken from our previous paper [62].

Table 4.23

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
PEG 200				
0.01	0.50	-0.22	-0.21	-0.64
0.02	0.13	-0.68	0.29	-1.33
0.03	-0.50	-0.90	0.33	-1.52
PEG 600				
0.01	-0.99	-0.21	0.43	-1.31
0.02	-3.33	-2.95	-2.32	-3.98
0.03	-3.80	-3.94	-4.88	-5.24

$^{a}m_B$ is the molality of Niacin; standard uncertainties u are $u_r(m) = 0.01$, $u(T)=0.01$ *K*, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)= 0.01$ *MPa*

Table 4.24

Values of empirical parameters of Eq., of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

$^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
PEG 200					
0.01	173.40	-0.03	0.00	0.9999	0.00103
0.02	173.42	0.02	-0.01	0.9999	0.00388
0.03	173.26	0.09	-0.01	0.9999	0.00308
PEG 600					
0.01	515.62	0.64	-0.04	0.9999	0.00318
0.02	512.93	0.60	-0.03	0.9999	0.00298
0.03	511.35	0.43	-0.01	0.9999	0.00212

$^{a}m_B$ is the molality of Niacin; standard uncertainties u are $u_r(m)$ = 0.01, *u(T)=0.01 K, u(ρ)*= $\pm$5.0 $kg \cdot m^{-3}$, *u(c)*= $\pm$2.0 $m \cdot s^{-1}$ and *u(p)*= 0.01 *MPa*

Table 4.25

Partial molar expansibilities, E_{ϕ}^{0}, of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

${}^{a}m_B$/ (mol·kg^{-1})	E_{ϕ}^{0} ×10^{6}/(m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K	
PEG 200					
0.01	-0.1183	-0.0327	0.0530	0.1386	0.0086
0.02	0.1598	0.0228	-0.1143	-0.2514	-0.0137
0.03	0.3482	0.0856	-0.1771	-0.4397	-0.0263
PEG 600					
0.01	1.3736	0.6397	-0.0941	-0.8280	-0.0734
0.02	1.2353	0.5959	-0.0435	-0.6828	-0.0639
0.03	0.7027	0.4261	0.1496	-0.1269	-0.0277

${}^{a}m_B$ is the molality of Niacin; standard uncertainties u are $u_r(m) = 0.01$, $u(T)=0.01$ K, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)= 0.01$ *MPa*

Table 4.26

Values of speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,s}$ of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^6$/(m^3·mol^{-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
0.00 mol·kg^{-1} Niacin + PEG 200								
0.00000	1481.14	1495.85	1508.84	1519.84^{b}				
0.10649	1491.35	1506.28	1519.04	1529.71	-45.28	-44.40	-43.63	-43.57^{b}
0.20264	1500.57	1515.70	1528.25	1538.62	-45.61	-44.71	-43.95	-43.88
0.30183	1510.08	1525.42	1537.75	1547.81	-45.80	-44.91	-44.13	-44.06
0.40099	1519.58	1535.13	1547.25	1557.00	-45.96	-45.06	-44.29	-44.22
0.50154	1529.22	1544.99	1556.88	1566.32	-46.11	-45.21	-44.43	-44.36
0.01 mol·kg^{-1} Niacin + PEG 200								
0.00000	1483.63	1497.22	1509.42	1519.97				
0.10009	1492.90	1506.97	1519.27	1529.82	-45.10	-44.29	-43.58	-42.97
0.20057	1502.75	1516.72	1528.87	1538.93	-45.46	-44.64	-43.92	-43.31
0.29997	1512.19	1526.40	1538.37	1548.33	-45.65	-44.83	-44.11	-43.50
0.40054	1521.85	1536.19	1548.04	1557.61	-45.82	-44.99	-44.26	-43.65

0.50090	1531.82	1546.02	1557.66	1566.89	-45.96	-45.13	-44.40	-43.79
0.02 mol·kg^{-1} Niacin + PEG 200								
0.00000	1484.77	1498.09	1510.21	1520.48				
0.10001	1494.07	1508.09	1520.23	1530.31	-45.04	-44.24	-43.53	-42.95
0.20056	1504.12	1517.81	1529.77	1539.58	-45.39	-44.58	-43.87	-43.28
0.29991	1513.62	1527.61	1539.32	1549.03	-45.58	-44.78	-44.06	-43.48
0.40071	1523.23	1537.26	1548.99	1558.31	-45.75	-44.93	-44.22	-43.63
0.49994	1533.28	1547.11	1558.54	1567.58	-45.89	-45.08	-44.36	-43.77
0.03 mol·kg^{-1} Niacin + PEG 200								
0.00000	1485.65	1498.79	1511.15	1521.47				
0.09743	1494.95	1508.65	1520.85	1530.96	-44.97	-44.19	-43.46	-42.88
0.21003	1506.22	1519.69	1531.69	1541.34	-45.36	-44.57	-43.84	-43.25
0.31962	1516.47	1530.55	1542.15	1551.69	-45.57	-44.77	-44.04	-43.45
0.40405	1524.84	1538.76	1550.36	1559.58	-45.70	-44.90	-44.17	-43.58
0.49999	1534.55	1548.22	1559.52	1568.47	-45.84	-45.04	-44.30	-43.71
0.00 mol·kg^{-1} Niacin + PEG 600								
0.00000	1481.14	1495.85	1508.84	1519.84[b]				
0.10411	1510.65	1525.11	1536.98	1547.04	-45.56	-44.66	-43.88	-43.24[b]
0.19978	1537.77	1551.99	1562.84	1572.04	-46.16	-45.23	-44.44	-43.79

0.30099	1566.45	1580.42	1590.19	1598.48	-46.09	-45.69	-44.89	-44.23
0.40249	1595.22	1608.94	1617.62	1625.02	-47.09	-46.12	-45.30	-44.63
0.50775	1625.06	1638.52	1646.07	1652.50	-47.53	-46.55	-45.71	-45.03
0.01 mol·kg^{-1} Niacin + PEG 600								
0.00000	1483.63	1497.22	1509.42	1519.97				
0.10515	1513.26	1527.06	1538.26	1549.08	-45.45	-44.61	-43.88	-43.27
0.19524	1539.67	1552.40	1563.32	1572.65	-46.01	-45.16	-44.41	-43.79
0.30210	1569.55	1582.36	1591.85	1600.58	-46.51	-45.64	-44.88	-44.26
0.40600	1599.25	1611.68	1620.50	1628.32	-46.97	-46.08	-45.31	-44.67
0.49904	1626.00	1638.63	1646.09	1653.16	-47.37	-46.47	-45.69	-45.02
0.02 mol·kg^{-1} Niacin + PEG 600								
0.00000	1484.77	1498.09	1510.21	1520.48				
0.10384	1514.48	1528.24	1539.99	1550.73	-45.37	-44.55	-43.83	-43.25
0.20696	1544.13	1557.40	1568.66	1577.96	-46.00	-45.17	-44.43	-43.83
0.30368	1570.42	1584.96	1594.23	1603.07	-46.46	-45.61	-44.85	-44.24
0.39971	1599.42	1612.00	1620.75	1628.65	-46.86	-45.99	-45.24	-44.63
0.50857	1632.61	1644.08	1650.63	1658.26	-47.29	-46.42	-45.66	-45.04
0.03 mol·kg^{-1} Niacin + PEG 600								
0.00000	1485.65	1498.79	1511.15	1521.47				

0.10409	1516.39	1530.22	1541.60	1551.65	-45.33	-44.52	-43.79	-43.20
0.20554	1546.43	1559.21	1569.69	1578.76	-45.95	-45.13	-44.39	-43.77
0.29967	1572.46	1585.89	1595.76	1603.78	-46.39	-45.56	-44.80	-44.18
0.40272	1602.99	1615.00	1623.34	1631.48	-46.84	-46.00	-45.22	-44.59
0.50316	1634.93	1645.10	1651.87	1659.02	-47.28	-46.41	-45.61	-44.97

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[a] m_A is the molality of polyethylene glycols in the aqueous solution Niacin; standard uncertainities u are $u_r(m) = 0.01$, $u(T)$=0.01K, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)$=0.01 MPa [b]Values of velocity and $K_{\phi,s}$ for (PEG 200 + water and PEG 600 + water) at temperature 298.15 and 308.15 K have been taken from our previous paper [62].

Table 4.27

Partial molar isentropic compression, $K_{\phi,s}^{0}$, and experimental slopes, S_K^*, of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

[a]m_B/ (mol·kg^{-1})	$K_{\phi,s}^{0}$ ×10^6/(m^3·mol^{-1}· GPa^{-1})				S_K^* ×10^6/(kg·m^3·mol^{-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
PEG 200								
0.00	-45.14(±0.07)	-44.25(±0. 07)	-43.50(±0. 07)	-43.91(±0. 07)[b]	-2.03(±0.21)	-1.99(±0. 21)	-1.95(±0. 21)	-1.94(±0. 21)
0.01	-44.98(±0.07)	-44.17(±0.07)	-43.45(±0.07)	-42.85(±0.07)	-2.07(±0.23)	-2.03(±0.22)	-2.00(±0.22)	-1.97(±0.22)
0.02	-44.91(±0.07)	-44.12(±0.07)	-43.40(±0.07)	-42.83(±0.07)	-2.06(±0.23)	-2.02(±0.22)	-2.00(±0.22)	-1.98(±0.22)
0.03	-44.84(±0.07)	-44.06(±0.07)	-43.34(±0.07)	-42.76(±0.07)	-2.10(±0.23)	-2.06(±0.23)	-2.04(±0.23)	-2.02(±0.)
PEG 600								
0.00	-45.13(±0. 07)	-44.25(±0. 07)	-43.49(±0. 07)	-42.86(±0. 07)[b]	-4.82(±0. 22)	-4.62(±0. 21)	-4.48(±0. 21)	-4.38(±0. 21)
0.01	-45.01(±0.6)	-44.19(±0.6)	-43.47(±0.6)	-42.88(±0.6)	-4.82(±0.20)	-4.64(±0.20)	-4.51(±0.19)	-4.38(±0.20)
0.02	-44.97(±0.08)	-44.16(±0.08)	-43.45(±0.07)	-42.87(±0.07)	-4.69(±0.25)	-4.55(±0.24)	-4.46(±0.22)	-4.37(±0.21)
0.03	-44.90(±0.07)	-44.11(±0.07)	-43.40(±0.07)	-42.81(±0.07)	-4.82(±0.21)	-4.66(±0.22)	-4.49(±0.22)	-4.38(±0.22)

[a]m_B is the molality of Niacin; standard uncertainties u are $u_r(m) = 0.01$, *u(T)=0.01 K, u(ρ)=* $\pm 5.0\ kg \cdot m^{-3}$, *u(c)=* $\pm 2.0\ m \cdot s^{-1}$ and *u(p)=* 0.01 *MPa*, [b]Values of $K_{\phi,s}^{0}$ and S_K^* for (PEG 200 + water and PEG 600 + water) at temperature 298.15 and 308.15 K have been taken from our previous paper [62].

Table 4.28

Partial molar isentropic compression transfer, $\Delta K_{\phi,s}^{0}$, of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

${}^{a}m_B$/ (mol·kg^{-1})	$\Delta K_{\phi,s}^{0}$ × 10^{6}/(m^{3}·mol^{-1}· GPa^{-1})			
	T=293.15 K	T=298.15 K	T =303.15 K	T =308.15 K
PEG 200				
0.01	0.16	0.08	0.05	1.06
0.02	0.23	0.13	0.10	1.08
0.03	0.30	0.19	0.16	1.15
PEG 600				
0.01	0.12	0.06	0.02	-0.02
0.02	0.16	0.09	0.04	-0.01
0.03	0.23	0.14	0.09	0.05

${}^{a}m_B$ is the molality of Niacin; standard uncertainties u are $u_r(m)$ = 0.01, $u(T)=0.01$ *K*, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)$= 0.01 *MPa*

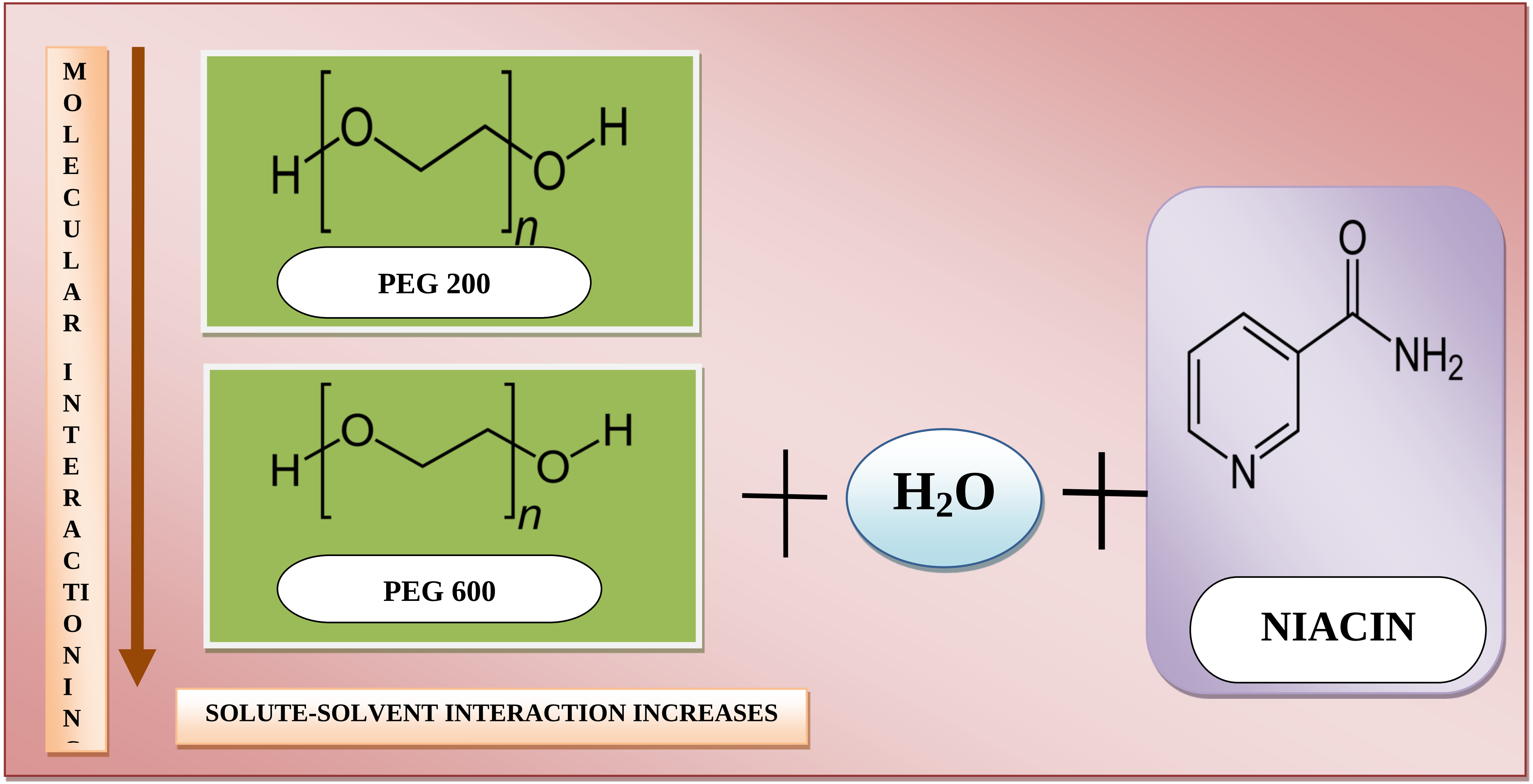
Table 4.29

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of polyethylene glycols in aqueous solutions of Niacin at different temperatures and experimental pressure 0.1 *MPa*.

T/K	V_{AB} ×10^{6}/(m^{3}·mol^{-2}· kg)	V_{ABB} ×10^{6}/(m^{3}·mol^{-3}·kg^{2})	K_{AB} ×10^{6}/(m^{3}·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^{6}/(m^{3}·mol^{-3}·kg^{2} GPa^{-1})
PEG 200				
293.15	34.41	-960.32	8.75	-86.45
298.15	-14.58	-18.61	4.30	-27.08
303.15	-5.33	263.56	1.94	17.16
308.15	-41.58	350.66	57.46	-870.39
PEG 600				
293.15	-79.30	292.65	5.81	-45.15
298.15	-31.85	-832.94	2.59	-7.89
303.15	34.57	-2639.75	0.39	24.74
308.15	-86.17	-81.77	-2.06	63.05

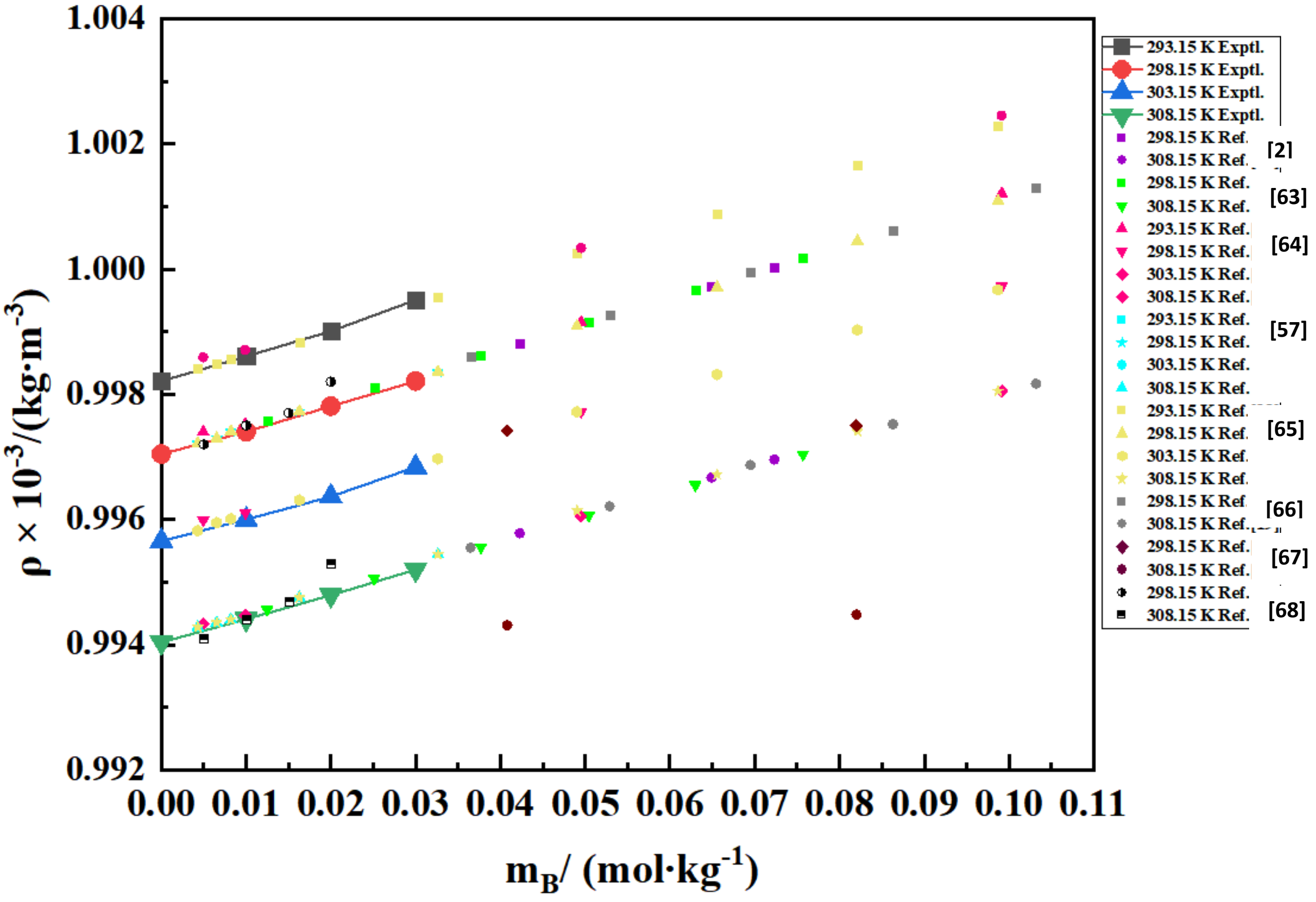
T/K is the temperatures; standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.01K, $u(\rho)= \pm 5.0\ kg \cdot m^{-3}$, $u(c)= \pm 2.0\ m \cdot s^{-1}$ and $u(p)$=0.01 MPa

Figure 4.15



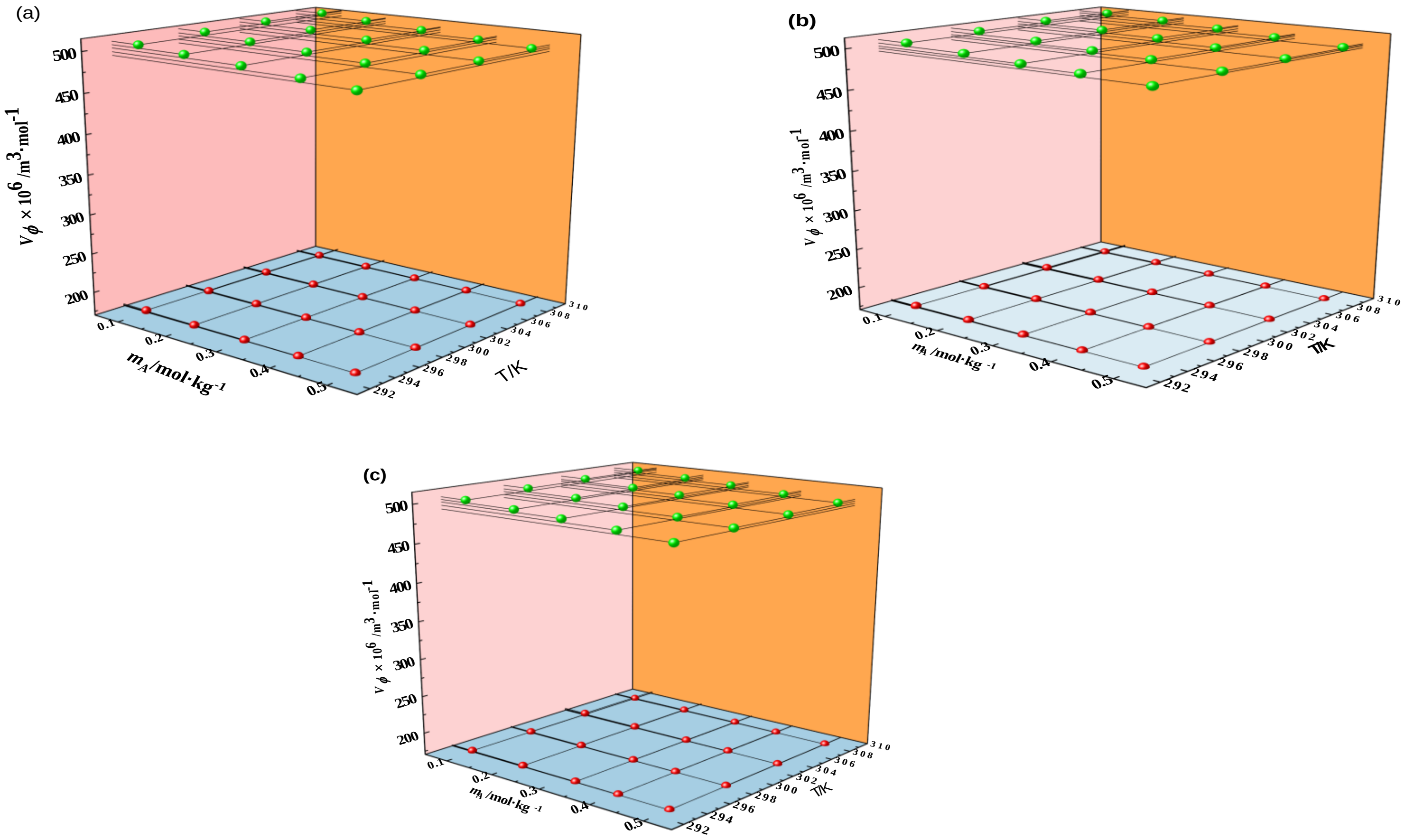
PEG 200/ PEG 600 and Niacin interactions.

Figure 4.16



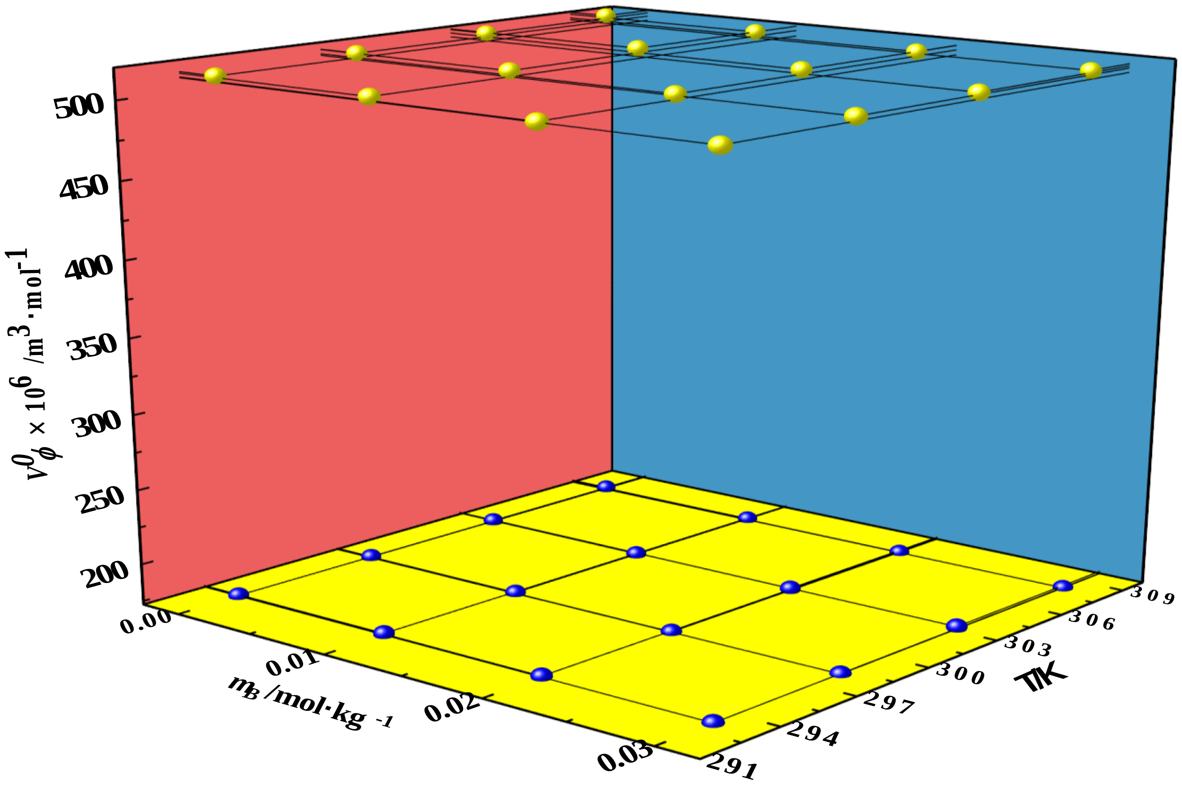
Variation of density for experimental and literature values [2, 57, 63-68] for (Niacin +Water) at T= 298.15K and T= 308.15 K.

Figure 4.17



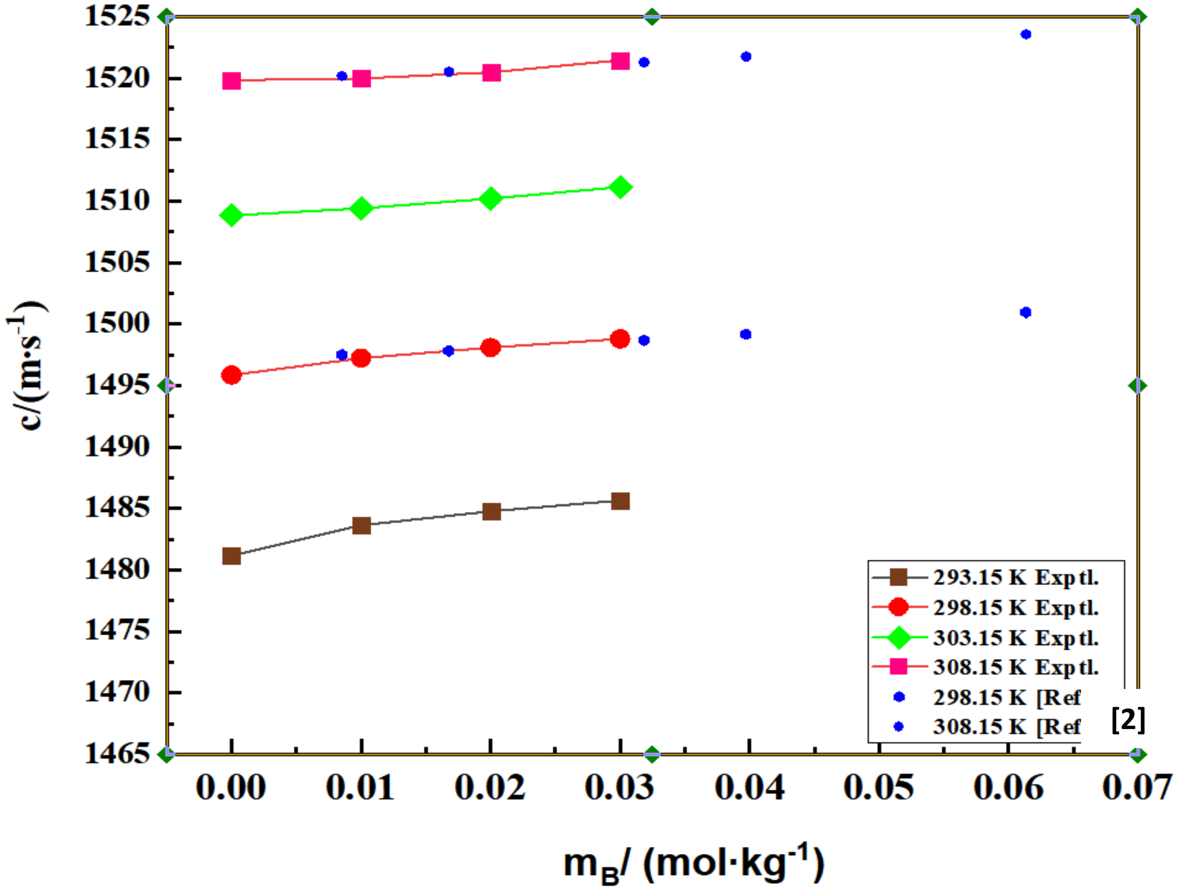
Variation of apparent molar volume, V_ϕ (a) 0.01 Niacin, (b) 0.02 Niacin, (c) 0.03 Niacin, against molality at different temperature [red, PEG 200 and green PEG 600].

Figure 4.18



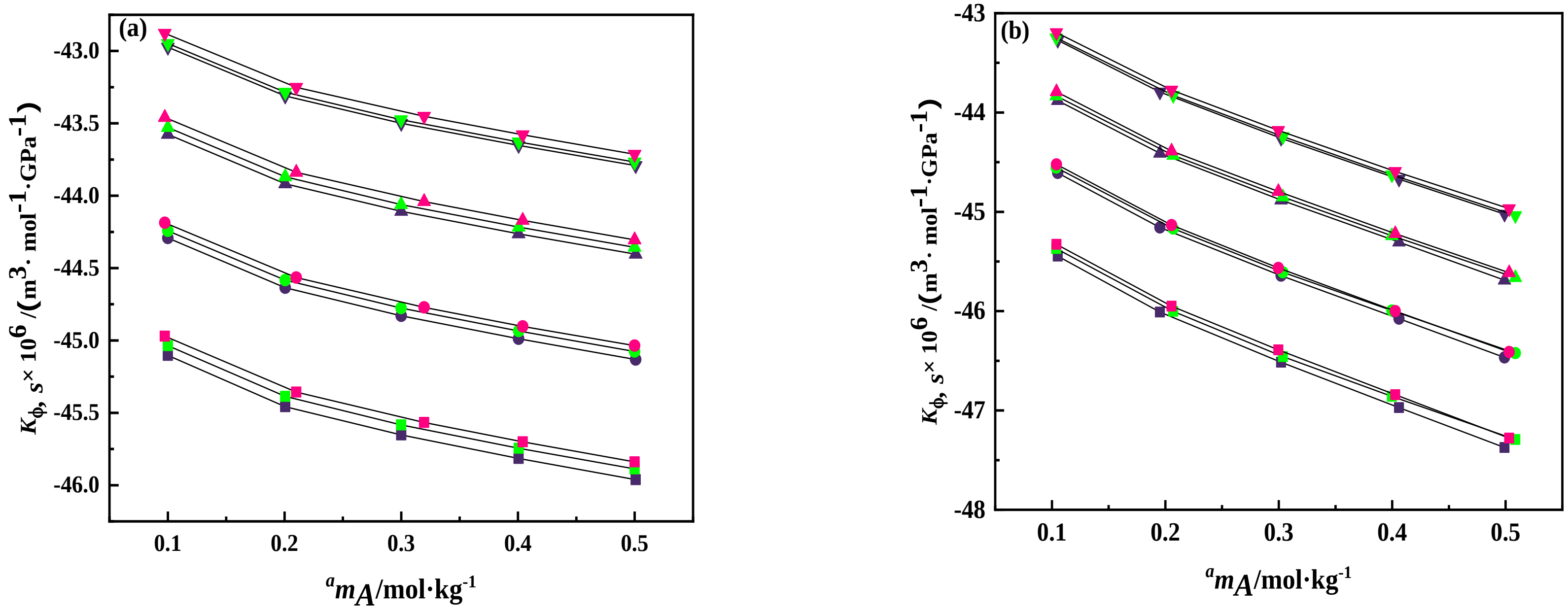
Variation of partial molar volumes, V_ϕ^0, of, PEG 200 (color blue) and PEG 600 (color yellow) in different concentration of aqueous Niacin solutions at different temperature.

Figure 4.19



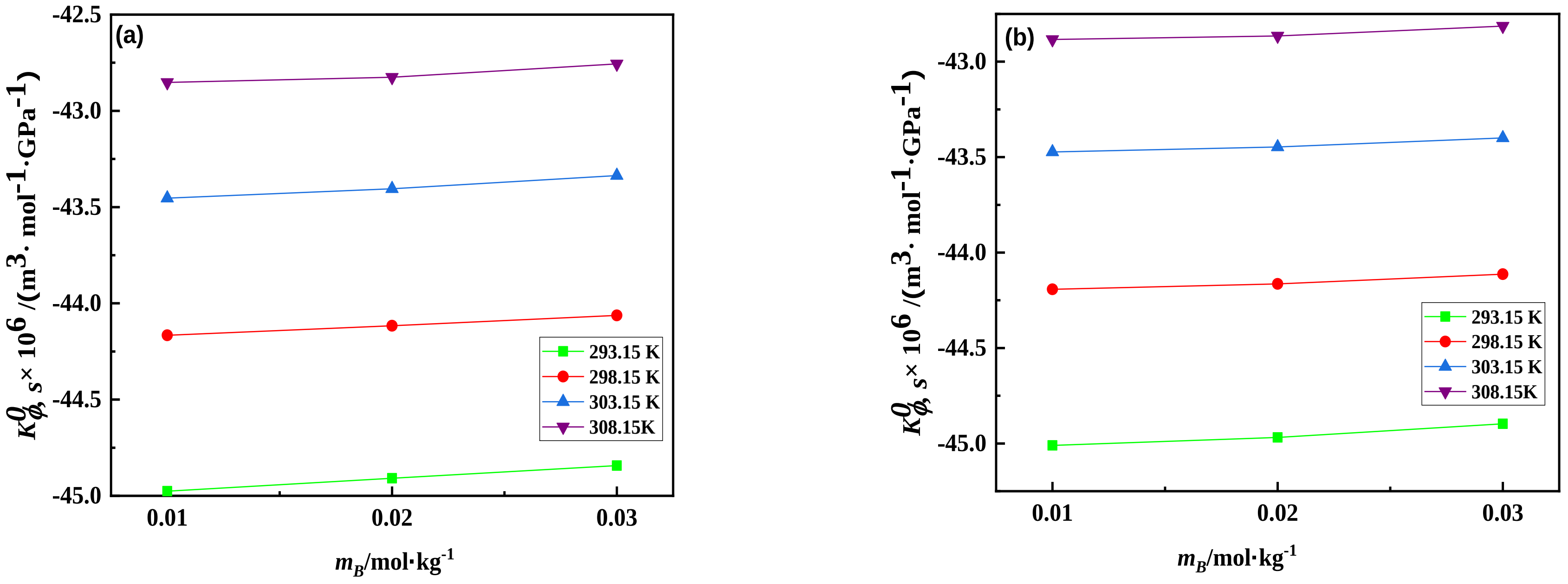
Variation of the speed of sounds for experimental and literature values [2] for (Niacin +Water) at T= 298.15K and T= 308.15 K.

Figure 4.20



Variation of apparent molar isentropic compression, $K_{\phi,s,}$ of (a) PEG 200 and (b) PEG 600 in aqueous solutions of **(**pink, 0.01 Niacin; green, 0.02 Niacin; purple**,** 0.03 Niacin**)** against molality at a different temperature [inverted triangle, 308.15 K; triangle, 303.15 K, circle 298.15 K; square, 293.15 K]

Figure 4.21



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, of (a) PEG 200, and (b) PEG 600 in aqueous Niacin solutions at different temperatures.

Problem 4

Volumetric and Ultrasonic Studies of Molecular Interactions of PEG 400 and PEG 4000 in aqueous niacin solutions at Different Temperatures.

In this section, we have reported the densities, ρ and speed of sound c of polyethylene glycol 400 (PEG 400), and polyethylene glycol 4000 (PEG 4000) in (0.00, 0.07, 0.08, 0.09) mol·kg^{-1} aqueous solutions of niacin at temperatures T = (288.15, 298.15, 308.15, 318.15) K.

4.32 Density

The density values for polyethylene glycols (400/4000) in 0.00 mol·kg^{-1} aqueous niacin solution at (288.15-318.15) K is taken from our previous paper [51] and are graphically compared with literature [7, 76-80] in **Figure 4.23** from which it is evident that they are following the same trend corresponding to their temperatures and concentrations. In **Table 4.31** the experimentally obtained density values for polyethylene glycols (400/4000) in the aqueous solution of niacin in (0.07, 0.08, and 0.09) mol·kg^{-1} at multiple temperatures are mentioned. The comparison graph of experimental and literature density [63, 66, 81] values for (Niacin+ water) is represented in **Figure 4.24,** which are in good agreement with each other i.e. the values are increasing with the glycol molality and niacin concentration but decreasing with the experimental temperatures.

4.33 Apparent molar volume

Equation **4.1** is used to calculate the values of apparent molar volume (V_ϕ) using the experimental density data where, M, m_A, ρ, and ρ_0 are representing the molar mass of the solute, the molality of the solute per one kilogram of the solvent (Niacin+ water), the densities of the solution and the solvent respectively. In **Table 4.31** the calculated V_ϕ values are reported, which are all positive thus implying the presence of strong solute-solvent interactions inside the liquid mixture due to the large intrinsic volume of solute. It can be seen that the V_ϕ values are increasing with the increase in the experimental temperatures, molality of polyethylene glycols, and niacin concentrations. This trend suggests that the niacin molecules combine with the water molecules constructively to strengthen the hydrogen bond in the solvent as in the first hydration shell of the water molecules associates with the OH group on niacin [48, 82]. Also, this upsurge of V_ϕ values with temperatures and concentrations is visible in **Figure 4.25,** which establishes the presence of dipole-dipole, dipole-induced dipole interactions, hydrophilic interactions in the water-rich region, and hydrophilic effect [46]. The extent of interactions of niacin with polyethylene glycols with temperatures is presented in **Figure 4.22** which suggests the accession of the molecular interaction in the mixture from PEG 400 to PEG 4000 due to a tenfold increase of average molecular weight and considerably longer chain length of PEG 4000 as compared to PEG 400 which increases ether hydrogen bond acceptors.

4.34 Partial Molar volume

Equation **4.2** is applied to retrieve the partial molar volume of polyethylene glycols in aqueous niacin solutions. The partial molar volume is attained applying the least square fitting of apparent molar volume (V_ϕ) values and the values of intercept V_ϕ^0 including the standard errors which are calculated from least-squares fitting are attributed in **Table 4.32**. The positive values of V_ϕ^0 escalate along with the molar mass of polyethylene glycols, from PEG 400 to PEG 4000, as graphically represented in **Figure 4.26**, thus suggesting the presence of a strong hydrogen bond interaction in the oxygen atoms of polyethylene glycols hydrogen atoms of water [1, 13]. The survival of solvent-solvent interaction is recommended by the positive V_ϕ^0 values wherein the co-spheres of two ionic species overlap with one another. This increases the volume, whereas when the (hydrophobic and hydrophobic) and (ion and hydrophobic) group overlaps on each other, a decrease in the volume is observed, as stated by the overlap model co-sphere [20, 41, 28]. Further, the positive values of V_ϕ^0 data describe the dominance of ion-hydrophilic interaction upon hydrophobic-hydrophobic interaction. The experimental slope S_V^* is defined as the semi-empirical solute-solute interaction parameter which is the fitting slope parameter indicating the nature of solute-solute interactions surviving in the liquid system, are reported in Table 3, along with the standard error. It describes the nature of solute-solute interactions concerning the asymmetric S_V^* values which are both positive and negative values that are smaller than the V_{ϕ}^{0} values. This implies the dominance of solute-solvent interactions over the solute and solute interactions [21].

4.35 Partial molar volume of transfer

Transfer of standard molar volume of glycols from water to niacin aqueous solutions at infinite dilution is computed employing equation **4.3**. In **Table 4.33** the ΔV_{ϕ}^{0} values are listed which are all positive and increasing with the temperature and concentration of niacin. This trend is due to the presence of strong (ion-ion) interaction of polyethylene glycols and niacin. Pauling [14, 15] gave the model for pure water structure which states that space is present in the water structure which is called clathrates in which any diverse molecules penetrates easily thus a very small portion of polyethylene glycols molecules gets placed in the cages of water structure such that the cage network is not eradicated. Due to the formation of the new structure and hydrogen bond among water and organic molecules in the solution, the higher content of polyethylene glycols destroys the cage arrangement of water. The complex-forming capability of solute increases in the solution as a result of interaction between solute and solvent molecules as the structural component of niacin and glycol contain polar group [83].

4.36 Temperature-dependent partial molar volume

Utilizing equation **4.4**, the variation in the apparent molar volume at infinite dilution with temperatures is determined. Here, $a, b, c,$ are empirical constants listed in **Table 4.34**, T_{ref}=298.15 K, and the temperature in Kelvin is represented as T. The V_{ϕ}^{0} values are obtained from the empirical constants which are mentioned in the same table S2 along with the aberrations obtained from the experimental data. The coefficient c values are all positive for PEG 400 but negative for PEG 4000. These positive c values define the deviation in the V_{ϕ}^{0} values and the values of R^2 are found to be the best fit of data[5]. The main purpose of V_{ϕ}^{0} was to obtain partial molar expansibilities values, which are computed using equation **4.5**. The extent of solute-solvent interactions in the fluid system is depicted from this parameter and the evaluation of structure making or structure breaking capability of the liquid system is established using the thermodynamic equation **4.6**. The structure making/breaking ability of solution is depicted with the sign of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$. The minute negative values of this parameter, along with the positive values of E_{ϕ}^{0} are ascribed in **Table 4.35**, indicating the structure making ability. The E_{ϕ}^{0} values are all positive, showing a decrement trend with temperatures, molality of polyethylene glycols, and niacin concentrations, suggesting the existence of interactions among solute-solvent as previously analyzed from the V_{ϕ}^{0} values. These positive values of E_{ϕ}^{0} infer the interaction among the polyethylene glycols and niacin molecules due to caging or packing effect [84].

4.37 Ultrasonic Speed

The speed of sound values has been experimentally obtained at (288.15, 298.15, 308.15, and 318.15) K for the aqueous niacin solutions as well as the ternary mixture (Niacin+ distilled water+ polyethylene glycols) at the concentrations of (0.07, 0.08, and 0.09) mol·kg^{-1} and are depicted in **Table 4.36.** The values for the speed of sound of (distilled water + Polyethylene glycols) is directly taken from our previous paper [51] and is compared with literature [7, 76, 78] for (PEG 400+ distilled water) that is represented in **Figure 4.23** [(b)] from which it can be deduced that the nature of the increment in the speed of sound values against its respective temperatures and concentrations in both the cases are in a similar pattern. The experimental c (speed of sound) values for (distilled water + Niacin) are compared beside the literature values [81, 85] at temperatures 298.15 K and 308.15 K which are represented graphically in **Figure 4.27,** and it is observed that the speed of sound values are rising along with the concentrations of niacin from (0.07 to 0.08 to 0.09) mol·kg^{-1} and temperatures, hence exhibiting the similar trend as the literature. This happens for the 3-dimensional networks in hydrogen bonds in the structure of water. This upsurge in the values of speed of sound for the polyethylene glycol and niacin mixture is due to intermolecular and intramolecular hydrogen bonding in solute-solvent molecules [23]. The increase in these values with the molality of polyethylene glycols suggests the H-bond network in the aqueous Niacin molecule. Also, by the rise of the molar mass of the polyethylene glycol, the H-bond in the water and niacin molecules degrades and ultimately gets suppressed but simultaneously fresh hydrogen bonds are produced between molecules of Niacin and polyethylene glycol [42].

4.38 Apparent molar isentropic compression

Apparent molar isentropic compression for polyethylene glycols in aqueous niacin solution is captured applying equation **4.7.** Equation **4.8** is used to calculate the isentropic compressibility. In **Table 4.36** the $K_{\phi,S}$ values are listed which are found to be negative**,** thus implying that the molecules of water are more compressible in the bulk solution comparatively than the water molecules over solute. The negative $K_{\phi,S}$ values are reducing with the increment in the concentration of niacin and the thermal reading, which is graphically expressed in **Figure 4.28** for polyethylene glycols at all temperatures [47, 56]. Therefore, as the outcome of hydrophobic interactions in non-polar groups, the water molecules contract. This variation in the values of $K_{\phi,S}$ suggests low compressibility of water molecules over the ionic charge group of solute and shows the alignment of water molecules in a distinct order overall the solute. Moreover, extra loss of structural compressibility of water is detected due to negative values of $K_{\phi,S}$ due to more aligning effect caused by solute and solvent [44].

4.39 Partial molar isentropic compression

With equation **4.9** the partial molar isentropic compression is calculated by considering the divergence of apparent molar isentropic compression along with the molality. The calculated $K^0_{\phi,S}$ values are recorded in **Table 4.37** along with the graphical description in **Figure 4.29.** From least square fitting, the intercept values $K^0_{\phi,S}$, and the experimental slope S^*_K are mentioned with their standard errors in Table 6. With the niacin concentration, the $K^0_{\phi,S}$ values are detected to be less negative and increases with the temperature, thus signifying the interactions are strong and attractive among the molecules of water and molecules of polyethylene glycols [55]. The reduction of electrostriction and ejection of molecules of water to bulk is observed, which is confirmed due to the negative values of $K^0_{\phi,S}$. Moreover, at high concentrations, water molecules around polyethylene glycols are more compressible than at lower concentrations which results due to dehydration of polyethylene glycols between niacin molecules [17]. The negative values of S_K^* confirms the existence of solute-solvent interactions at infinite dilution in the liquid mixture [58].

4.40 Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer for polyethylene glycol from water to aqueous niacin solutions at infinite dilution is determined using equation **4.10.** In **Table 4.38** the values of $\Delta K_{\phi,s}^0$ are listed**,** which are all positive and the values are decreasing with the temperatures but increasing with the niacin concentration and molality of polyethylene glycol. There exists structure making capability of solute due to the positive $\Delta K_{\phi,s}^0$ values which is evident from the table and this shows the interaction dominance between the zwitterionic center of glycol and niacin. The extent of structure making ability increases along with the solute-solvent interactions in the ternary system as with the polyethylene glycol molality, the $\Delta K_{\phi,s}^0$ values increases [16].

4.41 Pair and triplet interaction coefficients

The partial molar volume of transfer and the partial molar isentropic compression of transfer is obtained from equations **4.11** and **4.12.** *A* represents polyethylene glycols and *B* represents niacin. The pair and triplet interaction coefficient are represented by the parameters V_{AB} and V_{ABB}; $K_{AB},$ K_{ABB} for volume and isentropic compression respectively which are reported in **Table 4.39** for all the temperatures**.** As per McMillan-Mayer [34] theory, the pair and triplet interaction are formulated for the liquid mixtures to analyze the parting of effects which was later discussed by Friedman and Krishnan [35] and Franks et al [36]. The values of pair interaction coefficient V_{AB} are all positive and triplet interaction coefficient V_{ABB} is all positive throughout all the temperatures for all polyethylene glycols molality. While on the other hand, the pair interaction coefficient K_{AB} are all positive except at temperature 318.15. In the case of triplet coefficient K_{ABB} all the values are positive. Due to positive values of pair interaction coefficients; it suggests the dominance of pairwise interaction in (Niacin+ water) and (Niacin+ water + polyethylene glycols) mixtures for compressibility and volumetric measurements [5, 86].

Table 4.30

Values of the total mass of polyethylene glycols (PEG 400/ PEG 4000) corresponding to their molality in aqueous niacin solutions.

0.07 mol·kg^{-1} Niacin			
PEG 400		PEG 4000	
$^{a}m_A$/(mol·kg^{-1})	Weight (g)	$^{a}m_A$/(mol·kg^{-1})	Weight (g)
0.00998	0.015968	0.00999	0.15984
0.02005	0.032080	0.02008	0.32128
0.02900	0.046400	0.02990	0.47840
0.04021	0.064336	0.04000	0.64000
0.05005	0.080080	0.05011	0.80176
0.08 mol·kg^{-1} Niacin			
PEG 400		PEG 4000	
$^{a}m_A$/(mol·kg^{-1})	Weight (g)	$^{a}m_A$/(mol·kg^{-1})	Weight (g)
0.01011	0.016176	0.01003	0.16048
0.02000	0.032000	0.01999	0.31984
0.02990	0.047840	0.03000	0.48000
0.04003	0.064048	0.03999	0.63984
0.05100	0.081600	0.04990	0.79840
0.09 mol·kg^{-1} Niacin			
PEG 400		PEG 4000	
$^{a}m_A$/(mol·kg^{-1})	Weight (g)	$^{a}m_A$/(mol·kg^{-1})	Weight (g)

0.01027	0.016432	0.00999	0.15984
0.01989	0.031824	0.01992	0.31872
0.03021	0.048336	0.03031	0.48496
0.04092	0.065472	0.04101	0.65616
0.04990	0.079840	0.04998	0.79968

[a] m_A is the molality of polyethylene glycols in the aqueous solution Niacin; standard uncertainties u are $u_r(m) = 0.01$.

Table 4.31

Values of densities, ρ, apparent molar volumes, V_ϕ of polyethylene glycols in aqueous solutions of Niacin at different temperatures, and 0.1 MPa pressure.

$^{a}m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.00 mol·kg^{-1} Niacin + PEG 400								
0.00000	0.99926	0.99705	0.99404	0.99036[b]				
0.01000	0.99997	0.99774	0.99471	0.99101[b]	328.89	331.37	334.34	336.93[b]
0.01992	1.00064	0.99839	0.99534	0.99162[b]	330.16	332.78	335.91	338.56[b]
0.03006	1.00130	0.99903	0.99595	0.99222[b]	331.51	334.26	337.45	340.09[b]
0.03992	1.00191	0.99961	0.99651	0.99277[b]	332.91	335.65	338.89	341.46[b]
0.05009	1.00252	1.00020	0.99707	0.99331	334.06	336.83	340.06	342.78
0.07 mol·kg^{-1} Niacin + PEG 400								
0.00000	1.00221	1.00012	0.99689	0.99315				
0.00998	1.00290	1.00078	0.99755	0.99380	330.22	332.69	334.85	336.95
0.02005	1.00357	1.00144	0.99819	0.99442	331.22	333.62	335.76	337.98
0.02900	1.00414	1.00200	0.99873	0.99496	332.05	334.49	336.69	338.90
0.04021	1.00483	1.00267	0.99939	0.99561	333.26	335.65	337.86	339.89
0.05005	1.00542	1.00323	0.99994	0.99615	334.19	336.73	338.85	340.88
0.08 mol·kg^{-1} Niacin + PEG 400								

0.00000	1.00275	1.00061	0.99733	0.99367				
0.01011	1.00342	1.00127	0.99798	0.99431	332.67	334.76	336.81	338.67
0.02000	1.00406	1.00188	0.99859	0.99490	333.52	335.68	337.68	339.65
0.02990	1.00467	1.00248	0.99917	0.99548	334.52	336.62	338.52	340.60
0.04003	1.00527	1.00307	0.99975	0.99604	335.43	337.60	339.62	341.73
0.05100	1.00589	1.00367	1.00034	0.99663	336.53	338.76	340.71	342.73
0.09 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1.00327	1.00118	0.99782	0.99410				
0.01027	1.00393	1.00183	0.99845	0.99473	334.61	336.38	338.68	340.34
0.01989	1.00453	1.00241	0.99903	0.99530	335.50	337.30	339.56	341.20
0.03021	1.00514	1.00302	0.99962	0.99588	336.43	338.27	340.54	342.24
0.04092	1.00576	1.00362	1.00020	0.99646	337.46	339.31	341.52	343.21
0.04990	1.00625	1.00410	1.00068	0.99693	338.32	340.21	342.34	344.00
0.00 mol·kg^{-1} Niacin + PEG 4000								
0.00000	0.99926	0.99705	0.99404	0.99036[b]				
0.01003	1.00568	1.00350	1.00055	0.99694[b]	3340.48	3342.64	3344.86	3347.26[b]
0.02001	1.01164	1.00950	1.00661	1.00307[b]	3341.82	3343.89	3345.90	3348.39[b]
0.02929	1.01684	1.01474	1.01189	1.00841[b]	3343.02	3345.02	3347.23	3349.63[b]
0.03994	1.02243	1.02037	1.01758	1.01416[b]	3344.26	3346.11	3348.32	3350.75[b]
0.05012	1.02745	1.02542	1.02267	1.01931	3345.29	3347.17	3349.42	3351.84
0.07 mol·kg^{-1} Niacin + PEG 4000								

0.00000	1.00221	1.00012	0.99689	0.99315				
0.00999	1.00848	1.00642	1.00326	0.99960	3344.77	3346.93	3348.92	3350.93
0.02008	1.01441	1.01238	1.00928	1.00569	3345.59	3347.85	3349.83	3351.84
0.02990	1.01981	1.01781	1.01477	1.01125	3346.37	3348.64	3350.61	3352.58
0.04000	1.02502	1.02305	1.02006	1.01662	3347.22	3349.52	3351.52	3353.51
0.05011	1.02992	1.02798	1.02505	1.02166	3348.01	3350.28	3352.30	3354.39
0.08 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1.00275	1.00061	0.99733	0.99367				
0.01003	1.00900	1.00690	1.00368	1.00010	3348.32	3350.72	3352.90	3354.98
0.01999	1.01480	1.01272	1.00957	1.00606	3349.32	3351.73	3353.88	3355.91
0.03000	1.02025	1.01821	1.01512	1.01167	3350.38	3352.76	3354.95	3356.90
0.03999	1.02535	1.02333	1.02030	1.01692	3351.43	3353.92	3356.04	3357.99
0.04990	1.03010	1.02811	1.02513	1.02182	3352.42	3354.93	3357.09	3358.94
0.09 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1.00327	1.00118	0.99782	0.99410				
0.00999	1.00944	1.00739	1.00410	1.00047	3352.75	3354.74	3356.31	3358.03
0.01992	1.01517	1.01315	1.00993	1.00637	3353.79	3355.83	3357.41	3359.01
0.03031	1.02077	1.01878	1.01564	1.01216	3354.73	3356.84	3358.40	3360.03
0.04101	1.02617	1.02421	1.02113	1.01772	3355.66	3357.84	3359.43	3361.10
0.04998	1.03042	1.02849	1.02546	1.02211	3356.41	3358.58	3360.33	3362.05

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[a] m_A is the molality of polyethylene glycols in the aqueous solution of Niacin (solvent); standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.001K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1} and $u(V_\phi)$ = (0.05-0.07) × 10^{6}/ (m^{3}·mol^{-1}), [b]Values of densities and apparent

molar volumes, V_{ϕ} for (PEG 400 + water and PEG 4000 + water) at temperature 288.15 and 318.15 K have been taken from our previous paper [51].

Table 4.32

Partial molar volumes, V_ϕ^0, and experimental slopes, S_V^*, of polyethylene glycols in the aqueous solution of Niacin at different temperatures and 0.1 MPa pressure.

[a]m_B/ (mol·kg^{-1})	$V_\phi^0 \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-2})			
	T=288.15 K	T =298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				PEG 400				
0.00	327.56(±0.04)	329.98(±0.03)	332.86(±0.02)	335.44(±0.06)[b]	132.24(±1.40)	141.54(±1.21)	151.85(±0.80)	153.02(±2.37)[b]
0.07	329.22(±0.04)	331.62(±0.06)	333.80(±0.04)	336.01(±0.04)	99.62(±1.29)	101.08(±2.03)	100.60(±1.44)	97.27(±1.41)
0.08	331.68(±0.04)	333.74(±0.04)	335.78(±0.08)	337.65(±0.05)	94.50(±1.32)	97.56(±1.40)	95.71(±2.63)	100.18(±1.57)
0.09	333.64(±0.02)	335.38(±0.02)	337.73(±0.01)	339.39(±0.03)	93.53(±0.67)	96.31(±0.66)	92.58(±0.49)	93.01(±1.15)
				PEG 4000				
0.00	3339.16(±0.06)	3341.42(±0.07)	3343.65(±0.06)	3346.00(±0.06)[b]	130.74(±2.49)	120.34(±2.61)	117.74(±2.24)	120.70(±2.29)[b]
0.07	3343.96(±0.01)	3346.14(±0.04)	3348.11(±0.04)	3350.08(±0.04)	81.17(±0.43)	83.55(±1.47)	84.26(±1.27)	85.76(±1.39)
0.08	3347.27(±0.02)	3349.63(±0.04)	3351.80(±0.03)	3353.94(±0.04)	103.43(±0.65)	106.31(±1.43)	105.69(±1.09)	100.26(±1.45)
0.09	3351.91(±0.07)	3353.87(±0.08)	3355.36(±0.05)	3357.02(±0.02)	91.18(±2.25)	95.78(±2.68)	99.64(±1.51)	100.02(±0.84)

[a] m_B is the molality of aqueous Niacin, standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.001K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(V_\phi^0)$ =0.01 × 10^6/ (m^3·mol^{-1}) and $u(S_V^*)$ =0.03 × 10^6/ (m^3·mol^{-2}), [b]Values of partial molar volumes, V_ϕ^0 and experimental slopes, S_V^*, for (PEG 400 + water and PEG 4000 + water) at temperature 288.15 and 318.15 K have been taken from our previous paper [51]

Table 4.33

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in the aqueous solution of Niacin at different temperatures and 0.1 MPa pressure.

[a]m_B/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 400		
0.07	1.66	1.64	0.94	0.57
0.08	4.12	3.76	2.92	2.21
0.09	6.08	5.40	4.87	3.95
		PEG 4000		
0.07	4.80	4.72	4.46	4.08
0.08	8.11	8.21	8.15	7.94
0.09	12.75	12.45	11.71	11.02

[a] m_B is the molality of aqueous Niacin

Table 4.34

Values of empirical parameters of Eq., of glycols in the aqueous solution of Niacin at different temperatures and 0.1 MPa pressure.

$^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	ARD
			PEG 400		
0.07	331.578	0.230	0.000	0.9999	0.000
0.08	333.762	0.204	0.000	0.9999	0.000
0.09	335.574	0.198	0.000	0.9999	0.003
			PEG 4000		
0.07	3346.105	0.209	-0.001	0.9999	0.000
0.08	3349.606	0.227	-0.001	0.9999	0.000
0.09	3353.774	0.176	-0.001	0.9999	0.000

$^{a}m_B$ is the molality aqueous of Niacin

Table 4.35

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in the aqueous solution of Niacin at different temperatures and 0.1 MPa pressure.

${}^{a}m_{B}$/ (mol·kg^{-1})	$E_{\phi}^{0}\times10^{6}$/(m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			PEG 400		
0.07	0.240	0.230	0.221	0.212	-0.001
0.08	0.214	0.204	0.195	0.185	-0.001
0.09	0.202	0.198	0.194	0.190	0.000
			PEG 4000		
0.07	0.219	0.209	0.198	0.188	-0.001
0.08	0.238	0.227	0.216	0.206	-0.001
0.09	0.191	0.176	0.161	0.146	-0.002

${}^{a}m_{B}$ is the molality aqueous of Niacin

Table 4.36

Values of the speed of sound, *c,* apparent molar isentropic compression, $K_{\phi,s}$ of polyethylene glycols in aqueous solutions of Glycerol at different temperatures and 0.1 MPa pressure.

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^6$/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.00 mol·kg^{-1} Niacin + PEG 400								
0.00000	1466.59	1495.85	1519.14	1536.02^b				
0.01000	1469.00	1498.22	1521.23	1538.17^b	-41.89	-40.25	-38.99	-38.11^b
0.01992	1471.38	1500.57	1523.31	1540.32^b	-44.24	-42.52	-41.20	-40.29^b
0.03006	1473.80	1502.98	1525.43	1542.52^b	-45.06	-43.30	-41.97	-41.04^b
0.03992	1476.16	1505.32	1527.49	1544.65^b	-45.47	-43.70	-42.36	-41.42^b
0.05009	1478.82	1507.62	1529.78	1546.82	-45.82	-44.12	-42.87	-41.95
0.07 mol·kg^{-1} Niacin + PEG 400								
0.00000	1472.13	1502.03	1524.41	1540.75				
0.00998	1474.68	1504.53	1526.63	1542.97	-41.60	-39.94	-38.74	-37.89
0.02005	1477.18	1506.83	1528.83	1545.17	-43.94	-42.19	-40.95	-40.07
0.02900	1479.31	1509.19	1530.69	1547.08	-44.67	-42.90	-41.64	-40.75
0.04021	1482.12	1511.93	1533.09	1549.64	-45.14	-43.36	-42.08	-41.18
0.05005	1484.70	1514.24	1535.22	1551.73	-45.39	-43.60	-42.32	-41.42

0.08 mol·kg^{-1} Niacin + PEG 400								
0.00000	1473.33	1503.16	1525.69	1542.05				
0.01011	1475.82	1505.65	1528.07	1544.29	-41.59	-39.94	-38.74	-37.89
0.02000	1478.41	1508.08	1530.21	1546.45	-43.86	-42.12	-40.87	-39.99
0.02990	1480.75	1510.66	1532.33	1548.59	-44.64	-42.88	-41.61	-40.72
0.04003	1483.35	1513.11	1534.49	1550.87	-45.06	-43.28	-42.00	-41.11
0.05100	1486.21	1515.75	1536.85	1553.25	-45.34	-43.55	-42.26	-41.36
0.09 mol·kg^{-1} Niacin + PEG 400								
0.00000	1474.70	1504.47	1526.85	1543.21				
0.01027	1477.39	1507.05	1529.23	1545.39	-41.59	-39.94	-38.75	-37.90
0.01989	1479.72	1509.48	1531.32	1547.52	-43.76	-42.04	-40.80	-39.92
0.03021	1482.25	1512.09	1533.63	1549.74	-44.58	-42.82	-41.56	-40.68
0.04092	1485.05	1514.78	1536.01	1552.14	-45.00	-43.23	-41.96	-41.07
0.04990	1487.41	1516.85	1537.95	1554.15	-45.22	-43.45	-42.17	-41.27
0.00 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1466.59	1495.85	1519.14	1536.02[b]				
0.01003	1486.47	1515.48	1539.01	1555.56[b]	-42.33	-40.67	-39.41	-38.52[b]
0.02001	1506.24	1535.26	1558.78	1575.35[b]	-44.92	-43.17	-41.85	-40.93[b]
0.02929	1524.63	1553.66	1577.16	1593.75[b]	-45.89	-44.11	-42.77	-41.83[b]
0.03994	1545.74	1574.78	1598.26	1614.86[b]	-46.57	-44.77	-43.41	-42.47[b]

0.05012	1565.07	1593.89	1617.27	1635.86	-47.05	-45.31	-44.01	-43.14
0.07 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1472.13	1502.03	1524.41	1540.75				
0.00999	1492.57	1522.44	1544.59	1560.93	-42.01	-40.34	-39.14	-38.28
0.02008	1512.49	1543.05	1564.52	1580.93	-44.59	-42.83	-41.57	-40.69
0.02990	1531.56	1562.61	1583.82	1600.06	-45.58	-43.79	-42.51	-41.61
0.04000	1552.81	1582.89	1604.12	1620.56	-46.21	-44.39	-43.10	-42.20
0.05011	1573.12	1602.02	1623.16	1640.91	-46.66	-44.82	-43.53	-42.62
0.08 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1473.33	1503.16	1525.69	1542.05				
0.01003	1494.48	1523.76	1546.23	1562.04	-41.97	-40.30	-39.10	-38.24
0.01999	1514.25	1544.16	1566.03	1582.03	-44.50	-42.75	-41.49	-40.60
0.03000	1534.09	1564.22	1585.64	1602.01	-45.51	-43.72	-42.44	-41.55
0.03999	1555.02	1584.31	1606.01	1622.21	-46.12	-44.31	-43.02	-42.12
0.04990	1575.08	1603.03	1624.59	1642.03	-46.56	-44.74	-43.44	-42.53
0.09 mol·kg^{-1} Niacin + PEG 4000								
0.00000	1474.70	1504.47	1526.85	1543.21				
0.00999	1496.51	1525.02	1548.02	1564.04	-41.88	-40.21	-39.02	-38.17
0.01992	1516.01	1545.26	1567.54	1584.03	-44.41	-42.66	-41.41	-40.53
0.03031	1537.09	1566.33	1588.15	1604.31	-45.44	-43.66	-42.39	-41.50

0.04101	1559.61	1588.11	1610.02	1626.21	-46.08	-44.28	-42.99	-42.10
0.04998	1578.08	1605.11	1626.61	1644.03	-46.47	-44.65	-43.36	-42.46

[a] m_A is the molality of polyethylene glycols in the aqueous solution of Niacin (solvent); standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.001K, $u(\rho)=0.06$(kg·m^{-3}), $u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K_{\phi,S})$ =0.25 × 10^6/ (m^3·mol^{-1}· GPa^{-1}), [b] Values of speed of sound and apparent molar isentropic compression, $K_{\phi,s}$ for (PEG 400 + water and PEG 4000 + water) at temperature 288.15 and 318.15 K have been taken from our previous paper [51].

Table 4.37

Partial molar isentropic compression, $K^0_{\phi,s}$, and experimental slopes, S_K^*, of polyethylene glycols in the aqueous solution of Glycerol at different temperatures and 0.1 MPa pressure.

$^{a}m_B$/ (mol·kg^{-1})	$K^0_{\phi,s}$ ×10^6/(m^3·mol^{-1}· GPa^{-1})				S_K^* ×10^6/(kg·m^3·mol^{-2}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
PEG 400								
0.00	-39.13(±1.26)	-37.59(±1.22)	-36.40(±1.19)	-35.55(±1.17)^{b}	-190.51(±49.92)	-183.84(±48.20)	-179.21(±47.02)	-176.53(±46.33)^{b}
0.07	-41.54(±0.78)	-39.89(±0.75)	-38.69(±0.74)	-37.85(±0.73)	-87.23(±23.82)	-84.05(±22.97)	-82.07(±22.45)	-80.90(±22.14)
0.08	-41.53(±0.77)	-39.87(±0.74)	-38.68(±0.72)	-37.84(±0.71)	-84.72(±23.10)	-81.66(±22.29)	-79.71(±21.77)	-78.57(±21.47)
0.09	-41.47(±0.73)	-39.82(±0.71)	-38.63(±0.69)	-37.79(±0.68)	-84.80(±22.06)	-81.76(±21.26)	-79.86(±20.77)	-78.74(±20.49)
PEG 4000								
0.00	-39.34(±1.26)	-37.78(±1.22)	-36.59(±1.19)	-35.74(±1.17)^{b}	-213.82(±50.06)	-206.63(±48.35)	-201.66(±47.14)	-198.98(±46.48)^{b}
0.07	-41.74(±0.80)	-40.08(±0.77)	-38.88(±0.75)	-38.03(±0.74)	-108.88(±24.10)	-105.08(±23.29)	-102.87(±22.74)	-101.69(±22.43)
0.08	-41.69(±0.78)	-40.03(±0.76)	-38.82(±0.74)	-37.97(±0.73)	-108.34(±23.77)	-104.63(±22.99)	-102.41(±22.45)	-101.28(±22.15)
0.09	-41.60(±0.78)	-39.95(±0.75)	-38.76(±0.73)	-37.91(±0.72)	-107.59(±23.38)	-103.98(±22.64)	-101.76(±22.09)	-100.63(±21.80)

$^{a}m_B$ is the molality of aqueous Niacin, standard uncertainties u are $u_r(m) = 0.01$, $u(T)$=0.001K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K^0_{\phi,s})$ =0.01 × 10^6/(m^3·mol^{-1}· GPa^{-1})and $u(S_k^*)$ =0.24 × 10^6/(m^3·mol^{-2}· GPa^{-1}), ^{b}Values of Partial molar isentropic compression, $K^0_{\phi,s}$, and experimental slopes, S_K^*, for (PEG 400 + water and PEG 4000 + water) at temperature 288.15 and 318.15 K have been taken from our previous paper [51].

Table 4.38

Partial molar isentropic compression transfer, $\Delta K_{\phi,s}^{0}$, of glycols in the aqueous solution of Niacin at different temperatures and 0.1 MPa pressure.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta K_{\phi,s}^{0}$ × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 400		
0.07	0.23	0.22	0.11	0.08
0.08	0.24	0.22	0.12	0.09
0.09	0.31	0.29	0.17	0.14
		PEG 4000		
0.07	0.32	0.29	0.21	0.14
0.08	0.37	0.35	0.27	0.20
0.09	0.45	0.43	0.33	0.26

$^{a}m_B$ is the molality of aqueous niacin

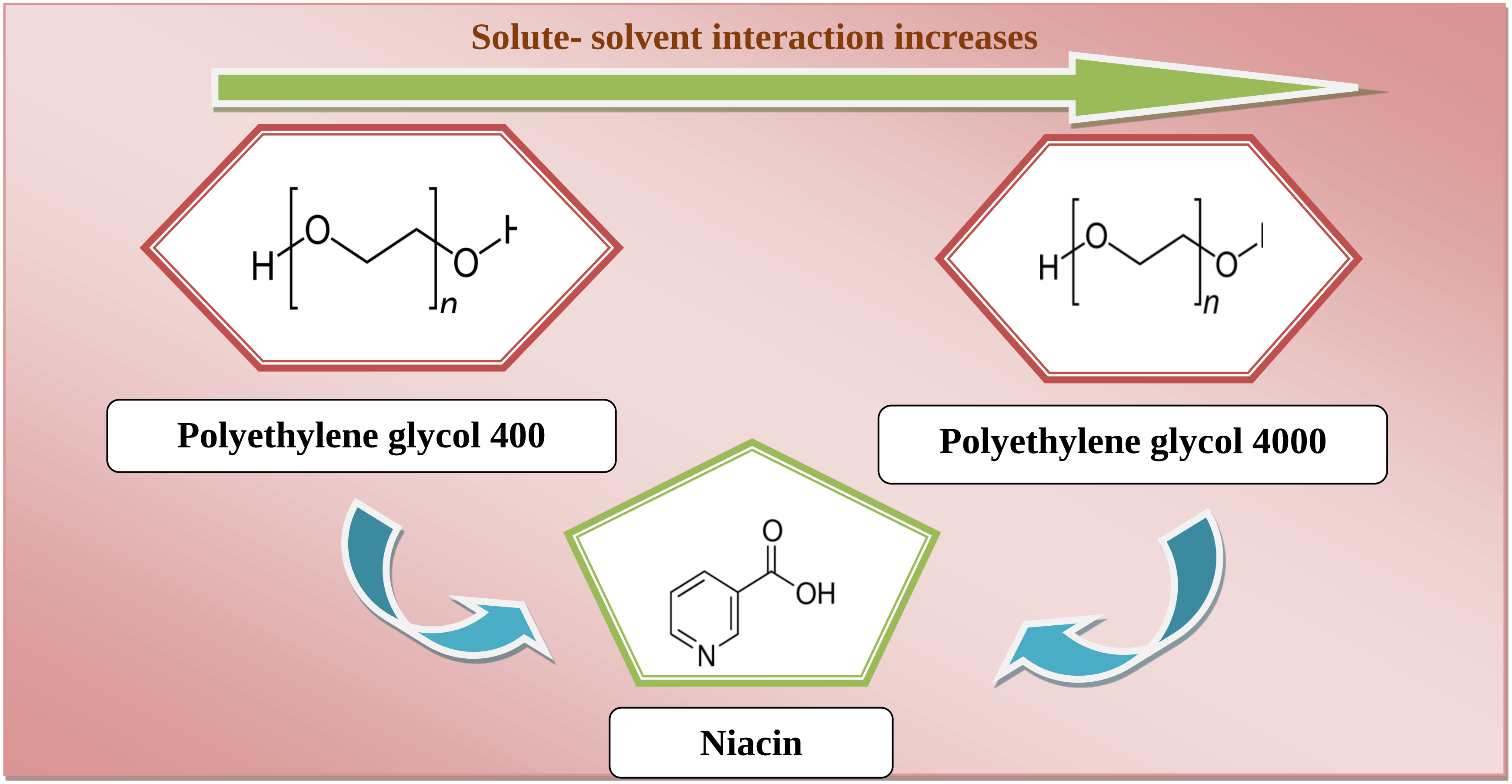
Table 4.39

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of Niacin at different temperatures and 0.1 MPa pressure.

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		PEG 400		
288.15	-61.94	714.58	1.27	2.97
298.15	-49.66	595.13	1.40	1.05
308.15	-63.15	670.75	0.12	5.96
318.15	-57.44	589.35	-0.26	7.42
		PEG 400		
288.15	-95.67	1229.81	1.24	9.43
298.15	-90.58	1182.97	1.14	8.95
308.15	-81.91	1093.58	0.33	11.23
318.15	-78.65	1044.62	-0.47	14.33

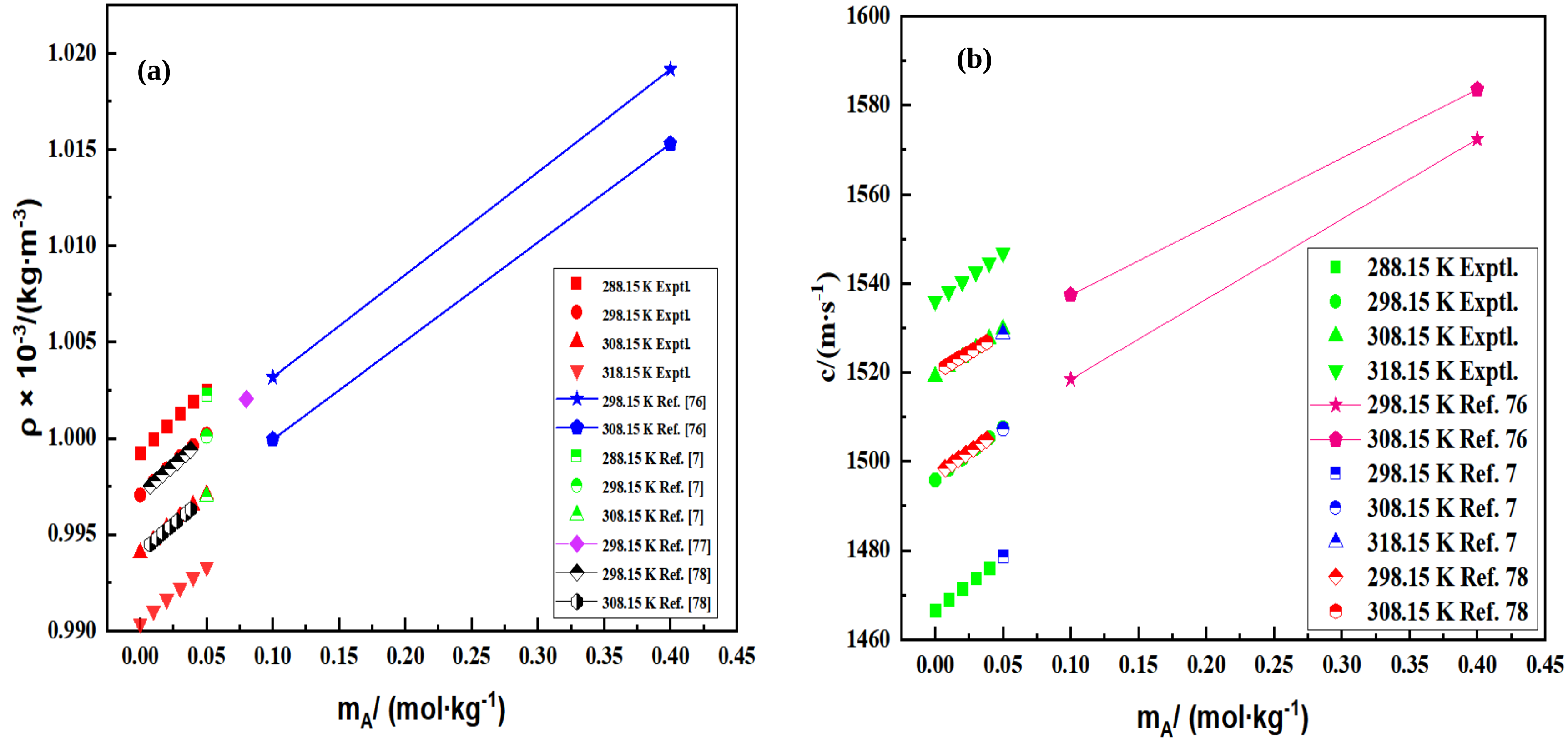
T/K is the temperatures

Figure 4.22

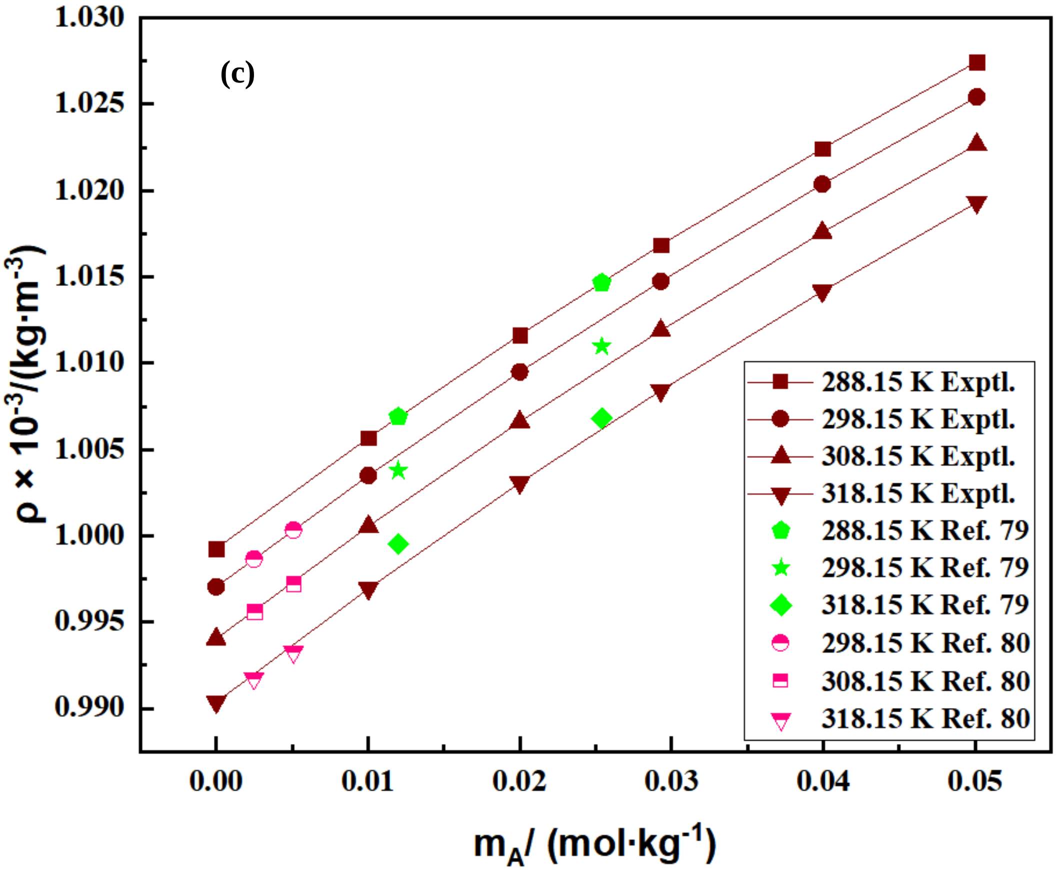


PEG 200/ PEG 600 and Niacin interactions.

Figure 4.23

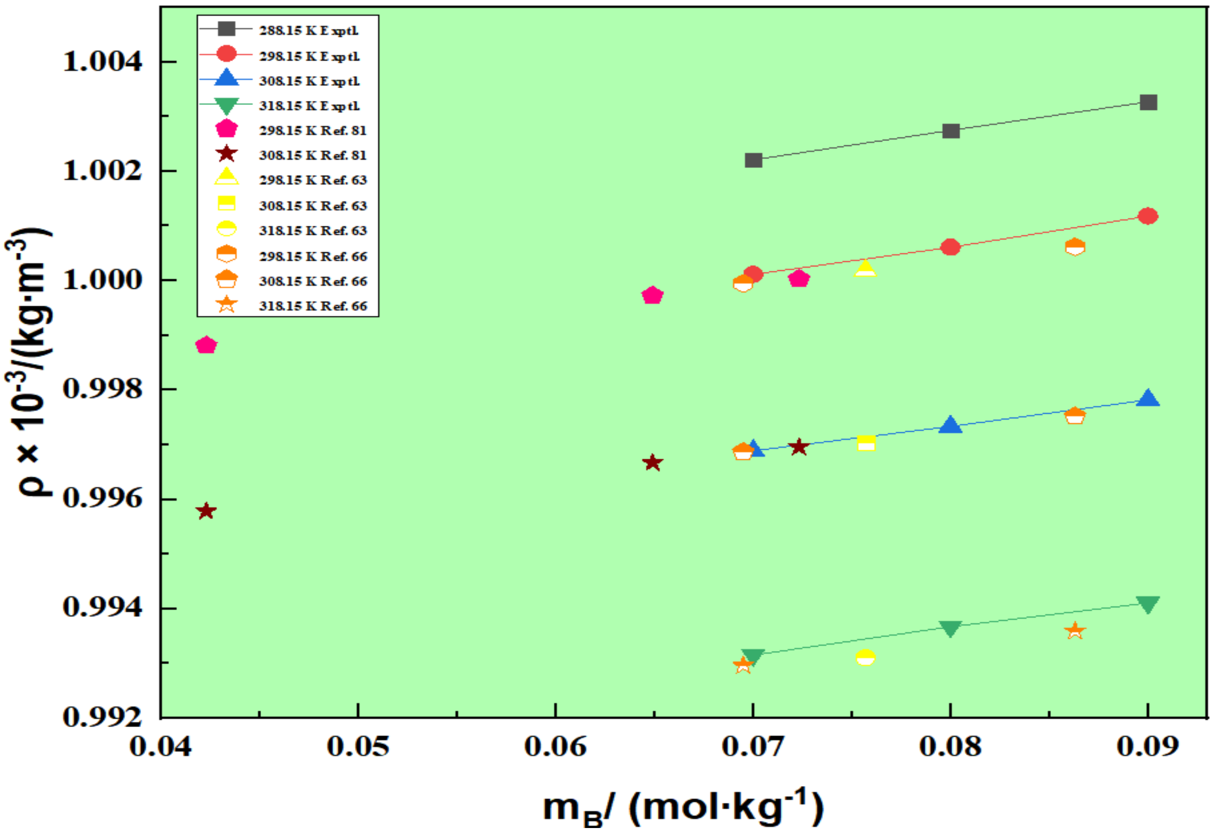


Variation of experimental (a) density and (b) speed of sound with literature values for (PEG 400 +Water) at T= 298.15 K and T= 308.15 K [■, 288.15 Exptl.; ●, 298.15 Exptl.; ▲, 308.15 K Exptl.;▼, 318.15 K Exptl; *, 298.15 K Lit. [76];⬟, 308.15 K Lit. [76]; ⬒ , 288.15 K Lit. [7]; ◓, 298.15 K Lit. [7], △, 308.15 K Lit. [7], ♦, 298.15 K Lit. [77], ⬘, 298.15 Lit. [78], ◑, 308.15 K Lit. [78].



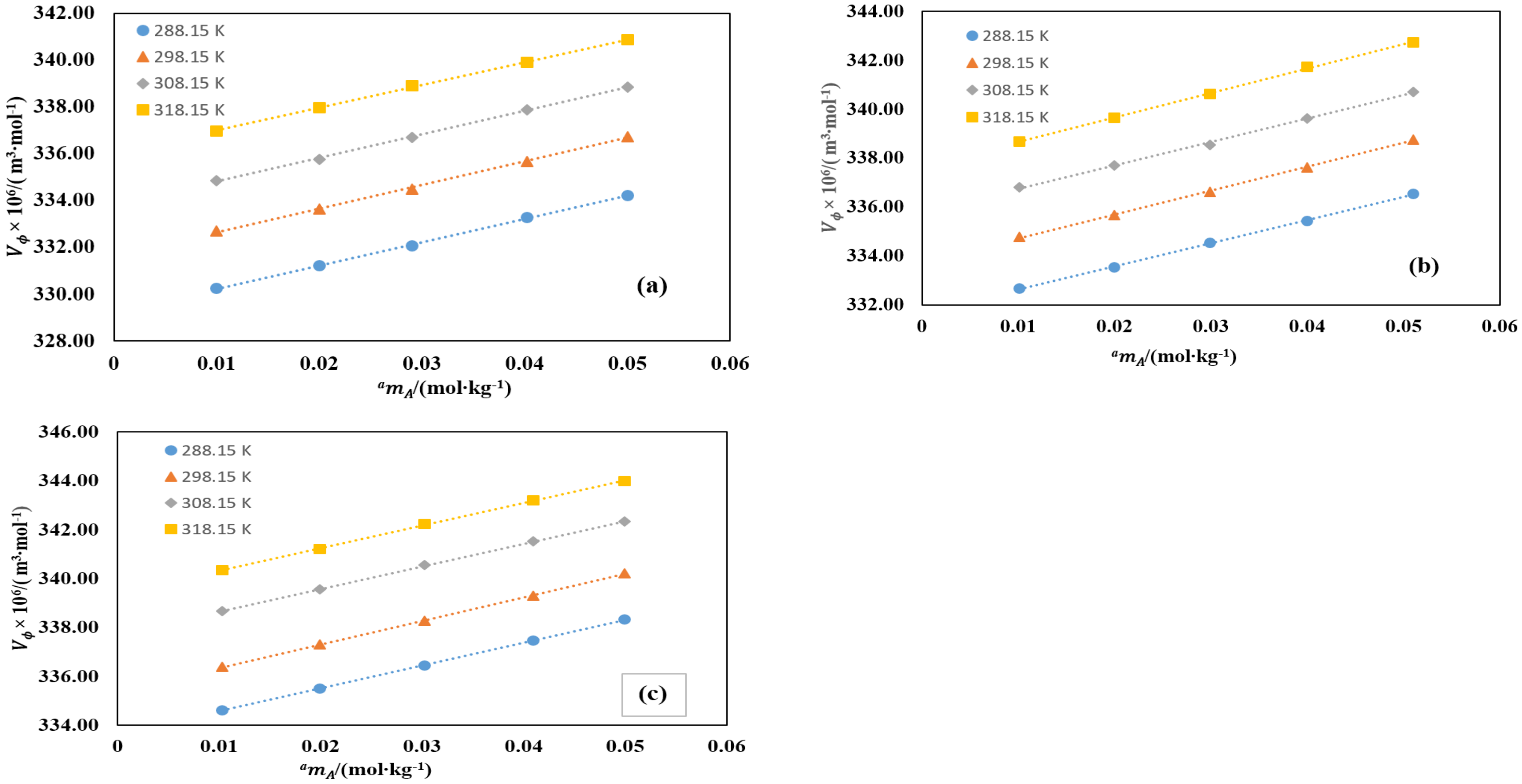
Variation of (c) experimental density with literature values for (PEG 4000 +Water) at T= 288.15 K, 298.15K, and 318.15 K [■, 288.15 Exptl.; ●, 298.15 Exptl.; ▲, 308.15 K Exptl;▼, 318.15 K Exptl; ⬟, 288.15 K Lit. [79]; *, 298.15 K Lit. [79]; ♦, 308.15 K Lit. [77]; ◒, 298.15 K Lit. [80]; ⬒, 308.15 K Lit. [80]; ▽, 318.15 K Lit. [80]]

Figure 4.24

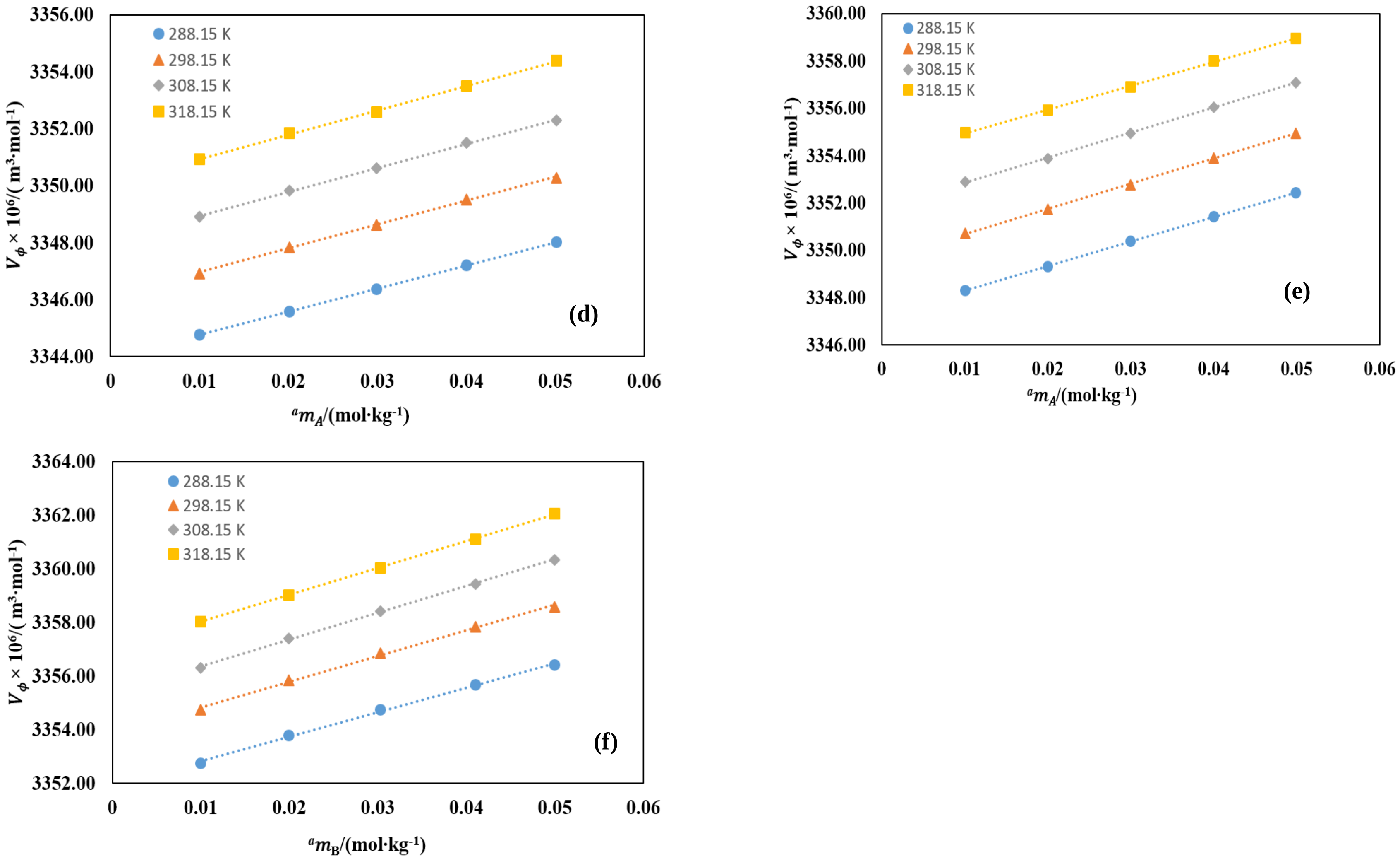


Variation of density for experimental and literature values for (Niacin +Water) at T= 298.15K and T= 308.15 K. [■, 288.15 Exptl.; ●, 298.15 Exptl.; ▲, 308.15 K Exptl.; ▼, 318.15 K Exptl; ⬟, 298.15 K Lit. [81]; *, 308.15 K Lit. [81]; △, 298.15 K Lit. [63]; ⬒, 308.15 K Lit. [63]; ◓, 318.15 K Lit. [63]; ⬟, 298.15 K Lit. [66]; ⬟, 308.15 K Lit. [66]; ★, 318.15 K Lit. [66]]

Figure 4.25

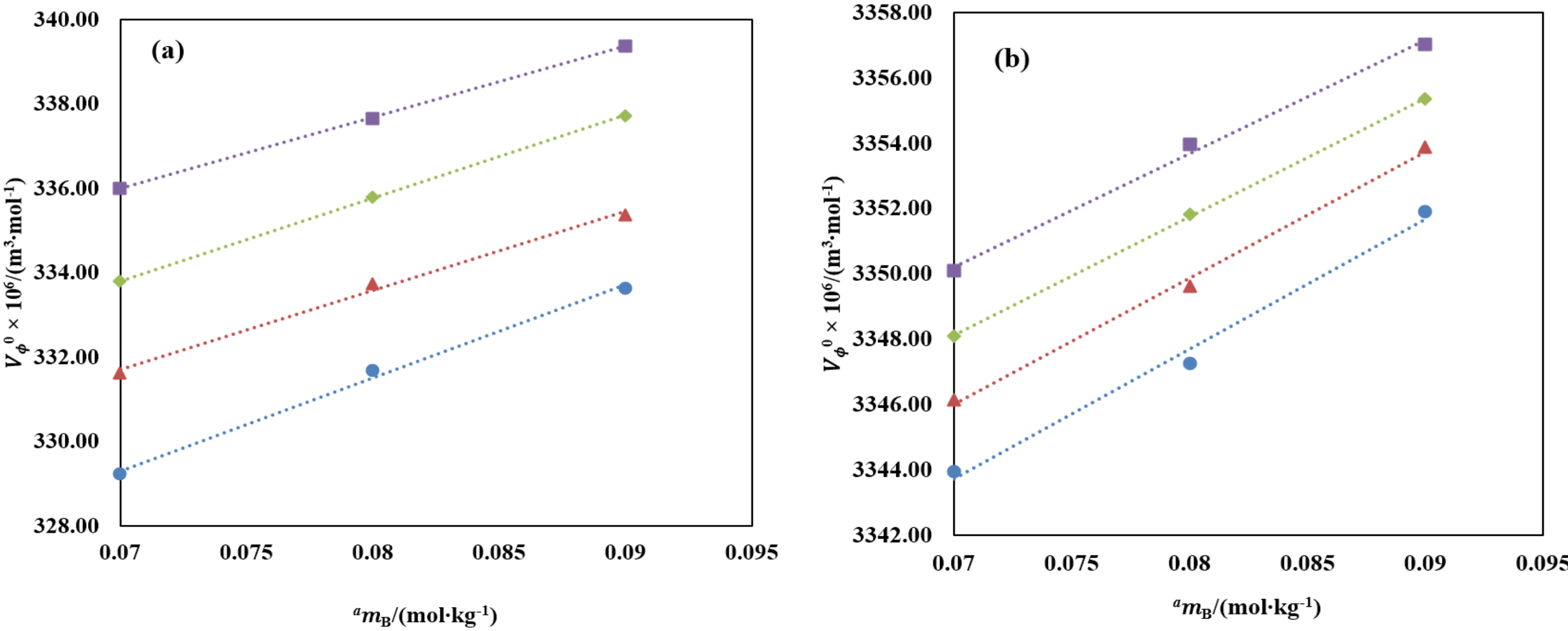


Variation of apparent molar volume(V_ϕ) of Polyethylene glycol 400 in (a) 0.07 Niacin, (b) 0.08 Niacin, (c) 0.09 Niacin, against molality at different temperatures [●, 288.15 K; ▲, 298.15 K; ♦, 308.15 K; ■, 318.15 K].



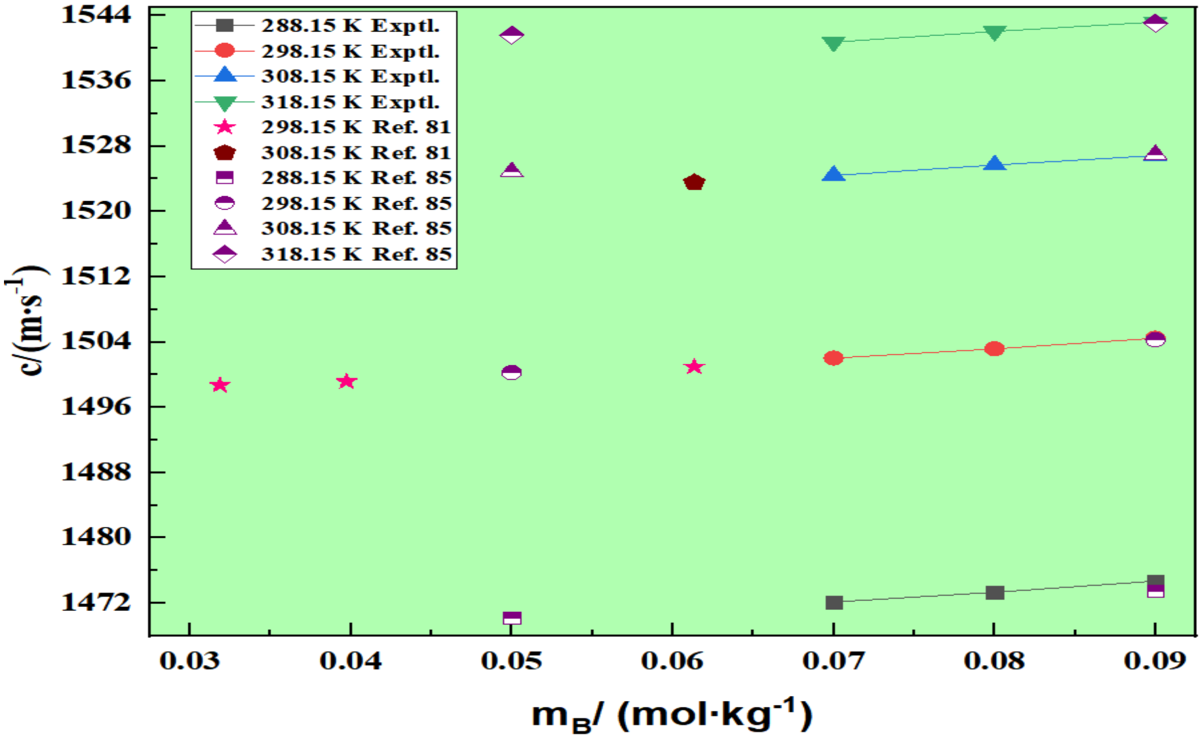
Variation of apparent molar volume(V_ϕ) of Polyethylene glycol 4000 in (d) 0.07 Niacin, (e) 0.08 Niacin, (f) 0.09 Niacin, against molality at different temperatures [●, 288.15 K; ▲, 298.15 K; ♦, 308.15 K; ■, 318.15 K].

Figure 4.26



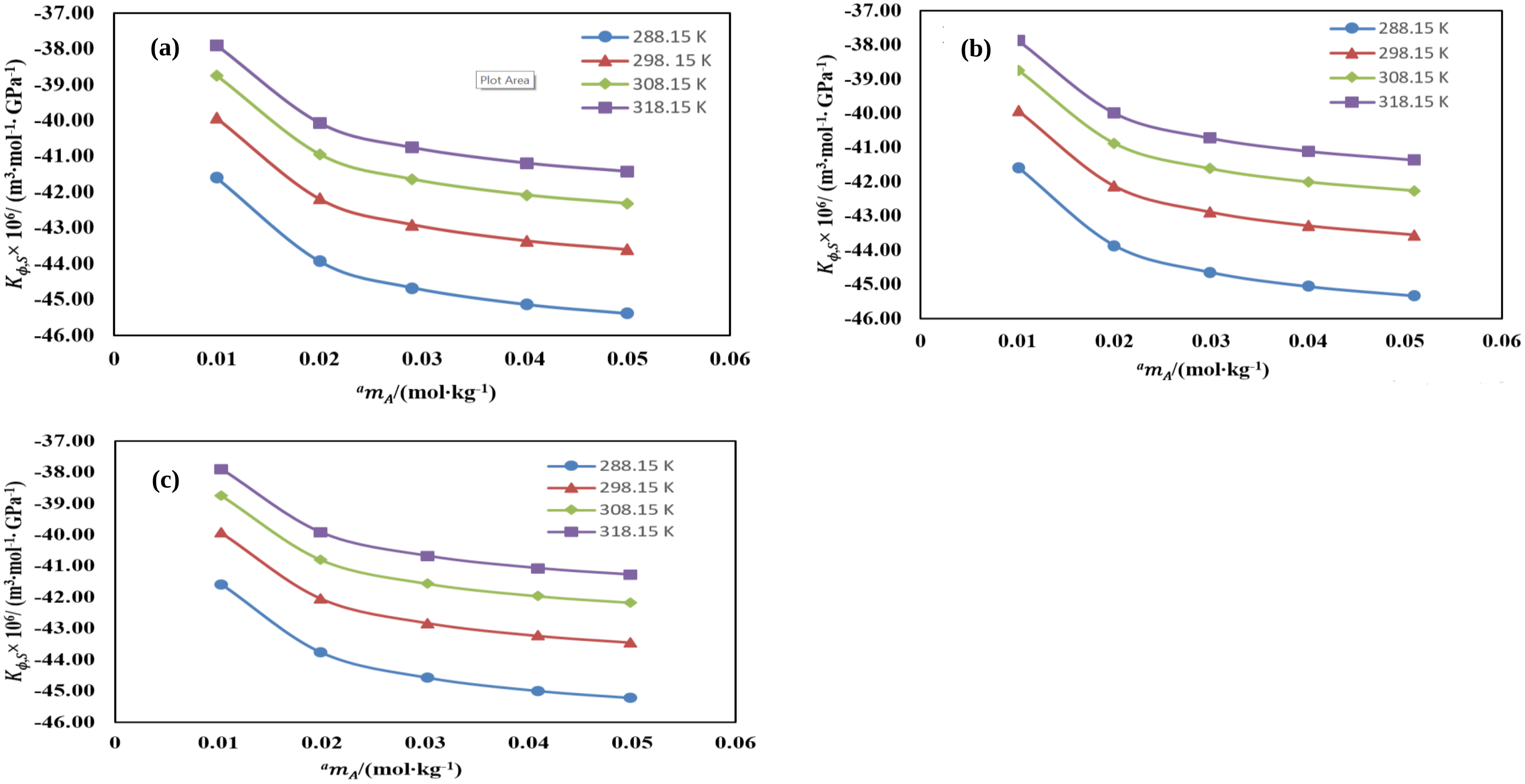
Variation of partial molar volumes, V_ϕ^0, of, (a) Polyethylene glycol 400 and (b) Polyethylene glycol 4000 in different concentrations of aqueous Niacin solutions at different temperatures (●, 288.15 K; ▲, 298.15 K; ♦, 308.15 K; ■, 318.15 K).

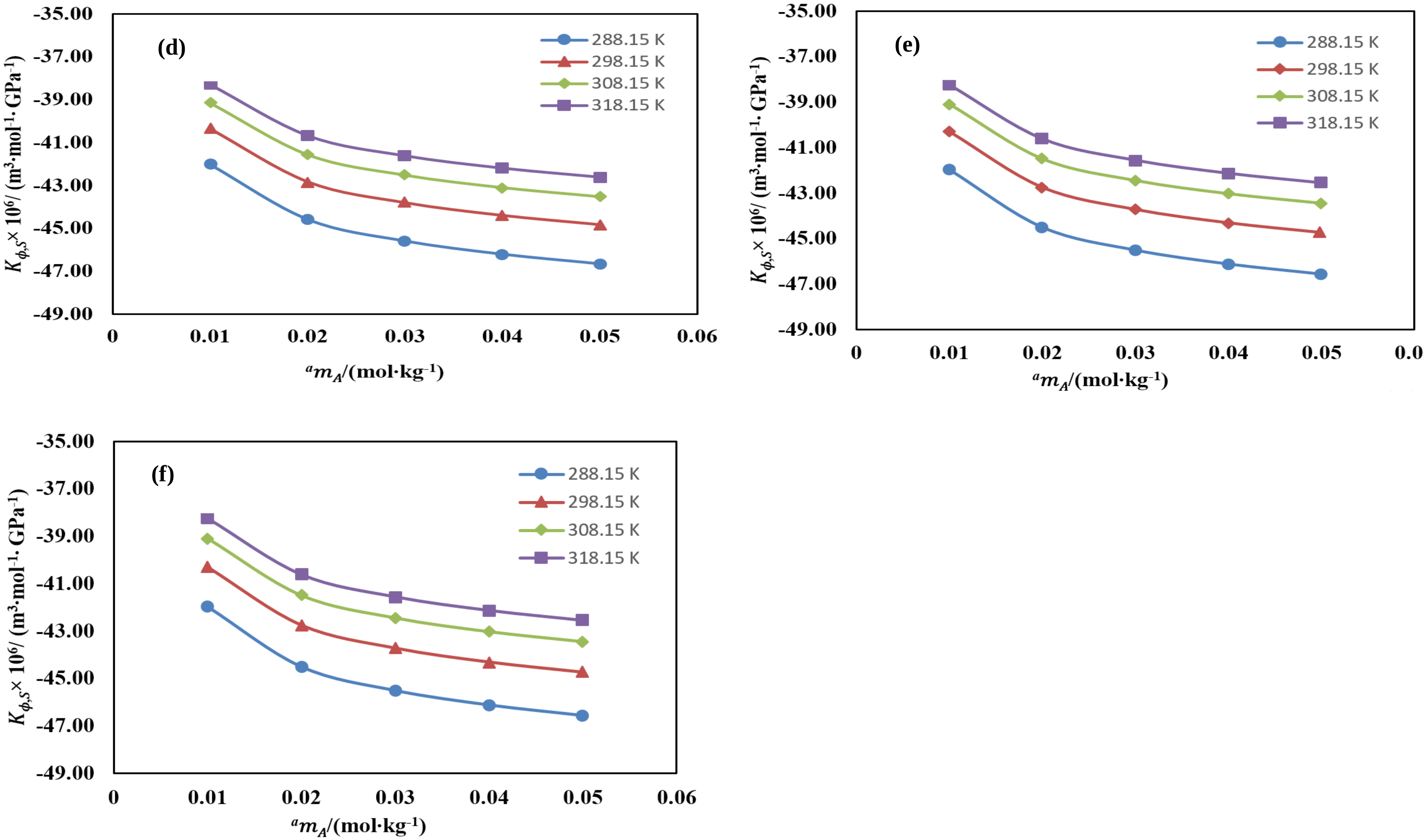
Figure 4.27



Variation of the speed of sounds for experimental and literature values^{22} for (Niacin +Water) at T= 298.15K and T= 308.15 K [■, 288.15 Exptl.; ●, 298.15 Exptl.; ▲, 308.15 K Exptl.; ▼, 318.15 K Exptl.; *, 298.15 K Lit. [81]; ⬟, 308.15 K Lit. [81]; ⬒, 288.15 K Lit. [85]; ◓ 298.15 K Lit. [85]; △, 308.15 K Lit. [85]; ⬘, 318.15 K Lit. [85]]

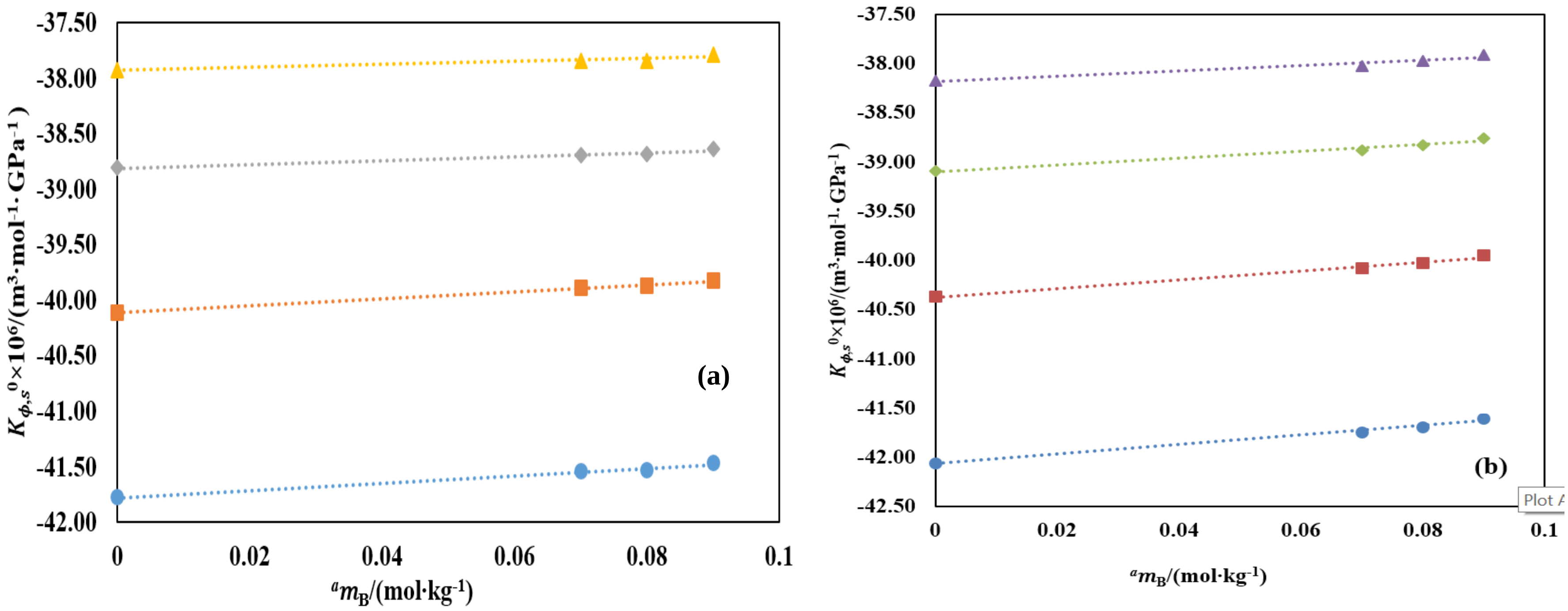
Figure 4.28


(a)
(b)
(c)
288.15 K
298. 15 K
298.15 K
308.15 K
318.15 K
Plot Area
$K_{\phi,S} \times 10^6$/ (m^3·mol^{-1}· GPa^{-1})
$^a m_A$/(mol·kg^{-1})
-37.00
-38.00
-39.00
-40.00
-41.00
-42.00
-43.00
-44.00
-45.00
-46.00
0
0.01
0.02
0.03
0.04
0.05
0.06



Variation of apparent molar isentropic compression ($K_{\phi,s}$), Polyethylene glycol 400 in (a) 0.07 Niacin, (b) 0.08 Niacin, (c) 0.09 Niacin, and Polyethylene glycol 4000 in (d) 0.07 Niacin, (e) 0.08 Niacin, (f) 0.09 Niacin, against molality at different temperatures [●, 288.15 K; ▲, 298.15 K; ♦, 308.15 K; ■, 318.15 K].

Figure 4.29



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, of (a) Polyethylene glycol 400 and (b) Polyethylene glycol 4000 in different concentrations of aqueous Niacin solutions at different temperatures (●, 288.15 K; ■, 298.15 K; ♦, 308.15 K; ▲, 318.15 K).

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Section II

Problem 5

Acoustic and thermodynamic study of D-Panthenol in aqueous solutions of glycol at different temperatures.

In this section, we have reported the densities, ρ and speed of sound c of ethylene glycol (EG), diethylene glycol (DEG) and triethylene glycol (TEG) in (0.00, 0.05, 0.10, 0.15) mol·kg^{-1} aqueous solutions of d-Panthenol at temperatures T = (293.15, 298.15, 303.15 and 308.15) K.

4.42 Apparent molar volume

From the experiment, the values of densities, ρ, of EG, DEG and TEG in (0.05, 0.10 and 0.15) mol·kg^{-1} in aqueous solutions of D-Panthenol are obtained at the temperatures of T= (293.15, 298.15, 303.15 and 308.15) K. The equation **4.1** is used to determine the apparent molar volumes (V_{ϕ}) from the values of densities. In **table 4.40**, the values of densities along with the apparent molar volumes are stated and with the increase in the temperature, the density values decrease. The calculated apparent molar volume values for EG, DEG and TEG in aqueous solution of D-Panthenol at different temperatures shows the positive values of V_{ϕ} imply the strong solute-solvent interaction [1, 2] and is graphically represented in **Figure 4.31**. The molecular interaction increases from EG, DEG and TEG in aqueous solution of D-Panthenol as shown in **Figure 4.32**.

4.43 Partial molar volume

The limiting value of the apparent molar volume is the partial molar volume V_{ϕ}^{0}, which is calculated by equation **4.2**. By the method of least square fitting of V_{ϕ}, and S_{V}^{*} is the slope of experimental data, which is coefficient of volumetric pair wise interaction and m_{A} represent the molality of solute. The calculated values of V_{ϕ}^{0} and S_{V}^{*} are reported in **table 4.41**, which are the standard errors. The presence of solvent-solvent interaction is indicated by the positive values of V_{ϕ}^{0} [2]. In accordance with co-sphere overlap model, the increase in the volume is by reason of the overlap of the co-spheres of two ionic species, whereas the volume decrease is the resultant of overlap ion-hydrophobic and the hydrophobic-hydrophobic groups [3, 4]. The hydrophobic-hydrophobic interactions are dominated by the ion-hydrophilic interactions which are responsible for he observed positive V_{ϕ}^{0} values. At infinite dilution the solute-solute interactions for example zwitterions- zwitterions or ion-ion interactions are negligible. As the crucial information on the solvent-solvent interaction is attained from the dependency of the standard partial molar property on the temperature. The calculated value of V_{ϕ}^{0} increases with the increase in molar mass [5]. In the table the values of S_{V}^{*} are noted and the magnitude of few observed values are negative at the different concentrations of D-Panthenol. This implies the weak solute and the solute interaction in these systems. As there is no regular pattern is the observed value of S_{V}^{*} it can be said that the solute and the solute interaction is affected by different factors. The solute and the solvent interaction dominate the solute and the solute interaction which is observed due to the comparison of the negative values of S_{V}^{*} to the positive values of V_{ϕ}^{0} [6, 7].

4.44 Partial molar volume of transfer

The transfer volume of glycols from water to the aqueous D-Panthenol solutions at infinite dilutions was computed with the equation **4.3**. In **table 4.42**, the calculated ΔV_{ϕ}^{0} values are reported and it is perceived that there exists strong ion-ion interaction of D-Panthenol and glycols which is indicated by the values of ΔV_{ϕ}^{0} [1]. As per the co-sphere overlap model, the solvophobic salvation and the structural interaction suggest the structure promoter character of these solutes as a result of their values [3, 4]. For the values of ΔV_{ϕ}^{0}, in agreement with co-sphere overlap model, from the solute and the solute interaction, the contribution is negligible and the information concerning the solute and the solvent interaction can be attained from it. The number of interactions which are taking place between glycols and D-Panthenol is listed as follows-

(i) ion-hydrophilic interactions
(ii) ion-hydrophobic interactions
(iii) hydrophilic- hydrophilic interactions

(iv) hydrophobic- hydrophobic interactions

Accordance with co-sphere overlap model, the negative contribution is given by the ion-hydrophobic interactions and hydrophobic-hydrophobic interactions while the positive contribution is due to the ion-hydrophilic interactions and hydrophilic-hydrophilic interactions, to the ΔV_{ϕ}^{0} values. Hence in our current study of D-Panthenol +water +glycols, it is analyzed that the ion-hydrophilic interactions and hydrophilic- hydrophilic interactions are imperious over the last two interactions [8, 9].

4.45 Temperature dependent partial molar volume

The variation of the apparent molar volume i.e V_{ϕ}^{0} with temperature at finite dilution is given by the equation **4.4**. Where T represent the temperature, T_{ref}=298.15 K, a, b and c represent the empirical constants. In **table 4.43**, the values of the constants of EG, DEG and TEG have been reported. The coefficient c is hardly statistically important and has the positive values for all glycols except for the few cases [1]. The positive values of c are the proof of the scatter in the values of V_{ϕ}^{0} and from R^{2} values it is evident that very small values are the best fit of the data. Apparently for glycols if the V_{ϕ}^{0} values are estimated over broad range of temperature, then the positive value of c would appear. The V_{ϕ}^{0} results are assumed sufficient, as the basic objective of the V_{ϕ}^{0} study was to achieve the limiting apparent molar expansibilities [2]. The limiting apparent molar expansibilities are determined by equation **4.5**. At infinite dilution the partial molar expansibilities is given as $E_{\phi}^{0} = \left(\partial E_{\phi}^{0}/\partial T\right)_{P}$, which is regarded a significant measure of solute and the solvent interactions exist among the solutions. A general thermodynamic equation was developed to measure the amount of solute as a structure maker or structure beaker in the system which was given by equation **4.6**. The tendency of the solute to be a structure maker or structure breaker in the solvent is estimated by the sign $\left(\partial E_{\phi}^{0}/\partial T\right)_{P}$. The positive and small negative $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ values suggest that the solute is having a structure making ability, while the negative values imply the structure breaking ability. In **table 4.44**, the values of limiting apparent molar expansibilities E_{ϕ}^{0} and $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$are noted. For all concentrations and temperatures, the values of E_{ϕ}^{0} are positive except for few values, which are suggesting the presence of solute and solvent interaction for the positive values of E_{ϕ}^{0}. An irregular behaviour is observed in the E_{ϕ}^{0}values [10].

4.46 Apparent molar isentropic compression

By using the equation **4.7**, apparent molar isentropic compression of EG, DEG and TEG in the aqueous solution of D-Panthenol is calculated, where $m_{A,}$ $M,$ $\rho,$ $\rho_{0,}$ $k_{s.0}$ and k_s are the molality of solute, the molar mass of solute, densities of the solvent and the solution, isentropic compressibility of the pure solvent and the solution accordingly. The isentropic compressibility is calculated by the equation **4.8** where c and ρ are the ultrasonic velocity and density of the solution respectively. In **table 4.45**, the values of ultrasonic velocity along with the calculated values of $K_{\phi,s}$ in different temperature are reported and are graphically represented in **Figure 4.32** and **Figure 4.33**. The values of experimental speeds of EG, DEG and TEG in aqueous D-Panthenol increases with the temperature. From experimental data, the calculated values of $K_{\phi,s}$ they are found to be negative at all concentrations and temperatures. With the increase in the temperatures, the values of $K_{\phi,s}$ are becoming less negative, whereas the negativity increases with the increase in the concentration of glycols in the solution and these negative values of $K_{\phi,s}$ suggest that around the ionic charge groups of solute, the water molecules are less compressible as compared to the molecules of water present in the bulk solution and this shows the arrangement of water molecules in particular order throughout the solute [11-14]. Also the larger loss of structural compressibility of water is suggested by the negative values of $K_{\phi,s}$ which denote the greater aligning effect caused by the solute on solvent [15].

4.47 Partial molar isentropic compression

By the equation **4.9**, the variation of apparent molar isentropic compression $K_{\phi,s}$ with the molar concentration is calculated where, $K_{\phi,s}^{0}$, S_K^{*} and m_A are the limiting isentropic compression, experimental slope of solute and the solute interactions and the molality of the solute in the aqueous D-Panthenol solutions. By the least square fitting method, the values of $K_{\phi,s}^0$ and S_K^* are the derived standard errors. In **table 4.46**, the calculated values of $K_{\phi,s}^0$ and S_K^* are reported. Due to the small size of S_K^* values, the solute and solute interactions at infinite dilution are insignificant [1]. The strong attractive interactions among glycols and water are observed due the less negative values of $K_{\phi,s}^0$ with the increase in temperature [16]. With this trend of decreasing of the negativity of the $K_{\phi,s}^0$ values, there is increase in the temperature, it implies the reduction of electrostriction and the emission of molecules of water to bulk. In addition to this , between the ions of D-Panthenol there attractive interaction and there are dehydration of the glycols which is caused by the water molecules and that is why the water molecules around glycols at high concentrations are more compressible as compared to the lower concentrations [17]. At infinite dilution, the partial molar isentropic compressions $\Delta K_{\phi,s}^0$ of glycols in aqueous solution of D-Panthenol is calculated with the equation **4.10**. In **table 4.47**, the calculated values of $\Delta K_{\phi,s}^0$ are reported. The values of $\Delta K_{\phi,s}^0$ are positive except for few values and it is observed that with the increase in the temperature the $\Delta K_{\phi,s}^0$ values decrease. In **Figure 4.34** the calculated values of $\Delta K_{\phi,s}^0$ are represented graphically [18]. At all concentrations of glycols as well as D-Panthenol, the values of $\Delta K_{\phi,s}^0$ are increasing. There is the tendency of the ions to make structure due to the interactions among positive zwitterionic centre of glycols and D-Panthenol is dominating, caused by the positive values of $\Delta K_{\phi,s}^0$. With the increase in concentration of D-Panthenol, the interaction between the zwitterionic centre of glycols and D-Panthenol increases. The electrostriction decreases with the increase in the concentration of D-Panthenol and thus the tendency of the ions to make structure increases. Due to this, the compressibility of electrostricted water is less than the bulk water and results in the huge decrease of the compressibility with the increase in the concentration of D-Panthenol [19, 20]. At lower concentrations and temperatures of D-Panthenol, the more molecules of water are combined with the ions of glycols due to the negative $K_{\phi,s}^0$ and positive values of $\Delta K_{\phi,s}^0$. This implies that the greater amount of molecules of water of solute is collaborated with the molecules of solvent that increase the interactions between the ions [8].

4.48 Pair and triplet interaction coefficients

The formula to calculate the interactions coefficients which was given by McMilan [21] theory which was later more discussed by Friedman and Krishnan [22], allows the splitting of effects caused by the interactions among two or more molecules of solute. From the equation **4.11** and **4.12**, the partial molar volume of transfer and the partial molar isentropic compression of transfer are obtained where A represent glycols and B represent D-Panthenol and m_B denotes the molality of the aqueous D-Panthenol solutions. The pair and triplet interaction coefficient are represented by the parameters V_{AB} and V_{ABB} for volume, and $K_{AB,}$ K_{ABB} for isentropic compression. By fitting the values of ΔV_{ϕ}^{0} and $\Delta K_{\phi,s}^{0}$, these constants are calculated and in **table 4.48**, these calculated values are reported [10]. The value of the pair interaction coefficients V_{AB} and triplet interaction coefficient V_{ABB}consists of both positive and negative values. The compressibility is both positive and negative for EG and for the rest is positive, corresponding pair interaction coefficient K_{AB}. For DEG and TEG the triplet coefficient K_{ABB} has negative values for all the temperatures. As per this theory, due to the overlapping of spheres, there is the release of the water molecules to bulk from hydration co-spheres, when the occurred interaction is non-bonding favourable [4]. The volume changes would be positive when there is the release of the water from a co-sphere we bulk is more structured and negative when the co-sphere is more structured due to the difference in the structural organization of the water molecules. In our present study, the pair interaction coefficient foe EG, DEG and TEG are decreasing with the increasing temperature [23].

Table 4.40

Values of densities, ρ, apparent molar volumes, V_ϕ of glycols in aqueous solutions of D-Panthenol at different temperatures

$^a m_A$/(mol·kg^{-1})	$\rho \times 10^3$/(kg·m^{-3})				$V_\phi \times 10^6$/(m^3·mol^{-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
EG+0.05 mol·kg^{-1} D-Panthenol								
0.00000	0.999509	0.998191	0.996926	0.995295				
0.09927	1.000360	0.999079	0.997693	0.996072	53.47	53.16	54.45	54.42
0.20001	1.001190	0.999849	0.998511	0.996857	53.60	53.77	54.20	54.39
0.29453	1.001910	1.000620	0.999252	0.997595	53.81	53.77	54.19	54.35
0.39970	1.002710	1.001495	1.000058	0.998393	53.91	53.71	54.21	54.37
0.49986	1.003490	1.002199	1.000808	0.999200	53.91	53.92	54.24	54.26
EG+0.10 mol·kg^{-1} D-Panthenol								
0.00000	1.001621	1.000221	0.998987	0.997338				
0.09994	1.002379	1.001055	0.999706	0.998038	54.37	53.67	54.88	55.16
0.19887	1.003085	1.001790	1.000400	0.998757	54.55	54.09	54.94	54.98
0.30277	1.003790	1.002510	1.001168	0.999521	54.71	54.37	54.80	54.87
0.38547	1.004410	1.003110	1.001821	1.000199	54.61	54.41	54.61	54.62
0.51235	1.005290	1.004069	1.002730	1.001178	54.63	54.34	54.61	54.49
EG+0.15 mol·kg^{-1} D-Panthenol								

0.00000	1.003341	1.002090	1.000580	0.998985				
0.09940	1.004060	1.002830	1.001284	0.999746	54.64	54.49	54.92	54.42
0.19930	1.004837	1.003537	1.002021	1.000454	54.33	54.63	54.73	54.67
0.30448	1.005571	1.004273	1.002757	1.001160	54.47	54.68	54.77	54.86
0.39600	1.006218	1.004917	1.003418	1.001887	54.49	54.68	54.72	54.63
0.50151	1.006939	1.005620	1.004076	1.002612	54.54	54.74	54.88	54.69
DEG+0.05 mol·kg^{-1} D-Panthenol								
0.00000	0.999509	0.998191	0.996926	0.995295				
0.09797	1.000883	0.999604	0.998259	0.996609	92.01	91.71	92.63	92.96
0.19870	1.002371	1.000992	0.999700	0.998000	91.49	91.91	92.14	92.63
0.29915	1.003700	1.002350	1.000990	0.999300	91.76	91.98	92.40	92.73
0.40094	1.005090	1.003705	1.002341	1.000628	91.73	92.00	92.36	92.70
0.49695	1.006300	1.004932	1.003507	1.001774	91.87	92.08	92.51	92.86
DEG+0.10 mol·kg^{-1} D-Panthenol								
0.00000	1.001621	1.000221	0.998987	0.997338				
0.09947	1.002914	1.001643	1.000328	0.998676	92.87	91.68	92.59	92.75
0.20205	1.004283	1.002986	1.001642	0.999990	92.57	92.16	92.81	92.96
0.30629	1.005596	1.004344	1.002997	1.001300	92.64	92.26	92.74	93.03
0.39789	1.006838	1.005603	1.004189	1.002565	92.40	92.08	92.64	92.71
0.50044	1.008224	1.006862	1.005536	1.003849	92.19	92.22	92.51	92.72

DEG+0.15 mol·kg^{-1} D-Panthenol								
0.00000	1.003341	1.002120	1.000580	0.998985				
0.10470	1.004667	1.003379	1.001779	1.000153	93.06	93.80	94.51	94.94
0.19784	1.005991	1.004647	1.003041	1.001459	92.22	92.94	93.40	93.47
0.29933	1.007372	1.006057	1.004416	1.002756	92.02	92.44	92.90	93.25
0.39620	1.008754	1.007448	1.005714	1.004047	91.70	92.02	92.64	92.95
0.49900	1.010031	1.008772	1.007140	1.005430	91.84	92.01	92.32	92.69
TEG+0.05 mol·kg^{-1} D-Panthenol								
0.00000	0.999509	0.998191	0.996926	0.995295				
0.10106	1.001710	1.000402	0.999053	0.997387	128.17	128.21	129.19	129.72
0.19881	1.003768	1.002419	1.001034	0.999337	128.26	128.56	129.32	129.84
0.30095	1.005808	1.004516	1.003094	1.001263	128.49	128.54	129.22	130.09
0.41255	1.008058	1.006818	1.005252	1.003482	128.41	128.36	129.26	129.79
0.49633	1.009694	1.008422	1.006825	1.004928	128.40	128.45	129.29	130.04
TEG+0.10 mol·kg^{-1} D-Panthenol								
0.00000	1.001621	1.000221	0.998987	0.997338				
0.10454	1.003797	1.002153	1.000817	0.999247	128.91	131.42	132.55	131.97
0.20136	1.005781	1.004160	1.002800	1.001053	128.81	130.08	130.86	131.54
0.30052	1.007841	1.006228	1.004851	1.002846	128.51	129.39	130.02	131.43
0.39983	1.009888	1.008240	1.006762	1.004800	128.27	129.06	129.84	130.84

0.50238	1.012050	1.010229	1.008890	1.006684	127.91	128.94	129.30	130.65
TEG+0.15 mol·kg^{-1} D-Panthenol								
0.00000	1.003341	1.002120	1.000580	0.998985				
0.09973	1.005351	1.004109	1.002580	1.001034	129.40	129.75	129.80	129.48
0.19904	1.007456	1.006135	1.004579	1.002860	128.62	129.26	129.51	130.32
0.30436	1.009537	1.008136	1.006557	1.004811	128.66	129.40	129.70	130.39
0.40056	1.011551	1.010167	1.008569	1.006641	128.27	128.82	129.14	130.18
0.49370	1.013536	1.011813	1.010335	1.008489	127.87	129.06	129.10	129.81

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainities *u* are *u(m)* $= 2 \times 10^{-5}$ mol·kg^{-1}, *u(T)*=0.01K, *u(ρ)=0.05*(kg·m^{-3}),*u(p)*=0.01MPa and at the experimental pressure=0.1 MPa

Table 4.41

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_V^*, of glycols in aqueous solution of D-Panthenol at different temperatures.

$^a m_A$/ (mol·kg^{-1})	$V_{\phi}^{0} \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-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
EG								
0.00	53.42 [24]	53.66[24]	53.88[24]	54.08 [24]				
0.05	53.39(±0.07)	53.23(±0.22)	54.38(±0.10)	54.46(±0.03)	1.19(±0.22)	1.45(±0.67)	-0.41(±0.31)	-0.33(±0.10)
0.10	54.39(±0.08)	53.66(±0.18)	55.02(±0.08)	55.32(±0.02)	0.58(±0.24)	1.66(±0.53)	-0.88(±0.23)	-1.70(±0.07)
0.15	54.49(±0.15)	54.47(±0.05)	54.82(±0.13)	54.49(±0.12)	-0.08(±0.46)	0.51(±0.15)	-0.14(±0.38)	0.46(±0.37)
DEG								
0.00	91.52 [24]	91.81 [24]	91.81[24]	92.06 [24]				
0.05	91.79(±0.23)	91.68(±0.06)	92.42(±0.22)	92.82(±0.16)	-0.05(±0.69)	0.83(±0.18)	-0.03(±0.67)	-0.14(±0.48)
0.10	93.00(±0.11)	91.78(±0.21)	92.77(±0.13)	92.93(±0.17)	-1.56(±0.32)	1.00(±0.63)	-0.36(±0.40)	-0.33(±0.52)
0.15	92.58(±0.14)	93.54(±0.16)	94.26(±0.13)	94.54(±0.26)	-1.79(±0.44)	-3.40(±0.50)	-4.07(±0.39)	-3.97(±0.78)
TEG								
0.00	128.26 [24]	128.55 [24]	128.78 [24]	129.10 [24]				
0.05	128.16(±0.10)	128.34(±0.17)	129.21(±0.06)	129.72(±0.16)	0.63(±0.31)	0.27(±0.51)	0.14(±0.18)	0.59(±0.49)
0.10	128.45(±0.40)	130.87(±0.19)	132.10(±0.29)	131.59(±0.30)	-0.70(±1.22)	-4.34(±0.56)	-5.98(±0.87)	-1.71(±0.90)

0.15	129.54(±0.21)	129.75(±0.24)	129.93(±0.09)	129.82(±0.39)	-3.48(±0.65)	-1.86(±0.72)	-1.83(±0.26)	0.51(±1.19)

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainities u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.01K, $u(\rho)=0.05$(kg·m^{-3}),$u(p)$=0.01MPa and at the experimental pressure=0.1 MPa

Table 4.42

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in aqueous solution of D-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^6$/(m^3·mol^{-1})			
	T =293.15 K	T =298.15 K	T =303.15 K	T =308.15 K
EG				
0.05	-0.03	-0.43	0.50	0.38
0.10	0.97	0.00	1.14	1.24
0.15	1.07	0.81	0.94	0.41
DEG				
0.05	0.27	-0.13	0.60	0.76
0.10	1.48	-0.03	0.95	0.87
0.15	1.06	1.73	2.44	2.48
TEG				
0.05	-0.10	-0.21	0.43	0.62
0.10	0.19	2.32	3.32	2.49
0.15	1.28	1.20	1.15	0.72

$^{a}m_B$ is the molality of D-Panthenol; standard uncertainties u are $u(m)$=2×10^{-5} mol·kg^{-1}, $u(T)$=0.01 K, $u(\rho)$= 0.05 kg·m^{-3}, $u(p)$= 0.01 MPa and at the experimental pressure=0.1 MPa

Table 4.43

Values of empirical parameters of Eq.4, of glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
EG					
0.05	53.59	0.08	0.00	0.9999	0.00385
0.10	54.13	0.03	0.01	0.9999	0.00503
0.15	54.63	0.02	0.00	0.9999	0.00225
DEG					
0.05	91.86	0.05	0.00	0.9999	0.00112
0.10	92.23	-0.05	0.01	0.9999	0.00288
0.15	93.57	0.17	-0.01	0.9999	0.00458
TEG					
0.05	128.50	0.09	0.00	0.9999	0.00385
0.10	130.95	0.36	-0.03	0.9999	0.00037
0.15	129.79	0.04	0.00	0.9999	0.00084

${}^{a}m_B$ is the molality of D-Panthenol; standard uncertainties *u* are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.01K, $u(\rho)=0.05$kg·m^{-3}, $u(p)$=0.01MPa and at the experimental pressure=0.1 MPa

Table 4.44

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	$E_{\phi}^{0} \times 10^{6}$/(m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T =293.15 K	T =298.15 K	T =303.15 K	T =308.15 K	
EG					
0.05	0.05	0.08	0.10	0.12	0.00
0.10	-0.07	0.03	0.13	0.24	0.02
0.15	0.05	0.02	-0.01	-0.04	0.05
DEG					
0.05	0.00	0.05	0.10	0.15	0.01
0.10	-0.19	-0.05	0.09	0.22	0.03
0.15	0.23	0.17	0.10	0.03	-0.01
TEG					
0.05	0.06	0.09	0.13	0.16	0.01
0.10	0.65	0.36	0.07	-0.23	-0.06
0.15	0.07	0.04	0.00	-0.03	-0.01

${}^{a}m_B$ is the molality of D-Panthenol; standard uncertainties u are $u(m)=2 \times 10^{-5}$ mol·kg^{-1}, $u(T)=0.01$ K, $u(\rho)= 0.05$ kg·m^{-3}, $u(p)=$ 0.01 MPa and at the experimental pressure=0.1 MPa

Table 4.45

Values of speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,S}$, of glycols in aqueous solutions of D-Panthenol at different temperatures

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s}$ × 10^6/(m^3·mol^{-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
EG+0.05 mol·kg^{-1} D-Panthenol								
0.00000	1489.41	1503.02	1515.97	1525.19				
0.09927	1492.40	1505.57	1518.19	1527.21	-44.67	-43.86	-43.11	-42.59
0.20001	1495.75	1508.13	1520.46	1529.49	-44.93	-44.12	-43.37	-42.85
0.29453	1498.66	1510.69	1522.73	1531.60	-45.04	-44.23	-43.47	-42.95
0.39970	1502.10	1513.95	1525.64	1534.00	-45.11	-44.30	-43.54	-43.02
0.49986	1505.32	1516.79	1528.19	1536.20	-45.17	-44.36	-43.60	-43.08
EG+0.10 mol·kg^{-1} D-Panthenol								
0.00000	1494.13	1507.57	1517.93	1529.07				
0.09994	1497.01	1509.93	1519.98	1531.31	-44.12	-43.36	-42.71	-42.19
0.19887	1499.88	1512.58	1522.14	1533.54	-44.38	-43.61	-42.96	-42.43
0.30277	1502.98	1515.24	1524.63	1535.70	-44.49	-43.72	-43.07	-42.54
0.38547	1505.57	1517.78	1527.05	1537.80	-44.55	-43.78	-43.13	-42.60
0.51235	1509.12	1521.39	1530.62	1540.74	-44.60	-43.83	-43.18	-42.65

EG+0.15 mol·kg^{-1} D-Panthenol								
0.00000	1498.55	1511.64	1522.94	1532.45				
0.09940	1501.43	1514.38	1525.28	1534.80	-44.12	-43.36	-42.71	-42.19
0.19930	1504.08	1516.70	1527.44	1537.10	-44.38	-43.61	-42.96	-42.43
0.30448	1507.01	1519.41	1530.10	1539.20	-44.48	-43.71	-43.07	-42.53
0.39600	1509.56	1521.98	1532.67	1541.31	-44.55	-43.78	-43.13	-42.60
0.50151	1512.28	1524.67	1535.57	1543.48	-44.60	-43.83	-43.18	-42.65
DEG+0.05 mol·kg^{-1} D-Panthenol								
0.00000	1489.41	1503.02	1515.47	1525.19				
0.09797	1494.71	1508.32	1519.57	1529.39	-44.30	-43.51	-42.86	-42.31
0.19870	1500.04	1513.41	1524.16	1533.78	-44.60	-43.80	-43.15	-42.60
0.29915	1505.77	1518.68	1528.73	1538.06	-44.74	-43.93	-43.28	-42.73
0.40094	1511.01	1523.81	1533.56	1542.71	-44.84	-44.03	-43.38	-42.82
0.49695	1516.02	1528.63	1537.98	1546.71	-44.92	-44.10	-43.45	-42.89
DEG+0.10 mol·kg^{-1} D-Panthenol								
0.00000	1494.13	1507.57	1519.53	1529.07				
0.09947	1499.73	1512.67	1524.03	1533.47	-44.02	-43.27	-42.62	-42.10
0.20205	1505.41	1517.85	1528.81	1537.95	-44.30	-43.55	-42.90	-42.37
0.30629	1511.17	1523.21	1533.77	1542.71	-44.44	-43.68	-43.03	-42.50
0.39789	1515.98	1528.12	1538.08	1546.92	-44.53	-43.77	-43.11	-42.59

0.50044	1521.36	1533.37	1543.06	1551.43	-44.61	-43.85	-43.20	-42.66
DEG+0.15 mol·kg^{-1} D-Panthenol								
0.00000	1498.55	1511.64	1522.94	1532.45				
0.10470	1504.25	1516.84	1527.64	1537.05	-43.78	-43.05	-42.44	-41.92
0.19784	1509.84	1521.73	1532.23	1541.44	-44.03	-43.30	-42.69	-42.17
0.29933	1515.47	1527.16	1536.86	1546.07	-44.17	-43.44	-42.82	-42.30
0.39620	1520.54	1532.03	1541.33	1550.42	-44.27	-43.53	-42.91	-42.39
0.49900	1525.89	1537.29	1546.59	1554.96	-44.35	-43.61	-43.00	-42.47
TEG+0.05 mol·kg^{-1} D-Panthenol								
0.00000	1489.41	1503.02	1515.47	1525.19				
0.10106	1497.66	1510.95	1522.11	1531.58	-44.14	-43.37	-42.73	-42.21
0.19881	1505.66	1518.52	1529.21	1537.73	-44.45	-43.67	-43.03	-42.50
0.30095	1513.34	1525.88	1536.38	1543.98	-44.62	-43.84	-43.20	-42.66
0.41255	1521.92	1534.29	1543.86	1551.05	-44.76	-43.98	-43.33	-42.79
0.49633	1528.75	1540.13	1550.00	1556.57	-44.85	-44.07	-43.42	-42.87
TEG+0.10 mol·kg^{-1} D-Panthenol								
0.00000	1494.13	1507.57	1519.53	1529.07				
0.10454	1502.37	1515.48	1526.38	1535.23	-43.88	-43.13	-42.51	-42.02
0.20136	1510.41	1523.22	1533.37	1541.48	-44.18	-43.42	-42.80	-42.30
0.30052	1517.80	1530.56	1540.25	1547.67	-44.34	-43.58	-42.96	-42.44

0.39983	1525.30	1538.21	1547.58	1554.06	-44.47	-43.70	-43.07	-42.56
0.50238	1533.29	1545.21	1554.83	1560.71	-44.59	-43.81	-43.19	-42.66
TEG+0.15 mol·kg^{-1} D-Panthenol								
0.00000	1498.55	1511.64	1522.94	1532.45				
0.09973	1507.06	1520.09	1529.94	1538.73	-43.59	-42.85	-42.30	-41.81
0.19904	1515.15	1528.07	1537.21	1545.35	-43.91	-43.15	-42.60	-42.10
0.30436	1522.69	1535.48	1544.03	1551.79	-44.07	-43.31	-42.76	-42.26
0.40056	1530.18	1542.95	1551.51	1558.06	-44.20	-43.44	-42.88	-42.37
0.49370	1537.45	1549.61	1558.29	1564.02	-44.30	-43.53	-42.97	-42.47

$^{a}m_A$ is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainities *u* are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.01K, $u(\rho)=0.05$(kg·m^{-3}),$u(p)$=0.01MPa and at the experimental pressure=0.1 MP

Table 4.46

Partial molar isentropic compression, $K_{\phi,s}^{0}$ and experimental slopes, S_{k}^{*}, of glycols in aqueous solution of D-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$K_{\phi,s}^{0}$ ×10^{6}/(m^{3}·mol^{-1}· GPa^{-1})				S_{K}^{*} ×10^{6}/(kg·m^{3}·mol^{-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
EG								
0.05	-44.63(±0.08)	-43.82(±0.08)	-43.07(±0.08)	-42.56(±0.07)	-1.19(±0.24)	-1.17(±0.23)	-1.15(±0. 23)	-1.14(±0. 23)
0.10	-44.73(±0.08)	-44.68(±0.08)	-44.62(±0.07)	-44.55(±0.07)	-1.13(±0. 23)	-1.12(±0. 23)	-1.12(±0. 23)	-1.12(±0. 22)
0.15	-44.09(±0.08)	-43.32(±0.08)	-42.68(±0.08)	-42.15(±0.07)	-1.14(±0. 23)	-1.12(±0. 23)	-1.10(±0. 23)	-1.10(±0. 22)
DEG								
0.05	-44.24(±0. 08)	-43.45(±0. 08)	-42.81(±0. 08)	-42.26(±0. 08)	-1.46(±0.25)	-1.43(±0.24)	-1.40(±0. 24)	-1.38(±0. 24)
0.10	-43.95(±0. 08)	-43.20(±0. 08)	-42.56(±0. 07)	-42.04(±0. 07)	-1.42(±0.23)	-1.39(±0. 23)	-1.37(±0.22)	-1.36(±0. 22)
0.15	-43.69(±0. 08)	-42.97(±0. 07)	-42.36(±0. 07)	-41.84(±0. 07)	-1.42(±0. 23)	-1.40(±0. 24)	-1.37(±0. 22)	-1.35(±0. 22)
TEG								
0.05	-44.05(±0.08)	-43.27(±0. 07)	-42.64(±0. 07)	-42.12(±0. 07)	-1.72(±0.23)	-1.70(±0.22)	-1.65(±0.22)	-1.61(±0.22)
0.10	-43.77(±0.07)	-43.01(±0. 07)	-42.40(±0. 07)	-41.92(±0. 07)	-1.73(±0.22)	-1.69(±0.23)	-1.67(±0.22)	-1.59(±0.21)
0.15	-43.50(±0.08)	-42.76(±0.08)	-42.21(±0. 07)	-41.73(±0. 07)	-1.74(±0.23)	-1.66(±0.23)	-1.65(±0.22)	-1.60(±0.22)

$^{a}m_B$ is the molality of D-Panthenol; standard uncertainities u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.01K, $u(\rho)=0.05$kg·m^{-3},$u(p)$=0.01MPa and at the experimental pressure=0.1 MPa

Table 4.47

Partial molar isentropic compression transfer, $\Delta K_{\phi,s}^{0}$, of glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	$\Delta K_{\phi,s}^{0}$ × 10^{6}/(m^{3}·mol^{-1}· GPa^{-1})			
	T =293.15 K	T =298.15 K	T =303.15 K	T =308.15 K
EG				
0.05	0.50	0.41	0.41	0.32
0.10	0.40	-0.45	-1.14	-1.67
0.15	1.04	0.91	0.80	0.73
DEG				
0.05	0.89	0.80	0.68	0.64
0.10	1.18	1.05	0.93	0.86
0.15	1.44	1.28	1.13	1.06
TEG				
0.05	1.08	0.98	0.84	0.78
0.10	1.36	1.24	1.08	0.98
0.15	1.63	1.49	1.27	1.17

${}^{a}m_B$ is the molality of D-Panthenol; standard uncertainties u are $u(m)=2 \times 10^{-5}$ mol·kg^{-1}, $u(T)=0.01$ K, $u(\rho)=0.05$ kg·m^{-3}, $u(p)=$ 0.01 MPa, and at the experimental pressure=0.1 MPa

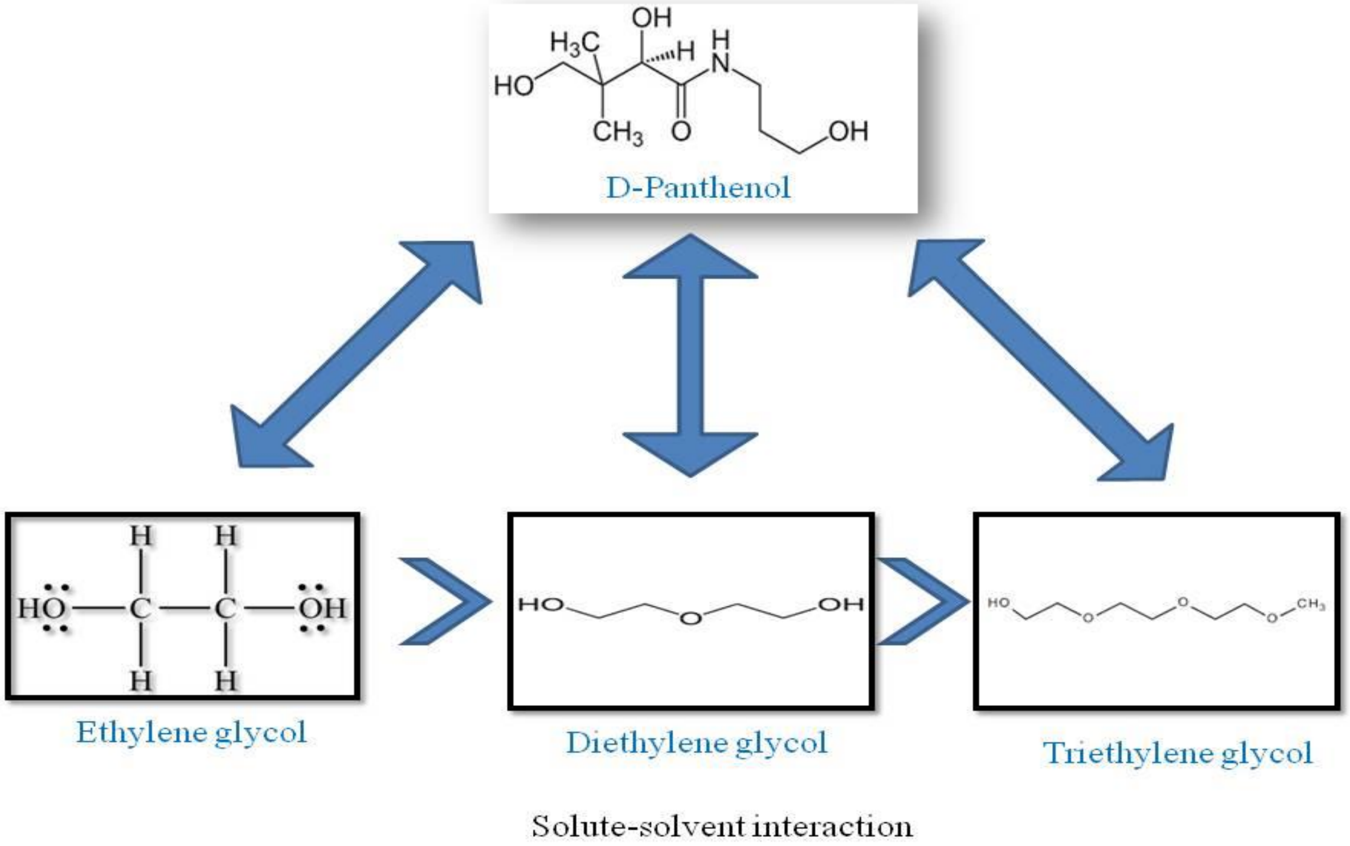
Table 4.48

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) interaction coefficient of glycols in aqueous solutions of D-Panthenol at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
EG				
293.15	2.12	7.94	2.69	2.46
298.15	-6.64	41.82	-3.31	25.43
303.15	8.12	-21.39	-7.62	41.46
308.15	9.95	-36.46	-11.64	57.30
DEG				
293.15	8.11	-18.27	9.62	-21.86
298.15	-8.09	60.51	8.65	-19.86
303.15	1.71	27.47	7.48	-16.79
308.15	2.34	24.66	6.98	-15.69
TEG				
293.15	-4.54	38.78	11.71	-28.45
298.15	9.42	-19.11	10.53	-25.26
303.15	21.69	-73.47	9.18	-22.35
308.15	19.22	-70.91	8.47	-20.66

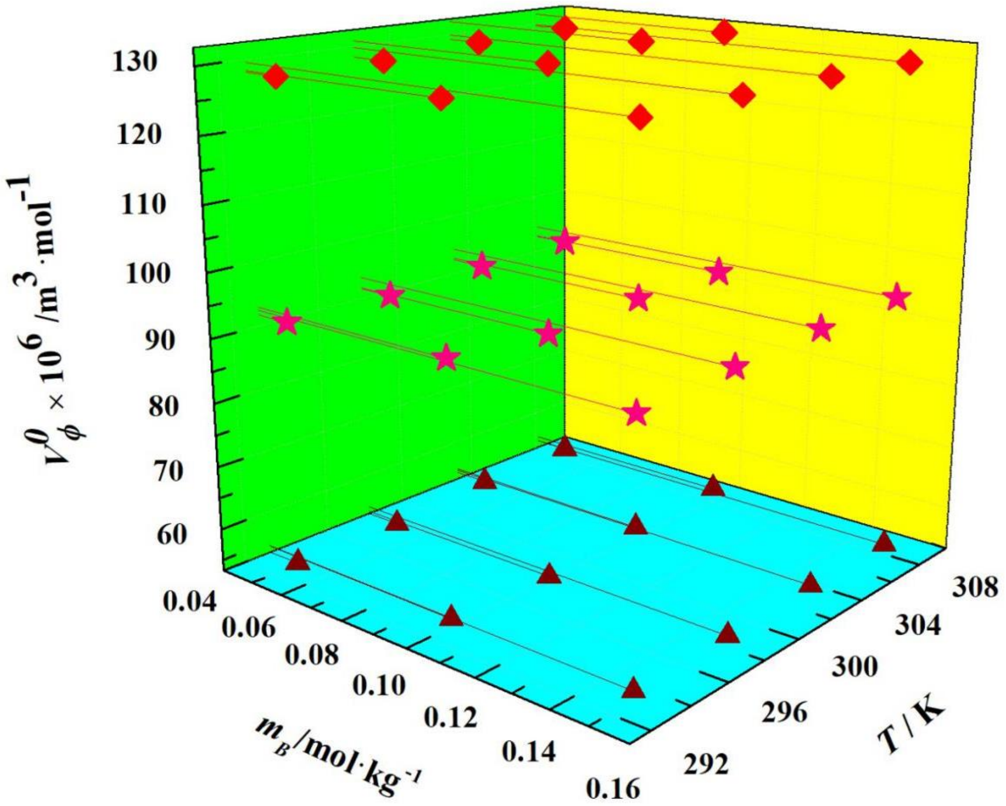
T/K is the temperatures; standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.01K, *u(ρ)=0.05*(kg·m^{-3}),*u(p)*=0.01MPa and at the experimental pressure=0.1 MPa

Figure 4.30



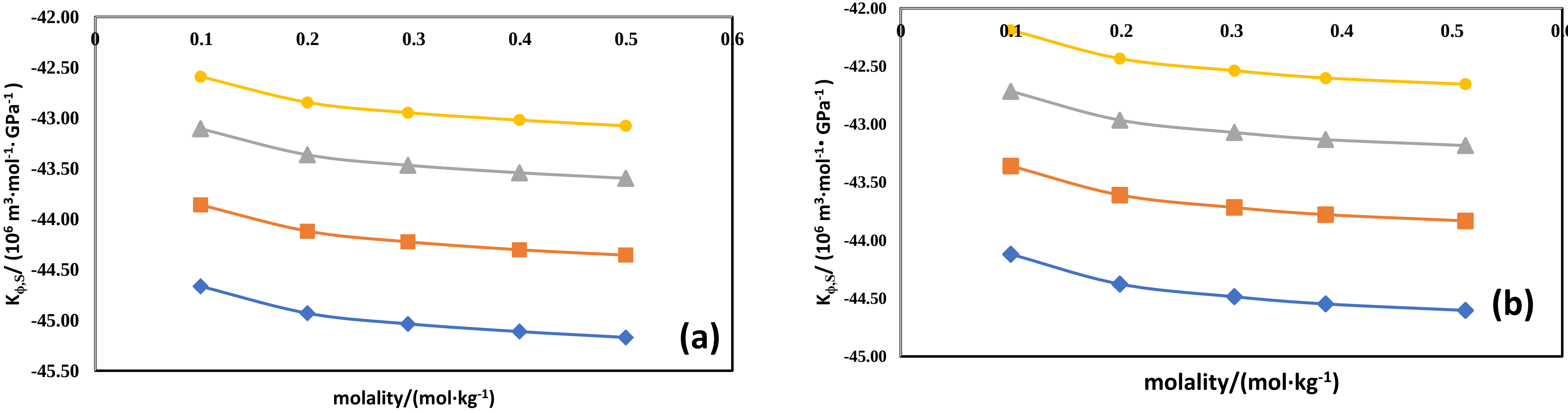
EG/ DEG/ TEG and D-Panthenol interactions.

Figure 4.31



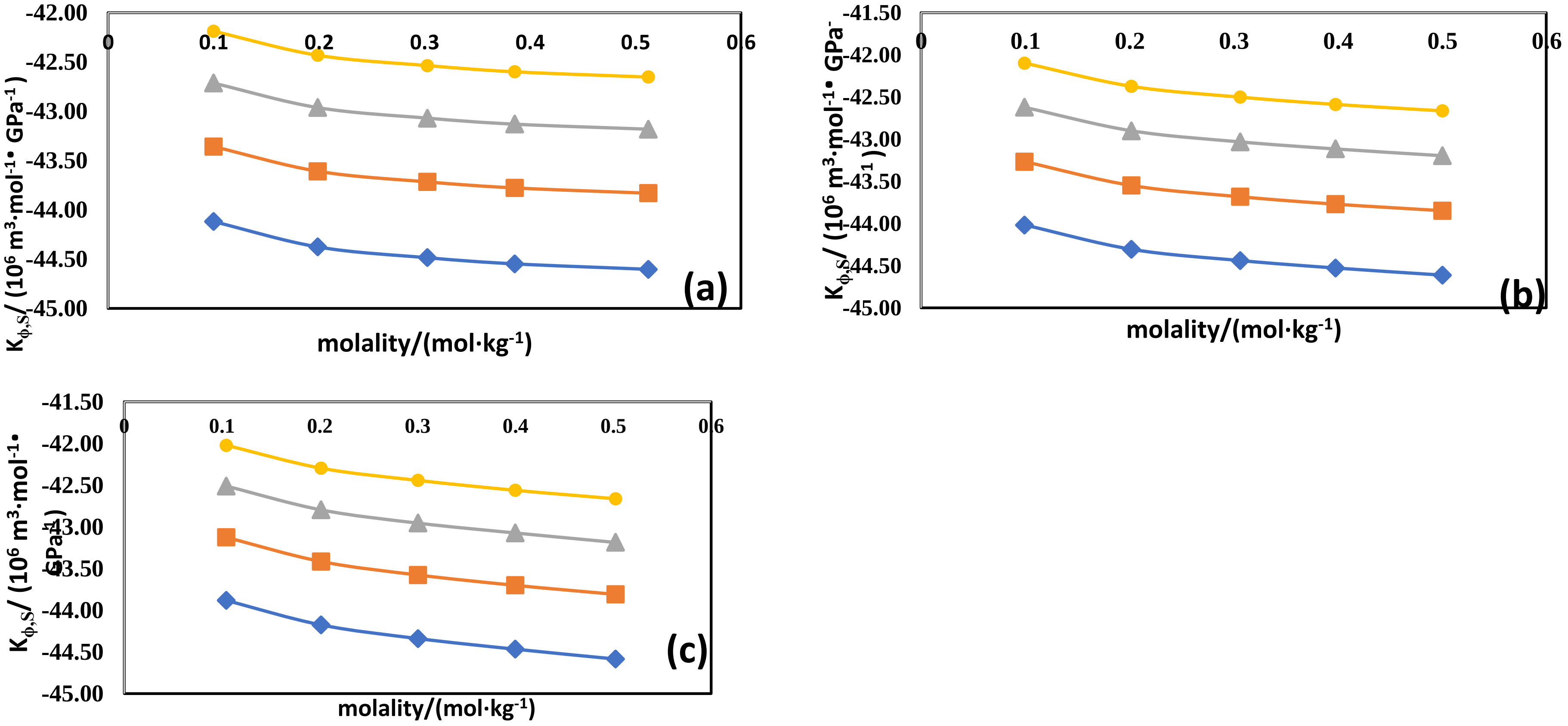
Variation of partial molar volumes, V_{ϕ}^{0}, of, ethylene glycol (filled with triangle), diethylene glycol (filled with circle) and triethylene glycol (filled with square) in different concentration of aqueous D-Panthenol solutions at different temperature.

Figure 4.32



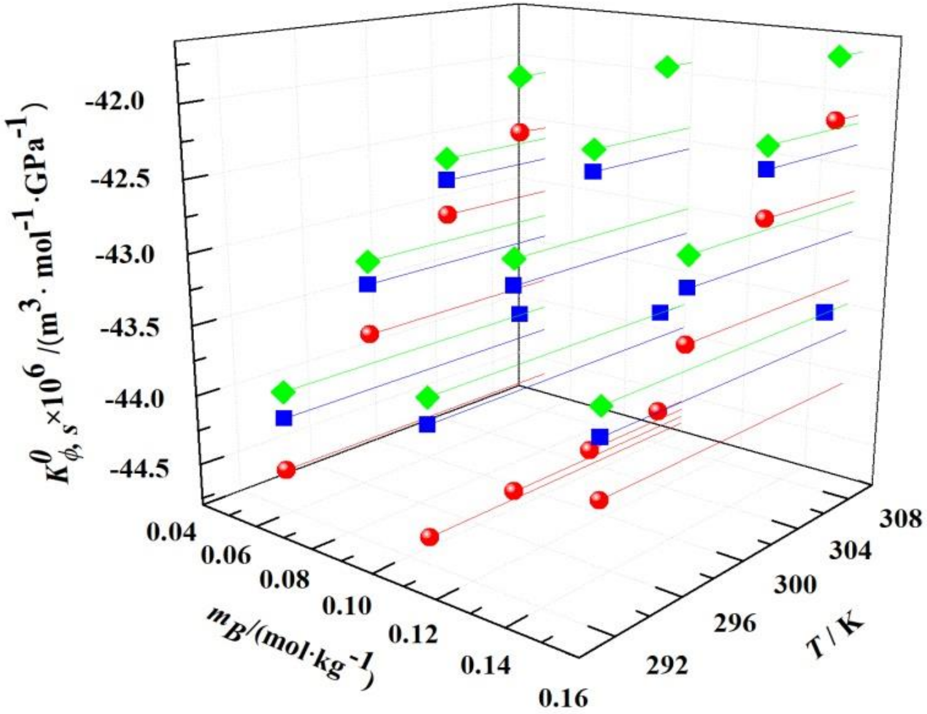
Variation of apparent molar isentropic compression, $K_{\phi,s,}$ of ethylene glycol in aqueous solutions of **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, against molality at different temperature [circle, 308.15 K; triangle, 303.15 K; square, 298.15 K; diamond, 293.15 K]

Figure 4.33



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, of ethylene glycol in aqueous solutions of **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol against molality at different temperature [circle, 308.15 K; triangle, 303.15 K; square, 298.15 K; diamond, 293.5 K]

Figure 4.34



Variation of Limiting apparent molar isentropic compression, $\Delta K^0_{\phi,s}$, of, ethylene glycol (filled with triangle), diethylene glycol (filled with circle) and triethylene glycol (filled with square) in different concentration of aqueous D-Panthenol solutions at different temperature.

Problem 6

Investigation on temperature-dependent volumetric and acoustical properties of homologous series of glycols containing d-panthenol

In this section, we have extended the previous work with the densities, ρ and speed of sound c of ethylene glycol (EG), diethylene glycol (DEG) and triethylene glycol (TEG) in (0.00, 0.05, 0.10, 0.15) mol·kg^{-1} aqueous solutions of d-Panthenol at temperatures T = (293.15, 298.15, 303.15 and 308.15) K and calculated the basic acoustic parameters.

4.49 Acoustic parameters

The following equations are used to find the Acoustic impedance (4.15), adiabatic compressibility (4.16), intermolecular free length (4.17), Wada’s constant (4.18), Rao’s constant (4.19), and Vander Waal’s constant (4.20), in the liquid mixture

$$Z = \rho \text{ x } c \tag{4.15}$$

$$\beta = {}^{1}\!/_{[\rho(c^2)]} \tag{4.16}$$

$$L_f = K_T\,(\beta)^{1/2} \tag{4.17}$$

$$W = (\beta)^{-\frac{1}{7}}\left(\frac{M}{\rho}\right) \tag{4.18}$$

$$R = {}^{[(c^{\frac{1}{3}})M]}\!/_{\rho} \tag{4.19}$$

$$b = \left(\frac{M}{\rho}\right)\left[1 - (RT/Mc^2)\sqrt{1 + (Mc^2/3RT)}\text{-}1\right] \tag{4.20}$$

Where,

Z= Acoustic impedance, β=Adiabatc compressibility, L_f= Intermolecular free length, W= Wada’s constant (independent of temperature), R=Rao’s constant, b= Vander Waal constant, M=Effective molecular weight, K_T= Temperature of dependent Jacobson’s constant, ρ=Density of mixture and c = Ultrasonic velocity in the medium. From the experimental density and velocity data the thermodynamical parameters such as Acoustic impedance **(Z)**, Adiabatic compressibility **(β)**, Intermolecular free length **(L_f)**, Wa da’s constant **(W)**, Rao’s constant **(R)** and Vander Waal’s constant **(b)** in the liquid mixture has been calculated which has suggested the intermolecular interactions among the glycols and vitamin B_5 D-Panthenol. The acoustic impedance and adiabatic compressibility are mentioned in Table 4.49, Wada’s constant and Rao’s constant in Table 4.50 and in Table 4.51 the intermolecular free length and Vander Waal constant are indexed. In Figure 4.35 the interaction of solute and solvent in sedcribed. The impedance values increases with the molality as well as with the temperature, shown in Figure 4.36, which suggest there is no complex formation inside the liquid mixture. With the concentration, the decrease in the adiabatic compressibility proves the greater bond strength among the molecules and in the intermolecular free length indicates that the molecules are much more closely packed, thus implying the existence of the strong solute-solvent interaction inside the mixture, evident from the Figure 4.37 and Figure 4.38 respectively. Figure 4.39, Figure 4.40 and Figure 4.41 shows the variations of Wada’s constant, Rao’s constant and Vander Waal’s constant respectively. The variation of the Wada’s constant with the temperature, in accordance with the concentration, depicts that the space between the solute and solvent molecules decreases, thus implying that the molecules are coming closer to each other, suggesting the strong solute-solvent interaction in the solution. The presence of the strong binding forces inside the liquid system between solute and solvent is confirmed by the increasing values of Vander waal’s constants with the temperature [25-27].

Table 4.49 Values of Acoustic Impedence, (*Z*) and Adiabatic Compressibility, (*β*), of glycols in aqueous solution of D-Panthenol at different temperature and at experimental temperature =0.1MPa

Molality	Z/ (kg $m^{-2}S^{-1}$)				β× 10^{-10}/(N/m^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
EG + 0.05 m D-Panthenol								
0.00000	1488.679	1500.301	1511.314	1518.014	4.510085	4.434624	4.364714	4.319171
0.09927	1492.937	1504.183	1514.688	1521.211	4.488210	4.415687	4.348613	4.304391
0.20001	1497.531	1507.902	1518.196	1524.683	4.464424	4.397324	4.332086	4.288188
0.29453	1501.522	1511.627	1521.591	1527.917	4.443908	4.379052	4.315977	4.273218
0.39970	1506.171	1516.213	1525.728	1531.535	4.420048	4.356404	4.296063	4.256452
0.49986	1510.574	1520.125	1529.425	1534.971	4.397737	4.337057	4.278529	4.240842
EG + 0.10 m D-Panthenol								
0.00000	1496.552	1507.903	1516.392	1525.000	4.472185	4.398950	4.344468	4.288475
0.09994	1500.571	1511.523	1519.533	1528.306	4.451626	4.381557	4.329641	4.272939
0.19887	1504.507	1515.288	1522.749	1531.634	4.431485	4.363014	4.314367	4.257454

0.30277	1508.676	1519.043	1526.411	1534.964	4.410123	4.344586	4.296987	4.242241
0.38547	1512.210	1522.50	1529.831	1538.106	4.392250	4.327467	4.280587	4.227795
0.51235	1517.103	1527.581	1534.799	1542.555	4.367783	4.302841	4.256780	4.207557
EG + 0.15 m D-Panthenol								
0.00000	1503.557	1514.799	1523.823	1530.895	4.438221	4.367134	4.309060	4.262539
0.09940	1507.526	1518.666	1527.238	1534.41	4.418045	4.348134	4.292828	4.246262
0.19930	1511.355	1522.065	1530.527	1537.798	4.399087	4.331788	4.277547	4.230568
0.30448	1515.406	1525.902	1534.318	1540.985	4.378799	4.313187	4.259559	4.216056
0.39600	1518.946	1529.464	1537.909	1544.218	4.361212	4.295878	4.242489	4.20147
0.50151	1522.774	1533.239	1541.829	1547.512	4.342426	4.277740	4.223710	4.186635
DEG + 0.05 m D-Panthenol								
0.00000	1488.679	1500.301	1510.811	1518.014	4.510085	4.434624	4.367595	4.31917
0.09797	1496.03	1507.723	1516.924	1524.204	4.472010	4.397289	4.338257	4.289816
0.19870	1503.597	1514.911	1523.703	1530.712	4.433695	4.361704	4.305952	4.259350
0.29915	1511.341	1522.249	1530.243	1536.983	4.394190	4.325617	4.274729	4.230167

0.40094	1518.701	1529.456	1537.15	1543.679	4.357731	4.290741	4.242120	4.199125
0.49695	1525.571	1536.169	1543.374	1549.454	4.323771	4.258519	4.212871	4.172655
DEG + 0.10 m D-Panthenol								
0.00000	1496.552	1507.903	1517.991	1525.000	4.472185	4.398950	4.335324	4.288475
0.09947	1504.100	1515.155	1524.530	1531.440	4.433127	4.363135	4.303982	4.258187
0.20205	1511.858	1522.382	1531.320	1537.935	4.393739	4.327603	4.271500	4.227853
0.30629	1519.627	1529.827	1538.367	1544.716	4.354616	4.291390	4.238184	4.196306
0.39789	1526.346	1536.682	1544.523	1550.888	4.321688	4.258518	4.209462	4.168231
0.50044	1533.872	1543.892	1551.602	1557.401	4.285278	4.224119	4.176733	4.138731
DEG + 0.15 m D-Panthenol								
0.00000	1503.557	1514.845	1523.823	1530.895	4.438221	4.367003	4.309060	4.262539
0.10470	1511.270	1521.965	1530.358	1537.285	4.398837	4.331671	4.277460	4.232116
0.19784	1518.885	1528.801	1536.890	1543.689	4.360578	4.298444	4.246522	4.202557
0.29933	1526.642	1536.410	1543.647	1550.331	4.322305	4.261950	4.215195	4.172020
0.39620	1533.851	1543.441	1550.137	1556.695	4.287647	4.229050	4.185373	4.143308

0.49900	1541.196	1550.775	1557.633	1563.403	4.252251	4.194647	4.151067	4.113483

TEG + 0.05 m D-Panthenol

0.00000	1488.679	1500.301	1510.811	1518.014	4.510085	4.434624	4.367595	4.319170
0.10106	1500.221	1511.557	1520.669	1527.578	4.450733	4.378499	4.320355	4.274221
0.19881	1511.333	1522.193	1530.791	1536.710	4.394534	4.326231	4.271859	4.231827
0.30095	1522.129	1532.771	1541.134	1545.930	4.341221	4.275652	4.223389	4.189561
0.41255	1534.184	1544.751	1551.968	1556.451	4.282830	4.219239	4.173585	4.142274
0.49633	1543.570	1553.101	1560.579	1564.241	4.237769	4.180641	4.134116	4.107029

TEG + 0.10 m D-Panthenol

0.00000	1496.552	1507.903	1517.991	1525.000	4.472185	4.398950	4.335324	4.288475
0.10454	1508.074	1518.743	1527.627	1534.074	4.413674	4.344758	4.288644	4.246003
0.20136	1519.142	1529.556	1537.663	1543.103	4.358197	4.292121	4.241229	4.204043
0.30052	1529.701	1540.092	1547.722	1552.075	4.307040	4.242315	4.194845	4.163025
0.39983	1540.382	1550.885	1558.045	1561.519	4.256143	4.191841	4.147314	4.120831
0.50238	1551.766	1561.016	1568.652	1571.142	4.202904	4.145769	4.100061	4.078143

TEG + 0.15 m D-Panthenol								
0.00000	1503.557	1514.845	1523.823	1530.895	4.438221	4.367003	4.309061	4.262539
0.09973	1515.124	1526.336	1533.887	1540.321	4.379466	4.310032	4.261202	4.219163
0.19904	1526.447	1537.445	1544.249	1549.770	4.323771	4.256545	4.212593	4.175476
0.30436	1537.212	1547.973	1554.154	1559.256	4.272231	4.207194	4.167256	4.132851
0.40056	1547.855	1558.637	1564.805	1568.407	4.222087	4.158178	4.118938	4.092202
0.49370	1558.261	1567.916	1574.395	1577.297	4.174061	4.115806	4.076036	4.053631

Table 4.50 Values of Waada's constant, *W* and Rao's constant, *R*, of glycols in aqueous solution of D-Panthenol at different temperature and at experimental temperature =0.1MPa

Molality	$W/(m^3/mol)(Pa)^{1/7}$				$R/\ (m^3/mol)(m/s)^{1/3}$			
	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
EG + 0.05 m D-Panthenol								
0.00000	50.07720	50.26434	50.44249	50.60092	709.1963	712.2892	715.2354	717.8569
0.09927	50.06937	50.25037	50.43033	50.58622	709.0668	712.0583	715.0343	717.6135
0.20001	50.06585	50.24158	50.41644	50.57362	709.0087	711.913	714.8044	717.4051
0.29453	50.06280	50.23274	50.40587	50.56146	708.9584	711.7667	714.6296	717.2038
0.39970	50.06135	50.22604	50.39853	50.54943	708.9343	711.6560	714.5082	717.0047
0.49986	50.05861	50.22268	50.39020	50.53512	708.8891	711.6005	714.3704	716.7679
EG + 0.10 m D-Panthenol								
0.00000	50.03189	50.22024	50.37187	50.54875	708.4477	711.5601	714.0673	716.9934
0.09994	50.02698	50.20681	50.36023	50.53949	708.3665	711.3381	713.8748	716.8402
0.19887	50.02416	50.20038	50.35071	50.52931	708.3200	711.2318	713.7174	716.6717

0.30277	50.02355	50.19466	50.34111	50.51651	708.3098	711.1374	713.5585	716.4600
0.38547	50.02168	50.19294	50.33579	50.50687	708.279	711.1089	713.4705	716.3005
0.51235	50.01779	50.18590	50.33024	50.49209	708.2148	710.9925	713.3788	716.0559
EG + 0.15 m D-Panthenol								
0.00000	50.00055	50.17858	50.35051	50.50916	707.9299	710.8716	713.714	716.3384
0.09940	49.99728	50.17279	50.34224	50.49831	707.8759	710.7759	713.5772	716.1588
0.19930	49.98932	50.16443	50.33085	50.48927	707.7444	710.6377	713.3888	716.0093
0.30448	49.98582	50.15849	50.32419	50.47844	707.6867	710.5396	713.2788	715.8301
0.39600	49.98241	50.15515	50.3199	50.46679	707.6304	710.4844	713.2078	715.6374
0.50151	49.97743	50.1504	50.3188	50.45579	707.5481	710.4057	713.1896	715.4553
DEG + 0.05 m D-Panthenol								
0.00000	85.61612	85.93607	86.23253	86.51152	1212.501	1217.788	1222.691	1227.308
0.09797	85.60221	85.9183	86.20034	86.48167	1212.271	1217.495	1222.159	1226.813
0.19870	85.58027	85.89882	86.16804	86.44911	1211.908	1217.173	1221.625	1226.275
0.29915	85.57630	85.88431	86.14651	86.42148	1211.843	1216.933	1221.268	1225.817

0.40094	85.55972	85.86761	86.12456	86.39765	1211.569	1216.657	1220.905	1225.423
0.49695	85.55241	85.85518	86.10956	86.37680	1211.448	1216.451	1220.657	1225.078
DEG + 0.10 m D-Panthenol								
0.00000	85.53866	85.86067	86.14584	86.42231	1211.221	1216.542	1221.257	1225.831
0.09947	85.53550	85.83897	86.11958	86.39394	1211.169	1216.183	1220.823	1225.362
0.20205	85.52787	85.82422	86.09973	86.36860	1211.043	1215.940	1220.495	1224.942
0.30629	85.52541	85.81113	86.07965	86.34794	1211.002	1215.723	1220.163	1224.601
0.39789	85.51258	85.79789	86.06103	86.32174	1210.790	1215.504	1219.855	1224.167
0.50044	85.49830	85.78995	86.04163	86.29884	1210.554	1215.373	1219.534	1223.788
DEG + 0.15 m D-Panthenol								
0.00000	85.48507	85.78725	86.08339	86.35463	1210.335	1215.328	1220.224	1224.711
0.10470	85.48102	85.77909	86.07081	86.34209	1210.269	1215.194	1220.016	1224.504
0.19784	85.47512	85.76512	86.05171	86.31588	1210.171	1214.963	1219.701	1224.070
0.29933	85.46551	85.74930	86.02485	86.29409	1210.012	1214.701	1219.256	1223.710
0.39620	85.44664	85.72576	86.00101	86.26820	1209.701	1214.312	1218.862	1223.281

0.49900	85.43973	85.71321	85.98028	86.23849	1209.587	1214.105	1218.519	1222.790
TEG + 0.05 m D-Panthenol								
0.00000	121.1631	121.6159	122.0354	122.4303	1715.919	1723.402	1730.341	1736.874
0.10106	121.1259	121.5681	121.9650	122.3562	1715.304	1722.612	1729.175	1735.648
0.19881	121.0972	121.5318	121.9201	122.2915	1714.83	1722.013	1728.432	1734.577
0.30095	121.0625	121.4820	121.8682	122.2314	1714.257	1721.190	1727.574	1733.582
0.41255	121.0262	121.4345	121.8128	122.1590	1713.657	1720.403	1726.659	1732.385
0.49633	121.0128	121.4006	121.7877	122.1322	1713.436	1719.843	1726.243	1731.942
TEG + 0.10 m D-Panthenol								
0.00000	121.0535	121.5092	121.9128	122.304	1714.108	1721.638	1728.312	1734.784
0.10454	121.0185	121.4899	121.8782	122.2441	1713.531	1721.319	1727.740	1733.792
0.20136	120.9983	121.4584	121.8305	122.1968	1713.196	1720.799	1726.951	1733.010
0.30052	120.9548	121.4110	121.7730	122.1493	1712.478	1720.016	1726.000	1732.224
0.39983	120.9148	121.3761	121.7399	122.0893	1711.817	1719.439	1725.452	1731.231
0.50238	120.8737	121.3285	121.6821	122.0422	1711.137	1718.653	1724.498	1730.452

TEG + 0.15 m D-Panthenol								
0.00000	120.9776	121.4053	121.8244	122.2082	1712.855	1719.921	1726.850	1733.200
0.09973	120.9659	121.3923	121.7755	122.1364	1712.660	1719.707	1726.041	1732.011
0.19904	120.9340	121.3642	121.7325	122.0955	1712.135	1719.242	1725.331	1731.334
0.30436	120.8917	121.3252	121.6813	122.0371	1711.435	1718.598	1724.483	1730.369
0.40056	120.8546	121.2842	121.641	121.9874	1710.823	1717.920	1723.818	1729.546
0.49370	120.8152	121.2642	121.6102	121.9287	1710.173	1717.589	1723.308	1728.576

Table 4.51 Values of Intermolecular free length, (L_f) and Vandar Waal's constant, (*b*), of glycols in aqueous solution of D-Panthenol at different temperature and at experimental temperature =0.1MPa

Molality	Intermolecular free length				Vandar Waal's constant			
	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
EG + 0.05 m D-Panthenol								
0.00000	4.327031	4.330163	4.335069	4.351359	122.8050	122.9650	123.1185	123.3146
0.09927	4.316525	4.320908	4.327065	4.343909	122.7035	122.8583	123.0261	123.2206
0.20001	4.305071	4.311912	4.318835	4.335725	122.6049	122.7662	122.9276	123.1258
0.29453	4.295168	4.302946	4.310798	4.328150	122.5196	122.6741	122.8387	123.0369
0.39970	4.283622	4.291805	4.300841	4.319651	122.4250	122.5701	122.7425	122.941
0.49986	4.272797	4.282264	4.292055	4.311723	122.3329	122.4866	122.6530	122.8439
EG + 0.10 m D-Panthenol								
0.00000	4.308812	4.312711	4.325003	4.335870	122.5512	122.7204	122.8674	123.0665
0.09994	4.298896	4.304177	4.317616	4.328009	122.4613	122.6205	122.7812	122.9824
0.19887	4.289160	4.295059	4.309994	4.320160	122.3778	122.5331	122.6981	122.8961

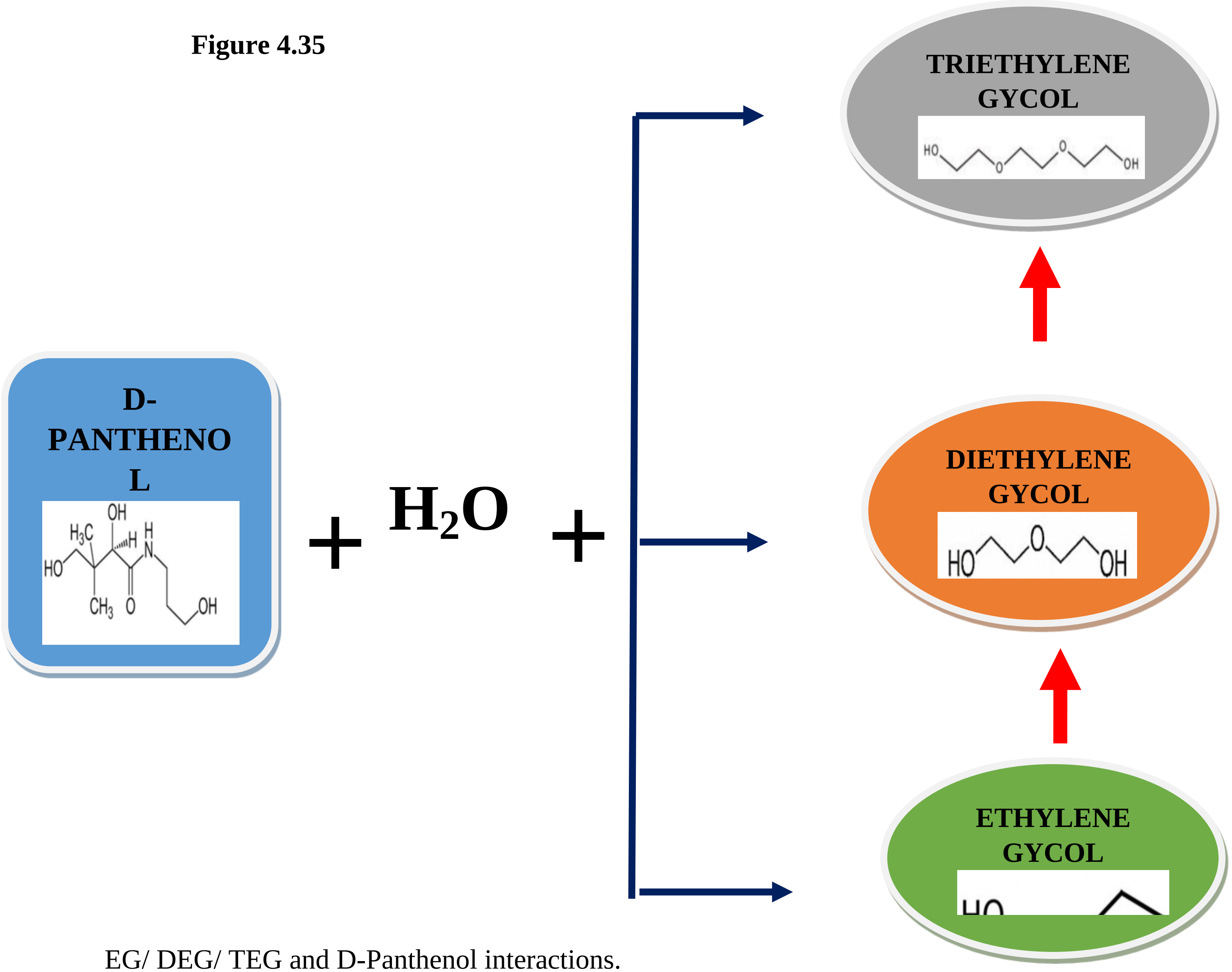
0.30277	4.278810	4.285979	4.301304	4.312434	122.2947	122.4477	122.6064	122.8043
0.38547	4.270131	4.277527	4.293087	4.305085	122.2217	122.3768	122.5288	122.7231
0.51235	4.258221	4.265339	4.281132	4.294769	122.1180	122.2633	122.4211	122.6060
EG + 0.15 m D-Panthenol								
0.00000	4.292419	4.297087	4.307342	4.322739	122.3457	122.4959	122.6768	122.8673
0.09940	4.282651	4.287729	4.299222	4.314477	122.2608	122.4081	122.5928	122.7761
0.19930	4.273452	4.279662	4.291563	4.306497	122.1689	122.3242	122.5048	122.6915
0.30448	4.263587	4.270463	4.282530	4.299105	122.0824	122.2371	122.4174	122.6071
0.39600	4.255016	4.261886	4.273940	4.291661	122.0063	122.1611	122.3392	122.5202
0.50151	4.245842	4.252879	4.264471	4.284078	121.9215	122.0782	122.2616	122.4337
DEG + 0.05 m D-Panthenol								
0.00000	4.327031	4.330164	4.336499	4.351359	209.9576	210.2311	210.4929	210.8289
0.09797	4.308727	4.311898	4.321911	4.336548	209.6781	209.9427	210.2188	210.5581
0.19870	4.29023	4.294415	4.305789	4.321122	209.3756	209.6599	209.9235	210.2720
0.29915	4.271073	4.276613	4.290150	4.306293	209.1075	209.3843	209.6605	210.0056

0.40094	4.253317	4.259337	4.273755	4.290463	208.8267	209.1099	209.3857	209.7345
0.49695	4.236712	4.243314	4.258996	4.276919	208.5835	208.8622	209.1495	209.5010
DEG + 0.10 m D-Panthenol								
0.00000	4.308812	4.312712	4.320449	4.335870	209.5237	209.8129	210.0664	210.4046
0.09947	4.289955	4.295119	4.304804	4.320532	209.2625	209.5234	209.7923	210.1301
0.20205	4.270854	4.277595	4.288529	4.305115	208.9863	209.2512	209.5249	209.8614
0.30629	4.251797	4.259660	4.271772	4.289023	208.7225	208.9768	209.2498	209.5945
0.39789	4.235692	4.243314	4.257272	4.274651	208.4726	208.7230	209.0084	209.3370
0.50044	4.217811	4.226141	4.240690	4.259498	208.1945	208.4701	208.7363	209.0765
DEG + 0.15 m D-Panthenol								
0.00000	4.292419	4.297023	4.307342	4.322739	209.1724	209.4229	209.7384	210.0642
0.10470	4.273331	4.279605	4.291520	4.307285	208.9054	209.1684	209.4949	209.8262
0.19784	4.254707	4.263159	4.275971	4.292216	208.6392	208.9122	209.2387	209.5598
0.29933	4.235994	4.245023	4.260171	4.276594	208.3621	208.6281	208.9598	209.2962
0.39620	4.218977	4.228607	4.245074	4.261853	208.0847	208.3478	208.6974	209.0342

0.49900	4.201526	4.211372	4.227640	4.246486	207.8298	208.0826	208.4102	208.7540
TEG + 0.05 m D-Panthenol								
0.00000	4.327031	4.330164	4.336499	4.351359	297.1300	297.5170	297.8875	298.3630
0.10106	4.298465	4.302675	4.312984	4.328658	296.4963	296.8781	297.2693	297.7527
0.19881	4.271241	4.276916	4.288709	4.307138	295.9067	296.2981	296.6974	297.1864
0.30095	4.245253	4.251842	4.264309	4.285575	295.3241	295.6965	296.1046	296.6294
0.41255	4.216606	4.223699	4.239091	4.261321	294.6841	295.0394	295.4860	295.9899
0.49633	4.194365	4.204336	4.218999	4.243153	294.2215	294.5831	295.0379	295.5763
TEG + 0.10 m D-Panthenol								
0.00000	4.308812	4.312712	4.320449	4.33587	296.5159	296.9252	297.2840	297.7626
0.10454	4.280532	4.286064	4.297126	4.314346	295.8922	296.3707	296.7562	297.2084
0.20136	4.253545	4.260023	4.273306	4.292975	295.3266	295.7960	296.1855	296.6867
0.30052	4.228507	4.235233	4.249874	4.271981	294.7398	295.2047	295.5968	296.1705
0.39983	4.203449	4.209963	4.225728	4.250277	294.1592	294.6326	295.0519	295.6092
0.50238	4.177076	4.186764	4.201586	4.228205	293.5484	294.0681	294.4459	295.0709

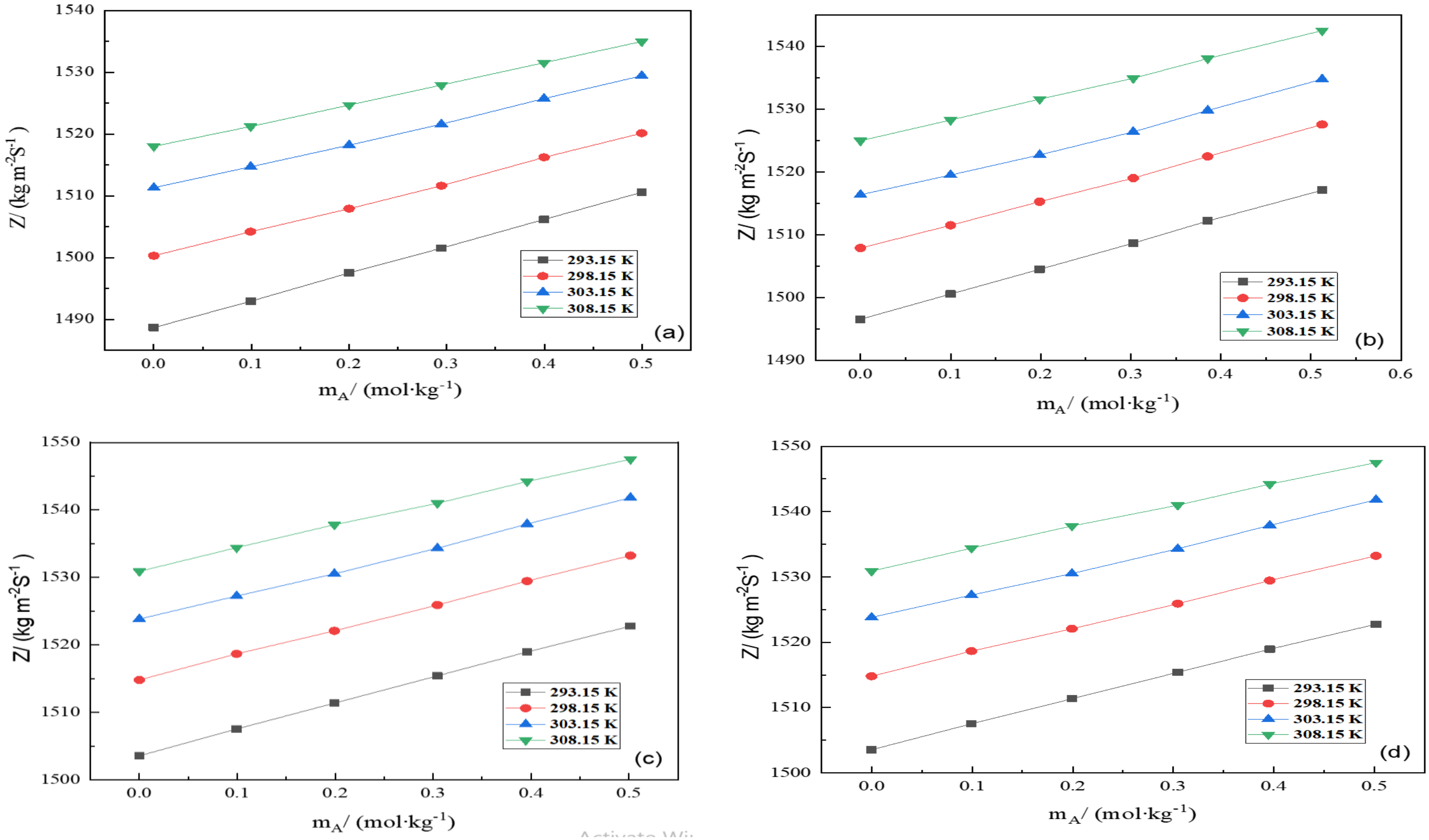
TEG + 0.15 m D-Panthenol								
0.00000	4.292419	4.297023	4.307342	4.322739	296.0188	296.3733	296.8197	297.2808
0.09973	4.263912	4.268902	4.283356	4.300689	295.446	295.8051	296.2438	296.6873
0.19904	4.236712	4.242331	4.258855	4.278365	294.847	295.2273	295.6709	296.1622
0.30436	4.211386	4.217666	4.235875	4.256471	294.2562	294.6579	295.1054	295.6019
0.40056	4.186597	4.193025	4.211247	4.235487	293.6869	294.0821	294.5332	295.0787
0.49370	4.162718	4.171607	4.189258	4.215479	293.1277	293.618	294.0332	294.5516

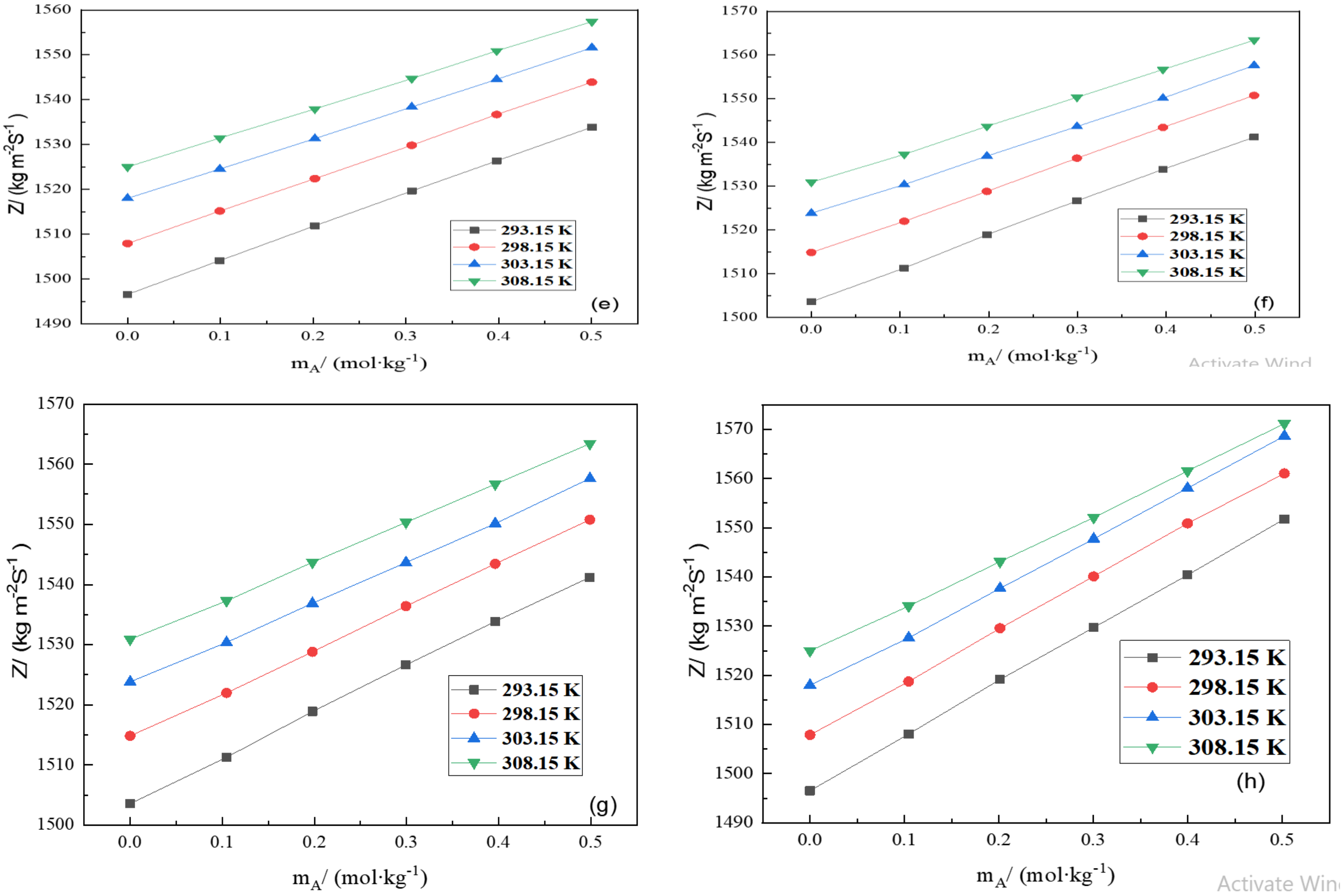
Figure 4.35

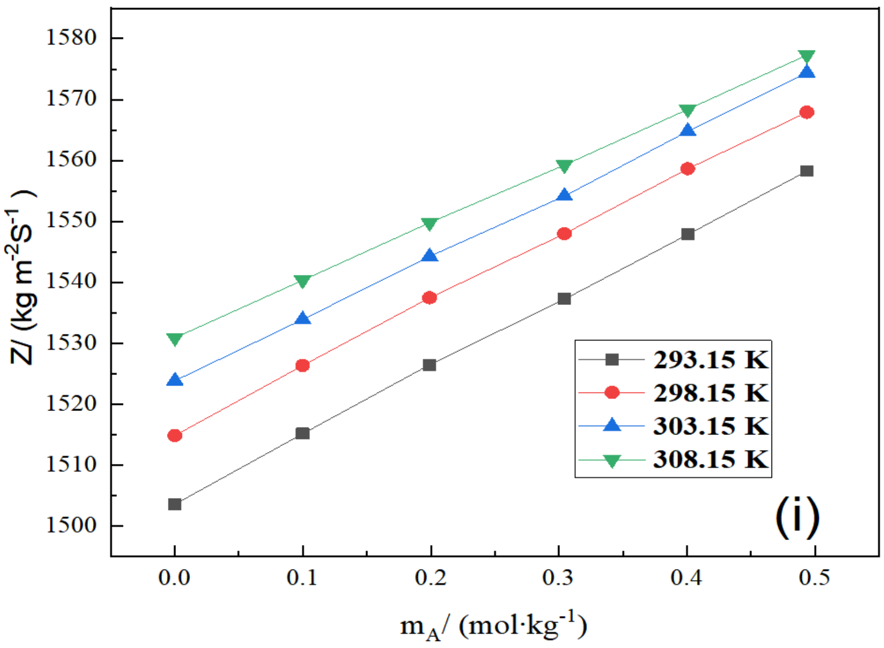


EG/ DEG/ TEG and D-Panthenol interactions.

Figure 4.36

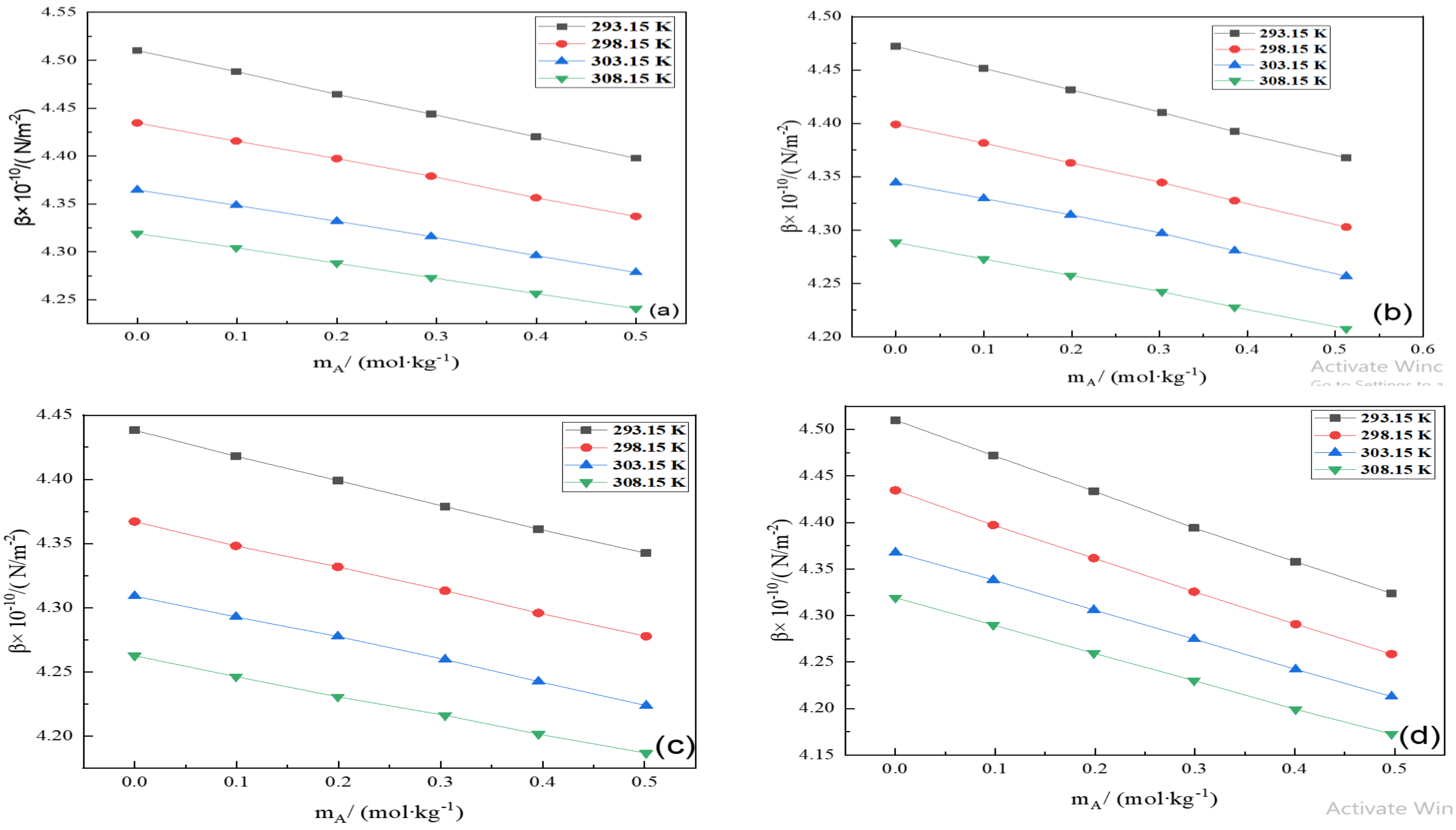

1540
1530
1520
1510
1500
1490
Z/ (kg m-2S-1)
0.0
0.1
0.2
0.3
0.4
0.5
mA/ (mol·kg-1)
293.15 K
298.15 K
303.15 K
308.15 K
(a)
1540
1530
1520
1510
1500
1490
Z/ (kg m-2S-1)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
mA/ (mol·kg-1)
293.15 K
298.15 K
303.15 K
308.15 K
(b)
1550
1540
1530
1520
1510
1500
Z/ (kg m-2S-1)
0.0
0.1
0.2
0.3
0.4
0.5
mA/ (mol·kg-1)
293.15 K
298.15 K
303.15 K
308.15 K
(c)
1550
1540
1530
1520
1510
1500
Z/ (kg m-2S-1)
0.0
0.1
0.2
0.3
0.4
0.5
mA/ (mol·kg-1)
293.15 K
298.15 K
303.15 K
308.15 K
(d)


1560
1550
1540
1530
1520
1510
1500
1490
Z/ (kg m^{-2}S^{-1})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(e)
1570
1560
1550
1540
1530
1520
1510
1500
Z/ (kg m^{-2}S^{-1})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(f)
1570
1560
1550
1540
1530
1520
1510
1500
Z/ (kg m^{-2}S^{-1})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(g)
1570
1560
1550
1540
1530
1520
1510
1500
1490
Z/ (kg m^{-2}S^{-1})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(h)

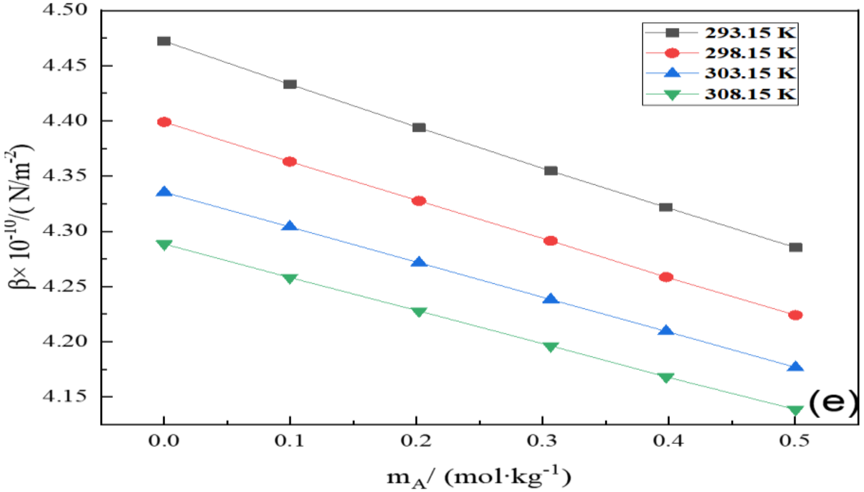


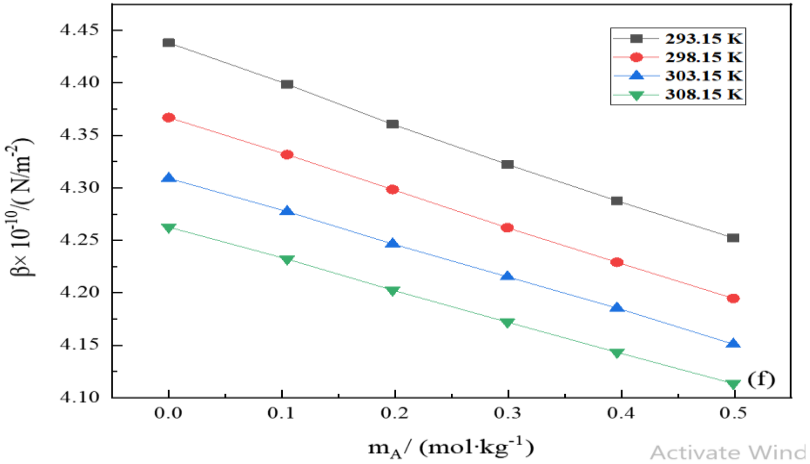
Variation of Acoustic Impedance, Z, of, ethylene glycol **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, diethylene glycol **(d)** 0.05 D-Panthenol, **(e)** 0.10 D-Panthenol and **(f)** 0.15 D-Panthenol and triethylene glycol **(g)** 0.05 D-Panthenol, **(h)** 0.10 D-Panthenol and **(i)** 0.15 D-Panthenol in different concentration of aqueous D-Panthenol solutions at different temperature.

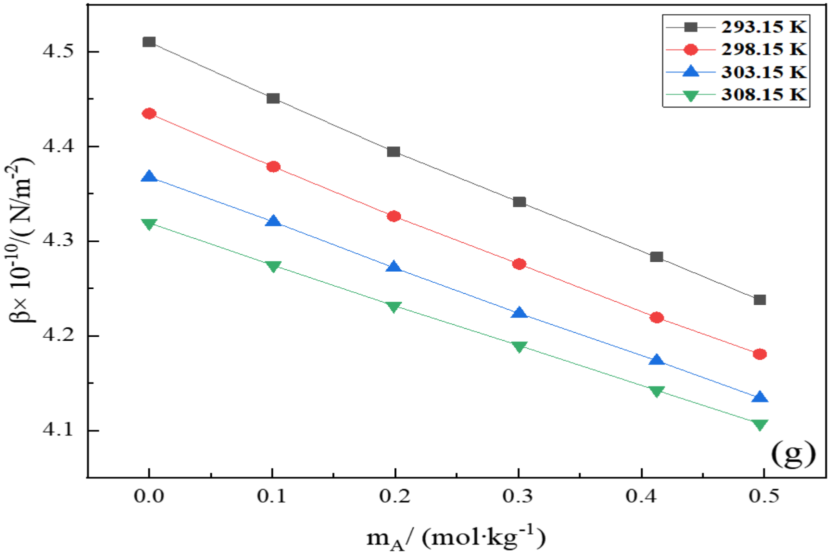
Figure 4.37

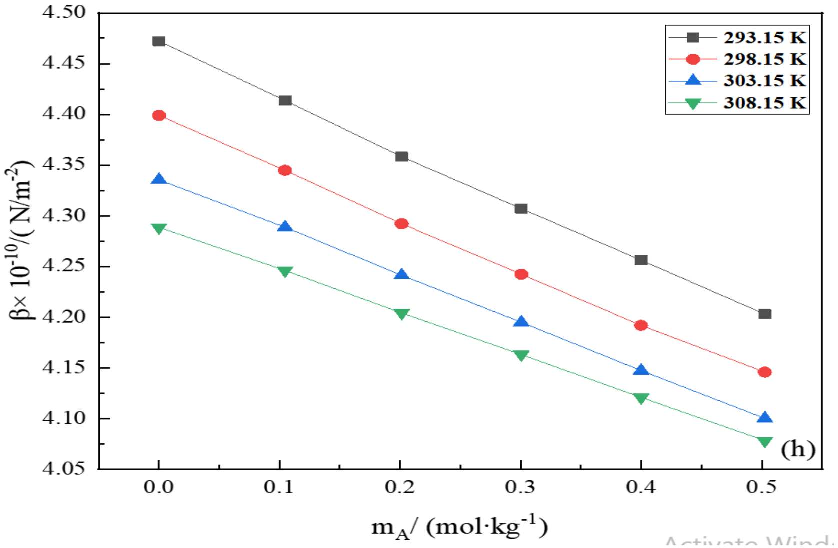


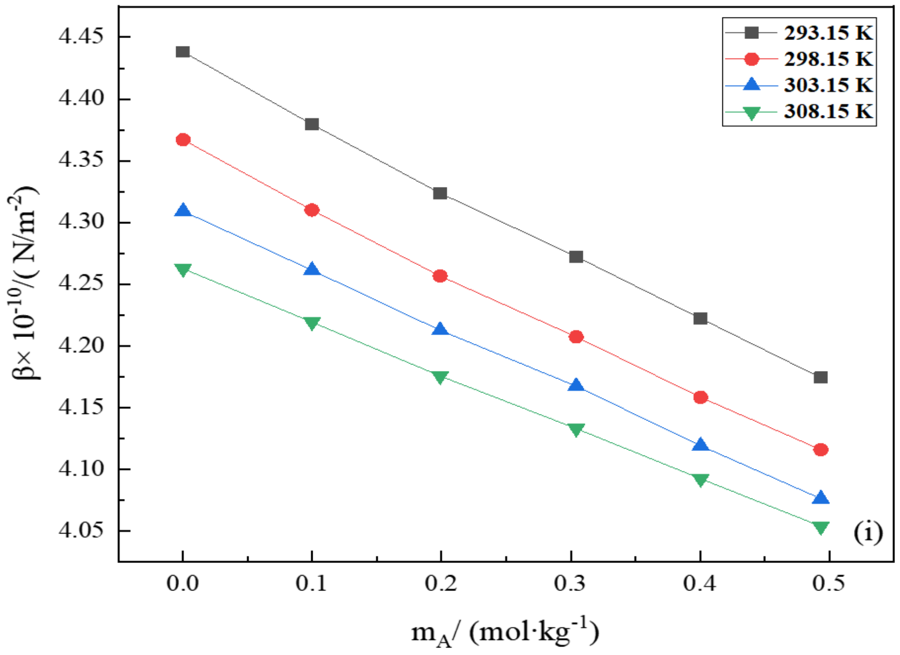
4.55
4.50
4.45
4.40
4.35
4.30
4.25
β× 10^{-10}/(N/m^{-2})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(a)
4.50
4.45
4.40
4.35
4.30
4.25
4.20
β× 10^{-10}/(N/m^{-2})
0.0
0.1
0.2
0.3
0.4
0.5
0.6
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(b)
4.45
4.40
4.35
4.30
4.25
4.20
β× 10^{-10}/(N/m^{-2})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(c)
4.50
4.45
4.40
4.35
4.30
4.25
4.20
4.15
β× 10^{-10}/(N/m^{-2})
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(d)


4.50
4.45
4.40
4.35
4.30
4.25
4.20
4.15
$\beta \times 10^{-10}/(\mathrm{N/m^{-2}})$
0.0
0.1
0.2
0.3
0.4
0.5
$m_A/\ (\mathrm{mol \cdot kg^{-1}})$
293.15 K
298.15 K
303.15 K
308.15 K
(e)


4.45
4.40
4.35
4.30
4.25
4.20
4.15
4.10
$\beta \times 10^{-10}/(\mathrm{N/m^{-2}})$
0.0
0.1
0.2
0.3
0.4
0.5
$m_A/\ (\mathrm{mol \cdot kg^{-1}})$
293.15 K
298.15 K
303.15 K
308.15 K
(f)

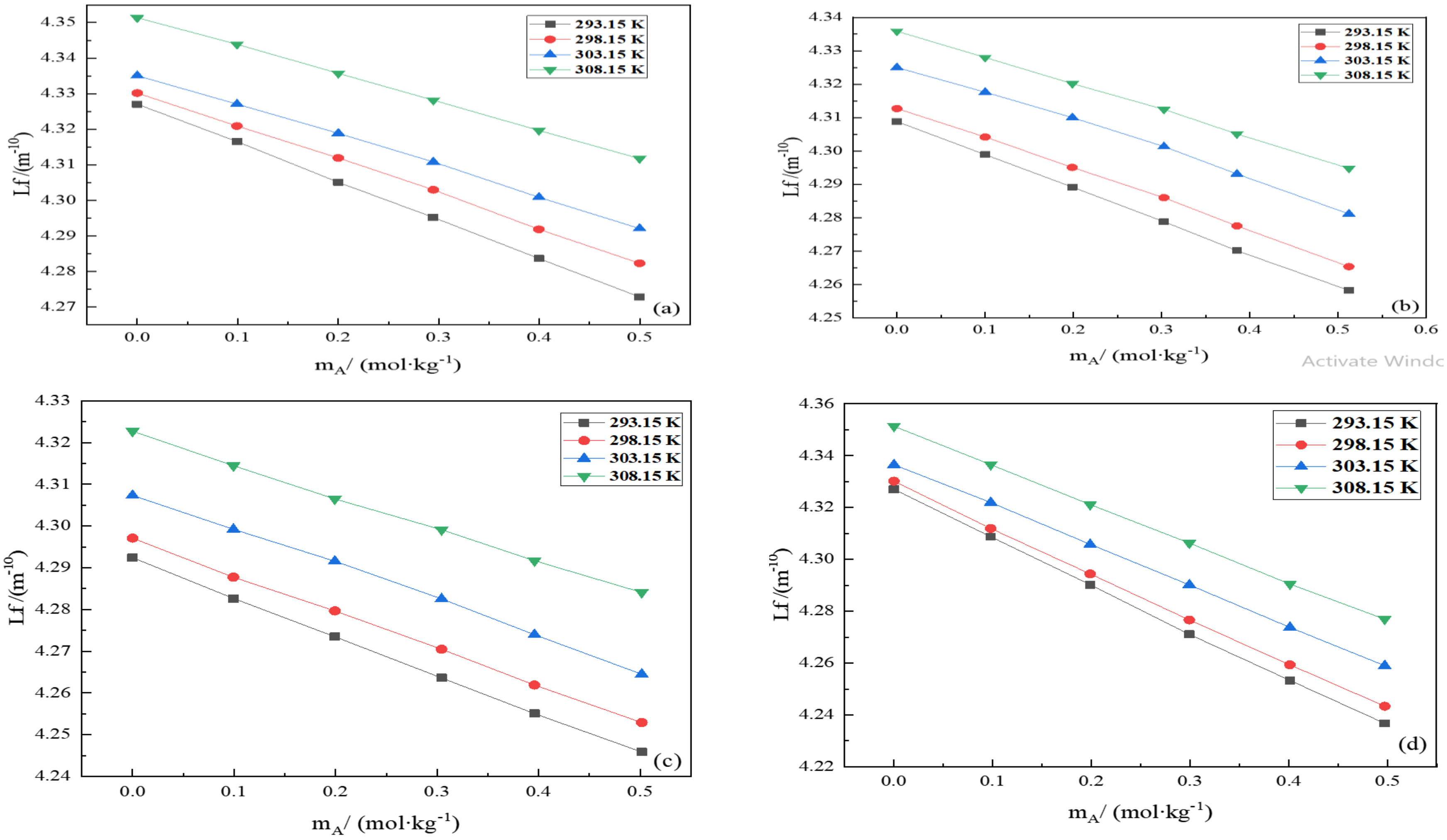

4.5
4.4
4.3
4.2
4.1
$\beta \times 10^{-10}/(\mathrm{N/m^{-2}})$
0.0
0.1
0.2
0.3
0.4
0.5
$m_A/\ (\mathrm{mol \cdot kg^{-1}})$
293.15 K
298.15 K
303.15 K
308.15 K
(g)

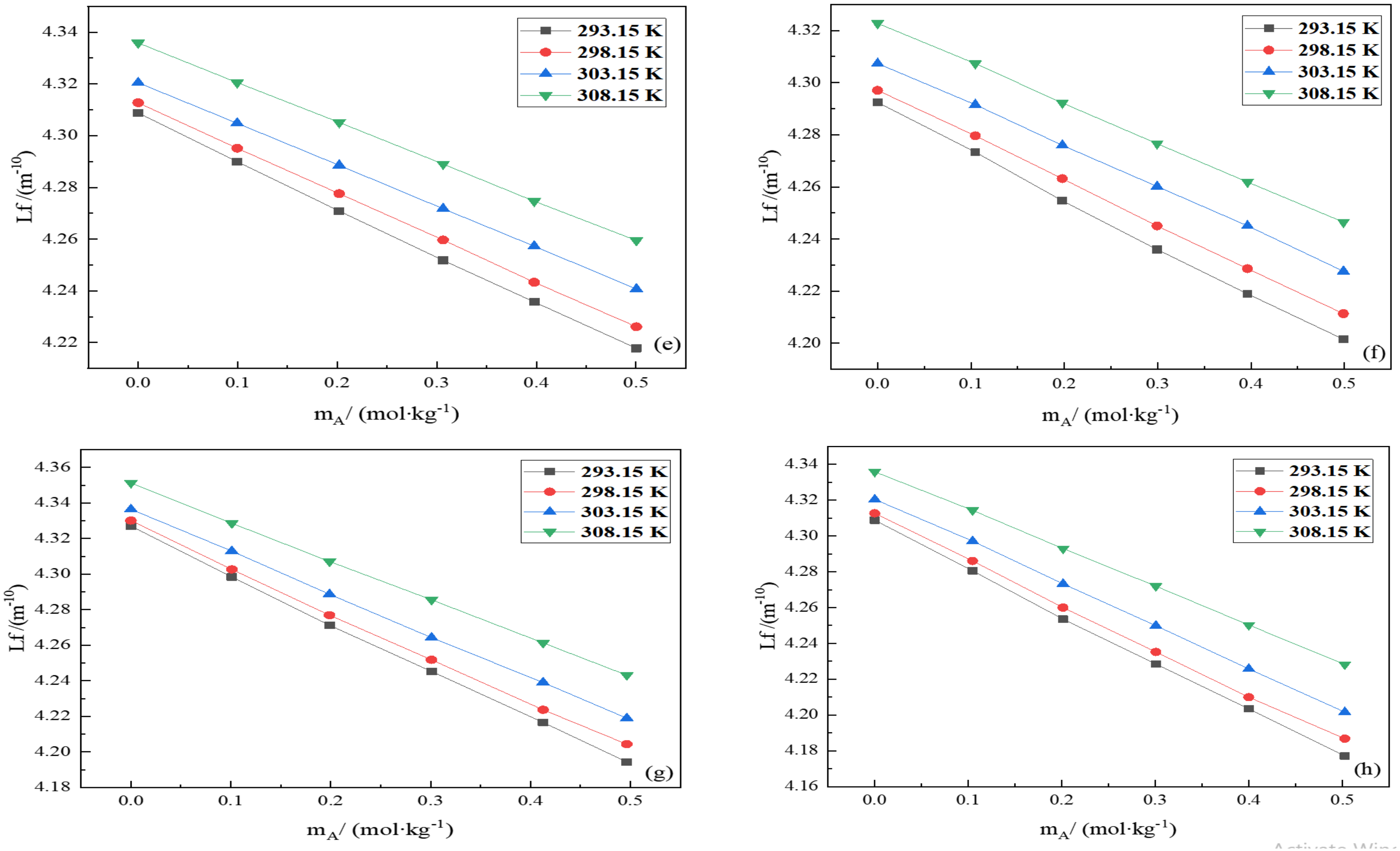

4.50
4.45
4.40
4.35
4.30
4.25
4.20
4.15
4.10
4.05
$\beta \times 10^{-10}/(\mathrm{N/m^{-2}})$
0.0
0.1
0.2
0.3
0.4
0.5
$m_A/\ (\mathrm{mol \cdot kg^{-1}})$
293.15 K
298.15 K
303.15 K
308.15 K
(h)



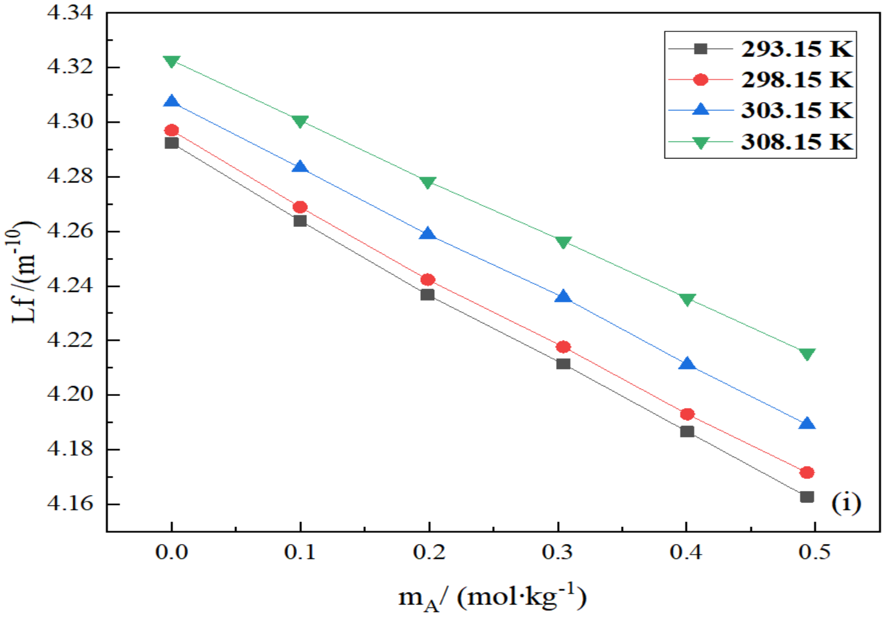
Variation of adiabatic compressibility, β , ethylene glycol **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, diethylene glycol **(d)** 0.05 D-Panthenol, **(e)** 0.10 D-Panthenol and **(f)** 0.15 D-Panthenol and triethylene glycol **(g)** 0.05 D-Panthenol, **(h)** 0.10 D-Panthenol and **(i)** 0.15 D-Panthenol in different concentration of aqueous D-Panthenol solutions at different temperature.

Figure 4.38


Lf /(m^{-10})
m_A/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(a)
4.27
4.28
4.29
4.30
4.31
4.32
4.33
4.34
4.35
0.0
0.1
0.2
0.3
0.4
0.5
(b)
4.25
4.26
4.27
4.28
4.29
4.30
4.31
4.32
4.33
4.34
0.6
(c)
4.24
4.25
4.26
4.27
4.28
4.29
4.30
4.31
4.32
4.33
(d)
4.22
4.24
4.26
4.28
4.30
4.32
4.34
4.36

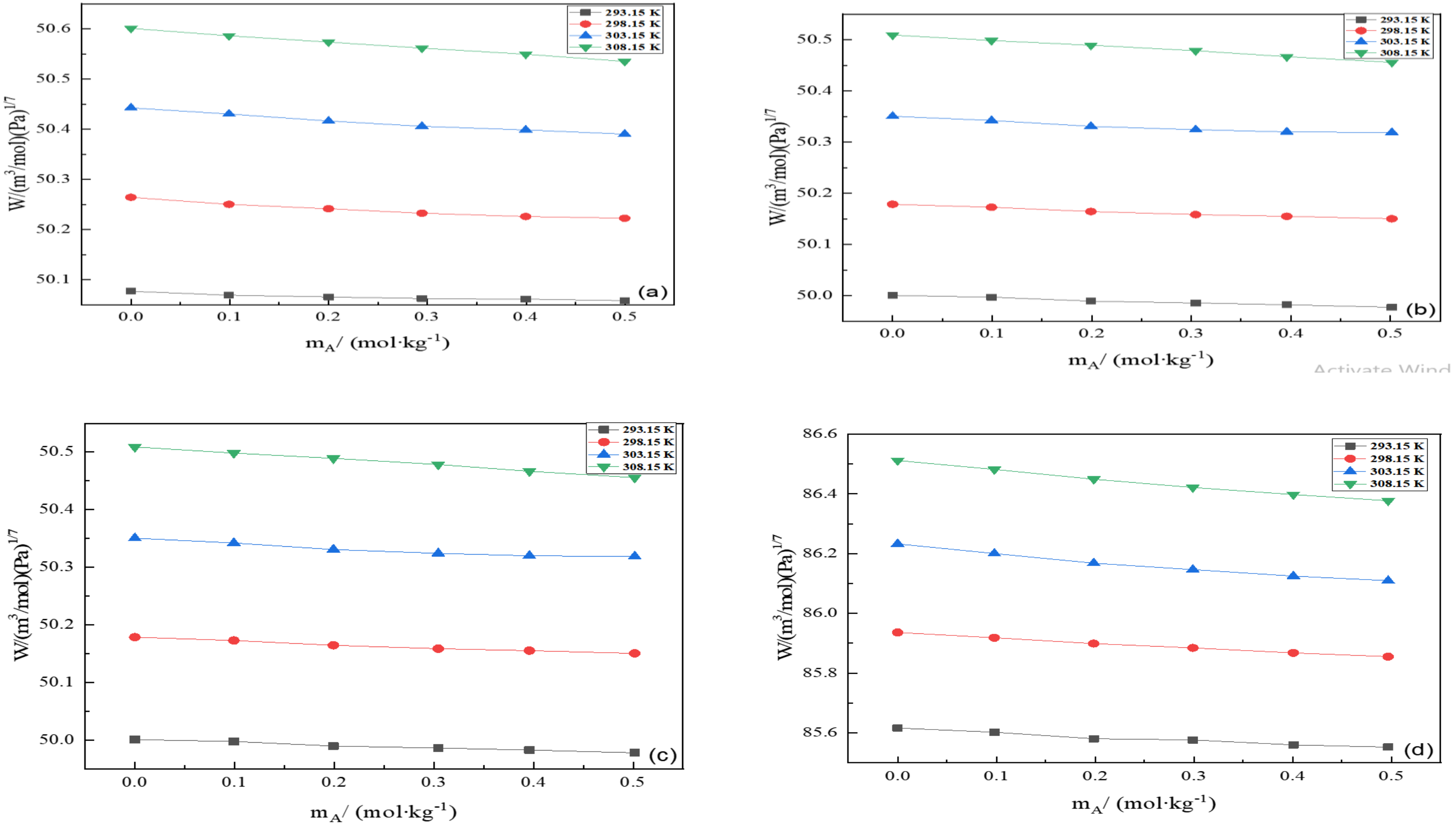


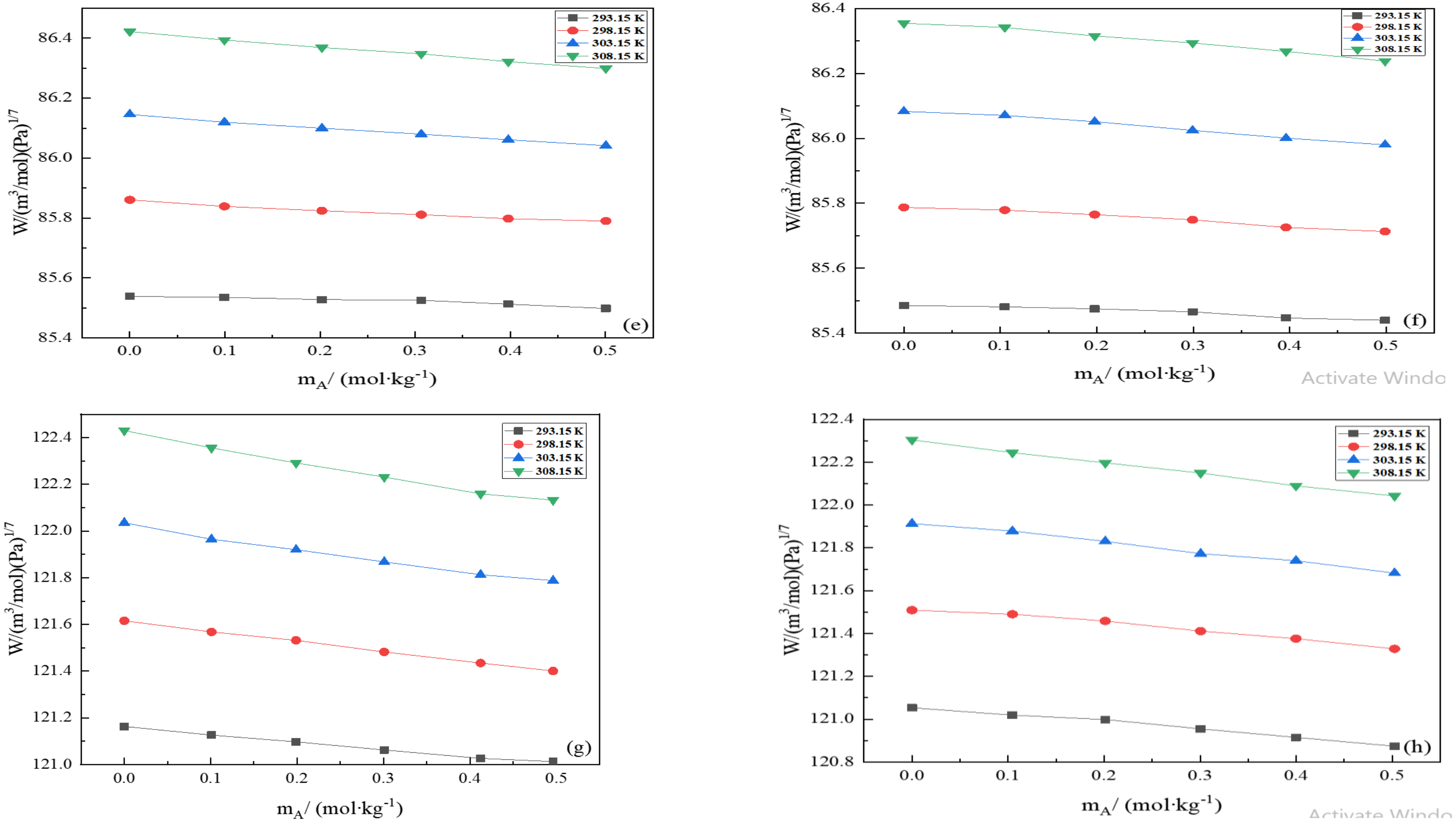
Lf /(m^{-10})
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(e)
4.22
4.24
4.26
4.28
4.30
4.32
4.34
0.0
0.1
0.2
0.3
0.4
0.5
(f)
4.20
4.22
4.24
4.26
4.28
4.30
4.32
(g)
4.18
4.20
4.22
4.24
4.26
4.28
4.30
4.32
4.34
4.36
(h)
4.16
4.18
4.20
4.22
4.24
4.26
4.28
4.30
4.32
4.34

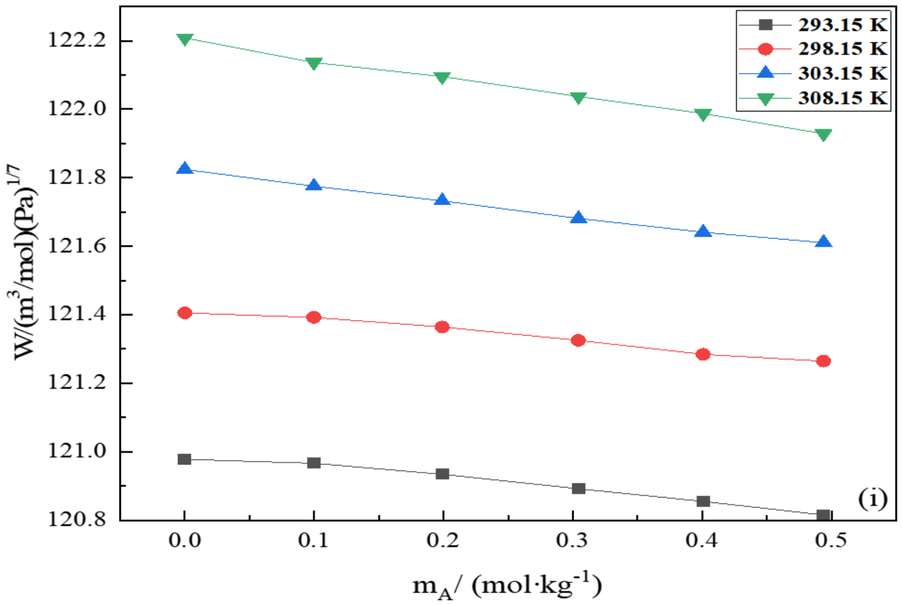


Variation of intermolecular free length, L_f , ethylene glycol **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, diethylene glycol **(d)** 0.05 D-Panthenol, **(e)** 0.10 D-Panthenol and **(f)** 0.15 D-Panthenol and triethylene glycol **(g)** 0.05 D-Panthenol, **(h)** 0.10 D-Panthenol and **(i)** 0.15 D-Panthenol in different concentration of aqueous D-Panthenol solutions at different temperature

Figure 4.39

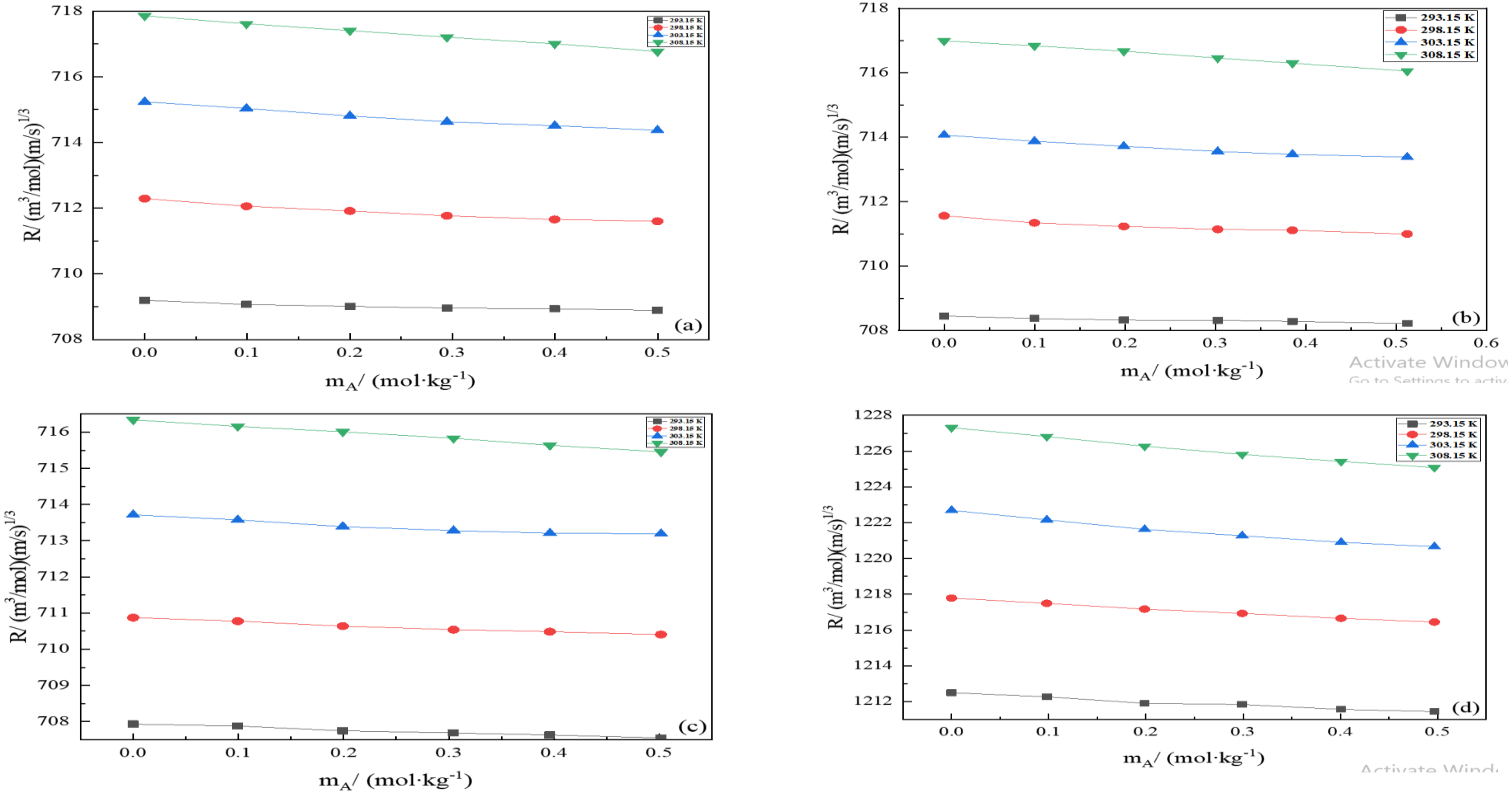

293.15 K
298.15 K
303.15 K
308.15 K
W/(m^3/mol)(Pa)^1/7
50.6
50.5
50.4
50.3
50.2
50.1
0.0
0.1
0.2
0.3
0.4
0.5
m_A/ (mol·kg^-1)
(a)
50.5
50.4
50.3
50.2
50.1
50.0
(b)
(c)
86.6
86.4
86.2
86.0
85.8
85.6
(d)

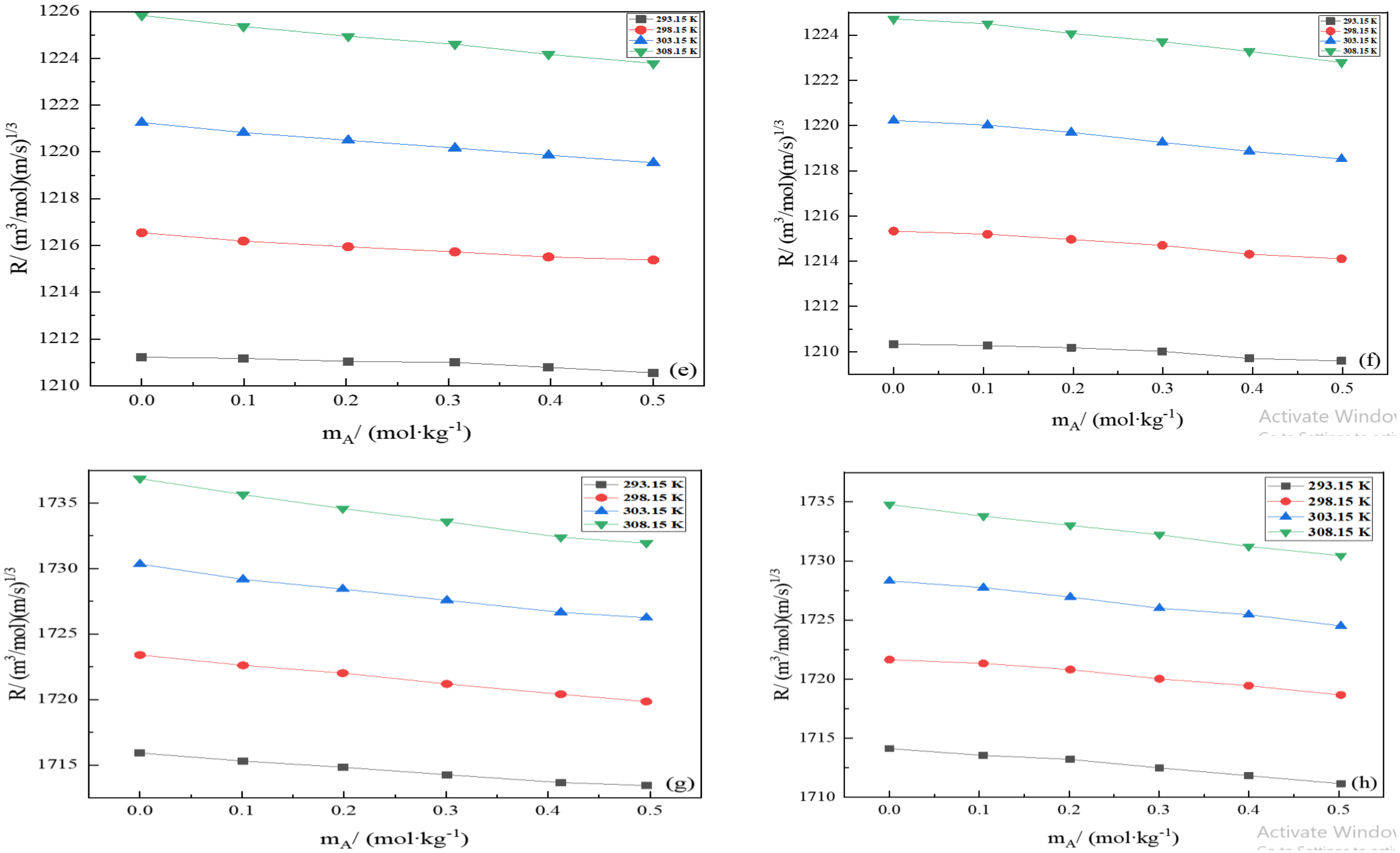

293.15 K
298.15 K
303.15 K
308.15 K
(e)
W/(m^3/mol)(Pa)^1/7
85.4
85.6
85.8
86.0
86.2
86.4
0.0
0.1
0.2
0.3
0.4
0.5
m_A/ (mol·kg^-1)
(f)
W/(m^3/mol)(Pa)^1/7
85.4
85.6
85.8
86.0
86.2
86.4
m_A/ (mol·kg^-1)
(g)
W/(m^3/mol)(Pa)^1/7
121.0
121.2
121.4
121.6
121.8
122.0
122.2
122.4
m_A/ (mol·kg^-1)
(h)
W/(m^3/mol)(Pa)^1/7
120.8
121.0
121.2
121.4
121.6
121.8
122.0
122.2
122.4
m_A/ (mol·kg^-1)

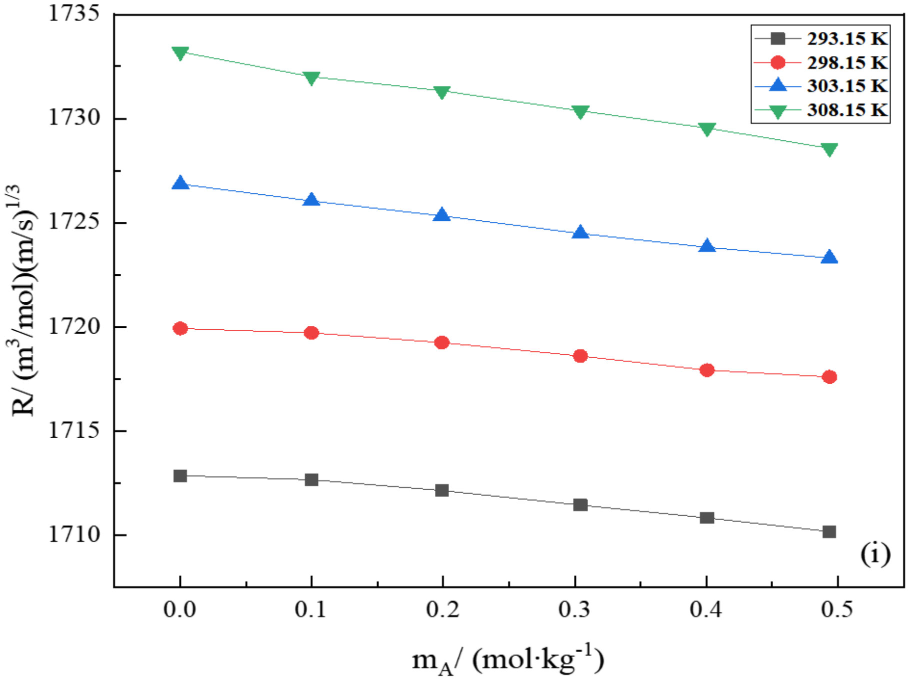


Variation of Wada's constant, W, of, ethylene glycol **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, diethylene glycol **(d)** 0.05 D-Panthenol, **(e)** 0.10 D-Panthenol and **(f)** 0.15 D-Panthenol and triethylene glycol **(g)** 0.05 D-Panthenol, **(h)** 0.10 D-Panthenol and **(i)** 0.15 D-Panthenol in different concentration of aqueous D-Panthenol solutions at different temperature

Figure 4.40

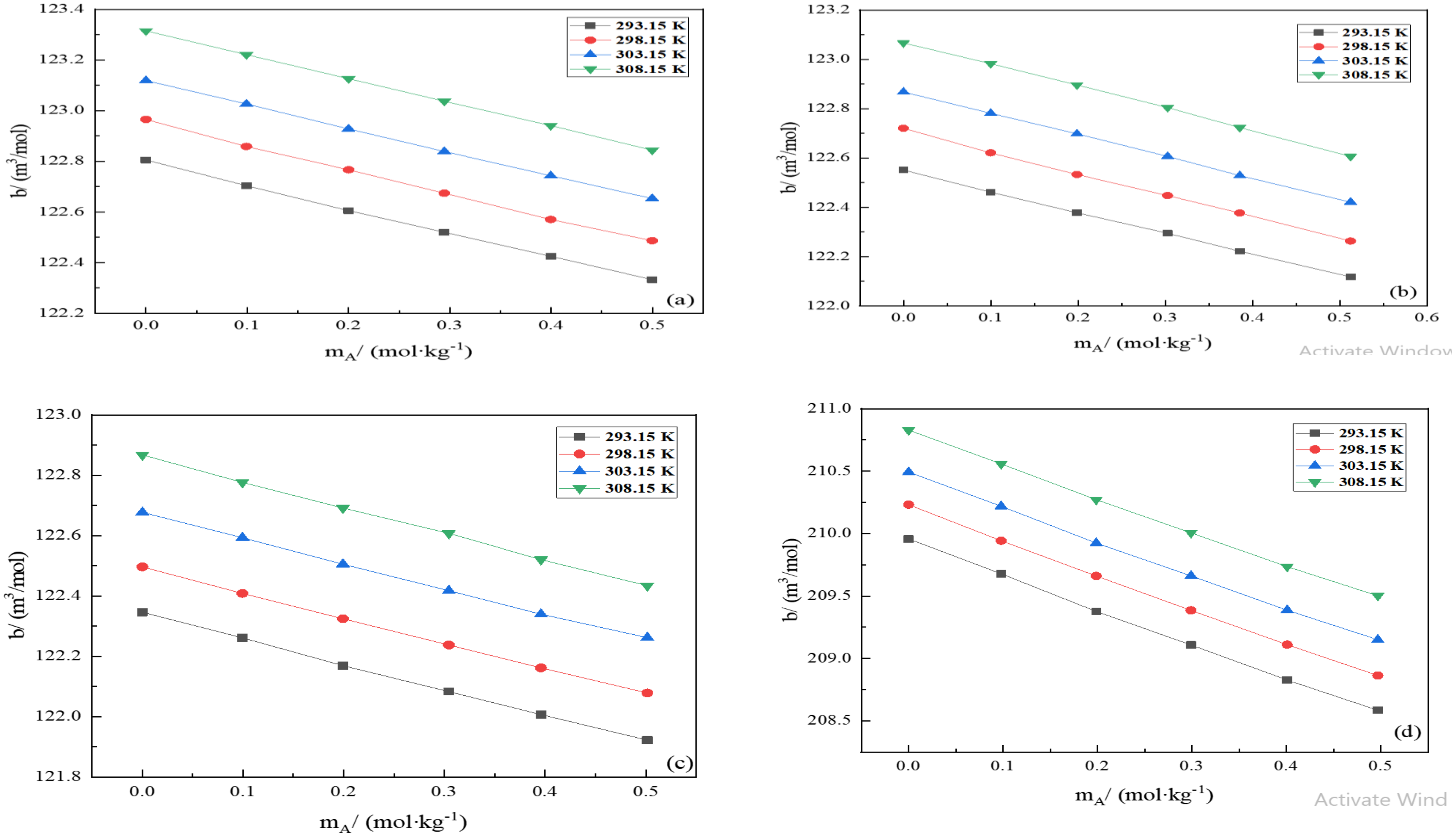

R/ (m^3/mol)(m/s)^1/3
m_A/ (mol·kg^-1)
293.15 K
298.15 K
303.15 K
308.15 K
(a)
708
710
712
714
716
718
(b)
0.0
0.1
0.2
0.3
0.4
0.5
0.6
(c)
709
711
713
715
(d)
1212
1214
1216
1218
1220
1222
1224
1226
1228


1226
1224
1222
1220
1218
1216
1214
1212
1210
R/ (m^3/mol)(m/s)$^{1/3$}
0.0
0.1
0.2
0.3
0.4
0.5
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(e)
1224
1222
1220
1218
1216
1214
1212
1210
R/ (m^3/mol)(m/s)$^{1/3}$
m$_A$/ (mol·kg^{-1})
(f)
1735
1730
1725
1720
1715
R/ (m^3/mol)(m/s)$^{1/3}$
m$_A$/ (mol·kg^{-1})
(g)
1735
1730
1725
1720
1715
1710
R/ (m^3/mol)(m/s)$^{1/3}$
m$_A$/ (mol·kg^{-1})
(h)

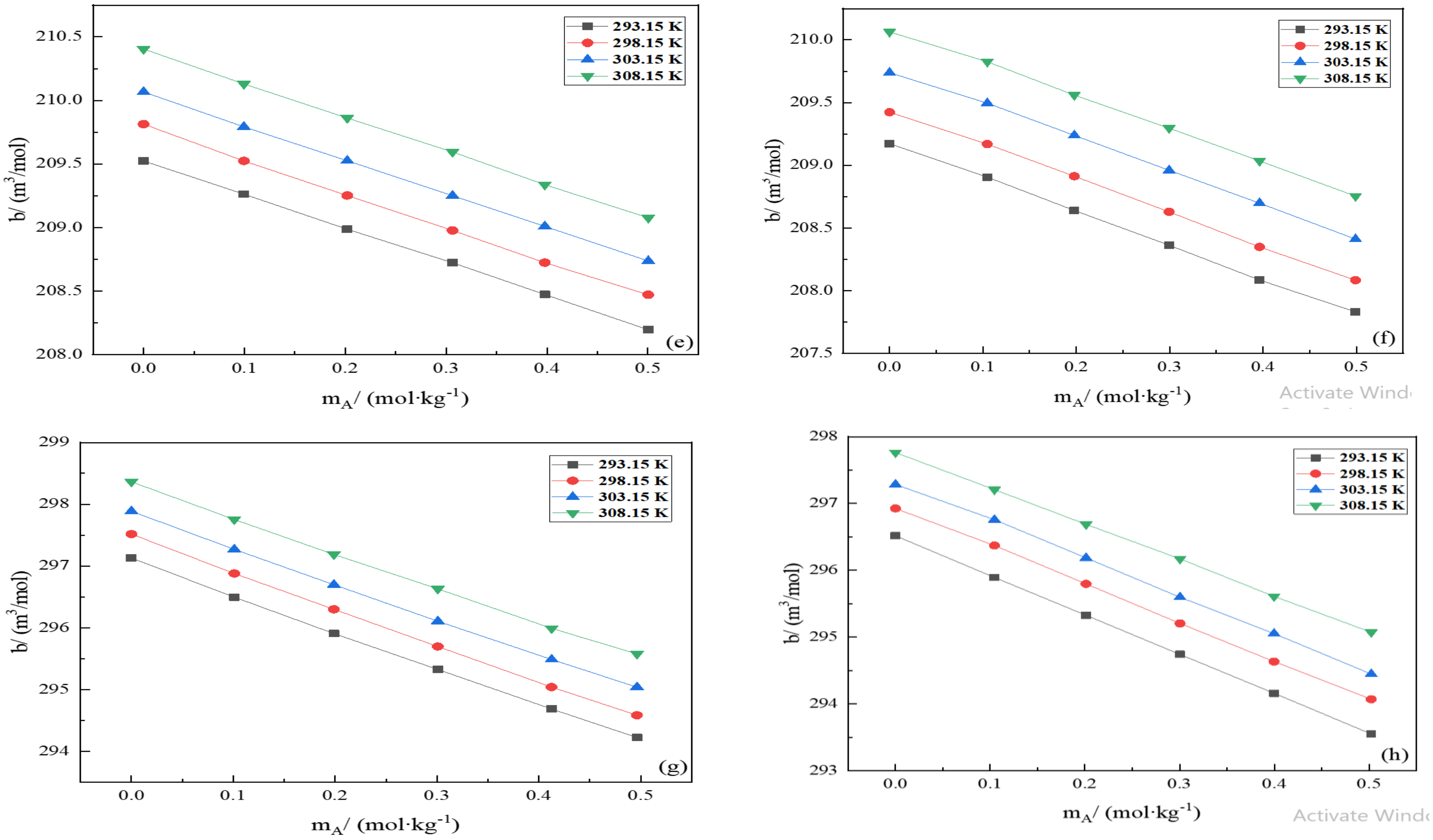


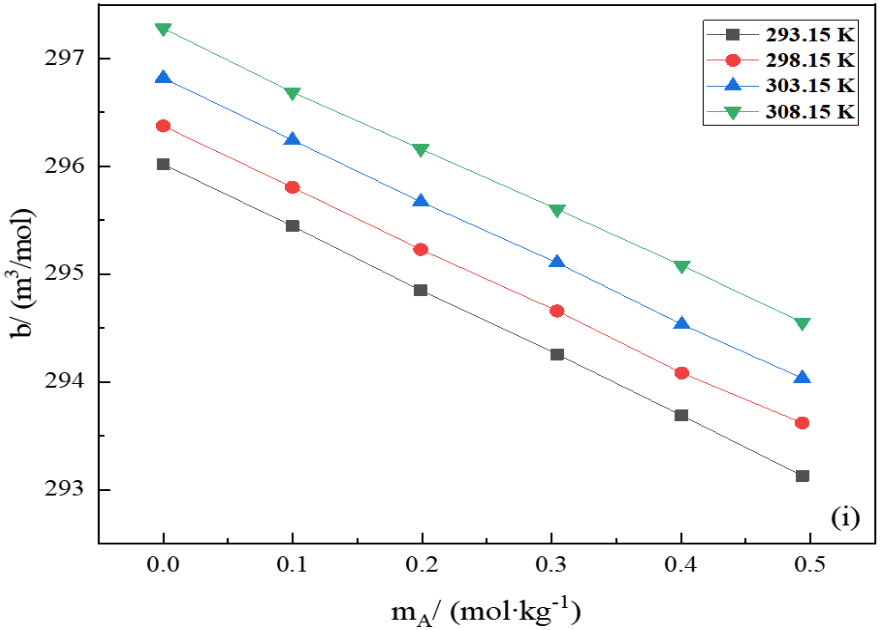
Variation of Rao's constant, R, of, ethylene glycol **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, diethylene glycol **(d)** 0.05 D-Panthenol, **(e)** 0.10 D-Panthenol and **(f)** 0.15 D-Panthenol and triethylene glycol **(g)** 0.05 D-Panthenol, **(h)** 0.10 D-Panthenol and **(i)** 0.15 D-Panthenol in different concentration of aqueous D-Panthenol solutions at different temperature

Figure 4.41



b/ (m^3/mol)
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
(a)
123.4
123.2
123.0
122.8
122.6
122.4
122.2
0.0
0.1
0.2
0.3
0.4
0.5
(b)
123.2
123.0
122.8
122.6
122.4
122.2
122.0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
(c)
123.0
122.8
122.6
122.4
122.2
122.0
121.8
0.0
0.1
0.2
0.3
0.4
0.5
(d)
211.0
210.5
210.0
209.5
209.0
208.5
0.0
0.1
0.2
0.3
0.4
0.5


b/ (m^3/mol)
m$_A$/ (mol·kg^{-1})
293.15 K
298.15 K
303.15 K
308.15 K
210.5
210.0
209.5
209.0
208.5
208.0
0.0
0.1
0.2
0.3
0.4
0.5
(e)
207.5
(f)
299
298
297
296
295
294
293
(g)
(h)



Variation of Vander waal's constant, b, of, ethylene glycol **(a)** 0.05 D-Panthenol, **(b)** 0.10 D-Panthenol and **(c)** 0.15 D-Panthenol, diethylene glycol **(d)** 0.05 D-Panthenol, **(e)** 0.10 D-Panthenol and **(f)** 0.15 D-Panthenol and triethylene glycol **(g)** 0.05 D-Panthenol, **(h)** 0.10 D-Panthenol and **(i)** 0.15 D-Panthenol in different concentration of aqueous D-Panthenol solutions at different temperature

Problem 7

Volumetric and ultrasonic studies of molecular interactions propylene glycol and hexylene glycol in aqueous D-Panthenol solutions at various temperatures

In this section, we have reported the densities, ρ and speed of sound c of propylene glycol (PG) and hexylene glycol (HG) in (0.00, 0.04, 0.08, 0.12) mol·kg^{-1} aqueous solutions of d-Panthenol at temperatures T = (288.15, 298.15, 308.15 and 318.15) K.

4.50 Density

The density values for glycols (PG/HG) in (0.00, 0.04, 0.08 and 0.12) mol·kg^{-1}aqueous d-Panthenol solution at (288.15-318.15) K are presented in **Table 4.52.** The comparison graph of experimental and literature density [28] values for (glycols+ water) is represented in **Figure 4.43,** which are in good agreement with each other i.e. the values are increasing with the glycol molality and decreasing with the experimental temperatures.

4.51 Apparent molar volume

The equation **4.1** is used to calculate the values of apparent molar volume (V_ϕ) using the experimental density data. Here, M, m_A, ρ, and ρ_0 are representing the molar mass of the solute, the molality of the solute per one kilogram of the solvent (d-Panthenol+ water), the densities of the solution and the solvent respectively. The computed V_ϕ values are reported in **Table 4.52** and it can be seen that all the values are positive and are increasing with the temperature as well as with the concentration of d-Panthenol which is graphically represented in **Figure 4.44**. This trend refers to the large intrinsic volume of the solute in the mixture thus establishes the presence of strong solute-solvent interactions. The upsurge of the V_ϕ values with the d-Panthenol concentration implies the association of OH- molecules insolvent with the water molecules in its first hydration shell. This is the reason for the constructive interaction of the d-Panthenol molecules with water which leads to the strong hydrogen bond in the solvent [29, 30]. The existence of hydrophobic hydration in the water-rich region, hydrophilic effect, dipole-induced-dipole, and dipole-dipole interactions are confirmed due to increase in V_ϕ values with the increment in the molar mass of the glycols from propylene glycol to hexylene glycol which is represented in **Figure 4.42** to show the upsurge of the extent of the intermolecular interaction in the liquid mixture [31].

4.52 Partial Molar volume

The equation **4.2** is used to obtain the partial molar volume of the liquid mixtures containing d-Panthenol and glycol. Here m_A is the molality of the solute. The partial molar volume (V_ϕ^0) and their experimental slope (S_V^*) is calculated from the least square fitting method, are reported in **Table 4.53** along with their standard errors. The obtained V_ϕ^0 and S_V^* values are all positive which establishes the existence of ion-hydrophilic interactions dominating the hydrophilic- hydrophilic interactions with the strong solute-solvent interactions inside the mixture. The variation of V_ϕ^0 values against the temperatures and solvent concentrations are graphically represented in **Figure 4.45** from which its increment with the upsurge in temperatures and d-Panthenol concentration is observed. This suggests the superposition of hydration co-sphere of two ionic species on each other leading to the increase in the volume but decreases upon the overlapping of hydrophobic groups over hydrophobic-hydrophobic groups as given by the co-sphere overlap model [32, 33]. The strength of the hydrogen bond in the solvent increases with the concentration of d-Panthenol due to constructive interaction between the water and d-Panthenol molecules [30]. The S_V^* values in the table show the presence of solute-solute interactions among the molecules of glycols and d-Panthenol which are influenced by some other factors as implied by the irregular pattern of S_V^* values [5].

4.53 Partial molar volume of transfer

Transfer of standard molar volume of glycols from water to d-Panthenol aqueous solutions at infinite dilution is computed employing the equation **4.3**. The positive ΔV_ϕ^0 values are observed in the mixture of glycols in aqueous d-Panthenol solution which are indexed in **Table 4.54**. From the table, it can be seen that the ΔV_ϕ^0 values are positive and are increasing with the d-Panthenol concentrations while an irregular trend is noticed concerning the temperatures. The theory of pure water's structure, as defined by Pauling [34, 35] states the availability of empty spaces inside the water structure which are known as clathrates, is easily penetrable by other molecules. That is why presumably a very little amount of glycols can be installed inside the water cage structure to demolish the network structure of water. There is a probability of new structure creation when a hydrogen bond is formed between the water and organic molecules due to the destruction of the cage structure by more glycol contents [36, 37]. The interactions among the solute and solvent molecules enhance the structure-making capability of solute in the solution due to the structural moiety of d-Panthenol and glycols consists of the polar group [38].

4.54 Temperature-dependent partial molar volume

Utilizing the equation **4.4**, the variation in the apparent molar volume at infinite dilution with temperatures is determined. Here, $a, b, c,$ are empirical constants listed in **Table 4.55**, T_{ref}=298.15 K, and the temperature in Kelvin is represented as T. The deviations in the calculated and experimental V_{ϕ}^{0} values are also mentioned in the same table and these deviations are evaluated using the equation **4.14**. Here, $\mathrm{Y} = V_{\phi}^{0}$ (apparent molar volume at infinite dilution). In the current study, the deviation values are very small which perfectly fits into the polynomial equation that is manifested from R^2values [39]. The positive c values in the table suggest the scatter in the V_{ϕ}^{0} values. The main objective to study the V_{ϕ}^{0} values was to attain the partial molar expansibilities using the equation **4.5.** The partial molar expansibility at infinite dilution is given by E_{ϕ}^{0}=$\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$. This parameter is considered as an essential measure of the interactions for solute and solvents inside the mixture. The structure making and breaking capability of the solute in the solution is determined using the following general thermodynamic equation **4.6**. Depending upon the sign of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ the structure making and breaking capability is estimated. The less negative and positive values of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ refers to the structure making ability while the negative values imply the structure breaking ability of solute in the mixture. In **Table 4.56** the E_{Φ}^{0} and $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ are ascribed and it can be observed that these values are all positive and in an irregular pattern over the entire range of d-Panthenol concentrations and experimental temperatures, thus implying the presence of structure making ability of glycols in aqueous d-Panthenol solution [40].

4.55 Ultrasonic speed

The speed of sound values has been experimentally obtained at (288.15, 298.15, 308.15, and 318.15) K for (d-Panthenol + distilled water+ glycols) at (0.00, 0.07, 0.08 and 0.09) mol·kg^{-1} concentrations and are reported in **Table 4.57**. The experimental speed of sound values for (glycols+ water) are compared with the literature values [28] for temperature 298.15 K and 308.15 K and are graphically represented in **Figure 4.46,** and it is observed that the speed of sound values are increasing along with the temperatures, thus showing the same trend as the literature values. This is due to the 3D networks of hydrogen bonds in water structure and the upsurge in the speed of sound values for the glycol and vitamin mixture is due to the intermolecular and intramolecular hydrogen bonding in solute-solvent molecules. The increment in the values of speed of sound with the molality of glycols refers to the hydrogen bond network insolvent with the aqueous d-Panthenol molecule. Also, with the rise in the molar mass of the glycol, the hydrogen bond among the water and d-Panthenol molecules degrades and eventually gets abolished but simultaneously fresh H-bonds are produced between molecules of d-Panthenol and glycol [18, 41].

4.56 Apparent molar isentropic compression

The Apparent molar isentropic compression for glycols in aqueous d-Panthenol solution is obtained using the equation **4.7.** Here, the densities of the solvent, densities of the solution, molar mass of solute, the molality of solute, and isentropic compressibility of the pure solvent and the solution are represented as ρ, ρ_0, M, m_A, $k_{s.0}$ and k_s respectively. Equation **4.8** is used to calculate the isentropic compressibility. Here, ρ represents the density of the solution. The values of speed of sound (c) and apparent molar isentropic compression ($k_{\phi,s}$) are listed in **Table 4.57.** The variation of $k_{\phi,s}$ values against the glycol molalities are presented in **Figure 4.47**, from which it is noticed that the values are negative and shows a symmetric behavior i.e. with the upsurge in the temperatures, the $k_{\phi,s}$ values become less negative but with the molality of glycols the negativity increases. This results in more alignment of the solvent due to solute as large loss of structure compressibility of water is observed since the $k_{\phi,s}$ values are negative. In the bulk solution, the water molecules are arranged in a particular order while they are less compressible in the region of charged groups due to negative $k_{\phi,s}$ values [42, 43].

4.57 Partial molar isentropic compression

With equation **4.9**, the partial molar isentropic compression is computed by contemplating the divergence of apparent molar isentropic compression along with the molality. Using the values of apparent molar isentropic compression($k_{\phi,s}$), the partial molar isentropic compression ($K^0_{\phi,S}$) and their experimental slope (S^*_k) are evaluated by the least square fitting method. The calculated parameters along with their standard errors are mentioned in **Table 4.58** and in **Figure 4.48** the $K^0_{\phi,S}$ values are graphically represented. The negative $K^0_{\phi,S}$ values are varying in regular order with temperatures and glycol molality. The attractive interactions among the d-Panthenol and glycols molecules occur due to decrement of negativity in $K^0_{\phi,S}$ values with temperature, and glycol molality. This behavior tends the water molecules to be less compressible around glycol molecules. Further, the negative S^*_k values suggest the existence of weak solute-solute interactions in the liquid system [44, 45].

4.58 Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer for glycol from water to aqueous d-Panthenol solutions at infinite dilution is determined using the equation **4.10**. In **Table 4.59** the calculated $\Delta K^0_{\phi,s}$ values are ascribed which are all positive and are increasing with the concentration of d-Panthenol. This characteristic indicates the upsurge of structure making ability of solute with the d-Panthenol concentration and the domination of zwitterionic center of glycols in d-Panthenol solutions [46].

4.59 Pair and triplet coefficients

The partial molar volume of transfer and the partial molar isentropic compression of transfer is obtained from the equation **4.11** and **4.12.** Where m_B denotes the molality of the aqueous d-Panthenol solutions, A represents glycols and B represents d-Panthenol. The pair and triplet interaction coefficients are represented by the parameters $V_{AB,}$ V_{ABB}; $K_{AB\,,}$ K_{ABB} for volume and isentropic compression respectively which are reported in **Table 4.60** for all the temperatures**.** For PG the triplet coefficient K_{ABB} is negative and for HG the pair coefficient V_{AB} and triplet coefficient K_{ABB} is negative at all temperatures. The rest of the coefficients i.e. K_{AB} and V_{ABB} are positive for both the glycols and V_{AB} is positive only for PG [47]. As per the theory given by McMillan [21], which was later conferred by Friedman and Krishnan [22] states the interaction of solute leads to splitting effects. By the overlapping of spheres from hydration co-spheres, the water molecules are released to the bulk resulting in non-bonding interactions [48].

4.60 Hydration number

Passynsky [49] developed an equation **4.13** to calculate the hydration number for the liquid mixtures. Here, n_1 is the number moles of solvent, n_2 is the number moles of solute, k_s is the isentropic compressibility of solution, and k_s^0 is the isentropic compressibility of solvent. It is considered that ions contain two hydration spheres: primary hydration spheres and secondary hydration spheres. The primary hydration sphere consist water molecules which strongly combine with the ion through an electrostatic ion-dipole attraction. The secondary hydration sphere is made up of water molecules which interacts partially with primary hydration sphere ion and partially with the water structure in the surroundings which merge into the bulk after extending an undefined length from the ion. The calculated hydration numbers using various techniques can be classified into two groups where low values indicate the primary hydration number and larger values implies the primary hydration along with overall or fractional part of secondary hydration sphere. These hydration numbers are further used to determine the solvation property of ions with some other properties of solvent in the mixture [50, 51]. The calculated hydration numbers at various concentrations and temperatures are mentioned in **Table 4.61.** These values are large ranging from

111 to 555.12 and thus indicating the presence of hydrophobic hydration and electrostatic hydration due to co-operative hydrogen bonding in aqueous d-Panthenol solutions. The decrement of the hydration numbers with the corresponding concentration shows the ion-association and implies that the calculated hydration numbers from the compressibility data is due to both electrostriction and secondary hydration shell which contributes hydrophobic hydration. Also, the high hydration numbers are attributed due to presence of co-operative hydrogen bonding and decrease in the solvating molecules due to replacement of water molecules by glycol molecules in the coordination sphere of ions inside the mixture [24, 52].

Table 4.52

Values of densities, ρ, apparent molar volumes, V_ϕ of glycols in aqueous solutions of d-Panthenol at different temperatures

$^a m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^6$/(m^3·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				0.00 mol·kg^{-1} d-Panthenol + PG				
0.00000	0.99926	0.99705	0.99404	0.99036				
0.10028	0.99953	0.99732	0.99433	0.99066	73.44	73.52	73.60	73.67
0.20000	0.99978	0.99758	0.99460	0.99096	73.50	73.58	73.66	73.73
0.30017	1.00001	0.99783	0.99486	0.99123	73.57	73.64	73.71	73.78
0.40905	1.00026	0.99808	0.99513	0.99152	73.63	73.70	73.77	73.84
0.50000	1.00045	0.99828	0.99534	0.99175	73.67	73.75	73.82	73.89
				0.04 mol·kg^{-1} d-Panthenol + PG				
0.00000	1.00083	0.99875	0.99571	0.99187				
0.10093	1.00108	0.99901	0.99599	0.99216	73.49	73.56	73.64	73.71
0.20010	1.00132	0.99926	0.99625	0.99244	73.55	73.62	73.70	73.77
0.30272	1.00155	0.99949	0.99650	0.99270	73.60	73.68	73.76	73.83
0.40065	1.00175	0.99970	0.99672	0.99295	73.66	73.74	73.81	73.89
0.50007	1.00195	0.99990	0.99693	0.99317	73.71	73.79	73.88	73.96
				0.08 mol·kg^{-1} d-Panthenol + PG				

0.00000	1.00233	1.00022	0.99715	0.99328				
0.10102	1.00257	1.00046	0.99741	0.99356	73.56	73.63	73.70	73.77
0.20006	1.00279	1.00069	0.99765	0.99382	73.62	73.69	73.77	73.84
0.30012	1.00299	1.00090	0.99787	0.99406	73.68	73.76	73.83	73.91
0.40001	1.00318	1.00110	0.99808	0.99429	73.74	73.82	73.89	73.97
0.49990	1.00336	1.00128	0.99828	0.99451	73.80	73.88	73.96	74.03
0.12 mol·kg^{-1} d-Panthenol + PG								
0.00000	1.00362	1.00147	0.99838	0.99448				
0.09993	1.00383	1.00170	0.99862	0.99475	73.65	73.71	73.78	73.84
0.20010	1.00404	1.00191	0.99885	0.99499	73.70	73.77	73.83	73.90
0.29998	1.00423	1.00211	0.99906	0.99523	73.74	73.82	73.89	73.95
0.39900	1.00441	1.00229	0.99925	0.99544	73.80	73.87	73.95	74.01
0.50015	1.00457	1.00246	0.99944	0.99565	73.85	73.93	74.00	74.07
0.00 mol·kg^{-1} d-Panthenol + HG								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.09976	0.99944	0.99725	0.99428	0.99063	116.37	116.41	116.45	116.49
0.20012	0.99962	0.99745	0.99450	0.99090	116.40	116.43	116.47	116.51
0.30214	0.99979	0.99765	0.99473	0.99115	116.42	116.46	116.50	116.54
0.39996	0.99995	0.99782	0.99493	0.99139	116.44	116.48	116.52	116.56
0.50067	1.00010	0.99800	0.99513	0.99163	116.46	116.50	116.55	116.59

0.04 mol·kg^{-1} d-Panthenol + HG								
0.00000	1.00083	0.99875	0.99571	0.99187				
0.09964	1.00099	0.99894	0.99593	0.99212	116.37	116.41	116.45	116.49
0.20120	1.00115	0.99911	0.99614	0.99237	116.40	116.43	116.47	116.51
0.30061	1.00130	0.99928	0.99633	0.99260	116.42	116.46	116.50	116.54
0.40004	1.00144	0.99944	0.99652	0.99282	116.44	116.48	116.52	116.56
0.49782	1.00157	0.99958	0.99669	0.99303	116.46	116.50	116.55	116.59
0.08 mol·kg^{-1} d-Panthenol + HG								
0.00000	1.00233	1.00022	0.99715	0.99328				
0.09997	1.00248	1.00039	0.99735	0.99352	116.40	116.44	116.47	116.51
0.19988	1.00262	1.00055	0.99754	0.99375	116.42	116.46	116.50	116.53
0.30011	1.00276	1.00070	0.99772	0.99397	116.45	116.48	116.52	116.56
0.40025	1.00288	1.00085	0.99790	0.99418	116.47	116.50	116.54	116.58
0.50101	1.00300	1.00098	0.99806	0.99438	116.49	116.53	116.57	116.61
0.12 mol·kg^{-1} d-Panthenol + HG								
0.00000	1.00362	1.00147	0.99838	0.99448				
0.10014	1.00375	1.00162	0.99856	0.99471	116.43	116.47	116.50	116.53
0.20220	1.00388	1.00177	0.99874	0.99493	116.45	116.49	116.52	116.55
0.30005	1.00399	1.00190	0.99890	0.99513	116.47	116.51	116.54	116.58
0.40000	1.00410	1.00203	0.99906	0.99533	116.49	116.53	116.57	116.60

0.49899	1.00420	1.00216	0.99921	0.99551	116.51	116.55	116.59	116.62

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1} and $u(V_\phi)$ =±(0.05-0.07) × 10^6/ (m^3·mol^{-1}).

Table 4.53

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_{V}^{*}, of glycols in the aqueous solution of d-Panthenol at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})				$S_{V}^{*} \times 10^{6}$/(m^{3}·kg·mol^{-2})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
				PG				
0.00	73.39(±0.004)	73.46(±0.002)	73.55(±0.001)	73.62(±0.002)	0.59(±0.014)	0.58(±0.007)	0.55(±0.004)	0.55(±0.007)
0.04	73.44(±0.001)	73.51(±0.002)	73.58(±0.003)	73.65(±0.002)	0.55(±0.003)	0.58(±0.007)	0.59(±0.010)	0.60(±0.006)
0.08	73.50(±0.001)	73.57(±0.003)	73.64(±0.002)	73.71(±0.002)	0.60(±0.004)	0.62(±0.009)	0.65(±0.007)	0.64(±0.006)
0.12	73.59(±0.001)	73.66(±0.002)	73.72(±0.002)	73.78(±0.002)	0.50(±0.005)	0.54(±0.007)	0.56(±0.006)	0.58(±0.006)
				HG				
0.00	116.35(±0.000)	116.39(±0.000)	116.42(±0.001)	116.46(±0.001)	0.23(±0.001)	0.23(±0.001)	0.24(±0.004)	0.24(±0.003)
0.04	116.35(±0.000)	116.39(±0.000)	116.43(±0.001)	116.46(±0.001)	0.23(±0.001)	0.23(±0.001)	0.24(±0.004)	0.24(±0.004)
0.08	116.38(±0.001)	116.41(±0.001)	116.45(±0.000)	116.48(±0.000)	0.23(±0.004)	0.24(±0.003)	0.24(±0.002)	0.25(±0.002)
0.12	116.41(±0.000)	116.44(±0.000)	116.48(±0.000)	116.51(±0.000)	0.21(±0.001)	0.22(±0.001)	0.22(±0.002)	0.22(±0.001)

$^{a}m_{B}$ is the molality of aqueous D-Panthenol, standard uncertainties *u* are *u(m)* $= 2 \times 10^{-5}$ mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}, *u*(V_{ϕ}^{0}) =±0.01 × 10^{6}/ (m^{3}·mol^{-1}) and *u*(S_{V}^{*}) =±0.03 × 10^{6}/ (m^{3}·mol^{-2}).

Table 4.54

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in the aqueous solution of d-Panthenol at different temperatures.

[a]m_B/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^6$/(m^3·mol^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
		PG		
0.04	0.05	0.04	0.03	0.03
0.08	0.11	0.11	0.09	0.09
0.12	0.21	0.19	0.18	0.16
		HG		
0.04	0.00	0.00	0.00	0.00
0.08	0.02	0.02	0.02	0.02
0.12	0.06	0.06	0.05	0.05

[a]m_B is the molality of aqueous D-Panthenol, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa and *u(c)*= 0.6 m·s^{-1}.

Table 4.55

Values of empirical parameters of Eq., of glycols in the aqueous solution of d-Panthenol at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
			PG		
0.04	73.506	0.007	0.000	0.9999	0.0007
0.08	73.569	0.007	0.000	0.9999	0.0000
0.12	73.659	0.006	0.000	0.9999	0.0004
			HG		
0.04	116.387	0.004	0.000	0.9999	0.0000
0.08	116.412	0.004	0.000	0.9999	0.0000
0.12	116.444	0.003	0.000	0.9999	0.0001

${}^{a}m_B$ is the molality aqueous of D-Panthenol, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}.

Table 4.56

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in the aqueous solution of d-Panthenol at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	$E_{\phi}^{0}\times10^{6}$/(m^3· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^3·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			PG		
0.04	0.0068	0.0071	0.0073	0.0075	0.0000
0.08	0.0070	0.0070	0.0070	0.0070	0.0000
0.12	0.0066	0.0064	0.0062	0.0060	0.0000
			HG		
0.04	0.0036	0.0037	0.0038	0.0039	0.0000
0.08	0.0037	0.0036	0.0036	0.0035	0.0000
0.12	0.0036	0.0034	0.0033	0.0031	0.0000

${}^{a}m_B$ is the molality aqueous of D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}.

Table 4.57

Values of the speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,s}$ of glycols in aqueous solutions of d-Panthenol at different temperatures

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^6$/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.00 mol·kg^{-1} d-Panthenol + PG								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.10028	1471.03	1500.79	1523.09	1539.09	-46.04	-44.26	-42.91	-41.97
0.20000	1475.50	1504.61	1526.29	1542.06	-46.29	-44.49	-43.14	-42.20
0.30017	1479.61	1508.02	1529.50	1545.03	-46.38	-44.58	-43.22	-42.28
0.40905	1483.28	1511.16	1532.52	1548.34	-46.43	-44.63	-43.27	-42.33
0.50000	1486.61	1513.99	1535.04	1550.83	-46.46	-44.66	-43.30	-42.36
0.04 mol·kg^{-1} d-Panthenol + PG								
0.00000	1471.19	1501.03	1523.15	1539.51				
0.11093	1475.95	1505.62	1526.84	1542.70	-45.76	-43.96	-42.69	-41.78
0.20010	1480.19	1509.40	1530.24	1545.65	-46.00	-44.19	-42.91	-42.00
0.31229	1484.15	1512.75	1533.50	1548.81	-46.09	-44.27	-43.00	-42.09
0.41165	1487.85	1515.85	1536.08	1551.61	-46.13	-44.32	-43.04	-42.13
0.51261	1491.33	1518.94	1539.05	1554.60	-46.16	-44.35	-43.07	-42.16

0.08 mol·kg^{-1} d-Panthenol + PG								
0.00000	1476.13	1504.84	1526.84	1542.51				
0.10102	1481.19	1509.61	1530.58	1545.67	-45.46	-43.74	-42.48	-41.62
0.20006	1485.53	1513.51	1533.83	1548.73	-45.69	-43.96	-42.70	-41.84
0.30012	1489.63	1516.95	1536.97	1551.74	-45.77	-44.04	-42.79	-41.92
0.40001	1493.26	1520.03	1539.91	1554.87	-45.82	-44.09	-42.83	-41.97
0.49990	1496.47	1523.07	1542.69	1557.74	-45.85	-44.12	-42.86	-42.00
0.12 mol·kg^{-1} d-Panthenol + PG								
0.00000	1480.25	1508.46	1529.91	1545.16				
0.09993	1485.36	1513.25	1533.68	1548.43	-45.20	-43.52	-42.31	-41.47
0.20010	1489.75	1517.19	1537.04	1551.52	-45.43	-43.75	-42.53	-41.70
0.29998	1493.85	1520.56	1540.16	1554.58	-45.52	-43.83	-42.61	-41.78
0.39900	1497.34	1524.04	1543.35	1557.58	-45.56	-43.88	-42.66	-41.82
0.50015	1500.48	1527.06	1545.84	1560.54	-45.59	-43.91	-42.69	-41.85
0.00 mol·kg^{-1} d-Panthenol + HG								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.09976	1476.42	1504.09	1526.06	1542.03	-46.04	-44.26	-42.91	-41.97
0.20012	1485.99	1513.18	1532.68	1549.03	-46.28	-44.49	-43.14	-42.20
0.30214	1495.08	1521.73	1540.15	1555.44	-46.37	-44.57	-43.22	-42.28
0.39996	1503.80	1529.03	1545.50	1560.44	-46.41	-44.62	-43.26	-42.32

0.50067	1510.68	1536.10	1550.22	1565.35	-46.44	-44.65	-43.30	-42.36
			0.04 mol·kg^{-1} d-Panthenol + HG					
0.00000	1471.19	1501.03	1523.15	1539.51				
0.09964	1480.33	1508.45	1529.75	1545.28	-45.75	-43.95	-42.68	-41.78
0.20120	1489.99	1517.76	1536.67	1552.41	-45.99	-44.18	-42.91	-42.00
0.30061	1499.19	1525.93	1543.75	1558.61	-46.08	-44.26	-42.99	-42.08
0.40004	1507.97	1533.23	1548.87	1563.71	-46.12	-44.31	-43.03	-42.13
0.49782	1514.95	1540.34	1553.68	1568.21	-46.15	-44.34	-43.06	-42.16
			0.08 mol·kg^{-1} d-Panthenol + HG					
0.00000	1476.13	1504.84	1526.84	1542.51				
0.09997	1485.65	1513.47	1533.96	1548.75	-45.45	-43.73	-42.48	-41.62
0.19988	1494.99	1522.27	1540.68	1555.95	-45.68	-43.96	-42.70	-41.84
0.30011	1504.36	1530.61	1547.90	1561.97	-45.77	-44.04	-42.78	-41.92
0.40025	1512.96	1537.91	1552.89	1566.79	-45.81	-44.08	-42.82	-41.96
0.50101	1520.13	1545.13	1558.21	1571.60	-45.84	-44.11	-42.85	-41.99
			0.12 mol·kg^{-1} d-Panthenol + HG					
0.00000	1480.25	1508.46	1529.91	1545.16				
0.10014	1490.02	1517.13	1537.14	1551.83	-45.20	-43.52	-42.31	-41.47
0.20220	1499.62	1526.43	1544.14	1559.06	-45.43	-43.75	-42.53	-41.70
0.30005	1509.08	1534.27	1551.01	1565.01	-45.51	-43.83	-42.61	-41.77

0.40000	1517.54	1541.59	1556.11	1569.71	-45.55	-43.87	-42.65	-41.82
0.49899	1524.46	1548.63	1561.46	1574.44	-45.58	-43.89	-42.68	-41.85

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, , $u(T)$=0.05K, $u(\rho)=0.06$(kg·m^{-3}),, $u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K_{\phi,S})$ =$\pm$0.25 × 10^{6}/ (m^{3}·mol^{-1}· GPa^{-1}).

Table 4.58

Partial molar isentropic compression, $K^{0}_{\phi,s}$, and experimental slopes, S^{*}_{K}, of glycols in the aqueous solution of d-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$K^{0}_{\phi,s}$ ×10^{6}/(m^{3}·mol^{-1}· GPa^{-1})				S^{*}_{K} ×10^{6}/(kg·m^{3}·mol^{-2}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				PG				
0.00	-46.03(±0.079)	-44.24(±0.076)	-42.89(±0.074)	-41.95(±0.073)	-0.96(±0.236)	-0.93(±0.228)	-0.91(±0.222)	-0.91(±0.219)
0.04	-45.74(±0.077)	-43.94(±0.074)	-42.67(±0.073)	-41.77(±0.072)	-0.95(±0.233)	-0.91(±0.225)	-0.90(±0.220)	-0.90(±0.217)
0.08	-45.44(±0.077)	-43.72(±0.074)	-42.47(±0.072)	-41.60(±0.071)	-0.93(±0.232)	-0.90(±0.224)	-0.88(±0.219)	-0.88(±0.216)
0.12	-45.19(±0.077)	-43.51(±0.075)	-42.29(±0.073)	-41.46(±0.072)	-0.92(±0.234)	-0.89(±0.226)	-0.88(±0.221)	-0.88(±0.219)
				HG				
0.00	-46.03(±0.079)	-44.24(±0.077)	-42.89(±0.075)	-41.95(±0.074)	-0.94(±0.240)	-0.92(±0.232)	-0.90(±0.226)	-0.91(±0.223)
0.04	-45.74(±0.079)	-43.94(±0.076)	-42.67(±0.074)	-41.76(±0.073)	-0.93(±0.239)	-0.90(±0.231)	-0.89(±0.225)	-0.90(±0.223)
0.08	-45.44(±0.078)	-43.72(±0.075)	-42.47(±0.073)	-41.60(±0.073)	-0.90(±0.235)	-0.88(±0.227)	-0.87(±0.222)	-0.88(±0.219)
0.12	-45.19(±0.077)	-43.51(±0.075)	-42.30(±0.073)	-41.46(±0.072)	-0.89(±0.233)	-0.87(±0.226)	-0.86(±0.221)	-0.87(±0.218)

$^{a}m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K^{0}_{\phi,s})$ =$\pm$0.01 × 10^{6}/(m^{3}·mol^{-1}· GPa^{-1})and $u(S^{*}_{K})$ =$\pm$0.24 × 10^{6}/(m^{3}·mol^{-2}· GPa^{-1}).

Table 4.59

Partial molar isentropic compression transfer, $\Delta K_{\phi,s}^{0}$, of glycols in the aqueous solution of d-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta K_{\phi,s}^{0}$ × 10^{6}/(m^{3}·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PG		
0.04	0.28	0.30	0.22	0.19
0.08	0.59	0.52	0.43	0.35
0.12	0.84	0.73	0.60	0.49
		HG		
0.04	0.29	0.31	0.23	0.19
0.08	0.59	0.52	0.43	0.35
0.12	0.84	0.73	0.60	0.49

$^{a}m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}

Table 4.60

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of d-Panthenol at different temperatures

T/K	V_{AB} ×10^{6}/(m^{3}·mol^{-2}· kg)	V_{ABB} ×10^{6}/(m^{3}·mol^{-3}·kg^{2})	K_{AB} ×10^{6}/(m^{3}·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^{6}/(m^{3}·mol^{-3}·kg^{2} GPa^{-1})
		PG		
288.15	0.45	2.31	3.77	-1.36
298.15	0.38	2.41	3.93	-4.92
308.15	0.25	2.68	2.97	-2.59
318.15	0.32	2.00	2.46	-2.26
		HG		
288.15	-0.07	1.75	3.82	-1.69
298.15	-0.06	1.68	3.97	-5.22
308.15	-0.06	1.58	3.01	-2.88
318.15	-0.05	1.40	2.50	-2.55

T/K is the temperatures, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}.

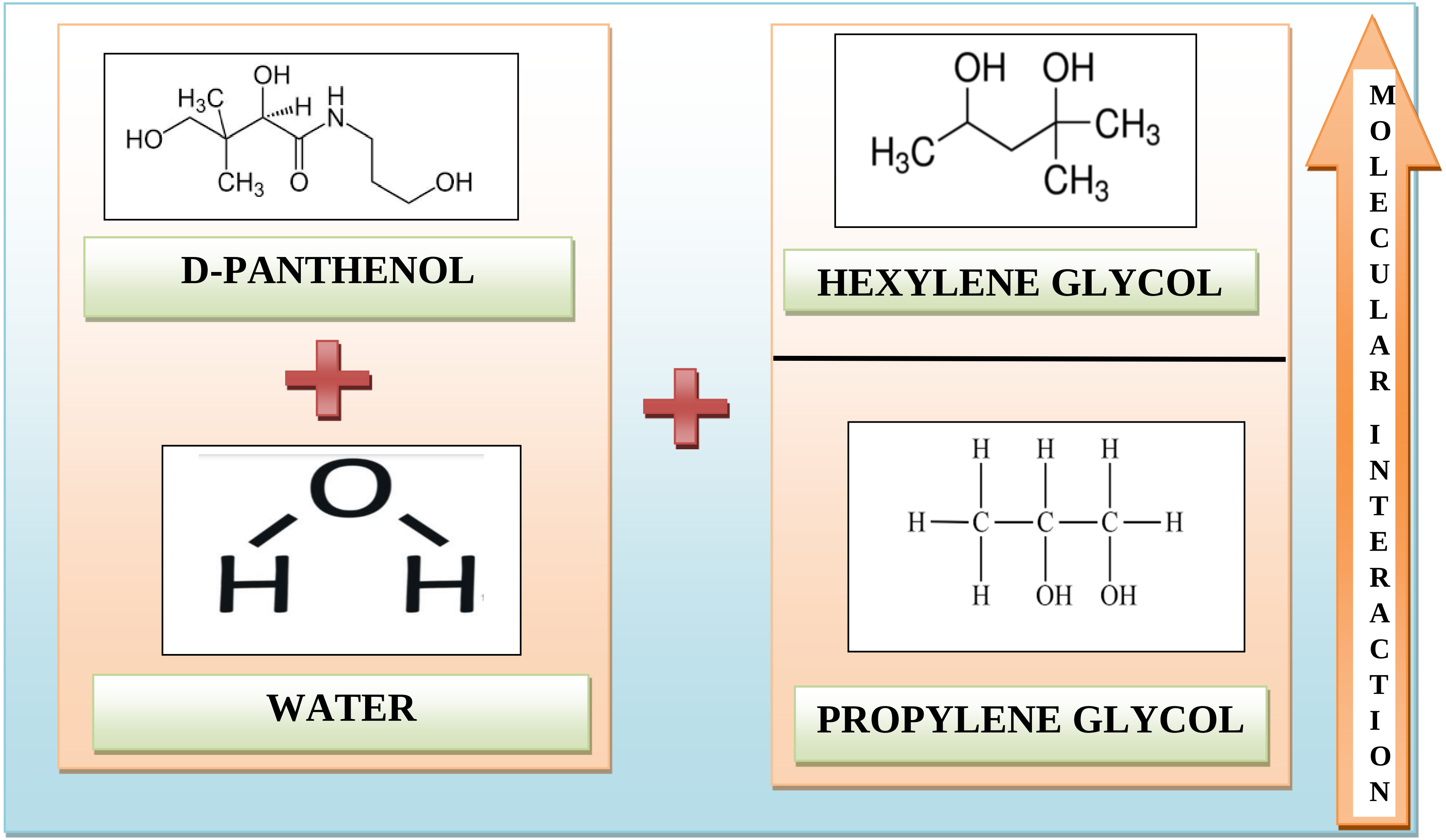
Table 4.61

Hydration number for glycols in aqueous solutions of d-Panthenol at different temperatures

$^{a}m_{A}$/(mol·kg^{-}	n_h			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
PG+0.00 mol·kg^{-1} d-Panthenol				
0.09917	554.9979	554.9983	554.9975	554.9968
0.19801	277.5007	277.5006	277.5000	277.4996
0.30136	185.0015	185.0013	185.0008	185.0005
0.39826	138.7519	138.7516	138.7512	138.7510
0.51059	111.0020	111.0017	111.0013	111.0012
PG+0.04 mol·kg^{-1} d-Panthenol				
0.10093	555.0381	555.0379	555.0372	555.0369
0.20010	277.5207	277.5204	277.5199	277.5196
0.30272	185.0148	185.0145	185.0141	185.0138
0.40065	138.7618	138.7614	138.7611	138.7609
0.50007	111.0100	111.0096	111.0093	111.0092
PG+0.08 mol·kg^{-1} d-Panthenol				
0.10102	555.0783	555.0780	555.0772	555.0768
0.20006	277.5408	277.5405	277.5398	277.5396
0.30012	185.0283	185.0279	185.0274	185.0271
0.40001	138.7719	138.7715	138.7711	138.7709
0.49990	111.0180	111.0176	111.0173	111.0172
PG+0.12 mol·kg^{-1} d-Panthenol				
0.09993	555.1183	555.1180	555.1172	555.1168
0.20010	277.5608	277.5605	277.5599	277.5596
0.29998	185.0416	185.0412	185.0407	185.0405
0.39900	138.7818	138.7815	138.7811	138.7809
0.50015	111.0259	111.0257	111.0253	111.0252
HG+0.00 mol·kg^{-1} d-Panthenol				
0.09903	555.0019	555.0006	554.9996	554.9989

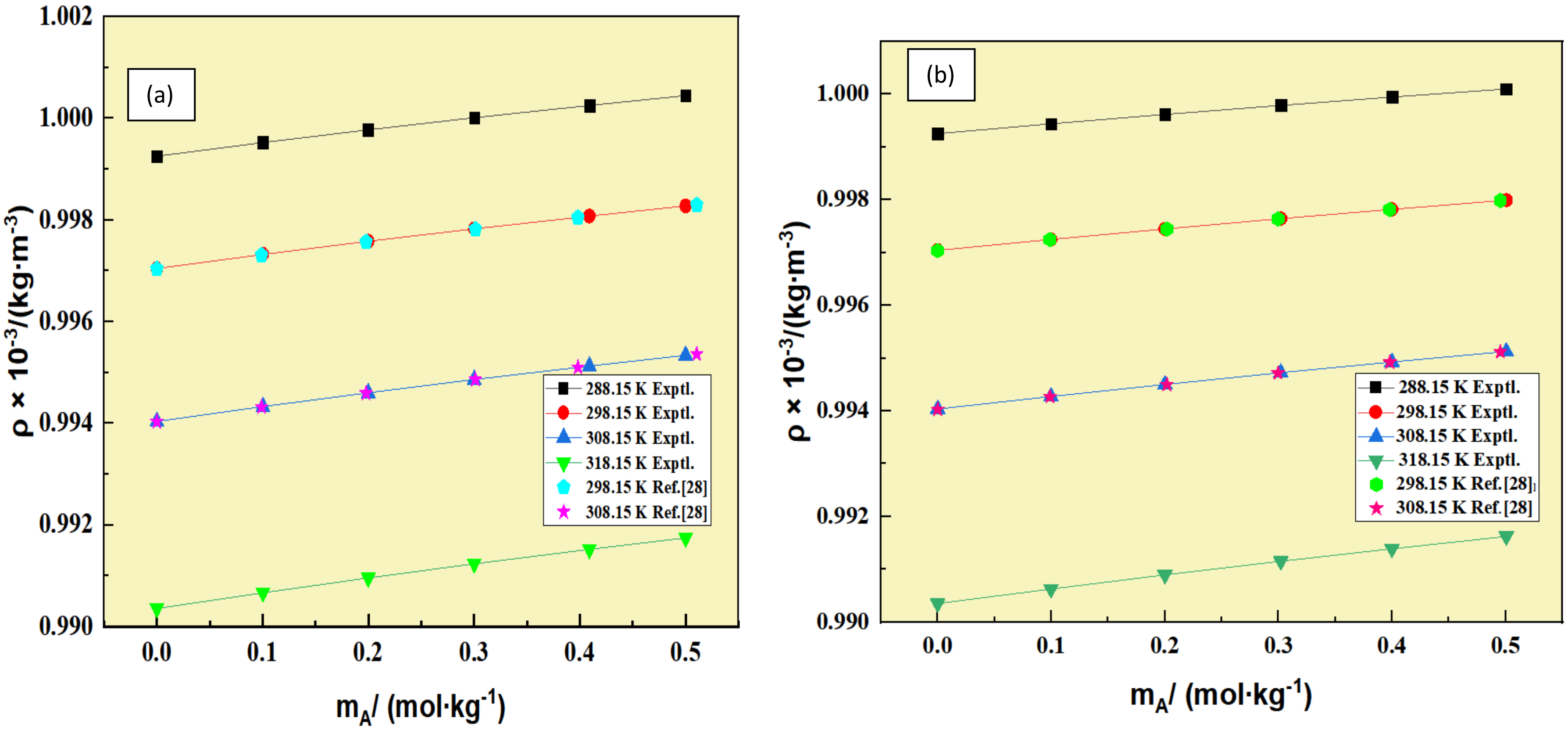
0.20184	277.5045	277.5037	277.5022	277.5020
0.29963	185.0052	185.0045	185.0033	185.0029
0.39805	138.7555	138.7547	138.7534	138.7531
0.49538	111.0054	111.0047	111.0034	111.0032
HG+0.04 mol·kg^{-1} d-Panthenol				
0.09964	555.0413	555.0400	555.0393	555.0387
0.20120	277.5243	277.5234	277.5222	277.5219
0.30061	185.0184	185.0176	185.0165	185.0161
0.40004	138.7654	138.7645	138.7633	138.7630
0.49782	111.0133	111.0126	111.0113	111.0110
HG+0.08 mol·kg^{-1} d-Panthenol				
0.09997	555.0815	555.0808	555.0796	555.0790
0.19988	277.5442	277.5436	277.5423	277.5421
0.30011	185.0318	185.0311	185.0299	185.0295
0.40025	138.7753	138.7746	138.7733	138.7730
0.50101	111.0213	111.0207	111.0194	111.0191
HG+0.12 mol·kg^{-1} d-Panthenol				
0.10014	555.1217	555.1207	555.1196	555.1192
0.20220	277.5644	277.5637	277.5624	277.5622
0.30005	185.0452	185.0444	185.0432	185.0429
0.40000	138.7854	138.7846	138.7833	138.7830
0.49899	111.0293	111.0286	111.0274	111.0271

Figure 4.42



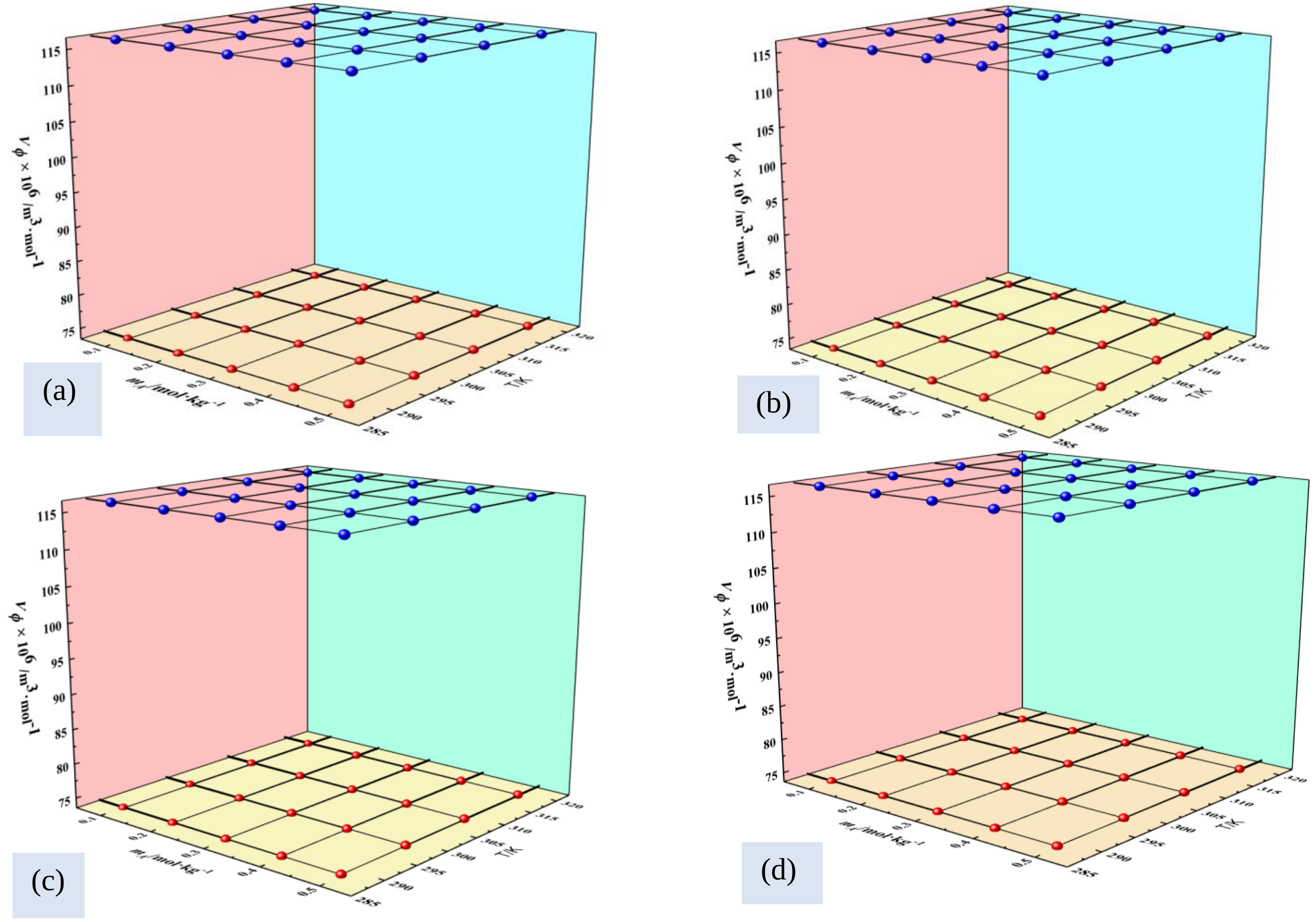
PG / HG and d-Panthenol interactions.

Figure 4.43



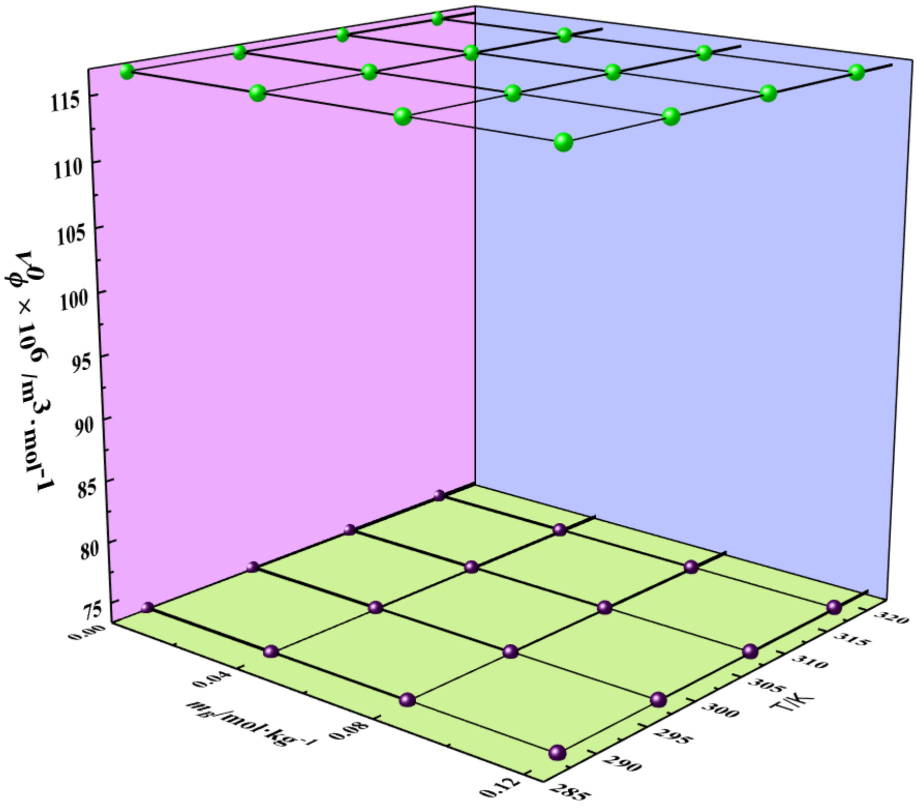
Variation of experimental and literature density values [28] of (a) (propylene glycol +Water) and (b) (hexylene glycol +Water) corresponding to the molality (m_A) of glycols at T= (298.15 and 308.15) K.

Figure 4.44



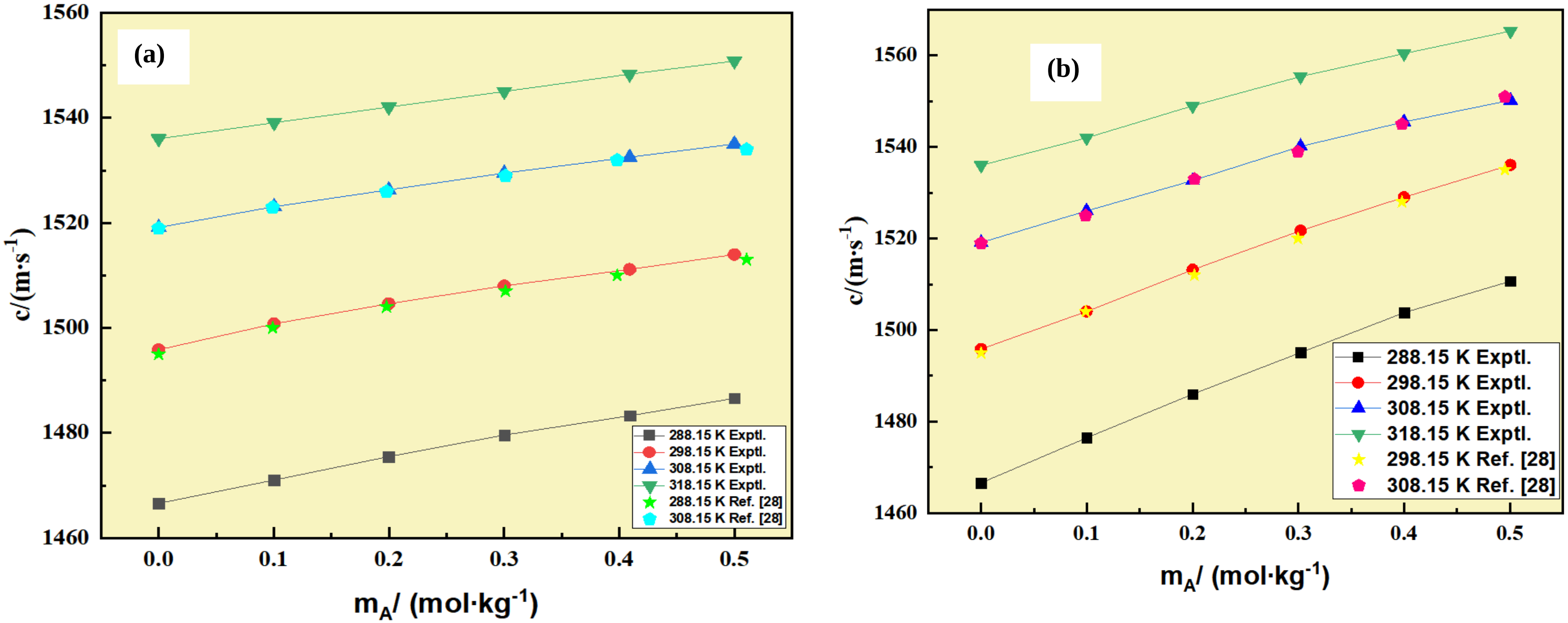
Variation of apparent molar volume, V_ϕ, corresponding to the molality (m_A) of glycols in d-Panthenol. (a) 0.00 d-Panthenol, (b) 0.04 d-Panthenol, (c) 0.08 d-Panthenol, (d) 0.12 d-Panthenol, against molality at a different temperature [red, Propylene glycol and blue, hexylene glycol]

Figure 4.45



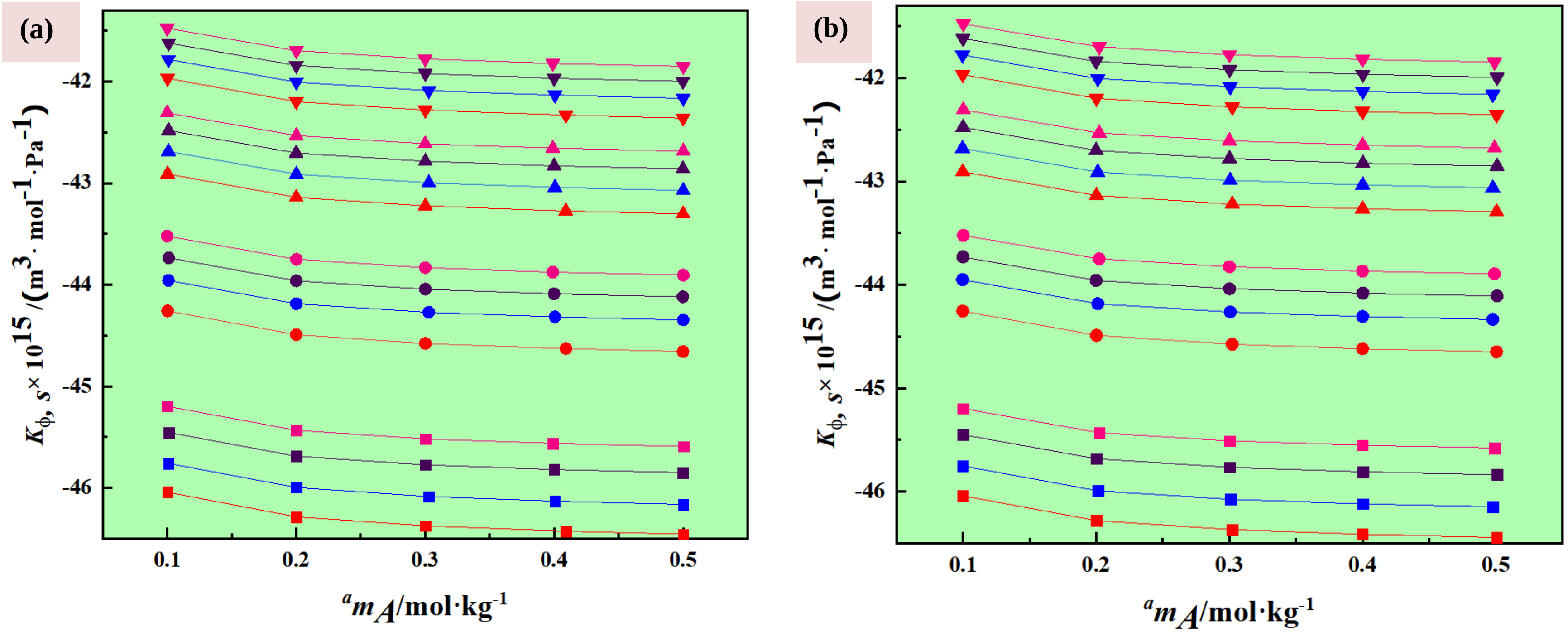
Variation of partial molar volumes, V_ϕ^0, corresponding to the molality (m_B) of d-Panthenol. Propylene glycol (color purple) and hexylene glycol (color green) in different concentrations of aqueous d-Panthenol solutions at different temperatures.

Figure 4.46



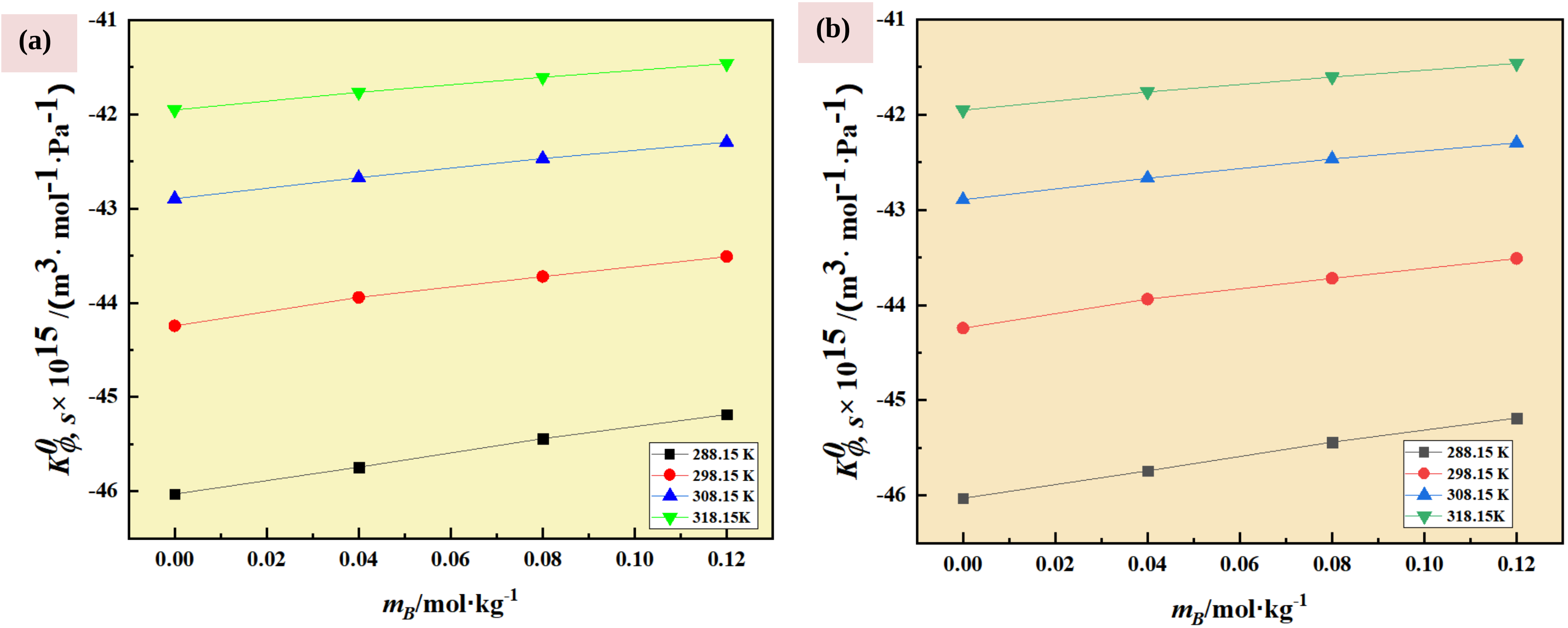
Variation of experimental and literature speed of sound values [28] of (a) (propylene glycol +Water) and (b) (hexylene glycol +Water) corresponding to the molality (m_A) of glycols at T= (298.15 and 308.15) K.

Figure 4.47



Variation of apparent molar isentropic compression, $K_{\phi,s,}$ corresponding to the molality (m_A) of glycols in d-Panthenol. (a) Propylene glycol and (b) Hexylene glycol in aqueous solutions of **(**red, 0.00 d-Panthenol; blue, 0.04 d-Panthenol; purple, 0.08 d-Panthenol; pink**,** 0.12 d-Panthenol**)** against molality at a different temperature [inverted triangle, 318.15 K; triangle, 308.15 K, circle 298.15 K; square, 288.15 K]

Figure 4.48



Variation of partial molar isentropic compression,$K^0_{\phi,s}$, corresponding to the molality (m_A) of glycols in d-Panthenol. (a) Propylene glycol, and (b) Hexylene glycol in aqueous d-Panthenol solutions at different temperatures.

Problem 8

Thermodynamics of various interactions in homologous series of polyethylene glycols in aqueous medium of d-panthenol at t= (288.15, 298.15, 308.15 and 318.15) k: a volumetric and acoustic approach

In this section, we have reported the densities, ρ and speed of sound c of polyethylene glycol 200 (PEG 200) and polyethylene glycol 400 (PEG 400) in (0.00, 0.03, 0.06 and 0.09) $\mathrm{mol \cdot kg^{-1}}$ aqueous solutions of d-Panthenol at temperatures T = (288.15, 298.15, 308.15 and 318.15) K.

4.61 Density

The experimental densities of (d-Panthenol + water) and (d-Panthenol + water + polyethylene glycols) at T= (288.15, 298.15, 308.15 and 318.15) K and concentrations of (0.00, 0.03, 0.06 and 0.09) $\mathrm{mol.kg^{-1}}$ are listed in **Table 4.62** from which it is evident that the density values are in a linear relationship with the polyethylene glycol molality and d-Panthenol concentrations but decreases with the temperature. The comparison of density values for (water + polyethylene glycols) with literature [39, 53] is provided in **Figure 4.50[a]** for (water + PEG 200) and **Figure 4.50[b]** for (water + PEG 400). From these figures it is observed that the experimental density values and the literature density values are in good agreement with each other i.e. they are following the same trend corresponding to the molality and temperatures [54-56].

4.62 Apparent molar volume

The equation **4.1** is used to calculate the values of apparent molar volume (V_{ϕ}) using the experimental density data. Here, M, m_A, ρ, and ρ_0 are representing the molar mass of the solute, the molality of the solute per one kilogram of the solvent (d-Panthenol+ water), the densities of the solution and the solvent respectively. The calculated V_{ϕ} values are incorporated in **Table 4.62,** where it can be seen that the values tend to increase with the experimental temperatures and molality of polyethylene glycols. Also, there is the rise in the V_{ϕ} values with the increase in the molar mass of the glycols as well as with the d-Panthenol concentration which is graphically represented in **Figure 4.51** [24]. The presence of strong solute-solvent interactions among the mixtures is observed due to positive V_ϕ values. This increment in the values results in more interactions among the solute and solvent molecules due to great affinity for the solvent molecules. Further, the apparent molar volume values increase from PEG 200 to PEG 400 and thus suggest the upsurge of solute-solvent interaction in the case of PEG 400 than PEG 200, which is clearly demonstrated in **Figure 4.49** [9]. This escalation is subjected due to few aspects such as hydrophobic hydration in the water-rich region, hydrophilic effect along some physical forces like dipole induced dipole and dipole-dipole interactions [38, 57].

4.63 Partial Molar volume

The equation **4.2** is used to obtain the partial molar volume of the liquid mixtures containing d-Panthenol and glycol. Here m_A is the molality of the solute. In **Table 4.63** the partial molar volume (V_ϕ^0) and their experimental slope (S_V^*) are reported along with their standard errors which are calculated from the least square fitting method. The partial molar volume is a crucial parameter that describes the solute-solvent interactions as this parameter is definitely independent of solute-solute interactions. From the table, it can be noticed that the V_ϕ^0 values are all positive and increase with the temperatures and d-Panthenol concentrations which is graphically represented in **Figure 4.52**. This trend indicates the existence of strong solute-solvent interactions inside the liquid mixture which gets strengthened with the elevating concentration of d-Panthenol and increasing temperature. Moreover, the V_ϕ^0 values increase from PEG 200 to PEG 400 which implies that V_ϕ^0 is linearly dependent on the molar mass of the polyethylene glycols due to hydrogen bond interactions between the hydrogen atom of water and OH group of polyethylene glycols [41, 58]. According to co-sphere overlap model [Mishra et al 1984 and Iqbal et al], there exist hydrophilic-hydrophilic, hydrophobic- hydrophobic, and hydrophilic-hydrophobic interactions in the liquid mixture which is the result for positive values of V_ϕ^0. The experimental slope S_V^* in the same table is found to be positive which again refers to the superiority of solute-solvent interactions in the liquid mixture [45].

4.64 Partial molar volume of transfer

Transfer of partial molar volume of polyethylene glycols from water to d-Panthenol aqueous solutions at infinite dilution is computed employing the equation **4.3**. Partial thermodynamic transfer properties give the information regarding the solute-cosolute interactions since at minuscule concentration the interactions among individual molecules of solute are insignificant [59]. The positive ΔV_{ϕ}^{0} values are observed in the mixture of polyethylene glycols in the aqueous d-Panthenol solution that is increasing with the upsurge in the concentration of d-Panthenol and molar mass of polyethylene glycols which are indexed in **Table 4.64**. As per Pauling's model for pure water structure [34, 35], there exists enough unoccupied space in water which is termed as clathrates, that is easily susceptible to other molecules. Therefore, to maintain the cage structure of the water very small amount of polyethylene glycols enters the cage but eventually, a high quantity of polyethylene glycol molecules abolishes the water structure and develops the hydrogen bond to provide the new structure [37].

4.65 Temperature-dependent partial molar volume

Using the equation **4.4**, the variation in the apparent molar volume at infinite dilution with temperatures is determined. Here, $a, b, c,$ are empirical constants listed in **Table 4.65**, T_{ref}=298.15 K, and the temperature in Kelvin is represented as T. The deviations in the calculated and experimental V_{ϕ}^{0} values are also mentioned in the same table and these deviations are evaluated using the equation **4.14**. Here, $\mathrm{Y} = V_{\phi}^{0}$ (apparent molar volume at infinite dilution). The deviation values are very minute which completely fits into the polynomial equation that is illustrated from R^{2}values in the present study. The empirical constant c in the table indicates the scatter in the values of V_{ϕ}^{0}. The main objective to study the V_{ϕ}^{0} values was to attain the partial molar expansibilities using the equation **4.5**. The partial molar expansibility at infinite dilution is given by E_{ϕ}^{0}=$\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$. The interactions for solute and solvents inside the mixture are analyzed by this parameter. The structure making and breaking capability of the solute in the solution is determined using the following general thermodynamic equation **4.6**. Utilizing the sign of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ the capability of solute for structure making and structure breaking in the solvent is analyzed. The observed $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ values propose the existence of the structure-making ability of polyethylene glycols in aqueous d-Panthenol solutions due to less negative and more positive values of the above parameter [60]. In **Table 4.66** the values of E_{ϕ}^{0} are attributed along with its first derivative which is equal to $\left(\partial^{2}\mathrm{V}_{\Phi}/\partial \mathrm{T}^{2}\right)_{p}$, which are all positive over the entire range of d-Panthenol concentrations and experimental temperatures, which reveal the solute-solvent interactions, as previously pointed by apparent molar volume properties. An irregular pattern is observed in the case of E_{ϕ}^{0} values corresponding to the concentration of d-Panthenol and temperatures [44].

4.66 Ultrasonic speed

The experimental speed of sound values of (d-Panthenol + water) and (d-Panthenol + water + polyethylene glycols) at T= (288.15, 298.15, 308.15 and 318.15) K and concentrations of (0.00, 0.03, 0.06 and 0.09) mol.kg^{-1} are listed in **Table 4.67**. The experimental speed of sound values for (water+ PEG 200) and (water+ PEG 400) are compared with the literature values [39, 53] for all temperatures and are graphically represented in **Figure 4.53 [a]** and **Figure 4.53 [b]** respectively. It is observed that the speed of sound values are increasing along with the temperatures and the concentrations of niacin from (0.03 to 0.06 to 0.09) mol·kg^{-1}, thus showing the same trend as the literature values. This behavior of the speed of sound values is due to intermolecular and intramolecular hydrogen bonding in solute-solvent molecules because of the three-dimension structure of hydrogen bonds in the water. Moreover, with the upsurge in the molar mass of the polyethylene glycols, the hydrogen bond present in the aqueous d-Panthenol solution reduces and eventually gets terminated but concurrently new hydrogen bonds are created among d-Panthenol and polyethylene glycol molecules [18, 41].

4.67 Apparent molar isentropic compression

The Apparent molar isentropic compression for polyethylene glycols in aqueous d-Panthenol solution is obtained using the equation **4.7**. Here, the densities of the solvent, densities of the solution, molar mass of solute, the molality of solute, and isentropic compressibility of the pure solvent and the solution are represented as ρ, ρ_{0}, M, m_A, $k_{s.0}$ and k_s respectively. The equation **4.8** is used to calculate the isentropic compressibility. Here, ρ represents the density of the solution. The calculated values of $K_{\phi,S}$ at different d-Panthenol concentrations and temperatures are ascribed in **Table 4.67**. From the table, it is observed that the $K_{\phi,S}$ values are all negative and the negativity increases with the temperature and concentration of d-Panthenol but became less negative with the polyethylene glycol molality which is clearly represented in **Figure 4.54**. This behavior of $K_{\phi,S}$ values against the experimental parameters (i.e. temperatures, molality of polyethylene glycol, and concentration of d-Panthenol) establishes that around the ionic charge group of solute the water molecules are less compressible than the bulk solution. Throughout the solute, the water molecules arrange themselves in a particular order due to the nature of $K_{\phi,S}$ values. Further, the larger loss of structural compressibility of water is observed as the consequence of the more aligning effect of the negative values to solute [16, 46, 61].

4.68 Partial molar isentropic compression

With the equation **4.9**, the partial molar isentropic compression is computed by contemplating the divergence of apparent molar isentropic compression along with the molality. Where m_A is the molality of the solute in the aqueous d-Panthenol solution. By the means of the least square fitting method, the partial molar isentropic compression ($K^0_{\phi,S}$) and the experimental slope (S^*_k) are calculated which are reported in **Table 4.68** along with their standard errors. The $K^0_{\phi,S}$ values show a regular trend where the values become more negative with the rise in the temperature and concentration of d-Panthenol while the negativity decreases with the upsurge in the molar mass of the polyethylene glycols. This trend is graphically represented in **Figure 4.55**, which occurs due to interactions among the polyethylene glycols and water molecules as the water molecules are released to bulk which is less compressible around polyethylene glycols due to strong interactions between the d-Panthenol and water molecules that increases the dehydration of polyethylene glycols. Also, the solute-solute is predominated by solute-solvent interactions because of the negative S^*_k values which show a symmetric pattern corresponding to the temperatures and d-Panthenol concentrations [14, 26].

4.69 Partial molar isentropic compression of transfer

The partial molar isentropic compression of transfer for polyethylene glycol from water to aqueous d-Panthenol solutions at infinite dilution is determined using the equation **4.10**. In **Table 4.69** the partial molar isentropic compression of transfer ($\Delta K_{\phi,s}^{0}$) are mentioned which are found to be positive and at each temperature the $\Delta K_{\phi,s}^{0}$ values increases with the elevating concentration of d-Panthenol which implies the structure making tendency in the solution. This is due to the decrement in the electrostriction with the rise of the d-Panthenol concentration which results in the enhancement of the structure-making property. Due to positive $\Delta K_{\phi,s}^{0}$ values the water molecules combine with the polyethylene glycols which indicates that the water molecules of the solute collaborate with the solvent molecules that increase with the molecular interaction [8, 20, 23].

4.70 Pair and triplet coefficients

The partial molar volume of transfer and the partial molar isentropic compression of transfer is obtained from the equation **4.11** and **4.12.** A represents polyethylene glycols and B represents d-Panthenol. The pair and triplet interaction coefficients are represented by the parameters $V_{AB,}$ V_{ABB}; $K_{AB,}$ K_{ABB} for volume and isentropic compression respectively which are reported in **Table 4.70** for all the temperatures**.** The pair and triplet coefficients of the liquid systems to investigate the parting effect were studied using the theory given by McMillan and Mayer [21] which was later reviewed by Friedman and Krishnan [22] and Franks et al [62]. The pair interaction coefficient values V_{AB} and K_{AB} are all positive except for PEG 200 at 318.15 K V_{AB} is negative. The triplet interaction coefficient V_{ABB} is positive only at 318.15 K for PEG 200 and at (308.15 and 318.15) K for PEG 400, while in the case of K_{ABB} all the values are negative. More positive values of V_{AB} and K_{AB} as compared to V_{ABB} and K_{ABB} against the temperatures imply the dominance of pairwise interactions in (d-Panthenol+ water) and (d-Panthenol+ water+ polyethylene glycols) mixtures for volumetric and compressibility measurements [42]. From the hydration co-spheres, the water molecules release to the bulk due to the overlapping of the spheres as per this theory. When the water releases from the co-spheres where the bulk is more structured the volume changes would be positive while it will be negative when due to the variation in the structural organization of the water molecules the co-spheres is more structured [33, 47].

Table 4.62

Values of densities, ρ, apparent molar volumes, V_{ϕ} of glycols in aqueous solutions of D-Panthenol at different temperatures

${}^{a}m_{A}$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_{\phi} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.00 mol·kg^{-1} D-Panthenol + PEG 200								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.10009	1.00221	1.00001	0.99701	0.99335	170.10	170.33	170.61	170.96
0.20044	1.00504	1.00284	0.99986	0.99621	170.28	170.52	170.83	171.18
0.30136	1.00777	1.00558	1.00260	0.99897	170.42	170.66	170.97	171.32
0.40026	1.01032	1.00815	1.00519	1.00157	170.58	170.79	171.10	171.44
0.49999	1.01280	1.01062	1.00767	1.00408	170.71	170.95	171.26	171.59
0.03 mol·kg^{-1} D-Panthenol + PEG 200								
0.00000	1.00045	0.99832	0.99535	0.99151				
0.09934	1.00335	1.00121	0.99826	0.99446	170.27	170.59	170.86	171.07
0.20021	1.00617	1.00404	1.00110	0.99733	170.38	170.70	170.96	171.18
0.30010	1.00886	1.00672	1.00380	1.00006	170.49	170.82	171.07	171.28
0.39977	1.01142	1.00928	1.00638	1.00266	170.61	170.95	171.19	171.41
0.50000	1.01390	1.01176	1.00887	1.00518	170.74	171.06	171.32	171.55
0.06 mol·kg^{-1} D-Panthenol + PEG 200								

0.00000	1.00165	0.99955	0.99650	0.99264				
0.10210	1.00459	1.00249	0.99945	0.99561	170.48	170.80	171.10	171.37
0.20006	1.00729	1.00518	1.00215	0.99835	170.61	170.95	171.26	171.53
0.30009	1.00993	1.00781	1.00479	1.00102	170.77	171.12	171.44	171.70
0.39991	1.01245	1.01031	1.00730	1.00356	170.92	171.31	171.63	171.87
0.50058	1.01487	1.01272	1.00972	1.00599	171.08	171.50	171.82	172.10
0.09 mol·kg^{-1} D-Panthenol + PEG 200								
0.00000	1.00268	1.00055	0.99747	0.99360				
0.10001	1.00552	1.00339	1.00033	0.99648	170.69	171.00	171.33	171.61
0.19950	1.00822	1.00609	1.00303	0.99920	170.90	171.22	171.56	171.86
0.30007	1.01082	1.00868	1.00563	1.00182	171.09	171.43	171.78	172.10
0.40046	1.01329	1.01114	1.00810	1.00432	171.29	171.65	172.00	172.31
0.50008	1.01563	1.01347	1.01044	1.00669	171.48	171.86	172.21	172.49
0.00 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.10015	1.00577	1.00349	1.00044	0.99673	333.00	334.28	335.56	336.82
0.20004	1.01179	1.00945	1.00636	1.00264	333.35	334.65	335.90	337.09
0.29995	1.01739	1.01499	1.01188	1.00813	333.69	334.99	336.18	337.42
0.40100	1.02267	1.02019	1.01705	1.01330	334.01	335.34	336.53	337.74
0.50006	1.02747	1.02496	1.02180	1.01804	334.35	335.64	336.82	338.00

0.03 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1.00045	0.99832	0.99535	0.99151				
0.10141	1.00681	1.00469	1.00175	0.99796	334.97	335.50	336.03	336.60
0.20037	1.01257	1.01045	1.00754	1.00379	335.30	335.82	336.35	336.92
0.29982	1.01796	1.01585	1.01294	1.00923	335.58	336.11	336.69	337.28
0.40009	1.02302	1.02091	1.01803	1.01435	335.88	336.41	336.96	337.59
0.49996	1.02771	1.02560	1.02274	1.01910	336.18	336.72	337.28	337.91
0.06 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1.00165	0.99955	0.99650	0.99264				
0.09920	1.00782	1.00570	1.00266	0.99883	335.29	336.06	336.80	337.53
0.19000	1.01308	1.01095	1.00791	1.00411	335.56	336.31	337.05	337.80
0.30007	1.01901	1.01686	1.01383	1.01006	335.87	336.61	337.37	338.09
0.40150	1.02409	1.02191	1.01889	1.01515	336.10	336.90	337.65	338.38
0.50006	1.02871	1.02649	1.02349	1.01977	336.33	337.16	337.90	338.63
0.09 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1.00268	1.00055	0.99747	0.99360				
0.10091	1.00884	1.00667	1.00359	0.99975	336.19	337.15	337.95	338.68
0.20034	1.01447	1.01226	1.00919	1.00538	336.42	337.42	338.26	338.95
0.30007	1.01972	1.01747	1.01440	1.01063	336.71	337.75	338.56	339.27
0.39977	1.02461	1.02231	1.01924	1.01551	337.00	338.06	338.90	339.56

0.50015	1.02916	1.02683	1.02379	1.02010	337.36	338.40	339.17	339.83

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 1.0 m·s^{-1} and $u(V_\phi)$ =±(0.05-0.07) × 10^{6}/ (m^{3}·mol^{-1}).

Table 4.63

Partial molar volumes, V_ϕ^0, and experimental slopes, S_V^*, of glycols in aqueous solution of D-Panthenol at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$V_\phi^0 \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-2})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				PEG 200				
0.00	169.96(±0.01)	170.20(±0.01)	170.48(±0.03)	170.85(±0.03)	1.52(±0.05)	1.51(±0.04)	1.57(±0.09)	1.50(±0.09)
0.03	170.15(±0.01)	170.46(±0.00)	170.73(±0.01)	170.94(±0.01)	1.16(±0.03)	1.20(±0.02)	1.15(±0.03)	1.19(±0.04)
0.06	170.31(±0.00)	170.61(±0.01)	170.91(±0.01)	171.18(±0.02)	1.52(±0.02)	1.75(±0.03)	1.81(±0.03)	1.79(±0.07)
0.09	170.50(±0.00)	170.79(±0.00)	171.12(±0.00)	171.41(±0.02)	1.97(±0.02)	2.15(±0.01)	2.20(±0.02)	2.21(±0.08)
				PEG 400				
0.00	332.68(±0.01)	333.96(±0.02)	335.25(±0.01)	336.51(±0.02)	3.34(±0.03)	3.41(±0.06)	3.14(±0.05)	3.00(±0.07)
0.03	334.68(±0.01)	335.20(±0.01)	335.73(±0.01)	336.27(±0.01)	3.01(±0.03)	3.03(±0.03)	3.10(±0.05)	3.29(±0.05)
0.06	335.06(±0.03)	335.78(±0.00)	336.53(±0.01)	337.26(±0.01)	2.58(±0.09)	2.77(±0.01)	2.76(±0.03)	2.76(±0.03)
0.09	335.85(±0.04)	336.81(±0.02)	337.64(±0.01)	338.39(±0.01)	2.95(±0.12)	3.15(±0.06)	3.08(±0.04)	2.89(±0.04)

$^a m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 1.0 m·s^{-1}, $u(V_\phi^0)$ =±0.01 × 10^6/ (m^3·mol^{-1}) and $u(S_V^*)$ =±0.03 × 10^6/ (m^3·mol^{-2}).

Table 4.64

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in aqueous solution of D-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 200		
0.03	0.19	0.27	0.25	0.10
0.06	0.35	0.41	0.42	0.33
0.09	0.54	0.59	0.63	0.56
		PEG 400		
0.03	2.00	1.24	0.47	-0.24
0.06	2.39	1.82	1.28	0.75
0.09	3.18	2.85	2.39	1.88

$^{a}m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 1.0 m·s^{-1}

Table 4.65

Values of empirical parameters of Eq., of glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
			PEG 200		
0.03	170.466	0.029	0.000	0.9999	0.000
0.06	170.614	0.029	0.000	0.9999	0.000
0.09	170.798	0.030	0.000	0.9999	0.001
			PEG 400		
0.03	335.199	0.053	0.000	0.9999	0.000
0.06	335.789	0.073	0.000	0.9999	0.000
0.09	336.806	0.090	-0.001	0.9999	0.001

${}^{a}m_B$ is the molality aqueous of D-Panthenol, standard uncertainties *u* are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}) ,$u(p)$=0.01MPa, $u(c)$=1.0 m·s^{-1}.

Table 4.66

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in aqueous solution of D-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	E_{ϕ}^{0} ×10^{6}/(m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			PEG 200		
0.03	0.035	0.029	0.024	0.018	-0.001
0.06	0.031	0.029	0.028	0.027	0.000
0.09	0.030	0.030	0.031	0.031	0.000
			PEG 400		
0.03	0.051	0.053	0.054	0.055	0.000
0.06	0.073	0.073	0.074	0.074	0.000
0.09	0.101	0.090	0.079	0.068	-0.001

$^{a}m_B$ is the molality aqueous of D-Panthenol, standard uncertainties *u* are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1} $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}) ,$u(p)$=0.01MPa, $u(c)$=1.0 m·s^{-1}.

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Table 4.67

Values of speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,s}$ of glycols in aqueous solutions of D-Panthenol at different temperatures

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^6$/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
				0.00 mol·kg^{-1} D-Panthenol + PEG 200				
0.00000	1466.59	1495.85	1519.14	1536.02				
0.10009	1477.01	1506.54	1529.35	1544.22	-46.17	-44.38	-43.03	-42.09
0.20044	1486.41	1516.04	1537.95	1553.92	-46.54	-44.74	-43.37	-42.43
0.30136	1496.73	1526.26	1548.14	1563.27	-46.74	-44.93	-43.57	-42.62
0.40026	1506.23	1534.26	1556.14	1572.27	-46.90	-45.08	-43.72	-42.76
0.49999	1515.44	1544.73	1567.02	1581.57	-47.04	-45.22	-43.85	-42.89
				0.03 mol·kg^{-1} D-Panthenol + PEG 200				
0.00000	1469.97	1499.54	1522.22	1538.53				
0.09934	1480.52	1509.55	1531.94	1546.78	-45.96	-44.16	-42.85	-41.95
0.20021	1489.89	1519.45	1540.89	1556.48	-46.32	-44.51	-43.20	-42.29
0.30010	1499.99	1529.15	1550.75	1565.97	-46.52	-44.71	-43.39	-42.47
0.39977	1509.76	1537.89	1559.02	1574.77	-46.68	-44.86	-43.53	-42.62
0.50000	1518.61	1548.26	1569.54	1584.06	-46.82	-44.99	-43.66	-42.75

0.06 mol·kg^{-1} D-Panthenol + PEG 200								
0.00000	1473.99	1503.04	1525.21	1541.11				
0.10210	1484.97	1512.86	1534.85	1550.04	-45.72	-43.97	-42.70	-41.82
0.20006	1494.24	1522.76	1543.79	1559.04	-46.07	-44.30	-43.02	-42.14
0.30009	1504.14	1532.71	1553.35	1568.57	-46.26	-44.49	-43.21	-42.33
0.39991	1513.94	1541.69	1561.75	1577.57	-46.42	-44.64	-43.35	-42.47
0.50058	1522.68	1551.77	1572.37	1587.01	-46.55	-44.77	-43.48	-42.59
0.09 mol·kg^{-1} D-Panthenol + PEG 200								
0.00000	1477.06	1506.19	1527.97	1543.25				
0.10001	1487.81	1515.66	1537.05	1552.04	-45.52	-43.77	-42.53	-41.69
0.19950	1497.23	1525.76	1546.19	1561.04	-45.87	-44.11	-42.86	-42.02
0.30007	1507.25	1535.52	1555.89	1570.82	-46.06	-44.30	-43.05	-42.20
0.40046	1517.24	1544.69	1564.75	1580.06	-46.22	-44.44	-43.19	-42.34
0.50008	1525.65	1554.59	1575.22	1589.54	-46.34	-44.57	-43.31	-42.46
0.00 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.10015	1487.57	1517.76	1539.62	1558.49	-46.35	-44.55	-43.19	-42.24
0.20004	1507.37	1537.69	1559.79	1578.91	-46.86	-45.04	-43.67	-42.71
0.29995	1527.36	1556.84	1578.93	1598.35	-47.20	-45.36	-43.98	-43.02
0.40100	1547.96	1576.84	1599.32	1617.80	-47.48	-45.63	-44.24	-43.27

0.50006	1569.69	1595.78	1617.05	1635.80	-47.73	-45.87	-44.47	-43.50
0.03 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1469.97	1499.54	1522.22	1538.53				
0.10141	1490.96	1521.81	1543.57	1561.79	-46.14	-44.33	-43.02	-42.11
0.20037	1510.96	1541.37	1563.88	1582.19	-46.63	-44.81	-43.48	-42.57
0.29982	1530.27	1560.16	1582.86	1601.67	-46.95	-45.12	-43.79	-42.87
0.40009	1551.27	1580.36	1603.24	1620.87	-47.22	-45.38	-44.05	-43.13
0.49996	1572.72	1599.15	1620.97	1638.74	-47.46	-45.61	-44.27	-43.35
0.06 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1473.99	1503.04	1525.21	1541.11				
0.09920	1494.68	1524.76	1545.92	1564.36	-45.87	-44.11	-42.83	-41.95
0.19000	1512.99	1543.01	1565.26	1583.26	-46.33	-44.55	-43.27	-42.38
0.30007	1534.39	1563.86	1586.85	1604.71	-46.69	-44.90	-43.61	-42.72
0.40150	1555.95	1583.93	1606.85	1624.66	-46.96	-45.16	-43.86	-42.97
0.50006	1577.09	1602.42	1623.99	1641.72	-47.19	-45.38	-44.08	-43.18
0.09 mol·kg^{-1} D-Panthenol + PEG 400								
0.00000	1477.06	1506.19	1527.97	1543.25				
0.10091	1499.03	1528.14	1549.06	1567.13	-45.68	-43.93	-42.69	-41.84
0.20034	1518.84	1548.31	1570.26	1587.76	-46.16	-44.39	-43.14	-42.29
0.30007	1538.32	1567.36	1590.15	1607.22	-46.48	-44.69	-43.43	-42.58

0.39977	1559.75	1586.93	1609.85	1627.06	-46.74	-44.94	-43.67	-42.82
0.50015	1581.20	1605.65	1627.38	1644.04	-46.97	-45.16	-43.89	-43.04

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainties *u* are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}) ,$u(p)$=0.01MPa, $u(c)$=1.0 m·s^{-1}, $u(K_{\phi,S}) = \pm 0.25 \times 10^{6}$/ (m^3·mol^{-1}· GPa^{-1}).

Table 4.68

Partial molar isentropic compression, $K^0_{\phi,s}$, and experimental slopes, S^*_K, of glycols in aqueous solution of D-Panthenol at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$K^0_{\phi,s}$ ×10^6/(m^3·mol^{-1}· GPa^{-1})				S^*_K ×10^6/(kg·m^3·mol^{-2}· GPa^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
				PEG 200				
0.00	-46.05(±0.08)	-44.26(±0.08)	-42.91(±0.07)	-41.97(±0.07)	-2.09(±0.25)	-2.02(±0.24)	-1.97(±0.23)	-1.95(±0.23)
0.03	-45.84(±0.08)	-44.04(±0.08)	-42.74(±0.07)	-41.83(±0.07)	-2.08(±0.25)	-2.00(±0.24)	-1.96(±0.24)	-1.94(±0.23)
0.06	-45.60(±0.08)	-43.85(±0.07)	-42.58(±0.07)	-41.71(±0.07)	-2.01(±0.24)	-1.94(±0.23)	-1.89(±0.23)	-1.88(±0.22)
0.09	-45.40(±0.08)	-43.66(±0.08)	-42.42(±0.07)	-41.59(±0.07)	-2.00(±0.25)	-1.92(±0.24)	-1.88(±0.23)	-1.86(±0.23)
				PEG 400				
0.00	-46.11(±0.09)	-44.32(±0.09)	-42.97(±0.09)	-42.03(±0.09)	-3.38(±0.29)	-3.23(±0.28)	-3.13(±0.27)	-3.07(±0.27)
0.03	-45.90(±0.09)	-44.11(±0.09)	-42.80(±0.08)	-41.90(±0.08)	-3.26(±0.28)	-3.14(±0.27)	-3.07(±0.27)	-3.03(±0.26)
0.06	-45.64(±0.09)	-43.89(±0.09)	-42.62(±0.08)	-41.75(±0.08)	-3.24(±0.28)	-3.11(±0.27)	-3.04(±0.26)	-3.00(±0.26)
0.09	-45.46(±0.09)	-43.72(±0.09)	-42.48(±0.08)	-41.64(±0.08)	-3.16(±0.28)	-3.02(±0.27)	-2.95(±0.26)	-2.92(±0.26)

$^a m_B$ is the molality of aqueous D-Panthenol, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1} *u(T)*=0.001 K, *u(ρ)*=0.15(kg·m^{-3}) ,*u(p)*=0.01MPa, *u(c)*=1.0 m·s^{-1}, *u*($K^0_{\phi,s}$) =±0.01 × 10^6/(m^3·mol^{-1}· GPa^{-1})and *u*(S^*_k) =±0.24 × 10^6/(m^3·mol^{-2}· GPa^{-1}).

Table 4.69

Partial molar isentropic compression transfer, $\Delta K^0_{\phi,s}$, of glycols in aqueous solution of D-Panthenol at different temperatures.

${}^a m_B$/ (mol·kg^{-1})	$\Delta K^0_{\phi,s}$ × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 200		
0.03	0.21	0.22	0.18	0.14
0.06	0.45	0.41	0.33	0.27
0.09	0.65	0.60	0.49	0.39
		PEG 400		
0.03	0.21	0.21	0.17	0.13
0.06	0.47	0.43	0.35	0.28
0.09	0.65	0.60	0.49	0.39

${}^a m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}) ,$u(p)$=0.01MPa, $u(c)$=1.0 m·s^{-1}

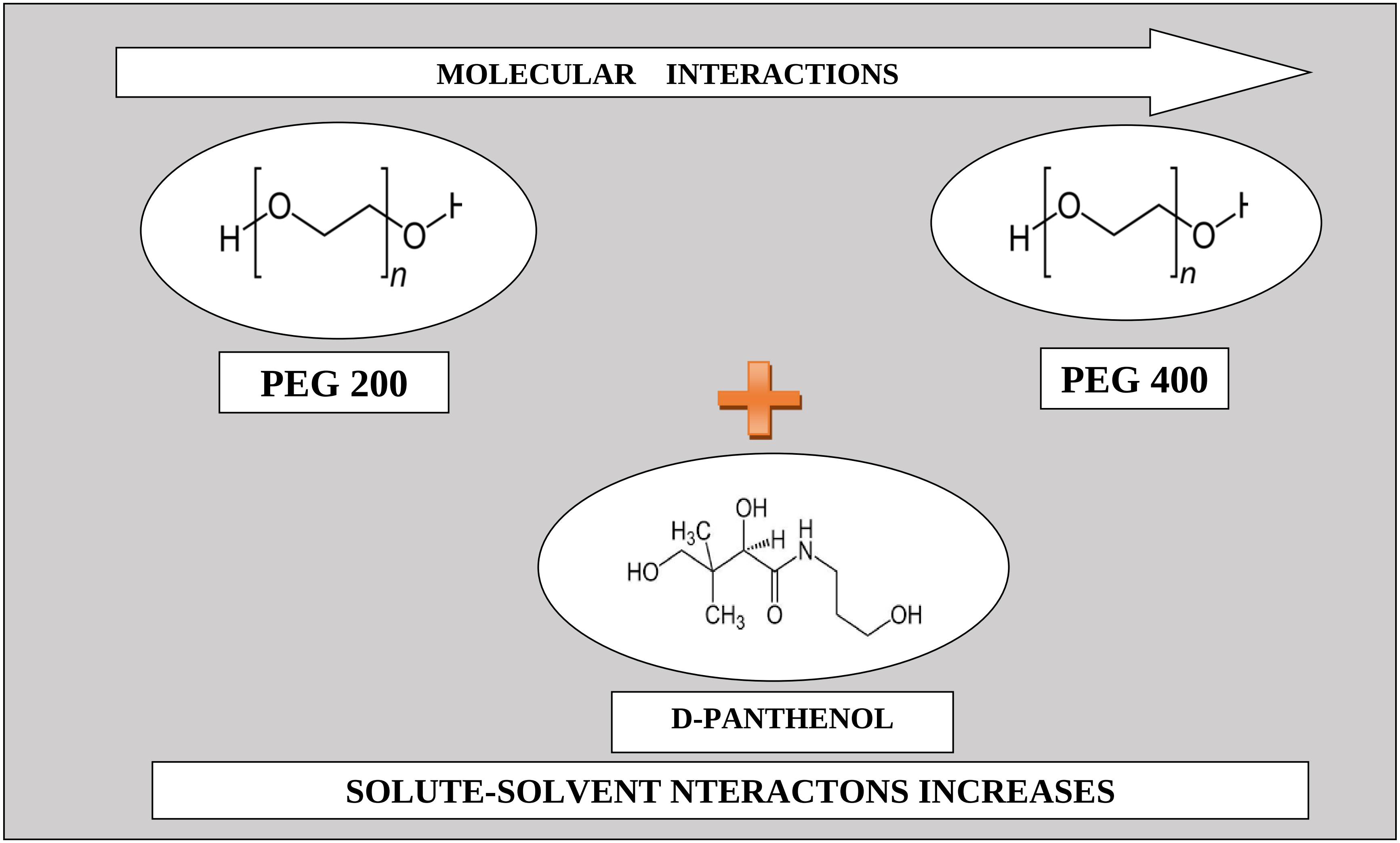
Table 4.70

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of D-Panthenol at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		PEG 200		
288.15	3.02	-0.27	3.80	-1.43
298.15	4.47	-9.19	3.75	-3.03
308.15	4.07	-4.43	2.94	-1.66
318.15	1.36	13.33	2.38	-1.74
		PEG 400		
288.15	33.53	-122.03	3.92	-1.99
298.15	18.91	-25.03	3.83	-3.39
308.15	5.30	59.17	2.99	-1.83
318.15	-7.06	131.86	2.41	-1.73

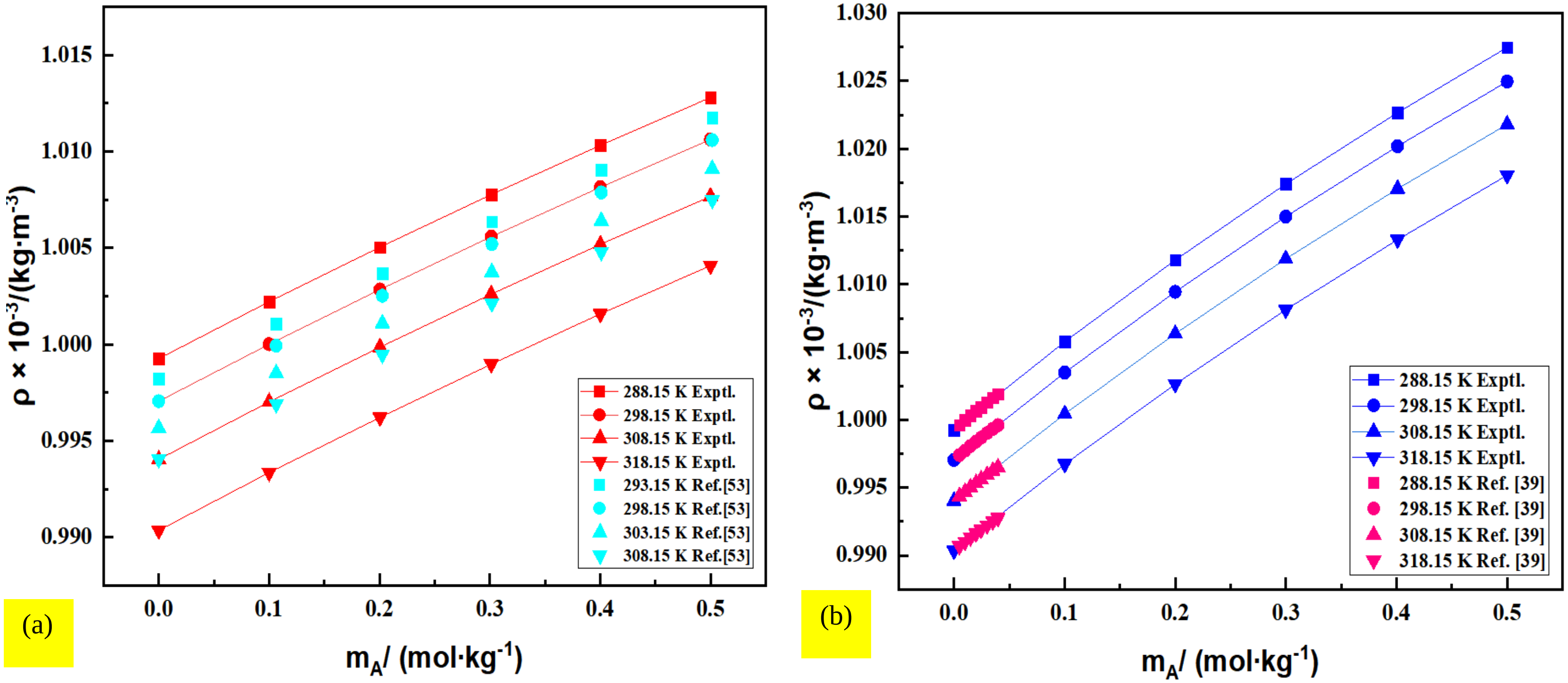
T/K is the temperatures.

Figure 4.49



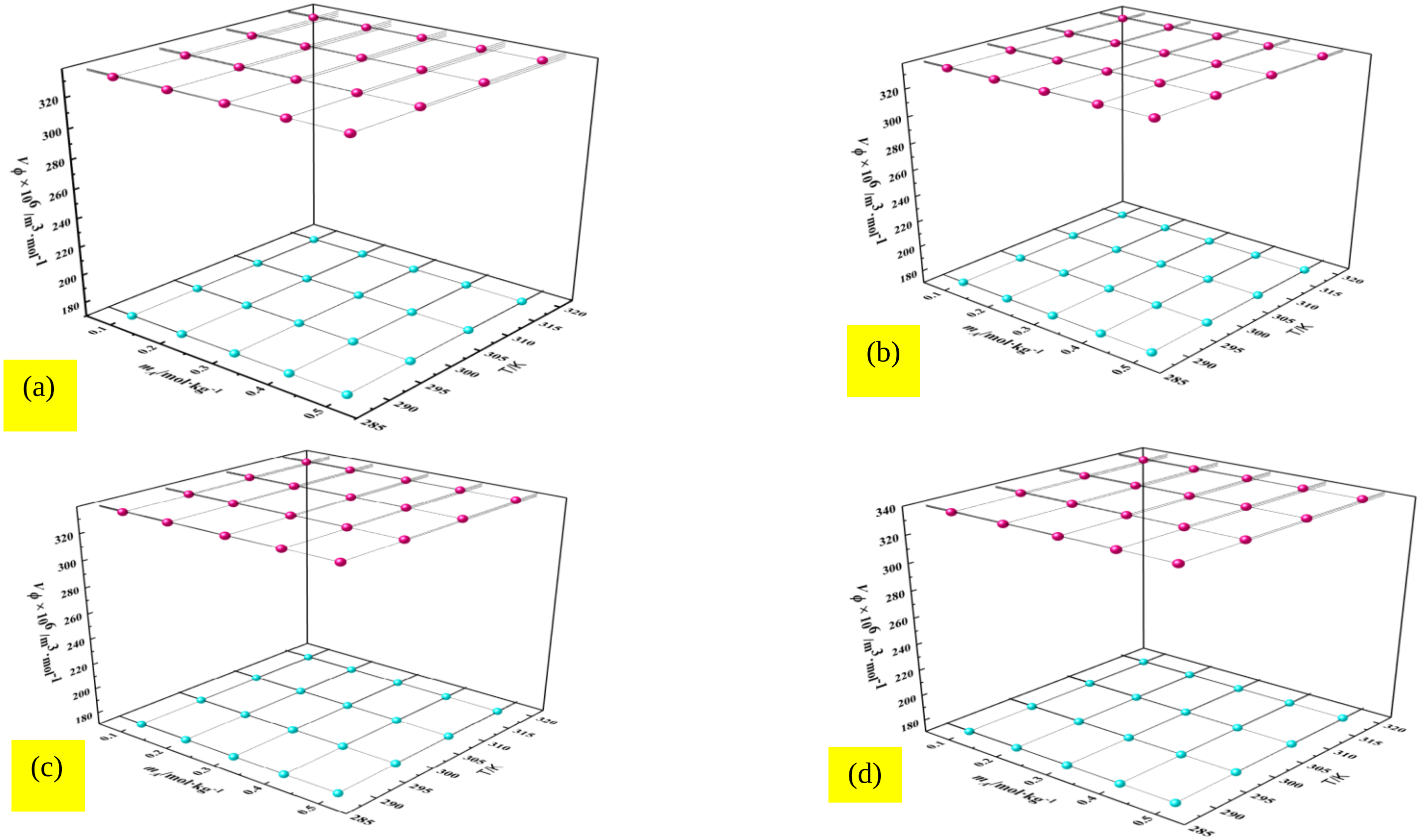
PEG 200 / PEG 400 and d-Panthenol interactions

Figure 4.50



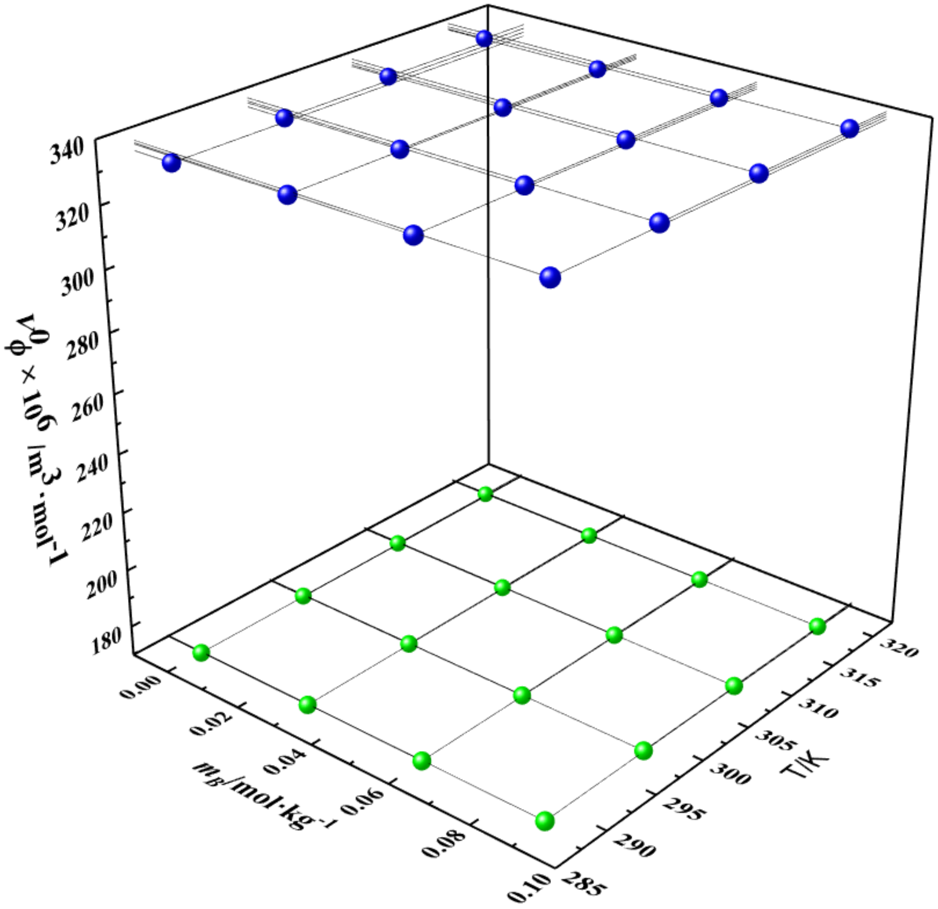
Variation of experimental and literature density values of (a) (polyethylene glycol 200+Water) [53] and (b) (polyethylene glycol 400 +Water) [39]corresponding to the molality (m_A) of glycols at different temperatures.

Figure 4.51



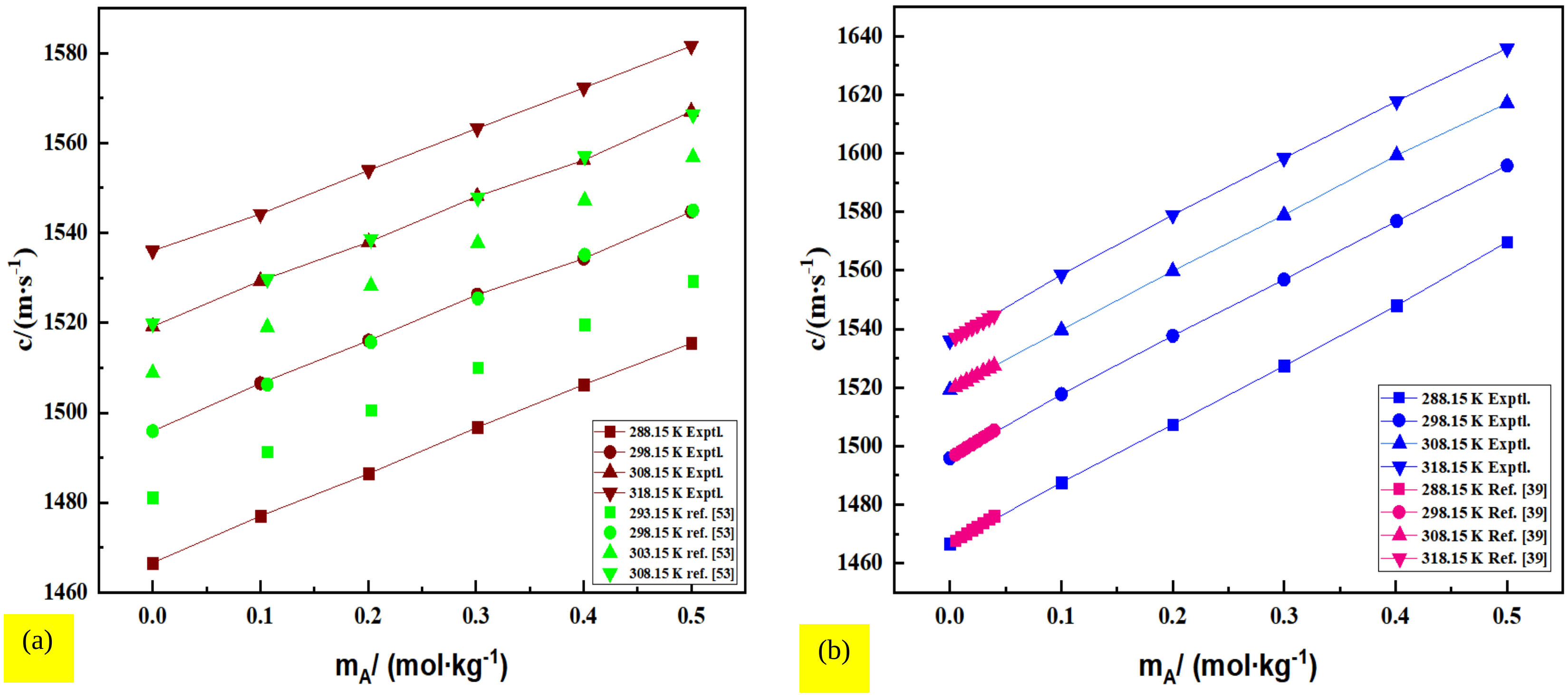
Variation of apparent molar volume, V_{ϕ}, corresponding to the molality (m_A) of glycols in d-Panthenol. (a) 0.00 d-Panthenol, (b) 0.03 d-Panthenol, (c) 0.06 d-Panthenol, (d) 0.09 d-Panthenol, against molality at a different temperature [cyan, polyethylene glycol 200 and magenta, polyethylene glycol 400]

Figure 4.52



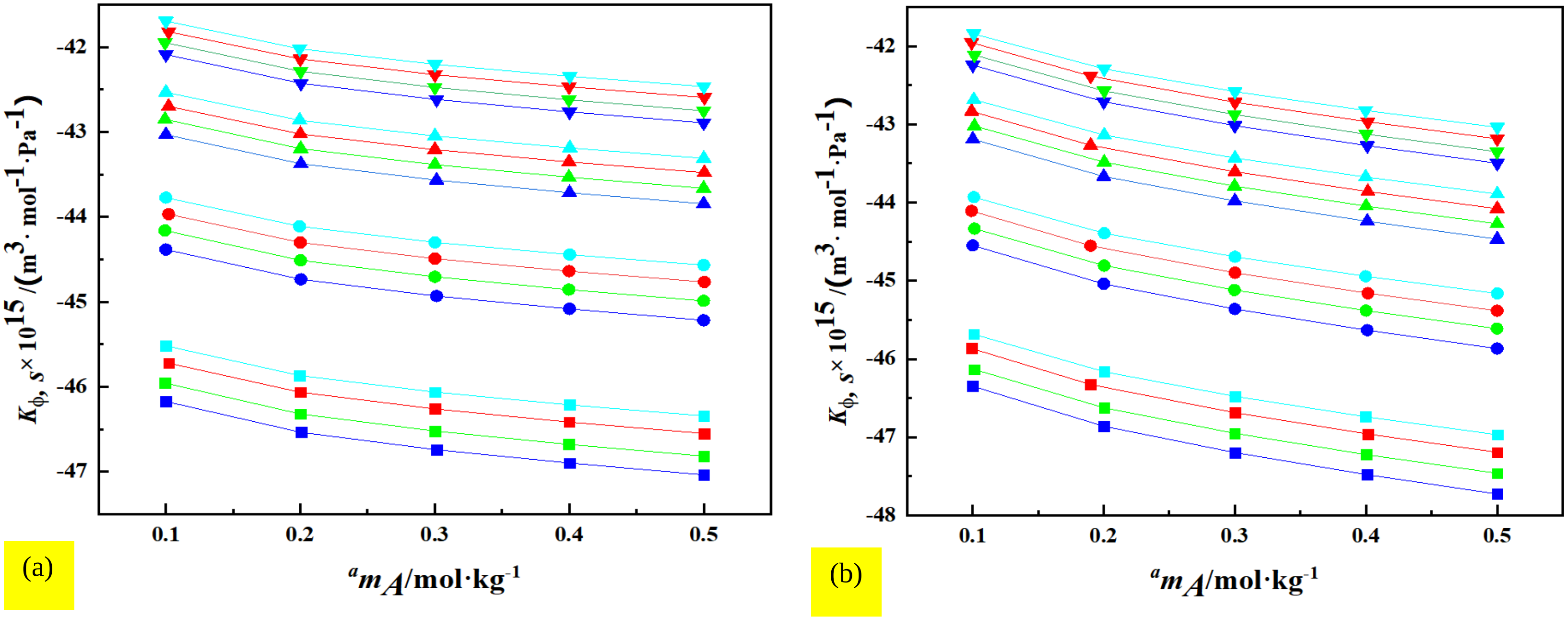
Variation of partial molar volumes, V_ϕ^0, corresponding to the molality (m_B) of d-Panthenol. Polyethylene glycol 200 (color green) and polyethylene glycol 400 (color blue) in different concentrations of aqueous d-Panthenol solutions at different temperatures.

Figure 4.53



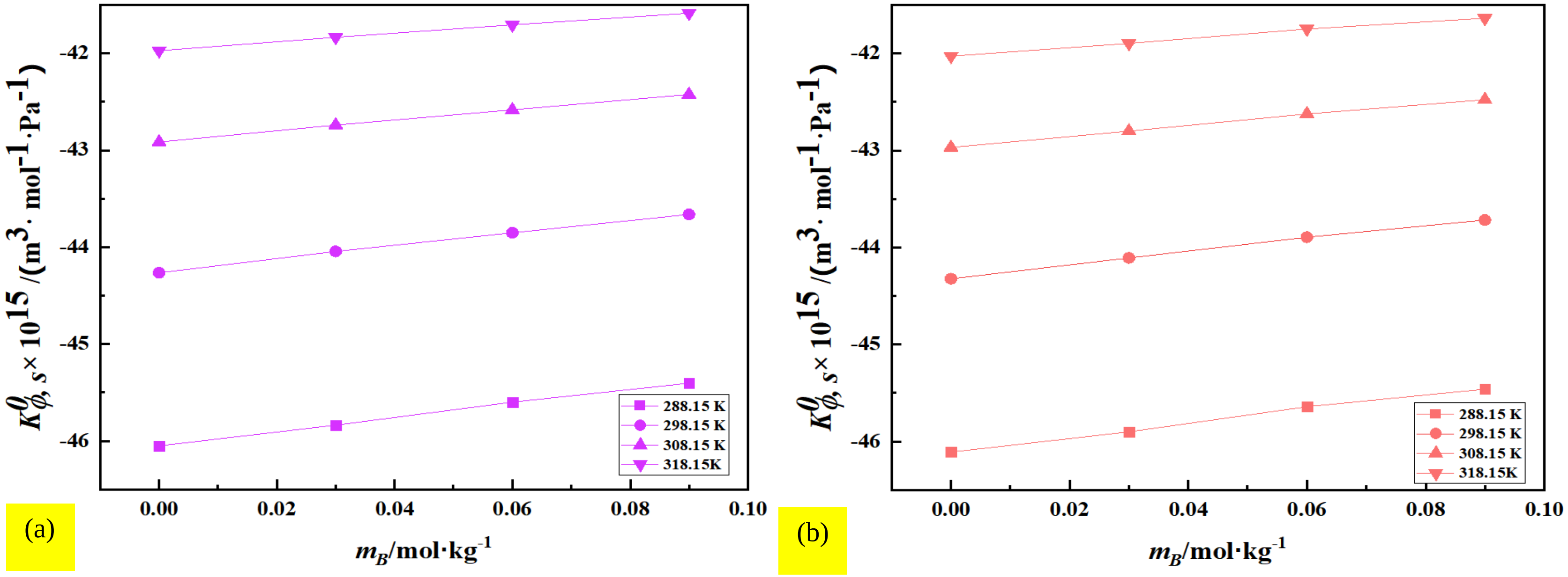
Variation of experimental and literature velocity values of (a) (polyethylene glycol 200+Water) [53] and (b) (polyethylene glycol 400 +Water) [39] corresponding to the molality (m_A) of glycols at different temperatures.

Figure 4.54



Variation of apparent molar isentropic compression, $K_{\phi,s}$, corresponding to the molality (m_A) of glycols in d-Panthenol. (a) polyethylene glycol 200 and (b) polyethylene glycol 400 in aqueous solutions of **(**blue, 0.00 d-Panthenol; green, 0.03 d-Panthenol; red, 0.06 d-Panthenol; cyan**,** 0.09 d-Panthenol**)** against molality at a different temperature [inverted triangle, 318.15 K; triangle, 308.15 K, circle 298.15 K; square, 288.15 K].

Figure 4.55



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, corresponding to the molality (m_A) of glycols in d-Panthenol. (a) Polyethylene glycol 200, and (b) polyethylene glycol 400 in aqueous d-Panthenol solutions at different temperatures.

Problem 9

Measurement of density and ultrasonic speed of sound of polyethylene glycols (600 and 6000) in aqueous vitamin B_5 solutions at different temperatures

In this section, we have reported the densities, ρ and speed of sound c of polyethylene glycol 600 (PEG 600) and polyethylene glycol 6000 (PEG 6000) in (0.00, 0.02, 0.07, and 0.12) mol·kg^{-1} aqueous solutions of d-Panthenol at temperatures T = (288.15, 298.15, 308.15 and 318.15) K.

4.71 Density

For the mixture of liquids (water + d-Panthenol + PEG 600/PEG 6000), the values of density are retrieved at the temperature of T= (288.15 K, 298.15 K, 308.15 K and 318.15 K) and 0.01 MPa pressure as the function of d-Panthenol concentrations (0.00, 0.02, 0.07 and 0.12) mol·Kg^{-1}. These experimental density values are indexed in **Table 4.71** and are compared with the literature values [63, 64] for the binary mixture of (water + PEG 600/PEG 6000) in **Figure 4.57**. At a constant d-Panthenol concentration, the density values are found to be decreasing along the temperature but with the rise in the molality of the polyethylene glycol, these values tend to increase. This trend of the experimental values is in accordance with the literature. Further, as the concentration of d-Panthenol escalates, the values of density upsurges and also as the molecular mass of the polyethylene glycol gets higher i.e. from PEG 600 to PEG 6000, an acceleration in the density is observed which is caused due to the increment in the chain length of the solute [42, 44].

4.72 Apparent molar volume

The density values are used to calculate the apparent molar volume (V_{ϕ}) values from the equation **4.1**. **Table 4.71** constitutes the values of apparent molar volume (V_{ϕ}), which are all positive. This trend manifests the existence of strong (solute-solvent) interaction in the liquid system which increases with the rise in the molecular mass of the polyethylene glycols from PEG 600 to PEG 6000, which signifies the increment in the molecular interaction in the same order and is represented in **Figure 4.56**. At a specific concentration value of d-Panthenol, with the escalation in the temperature and polyethylene glycol molality, the V_ϕ values shows an increment accordingly which is graphically illustrated in **Figure 4.58**. The phenomenon of solvation and great affinity in the solvent creates a strong linear relationship between the values of V_ϕ and temperature as well as polyethylene glycol molality, which explains the nature of molecular interaction in the composition. In the presence of water, the existence of inter-intramolecular hydrogen bonding, hydrophobic effect, hydrophobic hydration, (dipole-induced-dipole) and (dipole-dipole) interactions are established. The low V_ϕ values implies that the molecules of solutes are highly hydrated as in the water molecules its hydrogen bond structure intensifies the packing efficiency whereas the strong (solute-cosolute) interactions are observed due to high values of V_ϕ [1, 46, 55, 56, 65-67].

4.73 Partial Molar volume

To retrieve the values of partial molar volume of the liquid mixtures at infinite dilution containing d-Panthenol and polyethylene glycol, equation **4.2** is applied. m_A denotes the molality of the solute. More valuable information regarding the interactions occurring in (solute-solvent) molecules is imparted by the values of partial molar volume (V_ϕ^0) which is calculated by applying the method of least square fitting. The experimental fitting slope parameter (S_V^*), which is also termed as semi-empirical (solute- solute) interaction parameter and its standard errors are obtained from the same method. The V_ϕ^0 and S_V^* values are provided in **Table 4.72** along with their standard errors. Here the values of V_ϕ^0 are positive that increases with the upsurge in d-Panthenol concentration and temperature as well as with the increment in molecular mass of the polyethylene glycols and is graphically expressed in **Figure 4.59**. According to the model of co-sphere overlap [32, 68], the volume expands when the hydration co-sphere of two ionic species overlaps, but when (ion-hydrophobic) and (hydrophobic- hydrophobic) groups overlap the volume contracts. These positive values of V_ϕ^0 implies the existence of hydrophobic effects and strong hydrogen bond between the (hydroxyl groups of polyethylene glycols and molecules of water) and its variation with the temperature suggests the phenomenon of thermal expansion, hydrogen bond formation, discharge of molecules in solvation layers etc.

since, from the solvation layer of solute the solvation molecules are released in the mixture. The S_V^* parameter is a volumetric coefficient that characterizes the pair-wise interactions within the solvated species and interactions among solute species. The sign of S_V^* values are positive in the current study at all temperatures for all compositions of solution and thus, refers to the pair-wise interaction between (solute-solute) molecules and their constituent ions where the charged functional groups dominates these interactions. However, due to small values of S_V^* as compared to V_ϕ^0 values, the (solute-solvent) interaction dominates in the solution and characterizes the volumetric properties of the liquid mixture [5, 24, 41, 56, 69-74].

4.74 Partial molar volume of transfer

Equation **4.3** is employed to calculate the partial molar volume of Transfer for polyethylene glycols from water to aqueous solutions of d-Panthenol at infinite dilution**.** The partial molar volume of transfer (ΔV_ϕ^0) at infinite dilution provides the knowledge about (solute-solvent) interactions only, because at the small concentrations the interactions within the single molecules of solute becomes negligible and thus supply the information excluding the (solute-solute) interactions. In **Table 4.73** the ΔV_ϕ^0 values reported which are all positive and at a constant temperature, for a polyethylene glycol the values rises with the elevated d-Panthenol concentration. As per the co-sphere theory by Friedman and Krishnan [22] the [(ion-hydrophilic interaction within the zwitterionic groups of polyethylene glycols and –OH groups of d-Panthenol) and (hydrophilic-hydrophilic interactions between the –OH groups of polyethylene glycol and –OH groups of d-Panthenol)], leads to the positive values of ΔV_ϕ^0, whereas the negative values are due to the contribution of [(hydrophilic-hydrophobic interactions among the –OH groups of polyethylene glycols/d-Panthenol and the non-polar groups of d-Panthenol/polyethylene glycols) and (hydrophobic- hydrophobic interactions within the non-polar groups of polyethylene glycol and d-Panthenol)]. Therefore, in the present study the positive values of ΔV_ϕ^0 indicates the dominance of (ion-hydrophilic) and (hydrophilic-hydrophilic) interactions over the (hydrophilic-hydrophobic) and (hydrophobic-hydrophobic) interactions in the liquid system, that surges from PEG 600 to PEG

6000, in the same order as the ΔV_{ϕ}^{0} values increases for the polyethylene glycols, i.e. ΔV_{ϕ}^{0} (PEG 600) $<\Delta V_{\phi}^{0}$ (PEG 6000) at constant temperature and d-Panthenol concentration. Further, the positive nature of ΔV_{ϕ}^{0} values is attributed due to the decrement in the shrinkage volume in aqueous solution of d-Panthenol which is evaluated by the following equation given by Shahidi [75]

$$V_{\phi}^{0} = V_{v.w} + V_{void} - V_{shrinkage} \tag{4.15}$$

Here, $V_{v.w}$ represents the Vander Waal's equation volume, V_{void} represents the empty or void volume, and $V_{shrinkage}$ represents the volume due to change in (solute-solvent) interactions. In water and aqueous d-Panthenol solutions, the $V_{v.w}$ and V_{void} are considered to have same magnitudes, then the decline in $V_{shrinkage}$ alone contributes to the positive values of ΔV_{ϕ}^{0} and implies that on the hydrated polyethylene glycols there is a dehydration effect due to d-Panthenol [55, 66, 76-81].

4.75 Temperature-dependent partial molar volume

The effect of temperature on V_{ϕ}^{0} is very well studied by the values of partial molar expansibilities (E_{ϕ}^{0}) and its first derivative $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$which are calculated with the equation **4.4** by the method of least squares where the data is fitted. T is the temperature in Kelvin, T_{ref}=298.15 K and ($a, b,$ and c) are the empirical constants that are listed in **Table 4.74.** The deviations in the experimental and calculated V_{ϕ}^{0} values are mentioned in the same table and these deviations are evaluated using the equation **4.14**. Here, $\mathrm{Y} = V_{\phi}^{0}$ (apparent molar volume at infinite dilution). The deviation values are very low that perfectly satisfies the polynomial equation that is demonstrated from R^{2}values in the current study [3]. In the table, the empirical constant c describes the scatter in V_{ϕ}^{0} values. The primary objective to analyze the V_{ϕ}^{0} values was to retrieve the partial molar expansibilities using the equation **4.5**. In **Table 4.75** the values of E_{ϕ}^{0} are incorporated with $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ values which are all positive throughout the experimental temperatures for all concentrations of d-Panthenol. This implies the existence of (solute-solvent) interaction in the mixture with the accumulation of d-Panthenol molecules in the interstitial spaces of mixture and as a consequence the structure making property of the solutes are observed. Furthermore, the E_{ϕ}^{0} values shows a symmetric pattern with temperature i.e. the E_{ϕ}^{0} values enhances with the elevation in the temperature, where this trend is associated with the caging or packing effect [82, 83]. These values expands with the temperature as the molecules of the outer hydrated water is affected with the surge in the temperature. Hence, the qualitative information of (solute-solvent) interaction in the system is obtained from the E_{ϕ}^{0} values where Hepler [60] has developed a thermodynamic equation **4.6** that reveals the structure making and structure breaking tendency of solute. The values of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ are ascribed in **Table 4.76,** which evaluates the tendency of structure making or structure breaking property of the solute which is dissolved in solvent by its polarity. If the values of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ are positive it means that solute possess the structure making ability while the negative values infer the structure breaking property of solute in the mixture. In the current study the values of $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ are all positive which suggests the existence of structure making tendency in the solutes [42, 59, 84-87]

4.76 Ultrasonic speed

For the mixture of liquids (water + d-Panthenol + PEG 600/PEG 6000), the values of speed of sound are retrieved at the temperature of T= (288.15 K, 298.15 K, 308.15 K and 318.15 K) and 0.01 MPa pressure as the function of d-Panthenol concentrations (0.00, 0.02, 0.07 and 0.12) mol·Kg^{-1}. These experimental speed of sound values are indexed in **Table 4.76** and are compared with the literature values [63, 64] for the binary mixture of (water + PEG 600/PEG 6000) in **Figure 4.60**. At a constant d-Panthenol concentration, the speed of values are found to be increasing along the temperature and the molality of the polyethylene glycol. This trend of the experimental values is in accordance with the literature. Further, as the concentration of d-Panthenol escalates, the values of speed of sound upsurges and also as the molecular mass of the polyethylene glycol gets higher i.e. from PEG 600 to PEG 6000, the values get elevated. This linear relationship of speed of sound with the temperature implies the formation of inter-intramolecular hydrogen bond between (solute-solvent) interactions which is due to the great association within the molecules of solution and thus leads to the high rate of the combination for the constituent molecules in the mixture. This trend of the speed of sound of the ternary mixture with respect to the temperature is similar to the variation of pure water along the temperature due to the monomeric molecules of water formation and degradation of hydrogen bonds in the water molecules where these depleted molecules of water enters the free space and get stuck in the cage-like structure of the water molecules that results in increase in the close-packed structure numbers with the rise in temperature. The material medium in which the ultrasonic waves are propagating, a closed-packed structure of water is created along the temperature which cause the speed of sound of the ternary mixture to increase with the temperature as the pure water [40, 88, 89].

4.77 Apparent molar isentropic compression

For polyethylene glycols in aqueous d-Panthenol solution, the apparent molar isentropic compression is determined with the equation **4.7**. Here, the densities of the solvent, densities of the solution, molar mass of solute, the molality of solute, and isentropic compressibility of the pure solvent and the solution are symbolized as ρ, $\rho_{0,}$ M, $m_{A,}$ $k_{s.0}$ and k_s respectively. The Laplace-Newton's equation **4.8** [90] is used to calculate the isentropic compressibility where c is the speed of sound. In **Table 4.76** the negative values of apparent molar isentropic compression ($K_{\phi,S}$) are mentioned, where at a constant d–Panthenol concentration the negativity of $K_{\phi,S}$ values decreases with the temperature but increases with the polyethylene glycol molality which is graphically illustrated in **Figure 4.61.** The $K_{\phi,S}$ values become positive due to the hydrophobic solutes and negative due to the ionic compounds in water and hydrophilic solutes. Thus in the present investigation, the negative values of $K_{\phi,S}$ implies the hydration of solutes in the proximity of hydrophilic groups of their molecules, the electrostriction of water occurs. But when the temperature gets higher around the molecules of solute, the electrostriction water gets removed which decreases the negativity of the $K_{\phi,S}$ values with temperature. Further, it is noticed that as the concentration of d-Panthenol is accelerated, the negativity of $K_{\phi,S}$ values decreases which indicates that the molecules of water are less compressible than the water molecules in bulk around any ionic charge groups of polyethylene glycols and thus as a consequence the structural compressibility of water is lost which forms an arrangement around the solute with the water molecules. This behavior establishes the survival of (solute-solvent) interactions in the ternary mixture along with the (dipole-dipole) interactions within the –OH groups of polyethylene glycols and water molecules in its close vicinity [2, 6, 45, 84, 86, 91, 92, 93, 94,].

4.78 Partial molar isentropic compression

With the equation **4.9**, the partial molar isentropic compression is determined by contemplating the divergence of apparent molar isentropic compression corresponding to the molality. The partial molar isentropic compression ($K_{\phi,S}^{0}$) and the experimental fitting slope parameter (S_k^*), with its standard errors are obtained by applying the method of least square fitting which are provided in **Table 4.77**. Here the values of $K_{\phi,S}^{0}$ are all negative that decreases with the upsurge in d-Panthenol concentration and temperature which is graphically expressed in **Figure 4.62**. The negative nature of $K_{\phi,S}^{0}$ values refers to the (hydrophobic and hydrophilic) effects and the existence of strong (solute-solvent) interactions in the sample which makes the solutions less compressible as the electrostriction of the water is reduced due to its release in bulk. Kirkwood [63] had developed a model that explains the variation of negative $K_{\phi,S}^{0}$ values with the temperatures and d-Panthenol concentrations. This theory states that due to more open structure of bulk water as compared the electrostriction water which is more compressible, suppresses the electrostriction interaction among (water and polyethylene glycols) molecules since the interactions with the (polyethylene glycol and d-Panthenol) molecules intensifies. This makes the solute more compressible as the electrostriction water is released from the solvation layer of the bulk. The S_k^* parameter, is the indicative of (solute-solute) interactions in the mixtures which is very small as compared to the values of $K_{\phi,S}^{0}$. These diminished values of S_k^* suggests that the contribution of (solute-solute) interactions in the system is completely insignificant and (solute-solvent) interactions in prominent in the liquid system [59, 84-86, 95-97].

4.79 Partial molar isentropic compression of transfer

At infinite dilution, the partial molar isentropic compression of transfer is computed with the equation **4.10** for polyethylene glycol from water to aqueous d-Panthenol solutions. The partial molar isentropic compression of transfer ($\Delta K_{\phi,s}^{0}$) values are reported in **Table 4.78,** which are all positive and at a constant temperature, for a polyethylene glycol, the $\Delta K_{\phi,s}^{0}$ values increases with the concentration of d-Panthenol. Along the d-Panthenol concentration, the electrostriction water becomes compressible than the bulk due to reduction in compressibility. This leads to the positive values of $\Delta K_{\phi,s}^{0}$ even though the $K_{\phi,s}^{0}$ values are negative throughout the temperatures and d-Panthenol concentrations. The increment in the values of $\Delta K_{\phi,s}^{0}$ with the concentration of d-Panthenol indicates the presence of strong interactions between d-Panthenol and zwitterionic center of polyethylene glycols which cause the reduction in the electrostriction and thus leads to the structure making tendency in solutes. At low temperature and d-Panthenol concentrations, due to the merging of water molecules with solvent make the water molecules associate with the ions in the mixture [1, 19, 88, 97-99].

4.80 Pair and triplet coefficients

Pair-triplet volumetric coefficients (V_{AB}; V_{ABB}) and pair-triplet acoustic coefficients (K_{AB}; K_{ABB}) are obtained from ΔV_{ϕ}^{0} and ΔK_{ϕ}^{0} respectively with the equation **4.11** and **4.12** where m_B denotes the molality of the aqueous d-Panhenol solutions, A represents polyethylene glycols and B represents d-Panthenol. McMillian –Mayer theory [21] helps to study the separation effects in the liquid due to (pair-triplet) interactions in the molecules and is used to calculate these interaction coefficients which was later discussed by Friedman and Krishnan [22] and Franks et al [62]. From the **Table 4.79** it can be observed that the pair-wise interaction coefficients (V_{AB}; K_{AB}) are all positive throughout the temperatures whereas the triplet interaction coefficients (V_{ABB}; K_{ABB}) are almost negative. This trend establishes the dominance of pair-wise interaction coefficient in the ternary mixture. This theory states that water is released to the bulk from the co-sphere which results in the change of volume and this change is positive when the bulk is more structured than the co-sphere but negative change in the volume is observed due to the co-sphere being more structured than the bulk since the molecules of water organized themselves in different structures [68, 69, 95, 100].

Table 4.71

Values of densities, ρ, apparent molar volumes, V_ϕ of polyethylene glycols in aqueous solutions of D-Panthenol at different temperatures

$^a m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^6$/(m^3·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.00 mol·kg^{-1} D-Panthenol + PEG 600								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.01001	1.00095	0.99871	0.99567	0.99195	430.36	434.01	438.06	442.53
0.02000	1.00258	1.00031	0.99724	0.99349	432.58	436.29	440.22	444.48
0.03001	1.00416	1.00186	0.99876	0.99498	434.68	438.30	442.40	446.50
0.03999	1.00568	1.00335	1.00022	0.99642	436.76	440.34	444.44	448.47
0.05011	1.00718	1.00481	1.00165	0.99781	438.65	442.52	446.38	450.76
0.02 mol·kg^{-1} D-Panthenol + PEG 600								
0.00000	0.99999	0.99787	0.99489	0.99117				
0.00999	1.00164	0.99949	0.99647	0.99272	434.20	438.22	442.19	446.15
0.02004	1.00324	1.00106	0.99801	0.99423	436.46	440.32	444.44	448.35
0.03011	1.00479	1.00257	0.99950	0.99569	438.33	442.34	446.30	450.18
0.03999	1.00626	1.00401	1.00091	0.99708	440.40	444.48	448.23	452.18
0.04899	1.00756	1.00528	1.00214	0.99828	442.08	446.20	450.22	454.17
0.07 mol·kg^{-1} D-Panthenol + PEG 600								

0.00000	1.00200	0.99991	0.99679	0.99297				
0.01002	1.00360	1.00148	0.99833	0.99448	438.51	442.70	446.63	450.05
0.02001	1.00515	1.00299	0.99981	0.99594	440.59	444.78	448.52	452.01
0.03002	1.00664	1.00445	1.00125	0.99735	442.53	446.75	450.43	454.08
0.04041	1.00814	1.00592	1.00268	0.99877	444.58	448.70	452.45	456.01
0.05012	1.00950	1.00723	1.00398	1.00003	446.37	450.59	454.29	458.04
0.12 mol·kg^{-1} D-Panthenol + PEG 600								
0.00000	1.00362	1.00147	0.99838	0.99448				
0.01012	1.00520	1.00302	0.99989	0.99597	442.32	446.30	450.33	454.28
0.01990	1.00667	1.00446	1.00130	0.99735	444.45	448.29	452.29	456.32
0.02999	1.00813	1.00589	1.00270	0.99873	446.40	450.25	454.32	458.36
0.04031	1.00958	1.00730	1.00408	1.00008	448.36	452.25	456.37	460.39
0.05007	1.01089	1.00858	1.00534	1.00130	450.33	454.27	458.26	462.55
0.00 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.01002	1.00850	1.00628	1.00331	0.99970	5034.83	5044.35	5052.99	5060.62
0.02003	1.01680	1.01458	1.01165	1.00810	5038.88	5048.43	5056.39	5064.15
0.02999	1.02427	1.02205	1.01916	1.01566	5042.89	5052.48	5060.31	5068.68
0.04002	1.03110	1.02887	1.02600	1.02257	5046.78	5056.57	5064.91	5072.65
0.05014	1.03736	1.03513	1.03231	1.02891	5050.83	5060.44	5068.37	5076.72

0.02 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	0.99999	0.99787	0.99489	0.99117				
0.00998	1.00909	1.00696	1.00402	1.00036	5042.46	5052.71	5060.09	5068.93
0.02006	1.01736	1.01522	1.01231	1.00872	5046.53	5056.11	5064.83	5072.47
0.03008	1.02478	1.02263	1.01977	1.01622	5050.68	5060.70	5068.59	5077.24
0.04024	1.03160	1.02945	1.02659	1.02308	5054.68	5064.42	5073.31	5082.42
0.05001	1.03757	1.03539	1.03252	1.02903	5058.38	5068.85	5078.37	5088.31
0.07 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	1.00200	0.99991	0.99679	0.99297				
0.01041	1.01130	1.00922	1.00616	1.00241	5051.00	5058.79	5066.25	5074.64
0.01988	1.01893	1.01685	1.01383	1.01013	5054.15	5062.23	5070.17	5078.89
0.03005	1.02633	1.02427	1.02129	1.01766	5058.75	5066.52	5074.22	5082.91
0.04007	1.03294	1.03088	1.02792	1.02436	5062.45	5070.34	5078.72	5086.86
0.05022	1.03903	1.03697	1.03405	1.03056	5066.37	5074.45	5082.61	5090.65
0.12 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	1.00362	1.00147	0.99838	0.99448				
0.01032	1.01271	1.01057	1.00752	1.00371	5058.27	5066.58	5074.81	5082.19
0.02007	1.02042	1.01829	1.01529	1.01155	5062.58	5070.48	5078.46	5086.20
0.03004	1.02756	1.02544	1.02248	1.01880	5066.41	5074.14	5082.28	5090.47

0.03998	1.03401	1.03189	1.02896	1.02536	5070.11	5078.27	5086.32	5094.11
0.04990	1.03984	1.03772	1.03485	1.03130	5074.59	5082.80	5090.52	5098.41

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1} and $u(V_\phi)$ =±(0.05-0.07) × 10^{6}/ (m^{3}·mol^{-1}.

Table 4.72

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_V^*, of polyethylene glycols in aqueous solution of D-Panthenol at different temperatures.

[a]m_B/ (mol·kg^{-1})	$V_{\phi}^{0} \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-2})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
				PEG 600				
0.00	428.39(±0.11)	431.98(±0.08)	436.05(±0.10)	440.42(±0.10)	207.17(±3.57)	210.30(±2.50)	208.27(±3.14)	204.18(±3.26)
0.02	432.29(±0.11)	436.19(±0.06)	440.23(±0.12)	444.15(±0.11)	201.16(±3.59)	205.34(±1.87)	202.59(±3.81)	202.89(±3.61)
0.07	436.61(±0.07)	440.81(±0.06)	444.70(±0.01)	448.05(±0.05)	196.10(±2.25)	195.79(±2.05)	191.33(±0.55)	198.73(±1,73)
0.12	440.39(±0.08)	444.30(±0.04)	448.33(±0.02)	452.20(±0.06)	198.81(±2.64)	198.40(±1.27)	198.89(±0.77)	205.45(±2.08)
				PEG 6000				
0.00	5030.89(±0.05)	5040.37(±0.09)	5048.82(±0.37)	5056.36(±0.24)	398.03(±1.54)	402.27(±2.88)	392.00(±1.22)	406.13(±7.51)
0.02	5038.54(±0.12)	5048.38(±0.37)	5055.53(±0.43)	5063.26(±0.87)	399.03(±3.80)	404.83(±1.14)	449.21(±3.22)	485.88(±2.31)
0.07	5046.75(±0.29)	5054.57(±0.14)	5061.94(±0.16)	5070.73(±0.25)	391.40(±8.79)	395.05(±4.47)	413.53(±5.10)	400.50(±7.59)
0.12	5054.21(±0.26)	5062.24(±0.30)	5070.56(±0.02)	5078.04(±0.18)	405.39(±7.92)	406.16(±9.15)	396.58(±5.81)	407.26(±5.45)

[a] m_B is the molality of aqueous D-Panthenol, standard uncertainties *u* are *u(m)* $= 2 \times 10^{-5}$ mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}, *u(*V_{ϕ}^{0}*)* =±0.01 × 10^6/ (m^3·mol^{-1}) and *u(* S_V^**)* =±0.03 × 10^6/ (m^3·mol^{-2}).

Table 4.73

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of polyethylene glycols in aqueous solution of D-Panthenol at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 600		
0.02	3.91	4.21	4.18	3.73
0.07	8.22	8.83	8.66	7.63
0.12	12.00	12.33	12.28	11.78
		PEG 6000		
0.02	7.66	8.01	6.71	6.90
0.07	15.87	14.20	13.12	14.36
0.12	23.32	21.87	21.74	21.67

[a] m_B is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa and $u(c)$= 0.6 m·s^{-1}.

Table 4.74

Values of empirical parameters of Eq., of polyethylene glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	ARD
			PEG 600		
0.02	436.2279	0.3955	0.0001	0.9999	0.0001
0.07	440.8446	0.4034	-0.0021	0.9999	0.0000
0.12	444.3445	0.3956	-0.0001	0.9999	0.0045
			PEG 6000		
0.02	5047.8929	0.8657	-0.0053	0.9999	0.0001
0.07	5054.2863	0.7686	0.0024	0.9999	0.0000
0.12	5062.4095	0.8119	-0.0014	0.9999	0.0008

${}^{a}m_B$ is the molality aqueous of D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}.

Table 4.75

Partial molar expansibilities, E_ϕ^0, for polyethylene glycols in aqueous solution of D-Panthenol at different temperatures.

${}^a m_B$/ (mol·kg^{-1})	E_ϕ^0 ×10^6/(m^3· mol^{-1} ·K^{-1})				$(\partial E_\phi^0/\partial T)_p$/ (m^3·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			PEG 600		
0.02	0.3940	0.3955	0.3969	0.3984	0.0001
0.07	0. 3186	0. 3610	0. 4034	0. 4459	0.0042
0.12	0.3978	0.3956	0.3934	0.3912	0.0002
			PEG 6000		
0.02	0. 6548	0. 7602	0. 8657	0.9712	0.0105
0.07	0.7198	0.7686	0.8173	0.8661	0.0049
0.12	0. 7562	0. 7841	0. 8119	0. 8397	0.0028

${}^a m_B$ is the molality aqueous of D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}.

Table 4.76

Values of speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,s}$ of polyethylene glycols in aqueous solutions of D-Panthenol at different temperatures

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^6$/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
	0.00 mol·kg^{-1} D-Panthenol + PEG 600							
0.00000	1466.59	1495.85	1519.84	1536.02				
0.01001	1472.95	1501.99	1524.61	1540.11	-41.98	-40.33	-39.03	-38.17
0.02000	1478.91	1508.01	1529.15	1544.25	-44.37	-42.64	-41.28	-40.39
0.03001	1485.44	1513.47	1533.97	1549.05	-45.22	-43.46	-42.08	-41.18
0.03999	1490.96	1518.55	1538.85	1553.77	-45.68	-43.90	-42.50	-41.60
0.05011	1496.77	1523.84	1543.80	1559.02	-45.98	-44.19	-42.79	-41.88
	0.02 mol·kg^{-1} D-Panthenol + PEG 600							
0.00000	1468.57	1498.22	1521.09	1537.55				
0.00999	1474.85	1504.46	1526.01	1541.68	-41.86	-40.19	-38.96	-38.09
0.02004	1480.91	1510.55	1530.55	1545.95	-44.26	-42.51	-41.22	-40.32
0.03011	1487.67	1516.02	1535.61	1550.84	-45.10	-43.32	-42.01	-41.10
0.03999	1493.16	1521.07	1540.49	1555.59	-45.55	-43.75	-42.43	-41.51
0.04899	1498.37	1525.66	1544.79	1560.17	-45.82	-44.01	-42.68	-41.76

0.07 mol·kg^{-1} D-Panthenol + PEG 600								
0.00000	1475.01	1504.05	1526.01	1541.99				
0.01002	1480.81	1509.94	1530.71	1545.81	-41.52	-39.91	-38.74	-37.90
0.02001	1487.15	1515.69	1535.52	1550.19	-43.87	-42.18	-40.95	-40.09
0.03002	1493.72	1521.37	1540.51	1555.07	-44.70	-42.98	-41.73	-40.86
0.04041	1499.55	1526.68	1545.77	1560.21	-45.16	-43.42	-42.17	-41.28
0.05012	1505.17	1531.66	1550.41	1565.08	-45.44	-43.69	-42.43	-41.54
0.12 mol·kg^{-1} D-Panthenol + PEG 600								
0.00000	1480.25	1508.46	1529.91	1545.16				
0.01012	1485.81	1514.21	1534.45	1549.15	-41.28	-39.73	-38.59	-37.80
0.01990	1491.97	1519.96	1539.09	1553.48	-43.55	-41.92	-40.73	-39.91
0.02999	1498.85	1525.78	1543.96	1558.69	-44.38	-42.73	-41.52	-40.69
0.04031	1505.05	1531.12	1549.41	1563.99	-44.83	-43.16	-41.94	-41.11
0.05007	1510.34	1536.18	1554.15	1568.86	-45.11	-43.43	-42.20	-41.36
0.00 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	1466.59	1495.85	1519.84	1536.02				
0.01002	1497.97	1525.98	1547.01	1559.56	-42.55	-40.87	-39.55	-38.68
0.02003	1529.94	1555.26	1568.88	1579.85	-45.24	-43.47	-42.08	-41.17
0.02999	1558.63	1580.99	1591.96	1601.75	-46.35	-44.54	-43.12	-42.21
0.04002	1585.74	1604.98	1614.26	1622.86	-47.04	-45.20	-43.77	-42.86

0.05014	1610.07	1626.89	1637.27	1646.86	-47.55	-45.70	-44.26	-43.34
0.02 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	1468.57	1498.22	1521.09	1537.55				
0.00998	1499.71	1529.08	1548.31	1561.01	-42.41	-40.73	-39.47	-38.58
0.02006	1532.01	1558.45	1570.23	1581.43	-45.12	-43.33	-42.00	-41.09
0.03008	1561.11	1584.03	1593.65	1603.32	-46.22	-44.39	-43.04	-42.12
0.04024	1588.07	1608.69	1616.31	1625.06	-46.91	-45.05	-43.69	-42.76
0.05001	1612.05	1629.02	1638.05	1648.05	-47.39	-45.52	-44.16	-43.22
0.07 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	1475.01	1504.05	1526.01	1541.99				
0.01041	1506.78	1535.95	1554.72	1566.27	-42.25	-40.62	-39.32	-38.56
0.01988	1536.55	1563.61	1575.21	1585.52	-44.69	-42.96	-41.62	-40.82
0.03005	1565.88	1589.44	1598.92	1608.01	-45.79	-44.03	-42.80	-41.86
0.04007	1593.15	1613.21	1621.01	1629.01	-46.46	-44.67	-43.53	-42.49
0.05022	1617.89	1634.73	1644.01	1652.97	-46.96	-45.15	-44.06	-42.96
0.12 mol·kg^{-1} D-Panthenol + PEG 6000								
0.00000	1480.25	1508.46	1529.91	1545.16				
0.01032	1512.12	1539.99	1559.04	1569.58	-41.92	-40.35	-39.19	-38.37
0.02007	1542.55	1569.21	1579.91	1589.46	-44.39	-42.73	-41.51	-40.68
0.03004	1571.22	1594.52	1603.91	1612.08	-45.45	-43.75	-42.52	-41.67

0.03998	1598.55	1618.45	1625.63	1633.06	-46.10	-44.39	-43.14	-42.29
0.04990	1622.02	1638.47	1648.17	1656.07	-46.58	-44.85	-43.60	-42.75

[a] m_A is the molality of glycols in the aqueous solution D-Panthenol; standard uncertainties *u* are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, , $u(T)$=0.05K, $u(\rho)=0.06$(kg·m^{-3}),, $u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K_{\phi,S})$ =±0.25 × 10^{6}/ (m^{3}·mol^{-1}· GPa^{-1}).

Table 4.77

Partial molar isentropic compression, $K_{\phi,s}^{0}$, and experimental slopes, S_K^*, of polyethylene glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	$K_{\phi,s}^{0}$ ×10^{6}/(m^{3}·mol^{-1}· GPa^{-1})				S_K^* ×10^{6}/(kg·m^{3}·mol^{-2}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				PEG 600				
0.00	-41.86(±0.79)	-40.21(±0.76)	-38.92(±0.74)	-38.06(±0.73)	-92.97(±23.87)	-89.57(±23.06)	-87.25(±22.45)	-85.97(±22.15)
0.02	-41.69(±0.78)	-40.04(±0.75)	-38.81(±0.73)	-37.94(±0.72)	-94.82(±23.82)	-91.24(±22.98)	-89.01(±22.42)	-87.71(±22.12)
0.07	-41.40(±0.77)	-39.80(±0.74)	-38.63(±0.73)	-37.80(±0.72)	-90.82(±23.32)	-87.46(±22.50)	-85.45(±22.00)	-84.29(±21.72)
0.12	-41.15(±0.75)	-39.61(±0.73)	-38.47(±0.71)	-37.68(±0.70)	-89.04(±22.72)	-85.86(±21.46)	-83.93(±21.46)	-82.84(±21.21)
				PEG 6000				
0.00	-42.21(±0.82)	-40.55(±0.79)	-39.23(±0.77)	-38.36(±0.76)	-117.59(±24.86)	-113.38(±23.95)	-110.76(±23.19)	-109.69(±22.92)
0.02	-42.08(±0.82)	-40.41(±0.79)	-39.15(±0.77)	-38.27(±0.76)	-117.33(±24.82)	-112.91(±23.88)	-110.47(±23.18)	-109.33(±22.93)
0.07	-41.87(±0.76)	-40.25(±0.73)	-38.97(±0.71)	-38.19(±0.70)	-111.55(±22.90)	-107.44(±22.05)	-103.73(±21.36)	-104.49(±21.19)
0.12	-41.54(±0.76)	-39.98(±0.74)	-38.82(±0.71)	-38.01(±0.71)	-111.27(±23.09)	-107.38(±22.31)	-105.30(±21.62)	-104.61(±21.44)

${}^{a}m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)$=0.06(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K_{\phi,s}^{0})$ =±0.01 × 10^{6}/(m^{3}·mol^{-1}· GPa^{-1})and $u(S_k^*)$ =±0.24 × 10^{6}/(m^{3}·mol^{-2}· GPa^{-1}).

Table 4.78

Partial molar isentropic compression transfer, $\Delta K_{\phi,s}^{0}$, of polyethylene glycols in aqueous solution of D-Panthenol at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	$\Delta K_{\phi,s}^{0}$ × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 600		
0.02	0.16	0.18	0.11	0.12
0.07	0.45	0.41	0.29	0.27
0.12	0.70	0.60	0.44	0.38
		PEG 6000		
0.02	0.13	0.14	0.08	0.09
0.07	0.34	0.30	0.26	0.17
0.12	0.67	0.56	0.40	0.35

${}^{a}m_B$ is the molality of aqueous D-Panthenol, standard uncertainties u are $u(m)$ = 2×10^{-5} mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}.

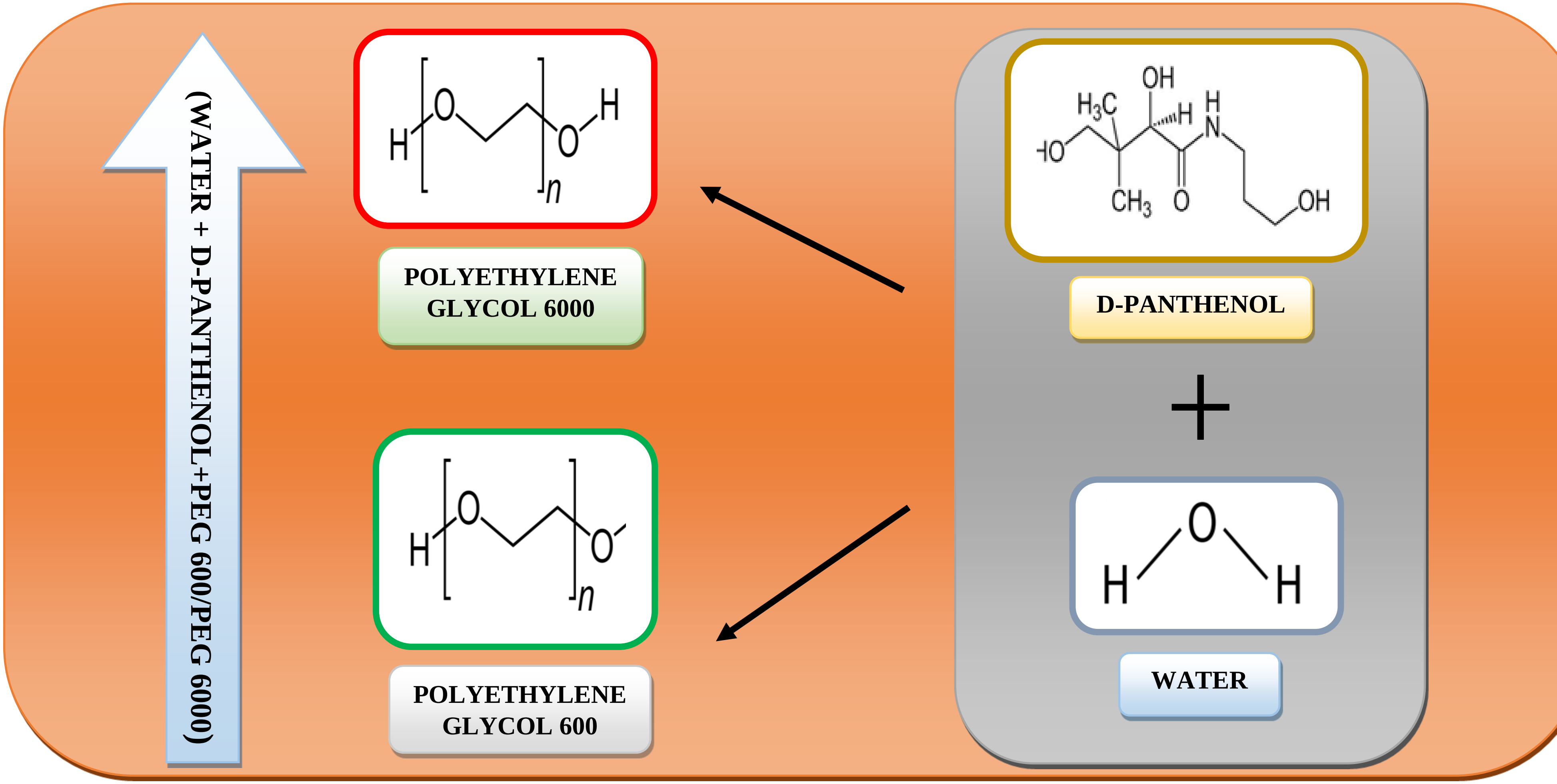
Table 4.79

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of polyethylene glycols in aqueous solutions of D-Panthenol at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		PEG 600		
288.15	80.57	-173.16	3.82	-5.08
298.15	89.14	-213.37	3.85	-7.58
308.15	86.95	-202.42	2.49	-3.62
318.15	72.73	-135.17	2.63	-5.87
		PEG 6000		
288.15	155.66	-331.99	2.37	2.21
298.15	143.97	-303.63	2.35	-0.16
308.15	120.65	-175.20	2.09	-2.24
318.15	138.09	-272.10	1.22	1.17

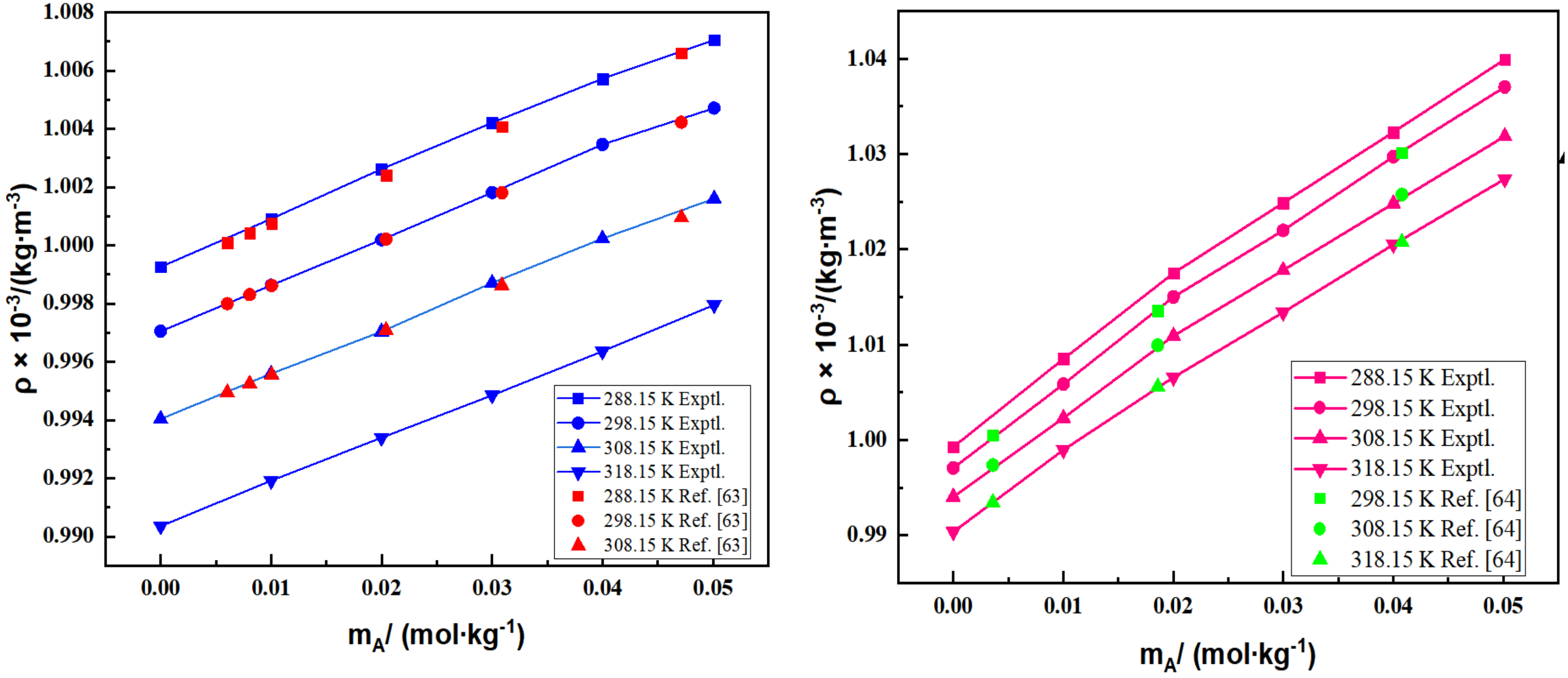
T/K is the temperatures.

Figure 4.56



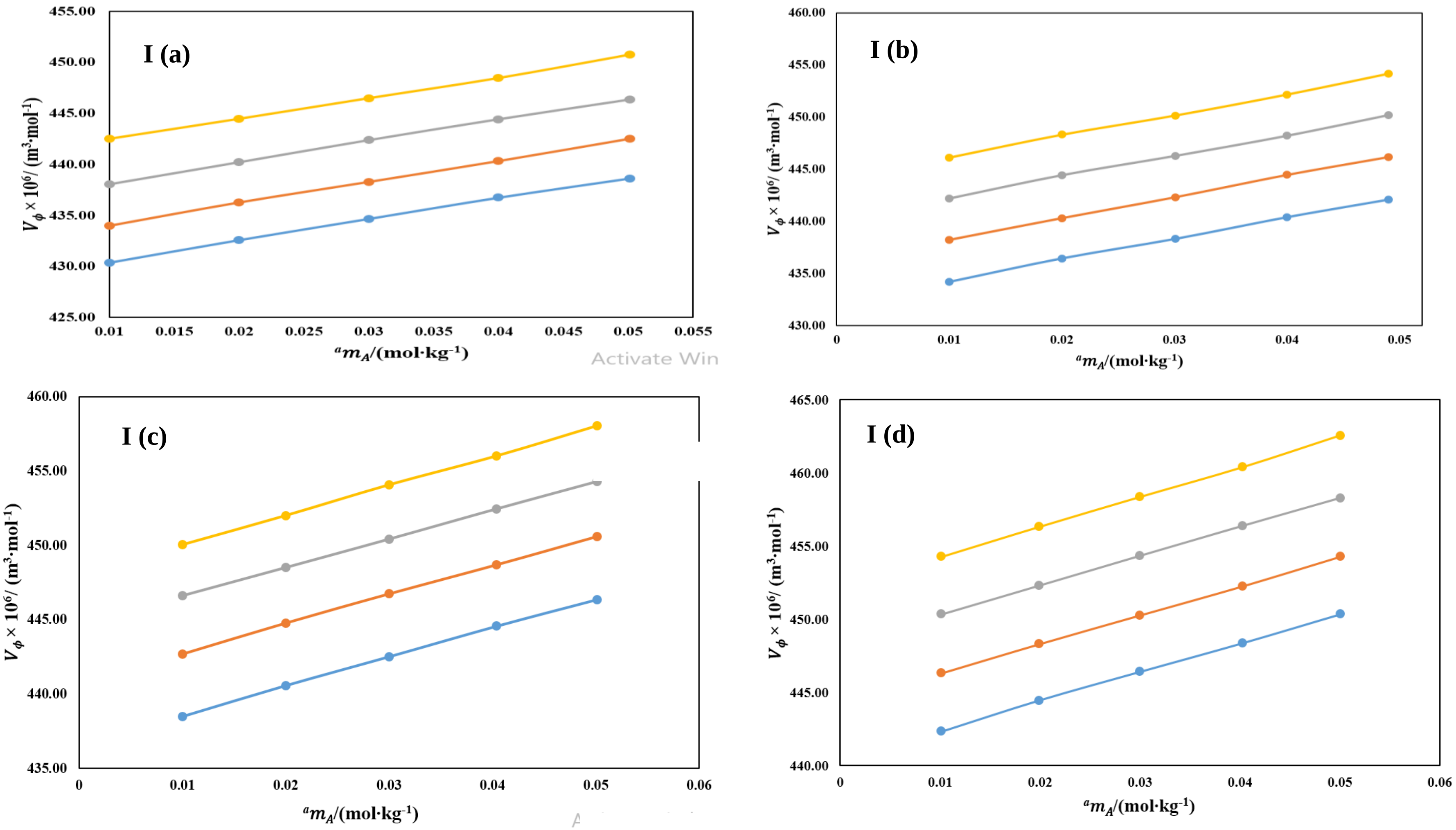
PEG 600 / PEG 6000 and d-Panthenol interactions.

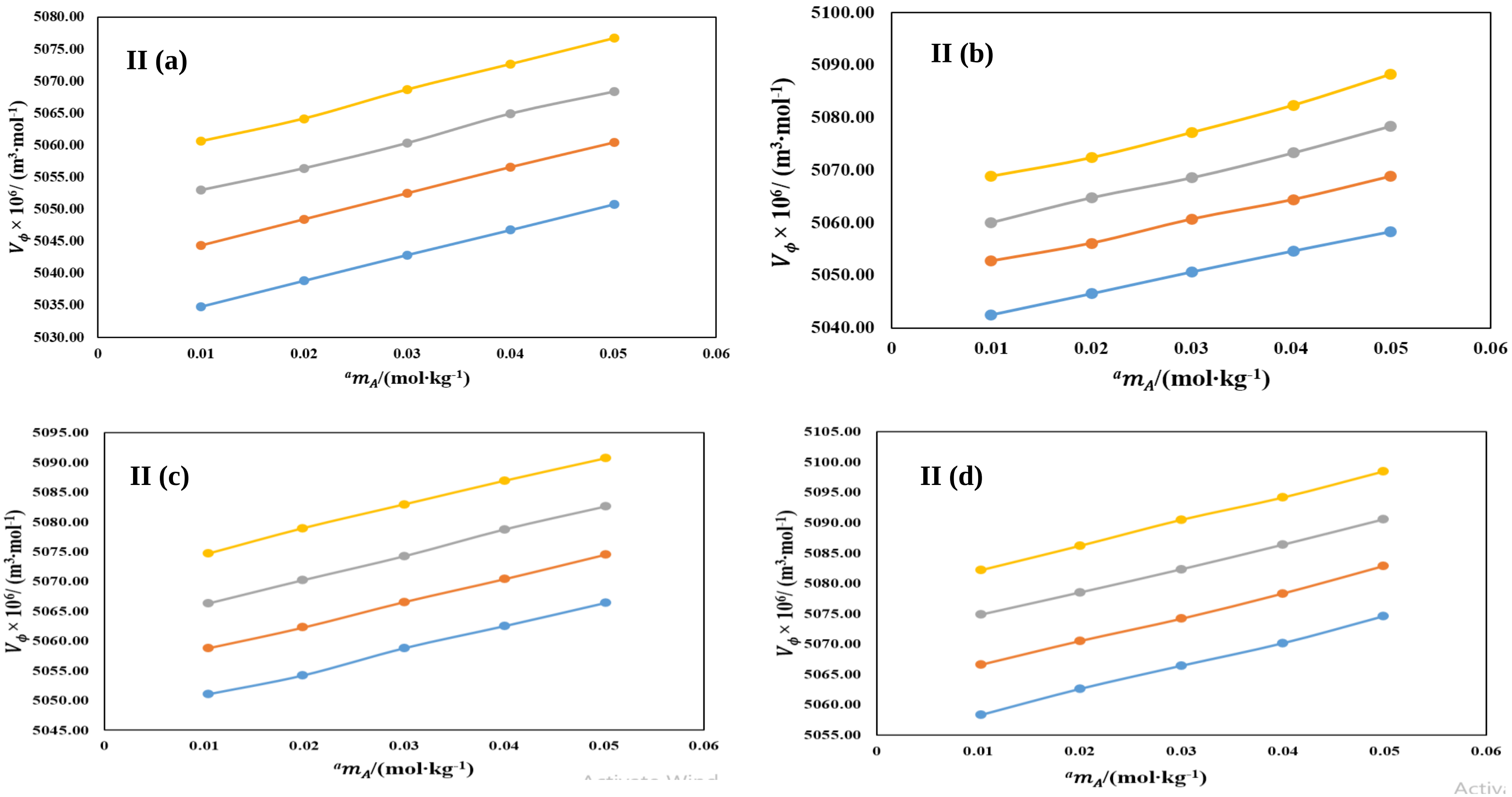
Figure 4.57



Variation of experimental and literature density values [63, 64] of (a) (Polyethylene glycol 600 +Water) and (b) (Polyethylene glycol 6000 +Water) corresponding to the molality (m_A) of glycols at different T.

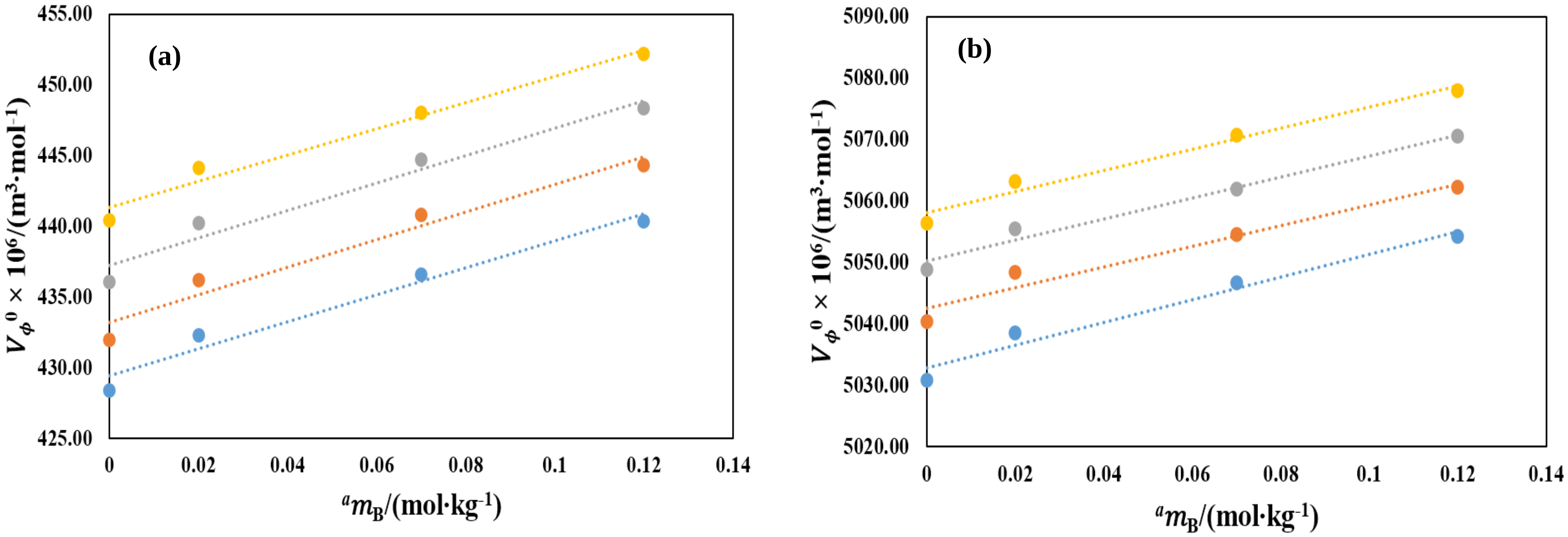
Figure 4.58


I (a)
455.00
450.00
445.00
440.00
435.00
430.00
425.00
0.01
0.015
0.02
0.025
0.03
0.035
0.04
0.045
0.05
0.055
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
I (b)
460.00
455.00
450.00
445.00
440.00
435.00
430.00
0
0.01
0.02
0.03
0.04
0.05
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
I (c)
460.00
455.00
450.00
445.00
440.00
435.00
0
0.01
0.02
0.03
0.04
0.05
0.06
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
I (d)
465.00
460.00
455.00
450.00
445.00
440.00
0
0.01
0.02
0.03
0.04
0.05
0.06
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)



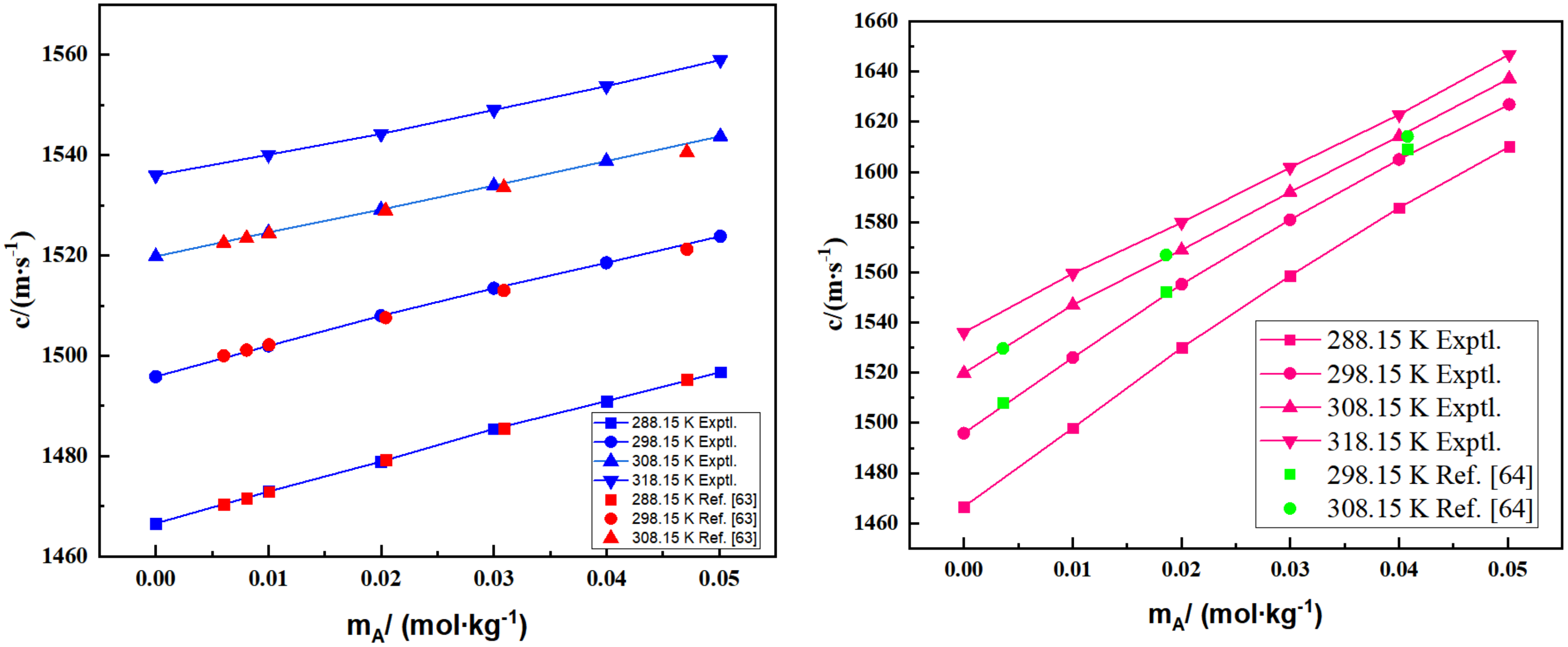
Variation of partial molar volumes, V_ϕ, of, (I) Polyethylene glycol 600 and (II) Polyethylene glycol 6000 in different concentration of aqueous d-Panthenol solutions at different temperatures [blue, 288.15 K; orange, 298.15 K; grey, 308.15 K; yellow 318.15 K]

Figure 4.59



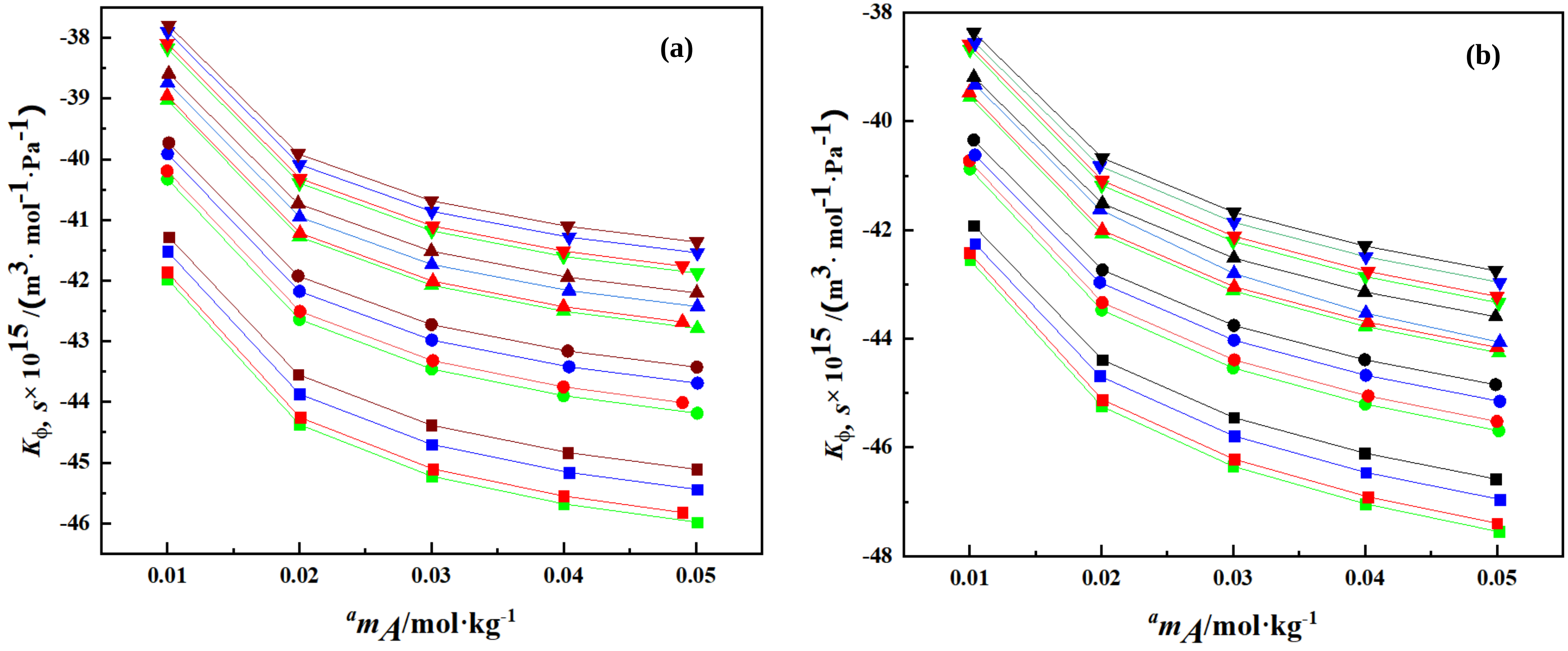
Variation of partial molar volumes, V_ϕ^0, of, (a) Polyethylene glycol 600 and (b) Polyethylene glycol 6000 in different concentration of aqueous d-Panthenol solutions at different temperatures [blue, 288.15 K; orange, 298.15 K; grey, 308.15 K; yellow 318.15 K]

Figure 4.60



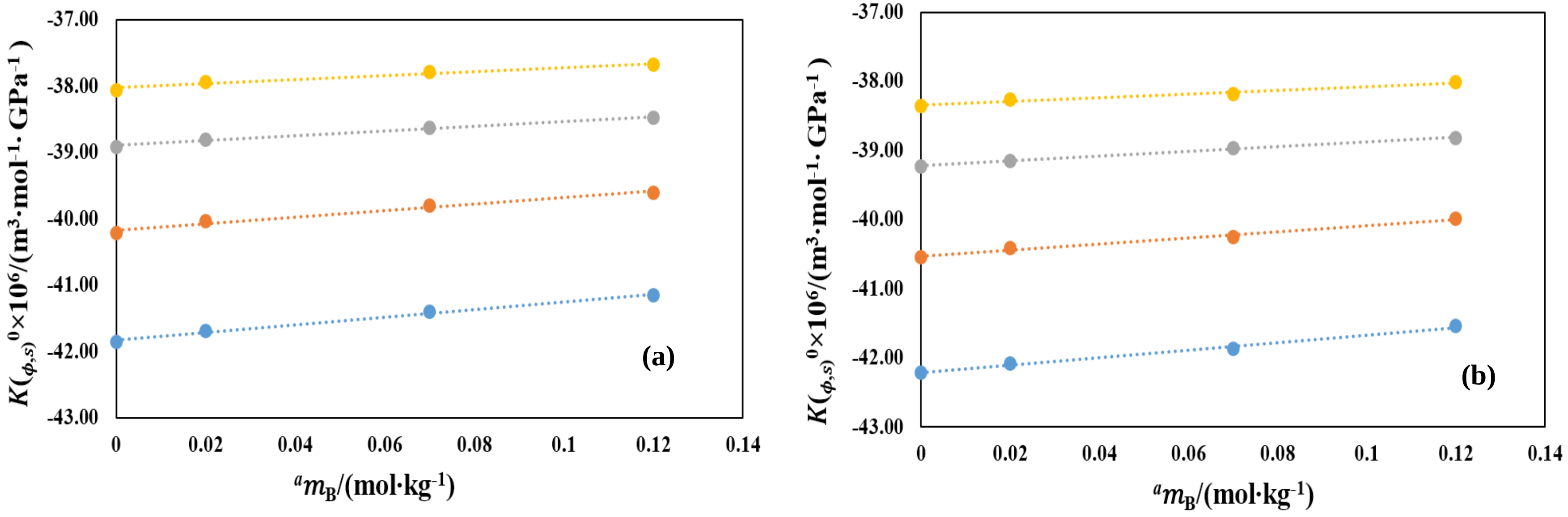
Variation of experimental and literature velocity values [63, 64] of (a) (Polyethylene glycol 600 +Water) and (b) (Polyethylene glycol 6000 +Water) corresponding to the molality (m_A) of glycols at different T.

Figure 4.61



Variation of apparent molar isentropic compression, $K_{\phi,s,}$ of (a) Polyethylene glycol 600 and (b) Polyethylene glycol 6000, against molality [green, 0.00 d-Panthenol; red, 0.02 d-Panthenol; blue, 0.07 d-Panthenol; olive, 0.12 d-Panthenol]at different temperatures [square, 288.15 K; circle, 298.15 K; triangle, 308.15 K; inverted triangle, 318.15 K]

Figure 4.62



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, of (a) Polyethylene glycol 600, and (b) Polyethylene glycol 6000, in aqueous d-Panthenol solutions at different temperatures [blue, 288.15 K; orange, 298.15 K; grey, 308.15 K; yellow 318.15 K]

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Section III

Problem X

Effect of ethylene glycol/diethylene glycol/triethylene glycol on the thermodynamics of the aqueous biotin solutions at various temperatures

In this section, we have reported the densities, ρ and speed of sound c of ethylene glycol (EG), diethylene glycol (DEG) and triethylene glycol (TEG) in (0.0000, 0.0015, 0.0025, and 0.0035) mol·kg^{-1} aqueous solutions of biotin at temperatures T = (288.15, 298.15, 308.15 and 318.15) K.

4.81 Density

The experimental density values for (EG, DEG and TEG) in (0.0000, 0.0015, 0.0025, and 0.0035) mol·Kg^{-1} aqueous biotin solutions are obtained at 0.1 MPa pressure as the function of experimental temperature T= (288.15 K, 298.15 K, 308.15 K, and 318.15 K) and are indexed in **Table 4.80**. The values of density for (water + EG/DEG/TEG) are directly taken from the previous paper [1] and are also compared with the literature values [2] that is graphically described in **Figure 4.64**. From the figure it is observed that the experimental density values and the literature values are consistent with each other throughout the temperatures and molality of glycols. It can be noted that the density values for a particular concentration of biotin, decreases with the rise in the temperature but as the glycol molality increases, the density too increases. Further, with the upsurge in the concentration of biotin, these values also tends to increase. Another behavior of density values which are noticeable is the escalation of these values with the increment in the molar mass of the glycols from EG to DEG to TEG [3, 4].

4.82 Apparent molar volume

The density values are used to calculate the apparent molar volume (V_{ϕ}) values from the equation **4.1**. M, m_A, ρ, and ρ_0 are the molar mass of the solute, molality of the solute per kg of the solvent (water + biotin), densities of the solution, and the solvent respectively. In **Table 4.80** the apparent molar volume (V_{ϕ}) for the liquid combination (water + EG/DEG/TEG) and (water + biotin + EG/DEG/TEG) are provided as the function of temperatures. Although, the V_ϕ values for (water + EG/DEG/TEG) are directly taken from the previous paper [1]. The values of V_ϕ are all positive that increases with the temperatures and molality of glycols at the specific concentration of biotin which is graphically represented in **Figure 4.65**. Also, the V_ϕ values increases with respect to the escalation in the biotin concentration. From the table it is observed that as the molecular mass of the glycol increases from EG to DEG to TEG, the values of apparent molar volume also accelerates along with the molecular interaction that is depicted in **Figure 4.63**. The existence of (solute-solvent) interaction is inferred from the positive values of V_ϕ that has strong linear relationship with the rising temperature and glycol molality. This occurs due to the phenomenon of solvation and great affinity in solvent which describes the nature of the molecular interaction in the composition. The inter-intramolecular hydrogen bond, hydrophobic hydration, hydrophobic effect, (dipole-dipole) and (dipole-induced-dipole) interactions by the glycols (EG, DEG and TEG) are remarked in the solution in presence of water. Thus, significant information are attained from the V_ϕ values and more clear details can be obtained from the partial molar volumes at infinite dilution about the (solute-solvent) and (solute-solute) interactions [5-11].

4.83 Partial Molar volume

To retrieve the values of partial molar volume of the liquid mixtures at infinite dilution containing biotin and glycol, the equation **4.2** is applied. The partial molar volume (V_ϕ^0) and the experimental slope (S_V^*) are calculated using the method of least square fitting that are ascribed in **Table 4.81** along with their standard errors. For (water + EG/DEG/TEG), the values of V_ϕ^0, S_V^* and their standard errors are directly taken from the literature [1]. It can be perceived from the table that the V_ϕ^0 values are all positive and increases as the temperature and biotin concentration rises, which is graphically portrayed in **Figure 4.66**. This trend suggests the presence of strong (solute-solvent) interactions in the sample that accelerates with the biotin concentration and temperatures. This variation of V_ϕ^0 values with the temperature occurs due to the thermal expansion, hydrogen bond formation and the exemption of the solvation molecules from the solvation layer of solute to the solution. Also, with the escalation in the molecular mass of the glycols (EG< DEG< TEG), the (solute-solvent) interaction strengthens since the V_{ϕ}^{0} values shows an upsurge with the rise in the chain length of the solutes. The existence of strong hydrogen bond between the molecules of water and the hydroxyl (-OH) group of glycols and the hydrophobic effects are verified by the positive values of V_{ϕ}^{0} , along with the dominance of (ion-hydrophilic) interactions over (hydrophobic- hydrophobic) interactions. As stated by model of co-sphere overlap [13, 14], an expansion in volume is observed when in two ionic species the hydration co-sphere overlaps while due to the overlapping of (ion-hydrophobic) and (hydrophobic- hydrophobic) groups, a contraction in volume is experienced. The S_{V}^{*} values in table are found to be positive corresponding each temperature and biotin concentrations. This experimental fitting slope parameter, which is also termed as semi-empirical (solute-solute) interaction parameter, represents the (solute-solute) interactions present in the solution, but since the values of V_{ϕ}^{0} are much larger than the S_{V}^{*} values, the preeminence of (solute-solvent) interaction in the sample is established [5, 9,14, 15].

4.84 Partial molar volume of transfer

The equation **4.3** is employed to calculate the partial molar volume of Transfer for glycols from water to aqueous solutions of biotin at infinite dilution**.** Excluding the (solute-solute) interactions in the liquid system, the qualitative details about the (solute-solvent) interaction are deduced from the values of partial molar volume of transfer (ΔV_{ϕ}^{0}) at infinite dilution. The calculated ΔV_{ϕ}^{0} values are found to be positive that are reported in **Table 4.82**. This refers to the presence of (ion-hydrophilic) and (hydrophilic- hydrophilic) interactions in the mixtures that occurs due to the discharge of few molecules of water into bulk as the electrostriction in the water molecules have decreased in the close proximity of the glycols. The increment of ΔV_{ϕ}^{0} values is noticed in the table at a constant temperature along the biotin concentration for each glycol. This nature indicates the formation of hydrogen bond between the hydrophilic groups of glycols and –OH group of biotin as the hydrophilic interactions amidst the molecules of (solute and water) reduces which results in the (hydrophilic-hydrophilic), (ion-hydrophilic) and (hydrophobic- hydrophobic) interactions in the ternary mixture. Thus the co-sphere overlap model [12, 13], predicts the interactions occurring in the sample that are illustrated as- (ion-hydrophilic) interactions within the zwitterionic groups of glycols and –OH groups of biotin ; (ion-hydrophobic) interactions among zwitterionic groups of glycols and alkyl groups of biotin; (hydrophilic- hydrophilic) interactions within hydrophilic groups of glycols and –OH groups of biotin; (hydrophilic- hydrophobic) interactions among alkyl groups of glycols and –OH groups of biotin; hydrophilic groups of glycols and –OH groups of biotin; (hydrophobic- hydrophobic) interactions among alkyl groups of glycols and alkyl groups of biotin. Though, in the mixture the dominance of (ion-hydrophilic) interaction is accomplished above all the other interactions that surges from EG to DEG to TEG, in the same order as the ΔV_{ϕ}^{0} values increases for the glycols, i.e. ΔV_{ϕ}^{0} (EG) <ΔV_{ϕ}^{0} (DEG) <ΔV_{ϕ}^{0} (TEG) at constant temperature and biotin concentration [16-19].

4.85 Temperature-dependent partial molar volume

The variation in the apparent molar volumes at infinite dilution with temperatures are obtained with the equation **4.4**. T is the temperature in Kelvin, T_{ref}=298.15 K and ($a, b,$ and c) are the empirical constants that are listed in **Table 4.83.** The deviations in the experimental and calculated V_{ϕ}^{0} values are mentioned in the same table and these deviations are evaluated using the equation **4.14.** Here, $\mathrm{Y} = V_{\phi}^{0}$ (apparent molar volume at infinite dilution). The deviation values are very low that perfectly satisfies the polynomial equation that is demonstrated from R^2values in the current study [20]. In the table, the empirical constant c describes the scatter in V_{ϕ}^{0} values. The primary objective to analyze the V_{ϕ}^{0} values was to retrieve the partial molar expansibilities using the equation **4.5**. The partial molar expansibility at infinite dilution is denoted as E_{ϕ}^{0} that is calculated as E_{ϕ}^{0}=$\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$, and are mentioned in **Table 4.84** which provides the qualitative information about the (solute-solvent) interactions occurring in the experimental sample. These values are all positive throughout the temperatures as well as biotin concentrations and this behavior implies that the molecules of biotin acquires the interstitial spaces in the sample which causes the property of the structure making in the solutes. For a specific glycol, the E_{ϕ}^{0} values are shows a symmetric trend i.e. the values intensifies as the corresponding temperatures and biotin concentration escalates and hence, suggest the presence of strong (solute-solvent) interactions in the system which increases with the temperature due to caging or packing effect [21, 21], where the molecules of outer hydrated water expands the values of E_{ϕ}^{0} at higher temperatures. Hepler's equation **4.6** [23] is utilized to determine the structure making/breaking ability of the solute in the solution. The structure making or structure breaking ability of the solute is evaluated by the sign of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$. If the value of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ is positive, then the solute possess the structure making property, while, the negative values infers the tendency of structure breaking in the solute. In the current study of (water + Biotin + EG/ DEG /TEG), the values of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ are observed to be positive for all the glycols corresponding each biotin concentration that are indexed in **Table 4.84**. Therefore, the values indicates the structure making capability of the solutes (EG, DEG and TEG) in the solution [24, 25].

4.86 Ultrasonic speed

At multiple temperatures T= (288.15 K, 298.15 K, 308.15 K, and 318.15 K), the speed of sound for the mixtures (water +biotin + EG/DEG/TEG) as the function of biotin concentrations (0.0000, 0.0015, 0.0025, and 0.0035) mol·Kg^{-1}, by keeping a constant pressure of 0.1 MPa, is measured by using Anton Paar DSA 5000 M and the values are reported in **Table 4.85**. The speed of sound values for (water + EG/DEG/TEG) are directly taken from the previous paper [1] and are also compared with the literature values [2] that is graphically described in **Figure 4.76**. From the figure it is observed that the experimental values of speed of sound and the literature values are consistent with each other throughout the temperatures and molality of glycols. It can be noted that the speed of sound values for a particular concentration of biotin, increases with the rise in the temperature and the glycol molality. Also, with the upsurge in the concentration of biotin, these values tend to increase. The intermolecular hydrogen bond in the (solute-solvent) molecules and intramolecular hydration bond in the molecules of glycol creates strong association in the molecules of solutes that increases with the speed of sound and results in high rate of combination in the mixture molecules. The similar trend of increasing with the temperature, is followed by the pure water due to the depletion of hydrogen bond in the water molecules and the development of more monomeric molecules of water. These depleted molecules of water enters the free space and get trapped in the cage-like structure of water which causes the increment in the number of closed-packed structures with the escalation in the temperature. As the ultrasonic waves propagate, the material medium is created due to the development of a close-packed structure of water with temperatures. That is why with the upsurge in the temperature the speed of sound values increases for pure water and in a similar way for glycols in aqueous biotin solutions [26-28].

4.87 Apparent molar isentropic compression

For glycols in aqueous biotin solution, the apparent molar isentropic compression is determined with the equation **4.7**. Here, the densities of the solvent, densities of the solution, molar mass of solute, the molality of solute, and isentropic compressibility of the pure solvent and the solution are symbolized as ρ, $\rho_{0,}$ M, $m_{A,}$ $k_{S.0}$ and k_S respectively. The undermentioned Laplace-Newton's formula **4.8** [29] is used to calculate the isentropic compressibility where c is the speed of sound. In (0.0000, 0.0015, 0.0025, and 0.0035) mol·Kg^{-1} biotin, the apparent molar isentropic compressibility ($K_{\phi,S}$) is calculated at different temperatures for glycols (EG/DEG/TEG) that are mentioned in **Table 4.85** and are graphically illustrated in **Figure 4.68**. The $K_{\phi,S}$ values for (water + EG/DEG/TEG) are directly taken from the previous paper [1]. It is noteworthy that the values of $K_{\phi,S}$ are negative throughout the glycol molalities and temperatures, where this negativity decreases with the rise in temperature but as the molality increases, the $K_{\phi,S}$ values become more negative at constant biotin concentration. Further, with the increment in the concentration of biotin, the $K_{\phi,S}$ values tends to become less negative. This nature of compressibility values implies that the water molecules in the vicinity of the ionic charges groups of glycols are less compressible than the water molecules around the bulk due to which the structural compressibility of the water reduces and forms an arrangement of water molecules over solute [30-32]. With the biotin molecules the glycols constitute compact structures through intermolecular hydrogen bonding that results in the decrement of compressibility. The existence of strong (solute-solvent) interactions are confirmed with the (dipole-dipole) interactions between the –OH groups of glycols and molecules of water present in its proximity [33-35].

4.88 Partial molar isentropic compression

With the equation **4.9**, the partial molar isentropic compression is determined by contemplating the divergence of apparent molar isentropic compression corresponding to the molality. The partial isentropic compression ($K_{\phi,S}^{0}$) and the experimental slope (S_{k}^{*}) are calculated using the method of least square fitting that are ascribed in **Table 4.86** along with their standard errors. For (water + EG/DEG/TEG), the values of $K_{\phi,S}^{0}$, S_{k}^{*} and their standard errors are directly taken from the literature [1]. It can be perceived from the table that the $K_{\phi,S}^{0}$ values are all negative, which decreases as the temperature and biotin concentration rises, which is graphically portrayed in **Figure 4.69**. With the upsurge in the molecular mass of the glycols i.e. from EG to DEG to TEG, the $K_{\phi,S}^{0}$ values also accelerates that indicates the survival of strong attractive interactions amidst the molecules of water and glycols where the devaluation in the electrostriction makes the water molecules release in the bulk which is described with the model given by Kirkwood [36]. This model states that electrostriction water has a less open structure as compared to the bulk water that makes the former more compressible, thus as a consequence, the molecules of glycols and water suppresses the electrostriction interaction in the system which increases the interaction among the biotin and glycol molality. The solute become more compressible as the electrostriction water is discharged from the solvation layer into bulk. The (solute-solute) interactions in the mixture are approximately insignificant as the S_{k}^{*} values in the table are very small as compared to the $K_{\phi,S}^{0}$ values which implies the dominance of (solute-solvent) interactions in the sample mixture [7, 37].

4.89 Partial molar isentropic compression of transfer

At infinite dilution, the partial molar isentropic compression of transfer is computed with the equation **4.10** for glycol from water to aqueous biotin solutions. In **Table 4.87** the calculated values of partial molar isentropic compression of transfer ($\Delta K_{\phi,S}^{0}$) is indexed, which are positive at all temperatures and biotin concentrations. A regular pattern emerges for $\Delta K_{\phi,S}^{0}$ values, where at a constant temperature of glycol, the values appears to be increasing with the biotin concentration, whereas along the variation in the temperature an asymmetric nature is observed, this trend of positive $\Delta K_{\phi,s}^{0}$ values indicates the habitation of strong interactions in zwitterionic centers of glycols and biotin that enhances corresponding the biotin concentration as the structure making ability of the solute is realized due to the reduction in the electrostriction. Since, the electrostriction water is compressible as compared to the bulk, this leads to the decrement in the compressibility of the mixture with the biotin concentration which makes the $\Delta K_{\phi,s}^{0}$values positive while the $K_{\phi,s}^{0}$values are negative for (EG /DEG/ TEG) at various temperatures and biotin concentrations. The water molecules associates with the ions at low temperatures and biotin concentrations as the solvent molecules are merged with the water molecules [11, 38-40].

4.90 Pair and triplet coefficients

The partial molar volume of transfer and the partial molar isentropic compression of transfer is obtained from the equation **4.11** and **4.12**. Where m_B denotes the molality of the aqueous biotin solutions, A represents glycols and B represents biotin. V_{AB}; V_{ABB} and K_{AB}; K_{ABB} represents the pair and triplet coefficients for volume and isentropic compression respectively which are mentioned in **Table 4.88.** These values are calculated using the theory of McMillian and Mayer [41] by fitting the partial molar values for volumes and isentropic compression (ΔV_{ϕ}^{0}; ΔK_{ϕ}^{0}). This theory investigates the separation of effects in the liquid mixture due to the pair and triplet interactions among the molecules. Friedman and Krishnan [42] and Franks et al [43] had discussed the same theory further. From the table it can be seen that the pair interaction coefficient (V_{AB}; K_{AB}) are positive throughout the temperatures. On the other hand, the triplet interaction coefficients (V_{ABB}; K_{ABB}) are all positive except at 318.15 K, V_{ABB} is negative for EG and at (288.15 K, K_{ABB}; 298.15 K and 318.15 K, V_{ABB}) is negative for DEG. Following this model, the water is discharged to the bulk from the co-sphere which changes the volume. This change is positive when the bulk is more structured than the co-sphere while if the co-sphere is more structured than the bulk, the change is negative since the molecules of water are organized in different structures which are released from the hydration co-spheres to the bulk when non-bonding interaction is developed. Thus, due to more negative values of triplet wise interaction coefficient in the solution, the dominance of pair-wise interaction coefficient is established [44-46].

Table 4.80

Values of densities, ρ, apparent molar volumes, V_ϕ of glycols in aqueous solutions of biotin at different temperatures and at the experimental pressure=0.1 MPa

$^a m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^6$/ (m^3·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				EG+0.0000 mol·kg^{-1} biotin				
0.00000	0.99926	0.99705	0.99404	0.99036^a				
0.09889	1.00012	0.99788	0.99484	0.99113	53.36	53.77	54.20	54.61^a
0.19894	1.00096	0.99869	0.99561	0.99188	53.45	53.87	54.35	54.78
0.29967	1.00179	0.99947	0.99636	0.99261	53.53	53.98	54.47	54.89
0.39481	1.00253	1.00018	0.99704	0.99326	53.64	54.09	54.59	55.01
0.50155	1.00335	1.00096	0.99776	0.99397	53.73	54.19	54.72	55.12
				EG+0.0015 mol·kg^{-1} biotin				
0.00000	0.99966	0.99755	0.99463	0.99098				
0.10045	1.00053	0.99839	0.99543	0.99175	53.41	53.79	54.27	54.77

0.19785	1.00132	0.99916	0.99617	0.99246	53.58	53.97	54.45	54.92
0.30036	1.00212	0.99993	0.99690	0.99317	53.76	54.15	54.62	55.08
0.39888	1.00284	1.00062	0.99756	0.99380	53.94	54.32	54.82	55.27
0.50340	1.00355	1.00131	0.99822	0.99442	54.14	54.51	54.99	55.48
EG+0.0025 mol·kg^{-1} biotin								
0.00000	0.99984	0.99778	0.99481	0.99130				
0.09790	1.00067	0.99859	0.99558	0.99204	53.55	53.89	54.38	54.90
0.20050	1.00150	0.99939	0.99636	0.99278	53.70	54.04	54.53	55.04
0.30008	1.00227	1.00014	0.99707	0.99346	53.84	54.19	54.67	55.17
0.39919	1.00300	1.00084	0.99774	0.99409	53.99	54.34	54.83	55.34
0.50201	1.00371	1.00152	0.99837	0.99470	54.16	54.52	55.03	55.53
EG+0.0035 mol·kg^{-1} biotin								
0.00000	1.00000	0.99798	0.99507	0.99165				
0.09926	1.00083	0.99879	0.99584	0.99239	53.62	54.00	54.46	54.96

0.20053	1.00164	0.99957	0.99660	0.99312	53.77	54.14	54.59	55.09
0.30031	1.00240	1.00031	0.99731	0.99380	53.92	54.29	54.73	55.22
0.39897	1.00312	1.00099	0.99797	0.99443	54.08	54.46	54.87	55.37
0.50012	1.00381	1.00166	0.99861	0.99503	54.24	54.62	55.03	55.54
DEG+0.0000 mol·kg^{-1} biotin								
0.00000	0.99926	0.99705	0.99404	0.99036[a]				
0.09849	1.00069	0.99846	0.99544	0.99176	91.51	91.89	92.23	92.51[a]
0.19736	1.00206	0.99978	0.99678	0.99310	91.72	92.25	92.46	92.71
0.29505	1.00336	1.00103	0.99805	0.99437	91.90	92.50	92.64	92.92
0.41013	1.00484	1.00249	0.99947	0.99579	92.06	92.58	92.85	93.14
0.50063	1.00596	1.00358	1.00053	0.99685	92.17	92.69	93.02	93.31
DEG+0.0015 mol·kg^{-1} biotin								
0.00000	0.99966	0.99755	0.99463	0.99098				
0.09919	1.00109	0.99895	0.99602	0.99237	91.62	92.10	92.35	92.63

0.20021	1.00247	1.00030	0.99737	0.99373	91.85	92.33	92.58	92.84
0.29895	1.00376	1.00156	0.99863	0.99499	92.05	92.53	92.78	93.04
0.40040	1.00504	1.00281	0.99988	0.99624	92.21	92.69	92.95	93.21
0.49893	1.00622	1.00398	1.00105	0.99742	92.38	92.84	93.08	93.34
DEG+0.0025 mol·kg^{-1} biotin								
0.00000	0.99984	0.99778	0.99481	0.99130				
0.10012	1.00128	0.99918	0.99620	0.99270	91.68	92.19	92.51	92.72
0.20003	1.00263	1.00050	0.99752	0.99402	91.94	92.44	92.74	92.96
0.29829	1.00389	1.00174	0.99875	0.99526	92.19	92.66	92.97	93.18
0.38999	1.00502	1.00284	0.99985	0.99636	92.38	92.86	93.16	93.38
0.50015	1.00632	1.00411	1.00111	0.99763	92.58	93.05	93.35	93.57
DEG+0.0035 mol·kg^{-1} biotin								
0.00000	1.00000	0.99798	0.99507	0.99165				
0.10109	1.00143	0.99938	0.99646	0.99305	91.79	92.29	92.63	92.86

0.19943	1.00276	1.00067	0.99774	0.99433	92.02	92.52	92.87	93.10
0.29798	1.00401	1.00190	0.99896	0.99555	92.26	92.76	93.10	93.35
0.40053	1.00524	1.00311	1.00015	0.99676	92.53	92.99	93.35	93.57
0.49952	1.00637	1.00422	1.00125	0.99786	92.76	93.22	93.56	93.80
TEG+0.0000 mol·kg^{-1} biotin								
0.00000	0.99926	0.99705	0.99404	0.99036[a]				
0.09650	1.00137	0.99913	0.99610	0.99241	128.13	128.69	129.25	129.73a
0.20020	1.00355	1.00127	0.99822	0.99452	128.26	128.85	129.42	129.89
0.29205	1.00542	1.00311	1.00001	0.99632	128.38	128.97	129.60	130.03
0.39856	1.00750	1.00514	1.00203	0.99833	128.53	129.15	129.76	130.19
0.49879	1.00937	1.00699	1.00385	1.00015	128.69	129.28	129.89	130.34
TEG+0.0015 mol·kg^{-1} biotin								
0.00000	0.99966	0.99755	0.99463	0.99098				
0.10091	1.00185	0.99971	0.99675	0.99310	128.23	128.79	129.42	129.85

0.20008	1.00391	1.00174	0.99876	0.99510	128.41	128.97	129.58	129.99
0.29899	1.00589	1.00368	1.00067	0.99702	128.56	129.15	129.76	130.15
0.39790	1.00779	1.00555	1.00252	0.99887	128.73	129.31	129.89	130.31
0.50005	1.00967	1.00741	1.00437	1.00071	128.90	129.45	130.02	130.43
TEG+0.0025 mol·kg^{-1} biotin								
0.00000	0.99984	0.99778	0.99481	0.99130				
0.09979	1.00200	0.99990	0.99690	0.99338	128.31	128.86	129.53	130.03
0.19930	1.00406	1.00193	0.99890	0.99537	128.50	129.04	129.69	130.18
0.30041	1.00606	1.00391	1.00085	0.99731	128.70	129.23	129.86	130.36
0.39983	1.00794	1.00577	1.00269	0.99914	128.88	129.41	130.02	130.50
0.49997	1.00978	1.00757	1.00446	1.00091	129.03	129.57	130.19	130.66
TEG+0.0035 mol·kg^{-1} biotin								
0.00000	1.00000	0.99798	0.99507	0.99165				
0.10007	1.00214	1.00009	0.99715	0.99372	128.44	129.00	129.65	130.17

0.19897	1.00417	1.00209	0.99912	0.99568	128.64	129.19	129.82	130.32
0.29896	1.00613	1.00403	1.00103	0.99759	128.85	129.38	130.00	130.48
0.40000	1.00803	1.00592	1.00289	0.99944	129.04	129.52	130.14	130.62
0.50011	1.00986	1.00771	1.00466	1.00119	129.18	129.68	130.28	130.78

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[a] m_A is the molality of glycols in the aqueous solution biotin; standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1},[a]Values of densities for (EG + water, DEG + water and TEG + water) at temperature 288.15 to 318.15 K have been taken from our previous paper [1].

Table 4.81

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_{V}^{*}, of glycols in the aqueous solution of biotin at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})				$S_{V}^{*} \times 10^{6}$/(m^{3}·kg·mol^{-2})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				EG				
0.0000	53.27(±0.01)	53.66(±0.00)	54.08(±0.00)	54.51(±0.02)^{a}	0.92(±0.03)	1.06(±0.01)	1.28(±0.02)	1.25(±0.06)^{a}
0.0015	53.34(±0.00)	53.71(±0.00)	54.14(±0.00)	54.64(±0.02)	1.80(±0.02)	1.77(±0.01)	1.80(±0.02)	1.78(±0.066)
0.0025	53.40(±0.00)	53.76(±0.01)	54.21(±0.01)	54.71(±0.02)	1.50(±0.02)	1.54(±0.03)	1.59(±0.06)	1.55(±0.06)
0.0035	53.46(±0.00)	53.84(±0.00)	54.31(±0.00)	54.80(±0.01)	1.56(±0.00)	1.55(±0.02)	1.41(±0.02)	1.46(±0.05)
				DEG				
0.0000	91.38(±0.03)	91.81(±0.11)	92.06(±0.01)	92.32(±0.00)^{a}	1.64(±0.11)	1.89(±0.34)	1.94(±0.04)	2.00(±0.02)^{a}
0.0015	91.45(±0.02)	91.94(±0.03)	92.20(±0.03)	92.48(±0.03)	1.90(±0.07)	1.84(±0.10)	1.83(±0.10)	1.77(±0.09)
0.0025	91.48(±0.03)	91.99(±0.02)	92.31(±0.02)	92.52(±0.02)	2.27(±0.11)	2.17(±0.08)	2.13(±0.08)	2.14(±0.05)
0.0035	91.54(±0.00)	92.06(±0.00)	92.40(±0.01)	92.63(±0.01)	2.46(±0.02)	2.33(±0.01)	2.35(±0.01)	2.36(±0.03)

				TEG				
0.0000	127.99(±0.01)	128.55(±0.01)	129.11(±0.02)	129.58(±0.00)[a]	1.38(±0.04)	1.48(±0.03)	1.61(±0.06)	1.52(±0.01)[a]
0.0015	128.07(±0.00)	128.63(±0.01)	129.28(±0.02)	129.70(±0.01)	1.65(±0.02)	1.67(±0.05)	1.52(±0.06)	1.48(±0.03)
0.0025	128.14(±0.01)	128.69(±0.00)	129.36(±0.00)	129.87(±0.00)	1.80(±0.04)	1.78(±0.02)	1.65(±0.00)	1.58(±0.02)
0.0035	128.27(±0.02)	128.85(±0.01)	129.50(±0.01)	130.02(±0.00)	1.88(±0.08)	1.68(±0.05)	1.58(±0.05)	1.53(±0.01)

[a] m_B is the molality of aqueous biotin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}, $u(V_\phi^0)$= ±0.01 × 10^6/(m^3·mol^{-1}) and $u(S_V^*)$=±0.03 × 10^6/(m^3·kg·mol^{-2}), [a]Values of Partial molar volumes (V_ϕ^0) and experimental slopes (S_V^*) for (EG + water, DEG + water and TEG + water) at temperature 288.15 to 318.15 K have been taken from our previous paper [1].

Table 4.82

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in the aqueous solution of biotin at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		EG		
0.0015	0.07	0.05	0.06	0.13
0.0025	0.13	0.10	0.13	0.20
0.0035	0.19	0.18	0.23	0.29
		DEG		
0.0015	0.07	0.13	0.14	0.16
0.0025	0.10	0.18	0.25	0.20
0.0035	0.16	0.25	0.34	0.31
		TEG		
0.0015	0.08	0.08	0.17	0.12
0.0025	0.15	0.14	0.25	0.29
0.0035	0.28	0.30	0.39	0.44

$^{a}m_{B}$ is the molality of aqueous biotin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}.

Table 4.83

Values of empirical parameters of Eq. 4, of glycols in the aqueous solution of biotin at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/ (m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
			EG		
0.0015	53.706	0.039	0.000	0.9999	0.0000
0.0025	53.767	0.040	0.000	0.9999	0.0001
0.0035	53.851	0.042	0.000	0.9999	0.0040
			DEG		
0.0015	91.905	0.039	-0.001	0.9999	0.0002
0.0025	91.978	0.042	-0.001	0.9999	0.0001
0.0035	92.048	0.043	-0.001	0.9999	0.0024
			TEG		
0.0015	128.678	0.058	0.000	0.9999	0.0002
0.0025	128.733	0.059	0.000	0.9999	0.0002
0.0035	128.882	0.061	0.000	0.9999	0.0025

${}^{a}m_B$ is the molality aqueous of biotin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}

Table 4.84

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in aqueous solution of biotin at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$E_{\phi}^{0}\times10^{6}$/ (m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_{p}$/ (m^{3}·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			EG		
0.0015	0.0329	0.0399	0.0468	0.0529	0.0007
0.0025	0.0338	0.0404	0.0470	0.0537	0.0007
0.0035	0.0370	0.0423	0.0476	0.0538	0.0005
			DEG		
0.0015	0.0489	0.0386	0.0273	0.0121	0.0010
0.0025	0.0570	0.0420	0.0281	0.0122	0.0015
0.0035	0.0581	0.0434	0.0288	0.0179	0.0015
			TEG		
0.0015	0.0604	0.0587	0.0520	0.0454	0.0007
0.0025	0.0612	0.0595	0.0572	0.0536	0.0002
0.0035	0.0644	0.0608	0.0577	0.0560	0.0004

$^{a}m_{B}$ is the molality aqueous of biotin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}.

Table 4.85

Values of the speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,S}$ of glycols in aqueous solutions of biotin at different temperatures and at the experimental pressure=0.1 MPa

[a]m_A/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,S}$ × 10^{6}/ (m^{3}·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
EG+0.0000 mol·kg^{-1} biotin								
0.00000	1466.59	1495.85	1519.14	1536.02[a]				
0.09889	1469.57	1498.92	1521.84	1539.17	−46.06	−44.28	−42.93	−41.98[a]
0.19894	1472.72	1501.72	1524.03	1542.24	−46.34	−44.54	−43.18	−42.23
0.29967	1475.45	1504.29	1526.18	1544.95	-46.46	−44.65	−43.29	−42.34
0.39481	1478.57	1506.64	1528.28	1547.87	−46.53	−44.72	−43.35	−42.40
0.50155	1481.17	1509.09	1530.34	1550.65	-46.59	−44.78	−43.41	−42.46
EG+0.0015 mol·kg^{-1} biotin								
0.00000	1469.95	1499.13	1521.92	1538.78				
0.10045	1472.92	1501.97	1524.57	1541.84	-45.86	-44.09	-42.78	-41.84

0.19785	1475.97	1504.75	1526.68	1544.75	-46.13	-44.34	-43.02	-42.08
0.30036	1478.98	1507.39	1528.95	1547.57	-46.24	-44.46	-43.13	-42.19
0.39888	1482.03	1509.97	1531.08	1550.51	-46.31	-44.52	-43.19	-42.25
0.50340	1484.54	1512.34	1533.19	1553.14	-46.37	-44.58	-43.24	-42.30
EG+0.0025 mol·kg^{-1} biotin								
0.00000	1472.25	1501.08	1524.43	1542.06				
0.09790	1474.97	1503.76	1526.81	1544.90	-45.71	-43.96	-42.62	-41.65
0.20050	1478.15	1506.71	1529.12	1547.79	-45.98	-44.23	-42.88	-41.90
0.30008	1481.09	1509.25	1531.28	1550.58	-46.10	-44.34	-42.99	-42.00
0.39919	1484.12	1511.69	1533.41	1553.51	-46.17	-44.41	-43.05	-42.07
0.50201	1486.49	1513.98	1535.37	1556.01	-46.22	-44.46	-43.10	-42.11
EG+0.0035 mol·kg^{-1} biotin								
0.00000	1475.05	1504.29	1527.17	1545.19				
0.09926	1477.85	1506.97	1529.59	1548.01	-45.54	-43.78	-42.48	-41.49

0.20053	1480.89	1510.01	1531.77	1550.81	-45.81	-44.04	-42.73	-41.73
0.30031	1484.04	1512.57	1533.99	1553.65	-45.92	-44.15	-42.83	-41.83
0.39897	1487.19	1514.94	1535.99	1556.45	-45.99	-44.22	-42.90	-41.90
0.50012	1489.51	1517.29	1537.94	1559.01	-46.05	-44.27	-42.94	-41.94
DEG+0.0000 mol·kg^{-1} biotin								
0.00000	1466.59	1495.85	1519.14	1536.02[a]				
0.09849	1472.11	1501.24	1523.52	1541.59	−46.09	−44.30	−42.95	−42.01[a]
0.19736	1478.01	1506.01	1527.52	1547.17	−46.39	−44.59	−43.23	−42.29
0.29505	1483.78	1510.78	1531.47	1552.68	−46.53	−44.72	−43.36	−42.41
0.41013	1489.36	1516.15	1536.11	1558.07	−46.64	−44.83	−43.46	−42.52
0.50063	1494.73	1520.34	1541.59	1563.21	−46.72	−44.90	−43.53	−42.58
DEG+0.0015 mol·kg^{-1} biotin								
0.00000	1469.95	1499.13	1521.92	1538.78				
0.09919	1475.40	1504.57	1525.85	1544.23	-45.85	-44.11	-42.80	-41.86

0.20021	1481.54	1509.51	1529.91	1549.92	-46.15	-44.40	-43.08	-42.14
0.29895	1487.21	1514.23	1533.77	1555.59	-46.28	-44.53	-43.20	-42.26
0.40040	1491.99	1518.96	1537.98	1560.15	-46.38	-44.62	-43.30	-42.35
0.49893	1498.25	1523.70	1543.77	1565.84	-46.46	-44.70	-43.37	-42.42
DEG+0.0025 mol·kg^{-1} biotin								
0.00000	1472.25	1501.08	1524.43	1542.06				
0.10012	1478.16	1506.35	1528.15	1547.54	-45.75	-44.00	-42.66	-41.69
0.20003	1484.36	1511.15	1532.13	1553.18	-46.04	-44.28	-42.93	-41.96
0.29829	1490.17	1516.01	1536.09	1558.49	-46.17	-44.41	-43.06	-42.08
0.38999	1494.51	1520.19	1540.09	1562.49	-46.26	-44.50	-43.14	-42.16
0.50015	1501.25	1525.41	1546.52	1568.82	-46.35	-44.58	-43.22	-42.24
DEG+0.0035 mol·kg^{-1} biotin								
0.00000	1475.05	1504.29	1527.17	1545.19				
0.10109	1480.71	1509.42	1530.98	1550.72	-45.58	-43.82	-42.51	-41.52

0.19943	1486.95	1514.14	1534.99	1555.85	-45.86	-44.09	-42.78	-41.79
0.29798	1493.01	1519.26	1538.73	1560.84	-46.00	-44.22	-42.90	-41.91
0.40053	1497.81	1524.01	1543.57	1565.61	-46.09	-44.31	-42.99	-42.00
0.49952	1504.38	1528.76	1549.60	1571.41	-46.17	-44.38	-43.06	-42.06
TEG+0.0000 mol·kg^{-1} biotin								
0.00000	1466.59	1495.85	1519.14	1536.02[a]				
0.09650	1474.72	1503.48	1525.09	1543.95	−46.12	−44.33	−42.97	−42.03[a]
0.20020	1483.26	1511.04	1531.28	1552.21	−46.47	−44.66	−43.30	−42.35
0.29205	1491.74	1517.62	1536.87	1560.57	−46.63	−44.82	−43.45	−42.50
0.39856	1499.22	1525.38	1543.31	1567.78	−46.77	−44.95	−43.57	−42.62
0.49879	1508.48	1532.21	1550.94	1576.89	−46.88	−45.05	−43.68	−42.72
TEG+0.0015 mol·kg^{-1} biotin								
0.00000	1469.95	1499.13	1521.92	1538.78				
0.10091	1478.31	1506.83	1527.95	1547.29	-45.93	-44.16	-42.84	-41.90

0.20008	1486.53	1513.99	1533.76	1555.23	-46.25	-44.47	-43.14	-42.20
0.29899	1495.59	1521.37	1539.77	1564.31	-46.42	-44.63	-43.29	-42.35
0.39790	1502.23	1528.51	1545.88	1571.09	-46.55	-44.75	-43.41	-42.47
0.50005	1511.54	1535.24	1554.03	1580.58	-46.66	-44.85	-43.51	-42.57
TEG+0.0025 mol·kg^{-1} biotin								
0.00000	1472.25	1501.08	1524.43	1542.06				
0.09979	1480.65	1508.63	1530.51	1550.54	-45.78	-44.03	-42.69	-41.72
0.19930	1489.29	1515.99	1536.16	1558.64	-46.11	-44.35	-43.00	-42.02
0.30041	1498.55	1523.74	1542.41	1567.89	-46.28	-44.51	-43.15	-42.17
0.39983	1505.18	1531.04	1548.79	1574.71	-46.40	-44.63	-43.27	-42.28
0.49997	1514.14	1537.61	1556.88	1584.53	-46.51	-44.73	-43.37	-42.38
TEG+0.0035 mol·kg^{-1} biotin								
0.00000	1475.05	1504.29	1527.17	1545.19				
0.10007	1482.97	1512.19	1533.29	1553.59	-45.61	-43.85	-42.54	-41.55

0.19897	1492.12	1519.45	1538.89	1562.05	-45.93	-44.16	-42.84	-41.84
0.29896	1500.72	1527.21	1545.21	1570.99	-46.10	-44.32	-42.99	-42.00
0.40000	1507.88	1534.27	1551.87	1578.53	-46.22	-44.44	-43.11	-42.11
0.50011	1517.07	1541.19	1560.22	1588.18	-46.33	-44.54	-43.21	-42.21

[a] m_A is the molality of glycols in the aqueous solution biotin; standard uncertainties *u* are $u(m)$ = 1%, $u(T)$=0.001 K, $u(\rho)$=0.15(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1},[a]Values of speed of sound for (EG + water, DEG + water and TEG + water) at temperature 288.15 and 318.15 K have been taken from our previous paper [1].

Table 4.86

Partial molar isentropic compression, $K_{\phi,s}^{0}$, and experimental slopes, S_k^*, of glycols in the aqueous solution of biotin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$K_{\phi,s}^{0}\times10^{6}$/(m^{3}·mol^{-1}· GPa^{-1})				$S_k^*\times10^{6}$/(kg·m^{3}·mol^{-2}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				EG				
0.0000	-46.03(±0.08)	-44.23(±0.07)	-42.89(±0.07)	-42.01(±0.07)[a]	-1.24(±0.24)	-1.18(±0.23)	-1.13(±0.23)	-1.13(±0.23)[a]
0.0015	-45.82(±0.08)	-44.05(±0.07)	-42.74(±0.07)	-41.81(±0.07)	-1.19(±0.24)	-1.14(±0.23)	-1.10(±0.22)	-1.07(±0.22)
0.0025	-45.67(±0.08)	-43.93(±0.08)	-42.59(±0.07)	-41.62(±0.07)	-1.22(±0.25)	-1.16(±0.24)	-1.12(±0.23)	-1.08(±0.23)
0.0035	-45.50(±0.08)	-43.75(±0.07)	-42.44(±0.07)	-41.46(±0.07)	-1.20(±0.24)	-1.14(±0.23)	-1.10(±0.22)	-1.07(±0.22)
				DEG				
0.0000	-46.03(±0.08)	-44.25(±0.07)	-42.90(±0.07)	-41.95(±0.07)[a]	-1.47(±0.24)	-1.40(±0.23)	-1.36(±0.23)	-1.34(±0.23)[a]
0.0015	-45.79(±0.08)	-44.06(±0.07)	-42.74(±0.07)	-41.81(±0.07)	-1.46(±0.24)	-1.39(±0.23)	-1.36(±0.23)	-1.34(±0.23)
0.0025	-45.69(±0.08)	-43.94(±0.07)	-42.61(±0.07)	-41.63(±0.07)	-1.44(±0.24)	-1.37(±0.23)	-1.34(±0.23)	-1.32(±0.23)
0.0035	-45.52(±0.08)	-43.76(±0.07)	-42.46(±0.07)	-41.47(±0.07)	-1.41(±0.24)	-1.35(±0.23)	-1.31(±0.22)	-1.29(±0.22)

TEG								
0.0000	-46.03(±0.08)	-44.25(±0.08)	-42.90(±0.08)	-41.96(±0.08)[a]	-1.81(±0.26)	-1.73(±0.25)	-1.68(±0.25)	-1.64(±0.24)[a]
0.0015	-45.74(±0.08)	-44.07(±0.07)	-42.75(±0.07)	-41.82(±0.07)	-1.76(±0.24)	-1.68(±0.23)	-1.63(±0.23)	-1.60(±0.22)
0.0025	-45.69(±0.08)	-43.95(±0.07)	-42.61(±0.07)	-41.64(±0.07)	-1.75(±0.24)	-1.68(±0.24)	-1.62(±0.23)	-1.59(±0.22)
0.0035	-45.52(±0.08)	-43.77(±0.07)	-42.46(±0.07)	-41.47(±0.07)	-1.73(±0.24)	-1.66(±0.23)	-1.61(±0.23)	-1.57(±0.22)

[a] m_B is the molality of aqueous biotin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}, $u(K_{\phi,s}^{0})$= ±0.01 ×10^{6}/(m^{3}·mol^{-1}·GPa^{-1}) and $u(S_k^{*})$= ±0.24×10^{6}/(kg·m^{3}·mol^{-2}· GPa^{-1}), [a]Values of Partial molar isentropic compression, ($K_{\phi,s}^{0}$) and experimental slopes (S_k^{*}) for (EG + water, DEG + water and TEG + water) at temperature 288.15 to 318.15 K have been taken from our previous paper [1].

Table 4.87

Partial molar isentropic compression transfer, $\Delta K_{\phi,s}^{0}$, of glycols in aqueous solution of biotin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta K_{\phi,s}^{0}$, × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		EG		
0.0015	0.21	0.17	0.15	0.20
0.0025	0.36	0.30	0.30	0.39
0.0035	0.53	0.48	0.45	0.55
		DEG		
0.0015	0.24	0.20	0.16	0.14
0.0025	0.34	0.31	0.29	0.32
0.0035	0.51	0.49	0.44	0.48
		TEG		
0.0015	0.19	0.18	0.15	0.14
0.0025	0.34	0.30	0.29	0.32
0.0035	0.51	0.49	0.44	0.49

$^{a}m_B$ is the molality of aqueous biotin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}.

Table 4.88

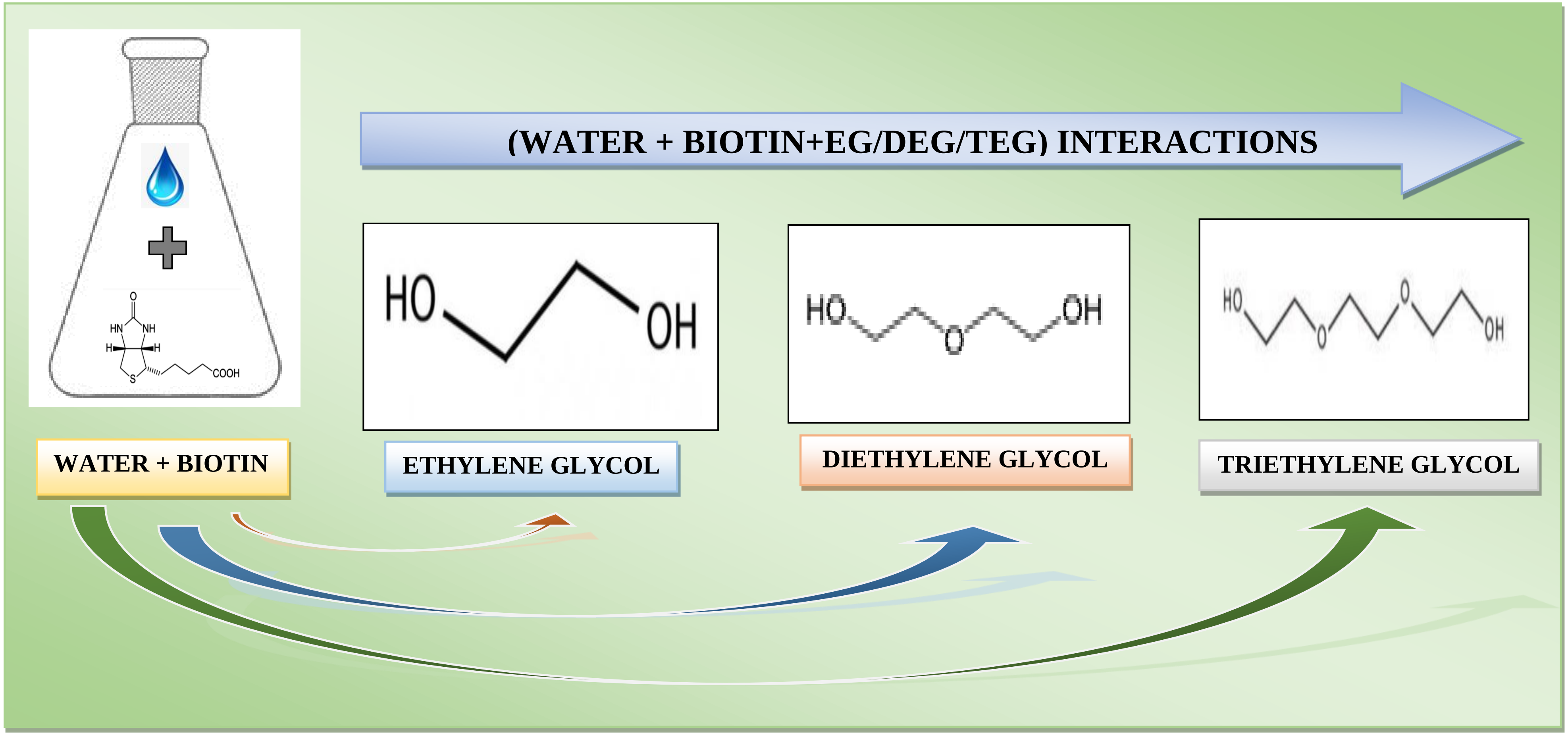
Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of biotin at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		EG		
288.15	22.62	822.70	63.04	2349.35
298.15	7.51	3384.09	45.33	4365.78
308.15	9.73	4492.75	41.38	4327.48
318.15	42.29	-296.91	63.60	3045.42
		DEG		
288.15	21.50	71.86	76.71	-851.40
298.15	47.28	-2364.75	53.72	2900.05
308.15	48.11	122.36	46.06	3324.94
318.15	52.08	-1789.61	37.87	5986.05
		TEG		

288.15	15.34	4521.52	57.42	2994.19
298.15	6.37	6750.87	48.69	3861.19
308.15	49.01	1236.15	41.33	4246.71
318.15	33.65	5631.19	37.30	6384.54

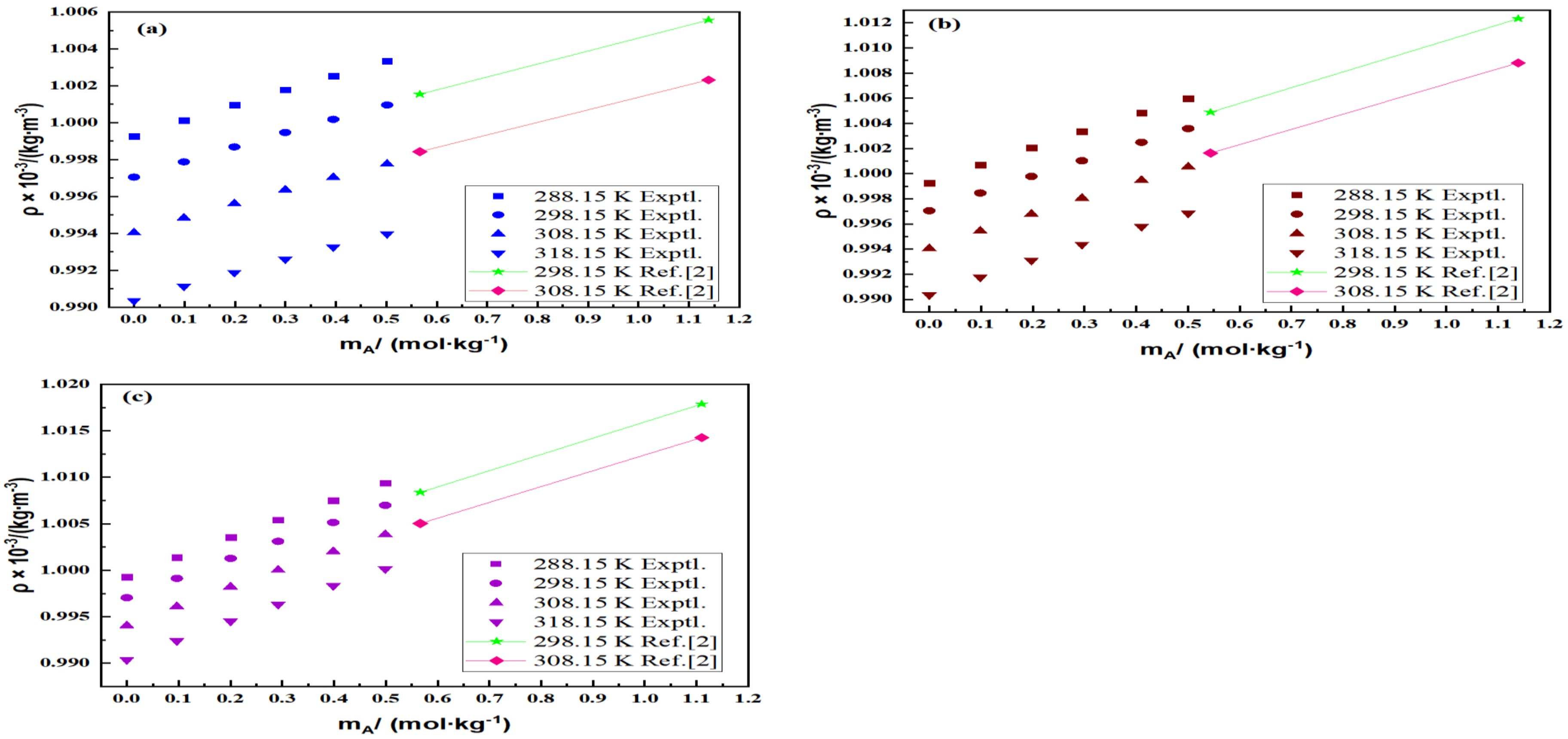
T/K is the temperatures, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}.

Figure 4.63



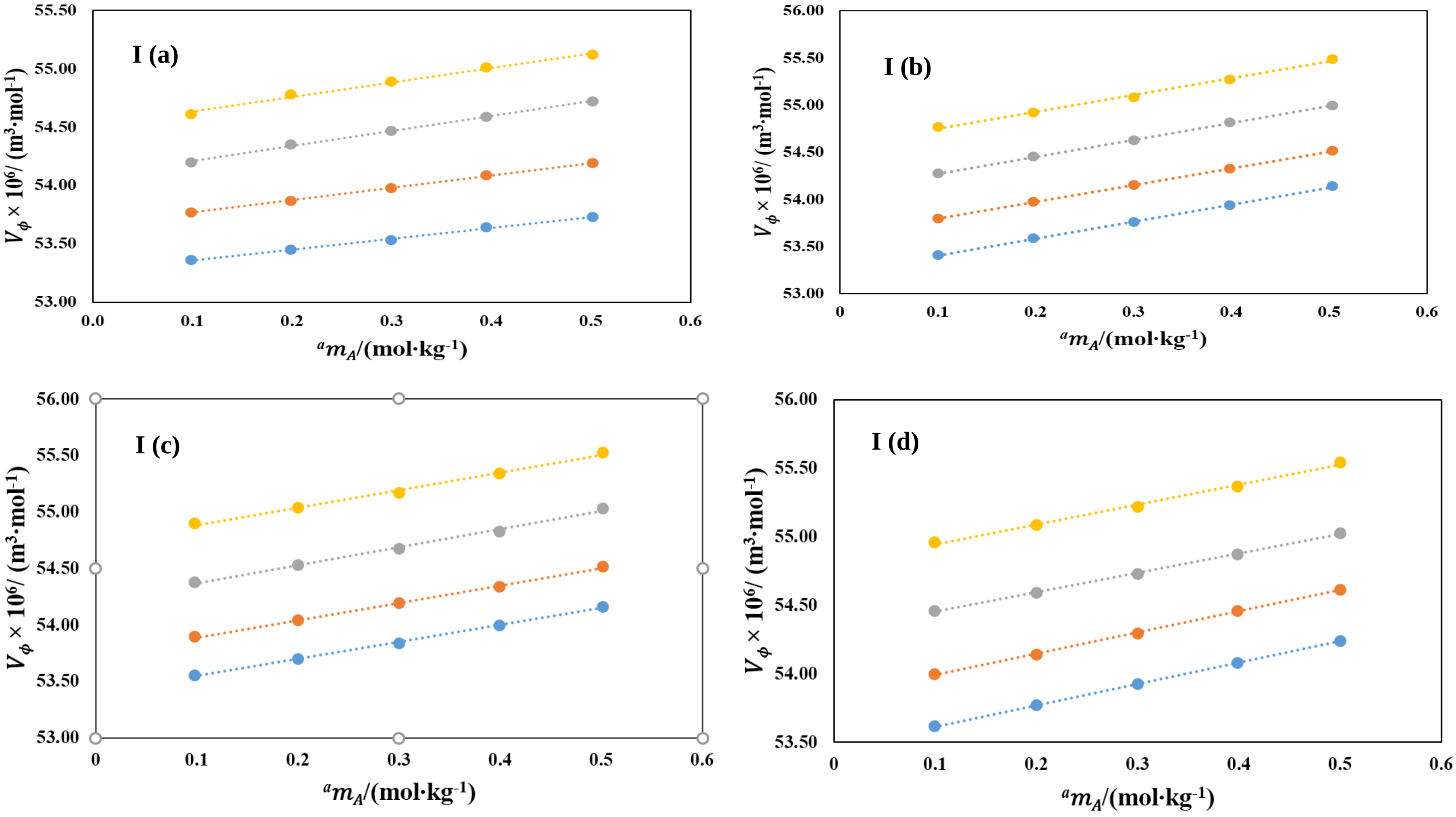
EG/ DEG/ TEG and biotin interactions.

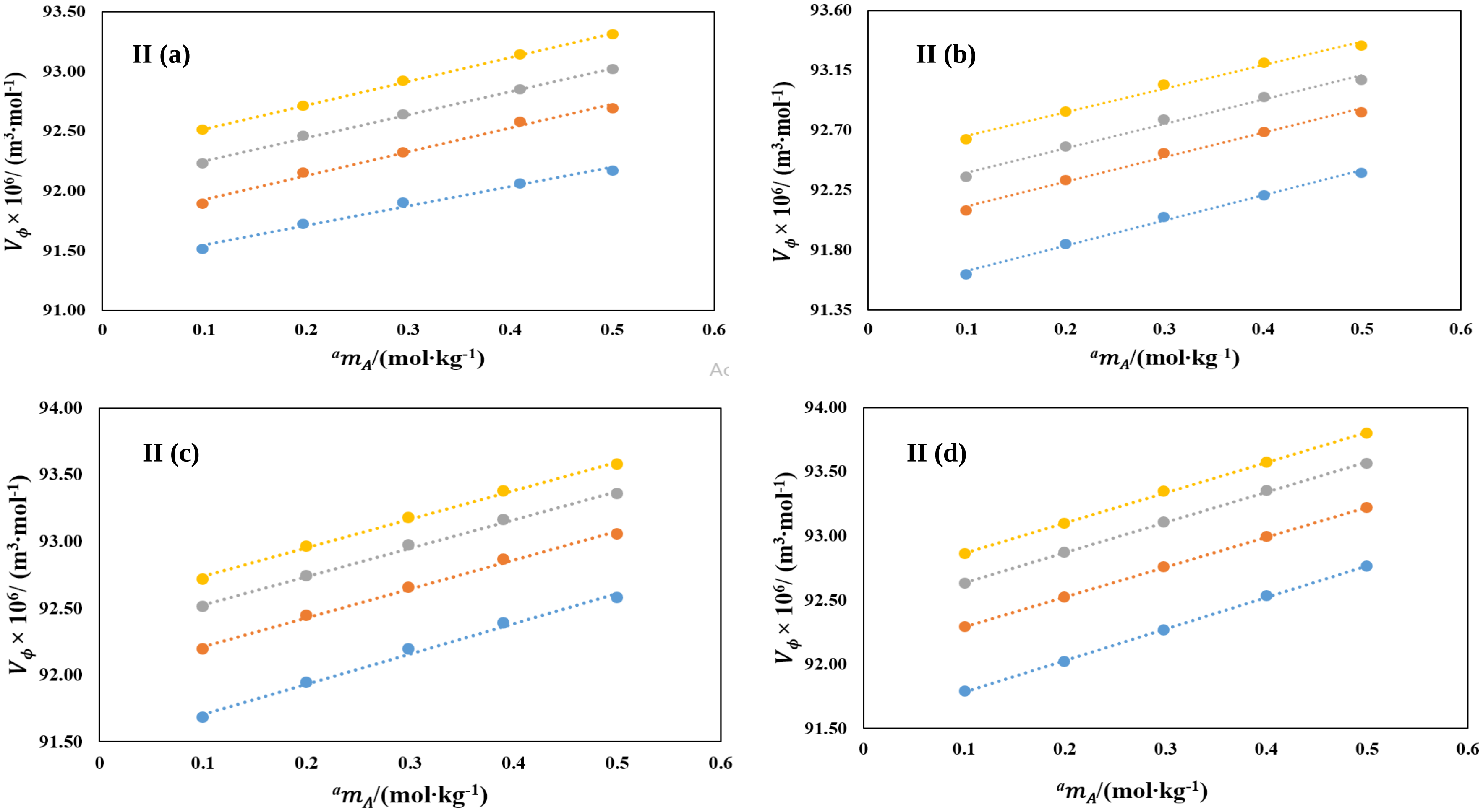
Figure 4.64

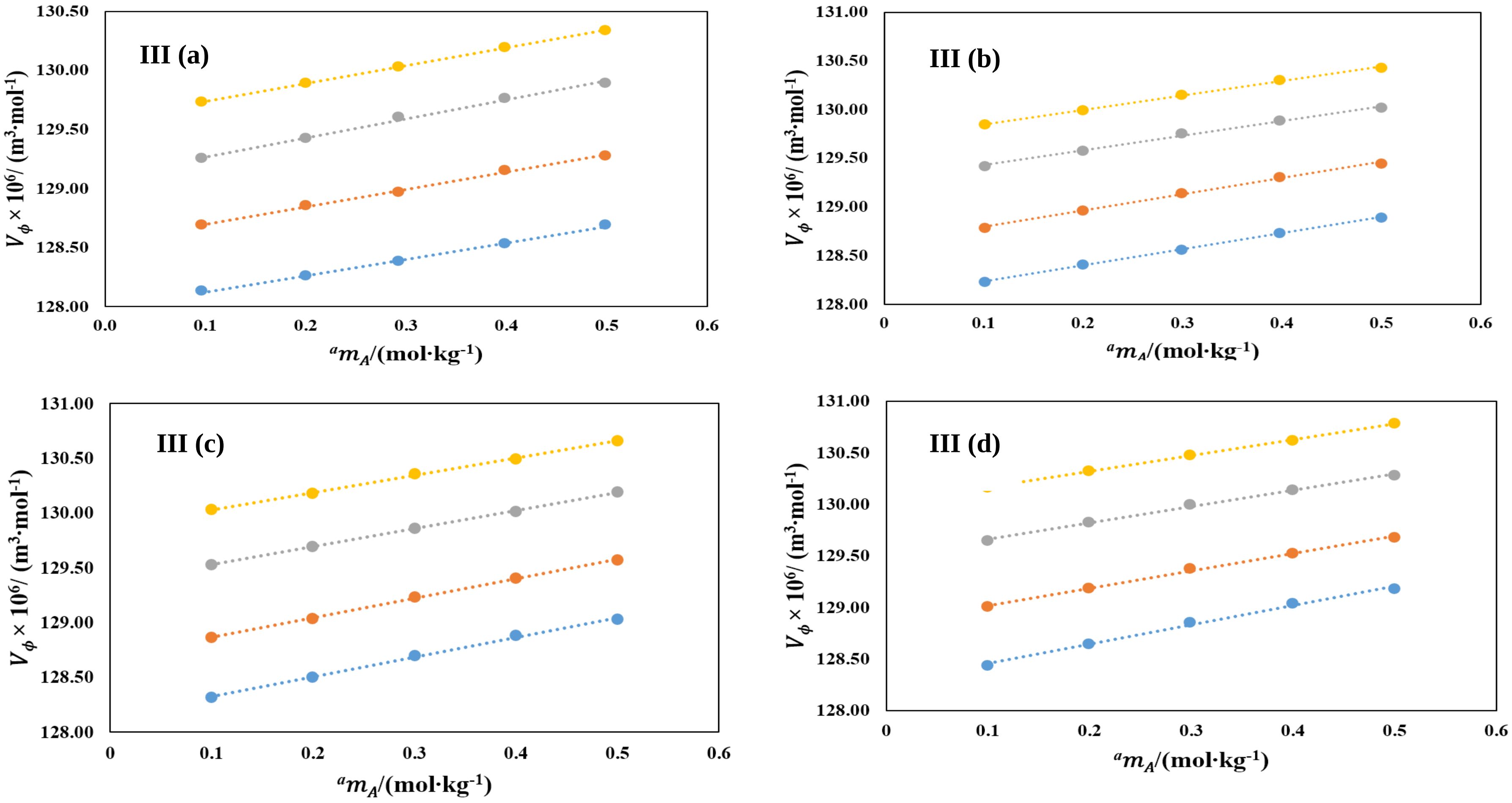


Variation of experimental and literature density values [2] of (a) (Water + EG), (b) (Water + DEG) and (c) (Water + TEG) corresponding to the molality (m_A) of glycols at different T.

Figure 4.65

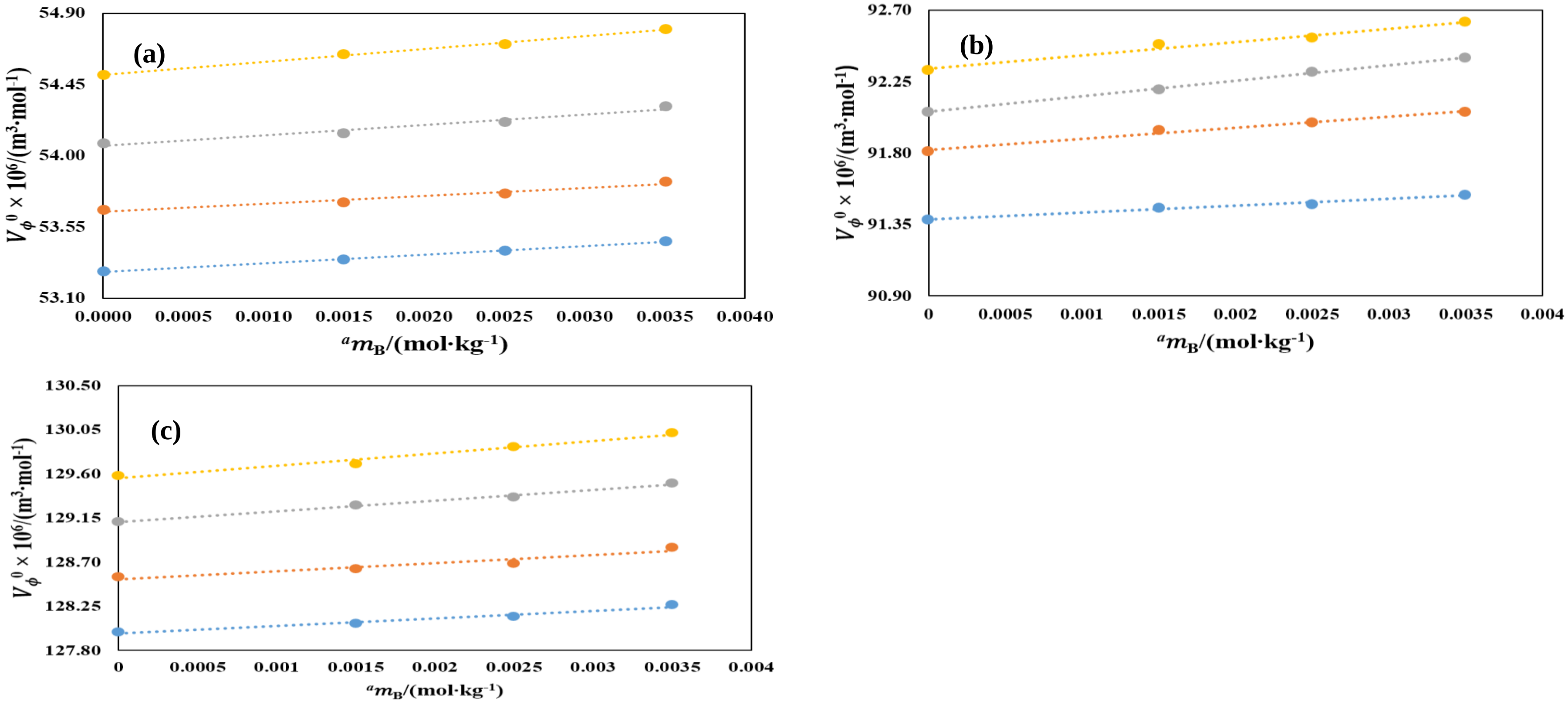

I (a)
I (b)
I (c)
I (d)
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
53.00
53.50
54.00
54.50
55.00
55.50
56.00
0.0
0
0.1
0.2
0.3
0.4
0.5
0.6


II (a)
93.50
93.00
92.50
92.00
91.50
91.00
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
0
0.1
0.2
0.3
0.4
0.5
0.6
$^a m_A$/(mol·kg^{-1})
II (b)
93.60
93.15
92.70
92.25
91.80
91.35
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
0
0.1
0.2
0.3
0.4
0.5
0.6
$^a m_A$/(mol·kg^{-1})
II (c)
94.00
93.50
93.00
92.50
92.00
91.50
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
0
0.1
0.2
0.3
0.4
0.5
0.6
$^a m_A$/(mol·kg^{-1})
II (d)
94.00
93.50
93.00
92.50
92.00
91.50
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
0
0.1
0.2
0.3
0.4
0.5
0.6
$^a m_A$/(mol·kg^{-1})



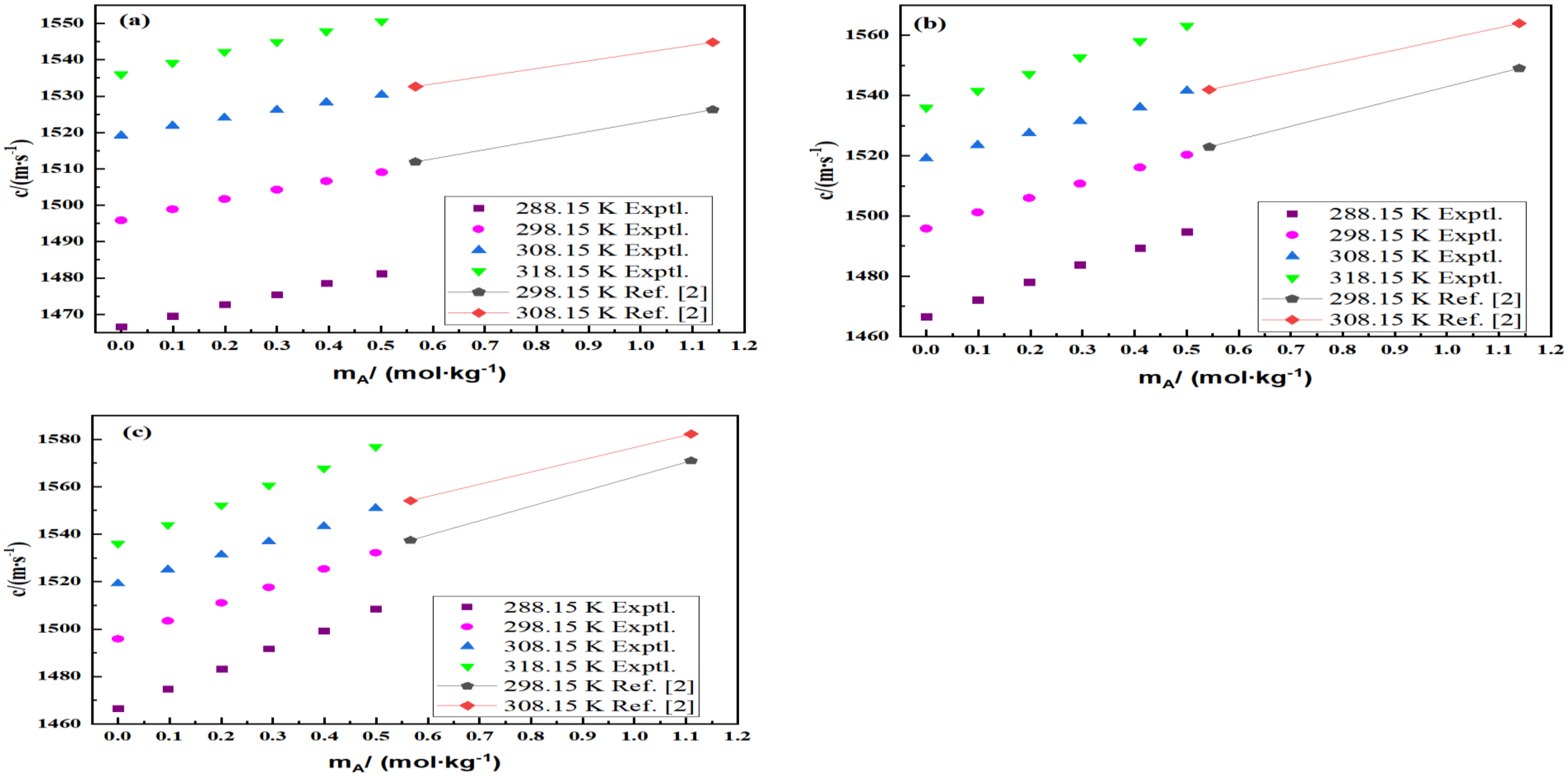
Variation of apparent molar volume, V_ϕ of EG (I), DEG (II) and TEG (III) (a) 0.0000 biotin, (b) 0.0015 biotin, (c) 0.0025 biotin, (d) 0.0035 biotin, against molality at different temperatures [blue, 288.15 K; red, 298.15 K; grey, 308.15 K; orange 318.15 K]

Figure 4.66



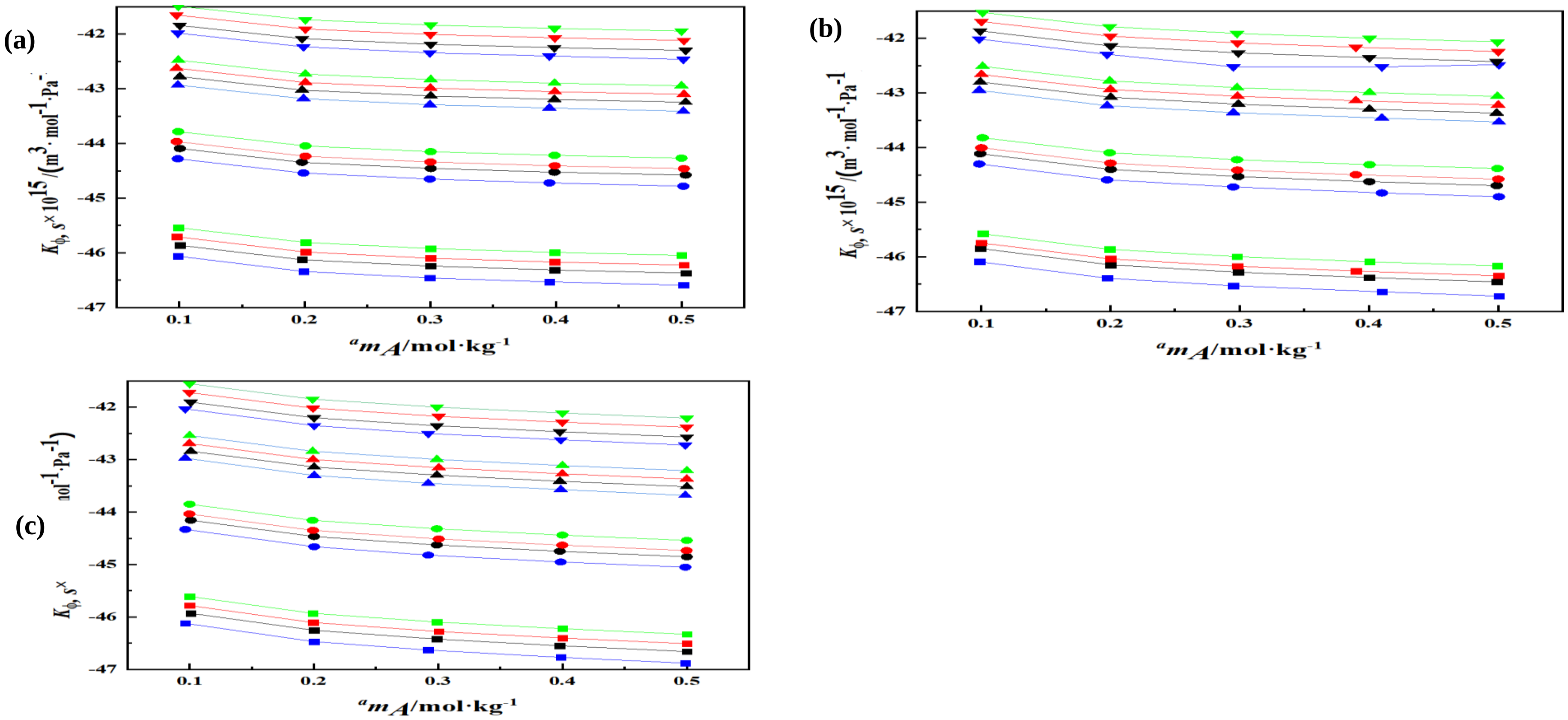
Variation of partial molar volumes, V_ϕ^0, of, (a) EG, (b) DEG and (c) TEG in different concentration of aqueous biotin solutions at different temperatures [blue, 288.15 K; red, 298.15 K; grey, 308.15 K; orange 318.15 K]

Figure 4.67



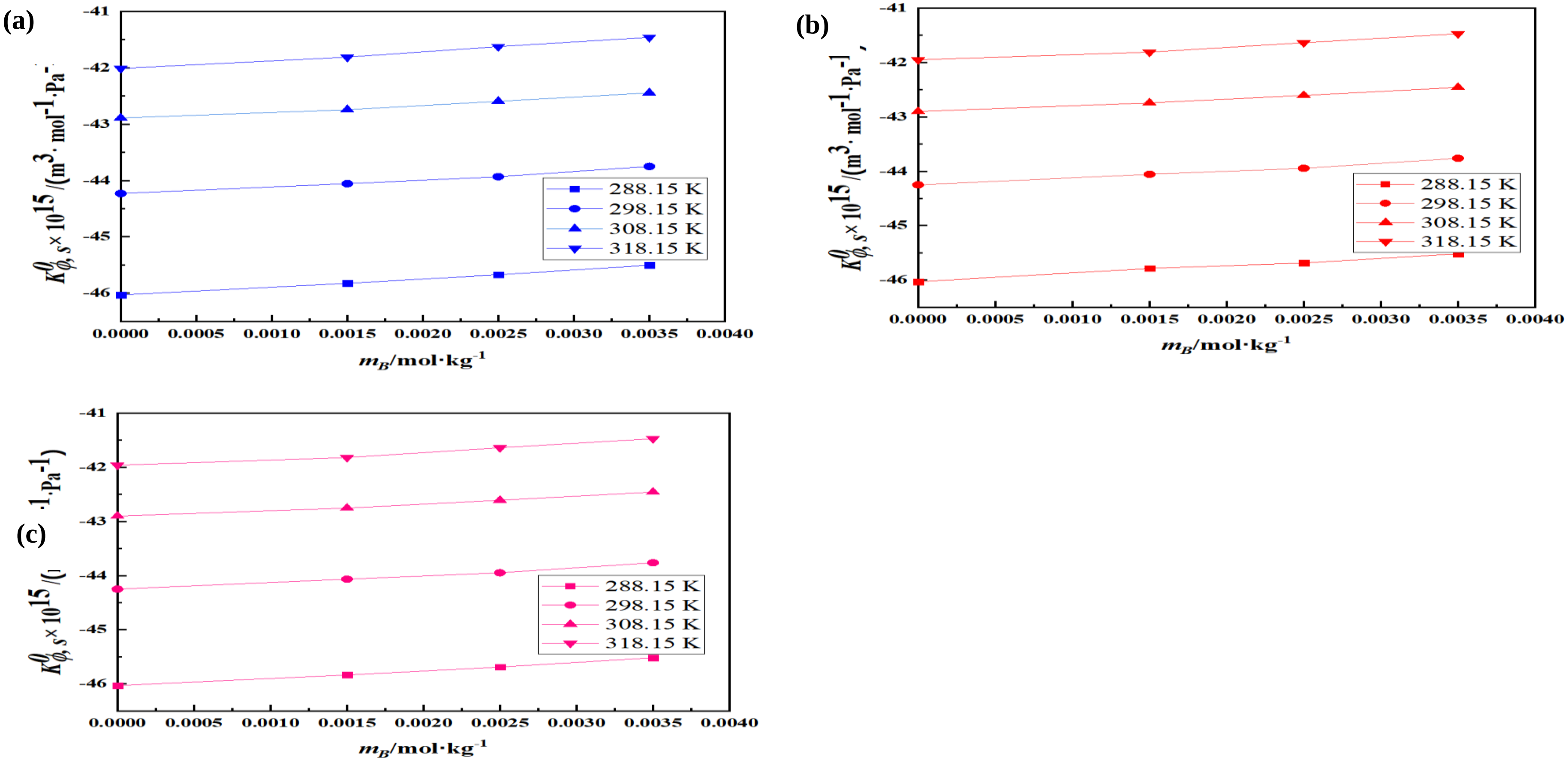
Variation of experimental and literature velocity values [2] EG), (b) (Water + DEG) and (c) (Water + TEG) corresponding to the molality (m_A) of glycols at different T.

Figure 4.68



Variation of apparent molar isentropic compression, $K_{\phi,s}$, of (a) EG, (b) DEG and (c) TEG against molality [blue, 0.0000 biotin; black, 0.0015 biotin; red, 0.0025 biotin; green, 0.0035 biotin]at different temperatures [square, 288.15 K; circle, 298.15 K; triangle, 308.15 K; inverted triangle, 318.15 K]

Figure 4.69



Variation of partial molar isentropic compression, $K^0_{\phi,s}$, of (a) EG, (b) DEG and (c) TEG in aqueous biotin solutions at different temperatures.

Problem XI

Temperature-dependent thermodynamic and physicochemical studies of glycols in aqueous biotin solutions

In this section, we have reported the densities, ρ and speed of sound c of propylene glycol (PG) and hexylene glycol (HG) in (0.000, 0.001, 0.002 and 0.003) mol·kg^{-1} aqueous solutions of biotin at temperatures T = (288.15, 298.15, 308.15 and 318.15) K.

4.91 Density

The values of experimental density for propylene glycol and hexylene glycol in aqueous (0.000, 0.001, 0.002 and 0.003) mol·Kg^{-1} biotin solutions has been obtained at multiple temperatures T= (288.25, 298.15, 308.15, 318.15) K and constant 0.1 MPa pressure. In the case of PG/HG with the molecular formula ($C_3H_8O_2$) and ($C_6H_{14}O_2$) respectively, contains two kinds of (-OH) alcohol functional groups named as primary and secondary alcohol that further gets attached to the carbon besides it. In **Table 4.89** the values of density are indexed as the function of experimental temperatures and glycol molality from which it can be noticed that for particular concentration biotin, the density of the ternary mixture escalates with the glycol molality but reduces with the upsurge in the temperatures. The experimental values of density for (water + PG) and (water + HG) are correlated beside the literature values [4] at (298.15 K and 308.15 K) which is graphically expressed in **Figure 4.71**. From the figure, it can be professed that both the literature and experimental values are consistent with each other.

4.92 Apparent molar volume

The values of density were utilized to determine the apparent molar volume (V_ϕ) values with the equation **4.1** where M, m_A, ρ, and ρ_0 are symbolizing the molar mass of the solute, molality of the solute per kg of the solvent (water + biotin), densities of the solution and the solvent respectively. In **Table 4.89** the values of apparent molar volume (V_ϕ) for the binary mixture (water+ glycols) and the ternary mixture (biotin+ water+ glycols) are provided. These calculated V_ϕ values are positive and vary with respect to the molality of glycols and temperatures. As the experimental temperatures and glycol molality increases for specific biotin concentrations, the V_{ϕ} values accelerate accordingly. This behavior explains the strong solute-solvent interaction in the mixture that is graphically elaborated in **Figure 4.72**. This increment of the values with the temperatures implies more affinity in the solvent and thus raise the interaction of solute and solvent, which increases from PG to HG due to an increase in the molar mass of the glycol as depicted in **Scheme 1** [9, 16, 47]. Glycols in the mixture in presence of water exhibits both inter-intramolecular hydrogen bond in addition with hydrophobic hydration, hydrophobic effect, (dipole-dipole) and (dipole induced dipole) interactions [10, 11, 48].

4.93 Partial Molar volume

In order to retrieve the values of partial molar volume of the liquid mixtures containing biotin and glycol, the equation **4.2** is applied where m_A denotes the molality of the solute. In **Table 4.90,** the partial molar volume (V_{ϕ}^{0}) with the experimental slope (S_V^*) is indexed corresponding to their experimental temperatures and biotin concentrations. In the same table, the standard errors are also reported. All these parameters are computed using the method of least square fitting. The values V_{ϕ}^{0} are all positive which is rising with the upsurge in the concentration of biotin and the temperatures. This is demonstrated in **Figure 4.73**. The trend of V_{ϕ}^{0} values is caused by the solute-solvent interactions in the liquid mixture. Further, as the chain length of glycols strengthens i.e. with the increment in the size of the glycols from propylene glycol to hexylene glycol, the partial molar volume increases indicating the dominance of ion-hydrophilic interactions than the hydrophobic-hydrophobic interactions in the system. The co-sphere overlap model [20, 49, 50] states that when in two ionic species the hydration co-sphere overlaps, the volume increases, but when the ion-hydrophobic group and hydrophobic- hydrophobic group overlap, there is a reduction in the volume. Thus the calculated positive values of V_{ϕ}^{0} are the result of ion-hydrophilic interactions which predominate the hydrophobic- hydrophobic and ion- hydrophobic interactions. The variation of V_{ϕ}^{0} values with the temperature includes different reasons, for example- exemption of the molecules in the solvation layers, thermal expansion, hydrogen bond, etc. The increment in the V_ϕ^0 values with the temperatures in the present study can be accounted for due to the discharge of solvation molecules from the relaxed solvation layers of solute into the mixture. Moreover, the partial molar volumes are sensitive to the solvation of solute since as the temperature increases, from the secondary solvation layer the solvent is discharged into the bulk and thus results in the expansion of the solution. This behavior contributes to the information regarding the change of the volume in the solvent due to the formation of the layer around it and the structural volume of the solute in the solvent [51, 52]. The S_V^* values, which are also termed as semi-empirical solute-solute interaction parameter, explains the presence of solute-solute interactions inside the mixture due to its positive values which are not following any particular pattern corresponding to the experimental temperatures and concentrations of the solvent. Although, the S_V^* values are very small in comparison to the values of V_ϕ^0 indicating that the solute-solute interaction is dominated by solute-solvent interaction in the solution [1, 9, 14, 15].

4.94 Partial molar volume of transfer

The equation **4.3** is employed to calculate the Transfer of partial molar volume of glycols from water to aqueous solutions of biotin at infinite dilution. The calculated values of partial molar volume of transfer (ΔV_ϕ^0) are mentioned in **Table 4.91** which are found to be all positive and increases with the rise in the concentration of biotin. This implies the strong ion-ion interactions of biotin with glycols as both of them consist of polar groups. The structure-making ability of the solute is enhanced due to their interactions in the solution. Therefore, the positive ΔV_ϕ^0 values attribute to the structure composition which is the consequence of solvophobic solvation and the structural interactions between the two co-spheres as stated by the co-spheres overlap theory [20, 49]. The mentioned ΔV_ϕ^0 value contributes to the solute-solute interactions which are almost negligible and thus administer various types of interactions in the solution such as (i) ion-hydrophilic interactions, (ii) ion-hydrophobic interactions, (iii) hydrophilic- hydrophilic interactions, and (iv) hydrophobic- hydrophobic interactions. Following the co-sphere overlap model, the positive values are associated with the ion-hydrophilic interactions and hydrophilic- hydrophilic interactions whereas the ion-hydrophobic interactions and hydrophobic-hydrophobic interactions attribute negatively to partial molar volume of transfer. Hence, in the current study (biotin+ water+ glycols), the existence of ion-hydrophilic and hydrophilic- hydrophilic interactions are depicted [53, 54].

4.95 Temperature-dependent partial molar volume

The variation in the apparent molar volumes at infinite dilution with temperatures are obtained with the equation **4.4**. In **Table 4.92** the empirical constants are listed which are represented as a, b and c. The temperature in Kelvin is represented as T where T_{ref}=298.15 K. The deviations in the experimental and calculated V_{ϕ}^{0} values are mentioned in the same table and these deviations are evaluated using the equation **4.14**. Here, $\mathrm{Y} = V_{\phi}^{0}$ (apparent molar volume at infinite dilution). The deviation values are very minute that perfectly satisfy the polynomial equation that is demonstrated from R^2values in the current study [20]. In the table, the empirical constant c describes the scatter in V_{ϕ}^{0} values. The primary objective to analyze the V_{ϕ}^{0} values was to retrieve the partial molar expansibilities using the equation **4.5.** The partial molar expansibility at infinite dilution is calculated using E_{ϕ}^{0}=$\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_P$ which is used to investigate the interactions for solute-solvent in the mixture. The structure making and breaking capability of the solute in the solution is determined with the following thermodynamical equation **4.6** given by Hepler [23]. The tendency of a solute blended in a solvent to be a structure maker or breaker is determined by the sign of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_P$ [25, 55]. The positive values of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_P$ indicate the structure-making capacity of the solute while the structure breaking capacity is attributed by the negative values. In **Table 4.93** the partial molar expansibility (E_{ϕ}^{0}) values along with its first derivative $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_P$ is mentioned and it can be seen that at all the temperatures the E_{ϕ}^{0} values are all positive but shows an irregular pattern corresponding to the biotin concentrations and is decreasing with the rise in the temperatures. The phenomenon of caging or packaging effect [56, 57] in the solution causes the positive E_{ϕ}^{0} values that also imply the existence of strong solute-solvent interactions which is already suggested by the apparent molar volumes. Further, the $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ values are slightly negative, thus refers to the structure-making tendency of solute in all aqueous solutions of biotin [11, 31].

4.96 Ultrasonic speed

The speed of sound (c) of glycols in (0.000, 0.001, 0.002, and 0.003) mol·Kg^{-1} aqueous biotin solutions have been experimentally obtained as the function of temperatures (288.25 K, 298.15 K, 308.15 K and 318.15 K) and constant 0.1MPa pressure. In **Table 4.94** the experimental *c* values are reported. In **Figure 4.74** the comparison graph between the experimental and literature [4] speed of sound values is presented for (water + PG) and (water + HG) respectively at (298.15 K and 308.15 K). This can be observed from the graph that the experimental values are consistent with the literature values i.e. the values are increasing with the temperature and glycol molality. Also, as the concentration of biotin rises (0.001 to 0.002 to 0.003) mol·Kg^{-1}, the speed of sound values increases. This occurs due to the presence of a 3-D network of hydrogen bonds in the water structure. Further, the intramolecular hydrogen bond in the solute molecules and intermolecular hydrogen bond in the solute-solvent molecules causes the surge in the values of speed of sound in the mixture and thus suggests a greater combination rate of the molecules. Between the molecules of water and biotin, the formation of the hydrogen bond degrades with the acceleration in the molar mass of the glycols i.e. from propylene glycol to hexylene glycol. The hydrogen bond network formation in the solute with the aqueous molecules of biotin results in the surge of the speed of sound values with the molality of glycols. Moreover, the bond formation among the molecules of water and biotin are destroyed eventually where simultaneously new hydrogen bonds are developed between the glycols and biotin molecules [5, 26, 58].

4.97 Apparent molar isentropic compression

For glycols in aqueous biotin solution the apparent molar isentropic compression is determined with the equation **4.7** where, the densities of the solvent, densities of the solution, molar mass of solute, the molality of solute, and isentropic compressibility of the pure solvent and the solution are symbolized as ρ, ρ_0, M, m_A, $k_{s.0}$ and k_s respectively. The undermentioned Laplace-Newton's formula **4.8** [29] is used to calculate the isentropic compressibility. The isentropic compressibility (k_s) consists of two different phrases- (i) solute isentropic compressibility and, (ii) solvent isentropic compressibility. The first term appears due to the compression in the hydration shell of solute i.e. glycols, and the second term emerges because of the compression of solvent molecules i.e. biotin, in the mixture. In **Table 4.94** the values of apparent molar isentropic compressibility $(K_{\phi,S})$ is provided as the function of temperatures (288.15-318.15) K, molality of glycols (m_A) and biotin concentrations (0.001 to 0.002 to 0.003) mol·Kg^{-1}, which is graphically demonstrated in **Figure 4.75**. It can be noticed that the $K_{\phi,S}$ values are all negative and the negativity decreases with the temperatures and biotin concentrations but increases as the molality of the glycols rise. This occurs due to the expulsion of the solute molecules in the solvent because of thermal agitation which results in the expansion of the volume and more compressibility. Also, the disrupted molecules of solvent and the hydration shell of solute contribute to this behavior of $K_{\phi,S}$ values. These negative values also reveal that inside the bulk, the water molecules are more compressible as compared to the solute. Due to hydrophobic-hydrophobic interactions in the non-polar groups, the molecules of water contract and suggest that over the ionic charge groups of solute the water molecules are less compressible and they arrange themselves in particular order around the solute. Besides, the structural compressibility of water is reduced as solute and solvent create a greater aligning effect since the values of $K_{\phi,S}$ is negative [24, 59-62].

4.98 Partial molar isentropic compression

With the equation **4.9**, the partial molar isentropic compression is determined by contemplating the divergence of apparent molar isentropic compression corresponding the molality. Here m_A is the molality of the solute. In **Table 4.95,** the partial molar isentropic compression ($K_{\phi,S}^0$) with the experimental slope (S_k^*) is indexed corresponding to their experimental temperatures and biotin concentrations. In the same table, the standard errors are also reported. All these parameters are computed using the method of least square fitting. The $K_{\phi,S}^0$ values are all negative which is reducing with the upsurge in the concentration of biotin and the temperatures. This is demonstrated in **Figure 4.76**. The reduction in the negative values of $K_{\phi,S}^0$ with temperature implies that some of the water molecules are discharged into bulk and thus there exists strong interaction among the molecules of water and glycols. The water molecules around the glycols are less compressible at lower concentrations of biotin but it is more compressible at higher biotin concentrations due to the dominant combination within the biotin and water molecules which dehydrates the glycol molecules. The S_k^* values in the table provide the information regarding solute-solute interactions in the mixture of aqueous biotin and glycols. As S_k^* values are very minimal as compared to the $K_{\phi,S}^0$ values, the solute-solute interaction are almost negligible in the liquid mixture and indicates that solute-solvent interaction is prevailing in the solution [57, 63].

4.99 Partial molar isentropic compression of transfer

At infinite dilution the partial molar isentropic compression of transfer is computed with the equation **4.10** for glycol from water to aqueous biotin solutions. The calculated values of $\Delta K_{\phi,s}^0$ are recorded in **Table 4.96** for propylene glycol and hexylene glycol at all concentrations of biotin as well as different temperatures. All $\Delta K_{\phi,s}^0$ values are found to be positive and increases with the biotin concentration but show no regular trend with the temperature. This pattern implies the tendency of structure making in the ions due to strong interactions amid the zwitterionic center of glycols and biotin where the interactions of the zwitterionic center increase with the surge in the biotin concentrations as the electrostriction decreases which increases the structure making tendency. The bulk water becomes more compressible as compared to the electrostriction water which causes a huge decrement in the compressibility with the concentration of biotin. This is the reason why $\Delta K_{\phi,s}^{0}$ values are positive while $K_{\phi,s}^{0}$ are negative for (PG/HG) at different concentrations of biotin as more amount of water molecules of solute are incorporated with the molecules of solvent that leads to more interactions within the ions since at lower concentrations of biotin and lower temperatures, the molecules of water constitute with the ions [11, 38-40].

4.100 Pair and triplet coefficients

The partial molar volume of transfer and the partial molar isentropic compression of transfer is obtained from the equation **4.11** and **4.12** where m_B denotes the molality of the aqueous biotin solutions, A represents glycols and B represents biotin. V_{AB}; V_{ABB} and K_{AB}; K_{ABB} represents the pair and triplet coefficients for volume and isentropic compression respectively which are mentioned in **Table 4.97.** These values are calculated by fitting ΔV_{ϕ}^{0} and ΔK_{ϕ}^{0} values for volume and isentropic compression respectively. Mcmillan-Mayer [41] provided the theory to calculate the pair-triplet interaction coefficients to investigate the parting of effects in the liquid mixture which was further discussed by Friedman and Krishnan [42] and Franks et al [43]. The values of pair interaction coefficients i.e. V_{AB} and K_{AB}, are found to be positive except for PG at 318.15K V_{AB} is negative. Similarly, in the case of triplet interaction coefficients i.e V_{ABB} and K_{ABB}, all values are positive throughout the temperatures for both propylene and hexylene glycol. From the hydration co-spheres, the water molecules are discharged to the bulk as they overlap when non-bonding favorable interactions occur. As per this theory, the water released from a co-sphere to bulk causes a change in the volume, which would be positive when the bulk is more structured than the co-sphere but would be negative when the co-sphere is more structured than the bulk due to the various structural arrangement of water molecules. The positive values of triplet interaction coefficient as compared to the pair interaction coefficient for volumetric and isentropic compression data manifest that the pair-wise interaction is dominated by triplet-wise interaction in the mixture of (biotin+ water+ PG/HG) [47, 64].

4.101 Hydration number

The hydration number for the liquid mixtures is calculated using the equation **4.13** which was developed by Passynsky [65]. Here, n_1 is the number of moles of solvent, n_2 is the number moles of solute, k_s is the isentropic compressibility of the solution, and k_s^0 is the isentropic compressibility of solvent. It is considered that ions contain two hydration spheres: primary hydration spheres and secondary hydration spheres. The primary hydration sphere consists of water molecules that strongly combine with the ion through an electrostatic ion-dipole attraction. The secondary hydration sphere is made up of water molecules that interact partially with the primary hydration sphere ion and partially with the water structure in the surroundings which merge into the bulk after extending an undefined length from the ion. The calculated hydration numbers using various techniques can be classified into two groups where low values indicate the primary hydration number and larger values implies the primary hydration along with the overall or fractional part of the secondary hydration sphere. These hydration numbers are further used to determine the solvation property of ions with some other properties of solvent in the mixture [66, 67]. The calculated hydration numbers at various concentrations and temperatures are mentioned in **Table 4.98.** These values are large ranging from 111.0012 to 555.0102 and thus indicating the presence of hydrophobic hydration and electrostatic hydration due to co-operative hydrogen bonding in aqueous biotin solutions. The decrement of the hydration numbers with the corresponding molality of glycols shows the ion-association and implies that the calculated hydration numbers from the compressibility data are due to both electrostriction and secondary hydration shell which contributes to hydrophobic hydration. Also, the high hydration numbers are attributed due to the presence of co-operative hydrogen bonding and a decrease in the solvating molecules due to the replacement of water molecules by glycol molecules in the coordination sphere of ions inside the mixture [1, 68].

Table 4.89

Values of densities, ρ, apparent molar volumes, V_ϕ of glycols in aqueous solutions of biotin at different temperatures

${}^{a}m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^{6}$/(m^3·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				0.000 mol·kg^{-1} biotin + PG				
0.00000	0.99926	0.99705	0.99404	0.99036				
0.10028	0.99953	0.99732	0.99433	0.99066	73.44	73.52	73.60	73.67
0.20000	0.99978	0.99758	0.99460	0.99096	73.50	73.58	73.66	73.73
0.30017	1.00001	0.99783	0.99486	0.99123	73.57	73.64	73.71	73.78
0.40905	1.00026	0.99808	0.99513	0.99152	73.63	73.70	73.77	73.84
0.50000	1.00045	0.99828	0.99534	0.99175	73.67	73.75	73.82	73.89
				0.001 mol·kg^{-1} biotin + PG				
0.00000	0.99955	0.99737	0.99442	0.99079				
0.09990	0.99981	0.99764	0.99471	0.99109	73.46	73.54	73.62	73.69
0.20045	1.00006	0.99790	0.99498	0.99138	73.52	73.60	73.68	73.75
0.29880	1.00029	0.99814	0.99523	0.99165	73.58	73.66	73.74	73.80
0.40084	1.00051	0.99837	0.99547	0.99191	73.65	73.72	73.80	73.87
0.50009	1.00071	0.99857	0.99569	0.99215	73.71	73.79	73.86	73.93
				0.002 mol·kg^{-1} biotin + PG				

0.00000	0.99974	0.99767	0.99474	0.99111				
0.10071	1.00000	0.99794	0.99502	0.99141	73.49	73.56	73.64	73.70
0.19991	1.00025	0.99819	0.99528	0.99169	73.54	73.62	73.71	73.77
0.30027	1.00048	0.99842	0.99553	0.99196	73.61	73.69	73.77	73.83
0.40010	1.00069	0.99864	0.99576	0.99221	73.67	73.75	73.83	73.89
0.49000	1.00087	0.99882	0.99595	0.99242	73.73	73.81	73.89	73.96
0.003 mol·kg^{-1} biotin + PG								
0.00000	0.99989	0.99787	0.99494	0.99145				
0.10087	1.00015	0.99814	0.99522	0.99175	73.51	73.60	73.68	73.74
0.20004	1.00039	0.99838	0.99548	0.99202	73.57	73.65	73.73	73.80
0.29996	1.00062	0.99861	0.99572	0.99228	73.63	73.71	73.79	73.86
0.40230	1.00083	0.99884	0.99596	0.99254	73.69	73.77	73.85	73.92
0.50006	1.00103	0.99904	0.99616	0.99276	73.74	73.83	73.91	73.98
0.000 mol·kg^{-1} biotin + HG								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.09976	0.99944	0.99725	0.99428	0.99063	116.37	116.41	116.45	116.49
0.20012	0.99962	0.99745	0.99450	0.99090	116.40	116.43	116.47	116.51
0.30214	0.99979	0.99765	0.99473	0.99115	116.42	116.46	116.50	116.54
0.39996	0.99995	0.99782	0.99493	0.99139	116.44	116.48	116.52	116.56
0.50067	1.00010	0.99800	0.99513	0.99163	116.46	116.50	116.55	116.59

0.001 mol·kg^{-1} biotin + HG								
0.00000	0.99955	0.99737	0.99442	0.99079				
0.10100	0.99973	0.99758	0.99466	0.99106	116.40	116.44	116.47	116.51
0.20035	0.99990	0.99777	0.99487	0.99131	116.42	116.46	116.50	116.53
0.29989	1.00006	0.99795	0.99508	0.99156	116.45	116.49	116.52	116.56
0.40002	1.00022	0.99812	0.99529	0.99180	116.47	116.51	116.55	116.59
0.50210	1.00037	0.99829	0.99548	0.99202	116.50	116.54	116.58	116.62
0.002 mol·kg^{-1} biotin + HG								
0.00000	0.99974	0.99767	0.99474	0.99111				
0.10002	0.99992	0.99786	0.99496	0.99138	116.42	116.45	116.48	116.52
0.20378	1.00009	0.99806	0.99519	0.99164	116.44	116.48	116.51	116.55
0.30087	1.00025	0.99823	0.99539	0.99187	116.47	116.50	116.53	116.57
0.39890	1.00039	0.99839	0.99558	0.99210	116.49	116.53	116.56	116.60
0.50010	1.00054	0.99856	0.99577	0.99232	116.52	116.55	116.59	116.63
0.003 mol·kg^{-1} biotin + HG								
0.00000	0.99989	0.99787	0.99494	0.99145				
0.10072	1.00007	0.99807	0.99516	0.99171	116.43	116.47	116.51	116.54
0.20054	1.00023	0.99825	0.99537	0.99196	116.46	116.50	116.54	116.56
0.30341	1.00039	0.99843	0.99558	0.99220	116.49	116.52	116.56	116.59
0.40009	1.00053	0.99859	0.99577	0.99242	116.51	116.55	116.59	116.62

0.49981	1.00067	0.99874	0.99595	0.99263	116.54	116.58	116.62	116.64

[a] m_A is the molality of glycols in the aqueous solution biotin; standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1},

Table 4.90

Partial molar volumes, V_{ϕ}^{0}, and experimental slopes, S_V^*, of glycols in the aqueous solution of biotin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$V_{\phi}^{0} \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-2})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				PG				
0.000	73.39(±0.004)	73.46(±0.002)	73.55(±0.001)	73.62(±0.002)	0.59(±0.014)	0.58(±0.007)	0.55(±0.004)	0.55(±0.007)
0.001	73.39(±0.003)	73.48(±0.002)	73.56(±0.003)	73.63(±0.001)	0.63(±0.012)	0.62(±0.008)	0.60(±0.009)	0.60(±0.005)
0.002	73.42(±0.003)	73.50(±0.002)	73.58(±0.002)	73.64(±0.002)	0.63(±0.009)	0.64(±0.008)	0.64(±0.007)	0.64(±0.008)
0.003	73.45(±0.000)	73.54(±0.001)	73.61(±0.002)	73.68(±0.001)	0.59(±0.002)	0.59(±0.004)	0.60(±0.007)	0.60(±0.005)
				HG				
0.000	116.35(±0.000)	116.39(±0.000)	116.43(±0.001)	116.46(±0.001)	0.23(±0.001)	0.23(±0.001)	0.24(±0.004)	0.24(±0.003)
0.001	116.37(±0.000)	116.41(±0.002)	116.44(±0.002)	116.48(±0.002)	0.25(±0.002)	0.26(±0.006)	0.27(±0.007)	0.27(±0.006)
0.002	116.39(±0.001)	116.42(±0.001)	116.46(±0.001)	116.49(±0.001)	0.25(±0.005)	0.26(±0.004)	0.26(±0.004)	0.27(±0.004)
0.003	116.41(±0.000)	116.45(±0.000)	116.48(±0.001)	116.51(±0.001)	0.26(±0.002)	0.26(±0.001)	0.26(±0.003)	0.26(±0.004)

$^{a}m_B$ is the molality of aqueous biotin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}, $u(V_{\phi}^{0})$= ±0.01 × 10^6/(m^3·mol^{-1}) and $u(S_V^*)$=±0.03 × 10^6/(m^3·kg·mol^{-2})

Table 4.91

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of glycols in the aqueous solution of biotin at different temperatures.

[a]m_B/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
		PG		
0.001	0.01	0.01	0.01	0.01
0.002	0.03	0.03	0.03	0.02
0.003	0.07	0.07	0.07	0.06
		HG		
0.001	0.02	0.02	0.02	0.02
0.002	0.04	0.04	0.03	0.03
0.003	0.06	0.06	0.06	0.05

[a]m_B is the molality of aqueous biotin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}

Table 4.92

Values of empirical parameters of Eq., of glycols in aqueous solution of biotin at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	ARD
			PG		
0.001	73.480	0.008	0.000	0.9999	0.0000
0.002	73.500	0.008	0.000	0.9999	0.0000
0.003	73.537	0.008	0.000	0.9999	0.0006
			HG		
0.001	116.408	0.004	0.000	0.9999	0.0000
0.002	116.423	0.003	0.000	0.9999	0.0000
0.003	116.448	0.004	0.000	0.9999	0.0002

${}^{a}m_B$ is the molality of aqueous biotin, standard uncertainties *u* are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}

Table 4.93

Partial molar expansibilities, E_{ϕ}^{0}, for glycols in the aqueous solution of biotin at different temperatures.

${}^{a}m_B$/ (mol·kg^{-1})	$E_{\phi}^{0}\times10^{6}$/(m^3· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^3·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			PG		
0.001	0.0091	0.0082	0.0074	0.0066	-0.0001
0.002	0.0087	0.0078	0.0070	0.0061	-0.0001
0.003	0.0090	0.0081	0.0072	0.0062	-0.0001
			HG		
0.001	0.0037	0.0036	0.0036	0.0035	0.0000
0.002	0.0031	0.0033	0.0034	0.0035	0.0000
0.003	0.0043	0.0037	0.0031	0.0025	-0.0001

${}^{a}m_B$ is the molality of aqueous biotin, standard uncertainties *u* are *u(m) = 1%*, *u(T)*=0.001 K, *u(ρ)=0.15*(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}

Table 4.94

Values of the speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,s}$ of glycols in aqueous solutions of biotin at different temperatures

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^{6}$/(m^{3}·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.000 mol·kg^{-1} biotin + PG								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.10028	1471.03	1500.79	1523.09	1539.09	-46.04	-44.26	-42.91	-41.97
0.20000	1475.50	1504.61	1526.29	1542.06	-46.29	-44.49	-43.14	-42.20
0.30017	1479.61	1508.02	1529.50	1545.03	-46.38	-44.58	-43.22	-42.28
0.40905	1483.28	1511.16	1532.52	1548.34	-46.43	-44.63	-43.27	-42.33
0.50000	1486.61	1513.99	1535.04	1550.83	-46.46	-44.66	-43.30	-42.36
0.001 mol·kg^{-1} biotin + PG								
0.00000	1468.41	1497.41	1521.14	1538.02				
0.09990	1473.04	1502.29	1525.12	1541.08	-45.93	-44.16	-42.80	-41.86
0.20045	1477.58	1506.12	1528.31	1544.08	-46.17	-44.40	-43.03	-42.09
0.29880	1481.57	1509.51	1531.45	1546.96	-46.26	-44.49	-43.11	-42.17
0.40084	1485.00	1512.56	1534.27	1550.12	-46.31	-44.53	-43.16	-42.22
0.50009	1488.86	1515.49	1537.07	1553.02	-46.34	-44.56	-43.19	-42.25

0.002 mol·kg^{-1} biotin + PG								
0.00000	1470.55	1499.55	1522.99	1540.24				
0.10071	1475.43	1504.48	1526.98	1543.27	-45.80	-44.04	-42.69	-41.74
0.19991	1479.81	1508.31	1530.16	1546.09	-46.04	-44.27	-42.92	-41.96
0.30027	1483.71	1511.62	1533.52	1549.10	-46.13	-44.36	-43.00	-42.05
0.40010	1487.13	1514.65	1536.15	1552.28	-46.17	-44.41	-43.05	-42.09
0.49000	1490.80	1517.26	1538.85	1554.91	-46.20	-44.43	-43.08	-42.12
0.003 mol·kg^{-1} biotin + PG								
0.00000	1473.64	1501.64	1525.68	1543.35				
0.10087	1478.39	1506.54	1529.64	1546.13	-45.61	-43.92	-42.55	-41.57
0.20004	1482.66	1510.30	1532.69	1548.99	-45.84	-44.15	-42.77	-41.80
0.29996	1486.29	1513.78	1536.03	1551.97	-45.93	-44.23	-42.85	-41.88
0.40230	1490.03	1516.81	1538.83	1555.17	-45.98	-44.28	-42.90	-41.92
0.50006	1494.24	1519.79	1541.79	1557.96	-46.01	-44.31	-42.93	-41.95
0.000 mol·kg^{-1} biotin + HG								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.09976	1476.42	1504.09	1526.06	1542.03	-46.04	-44.26	-42.91	-41.97
0.20012	1485.99	1513.18	1532.68	1549.03	-46.28	-44.49	-43.14	-42.20
0.30214	1495.08	1521.73	1540.15	1555.44	-46.37	-44.57	-43.22	-42.28
0.39996	1503.80	1529.03	1545.50	1560.44	-46.41	-44.62	-43.26	-42.32

0.50067	1510.68	1536.10	1550.22	1565.35	-46.44	-44.65	-43.30	-42.36
$0.001\ mol\cdot kg^{-1}$ biotin + HG								
0.00000	1468.41	1497.41	1521.14	1538.02				
0.10100	1478.35	1506.04	1528.33	1544.45	-45.93	-44.17	-42.80	-41.86
0.20035	1488.32	1514.82	1535.13	1551.55	-46.17	-44.40	-43.02	-42.09
0.29989	1496.91	1523.31	1542.56	1557.66	-46.25	-44.48	-43.10	-42.17
0.40002	1506.31	1530.61	1547.86	1562.78	-46.30	-44.52	-43.15	-42.21
0.50210	1513.33	1537.78	1552.59	1567.73	-46.33	-44.55	-43.18	-42.24
$0.002\ mol\cdot kg^{-1}$ biotin + HG								
0.00000	1470.55	1499.55	1522.99	1540.24				
0.10002	1480.71	1508.14	1530.19	1546.54	-45.79	-44.04	-42.69	-41.74
0.20378	1491.11	1517.16	1537.49	1553.94	-46.04	-44.27	-42.92	-41.97
0.30087	1499.45	1525.41	1544.59	1559.92	-46.12	-44.35	-43.00	-42.05
0.39890	1508.95	1532.51	1549.79	1564.72	-46.16	-44.40	-43.04	-42.09
0.50010	1515.81	1539.60	1554.33	1569.78	-46.19	-44.43	-43.07	-42.12
$0.003\ mol\cdot kg^{-1}$ biotin + HG								
0.00000	1473.64	1501.64	1525.68	1543.35				
0.10072	1483.93	1510.35	1533.20	1550.04	-45.61	-43.92	-42.54	-41.57
0.20054	1493.89	1519.25	1540.20	1557.40	-45.84	-44.15	-42.77	-41.80
0.30341	1502.99	1527.80	1547.65	1563.56	-45.93	-44.23	-42.85	-41.88

0.40009	1512.17	1534.80	1552.15	1568.56	-45.97	-44.27	-42.89	-41.92
0.49981	1519.07	1541.96	1556.71	1573.18	-46.00	-44.30	-42.92	-41.95

$^{a}m_A$ is the molality of glycols in the aqueous solution biotin; standard uncertainties *u* are *u(m)* = 1%, *u(T)*=0.001 K, *u(ρ)*=0.15(kg·m^{-3}), *u(c)*= 1.0 m·s^{-1}.

Table 4.95

Partial molar isentropic compression, $K^0_{\phi,s}$, and experimental slopes, S^*_K, of glycols in the aqueous solution of biotin at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$K^0_{\phi,s}$ ×10^6/(m^3·mol^{-1}· GPa^{-1})				S^*_K ×10^6/(kg·m^3·mol^{-2}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
PG								
0.000	-46.03(±0.079)	-44.24(±0.076)	-42.89(±0.074)	-41.95(±0.073)	-0.96(±0.236)	-0.93(±0.228)	-0.91(±0.222)	-0.91(±0.219)
0.001	-45.91(±0.079)	-44.15(±0.077)	-42.78(±0.075)	-41.84(±0.074)	-0.96(±0.240)	-0.93(±0.232)	-0.91(±0.226)	-0.91(±0.223)
0.002	-45.78(±0.077)	-44.02(±0.074)	-42.68(±0.073)	-41.72(±0.071)	-0.97(±0.235)	-0.94(±0.227)	-0.92(±0.222)	-0.92(±0.218)
0.003	-45.59(±0.077)	-43.91(±0.075)	-42.53(±0.073)	-41.56(±0.072)	-0.94(±0.233)	-0.91(±0.226)	-0.90(±0.220)	-0.89(±0.217)
HG								
0.000	-46.03(±0.079)	-44.24(±0.077)	-42.89(±0.075)	-41.95(±0.074)	-0.94(±0.240)	-0.92(±0.232)	-0.90(±0.226)	-0.91(±0.223)
0.001	-45.92(±0.078)	-44.16(±0.075)	-42.79(±0.073)	-41.85(±0.072)	-0.92(±0.235)	-0.90(±0.227)	-0.89(±0.222)	-0.89(±0.219)
0.002	-45.78(±0.079)	-44.03(±0.077)	-42.68(±0.075)	-41.72(±0.074)	-0.93(±0.240)	-0.90(±0.232)	-0.89(±0.226)	-0.90(±0.223)
0.003	-45.59(±0.077)	-43.91(±0.075)	-42.53(±0.073)	-41.56(±0.072)	-0.92(±0.233)	-0.89(±0.226)	-0.88(±0.220)	-0.88(±0.217)

$^a m_B$ is the molality of aqueous niacin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}, $u(K^0_{\phi,s})$= ±0.01 ×10^6/(m^3·mol^{-1}·GPa^{-1}) and $u(S^*_k)$= ±0.24×10^6/(kg·m^3·mol^{-2}· GPa^{-1})

Table 4.96

Partial molar isentropic compression transfer, $\Delta K^0_{\phi,s}$, of glycols in the aqueous solution of biotin at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$\Delta K^0_{\phi,s}$ × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PG		
0.001	0.11	0.09	0.11	0.11
0.002	0.25	0.22	0.22	0.23
0.003	0.44	0.34	0.36	0.40
		HG		
0.001	0.11	0.09	0.11	0.10
0.002	0.25	0.22	0.22	0.23
0.003	0.44	0.34	0.36	0.39

$^a m_B$ is the molality of aqueous niacin, standard uncertainties u are $u(m) = 1\%$, $u(T)$=0.001 K, $u(\rho)=0.15$(kg·m^{-3}), $u(c)$= 1.0 m·s^{-1}.

Table 4.97

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of glycols in aqueous solutions of biotin at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		PG		
288.15	1.35	2151.06	46.02	5894.13
298.15	2.57	2062.40	46.62	2255.77
308.15	3.41	1747.72	49.14	2484.97
318.15	-1.69	2594.07	46.06	4344.48
		HG		
288.15	10.50	183.53	42.38	6686.46
298.15	9.19	115.76	42.92	3056.73
308.15	6.62	689.21	45.60	3250.97
318.15	7.16	104.47	42.53	5102.28

T/K is the temperatures.

Table 4.98

Hydration number for glycols in aqueous solutions of biotin at different temperatures

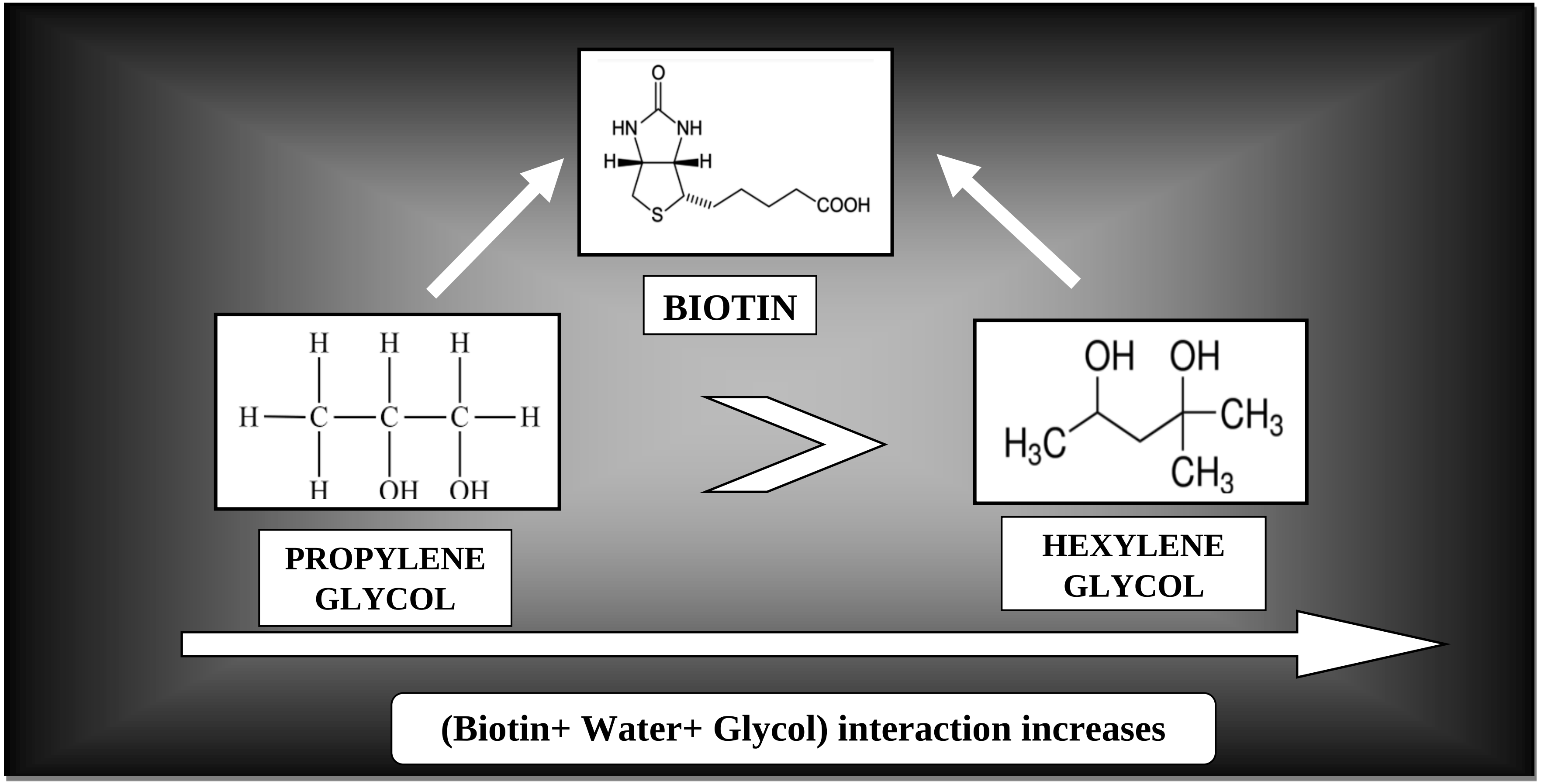
$^{a}m_A$/(mol·kg^{-1}	n_h			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
PG+0.000 mol·kg^{-1} biotin				
0.09917	554.9979	554.9983	554.9975	554.9968
0.19801	277.5007	277.5006	277.5000	277.4996
0.30136	185.0015	185.0013	185.0008	185.0005
0.39826	138.7519	138.7516	138.7512	138.7510
0.51059	111.0020	111.0017	111.0013	111.0012
PG+0.001 mol·kg^{-1} biotin				
0.09990	555.0041	555.0042	555.0035	555.0028
0.20045	277.5038	277.5036	277.5030	277.5026
0.29880	185.0036	185.0032	185.0028	185.0024
0.40084	138.7533	138.7530	138.7526	138.7524
0.50009	111.0032	111.0029	111.0025	111.0024
PG+0.002 mol·kg^{-1} biotin				
0.10071	555.0053	555.0052	555.0045	555.0038
0.19991	277.5043	277.5041	277.5035	277.5030

0.30027	185.0039	185.0036	185.0032	185.0027
0.40010	138.7536	138.7532	138.7529	138.7527
0.49000	111.0034	111.0030	111.0027	111.0025
PG+0.003 mol·kg^{-1} biotin				
0.10087	555.0063	555.0062	555.0055	555.0048
0.20004	277.5048	277.5046	277.5040	277.5035
0.29996	185.0042	185.0039	185.0035	185.0031
0.40230	138.7538	138.7535	138.7531	138.7529
0.50006	111.0036	111.0032	111.0029	111.0027
HG+0.000 mol·kg^{-1} biotin				
0.09903	555.0019	555.0006	554.9996	554.9989
0.20184	277.5045	277.5037	277.5022	277.5020
0.29963	185.0052	185.0045	185.0033	185.0029
0.39805	138.7555	138.7547	138.7534	138.7531
0.49538	111.0054	111.0047	111.0034	111.0032
HG+0.001 mol·kg^{-1} biotin				
0.10100	555.0080	555.0069	555.0058	555.0052
0.20035	277.5077	277.5067	277.5054	277.5052
0.29989	185.0072	185.0065	185.0054	185.0049
0.40002	138.7571	138.7562	138.7550	138.7546

0.50210	111.0067	111.0059	111.0047	111.0044
HG+0.002 mol·kg^{-1} biotin				
0.10002	555.0091	555.0079	555.0068	555.0061
0.20378	277.5084	277.5072	277.5061	277.5057
0.30087	185.0076	185.0068	185.0057	185.0053
0.39890	138.7574	138.7564	138.7552	138.7548
0.50010	111.0069	111.0061	111.0048	111.0046
HG+0.003 mol·kg^{-1} biotin				
0.10072	555.0102	555.0089	555.0080	555.0074
0.20054	277.5088	277.5077	277.5066	277.5063
0.30341	185.0081	185.0072	185.0062	185.0057
0.40009	138.7577	138.7566	138.7554	138.7552
0.49981	111.0071	111.0063	111.0050	111.0048

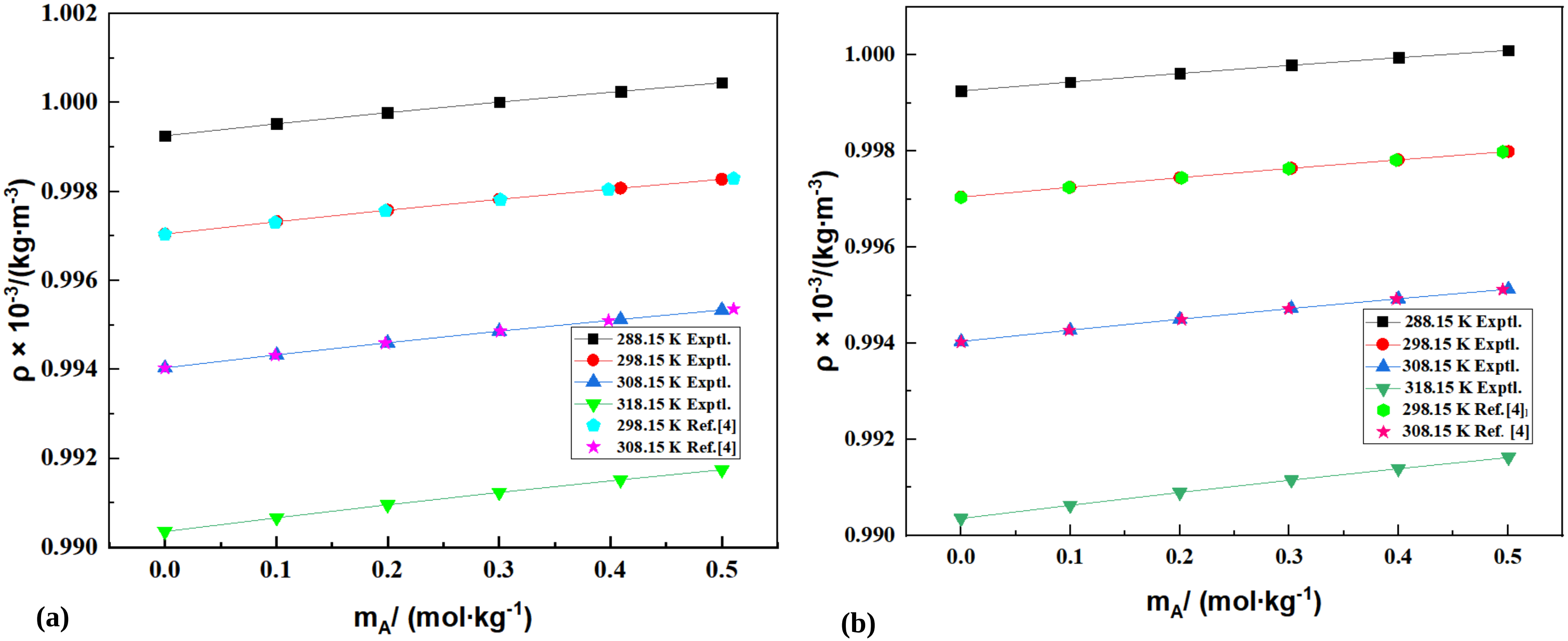
[a] m_A is the molality of glycols in the aqueous solution biotin

Figure 4.70



PG / HG and biotin interactions.

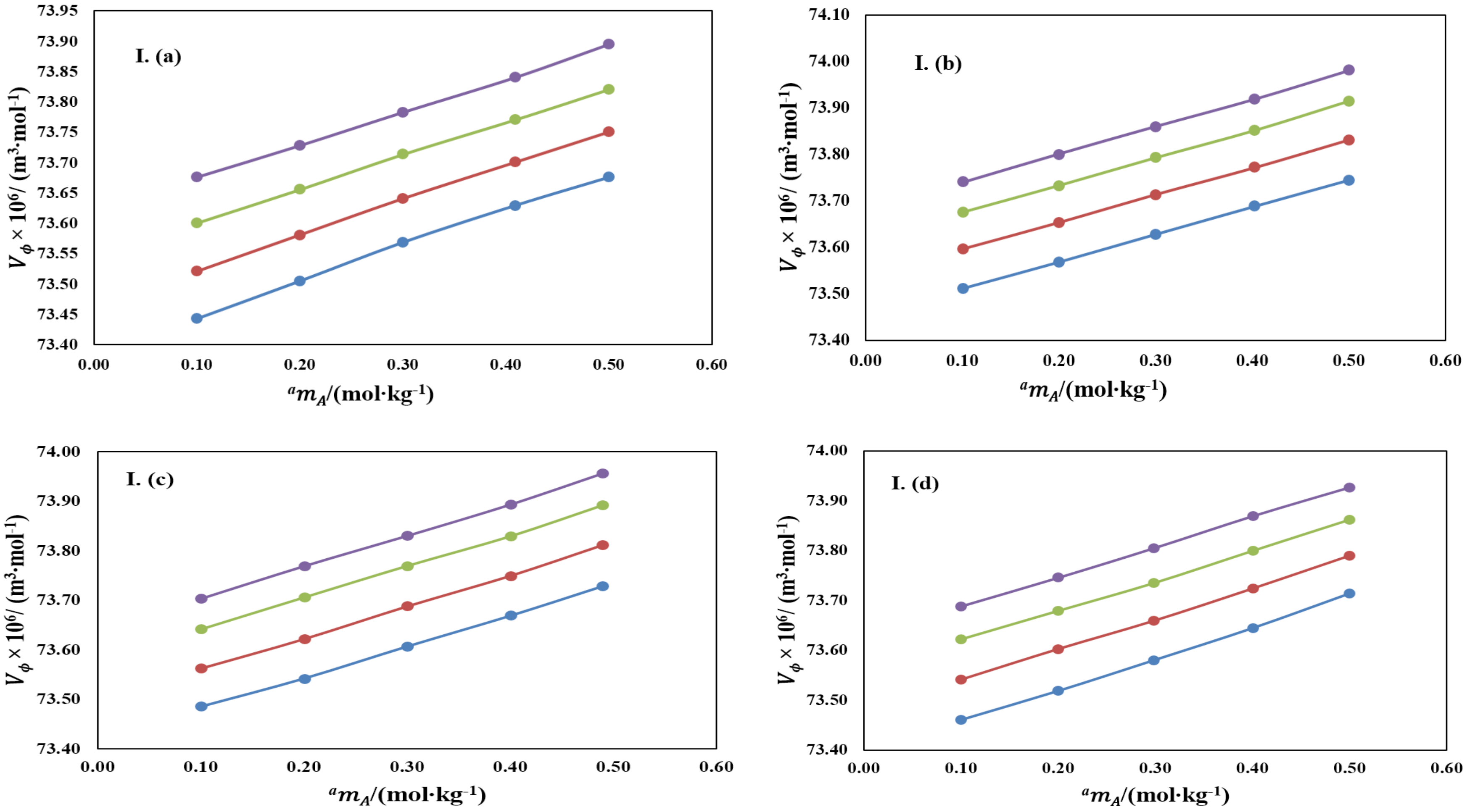
Figure 4.71

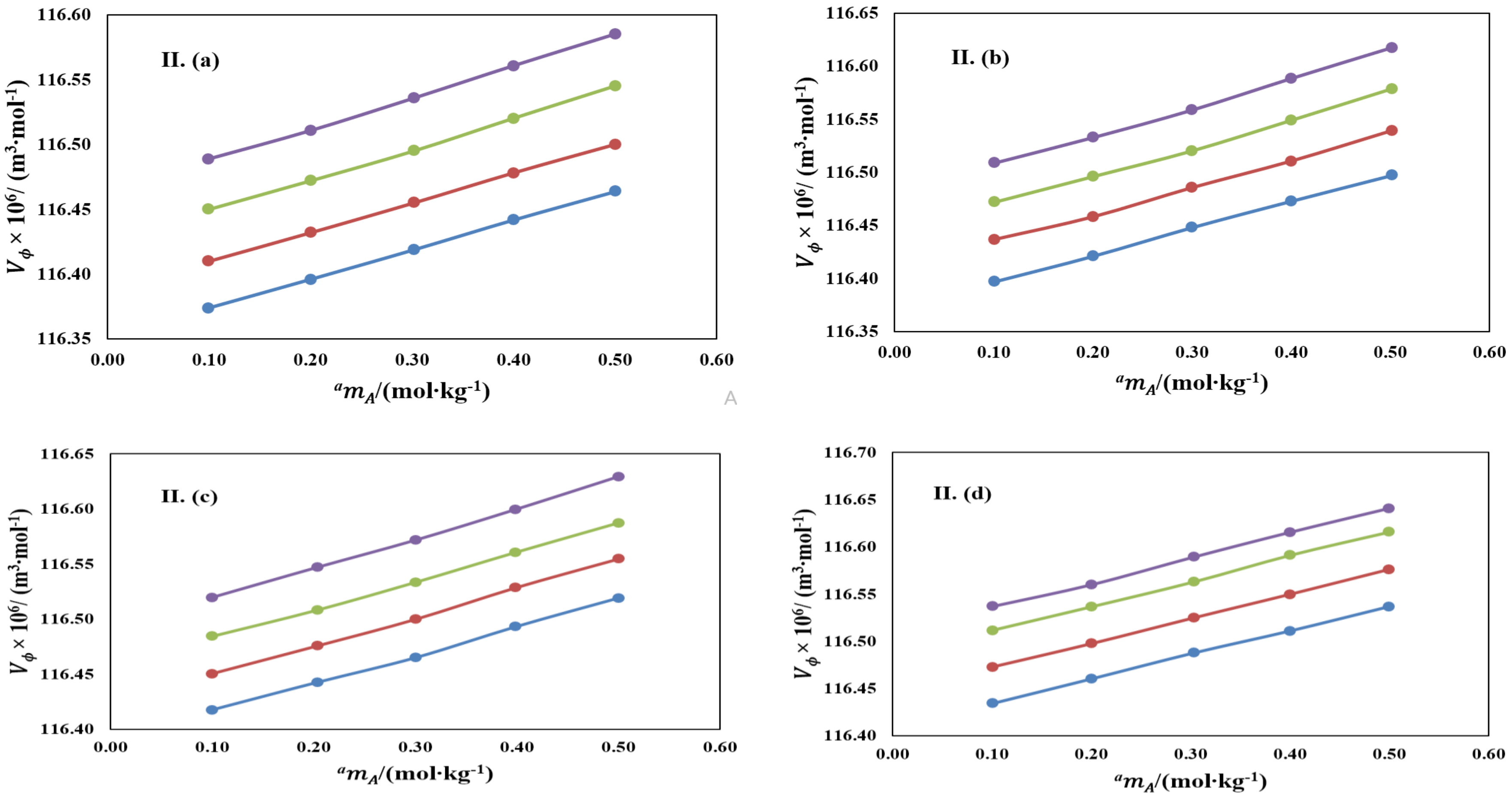


(a) (b)

Variation of experimental and literature density values [4] of (a) (Propylene glycol+Water) and (b) (Hexylene glycol +Water) corresponding to the molality (m_A) of glycols at different T.

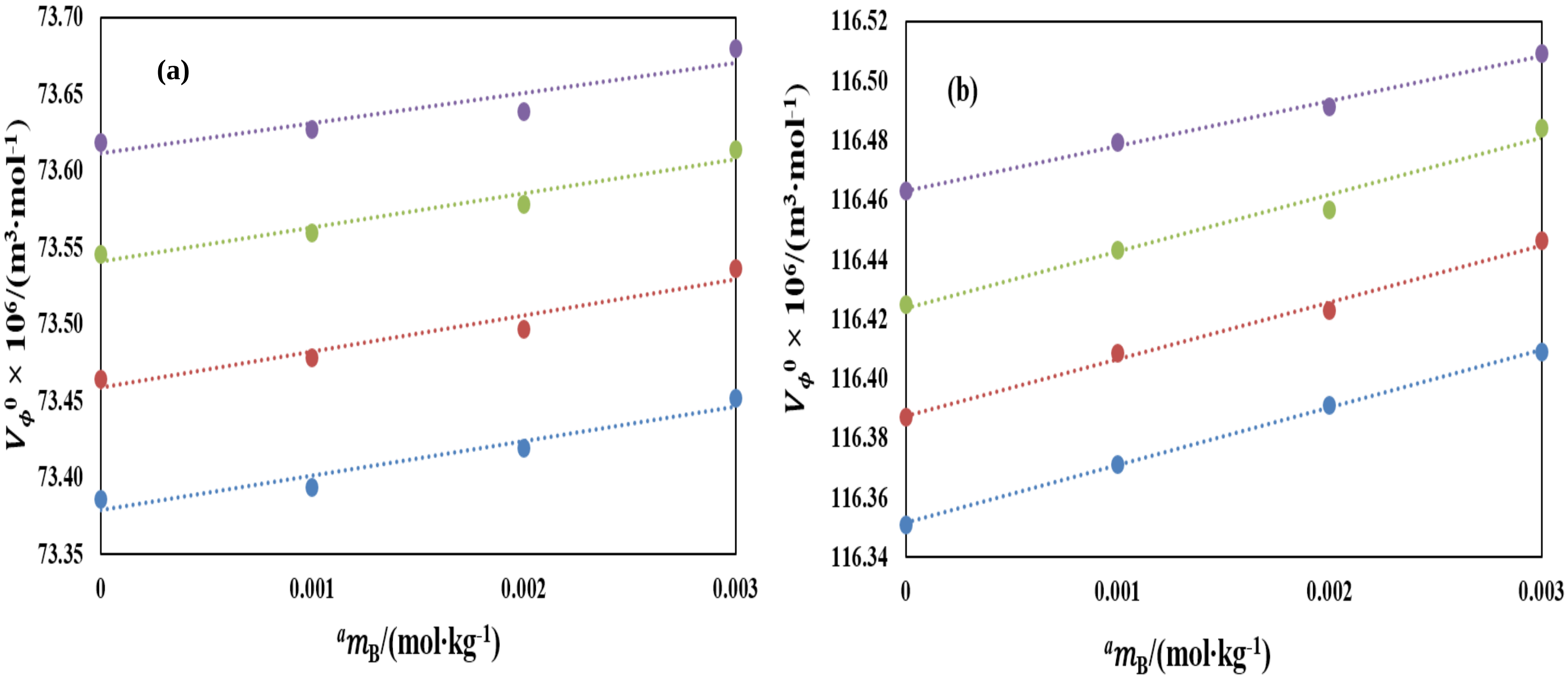
Figure 4.72


I. (a)
73.95
73.90
73.85
73.80
73.75
73.70
73.65
73.60
73.55
73.50
73.45
73.40
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
I. (b)
74.10
74.00
73.90
73.80
73.70
73.60
73.50
73.40
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
I. (c)
74.00
73.90
73.80
73.70
73.60
73.50
73.40
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)
I. (d)
74.00
73.90
73.80
73.70
73.60
73.50
73.40
0.00
0.10
0.20
0.30
0.40
0.50
0.60
$V_\phi \times 10^6$/ ($m^3 \cdot mol^{-1}$)
$^a m_A$/($mol \cdot kg^{-1}$)



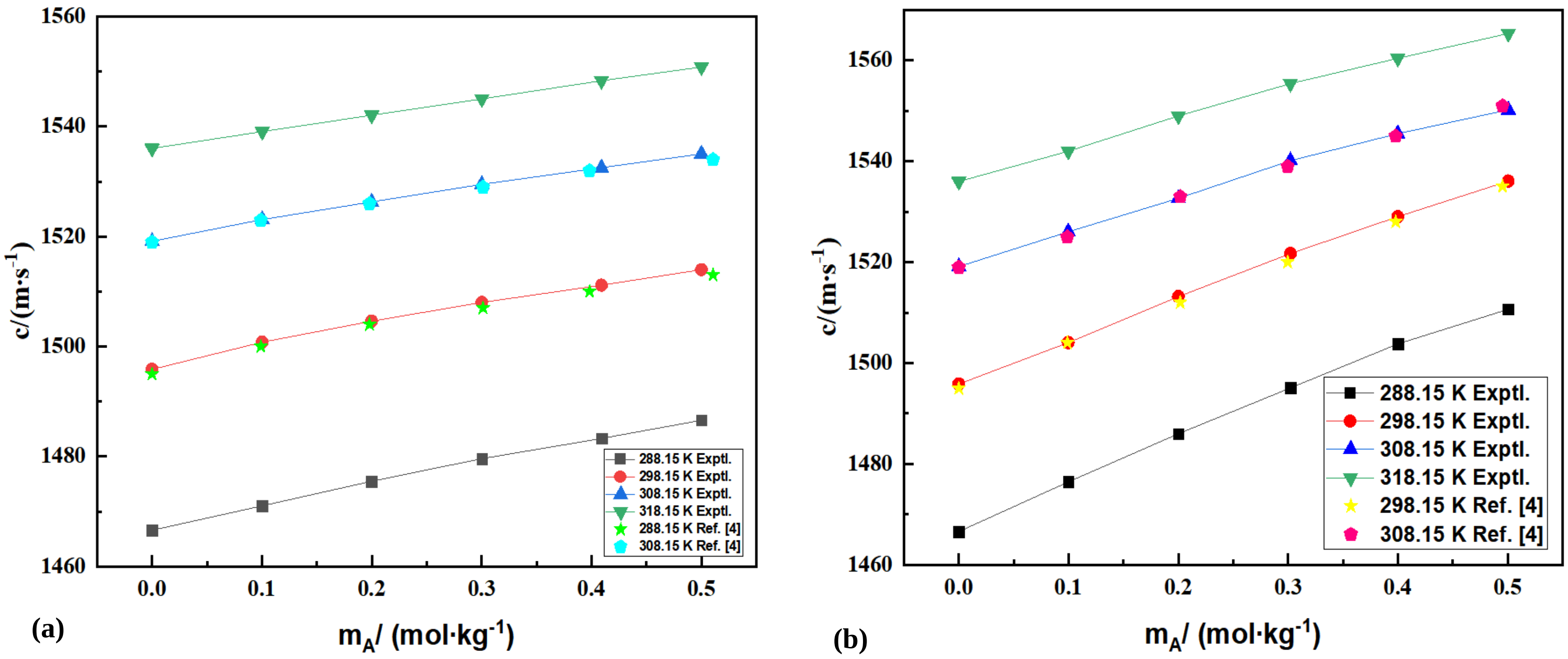
Variation of apparent molar volume, V_ϕ of Propylene glycol (I) and hexylene glycol (II) (a) 0.000 biotin, (b) 0.001 biotin, (c) 0.002 biotin, (d) 0.003 biotin, against molality at different temperatures [blue, 288.15 K; red, 298.15 K; green, 308.15 K; purple 318.15 K]

Figure 4.73



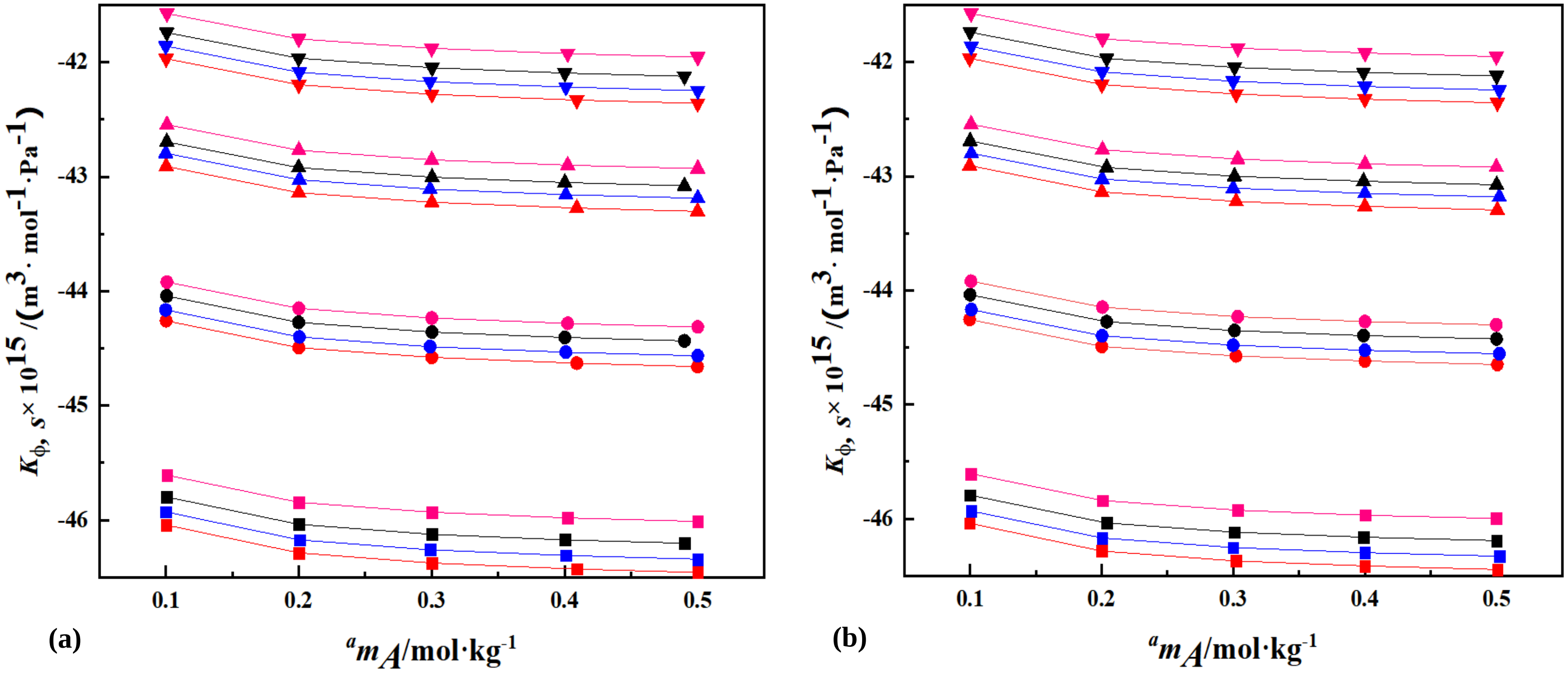
Variation of partial molar volumes, V_ϕ^0, of, (a) Propylene glycol and (b) hexylene glycol in different concentration of aqueous biotin solutions at different temperatures [blue, 288.15 K; red, 298.15 K; green, 308.15 K; purple 318.15 K]

Figure 4.74



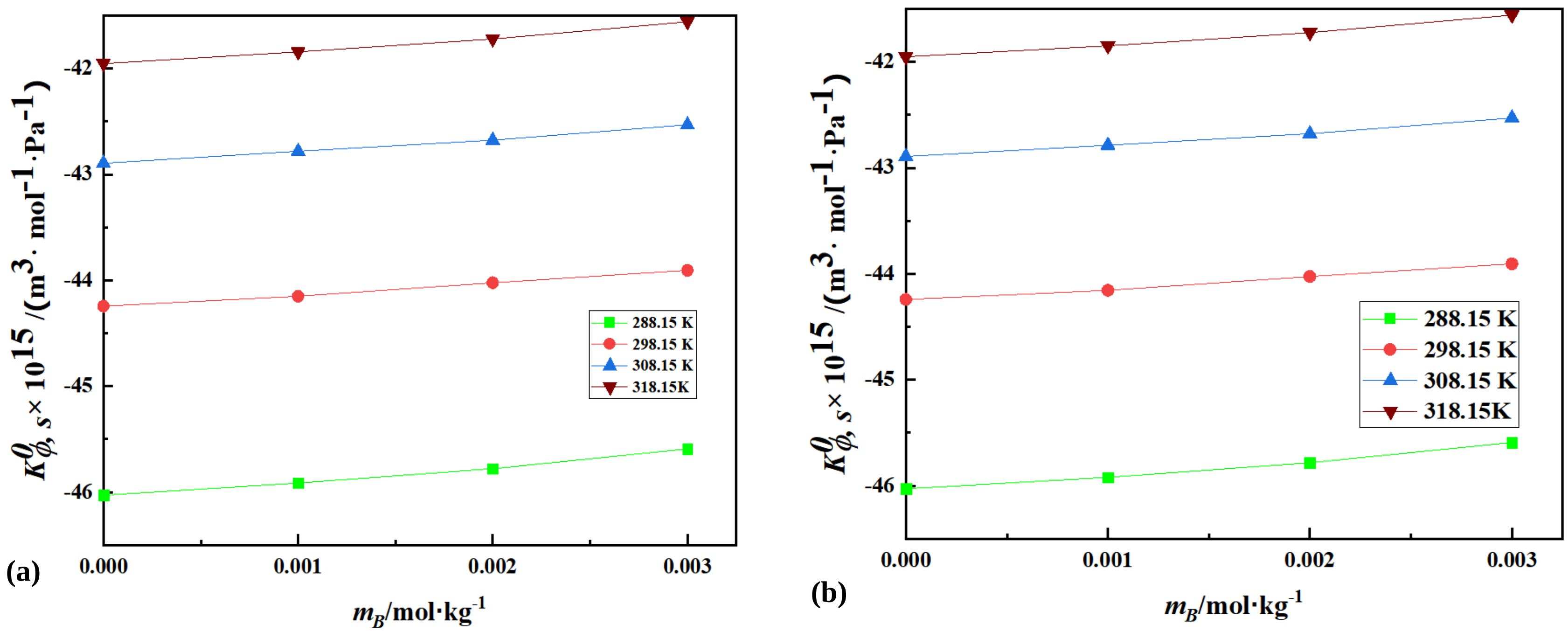
Variation of experimental and literature velocity values [4] of (a) (propylene glycol +Water) and (b) (hexylene glycol +Water) corresponding to the molality (m_A) of glycols at different T.

Figure 4.75



Variation of apparent molar isentropic compression, $K_{\phi,s}$, of (a) propylene glycol and (b) hexylene glycol, against molality [red, 0.000 biotin; blue, 0.001 biotin; black, 0.002 biotin; pink, 0.003 biotin]at different temperatures [square, 288.15 K; circle, 298.15 K; triangle, 308.15 K; inverted triangle, 318.15 K]

Figure 4.76



Variation of partial molar isentropic compression, $K^{0}_{\phi,s}$, of (a) propylene glycol, and (b) hexylene glycol in aqueous biotin solutions at different temperatures.

Problem XII

Densities and speed of sounds of (biotin + water + polyethylene glycols) solutions at different temperatures and atmospheric pressure

In this section, we have reported the densities, ρ and speed of sound c of polyethylene glycol 200 (PEG 200) and polyethylene glycol 400 (PEG 400) in (0.0000, 0.0024, 0.0032, and 0.0040) mol·kg^{-1} aqueous solutions of biotin at temperatures T = (288.15, 298.15, 308.15 and 318.15) K.

4.102 Density

Densities of the ternary mixture (biotin + water + PEG 200/PEG 400) and binary mixtures (water + biotin); (water + PEG 200/PEG 400) as the function of temperature (288.15 K, 298.15 K, 308.15 K, and 318.15 K) at atmospheric pressure 0.1MPa are reported in **Table 4.99**. The binary solutions were prepared by dissolving biotin in water at different concentrations of (0.0000, 0.0024, 0.0032, and 0.0040) mol·Kg^{-1} and the ternary solutions were prepared by dissolving the polyethylene glycols in aqueous biotin solutions at the mentioned concentrations. The values of density are scrutinized and it can be perceived that at particular biotin concentration when the temperature rises, the density values decrease but with the upsurge in the molality of the polyethylene glycols these values increases. Further, when the concentration of biotin escalates, the density values show increment accordingly. For (water + PEG 200) and (water + PEG 400), the density values are compared with the literature values [69, 70] and are observed to be in good agreement with each other i.e. the experimental values follows the same pattern as literature values corresponding to the temperatures, which is perfectly represented in **Figure 4.78** [4, 50, 54].

4.103 Apparent molar volume

The values of density were utilized to determine the apparent molar volume (V_ϕ) values with the equation **4.1** where M, m_A, ρ, and ρ_0 are symbolizing the molar mass of the solute, molality of the solute per kg of the solvent (water + biotin), densities of the solution, and the solvent respectively. The calculated values of the apparent molar volumes (V_ϕ) are indexed in **Table 4.99** for the ternary mixture (biotin + water + PEG 200/PEG 400) and binary mixtures (water + biotin); (water + PEG 200/PEG 400) as the function of temperatures. From the table, it can be remarked that all the V_ϕ values are constant and at a constant concentration of biotin, the V_ϕ values escalate with the increment of the temperatures and polyethylene glycol molality. Also, it is noteworthy, that when the biotin concentration accelerated along with the molar mass of the polyethylene glycols, V_ϕ values increases in the order from PEG 200<PEG 400 which is expressed in **Figure 4.79** [16]. This behavior of V_ϕ values with temperature refers to the phenomenon of solvation in the mixture at high temperatures and more affinity in the solvent which causes strong solute-solvent interactions in the sample compositions that increases from PEG 200 to PEG 400 as depicted in **Figure 4.77**. The nature of molecular interactions present in the composition is described by the values of V_ϕ which makes it very significant for investigations. In the presence of water, the polyethylene glycols display inter-intramolecular hydrogen bond, hydrophobic effect, hydrophobic hydration, (dipole-dipole) and (dipole-induced-dipole) interactions. Nonetheless, more clear details can be attained from the partial molar volumes at infinite dilution concerning the (solute-solvent) and (solute-solute) interactions [8-11, 47].

4.104 Partial Molar volume

To retrieve the values of partial molar volume of the liquid mixtures containing biotin and glycol, the equation **4.2** is applied where m_A denotes the molality of the solute. With the help of the least square fitting method, the partial molar volume (V_ϕ^0), the experimental slope (S_V^*) along with the standard errors are evaluated and reported in **Table 4.100**. These V_ϕ^0 values are graphically represented in **Figure 4.80** and it can be observed that these values tend to increase with the upsurge in the experimental temperatures and biotin concentrations corresponding to the raise in the molar mass of the polyethylene glycols from PEG 200 to PEG 400. The positive values of V_ϕ^0 for solutes in water refer to the hydrophobic effects and strong hydrogen between the hydroxyl (-OH) groups of polyethylene glycols and molecules of water [71]. The existence of strong (solute-solvent) interaction is attributed to the dominance of ion-hydrophilic interactions over hydrophobic- hydrophobic interactions in the liquid mixtures which escalate with the increase in the chain length of polyethylene glycols.

According to the model of co-sphere overlap [12, 13], the volume expands when the hydration co-sphere of two ionic species overlaps, but when (ion-hydrophobic) and (hydrophobic- hydrophobic) groups overlap the volume contracts. Along with the temperature, the variation pattern of V_{ϕ}^{0} values is associated with the thermal expansion, hydrogen bond, discharge of molecules in solvation layers, etc., as the solvation molecules are released from the solvation layers of solute into mixture [51, 52]. For all concentrations of biotin, the magnitude of S_{V}^{*} is positive for all temperatures, and at a specific temperature, they are appeared to be decreasing corresponding to the biotin concentrations. This establishes the (solute-solute) interactions in the mixture but being smaller as compared to the V_{ϕ}^{0} values, the (solute-solvent) interaction remains stronger and overshadows (solute-solute) interaction in the sample [1, 5, 9, 14, 15].

4.105 Partial molar volume of transfer

Equation **4.3** is employed to calculate the Transfer of partial molar volume of glycols from water to aqueous solutions of biotin at infinite dilution**.** In **Table 4.101** the transfer partial molar volume (ΔV_{ϕ}^{0}) is reported. These properties contribute the qualitative information regarding the (solute-solvent) interactions inside the liquid mixture without considering (solute-solute) interactions. The co-sphere overlap model [12, 13] articulates the interactions occurring inside the polyethylene glycols and biotin molecules. The positive values of ΔV_{ϕ}^{0} are attributed due to the (ion-hydrophilic) and (hydrophilic-hydrophilic) interactions which result in the reduction of the electrostriction of molecules of water that are in the close vicinity of the polyethylene glycol molecules and leads to the exemption of some molecules of water into bulk. Further, it can be noticed from the table that the positive ΔV_{ϕ}^{0} values intensify with the biotin concentrations at a particular temperature which refers to the decrement of the hydrophilic interactions between (solute and water) molecules and forms hydrogen bond amidst the –OH group of biotin and a hydrophilic group of polyethylene glycols and thus give rise to (hydrophilic-hydrophobic), (ion-hydrophobic) and (hydrophobic- hydrophobic) interactions in (biotin + water + PEG 200/PEG 400) mixture. Therefore, the transfer volume values are inspected and analyzed through co-sphere overlap model and are interpreted as the following interactions-

(i) (ion-hydrophilic) interactions within the zwitterionic groups of polyethylene glycols and –OH groups of biotin,

(ii) (ion-hydrophobic) interactions among zwitterionic groups of polyethylene glycols and alkyl groups of biotin,

(iii) (hydrophilic- hydrophilic) interactions within hydrophilic groups of polyethylene glycols and –OH groups of biotin,

(iv) (hydrophilic- hydrophobic) interactions among alkyl groups of polyethylene glycols and –OH groups of biotin; hydrophilic groups of polyethylene glycols and –OH groups of biotin,

(v) (hydrophobic- hydrophobic) interactions among alkyl groups of polyethylene glycols and alkyl groups of biotin.

Although, the (ion-hydrophilic) interactions dominate all the other interactions in the mixture that increases from PEG 200 to PEG 400 as the partial molar of volume transfer increases in the same order i.e. ΔV_{ϕ}^{0} (PEG 400) $>\Delta V_{\phi}^{0}$ (PEG 200) at constant temperature and biotin concentration [8, 16-19].

4.106 Temperature-dependent partial molar volume

The variations in the apparent molar volumes at infinite dilution with temperatures are obtained with the equation **4.4**. The temperature in Kelvin is represented as T where T_{ref}=298.15 K and $(a, b,$ and $c)$ denotes the empirical constants which are listed in **Table 4.102**. The deviations in the experimental and calculated V_{ϕ}^{0} values are mentioned in the same table and these deviations are evaluated using the equation **4.14.** Here, $\mathrm{Y} = V_{\phi}^{0}$ (apparent molar volume at infinite dilution). The deviation values are very low that perfectly satisfies the polynomial equation that is demonstrated from R^2values in the current study [20]. In the table, the empirical constant c describes the scatter in V_{ϕ}^{0} values. The primary objective to analyze the V_{ϕ}^{0} values was to retrieve the partial molar expansibilities using the equation **4.5.** The partial molar expansibility at infinite dilution is calculated using E_{ϕ}^{0}=$\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$. The E_{ϕ}^{0} values in **Table 4.103** are observed to be all positive throughout different temperatures and biotin concentrations for (biotin + water + PEG 200/PEG 400) mixture. These values prove to be a valuable measure of (solute-solvent) interactions and exhibit the prominence of temperature on the interactions occurring among polyethylene glycols in aqueous biotin solutions over aqueous polyethylene glycol solutions. With the upsurge in temperatures, the E_{ϕ}^{0} values increase as a consequence of caging or packing effect [21, 22]. Since, as the temperature rises, the molecules of outer hydrated water are affected due which the E_{ϕ}^{0} values expand along with the higher temperature. Also, the positive values of E_{ϕ}^{0} suggest that the biotin molecules accumulate in the interstitial spaces of the mixture and lead to the structure-making property of solutes though these values are asymmetric in nature corresponding to the biotin concentrations. Thus E_{ϕ}^{0} values provide the qualitative information regarding (solute-solvent) interactions in the mixture. The structure making and breaking capability of the solute in the solution is determined with the following thermodynamical equation **4.6** given by Hepler [23]. The sign of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ determines the structure making and structure breaking tendency of the solute dissolved in the solvent. The positive $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ values infer the capability of structure making of solutes, whereas, when the values of $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ are negative, it indicates the structure breaking ability of solute in the mixture. These values are displayed in **Table 6** where all the values are positive except for PEG 200 in 0.040 mol·Kg^{-1} biotin, which reveals that both the polyethylene glycols in aqueous biotin solutions are structure maker in nature [7, 24, 25].

4.107 Ultrasonic speed

Speed of sound for the ternary mixture (biotin + water + PEG 200/PEG 400) and binary mixtures (water + biotin); (water + PEG 200/PEG 400) as the function of temperature (288.15 K, 298.15 K, 308.15 K and 318.15 K) and different biotin concentrations (0.0000, 0.0024, 0.0032 and 0.0040) mol·Kg^{-1} at atmospheric pressure 0.1MPa are reported in **Table 4.104**. A comparison graph has been plotted between the literature [69, 70] and experimental values of speed of sound for (water + PEG 200) and (water + PEG 400) at temperature (298.15 and 308.15) K, which is demonstrated in **Figure 4.81** and it can be noted that both the values are in good agreement with each other i.e. both the values are symmetric to each other. From the table, it is observed that the speed of sound values at a constant biotin concentration, accelerates with the rise in the experimental temperatures and polyethylene glycol molality. This behavior implies the greater association among the solution molecules which occurs as a result of intramolecular hydration bond in the polyethylene glycol molecules and intermolecular hydrogen bond formation between (solute-solvent) molecules that increases with the speed of sound in the sample and infers the high rate of combination for molecules in the mixture. The speed of sound in pure water also follows the same trend i.e. increases with the temperatures, which occurs due to the formation of more monomeric molecules of water and depletion of the hydrogen bonds in the water molecules. These depleted molecules of water penetrate the free space and get trapped in the cage-like structure of water which causes the increment in the number of closed-packed structures with the escalation in the temperature. As the ultrasonic waves propagate, the material medium is created due to the development of a close-packed structure of water with temperatures. That is why with the upsurge in the temperature the speed of sound values increases for pure water and in a similar way for polyethylene glycols in aqueous biotin solutions [26-28].

4.108 Apparent molar isentropic compression

For polyethylene glycols in aqueous biotin solution, the apparent molar isentropic compression is determined with the equation **4.7 w**here, the densities of the solvent, densities of the solution, molar mass of solute, the molality of solute, and isentropic compressibility of the pure solvent and the solution are symbolized as ρ, $\rho_{0,}$ M, $m_{A,}$ $k_{s.0}$ and k_s respectively. The Laplace-Newton's formula **4.8** [29] is used to calculate the isentropic compressibility where c is the speed of sound. In (0.0000, 0.0024, 0.0032, and 0.0040) mol·Kg^{-1} biotin, the apparent molar isentropic compressibility ($K_{\phi,S}$) is calculated at different temperatures for polyethylene glycols (PEG 200/PEG 400). These values are listed in **Table 4.104** which are found to be all negative. At a specific concentration of biotin, the negativity of $K_{\phi,S}$ values increases with the upsurge in the polyethylene glycol molality but reduces as the temperature gets higher. Also, with the rise in the biotin concentration the negativity of $K_{\phi,S}$ values minimize which is graphically expressed in **Figure 4.82**. This trend suggests that around ionic charge groups of polyethylene glycols, the molecules of water are less compressible as compared to the molecules of water in bulk. This results in the huge loss of structural compressibility of water which creates an arrangement of water molecules around the solute [30-32]. Through intermolecular hydrogen bonding, the polyethylene glycols form compact structures with biotin molecules which reduce the compressibility. Further, the average distance among the molecules increases with the surge in compressibility at high temperatures. The existence of strong (solute-solvent) interactions are confirmed with the (dipole-dipole) interactions between the –OH groups of polyethylene glycols and molecules of water present in its proximity [33-35].

4.109 Partial molar isentropic compression

With equation **4.9**, the partial molar isentropic compression is determined by contemplating the divergence of apparent molar isentropic compression corresponding to the molality. With the help of the least square fitting method, the partial molar isentropic compressibility ($K^0_{\phi,S}$), the experimental slope (S^*_k) along with the standard errors are evaluated and reported in **Table 4.105**. These $K^0_{\phi,S}$ values are graphically represented in **Figure 4.83** and it can be observed that these values are all negative and the negativity tends to decrease along with the temperature but rises with the increment in the biotin concentration. As the molar mass of the polyethylene glycol increases from PEG 200 to PEG 400, the negativity of $K^0_{\phi,S}$ values also intensifies. This implies the habitation of strong attractive interactions among the polyethylene glycols and water with the discharge of water molecules in bulk due to the reduction of electrostriction. This behavior of $K^0_{\phi,S}$ values with the biotin concentrations is explained by the Kirkwood model [36], which states that electrostriction water has a less open structure as compared to the bulk water that makes the former more compressible. As a result, the electrostriction interactions are oppressed among the molecules of water and polyethylene glycols as the interaction increases between the polyethylene glycols and biotin. Thus, from the solvation layer, the electrostriction water is discharged into the bulk by making the solute further compressible [7]. The (solute-solute) interactions in the mixture are approximately insignificant as the S^*_k values in the table are very small as compared to the $K^0_{\phi,S}$

values which implies the dominance of (solute-solvent) interactions in the sample mixture [37].

4.110 Partial molar isentropic compression of transfer

At infinite dilution, the partial molar isentropic compression of transfer is computed with the equation **4.10** for glycol from water to aqueous biotin solutions. The calculated $\Delta K_{\phi,s}^{0}$ values appear to be positive in nature throughout the experimental temperatures and biotin concentrations which are recorded in **Table 4.106**. It is observed that as the concentration of biotin rises, the $\Delta K_{\phi,s}^{0}$ values enhance along at a particular temperature but show asymmetric behavior corresponding to the experimental temperatures. Strong interaction occurs between the zwitterionic center of polyethylene glycols and biotin which increases with the increment in the biotin concentration as the electrostriction is reduced and results in the tendency of structure making in solute. The compressibility decreases along with the biotin concentration as the electrostriction water is compressible as compared to the bulk and as a consequence to which the values of $\Delta K_{\phi,s}^{0}$ are positive whereas $K_{\phi,s}^{0}$values are negative for (PEG 200/PEG 400) at various temperatures and biotin concentrations. The water molecules associates with the ions at low temperatures and biotin concentrations as the solvent molecules are merged with the water molecules [11, 38-40].

4.111 Pair and triplet coefficients

The partial molar volume of transfer and the partial molar isentropic compression of transfer is obtained from the equation **4.11** and **4.12** where m_B denotes the molality of the aqueous biotin solutions, A represents glycols and B represents biotin. V_{AB}; V_{ABB} and K_{AB}; K_{ABB} represents the pair and triplet coefficients for volume and isentropic compression respectively which are mentioned in **Table 4.107.** Applying McMillian-Mayer theory [41], the pair and triplet interaction coefficients ($V_{AB,}$ K_{AB}; V_{ABB}, K_{ABB}) are calculated by fitting the values of partial molar properties for volume and isentropic compression (ΔV_{ϕ}^{0}; ΔK_{ϕ}^{0}) respectively. This theory investigates the separation of effects in the liquid mixture due to the pair and triplet interactions among the molecules. Friedman and Krishnan [42] and Franks et al [43] had discussed the same theory further. It can be noted from the table that the pair-interaction coefficient V_{AB} is negative at all temperatures for PEG 200 but for PEG 400 it is positive at (288.15 and 298.15) K and negative at (308.15 and 318.15) K. Throughout all the temperatures the pair interaction coefficient K_{AB} is positive. Moreover, the triplet interaction coefficients (V_{ABB}; K_{ABB}) are all positive except for V_{ABB} that is negative at 288.15 K for PEG 400. Following this theory, from the co-sphere, the water is released to the bulk that changes the volume. When the bulk is more structured than the co-sphere, then the change would be positive whereas negative change is observed when the co-sphere is more structured than the bulk as the water molecules are arranged in different structures. Also, the water molecules are discharged to the bulk from the hydration co-spheres since the occurred interaction is non-bonding. Therefore, more positive values of triplet interaction coefficients in the mixture of (biotin + water + PEG 200/PEG 400) as compared to the pair interaction coefficients, establishes the dominance of triplet-wise interactions in the present study [64, 72].

Table 4.99

Values of densities, ρ, apparent molar volumes, V_ϕ of polyethylene glycols in aqueous solutions of Biotin at different temperatures

$^{a}m_A$/(mol·kg^{-1})	$\rho \times 10^{-3}$/(kg·m^{-3})				$V_\phi \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
0.0000 mol·kg^{-1} Biotin + PEG 200								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.10009	1.00221	1.00001	0.99701	0.99335	170.10	170.33	170.61	170.96
0.20044	1.00504	1.00284	0.99986	0.99621	170.28	170.52	170.83	171.18
0.30136	1.00777	1.00558	1.00260	0.99897	170.42	170.66	170.97	171.32
0.40026	1.01032	1.00815	1.00519	1.00157	170.58	170.79	171.10	171.44
0.49999	1.01280	1.01062	1.00767	1.00408	170.71	170.95	171.26	171.59
0.0024 mol·kg^{-1} Biotin + PEG 200								
0.00000	0.99982	0.99773	0.99479	0.99124				
0.10067	1.00276	1.00067	0.99774	0.99421	170.30	170.60	170.89	171.20
0.20520	1.00556	1.00355	1.00066	0.99716	170.51	170.82	171.09	171.41
0.30009	1.00818	1.00609	1.00320	0.99970	170.72	171.03	171.28	171.62
0.39863	1.01068	1.00858	1.00571	1.00222	170.93	171.23	171.50	171.84
0.50062	1.01315	1.01106	1.00818	1.00470	171.11	171.42	171.72	172.07
0.0032 mol·kg^{-1} Biotin + PEG 200								

0.00000	0.99994	0.99793	0.99501	0.99154				
0.09879	1.00280	1.00078	0.99788	0.99443	170.60	170.93	171.18	171.48
0.19893	1.00566	1.00358	1.00067	0.99723	170.80	171.09	171.35	171.65
0.30302	1.00821	1.00624	1.00337	1.00000	170.98	171.29	171.54	171.84
0.40049	1.01075	1.00873	1.00587	1.00248	171.18	171.47	171.74	172.03
0.50208	1.01316	1.01116	1.00830	1.00494	171.36	171.68	171.96	172.24
0.0040 mol·kg^{-1} Biotin + PEG 200								
0.00000	1.00007	0.99811	0.99519	0.99181				
0.09892	1.00290	1.00094	0.99804	0.99467	170.90	171.19	171.46	171.73
0.20019	1.00567	1.00370	1.00081	0.99747	171.08	171.39	171.67	171.91
0.29783	1.00830	1.00629	1.00341	1.00005	171.26	171.57	171.85	172.10
0.40412	1.01086	1.00889	1.00602	1.00272	171.43	171.75	172.04	172.29
0.50056	1.01319	1.01118	1.00831	1.00504	171.59	171.92	172.23	172.47
0.0000 mol·kg^{-1} Biotin + PEG 400								
0.00000	0.99926	0.99705	0.99404	0.99036				
0.10015	1.00577	1.00349	1.00044	0.99673	333.00	334.28	335.56	336.82
0.20004	1.01179	1.00945	1.00636	1.00264	333.35	334.65	335.90	337.09
0.29995	1.01739	1.01499	1.01188	1.00813	333.69	334.99	336.18	337.42
0.40100	1.02267	1.02019	1.01705	1.01330	334.01	335.34	336.53	337.74
0.50006	1.02747	1.02496	1.02180	1.01804	334.35	335.64	336.82	338.00

0.0024 mol·kg^{-1} Biotin + PEG 400								
0.00000	0.99982	0.99773	0.99479	0.99124				
0.10046	1.00621	1.00411	1.00117	0.99760	334.30	334.92	335.73	336.98
0.19982	1.01208	1.00998	1.00704	1.00344	334.59	335.21	336.01	337.26
0.30204	1.01765	1.01558	1.01264	1.00903	334.92	335.52	336.34	337.55
0.40005	1.02269	1.02058	1.01764	1.01400	335.22	335.84	336.66	337.89
0.49989	1.02757	1.02530	1.02234	1.01869	335.54	336.22	337.08	338.29
0.0032 mol·kg^{-1} Biotin + PEG 400								
0.00000	0.99994	0.99793	0.99501	0.99154				
0.10002	1.00627	1.00426	1.00134	0.99784	334.61	335.15	336.00	337.18
0.20005	1.01214	1.01015	1.00722	1.00371	334.81	335.39	336.23	337.42
0.29993	1.01768	1.01562	1.01268	1.00915	335.03	335.64	336.53	337.68
0.40042	1.02278	1.02074	1.01780	1.01426	335.31	335.94	336.80	337.95
0.49899	1.02765	1.02541	1.02247	1.01889	335.61	336.27	337.11	338.33
0.0040 mol·kg^{-1} Biotin + PEG 400								
0.00000	1.00007	0.99811	0.99519	0.99181				
0.10305	1.00655	1.00459	1.00167	0.99827	334.94	335.49	336.32	337.30
0.19872	1.01217	1.01019	1.00726	1.00386	335.16	335.69	336.55	337.52
0.30020	1.01769	1.01573	1.01279	1.00938	335.36	335.93	336.80	337.80
0.40065	1.02280	1.02082	1.01787	1.01447	335.61	336.21	337.10	338.07

0.50321	1.02773	1.02568	1.02271	1.01929	335.89	336.48	337.39	338.40

[a] m_A is the molality of polyethylene glycols in the aqueous solution Biotin; standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1} and $u(V_{\phi})$ =±(0.05-0.07) × 10^{6}/ (m^{3}·mol^{-1}.

Table 4.100

Partial molar volumes, V_ϕ^0, and experimental slopes, S_V^*, of polyethylene glycols in the aqueous solution of Biotin at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$V_\phi^0 \times 10^6$/(m^3·mol^{-1})				$S_V^* \times 10^6$/(m^3·kg·mol^{-2})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
				PEG 200				
0.0000	169.96(±0.01)	170.20(±0.01)	170.48(±0.03)	170.85(±0.03)	1.52(±0.05)	1.51(±0.04)	1.57(±0.09)	1.50(±0.09)
0.0024	170.10(±0.01)	170.40(±0.01)	170.67(±0.01)	170.97(±0.01)	2.05(±0.04)	2.07(±0.04)	2.07(±0.0)	2.18(±0.0)
0.0032	170.42(±0.00)	170.73(±0.01)	170.97(±0.01)	171.28(±0.01)	1.87(±0.02)	1.87(±0.03)	1.94(±0.0)	1.88(±0.0)
0.0040	170.73(±0.00)	171.02(±0.01)	171.28(±0.01)	171.55(±0.00)	1.73(±0.02)	1.80(±0.0)	1.89(±0.0)	1.84(±0.0)
				PEG 400				
0.0000	332.68(±0.01)	333.96(±0.02)	335.25(±0.01)	336.51(±0.02)	3.34(±0.03)	3.41(±0.06)	3.14(±0.05)	3.00(±0.07)
0.0024	333.98(±0.00)	334.58(±0.03)	335.36(±0.04)	336.62(±0.05)	3.11(±0.02)	3.21(±0.09)	3.34(±0.14)	3.25(±0.15)
0.0032	334.33(±0.04)	334.84(±0.03)	335.69(±0.02)	336.86(±0.04)	2.50(±0.13)	2.79(±0.11)	2.80(±0.07)	2.85(±0.14)
0.0040	334.69(±0.02)	335.21(±0.02)	336.02(±0.02)	336.99(±0.02)	2.34(±0.08)	2.50(±0.03)	2.69(±0.07)	2.75(±0.08)

$^a m_B$ is the molality of aqueous Biotin, standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(V_\phi^0) = \pm 0.01 \times 10^6$/ (m^3·mol^{-1}) and $u(S_V^*) = \pm 0.03 \times 10^6$/ (m^3·mol^{-2}).

Table 4.101

Partial molar volumes of transfer ΔV_{ϕ}^{0}, of polyethylene glycols in the aqueous solution of Biotin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$\Delta V_{\phi}^{0} \times 10^{6}$/(m^{3}·mol^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
		PEG 200		
0.0024	0.14	0.20	0.12	0.10
0.0032	0.46	0.53	0.44	0.34
0.0040	0.77	0.82	0.77	0.48
		PEG 400		
0.0024	1.30	0.62	0.19	0.12
0.0032	1.65	0.88	0.49	0.43
0.0040	2.01	1.25	0.80	0.70

$^{a}m_B$ is the molality of aqueous Biotin, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa and *u(c)*= 0.6 m·s^{-1}.

Table 4.102

Values of empirical parameters of Eq., of polyethylene glycols in aqueous solution of Biotin at different temperatures.

${}^{a}m_B$/(mol·kg^{-1})	$a \times 10^6$/(m^3·mol^{-1})	$b \times 10^6$/(m^3·mol^{-1}·K^{-1})	$c \times 10^6$/(m^3·mol^{-1} ·K^{-2})	R^2	*ARD*
PEG 200					
0.0024	170.3909	0.0290	0.0000	0.9999	0.0000
0.0032	170.7108	0.0283	0.0000	0.9999	0.0001
0.0040	171.0162	0.0276	-0.0001	0.9999	0.0008
PEG 400					
0.0024	334.5327	0.0704	0.0017	0.9999	0.0001
0.0032	334.8457	0.0683	0.0016	0.9999	0.0000
0.0040	335.2273	0.0659	0.0011	0.9999	0.0010

${}^{a}m_B$ is the molality aqueous of Biotin, standard uncertainties *u* are *u(m)* $= 2 \times 10^{-5}$ mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}.

Table 4.103

Partial molar expansibilities, E_{ϕ}^{0}, for polyethylene glycols in the aqueous solution of Biotin at different temperatures.

$^{a}m_B$/ (mol·kg^{-1})	$E_{\phi}^{0}\times10^{6}$/(m^{3}· mol^{-1} ·K^{-1})				$(\partial E_{\phi}^{0}/\partial T)_p$/ (m^{3}·mol^{-1}·K^{-2})
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K	
			PEG 200		
0.0024	0.0288	0.0289	0.0290	0.0291	0.0000
0.0032	0.0280	0.0281	0.0283	0.0284	0.0000
0.0040	0.0255	0.0265	0.0276	0.0286	-0.0001
			PEG 400		
0.0024	0.0374	0.0704	0.1035	0.1365	0.0033
0.0032	0.0360	0.0683	0.1007	0.1330	0.0032
0.0040	0.0433	0.0659	0.0885	0.1111	0.0023

$^{a}m_B$ is the molality aqueous of Biotin, standard uncertainties u are $u(m) = 2\times10^{-5}$ mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}.

Table 4.104

Values of the speed of sound, *c*, apparent molar isentropic compression, $K_{\phi,s}$ of polyethylene glycols in aqueous solutions of Biotin at different temperatures

$^{a}m_A$/(mol·kg^{-1})	c/(m·s^{-1})				$K_{\phi,s} \times 10^6$/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
0.0000 mol·kg^{-1} Biotin + PEG 200								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.10009	1477.01	1506.54	1529.35	1544.22	-46.17	-44.38	-43.03	-42.09
0.20044	1486.41	1516.04	1537.95	1553.92	-46.54	-44.74	-43.37	-42.43
0.30136	1496.73	1526.26	1548.14	1563.27	-46.74	-44.93	-43.57	-42.62
0.40026	1506.23	1534.26	1556.14	1572.27	-46.90	-45.08	-43.72	-42.76
0.49999	1515.44	1544.73	1567.02	1581.57	-47.04	-45.22	-43.85	-42.89
0.0024 mol·kg^{-1} Biotin + PEG 200								
0.00000	1471.75	1500.62	1523.72	1541.36				
0.10067	1482.02	1510.62	1533.23	1550.30	-45.85	-44.10	-42.77	-41.80
0.20520	1492.09	1521.05	1543.03	1560.22	-46.22	-44.46	-43.12	-42.14
0.30009	1501.94	1530.41	1552.21	1568.93	-46.41	-44.64	-43.30	-42.31
0.39863	1511.47	1538.39	1560.39	1578.41	-46.56	-44.79	-43.44	-42.46
0.50062	1521.12	1550.01	1572.12	1588.30	-46.70	-44.92	-43.57	-42.58

0.0032 mol·kg^{-1} Biotin + PEG 200								
0.00000	1474.31	1503.13	1526.04	1544.08				
0.09879	1484.58	1513.11	1535.40	1553.16	-45.68	-43.94	-42.63	-41.64
0.19893	1494.19	1523.16	1545.09	1562.41	-46.05	-44.29	-42.97	-41.98
0.30302	1504.95	1533.19	1555.03	1571.94	-46.24	-44.49	-43.17	-42.17
0.40049	1514.48	1541.69	1563.24	1581.70	-46.40	-44.64	-43.31	-42.31
0.50208	1524.28	1553.12	1574.99	1591.69	-46.53	-44.77	-43.44	-42.43
0.0040 mol·kg^{-1} Biotin + PEG 200								
0.00000	1476.47	1505.75	1528.65	1546.66				
0.09892	1486.86	1516.04	1538.07	1555.47	-45.55	-43.79	-42.49	-41.50
0.20019	1497.03	1525.73	1547.70	1564.69	-45.91	-44.14	-42.83	-41.84
0.29783	1507.05	1535.40	1556.98	1573.94	-46.10	-44.33	-43.01	-42.02
0.40412	1517.39	1544.88	1566.36	1584.40	-46.26	-44.48	-43.16	-42.17
0.50056	1526.55	1556.12	1577.43	1593.70	-46.39	-44.60	-43.28	-42.28
0.0000 mol·kg^{-1} Biotin + PEG 400								
0.00000	1466.59	1495.85	1519.14	1536.02				
0.10015	1487.57	1517.76	1539.62	1558.49	-46.35	-44.55	-43.19	-42.24
0.20004	1507.37	1537.69	1559.79	1578.91	-46.86	-45.04	-43.67	-42.71
0.29995	1527.36	1556.84	1578.93	1598.35	-47.20	-45.36	-43.98	-43.02
0.40100	1547.96	1576.84	1599.32	1617.80	-47.48	-45.63	-44.24	-43.27

0.50006	1569.69	1595.78	1617.05	1635.80	-47.73	-45.87	-44.47	-43.50
0.0024 mol·kg^{-1} Biotin + PEG 400								
0.00000	1471.75	1500.62	1523.72	1541.36				
0.10046	1493.05	1522.99	1543.25	1563.71	-46.02	-44.27	-42.93	-41.95
0.19982	1513.01	1541.99	1563.85	1583.99	-46.52	-44.75	-43.40	-42.41
0.30204	1533.62	1561.80	1583.36	1603.80	-46.85	-45.07	-43.72	-42.72
0.40005	1553.39	1582.08	1602.34	1622.49	-47.12	-45.33	-43.97	-42.97
0.49989	1574.93	1600.08	1621.46	1641.80	-47.37	-45.56	-44.19	-43.19
0.0032 mol·kg^{-1} Biotin + PEG 400								
0.00000	1474.31	1503.13	1526.04	1544.08				
0.10002	1495.82	1525.44	1546.88	1566.72	-45.86	-44.11	-42.80	-41.80
0.20005	1515.79	1545.11	1567.06	1587.72	-46.36	-44.60	-43.27	-42.26
0.29993	1535.58	1564.18	1587.03	1607.07	-46.69	-44.91	-43.57	-42.56
0.40042	1556.51	1585.18	1606.19	1626.86	-46.96	-45.18	-43.83	-42.81
0.49899	1577.01	1603.05	1626.03	1646.12	-47.21	-45.40	-44.05	-43.03
0.0040 mol·kg^{-1} Biotin + PEG 400								
0.00000	1476.47	1505.75	1528.65	1546.66				
0.10305	1499.20	1528.52	1550.37	1570.21	-45.74	-43.98	-42.67	-41.68
0.19872	1518.20	1548.61	1569.41	1589.92	-46.21	-44.43	-43.11	-42.11
0.30020	1538.11	1567.86	1590.15	1609.99	-46.54	-44.75	-43.42	-42.42

0.40065	1558.91	1589.11	1609.19	1629.81	-46.82	-45.01	-43.68	-42.67
0.50321	1580.96	1607.05	1630.32	1650.19	-47.07	-45.25	-43.91	-42.89

$^{a}m_A$ is the molality of polyethylene glycols in the aqueous solution Biotin; standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.05K, $u(\rho)=0.06$(kg·m^{-3}),, $u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}, $u(K_{\phi,S}) = \pm 0.25 \times 10^{6}$/ (m^{3}·mol^{-1}· GPa^{-1}).

Table 4.105

Partial molar isentropic compression, $K_{\phi,s}^{0}$, and experimental slopes, S_{K}^{*}, of polyethylene glycols in the aqueous solution of Biotin at different temperatures.

$^{a}m_{B}$/ (mol·kg^{-1})	$K_{\phi,s}^{0}$ ×10^{6}/(m^{3}·mol^{-1}· GPa^{-1})				S_{K}^{*} ×10^{6}/(kg·m^{3}·mol^{-2}· GPa^{-1})			
	T=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K	*T*=288.15 K	*T*=298.15 K	*T* =308.15 K	*T* =318.15 K
				PEG 200				
0.0000	-46.05(±0.08)	-44.26(±0.08)	-42.91(±0.07)	-41.97(±0.07)	-2.09(±0.25)	-2.02(±0.24)	-1.97(±0.23)	-1.95(±0.23)
0.0024	-45.73(±0.08)	-43.99(±0.08)	-42.66(±0.07)	-41.69(±0.07)	-2.05(±0.25)	-1.98(±0.24)	-1.93(±0.24)	-1.90(±0.23)
0.0032	-45.57(±0.08)	-43.83(±0.08)	-42.53(±0.08)	-41.53(±0.07)	-2.03(±0.25)	-1.97(±0.24)	-1.92(±0.24)	-1.90(±0.23)
0.0040	-45.43(±0.08)	-43.68(±0.08)	-42.38(±0.08)	-41.40(±0.07)	-2.02(±0.25)	-1.95(±0.24)	-1.90(±0.24)	-1.88(±0.23)
				PEG 400				
0.0000	-46.11(±0.09)	-44.32(±0.09)	-42.97(±0.09)	-42.03(±0.09)	-3.38(±0.29)	-3.23(±0.28)	-3.13(±0.27)	-3.07(±0.27)
0.0024	-45.78(±0.09)	-44.04(±0.09)	-42.71(±0.09)	-41.74(±0.08)	-3.31(±0.28)	-3.17(±0.28)	-3.09(±0.27)	-3.02(±0.27)
0.0032	-45.62(±0.09)	-43.89(±0.09)	-42.58(±0.09)	-41.59(±0.08)	-3.31(±0.28)	-3.17(±0.28)	-3.08(±0.27)	-3.01(±0.27)
0.0040	-45.50(±0.09)	-43.75(±0.08)	-42.45(±0.08)	-41.46(±0.08)	-3.24(±0.28)	-3.11(±0.26)	-3.02(±0.26)	-2.96(±0.25)

$^{a}m_{B}$ is the molality of aqueous Biotin, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}, *u*($K_{\phi,s}^{0}$) =±0.01 × 10^{6}/(m^{3}·mol^{-1}· GPa^{-1})and *u*(S_{k}^{*}) =±0.24 × 10^{6}/(m^{3}·mol^{-2}· GPa^{-1}).

Table 4.106

Partial molar isentropic compression transfer, $\Delta K^0_{\phi,s}$, of polyethylene glycols in the aqueous solution of Biotin at different temperatures.

$^a m_B$/ (mol·kg^{-1})	$\Delta K^0_{\phi,s}$ × 10^6/(m^3·mol^{-1}· GPa^{-1})			
	T=288.15 K	T=298.15 K	T =308.15 K	T =318.15 K
		PEG 200		
0.0024	0.32	0.28	0.25	0.29
0.0032	0.48	0.43	0.39	0.44
0.0040	0.62	0.58	0.53	0.58
		PEG 400		
0.0024	0.33	0.28	0.26	0.29
0.0032	0.49	0.43	0.39	0.44
0.0040	0.61	0.57	0.52	0.57

$^a m_B$ is the molality of aqueous Biotin, standard uncertainties u are $u(m) = 2 \times 10^{-5}$ mol·kg^{-1}, $u(T)$=0.03K, $u(\rho)=0.06$(kg·m^{-3}),$u(p)$=0.01MPa, $u(c)$= 0.6 m·s^{-1}

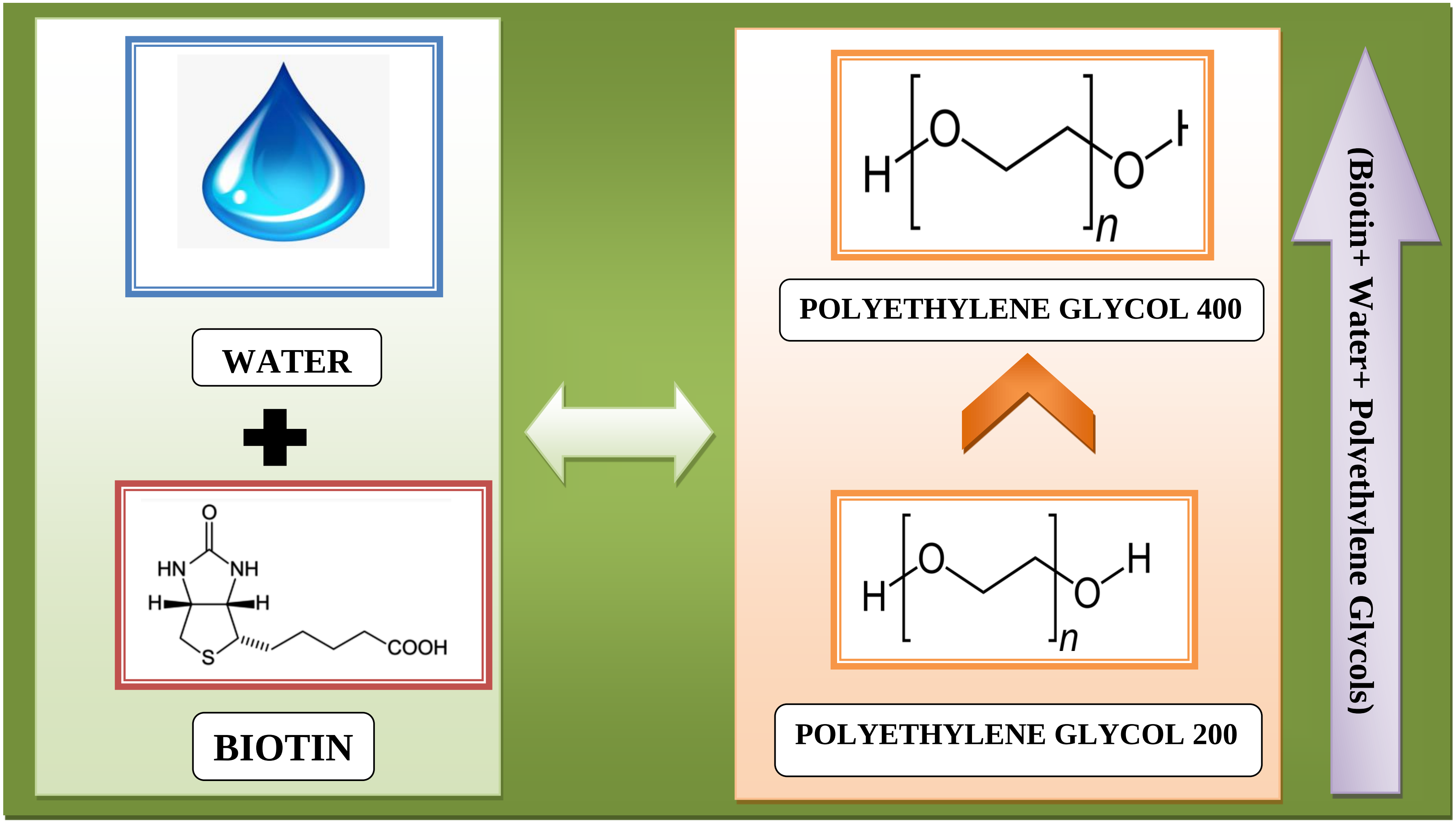
Table 4.107

Pair (V_{AB}, K_{AB}) and triplet (V_{ABB}, K_{ABB}) of polyethylene glycols in aqueous solutions of Biotin at different temperatures

T/K	V_{AB} ×10^6/(m^3·mol^{-2}· kg)	V_{ABB} ×10^6/(m^3·mol^{-3}·kg^2)	K_{AB} ×10^6/(m^3·mol^{-2}· kg GPa^{-1})	K_{ABB} ×10^6/(m^3·mol^{-3}·kg^2 GPa^{-1})
		PEG 200		
288.15	-140.982	46406.23	40.82	7198.47
298.15	-112.41	42307.18	20.98	10090.61
308.15	-109.947	40847.54	18.81	9287.71
318.15	-129.15	42568.48	27.71	8728.00
		PEG 400		
288.15	321.94	-13836.97	46.99	5902.92
298.15	63.52	17511.94	26.21	8884.81
308.15	-163.21	50579.52	24.11	8035.56
318.15	-77.27	27335.95	33.73	7335.49

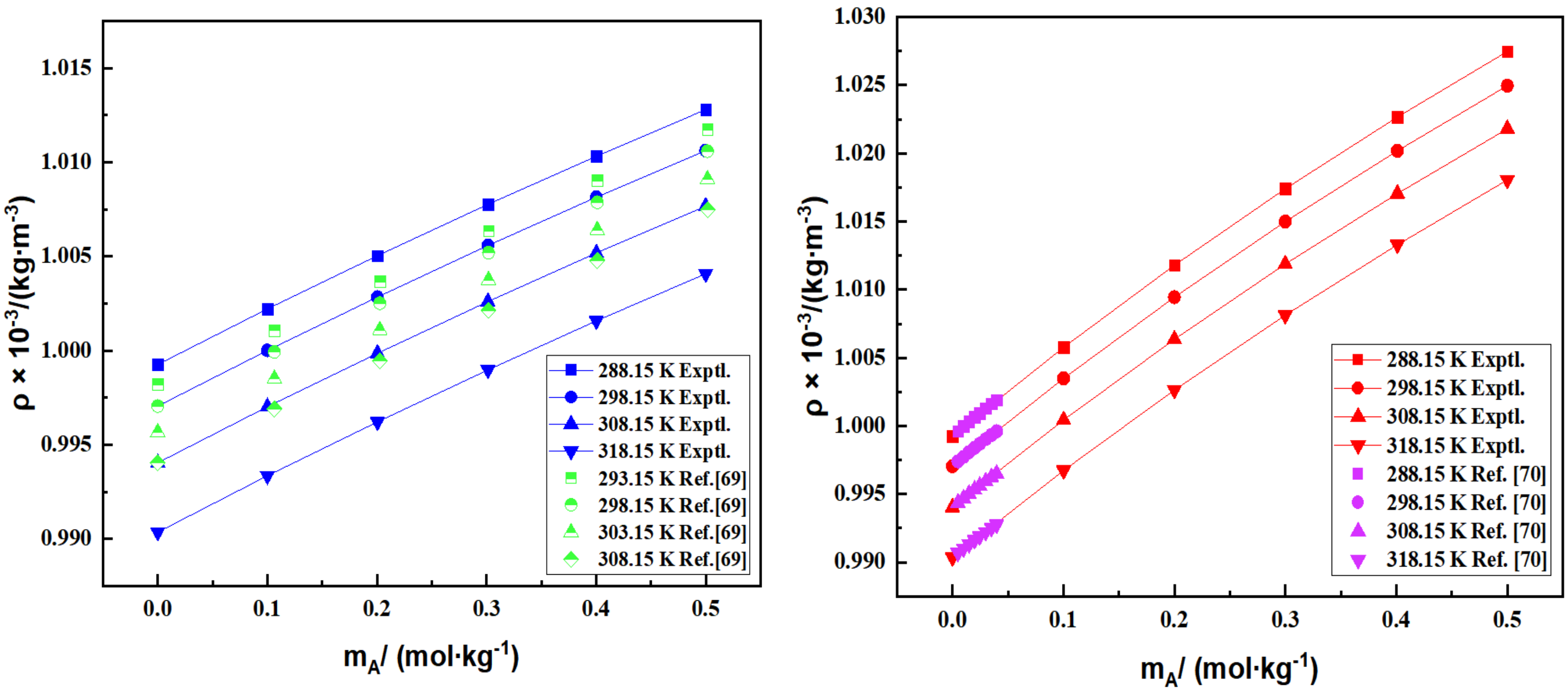
T/K is the temperatures, standard uncertainties *u* are *u(m)* = 2×10^{-5} mol·kg^{-1}, *u(T)*=0.03K, *u(ρ)=0.06*(kg·m^{-3}),*u(p)*=0.01MPa, *u(c)*= 0.6 m·s^{-1}.

Figure 4.77



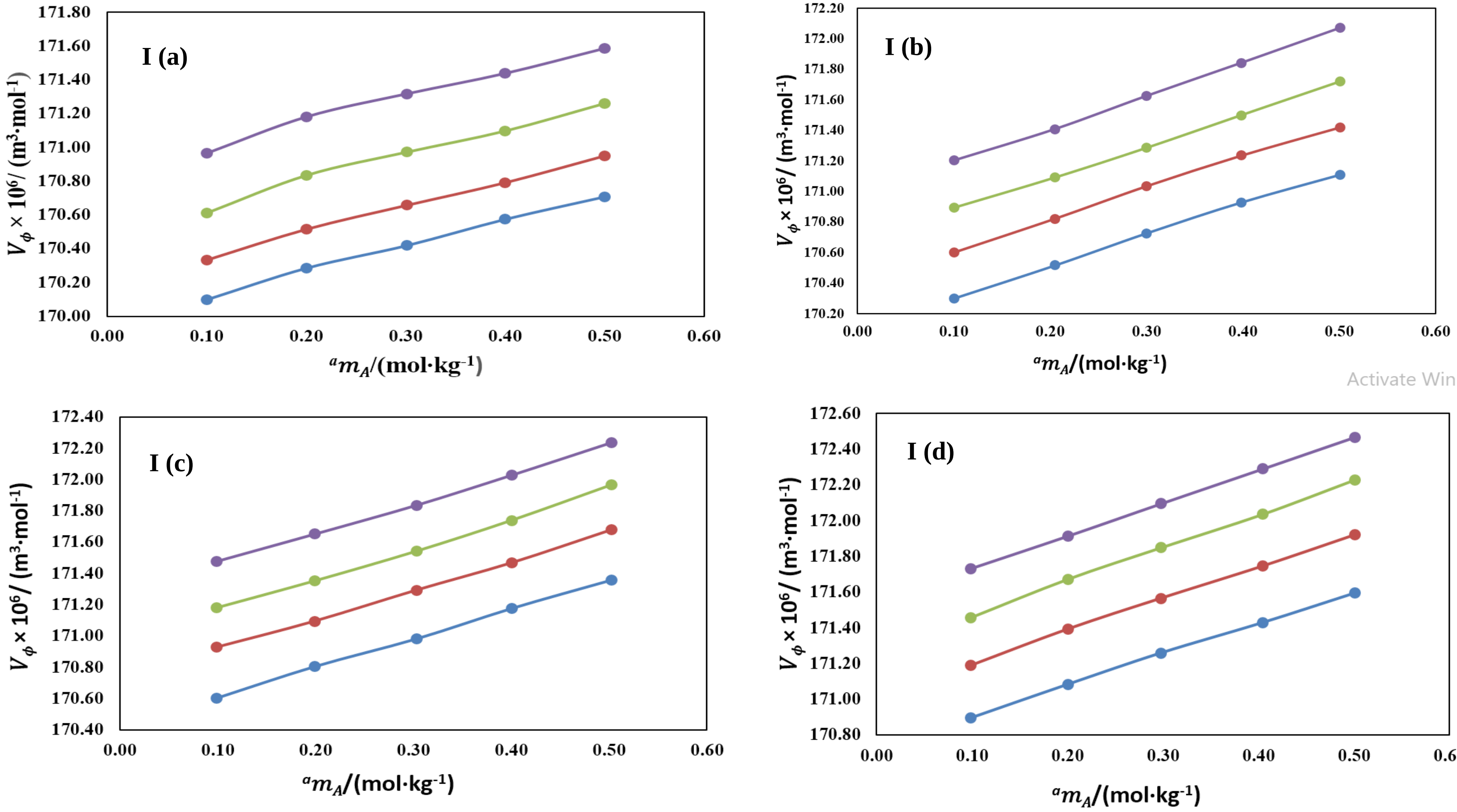
PEG 200 / PEG 400 and biotin interactions.

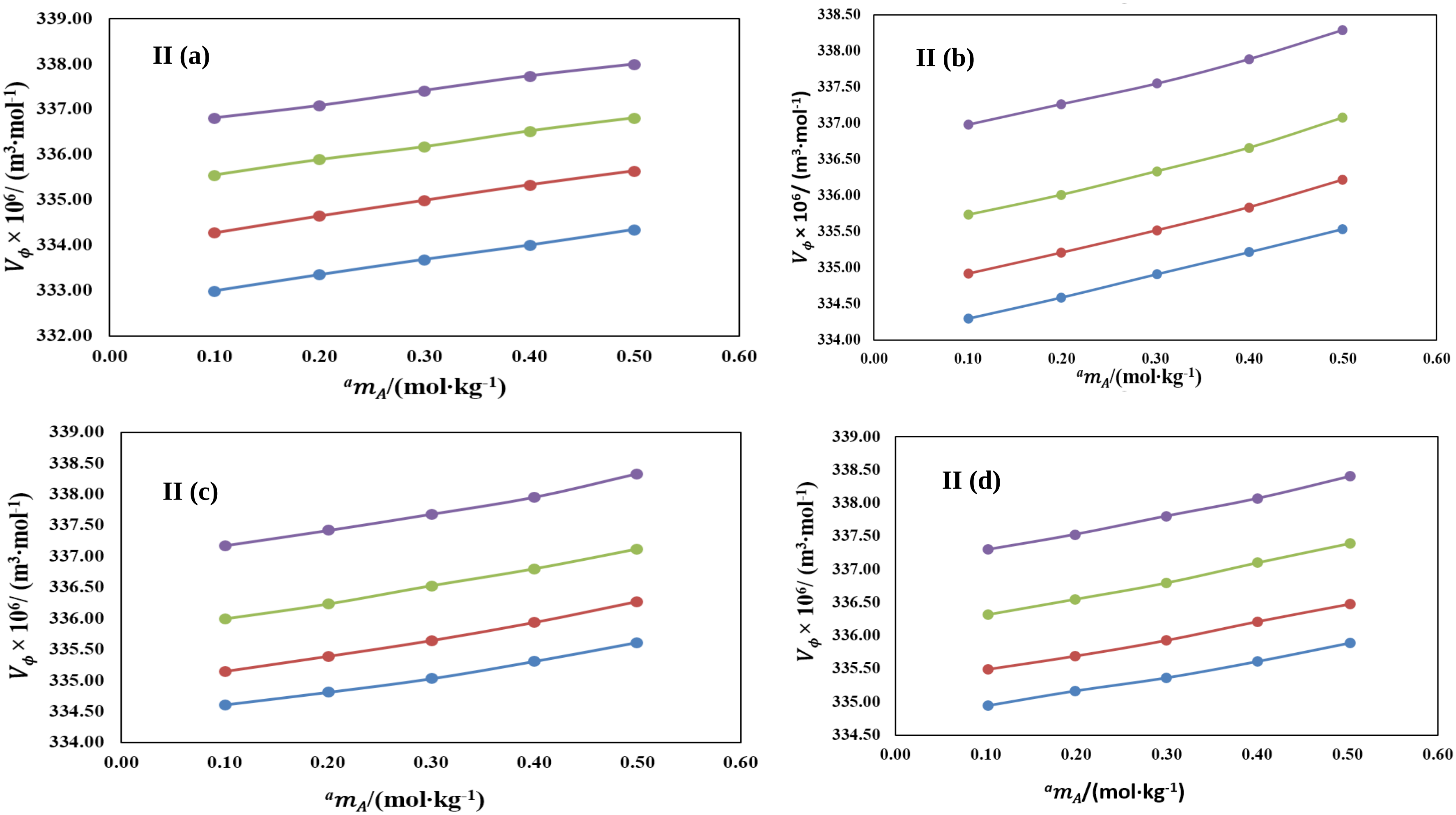
Figure 4.78



Variation of experimental and literature density values [69, 70] of (a) (Polyethylene glycol 200 +Water) and (b) (Polyethylene glycol 400 +Water) corresponding to the molality (m_A) of glycols at different T.

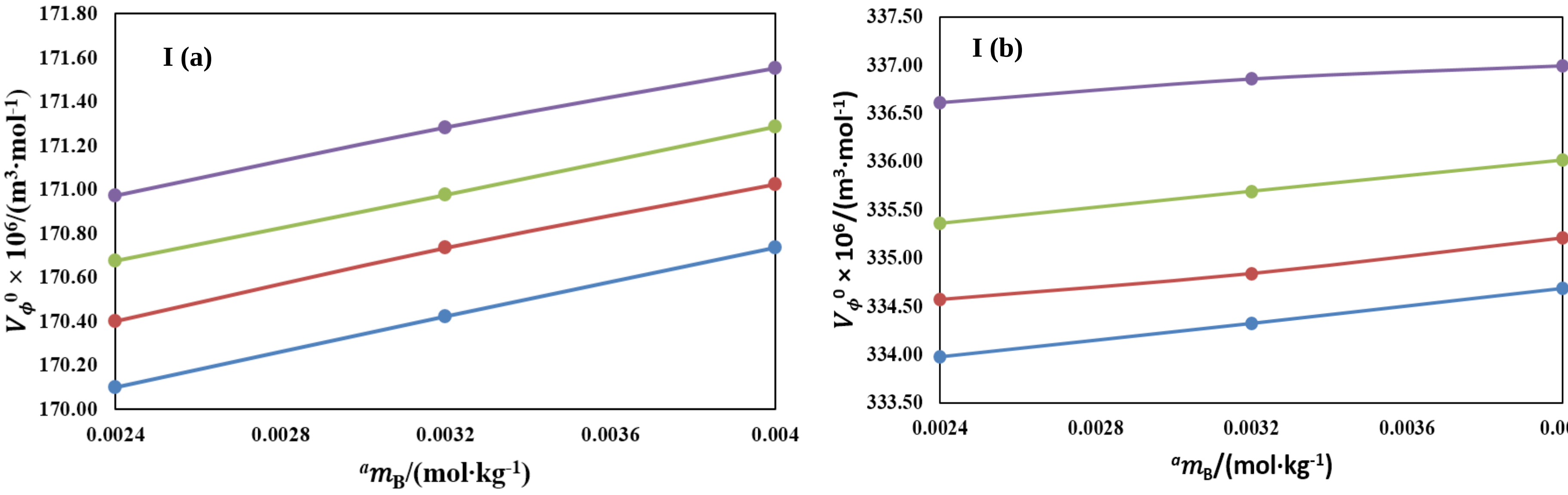
Figure 4.79


I (a)
I (b)
I (c)
I (d)
$V_\phi \times 10^6$/ (m^3·mol^{-1})
$^a m_A$/(mol·kg^{-1})
170.00
170.20
170.40
170.60
170.80
171.00
171.20
171.40
171.60
171.80
172.00
172.20
172.40
172.60
0.00
0.10
0.20
0.30
0.40
0.50
0.60



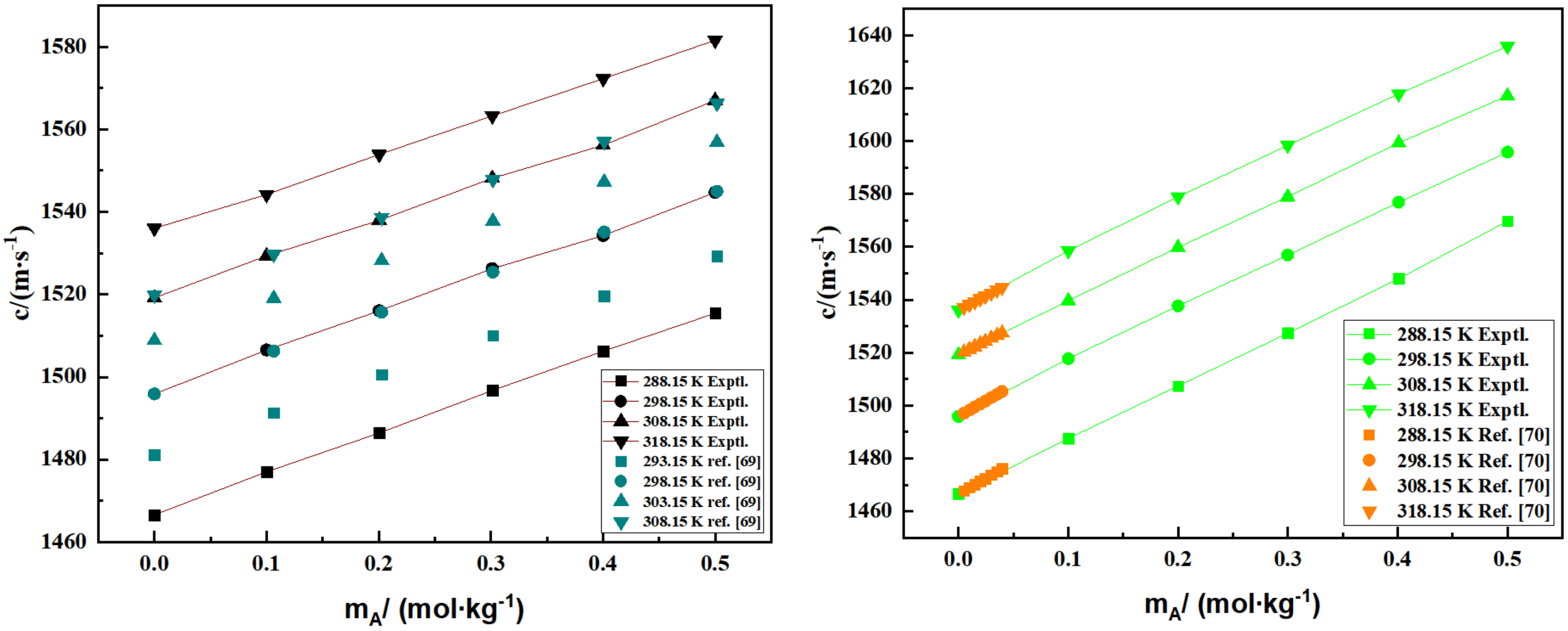
Variation of apparent molar volume, V_ϕ of Polyethylene glycol 200 (I) and Polyethylene glycol 400 (II) (a) 0.0000 biotin, (b) 0.0024 biotin, (c) 0.0032 biotin, (d) 0.0040 biotin, against molality at different temperatures [blue, 288.15 K; red, 298.15 K; green, 308.15 K; purple 318.15 K]

Figure 4.80



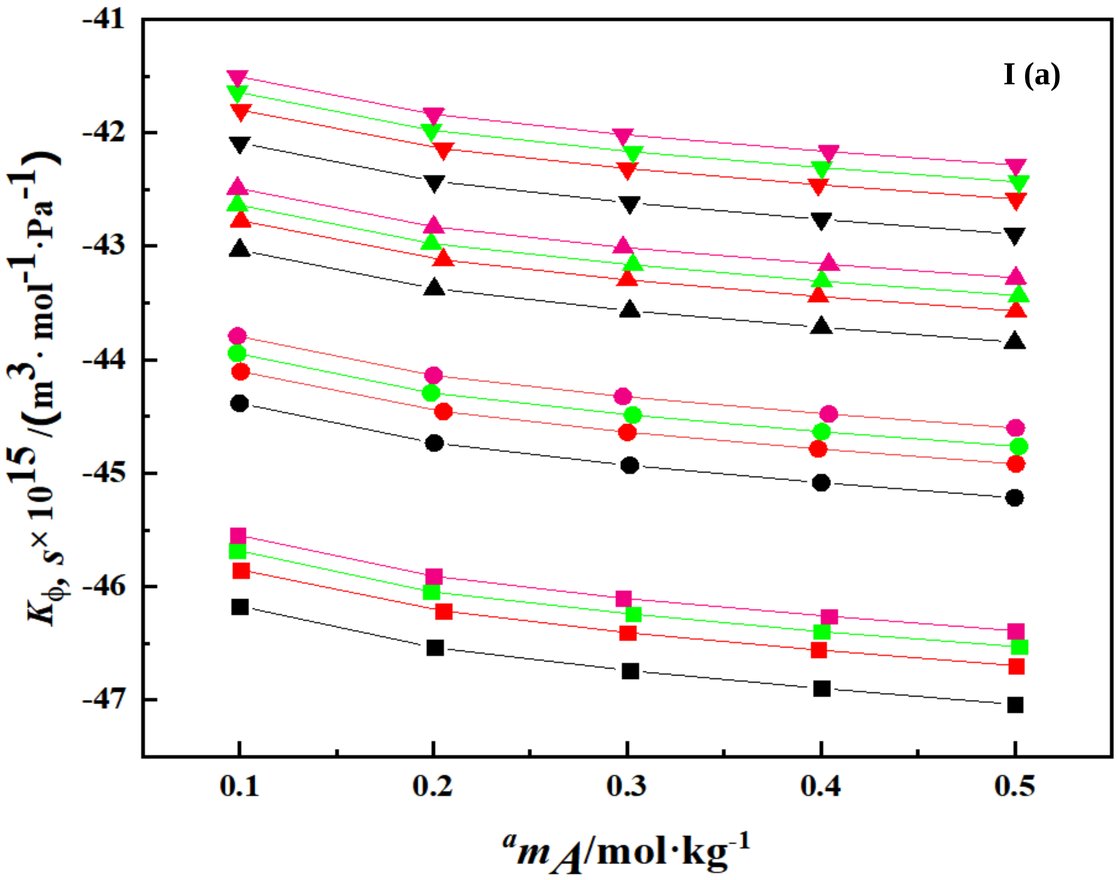
Variation of partial molar volumes, V_ϕ^0, of, (a) Polyethylene glycol 200 and (b) Polyethylene glycol 400 in different concentration of aqueous biotin solutions at different temperatures [blue, 288.15 K; red, 298.15 K; green, 308.15 K; purple 318.15 K]

Figure 4.81

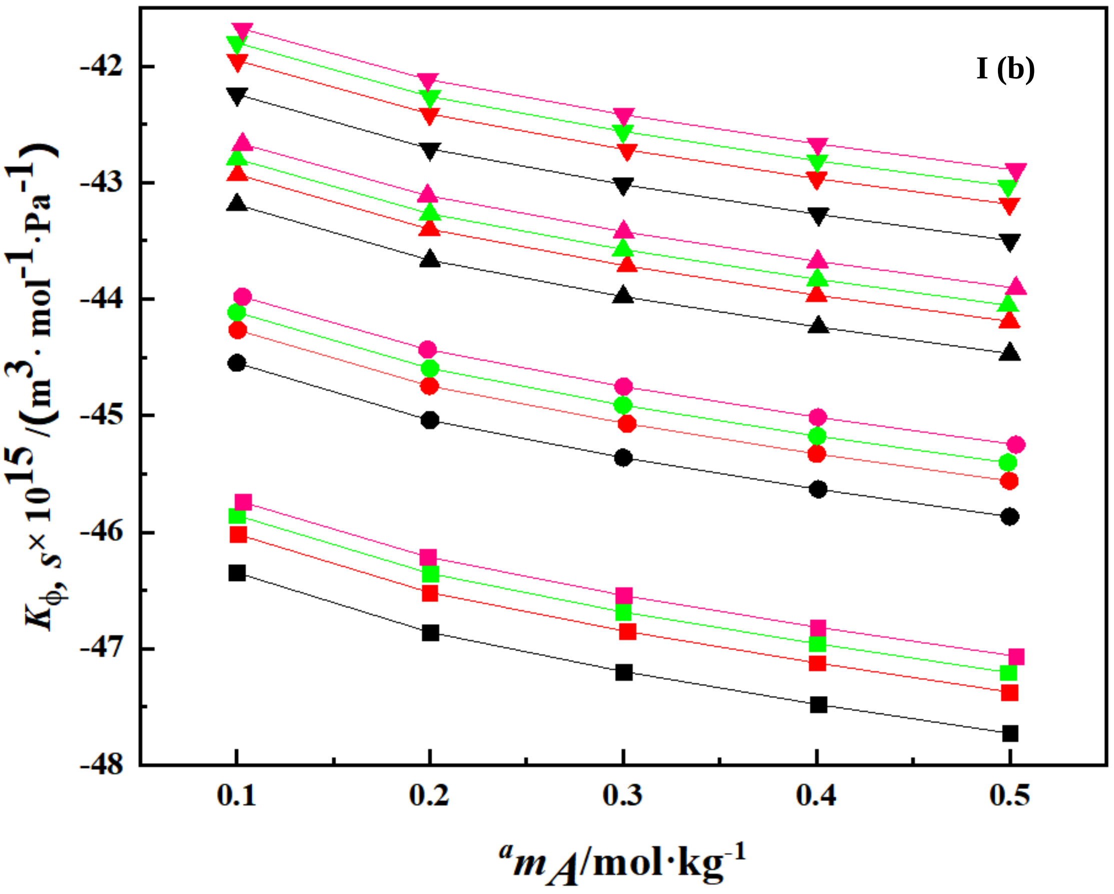


Variation of experimental and literature velocity values [69, 70] of (a) (Polyethylene glycol 200 +Water) and (b) (Polyethylene glycol 400 +Water) corresponding to the molality (m_A) of glycols at different T.

Figure 4.82

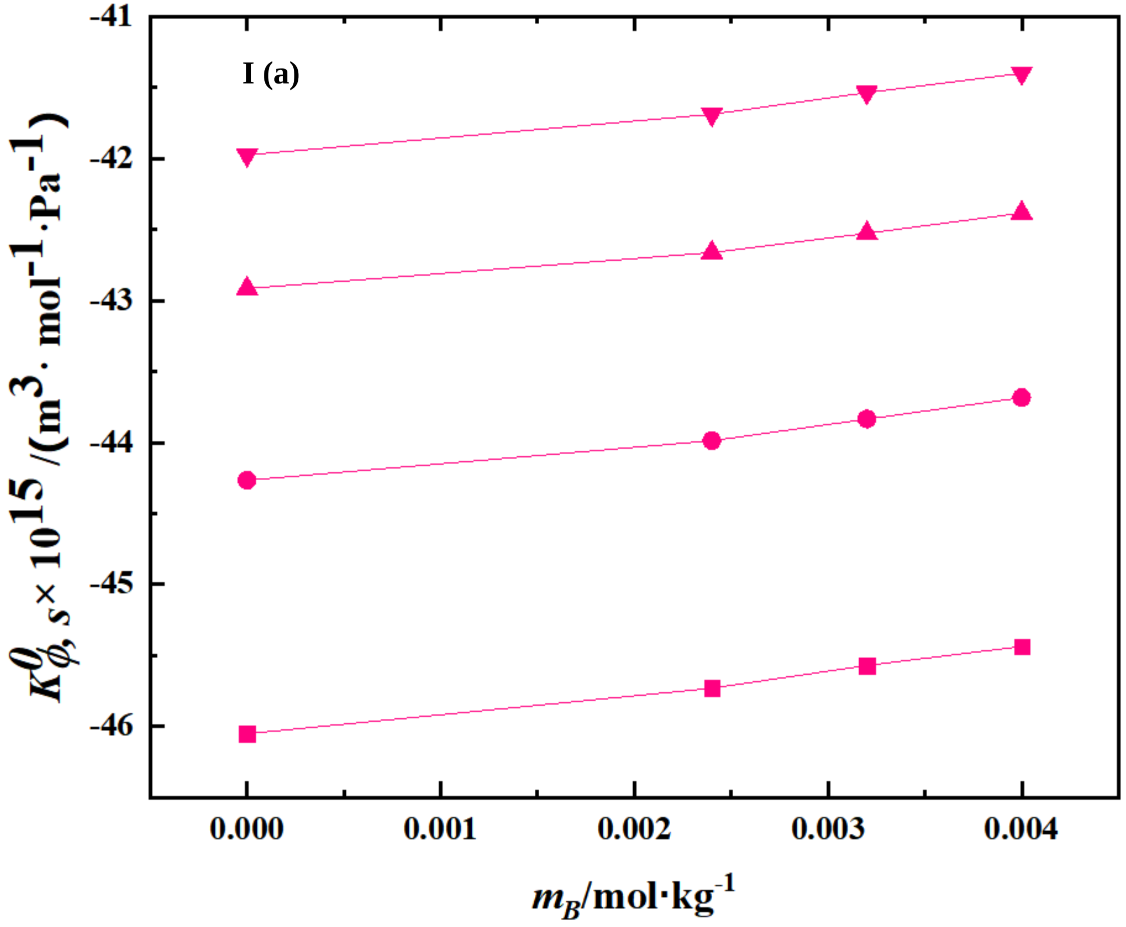


I (a)
-41
-42
-43
-44
-45
-46
-47
$K_{\phi,s} \times 10^{15}/(\mathrm{m^3 \cdot mol^{-1} \cdot Pa^{-1}})$
0.1
0.2
0.3
0.4
0.5
${}^a m_A/\mathrm{mol \cdot kg^{-1}}$

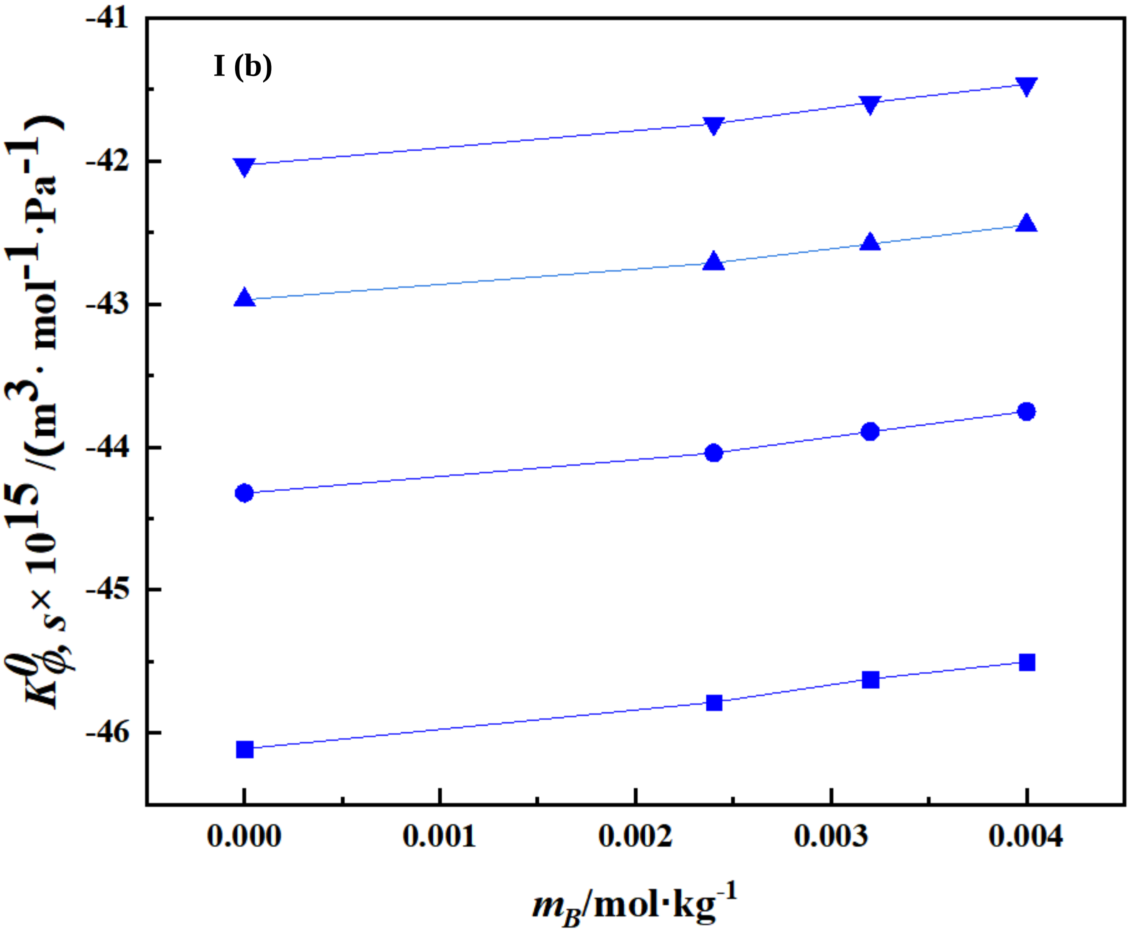


Variation of apparent molar isentropic compression, $K_{\phi,s,}$ of (a) Polyethylene glycol 200 and (b) Polyethylene glycol 400, against molality [black, 0.0000 biotin; red, 0.0024 biotin; green, 0.0032 biotin; pink, 0.0040 biotin]at different temperatures [square, 288.15 K; circle, 298.15 K; triangle, 308.15 K; inverted triangle, 318.15 K]

Figure 4.83



I (a)
-41
-42
-43
-44
-45
-46
0.000
0.001
0.002
0.003
0.004
$K^0_{\phi,s} \times 10^{15}/(m^3 \cdot mol^{-1} \cdot Pa^{-1})$
$m_B/mol \cdot kg^{-1}$



Variation of partial molar isentropic compression, $K^{0}_{\phi,s}$, of (a) Polyethylene glycol 200, and (b) Polyethylene glycol 400, in aqueous biotin solutions at different temperatures.

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Summary and Conclusions

The thesis titled **Acoustic and thermodynamic parameter investigations in the mixture containing vitamin B with glycols using ultrasonic technique** describes the thermodynamic and ultrasonic properties of the mixture for aqueous vitamin B (niacin, vitamin B_3; d-Panthenol, vitamin B_5; biotin, vitamin B_7) with glycols at multiple temperatures and constant pressure as the function of solvent concentration. With Anton Paar DSA 5000 M the density and speed of sound of liquid mixtures are measured with which acoustic and thermodynamic parameters are calculated. The volumetric and acoustical properties have been studied for the ternary liquid combination of (EG/DEG/TEG) in (0.00, 0.02, 0.04 and 0.06) $mol\cdot kg^{-1}$ aqueous niacin solution at the temperature variation of (293.15, 298.15, 303.15 and 308.15) K and atmospheric pressure in problem 1. The calculations of various thermodynamic and acoustical parameters predict the significant information regarding the interactions in the present ternary liquid combination such as the existence of ion-hydrophilic; hydrophobic-hydrophobic interaction from the acoustical properties and (dipole-induced-dipole); (dipole-dipole) interactions from the volumetric properties. The structure making ability of the solute in the solution is observed from the positive E_{ϕ}^{0} values. The pair and triplet coefficients are calculated using the partial molar parameters and show the subjugation of the pairwise interactions among the glycols and niacin molecules. The hydrogen bond network is also formed in the mixture which is justified by the speed of sound values for glycols in aqueous niacin.For the liquid combination of [Propylene glycol (PG)/Hexylene glycol (HG) + niacin+ water], the volumetric and acoustical properties have been studied through the calculations of various thermodynamic parameters at the temperature variation of (293.15, 298.15, 303.15, and 308.15) K over the solvent concentrations of (0.01, 0.03 and 0.05) $mol\cdot kg^{-1}$ at atmospheric pressure in problem 2. Significant information regarding the interactions in the present ternary liquid combination has been revealed through the calculated parameters. The existence of strong solute-solvent interactions along with (dipole and dipole) interactions, (dipole-induced-dipole), hydrophilic effect, and hydrophobic hydration has been confirmed from volumetric properties. The domination of ion-hydrophilic interaction over hydrophobic-hydrophobic interaction, strong ion-ion interaction of glycols and niacin, solute-solvent interactions is revealed from the acoustical properties. At the temperature range of T=(293.15, 298.15, 303.15 and 308.15) *K*, the speed of sound and density for the ternary solution (Niacin+ water + PEG 200 / PEG 600) were measured in 0.1 *MPa* pressure and concentrations of (0.01, 0.02 and 0.03) $mol{\cdot}kg^{-1}$ to analyze the volumetric and acoustical properties through the calculations of various thermodynamic parameters are provided in problem 3. The V_{ϕ} values show the solute-solvent interaction with the strong hydrogen bond, hydrophilic effect, hydrophobic hydration, and (dipole-dipole) interactions. At higher temperatures, less negative $K_{\phi,s}$ values establish the presence of hydrophobic interactions of polar groups. Calculated E_{ϕ}^{0} values suggest the solute-solvent interactions with the structure breaking ability due to $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ negative values._Further, pairwise interaction is indicated by_V_{AB} and K_{AB} between PEGs and niacin molecules. The values of E_{ϕ}^{0}, indicates the structure making ability of the molecules inside the mixture. The formation of hydrogen bond network insolvent with aqueous niacin molecule, the strong attractive interactions among the molecules of water and molecules of glycols, the dominance of pairwise interaction is also observed which is justified from the experimental speed of sound values and pair and triplet coefficients. The volumetric and acoustical properties have been studied through the calculations of various thermodynamic parameters for the liquid combination of (Polyethylene glycol 400 (PEG 400)/ Polyethylene glycol (PEG 4000) + Niacin+ water) at the temperature variation of (288.15, 298.15, 308.15 and 318.15)K over the solvent concentrations of (0.07, 0.08 and 0.09) $\mathrm{mol{\cdot}kg^{-1}}$ at atmospheric pressure in problem 4. In the present ternary liquid combination, the existence of (dipole and dipole) interactions, (dipole-induced-dipole), hydrophilic effect, and hydrophobic hydration has been confirmed from apparent molar values. Significant information regarding the interactions has been revealed through the calculated parameters. From the acoustical properties, the dominance of ion-hydrophilic interaction over hydrophobic-hydrophobic interaction, strong ion-ion interaction of polyethylene glycols and niacin along with the solute-solvent interactions are revealed. The E_{ϕ}^{0} values indicate the structure-making ability of the molecules inside the mixture. The formation of hydrogen bond network with aqueous niacin molecule, the strong attractive interactions among the molecules of water and molecules of polyethylene glycols, the dominance of pairwise interaction is also observed which is justified from the experimental speed of sound values and pair and triplet coefficients. The measurements of density and ultrasonic velocity of EG, DEG and TEG in aqueous D-Panthenol solution are reported in problem 5. From the experimental data, apparent molar properties and partial molar properties of transfer have been calculated. After the interpretation of the experimental data, it is evident that there are interactions among glycols and D-Panthenol molecules. Along with increase in the concentration of D-Panthenol and the increase in molar mass of glycols, the interaction extent increases. The pair wise interaction between glycols and D-Panthenol is suggested by the V_{AB} and K_{AB} values. It is concluded from the results that (ion-hydrophilic) and (hydrophilic- hydrophilic) interactions are present. The investigated binary solution consisting of ethylene, diethylene and triethylene glycols as solute and D-Panthenol as solvent was chosen in order to obtain the information about the inter-molecular interaction between their constituent particles are provided in problem 6. The variations in the experimentally obtained and derived parameters indicate the presence of molecular interactions between the molecules of the given solution. The trend obtained with respect to fundamental parameters, that is, ultrasonic density and ultrasonic velocity at different temperatures and different concentrations was obtained linear in nature. The ultrasonic velocity increases with the increase in the mole fraction/concentration and decreases with the increase in the temperature and density increases with the increase in the mole fraction/concentration as well as with the increase in the temperature. The derived parameters such as acoustic impedance, adiabatic compressibility, intermolecular free length, Wada's constant, Rao's constant and Vander Waal's constant varies linearly with the different concentrations which show the absence of complex formations. In all the cases of ethylene, diethylene and triethylene glycols, the acoustic impedance shows the linearly increasing trend which increases as the temperature and concentration increases, the adiabatic compressibility shows the linearly decreasing trend which increases with increase in the concentration and decreases with the temperature, the inter molecular free length shows the decreasing trend which decreases with the concentration and increases with temperature and Wada's constant, Rao's constant and Vander Waal's constant shows decreasing trend which decreases with increasing concentration and increases with Increasing temperature, which is because of absence of heavy molecules in the solution. The volumetric and acoustic results for PG and HG in aqueous solutions of d-Panthenol at temperatures T= (288.15, 298.15, 308.15, and 318.15) K and concentrations (0.04, 0.08, and 0.12) mol·kg^{-1} has been determined. From the experimental density and speed of sound values, the apparent and partial molar properties are evaluated in problem 7. The apparent molar properties manifest the presence of strong solute-solvent interactions among the d-Panthenol and glycol molecules. With the rise in the molar mass of the glycols from PG to HG, an increase in V_{ϕ} and V_{ϕ}^{0} values is observed that validates the presence of strong intermolecular interactions in the liquid system which is increasing from PG to HG as shown in scheme 1. The volumetric properties confirm the existence of dipole-dipole, dipole induced dipole interactions, hydrophobic hydration, and hydrophilic effect along with the hydrophobic- hydrophobic interaction predominating by ion-hydrophilic interactions is deduced from acoustic parameters. The hydrogen bond is created in the aqueous d-Panthenol with strong attractive interactions due to structure making ability of solute, is noted in the solution. The estimated hydration numbers for glycols in aqueous d-Panthenol solutions which are utilized from Passynski's formula are very large and are attributed due to cooperative hydrogen bonding in the liquid mixture. The volumetric and acoustic investigations of the ternary solution (d-Panthenol+ water+ PEG 200/PEG 400) has been done at (0.00, 0.03, 0.06 and 0.09) mol.kg^{-1} as the function of temperatures T=(288.15, 298.15, 308.15 and 3 18.15)K and constant pressure of 0.1 MPa in problem 8. The density and speed of sounds are experimentally obtained by Anton Paar DSA 5000 M, which are used to calculate the various thermodynamic parameters such as apparent molar properties, partial molar properties and pair/triplet interaction coefficients. These calculated parameters are scrutinized corresponding to their experimental temperatures and solvent concentrations where the molecular interactions are occurring inside the mixtures are analyzed. From the apparent molar and partial molar properties the presence of strong solute-solvent interactions are observed along with the dipole induced dipole and dipole-dipole interactions. Also, the hydrophilic effect, hydrophobic hydration in water rich region, hydrophilic-hydrophilic, hydrophobic-hydrophobic and hydrophilic- hydrophobic interactions are found in the ternary mixture. The strong attractive molecular interactions among the molecules of water and polyethylene glycols are realized due to development of hydrogen bond network within the aqueous d-Panthenol solution which increases from PEG 200 to PEG 400 as the molar mass of the polyethylene glycols increases. This characteristic is perfectly interpreted in Scheme 1. The partial molar expansibility (E_{ϕ}^{0}) values are all positive, thus refers to the structure making ability of the solute in the liquid system. Likewise, the pair and triplet interaction coefficients (V_{AB},K_{AB}, V_{ABB} and K_{ABB}) anticipated the supremacy of pairwise interaction in (d-Panthenol+ water+ polyethylene glycols). Thermodynamic investigations have been done for the polyethylene glycols (PEG 600/PEG 6000) in aqueous solution of d-Panthenol at different temperatures (288.15 K, 298.15 K, 308.15 K, and 318.15 K) and as a function of d-Panthenol concentration (0.00, 0.02, 0.07 and 0.12) mol·Kg^{-1} in problem 9. Different volumetric and acoustic parameters are calculated from the experimental density and speed of sound values, which provides the better insight to the ternary mixture. The volumetric parameters (apparent molar volume, V_{ϕ}; partial molar volume, V_{ϕ}^{0}; partial molar volume of transfer, ΔV_{ϕ}^{0}) and acoustic parameters (apparent molar isentropic compression,$K_{\phi,S}$; partial molar isentropic compression,$K_{\phi,S}^{0}$; partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^{0}$) depicts the existence of (solute-solvent) interactions, (inter-intramolecula r hydrogen bond), (hydrophobic effect), (hydrophobic hydration), (dipole-dipole) interaction, (dipole-induced-dipole) interaction, (ion-hydrophilic) interaction and (hydrophilic- hydrophilic) interaction. The partial molar expansibility(E_{ϕ}^{0}) and its first derivative $\left(\partial \mathrm{E}_{\Phi}^{0}/\partial \mathrm{T}\right)_{P}$ are calculated using the thermodynamic derived parameters which suggests the strong (solute-solvent) interactions with the structure-making property of the solutes and the pair-triplet interaction coefficients (V_{AB}, K_{AB}; V_{ABB}, K_{ABB}) are calculated using the partial molar transfer properties which indicates the dominance of pair-wise interaction coefficient in the ternary system. Measurement of density and speed of sound for the ternary mixture of (water + biotin + EG /DEG/ TEG) as the function of biotin concentrations (0.0000, 0.0015, 0.0025 and 0.0035) mol·Kg^{-1} and experimental temperat ures (288.15 K, 298.15 K, 308.15 K, and 318.15 K) at 0.1 MPa atmospheric pressure has been done using Anton Paar DSA 5000 M in problem 10. From these experimental data, various properties such as apparent molar properties (apparent molar volume, V_ϕ; apparent molar isentropic compression,$K_{\phi,S}$), the partial molar properties (partial molar volume, V_ϕ^0; partial molar isentropic compression, $K_{\phi,S}^0$), and the partial molar transfer properties (partial molar volume of transfer, ΔV_ϕ^0; partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^0$) are evaluated. The presence of strong (solute-solvent) interactions, (hydrophilic-hydrophilic) interaction, (ion-hydrophilic) interaction, (hydrophobic-hydration), (dipole-induced-dipole) interaction, (dipole-dipole) interaction, (hydrophobic effect), (intermolecular hydrogen bond) and (intramolecular hydrogen bond) are deduced from the volumetric and acoustic parameters. The partial molar expansibility(E_ϕ^0) and its first derivative $\left(\partial \mathrm{E}_\phi^0/\partial \mathrm{T}\right)_P$ are determined from these derived thermodynamic parameter along with the pair-triplet interaction coefficients (V_{AB}, K_{AB}; V_{ABB}, K_{ABB}). The strong (solute-solvent) interactions are depicted along with the structure-making property of the solutes from the expansibility data, and the dominance of pair-wise interaction is noticed from the coefficients of pair-triplet interactions. A systematic study of volumetric and acoustic properties of (biotin+ water+ PG/HG) has been carried out at different temperatures (288.15, 298.15, 308.15, and 318.15) K, constant pressure 0.1 MPa, and over the entire range of biotin concentrations (0.000, 0.001 to 0.002 to 0.003) mol·Kg^{-1} in problem 11. The volumetric parameters (apparent molar volume, V_ϕ; partial molar volume, V_ϕ^0; partial molar volume of transfer, ΔV_ϕ^0) are calculated using experimental density (ρ) values and acoustic parameters (apparent molar isentropic compression, $K_{\phi,s}$;

partial molar isentropic compression, $K_{\phi,s}^{0}$; partial molar isentropic compression of transfer, $\Delta K_{\phi,s}^{0}$) are calculated with experimental values of speed of sound (c). These derived parameters were later utilized to determine the partial molar expansibility (E_{ϕ}^{0}) along with its first derivative $(\partial E_{\phi}^{0}/\partial T)_p$ and pair-triplet interaction coefficients (V_{AB}, K_{AB}; V_{ABB}, K_{ABB}). The hydration numbers (n_h) were also estimated for this liquid combination by Passynski's formula using isentropic compressibility data. From the apparent molar properties, it is deduced that there exist strong solute-solvent interactions inside the liquid system along with the inter-intramolecular hydrogen bond, dipole-dipole , and dipole-induced-dipole interactions. The presence of hydrophobic hydration and hydrophobic effect is also observed from these parameters. The partial molar properties of the current solution suggest the dominance of ion-hydrophilic interactions over hydrophobic-hydrophobic and ion-hydrophobic interactions. The strong ion-ion interactions with insignificant solute-solute interactions and ion-hydrophilic; hydrophilic-hydrophilic interactions are manifested by the partial molar transfer properties. The partial molar expansibility and its first derivative reveal the structure-making capacity in solutes along with the strong solute-solvent interactions which were already depicted by apparent molar properties. Also, the triplet-wise interaction is sustained in the liquid mixture as per the positive values of (V_{ABB}, K_{ABB}) over (V_{AB}, K_{AB}). The estimated hydration numbers are very large and are attributed due to cooperative hydrogen bonding in the liquid mixture. Problem 12 comprises the measurement of density and speed of sound for the ternary mixture of (biotin + water + PEG 200/PEG 400) as the function of biotin concentrations (0.0000, 0.0024, 0.0032 and 0.0040) mol·Kg^{-1} and experimental temperatures (288.15 K , 298.15K, 308.15K, and 318.15 K) at 0.1 MPa atmospheric pressure. These experimental data are utilized to evaluate the apparent molar properties (apparent molar volume, V_{ϕ}; apparent molar isentropic compression,$K_{\phi,S}$), the partial molar properties (partial molar volume, V_{ϕ}^{0}; partial molar isentropic compression, $K_{\phi,S}^{0}$), and the partial molar transfer properties (partial molar volume of transfer, ΔV_{ϕ}^{0}; partial molar isentropic compression of transfer, $\Delta K_{\phi,S}^{0}$). The volumetric and acoustic parameters of the mixtures suggest the existence of strong (solute-solvent) interactions, (intermolecular hydrogen bond), (intra molecular hydrogen bond), (hydrophobic effect), (hydrophobic hydration), (dipole-dipole) interaction, (dipole-induced-dipole) interaction, (ion-hydrophilic) interaction and (hydrophilic- hydrophilic) interaction. These derived thermodynamic parameters (i.e. app arent molar parameters, partial molar parameters, and partial molar transfer parameters) are further applied to determine the partial molar expansibility(E_{ϕ}^{0})with its first derivative $\left(\partial \mathrm{E}_{\phi}^{0}/\partial \mathrm{T}\right)_{P}$ and the pair-triplet interaction coefficients ($V_{AB,}$ K_{AB}; V_{ABB}, K_{ABB}). From the expansibility data, the strong (solute-solvent) interactions are depicted along with the structure-making property of the solutes, and the dominance of triplet-wise interaction is observed from the coefficients of pair-triplet interactions.

List of publications

1. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "**Temperature-dependent thermodynamic and physicochemical studies of glycols in aqueous biotin solutions**" (2021) 116605, published in ***Journal of Molecular Liquids*** **(Elsevier publications)** with impact factor **5.065**
https://doi.org/10.1016/j.molliq.2021.116605

2. **Nabaparna Chakraborty,** K. C. Juglan and Harsh Kumar "**Volumetric and ultrasonic studies of molecular interactions of glycols in aqueous Niacin (vitamin B3) at different temperatures.**" (2021) 115869, published in ***Journal of Molecular Liquids*** **(Elsevier publications)** with impact factor **5.065**
https://doi.org/10.1016/j.molliq.2021.115869

3. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "**Volumetric and Ultrasonic Studies of Molecular Interactions of PEG 400 and PEG 4000 in aqueous niacin solutions at Different Temperatures**" (2021) published in ***Journal of Chemical Engineering and Data*** **(ACS publications)** with impact factor **2.396.**
https://doi.org/10.1021/acs.jced.0c01091

4. **Nabaparna Chakraborty,** K. C. Juglan and Harsh Kumar "**Volumetric and Ultrasonic study of polyethylene glycols in aqueous solutions of Niacin at different temperatures.**" 154 (2021) 106326, published in ***Journal of Chemical Thermodynamics*** **(Elsevier publications)** with impact factor **2.888.**
https://doi.org/10.1016/j.jct.2020.106326

5. **Nabaparna Chakraborty,** K. C. Juglan and Harsh Kumar "**Study of Thermodynamic and Acoustic Properties of Niacin in Aqueous Hexylene Glycol and Propylene Glycol at Different Temperatures.**" 5, 32357–32365 (2020) published in ***ACS Omega*** **(ACS publications)** with impact factor **2.87**.
https://doi.org/10.1021/acsomega.0c04292

6. **Nabaparna Chakraborty**, Kirandeep Kaur, Harsh Kumar and K. C. Juglan, "**Acoustic and thermodynamic study of D-Panthenol in aqueous**

solutions of glycol at different temperatures." 126, 137-146 (2018) published in ***Journal of Chemical Thermodynamics*** **(Elsevier publications)** with impact factor **2.888.**

https://doi.org/10.1016/j.jct.2018.07.006

7. **Nabaparna Chakraborty**, Kirandeep Kaur, Harsh Kumar and K. C. Juglan, "**Volumetric and Ultrasonic studies on interaction of glycols in aqueous solution of xylitol at different temperatures.**" 65, 1435–1446 (2020) published in ***Journal of Chemical Engineering and Data*** **(ACS publications)** with impact factor **2.396.**

https://doi.org/10.1021/acs.jced.9b00869

8. Parminder Kaur, **Nabaparna Chakraborty**, K. C. Juglan and Harsh Kumar, "**Volumetric and Ultrasonic studies of molecular interations of glycols in aqueous glutaraldehyde solutions at different temperatures**." 315 (2020) 113763 published in ***Journal of Molecular liquids*** **(Elsevier publications)** with impact factor **5.065.**

https://doi.org/10.1016/j.molliq.2020.113763

9. Diksha Chawla, **Nabaparna Chakraborty**, Kailash Chandra Juglan, Harsh Kumar "**Temperature-dependent physicochemical studies of some Glycols in aqueous D-Mannitol solution**" 75, 1497–1506 (2021) published in ***Chemical Papers*** **(Springer publications)** with impact factor **2.369.**

https://doi.org/10.1007/s11696-020-01403-y

10. Harsimran Kaur, **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "**Volumetric and acoustical investigation of molecular interactions of PEG-200 and PEG-600 in aqueous solutions of D-Mannitol at different temperature**" (2021) published in J***ournal of Solution Chemistry*** with impact factor **1.273**.

11. **Nabaparna Chakraborty**, Parminder Kaur, Kirandeep Kaur, Harsh Kumar and K. C. Juglan, "**Theoretical and experimental ultrasonic velocities comparison of binary mixtures of triethylene glycol and glycerol at different**

temperatures” (2020) published in ***Journal of Physics: Conference Series*** **(IOP publications).**

12. Parminder Kaur, **Nabaparna Chakraborty**, Satnam Singh, K. C. Juglan and Harsh Kumar, “**Study of intermolecular interaction of binary mixture of adrenaline and KOH**” (2020) published in ***Journal of Physics: Conference Series*** **(IOP publications).**

13. Ashima Thakur, Harsimran Kaur, **Nabaparna Chakraborty**, K. C. Juglan and Harsh Kumar, “**Molecular interactions in ternary system of ethane-1,2-diol with methanol and methyl-4-hydoxybenzoate at 298 K: An acoustic approach**” (2020) published in ***Journal of Physics: Conference Series*** **(IOP publications).**

14. **Nabaparna Chakraborty** and K.C. Juglan, “**Investigation on temperature-dependent volumetric and acoustical properties of homologous series of glycols containing d-panthenol**” 20, 3089-3102 (2020) published in ***Journal of Plant Archives*** **(Indexed Scopus and web of Science).**

15. **Nabaparna Chakraborty**, Monica Rani and K.C. Juglan, “**Ultrasonic investigation of dichloromethane with ethanolamine at various temperatures**” 20, 2825-2829 (2020) published in ***Journal of Plant Archives*** **(Indexed Scopus and web of Science).**

16. **Nabaparna Chakraborty**, Priti, K.C. Juglan “**Measurement of density, velocity and viscosity of glyphosate with water at various frequencies**” 6, 147-155 (2019) published in ***Journal of Emerging Technologies and Innovative Research.***

17. **Nabaparna Chakraborty**, Priti, K.C. Juglan “**Comparison of basic thermodynamic parameters of glyphosate with water at various frequencies**” 6, 156-164 (2019) published in ***Journal of Emerging Technologies and Innovative Research.***

18. **Nabaparna Chakraborty**, K. G. Kaur, K.C. Juglan "**Volumetric and Viscometric studies for aqueous solution of Methyl Ester Glyphosate at different temperatures**" (2019) published in ***Think India Journal***.

19. **Nabaparna Chakraborty**, Mehar and K.C. Juglan *"***Acoustical and Thermodynamic Investigation of The Binary Mixture of Acetic Acid And Propan-2-Ol At Different Temperatures**" 22, 936-954 (2019) published in ***Think India Journal***.

20. **Nabaparna Chakraborty**, K.C. Juglan "**A Comparison Study Of Ultrasonic Velocities Binary Mixtures EG, DEG And TEG With Glycerol**" 7, 3580-3585 (2020) published in ***European Journal of Molecular & Clinical Medicine.***

List of communicated papers

1. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "Study of thermodynamic interactions of hexylene and propylene glycols in aqueous solutions of D-Panthenol at various temperatures" submitted to *Journal of molecular structure*.
2. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "Thermodynamics of various interactions in homologous series of polyethylene glycols in aqueous medium of d-panthenol at t= (288.15, 298.15, 308.15 and 318.15) k: a volumetric and acoustic approach" submitted to *Brazilian Journal of Chemical Engineering.*
3. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "Measurement of density and ultrasonic speed of sound of polyethylene glycols (600 and 6000) in aqueous vitamin B_5 solutions at different temperatures" submitted to *Food Chemistry*.
4. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "Densities and speed of sounds of (biotin + water + polyethylene glycols)

solutions at different temperatures and atmospheric pressure" submitted to *Physics and Chemistry of Liquids.*

5. **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "Effect of ethylene glycol/diethylene glycol/triethylene glycol on the thermodynamics of the aqueous biotin solutions at various temperatures" submitted to *Journal of Chemical Thermodynamics.*
6. Bhima Devi Neopaney, **Nabaparna Chakraborty**, K.C. Juglan, Harsh Kumar, "Investigation of acoustic and volumetric properties of liquid mixture containing glycols: A Review" submitted to *Journal of Chemical Thermodynamics..*
7. Parminder Kaur, **Nabaparna Chakraborty**, Harsh Kumar and Kailash Chandra Juglan, "Volumetric and ultrasonic studies on interactions of Hexylene and Propylene glycols in aqueous solutions of Glutaraldehyde at different temperatures" submitted to *Journal of Iranian Chemical Society.*
8. Ashima Thakur, Bhavna Rahal. Harsh Kumar, **Nabaparna Chakraborty**, Meenu Singla and Kailash Chandra Juglan, "Thermophysical characteristics of glycols in aqueous glycerin at several temperatures: Acoustic and Volumetric analysis" submitted to *Journal of Chemical and Engineering Data.*

List of Conferences/ Seminar/ Short term courses attended

Conferences

1. **106th Indian Science Congress**, Lovely Professional University, Phagwara, Punjab, 3rd January 2019 to 7th January 2019, “Ultrasonic Velocities of Binary Mixtures of Homologous Series of Diethylene Glycols and Glycerol at Different Temperatures”.
2. **Innovations in Applied Science and Engineering**, National Institute of Technology, Jalandhar, Punjab, 27th April 2019 and 28th April 2019, “Ultrasonic velocities of binary mixtures of glycols and glycerol at different temperatures”.
3. **Recent Advances in Fundamental and Applied Sciences** (RAFAS 2019), Lovely Professional University, Phagwara, Punjab, 5th November 2019 and 6th November 2019 Theoretical and experimental ultrasonic velocities comparison of binary mixtures of triethylene glycols and glycerol at different temperatures.

Short term courses

1. **Innovations in Applied Science and Engineering**, National Institute of Technology Jalandhar, Punjab, 16th April 2019 - 20th April 2019.
2. **Recent Trends in Advanced Materials and Devices,** National Institute of Technology Jalandhar, Punjab, 21st September 2020 - 25th September 2020.
3. **Advanced Energy Materials,** National Institute of Technology Jalandhar, Punjab, 12th October 2020- 16th October 2020

Future Scope of the work

Thermodynamic properties are of great importance in understanding the solvation behavior of liquids. Glycols are broadly used in plastic industry where they are used in the preparation of polyethylene terephthalate which is used further to make plastic bottles for pharmaceutical and food industry. B vitamins play a vital role in maintaining good health and well-being. As the building blocks of a healthy body, B vitamins have a direct impact on your energy levels, brain function, and cell metabolism. Niacin, D-Panthenol and Biotin have been studied with glycols in the present study, other vitamins can be studied with glycols to see the thermodynamic interaction among their molecules. Future studies with more vitamins and the chemicals which found their applications within them, needs to be conducted to establish and collaborate the problem of the present pilot study with the underlying aim of better understanding of the mechanism and innate utility of such a synergism in the realm of preclinical research and a part of future for its utility therapeutics.