International Journal of Advance and Applied Research
www.ijaar.co.in
ISSN – 2347-7075 **Impact Factor – 8.141**
Peer Reviewed **Bi-Monthly**
Vol. 12 No. 5 **May – June 2025**

Solubility and Molecular Interactions of Ferulic Acid in Polyethylene Glycol PEG-200 Solution

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DOI - 10.5281/zenodo.16397725

Abstract:

This study examines the ultrasonic velocities and densities of dilute solutions of polyethylene glycol (PEG-200) in ferulic acid at temperatures ranging from 293.15K to 308.15K. The experimental data are used to calculate various thermo-acoustical parameters, providing insights into the molecular structure and intermolecular interactions. The solubility of ferulic acid in PEG-200 solutions is measured at 293.15K and 308.15K. Activity coefficients are determined to assess the molecular interactions between ferulic acid and PEG-200, shedding light on the solvent-solute interactions. Ultrasonic velocities and densities are measured for PEG-200 solutions in ferulic acid at various temperatures. The data are used to compute thermo-acoustical parameters, exploring the effects of temperature and mole fraction on molecular interactions. The solubility and activity coefficients of ferulic acid in PEG-200 solutions are investigated to understand the molecular interactions between the solute and solvent. These findings provide valuable information on the solution's thermodynamic properties.

Keywords:* *Ultrasonic Velocities, Isentropic Compressibility, Intermolecular Free Length, Specific Acoustic Impedance And Thermo-Acoustic Parameters.

Introduction:

Polyethylene glycol (PEG) is a polyether compound with hydroxyl (-OH) groups, derived from petroleum. Its unique properties make it a valuable resource for various industries and research applications. PEG's low toxicity and high solubility in organic solvents have led to its widespread use in, Food industry, Cosmetic industry, Pharmaceutical industry and Chemical industry. PEG's benefits include:Enhancing biochemical activity and bioavailability of proteins and biological macromolecules, Serving as a dispersant in toothpaste and used in edible film preparations, preservatives, laxatives, and skincare products. PEG's hydrophilic nature makes it an essential tool in single-molecule fluorescence studies, helping to prevent protein sticking on microscopic glass slides. Overall, PEG's versatility and unique properties have made it a valuable compound in various fields [1−4].

Ferulic acid (FA), chemical name - 4-hydroxy-3-methoxycinnamic acid ; molecular formula: $C_{10}H_{10}O_4$; molar mass: 194.18 g/mol; and CAS registry number: 1325-24-6 occurs as white to off-white crystalline solid.[5-6] It is obtained from various parts of plants such as ‘fruits, grains, vegetables and leaves [7-8]. It is a phenolic compound which had various applications in biomedical, pharmaceutical and food industries.[Various kinds of therapeutic activity such as antioxidant, antimicrobial, anti-inflammatory, anti-allergi, cardioprotective and anticancer have been reported for FA in the literature [9-11].

By examining dilute solutions under varying concentrations and temperatures, researchers can gain a deeper understanding of the intricate relationships between molecules. This knowledge encompasses:Molecular packing and motion, Structural organization and changes, Molecular interactions and solvation, Hydrogen bonding dynamics, Polymer chain flexibility and movement, Mass and heat transfer mechanisms . The study of volumetric and ultrasonic properties is crucial for advancing various fields like Chemical engineering, Industrial processes and Biological systems. In non-polar solvents, the distance between polar molecules is significant, making solute-solvent interactions the dominant force. The choice of solvent is vital in these studies. As solute concentration or temperature changes, density fluctuations occur, impacting ultrasonic velocity. These changes, in turn, affect acoustical parameters and thermo-dynamic properties, providing valuable insights into the behavior of molecules in solution.

The literature survey has revealed that several earlier researchers have addressed these topics and subjects related to these parameters of aqueous solutions of poly(ethylene glycol) polymer. In the past, several attempts have been made to study acoustic properties of the solution of poly(ethylene glycol) with water. [12-14].

Significant Reckonings:

The following equations define key acoustic parameters for dilute solutions of PEG 200 in ferulic acid likes Isentropic Compressibility (β), Intermolecular Free Length (Lf), Acoustic Impedance (Z), Molar Volume (Vm), Schoff's Available Volume (Va), Rao's Constant (Ra) (Molar Sound Velocity), Wada's Constant (W) (Molar Compressibility). These parameters are calculated using ultrasonic velocity (u) and density (ρ) measurements of the solution.

$$b = 1/u2q \qquad 1)$$

$$Lf = Kb^{1/2} \qquad 2)$$

$$Z = uq \qquad 3)$$

$$Vm = (Mi/q) \qquad 4)$$

$$Va(s) = \{1 — (u/u\infty)\}Vm \qquad 5)$$

$$Ra = Vmu^{1/3} \qquad 6)$$

$$W = Vmb^{—1/7} \qquad 7)$$

The following parameters and constants are used to calculate acoustic properties such that Mole fraction of PEG 200 in ferulic acid (X1), Absolute temperature (T),Effective molecular mass of the solution (calculated as MpWp + MbWb) (Mi), Molecular mass of PEG 200 (Mp), Molecular mass of ferulic acid (Mb), Weight fraction of PEG 200 (Wp), Weight fraction of ferulic acid (Wb), Ultrasonic velocity constant (1,600 ms-1) (ui), Temperature-dependent Jacobson constant (calculated as (93.875 + 0.375T) × 10-8) (K).

Experimental:

The investigation utilized analytical reagent-grade poly(ethylene glycol) with an average molecular mass of 200 g mol-1. All chemicals, sourced from Loba Chemical Pvt. Ltd. India, were of the highest purity (> 0.99) and used without further purification. The solute and solvent were also used as is. Density measurements were taken for solutions of varying weight fractions at temperatures ranging from 293.15K to 313.15K, with an accuracy of ±0.0002 g cm-3. The measured densities were validated by comparing them to literature values, with deviations not exceeding 0.06%. Ultrasonic velocities were measured in binary solutions of PEG 200 in ferulic acid using an ultrasonic interferometer (M/S Mittal Enterprises, New Delhi) operating at 2.9979 MHz. The measurement accuracy was within ±0.3% at the specified temperatures. Temperature control was maintained using an electronically regulated thermostatic water bath with a precision of ±0.1 K.

Results and Discussion:

The speed of sound and density of polyethylene glycols (PEG 200) in ferulic acid solutions were measured at various concentrations (0.00 to 0.04 mol/kg) and temperatures (293.15K to 313.15K). The results, indexed in Table 1, show that density and speed of sound values increase with rising ferulic acid concentration and PEG content. However, at a specific concentration, these values decrease with increasing temperature.The measured densities were correlated with literature data [15-16]and plotted in Figs. 1, showing a satisfactory agreement. The increase in speed of sound indicates stronger molecular connections, attributed to intermolecular hydrogen bonding between solute and solvent molecules, as well as between solute molecules themselves.

As PEG is added to aqueous ferulic acid, the bonds between ferulic acid and water molecules are disrupted due to weakening of hydrogen bonds. New hydrogen bonds form between PEG, ferulic acid, and water molecules. The evaluated speed of sound data for PEGs in water mixtures were compared to literature results (Figs. 2 and 3), showing satisfactory agreement, except for one exception.[17-18].

Fig. 4 and 5 Table 1 reveal the nature of variation of Z and Vm with mole fraction X1 and temperature T. All the curves in each figure are found to increase quadratically with X1 at constant T. Coefficients of polynomial expression fitted to these variations are also reported in the Table 1. These correlation coefficients establish the validity of the linearity existing between Z and T. As X1 of solute in solution increases, effective molecular mass Mi increases and reciprocal of density decreases. Values of Vm are dependent on the product of Mi and (1/q). This product has the tendency to increase quadratically with X1 at given T. This means increasing tendency of Mi overshadows the decreasing tendency of (1/q). Hence, Vm has the tendency to increase with X1 at all T.

As temperature increases at a constant mole fraction, thermally agitated molecules tend to move away from each other, leading to decreased solute-solvent interactions and a less ordered structure. This results in increased spacing between molecules and volume expansion of the solution. Conversely, as temperature decreases, volume contraction occurs, causing the molecules to pack more tightly. The closest packing would theoretically occur at 0.0 K..The available volume, calculated using Eq. 5, increases with both mole fraction at constant temperature and temperature at constant mole fraction. [19-20].

The specific acoustic impedance (Z) of the dilute solution depends on the inertial and elastic properties of the medium, which are influenced by both concentration and temperature. As a parameter, Z is more significant in describing solute-solvent interactions than ultrasonic velocity (u) and density (q) individually, since it is the product of these two properties. The non-linear increase in Z with mole fraction at constant temperature suggests an increase in molecular interactions between unlike molecules. In contrast, Z decreases linearly with temperature at constant mole fraction, consistent with the decrease in ultrasonic velocity and density with temperature.

On the basis of above concept have arrived at simple expression for molar sound velocity Ra in the form of Eq. 6. They have come to conclusion that Ra is invariant with respect to temperature. In Table 1 and Figs. 6, clearly suggest that molar sound velocity Ra and molar adiabatic compressibility W values increase significantly with increase in mole fraction X1 of solute in the solution. Such an overlapping and readings in Table 1 suggest that Ra and W are almost invariant with respect to temperature [21].

Conclusions:

Dilute solution of PEG 200 in ferulic acid has a tendency to undergo volume expansion with a raise in the temperature. With increase in T of the solution of constant mole fraction, unfolding and chain expansion occurs due to decrease in the intramolecular and solute–solvent interactions. This results in structure alteration with increase in T. The PEG molecules on entering the solvent environment at constant temperature get their coiled structure loosened due to which unfolding of chains occur. As a result of this, more number of PEG 200 polymer segments comes close to ferulic acid molecules. Therefore, there occurs an increase in solute–solvent molecular interaction with increase in mole fraction at constant temperature.

Table 1: Ultrasonic velocity (u), density (q) and thermo-acoustic parameters like isentropic compressibility (b), intermolecular free length (L_f) acoustic impedance (Z), molar volume (Vm), Schoff's available volume Va(s), molar sound velocity or Rao's constant (Ra), and molar compressibility or Wada's constant (W) as a function of X_1 of of PEG 200 in ferulic acid at different T.

T (K)	X_1	u (ms^{-1})	q (kg m^{-3})	b(10^{-10} m^2N^{-1})	L_f(10^{-10} m)	Z (10^6 kg m^{-2} s^{-1})	V_m (10^{-3} m^3 mol^{-1})	R_a (10^{-4} $m^{10/3}s^{-1/3}$ mol^{-1})	W (10^{-3} m^3mol^{-1}) $(TPa)^{1/7}$
293.15K	0.00	1412.5	1.0012	5.2698	0.5425	0.0982	0.1093	09.8962	1.2298
	0.01	1456.1	1.0030	5.1604	0.5403	1.2118	0.1205	11.1300	1.4638
	0.02	1462.7	1.0056	5.0253	0.5450	1.2873	0.1328	12.4894	1.7219
	0.03	1478.1	1.0077	4.8903	0.5396	1.3445	0.1437	12.6954	1.9521
	0.04	1493.5	1.0092	4.7712	0.5248	1.3997	0.1552	13.9898	2.1985
298.15K	0.00	1410.5	1.0022	5.2598	0.5415	0.0972	0.1093	09.8962	1.2298
	0.01	1426.1	1.0031	5.2004	0.5403	1.2018	0.1205	11.1300	1.4638
	0.02	1432.7	1.0039	5.1853	0.5348	1.2073	0.1328	12.4894	1.7219
	0.03	1448.1	1.0041	4.1503	0.5350	1.2145	0.1437	12.6954	1.9521
	0.04	1453.5	1.0045	4.1212	0.5245	1.2197	0.1552	13.9898	2.1985
303.15 K	0.00	1409.5	1.0020	5.2588	0.5405	0.0970	0.1083	09.8932	1.2288
	0.01	1425.1	1.0030	5.2000	0.5403	1.2012	0.1185	11.1250	1.4628
	0.02	1430.7	1.0035	5.1843	0.5398	1.2068	0.1288	12.4884	1.7210
	0.03	1447.9	1.0039	4.1540	0.5340	1.2135	0.1247	12.6924	1.9511
	0.04	1452.5	1.0045	4.1235	0.5239	1.2177	0.1452	13.9878	2.1905
308.15 K	0.00	1409.5	1.0022	5.2598	0.5415	0.0972	0.1093	09.8962	1.2280
	0.01	1425.1	1.0031	5.2004	0.5403	1.2018	0.1205	11.1300	1.4622
	0.02	1430.7	1.0039	5.1853	0.5348	1.2073	0.1328	12.4894	1.7210
	0.03	1447.9	1.0041	4.1503	0.5350	1.2145	0.1437	12.6954	1.9518
	0.04	1452.5	1.0045	4.1212	0.5245	1.2197	0.1552	13.9898	2.1905
313.15 K	0.00	1410.5	1.0022	5.2598	0.5415	0.0972	0.1093	09.8962	1.2279
	0.01	1426.1	1.0031	5.2004	0.5403	1.2018	0.1205	11.1300	1.4635
	0.02	1432.7	1.0039	5.1853	0.5348	1.2073	0.1328	12.4894	1.7217
	0.03	1448.1	1.0041	4.1503	0.5350	1.2145	0.1437	12.6954	1.9515
	0.04	1453.5	1.0045	4.1212	0.5245	1.2197	0.1552	13.9898	2.1885

Fig.1

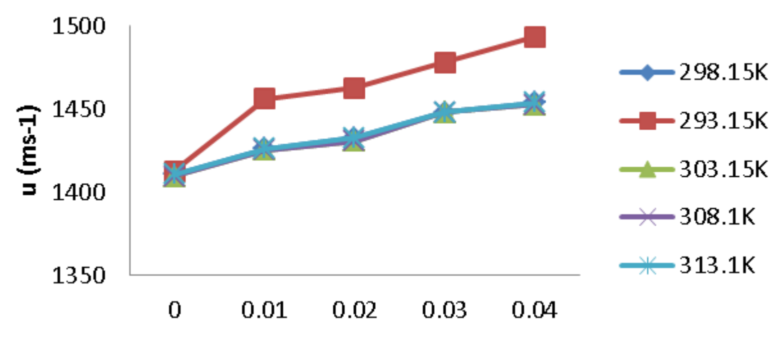


Fig.2

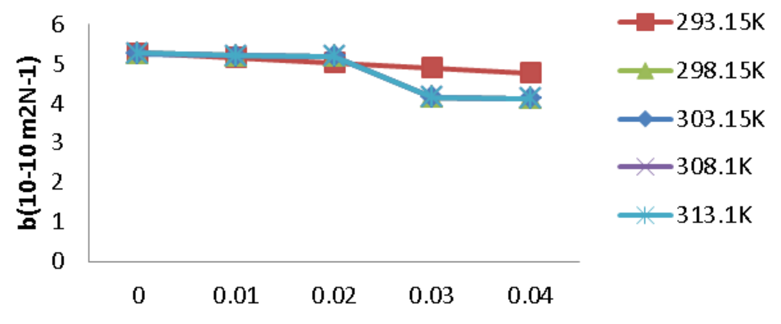


Fig.3

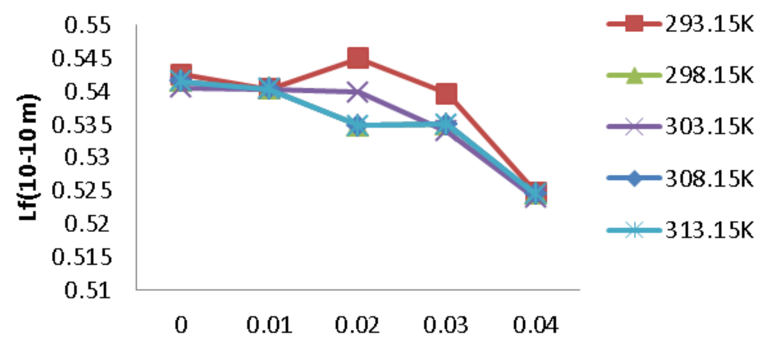
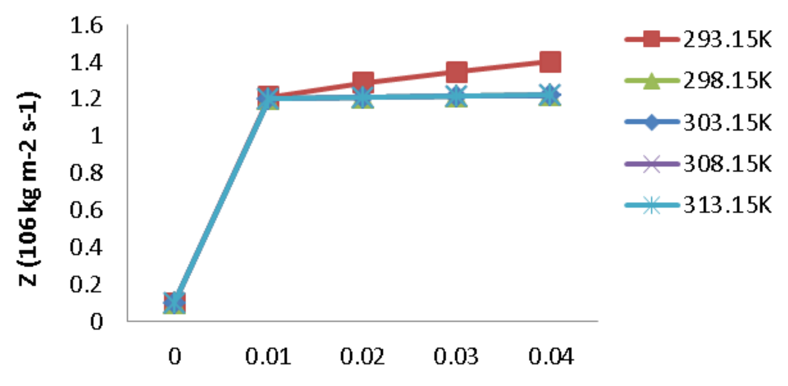


Fig.4



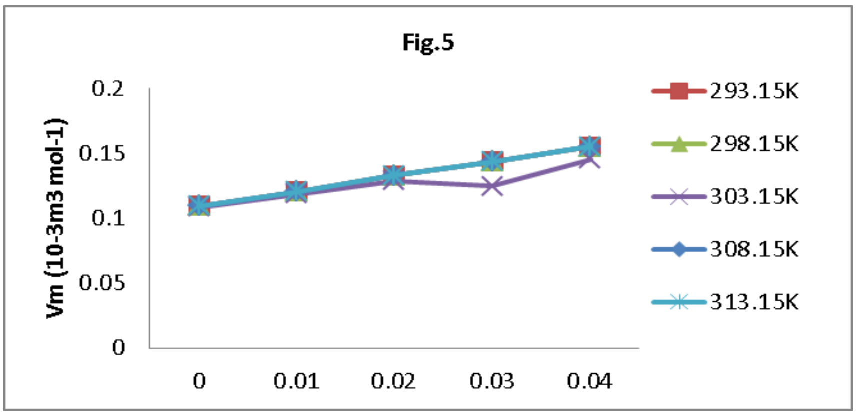


Fig.5

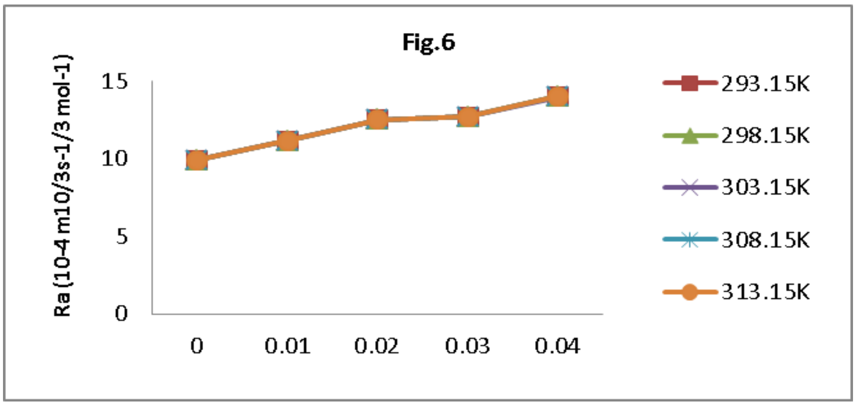


Fig.6

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