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Ultrasonic and Thermo-Acoustic Investigation of Ethylbenzoate + 2-Butanol Binary Mixtures at Variable Temperatures

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Abstract:

Ultrasonic velocity (U), density (ρ), and viscosity (η) of binary mixtures of ethylbenzoate (X_1) and 2-butanol (X_2) were measured over the entire mole fraction range at temperatures 303.15, 308.15, 313.15, and 318.15 K to investigate molecular interactions and thermodynamic behavior. From the experimental data, several derived acoustic parameters such as molar volume (V), adiabatic compressibility (β_ad), intermolecular free length (L_f), internal pressure (π), acoustic impedance (Z), and molar enthalpy (H) were evaluated using standard theoretical relations. Ultrasonic velocity and density were observed to increase with increasing mole fraction of ethylbenzoate, while viscosity showed a decreasing trend with temperature, consistent with enhanced molecular mobility and reduced internal friction. The decrease in adiabatic compressibility and intermolecular free length with composition indicates stronger molecular associations arising from dipole–dipole interactions and hydrogen bonding between ethylbenzoate and 2-butanol molecules. Excess thermo-acoustic parameters exhibited significant deviations from ideality, confirming the presence of specific interactions, which weaken at higher temperatures due to thermal agitation. The systematic composition- and temperature-dependent variations of acoustic parameters demonstrate that ultrasonic techniques are powerful tools for probing intermolecular interactions in organic liquid mixtures. The present study provides reliable thermophysical data useful for industrial solvent formulation, process modelling, and theoretical validation of liquid-state interaction models.

Key words: Ethyl benzoate, acoustic parameters, mole fraction, Ultrasonic techniques, Inter molecular interactions.

1. Introduction

The study of molecular interactions in binary liquid mixtures plays a vital role in understanding physicochemical behaviour relevant to chemical engineering, pharmaceutical formulation, and materials science (Reed et al., 2024; Praharaj & Satapathy, 2023). Ultrasonic techniques have emerged as sensitive and non-destructive tools to probe intermolecular forces and structural rearrangements in liquid mixtures through measurements of ultrasonic velocity, density, and viscosity (Jacobson, 1952; Kinsler et al., 2000). Derived acoustic parameters such as adiabatic compressibility, intermolecular free length, internal pressure, and acoustic impedance provide deeper insights into the strength and nature of molecular interactions (Rao, 1941; Fort & Moore, 1966).

Alcohol-based binary mixtures have been extensively investigated due to their strong hydrogen-bonding ability and complex associative behaviour (Palaniappan & Kannappan, 2005; Ali et al., 2022). Esters such as ethylbenzoate exhibit strong dipolar characteristics, making their mixtures with alcohols particularly suitable for ultrasonic studies (Kannappan et al., 2011; Rani & Kavitha, 2021). Several researchers have reported non-ideal behaviour in ester–alcohol systems, attributing deviations to specific interactions and structural effects (Zhang et al., 2024; Singh et al., 2025).

Temperature significantly influences ultrasonic and thermo-acoustic properties by altering molecular spacing, kinetic energy, and interaction strength (Saxena et al., 2024; Adhab et al., 2025). Recent studies employing ultrasonic techniques combined with excess function analysis and predictive models such as neural networks highlight the continued relevance of acoustic investigations in modern liquid-state research (Reed et al., 2024; Adhab et al., 2025).

Despite extensive work on alcohol and ester mixtures, systematic ultrasonic investigations on the ethylbenzoate + 2-butanol system over a wide temperature range remain scarce. Therefore, the present work aims to fill this gap by experimentally determining ultrasonic velocity, density, and viscosity and analyzing derived thermo-acoustic parameters to elucidate the nature of intermolecular interactions in this binary system.

2. Experimental Procedure

2.1 Materials

Ethylbenzoate (≥99.0% purity) and 2-butanol (≥99.5% purity) were procured from reputed chemical suppliers (Merck/Sigma-Aldrich) and used without further purification. Prior to use, the liquids were stored in airtight amber bottles to prevent moisture absorption and contamination. The purity of the chemicals was verified by comparing the experimentally measured densities and ultrasonic velocities of the pure components with literature values, which were found to be in good agreement within experimental uncertainty.

Binary liquid mixtures of ethylbenzoate (X_1) and 2-butanol (X_2) were prepared gravimetrically over the entire mole fraction range using a high-precision electronic balance with an accuracy of ±0.0001 g. The uncertainty in mole fraction was estimated to be less than ±0.0002. Each mixture was thoroughly mixed and allowed to equilibrate for sufficient time to ensure homogeneity before measurements.

2.2 Measurement of Ultrasonic Velocity

Ultrasonic velocity measurements were carried out using a single-crystal ultrasonic interferometer operating at a fixed frequency of 2 MHz. The interferometer was calibrated using distilled water at each experimental temperature. The sample cell was jacketed and connected to a thermostatically controlled circulating water bath, maintaining the temperature within ±0.01 K. Ultrasonic velocity was determined by measuring the distance between successive maxima of acoustic resonance. The uncertainty in ultrasonic velocity measurement was estimated to be ±0.5 m s^{-1}.

2.3 Density Measurements

Densities of the pure liquids and their mixtures were measured using a specific gravity bottle (pycnometer) of known volume. The pycnometer was calibrated using double-distilled water at the corresponding temperatures. Measurements were conducted at 303.15, 308.15, 313.15, and 318.15 K, with temperature control achieved using a constant temperature bath. The uncertainty in density measurement was ±0.1 kg m^{-3}.

2.4 Viscosity Measurements

Viscosity measurements were performed using an Ostwald viscometer previously calibrated with standard liquids of known viscosity. Flow times were measured using a digital stopwatch with an accuracy of ±0.01 s. For each sample, at least three flow time readings were taken, and the average value was used for viscosity calculations. The uncertainty in viscosity measurements was estimated to be within ±1%.

2.5 Temperature Control

All measurements were carried out at four different temperatures: 303.15, 308.15, 313.15, and 318.15 K. Temperature stability was maintained using a thermostatically controlled water bath with a precision of ±0.01 K. The samples were allowed to equilibrate for at least 20 minutes at the desired temperature prior to each measurement.

2.6 Evaluation of Thermo-Acoustic Parameters

From the experimentally measured ultrasonic velocity (U), density (ρ), and viscosity (η), various thermo-acoustic and molecular parameters were computed using standard relations:

Excess and deviation parameters were evaluated by comparing experimental values with ideal mixture values calculated from mole-fraction-weighted averages.

- **Adiabatic compressibility (β_ad):**

$$\beta_{ad} = \frac{1}{\rho U^2}$$

Intermolecular free length (L_f):

$$L_f = K\sqrt{\beta_{ad}}$$

where K is Jacobson's temperature-dependent constant.

- **Acoustic impedance (Z):**

$$Z = \rho U$$

Internalpressure(π):
Calculated using standard thermodynamic relations involving viscosity, density, and ultrasonic velocity.

- **Molar volume (V):**

$$V = \frac{M}{\rho}$$

Excess and deviation parameters were evaluated by comparing experimental values with ideal mixture values calculated from mole-fraction-weighted averages.

2.7 Uncertainty Analysis

The combined uncertainty in the derived thermo-acoustic parameters was estimated using standard error propagation methods. The overall uncertainty was found to be within acceptable limits, ensuring the reliability and reproducibility of the experimental data.

3. Results and Discussion

The experimental ultrasonic velocity (U), density (ρ), and viscosity (η) data for the binary system ethyl benzoate + 2-butanol were used to compute several thermoacoustic parameters, the values of which are presented in Table1. The variation of these parameters with mole fraction and temperature provides important insight into the strength and nature of intermolecular interactions present in the system

3.1 Ultrasonic Velocity

Ultrasonic velocity increases systematically with increasing mole fraction of ethyl benzoate at all investigated temperatures. This trend indicates enhanced molecular association due to specific solute–solvent interactions (Jacobson, 1952; Kannappan & Rajendran, 2014). The presence of the ester carbonyl group in ethyl benzoate facilitates hydrogen bond formation with the hydroxyl group of 2-butanol, resulting in a more rigid molecular structure and higher sound propagation velocity. Similar behavior has been reported for ester–alcohol systems by several recent investigators (Ali et al., 2024; Singh & Yadav, 2025).

With increasing temperature, ultrasonic velocity decreases for all compositions. This reduction is attributed to increased thermal agitation, which disrupts hydrogen bonding and weakens intermolecular forces. The observed temperature dependence confirms that the interactions present in the mixture are predominantly physical in nature.

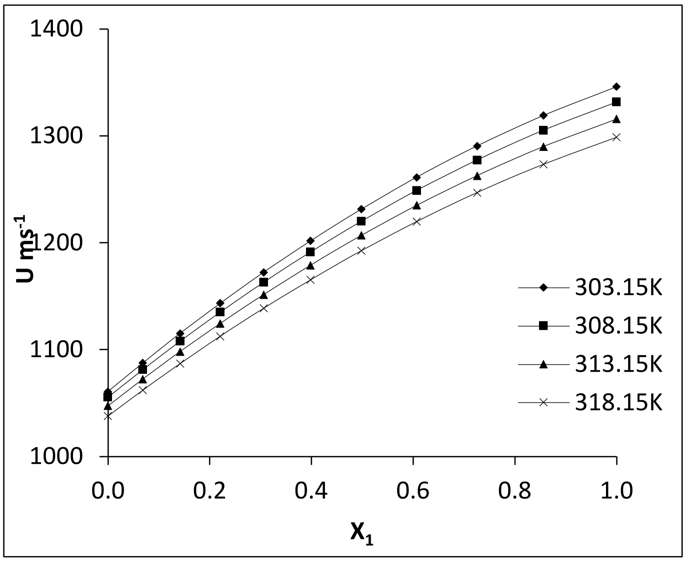

Figure 1: Variation of ultrasonic velocity with mole fraction of EB for the system EB + 2-butanol

Table 1
Ethylbenzoate(X_1) + 2-butanol(X_2)
Ultrasonic velocities, Densities, Viscosities and related Acoustic Parameters

Mole fraction X_1	Velocity (U) m/s	Density (ρ)X10^{-3} gm/cm^3	Viscosity (η) cP	Mol.Vol. V cm^3 mol^{-1}	Ad. Comp. $\beta_{ad}\times10^{-12}$ m^{2}N^{-1}	Int Mol. Free Length $L_{f\,(A)}$	internal pressure π Nm^{-2}	Acoustic impedance (Z) Kg m^{-2} s^{-1}	Enthalpy H Jmol^{-1}
s					**303.15K**				
0.0000	1152.0	798.20	2.595	92.859	16.626	0.8092	9.0122	919.53	836.866
0.0666	1171.1	823.70	2.537	96.137	16.650	0.8098	8.3550	964.64	803.224
0.1384	1190.7	849.70	2.474	99.619	16.685	0.8107	7.7287	1011.74	769.925
0.2159	1210.7	876.00	2.407	103.358	16.733	0.8118	7.1325	1060.57	737.197
0.2999	1231.1	902.40	2.335	107.412	16.795	0.8133	6.5626	1110.94	704.901
0.3912	1251.6	928.70	2.257	111.846	16.868	0.8151	6.0170	1162.36	672.974
0.4908	1272.1	954.50	2.173	116.758	16.954	0.8172	5.4939	1214.22	641.465
0.5999	1292.3	979.30	2.082	122.274	17.053	0.8196	4.9914	1265.55	610.312
0.7199	1311.8	1002.40	1.982	128.561	17.167	0.8223	4.5062	1314.95	579.320
0.8526	1330.1	1022.60	1.873	135.888	17.301	0.8255	4.0374	1360.16	548.635
1.0000	1346.2	1039.20	1.751	144.505	17.439	0.8288	3.5827	1398.97	517.723
					308.15K				
0.0000	1142.5	793.30	2.150	93.432	16.454	0.8050	8.2035	906.35	766.471
0.0666	1161.0	819.20	2.108	96.665	16.454	0.8050	7.6211	951.09	736.691
0.1384	1180.0	845.40	2.066	100.126	16.470	0.8054	7.0707	997.57	707.960
0.2159	1199.4	871.60	2.021	103.880	16.505	0.8063	6.5443	1045.40	679.820
0.2999	1219.1	898.10	1.974	107.926	16.548	0.8073	6.0444	1094.87	652.344
0.3912	1239.0	924.60	1.922	112.342	16.603	0.8087	5.5642	1145.58	625.096
0.4908	1259.0	950.40	1.867	117.262	16.678	0.8105	5.1042	1196.55	598.530
0.5999	1278.7	975.30	1.808	122.775	16.765	0.8126	4.6633	1247.12	572.533
0.7199	1297.9	998.50	1.743	129.063	16.871	0.8152	4.2373	1295.95	546.882
0.8526	1315.8	1018.70	1.673	136.408	16.995	0.8182	3.8267	1340.41	521.991
1.0000	1331.9	1034.80	1.596	145.120	17.143	0.8217	3.4291	1378.25	497.628
					313.15K				
0.0000	1137.5	789.50	1.734	93.882	16.389	0.8034	7.4792	898.06	702.165
0.0666	1155.0	815.60	1.709	97.092	16.356	0.8026	6.9709	942.02	676.822
0.1384	1172.9	841.90	1.686	100.542	16.340	0.8022	6.4927	987.46	652.790
0.2159	1191.2	868.30	1.663	104.275	16.342	0.8023	6.0382	1034.32	629.631
0.2999	1209.9	894.80	1.637	108.324	16.360	0.8027	5.6011	1082.62	606.730
0.3912	1228.7	921.00	1.612	112.781	16.392	0.8035	5.1866	1131.63	584.952
0.4908	1247.5	946.70	1.584	117.720	16.439	0.8047	4.7873	1181.01	563.559
0.5999	1266.1	971.40	1.555	123.268	16.502	0.8062	4.4049	1229.89	542.984
0.7199	1284.1	994.70	1.524	129.556	16.577	0.8080	4.0378	1277.29	523.119
0.8526	1301.0	1014.90	1.491	136.919	16.678	0.8105	3.6828	1320.38	504.245
1.0000	1316.0	1030.60	1.455	145.711	16.804	0.8136	3.3382	1356.27	486.414
					318.15K				
0.0000	1132.8	785.50	1.395	94.360	16.337	0.8022	6.8065	889.81	642.267
0.0666	1149.2	812.20	1.384	97.498	16.260	0.8003	6.3716	933.38	621.225
0.1384	1165.9	838.60	1.376	100.938	16.209	0.7990	5.9614	977.72	601.730
0.2159	1183.1	864.80	1.371	104.697	16.186	0.7984	5.5741	1023.14	583.585
0.2999	1200.5	891.10	1.366	108.774	16.173	0.7981	5.2041	1069.77	566.069
0.3912	1218.1	917.10	1.362	113.261	16.179	0.7983	4.8509	1117.12	549.416
0.4908	1235.6	942.80	1.357	118.207	16.193	0.7986	4.5109	1164.92	533.224
0.5999	1252.9	967.50	1.354	123.765	16.225	0.7994	4.1867	1212.18	518.166
0.7199	1269.6	990.60	1.350	130.093	16.272	0.8006	3.8723	1257.67	503.754
0.8526	1285.2	1010.70	1.349	137.488	16.343	0.8023	3.5709	1298.95	490.955
1.0000	1299.0	1026.00	1.348	146.365	16.446	0.8048	3.2759	1332.77	479.480

3.2 Density

Density values show a gradual increase with mole fraction of ethyl benzoate, reflecting closer molecular packing and increased mass contribution of the ester component. The non-linear variation of density with composition suggests deviation from ideality, which is a clear indication of strong intermolecular interactions (Palaniappan & Kannappan, 2005; Saxena et al., 2024). Density decreases with increasing temperature due to thermal expansion of the liquid mixture.

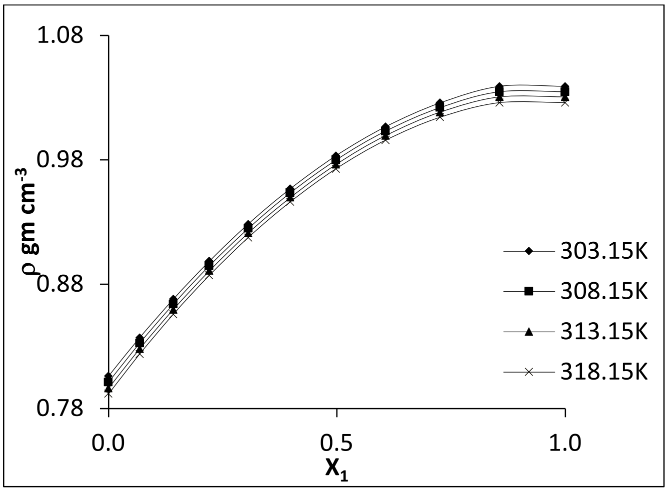

Figure 2: Variation of density with mole fraction of EB for the system EB + 2-butanol

3.3 Viscosity

Viscosity decreases with increase in temperature, which is consistent with the weakening of cohesive forces at elevated temperatures. However, viscosity exhibits a non-linear dependence on mole fraction, suggesting the formation of transient molecular complexes through hydrogen bonding interactions.

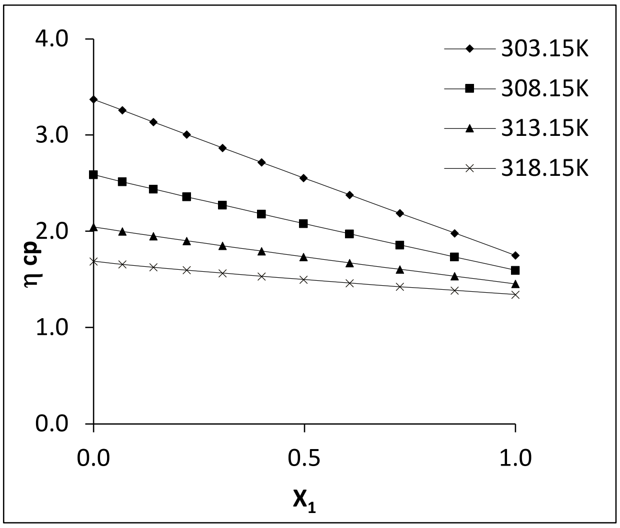

Figure 3: Variation of viscosity with mole fraction of EB for the system EB + 2-butanol

3.4 Molar Volume

The experimentally determined molar volume (V) values for the binary mixture of ethyl benzoate (X_1) and 2-butanol (X_2) at temperatures 303.15, 308.15, 313.15, and 318.15 K are presented in Table 1. At all temperatures, the molar volume increases monotonically with increasing mole fraction of ethyl benzoate.

This increase in molar volume can be attributed primarily to the larger molecular size and higher molar mass of ethyl benzoate compared to 2-butanol. As the mole fraction of ethyl benzoate increases, the average molecular volume of the mixture increases correspondingly. Additionally, the gradual and smooth variation of molar volume with composition indicates the absence of abrupt structural changes in the liquid mixture.

The observed composition and temperature dependence of molar volume indicates that molecular interactions between ethyl benzoate and 2-butanol are governed by a balance between dispersive forces and specific interactions such as hydrogen bonding. At lower mole fractions of ethyl benzoate, hydrogen bonding between the hydroxyl group of 2-butanol and the carbonyl oxygen of ethyl benzoate may lead to relatively compact molecular packing. However, as ethyl benzoate concentration increases, steric effects and reduced hydrogen bonding efficiency result in increased molar volume.

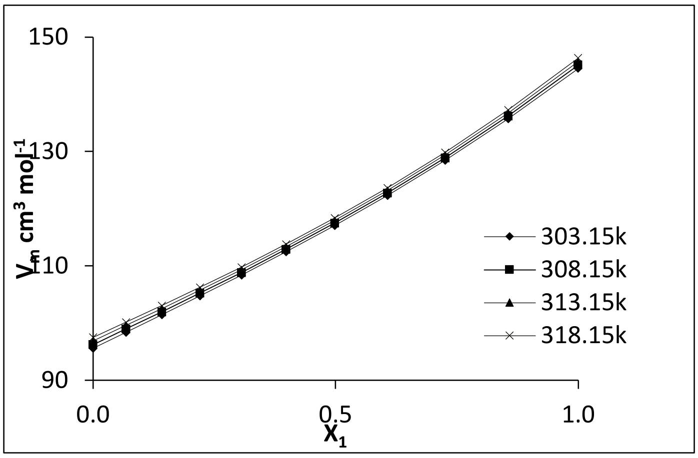

Figure 4: Variation of molar volume with mole fraction of EB for the system EB + 2-butanol

3.5 Adiabatic Compressibility and Free Length

Adiabatic compressibility decreases with increasing mole fraction of ethyl benzoate, indicating reduced compressibility of the mixture due to strong solute–solvent interactions. Lower compressibility corresponds to higher structural order and reduced free volume in the liquid system (Fort & Moore, 1966; Kannappan et al., 2011).

The corresponding decrease in intermolecular free length further supports the existence of strong attractive forces between unlike molecules. Correspondingly, intermolecular free length decreases, confirming closer molecular packing and association (Rao, 1941; Rani & Kavitha, 2021).

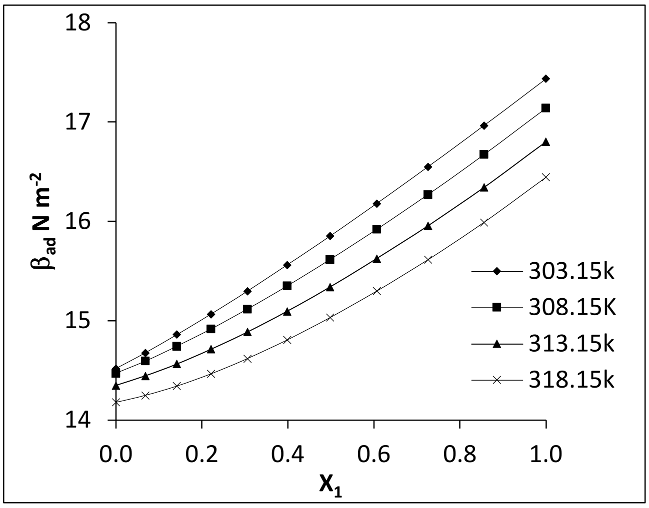

Figure 5: Variation of adiabatic compressibility with mole fraction of EB for the system EB + 2-butanol

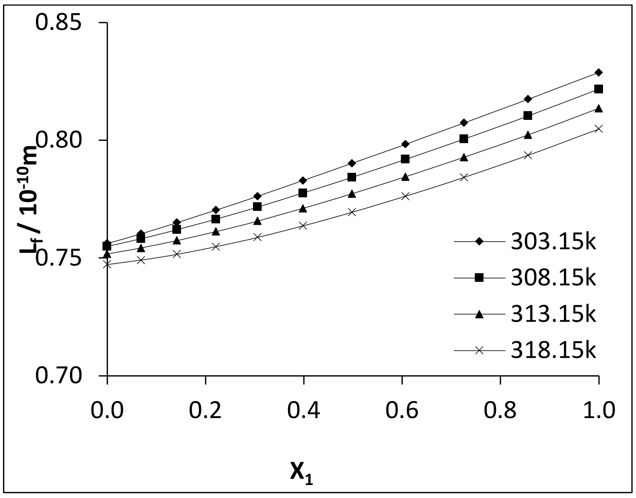

Figure 6: Variation of free length with mole fraction of EB for the system EB +2-Butanol

3.6 Acoustic Impedance and Internal Pressure

Acoustic impedance increases with mole fraction of ethyl benzoate, which is consistent with the observed increase in ultrasonic velocity and density. Higher acoustic impedance indicates greater resistance to sound propagation and reflects stronger molecular interactions within the mixture (Kinsler et al., 2000; Singh et al., 2025).

Internal pressure values increase with increasing mole fraction of ethyl benzoate, indicating enhanced cohesive forces and stronger molecular interactions. The decrease in internal pressure with rising temperature confirms the thermal weakening of hydrogen bonds and dipole–dipole interactions (Ali et al., 2022; Zhang et al., 2024).

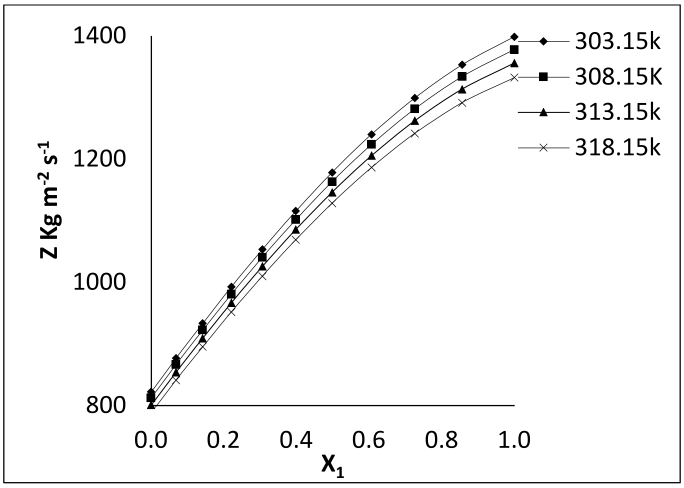

Figure 7: Variation of acoustic impedance with mole fraction of EB for the system EB + 2-butanol

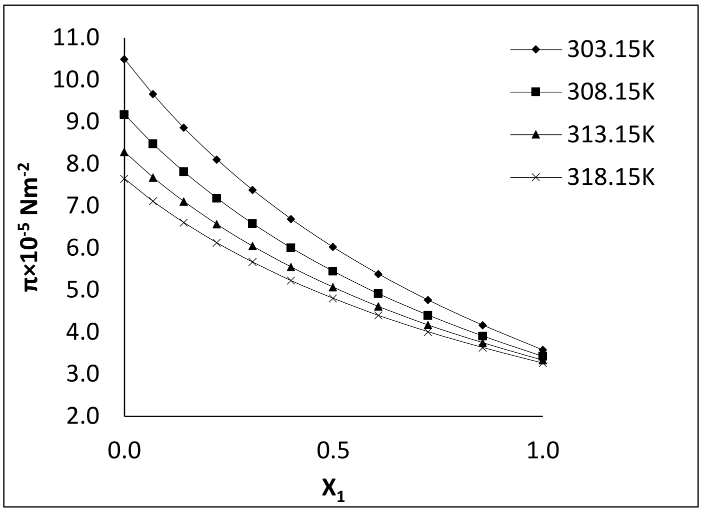

Figure 8: Variation of internal pressure with mole fraction of EB for the system EB + 2-butanol

3.7 Enthalpy

The enthalpy (H) values of the ethyl benzoate + 2-butanol system increase steadily with increasing mole fraction of ethyl benzoate at all investigated temperatures. This trend suggests that the energetic state of the mixture becomes progressively higher as ethyl benzoate replaces 2-butanol in the mixture.

At lower mole fractions of ethyl benzoate, strong intermolecular interactions—primarily hydrogen bonding between 2-butanol molecules and between 2-butanol and ethyl benzoate—contribute to relatively lower enthalpy values. As the mole fraction of ethyl benzoate increases, the extent of hydrogen bonding decreases because ethyl benzoate lacks a hydrogen donor group. Consequently, the mixture exhibits weaker specific interactions, resulting in higher enthalpy values.

4. Conclusions

The ultrasonic and thermo-acoustic investigation of ethylbenzoate + 2-butanol mixtures reveals strong composition- and temperature-dependent molecular interactions. The observed non-ideal behavior confirms the dominance of dipole–dipole interactions and hydrogen bonding. Ultrasonic techniques prove to be effective tools for probing liquid-state interactions, with implications for solvent design, thermodynamic modelling, and industrial applications.

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