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THE BEHAVIOR OF BENZENE WITH PARABENS IN ISOPROPANOL BY USING ULTRASONIC AND VOLUMETRIC EXPERIMENTS

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ABSTRACT
Benzene with Butyl/Pentyl Parabens is evaluated using the volumetric and acoustic study as a function of temperature. The properties such as partial and apparent molar volumeand partial and apparent molar compressibility of the mixtures were studied. The thermoacoustic properties of the mixture, such as acoustic impedanceand free lengthwere analyzed. These measurements were utilized to interpret the intermolecular interactions among the constituents.
Keywords: Acoustic Impedance, Intermolecular Free Length, Adiabatic Compressibility,Acoustic Study, Temperature Range.
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INTRODUCTION

Thermoacoustic characteristics of the chosen mixtures are used to study the physicochemical behavior, molecular packing, and numerous sorts of intermolecular interactions. Recent studies on ultrasonic velocity and their derived parameters with the variation in composition and temperature provide vital information about the intermolecular interaction among the constituents of the mixture.[1-9] The obtained outcomes are discussed in terms of intermolecular interactions. In continuation of ourresearch work on ultrasonic velocities, density, etc., the present work is to undertake volumetric and acoustical analysis of Benzene with Butyl/Pentyl parabens in Isopropanol medium at various temperatures varying from 298.15K to 323.15K at atmospheric pressure.[10,11] The acoustic parameters were computed based on the density,ultrasonic velocity, and viscosity data. This calculated data is utilized to interpret the intermolecular interactions of the selected constituents. Kumara Sastry *et al.* measured acoustic velocity, density, and viscosity of the ternary system containing Ethyl paraben along with 1-Propanol/2-Propanol and benzene and calculated the acoustic parameters derived from measured data at 303K.[12,13] The results are interpreted based on steric considerations. Ashima *et al.* studied the variation of sound speed, density, and viscosity of Ethane-1,2-diol, methyl, and methanol parabens at an operating temperature of 298K with various compositions.[14] The acoustic parameters were then calculated from the experimental data. The linear deviation of acoustic parameters infers the aggregate formation in the chosen ternary system. Ashima and Juglan studied the acoustic parameters of Ethylene Glycol (EG) and Propylene Glycol (PG) with sodium ethylparaben at 298.15K as determined by ultrasonic velocity, density, and viscosity.[15] Further, there are strong connections between the solvent and solute molecules. Ashima and Juglan analyzed the acoustic as well as volumetric behavior of the glycols with Ethyl paraben in the aqueous medium with operating temperatures ranging between 293.15K and 308.15 K at atmospheric pressure.[16,17] The findings were analyzed in terms of the extent of weakening tendencies among the solvents and co-solutes.Shaik Babu *et al.* measured Ultrasonic velocity at a frequency of 2 MHz for an Ethyl Benzoate mixture using 1-Propanol, 1-Butanol, and last 1-Pentanol, and the experimental values were compared with the theoretical values.[18]

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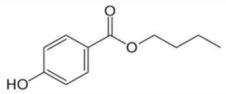
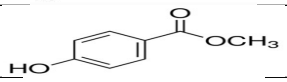
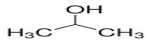
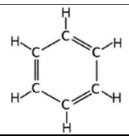
EXPERIMENTAL

Butyl p-hydroxy benzoate (Butylparaben) is a white powder that dissolves in polar solvents, used as an antimicrobial preservative in cosmetics, medication suspensions, and flavoring additive in food.[19-22] Pentyl p-hydroxybenzoate is a white solid that can be dispersed in organic solvents. Parabens belong to the family of para-hydroxybenzoic acid esters and have a para position on the benzene ring.The chemicals used in the present work, with aminimum assay of 99.9%, were obtained from Frinton Laboratories Inc., USA. All liquid mixtures have been prepared gravimetrically in sealed bottles appropriately. Care is taken to prevent evaporation losses. The compounds were first degassed via 0.4nm molecular sieves for 72 hours to remove moisture. The benzene is used as solute while the mixture of parabens with isopropanol is used as a solvent in the preparation of the solution. Butyl p-hydroxybenzoate (4HB) and pentyl p-hydroxybenzoate (5HB) were dissolved in isopropanol (IPA) at 0.01m and the solute compositions were then diluted with a varying molality of solvent. A digital electronic balance was used to conduct mass measurements with an error of 0.00001g (METTLER TOLEDO AB135, Switzerland). The Ostwald viscometer was used to measure the viscosities.[23] Double distilled water was used to calibrate the viscometer at each temperature. The measurement of viscosity has a margin of error of up to 0.0001mPa-s. After each mixture had reached the specified bath temperature, the flow time was measured. The flow measurements were taken using a 0.01s precision electronic stopwatch. 3-4 readings were done for each pure component and mixture, and the mean of these values was utilized in all computations. For robustness, a single crystal variable path interferometer was calibrated and operated at a frequency of 2 MHz to measure the speed of sound. Furthermore, with a consistent temperature, we could calculate accurate density measurements with an average error of 0.001 kg/m^3. Table 1 shows the compounds utilized in the present study alongwith purification method, molar mass and chemical structure.

Table-1: Specifications on Pureness of Compounds Utilized in the Present Study

Chemical name	CAS no.	Molar mass (g/mol)	Formula	Purification method	Chemical Structure
Butyl Paraben	94-26-8	194.227	$C_{11}H_{14}O_3$	Vacuum drying	
Pentyl Paraben	6521-29-5	208.25	$C_{12}H_{16}O_3$	Vacuum drying	
Isopropanol	67-63-0	60.1	$CH_3CHOHCH_3$	Used as such	
Benzene	71-43-2	78.11	C_6H_6	Used as such	

The density and acoustic velocity of pure compounds from the literature data are displayed in Table-2. The density and acoustic velocity for benzene in 0.01 molkg^{-1}, Isopropanol-BHB and Isopropanol were studied. Tables-3 to 4 shows the ultrasonic and volumetric characteristics of benzene with parabens in isopropyl alcohol medium.

Table-2: Contrast of Density (ρ) and Acoustic Velocity (U) of Pure Compounds at T = 298.15K to 323.15K

Compound	T/K	Densityx10^{-3} kg.m^{-3}		Ultrasonic velocity m.s^{-1}	
		Measured	Literature data	Measured	Literature data
Isopropanol	298.15	780.92	780.52[26]	1152.0	1152.63[24]
	303.15	776.25	777.47[24]	1117.8	1132.16[25]
	308.15	772.79	773.15[24]	1107.8	1114.33[25]
	313.15	767.29	768.45[24]	1091.4	1096.18[25]
	318.15	765.40	767.10[24]	1074.8	1075.5[25]

	323.15	758.61	758.9[25]	1052.0	1052.20
Benzene	298.15	873.48	873.61[27]	1296.0	1299.3[26]
	303.15	867.00	867.4[25]	1281.0	1280[27]
	308.15	862.75	862.9[20]	1256.0	1258.23[28]
	313.15	844.9	845.31[25]	1250.5	1251[29]
	318.15	851.95	852.23[19]	1212.0	1212.58[17]
	323.15	818.00	819.80[16]	1189.0	1189.91[17]

Standard Uncertainties is u(T) = ±0.01K, u(ρ)= ±0.15 kg.m^{-3}, u(U) = ±1.0m. s^{-1}

Table-3: Densities, ρ of Ternary System (Benzene +BP/ PP+ IPA) at Several Temperatures and at p = 0.1 MPa.

[a]m(mol.kg^{-1})	ρx10^{-3}/(kg.m^{-3})					
	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
0.00000	792.563	787.2	782.367	777.249	772.946	767.948
0.11325	796.441	790.963	786.108	780.773	776.047	770.928
0.223212	801.897	796.207	791.442	786.606	781.688	775.685
0.330032	809.897	804.042	798.481	793.631	788.692	782.144
0.433837	817.231	811.324	805.957	800.315	795.195	788.998
0.534756	825.182	819.15	814.048	807.882	802.649	796.343
0.632911	834.972	829.298	823.57	818.289	812.145	805.54
0.728406	845.053	839.272	833.443	827.069	821.247	815.172
0.821352	853.984	847.64	842.266	835.842	829.38	823.861
0.911856	863.414	858.053	852.658	846.227	839.756	834.243
1.00000	873.798	868.454	863.087	857.694	852.289	846.853
	Benzene+(1/100) mol.kg^{-1} PP in IPA					
0.00000	789.497	785.188	780.804	776.338	771.783	767.13
0.112393	796.303	791.531	787.292	782.269	777.961	773.157
0.221733	803.685	799.024	794.485	789.565	786.566	781.58
0.328142	810.505	805.72	800.874	795.941	791.933	786.839
0.431737	818.006	812.915	808.157	802.832	798.032	792.854
0.532628	826.206	821.151	816.035	810.859	806.615	801.3
0.630920	834.407	829.726	824.502	819.416	815.375	809.966
0.726711	843.032	838.068	832.776	827.427	823.026	817.569
0.820095	851.664	846.343	840.988	835.586	830.137	824.632
0.911163	861.62	856.24	850.833	845.39	839.912	834.392
1.00000	873.798	868.454	863.087	857.694	852.289	846.853

[a]m states the molality's of Benzene in the Isopropanol solution of Butyl/Pentyl Paraben.Standard Uncertainties u is u_r(m) = 1%, u(T)= 0.01%, u(ρ) = 0.15 kg.m^{-3}

Table-4: Ultrasonic Velocities, U of Ternary System (Benzene +BP/ PP+ IPA) at Various Degrees and Atmospheric Pressure, p = 0.1 MPa.

[a]m(mol.kg^{-1})	U/ (m.s^{-1})					
	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
0.00000	1160.27	1142.38	1124.25	1105.82	1087.33	1068.79
0.11325	1160.67	1142.77	1124.92	1107.01	1089.01	1070.97
0.223212	1165.19	1147.07	1129.14	1108.99	1090.75	1072.55
0.330032	1172.85	1153.70	1134.74	1115.54	1096.30	1077.00
0.433837	1184.94	1166.21	1146.22	1125.24	1106.27	1085.30
0.534756	1198.51	1178.25	1157.73	1137.27	1116.89	1096.55
0.632911	1213.28	1193.27	1172.56	1149.70	1129.92	1107.23
0.728406	1229.13	1207.67	1186.59	1165.38	1145.32	1122.37
0.821352	1246.13	1224.48	1203.18	1181.80	1160.54	1138.39
0.911856	1268.69	1245.91	1221.47	1201.96	1178.58	1158.29
1.00000	1299.22	1276.30	1252.16	1230.17	1207.38	1182.78

	Benzene+(1/100) mol.kg^{-1} PP in IPA					
0.00000	1151.59	1135	1116.56	1098.78	1080.91	1062.95
0.112393	1161.53	1144.51	1125.18	1105.8	1088.35	1069.86
0.221733	1171.28	1153.25	1132.13	1112.98	1094.83	1076.61
0.328142	1179.75	1162.20	1142.01	1121.39	1103.75	1084.14
0.431737	1190.02	1170.07	1150.34	1130.43	1110.53	1090.62
0.532628	1200.33	1181.78	1161.46	1140.97	1120.59	1100.20
0.630920	1212.59	1194.79	1173.85	1152.97	1133.26	1111.62
0.726711	1227.06	1208.04	1186.87	1165.76	1144.84	1124.01
0.820095	1242.93	1223.61	1201.13	1179.78	1158.60	1138.53
0.911163	1266.77	1243.53	1221.73	1200.06	1176.56	1157.16
1.00000	1299.22	1276.30	1252.16	1230.17	1207.38	1182.78

[a]m states the molality's of Benzene in the Isopropanol solution of Butyl/Pentyl Paraben. Standard uncertainties u is $u_r(m) = 1\%$, $u(T) = 0.01\%$, $u(U) = 1.0$ m.s^{-1}.

Table-5: Viscosities, η of Ternary System (Benzene +BP/ PP+ IPA) at Various Temperatures and Atmospheric Pressure,p = 0.1 MPa.

[a]m(mol.kg^{-1})	η/ (mPa-s)					
	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
0.00000	1.891626	1.698588	1.555801	1.375429	1.2256066	1.110062
0.11325	1.706075	1.533519	1.393354	1.225574	1.0968206	0.987144
0.223212	1.379903	1.267635	1.182255	1.04434	0.9299828	0.861913
0.330032	1.233769	1.126559	0.996428	0.894431	0.8176049	0.755605
0.433837	1.110641	1.010211	0.863801	0.766502	0.6883388	0.623101
0.534756	0.97473	0.875681	0.781468	0.703591	0.6404396	0.582041
0.632911	0.874391	0.745699	0.697639	0.613822	0.5667591	0.543849
0.728406	0.778805	0.674862	0.63239	0.573267	0.5193937	0.491417
0.821352	0.690784	0.627527	0.573476	0.52688	0.4907838	0.463254
0.911856	0.644214	0.604117	0.560972	0.515332	0.4718239	0.453949
1.00000	0.603	0.562	0.537	0.506	0.4525093	0.436
	Benzene+(1/100) mol.kg^{-1} PP in IPA					
0.00000	1.691152	1.581526	1.384348	1.218861	1.090967	0.982512
0.112393	1.212969	1.109281	1.021978	0.919982	0.806921	0.747461
0.221733	1.072751	0.965078	0.888652	0.803253	0.741637	0.692667
0.328142	0.892721	0.808218	0.761502	0.703437	0.662736	0.618274
0.431737	0.845957	0.770489	0.741681	0.670041	0.596828	0.567322
0.532628	0.76456	0.687184	0.637649	0.578535	0.517986	0.498197
0.630920	0.72679	0.63879	0.605973	0.550585	0.49967	0.490065
0.726711	0.681855	0.620623	0.563581	0.522018	0.487268	0.460074
0.820095	0.635373	0.596093	0.554095	0.509404	0.466789	0.449259
0.911163	0.628361	0.572927	0.542334	0.507118	0.459949	0.444829
1.00000	0.603	0.562	0.537	0.506	0.4525	0.436

Theory

Using the measured data of Ultrasonic velocity (U), density (ρ), and viscosity (η), the following acoustic parameters have been calculated.

Isentropic Compressibility (β_{ad})

$$\beta_{ad} = \frac{1}{\rho U^2} \qquad N^{-1}m^2 \qquad \ldots\ldots\ldots\ldots\ldots \quad (1)$$

Acoustic Impedance (Z)

$$Z = U\rho \qquad Kgm^{-2}s^{-1} \qquad \ldots\ldots\ldots \quad (2)$$

Free Length (L_f)

Sanghamitra, and Jacobson calculated the free length of the liquid as[30-32]

$$L_f = k\beta_{ad}^{1/2} \quad m \quad \ldots\ldots\ldots(3)$$

Where k denotes Jacobson's constant, a temperature-dependent variable provided by the value

$$k = (93.875 + 0.345T)\, x\, 10^{-8}$$

Relaxation time(τ)

$$\tau = \frac{4\beta\eta}{3} \quad s \quad \ldots\ldots\ldots\ldots\ldots(4)$$

Relative association (Ra)

$$Ra = \left[\frac{\rho}{\rho_0}\right]\left[\frac{U}{U_0}\right]^{1/3} \quad \ldots\ldots\ldots(5)$$

Apparent molar volume (V_ϕ)

$$V_\Phi = \left(\frac{M}{\rho}\right) - \left\{\frac{(\rho - \rho_0)}{m\rho\rho_0}\right\} \quad \ldots\ldots\ldots(6)$$

Partial molar volume (V_ϕ^0)

$$V_\Phi = V_\Phi^0 + S_v m \quad \ldots\ldots\ldots(7)$$

Apparent Molar Isentropic Compression ($K_{\phi,S}$)

The molar apparent property of isentropic compression ($K_{\phi,s}$) of benzene with butyl/pentylparaben immersed in isopropanol has been investigated in the following way[16]:

$$K_{\phi,S} = \left(\frac{M\beta_s}{\rho}\right) - (\beta_s\rho_0 - \beta_{s,0}\rho)m\rho\rho_0 \quad \ldots\ldots\ldots(8)$$

Laplace–Newton equation explained isentropic compressibility as:

$$\beta_s = \frac{1}{U^2\rho}$$

Isentropic Partial Molar Compression($K_{\phi,S}^0$)

$$K_{\phi,s} = K_{\phi,s}^0 + S_k m \quad \ldots\ldots\ldots(9)$$

Where ρ is the density of the solution, ρ_0 is the density of the solvent; U is the acoustic velocity of the solution and U_0 is the acoustic velocity of the solvent, M is the molecular weight of the solute and m is the molality of the solute. S_v and S_k are the experimental slopes. V_ϕ^0 is the partial molar volume at infinite dilution. β_s is the isentropic compressibility of the solution and β_s^0 is the isentropic compressibility of the solvent respectively.Tables 8 and 9 show the $K_{\phi,s}^0$ and S_k values attained using the least square befitting approach.

RESULTS AND DISCUSSION

Table-3 shows the reduction of the density of the mixture with the increase in temperature for a given molality of benzene, and at a particular temperature, as we increase the molality of benzene in both systems, we see a gradual increase in the density of the mixture.Table-4 shows the reduction of Ultrasonic velocity with the mixture's temperature rise for a given benzene molality. At one particular temperature of the given mixture, we observe a gradual increase in Ultrasonic velocity with the rise in the molality of benzene in both the systems. Table-5 shows the reduction of viscosity of the mixture with the increase in temperature for a given molality of benzene, but at a particular temperature, the viscosity asymptotically

reduces with an increase in the molality of benzene in both systems.The decreaseof ultrasonic velocity, density, and viscosity values of the mixture with temperature indicates the rupturing of hetero- and homo-molecular clusters at higher temperatures. Acoustic impedance (Z) is a measure of the bond energy in a system. Figures-1 and 2 show an increase in the acoustic impedance values with an increase in the molality of benzene in both systemsat a given temperature. For a given molality of benzene, the impedance values decrease with an increase in temperature.

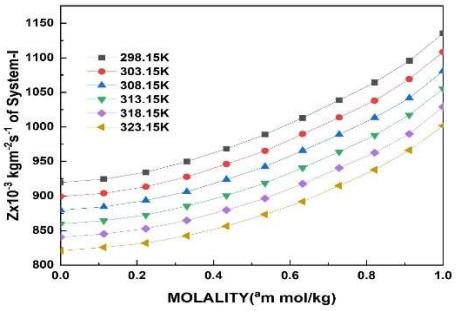


Fig.-1: Diversity of Acoustic Impedance of Benzene + 0.01m of Butyl Paraben in the Isopropanol solution

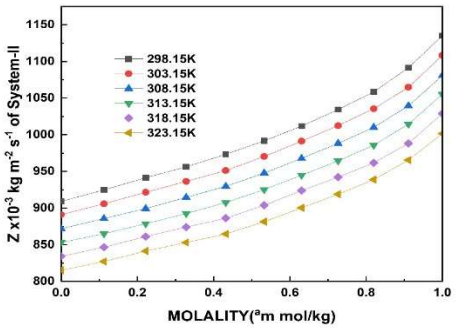


Fig.-2: Diversity of Acoustic Impedance of Benzene + 0.01m of Pentyl Paraben in the Isopropanol solution

Eyring and Kincaid reported that acoustic velocity could be usedto measure the molecular structures of substances.[33] As molecules get closer together, they move faster (and vice versa). Figures 3 and 4 show an increase in molecular free length with an increase in temperature, for a given molality of benzene in both systems.

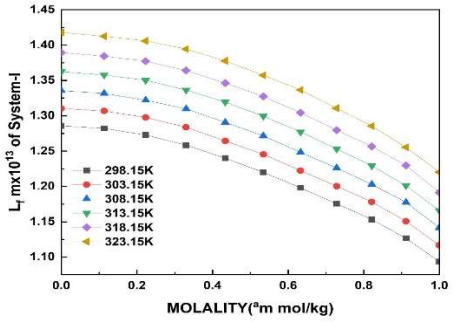


Fig.-3: Diversity of Free length of Benzene + 0.01m of Butyl Paraben in the Isopropanol Solution

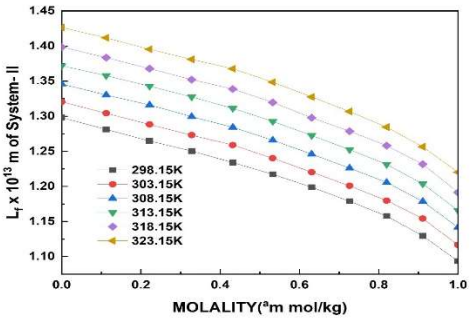


Fig.-4: Diversity of Free length of Benzene + 0.01m of Pentyl Paraben in the Isopropanol Solution

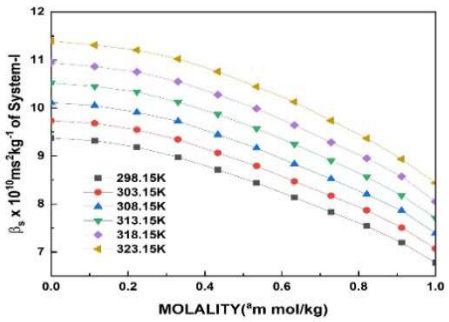


Fig.-5: Variation of Adiabatic Compressibility of Benzene + 0.01m of Butyl Paraben in the Isopropanol Solution

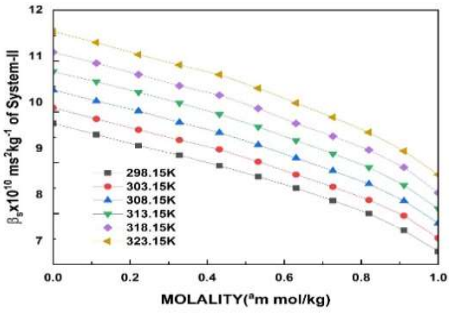


Fig.-6: Variation of Adiabatic Compressibility of Benzene + 0.01m of Pentyl Paraben in the Isopropanol Solution

In an ideal mixture in which the components are non-interacting, the variation of density, viscosity, and acoustic velocity of the mixture with the concentration is expected to be linear. The addition of another

molecule or a liquid changes the values, depending upon the nature of the components. The adiabatic compressibility reflects the degree of deviation from ideality and indicates the existence of interactions among the components. Figures-5 and 6 indicate the decrease in adiabatic compressibility with an increase in the molality of benzene in both systems. It is also perceived that for a given molality of benzene, adiabatic compressibility values increase with the increase in temperature, indicating the existence of intermolecular interactions among the components.

Figures-7 and 8 show the decreas of the relaxation time of the mixture with the increasein temperature for a given benzene molality, but at a particular temperature, the relaxation time of the mixture decreases with an increase in themolality of benzene in both the systems indicating the existence of a molecular association between the solute and solvent.

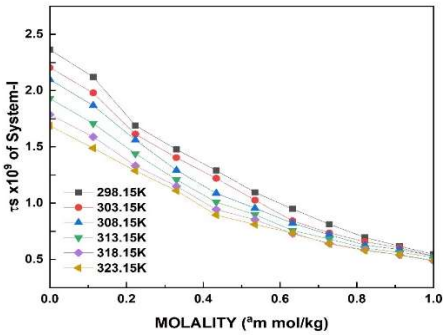


Fig.-7: Diversity of Relaxation time of Benzene + 0.01m of Butyl Paraben in the Isopropanol Solution

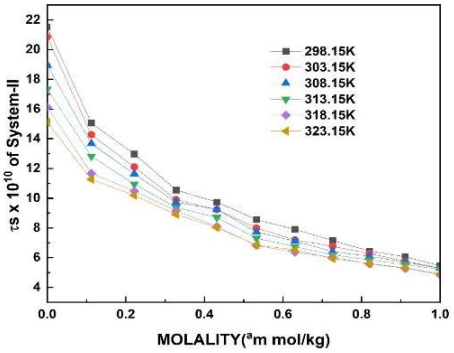


Fig.-8: Diversity of Relaxation time of Benzene + 0.01m of Pentyl Paraben in the Isopropanol Solution

The V_ϕ values are incorporated in Table 6 and shown in Fig.-9 and 10.The predicted error for V_ϕ is 0.07 x $10^{-6}m^3$/mol.

Table-6: Apparent Molar Volume, V_ϕ of Ternary System (Benzene +BP/ PP+ IPA) at Various Degrees with Different Atmospheric Pressure, p = 0.1 MPa.

^{a}m(mol.kg^{-1})	V_ϕ x10^{-6}/(m^3.mol^{-1})					
	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
0.11325	98.019558	98.69967	99.30923	99.99060551	100.6055	101.275
0.223212	97.340729	98.03825	98.62761	99.23146589	99.85996	100.6399
0.330032	96.362539	97.06604	97.74508	98.34058503	98.95913	99.79491
0.433837	95.491064	96.18767	96.82961	97.51359831	98.14404	98.9189
0.534756	94.564638	95.26229	95.85955	96.59368439	97.22573	97.99905
0.632911	93.446794	94.08621	94.74215	95.3533207	96.07874	96.87
0.728406	92.324479	92.96055	93.61213	94.33554225	95.007	95.7167
0.821352	91.354929	92.03969	92.62725	93.34086856	94.07161	94.70209
0.911856	90.352906	90.91664	91.4921	92.18882764	92.90223	93.51631
1.00000	89.27407	89.82258	90.38119	90.94910347	91.52688	92.11428
	Benzene+(1/100) mol.kg^{-1} PP in IPA					
0.112393	97.994481	98.59137	99.1196	99.76367	100.3119	100.9369
0.221733	97.088974	97.6573	98.2158	98.83057	99.19526	99.82989
0.328142	96.271965	96.84544	97.43314	98.03874	98.53161	99.17112
0.431737	95.386049	95.98569	96.55161	97.19462	97.77957	98.41955
0.532628	94.434927	95.01786	95.61512	96.22698	96.73173	97.37473
0.630920	93.503337	94.03116	94.62839	95.21666	95.68662	96.32688
0.726711	92.542976	93.09188	93.68474	94.29163	94.79486	95.42867
0.820095	91.601833	92.17897	92.76709	93.36794	93.98184	94.6102
0.911163	90.538451	91.10844	91.68846	92.27976	92.88249	93.49775
1.00000	89.26917	89.81933	90.37863	90.94759	91.52493	92.11289

[a]m states the molality's of Benzene in the Isopropanol solution of Butyl/Pentyl Paraben. Standard uncertainties u is $u_r(m) = 1\%$, $u(T) = 0.01\%$, $u(U) = 1.0\ m.s^{-1}$, $u(V_\phi) = \pm 0.07 \times 10^{-6} m^3.mol^{-1}$.

Table-7 indexes the value of V_ϕ^0 and S_v along with their typical inaccuracies reckoned by applying the least square fitting method for apparent molar volume.

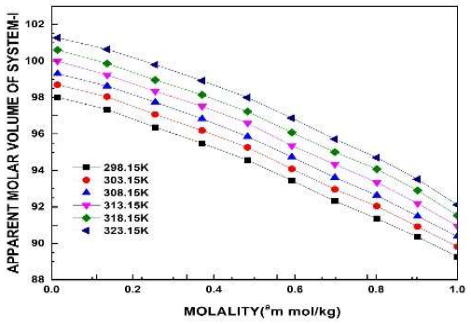


Fig.-9: Benzene Apparent Molar Volume Diversity + 0.01m of Butyl Paraben in the Isopropanol Solution

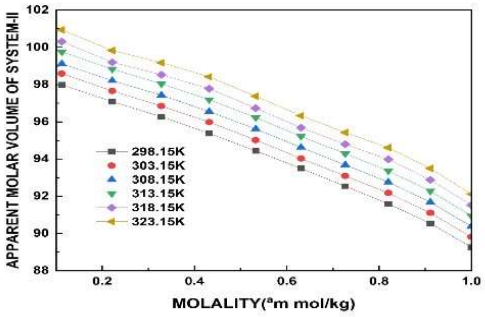


Fig.-10: Benzene Apparent Molar Volume Diversity + 0.01m of Pentyl Paraben in the Isopropanol Solution

Table-7: Partial Molar Volume and Experimental Slopes of Benzene with Butyl/Pentyl Paraben in Isopropanol

[a]m(mol.kg^{-1})	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
V_ϕx10^{-6}/ (m^3.mol^{-1})	89.12543912	89.77688789	90.35618018	90.95123274	91.52080825	92.24229757
S_v	-7.30383	-7.4117	-7.45113	-7.43959	-7.39109	-7.52549
	Benzene+(1/100) mol.kg^{-1} PP in IPA					
V_ϕx10^{-6}/ (m^3.mol^{-1})	97.51984	98.10345	98.66624	99.29693	99.77123	100.4122
S_v	-7.03748	-7.06457	-7.0401	-7.08461	-6.98459	-7.00802

The $K_{\phi,S}$ statistics are included in Table-8 and are shown in Figs.-11 and 12.

Table-8: ($K_{\phi,S}$) of a Ternary System (Benzene +BP/ PP+ IPA) at Different Temperatures and Atmospheric Pressure, p = 0.1 MPa.

[a]m(mol.kg^{-1})	$K_{\phi,s}$ x10^{-5}/(m^3.mol^{-1} GPa^{-1})					
	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
0.00000	9.236787	9.658625	10.09624	10.57347	11.05823	11.59467
0.11325	9.140807	9.560468	9.988528	10.45578	10.93627	11.45848
0.223212	8.947304	9.36462	9.781112	10.26481	10.7449	11.28529
0.330032	8.657904	9.078424	9.515432	9.966477	10.44895	11.00873
0.433837	8.331716	8.727096	9.154735	9.633535	10.09542	10.65451
0.534756	7.989562	8.38866	8.797729	9.256587	9.722817	10.24698
0.632911	7.616752	7.982228	8.381764	8.830922	9.281336	9.824269
0.728406	7.248428	7.611709	7.99481	8.416255	8.837252	9.33944
0.821352	6.908591	7.261981	7.617206	8.016563	8.442357	8.891501
0.911856	6.524555	6.849516	7.216016	7.565371	7.98928	8.380876
1.00000	6.080151	6.377559	6.707613	7.036595	7.396864	7.806056
	Benzene+(1/100) mol.kg^{-1} PP in IPA					
0.000000	9.449523	9.834847	10.27681	10.73454	11.22373	11.74743
0.112393	9.130566	9.517867	9.954022	10.43873	10.89584	11.41626
0.221733	8.815546	9.199699	9.655465	10.11543	10.5335	11.03244
0.328142	8.544655	8.909485	9.339211	9.806129	10.2248	10.73561
0.431737	8.245778	8.63632	9.040527	9.486214	9.947696	10.44922
0.532628	7.946351	8.298811	8.699598	9.130075	9.564894	10.05454

0.630920	7.636347	7.9544	8.345181	8.757565	9.154778	9.641779
0.726711	7.308257	7.629456	8.004443	8.404141	8.807226	9.258625
0.820095	6.982472	7.295124	7.666901	8.04944	8.455821	8.873424
0.911163	6.572229	6.905272	7.244514	7.604839	8.014352	8.394856
1.00000	6.081297	6.378507	6.708584	7.037461	7.397719	7.806838

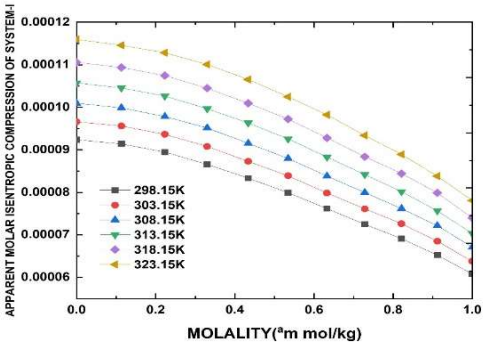


Fig.-11: Variation of Apparent Molar Isentropic Compression of Benzene + 0.01m of Butyl Paraben in the Isopropanol Solution

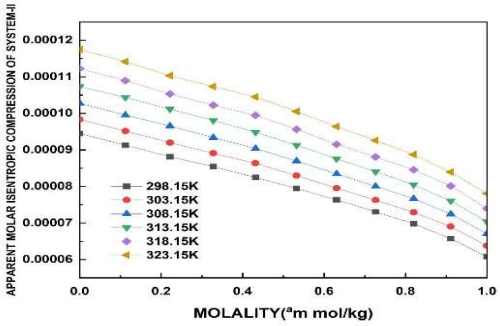


Fig.-12: Variation of Apparent Molar Isentropic Compression of Benzene + 0.01m of Pentyl Paraben in the Isopropanol Solution

Table -9 shows $K_{\phi,s}^0$ and S_k values obtained using the least square befitting approach

Benzene possesses the chemical formula C_6H_6. In Benzene, every Carbon atom is attached to two other Carbon atoms and one Hydrogen atom. The fourth bond electron pair from every Carbon atom is delocalized, creating a delocalized electron cloud over and beneath the plane. Benzene is a hexagonal ring having 120-degree bond angles between carbon atoms. In Benzene, all bond lengths are the same due to the subsistence of the delocalized electron system. Benzene is dynamically stable, and its extra stability is acknowledged as its delocalization energy. Owing to its amplified stability, Benzene does not readily engage in addition reactions; rather, it involves addition reactions in situations where a hydrogen atom is replaced by another atom or group. Alcohol molecules, because of their hydroxyl properties and the presence of hydrogen bonds and water molecules when absorbed, Isopropanol is polar. Because hydroxyl groups cause electrons to devote more time near the material's electronegative oxygen atom, any chemical containing hydroxyl groups is polar. It can dissolve various polar and non-polar materials because of their polarity. Isopropyl alcohol possesses hydroxyl groups, which are generated when an oxygen atom attaches to a hydrogen atom in covalent bonding. Water molecules, which are also polar molecules, can form hydrogen bonds with these groups. The hydroxyl group structure causes electrons to accumulate near the oxygen atom, attracting more of these particles than the other atoms. This makes the compound more polar. Butylparaben is made by esterifying 4-hydroxybenzoic acid with 1-butanol in sulfuric acid. Butyl Paraben is a popular bacteria killer and fungicide, often used in cosmetics. Short-chained parabens such as methyl and ethyl are more estrogenic than long-chained parabens such as butyl and pentyl. The distinction is related to the lipophilicity of the former. When compared to methyl, ethyl, and propyl parabens, butylparaben demonstrated the greatest competitive binding with rat estrogen receptors.

Table-9: $K_{\phi,s}^0$, S_k of Benzene with Butyl/Pentyl Parabens in Isopropanol at a Variety of Temperatures

^{a}m(mol.kg^{-1})	25^{0}C	30^{0}C	35^{0}C	40^{0}C	45^{0}C	50^{0}C
	Benzene+(1/100) mol.kg^{-1} BP in IPA					
$K_{\phi,s}^0$x10^{-6}/ (m^3.mol^{-1})	95.7256	100.15	104.658	109.712	114.736	120.491
S_k x 10^{-5}	-3.249	-3.36922	-3.46836	-3.6071	-3.7099	-3.8484
	Benzene+(1/100) mol.kg^{-1} PP in IPA					
$K_{\phi,s}^0$x10^{-6}/ (m^3.mol^{-1})	95.6335	99.6169	104.215	109.144	113.834	119.259
S_kx 10^{-5}	-3.23398	-3.32756	-3.447	-3.58574	-3.67367	-3.80963

CONCLUSION

The experimental results provide the existence of molecular interactions between the solute and solvent.

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CONFLICT OF INTERESTS

The authors declare that there is no conflict of interest.

AUTHOR CONTRIBUTIONS

All the authors contributed significantly to this manuscript, participated in reviewing/editing and approved the final draft for publication. The research profile of the authors can be verified from their ORCID ids, given below:

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REFERENCES

1. J. Panduranga Rao, K. Jyothi, K. Nanda Gopal and G. Srinivas, *Rasayan Journal of Chemistry,* **10(2)**, 488 (2017), http://dx.doi.org/10.7324/RJC.2017.1021610
2. C. Senthamil Selvi, C. Thillaiyadi Valliammai, P. Malliga, C. Thenmozhi and V. Kannappan, *Rasayan Journal of Chemistry,* **10(1)**, 271(2017).
3. S. Jagan Raj, V. Subha and S. Bangaru Sudarsan Alwar, *Rasayan Journal of Chemistry,***14(4)**, 2622 (2021), http://dx.doi.org/10.31788/RJC.2021.1445767
4. A.Saini, A. Prabhune, A. P. Mishra, and R. Dey, *Journal of Molecular Liquids*, **323**, 114593(2021), https://doi.org/10.1016/j.molliq.2020.114593
5. D. Chinnarao, Ch. V Padmarao, K. Raja, M.Srilatha and B. Venkateswara Rao, *International Journal of Engineering Research and Technology*, **9(4)**, 94(2020), http://dx.doi.org/10.17577/IJERTV9IS040093
6. Nabaparna Chakraborty, Monika Rani and K.C. Juglan, *Plant Archives*, **20(2)**, 2825(2020).
7. A. Suryanarayana Reddy and M. Satyanarayana, *European Journal of. Biomedical and Pharmaceutical Sciences,* **5(2)**, 1194(2018).
8. Suneel Kumar, Chandra Pal, and Dhirendra Kumar Sharma, *International Journal of Current Science Research and Review,***5(7)**, 2504, (2022), https://doi.org/10.47191/ijcsrr/V5-i7-34
9. Aditi Prabhune, Amrita Natekar, and Ranjan Dey, *Frontiers in Chemistry*, **10**, 868836(2022), https://doi.org/10.3389/fchem.2022.868836
10. J.V. Srinivasu, K. Narendra, Ch. Kavitha and R. Dey, *Physical Chemistry Research*, **9(4)**, 579(2021), https://doi.org/10.22036/PCR.2021.270810.1880
11. K. Srisanthi, Sk. Suriya Shihab, and S. Sreehari Sastry, *PONTE,* **76(5),** 51(2020), https://doi.org/10.21506/j.ponte.2020.5.4
12. K. Srisanthi, Sk. Suriya Shihab, T.Vishwam and S. Sreehari Sastry, *PONTE*, **76(9)**, 185 (2020), https://doi.org/10.21506/j.ponte.2020.9.14
13. S. V. Kumara Sastry, Shaik. Babu, Ha. Sie Tiong and S. Sreehari Sastry, *Journal of Chemical Pharmaceutical Research*, **4(4),** 2122 (2012).

14. S.V. Kumara Sastry, Shaik Babu, Ha Sie Tiong and S Sreehari Sastry, *Research Journal of Pharmacetical, Biological and Chemical Sciences,* **3(2),** 500(2012).
15. Ashima Thakur, Harsimran Kaur, Nabaparna, K.C. Juglan and Harsh Kumar, *RAFAS, Journal of Physics: Conference Series*, **1531**, 012017 (2020), https://doi.org/10.1088/1742-6596/1531/1/012017
16. Ashima and K.C. Juglan, *Plant Archives,* **20(2)**, 2801(2020). Ashima, K.C. Juglan and Harsh Kumar, *Results in Chemistry,* **2**, 100049(2020), https://doi.org/10.1016/j.rechem.2020.100049
17. Shaik Babu, S.V.Kumara Sastry, Ha Sie Tiong and S. Sreehari Sastry, *E-Journal of Chemistry*, **9(4)**, 2309 (2012), https://doi.org/10.1155/2012/147940
18. J.Lincho, R.C.Martins and J.Gomes, Paraben Compounds—Part I: An Overview of Their Characteristics, Detection, and Impacts. *Applied Sciences,* **11,** 2307(2021), https://doi.org/10.3390/app11052307
19. Priya Cherian, Jinqiu Zhu, Wilma F. Bergfeld, Donald V. Belsito, Ronald A. Hill, Curtis D. Klaassen, Daniel C. Liebler, James G. Marks, Jr., Ronald C. Shank, Thomas J. Slaga, Paul W. Snyder, and Bart Heldreth, *International Journal of Toxicology*, **39(1)**, 5S (2020), https://doi.org/10.1177/1091581820925001
20. Hadir M. Maher, Nourah Z. Alzoman, Munira Abdulaziz Almeshal, Hawazin Abdullah Alotaibi, Njoud Naif Alotaibi, and Hessa Al-Showiman, *Arabian Journal of Chemistry*, **13**, 2897(2020), https://doi.org/10.1016/j.arabjc.2018.07.019
21. Kabita Banik, Simanchala Rath and B.K Gupta, *Research & Reviews*: *Journal of Pharmaceutical Analysis*, **8(1)**, 11(2019).
22. Sana Rajgoli and Ashish Patil, *Internation.Research Journal of Engineering and Technolonogy*, **6(6),** 1310 (2019).
23. Akanksha Saini, Hrishikesh Joshi, Kratrika Kukreja and Ranjan Dey, *Journal of Molecular Liquids*, **10**, 1016(2016), https://doi.org/10.1016/j.molliq.2016.08.046
24. R.Velavan and P.Myvizhi, *International journal of Innovative Research in Science, Engineering and Technology,* **4(8)**, 7982(2015), https://doi.org/10.15680/IJIRSET.2015.0408279
25. Shaik.Babu, *E-Journal of Chemistry*, **8(S1)**, S330(2014), https://doi.org/10.1155/2011/202108
26. S. S. J. Srinivas, B. Tulasi Koteswari Bai, K. Babu Rao, K. Narendra and M. Sarath Babu, *International Letters of Chemistry, Physic and . Astronomy.*, **10(2)**, 151(2013), https://doi.org/10.18052/www.scipress.com/ILCPA.15.151
27. K. Saravanakumar, R. Baskaran and T.R. Kubendran, *Journal of Applied Sciences*, **10**, 1616 (2010), https://doi.org/10.3923/jas.2010.1616.1621
28. M. Srilatha, D. Chinnarao and Ch.V. Padmarao, *International Journal of Engineering Sciences & Research Technology*, **4(4)**, 584(2015).
29. Sanghamitra Pradhan, Manaswini Chhotaray and Sujata Mishra, *Materials International*, **2(2)**, 83 (2020), https://doi.org/10.33263/Materials22.083096
30. B.Jacobson, *Journal of Chemical Physics*, **20**, 927(1952)
31. B.Jacobson, *Acta Chemica Scandinavica*, **6**, 1485(1952).
32. H.Eyring and J.F.Kincaid, *Journal of Chemical Physics*, **6**, 620(1938). https://doi.org/10.1063/1.1750134

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