



International Journal for Innovative Engineering and Management Research

A Peer Reviewed Open Access International Journal

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IJIEMR Transactions, online available on 18th Feb 2022. Link

[:http://www.ijiemr.org/downloads.php?vol=Volume-12&issue=Issue 02](http://www.ijiemr.org/downloads.php?vol=Volume-12&issue=Issue 02)

DOI: 10.48047/IJIEMR/V12/ISSUE 02/71

Title Molecular Interaction and Thermodynamic Parameters in Certain Binary Liquid Mixtures with Variation of Temperature

Volume 12, ISSUE 02, Pages: 444-454

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Molecular Interaction and Thermodynamic Parameters in Certain Binary Liquid Mixtures with Variation of Temperature

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Abstract

The study of molecular interactions and the variations in these interactions due to structural changes has been carried out by numerous experimental techniques such as Infrared, Nuclear Magnetic Resonance and Raman Spectra and Dielectric property measurement. The three binary mixtures chosen for the investigation of molecular interactions are 1,2 Dichloroethane as a basic solvent which was mixed with cresols such as o-cresol, m-cresol and p-cresol. Ultrasonic sound velocity (u), density (ρ) and viscosity (η) were measured experimentally at four different temperatures namely 303K, 308K, 313K, 318K and at different compositions of 1,2-dichloroethane. The physical properties such as molar volume, adiabatic compressibility, mean free length, acoustic impedance, Rao's constant and free volume are calculated using these experimental values. The results obtained are utilised to analyse the interactions between the component molecules.

Key Words: Binary Mixtures, adiabatic compressibility, impedance, density, viscosity

Introduction

Introduction

The study of molecular interactions and the variations in these interactions due to structural changes has been carried out by numerous experimental techniques such as Infrared [1], Nuclear Magnetic Resonance [2] and Raman Spectra [3] and Dielectric property measurement [4]. The thorough understanding of the nature of intermolecular method. The successful use of acoustical methods to the physicochemical investigation of solutions has become possible after the development of adequate theoretical approaches and methods for precise ultrasonic velocity measurements. Lagemann and Dunbar [5] pointed out the sound velocity approach for the qualitative estimation of interaction in liquids. A parallel measurement of sound velocity and density of solution agree one to obtain information about their volume, elastic properties and changes in their properties. Composite formation in liquid mixtures has been extensively studied by ultrasonic methods by many workers. The formation of hydrogen bond in liquid mixtures and its effect on physical

properties of the mixtures have received much attention.

Experimental Details

By using jobs method of continuous variation, we have to prepare the mixture of required portion with the help of two separate burettes. The mixed proportions of the liquids are stored in the conical flasks and kept aside for nearly 24 hours. They are allowed to attain the thermal equilibrium.

The author has used antonpaar to measure the velocities and viscosity of the liquid and liquid mixtures. Comparing the relative merits of various techniques, the antonpaar viscometer is a simple and direct device to determine the ultrasonic velocity in pure liquids and liquid mixtures with high degree of accuracy. It is known for its easy operation and reliability

- Pulse excitation method (PEM): To determine the density and sound velocity using Antonpaar. The U-

shaped glass tube is made to oscillate to its stable state and gets excited. After the excitations the oscillations fades out freely. This sequence of excitation and fade out repeats continuously creating the pulsing oscillation pattern

- Rolling ball principle: To determine the viscosity of the liquid and liquid mixtures using micro capillary tube in which the gold coated ball is inserted for free flow of liquid within the tube.

Specification of Sound Velocity & Density Meter (DSA 5000 M):

Density range is
: 0 - 3 gm./cm³
Sound Velocity
: 1000 m/s to 2000 m/s
Measuring range of temperature
: 0-100°C
Pressure range
: 0-8 bar
Measuring time per sample
: 1 to 4 min
Sample volume
: approx. 3.5 ml

Before starting measurement with the instrument, make it sure of primary connections and settings as given in the manual. The measuring cell and syringe must be clean and dry. Then prepare the instrument for measurement, following the instructions on the screen. Following the instruction on the touch screen make the instrument necessary measurements. After measuring the process is completed we will get the display message 'Finish' on the screen and shows "Master Condition" output is "Valid".

After recording data measuring cells must be cleaned as directed in the manual and make them dry for the next measurement. We have taken the data of density, kinetic viscosity and the speed of sound parameters of pure, binary and ternary mixtures of liquid of study.

From the measured values of ultrasonic velocity (U), density (ρ) and viscosity (η). The Adiabatic Compressibility (β_{ad}), Internal Molecular Free Length (L_f), Acoustical Impedance (Z), Molar Volume (V_m), Rao's Constant (R), Wada's constant (W), Viscosity (η), internal pressure (π)

and free volume(V_f) were calculated by using the following standard relations.

Theoretical Parameters:

Number Of Gram Molecules of The Two Components:

If "v₁" of a liquid of density(ρ₁) and molecular weight(M₁) is mixed with "v₂" of liquid of density(ρ₂) and molecular weight (M₂) then the number of gram molecules of the first liquid(N₁) present in this mixture will be

$$N_1 = \frac{\rho_1 v_1}{M_1}$$

and for the second liquid it will be

$$N_2 = \frac{\rho_2 v_2}{M_2}$$

MOLE FRACTION OF THE TWO LIQUIDS (X₁, X₂):

The mole fraction of first liquid is given by

$$X_1 = \frac{N_1}{N_1 + N_2}$$

Mole fraction of second liquid is given by

$$X_2 = \frac{N_2}{N_1 + N_2}$$

Adiabatic Compressibility (β_{ad}):

$$\beta_{ad} = \frac{1}{\rho u^2} N^{-1} M^2$$

INTERMOLECULAR FREE LENGTH (L_f):

$$L_f = K \beta_{ad}^{\frac{1}{2}}$$

Where "K" is the temperature dependent constant known as Jacobson Constant. The value of "K" calculated for working temperatures of the experiment are given as

Temperature (K)	303.15	308.15	313.15	318.15
Value of K	627	631.5	636	640.5

Molar Volume (V):

$$V = \frac{M}{\rho} \text{ m}^3 \text{ mol}^{-1}$$

Impedance (Z):

The acoustic impedance (Z) of a material is defined as the product of its density (ρ) and acoustic velocity (u).

$$Z = u \rho \text{ Kgm}^{-2} \text{ s}^{-1}$$

Free Volume:

$$V_f = \left[\frac{\bar{M} \times u}{K\eta} \right]^{\frac{3}{2}}$$

Where “K” is constant and its value is 4.28 X 10⁹ for all liquids.

Rao’s Constant or Molar Sound Velocity(R):

Rao’s constant is calculated by using the formula

$$R = V_m u^{\frac{1}{3}}$$

Wada’s Constant (W):

Wada derived a relation between adiabatic compressibility (β_{ad}) and molar volume (V) of liquids. Wada’s constant of the solution is calculated by using the formula

$$W = V (\beta_{ad})^{-1/7} \quad 2.3.5.8.$$

Internal pressure
 $(\pi): \pi = b R T \left[\frac{K\eta}{u} \right]^{1/2} \left[\frac{\rho^{2/3}}{\bar{M}^{7/6}} \right] \text{ Nm}^{-1}$

Where ‘b’ is the packing factor (b = 2), “k” is a constant, and its value is 4.28 X 10⁹ for all liquids, “R” is Universal Gas Constant and “T” is absolute temperature

Enthalpy (H):

Enthalpy is determined by using the relation

$$H = \pi_i V_m \quad \text{Jmol}^{-1}$$

Where π_i is the internal pressure and V_m is the molar volume of the liquid solution.

Gibbs Free Energy for Activation Flow(ΔG)

The relaxation time is related to the activation free energy for a given transition. The variation of relaxation time with temperature can be expressed in the form of Eyring salt process theory and the equation is given as

$$\Delta G = RT \ln[\eta V_m]$$

Where “R” is universal Gas constant 8.31432 X 10⁷ JK⁻¹, and “T” is Absolute Temperature

Table 1 (a)

Binary Liquid Mixture – I: 1,2-Dichloroethane +M- Cresol at Temperature 303 K, 308 K, 313K 318 K and Density, Ultrasonic Velocity, Viscosity and some related acoustic parameters

Molefraction of 1,2-DCE	Density ρ Kgm ⁻³	Velocity U ms ⁻¹	Viscosity $\eta \times 10^{-3}$ Ns/m ²	$\beta \times 10^{-10}$ kg ⁻¹ m s ²	$V_m \times 10^{-5}$ m ³ /mol ⁻¹	$R \times 10^{-3}$ m ^{10/3} s ^{-1/3} mol ⁻¹	$W \times 10^{-6}$ m ³ .mol ⁻¹ (N/m ²) ^{1/7}	$L_f \times 10^{-11}$ m	$V_f \times 10^{-7}$ m ³ /mol ⁻¹
303 K									
0.0000	1028.24	1467.80	9.378	4.5141	104.8712	5.5477	8.4797	4.4086	0.0806
0.2081	1062.84	1396.51	7.423	4.8244	99.6845	5.1853	7.9823	4.5576	0.1405
0.3965	1096.18	1335.60	5.712	5.1140	95.1412	4.8727	7.5502	4.6924	0.2261
0.5679	1131.24	1284.84	4.225	5.3542	90.9804	4.5909	7.1588	4.8016	0.3440
0.7244	1163.93	1241.63	2.947	5.5729	87.1895	4.3497	6.8215	4.8984	0.5247
0.8679	1199.83	1207.61	1.785	5.7151	83.4815	4.1263	6.5079	4.9605	0.7474
1.0000	1236.67	1175.05	0.830	5.8564	80.0132	3.9190	6.2158	5.0215	0.9912
308 K									
0.0000	1022.10	1454.20	8.443	4.6265	105.4725	5.5637	8.5007	4.5062	0.1506
0.2081	1057.15	1380.54	6.488	4.9632	100.2871	5.1933	7.9928	4.6673	0.2317
0.3965	1091.19	1319.80	4.799	5.2663	95.6785	4.8748	7.5530	4.8077	0.3376
0.5679	1126.03	1267.94	3.421	5.5239	91.4010	4.5918	7.1600	4.9239	0.4925
0.7244	1157.85	1224.24	2.347	5.7625	87.6470	4.3520	6.8246	5.0291	0.7052
0.8679	1193.52	1189.16	1.425	5.9250	83.9227	4.1269	6.5087	5.0995	0.9512
1.0000	1229.51	1157.24	0.772	6.0732	80.6712	3.9218	6.2196	5.1629	1.2032

313K

318 K

0.0000	1014.12	1420.92	6.582	4.8839	106.6343	5.5644	8.5016	4.7182	0.3136
0.2081	1048.16	1348.47	4.627	5.2467	101.3520	5.1973	7.9981	4.8903	0.4232
0.3965	1081.18	1286.46	3.158	5.5886	96.6578	4.8794	7.5592	5.0472	0.5856
0.5679	1114.89	1232.74	1.984	5.9023	92.3230	4.5948	7.1641	5.1869	0.8054
0.7244	1145.90	1189.32	1.224	6.1695	88.5679	4.3555	6.8294	5.3030	1.0712
0.8679	1180.04	1152.97	0.723	6.3748	84.8852	4.1314	6.5149	5.3905	1.3556
1.0000	1214.70	1117.47	0.698	6.5926	81.4604	3.9236	6.2221	5.4818	1.6312

Table 1(b)

Binary Liquid Mixture – I: 1,2-Dichloroethane + M - Cresol at Temperature 303K, 308 K,313 K,318 K Some related acoustic parameter

Mole fraction of 1,2-DCE	$\pi_i \times 10^6$ N.m ⁻²	H x 10 ³ J.mol ⁻¹	$\Delta G \times 10^{-20}$ KJ.mol ⁻¹	Z x 10 ⁶ Kg.m ² s ⁻¹	$\tau \times 10^{-12}$ sec	α Np.m ⁻¹	$(\sigma/f^2) \times 10^{-14}$ Np.m ⁻¹ s ⁻²	$\chi_U \times 10^{-3}$
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303 K

0.0000	996.6741	119.6683	0.1145	1.5092	5.6444	312.2144	80.3199	0.0000
0.2081	921.3874	108.2744	0.1139	1.4842	4.7748	270.1826	56.5975	-0.0099
0.3965	847.3256	96.39013	0.1130	1.4640	3.8948	230.4385	39.2931	-0.0163
0.5679	772.6246	83.8507	0.1120	1.4507	3.0165	185.5251	26.7021	-0.0195
0.7244	689.2654	70.7305	0.1110	1.4386	2.1898	139.3653	17.2942	-0.0157
0.8679	597.3214	55.3755	0.1096	1.4285	1.3602	89.00541	9.9347	-0.0084
1.0000	474.5863	37.9732	0.1080	1.4197	0.6481	43.58461	4.3865	0.0000

308 K

0.0000	927.6542	106.5214	0.1158	1.4863	5.2082	287.6451	69.9003	0.0000
0.2081	845.6402	95.3244	0.1151	1.4594	4.2935	245.7566	47.5348	-0.0089
0.3965	768.2147	84.5122	0.1142	1.4394	3.3697	201.8579	31.6629	-0.0152
0.5679	692.2145	72.5402	0.1133	1.4257	2.5196	157.0308	20.6831	-0.0186
0.7244	619.3571	60.6782	0.1122	1.4126	1.8032	116.3962	13.1335	-0.0146
0.8679	547.5471	49.6712	0.1109	1.4027	1.1257	74.8070	7.5332	-0.0074
1.0000	467.0084	37.5844	0.1094	1.3944	0.6251	42.6867	3.8746	0.0000

313 K

0.0000	856.2410	93.3215	0.1170	1.4625	4.7521	262.2148	60.0154	0.0000
0.2081	766.5721	82.6215	0.1164	1.4376	3.7941	219.5344	39.4594	-0.0079
0.3965	683.2014	71.3214	0.1155	1.4150	2.8627	173.6459	25.0370	-0.0141
0.5679	611.1521	60.2145	0.1146	1.3993	2.0689	130.9009	15.5931	-0.0176
0.7244	547.2456	51.2445	0.1135	1.3867	1.4174	92.8095	9.5168	-0.0135
0.8679	498.1457	43.3141	0.1123	1.3754	0.9003	60.7504	5.5174	-0.0066
1.0000	472.2104	37.4102	0.1108	1.3654	0.6267	43.5760	3.5063	0.0000

318K

0.0000	788.3695	78.4245	0.1185	1.4409	4.2861	238.3623	50.4398	0.0000
0.2081	692.3154	68.1871	0.1178	1.4134	3.2368	189.6819	31.3234	-0.0069
0.3965	610.6702	58.4021	0.1170	1.3908	2.3532	144.5450	19.1477	-0.0129
0.5679	535.3820	49.0251	0.1160	1.3743	1.5613	100.0859	10.9145	-0.0166
0.7244	477.6712	41.0244	0.1149	1.3601	1.0068	66.8985	6.2150	-0.0124
0.8679	442.6841	36.4612	0.1137	1.3481	0.6145	42.1177	3.4443	-0.0058
1.0000	460.3523	37.2572	0.1122	1.3382	0.6135	43.3867	3.1163	0.0000

Table 2(a)

Binary Liquid Mixture – I: 1,2-Dichloroethene + O - Cresol at Temperature 303 and 308 K and Density, Ultrasonic Velocity, Viscosity and some related acoustic parameters

Molefraction of 1,2-DCE	Density ρ Kgm ⁻³	Velocity U ms ⁻¹	Viscosity $\eta \times 10^{-3}$ Ns/m ²	$\beta \times 10^{-10}$ kg ⁻¹ m s ²	$V_m \times 10^5$ m ³ /mol	$R \times 10^{-3}$ m ^{10/3} s ⁻¹ mol ¹	$W \times 10^{-5}$ m ³ .mol ⁻¹ (N/m ²) ^{1/7}	$L_f \times 10^{-11}$ m	$V_f \times 10^{-7}$ m ³ /mol
303 K									
0.0000	1036.93	1490.06	6.522	4.3435	104.2886	5.5288	8.4550	4.3245	0.0806
0.2067	1069.05	1418.03	5.123	4.6519	99.3776	5.1822	7.9783	4.4754	0.1405
0.3945	1101.95	1355.95	3.912	4.9357	94.8445	4.8725	7.5502	4.6099	0.2261
0.5658	1136.27	1298.92	2.914	5.2161	90.5944	4.5880	7.1552	4.7390	0.3440
0.7227	1169.10	1252.46	2.067	5.4528	86.8171	4.3437	6.8135	4.8453	0.5247
0.8669	1201.50	1213.13	1.345	5.6553	83.3729	4.1272	6.5092	4.9345	0.7474
1.0000	1236.67	1175.05	0.830	5.8564	80.0132	3.9190	6.2158	5.0215	0.9912
308 K									
0.0000	1032.56	1472.86	5.357	4.4265	104.7299	5.5308	8.4597	4.4265	0.1506
0.2067	1064.27	1400.89	4.158	4.5840	99.8262	5.1845	7.9854	4.5840	0.2317
0.3945	1096.72	1338.80	3.129	4.7252	95.34556	4.8752	7.5572	4.7252	0.3376
0.5658	1130.55	1281.24	2.310	4.8630	91.0559	4.5904	7.1603	4.8630	0.4925
0.7227	1163.06	1234.32	1.597	4.9768	87.2705	4.3452	6.8187	4.9768	0.7052
0.8669	1194.98	1194.28	1.085	5.0745	83.8292	4.1282	6.5125	5.0745	0.9512
1.0000	1229.51	1155.56	0.772	5.1704	80.6712	3.9199	6.2196	5.1704	1.2032
0.0000	1028.16	1455.61	4.462	4.5314	105.3875	5.5324	8.4597	4.5314	0.2265
0.2067	1059.46	1383.70	3.254	4.6959	100.3571	5.1868	7.9854	4.6959	0.3275
0.3945	1091.48	1321.47	2.314	4.8444	96.0125	4.8767	7.5572	4.8444	0.4529
0.5658	1124.81	1263.53	1.680	4.9909	91.6713	4.5925	7.1603	4.9909	0.6404
0.7227	1156.81	1216.32	1.185	5.11247	87.9742	4.3468	6.8187	5.1124	0.8806
0.8669	1188.21	1175.60	0.862	5.2192	84.3824	4.1303	6.5125	5.2192	1.1400
1.0000	1222.12	1136.51	0.742	5.3232	81.3458	3.9218	6.2196	5.3232	1.4162

Table 2 (b)

Binary Liquid Mixture – I: 1,2-Dichloroethene + O - Cresol at Temperature 303 K, 308 K, 313 K, 318 K Some related acoustic parameter

Mole fraction of 1,2-DCE	$\pi_i \times 10^6$ N.m ⁻²	H x 10 ³ J.mol ⁻¹	$\Delta G \times 10^{-20}$ KJ.mol ⁻¹	Z x 10 ⁶ Kg.m ² s ⁻¹	$\tau \times 10^{-12}$ sec	α Np.m ⁻¹	(α/f^2) $\times 10^{-14}$ Np.m ⁻¹ s ⁻²	$\gamma \times 10^{-3}$
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303 K

0.0000	996.6741	98.7729	0.1144	1.5450	3.7773	200.3171	58.9358	0.0000
0.2067	921.3874	89.0893	0.1137	1.5159	3.1775	177.0712	41.1335	-0.0099
0.3945	847.3256	79.0280	0.1129	1.4941	2.5744	150.0320	28.3080	-0.0163
0.5658	763.3337	69.1538	0.1121	1.4759	2.0266	123.2932	19.1133	-0.0195
0.7227	678.3326	58.8909	0.1109	1.4642	1.5027	94.8146	12.5055	-0.0157
0.8669	574.9586	47.9359	0.1096	1.4575	1.0141	66.0624	7.5995	-0.0084
1.0000	474.5863	37.9732	0.1080	1.4531	0.6481	43.5846	4.3865	0.0000

308 K

0.0000	919.6741	91.6506	0.1157	1.5208	3.1887	171.0802	46.5521	0.0000
0.2067	845.6402	82.2050	0.1150	1.4909	2.6543	149.7264	32.0454	-0.0089
0.3945	769.6716	72.4168	0.1142	1.4682	2.1223	125.2681	21.6903	-0.0152
0.5658	693.2301	63.1227	0.1133	1.4485	1.6595	102.3549	14.4680	-0.0186
0.7227	608.3917	53.0946	0.1122	1.4355	1.2016	76.9303	9.2004	-0.0146
0.8669	527.1225	44.1882	0.1109	1.4271	0.8487	56.1601	5.8173	-0.0074
1.0000	467.3477	37.6117	0.1094	1.4207	0.6269	42.8731	3.8578	0.0000

313 K

0.0000	850.7017	85.1671	0.1170	1.4965	2.7309	148.2558	37.2686	0.0000
0.2067	769.1025	74.8471	0.1164	1.4659	2.1388	122.1476	24.0572	-0.0079
0.3945	689.6741	65.1421	0.1155	1.4423	1.6187	96.7951	15.3521	-0.0141
0.5658	614.6679	56.0282	0.1146	1.4212	1.2473	78.0102	10.0406	-0.0176
0.7227	541.2203	46.9877	0.1135	1.4070	0.9232	59.9778	6.4974	-0.0135
0.8669	482.2801	40.4529	0.1123	1.3968	0.6998	47.0449	4.3832	-0.0066
1.0000	467.6144	37.4102	0.1108	1.3889	0.6267	43.5760	3.5063	0.0000

318K

0.0000	788.3695	78.4245	0.1185	1.472	2.1925	120.4552	27.9497	0.0000
0.2067	692.3154	68.1871	0.1178	1.441	1.5754	91.1027	16.4951	-0.0069
0.3945	610.6702	58.4021	0.1170	1.416	1.1318	68.5888	9.94797	-0.0129
0.5658	535.3820	49.0251	0.1160	1.394	0.8322	52.7916	6.17716	-0.0166
0.7227	477.6712	41.0244	0.1149	1.378	0.6332	41.7754	4.08325	-0.0124
0.8669	442.6841	36.4612	0.1137	1.366	0.5674	38.7568	3.24322	-0.0058
1.0000	460.3523	37.2572	0.1122	1.357	0.6135	43.3867	3.11637	0.0000

Table 3(a)

Binary Liquid Mixture – I: 1,2-Dichloroethene + P - Cresol at Temperature 303 and 308 K and Density, Ultrasonic Velocity, Viscosity and some related acoustic parameters

Molefraction of 1,2-DCE	Density ρ Kgm ⁻³	Velocity U ms ⁻¹	Viscosity $\eta \times 10^{-3}$ Ns/m ²	$\beta \times 10^{-10}$ kg ⁻¹ m s ²	$V_m \times 10^{-5}$ m ³ /mol	$R \times 10^{-3}$ m ^{10/3} s ⁻¹ mol ¹	$W \times 10^{-6}$ m ³ .mol ⁻¹ (N/m ²) ^{1/7}	$L_f \times 10^{-11}$ m	$V_f \times 10^{-7}$ m ³ /mol
303 K									
0.0000	1026.42	1473.56	7.275	4.48682	105.3467	5.5642	8.5013	4.3952	0.0957
0.2084	1062.63	1397.53	6.096	4.8183	99.9562	5.1871	7.9846	4.5547	0.1158
0.3969	1097.05	1335.36	4.912	5.1118	95.2424	4.8681	7.5440	4.6914	0.1592
0.5683	1132.80	1281.75	3.841	5.3732	90.8480	4.5805	7.1448	4.8099	0.2224
0.7247	1166.94	1239.62	2.827	5.5766	86.9596	4.3359	6.8028	4.9001	0.3090
0.8681	1201.68	1205.76	1.826	5.72386	83.3504	4.1177	6.4963	4.9643	0.4112
1.0000	1236.67	1175.05	0.830	5.8564	80.0132	3.9190	6.2158	5.0215	0.5302
308 K									
0.0000	1022.54	1457.81	6.289	4.6016	105.7464	5.5654	8.5028	4.4941	0.1352
0.2084	1058.22	1381.49	5.124	4.9514	100.3757	5.1889	7.9869	4.6617	0.1703
0.3969	1092.11	1322.56	4.097	5.2636	95.6773	4.8702	7.5469	4.8064	0.2282
0.5683	1127.27	1264.91	3.121	5.54437	91.2977	4.5829	7.1481	4.9329	0.3041
0.7247	1160.82	1222.36	2.328	5.76549	87.4212	4.3386	6.8065	5.0303	0.4045
0.8681	1195.16	1187.25	1.538	5.9359	83.8069	4.1190	6.4980	5.1042	0.5271
1.0000	1229.51	1155.56	0.772	6.0909	80.4792	3.9199	6.21707	5.1704	0.6582
313K									
0.0000	1018.64	1442.12	5.259	4.7203	106.1513	5.5666	8.5043	4.5951	0.1822
0.2084	1053.78	1365.5	4.181	5.0894	100.8018	5.1907	7.9894	4.7713	0.2306
0.3969	1087.14	1302.61	3.278	5.4210	96.1192	4.8724	7.5498	4.9243	0.3046
0.5683	1121.73	1248.1	2.475	5.7228	91.7530	4.5853	7.1513	5.0596	0.4022
0.7247	1154.70	1204.66	1.825	5.9676	87.8881	4.3406	6.8092	5.1666	0.5189
0.8681	1188.40	1169.25	1.222	6.1549	84.2856	4.1215	6.5014	5.2471	0.6456
1.0000	1222.12	1136.51	0.742	6.3348	80.9658	3.9218	6.2196	5.3232	0.7856
318 K									
0.0000	1014.72	1426.54	4.231	4.8426	106.5614	5.5679	8.5061	4.6983	0.2315
0.2084	1049.31	1349.64	3.301	5.23191	101.2344	5.1927	7.9921	4.8834	0.2945
0.3969	1082.14	1286.41	2.488	5.5841	96.5678	4.8748	7.5530	5.0451	0.3855
0.5683	1116.15	1231.31	1.865	5.9093	92.2163	4.5877	7.1546	5.1900	0.5071
0.7247	1148.64	1187.4	1.347	6.1747	88.3553	4.3427	6.8121	5.3052	0.6341
0.8681	1181.63	1151.21	0.944	6.3857	84.7705	4.1237	6.5045	5.3951	0.7752
1.0000	1214.70	1117.47	0.698	6.5926	81.4604	3.9236	6.2221	5.4818	0.9202

Table 3 (b)

Binary Liquid Mixture – I: 1,2-Dichloroethene + P - Cresol at Temperature 303 K, 308 K, 313 K, 318 K Some related acoustic parameter

Mole fraction of 1,2-DCE	$\pi_i \times 10^6$ N.m ⁻²	H x 10 ³ J.mol ⁻¹	$\Delta G \times 10^{-20}$ KJ.mol ⁻¹	Z x 10 ⁶ Kg.m ² s ⁻¹	$\tau \times 10^{-12}$ sec	α Np.m ⁻¹	(α/f^2) x10 ⁻¹⁴ Np.m ⁻¹ s ⁻²	$\chi U \times 10^{-3}$
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303 K

0.0000	1008.4782	106.3211	0.1149	1.5124	4.3522	233.3900	62.9331	0.0000
0.2084	981.3546	98.0925	0.1145	1.4850	3.9163	221.4407	46.5723	-0.0197
0.3969	938.3565	89.3714	0.1139	1.4649	3.3479	198.1138	33.7985	-0.0314
0.5683	876.8701	79.3104	0.1132	1.4519	2.7352	169.3844	23.6022	-0.0347
0.7247	796.6066	69.2726	0.1123	1.4465	2.1020	133.9952	16.5522	-0.0278
0.8681	672.1296	56.0223	0.1112	1.4489	1.3935	91.3287	10.1318	-0.0148
1.0000	474.5863	37.9732	0.1101	1.4531	0.6481	43.5846	4.3865	0.0000

308 K

0.0000	946.9960	100.1414	0.1164	1.4906	3.8586	209.1589	52.4786	0.0000
0.2084	917.2774	92.0723	0.1159	1.4619	3.3828	193.4941	37.6570	-0.0188
0.3969	873.8456	83.6072	0.1153	1.4404	2.8753	172.2671	27.0411	-0.0305
0.5683	809.6384	73.9181	0.1145	1.4258	2.3072	145.1395	18.7550	-0.0339
0.7247	737.3623	64.4611	0.1135	1.4189	1.7896	115.6907	13.0005	-0.0271
0.8681	629.5915	52.7641	0.1123	1.4189	1.2172	81.0180	8.1026	-0.0138
1.0000	467.3477	37.6117	0.1112	1.4207	0.6269	42.8731	3.8578	0.0000

313 K

0.0000	882.5565	93.6845	0.1178	1.4690	3.3099	181.3661	42.3200	0.0000
0.2084	844.5419	85.1313	0.1172	1.4389	2.8371	164.1848	29.5476	-0.0179
0.3969	796.8153	76.5892	0.1165	1.4161	2.3693	143.7335	20.7470	-0.0297
0.5683	735.1506	67.4523	0.1156	1.4000	1.8885	119.5684	14.2177	-0.0330
0.7247	665.9287	58.5272	0.1145	1.3910	1.4521	95.2529	9.7038	-0.0262
0.8681	572.4926	48.2529	0.1133	1.3895	1.0028	67.7742	6.1146	-0.0134
1.0000	467.6144	37.8608	0.1121	1.3889	0.6267	43.5760	3.5063	0.0000

318K

0.0000	806.5557	85.9477	0.1190	1.447	2.7319	151.3292	32.8291	0.0000
0.2084	764.6689	77.4108	0.1183	1.416	2.3027	134.8235	22.4295	-0.0168
0.3969	707.4845	68.3202	0.1174	1.392	1.8524	113.7906	15.0969	-0.0287
0.5683	650.5489	59.9912	0.11658	1.374	1.4694	94.3044	10.2357	-0.0320
0.7247	583.3771	51.5445	0.1154	1.363	1.1089	73.8024	6.8227	-0.0250
0.8681	513.2278	43.5065	0.1142	1.360	0.8037	55.1702	4.4826	-0.0124
1.0000	462.8056	37.7003	0.1131	1.357	0.6135	43.3867	3.1163	0.0000

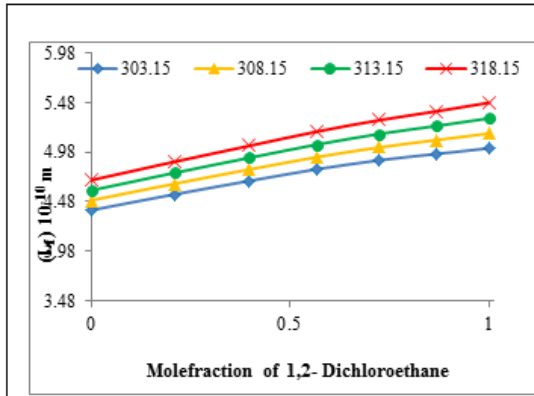


Fig 3.1.9 Variation of Intermolecular free length with Mole fraction of 1,2-Dichloroethane.

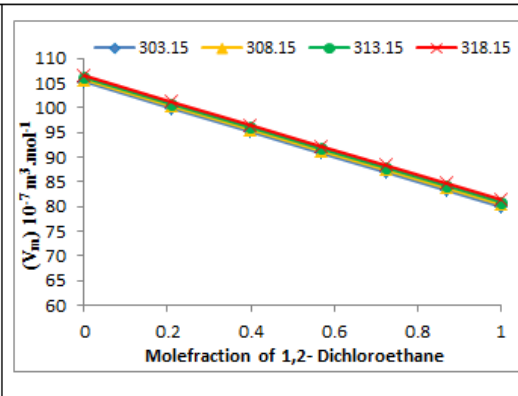
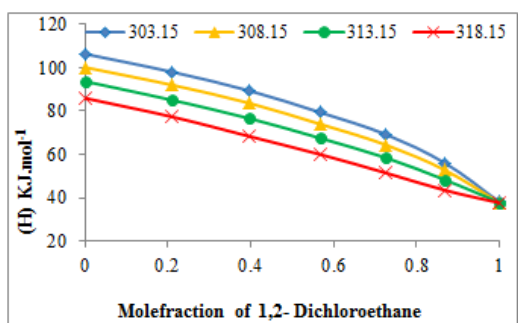
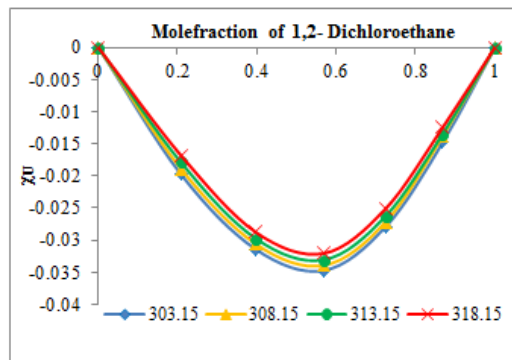
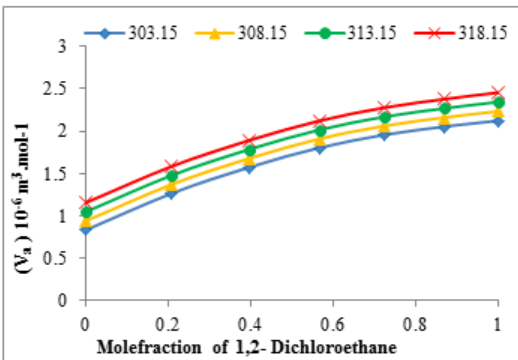
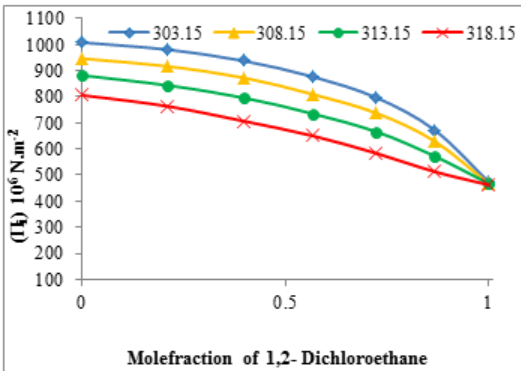
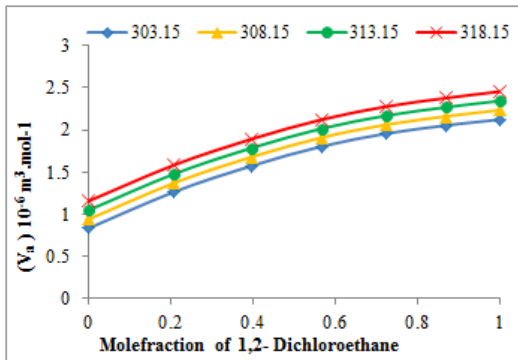
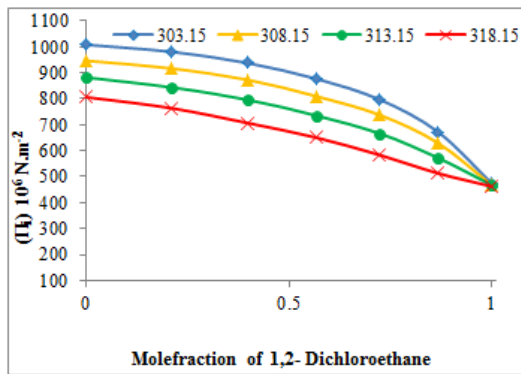
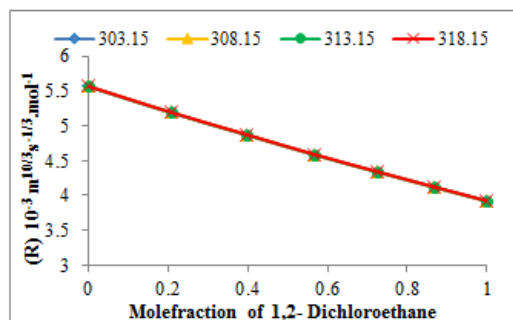
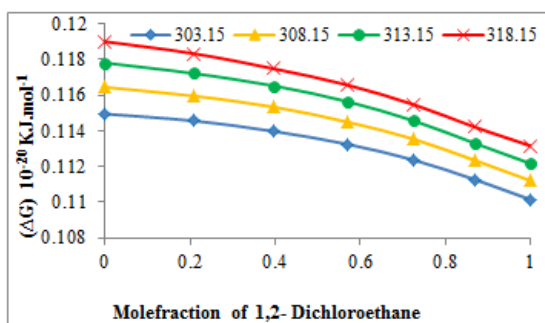


Fig 3.1.11 Variation of Molar volume with mole fraction of 1,2-Dichloroethane.





Results and Discussions

Ultrasonic velocity(u), viscosity(η) and density(ρ) were measured at a fixed frequency of 2MHz for the whole composition of 1,2 Dichloroethane at four different temperatures, 303.15k,308.15k,303.15k and 318.15k, are given in tables (3.1(a),3.2(a),3.3(a)). The other physical properties such as molar volume, adiabatic compressibility, mean free length, free volume, acoustic impedance, Rao's constant are calculated with the experimental data.

The variation of sound velocity with mole fraction of 1,2Dichloroethane at four different temperatures is shown in Fig(3.1.1,3.2.1,3.3.1). The sound velocity decreases as the mole fraction of 1,2 Dichloroethane increases. The similar trends are observed for the system at all the four temperature Density (ρ) is the measure of solvent- solvent interactions. Density increases with concentration indicates the increase in solvent- solvent and solvent- solute interactions whereas decrease in density indicates the lesser magnitude of interactions. The decrease in viscosity values of mixture could be explained by the strong electrostatic interactions between the molecules[6]. For all the three mixtures the same trend is observed.

The adiabatic compressibility increased with increase in temperature. This leads to structural reorientation of particles which increases the compressibility[7]. It is observed that in all the mixtures the molar volume decreases with increasing

the temperature and also with increase in the temperature[8]. It is clear that the interaction become weaker at higher temperatures. The Rao's constant (R) and Wada's constant (W) for the three systems at different temperatures are presented in tables (3.1(a),3.2(a),3.3(a)). The corresponding plots of Rao's constant vs. molefraction and Wada's constant vs. mole fraction are given respectively in figures (3.1.23,3.2.23,3.3.23,3.1.24,3.2.24,3.3.24) for all the three mixtures. The space between the molecules is decreasing with the increase of temperature. This behaviour of W and R , supports the possibility of weak interactions between the molecules of liquid mixture components[9]. In the present study the intermolecular free length (L_f) follows the same trend as that of Adiabatic Compressibility (β_{ad}). The free volume values are calculated and presented in tables(3.1(a),3.2(a),3.3(a)) for the three binary mixtures and the corresponding plots of free volume vs. mole fraction are given in fig(3.1.17,3.2.17,3.3.17). Thus increase in the value of free volume (V_f) decreases the intermolecular distance, making relatively less gap between the molecules[10]

In the present study the internal pressure values are decreased with an increase in the temperature for all the three binary mixtures and are presented in the tables (3.1(b),3.2(b),3.3(b)). It can be concluded that the decreasing trend suggests the strong interactions among the molecules of components of the system[11]. Gibb's free energy decreases with increase in

concentration which confirms the hydrogen bonding formation in binary liquid mixtures [12].

The decreasing values of acoustic impedance (Z), decreases the intermolecular distance, making relatively less gap between the molecules.[13]

The relaxation time (τ) values decrease with increase of mole fraction of 1,2Dichloroethane. This may be account for the decrease of dielectric constant of the medium and change of intermolecular and intramolecular interactions between the molecules[14]. In the present study, the absorption coefficient values decrease with increase in the mole fraction of first component in the three mixtures[15]. The corresponding plots of molecular interaction vs. mole fraction of the first component 1,2 Dichloroethane are given in fig(3.1.27,3.2.27,3.3.27). The trend is negative and negative values are increased up to 0.6 molefraction of 1,2-dichloroethane and then increases.

Conclusion

The ultrasonic velocity, density, viscosity and other related parameters were calculated. The existence of type of molecular interactions in solute-solvent is confirmed from the U , ρ , β_{ad} , L_f , Z , V_m , R , W , η , π and V_f data. All the experimental determinations of acoustic parameters are strongly correlated between 1,2 Dichloroethane and o cresol p cresol and m cresol.

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