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"Molecular Interaction Studies Of Ternary Mixtures Containing Acrylic Acid As Common Componant In Benzene, Toluene And 1, 4-dioxane Ultrasonically."

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Abstract: Ultrasound velocity, density and viscosity have been observed of acrylic acid in Benzene, Toluene and 1, 4-Dioxane at temp. 30ºC, 35ºC & 40ºC. The isentropic compressibility, intermolecular free length, molar volume, viscosity and their excess values also have been computed in these systems. The nature and extent of molecular interaction parameter (α) is also calculated and found to be useful in understanding the interaction in ternary liquid systems.

Key Words: Ultrasound, velocity, observed, Benzene, entropic, compressibility, intermolecular, molar volume.

The study of intermolecular interactions is of considerable importance in the elucidation of the formation of complexes and plays an important role in the liquid mixtures. The intermolecular interactions influence the structural arrangement along with the shape of molecules. Lagemann and Dunbar[1] was the first to point out the sound velocity approach for qualitative determination of the degree of association in liquids. There has been an increasing interest in the study of molecular in binary liquid mixtures by many experimental procedures[2-7] & applied it order to determine the nature and strength of molecular interaction.

Prakash et. al[8-11] determined ultrasound velocity and density experimentally of some ternary non-aqueous liquid - liquid systems and computed thermodynamic properties like isentropic compressibility intermolecular free length, available and free volumes and their excess values. Which decide the nature and extent of interaction in terms of excess properties. Recentaly Kannapann et.al[12] computed ultrasound velocity theoretically using Nomoto's relation, jacobson's free length theory and Schaff's Collision factor in ternary mixtures of (i) Acetone - Toluene - Carbon tetra chloride, (ii) Benzene – Acetone – Toluene and (iii) Cyclohexane – Carbon tetra chloride – Ethyl acetate.

The present paper reports the results of the ultrasound study of molecular interaction in the following ternary liquid mixtures : (i) Acrylic acid - Benzene - Toluene, (ii) Acrylic acid – Toluene - 1, 4-Dioxane and (iii) Acrylic acid - 1, 4 Dixone - at temp. 300C, 350C and 400C.

The molecular interaction terms ($\propto$) has also been calculated for all the mixtures and discussed in the light of interactions between molecules.

EXPERIMENTAL :

Ultrasound velocities were measured using single crystal ultrasound interferometer of 2MHz frequency and the data were accurate upto 0.2%. Densities of the mixtures have been determined by pyknometer and electrical valance. The viscosities have been determined by using ostwald viscometer. The temperature was maintained by an electronically controlled thermostat. Acrylic acid (B.D.H., Poole England), Benzene (A.R./B.D.H.), Toluene (E.Marck) and 1, 4-Dioxane (Reedal De Haen) were purified by standard methods.

The isentropic compressibility, intermolecular free length, molar volume were calculated using the following relations :

$$\beta_s = 1/u^2\rho$$

$$L_f = K.\sqrt{\beta_s}$$

$$V_m = \bar{M}/\rho^{-1}$$

where $\bar{M} = X_1M_1 + X_2M_2 + X_3M_3$

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X_1, X_2 & X_3 are mole fraction of component 1,2 & 3

The excess parameters A^E can be calculated from the relations :

$$A^E = A_{exp} - A_{ideal}$$

and

$$A_{ideal} = X_1A_1 + X_2A_2 + X_3A_3$$

Where the symbols have their usual significance.

Molecular interaction ($\propto$) the degree of intermolecular interaction ($\propto$) is given by :

$$\propto = \frac{U_{exp}^2}{U_{im}^2} - 1$$

Where, U_{im} is calculated following the equation suggested by Van Dael & Vangeel[13] given by –

$$\frac{1}{X_1M_1 + X_2M_2 + X_3M_3} \cdot \frac{1}{U_{im}^2} = \frac{X_1}{M_1U_1^2} + \frac{X_2}{M_2U_2^2} + \frac{X_3}{M_3U_3^2}$$

RESULTS and DISCUSSION :

Ultrasound velocity, density and viscosity have been observed of Acrylic acid as comman componant in Benzene, Toluene and 1, 4-Dioxane at temp 30ºC. The isentropic compressibility, intermolecular free length, specific acoustic impedence, molar volume, viscosity and their excess values also have been computed in these systems and tabulated (From 1 to 30). It is observed that ultrasound velocity decreases on increasing mole fraction of Acrylic acid in each system. It is also decrease with increasing temperature.

It is clear from plotted graphs (1 to 3) that excess isentropic compressibility of Acrylic acid with Benzene, Toluene and 1, 4-Dioxane are negative while excess viscosity of above acrylic acid in ternary system are positive. The excess negative values of β_s and positive values of η^E will favour for strong interaction between the molecules of ternary mixtures.

The increasing mole fraction of above liquids cause more deviation of β_s, L_f, V_m and opposite nature of n is due to polarization of non-polar molecules of benzene and toluene by the more diploe moment values of the acid. Benzene and Toluene are highly polarizable so these molecules polarized by acid molecules due to more value of dipole movement as observed by Joesten et.al.[14]

Adgaokar et.al[15] also observed the greater association of toluene substituted compound with non-polar molecules. The associating nature of acrylic acid with highly polarizable molecules acid at 0.5014 in system (i), while it is greater in other two system is which Toluene concentration is more. Therefore it is concluded that Toluene is most associating nature in comparision to benzene and 1, 4-Dioxane.

Ultrasound velocity (v), Density (P), Viscosity (η), Isentropic compressibility (β_s), Interaction free length (L_f), Molar volume (V_m) and Molecular interaction parameter ($\propto$) of Acrylic acid ternary systems at 30ºC, 35ºC and 40ºC.

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Table - I

Acrylic Acid + Tolune + Benzene

at temp. 30^0C

Mole fraction Acrylic Acid (X_1)	Mole fraction of Aromatic Hydrocar-Bon (X_2)	U m/s	ρ g/ml.	η C.P.	β 10^{12} cm^2/ dyne	L_f (A^0)	V_m Ml/mole	∝
0.0000	0.0000	1282	0.8610	0.4542	70.66	0.5304	90.72	0.00000
0.0000	1.0000	1287	0.8466	0.4402	71.31	0.5328	108.83	0.00000
0.0827	0.1789	1293	0.8625	0.4889	68.55	0.5224	91.96	0.00997
0.1717	0.2792	1294	0.8835	0.5271	67.59	0.5167	91.65	0.00045
0.2685	0.3880	1306	0.9025	0.5680	65.32	0.5099	90.77	0.00648
0.5014	0.3170	1325	0.9350	0.6939	60.48	0.4907	83.47	0.00860
1.0000	0.0000	1360	0.9985	0.8806	54.14	0.4842	72.16	0.00000

Table - II

Acrylic Acid + Toluene + 1, 4-Dioxan

Tem. 30°C

X_1	X_2	v	ρ	η	B_s	L_f	V_m	∝
0.0000	1.0000	1420	0.9669	1.2021	51.82	0.4542	92.07	0.00000
0.0000	0.0000	1287	0.8466	0.4402	71.31	0.5328	108.83	0.00000
0.0825	0.2110	1416	0.9608	1.0291	51.90	0.4545	091.91	0.04835
0.1673	0.3210	1410	0.9645	0.9112	52.15	0.4545	89.90	0.07413
0.2546	0.4340	1404	0.9680	0.7946	52.40	0.4567	88.59	0.09896
0.3443	0.5503	1400	0.9783	0.6777	52.51	0.4572	87.27	0.12577
0.6139	0.2543	1380	0.9783	0.8206	53.67	0.4622	80.98	0.04188
1.0000	0.0000	1360	0.9985	0.8806	54.14	0.4622	72.16	0.00000

Table - III

Acrylic Acid + Benzene + 1,4-Dioxane

Temp. 30°C

X_1	X_2	v	P	η	B_s	L_f	V_m	∝
0.0000	1.0000	1420	0.9569	1.2021	51.82	0.4542	92.07	0.00000
0.0000	0.0000	1282	0.8610	0.4542	70.66	0.5304	90.72	0.00000
0.0905	0.2216	1415	0.9610	1.0098	51.97	0.4548	87.76	0.05868
0.1803	0.3308	1409	0.9640	0.9011	52.25	0.4561	84.95	0.08493
0.2692	0.4384	1405	0.9670	0.7929	52.38	0.4566	82.10	0.10754
0.3572	0.5459	1399	0.9720	0.6840	52.56	0.4574	79.80	0.12540
0.5616	0.2861	1386	0.9790	0.8114	53.16	0.4600	77.91	0.06712
1.0000	0.0000	1360	0.9985	0.8606	54.14	0.4642	72.16	0.00000

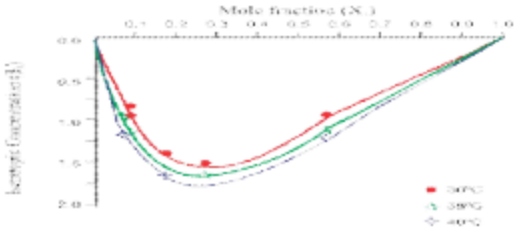

Fig.: Mole fraction of acrylic acid Vs Isentropic Compression for acrylic acid + toluene + Benzene (Curve I)

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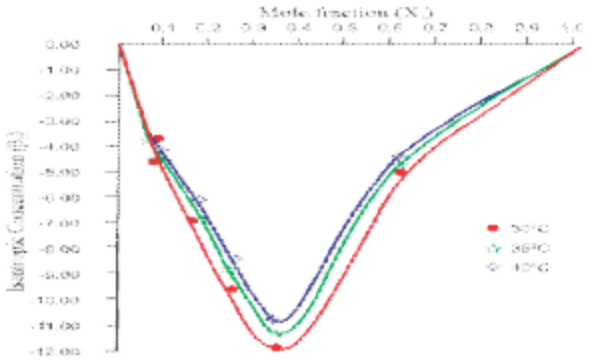

Fig.: Mole fraction of acrylic acid Vs Isentropic Concentration for acrylic acid + toluene + 1,4 - Dioxane [Curve III]

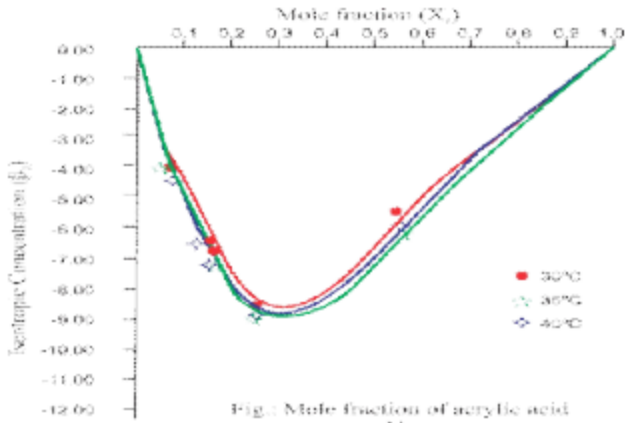

Fig.: Mole fraction of acrylic acid Vs Isentropic Concentrestibility for acrylic acid + benzene + 1,4 - Dioxane [Curve III]

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