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## The excess acoustic & thermodynamic properties based molecular interaction of alpha pyrone in methanol and acetone

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### Abstract

The physical properties like ultrasound velocity, density and viscosity determined in ternary ten samples of different mole fraction of Alpha pyrone in methanol & acetone. At 30C. Various acoustic and thermodynamic parameters were also computed in these ternary mixtures. The excess values of acoustic & thermodynamic parameters will have used to interpret the molecular interaction between the two component of ternary liquid mixtures. The negative deviation of isentropic compressibility and positive deviation of viscosity interpret the specific interaction.

**Keywords:** The excess acoustic, thermodynamic properties based, methanol

### Introduction

The ultrasound velocity, density and viscosity measurements find wide applications in defining the physico-chemical behaviour of liquid mixtures<sup>[1-3]</sup> and in the study of molecular interaction. The ultrasound velocity of a liquid is related to the binding forces between the atoms or molecules. Ultrasound velocity has been adequately employed in understanding the nature of molecular interactions in pure liquids<sup>4</sup> and binary mixtures. The method of studying the molecular interaction from the knowledge of variation of acoustic thermodynamic parameters and their excess values with composition gives an insight in to the molecular process<sup>[5-7]</sup>. The investigations regarding the molecular interactions in organic ternary mixtures having Alpha pyrone as polar and associating component with other polar solvent like methanol and Acetone can associate with high degree of interaction because unsaturated esters are polar as well as associating white non-benzonril component are also polar.

In view of the importance mentioned, an allemtt has been made to elucidate the molecular interactions in the mixtures of alpha pyrone with methanol and acetone at 303°K. Further, the excess value of density, viscosity and acoustic parameters of the mixtures are computed. The excess functions are used to explain intermolecular interaction in there ternary mixtures.

### Material and Methods

All the chemicals used in the present work are Analytical Reagent (A.R.) of minimum assey of 99.9% obtained and again purified. The purities of above chemicals used were checked by density measurements at 303K. The ternary liquid mixtures of different known composition were prepared in stopper measuring flasks. The density, viscosity and velocity were measured as a function of composition of ternary liquid mixture of alpha pyrone with methanol and acetone at 303K. The density was determined by bi capillary pyknometer. The weight of the samples was measured by electronic digital balance with an accuracy of  $\pm 0.1\text{mg}$ . An ubbelohde viscometer has used for viscosity measurements using a digital clock to within  $\pm 0.01\text{sec}$ . An ultrasonic interferometer having frequency of 2MHz (Mittal Enterprises, New Delhi, Model F-81) with an overall accuracy of  $\pm 0.1\%$  has been used for velocity measurements. An electronic water both has been used to circulate water through the double walled measuring cell.

### Formula Derivation

The various acoustic and thermodynamic parameters viz. isentropic compressibility ( $\beta_s$ ), intermolecular free length ( $L_f$ ), specific acoustic impedance ( $Z$ )<sup>[8]</sup>, molar volume ( $V_m$ ), available volume ( $V_a$ ), viscosity( $\eta$ ), wada constant (B), shear's relaxation time ( $\tau$ ) have been evaluated by using the following empirical formula:

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1.  $\beta_s = \frac{1}{v^2} \rho$
2.  $L_f = K(\beta_s)^{1/2}$
3.  $Z = v \times \rho \times 10^{-5}$
4.  $B = \left[ \frac{\bar{M}}{\rho} \right] \beta_s^{-1/7}$
5.  $V_m = \frac{\bar{M}}{\rho}$
6.  $V_a = V_r \left\{ 1 - \frac{V}{V_\infty} \right\}$
7.  $\eta = \rho \left( at - \frac{b}{t} \right)$
8.  $\tau = \frac{4}{3} \eta \times \beta_s$

The excess values of above parameters were computed by the formula

$$A^E = A_{\text{exp}} - (X_1 A_1 + X_2 A_2 + X_3 A_3)$$

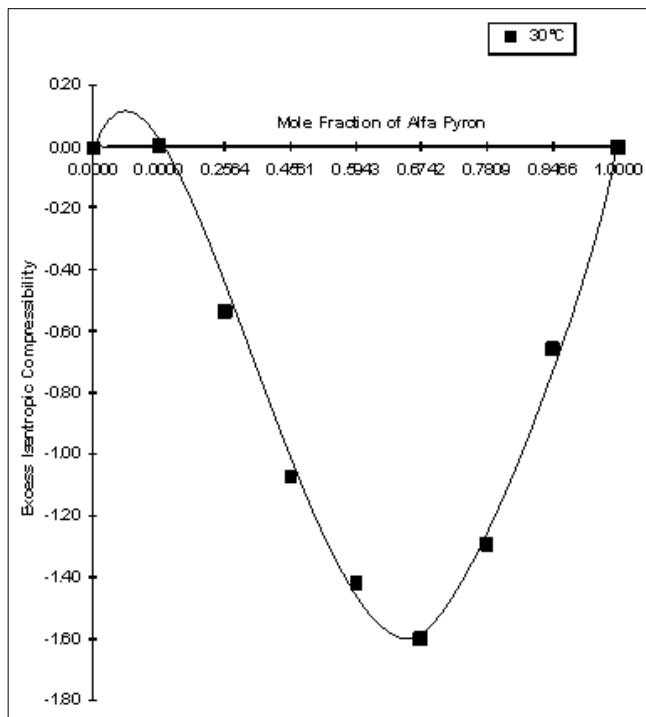
Where V,  $\rho$ ,  $\beta_s$ ,  $\eta$ , Z,  $L_f$ , M,  $V_a$ ,  $V_m$ ,  $\tau_s$ , Bare Ultrasonic velocity, Density, Isentropic Compressibility, Viscosity, Specific Acoustic Impedance, Intermolecular Free Length, Available Volume, Molar Volume, Shear's Relaxation Time, Wada constant respectively. Here

$$\bar{M} = \frac{M_1 X_1 + M_2 X_2 + M_3 X_3}{X_1 + X_2 + X_3}$$

Where  $M_1$ ,  $M_2$ ,  $M_3$ ,  $X_1$ ,  $X_2$  and  $X_3$  are the molecular weight and mole fraction of liquid component of 1, 2 and 3.

**Alpha Pyrone + Methanol + Acetone at Temp. 30 °C**

Mole Fraction of Alpha Pyrone	Mole Fraction of Methanol	Density (excess)	Ultrasound Velocity	Isent. Comp. (excess)	Intermo. Free Len. (excess)	Molar Volume (excess)	Available Volume (excess)	Viscosity (excess)	Shear's Relaxation Time	Specific Acoustic Impedance	Rao's Constant
0.0000	0.0000	0.0000	1160	0.00	0.0000	0.00	0.00	0.0000	40.1885	0.9018	13.55
0.0000	1.0000	0.0000	1100	0.00	0.0000	0.00	0.00	0.0000	74.1331	0.8609	422.31
0.2564	0.2638	0.0014	1142	-0.54	0.0037	5.33	3.18	0.0207	56.1035	1.0161	333.06
0.4561	0.1173	0.0018	1168	-1.07	0.0034	7.30	4.40	0.0247	53.7993	1.1385	439.42
0.5943	0.1834	0.0021	1179	-1.42	0.0036	5.86	4.21	0.0289	56.2619	1.2196	583.01
0.6742	0.1156	0.0018	1196	-1.60	0.0035	5.33	3.96	0.0317	54.5864	1.2772	623.86
0.7809	0.1148	0.0013	1220	-1.29	0.0012	3.68	2.88	0.0281	53.2603	1.3579	717.12
0.8466	0.0544	0.0007	1249	-0.66	-0.0030	2.72	1.78	0.0207	49.9512	1.4241	752.53
1.0000	0.0000	0.0000	1280	0.00	0.0005	0.00	0.00	0.0000	46.7423	1.5421	866.01



**Result & Discussion**

In the present study, used pure chemicals are alpha pyrone, methanol and acetone. The alpha pyrone is polar and associating while methanol and acetone are polar due to presence of ketonic and oxy group. The presence of unsaturation in the cyclic ring these are also electron with drawing group. Therefore the interaction will be discussed on

the observed facts as obtained by the results.

The density, ultrasound velocity and viscosity observed practically and results are tabulated on the tables. The acoustic and thermodynamic parameters also computed and tabulated on the tables. The excess values of almost parameters have also computed. The excess values of isentropic compressibility, intermolecular free length, molar volume and viscosity are also plotted on the graphs against mole fraction of allyl acetate in the ternary system as-

**1. Alpha pyrone + Methanol + Acetone**

It is seen from table that the curves of excess isentropic compressibility, intermolecular free length are negative over entire range of mole fraction while excess viscosity is positive for both mixtures at entire range of mole fraction. The positive excess viscosity and molar volume attributed to the existence of dispersion and dipolar forces between unlike molecules<sup>10-12</sup>. The other variation and extend of excess compressibility so negative trend while viscosity show positive trend indicating strong interaction between the molecules of chemicals.

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