Available online www.jocpr.com

Journal of Chemical and Pharmaceutical Research, 2012, 4(1):653-655

Research Article

ISSN : 0975-7384
CODEN(USA) : JCPRC5

Intermolecular Interaction studies on Ternary Liquid Mixtures at 303 K

R. Uvarani and J. Sivapragasam*

Department of Physics, KSR College of Engineering, Tiruchengode, India

---

ABSTRACT

The ultrasonic velocity, density and viscosity have been measured for the ternary liquid mixtures of cyclohexanone with 2-propanol and 2-methyl-2-propanol in carbontetrachloride at 303 K. The acoustical parameters such as adiabatic compressibility, free length, molar volume and internal pressure have been obtained from the experimental data for the liquid mixtures with a view to investigate the exact nature of the molecular interaction. The excess values of the above said parameters have also been calculated and found to be useful in estimating the strength of the interaction in the mixtures.

Keywords: Ternary liquid mixtures, acoustical parameters, molecular interaction.

INTRODUCTION

The study of molecular interaction has attracted the attention of many researchers and extensive investigations in both binary and ternary liquid mixtures have been carried out by different techniques [1]. The present investigation is concerned with the study of molecular interaction in the ternary mixtures of cyclohexanone with 2-propanol and 2-methyl-2-propanol in carbon tetrachloride at 303 K. A deeper knowledge of mixing properties of such multicomponent liquid system is essential in many industrial applications such as design calculation, mass transfer, fluid flow etc., [2]. Molecular interactions in different liquid mixtures changes depending upon the nature of solvent, the structure of molecule and the extent of solution taking place in the solution. [3]

EXPERIMENTAL SECTION

The ultrasonic velocities of the liquid and liquid mixtures were measured at 303 K, using a single crystal interferometer with a high degree of accuracy operating at a frequency of 2 MHz. An Oswald's viscometer calibrated with double distilled water is used for the measurement of viscosities in the mixtures. The values are accurate to ± 0.001 Nsm^{-2}.The densities of the mixture were measured using a specific gravity bottle and the accuracy in the measurement is 0.1Kgm^{-3}.The acoustical parameters such as adiabatic compressibility (β), free length (L_f), molar volume (V) and internal pressure (π_i) are calculated using the well known equations.

$$\beta = 1/U^2\rho$$

$$L_f = k\,(\beta)^{½}$$

$$V=(x_1m_1+x_2m_2)/\rho$$

$$\pi_i=bRT[(K\eta)/U]^{1/2}\,[\rho^{2/3}/\ M_{eff}^{7/6}]$$

The excess values are calculated as,

$$A^E = A_{exp} - [X_1A_1 + X_2A_2 + X_3A_3]$$

Where A is any acoustical parameter and X is the mole fraction of the liquid component.

RESULTS AND DISCUSSION

The values of ultrasonic velocity (U), density (ρ) and viscosity (η) are measured at 303 K and the excess values of acoustical parameters for the ternary liquid mixtures are furnished in the Table-1.

Table 1: Values of experimental density (ρ), Viscosity (η), and ultrasonic velocity (U) and their excess acoustical parameters(β^E, L_r^E, V^E, π_i^E) of the ternary mixtures at 303K.

Mole Fraction		ρ	η	U	β^E	L_f^E	V^E	π_i^E
X_1	X_2	(Kgm^{-3})	($x10^{-3}Nsm^{-2}$)	(ms^{-1})	($x10^{-11}N^{-1}m^2$)	($x10^{-12}m$)	($x10^{-7}m^3mol^{-1}$)	($x10^6Pa$)
Cyclohexanone (X_1) + 2- Propanol(X_2) + Carbon tetrachloride (X_3)								
0.0000	0.6999	1056.37	1.4648	994.6	1.092	-0.239	2.209	-127.76
0.1999	0.5000	1075.48	1.3789	1063.8	-4.906	-1.298	-2.382	-140.02
0.3499	0.3499	1090.73	1.4441	1113.0	-5.779	-1.609	-1.847	-110.38
0.3996	0.3000	1094.50	1.4703	1127.1	-5.443	-1.515	-1.534	-98.67
0.5999	0.1004	1111.13	1.6706	1184.8	-3.538	-1.032	-1.316	-32.57
0.6998	0.0000	1118.20	1.8976	1213.8	-2.088	-0.658	-0.486	18.94
Cyclohexanone (X_1) + 2-Methyl - 2 –Propanol (X2) + Carbon tetrachloride (X_3)								
0.0000	0.6999	1009.52	1.8516	973.2	3.088	1.130	4.397	-191.98
0.2000	0.4999	1045.72	1.7696	1060.1	-5.355	-1.316	-0.683	-157.74
0.3497	0.3503	1069.42	1.7275	1108.6	-6.074	-1.575	-2.330	-120.25
0.3999	0.3002	1077.14	1.7211	1124.9	-6.024	-1.596	-1.952	-105.82
0.6002	0.0997	1104.51	1.8006	1186.9	-4.034	-1.168	-0.819	-29.24
0.6998	0.0000	1118.20	1.8976	1213.8	-2.088	-0.658	-0.486	18.94

The results presented in Table-1 shows the non- ideal behaviour of the liquid mixture. If the mixtures are ideal, then all the excess values should have been zero. The deviations, either positive or negative, suggest the mixtures are non-ideal [4].

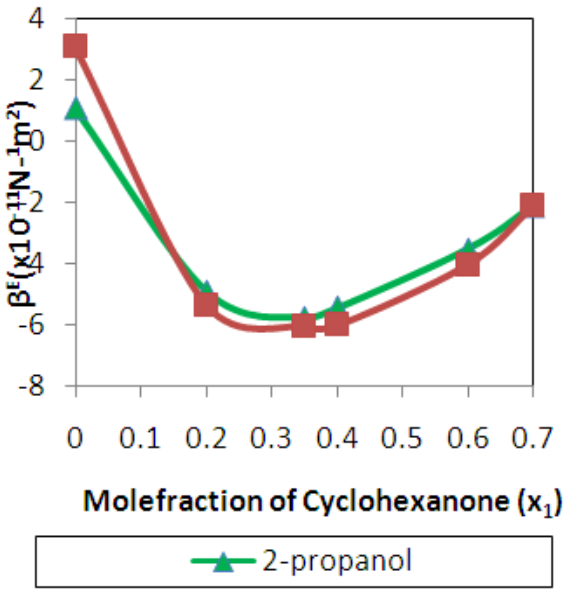

Fig 1: Variation of excess adiabatic compressibility Versus molefraction of cyclohexanone (x_1)

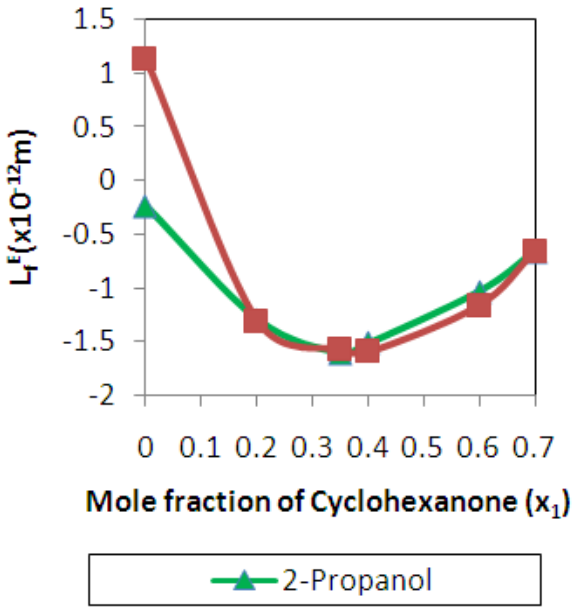

Fig 2 : Variation of excess free length versus molefraction of cyclohexanone(x_1)

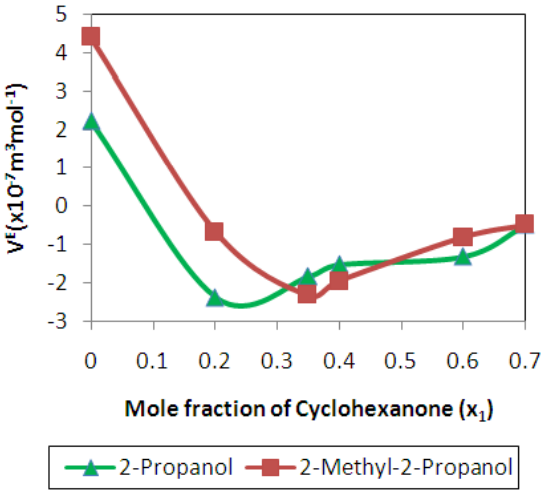

Fig 3: Variation of excess molar volume Versus molefraction of cyclohexanone (x_1)

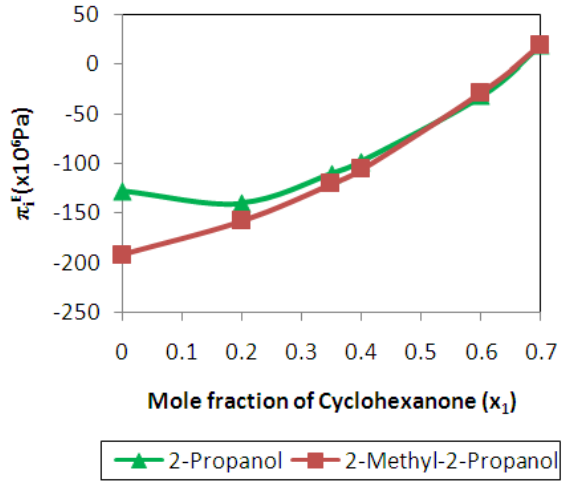

Fig 4 : Variation of excess internal pressure versus molefraction of cyclohexanone (x_1)

It can be observed from the Figure -1 that the β^E values are positive for the two systems of branched alcohol diluted with carbon tetrachloride and with zero concentration of cyclohexanone. The addition of carbon tetrachloride to the self associated alcohols breaks the self association and almost all the dipoles are freed due to the rupture of H-bonding. This results in an increase in volume and so greater compressibility for the systems. When cyclohexanone is added to these systems the dipoles of cyclohexanone interact with the free dipoles of alcohols. There will be dipole – dipole interaction as well as formation of new H – bonds between the unlike molecules.

In the systems studied, β^E values are more negative for 2-methyl-2-propanol system than for the system with 2-propanol.With increased branching in the former case, the –CO group of the alicyclic ketone is more hindered and less active to break the self association in 2-methyl-2-propanol system. The additional rigidity may be the reason for the negative values of β^E for the cyclohexanone +2-methyl-2-propanol system [5]. Since L_f is directly related to the β values similar trends are observed for L_f^E in both the systems [6]as shown in figure -2.

It can be observed from Figure-3, the excess molar volume V^E are found to be positive and negative with respect to the composition of the mixtures. Also the V^E values shows less variation with the increase in concentration of cyclohexanone .The negative values of V^E in all the systems may be attributed to the presence of dipole – dipole interaction.[7,8] The values of π_i^E are initially negative and as the concentration of cyclohexanone increases π_i^E becomes positive as shown in figure-4 for the systems studied .This suggests that dipole and dispersive forces are operative in these systems [9,10,11].

REFERENCES

[1] Alka Tadkalkar; Pravina pawar; and Govind K. Bichile; *J of Chem Pharm res*, **2011**, 3(3), 165 – 168.
[2] AJ Clement Lourduraj; and I Johnson; *J.pure Appl.Ultrasonics.*, **2008**, 30, 69-73.
[3] S Thirumaran; S Sudha; *J of Chem Pharm res*, **2010,** 2(1), 327.
[4] N Prasad; O Prakash; S Singh; and S Prakash; *Ultrasonics*, **1978**, 16(2**),** 77.
[5] Amalendu Pal; Harshkumar; BK Arbad; and AB Tekale; *Indian J Pure Appl. Phys.*, **2003**, 41, 113.
[6] GV Rama Rao;Viswanatha sarma; and C Rambabu;*Indian J Che*., **2004**, 43(A**)**, 752.
[7] A Ali, K Tiwari; AK Nain; and V Chakravortty; *Indian J Phys*., **2000**, 74 B(5), 351.
[8] KS Kumar; and PR Naidu; *J.Chem.Engg.Data*, **1994,** 39, 2.
[9] AN Kannanppan; and L Palaniappan; *Indian J Phys.*, **1999**, 73(B**)**, 531.
[10] AN Kannanppan; and R Palani; *Indian J Phys*., **1996**, 70(B), 59.
[11] S Thirumurugan; R Murugan; and N. Prakash; *J of Chem Pharm res*, **2010,** 2(1), 53.