



Excess Gibb's free energy function values at different temperatures in binary liquid mixture for the study of molecular interactions

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ABSTRACT

Density, ultrasonic velocity and viscosity values have been measured experimentally in the binary mixture containing quinolone and m-xylene at different temperatures at different mole fractions. These experimentally measured data have been used to calculate the excess Gibb's free energy function (G^{*E}). The obtained results have been used to explain the molecular interactions.

Keywords: Density, ultrasonic velocity, quinolone and excess Gibb's free energy function.

INTRODUCTION

When two or more liquids are mixed, there occur some changes in physical and thermodynamic properties because of change in molecular orientations. The study of molecular behavior of liquids is no longer a neglected branch of chemistry. Considerable amount of work has been done on the theories of liquids and liquid mixtures. As a part of ongoing research [1-5] on thermodynamic and excess properties of binary liquid mixtures, we report here the results of study on binary mixtures of heterocyclic aromatic compound such as quinoline with m-xylene over the entire range of composition at different temperatures ranging from $T = 303.15\text{K}$ to $T = 318.15\text{K}$. Quinoline is a colourless liquid with strong odor and widely used in manufacturing of dyes, pesticides and solvent for resins and terpenes. Xylene is very much useful in many agricultural applications. xylene is mostly useful as clearing agent. By using the experimentally measured values of ultrasonic velocity (u), density (ρ) and viscosity (η), excess thermodynamic function like excess Gibb's free energy function (G^{*E}) have been calculated for the binary mixture.

EXPERIMENTAL SECTION

All the chemicals used were obtained from SDFCL chemicals (quinoline) and Merck (m-xylene). The chemicals were purified by standard procedure [6]. The purity of samples was checked by comparing experimental values of density and ultrasonic velocity with the available literature. Job's method of continuous variation was used to prepare the mixtures of required proportions. The prepared mixtures were preserved in well-Stoppard conical flasks. After mixing the liquids thoroughly, the flasks were left undisturbed to allow them to attain thermal equilibrium. The ultrasonic velocities were measured by using single crystal ultrasonic pulse echo interferometer of Mittal enterprises, India with model number F-80X. The densities of pure liquids and liquid mixture were measured by using a specific gravity bottle with an accuracy of $\pm 0.5\%$. Viscosities were measured at the desired temperature using Ostwald's viscometer calibrated using water and benzene. The flow time has been measured after the attainment of bath temperature by each mixture. For all pure compounds and mixtures, 4 to 5 measurements were performed and the average of these values was used in all the calculations.

THEORY:

The excess free energy function is calculated by the following equation

$$G^{*E} = RT \left[\ln \left(\frac{\eta V_m}{\eta_2 V_{m2}} \right) - x_1 \ln \left(\frac{\eta_1 V_{m1}}{\eta_2 V_{m2}} \right) \right] \text{-----(1)}$$

and

It is fitted to Redlich-Kister polynomial equation

$$Y^E = X_1 \cdot X_2 \sum_{i=0}^n A_i (X_1 - X_2)^i \text{-----(2)}$$

RESULTS AND DISCUSSION

The values of ultrasonic velocities and densities for the two pure liquids are experimentally measured and are compared with the literature values and they are good agreement with each other as given in **Table-1**.

Table-1: Comparison of experimental densities ρ and ultrasonic velocities U of pure liquids with literature values

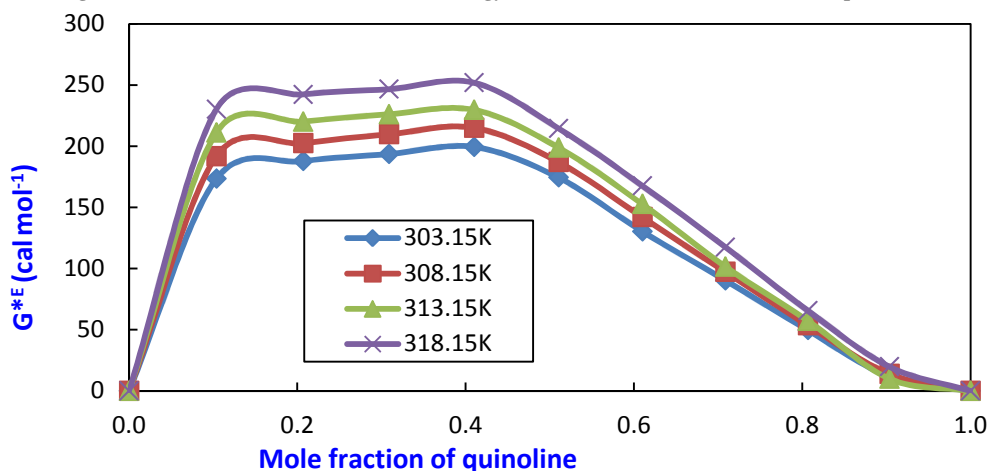
Liquids	Density ' ρ ' (kg . m ⁻³)		Ultrasonic Velocity ' U ' (m . s ⁻¹)	
	Expt	Lit	Expt	Lit
Quinoline	1085.45	1085.79[7]	1553.68	1547[7]
m-Xylene	855.70	855.47[8]	1304.21	1300.34 [8]

The values of excess Gibb's free energy function (G^{*E}) which are calculated from the experimentally measured values are given in **Table-2**. The variations in the measured values of excess Gibb's free energy function (G^{*E}) in the present binary mixture at different temperatures are represented in the **Figure-1**.

Table-2: Calculated Values of Excess Gibb's free energy function (G^{*E})

Excess Gibb's free energy function (G^{*E})			
At (T=303.15K)	At (T=308.15K)	At (T=313.15K)	At (T=318.15K)
0.00	0.00	0.00	0.00
173.45	191.86	211.25	230.34
187.78	202.42	220.08	242.34
193.60	209.82	226.15	246.66
199.42	215.05	229.79	251.89
174.40	186.99	198.92	214.56
130.40	142.07	152.68	167.74
90.37	97.35	101.58	117.56
49.72	53.71	57.42	65.67
11.69	13.86	9.98	19.78
0.00	0.00	0.00	0.00

Figure-1: Variations of excess Gibb's free energy function (G^{*E}) with mole fraction of quinoline



According to Oswalet *al.*[9] and Reed *et al.*[10] the positive G^{*E} may be attributed to specific interactions. It is observed from the figures that the G^{*E} values are positive in the present binary mixture. Similar like observations are made by Rathnam *al.*[11] according to them the positive values of G^{*E} show strong interactions.

CONCLUSION

From the variations of excess Gibb's free energy function with the mole fraction of quinoline at different temperatures. It is observed that there exists a strong molecular interaction between the components of the present binary liquid mixture.

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