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MOLECULAR INTERACTION STUDIES USING THERMO-ACOUSTICAL EXCESS PARAMETERS AND REDLICH-KISTER COEFFICIENTS ANALYSIS AT TEMPERATURES FROM 303.15K TO 318.15K

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Abstract - Molecular Interaction Studies are related with the Thermo-acoustical parameters and the present work is related to the analysis involved in the study of these excess values of thermo-acoustical parameters and their Redlich-Kister Coefficients at different temperatures range from 303.15K to 318.15K with variation of 5K temperature interval for each study and all these are explained in liquid mixtures containing functional chemical combination namely (Benzene mixed with ethanol).The obtained excess values of acoustical parameters namely Gibb's free energy (G^{*E}) , enthalpy (H^E) and internal pressure (π^E) have been computed from measured experimental data . The results have also been helpful to obtain Redlich-Kister coefficients from polynomial equation and also to obtain their deviations. Excess thermo-acoustical parameters are discussed along with Redlich-Kister coefficients generally for the study of interactions among the molecules of liquid species.

Keywords: Ethanol; Redlich-Kister Coefficients; Excess Enthalpy; Excess Gibb's function.

INTRODUCTION

Analysis of either thermo acoustical or excess factors thermo-acoustical parameters is very much useful tool in understanding the effect of interactions among the molecules of liquid mixture [1-7]. The study of structural packing, the study of shape and the study of size is generally effected by the molecular interactions. Speed of sound studies and related thermo acoustical excess parameters in liquids and liquid mixture are useful in explaining molecular activities with their typical behavior [8-14]. The author attempted a research work in the paper to report study in variations of thermo acoustical excess factors namely Gibb's free energy (G^E), Enthalpy (H^E) and internal pressure (π^E), in liquid mixtures functional materials namely (Benzene mixed with Ethanol) at known four temperatures range from 303.15K to 318.15K with variation of 5K temperature interval for each study for different range of molefraction of benzene. With these excess thermo-acoustical factors the author have allowed to fit to Redlich-Kister equation and the results are analyzed with their variations in coefficients of their respective thermo acoustical excess parameters of the liquid mixture [15]. The deviations that are produced during the study implies the existence of molecular interactions.

EXPERIMENTAL METHODS

Pulse echo type Ultrasonic interferometer (Making Mittal enterprises, India) is used for the measurements of ultrasonic velocities and the measurements are carried out at a frequency of 3MHz. The temperature adjustment carried out via temperature water bath viscometer of Ostwald's version were hired for the study of viscosities of liquid combinations. A Specific gravity bottle of 10 ml is used for the study of densities of liquid combinations. Digital Shimadzu AUY220 weighing balance (Making from Japan), having a precision of + or - 0.1 mg is applied for the measurements of masses of liquid combinations.

THEORY

The thermo acoustical excess factors namely internal pressure excess value (π^E), $\mathbf{G^{*E}}$ (Gibb's free energy excess value) and $\mathbf{H^E}$ (excess Enthalpy excess value) have been calculated.

$$\boldsymbol{\pi^E = \pi_{exp} - (x_1 \pi_1 + x_2 \pi_2)} \quad \text{J/mole}$$

Where $\boldsymbol{\pi^E}$ is excess Gibb's free energy.Here $\boldsymbol{\pi_1}$ **and** $\boldsymbol{\pi_2}$ are Internal energies of each pure liquid, and also here $\mathbf{x_1}$ **and** $\mathbf{x_2}$ molefractions of 1st component and 2nd component respectively.

$$\mathbf{G^{*E} = G_{exp} - (x_1 G_1 + x_2 G_2)} \quad \text{J/mole}$$

Where $\mathbf{G^{*E}}$ is excess Gibb's free energy .Here $\mathbf{G_1, G_2}$ are Gibb's free energies of each pure liquid, and also here $\mathbf{x_1}$ **and** $\mathbf{x_2}$ molefractions of 1st component and 2nd component respectively.

$$\mathbf{H^E = H_{exp} - (x_1 H_1 + x_2 H_2)} \quad \text{J/mole}$$

Where $\mathbf{H^E}$ is excess Enthalpy. Here $\mathbf{H_1, H_2}$ are the Enthalpies of each pure liquid, and also here $\mathbf{x_1}$ **and** $\mathbf{x_2}$ molefractions of 1st component and 2nd component respectively.

All the above thermo acoustical excess parameters for each mixture can be allowed to fit to the Redlich-Kister equation [16]

$$Y^E = X_1.X_2 \sum_{i=0}^{n} A_i \left(X_1 - X_2\right)^i$$

where, A_i is called co-efficient of Redlich-Kister equation. The coefficients are evaluated by using the least squares method. These coefficients are useful for a better fitting of excess parameters.

Further, standard deviation for any excess parameter Y^E is estimated by

$$\sigma(Y^E) = \left[\frac{\sum_{i=1}^{n} (Y^E_{\exp t} - Y^E_{cal})^2}{m-n} \right]^{1/2}$$

Based on the significance of the sign of a particular excess thermo-acoustical parameter, molecular interactions are analyzed between component moleules of present in liquid mixture.

RESULTS AND DISCUSSIONS

The coefficients of Redlich-Kister equation are computed using the excess parameters π^E, $\mathbf{G^{*E}}$ and $\mathbf{H^E}$ for the three liquid mixtures of functional materials namely (Benzene mixed with Ethanol) at known four temperatures range from 303.15K to 318.15K with variation of 5K temperature interval for each study are given in the from Table-1.The corresponding variations against the molefraction of Benzene are represented in the figures from Fig 1-3.

Table -1: Values of Redlich-Kister coefficients for the liquid mixture of binary combination namely **Benzene mixed with Ethanol** at four known temperatures 303.15K, 308.15K, 313.15K & 318.15 K.

Benzene mixed with 1-Propanol				
Co-efficients	**303.15K**	**308.15K**	**313.15K**	**318.15K**
Excess Internal Pressure (π^E)				
A_O	0.2424	0.2015	0.1873	0.2447
A_1	0.2497	0.2066	0.1917	0.2521
A_2	0.2569	0.2118	0.1962	0.2595
A_3	0.2642	0.217	0.2006	0.2669
A_4	0.2715	0.2221	0.205	0.2743

σ	0.2787	0.2273	0.2095	0.2817
Excess free Gibb's Energy (G^{*E})				
A_O	0.2552	0.1695	0.2158	0.2011
A_1	0.2605	0.1722	0.2199	0.2047
A_2	0.2659	0.1748	0.2239	0.2083
A_3	0.2712	0.1774	0.228	0.212
A_4	0.2765	0.18	0.2321	0.2156
σ	0.2819	0.1826	0.2362	0.2192
Excess Enthalpy (H^E)				
A_O	0.2101	0.2061	0.2688	0.1717
A_1	0.2147	0.2106	0.2757	0.1749
A_2	0.2194	0.2151	0.2827	0.178
A_3	0.224	0.2196	0.2897	0.1811
A_4	0.2287	0.2241	0.2966	0.1843
σ	0.2333	0.2286	0.3036	0.1874

Fig -1: Plots of excess internal pressure (π^E) with the molefraction of **Benzene** in the binary combination of functional materials namely **(Benzene mixed with Ethanol)** at known four temperatures range from 303.15K,308.15K,313.15K and 318.15K.

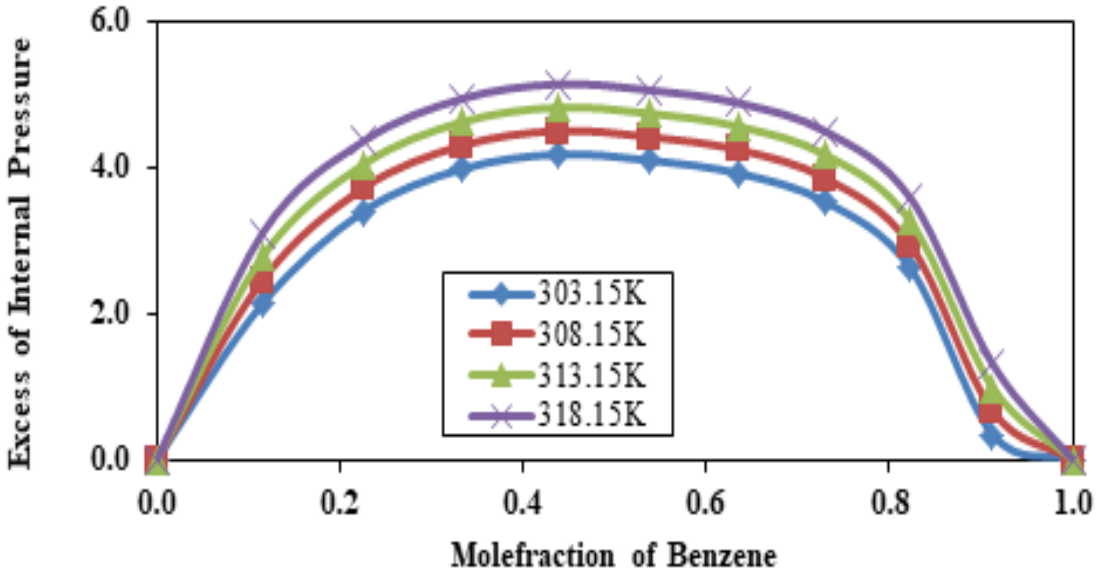

Fig 1: Excess Internal Pressure (π^E) variations with molefraction of Benzene in binary combination functional materials namely (Benzene mixed with Ethanol)

Fig -2: Plots of excess Gibb's free energy (G^{*E}) with the molefraction of **Benzene** in the binary combination of functional materials namely **(Benzene mixed with Ethanol)** at known four temperatures range from 303.15K,308.15K,313.15K and 318.15K.

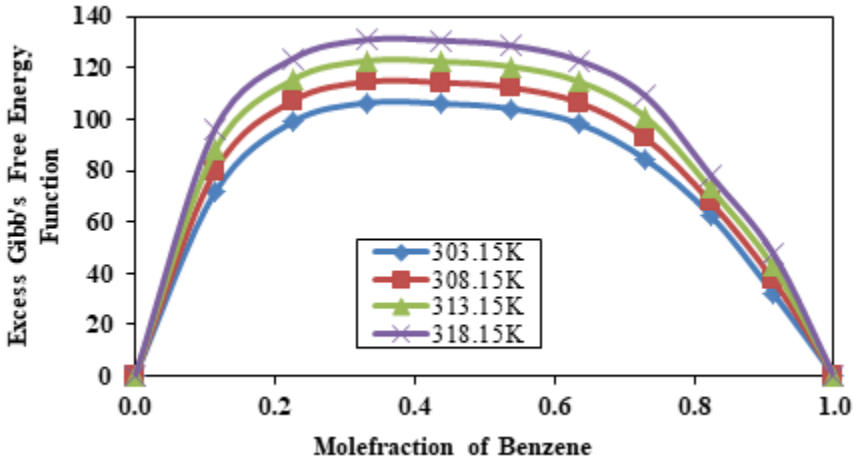

Fig 2: Excess Gibb's Free Energy of Activation(G^{*E}) variations with molefraction of Benzene in binary combination functional materials namely (Benzene mixed with Ethanol)

Fig -3: Plots of excess enthalpy (H^E) with the molefraction of **Benzene** in the binary combination of functional materials namely **(Benzene mixed with Ethanol)** at known four temperatures range from 303.15K,308.15K,313.15K and 318.15K.

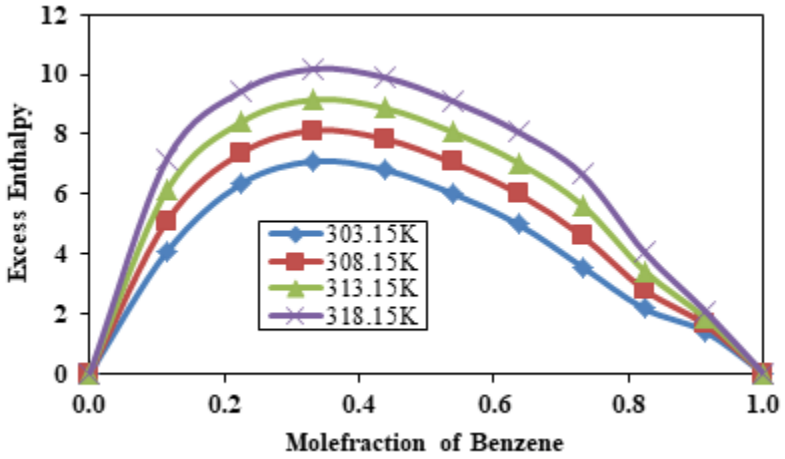

Fig 3: Excess Enthalpy (H^E) variations with molefraction of Benzene in binary combination functional materials namely (Benzene mixed with Ethanol)

The variations of Internal pressure excess value (π^E) with molefraction of Benzene in the functional chemical combination namely (Benzene mixed with Ethanol) at known four temperatures are as shown in Fig-1. These variations in excess internal pressure show positive trend entire molefraction of Benzene. Generally, positive values of excess internal pressure indicate existence of **strong type molecular interactions among the molecules** of liquid mixtures and negative values in excess internal pressure say that there is an existence of weak type of interactions among the molecules of liquid mixtures [17,18].

The variations of Gibb's free energy excess values (G^{*E}) with molefraction of Benzene in functional chemical combination namely (Benzene mixed with Ethanol) are represented in Fig-2. These variations from Fig-2 show positive trend. However positive excess Gibb's free energy function suggests the **occurrence of strong type of molecular interactions among the molecules of liquid mixtures** and the same result is supported by positive deviations in Redlich-Kister coefficients [19].

The variations of Enthalpy excess values (H^E) with molefraction of Benzene in functional chemical combination namely (Benzene mixed with Ethanol) liquid mixtures of binary combinations are represented in Fig-3.From Fig-3, H^E values are completely positive. The results suggest that, molecules are closely associated with each other in binary combinations when compared to individual pure liquids. It also implies that, **strong attractive type of molecular interactions** among component molecules such as hydrogen bonding, dipole-dipole type interactions and other type of interactions [20]. The Kind of same trend of result is observed in case of Redlich-Kister coefficients along with standard deviations The study of Redlich-Kister coefficients along with standard deviations also supports the variations of these figures at all the four known temperatures [21,22].

CONCLUSION

The excess thermo-acoustical factors namely excess free Gibb's energy (G^{*E}),excess internal pressure (π^E) and excess enthalpy (H^E) have been evaluated over the entire molefraction range of Benzene at four known temperatures range from 303.15K to 318.15K with an interval of 5K temperature difference. An analysis of these results suggests the **strong nature of Molecular interactions which is supported by Redlich –Kister coefficients with their standard deviations in functional chemical combination namely (Benzene mixed with Ethanol)** and also the interactions are becoming weak with the raise of temperature.

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