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Thermo-acoustic Redlich-Kister coefficients analysis in functional materials by excess parameters at temperatures 303.15K - 318.15K

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Acoustic thermodynamic analysis in the present work is an investigation of excess parameters and respective Redlich Kister coefficients at temperatures of 303.15K to 318.15K in liquid mixtures containing three different functional material groups of combinations such as benzene with toluene, benzene with o-xylene and benzene with mesitylene. The obtained corresponding excess acoustic parameters such as Gibbs free energy excess value (G^{*E}), enthalpy excess value (H^E) and internal pressure excess value (π^E) were computed from experimentally measured data. The results were helpful to obtain Redlich-Kister coefficients from a polynomial equation. Thermo acoustic excess parameters are discussed along with Redlich-Kister coefficients generally for investigating interactions among the molecules of liquid species.

Keywords*:* Redlich Kister coefficients; Benzene; Toluene; Mesitylene; Internal pressure.

INTRODUCTION

Clearly, the study of thermos-acoustic excess parameters is a highly important instrument in understanding interactions between molecules in a liquid mixture [1-9]. Molecular interactions frequently impact the study of shape and size. Research on the speed of sound and the corresponding thermo acoustic properties of liquids and liquid mixtures may help to understand molecular activity and their normal behavior [10-14]. The authors' purpose in this research is to study alterations in functional materials in three liquid compounds with binary combinations of thermo acoustic excess variables, Gibbs free energy (G^{*E}), enthalpy (H^E), and internal pressure (π^E) at four known temperatures ranging from 303.15K to 318.15K in liquid mixtures, namely, benzene with toluene, benzene with o-xylene, and benzene with mesitylene. Benzene may be used in glues, adhesives, cleaning products, paint strippers. xylene is also widely used as a cleaning agent, a thinner for paint, and in varnishes. Mesitylene is used in the laboratory as a specialty solvent. In the electronics industry, mesitylene is used as a developer for photopatternable silicones due to its solvent properties. Toluene is useful in paints, chemical reactants, rubber, adhesives (glues) and as a disinfectant. The irregularities of investigation indicate the presence of molecular interactions between the combination of distinct liquid molecules. Finally, the Redlich-Keister equation is allowed to apply. These findings were discussed in terms of molecular interactions along with the coefficients of thermo-acoustic parameters of their respective liquid mixture [15-17].

EXPERIMENTAL

To measure ultrasonic speeds, the ultrasonic pulse echo interferometer (Mittal Enterprises, India) was utilized; The measurements were made at a frequency of 3 MHz. The temperature was controlled using a thermal bath. For the research of liquid combination densities, a 10 mL specific gravity container was employed. To measure loads of liquid mixes, a computerized Shimadzu AUY220 (Japan) weight balance with an accuracy of $\pm$ 0.1 mg was used. An Ostwald's viscometer was utilized for evaluating the viscosities of liquid mixtures.

THEORY

Internal pressure excess value (π^E), Gibbs free energy excess value (G^{*E}), and excess enthalpy H^E were determined for the following individual combinations:

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

Internal pressure excess value is represented by π^E in this equation, π_1 and π_2 indicate the internal pressures of each pure liquid, respectively, whereas x_1 and x_2 represent the mole fractions of the first liquid and second liquid, respectively.

$$G^{*E} = G_{exp} - (x_1G_1 + x_2G_2) \qquad \text{Joule/mole}$$

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G^{*E} represents excess Gibbs free energy where G_1, G_2 are the free energies of the molecule of each pure liquid, and x_1 and x_2 are the mole fractions of the first liquid and second liquid, respectively.

$$H^E = H_{exp} - (x_1H_1 + x_2H_2)\ J/mole$$

where H^E stands for excess enthalpy. H_1, H_2 are the enthalpies of each pure liquid and the x_1 and x_2 are mole fractions of the first liquid and second liquid, respectively.

All of the following thermo-acoustic properties are allowed to fit the Redlich-Kister equation [18].

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

The Redlich-Kister equation's coefficient is A_i. The least squares approach was used to compute the coefficients. These coefficients are essential for improving excess parameter fit.

In addition, the standard deviation for each excess parameter Y^E was computed.

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

The sign of an excess thermo-acoustic parameter was utilized to analyze molecular interactions between the component molecules of liquid mixtures.

RESULTS AND DISCUSSION

The excess parameters π^E, G^{*E}, and H^E computed from the basic measurements and their Redlich-Kister coefficients, in benzene with toluene, benzene with o-xylene and benzene with mesitylene) are presented in Tables 1-3. The variations of these excess parameters with the mole fraction of benzene are presented in Fig, 1(a,b,c) to Fig. 3(a,b,c).

Figure 1 shows the variations in excess internal pressure (π^E) with mole fraction of benzene at four different temperatures. Excess internal pressure variations show a positive trend up to 0.8 mole fraction of benzene and negative trend above 0.8 mole fraction. It's worth noting that only the binary liquid mixture combination benzene and toluene has both positive and negative variations. That means both positive and negative trends for benzene and toluene liquid mixtures, whereas the other two binary liquid mixture combinations only have positive trends. The mixed trend of positive and negative variations in benzene-toluene combinations is caused by dispersive forces and dipole-induced dipole type interactions.

Table 1. Redlich-Kister coefficient values for a binary liquid mixture of benzene and toluene at four known temperatures: 303.15 K, 308.15 K, 313.15 K, and 318.15 K.

Benzene mixed with Toluene				
Co-efficient	**303.15K**	**308.15K**	**313.15K**	**318.15K**
Excess Internal Pressure (π^E)				
A_0	0.1499	0.1090	0.0948	0.1522
A_1	0.1572	0.1141	0.0992	0.1596
A_2	0.1644	0.1193	0.1037	0.1670
A_3	0.1717	0.1245	0.1081	0.1744
A_4	0.1790	0.1296	0.1125	0.1818
Σ	0.1862	0.1348	0.1170	0.1892
Excess free Gibb's Energy (G^{*E})				
A_0	0.1768	0.0911	0.1374	0.1227
A_1	0.1821	0.0938	0.1415	0.1263
A_2	0.1875	0.0964	0.1455	0.1299
A_3	0.1928	0.099	0.1496	0.1336
A_4	0.1981	0.1016	0.1537	0.1372
Σ	0.2035	0.1042	0.1578	0.1408
Excess Enthalpy (H^E)				
A_0	0.1270	0.1230	0.1857	0.0886
A_1	0.1316	0.1275	0.1926	0.0918
A_2	0.1363	0.132	0.1996	0.0949
A_3	0.1409	0.1365	0.2066	0.098
A_4	0.1456	0.141	0.2135	0.1012
Σ	0.1502	0.1455	0.2205	0.1043

Table 2. Redlich-Kister coefficient values for a binary liquid mixture, benzene mixed with o-xylene, at four different temperatures: 303.15 K, 308.15 K, 313.15 K, and 318.15 K.

Benzene mixed o-Xylene				
Co-efficient	**303.15K**	**308.15K**	**313.15K**	**318.15K**
Excess Internal Pressure (π^E)				
A_0	0.3545	0.3075	0.2407	0.1848
A_1	1.0823	0.856	0.8188	0.7831
A_2	0.4998	0.8181	0.9247	1.0891
A_3	0.2877	0.0798	0.0223	0.1165
A_4	0.2463	0.7814	1.0258	1.4343
σ	0.0235	0.024	0.025	0.0256
Excess free Gibb's Energy (G^{*E})				
A_0	0.9334	0.9302	0.9230	0.9193
A_1	0.1299	0.2323	0.2357	0.2750
A_2	-0.0060	0.1750	0.1972	0.3164
A_3	-0.5611	-0.7528	-0.6384	-0.7011
A_4	0.8779	0.4171	0.2708	0.2484
σ	0.0126	0.0126	0.0123	0.0126
Excess Enthalpy (H^E)				
A_0	0.4788	0.4447	0.4008	0.3786
A_1	0.5294	0.6819	0.7	0.7182
A_2	0.2327	0.0914	0.2138	0.313
A_3	0.9441	1.1863	1.1428	0.9815
A_4	1.0675	0.2979	0.0609	0.1381
σ	0.0208	0.021	0.0212	0.0214

Table 3. Redlich-Kister coefficient values for a binary liquid mixture of benzene and mesitylene at four known temperatures: 303.15 K, 308.15 K, 313.15 K, and 318.15 K.

Benzene mixed Mesitylene				
Co-efficient	**303.15K**	**308.15K**	**313.15K**	**318.15K**
Excess Internal Pressure (π^E)				
A_0	1.6357	1.5887	1.5219	1.466
A_1	0.1173	0.6436	0.4608	1.2165
A_2	1.781	2.0993	2.2059	2.3703
A_3	1.7689	1.2198	1.2773	1.3977
A_4	3.5275	1.5182	2.2138	2.8653
σ	1.3047	1.3052	1.3062	1.3068
Excess free Gibb's Energy (G^{*E})				
A_0	2.2146	2.2114	2.2042	4.1314
A_1	1.4111	1.5135	1.5169	3.1482
A_2	2.2173	1.4562	2.1204	1.5976
A_3	0.7201	2.2304	0.6428	0.5801
A_4	3.1679	1.6983	1.552	1.5296
σ	1.2938	1.2938	1.2935	1.2938
Excess Enthalpy (H^E)				
A_0	1.7600	1.7259	1.6820	1.6598
A_1	1.8106	1.9631	1.9812	1.7182
A_2	2.0669	1.3726	1.4950	1.5330
A_3	0.3455	0.1133	0.1568	0.3181
A_4	2.3487	1.5791	5.3421	1.1615
σ	3.3020	4.3022	1.3024	1.3026

Positive excess internal pressure values indicate the presence of a strong type of interactions between component molecules of the liquid mixture, whereas negative values indicate the presence of weak type interactions [19, 20]. Figure 2 depicts the changes in excess Gibbs free energy with mole fraction of benzene for all three functional materials combinations of liquid mixtures. For all three combinations, Fig. 2, variations are positive. Gibbs free energy function, which is confirmed by positive Redlich-Kister coefficients [21, 22], indicates the presence of strong molecular interactions among liquid mixture molecules. Excess enthalpy (H^E) changes in all three functional materials liquid mixtures of binary combinations with benzene mole fraction are presented in Fig. 3, according to which H^E values in the benzene-toluene combination are positive up to 0.8 mole fraction and negative for the remaining mole fraction ranges of benzene. The H^E values for the other binary combinations, on the other hand, are all positive. When compared to other pure fluids, the results show that the molecules in binary compounds interacted. It is also suggested that the most desirable types of interactions, such as hydrogen bonding, dipole-dipole type interchanges in excess actions, and others, take place between component molecules [23-25]. Redlich-Kiester coefficients and standard deviations follow the same pattern for benzene functional binary material combinations with toluene. Redlich-Kiester coefficients and standard deviations study at four known temperatures supports the latter two binary functional material combinations, with benzene-o-xylene and benzene-mesitylene liquid mixtures [26].

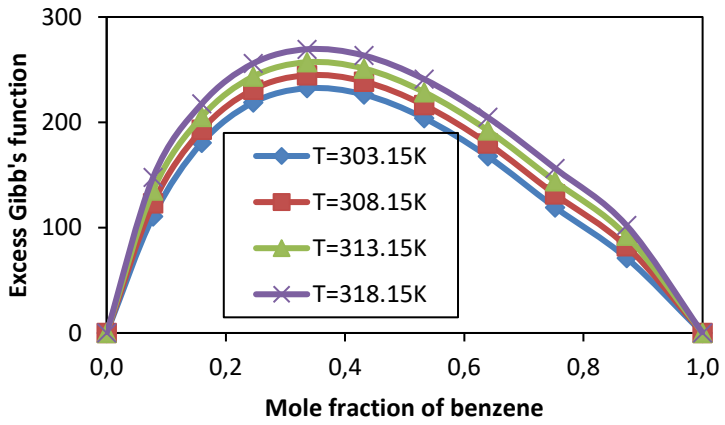

Fig. 2(a). Excess Gibbs free energy of activation (G^{*E}) varying with benzene mole fraction in the binary combination benzene mixed with toluene)

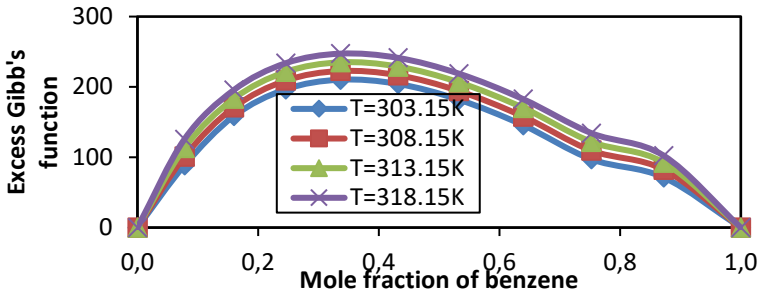

Fig. 2(b). Excess Gibbs free energy of activation (G^{*E}) varying with benzene mole fraction in the binary combination benzene mixed with o-xylene

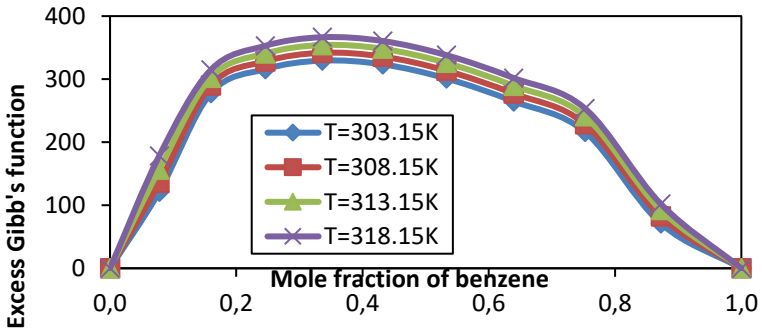

Fig. 2(c). Excess Gibbs free energy of activation (G^{*E}) varying with benzene mole fraction in the binary combination benzene mixed with mesitylene

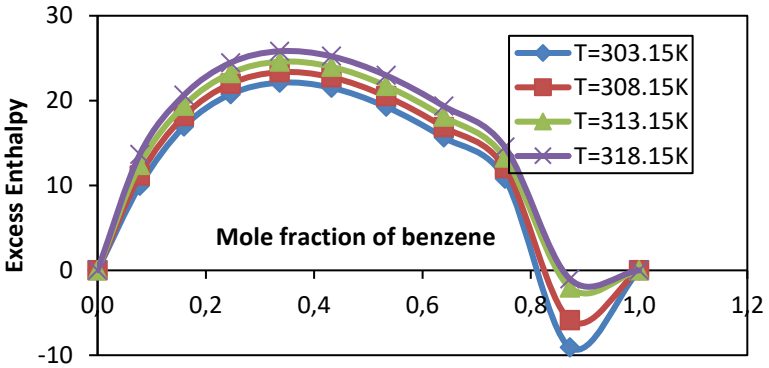

Fig. 3(a). Excess enthalpy (H^E) variations with benzene mole fraction in a binary combination of benzene mixed with toluene

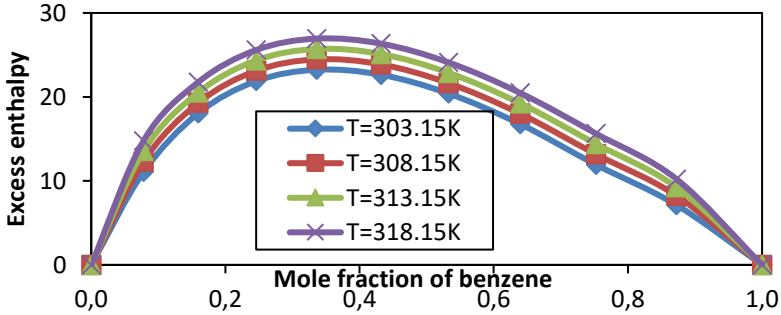

Fig. 3(b). Excess enthalpy (H^E) variations with benzene mole fraction in a binary combination of benzene mixed with o-xylene

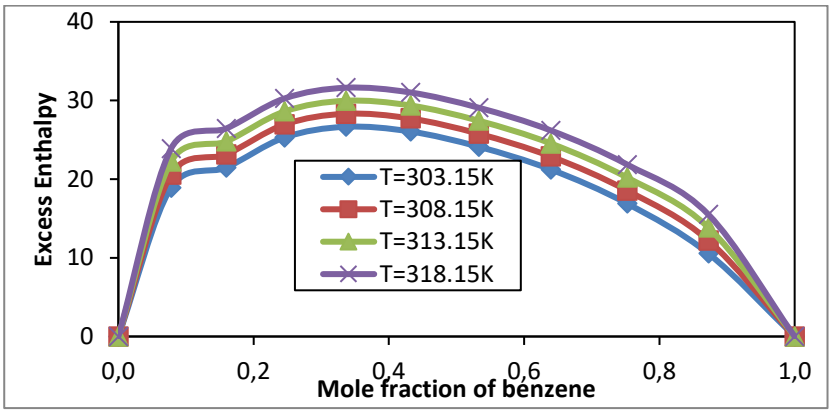

Fig. 3(c). Excess enthalpy (H^E) variations with benzene mole fraction in a binary combination of benzene mixed with mesitylene

CONCLUSION

Thermo-acoustic excess factors, namely excess free Gibbs energy (G^{*E}), excess internal pressure (π^E) and excess enthalpy (H^E), were determined across the total mole fraction of benzene at four known temperatures ranging from 303.15K to 318.15K. These findings show that interactions are strong in all three binary combinations of functional materials and become weak as temperature rises. The Redlich-Kister coefficient fluctuations and standard deviations back up these conclusions.

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