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MOLECULAR INTERACTIONS OF DIMETHYLSULFOXIDE WITH CHLOROBENZENE, BROMOBENZENE AND NITROBENZENE BY EVALUATION OF EXCESS ACOUSTICAL PARAMETERS AT 313K TEMPERATURES

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ABSTRACT:
Ultrasonic velocity (U), density (ρ) and viscosity (η) have been measured for binary mixtures of Dimethylsulfoxide with Chlorobenzene, Bromobenzene and Nitrobenzene at 313 K temperatures. The experimental data have been used to evaluate acoustical parameters such as adiabatic compressibility (β), free length (L_f), acoustic impedance (Z) and molar volume (Vm). Excess values of above parameters have been also evaluated, excess molar volume (V_m^E), excess intermolecular free length (L_f^E), excess adiabatic compressibility (β^E) and excess acoustic impedance (Z^E) at each temperature. These values are useful to understand molecular interactions of binary liquid mixtures.

***Keywords*:** *Excess acoustical Parameters, Acoustical properties, Molecular Interactions, Ultrasonic Technique.*

INTRODUCTION:

Molecular interactions play an important role in understanding the structures and properties of liquids. The molecular interaction study from the variation of acoustical parameters and their excess values with composition gives insight into the molecular process. In recent years, the theoretical and experimental investigations of excess and deviation functions are taken as interaction parameters to improve the results. This work is concerned to the systematic study of molecular interactions in the binary mixtures, which are important in many fields of industrial and biological processes. Mixed solvents find practical applications as they provide wide range of mixtures with desired properties.

In present work acoustical parameters of binary liquid mixtures of Dimethylsulfoxide with Chlorobenzene, Bromobenzene and Nitrobenzene are calculated at 313 K temperatures as a function of composition. A complete knowledge of thermodynamic and transport properties of these industrially imported mixtures are often required for their industrial applications. From the practical point of view the mixtures investigated are especially important because they are widely used as solvents for dyes, coloring raw materials in plastic industry used to make synthetic fibers and for aircraft and vehicles.

Experimental

All the chemicals were AR grade; purities of these chemicals were checked by density determination at 313 K which showed an accuracy of 0.0001 gm cm^{-3} as compared to reported values. Binary liquid mixtures were prepared in measuring flask. The density, viscosity and velocity were measured as a function of composition of binary liquid mixture at 293-313 K. The density of sample was measured using digital densitometer (Rudolph) with an accuracy of 0.0001. An Ostwald's viscometer was used for the viscosity measurements. An ultrasonic interferometer having the frequency 2 MHz was used for ultrasonic velocity measurements. An electronically operated constant temperature bath was used to circulate water through measuring cell made up of steel containing experimental solution at 293-313 K temperature.

Theoretical

Various acoustical parameters were calculated from measured data by using following equations

Adiabatic compressibility (β) = $1/U^2 . \rho$ … (1)

Intermolecular Free length (L_f) = K. $\beta^{1/2}$ (2)

Where K is temperature dependant constant, value of K is 642 X 10^{-6} at 313 k.

Acoustic impedance (Z) = $U\rho$ …….. (3)

Molar Volume (V) = $(M_{eff} . U / K.\eta)^{3/}$… (4)

Where M is mean molecular weight. It is calculated as

$M = X_1M_1 + X_2M_2$

X_1 and X_2 are mole fractions and M_1, M_2 are molecular weights of constituent components of binary liquid mixtures.

Excess parameters were calculated from following equations

$Y^E = Y_{exp.} - (X_1Y_1 + X_2Y_2)$ ………… (5)

Where,

$Y_{exp.}$ = experimental values of mixtures

Y_1 & Y_2 = values of parameters for liquids 1 and 2 respectively.

X_1 & X_2 = mole fractions of liquid 1 and 2 respectively.

Graphs:

The excess values of the intermolecular free length, adiabatic compressibility, acoustic impedance and molar volume plotted against mole fraction of Dimethylsulfoxide (DMSO) with Chlorobenzene (CB), Bromobenzene (BB) and Nitrobenzene (NB) at temperatures 313K.

MATERIALS AND METHODS:

1.1. Study site

In West Bengal, Asansol (23.673^{0}N, 86.952^{0}E) which is situated in the Western part of Burdwan district of West Bengal in the eastern India (Fig. 1), is the second largest city of the state. It is also known as 'coal mining city' because, the entire region of Asansol sits on layers and layers of coal. The coal is of high-quality superior coal.

Over the last ten years there was hectic develo pment in the area in terms of industrieslike Indian Iron and Steel Company (IISCO), Burnpur Cement Limited (BCL), Dishergarh Power Supply Company limited, Joy Balaji Sponge Iron Private Limited, Shyam Gel Limited (Power Divisions) etc. In Asansol the ambient air quality has rapidly deteriorated[19-21] due to mainly for industrialization, modernization and urbanization, which is affecting human population, other animals and plant communities.

1.2. Data sources and analysis

In this study, five parameters like CO, SO_2, NO_2, PM2.5 and PM10 have been considered to evaluate the deviation of air quality before and after lockdown period (January 1, 2020 to July 31, 2020). The secondary data of above-mentioned selected pollution parameters has been obtained from the Central Pollution Control Board (CPCB), Govt. of India. The maps regarding variation of NO_2 and aerosol concentration over India have been obtained from European space agency (ESA) and the National aeronautics and Space Administration (NASA) individually[22-23]. The five parameters

(CO, SO_2, NO_2, PM2.5 and PM10) measured from January 1, 2020 to July 31, 2020 were subject to ANOVA using SYSTAT.

Positive deviations of Lf^E, Vm^E, Z^E, and β^E in binary systems have been attributed to dispersion forces and negative deviation is due to dipole-dipole and induced dipole interactions. Dispersion forces are operative in all systems, but since more than one type of interactions are present between the components, the excess values are the net result of all type of contributions.

Fig.1, 2 and 3 shows β^Evalues for all the binary mixtures of DMSO. The values of β^E in the mixtures of DMSO are less negative for CB and BB but positive for NB. The observed facts are attributed mainly to strong dipole-dipole and dipole-induced dipole interactions of binary liquid mixtures of DMSO **[16]**.

Fig. 1, 2 and 3 shows L_f^Evalues for all the binary mixtures of DMSO. The values of L_f^E are positive for all binary liquid mixtures DMSO with CB, BB and NB. The positive values are attributed to the fact that the dispersive forces developed in the binary mixtures of DMSO.

V_m^E values are negative for all binary mixtures of DMSO with CB and BB except DMSO + NB. The negative V_m^E values are attributed to strong dipole-dipole interactions between the unlike molecules in the mixtures. The positive values of DMSO + NB may be due to the fact that Nitro group of nitrobenzene is electron withdrawing while in case of other groupsit is electron donating.

Z^E values are positive for almost all mixtures of DMSO with CB/BB/NB. The positive value reflects weak interactions between the unlike molecules.

CONCLUSION:

The values of all excess parameters show small deviations for the binary mixtures of DMSO with CB/BB/NB. From excess parameters following trends are observed in different solvents-

Chlorobenzene > Nitrobenzene > Bromobenzene

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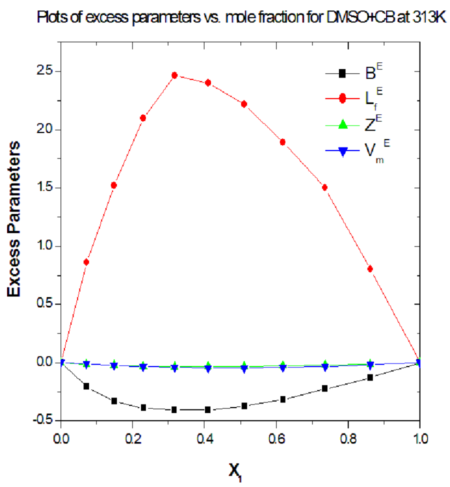

Fig.1. Plot for DMSO+CB

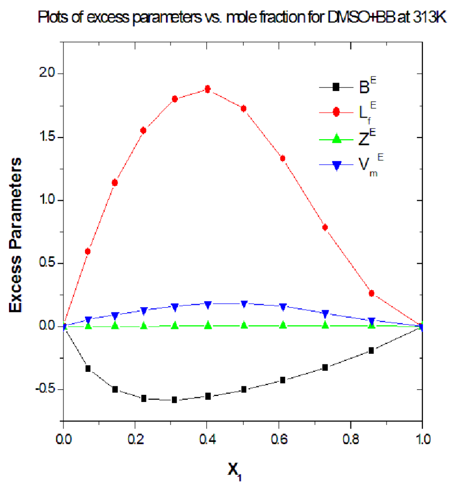

Fig.2. Plot for DMSO+BB

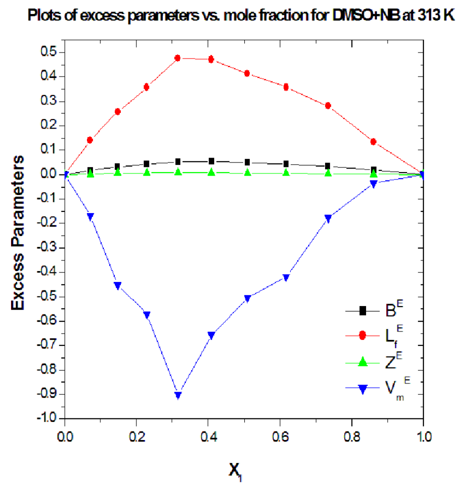

Fig.3 .Plot for DMSO+NB