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STUDY OF MOLECULAR INTERACTIONS THROUGH PHYSICO-CHEMICAL STUDY OF POLAR POLAR LIQUIDS

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ABSTRACT:

Excess parameters viz. excess viscosity and excess density of (DMSO) Dimethyl sulphoxide + iso-Butanol mixtures over the entire range of concentration at 303.15 K were calculated from experimental viscosity and density data. Excess density and excess viscosity reveals positive deviations due to strong heteromolecular interactions arised due to strong hydrogen bonding. Size and functional group differences of the unlike molecules. The excess parameters were fitted to the Redlich-Kister polynomial equation. These excess parameters plays vital role to reveal the effects of specific type of interactions. R K Fit equation shows good agreement between experimental and calculated data.

KEYWORDS: Excess Viscosity, Excess density, intermolecular interactions.

1. INTRODUCTION

Dimethyl sulfoxide (DMSO) is an organosulfur compound with the formula $(CH_3)_2SO$. It is an important polar aprotic solvent that dissolves both polar and nonpolar compounds.

DMSO is widely used as a solvent for various chemical reactions. It also entensively used in biopreservation especially stem cell banking. DMSO plays vital role in sample management and high-throughput screening operations in drug design. In medical research, DMSO is often used as a drug vehicle in vivo and in vitro experiments. DMSO is used to preserve organs, tissues, and cell suspensions.

iso-Butanol has a variety of technical and industrial applications. iso-Butanol is used in the production of lacquer and similar coatings, and in the food industry as a flavoring agent. Iso butanol is alcohol having hydroxyl group at secondary position. The investigations regarding the molecular association in organic binary mixtures having iso-Butanol as one of the components is of particular interest, since iso-Butanol is highly polar protic liquid and can associate with any other group having some degree of polar attractions. DMSO is aprotic, strongly associated due to highly polar molecule. Unsaturation character and presence of sulphoxide grope in DMSO and hydroxyl group in iso-Butanol creates remarkable interest in this system. Both the liquids have enormous applications in various fields at the same time both the liquids are also used in medicine and pharmacy. This also adds specific interest towards this system.

Physicochemical properties like density and viscosity for liquid mixtures are important from practical as well as theoretical points of view. Experimental measurements of these physicochemical properties for binary mixtures have increased much importance in many chemical industries and engineering fields [1-4]. Prediction of the complex structure, dynamics of butanol mixture is possible with the experimental findings. Therefore, experimental measurements are needed to understand the fundamental behavior of this property.

2. EXPERIMENTAL DETAILS

CHEMICALS

In the present system of DMSO + iso-Butanol binary mixture DMSO, iso-Butanol and both are of HPLC grade. Both the liquids are used without further purification. The liquid mixtures of different composition were prepared by measuring appropriate volumes of each composition.

DENSITY MEASUREMENT

The Density measurements were carried out by portable Digital Density meter (DMA-35, Anton Paar) for pure liquids and binary mixture. This

Digital Density meter uses the vibrating U-tube principle to calculate the Density of the sample. The required quantity of sample is approximately 2ml. (the temperature of the sample is controlled by environmental temp around U-tube/sample cell). The measured values of pure liquids are found to be in good agreement with standard values. Accuracy of the instrument used is =0.0001 g/cm^3. The instrument is calibrated by various pure liquids and found to be in good agreement with literature/standard values.

VISCOSITY MEASUREMENT

Viscosity of the sample in the present study were measured by using Brookfield Viscometer (Brookfield Viscometer, Model: LV DV-II+ Pro, Cone-plate Model with CPE-40 spindle).The required sample is very low in quantity (0.5ml). The device is calibrated using the doubly distilled water and other pure liquids of known viscosity at 25^{0}C room temperature and found to be in good agreement with standard value from literature. The accuracy of the instrument is =0.01cP. The sample cell of the instrument is double walled, and electronically operated programmable constant temperature water bath is used to circulate water through the double walled measuring cell made up of steel containing the experimental liquid at the desired temperature.

3. RESULTS AND DISCUSSION

Table 1 Density, viscosity of DMSO + iso- Butanol at 303K

Volume fraction of iso butanol	Density	Viscosity
0	1.093	2.97
0.1	1.081	2.9
0.2	1.071	2.83
0.3	1.048	2.75
0.4	1.021	2.65
0.5	0.978	2.51
0.6	0.935	2.36
0.7	0.898	2.23
0.8	0.865	2.11
0.9	0.832	2
1	0.801	1.88

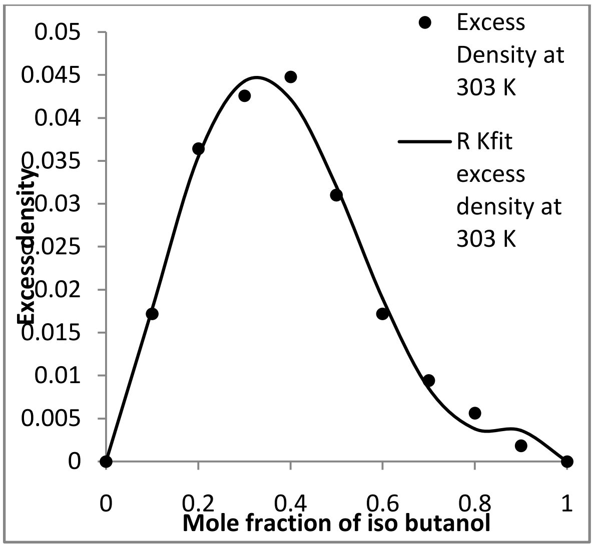

Fig. 1 *Excess Density of DMSO+iso-Butanol at 303K*

Fig 1 gives Excess Density of DMSO+iso-butanol. As concentration of iso-Butanol increases excess density becomes positive. Iso-butanol molecule cooperates with DMSO molecule. Positive values indicate that volume contraction takes place upon mixing due to strong association between dissimilar molecules via hydrogen bonding. Positive values also attributed to strong interaction between unlike molecules through hydrogen bonding[3-4].

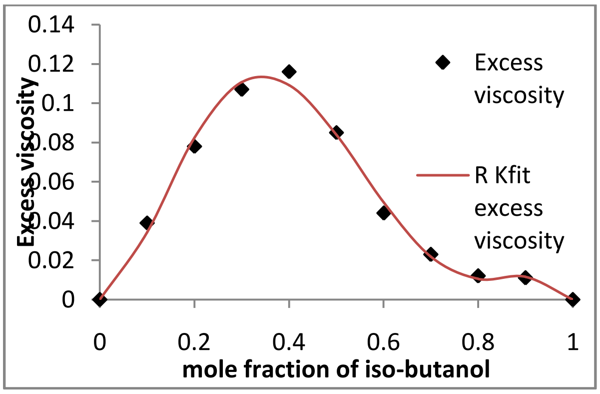

Fig. 2 *Excess Visocity of DMSO + iso-Butanol at 303K*

Fig 2 gives Excess Viscosity of DMA+ n-butanol. Positive values of η^E for the mixture can be explained on the basis of complex formation between unlike molecules through hydrogen bonding. Charge transfer, hydrogen bonding forces leading to the formation of complex species between unlike molecules results in positive deviation. Positive deviation of η^E indicates that the interaction between binary mixture is strong.

Electronegative oxygen atom from sulphoxide group of DMSO attracts hydrogen of iso butanol and forms hydrogen bonding between them. Probable hydrogen bonding structure of DMSO + iso-butanol is shown in fig 3.

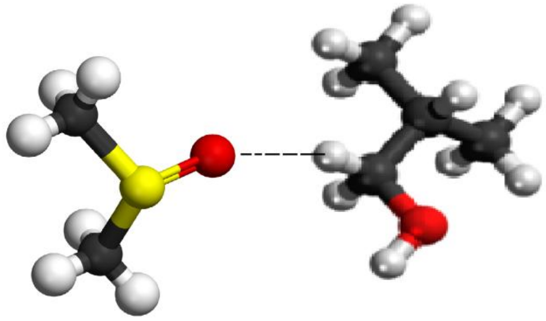

Fig. 3 *Hydrogen bonding structure of DMSO + iso-Butanol at 303K*

Table 2 Quantitative data R K coefficient and Standard error for Excess Density, Excess viscosity of DMSO + iso- Butanol at 303K

	a_0	a_1	a_2	a_3	Standard Error
Excess Density	0.12	-0.25	-0.014	0.23	1.79E-03
Excess viscosity	0.33	-0.65	-0.12	0.77	4.42E-03

4. Conclusions

In this study, the measurement of density, viscosity of DMSO in iso-Butanol solution was studied in different concentrations at 303K. The experimental data and excess parameters contain valuable information regarding the solute-solvent interactions in the measurements, it can be concluded that the concentration of the iso-Butanol affects and gives rise to strong hydrogen bonding interaction. Increase in concentration of iso-Butanol plays an important role in forming hydrogen bonding interactions in the solutions. Both the parameters supports each other and conforms that with increase in concentration of iso-Butanol the strength of hydrogen bonding in the system increases

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