



## THE STUDY OF EXCESS REFRACTIVE INDICES OF BENZENE+ETHANOL AND HEXANE+ETHANOL BINARY SYSTEMS

Dilbar Bozorova<sup>1</sup>, Shukur Gofurov<sup>2</sup>, Kokhkharov A. M.<sup>1</sup> & Oksana B. Ismailova <sup>3,4\*</sup>

<sup>1</sup>Ion-plasma and Laser Technologies Institute, Tashkent, Uzbekistan

<sup>2</sup>University of Tsukuba, Japan

<sup>3</sup>Turin Polytechnic University in Tashkent, Uzbekistan

<sup>4</sup>Uzbek-Japan Innovation Center of Youth, Tashkent, Uzbekistan

\*  [oismailova56@gmail.com](mailto:oismailova56@gmail.com)

 Oksana B. Ismailova: <https://orcid.org/0000-0001-8972-546X>

### ABSTRACT

*In many technological processes, ethanol solvents and their mixtures are actively used to prepare nanostructured matrices, substrates and devices. A change in the concentration of one of the components leads to a change in the structure as a whole, affecting a number of quantities, such as the electrical conductivity of solutions, the diffusion coefficient, and the thermodynamics of processes, which is important to take into account when selecting optimal systems that use new nanomaterials with predetermined properties and characteristics for targeted preparation. The most informative method in the study of structural processes associated with the cluster formation of molecules is the method of refractometry. In this work, the refractive indices measured for binary system benzene+ethanol and hexane+ethanol at the 298.15K and the atmospheric pressure are reported. The refractive indices were measured over a wide range of benzene, hexane and ethanol concentrations (0÷1.0 mole fractions). It has been shown that hetero-molecular complexes in binary solutions are formed through  $\pi \cdots HO$  bonding at concentration of ~0.4 a mole fraction of benzene and through H-bonding at concentration of ~0.5 mole fraction of hexane. Relatively weak interactions are determined at concentration of ~0.2 and ~0.7 mole fraction of benzene.*

**Keywords:** *Refractometer, Heteromolecular Structure, Cluster Formation, Binary System, Hydrogen Bond, Excess Refractive Index, Weak Molecular Interactions, Mole Fraction.*

## Introduction

Ethanol and its mixtures widely used for forming clathrate of hydrogen storage. The unique properties of ethanol, it can be used for creating both the clathrate cavities and the clathrate host lattice (Strobel *et al.*, 2008; Woo *et al.*, 2018). Benzene solutions are used in a variety of advanced functional materials, namely for metal catalyzed chemistry and for transition metal free synthesis (Panwar *et al.*, 2020). Benzene and hexane were found as typical adsorbents for ordered mesoporous carbon for further usage an adsorbent for volatile organic compound (VOC) disposal (Wang *et al.*, 2015). Their mixture with ethanol successfully used for different processes in creating materials for nano devices. For example, benzene-ethanol was explored to realize the enhanced textural properties of nano crystalline ZSM-5 (~20 nm) (Saxena *et al.*, 2016) and preparation of graphene/metal-organic composites and its adsorption quality for benzene and ethanol was examined (Liu *et al.*, 2015). Thermodynamic properties of binary solutions would be helpful in getting information about the molecular structure and molecular interactions in liquid mixtures.

Refractometry is a sensitive method to identify structural states of solutions. The advantages of this method are high accuracy and quick determinations of parameters of a substance. It is crucial to determine concentration at which cluster formation is stable. In this report, complex formation between the alcohol and solvent molecule and association of alcohol molecules are

studied from refractometry method. In this work, we present the new experiment measurements of refractive index for the binary mixtures of ethanol + benzene and hexane + ethanol. Deviation in refractive index has been identified to be an essential parameter for characterization and understanding the thermodynamic properties of solutions

## Materials and Methodology

Benzene, Ethanol (99.9%, Sigma-Aldrich, USA).

Ethanol solutions of benzene were prepared by gravimetric method (Yang *et al.*, 2018).

The data were obtained by using the RX-7000-alpha digital refractometer with the temperature recording function (Atago, Japan). The measurement error of  $n$  is less than 0.0001. The measurement time of both  $n$  and temperature of solutions took less than 20 seconds. For the refractive index measurements, benzene-ethanol solutions were prepared in a concentration range of 0÷1.0 mole fraction. For each solution, at least three values were measured at a fixed A temperature of  $298.15 \pm 0.05$  K. The final result was obtained by averaging over the entire series of measurements

## Results and Discussion

Experimental refractive indices  $n$  and excess refractive indices  $n^E$  at temperature of 298.15K and atmospheric pressure for benzene + ethanol binary liquid mixture are listed in **Table 2**. A comparison of our experimental values of refractive index with the data reported in literature for-

**Table 1: Comparison of experimental refractive indices with the literature data for pure liquids at 298.15K**

Liquid	Refractiveindex (n)	
	This work	Literature
Hexane	1.3734	1.3790 (Aliaj <i>et al.</i> , 2016)
		1.3721 (Blanco <i>et al.</i> , 2012)
		1.37234 (Orge <i>et al.</i> ,1997)
Ethanol	1.3581	1.3593 (Aliaj <i>et al.</i> , 2016)
		1.3592 (Blanco <i>et al.</i> , 2012)
		1.37234 (Orge <i>et al.</i> ,1997)
Benzene	1.4898	1.4966 (Aliaj <i>et al.</i> , 2016)

**Table 2: Experimental mole fraction  $x$ , refractive index  $n$ , excess refractive index  $n^E$  and excess refractive index for benzene + ethanol and hexane + ethanol.**

$x$ ,hexane	$n$	$n^E$	$x$ , benzene	$n$	$n^E$
0.000000	1.3600	0.0000	0.000000	1.3581	0.0000
0.046979	1.3612	0.0006	0.059661	1.3681	0.0021
0.099840	1.3620	0.0007	0.124922	1.3827	0.0081
0.159761	1.3628	0.0007	0.196608	1.3947	0.0107
0.228257	1.3638	0.0007	0.275719	1.4046	0.0102
0.307313	1.3655	0.0014	0.363471	1.4213	0.0153
0.399572	1.3681	0.0027	0.461361	1.4322	0.0133
0.508645	1.3683	0.0015	0.571253	1.4469	0.0136
0.639589	1.3722	0.0036	0.695501	1.4641	0.0144
0.799715	1.3731	0.0024	0.837112	1.4767	0.0084
1.000000	1.3734	0.0000	1.000000	1.4898	0.0000

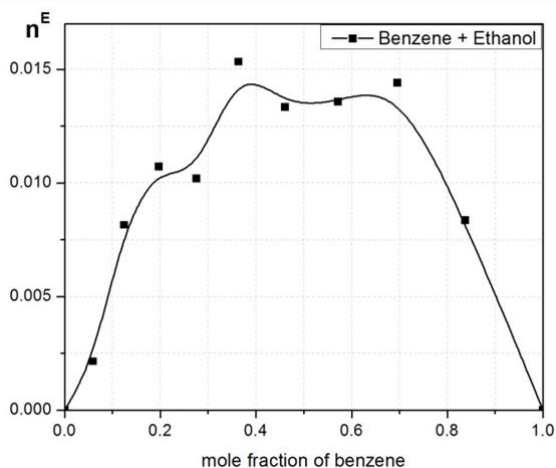
-the pure liquids at 298.15K is shown in **Table 1**. A good agreement is found between the values in our work and those reported in literature.

Evidently, the refractive index of the binary liquid mixture increases with increasing mole fraction of benzene. Excess refractive index  $n^E$  calculated by the formula [1]:

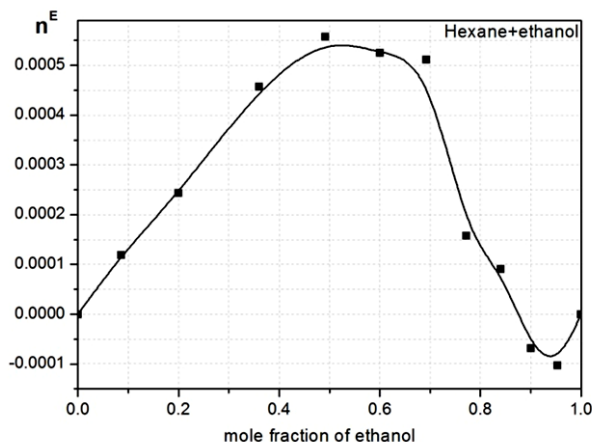
$$n^E = n_{solution} - (x \cdot n_1 + (1 - x) \cdot n_2) \quad [1]$$

The systems of hexane+ethanol in which only self-association between alcohol molecules occurs. In ethanol-rich **Fig. 1 & 2** represent experimental data of excess refractive index from different concentration binary mixtures of benzene-ethanol. The first peak at the ~0.2 mole fraction characterizes dispersive weak interaction between benzene molecules and corresponds to the stretching and breaking of molecular associates present in the pure liquids. In addition to these effects, the dispersion forces were also expected to operate

between unlike molecules. The maximum value of excess refractive index at ~0.4 mole fraction of benzene indicate that complex formation occurred through  $\pi \cdots \text{HO}$  bonding between the  $\pi$ -electron cloud of the aromatic ring of benzene and the proton of the hydroxyl group of ethanol.



**Figure 1: Changes of excess refractive index  $n^E$  on mixing for freshly prepared benzene-ethanol solutions.**



**Figure 2: Changes of excess refractive index  $n^E$  on mixing for freshly prepared hexane-ethanol solutions.**

The third peak at a concentration of ~0.7 mole fraction of describes the hydrogen bond between ethanol molecules and there are no strong specific interactions between components of the mixtures. This polar liquid is strongly self-associated through hydrogen bonding ( $\text{OH} \cdots \text{HO}$  interactions).

Significant structural effects are absent to due to lack of hydrogen bond. Stable heteromolecular complexes are formed in solutions with a concentration of ~0.5 mole fraction of hexane. This is confirmed by extreme values of excess refractive index of hexane-ethanol solutions (Fig. 2).

### Conclusion

It was shown that with a change in the concentration of benzene in ethanol solutions, a restructuring of the solution occurs, accompanied by a local reorganization of the formed complexes and associates. From the experimental results, the deviations in refractive index,  $n^E$ , were calculated and  $n^E$  was positive for the solution. Results on the excess refractive index gave information about heteromolecular structures due to  $\pi \cdots \text{HO}$  bond which occur at the concentration ~0.4 mole fraction of benzene. Also, the graphics showed that there are weaker complexes at the concentration ~0.2 and ~0.7 mole fractions of benzene, respectively.

### Acknowledgement

This work was financially supported by Grant No. OT-F2-51 for the fundamental investigations of the Academy of Sciences

of Uzbekistan and by Grant No.VA-FA-F6-010 Ministry of Science and Technology of the Republic of Uzbekistan.

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