Preferential Solvation in Binary Liquid Mixtures with Norbornadiene

Richa Verma1

1 Department of Physics JSS Academy of Technical Education , Dr. A.P.J. Abdul Kalam Technical University, C-20/1, Sector 62, NOIDA, Uttar Pradesh 201301, India

Email richaverma@jssaten.ac.in

**Abstract**. Norbornadiene has been found useful in organic and polymer synthesis and recently its mixtures have been found useful in solar energy storage. Concentration structure factors Scc(0 help to identify structure and binding at microscopic level and also play a significant role in understanding and characterizing exchanges in liquid systems. Preferential solvation Parameter ij provides information about deviation from ideal behavior for the solvent. In this work concentration concentration structure factors Scc(0) and preferential solvation Parameter ij were evaluated of binary Liquid Mixtures of Norbornadiene with Benzene, Cyclohexane, Decane, and Carbon Tetrachloride using Kirkwood Buff formalism. For the said binary mixtures experimental data pertaining to the calculations were taken from literature. Obtained results indicate that molecules which tend to form dipole interactions or hydrogen bonds form favourable interactions as seen in Norbornadiene + carbon tetrachloride where the small molecule of CCl4 is not sterically hindered to approach the polar Norbornadiene molecule. Long chain and ring structure of carbon have a negative influence on hetero interactions. Studying these parameters will develop predictive techniques to determine the right composition at which the binary system will give optimum efficiency.

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Excess thermodynamic properties are of great importance,  
especially in the development of new classical and statistical  
theories of solutions. Rarely are all the data necessary to test  
the new theories available in the literature. It is, therefore,  
very important to derive equations which interrelate the different excess thermodynamic functions; knowledge of some  
of these properties permits the evaluationof the others.

Density functional calculations with the hybrid B3LYP functional have been used to study the ground state of  
norbornadiene bound to the photosensitizer [Cu(8-oxoquinolinato)]. The main bonding interaction between the  
ligand and the metal is *π* back-donation, metal to ligand, which reduces the *π*-*π*\* band gap in norbornadiene.  
CIS calculations performed on free norbornadiene and on the system where norbornadiene interacts with the  
photosensitizer have shown that the photosensitizer reduces the excitation energy to promote the system to the  
first excited singlet state. In terms of wavelength, this difference implies that light with *λ* almost 100 nm longer  
can be used to photoactivate the norbornadiene with respect to free norbornadiene

**Kirkwood-Buff Integrals and structure factor for binary mixtures of ionic** 1  
**liquid with 1-alkanol** 2

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| **Zohrab Khedri, a Mohammad Almasi, \*b Afsaneh Maleki a** | 3 |
| ***a*** *Department of Chemistry, Islamic Azad University, Omidiyeh Branch, Omidiyeh, Iran* | 4 |
| ***b*** *Department of Applied Chemistry, Faculty of Science, Malayer University, Malayer, 65174, Iran.* | 5 |
| *Corresponding Author Email: m.almasi@malayeru.ac.ir* | 6 |
| **Abstract**: In this paper, we have tried to describe the factors affecting molecular interactions and | 7 |
| structure of binary systems including 1-Hexyl-3-methylimidazolium Nitrate ([Hmim][NO3]) and 1- | 8 |
| alkanol (1-hexanol, up to 1-decanol) using Kirkwood-Buff (KB) integrals and structure factor. | 9 |
| Obtained results indicate that unlike molecules tend to form favorable interactions via forming | 10 |
| hydrogen bonds or dipolar interactions and stay alongside, while an increase in the carbon chain of 1- | 11 |
| alkanols reduces the strength of bonds and tendency of the unlike molecules to stay together. | 12 |
| Moreover, the structure of mixtures was studied using the concentration-concentration structure | 13 |
| factor, *SCC* (0) . Results from the application of this parameter show that in all binary mixtures, | 14 |
| heterocoordination is predominant, ordering occurs in solutions and fluctuations are less than random | 15 |
| orientation. In addition, the chemical short-range order parameter α′, which is an important function to | 16 |
| understand the complex formation and phase segregation in the liquid mixtures, was calculated and | 17 |
| discussed for mentioned mixtures. For current binary mixtures, experimental data and theoretical | 18 |
| investigations are novel and reported for the first time. | 19 |
| Keywords: Molecular interactions, KB integrals, structural factor, ionic liquid |  |