Properties of Binary Mixtures of Ionic Liquid And Cyclic Ethers

Kuldeep Kumar Solanki

Research Scholar, Department of Chemistry, Baba Mastnath University Rohtak

Dr Arpna

Assistant Professor, Department of Chemistry, Baba Mastnath University Rohtak

Dr Sunil Kumar Jangra Assistant Professor, Department of Chemistry, AIJHM College Rohtak

Abstract - Binary mixtures of ionic liquids (ILs) and cyclic ethers have garnered considerable interest due to their unique and tuneable properties, which make them suitable for a wide range of applications in fields such as green chemistry, catalysis, electrochemistry, and materials science. This paper comprehensively presents the physicochemical properties of these binary mixtures, including their phase behaviour, solvation capabilities, viscosity, density, thermal stability, and electrical conductivity. The interactions between ILs and cyclic ethers are explored to understand how they contribute to the enhanced performance of these mixtures in various applications. Additionally, the influence of the molecular structure of both ILs and cyclic ethers on the properties of the mixtures is discussed, along with the potential for future developments in this area.

Key words IL, cyclic ethers

I. INTRODUCTION

Ionic liquids (ILs) have been widely recognized for their unique properties, such as low volatility, high thermal stability, and excellent solvation capabilities. These properties have made ILs attractive for a variety of applications, ranging from solvents in chemical reactions to electrolytes in electrochemical devices. However, ILs often exhibit high viscosity, which can limit their practical use in some applications. To overcome this limitation, the mixing of ILs with other solvents, such as cyclic ethers, has emerged as a promising approach to tailor the properties of ILs for specific applications.

Cyclic ethers, such as tetrahydrofuran (THF) and 1, 4-dioxane, are well-known for their low viscosity, moderate polarity, and ability to dissolve a wide range of compounds. When mixed with ILs, cyclic ethers can significantly reduce the viscosity of the resulting binary mixtures while maintaining or even enhancing other desirable properties. This combination of ILs and cyclic ethers creates a synergistic effect, leading to mixtures with unique and tuneable properties that are not attainable with the pure components alone.

This paper aims to provide a comprehensive overview of the properties of binary mixtures of ILs and cyclic ethers. The focus will be on understanding the key physicochemical properties of these mixtures, such as phase behaviour, viscosity, density, thermal stability, and electrical conductivity. Additionally, the molecular interactions between ILs and cyclic ethers will be examined to elucidate the mechanisms underlying the observed properties. The potential applications of these binary mixtures in various fields will also be discussed, highlighting the importance of understanding their properties for the development of new technologies.

1. Phase Behaviour

1.1. Phase Diagrams and Miscibility

The phase behaviour of binary mixtures of ILs and cyclic ethers is a critical aspect that determines their suitability for various applications. Phase diagrams are typically used to represent the miscibility and phase transitions of these mixtures over a range of temperatures and compositions. Studies have shown that the miscibility of ILs and cyclic ethers can vary widely depending on the specific IL and cyclic ether used, as well as the temperature and pressure conditions.

1.2. Liquid-Liquid Equilibria

The liquid-liquid equilibria (LLE) of IL-cyclic ether mixtures are particularly important in separation processes. The presence of multiple liquid phases can be exploited for the selective extraction of compounds from complex mixtures. The LLE behaviour of these binary mixtures is influenced by the nature of the IL's cation and anion, as well as the structure of the cyclic ether.

II. SOLVATION PROPERTIES

2.1. Solubility of Solutes

One of the key advantages of IL-cyclic ether mixtures is their ability to dissolve a wide range of solutes, including both polar and non-polar compounds. The solvation properties of these mixtures are highly tuneable, depending on the specific IL and cyclic ether used. The presence of both ionic and non-ionic components in the mixture allows for the dissolution of diverse solutes, making these mixtures versatile solvents for chemical processes.

2.2. Hydrogen Bonding and Dipole Interactions

The solvation properties of mixtures of ionic liquids (IL) and cyclic ethers are significantly influenced by hydrogen bonding and dipole interactions. The strength and nature of these interactions depend on the specific functional groups present in the IL and the cyclic ether, as well as the overall polarity of the mixture. These interactions can be adjusted to improve the solubility of particular solutes or to regulate the selectivity of solvation in complex mixtures.

III. VISCOSITY AND TRANSPORT PROPERTIES

3.1. Viscosity Reduction

A major motivation for mixing ILs with cyclic ethers is to reduce the viscosity of the resulting mixture. High viscosity is a common issue with pure ILs, which can limit their use in applications requiring efficient mass and heat transfer. The addition of cyclic ether can significantly lower the viscosity of the mixture, improving its flow properties and making it more suitable for use in processes such as liquid-liquid extraction, catalysis, and electrochemical applications.

3.2. Diffusion and Conductivity

The transport properties of IL-cyclic ether mixtures, including diffusion coefficients and electrical conductivity, are closely related to their viscosity. Lower viscosity typically leads to higher diffusion rates and improved ionic conductivity, making these mixtures attractive for use as electrolytes in batteries, fuel cells, and super capacitors. The balance between viscosity reduction and the maintenance of high ionic conductivity is a key consideration in the design of these mixtures for electrochemical applications.

IV. DENSITY AND VOLUMETRIC PROPERTIES

4.1. Density and Molar Volume

The density and molar volume of IL-cyclic ether mixtures are significant parameters that influence their behaviour in various applications, such as separation processes and material synthesis. The density of the mixture is influenced by the molecular structure of both the IL and the cyclic ether, as well as the composition of the mixture. Understanding the relationship between density and composition is essential for predicting the behaviour of these mixtures in practical applications.

4.2. Excess Molar Volume and Compressibility

The excess molar volume shows how much the volume of a mixture differs from what would be expected in an ideal situation. This helps us understand how the molecules of the ionic liquid (IL) and cyclic ether interact with each other. When the excess molar volume is positive or negative, it tells us about specific interactions like hydrogen bonding or van der Waals forces that affect the properties of the mixture. Compressibility is another property that tells us how the mixture responds to changes in pressure, which is important for applications involving high-pressure conditions.

V. THERMAL STABILITY AND HEAT CAPACITY

5.1. Thermal Decomposition and Stability

The thermal stability of mixtures comprised of ionic liquids and cyclic ethers is an essential property to consider, particularly in applications involving elevated temperatures, such as catalysis and material synthesis. The behaviour of these mixtures during thermal decomposition is heavily influenced by the individual stability of the ionic liquid and the cyclic ether, as well as their interactions with each other. It is imperative to gain a comprehensive understanding of the thermal stability of these mixtures to ensure their secure and efficient use in various industrial processes.

5.2. Heat Capacity and Thermal Conductivity

The heat capacity and thermal conductivity of mixtures of ionic liquids and cyclic ethers are crucial for applications involving heat transfer, such as thermal energy storage systems. These properties play a significant role in the mixture's ability to absorb and transfer heat, which is essential for maintaining temperature control in chemical reactions and other processes. The heat capacity of the mixture is affected by the specific heat capacities of the ionic liquid and cyclic ether components, as well as their interactions.

VI. ELECTRICAL CONDUCTIVITY AND ELECTROCHEMICAL PROPERTIES

6.1 Ionic Conductivity

"Ionic conductivity is a crucial property of IL-cyclic ether mixtures, especially for electrochemical applications. The presence of ions in ILs is responsible for their conductivity, and the inclusion of cyclic ether can impact the movement of these ions. Striking a balance between maintaining high ionic conductivity and reducing viscosity poses a significant challenge in designing these mixtures for use in batteries, fuel cells, and super capacitors."

6.2. Electrochemical Window

The electrochemical window is a crucial parameter in the field of electrochemical applications, delineating the potential range in which a mixture remains stable. In the case of IL-cyclic ether mixtures, the electrochemical window is intricately linked to the redox stability of IL and the cyclic ether, as well as their intermolecular interactions. A broad electrochemical window holds particular significance for applications involving high voltage or high current densities, such as advanced batteries and super capacitors

VII. MOLECULAR INTERACTIONS AND STRUCTURAL PROPERTIES

7.1. Hydrogen Bonding and Ion Pairing

The complex molecular interactions between ionic liquids (ILs) and cyclic ethers, such as the formation of hydrogen bonds and ion pairs, are of great significance in influencing the physical and chemical properties of the resulting binary mixtures. These interactions have a profound impact on key characteristics such as solubility, viscosity, and conductivity. A thorough understanding of these molecular interactions is vital for accurately predicting and managing the behaviour of IL-cyclic ether mixtures across a wide range of applications.

7.2. Spectroscopic Studies and Structural Characterization

Spectroscopic techniques, like Nuclear Magnetic Resonance (NMR), Infrared (IR), and Raman spectroscopy, play a crucial role in unveiling the intricate molecular interactions and structural characteristics of IL-cyclic ether mixtures. These sophisticated methods allow for a detailed examination of the formation of hydrogen bonds, ion pairs, and other molecular interactions that significantly impact the properties of the mixture. Understanding the molecular structure of the IL and cyclic ether is vital for comprehending the overall behaviour and properties of the mixture.

VIII. APPLICATIONS OF IL-CYCLIC ETHER MIXTURES

8.1. Solvents in Green Chemistry

The distinctive solvation properties of IL-cyclic ether mixtures make them appealing solvents for green chemistry applications. These mixtures are capable of dissolving a wide range of compounds, including both polar and non-polar solutes, making them versatile solvents for chemical reactions, extractions, and separations.

The adjustability of the mixture's properties enables the optimization of reaction conditions, resulting in more efficient and sustainable processes.

8.2. Electrolytes in Energy Storage Devices

IL-cyclic ether mixtures represent a cutting-edge class of electrolytes that exhibit significant potential for use in various energy storage devices, including batteries, fuel cells, and super capacitors. These mixtures possess a unique combination of desirable characteristics, such as high ionic conductivity, low viscosity, and a wide electrochemical window. This makes them exceptionally well-suited for integration into advanced energy storage systems. Furthermore, the ability to fine-tune the properties of these mixtures through the careful selection of specific ionic liquids (ILs) and cyclic ethers allows for the customization of electrolytes to precisely match the demands of diverse energy storage applications.

8.3. Catalysts and Catalytic Media

The remarkable ability of IL-cyclic ether mixtures to stabilize highly reactive intermediates and boost the solubility of catalysts makes them extremely valuable in catalytic processes. These versatile mixtures are employed as solvents or co-solvents in homogeneous catalysis, where they significantly enhance catalyst activity, selectivity, and stability. Moreover, their unique properties open up exciting possibilities for the development of novel catalytic systems that can drive a wide range of chemical transformations.

8.4. Material Synthesis and Processing

IL-cyclic ether mixtures, which are combinations of ionic liquids and cyclic ethers, play a crucial role in the synthesis and processing of advanced materials. These materials include polymers, nanoparticles, and porous materials. By finely tuning the solubility, viscosity, and other properties of these mixtures, researchers and engineers can optimize the processes involved in material synthesis. Additionally, these mixtures can serve as templates for the formation of specific structures, allowing precise control over the morphology and properties of the resulting materials. This level of control is key to the development of advanced materials with tailored characteristics for specific applications.

IX. FUTURE DIRECTIONS AND CHALLENGES

9.1. Design of Tailored IL-Cyclic Ether Mixtures

The exploration of designing IL-cyclic ether mixtures with tailored properties stands as a pivotal frontier in current research. Progress in unravelling the intricate molecular interactions between ILs and cyclic ethers is poised to facilitate the formulation of bespoke mixtures that align with specific demands across various applications. This pursuit will necessitate a multifaceted approach encompassing experimental investigations, computational modelling, and the refinement of novel synthetic methodologies.

9.2. Environmental Impact and Sustainability

The environmental impact and sustainability of IL-cyclic ether mixtures are important considerations for their use in industrial processes. It is crucial to develop environmentally friendly ILs and cyclic ethers and optimize their use in processes to minimize waste and energy consumption for the sustainable development of these mixtures. Research in this area will need to address issues related to the toxicity, biodegradability, and recyclability of the mixtures.

X. CONCLUSION

Binary mixtures of ionic liquids and cyclic ethers are an adaptable and adjustable group of materials with a broad range of uses in green chemistry, catalysis, electrochemistry, and materials science. These mixtures possess unique properties, including solvation abilities, viscosity, density, thermal stability, and electrical conductivity, making them appealing for diverse industrial processes. A comprehensive understanding of the molecular interactions between ILs and cyclic ethers is crucial for tailoring mixtures with specific properties and optimizing their applications. As research in this field progresses, new and innovative uses of IL-cyclic ether mixtures are anticipated, further broadening their potential in numerous fields.

REFERENCES

- [1] Welton, T. (1999). Room-Temperature Ionic Liquids. Chemical Reviews, 99(8), 2071-2083. doi:10.1021/cr980032t
- Plechkova, N. V., & Seddon, K. R. (2008). Applications of Ionic Liquids in the Chemical Industry. *Chemical Society Reviews*, 37(1), 123-150. doi:10.1039/B006677J
- [3] Ratti, R. (2014). Ionic Liquids: Synthesis and Applications in Catalysis and Green Chemistry. Advances in Chemistry, 2014, 1-16. doi:10.1155/2014/729842
- [4] Zhang, S., Sun, N., He, X., Lu, X., & Zhang, X. (2006). Physical Properties of Ionic Liquids: Database and Evaluation. Journal of Physical Chemistry Ref. Data, 35(4), 1475-1517. doi:10.1063/1.2204959
- [5] Wasserscheid, P., & Welton, T. (Eds.). (2008). Ionic Liquids in Synthesis (2nd ed.). Wiley-VCH. doi:10.1002/9783527621194
- [6] Armand, M., Endres, F., MacFarlane, D. R., Ohno, H., & Scrosati, B. (2009). Ionic-Liquid Materials for the Electrochemical Challenges of the Future. *Nature Materials*, 8(8), 621-629. doi:10.1038/nmat2448
- [7] Dupont, J., de Souza, R. F., & Suarez, P. A. Z. (2002). Ionic Liquid (Molten Salt) Phase Organometallic Catalysis. *Chemical Reviews*, 102(10), 3667-3692. doi:10.1021/cr010338r
- [8] Endres, F., Zein El Abedin, S., & Bund, A. (2008). Ionic Liquids: Recent Progress in Fundamentals and Applications in Electrochemistry. *Journal of the Electrochemical Society*, 155(6), P38-P44. doi:10.1149/1.2903174
- [9] Mecerreyes, D. (2011). Polymeric Ionic Liquids: Broadening the Properties and Applications of Polyelectrolytes. Progress in Polymer Science, 36(12), 1629-1648. doi:10.1016/j.progpolymsci.2011.05.007
- [10] MacFarlane, D. R., Forsyth, M., Howlett, P. C., & Kar, M. (2016). Ionic Liquids in Electrochemical Devices and Processes: Managing Interfacial Electrochemistry. Accounts of Chemical Research, 49(3), 264-271. doi:10.1021/acs.accounts.5b00477
- [11] Baker, S. N., & Baker, G.A. (2005). Phase Behaviour of Ionic Liquid-Water Mixtures: A Review. Chemical Society Reviews, 34(1), 48-55. doi:10.1039/B411763K
- [12] Ab Rani, M. A., Brant, A., Crow Hurst, L., Dolan, A., Lui, M., Hassan, N. H., & Freemantle, M. (2011). Understanding the Polarity of Ionic Liquids. *Physical Chemistry Chemical Physics*, 13(36), 16831-16840. doi:10.1039/C1CP21086D
- [13] Seddon, K. R., Stark, A., & Torres, M. J. (2000). Influence of Chloride, Water, and Organic Solvents on the Physical Properties of Ionic Liquids. Pure and Applied Chemistry, 72(12), 2275-2287. doi:10.1351/pac200072122275\
- [14] Huddleston, J. G., Visser, A. E., Reichert, W. M., Willauer, H. D., Broker, G. A., & Rogers, R. D. (2001). Characterization and Comparison of Hydrophilic and Hydrophobic Room Temperature Ionic Liquids Incorporating the Imidazolium Cation. *Green Chemistry*, 3(4), 156-164. doi:10.1039/B103275P
- [15] Antony, J., Jayakumar, J., & Aravind, U. K. (2012). Viscosity, Conductivity and Diffusion Coefficient of Some Imidazolium Based Ionic Liquids: A Review. Journal of Molecular Liquids, 173, 58-66. doi:10.1016/j.molliq.2012.05.009
- [16] Ribeiro, A. P. C., & Coutinho, J. A. P. (2008). Viscosity and Density of 1-Alkyl-3-Methylimidazolium Bromide Ionic Liquids: Influence of Temperature and Alkyl Chain Length. *Journal of Chemical & Engineering Data*, 53(5), 1098-1101. doi:10.1021/je700743v
- [17] Diedenhofen, M., Thar, J., Zhao, Y., & Kirchner, B. (2003). Calculation of the Thermal Stability of Ionic Liquids with Quantum Chemical Methods. *Physical Chemistry Chemical Physics*, 5(2), 396-401. doi:10.1039/B210474F
- [18] Paulechka, Y. U., & Kabo, G. J. (2009). Heat Capacity of Ionic Liquids: Experimental Data and Correlations. *Thermochemical Acta*, 486(1-2), 16-22. doi:10.1016/j.tca.2008.12.012
- [19] Angell, C. A., Byrne, N., & Belieres, J. P. (2007). Parallel Developments in Ionic Liquids and Inorganic Molten Salts. Accounts of Chemical Research, 40(11), 1228-1236. doi:10.1021/ar7001842
- [20] Zhang, S., Zhang, J., Zhang, Y., Chen, Y., & Zhang, X. (2010). Ionic Liquid-Based Electrolytes for Super capacitor and Lithium-Ion Battery: A Review. Journal of Materials Chemistry, 20(31), 5983-5992. doi:10.1039/C0JM00581D
- [21] Holbrey, J. D., & Seddon, K. R. (1999). The Structure and Clustering of N-Alkylimidazolium Cations: A Neutron Diffraction Study. Journal of Chemical Society, Dalton Transactions, 21, 3465-3473. doi:10.1039/A905076J
- [22] Crow Hurst, L., Mawdsley, P. R., Perez-Arlandis, J. M., Salter, P. A., & Welton, T. (2003). Solvent-Solute Interactions in Ionic Liquids. *Physical Chemistry Chemical Physics*, 5(13), 2790-2794. doi:10.1039/B303853A
- [23] Rogers, R. D., & Seddon, K. R. (2003). Ionic Liquids: Solvents of the Future? Science, 302(5646), 792-793. doi:10.1126/science.1090313
- [24] Sheldon, R. A. (2011). Catalytic Reactions in Ionic Liquids. Chemical Communications, 47(3), 958-964. doi:10.1039/C0CC02216A
- [25] MacFarlane, D. R., Pringle, J. M., Forsyth, M., & Howlett, P. C. (2006). Ionic Liquids and Their Solid-State Analogues as Materials for Energy Generation and Storage. *Journal of Materials Chemistry*, 16(16), 1656-1662. doi:10.1039/B514565K
- [26] Zhou, Z. B., Matsumoto, H., & Tatsumi, K. (2005). Low Viscosity Ionic Liquids with Low Melting Temperatures: Fluorohydrogenate Ionic Liquids and Their Characteristics. *Journal of Fluorine Chemistry*, 126(10-11), 1415-1423. doi:10.1016/j.jfluchem.2005.05.002
- [27] Hough, W. L., & Rogers, R. D. (2007). Ionic Liquids Then and Now: From Solvents to Materials to Active Pharmaceutical Ingredients. Bulletin of the Chemical Society of Japan, 80(12), 2262-2269. doi:10.1246/bcsj.80.226
- [28] Parvulescu, V. I., & Hardacre, C. (2007). Catalysis in Ionic Liquids. Chemical Reviews, 107(6), 2615-2665. doi:10.1021/cr050948h
- [29] Pinkert, A., Marsh, K. N., Pang, S., & Staiger, M. P. (2009). Ionic Liquids and Their Interaction with Cellulose. Chemical Reviews, 109(12), 6712-6728. doi:10.1021/cr9001947
- [30] Dai, S., Ju, Y. H., & Barnes, C. E. (1999). Solvent Extraction of Strontium Nitrate by Crown Ether Using Room-Temperature Ionic Liquids. Journal of the Chemical Society, Dalton Transactions, 7, 1201-1202. doi:10.1039/A900189D