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To Study the Concept of Deep Eutectic Solvent in Context of Water

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***Abstract*-- Deep Eutectic Solvents (DESs) are a class of environmentally friendly solvents formed by mixing a hydrogen bond acceptor (HBA) and a hydrogen bond donor (HBD), resulting in a eutectic mixture with a melting point much lower than that of the individual components. Due to their low toxicity, biodegradability, low vapor pressure, and simple preparation, DESs have gained significant attention as green alternatives to conventional organic solvents. However, DESs are highly hygroscopic and readily absorb water from the atmosphere. Water has a profound influence on the physical, chemical, and structural properties of DESs. Small amounts of water reduce viscosity and improve ionic conductivity without disrupting the hydrogen-bonding network. In contrast, excessive water weakens hydrogen bonding, alters solvent structure, and may transform the DES into an aqueous solution. Understanding the effect of water is essential for optimizing DES performance in biomass processing, catalysis, extraction, electrochemistry, pharmaceutical applications, and material synthesis.**

***Keywords*--Deep Eutectic Solvent (DES), Green Chemistry, Physicochemical Properties, Water– DES Interactions, Solubility, Sustainable Solvents.**

I. Introduction

Deep Eutectic Solvents (DESs) are a class of designer solvents formed by mixing two or more components, typically a hydrogen bond donor (HBD) and a hydrogen bond acceptor (HBA), in a specific molar ratio. The interaction between these components through hydrogen bonding causes a significant decrease in the melting point of the mixture compared to the individual components. DESs have attracted considerable attention as environmentally friendly alternatives to conventional organic solvents and ionic liquids. They are generally easy to prepare, biodegradable, cost-effective, and exhibit low volatility. Common examples include choline chloride mixed with urea, glycerol, or ethylene glycol

Deep Eutectic Solvents (DESs) were first introduced by Andrew Abbott and co workers in 2003. They are generally prepared by mixing a hydrogen bond acceptor (HBA), such as Choline chloride, with a hydrogen bond donor (HBD), such as Urea, Ethylene glycol, or Glycerol.

Strong hydrogen-bond interactions lower the melting point of the mixture, producing a liquid at room temperature.

DESs possess several attractive properties:

- Low volatility
- Non-flammability
- Low toxicity
- High thermal stability
- Easy synthesis
- Biodegradability
- Excellent solvating ability

One of the most important factors affecting DES performance is the presence of water. Since DESs readily absorb moisture from the atmosphere, water content is difficult to avoid and significantly influences their behavior.

➢ *Interaction Between Water and DES*

Water interacts strongly with DESs through hydrogen bonding.

- *At low water concentrations:* Water becomes incorporated into the hydrogen-bond network. The DES structure remains largely intact. Molecular mobility increases.
- *At high water concentrations:* Water competes with the HBD for hydrogen bonding. Original DES interactions weaken. The supra molecular structure gradually breaks down.

➢ *The Step-by-Step Structural Mechanism*

The mechanism of how water alters a DES is categorized into three distinct hydration regimes based on water mass fraction:

1. Low Water Content: < 5 to 10 wt%

When a small amount of water is introduced (or absorbed from the atmosphere due to the hygroscopic nature of DESs), the water molecules do not break the bulk structure. Instead, they are sequestered.

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- *Mechanism:* Water molecules insert themselves into the empty nano scale cavities of the DES matrix. They form localized hydrogen bonds with the HBA (e.g., chloride ions) and the HBD without separating them.
- *Result:* The core eutectic network remains completely intact. However, this small amount of water acts as a lubricant, weakening the overall cohesive energy just enough to drastically decrease the solvent's viscosity and increase its ionic conductivity.

2. Moderate Water Content: ~ 10 to 40 wt%

As more water is added, the system transitions into a complex ternary mixture.

- *Mechanism:* Water begins to actively compete for hydrogen bonding sites. It starts to solvate the individual components (like the cholinium cations and chloride anions), clustering them into nanostructured domains.
- *Result:* The pure DES structural integrity begins to non-linearly decline. Interestingly, the nanostructure is surprisingly resilient; around ***30*** to ***40 wt%***, the DES still retains roughly half of its original "pure" properties because the water is structurally sequestered into localized aqueousv pockets.

3. High Water Content: > 40 to 50 wt%

At this tipping point, the concentration of water forces a complete phase and structural transition.

- *Mechanism:* The sheer volume of water overcomes the cohesive hydrogen-bonding network between the HBA and HBD. Water-water and water-DES interactions completely dominate.
- *Result:* The eutectic nature is destroyed. The system is no longer a Deep Eutectic Solvent; itv behaves strictly as an **aqueous solution of its individual parent components** (e.g., a simple saltand- sugar water solution).

➢ *Impact on Physicochemical Properties*

Adjusting the water content is frequently used as a tool to "tailor" the properties of a DES for specific industrial and laboratory applications:

- *Viscosity Reduction:* DESs are inherently highly viscous due to their extensive hydrogen-bonding network. Small amounts of water (within the first regime) drastically decrease viscosity, significantly improving mass transfer and fluidics.

WATER CONTENT (%)	RELATIVE VISCOSITY
0	Very high
5	Lower
10	Much lower
20	Very low

- *Conductivity Enhancement:* Concurrently with the drop in viscosity, ionic mobility increases sharply, leading to a substantial rise in electrical conductivity, which is highly beneficial for electrochemical applications.

WATER CONTENT (%)	CONDUCTIVITY
0	Low
5	Higher
10	Much higher
20	Maximum
>40	May decrease because DES structure is lost

- *Density Modulation:* The mass-to-volume ratio changes non-linearly as the close-packed supra molecular structure is reconfigured by the inclusion of water molecules.
- *Polarity Shifts:* The overall polarity of the mixture shifts closer to that of pure water, modifying the solvent's affinity and capacity to dissolve target solutes or biomolecules selectively.

II. Conclusion

Water is one of the most influential factors governing the behaviour of Deep Eutectic Solvents. A small amount of water is generally beneficial because it decreases viscosity, improves conductivity, enhances mass transfer, and facilitates extraction and chemical reactions while preserving the hydrogen-bond network. However, excessive water disrupts the hydrogen-bond interactions responsible for DES formation, causing the solvent to lose its characteristic structure and properties.

Therefore, careful control of water content is essential for maximizing DES performance in scientific research and industrial applications.

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