Everything You Wanted to Know about Deep Eutectic Solvents but Were Afraid to Be Told

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From chemical synthesis to the extraction of value-added materials, solvents are ubiquitous in chemistry. Until recently, though, only liquids could be used as solvents. Deep eutectic solvents (DESs) shattered this status quo. A DES is a liquid mixture formed by physically mixing a solid hydrogen bond donor (HBD) and a solid hydrogen bond acceptor (HBA). There is no chemical reaction involved: the liquid phase of the DES arises due to solid-liquid equilibrium (SLE) that leads to a severe melting temperature depression.

While DESs are liquid mixtures of solids, not all liquid mixtures of solids are DESs. Thus, we composed a working definition of eutectic and deep eutectic solvents, grounded on thermodynamics, that can be summarized as:

> *"A eutectic solvent is a eutectic-type system that is a liquid at a given desired temperature where at least one of its components would, otherwise, be a solid unfit to be applied as a solvent. A deep eutectic solvent is a eutectic solvent whose components present enthalpic-driven negative deviations from thermodynamic ideality."*

We also formulated heuristic rules to anticipate which mixtures display negative deviations from ideality and, thus, yield DESs. These occur when intermolecular interactions across mixture components (A-B) are stronger than those between any of the pure components (A-A or B-B). Interactions of the A-B type can be maximized using asymmetric HBDs (compounds with little HBA capability, usually due to electron withdrawing effects from motifs such as aromatic rings) and/or lone HBAs (compounds without any HBD functional groups). A typical example of each class of compounds is given in Figure 1.

Leveraging the framework developed in this work, materials of interest, from powerful chelants such as trioctylphosphine oxide [2] or phenanthroline [3] to active pharmaceutical ingredients [4], can be readily liquefied and applied under the umbrella of DESs using cheap and sustainable asymmetric HBDs or lone HBAs.

References

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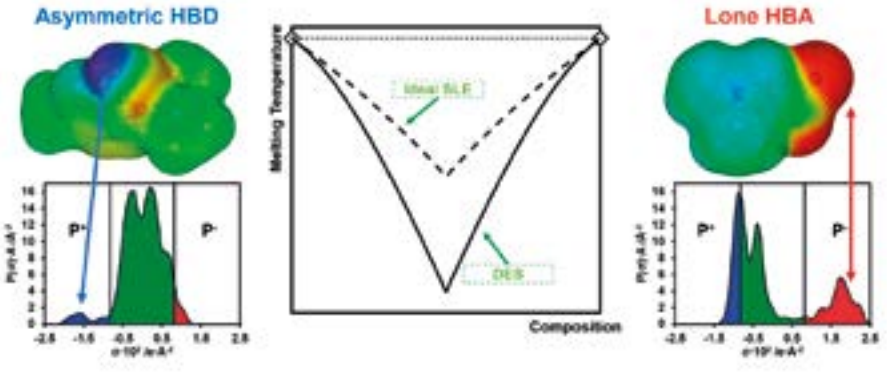

FIGURE 1
Example of an asymmetric HBD (thymol, left) and a lone HBA (betaine, right), highlighting their corresponding excess polarities, and the resulting SLE phase diagram (full line, middle).