Design of Low Viscosity Hydrophobic Deep Eutectic Solvents: Correlation with the Pure Constituent Molecular Structure and Liquid Phase Non-Ideality

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Eutectic mixtures have been recently regarded as a new promising category of tunable, green, and inexpensive solvents. Although many chemical substances can be used to form eutectic mixtures, those showing a significant deep depression in the mixture melting temperature at the eutectic point are of interest for research, usually referred to as deep eutectic solvents (DES) [1]. DESs usually possess higher viscosity compared to conventional solvents, which limits their applicability in many fields. Hydrophilic DESs are usually diluted with water to tune their viscosity, which is impossible for hydrophobic DESs. Therefore, it is crucial to design hydrophobic DESs with low viscosity. This work aims to study the effect of the molecular structure of DES constituents and the intermolecular interactions in the liquid phase on the viscosity of hydrophobic DES. DESs were treated as binary eutectic mixtures. The eutectic mixtures studied are either ideal eutectics, i.e., the intermolecular interactions in the liquid solution are not different from that in the pure liquid constituents, or non-ideal eutectics, i.e., strong intermolecular interactions between unlike molecules. The viscosity of the eutectic mixtures was measured over a wide range of temperatures and compositions. We found that the viscosity of the pure constituents correlates with the chemical functionality, molecular weight, and molecular structure. Constituents containing cyclic structures possess considerably higher viscosity compared to linear structures. We showed that ideal eutectics behave like supercooled liquids, where the viscosity of the mixture do not deviate considerably from ideal viscosity. In contrast, the deviation from ideal viscosity for non-ideal eutectics at low temperatures shows that these mixtures behave like glasses. This work provides a notable understanding of the rheological behavior of eutectic mixtures that will aid in designing and tuning the viscosity of hydrophobic DESs.

References

[1]. Alhadid, A.; Mokrushina, L.; Minceva, M., *Molecules* **2019**, *24*, 2334.