

Hydrogen-Bonded Anion Clusters in Choline Phenylalaninate, an Unexpected Origin of Nanostructure in Biocompatible Ionic Liquid

Thursday, 12 November 2020 12:17 (12 minutes)

Recently, a number of choline amino-acid salts have been reported to form ionic liquids (ChILs), creating the possibility of biocompatible ILs with a sustainable production cycle.[1,2] Since their discovery, these designer solvents have proven useful across many applications, including drug synthesis and delivery, electrochemistry, biomass processing and CO₂ capture, often in mixtures with water.[3] However, little is still known about how the structure of their constituent ions determines properties and performance of both the pure IL and its solutions, limiting the capacity to design task-specific ILs and optimise for large scale applications. In this study, we investigate choline DL-phenylalaninate (ChPhe) using time-of-flight neutron diffraction and modelled its structure with simulations. Our aim is to understand how its amphiphilic liquid nanostructure arises from atomic correlations. Surprisingly, we discovered the aromatic moieties of the phenylalaninate anion form distinct, small clusters or non-polar domains, but with no evidence for pi-pi stacking. Detailed analysis of the atomic correlations reveals that inter-anion hydrogen bonds are the main stabilisation factor of these non-polar clusters. This is the first example of self-assembled ionic liquid nanostructure not of solvophobic origin. The unusual suite of interactions also explains its water miscibility but inability to retain nanostructure upon water dilution,[4] as well as its poor performance for biomass pretreatment (relative to other nanostructured ChILs),[5] and provides a new strategy by which to engineer and tune ionic liquid nanostructure for the design of application-specific, renewable solvent systems.

References

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Level of Expertise

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Session Classification: Chemistry & Crystallography

Track Classification: Chemistry & Crystallography