Non-covalent Interactions and Morphologies as Tools for Structure Driven Informatics: Rationalizing the Behavior of Ionic Liquids

Dr Patrick C Hillesheim[1], Dr Arsalan Mirjafari[2], Dr Matthias Zeller[3], Sophia Bellia[1], Mairead Boucher[1]
[1]Ave Maria University, [2]SUNY Oswego, [3]Purdue University
patrick.hillesheim@avemaria.edu

Ionic liquids are a class of material that is classified as a liquid comprised entirely of ions. They are composed of large organic cations and small inorganic anions. Due to their unique properties such as low volatility, high conductivity, and tunable solubility, ionic liquids have found numerous applications in various fields including chemical synthesis, electrochemistry, and energy storage. One of the challenges in studying ionic liquids is their disordered structure, which makes it difficult to determine the precise arrangement of ions in the liquid state. However, recent advances in techniques such as X-ray diffraction coupled with computational methods, have provided insights into the structure and properties of ionic liquids by examining the solid-state structures.

As we continue to search for new ionic liquid structures, crystallography can be used to answer specific questions. In our groups work, we have applied the principles of crystallographic analysis to evaluate the properties of ionic compounds. Through careful evaluation of the solid-state structure of the salts, we were able to rationalize the physicochemical properties of these compounds. We supplement our evaluation of the compounds by coupling traditional crystallographic techniques (e.g., bond distance and angle analysis) with modern computational techniques. This coupling of experimental and theoretical analysis provides a wealth of information useful in developing the next generation of ionic materials.

Our recent investigation into thiazolium-based ionic liquids revealed unexpected thermal behavior. Through systematic variation of the cation structure, we were able to narrow down the set of non-covalent interactions which are responsible for the higher than anticipated melting points of these compounds. Specifically, interactions with the sulfur moiety were found to be key in forming higher melting salts. Hirshfeld surface analysis was crucial in revealing the different interactions in the thiazolium complexes when contrasted with the more commonly used imidazolium complexes. Through careful evaluation of the crystal structures, we were able to rationalize the physicochemical properties of the ionic compounds.

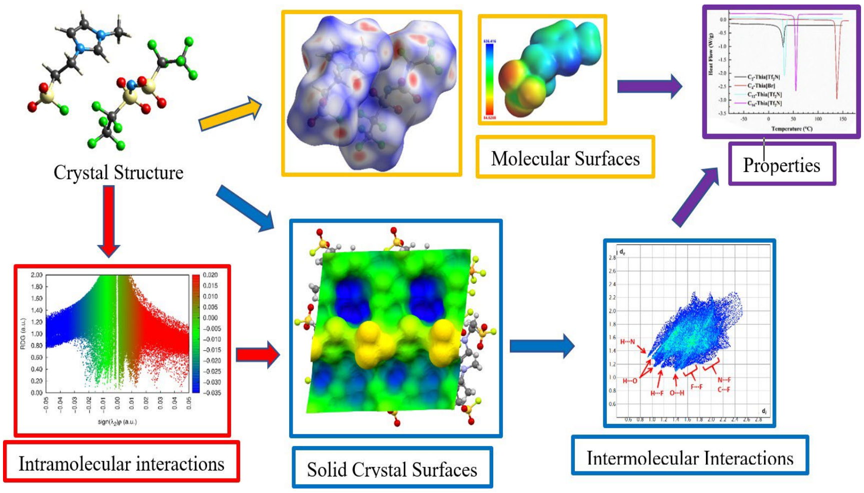

Figure 1

Acta Cryst. (2023). A79, a124