

*Crystallographic analysis of Ionic liquids*Manish Kumar Mishra¹, Steven P Kelley¹, Robin D Rogers¹¹Department Of Chemistry, McGill University, Montreal, Canada

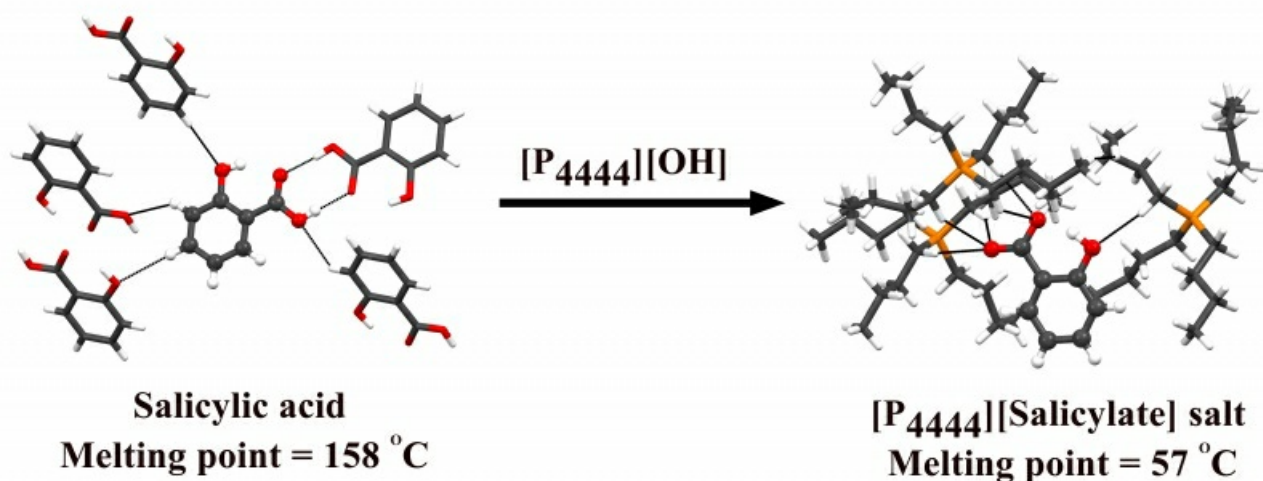
E-mail: manish.mishra@mcgill.ca

Within the last decade, the use of ionic liquids (salt melts below 100 °C) has extended from the more traditional fields of electrochemistry, separation or catalysis, to newer areas in materials chemistry and crystal engineering. Ionic liquids have also attracted the interest of pharmaceutical scientists because of the ease of tuning the physical, chemical, and biological properties, further providing a new strategy to overcome major problems such as polymorphism, bioavailability, and solubility. Our group has designed various bioactive ionic liquids formed from biologically active ions by utilizing anti-crystal engineering principles with the goal of decreasing the prominent intermolecular interactions between cations and anions that might yield common supramolecular synthons in a crystal. However, it is still challenging to understand the fundamental chemistry of liquids, where the system is more dynamic and harder to characterize. In this sense, the crystallographic study of crystalline salts containing ionic liquid ions provides a direct insight into the spatial relationship between the cations and anions including the strength, type and number of intermolecular interactions, all of which are major factors determining the lattice energies, viscosity, melting point, and general behavior of ionic liquids and salts. This presentation will discuss crystallographic details of low-melting bioactive salts, focusing on weak intermolecular interactions, ionic repulsion, structural flexibility, and packing. Further, such insights have been applied to produce unusual crystal structures of nucleobases to better understand their biological roles and reveal unknown interactions.

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