Crystal Structure of Protic Ionic Liquids and their hydrates

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Protic Ionic Liquids (PILs) are a class of tailorable solvents made up of fused salts with melting points below 100 °C, which are formed through a Brønsted acid-base reaction involving proton exchange[1]. These solvents have applications as lubricants, electrolytes, and many other uses[2]. Although they are quite similar to molten salts, their crystal structures have not been explored in-depth, with only ethylammonium nitrate (EAN) having a reported crystal structure[3, 4].

Ten alkylammonium-based protic ionic liquids at both neat (<1 wt% water) and 90 mol% PIL, 10 mol% water concentrations were selected. Diffraction patterns were collected at the Australian Synchrotron ANSTO while attempting to crystallise the samples by cooling to 120 K. Five samples crystallised (3 neat, 2 dilute), where the temperature of the system was then increased at a rate of 6 K/min to room temperature. From these patterns we have identified a number of crystal phases, identifying their stability ranges and lattice constant variation from 120 K to room temperature.

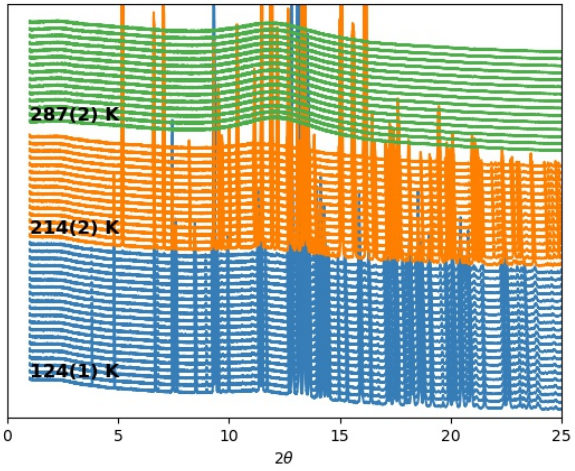

Figure 1. Waterfall plot of ethylammonium nitrate (EAN) crystal phase structure with increasing temperature. Three phases are visible: α-crystal in blue, β-crystal in orange, and liquid phase in green.

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