Poster Presentation

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Imaging H-atom behaviour on I19, diamond light source

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I19 at Diamond Light Source is a beamline dedicated to small molecule single crystal X-ray diffraction. Operating in the 5 to 25 KeV energy range with a choice between two specialised experiments hutches it can accommodate a wide variety of crystallographic experiments including variable temperature and high pressure work, time-resolved photo crystallography, gas cell and charge density studies.

The short data collection times in the recently upgraded experiments hutch 1 (EH1) equipped with a Pilatus 2M detector provides potential for the study of finer detail of crystal structure and its evolution; either as a function of an external variable, such as temperature, or across a set of related materials. In particular, the evolving behaviour of hydrogen atoms (H-atoms) across hydrogen bonds is of interest, enabling charge and energy transfer in a range of biological and chemical systems. [1] The study of this behaviour therefore allows insight into how it may be targeted and tuned in future materials.

Recent work has demonstrated the potential of single crystal X-ray diffraction (SCXD) to image the evolution of H-atom behaviour as a function of temperature, revealing equivalent trends to that found by neutron diffraction. [2] The development of appropriate methodology in the imaging of H-atom behaviour using synchrotron SCXD is important, particularly as previous studies have involved laboratory X-ray sources only. Here we study a number of systems with evolving H-atom behaviour using synchrotron SCXD including 3,5-dinitrobenzoic acid II (C2/c polymorph), known to exhibit proton disorder, and substituted urea organic acid molecular complexes with interesting proton migration behaviour. Efforts are focused on exploring data collection and refinement strategies for obtaining good quality Fourier difference maps in which H-atom behaviour may be determined. [3]

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