Cool structures from event-based single crystal neutron diffraction

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Neutron diffraction is sensitive to the nuclear density of atoms. Isotopes of the same element can have very different neutron scattering properties; for example, the scattering length is negative for hydrogen and positive for deuterium. Unlike X-rays form factors, neutron scattering lengths do not decrease for high Q reflections, advantageous for using neutron diffraction to locate light elements at the subatomic resolution, including hydrogen positions for the study of hydrogen bonding interactions. Neutron wavelength-resolved time-of-flight Laue technique expands the measured diffraction pattern from 2D on detector spaces to wavelength-resolved 3D volume in (x, y, λ) along the neutron transport direction. Neutron event data collection at Spallation Neutron Source uses an array of area detectors on TOPAZ with a fast detection time in the microsecond scale. A large number of reflections can be measured at one sample orientation. Metadata with 'real-time' parameter information are saved with event data, ideal for the study of temporal and stroboscopic structural changes induced by external stimuli such as temperature, pressure, electric and magnetic fields.

We have used the TOPAZ instrument to locate hydrides and deuterium atoms in transition metal complexes, study the phase transition and temperature dependence of hydrogen bonding in hybrid organic-inorganic perovskites (HOIPs) by collecting the 3D volume of diffraction patterns in neutron event mode. Variable temperature data from single-crystal neutron diffraction following the initiation of orthorhombic-tetragonal phase transition provided details for the change of hydrogen bonding pattern between the organic donor and the inorganic accepter in HOIP compounds. The corresponding neutron structures and hydrogen bonding interactions will be presented.

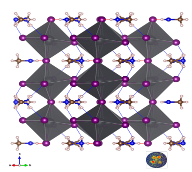

Figure 1