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Single-Crystal Neutron Diffraction Studies of Hydrogen-Bonded Proton Conductors. C.R.I. Chisholm¹, S.M. Haile¹, W.T. Klooster², ¹Materials Science, California Institute of Technology, Pasadena, CA; ²Bragg Institute, Australian Nuclear Science and Technology Organization, Menai, Australia.

Several alkali acid sulfates, phosphates and selenates are known to undergo “superprotonic” transitions in response to a change in temperature, at which the conductivity jumps 3-5 orders of magnitude. Examples include CsHSO₄, Cs₃(HSO₄)₂(H₂PO₄), CsH₂PO₄, and Rb₃H(SeO₄)₃. The high conductivities have generated interest in their potential application to fuel cells and other electrochemical devices. In order to assess the entropic driving force for the superprotonic transition and understand proton transport mechanisms, it is essential to completely describe both the room and high temperature structures. In particular, the details of the hydrogen bond network and the distribution of dissimilar anion groups (*e.g.* ordered vs. randomly arranged SO₄/PO₄ groups) must be established. In many cases, neutron diffraction is essential for obtaining such information. We present three examples from our laboratory: Cs₃Li(DSO₄)₄, CsNa₂(HSO₄)₃, and β-Cs₃(HSO₄)₂[H_{2-x}(P_{1-x}S_x)O₄]. In the first example, neutron diffraction studies led to corrections to the assigned stoichiometry, in the second, such studies aided in assessment of the space group, and in the third, to insight into local ordering phenomenon.