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Use of Neutron and X-ray Rietveld Refinement of Phase Transitions with Molecular Ions. Swainson, Ian P. Neutron Program for Materials Research, NRC, Chalk River Laboratories, Chalk River, ON KOJ 1J0 CANADA.

For many structural phase transitions, the ordering process is strongly coupled to strain. Where these transitions are strongly discontinuous, often the case in order-disorder transitions involving molecular ions, single crystals can suffer heavy twinning or explode. Powder diffraction then may be the only diffraction method available. Neutrons are highly sensitive to the isotopes of hydrogen; this is the atom that X-rays are least sensitive to. However, a high degree of deuteration is often required for neutron powder diffraction. For ammonium compounds use of neutrons can be essential, as it may be impossible to uniquely determine the orientation of ammonium, even from synchrotron data. I will give an example of a counterintuitive hydrogen-bonding situation where this was the case. Although usually difficult to tell between distinct site hopping and continuous librational growth from standard powder data, I will show that in some cases one can distinguish between the two mechanisms from neutron data when used in conjunction with spin models. Finally, I will show examples of organic-inorganic perovskites in which the use of both radiations can be highly helpful to obtaining a final solution and elucidating the nature of the transitions in these compounds.