Crystal Structure of the Superconducting Layered Cobaltate $Na_xCoO_2{\cdot}yD_2O$

Dimitri N. Argyriou[a], P.G. Radaelli[b], C. J. Milne[a], N. Aliouane[a*], L.C. Chapon[a], A. Chemseddine[a], J. Veira[a], S. Cox[c], N. D. Mathur[c], P. A. Midgley[c], *[a]Hahn-Meitner-Institut, Berlin, Germany. [b]ISIS Facility, Rutherford Appleton, U. K. [c]Department of Materials Science and Metallurgy, University of Cambridge, U.K.* E-mail: argyriou@hmi.de

Superconductivity in layered $Na_xCoO_2{\cdot}yH_2O$ occurs in CoO_2 sheets that have a quasi 2D triangular symmetry, analogous to that of geometrically frustrated systems. This is in stark contrast to the well know perovskite high-Tc cuprates, and makes the determination of the structural details of this novel superconductor essential in the understanding of its properties. However, due to the complexity of the intercalation of the H_2O between Na and CoO_2 sheets, details of the crystal structure of these materials has remained ambiguous. We have used electron and neutron powder diffraction to elucidate the structural properties of superconducting $Na_xCoO_2{\cdot}yD_2O$ over a wide compositional range. Our measurements show that superconducting samples exhibit a number of supercells ranging from 1/3a* to 1/15a*, but the predominant modulation, observed also in the neutron data, is a double hexagonal cell with dimensions 2*a* x 2 *a* x *c*. Rietveld analysis reveals that D_2O is inserted between CoO_2 sheets as to form a layered network of NaO_6 triangular prisms. Our model removes the need to invoke a 5K superconducting point compound and suggests that a solid solution of Na is possible within a constant amount of water *y*.

Keywords: oxide superconductors, powder neutron diffraction, bound water