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Sodium Ordering Phase Transition in Sodium Cobaltate D.J.P. MORRIS, HMI Berlin, Germany., M. ROGER, CEA Saclay, France., D.A. TENNANT, HMI Berlin and Technische Universitat Berlin, Germany, M.J. GUTMANN, ISIS Facility, UK., J.P. GOFF, Royal Holloway, University of London, UK., D. PRABHAKARAN, Clarendon Laboratory, Oxford, UK., J.-U. HOFFMANN, R. FEYERHERM, E. DUDZIK, K. KIEFER, HMI Berlin, Germany. — Na_xCoO_2 has emerged as a system of fundamental scientific interest because of its highly unusual electrical and magnetic properties. Using neutron and x-ray diffraction we have detected long-range 3D ordering of Na^+ ions in single crystals, and demonstrate a kaleidoscope of Na^+ ion patterns as a function of concentration and temperature [1]. Large scale numerical simulations reveal the ordering principle for this system, the formation of tri-vacancy charged droplets that then order long range, and the structure factors from these defect clusters are in good agreement with the observed neutron diffraction intensities. Superstructure transitions are observed in the diffraction data which are explained by a change from a stripe structure of tri-vacancies. The results readily explain many of the observed electrical and magnetic properties, including the formation of ferromagnetic sheets in the CoO_2 layers over this composition range, and the 3D nature of the magnetic excitations. [1] M. Roger et al. Nature 445, 631 (2007)

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