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### *Thermal expansion of monoclinic natrojarosite*

H. Brand<sup>1,2</sup>, N. Scarlett<sup>2</sup>, I. Grey<sup>2</sup>, K. Knight<sup>3,4</sup>

<sup>1</sup>Australian Synchrotron, Clayton, Australia, <sup>2</sup>CSIRO Process Science and Engineering, Clayton South, Australia, <sup>3</sup>ISIS neutron and Muon Facility, Science and Technologies Research council, Rutherford Appleton Laboratory, Harwell, Didcot, United Kingdom, <sup>4</sup>Natural History Museum, London, United Kingdom

Jarosites and related minerals are of great interest to a range of mineral processing and research applications. In some industrial settings jarosite formation is encouraged; for example to aid the removal of iron species from solutions in hydrometallurgical processes. In other environments such as bioleaching, jarosite formation can hinder the process by creating a kinetic barrier, in the form of a passivation layer, to the desired reaction. Jarosites are a major component of acidic soils and are present in significant amounts in acid mine drainage environments. There has been a recent resurgence in interest in jarosite minerals since their detection on Mars by the MER rover Opportunity. In this context, the presence of jarosite has been recognised as a likely indicator of the presence of water on Mars in the past. It is hoped that study of their formation mechanisms, stability and thermoelastic properties will provide insight into the environmental history of Mars as well as informing terrestrial industrial concerns. To this end we are engaged in a program to study jarosites and their formation and stability behaviour over a range of conditions. This contribution describes in situ powder diffraction experiments to determine the thermal expansion of a deuterated natrojarosite. Data were collected on the HRPD beamline at the ISIS spallation source where the natrojarosite sample was heated from 10–700K, and at the powder diffraction beamline at the Australian synchrotron where the sample was heated from 80-700K. Isothermal neutron and synchrotron datasets were refined simultaneously. Analysis of the lattice parameter variation with temperature shows that all cell edges increase smoothly to ~500 K where there is a discontinuity. This discontinuity represents the initially non-stoichiometric monoclinic jarosite converting to a stoichiometric, rhombohedral phase, shortly after which FeOHSO<sub>4</sub> peaks become visible. Thermal expansion coefficients have been fitted from 10-470K and show that there is most variation in the monoclinic c-axis. This direction is normal to the layers of sulphate tetrahedra and iron octahedra within the jarosite structure and contains more flexible hydrogen bond linkages which more easily accommodate expansion than the more rigid polyhedra. Details of the combined neutron-synchrotron diffraction approach will also be discussed.

**Keywords:** Jarosite, thermal expansion