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In Situ Neutron and Synchrotron X-ray Diffraction Studies of Jarosite at High-Temperature High-Pressure Conditions H. XU, Y. ZHAO, D. HICKMOTT, J. ZHANG, S. VOGEL, L. DAEMEN, M. HARTL, Los Alamos National Laboratory — Jarosite ($KFe_3(SO_4)_2(OH)_6$) occurs in acid mine drainage and epithermal environments and hot springs associated with volcanic activity. Jarosite is also of industrial interest as an iron-impurity extractor from zinc sulfide ores. In 2004, jarosite was detected by the Mars Exploration Rover Mössbauer spectrometer, which has been interpreted as a strong evidence for the existence of water (and possibly life) on ancient Mars. This discovery has spurred considerable interests in stability and structural behavior of jarosite and related phases at various temperature, pressure, and aqueous conditions. In this work, we have investigated the crystal structure and phase stability of jarosite at temperatures up to 900 K and/or pressures up to 9 GPa using *in situ* neutron and synchrotron X-ray diffraction. To avoid the large incoherent scattering of neutrons by hydrogen, a deuterated sample was synthesized and characterized. Rietveld analysis of the obtained diffraction data allowed determination of unit-cell parameters, atomic positions and atomic displacement parameters as a function of temperature and pressure. In addition, the coefficients of thermal expansion, bulk moduli and pressure-temperature stability regions of jarosite were determined.

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