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X-ray diffraction reveals two structural transitions in szomolnokite

Olivia S. Pardo[1,*], Vasilije V. Dobrosavljevic[1], Tyler Perez[1,2], Wolfgang Sturhahn[1], Zhenxian Liu[3], George R. Rossman[1], and Jennifer M. Jackson[1]

[1]Division of Geological and Planetary Sciences, California Institute of Technology, 1200 E. California Boulevard, Pasadena, California 91125, U.S.A.
[2]Now at Johns Hopkins University, 3400 N. Charles Street, Baltimore, Maryland 21218, U.S.A.
[3]Department of Physics, University of Illinois at Chicago, Chicago, Illinois 60607, U.S.A.

Abstract

Hydrated sulfates have been identified and studied in a wide variety of environments on Earth, Mars, and the icy satellites of the solar system. The subsurface presence of hydrous sulfur-bearing phases to any extent necessitates a better understanding of their thermodynamic and elastic properties at pressure. End-member experimental and computational data are lacking and are needed to accurately model hydrous, sulfur-bearing planetary interiors. In this work, high-pressure X-ray diffraction (XRD) and synchrotron Fourier-transform infrared (FTIR) measurements were conducted on szomolnokite ($FeSO_4 \cdot H_2O$) up to ~83 and 24 GPa, respectively. This study finds a monoclinic-triclinic ($C2/c$ to $P\bar{1}$) structural phase transition occurring in szomolnokite between 5.0(1) and 6.6(1) GPa and a previously unknown triclinic-monoclinic ($P\bar{1}$ to $P2_1$) structural transition occurring between 12.7(3) and 16.8(3) GPa. The high-pressure transition was identified by the appearance of distinct reflections in the XRD patterns that cannot be attributed to a second phase related to the dissociation of the $P\bar{1}$ phase, and it is further characterized by increased H_2O bonding within the structure. We fit third-order Birch-Murnaghan equations of state for each of the three phases identified in our data and refit published data to compare the elastic parameters of szomolnokite, kieserite ($MgSO_4 \cdot H_2O$), and blödite ($Na_2Mg(SO_4)_2 \cdot 4H_2O$). At ambient pressure, szomolnokite is less compressible than blödite and more than kieserite, but by 7 GPa both szomolnokite and kieserite have approximately the same bulk modulus, while blödite's remains lower than both phases up to 20 GPa. These results indicate the stability of szomolnokite's high-pressure monoclinic phase and the retention of water within the structure up to pressures found in planetary deep interiors.

Keywords: Szomolnokite, hydrated sulfates, high pressure, X-ray diffraction, infrared spectroscopy, equation of state