Lattice dynamics of an iron-bearing hydrated sulfate at high pressure

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Complex mixtures of ice, sulfates, silicates, and other mantle phases have been observed in a variety of planetary environments on Earth, Mars, and the icy satellites of the solar system. The presence of these complex mixtures of sulfates has demonstrated that characterizing the properties of the corresponding endmembers is important for understanding the interiors of a range of planetary bodies.[1,2,3,4,5] To measure the vibrational properties of the iron endmember, szomolnokite, ($FeSO_4 \bullet H_2O$), we have performed synchrotron infrared spectroscopy (SIR) and ^{57}Fe nuclear resonant (NR) inelastic and forward scattering experiments in the diamond anvil cell up to 24 GPa. This pressure range covers deep Earth interiors relevant to sulfur cycling in subduction zones and lower pressures of smaller body interiors like the icy satellites and larger icy, sulfate-rich interiors.[6,7]

The SIR and NR experiments were conducted at NSLS-II beamline 22-IR-1 and the Advanced Photon Source at sector 3-ID-B, respectively. In this work we focus on understanding the crystal structural environments of the H_2O and sulfate groups, as well as interactions involving the iron atoms within szomolnokite. The NR inelastic x-ray scattering measurements probe the Fe-participating vibrational properties, whereas the NR elastic scattering measurements (synchrotron Mössbauer spectroscopy) probe the electronic environment of the Fe-atoms. Combined with our previous identification of two structural transitions occurring in szomolnokite[8], we now present a detailed analysis of the vibrational and electronic properties of szomolnokite near both phase transitions. We quantify changes in bonding environments at high pressure, including retention of "water" across both phase transitions. This work contributes experimental data on an iron-endmember hydrated sulfate necessary for future modeling work to better describe the planetary environments in which these hydrated sulfates may be found.

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