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Thermal expansion of römerite under low-temperature conditions

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Abstract

Römerite, a triclinic hydrous sulfate in the $P\bar{1}$ space group with the chemical formula $Fe^{2+}Fe_2^{3+}(SO_4)_4{\cdot}14(H_2O)$, is of potential interest in studies of planetary environments, with particular relevance to Mars and the icy jovian satellites. Past work has indicated the presence of hydrous sulfates on said bodies, and the mixed-valence iron in römerite's structure makes the mineral a worthwhile end-member composition in thermodynamic models. Such models should be constrained by measurements at the low temperatures relevant to the planetary environments in question. We characterized single crystals of römerite with time-domain Mössbauer spectroscopy, Raman spectroscopy, and X-ray diffraction methods. Through our X-ray diffraction experiment, we refined the unit-cell parameters of the crystal between 100 and 300 K. The resulting temperature-variant lattice parameters and volumes are reported and are fit by physical and empirical models of the thermal expansion coefficient. The physical model considered, a Debye model of thermal expansion, provides estimates of additional thermodynamic parameters: the ratio of the bulk modulus at 0 K and 1 bar to the thermodynamic Grüneisen parameter ($K_{0,0K}/\gamma_{th}$), the volume at 0 K and 1 bar ($V_{0,0K}$), and the Debye temperature (θ_D).

Keywords: Römerite, hydrous sulfate, low temperature, X-ray diffraction, icy satellites, thermal expansion, Mössbauer spectroscopy, Raman spectroscopy