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Investigation of the kieserite–szomolnokite solid-solution series, $(Mg,Fe)SO_4 \cdot H_2O$, with relevance to Mars: Crystal chemistry, FTIR, and Raman spectroscopy under ambient and martian temperature conditions

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ABSTRACT

The investigation of hydrous sulfate deposits and sulfate-cemented soils on the surface of Mars is one of the important topics in the recent scientific endeavor to retrieve detailed knowledge about the planetary water budget and surface weathering processes on our neighbor planet. Orbital visible/near-IR spectra of the surface of Mars indicate kieserite, $MgSO_4 \cdot H_2O$, as a dominant sulfate species at lower latitudes. However, given the Fe-rich composition of the martian surface, it is very probable that its actual composition lies at an intermediate value along the solid-solution series between the kieserite and szomolnokite ($FeSO_4 \cdot H_2O$) end-members. Despite the known existence of significant lattice parameter changes and spectral band position shifts between the two pure end-members, no detailed crystal chemical and spectroscopic investigation along the entire kieserite–szomolnokite solid solution range has been done yet.

The present work proves for the first time the existence of a continuous kieserite–szomolnokite solid-solution series and provides detailed insight into the changes in lattice parameters, structural details, and positions of prominent bands in FTIR (5200–400 cm^{-1}) and Raman (4000–100 cm^{-1}) spectra in synthetic samples as the Fe/Mg ratio progresses, at both ambient as well as Mars-relevant lower temperatures. Additionally, an UV-Vis-NIR (29 000–3500 cm^{-1}) crystal field spectrum of szomolnokite is presented to elucidate the influence of Fe^{2+}-related bands on the overtone- and combination mode region.

The kieserite–szomolnokite solid-solution series established in this work shows Vegard-type behavior, i.e., lattice parameters as well as spectral band positions change along linear trends. The detailed knowledge of these trends enables semi-quantitative estimations of the Fe/Mg ratio that can be applied to interpret martian monohydrated sulfates in data from remote sensing missions on a global scale as well as from in situ rover measurements. Given the knowledge of the surface temperature during spectral measurements, the established temperature behavior allows quantitative conclusions concerning the Fe/Mg ratio. Our understanding of the kieserite–szomolnokite solid-solution series will be well applicable to the Mars 2020 and ExoMars 2020 rover missions that will focus on near IR (0.9 to 3.5 μm) and, for the first time on Mars, Raman spectroscopy.

Keywords: Kieserite–szomolnokite solid solution, Mars mineralogy, crystal chemistry, FTIR spectroscopy, Raman spectroscopy, UV-Vis-NIR spectroscopy