

CRYSTAL CHEMICAL AND IR-SPECTROSCOPIC INVESTIGATION OF THE KIESERITE - SZOMOLNOKITE SOLID SOLUTION SERIES WITH RELEVANCE TO MARS

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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 endeavour to retrieve detailed knowledge about the planetary water budget and surface weathering processes on our neighbour planet. Orbiter IR spectra of the Martian surface indicate that kieserite, $\text{MgSO}_4 \cdot \text{H}_2\text{O}$, is a dominant sulfate species at lower latitudes (CHRISTENSEN et al., 2004; CLARK et al., 2005). However, given its presumed formation by weathering of Fe-rich olivines and pyroxenes (CLARK & VAN HART, 1981), it is very probable that the actual composition lies at an intermediate value between the Mg- and Fe-kieserite (szomolnokite) endmembers. Although it is known that lattice parameters and spectral band positions differ significantly between these two endmembers, no detailed crystal chemical or spectroscopic investigation along the entire $(\text{Mg,Fe})\text{SO}_4 \cdot \text{H}_2\text{O}$ solid solution range was done so far.

We hereby present first results on structural and lattice parameter changes from single crystal X-ray diffraction measurements of hydrothermally synthesized crystals with variable Mg/Fe ratio. Furthermore, FTIR spectra reveal changes in the wavenumber positions of prominent bands at ambient and low temperature, as the Fe/Mg ratio progresses towards Fe-dominant compositions. The entire kieserite-szomolnokite solid solution shows Vegard-type behaviour, i.e. lattice parameters as well as spectral band positions change along linear trends with increasing Fe content ($a = 6.91\text{-}7.09$, $b = 7.63\text{-}7.55$, $c = 7.64\text{-}7.78$ Å; $\beta = 118.0\text{-}118.6^\circ$ from kieserite to szomolnokite). The changes observed for several absorption features in the IR spectra enable to roughly estimate the Fe/Mg ratio and its variation in Martian kieserite, by comparison with present and future remote sensing data on a global scale, as well as by in-situ rover measurements. Most suitable absorption features in this respect are the ν_1 vibration of the H_2O molecule, the H_2O bending vibration, the ν_3 and ν_1 stretching modes of the sulfate tetrahedron, as well as a band diagnostic for kieserite at around 850 cm^{-1} (LANE et al., 2015). The symmetric stretching mode of H_2O increases in wavenumber with increasing Fe content, while the SO_4^{2-} stretching modes decrease in energy, along with the H_2O bending vibration and the well-resolved band at $\sim 850\text{ cm}^{-1}$. However, apart from the band at 850 cm^{-1} and the symmetric stretching mode of H_2O , the changes are likely too small to be effectively interpreted from orbital remote sensing measurements showing a poor signal to noise ratio. We therefore recommend only the aforementioned two spectral features to be used for interpretation of the composition of kieserite on the Martian surface.

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