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Chemistry-dependent Raman spectral features of glauconite and nontronite: Implications for mineral identification and provenance analysis

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Abstract

This study provides a comprehensive Raman spectral characterization of nontronite and glauconite-nontronite mixed-layer phases from seafloor hydrothermal fields. These 2:1 phyllosilicates, which show isomorphous cation exchange between Mg^{2+}+Fe^{2+} and Fe^{3+}+Al^{3+} in the dioctahedral sheets, exhibit three diagnostic Raman peaks in the low wavenumber region (v1 ~241–257 cm^{-1}; v2 ~600–606 cm^{-1}; v3 ~690 cm^{-1}), and one peak at ~3548–3570 cm^{-1} (v4). With increasing $(Mg^{2+}+Fe^{2+})_{oct}$, the presumed stretching band of octahedral OH-O bonds (v1) is displaced to a higher wavenumber, whereas the stretching band of tetrahedral Si-O-Si bonds (v2) is shifted to a lower wavenumber. Peak v4, which relates to O-H bonds of hydroxyls linked to octahedral cations, shows a downshift with increasing $(Mg^{2+}+Fe^{2+})_{oct}$. The band v4 can be mathematically fitted by three bands, two of which strongly correlate with the cation occupancy in the octahedral sheets; i.e., vibrations of hydroxyls linked to trivalent cations (Fe^{3+} and Al^{3+}) are mainly represented by a band at ~3560–3573 cm^{-1}, whereas divalent cations (Mg^{2+} and Fe^{2+}) mainly contribute to a band at ~3538–3540 cm^{-1}. This result is consistent with theoretical considerations for dioctahedral phyllosilicates, which predict for the incorporation of Mg^{2+} and Fe^{2+} a weakening/lengthening of O-H bonds in the OH groups, accounting for a downshift of the O-H vibrations. Hence, this is one of the first studies that trace how even subtle chemical modifications in phyllosilicates influence Raman spectral features. The reported findings have implications for mineral identification and provenance analysis, such as during surface exploration on Mars, where compositionally diverse phyllosilicates occur.

Keywords: Phyllosilicates, glauconite, nontronite, peak shift