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Micro-Raman studies of gypsum in the temperature range between 9 K and 373 K

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ABSTRACT

Raman spectra were collected for synthetic gypsum ($CaSO_4 \cdot 2H_2O$) powder between 9 and 373 K under atmospheric pressure with special emphasis on the temperature dependence of the OH-stretching modes. The stretching bands of the water molecules in gypsum were found to shift in opposite directions as a result of the different degree of intermolecular hydrogen-bonding between nonequivalent water H atoms and the O atoms of nearby SO_4 ions. The anharmonic parameters of the OH-stretching modes are calculated using the temperature derivatives measured from the present investigation and existing pressure derivatives. These parameters are -4.7×10^{-6} K^{-1} and -0.6×10^{-6} K^{-1} for the 3407 and 3494 cm^{-1} bands, respectively. The dehydration of gypsum into γ-$CaSO_4$ and the subsequent rehydration of γ-$CaSO_4$ into hemihydrate are clearly identified in the Raman spectra by the observed variation in Raman shifts of the OH and $\nu_1(SO_4)$ bands. The latter increases as the mineral becomes increasingly anhydrous (1007 cm^{-1} in gypsum; 1014 cm^{-1} in hemihydrate; 1026 cm^{-1} in γ-$CaSO_4$), which can be used as a fingerprint for the remote detection of these minerals on planetary surfaces.