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LETTER

Theoretical infrared absorption coefficient of OH groups in minerals

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ABSTRACT

The integrated molar absorption coefficient of isolated and localized OH groups in selected minerals is theoretically investigated within the density functional theory framework. The overall decrease in absorption coefficient of stretching modes observed with increasing frequency is consistent with the experimental observations. It is related to a decrease in the magnitude of the hydrogen Born effective charge tensor projected along the OH bond as a function of increasing H-bonding. The scatter of theoretical data shows that the use of a general calibration of infrared absorbances in minerals cannot lead to accurate water contents. In contrast, the combination of theoretical modeling and experimental measurements should improve the determination of the hydrogen distribution among structurally distinct OH defects in nominally anhydrous minerals.

Keywords: Infrared, spectroscopy, DFT, hydroxyl