

Complex IR spectra of OH⁻ groups in silicate glasses: Implications for the use of the 4500 cm⁻¹ IR peak as a marker of OH⁻ groups concentration

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ABSTRACT

Previous studies of hydrous glasses and melts with infrared spectroscopy have led to the conclusion that the IR combination peaks near 4500 and 5200 cm⁻¹ reflect the existence of OH⁻ (hydroxyl) groups and H₂O_{mol} water molecules in those materials. Here, we show that the glass chemical composition can impact profoundly the intensities and frequencies of the fundamental O-H stretching signal and, therefore, potentially those of the 4500 and 5200 cm⁻¹ combination peaks. In alkali silicate glasses, compositional effects can give rise to peaks assigned to fundamental O-H stretching at frequencies as low as 2300 cm⁻¹. This expanded range of Raman intensity assigned to O-H stretch is increasingly important as the ionic radius of the alkali metal increases. As a result, the combination of the fundamental O-H stretch in OH⁻ groups with the Si-O-H stretch located near 910 cm⁻¹ gives rise to a complex combination signal that can extend to frequencies much lower than 4200 cm⁻¹. This combination signal then becomes unresolvable from the high-frequency limb of the band assigned to fundamental O-H stretch vibration in the infrared spectra. It follows that, when O-H stretch signals from OH⁻ groups extend to below 3000 cm⁻¹, the 4500 cm⁻¹ peak does not represent the total OH⁻ signal. Under such circumstances, this infrared peak may not be a good proxy for determining the concentration of OH⁻ hydroxyl groups for glassy silicate materials.

Keywords: Water speciation, FTIR spectroscopy, O-H stretch signal, silicate glasses