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LETTER

The 4500 cm^{-1} infrared absorption band in hydrous aluminosilicate glasses is a combination band of the fundamental (Si,Al)-OH and O-H vibrations

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ABSTRACT

The position of the infrared absorption band near 4500 cm^{-1} shifts from 4520 to 4440 cm^{-1} as the Al content increases along the SiO_2-$NaAlSiO_2$ join and closely follows the sum of the positions of the Raman bands near 900 and 3600 cm^{-1}. This confirms the idea that the 4500 cm^{-1} band is a combination band of the fundamental (Si,Al)-OH vibration near 900 cm^{-1} and the fundamental O-H stretching vibration near 3600 cm^{-1}. As a consequence, the 4500 cm^{-1} band should not be used to quantify the water speciation for glass compositions for which significant amounts of free hydroxyls are expected as these do not contribute to the band's intensity.

Keywords: Raman spectroscopy, infrared spectroscopy, FTIR, water speciation, silicate glasses, band assignment