The determination of sulfate and sulfide species in hydrous silicate glasses using Raman spectroscopy KEVIN KLIMM^{1,*} AND ROMAN E. BOTCHARNIKOV²

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ABSTRACT

Raman spectroscopy is used to identify the sulfur speciation (sulfur valence state) in "technical" iron-free soda-lime and potassium-silicate glasses and in "natural" glass compositions such as basalt, andesite, and rhyodacite. The presence of sulfate (S⁶⁺) is marked in Raman spectra of oxidized synthetic and natural glasses by bands at ~990 and ~1000 cm⁻¹, respectively. The presence of sulfide (S²⁻) in the reduced technical glasses is marked in Raman spectra by a band at 2574 cm⁻¹ indicating that S²⁻ is present as HS⁻ in these Fe-free glasses. Such a band is absent in the Raman spectra of reduced basaltic, and entited S-bearing "natural" glasses when compared to that of S-free reduced "natural" reference glasses indicating that S²⁻ is most likely complexed with Fe in these glasses. Thus, the dissolution mechanism of S²⁻ appears to be different in Fe-free and Fe-bearing glasses and S²⁻ is dissolved as either HS⁻-species or Fe-S complexes, respectively. The data shown here demonstrate the potential of Raman spectroscopy in identifying the sulfur valence state in silicate glasses. In addition, S²⁻ is dissolved as completely different complexes when comparing "technical" iron-free and "natural" iron-bearing, hydrous silicate glass compositions.

Keywords: Raman spectroscopy, silicate glass, sulfur speciation, sulfur valence state