

Effect of SiO₂, total FeO, Fe³⁺/Fe²⁺, and alkali elements in basaltic glasses on mid-infrared spectra

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ABSTRACT

A suite of basaltic glasses were examined to determine how subtle compositional changes affect mid-infrared spectra (650 to 5400 cm⁻¹). Glasses with different SiO₂, FeO_{total}, Fe³⁺/Fe²⁺, and alkali contents were synthesized in a gas-mixing furnace and analyzed using electron probe microanalysis, Mössbauer spectroscopy, and micro-reflectance Fourier transform infrared spectroscopy. The major mid-infrared spectral feature in silicate glasses is a broad peak located at ~900 to 1100 cm⁻¹ arising from Si-(Al)-O asymmetric stretching vibrational modes. To accurately compare spectra of different glass compositions, we have applied the Kramers-Kronig (KK) transform to our spectra and examined the resulting absorption peak (KK abs. peak). The location of the KK abs. peak shifts to higher wavenumbers as SiO₂ content increases (1031–1054 cm⁻¹ with SiO₂ from 47.18 to 55.57 wt%). For basaltic glasses with near-constant Al/(Al+Si), the full-width half maximum of the KK abs. peak decreases as alkali content increases (235–188 cm⁻¹ with Na₂O+K₂O contents from 0.07 to 3.74 wt%). In contrast, the location and shape of the KK abs. peak are not affected by variations in total FeO (6.06–16.30 wt%) and Fe³⁺/Fe²⁺ (0.05–1.17). Our results show that KK transformed mid-infrared spectra of basaltic glasses may be used to determine the SiO₂ contents in basaltic glasses, irrespective of FeO_{total} and Fe³⁺/Fe²⁺, and the alkali contents if Al/(Al+Si) is known. These observations will aid in the interpretation of laboratory and remotely sensed IR spectra.

Keywords: IR peak location and shape, glass composition, Mössbauer spectroscopy, oxygen fugacity