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Effect of SiO_2, total FeO, Fe^{3+}/Fe^{2+}, 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 SiO_2, FeO_{total}, Fe^{3+}/Fe^{2+}, 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 SiO_2 content increases (1031–1054 cm^{-1} with SiO_2 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 Na_2O+K_2O 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 Fe^{3+}/Fe^{2+} (0.05–1.17). Our results show that KK transformed mid-infrared spectra of basaltic glasses may be used to determine the SiO_2 contents in basaltic glasses, irrespective of FeO_{total} and Fe^{3+}/Fe^{2+}, 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