

LETTER

The speciation of carbon monoxide in silicate melts and glasses

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ABSTRACT

We have studied the speciation of carbon monoxide in both Fe-bearing and Fe-free basaltic glasses using Raman, FTIR, and Mössbauer spectroscopy. We show that a band at 2110 cm⁻¹ in the Raman spectrum and another band at 2210 cm⁻¹ in the FTIR spectrum occur both in the Fe-bearing and Fe-free samples, implying that they cannot be due to any Fe-bearing species. This observation is consistent with ⁵⁷Fe Mössbauer spectra, which do not show any evidence for Fe species with zero isomer shift, as expected for carbonyls. Thermodynamic calculations show that iron carbonyl in basaltic melts under crustal and upper mantle conditions may only be a trace species. Rather than being due to distinct chemical species, the range of vibrational frequencies observed for carbon monoxide in silicate glasses appears to be due to rather subtle interactions of the CO molecule with the matrix. Similar effects are known from the extensive literature on carbon monoxide adsorption on oxides and other surfaces. In the melt at high temperature, there is likely little interaction of the CO molecule with the silicate matrix and solubility may be largely controlled by pressure, temperature, and the overall polymerization or ionic porosity of the melt.

Keywords: Silicate melt, carbon monoxide, iron, carbonyl, Raman, Mössbauer