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A new approach to determine and quantify structural units in silicate glasses using micro-reflectance Fourier-Transform infrared spectroscopy

KIM N. DALBY* AND PENELOPE L. KING

Department of Earth Sciences, The University of Western Ontario, London, Ontario N6A 5B7, Canada

ABSTRACT

Eight silicate unit vibrational modes were identified in a suite of PbO-SiO_2 glasses using micro-reflectance Fourier Transform infrared (μR-FTIR) spectra that were transformed using the Kramers-Kronig relation. The transformed FTIR spectra, in the 800–1200 cm^{-1} range, were deconvolved systematically into eight Voigt-shaped bands at centers that were predicted from the second derivative of the spectra. The area of the eight bands varied as a function of SiO_2 content, and these trends were combined with theoretical constraints to identify and assign the bands to seven provisional silicate units: SiO_4^{4-} (830 and 860 cm^{-1}), $Si_2O_7^{6-}$ (900 cm^{-1}), $Si_6O_{18}^{12-}$ (950 cm^{-1}), $Si_2O_6^{4-}$ (980 cm^{-1}), $Si_4O_{11}^{6-}$ (1010 cm^{-1}), $Si_2O_5^{2-}$ (1050 cm^{-1}), and SiO_2 (1100 cm^{-1}). The provisional units were then grouped according to their NBO/T values: NBO/T = 4 (SiO_4^{4-}), NBO/T = 3 ($Si_2O_7^{6-}$), NBO/T = 2 ($Si_6O_{18}^{12-}$ and $Si_2O_6^{4-}$), NBO/T = 1 ($Si_4O_{11}^{6-}$ and $Si_2O_5^{2-}$) and NBO/T = 0 (SiO_2). The derived quantities of each NBO/T unit compare favorably with nuclear magnetic resonance data for PbO-SiO_2 glasses reported in the literature. This new approach for determining glass structure is advantageous because it may be performed on small Fe-bearing samples with minimal preparation, and analyses are rapid and relatively inexpensive.

Keywords: IR spectroscopy, glass structure, band fitting, PbO-SiO_2