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Coordination of Ti^{4+} in silicate glasses: A high-resolution XANES spectroscopy study at the Ti *K* edge

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Abstract

The coordination environment of Ti in eight Ti-bearing glasses of the $Na_2Si_4O_9$-$Na_2Ti_4O_9$ join (NTS) and in six ATY2 glasses ($A_2O{\cdot}TiO_2{\cdot}2YO_2$, with A = Na, K, or Rb and Y = Si or Ge) was determined using high-resolution, X-ray absorption near-edge structure (XANES) spectroscopy at the Ti *K* edge in ambient conditions.

Fivefold-coordinated Ti ($^{[5]}Ti$) is the dominant Ti species ($\geq 50 \pm 10\%$ of the total Ti) in all the glasses studied. Sixfold-coordinated Ti was detected mostly in sodic glasses (NTS, NTS2, NTG2), and it increases with TiO_2 content (as high as $40 \pm 10\%$ of the total of Ti in the most TiO_2-rich NTS glasses) and in the order Si < Ge. Fourfold-coordinated Ti was detected only in nonsodic ATY2 glasses, and its content increases in the order Na < K < Rb and Ge < Si. Fivefold-coordinated Ti^{4+} is probably present as square pyramidal, titanyl-bearing moieties, or $(^{[5]}Ti{=}O)O_4$.

A synthesis of Ti^{4+} coordination for oxide glasses derived using direct methods (X-ray absorption and neutron scattering) can be used, for instance, to help in the interpretation of Raman scattering spectra collected for Ti-bearing glasses and to estimate NBO/T ratios better for titanosilicate glasses and melts.