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Disordering during melting: An ^{17}O NMR Study of crystalline and glassy $CaTiSiO_5$ (titanite)

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ABSTRACT

Although titanite ($CaTiSiO_5$) has one of the highest known entropies of fusion among silicates, the corresponding melt is a relatively good glass-former, which provides an opportunity to investigate the structural origin of disorder in the liquid. Here we present an ^{17}O NMR study of $CaTiSiO_5$ glass, using detailed new results on the crystalline phase, collected at magnetic fields of 9.4, 14.1, 18.8, and 21.1 Tesla, to interpret the spectra. We find that the glass contains significant concentrations of Si-O-Si and Si-O-Ca sites in addition to the Ti-O-Ti and Ti-O-Si sites of the crystal, suggesting considerable network disorder. Simulations of the spectra for the crystal allow the derivation of isotropic chemical shifts and quadrupolar coupling constants (C_Q) for each of the five O atom sites. In addition the Ti-O-Ti site has an unusually large chemical shift anisotropy and an unusually small C_Q value.