Fe-tourmaline synthesis under different T and f_{o_2} conditions

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ABSTRACT

Mössbauer spectrometry of natural samples of tourmaline shows the presence of Fe^{2+} and Fe^{3+} either in the Y (9b) or the Z (18c) sites, with intervalent iron delocalized between these sites. To understand the distribution of iron in natural samples, tourmaline was synthesized at temperatures from 400 to 700 °C, under a pressure of 100 MPa, by the transformation of an Fe^{2+} -rich natural chlorite in the presence of $Na_{0.5}K_{0.5}$ -feldspar, boric acid, and H_2O in stoichiometric proportions. The oxygen fugacity, $f_{0.2}$, of most experiments was buffered by solid assemblages including hematite (HM), nickel-nickel oxide (NNO), and quartz-fayalite-iron (QFI). It was possible to synthesize tourmaline with Fe^{2+} in the Z site and Fe^{2+} or $Fe^{2+} + Fe^{3+}$ in the Y site. These site occupancies are similar to those observed in many natural samples.

For each f_{O_2} buffer, Mössbauer spectrometry shows that Fe³⁺/Fe²⁺ in the Y site is correlated positively with T and f_{O_2} for T <550 °C. For higher temperatures, a negative correlation is observed. These relationships reflect structural changes involving the localization of Fe²⁺ in the Z site and an increasing amount of Al in the Y site. Fe³⁺/total Fe can be represented by general equations of the type [%Fe³⁺] = e^(a log fo_2+b). The curves corresponding to each temperature are roughly parallel and equidistant. Thus, Fe tourmaline is a potential geothermometer and an f_{O_2} indicator.