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_{O_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 Fe^{3+}/Fe^{2+} 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 Fe^{2+} in the Z site and an increasing amount of Al in the Y site. Fe^{3+}/total Fe can be represented by general equations of the type $[\%Fe^{3+}] = e^{(a\ \log f_{O_2} + b)}$. The curves corresponding to each temperature are roughly parallel and equidistant. Thus, Fe tourmaline is a potential geothermometer and an f_{O_2} indicator.