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Fe-tourmaline synthesis under different T and f_{0} , conditions

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ABSTRACT

Mössbauer spectrometry of natural samples of tourmaline shows the presence of Fe²⁺ and Fe³⁺ 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 Fe²⁺-rich natural chlorite in the presence of Na_{0.5}K_{0.5}-feldspar, boric acid, and H₂O in stoichiometric proportions. The oxygen fugacity, $f_{0.5}$, 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 Fe²⁺ in the Z site and Fe²⁺ or Fe²⁺ + Fe³⁺ 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 logfO_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.