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High-temperature, high-pressure optical spectroscopic study of ferric-iron-bearing tourmaline

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ABSTRACT

The optical spectra of dravite (tourmaline) with an unusually high ratio of Fe^{3+} to Fe^{2+} and a synthetic elbaite with high Fe^{3+} content were studied at high temperature (297 to 600 K) and high pressure (to 10.51 GPa) conditions. Individual absorption bands derived from paired Fe atoms were identified in the spectra and their temperature and pressure dependence was studied. The most pronounced effects are the intensification of the two Fe^{2+}-related bands (~9090 cm^{-1} and ~14300 cm^{-1}) at pressure, their shift to higher energy at pressure, and their pronounced intensity decrease with increasing temperature. Such behavior is assumed to be caused by an electronic exchange interaction in an Fe^{2+}-Fe^{3+} pair at adjacent Y sites in the structure.

Temperature and pressure dependencies of the bands attributed to Fe^{3+}-Fe^{3+} exchange-coupled pairs are noticeably different from those of Fe^{2+}-Fe^{3+} pairs. This shows that the two types of pairs have different exchange interactions, and points to the need for further experimental and theoretical investigation.

The intensity of the intense **E⊥c**-polarized band at ~ 20580 cm^{-1} originating from the $^6A_{1g} \rightarrow (^4A_{1g}, {}^4E_g)$ transition of the Fe^{3+}(Y)-Fe^{3+}(Y) pair, depends moderately on temperature and pressure. The intensity of a weak shoulder at ~18350 cm^{-1} (**E⊥c**), also attributed to an Fe^{3+}(Y)-Fe^{3+}(Y) pair, decreases and nearly disappears between 5.44 and 9.55 GPa. The intensity of the **E||c**-polarized band at ~18500 cm^{-1}, attributed to an Fe^{3+}(Z)-Fe^{3+}(Z) pair, displays a strong inverse temperature dependence, whereas the energy of the band remains nearly constant.