INTRODUCTION

Tourmaline is a structurally and chemically complex boro-silicate mineral with the general formula $XY_3Z_6Si_6O_{18}(BO_3)_3W_4$, where $X = Na^+$, $Ca^{2+}$, $K^+$, vacancy ($\square$); $Y = Mg^{2+}$, $Fe^{2+}$, $Mn^{2+}$, $Al^{3+}$, $Fe^{3+}$, $Mn^{3+}$, $Cr^{3+}$, $Li^+$; $Z = Al^{3+}$, $Mg^{2+}$, $Fe^{3+}$, $Cr^{3+}$, $V^{3+}$, and $W = O^{2-}$, $OH^-$, $F^-$, $Cl^-$. In this structure, corner-sharing tetrahedra form hexagonal rings and are principally occupied by Si, although minor amount of $^{19}Al$ is found in some cases (Rosenberg and Foit 1979). Al, B and Na ions serve in different ways to tie together the central cores of composition $Y_3OH_4Si_6O_{21}$ (Fig. 1). OH groups occupy two structurally distinct positions: the center of the hexagonal rings and the corner of brucite-like fragments of three edge-sharing octahedra (Gonzalez et al. 1988). Although extensive solid solution is possible, the main compositional varieties in nature are Na- and Mg-rich dravite, Na- and Fe-rich schorl, Ca- and Mg-rich uvite and Na- and Li-rich elbaite (Dietrich 1985).

Since Merrit’s first observation of the infrared (IR) spectrum of tourmaline in 1895 (Dietrich 1985), it has been the subject of many investigations. For example, IR spectra of natural tourmaline of dravite-schorl and elbaite-schorl series were studied by Gonzalez et al. (1988) and O-H stretching bands were related to O-H environments. Blanco (1989) investigated IR spectra of red, blue, and colorless elbaite crystals and observed very similar data, however some differences in wavenumber and the intensity of the bands were attributed to different content in some elements. IR spectra of the O-H stretching region of synthetic tourmalines of the olenite-dravite and olenite-schorl series were studied by Mashkovtsev et al. (1989), who discussed the position and intensity of O-H bands in terms of crystallochemical features of tourmaline. Mashkovtsev and Lebedev (1991), interpreted the number and the positions of OH bands of natural tourmaline based on the spectral behavior of solid solutions. Grice and Ercit (1993) investigated elbaite, dravite, schorl, and uvite and observed a single absorption band in 3300–3800 cm$^{-1}$ region for all tourmaline samples, except elbaite, which has two bands. The proposed O-H stretching assignments are not in agreement (Table 1). This paper reports IR spectra of tourmaline from the elbaite-schorl series in the 3100–3800 cm$^{-1}$ region, and assigns bands on the basis of unit-cell parameter and the results of factor group analysis (Fateley et al. 1972). Fifteen tourmaline samples studied were selected from granitic pegmatites from the Araçú area, northeast Minas Gerais state, Brazil.

ABSTRACT

Two different behaviors controlled by local lattice environment of crystallization are observed in the IR spectra of polycrystalline natural tourmalines from the elbaite-schorl series in the O-H stretching region (3800–3100 cm$^{-1}$). The first case is characterized by the presence of three O-H stretching bands, and is observed in elbaite $[Na(Li,Al)_{3}Al_{6}(BO_3)_3Si_6O_{18}(OH)_4]$, schorl $[NaFe^{3+}Al_3(BO_3)Si_5O_{16}(OH)_4]$ and Fe-elbaite. The second case is observed in Li-rich schorl and is marked by four O-H stretching bands. This behavior is due to the presence of Li-rich and Fe-rich domains in schorl crystallized in Li-bearing pegmatites. Band assignments are discussed using the results of the factor group analysis for a $C_{3v}$ crystal structure and considering the interactions between the O-H and the atoms in the Y and Z sites in the crystal. The interpretation presented differs from previous conclusions.

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