

Structural and chemical response to varying ^{14}B content in zoned Fe-bearing olenite from Koralpe, Austria

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ABSTRACT

Tourmaline has recently been shown to incorporate large amounts of substituent B at the tetrahedral site. To characterize the response of the tourmaline atomic arrangement to differing amounts of substitution of B for Si, five samples were separated from a core-to-rim (~3 mm) section of an Fe-bearing olenite with a dark green core and a nearly colorless rim from Koralpe, Austria. Crystal structures of the five samples were refined to R values <0.018 using three-dimensional X-ray methods, and the compositions of the crystals were determined by electron microprobe, secondary ion mass spectrometric, and Mössbauer analyses. From core to rim, ^{14}B increases monotonically from 0.35 to 0.65 apfu, whereas the mean T-O distance decreases from 1.621 to 1.610 Å. Optimized formulae using chemical and structural data range from $^{\text{X}}(\text{Na}_{0.632}\text{Ca}_{0.145}\square_{0.223})^{\text{Y}}(\text{Al}_{1.320}\text{Fe}_{1.202}^{2+}\text{Li}_{0.190}\text{Mg}_{0.086}\text{Ti}_{0.028}\text{Mn}_{0.024}^{2+}\square_{0.150})^{\text{Z}}\text{Al}_{6.00}\text{B}_{3.00}\text{T}(\text{Si}_{5.525}\text{B}_{0.333}\text{Al}_{0.130}\text{Be}_{0.012})\text{O}_{27}[(\text{OH})_{3.19}\text{O}_{0.81}]$ (core composition) to $^{\text{X}}(\text{Na}_{0.408}\text{Ca}_{0.290}\text{K}_{0.002}\square_{0.300})^{\text{Y}}(\text{Al}_{2.338}\text{Li}_{0.365}\text{Fe}_{0.084}^{2+}\text{Mn}_{0.009}^{2+}\text{Mg}_{0.005}\text{Ti}_{0.005}\square_{0.194})^{\text{Z}}\text{Al}_{6.00}\text{B}_{3.00}(\text{Si}_{4.989}\text{B}_{0.615}\text{Al}_{0.362}\text{Be}_{0.034})\text{O}_{27}[(\text{OH})_{3.41}\text{O}_{0.59}]$ (rim composition). The variation of chemistry and structure, coupled with short-range order constraints, demonstrates that (1) the average tetrahedral bond length (<T-O>) reflects the substitution of ^{14}B , (2) tourmaline samples with relatively high Fe^{2+} contents (ca. 1 apfu Fe^{2+}) and <T-O> distances up to 1.621 Å can contain significant amounts of ^{14}B (up to ca. 0.3 apfu), (3) the presence of substantial ^{14}B is limited to, or more common in Al-rich tourmalines, (4) the presence of ^{14}B substituents favors OH at the O3 site, (5) the presence of Ca or Na at the X site is not simply correlated with occupancy of ^{14}B in the adjacent tetrahedral ring, and (6) no two B-substituted tetrahedra will link through bridging O atoms.