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Exploring the potential of Raman spectroscopy for crystallochemical analyses of complex hydrous silicates: II. Tourmalines

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Abstract

A detailed Raman spectroscopic, electron microprobe, and laser ablation-induced coupled plasma-mass spectrometric study of 46 natural tourmalines [$XY_3Z_6(T_6O_{18})(BO_3)_3V_3W$] from 10 subgroups was performed to evaluate the potential of the Raman scattering, in particular of the OH bond stretching vibrations, for the identification of tourmaline species and site-occupancy analysis. The widespread chemical variety of the studied samples is reflected in the different spectral shapes. The positions and intensities of the observed vibrational modes can be used for tourmaline species identification. Taking into account the charge of the Y- and Z-site cations as well as the X-site occupancy, the Raman peaks generated by the bond stretching mode of the ^{V}OH groups were attributed to different YZZ-YZZ-YZZ cationic configurations, while the peaks originating from ^{W}OH stretching is due to chemically different YYY triplets next to an X-site vacancy, ^{X}Na, or ^{X}Ca. It is shown that the integrated intensities of the ^{V}OH-stretching peaks can be used to calculate the contents of the major Y-site elements Mg, (Fe^{2+}+Mn^{2+}), Li, and Al. The analysis of the ^{V}OH-peak positions yields information on the X-site occupancy. The fitted linear equations can be used to determine the content of ^{X}(Na+Ca) and X-site vacancy per formula unit. Guidelines for how to gain crystallochemical information from the Raman spectra of tourmaline are suggested. This study, along with Part 1 dedicated to amphiboles (Leissner et al. 2015), reveals that Raman spectroscopy is well suited as a non-destructive, preparation-free, and easy-to-handle method for species identification and site-occupancy analysis in complex hydrous silicate. Our results demonstrate that the chemistry on the non-tetrahedral positions substantially influences the Raman-active H-O bond stretching phonon modes, which allows for quantitative compositional analysis, including the content of lithium.

Keywords: Tourmaline, Raman spectroscopy, electron microprobe analysis, LA-ICP-MS