Raman spectra of various types of tourmaline

BILIANA GASHAROVA*, BORIANA MIHAILOVA** and LUDMIL KONSTANTINOV**

*Forschungszentrum Karlsruhe GmbH, ITC-WGT, Department of Technical Mineralogy, P.O. Box 3640, D-76021 Karlsruhe, Germany e-mail: biliana.gasharova@itc-wgt.fzk.de
**Central Laboratory of Mineralogy and Crystallography, Bulgarian Academy of Sciences, Rakovski St. 92, 1000-Sofia, Bulgaria e-mail: mincryst@bgcict.acad.bg

Abstract: A large number of different tourmalines are investigated by Raman spectroscopy in the spectral range 150–1550 cm⁻¹. According to their chemical composition, the studied tourmalines can be classified into three main groups: buergerite-schorl, G1; elbaite-type, G2; and dravite-buergerite-uvite, G3. It is shown that the same classification of tourmalines can be established on the basis of their Raman spectra. Bands for G1 are centred at about 230 and 670 cm⁻¹, the spectra being characterized by a single peak at 238 ± 2 cm⁻¹ and three resolved peaks at 635 ± 3, 674 ± 3 and 697 ± 3 cm⁻¹; G2 has a sharp peak at 224 ± 2 and two well separated peaks, one at 638 ± 3 cm⁻¹ and the other higher than 707 cm⁻¹; G3 is characterized by two peaks at 215 ± 3 and 237 ± 3 cm⁻¹, with a smoothed spectral band centred at about 670 cm⁻¹.

Key-words: tourmaline, Raman spectroscopy.

Introduction

Tourmalines have recently attracted much interest due to the significant variations observed in their composition within one and the same type of structure. The tourmaline group of minerals has been most generally described by the formula XY₂Z₆(BO₃)₃[(Si,Al)₆O₁₈](O,OH)₃(OH,F), where X = Na,Ca,Mg,□; Y = Li,Mg,Fe²⁺/³⁺,Al, Ti, □ and Z = Mg,Fe³⁺,Al, etc.

Due to the large amount of substitutions in octahedral sites Y and Z, tourmalines have been usually considered in terms of the end-member components:

- schorl NaFe³⁺Al₆(BO₃)₃Si₆O₁₈(OH,F)₄;
- elbaite Na(Li,Al)₁₂Al₆(BO₃)₂Si₁₈O₁₈(OH,F)₄;
- buergerite NaFe⁺³Al₆(BO₃)₃Si₆O₁₈(F,O)₃;
- dravite NaMg₃Al₆(BO₃)₃Si₁₈O₁₈(OH,F)₃;
- uvite CaMg₃(Al₃Mg)(BO₃)₂Si₁₈O₁₈(OH,F)₄.

Although Raman spectroscopy has proved to be a powerful method for studying structural properties of minerals (especially the role of short- and intermediate-range ordering), it has been only sporadically applied to tourmalines. The reason is the complicated structure of these minerals, which requires sophisticated identification of the spectral peaks. So far, only the study of Griffith (1969) has systematized Raman shifts in tourmalines in terms of the vibrational modes of rings of SiO₄ tetrahedra. Alvarez & Coy-Yll (1978) have presented Raman spectra of four single crystals of tourmaline in the frequency range 100–1200 cm⁻¹, suggesting that the Si₆O₁₈ rings can hardly be considered as separate vibrational units. On the contrary, a relatively recent study by Peng et al. (1989) reported polarized Raman spectra of tourmalines from three geological occurrences in China, in which the major peaks in the spectral range below 1200 cm⁻¹ were related to modes of hexagonal [Si₆O₁₈]¹²⁻ rings.

The present study presents the results of a detailed study of tourmalines by Raman spectroscopy in the frequency range 150–1550 cm⁻¹, where cation-oxygen vibrational modes are Ra-