

**A CALIBRATION CURVE FOR THE OH CONTENT OF VESUVIANITE:
A POLARIZED SINGLE-CRYSTAL FTIR STUDY**

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A well-characterized suite of vesuvianite samples from the volcanic ejecta of Latium (Italy) was studied by SREF (single-crystal X-ray refinement), EMPA, SIMS (Secondary-Ion Mass Spectrometry) and single-crystal, polarized radiation, FTIR spectroscopy in the OH-stretching region. Light elements in particular were analyzed by SIMS using an ion microprobe (Cameca IMS 4f) at CNR-Istituto di Geoscienze e Georisorse (Pavia). A ¹⁶O⁻ primary ion beam accelerated at 12.5 kV, with a beam intensity of 3 nA and a beam diameter ≤ 5 μm was employed. The SiO₂ (wt%) content (from EMPA) was selected as an internal reference for H, Li, Be and B (OTTOLINI et al., 2002; OTTOLINI & OBERTI, 2000). Most samples are B- (up to 3.67 wt%) and F-rich (up to 2.38 wt%). All IR spectra consist of a rather well-defined triplet of broad bands at higher frequency (3700-3300 cm⁻¹), and a very broad, composite absorption below 3300 cm⁻¹. These spectra are characteristic of B-rich and F-rich vesuvianites (GROAT et al., 1995). Measurements with E//c or E.Lc show that all bands are strongly polarized with maximum absorption for E//c, and agree with previous band assignment to the two O(11)-H(1) and O(10)-H(2) groups in the structure (GROAT et al., 1995). Pleochroic measurements with changing direction of the E vector of the incident radiation shows that the orientation of the O(11)-H(1) dipole is OH[^]c ~ 35°, in excellent agreement with the neutron data of LAGER et al. (1999). A calibration curve, based on SIMS data on the same crystals used for FTIR analysis is presented. The integrated molar absorption coefficient for vesuvianite is ε_i = 97.000 ± 2000 l mol⁻¹ cm⁻². This value is in good agreement with the calibration curve for minerals established by LIBOWITZKY & ROSSMAN (1997). Preliminary data show that a quantitative determination of water in vesuvianites is also possible using powder IR spectroscopy, provided the sample is prepared in a well-standardized way.

References

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