

## **FTIR spectroscopy of Ti-rich pargasites from Lherz and the detection of O<sup>2-</sup> at the anionic O3 site in amphiboles**

**GIANCARLO DELLA VENTURA,<sup>1,2,\*</sup> ROBERTA OBERTI,<sup>2</sup> FRANK C. HAWTHORNE,<sup>3</sup>  
AND FABIO BELLATRECCIA<sup>1</sup>**

<sup>1</sup>Dipartimento di Scienze Geologiche, Università Roma Tre, Largo S. Leonardo Murialdo 1, I-00146 Roma, Italy

<sup>2</sup>CNR-Istituto di Geoscienze e Georisorse, Unità di Pavia, via Ferrata 1, I-27100 Pavia, Italy

<sup>3</sup>Department of Geological Sciences, University of Manitoba, Winnipeg, R3T 2N2 Canada

### **ABSTRACT**

This paper reports a single-crystal unpolarized-light FTIR study in the OH-stretching region of a suite of well-characterized Ti-rich pargasites from Lherz (French Pyrenees). All amphiboles studied have fairly constant M-site composition, with <sup>6</sup>Al<sub>tot</sub> ~0.55 atoms per formula unit (apfu), <sup>6</sup>Ti ~0.45 apfu, and <sup>6</sup>Fe<sup>3+</sup> ~0.40 apfu. SIMS and SREF data show all samples to have an O3 anion composition of OH ≈ O<sup>2-</sup> ≈ 1.0 apfu, with negligible F. The FTIR spectra show for all samples a broad absorption consisting of several overlapping bands; three main components can be recognized: ~3710, 3686, and 3660 cm<sup>-1</sup>, respectively, with an asymmetric tail extending to lower frequency. Six Gaussian components can be fitted to the spectra; comparison with spectra of both synthetic and natural pargasites allows five of these components to be assigned to local configurations involving OH-O<sup>2-</sup> at the O3 site, thus showing that coupling with an O<sup>2-</sup> anion through an A-cation significantly affects band position. Infrared spectroscopy can detect the presence of O<sup>2-</sup> in amphiboles in chemically favorable cases, i.e., in the absence of F. Moreover, the FTIR spectra show that all octahedral configurations involving <sup>M1</sup>Ti<sup>4+</sup> or <sup>M1</sup>Fe<sup>3+</sup> <sup>M3</sup>Fe<sup>3+</sup> are associated with O<sup>2-</sup> at both adjacent O3 sites, and that <sup>M3</sup>Al is locally associated with OH, confirming SRO models based on structure refinement results.

**Keywords:** Ti-rich pargasite, Lherz (French Pyrenees), single-crystal FTIR spectroscopy, anion occupancy