

## **Calibration for IR measurements of OH in apatite**

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### **ABSTRACT**

In this work, we have calibrated the infrared (IR) method for determining OH concentrations in apatite with absolute concentrations obtained through elastic recoil detection (ERD) analysis. IR spectra were collected on oriented, single-crystal apatite samples using polarized transmission infrared spectroscopy. The weight percent H<sub>2</sub>O is  $0.001199 \pm 0.000029$  (the error is given at  $1\sigma$  level hereafter) times  $A/d$ , where  $A$  is the linear absorbance peak height measured using polarized IR when the light vector  $\mathbf{E}$  is parallel to the  $\mathbf{c}$ -axis of the apatite crystal, and  $d$  is the sample thickness in centimeters. This corresponds to a linear molar absorptivity,  $\epsilon = 470 \pm 11$  L/mol/cm<sup>-1</sup>. The calibration using linear absorbance can be applied when there is only one dominant peak at 3540 cm<sup>-1</sup>. If other peaks are significant, then the integrated molar absorptivity,  $\epsilon = (2.31 \pm 0.06) \times 10^4$  L/mol/cm<sup>2</sup>, should be used. The detection limit of H<sub>2</sub>O concentration in apatite by IR approaches parts per million level for wafers of 0.1 mm thickness. The accuracy based on our calibration is 5–10% relative.

**Keywords:** Apatite, water concentration, IR spectroscopy, ERD analysis