

SPECIAL COLLECTION: APATITE: A COMMON MINERAL, UNCOMMONLY VERSATILE

## Quantification of CO<sub>2</sub> concentration in apatite

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### ABSTRACT

We have calibrated the infrared (IR) method for determining CO<sub>2</sub> concentrations in apatite with absolute concentrations obtained through nuclear reaction analysis (NRA). IR data were obtained on double-polished apatite wafers using polarized transmission IR spectroscopy. Due to the various sites and orientations of CO<sub>3</sub><sup>2-</sup> in apatite, the IR spectra are complicated and do not have the same shape in different apatite samples. Hence, simple peak heights are not used to characterize CO<sub>2</sub> concentrations in apatite. The total absorbance ( $A_{\text{total}}$ ) was derived using the integrated area under the curves in a given polarized spectral region. Then  $A_{\text{total}}$  is calculated as  $A_{\text{E}/\text{c}} + 2A_{\text{E}\perp\text{c}}$ . The calibration has been carried out for two wavenumber regions, one with high sensitivity and the other applicable to apatite with high CO<sub>2</sub> concentrations. The first calibration is for the fundamental asymmetric CO<sub>3</sub><sup>2-</sup> stretching at wavenumbers of 1600–1300 cm<sup>-1</sup>, and the CO<sub>2</sub> concentration in parts per million can be obtained as  $(0.0756 \pm 0.0036) A_{\text{total}}/d$  where  $d$  is sample thickness in centimeters. The fundamental stretching bands are strong and hence sensitive for measuring low CO<sub>2</sub> concentrations in apatite, down to parts per million level. The second calibration is for the CO<sub>3</sub><sup>2-</sup> bands at wavenumbers of 2650–2350 cm<sup>-1</sup>, and the CO<sub>2</sub> concentration in parts per million is  $(9.3 \pm 0.6) A_{\text{total}}/d$  where  $d$  is sample thickness in centimeters. These bands are weak and hence are useful for measuring high CO<sub>2</sub> concentrations in apatite without preparation of super-thin wafers. The anisotropy is significant. The difference between  $A_{\text{E}/\text{c}}$  and  $A_{\text{E}\perp\text{c}}$  can reach a factor of 2.73. Hence, for high accuracy, it is best to use polarized IR to determine CO<sub>2</sub> concentrations in apatite. For rough estimation, unpolarized IR spectra may be used by estimating  $A_{\text{total}} = 3A_{\text{unpol}}$ , where  $A_{\text{unpol}}$  is the integrated absorbance from unpolarized spectra.

**Keywords:** Carbonate in apatite, IR spectroscopy, nuclear reaction analysis, NRA