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Quantitative absorbance spectroscopy with unpolarized light: Part II. Experimental evaluation and development of a protocol for quantitative analysis of mineral IR spectra

István Kovács,[1,*] Jörg Hermann,[1] Hugh St.C. O'Neill,[1] John Fitz Gerald,[1] Malcolm Sambridge,[1] and Gábor Horváth[2,3]

[1]Research School of Earth Sciences, The Australian National University, Building 61, Mills Road, 0200, Canberra, ACT, Australia
[2]Centre for Computer Science and Informatics Research, University of Hertfordshire, College Lane, Hatfield, Hertfordshire, AL10 9AB, U.K.
[3]Department of Algebra and Number Theory, Eötvös Loránd University, Budapest, Pázmány Péter sétány 1/C, 1118, Hungary

Abstract

The predictions of the theory of light propagation in weakly absorbing anisotropic minerals are tested against systematic measurements of the infrared absorbance spectra of calcite, olivine, and topaz oriented in both principal and random sections, using both polarized and unpolarized light. We show that if the linear polarized maximum absorbance is smaller than ~0.3, or if the ratio of maximum and minimum absorbance is close to unity, then (1) the polarized maximum and minimum absorbances as well as the unpolarized absorbance are, to a good approximation, linearly proportional to thickness, regardless of the direction of the incident light; (2) the angular variation of polarized light absorption is indistinguishable from the theoretical predictions within the uncertainty of the measurements; (3) for any section the unpolarized absorbance is the mean of the polarized maximum and minimum absorbance; and (4) the average unpolarized absorbance of randomly oriented grains is one third of the Total Absorbance (defined as the sum of the three principal absorbances). Therefore, calibrations relating Total Absorbance to absorber concentration in minerals that have been developed from measurements with polarized light parallel to the principal axes may be applied to measurements with unpolarized light on a population of randomly oriented sections. We show that 10 such measurements are sufficient to achieve a petrologically useful accuracy. The method enables water concentrations in nominally anhydrous minerals to be determined from samples where the preparation of oriented specimens is not feasible, such as high-pressure experimental runs and fine-grained mantle xenoliths. The method may also be used for obtaining quantitative measurements on low-symmetry minerals.

Keywords: Infrared spectroscopy, absorbance spectroscopy, unpolarized light, olivine, calcite, topaz, nominally anhydrous minerals