American Mineralogist, Volume 103, pages 1176–1184, 2018

The inverse problem of unpolarized infrared spectroscopy of geological materials: Estimation from noisy random sampling of a quadratic form

Andrew Jackson[1,*,†], Robert L. Parker[2], Malcolm Sambridge[3], Catherine Constable[2], and Aaron S. Wolf[4]

[1]Institute for Geophysics, ETH Zurich, Sonneggstrasse 5, 8092 Zurich, Switzerland
[2]Institute of Geophysics and Planetary Physics, Scripps Institution of Oceanography, University of California, San Diego, U.S.A.
[3]Research School of Earth Sciences, Australian National University, Canberra, Australia
[4]Department of Earth and Environmental Sciences, University of Michigan, Ann Arbor, Michigan, U.S.A.

Abstract

We address the problem of unpolarized light spectroscopy of geological materials. Using infrared radiation, the aim of this technique is to learn about the absorbing species, such as hydroxyl. The use of unoriented samples leads to the need to perform a rigorous statistical analysis, so that the three principal absorbances of the crystal can be retrieved. We present here such an analysis based on a derivation of the probability density function for a single random measurement. Previous methods for retrieval of the absorbances are shown to be suboptimal, producing biased results that are sometimes even unphysical (e.g., negative estimates for an inherently positive quantity). The mathematical structure of the problem is developed to use the maximum likelihood estimation method, and we show how to optimize for the three absorbance parameters. This leads to good parameter retrieval on both synthetic and real data sets.

Keywords: Spectroscopy, hydroxyl, unpolarized, infrared; Water in Nominally Hydrous and Anhydrous Minerals