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Determining hematite content from NUV/Vis/NIR spectra: Limits of detection

William Balsam[1,*], Junfeng Ji[2], Devon Renock[1], Bobby C. Deaton[3] and Earle Williams[4]

[1]Department of Earth Sciences, Dartmouth College, Hanover, New Hampshire 03755, U.S.A.
[2]Key Laboratory of Surficial Geochemistry, Ministry of Education, School of Earth Sciences and Engineering, Nanjing University, Nanjing 210093, China
[3]Department of Physics, Texas Wesleyan University, Fort Worth, Texas 76105, U.S.A.
[4]Parsons Laboratory, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, U.S.A.

Abstract

Hematite occurs in various geologic settings including igneous, metamorphic, and sedimentary rocks as well as in soils. However, it frequently occurs at low concentrations, especially in soils, where it may be <1% by weight. Because hematite has the potential to be an indicator of oxidizing and climatic conditions in soils and paleosols, it is important to understand its limit of detection. In this paper we examine the limits of detection of hematite visually and with diffuse reflectance spectrophotometry (DRS) and X-ray diffraction (XRD). To accomplish this we used a sample set consisting of "knowns" or calibration samples. These known samples consisted of 15 different matrices of varying mineral composition into which hematite in 7 different concentrations ranging from 0.01 to 4% by weight were mixed. Including the 0% hematite, our calibration data set consisted of 120 samples. Visually, hematite can be detected at a concentration of 0.01% by weight in a light matrix and 0.5% in the darkest of our matrices. However, because of metamerism, visual techniques cannot specifically identify hematite. We find that for both DRS and XRD the limit of detection is also dependent on the matrix. For XRD the limit of detection for hematite in bulk samples is about 1%. For DRS the limit of detection depends on the data reduction technique used. The commonly used Kubelka-Munk remission function and its first and second derivatives can easily identify hematite at the 0.5% level. However, the first derivative of the percent reflectance curve can detect hematite at 0.01% by weight in a light matrix and 0.05% in a dark matrix. We suggest that the first derivative of DRS curves is the best currently available method for qualitatively detecting the mineral hematite at low concentrations found in soils, sediments, and rocks.

Work described in this paper may be applied in several situations. Our study of visual limits of hematite detection should aid field geologists in assessing hematite content. Analysis of color wavelength bands may also have application in remote sensing by indicating which bands are most sensitive to hematite, reported to be an important constituent of the martian surface. Furthermore, this study could help clarify remotely sensed terrestrial albedo changes, especially the Sahara/Sahel transition where the sediments change from light, quartz-dominated to dark, hematite-dominated. Our study also points out that with laboratory-based spectra the first derivative of the reflectance curve is the most sensitive transform for processing spectral data for hematite, thereby allowing concentrations as low as 0.01% to be detected.

Keywords: Hematite, first derivative transform, color, diffuse reflectance spectrophotometry, Kubelka-Munk remission function, XRD