

*AN INDEPENDENT ASSESSMENT OF DERIVATIVE ANALYSIS OF REFLECTANCE SPECTRA*

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We have been investigating the utility of derivative-based spectral analyses for reflectance spectroscopy, including the method of Huguenin and Jones (1986). The need for more objective and automatic analysis tools exists at present, and will become critical for the large amounts of spectral image data to be returned by future missions including Galileo, Mars Observer, and CRAF. Quantitative analysis techniques applied uniformly to laboratory and remotely-sensed data sets should produce consistent and reproducible results, including an estimate of uncertainty. A specific important need is an improved method for identifying and characterizing individual mineral absorptions in complicated, overlapping band envelopes.

We have examined the practical utility of recognizing absorption band positions, and the responsible mineralogies, through the characteristics of second and higher-order derivatives of reflectance spectra. This idea was proposed by Huguenin and Jones (1986) based on similar techniques commonly employed in laboratory absorption spectroscopy (e.g. Morrey, 1968). We have evaluated their method as closely as possible, using actual laboratory spectra of controlled binary mixtures of orthopyroxene, clinopyroxene, and olivine (from Singer, 1981), both from the point of view of internal self-consistency and by comparison with results of more traditional analyses. In addition we have considered alternate analysis schemes, concentrating primarily on the second derivative.

The concepts of spectral derivative analysis first appeared in the analytical chemistry literature 30 years ago (e.g. Hammond and Price, 1953; Morrison, 1953; French et al., 1954). Most of the chemical applications are in absorption spectroscopy, in which the data are typically less complicated and of higher signal/noise than for remote sensing applications. Spectral derivatives have been most commonly used for determining the energies of broad absorption maxima to greater precision. Less frequently they have been used to enhance small scale structure over a slowly varying background, and to resolve overlapping bands. The use of derivatives to actually identify absorption features has not become popular in analytical chemistry. Morrey (1968) derived conditions under which peaks in synthetic composite spectra could be detected from examining third and fourth derivatives. Huguenin and Jones (1986) modified and expanded the work of Morrey.

In the approach of Huguenin and Jones, bands are identified at positions where the 5th derivative crosses zero, the 4th derivative is negative, and the 2nd derivative is positive. As stated by those authors, the utility of this type of technique is critically dependent on proper smoothing of the data, since higher order derivatives are increasingly sensitive to small variations such as noise (although smoothing is essential for analysis of synthetic data, also). Huguenin and Jones (1986) refer to a proprietary "adaptive filtering" scheme used in their method, but do not provide enough information for others to reproduce it and test their technique exactly. Instead we analyzed our data over a large range of filtering parameters to see under what conditions the technique might succeed. As an initial test of our procedure we successfully duplicated Huguenin and Jones' results on synthetic spectra including multiple overlapping bands. This analysis succeeds only within a fairly narrow range of filtering severity, with the optimum filtering dependent on the width of each feature.

A new approach in the study reported here is the application of derivative analysis to actual laboratory spectra of well-characterized mineral endmembers and binary physical mixtures of these endmembers. For the endmember spectra we compared the results of derivative analysis to previous interpretive results obtained by visual analysis, gaussian band fitting (Roush and Singer, 1986) and band positions and crystal-field assignments obtained for related minerals from polarized spectroscopic observations (e.g. Burns, 1970). This approach provides a qualitative comparison among the various methods. It should also be noted that not all of the reference techniques above provide identical results. For endmember spectra we find the Huguenin-Jones rules pick reasonable band locations (based on the various reference techniques mentioned above) within a narrow range of filtering severity. This range depends on the width of each spectral feature. With less severe filtering the number of minor features associated with small inflections in the spectra rapidly proliferates. For mixture spectra we find that some diagnostic bands are missed, in some cases at all degrees of smoothing. We agree with Huguenin and Jones that for any high-order derivative technique to succeed the filtering parameters must be critically varied throughout the spectrum. We were unable to test their proprietary adaptive filtering procedure. Based on our results, however, we seriously question whether any filtering scheme could be developed to consistently and properly locate all the traditionally diagnostic  $\text{Fe}^{2+}$  bands in our relatively simple laboratory test suite, let alone higher-noise planetary observations.

It is possible that the derivative analysis methods examined here, or related techniques, could prove to be useful for identifying mineral compositions or classes of minerals based on internal self-consistency, rather than as a new way to find bands already known from crystal-field or other analyses. Any such new classification scheme would have to be statistically based, and would require consistent treatment of an enormous body of laboratory spectra of geologically important minerals for development and verification. It would also need to incorporate a measure of significance of detected spectral features, to avoid unduly weighting noisy spectra which simply have more features to be detected.

We feel that other applications of derivative analysis will prove more useful for remote sensing. A band criterion which is slightly more robust than the Huguenin-Jones technique is a local maximum in the second derivative. This is the lowest order derivative which can be used for band center identification, and is less sensitive to noise than higher orders. Results utilizing the second derivative alone are internally self consistent, but, as with the Huguenin-Jones method, they are not directly comparable with results of more conventional spectroscopic analyses. As is the case with absorption spectroscopy, the best immediate use for derivative analysis seems to be for localizing the center of a band which has already been identified by other criteria.

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