

DETERMINING TES DETECTION LIMITS FOR MINERALS. L. E. Kirkland¹, K. C. Herr², J. W. Salisbury³, J. M. McAfee⁴, P. B. Forney⁵. ¹Lunar and Planetary Institute, 3600 Bay Area Blvd., Houston, TX, 77058, kirkland@lpi.usra.edu; ²The Aerospace Corp., Kenneth.C.Herr@aero.org; ³Johns Hopkins (*retired*) salisbury@worldnet.att.net; ⁴Los Alamos National Lab, mcphi@lanl.gov; ⁵Lockheed Martin, paul.forney@lmco.com.

Introduction: Characteristic spectral bands recorded in remotely sensed infrared emission spectra may be used to examine which minerals are present in a target, such as the surface of Mars. However, lack of a well-established method to calculate the minimum contrast a spectral band must exhibit to be accepted as a detection has increased the difficulty of discussing mineral detection limits. For example, Figure 1 shows a typical spectrum measured of Mars by the 1996 Thermal Emission Spectrometer (TES, ~6.5-50 μm). How do we determine whether the example feature near 11.4 μm should be accepted as a detection?

Carbonate detection limits for TES have been given as 5-10% pixel coverage at $\sim 3 \times 5 \text{ km}^2$ [1], but the method used is uncertain. Here we will show how to calculate band detection limits, and why for TES spectra of massive carbonates, the narrower, weaker 11.2 μm calcite band provides a more sensitive detection than the stronger, wider $\sim 6.5 \mu\text{m}$ band. A well-defined method allows determinations of which features are most detectable by a given instrument, and quantification and discussion of the resulting detection limits.

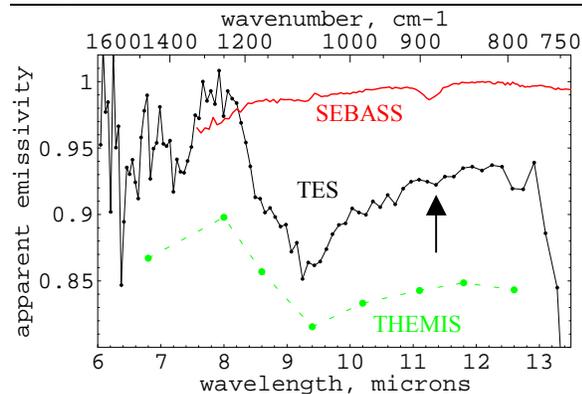


Figure 1: Typical TES spectrum. Transmission through the silicate aerosol dust is the main contributor to the broad $\sim 9 \mu\text{m}$ band. We desire to quantify which spectral features to accept as a detection relative to the local continuum. For example, should the marked $\sim 11.4 \mu\text{m}$ feature be accepted as a detection? TES spectrum 57023856, from the NASA-PDS archive, converted to apparent emissivity with respect to the brightness temperature at 7.75 μm , 270K. A SEBASS spectrum of calcite and a THEMIS spectrum simulated from the TES spectrum are shown for comparison [2].

TES wavelengths used: Carbonates have strong, broad bands near 1540 and 300 cm^{-1} (6.5 and 33 μm), and a weaker, sharper band near 890 cm^{-1} (11.2 μm). However, TES spectra consistently exhibit unexpected

and puzzling spectral behavior at long wavelengths (Figure 2), so until it can be determined whether a calibration problem causes the unexpected spectral shape, we exclude the $\sim 550\text{-}200 \text{ cm}^{-1}$ region. Possible calibration problems include stray light and uncertainties in the internal blackbody calibration target signature. Here we will focus on the 890 and 1540 cm^{-1} calcite bands, but the method can be applied to any region where the continuum shape is well understood.

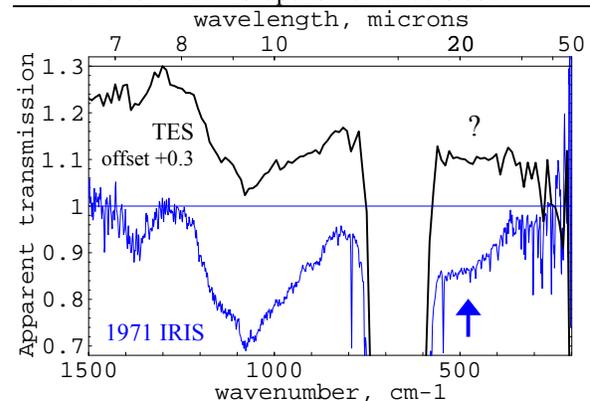


Figure 2: TES 20 μm question. The 1971 IRIS (blue) spectrum shows the ubiquitous aerosol silicate bands centered near ~ 9 and 20 μm (arrow). In contrast, TES spectra have a more sloping continuum toward longer wavelengths and lack a well-defined 20 μm band, which may be due to a calibration issue or other, unknown cause.

Background: Remotely sensed spectra are typically compared to laboratory spectra for interpretation. If a spectrum shows no evidence of a band known to exist in a material, then this may be used to place upper limits on the amount of material present. Several remote sensing studies have examined detection limits using linear spectral mixing models of laboratory spectra [3]. The success of this method is limited in main by three issues. First is how well the remotely sensed spectra can be converted to a unit (e.g. apparent emissivity) for comparison to laboratory spectra, and lack of accompanying ground truth decreases confidence in the conversion. Second, spectral shape varies with particle size, weathering, surface properties, and composition, so the accuracy of the result depends on how inclusively the laboratory endmembers represent the variations present in the target. Third, the result also depends on whether the remotely sensed spectra have the spectral resolution, range, and signal-to-noise (SNR) to discriminate between all the endmembers present.

Given these complications, rather than focusing on linear mixture models, we desire first to quantify whether any given spectral feature may be accepted as a detection relative to the local continuum (Figure 1).

Method: The *band detection limit* is the minimum percent band depth that a feature must have in a single spectrum to be accepted with the desired confidence relative to the noise and local continuum. It depends on the (1) SNR; (2) instrument spectral resolution and sampling interval; (3) target spectral band depth; (4) band width; and (5) the *confidence factor*, which sets the contrast relative to the peak-to-peak noise necessary for acceptance.

The band detection limit (*DL*) is calculated using:

$$DL = \frac{100 \times \text{Confidence Factor}}{\frac{\text{signal}}{\text{noise}_{P_{top}}/2} \times \sqrt{\frac{\text{Band FWHM}}{\text{Sampling Interval}}} \quad (1)$$

where *signal* = signal used in the SNR calculation; *noise_{P_{top}}* = peak-to-peak noise. Dividing the noise by 2 accounts for the measurement being made relative to the local continuum, so the deflection is referenced to one-half the peak-to-peak noise; *Band FWHM* = target band full width at the half maximum of the band depth; and *Sampling Interval* = spacing of points measured (10.58 cm⁻¹ for TES). The square root accounts for the increase in SNR that occurs with the square root of the number of points measured on the band.

Lower numbers for the detection limit indicate lower spectral contrast is required for detection. Thus a more sensitive detection results from a higher SNR, denser wavenumber sampling interval, and a material with a wider and deeper band. A higher confidence factor requires a greater band contrast for acceptance. Values most commonly used are 1, 2, and 3 [4], and it may be varied to account for confidence in the atmospheric compensation and other uncertainties.

Results: Figure 3 shows the detection limit for TES for a band with FWHM=30 cm⁻¹. It illustrates the large detection limit variation with wavelength caused by the variation in SNR with wavelength.

Table 1 gives the measured band depths and the band detection limit values for the 890 and 1540 cm⁻¹ bands exhibited by a limestone and calcrete from the Mormon Mesa, Nevada [5]. These band detection limits assume TES measures the material under similar conditions as those present for the laboratory measurement (the target surface is smooth for areas larger than the sample and fills the field of view, and no atmospheric effects). It should be kept in mind that this calculation does not directly account for atmospheric effects.

For limestone, Table 1 shows that because of the varying TES SNR with wavelength, the 1540 cm⁻¹ band would need to have 6.6 times stronger contrast than the

890 cm⁻¹ band for it to be as detectable in TES spectra. However, the 1540 cm⁻¹ band is only 1.6 times stronger. Thus for TES, the narrower, weaker 890 cm⁻¹ limestone band is actually more detectable than the 1540 cm⁻¹ band. A similar result is obtained for the calcrete (Table 1). This critical but often-overlooked point should be considered when determining and stating detection limits, and when searching a data base for mineral signatures.

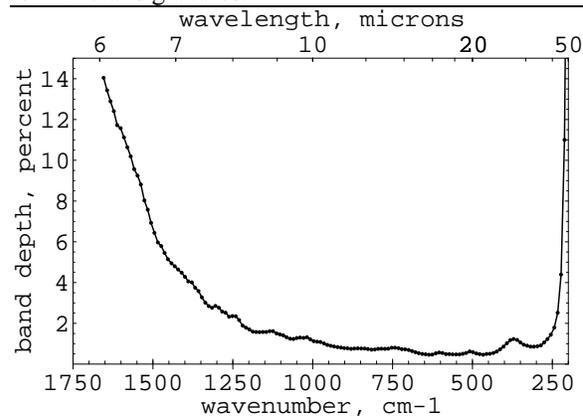


Figure 3: TES band detection limits. This shows the band detection limits calculated using Equation 1, with FWHM=30 cm⁻¹, and confidence factor=2. It shows the percent band depth that a feature must exhibit relative to the local continuum to be accepted as a detection, and it illustrates the variation in sensitivity with wavelength.

Table 1: Limestone and calcrete detection limits

	limestone	calcrete
890 cm ⁻¹ band width (cm ⁻¹)	40	30
890 cm ⁻¹ band depth	14.2%	4.8%
890 cm ⁻¹ detection limit	0.7%	0.8%
1540 cm ⁻¹ band width (cm ⁻¹)	118	110
1540 cm ⁻¹ band depth	23.4%	11%
1540 cm ⁻¹ detection limit	4.4%	4.6%
detection limit ratio, 1540:890 cm⁻¹	6.6	6.0
band depth ratio, 1540:890 cm⁻¹	1.6	2.3

where *detection limit ratio* is the ratio of the 1540 to the 890 cm⁻¹ band detection limit; and *band depth ratio* is the ratio of the 1540 to 890 cm⁻¹ band depths. Detection limits calculated for a confidence factor of 2.

References: [1] e.g. Christensen P. R. et al. (1998), *Science* 279, 1692-1698; Christensen, P. R. et al. (2000), *JGR* 105, 9609-9621. [2] Keim E. R. et al. (2000) and Kirkland L. E. et al. (2000), submitted to *LPSC XXXII*. [3] e.g. Sabol D. E. et al. (1992), *JGR* 97, 2659-2672; Adams J. B. et al. (1993) *Ch.7 in Remote Geochemical Analysis: Elemental and Mineralogical Composition*, C. Pieters and P. Englert ed. [4] Ingle J. D. and S. T. Crouch (1988), *Spectrochemical Analysis*, pp. 172-174. [5] Kirkland L. E. et al. (2000), *LPSC XXXI Abs. 1876 and Abs. 1915*.