

Martian spectra based on the new linear deconvolution results, using the classification techniques described by *Wyatt et al.* [this issue].

## 2. Data and Methods

### 2.1. Laboratory Rock and Mineral Spectra

Thermal infrared (2000–400  $\text{cm}^{-1}$ , or  $\sim 5\text{--}25\ \mu\text{m}$ ) emission spectra of 32 terrestrial volcanic rocks were acquired at  $2\ \text{cm}^{-1}$  sampling with Arizona State University's (ASU) Mattson Cygnus 100 fourier transform infrared (FTIR) interferometric spectrometer [*Ruff et al.*, 1997]. Although the TES instrument covers an additional portion of the spectrum, from 400 to  $200\ \text{cm}^{-1}$  (25–50  $\mu\text{m}$ ), we were unable to cover this region in the laboratory with the Mattson instrument. At the time the present work was completed, ASU's Thermal Emission Spectroscopy lab had just purchased a new spectrometer that will permit coverage of the full TES wavelength range, and we anticipate using this new spectrometer to update our study. Details of the sample mineralogies and chemistries and spectral data acquisition and calibration are presented in paper 1 [*Wyatt et al.*, this issue]. For this study the terrestrial rock spectra were convolved to the exact  $10\ \text{cm}^{-1}$  sampling of the TES. Similarly, end-member mineral spectra from the ASU spectral library (also described in paper 1) [*Christensen et al.*, 2000c] were convolved to TES resolution prior to their use in linear deconvolution models of the terrestrial and Martian spectra.

### 2.2. TES Martian Surface Spectra

TES spectra of the Martian surface shown in this study are the “surface type 1” and “surface type 2” spectra from *Bandfield et al.* [2000a] and represent the averages of four to seven regional, low-albedo locations. Detailed descriptions of the methodology used for separating the surface and atmospheric components in TES-measured spectra are provided by *Bandfield et al.* [2000a, 2000b] and *Smith et al.* [2000]. Calibration of the TES and instrument-related errors are described by *Christensen et al.* [2000a]. Although *Bandfield et al.* [2000a] describe the bulk mineralogy of Martian dark regions in terms of two primary components, additional local-scale variations on the surface have been identified [e.g., *Christensen et al.*, 2000b; *Hoefen et al.*, 2000; *Clark and Hoefen*, 2000; *Christensen et al.*, 2001] that were not identified in the locally averaged spectra, and it is likely that further variations will become apparent as the entire TES data set is analyzed in detail. Small-scale chemical or spatial variations are not addressed here. As new and revised results are presented, we will examine them in the context of our classification schemes.

Initial examinations of the Martian surface spectra show general matches to laboratory spectra of both particulate rock samples and linear mixtures of minerals, with no evidence for unusual particle size or environmental effects [*Christensen et al.*, 2000a]. These similarities support comparisons of Martian surface spectra with thermal emission spectra of terrestrial volcanic rocks. However, Martian surface materials analyzed by TES are thought to be sand-sized particulates [*Christensen et al.*, 2000a; *Bandfield et al.*, 2000a] not bedrock, so their spectral contrast will be less than that exhibited by our laboratory rock samples [*Ruff*, 1998; *Hamilton*, 1998; *Hamilton and Christensen*, 2000]. Thus, only for visual comparison of the Martian surface spectra and laboratory spectra (e.g., Figure 4 below), we have contrast enhanced the TES spectra by 40% to

simulate solid rock spectra [*Ruff*, 1998; *Hamilton and Christensen*, 2000]. Note that contrast enhancement is a cosmetic change equally affecting the entire spectrum; it does not change the shape of spectral features and was not applied to the deconvolved TES spectra.

### 2.3. Linear Deconvolution

The linear deconvolution technique for emission spectra is fully described by *Ramsey and Christensen* [1998], and its application to the present work is outlined in paper 1 (section 3.3). Briefly stated, the spectrum of a rock is a linear combination of the spectra of the minerals composing the rock in proportion to their abundance [*Lyon*, 1965; *Christensen et al.*, 1986; *Crown and Pieters*, 1987; *Thomson and Salisbury*, 1993]. A linear deconvolution algorithm uses a library of pure mineral spectra (“end-members”) to perform a linear least squares fit to the spectrum of an unknown mixture, such as a rock [*Ramsey and Christensen*, 1998]. Upon obtaining a fit to the unknown spectrum, the algorithm supplies the user with a model-derived spectrum and the specific end-members used in the fit along with the percentage of the model represented by each end-member. The percentages are based on areal abundances (as measured by the spectrometer) and are thus comparable to percentages obtained by viewing a rock in thin section; therefore percentages are reported as vol %. The quality of the fit and resultant mineralogy can be judged by the degree of difference between the model-derived spectrum and the unknown spectrum and by the root-mean-square (RMS) error value provided as part of the output of the algorithm [*Ramsey and Christensen*, 1998; *Hamilton et al.*, 1997; *Feely and Christensen*, 1999; *Hamilton and Christensen*, 2000]. However, because RMS error values are valid only for comparing deconvolution runs for a given sample not the fits of different samples [*Hamilton and Christensen*, 2000; *Christensen et al.*, 2000], we have determined a more robust measure of uncertainty by calculating the standard deviation of the absolute differences between measured and modeled abundances [*Wyatt et al.*, this issue]. Commonly, a blackbody end-member (unit emissivity at all wavelengths) is included in the end-member set to account for differences in spectral contrast between the end-members and the mixture spectrum [*Hamilton et al.*, 1997; *Feely and Christensen*, 1999; *Hamilton and Christensen*, 2000]. Unlike continuum removal, the addition of a blackbody end-member does not change spectral shape; it only changes spectral contrast uniformly across a spectrum. Deconvolution results are typically normalized to remove any blackbody percentage so that mineral phases sum to  $\sim 100$  vol %; this is how modal abundances are presented in this work.

### 2.4. Calculation of Bulk Oxides From Deconvolution Results

Bulk oxides for unknown spectra can be derived by summing the known chemistries of the end-members used in the best fit model in proportion to their modeled abundance [*Ruff*, 1998; *Hamilton*, 1998; *Hamilton and Christensen*, 2000]. The uncertainties associated with modeled bulk oxides derived from  $10\ \text{cm}^{-1}$  data were determined by calculating the  $1\ \sigma$  standard deviation of the absolute differences between the measured and modeled bulk oxide values [*Wyatt et al.*, this issue]; these are the uncertainties shown on all plots. Oxide values are generally reported to two significant figures but typically have associated uncertainties at the hundredths of a percent level that vary by oxide. Using these known values for each end-