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TES Data Analysis: Index Mapping and Deconvolution

TES data in this work were mapped using the Glotch and Rogers (2013) spectral index, which highlights long-wavelength spectral features due to Fe/Mg-carbonates and their decomposition products, in order to discriminate potential carbonatebearing localities to perform TES quantitative analysis. Data for mapping and quantitative analysis were limited to locations with well-calibrated, clear atmosphere and warm surface temperatures (>250K, 9µm dust extinction <0.17. 11µm ice extinction <0.04, TES Lambert albedo <0.18, emission angles <5°, no solar panel or mirror motion, and orbit counter keeper (OCK) values <7000). Mineral abundance determination and atmospheric correction was performed by modeling each TES emissivity spectrum with a library of mineral spectra (Table DR3) and atmospheric components (Bandfield et al., 2000), using non-negative linear leastsquares fitting (Rogers and Aharonson, 2008; Smith et al., 2000). This atmospheric/surface separation technique and endmember mineral deconvolution is commonly employed to determine mineral abundances to ~5-10% absolute areal abundance for minerals above the typical $\sim 10\%$ detection limit (Table DR1: Feely and Christensen, 1999; Ramsey and Christensen, 1998).

CRISM Data Analysis: Selection and Non-Linear Mixing

CRISM I/F data were atmospherically corrected using the volcano scan method (Murchie et al., 2009) and processed into spectral index parameters (Pelkey et al., 2007) to map the spatial distribution of carbonate (D2300, 2.3µm absorption; BD2500, 2.5µm absorption; Pelkey et al., 2007; Ehlmann et al., 2008) and olivine (OLINDEX2; Salvatore et al., 2010) and to identify locations with the strongest absorptions from which spectra were then extracted (Fig. 2). A single CRISM image (FRT0000C968) was processed through the discrete ordinates radiative transfer (DISORT) atmospheric retrieval algorithm, solving for carbon dioxide, water vapor, carbon monoxide, and associated Rayleigh scattering and discrete gas absorptions for CO₂, H₂O, and CO (Arvidson et al., 2014; Stamnes et al., 1988; Wiseman et al., 2012). These data were processed to single scattering albedo (SSA) to enable numerical modeling of the spectra by two methods (Ehlmann et al., 2011b): (1) a Hapke -style (Hapke, 1993) radiative transfer unmixing model that uses the optical constants of phases of interest (Table DR4) to simultaneously solve for phase abundance and grain size by downhill simplex minimization of error between measured and modeled spectra over the 1.20 to 2.56 µm wavelength range (Table DR2); and (2) a forward model that uses laboratory-derived optical constants for magnesite with a scene-derived olivine-basalt spectrum to establish a relationship between band depth, single scattering albedo, and abundance for given mixing ratios and grain sizes of olivine-basalt and carbonate. Approach 2 assumes that the major compositional difference between the olivine-basalt bedrock and the carbonate-bearing materials is the addition of carbonate, an assumption warranted by TES and approach 1 results, discussed further herein. Note that in Approach 2,

band depth at 2.3 μ m, band depth at 2.5 μ m, and SSA each bound the maximum possible carbonate. They must also produce simultaneously consistent values. Thus, while the albedo of the deposit permits up to 25 wt.% Mg-carbonate mixed with basalt, the observed depth of the 2.5- μ m absorption in carbonate suggests the upper bound to be about 5 wt.%.

THEMIS Data Analysis: Composition and Thermophysics

Spectral ratios are commonly used when analyzing CRISM data but are rarely calculated with THEMIS data. Spectral ratios do not require fully atmospherically corrected THEMIS images, which is advantageous in this region because coincident THEMIS and TES data that meet the requirements for a high quality correction are limited (Bandfield et al., 2004). All other THEMIS standard processing procedures were followed (Edwards et al., 2011). Due to the low signal-to-noise ratios (SNR) of bands 1 & 2 (6.78µm), originally designed to map carbonates (Christensen et al., 2004), our use of THEMIS spectral data is limited to spectral ratios and not quantitative unmixing; THEMIS is used primarily to highlight spectral differences between terrains. Two spectral indices, band 1/2 downturn and band 7 band depth, were developed to map olivine and carbonate-related spectral parameters over the region.

THEMIS thermal inertia data were also modeled over the entire region (Fergason et al., 2006). Thermal inertia data are sensitive to small changes in particle size (Piqueux and Christensen, 2011; Presley and Christensen, 1997) and are exceptionally sensitive to small volumes of pore filling cements (Piqueux and Christensen, 2009). We use these data in conjunction with spectral data to identify and map distinct compositional and thermophysical groupings.



Figure DR1. Modeled infrared single scattering albedo (SSA), 2.3 µm absorption band depth (BD2300), and 2.5 µm absorption band depth (BD2500) for mixtures of carbonate with the olivine-enriched rock at Nili Fossae. Forward modeling was performed to generate simulated mixture spectra. The derived SSA olivine rock endmember spectrum from the CRISM scene was mixed with the SSA spectrum of magnesium carbonate from our optical constant library at different abundances. Grain size of the olivine-bearing rocks was assumed to be 1mm, based on Hapke inverse modeling results and THEMIS thermal inertia. The carbonate grain size was varied. All runs with the three parameters indicate carbonate abundances are lower than 25%. Observed BD2500 suggests abundances ≤5%.



Figure DR2. CRISM BD2500 and OLINDEX2 band parameter maps over the same region as Fig. 4A. Linear streaks are artifacts in the image and not associated with surface features.



Figure DR3. Density plots of THEMIS band indices (Fig. 4A) for A: band 1 & 2 index and B: band 7. THEMIS TI over the region shown. Only the locations where both datasets were present are plotted.

Mineral	TES ^{A&B}	TESC	Syrtis Type ^b	
Pyroxene	21 (8)	27 (7)	32 (3)	
Olivine	21 (4)	4 (5)	5 (3)	
High-Si Phases	24 (8)	20 (7)	19 (10)	
Carbonate	15 (4)	10(1)	7 (1)	
Feldspar	11 (7)	30 (10)	27 (6)	
Other ^a	8 (3)	9 (3)	10 (2)	
RMS Fit Error	0.35	0.35	0.14	

Table DR1: TES model mineral abundances (%), Values reported in parentheses are $\pm 1\sigma$ for derived abundances.

^aValues reported in the "Other" category include phases like hematite, sulfate, and quartz. ^bValues from *Rogers and Christensen* (2007) of nearby Hesperian basalt for comparison

Table DR2: CRISM Deri	ived abundances	(wt % & grain size)
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Phase	Carbonat e Bedrock	Dark Bedrock	Dunes	Capping Unit
Carbonata	15	1	8	1#
Carbonate	(1 mm)	(12µm)	(1mm)	(23µm)
Olivine	24 (~1mm)	26 (~1mm)	25 (~1mm)	5 (384µm)
Basalt	59 (950μm)	70 (560 μm)	65 (770μm)	89 (394µm)
Other*	2	2	2	5
RMS Fit Error	0.0038	0.0023	0.0033	0.0023
TI-Derived Grain Size^	≳1 mm	≳1 mm	≳1 mm	~300- 700 μm

*Values reported in the "Other" category include phases like dust, additional feldspar & nontronite.

#Ill-fit; carbonate and nontronite introduce an absorption not present in the data. A hydrated phase not in our optical constant libraries is needed to account for the overall continuum shape. ^Grain Sizes

Mineral	Group
Quartz BUR-4120	Quartz
Microcline BUR-3460	Feldspar
Albite WAR-0235	Feldspar
Oligoclase BUR-060D	Feldspar
Andesine WAR-0024	Feldspar
Labradorite BUR-3080A	Feldspar
Bytownite WAR-1384	Feldspar
Anorthite BUR-340	Feldspar
Shocked An 17 GPa ^b	Feldspar
Shocked An 21 GPa ^b	Feldspar
Shocked An 25.5 GPa ^b	Feldspar
Shocked An 27 GPa ^b	Feldspar
Shocked An 38.2 GPa ^b	Feldspar
Shocked An 56.3 GPa ^b	Feldspar
Bronzite NMNH-93527	Pyroxene
Enstatite HS-9.4B	Pyroxene
Hypersthene NMNH-B18247	Pyroxene
Pigeonite ^c	Pyroxene
Diopside	Pyroxene
Augite NMNH-9780 ^c	Pyroxene
Augite NMNH-122302 ^c	Pyroxene
Hedenbergite DSM-HED01	Pyroxene
Forsterite BUR-3720A	Olivine
Fayalite WAR-RGFAY01	Olivine
Olivine Fo60 KI3362 ^d	Olivine
Olivine Fo68 KI3115 ^d	Olivine
Olivine Fo35 KI3373 ^d	Olivine
Olivine Fo10 KI3008 ^d	Olivine
Illite IMt-1	High-Si Phase
Montmorillonite STx-1	High-Si Phase
Saponite SpNv-1	High-Si Phase
Montmorillonite SWy-1	High-Si Phase
K-rich glass ^e	High-Si Phase
SiO2 glass ^e	High-Si Phase
Opal-A 02-011 ^f	High-Si Phase
Aluminous opal ^g	High-Si Phase
Heulandite ^h	High-Si Phase
Stilbite ^h	High-Si Phase
Avg. Martian hematite ⁱ	Hematite
Anhydrite S9	Sulfate

Table DR3: Library Mineral Endmembers for Linear Spectral Mixture Analysis of TES Data^a

Sulfate
Sulfate
Carbonate
Carbonate
Carbonate
Carbonate

a) All samples are from the ASU spectral library available at http://speclib.asu.edu Christensen et al. (2000) unless otherwise noted

b) Johnson et al. (2002)

c) Provided by V. E. Hamilton, described by Hamilton (2000)

d) Described by Koeppen and Hamilton (2008)

e) Described by Wyatt et al. (2001)

f) Described by Michalski et al. (2003)

g) Provided by M. D. Kraft

h) *Described by Ruff (2004)*

i) Derived from TES data, described by Glotch et al. (2004)

j) Described by Glotch and Rogers (2013)

Table DR4: Optical constants used for Hapke spectral unmixing of CRISM data. A variety of runs with greater and fewer constants (max of 7 per run) were executed with fitting over the wavelength range 1200-2560 nm. Those used in the final best-fit presented in the paper are indicated in the main text. The cap unit cannot be wellmodeled with the same set as the olivine-bearing materials to produce an acceptable fit, pointing to a substantially different composition. Specifically, the continuum shape requires a hydrated phase, but inclusion of carbonate and nontronite leads to absorptions in modeled data that are not present in the actual data. The basaltic cap spectrum remained relatively ill-fit (Fig. 2) at the longest wavelengths (3- μ m downturn) due to lack of an appropriate library optical constant match of the hydrated phase.

Phase	References
Olivine	Ehlmann et al. (2011a; 2011b)
Magnesite	Ehlmann et al. (2011a; 2011b)
Basalt	Ehlmann et al. (2011a; 2011b)
Feldspar (w/ magnetite	Poulet et al. (2008)
inclusions)	
Pyroxene	Poulet et al. (2008)
Dust	Wolff et al. (2009)
Nontronite (NG-1)	Ehlmann et al. (2011a; 2001b)

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