MARS INFRARED SPECTROSCOPY:
FROM THEORY AND THE LABORATORY TO FIELD OBSERVATIONS

June 4-6, 2002
at the Lunar and Planetary Institute

Edited by
Laurel Kirkland, John Mustard, John McAfee, Bruce Hapke, Michael Ramsey

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- **S. Saunders**: Science Involvement in Mars Exploration in the First Decade of the Twenty-First Century [abs. 2012]
- **B. Schmidt, Doué, Erard, Langevin**: Discrimination Between Solid, Liquid and Gaseous H₂O, and Assessment of H₂O Temperature by Spectroscopy Using the OMEGA Imaging Spectrometer [abs. 2005]
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F. Seelos, R. Arvidson: Mantled and Exhumed Terrains in Terra Meridiani \textit{[abs. 2006]}

G. Sellar, L. Kirkland, G. Boreman and D. Wang, Novel Imaging Spectrometer With High Signal Collection Ability and No Moving Parts \textit{[abs. 2011]}
INTRODUCTION

MARS INFRARED SPECTROSCOPY:
From Theory and the Laboratory to Field Observations

The continuity and timely implementation of the Mars exploration strategy relies heavily on the ability of the planetary community to interpret infrared spectral data. However, the increasing mission rate, data volume, and data variety, combined with the small number of spectroscopists within the planetary community, will require a coordinated community effort for effective and timely interpretation of the newly acquired and planned data sets. Relevant spectroscopic instruments include the 1996 TES, 2001 THEMIS, 2003 Pancam, 2003 Mini-TES, 2003 Mars Express OMEGA, 2003 Mars Express PFS, and 2005 CRISM.

In light of that, leaders of the Mars spectral community met June 4–6 to address the question:
What terrestrial theoretical, laboratory, and field studies are most needed to best support timely interpretations of current and planned visible/infrared spectrometer data sets, in light of the Mars Program goals?

A primary goal of the spectral community is to provide a reservoir of information to enhance and expand the exploration of Mars. Spectroscopy has a long history of providing the fundamental compositional discoveries in the solar system, from atmospheric constituents to surface mineralogy, from earth-based to spacecraft-based observations. However, such spectroscopic compositional discoveries, especially surface mineralogies, have usually come after long periods of detailed integration of remote observations, laboratory analyses, and field measurements. Spectroscopic information of surfaces is particularly complex and often is confounded by interference of broad, overlapping absorption features as well as confusing issues of mixtures, coatings, and grain size effects. Thus some spectroscopic compositional discoveries have come only after many years of research.

However, we are entering an era of Mars exploration with missions carrying sophisticated spectrometers launching about every 2 years. It is critical that each mission provide answers to relevant questions to optimize the success of the next mission. That will not occur effectively unless the spectroscopic remote sensing data can be processed and understood on an approximate 2-year rate. Our current knowledge of spectral properties of materials and confounding effects of the natural environment are not well enough understood for the accurate interpretations needed for such ambitious and time critical exploration objectives. This workshop focused on identifying critical gaps in moving the field towards the goal of rapid and accurate analysis and interpretation.
RECOMMENDATIONS

SUMMARY
This report focuses on identification of critical gaps, particularly those that cannot be filled by individual researchers alone, and does not discuss the relative importance of ongoing research. The two most critical gaps are in coordinated end-to-end field testing and in libraries of spectroscopic data. Three related gaps are in data from terrestrial sites to aid TES and CRISM interpretations, lack of high quality development data to support landers, and delays in funding owing to lack of coordination between R&A proposal due dates and mission data releases.

CRITICAL GAPS
1. End-to-end testing. Field/rover, airborne/satellite, and telescopic measurements are sensitive to very different effects, and these differ from those present in the laboratory. Thus a convincing determination of uncertainties as related to studies of Mars requires demonstration through coordinated “end-to-end” field testing. This should proceed in light of our current best understanding of martian mineralogy and environment, using:
   (1) Data sets of appropriate terrestrial analog sites that are measured with both geometric and spectral fidelity as close as possible to landed and orbital flight instruments;
   (2) Interpretation using spectral libraries and theoretical work as applied to data of Mars;
   (3) Reporting interpretations at a community workshop, including a “blind test” (with minimal foreknowledge of the test site or ground truth);
   (4) Validation through ground truth.
This will:
   (1) Test mission protocols and interpretation methods used for flight data;
   (2) Develop theoretical ties and address critical current uncertainties in detectability, uniqueness of identifications, abundance mapping, and atmospheric compensations;
   (3) Prepare the community to interpret flight data in a timely manner;
   (4) Help define and highlight gaps in public spectral libraries, and the importance of the libraries and theoretical work to the interpretation chain.
Coordination through an independent steering group is critical in order to maintain and facilitate a clear focus on addressing the central questions. This is imperative to support timely interpretations and to plan and manage future flight instruments, but it cannot be achieved by individual researchers alone. Further, in order to achieve results in time to support the current suite of missions, this program needs to begin as soon as possible with adequate and focused funding.

2. Public libraries of spectroscopic data. Interpretation quality is limited to the quality of the accessible spectral libraries. Current public libraries focus on specific issues or conditions (such as major groups of igneous minerals and terrestrial weathering products, and large particles). Primary gaps include (1) systematic measurements of other weathering products, coatings, a range of surface textures, full particle size ranges; (2) measurements made under simulated Martian conditions; (3) motivating and facilitating a conversion of private libraries into the public domain; and (4) systematic development of fundamental optical constants for modeling. Currently there is insufficient funding and staffing to measure, document and prepare for public release documented digital spectral libraries. It is unclear which R&A program is responsible for developing strong public libraries, and this should be clarified in the appropriate Announcement of Opportunity. Additions and public access should be fostered in cooperation with NASA’s Planetary Data System.
ADDITIONAL GAPS

3. High fidelity data. There are gaps in terrestrial hyperspectral airborne/satellite data sets for CRISM and OMEGA (mainly 2.5–5 μm), and essentially no thermal-IR hyperspectral airborne or satellite data sets comparable to TES exist in the NASA community. Data should be identified and made publicly available to allow validation of methods, interpretations, and uncertainties.

4. Lander development data. The NASA community has essentially no field data sets available measured with high fidelity to the lander Mini-TES or Pancam or similar to future landers. Data should be identified and made available to allow development and validation of methods, and to expedite community contributions after the flight data sets are released.

5. Mismatch of flight data release and R&A cycle timing delays community research. When the first public release of flight data occurs after the relevant Research and Analysis (R&A) program deadlines, it can delay funding non-team member research ~2 years from initial data return. For example, this delay will occur for Odyssey research. This is a significant weakness given the rapid turnover rate of current missions. R&A management should coordinate with flight teams and the PDS to officially release demonstration flight data timed to prevent this additional delay.

Participants of the workshop,

*Mars Infrared Spectroscopy: From Theory and the Laboratory to Field Observations*

Raymond Arvidson  Donal2 Barker  Janice Bishop  Diana Blaney
Don Burt  John Cipar  Roger Clark  Kim Deal
Sergio Fonti  Bruce Hapke  Laurel Kirkland  John McAfee
Daniel McCleese  Richard Morris  Scott Murchie  John Mustard
Carlé Pieters  Michael Ramsey  Steve Saunders  Bernard Schmitt
Frank Seelos  R. Glenn Sellar  Maria Sgavetti  Ann Sprague
Shawn Wright
Spectroscopic Data for Mars

The missions associated with the Mars Exploration Program (MEP) as well as missions from other countries and international agencies, will acquire abundant spectroscopic observations to determine surface composition. Below is a short summary of the existing and expected data sets:

1) Defined Spectroscopic Instruments
   - Continued analysis and interpretation of TES/MGS data and THEMIS/Odyssey
   - New data from Pancam and Mini-TES on the MER rovers (2004)
   - New data from PFS and OMEGA on Mars Express (2004–2007)

2) Planning for 2007–2020
   - Possible instruments proposed for Scout mission (2007)
   - Planned NASA contribution to CNES orbiter (2007)
   - Instruments on the Mars Smart Lander (MSL) (2009)
   - Beyond MSL are possible additional Scout missions, landers, and Sample Return

3) How will IR Spectroscopy contribute in the next decade
   - Data analysis and interpretation of orbital assets
   - Data analysis and interpretation of landed assets
   - Integration of orbital and lander data for sample return targeting, investigation of planet
Specific Gaps and Recommendations

1. **Terrestrial analog testing of the complete theory-lab-field-airborne/satellite chain.**
   
   The steering group's critical role is to facilitate and maintain a strong focus on addressing the central questions outlined in the summary. The steering group should:
   
   (1) Facilitate and collect community input.
   
   (2) Select appropriate terrestrial field sites.
   
   (3) Facilitate making appropriate data publicly available. This may draw on data sets measured for other studies.
   
   (4) Facilitate reporting at a community workshop, including discussion of what the results indicate for meshing current and future measurements with the Mars exploration program.

   End-to-end spectroscopy research of terrestrial analog sites that includes field/rover, airborne/satellite, laboratory work, and theory is important. The specific implementation could take several forms but must be designed to address fundamental problems in field/rover, airborne/satellite, telescopic, and theoretical work as applied to interpretations of data sets of Mars. Interlinking of the perspectives through theoretical work is also important. However, it is not sufficient to collect and release the data; analysis must be funded. In addition, collaboration between the Space Science enterprises and terrestrial communities in spectroscopy should be encouraged and facilitated.

2a. **Community spectral libraries.**

   **Data gaps:** There is an insufficient range of weathering products, coatings, textures, small particle size ranges (<50–100 μm), pure as well as mixed materials (composition and size distribution), transmission, optical constants, packing effects, and measurements at low temperature and in low pressure CO₂ using well-characterized samples.

   **Well-characterized** includes (1) location or origin of sample; (2) chemical characterization, including major element analyses, solution pH and electrical conductivity, thermal and evolved gas analyses (e.g., differential scanning calorimetry (DSC) integrated with a mass spectrometer); (3) mineralogical characterization, including from Moessbauer and Raman spectroscopy, magnetic properties (magnetic susceptibility and saturation magnetization), powder X-ray diffraction, petrographic analyses of thin sections; (4) physical characterization, including bulk density, porosity, fabric, surface texture, and particle size distribution analysis. Chemical and mineralogical characterization can be done for each size separate, and magnetic separate analysis for soils. Chemical and mineralogical characterization can be done for each magnetic separate. However, not all these need be done on each sample. Sample characterization is the most time consuming step: it is estimated that it takes 2 to 3 weeks per sample to provide all the verification listed here.

   **Production gap:** Researchers typically measure spectra to examine a particular question, not to create a public data base. Although it is highly desired to make data publicly accessible, the motivation for researchers to spend unfunded time to do so is unclear, particularly when the spectra were measured through unfunded or non-NASA funded means.

   **Distribution gap:** No central location coordinates linking to the available public libraries, and no guidelines exist for individuals the archive their own data on-line.

   **Recommendation:** The PDS Geoscience Node should maintain a web page with links to the currently available libraries of spectroscopic data and solicit or create links for additional data sites. PDS should provide guidelines and options for organizing (along with appropriate supplemental information/comments), posting, and referencing spectral libraries acquired or assembled under the R&A program. For continuity, PDS should also maintain a mirror site and back-up capabilities.
**R&A gap:** It is unclear which R&A program is responsible for funding spectral library development specifically intended for public access.

**Recommendation:** The appropriate R&A program associated with the Mars program (e.g. MDAP) should state in the AO an interest in funding VIS/IR public spectral libraries to support interpretation of current and planned data sets, and specifically include public production both of data already measured and to be measured. This will clarify where and what to propose. Additionally, PI's funded to produce public spectral libraries should have that funding continued only when they make the spectroscopic data public on schedule as proposed.

**Theoretical studies and links with spectral libraries:** The surface and atmosphere of Mars very probably contain an abundance of micrometer-sized particles, which are much smaller than the wavelengths used in thermal remote sensing. The small size regime is poorly understood for two reasons: (1) Coherent interactions between particles are important. (2) Weak bands are strongly displayed in the spectra of small particles; however, the spectra in some libraries were made using large particles, in which weak bands are poorly displayed.

**Recommendations:** Extend spectral libraries to include media of micrometer-sized particles, including mixed media with a range of size distributions. Publishing complex refractive indices would be extremely valuable, provided that measurement methods, such as transmission are used that are sensitive to weak as well as strong bands. Laboratory spectral measurements designed to study coherent effects (e.g. intimate mixtures, packing effects) are also needed.

**2b. Laboratory instrumentation.** There are important gaps in attachments and environmental chambers for laboratory instrumentation:

**Facility gap:** Hemispherical reflectance measurements may be necessary in the thermal-infrared for small particle size ranges, because they typically have a temperature gradient that causes spectral artifacts when measured in emission. However, a gap in hemispherical reflectance capabilities exists from 25–50 μm.

**Facility gap:** Insufficient environmental capabilities exist to mimic the low pressure, desiccating, and cold (<150 K) conditions on Mars, and at high temperature to drive off bound water (>380 K).

**Funding gap:** Ensure sustained funding to upgrade current equipment

**3a. TIR airborne/satellite data.** There are essentially no publicly available airborne/satellite TIR hyperspectral data sets. Hyperspectral data are required to address uniqueness, quantification, and detectability questions for satellite and airborne hyperspectral studies of Mars.

**Data gap:** Hyperspectral TIR data are largely in the DoD community. Desired data include surface measurements and upward emission function (emission phase function, EPF) data.

**Recommendation:** The planetary community should make its needs known to communities who have hyperspectral TIR data. Hyperspectral data sets may be available if asked for.

**Options:** Options to allow validation of hyperspectral methods include:

A. Develop and purchase a community spectrometer
B. Sponsor a group that has the instrumentation to measure data and make it publicly available (full NASA funding)
C. Propose joint measurements with a group that has the instrumentation (shared funding)
D. Request piggyback measurements on other work performed by a group that has the instrumentation (no NASA funding provided, making availability unpredictable)
E. Interpret Mars hyperspectral data sets without benefit of similar terrestrial hyperspectral experience validated by ground truth.

Research gaps:
A. Uniqueness of mineral identification when ground truth is not available
B. There is no terrestrial hyperspectral study that validates the main atmospheric compensation technique used for TES data
C. Testing and validation of current quantitative abundance mapping methods using terrestrial hyperspectral data validated by ground truth.

3b. VIS/NIR airborne or satellite instrumentation.

Data gaps: The ~2.5–5 μm range has both reflected and emitted light, which requires development and testing of techniques for interpretation to support CRISM. No data in the NASA community covering this range was identified, but other communities have instrumentation that covers this range.

Data gaps for atmospheric compensation studies: CRISM plans to compensate for atmospheric interference using upward emission function (emission phase functions, EPF), but no public data sets exist to study this technique over the 1–5 μm range. However, it was unclear how important this gap is, since coverage of shorter and longer wavelength regions is available that could be used to develop and test techniques.

3c. Ground-based telescopic spectroscopy: Measuring atmospheric constituents like ozone and water vapor, and clouds and circulation have an important role in the Mars program. Ground-based measurements provide global coverage and long term systematic baseline measurements that the current Mars flight program is not designed to provide.

4a. TIR field spectrometers.

Data gap: Almost no NASA research exists using data measured with high fidelity to the 2003 lander spectrometer. Nearly all NASA data sets are measured looking straight down at the surface, while lander spectrometers will measure more horizontally and over a wide range of angles.

Facility gap (high fidelity): Options to allow high fidelity testing and to prepare the community include:
A. Develop and purchase a community TIR imaging field spectrometer
B. Sponsor a group that has the instrumentation to measure data and make it publicly available (full NASA funding)
C. Propose joint measurements with a group that has the instrumentation (shared funding)
D. Request piggyback measurements on other work performed by a group that has the instrumentation (no NASA funding provided, making availability unpredictable)
E. Interpret Mars data sets without benefit of similar terrestrial experience validated by ground truth.

Facility gap (low-fidelity): Three groups can make point (non-imaging) measurements, with one instrument shared among three universities, so five research groups have access to a non-imaging instrument. Although these are low fidelity to the flight instruments, they are important for research and teaching.

Recommendation: Modest investment in a point-measuring spectrometer is warranted, if the instrument is managed in a manner to make it openly available to the community.
4b. VIS/NIR field spectrometers.

*Facility gap:* No facility to cover the 2.5–5 μm range was identified in the NASA community.

*Data gap:* Too little research has occurred using data measured in a geometry similar to landers. Most data sets are measured looking straight down at the surface, while lander spectrometers will view the scene more horizontally and over a wide range of angles. No field data covering the 2.5–5 μm range was identified in the NASA community.

5. Mesh first community access to flight data with the R&A cycle.

*Gap:* The period where only the instrument team has access to Odyssey data ends in October 2002, after the deadline for Mars-related R&A programs has passed (e.g. MDAP is due in Aug). Thus non-team members must wait until the following year’s R&A to propose on even footing (~Aug 2003); followed by at least a ~6 month delay in funding (~Feb 2004). The total can delay R&A funded non-team member research by at least ~2 years from initial Odyssey data return (Feb 2002). This is a significant delay in light of the 26 month Mars mission cycle, and it reduces the community’s engagement and capacity to address gaps in research that would aid the Mars program goals.

*Recommendation:* Officially release sufficient demonstration data and documentation in time to support proposals on an even footing. This requires coordination between R&A management, instrument teams, and the PDS to define:

A. When the data have to be available to mesh with the most relevant R&A program deadline(s)

B. The volume/type of preliminary data (e.g. how many images?).

C. Completeness (e.g. are full band THEMIS data needed?).

D. Who would release the data (PDS or PI).

E. How to announce it is available (e.g. through the R&A program).
TUESDAY, June 4, 2002

Doors open at 7:45. Posters can be put up, and we will have a table for reprints and handouts.

7:45–8:15 Registration ($15)
8:25 Welcome
* = speaker

8:30 Mars Program: Current and Future Goals
Chair: Bishop
8:30–8:55 *S. Saunders: Science Involvement in Mars Exploration in the First Decade of the Twenty-First Century
9:20–9:45 *R. Arvidson: Mars Exploration and Importance of Spectroscopic Observations

9:45 Discussion: Program Goals and Spectral Observations
Moderator: Bishop
How do spectral observations fit into the Mars program?

10:15–10:35 Break

10:35 Current and Planned Data Sets of Mars’ Surface
Chair: Pieters
10:35–11:00 telescopic: *A. Sprague
11:00–11:20 ISM: *J. Mustard: Review of the ISM Instrument and Results
11:50–1:15 Lunch
1:15–1:55 TES: *R. Clark Spectral Feature Mapping and Analysis of Mars Global Surveyor Thermal Emission Spectrometer Data
1:55–2:20 THEMIS: *S. Saunders
2:20–2:40 Mini-TES
2:40–3:00 Break
3:00–3:20 Pancam: *D. Morris
3:20–3:45 Mars Express OMEGA: *B. Schmidt, Douté, Erard, Langevin: Discrimination Between Solid, Liquid and Gaseous H2O, and Assessment of H2O Temperature by Spectroscopy Using the OMEGA Imaging Spectrometer
3:45–4:05 Mars Express PFS: V. Formisano, *S. Fonti et al.: The Planetary Fourier Spectrometer (PFS) Onboard the European Mars Express Mission
4:05–4:25 CRISM: *S. Murchie et al.: CRISM: Compact Reconnaissance Imaging Spectrometer for Mars on the Mars Reconnaissance Orbiter

4:30–5:00 Discussion: How to mesh instrument data release with the R&A cycle
Moderator: Saunders

5:00–6:00 Reception and Posters
Beer and Light Refreshments Served
Doors open at 7:45

WEDNESDAY Morning, June 5

8:15 Theory and Laboratory
Chair: Murchie

8:15–8:55 *B. Hapke: Status of Reflectance and Emissivity Models Relevant to Mars Studies
8:55–9:20 *R. Morris: Martian Analogue Sample Characterization and Spectral Library Development at the Johnson Space Center
9:20–9:45 *S. Fonti et al.: A Coordinated Laboratory Program in Support of the Spectroscopic Experiments on Board Martian Missions

9:45–10:05 Break

10:05–10:30 *C. Pieters: Mid-Infrared Reflectance Spectroscopy: Where Are We, Where Are We Going, and Why?
10:30–10:55 *J. Mustard: Methods of Spectral Analysis

10:55–12:10 Break-Out Groups: Theory and Laboratory through lunch (brought in at 11:30)

* = present results in the panel discussion
All questions are open to all groups, but each group should address their question(s) in-depth first.

Group 1: Granahan, Murchie, *Pieters, Saunders, Schneebeli, Sprague
VIS/NIR theoretical and lab studies: What are the critical gaps, and what studies are most needed to address those gaps?

Group 2: Bishop, *Fonti, McCleese, Ramsey, Hapke, Wright
Thermal-IR theoretical and lab studies: What are the critical gaps, and what studies are most needed to address those gaps?

Group 3: Arvidson, Barker, Deal, Kirkland, *Morris, Sellar
What community spectral libraries are most needed?
What lab instrumentation is available?
What lab instrumentation is most needed?

Group 4: Blaney, Cipar, *Clark, Mustard, Schmidt, McAfee, Seelos
Getting lab data to the community:
Who should deliver it (e.g. PI, PDS...)?
Who should fund distribution (e.g. R&A, PDS...)?
Who should define what is needed (samples, wavelength range, reflectance vs. emission,...?)
How does and should the community have input?

12:10–1:10 Theory and Laboratory Panel Discussion
Moderator: Sprague
WEDNESDAY Afternoon, June 5
1:10 Field and Airborne
Chair: Clark

1:10–1:35 field-rover VIS/NIR: *D. Blaney: Visible To Short Wavelength Infrared Spectroscopy On Rovers: Why We Need It On Mars and What We Need To Do On Earth

1:35–2:00 field-rover thermal: *J. McAfee, L. Kirkland: Thermal Infrared Field Spectroscopy

2:00–2:20 Break


3:35–4:00 *Schneebeli: Quantification of Near-Infrared Photography of Snow Surfaces on Earth and Mars

4:00–4:15 Break

4:15–5:15 Break-Out Groups: Field and Airborne

* = present results in the panel discussion
All questions are open to all groups, but each group should address their question(s) first.

Group 1: Arvidson, Hapke, Mustard, *Ramsev, Fonti, Sellar, Wright
Thermal-IR field/airborne studies: What are the critical gaps, and what studies are most needed? Thermal-IR current capabilities: What field and airborne data sets should be measured specifically for release to the community using current instruments? Who should define what to measure (field sites, wavelength range, multi-vs. hyperspectral, imaging vs. point measurements,...)? How does and should the community have input? Who should deliver it (e.g. PI, PDS...)? Who should fund distribution (e.g. R&A, PDS...)?

Group 2: *Blaney, Cipar, Kirkland, McAfee, McCleese, Seelos
Thermal-IR field/airborne studies: What are the critical gaps, and what studies are most needed? Thermal-IR field/airborne future capabilities: What additional instrumentation is most needed (if any)?

Group 3: Barker, Bishop, Clark, McAfee, Morris, *Murchie, Schmidt
VIS/NIR field/airborne studies: What are the critical gaps, and what studies are most needed? VIS/NIR current capabilities: What field and airborne data sets should be measured specifically for release to the community using current instruments? Who should define what to measure (field sites, wavelength range, multi-vs. hyperspectral, imaging vs. point measurements,...)? How does and should the community have input? Who should deliver it (e.g. PI, PDS...)? Who should fund distribution (e.g. R&A, PDS...)?

Group 4: Deal, *Granahan, Pieters, Saunders, Schneebeli, Sprague
VIS/NIR field/airborne studies: What are the critical gaps, and what studies are most needed? VIS/NIR field/airborne future capabilities: What additional instrumentation is most needed (if any)?

6:00 Group dinner (Italian Cafe)
DOORS OPEN AT 7:45

8:15–9:30 Field and Airborne Panel
Moderator: Mustard

9:30–9:50 Break

* = present results in the panel discussion
All questions are open to all groups, but each group should address their question(s) in-depth first.

Group 1: Barker, Bishop, Clark, Fonti, Ramsey, *Saunders
What studies are most needed to attain the critical goals of the Mars Program to support searching for possible mineral biomarkers and environments that could preserve signatures of life?

Group 2: Deal, *Hapke, Morris, Murchie, Schneebeli, Sprague
What studies are most needed to attain the critical goals of the Mars Program to support interpretations for answering basic questions in geology and volatile budget?

Group 3: Blaney, Granahan, *McCleese, Mustard, Schmidt, Wright
Contingency plans: If a currently slated spectral data set is not returned or is not as productive as planned, would requirements or priorities for supporting studies change?

Group 4: *Arvidson, Cipar, Kirkland, McAfee, Pieters, Seelos, Sellar
What lab, field, airborne instrumentation is most needed?
What community spectral libraries are most needed?
What field and airborne data sets should be measured specifically for release to the community?
How to get data to the community?
How to mesh data release with the R&A cycle?

10:50–12:10 Panel discussion for the report
Moderator: Kirkland
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MARS EXPLORATION AND IMPORTANCE OF SPECTROSCOPIC OBSERVATIONS. R. E. Arvidson, Department of Earth and Planetary Sciences, McDonnell Center for the Space Sciences, Washington University, St. Louis, Missouri, 63130; arvidson@wunder.wustl.edu

An update will be given based on the work by the Pathways Science Steering Subgroup of the Mars Exploration Payload Analysis Group (MEPAG), focusing on planned and needed spectroscopic investigations from orbit and from the surface that would pursue science objectives associated with climate, life, resources, and the role of water. This Subgroup is chartered to examine the mission set and expected results through the 2009 Mars Smart Lander (MSL) Mission and to postulate alternate discovery-driven investigation pathways that NASA might take in exploring Mars during the next decade. An emphasis will be on global understanding of the tectonic and climatic cycles and whether or not they conspired to produce suitable habitats for life of Mars. Summaries will be provided for observation capabilities associated with existing and planned spectroscopic systems through MSL and requirements derived and presented for several investigation-driven pathways for the next decade.

Introduction: Martian surface composition analysis should include multiple types of spectral measurements in order to maximize the information to be gained. Mars research is utilizing this concept in combining thermal IR (TES and THEMIS) with visible/NIR (Omega and CRISM) global spectral measurements in current and upcoming missions, as well as a combination of multispectral visible/NIR and hyperspectral thermal IR on the 2003 MERs. What we need urgently to support these missions are studies of analog materials, both in the lab and in situ. These studies should include hyperspectral visible/NIR, mid-IR and Raman data in order to be applicable to future missions where these data will hopefully be collected on Mars.

Current Study: Results are summarized here for a spectral study of two hydrothermal rocks from Yellowstone. Many of the minerals present in hydrothermal samples may be associated with organisms and may be useful as indicators of life or environments supportive of life on Mars. Spectra so far on this project have been performed in the laboratory on rock samples and powders. Samples such as these need to be studied in situ in the field as well in order to address a broader range of measurement concerns.

Preliminary work on this project was reported at the 2001 Mars technology workshop [1]. The samples were provided by Rocco Mancinelli. X-ray diffraction of the silicate rock indicates the presence of a combination of silicate species including opal-A and cristobalite, as well as poorly crystalline phases of tridymite or other SiO4 polymorphs.

Visible/NIR Spectra: Two visible/NIR spectra are shown in Figure 1 of <125 μm powders of a hydrothermal rock collected at the Mammoth Formation. One spectrum (331) is dominated by calcite spectral bands and the other contains spectral features characteristic of both calcite and gypsum. Spectra of these minerals are shown for comparison. The calcite and gypsum samples are described in a previous study [2].

Two visible/NIR spectra are shown in Figure 1 of <125 m powders of a hydrothermal rock collected at Octopus Springs. The spectral bands near 1.41, 1.9 and 2.2 μm are consistent with the presence of montmorillonite, but could also be due to some other Al-OH species. The weak bands near 1.37 and 2.22 μm are attributed to Si-OH species based on work by [3]. Spectra of montmorillonite [4] and quartz [5] are shown for comparison. The finely ground quartz sample contains features near 1.4 and 2.2 μm attributed to Si-OH groups formed on the surface through grinding, and near 1.9 and 2.9 μm attributed to H2O adsorbed on the surface.

Mid-IR & Raman Spectra: Emission, reflectance and Raman spectra are shown in Figure 2 of the same particulate sample (331) of the Mammoth Formation rock. These spectra all exhibit features characteristic of calcite. In addition, an emission spectrum is shown of the rock surface that exhibits spectral bands due to calcite and gypsum. Black lines are shown near 1150, 870 and 710 cm⁻¹ where strong calcite IR bands are observed. Strong Raman bands due to calcite are observed at 1085, 712, 285 and 158 cm⁻¹. Gray lines are shown near 680 and 600 cm⁻¹ where characteristic gypsum bands are present.
MINERAL DETECTION ON MARS: J. L. Bishop et al.

Figure 2. Mid-IR reflectance, emission, and Raman spectra of a carbonate rock from Mammoth Formation, Yellowstone.

Figure 3. Mid-IR reflectance, emission, and Raman spectra of a silicate rock from Octopus Springs, Yellowstone.

The strongest Raman band is present near 2800 cm\(^{-1}\) for sample 329 and is characteristic of CH stretching vibrations [6]. The Raman spectrum for sample 270 contains weak bands near 800 and 430-470 cm\(^{-1}\) that are attributed to Si-OH bending at 800 cm\(^{-1}\), and bending in distorted SiO\(_4\) groups near 470 cm\(^{-1}\), e.g. [7]. Raman bands are observed near 710, 430 and 200 cm\(^{-1}\) in montmorillonite (Figure 4 and [7, 8]) and may explain weaker bands and shoulders at these positions.

Figure 4. Mid-IR reflectance and Raman spectra of three montmorillonite samples from the Clay Minerals Society. All are dry sieved to <45 \(\mu\)m and contain carbonate, silica and/or quartz impurities. The STx-1 and SWy-1 reflectance spectra are offset by +0.1 for clarity.

Summary: Spectroscopic studies of Mars analog materials need to be pursued that combine multiple spectral ranges and techniques in order to gain the ground truth necessary for interpretation of rocks and soils on Mars. These studies need to be performed on samples in the lab and in the field.

VISIBLE TO SHORT WAVELENGTH INFRARED SPECTROSCOPY ON ROVERS: WHY WE NEED IT ON MARS AND WHAT WE NEED TO DO ON EARTH. D. L. Blaney, Jet Propulsion Laboratory, 4800 Oak Grove Dr., MS183-501, Email: Diana.Blaney@jpl.nasa.gov

Introduction: The next stage of Mars exploration will include the use of rovers to seek out specific mineralogies. Understanding the mineralogical diversity of the locale will be used to determining which targets should be investigated with the full suite of in situ capability on the rover. Visible to Short Wavelength Infrared (VSWIR) spectroscopy is critical in evaluating the mineralogical diversity and to validate the global remote sensing data sets to be collected by Mars Express and the Mars Reconnaissance Orbiter. However, spectroscopy on mobile platforms present challenges in both the design of instruments and in the efficient operation of the instrument and mission. Field-testing and validation on Earth can be used to develop instrument requirements analysis tools needed for used on Mars.

VSWIR Spectroscopy: To fully address the evolution of the Martian surface, the mineralogy and geologic context of both the original igneous material and the alteration products must be determined. Many unanswered questions remain about how the fresh igneous material on the Martian surface evolved into the alteration products seen today. The answers to these questions will tell us about weathering environments, rates of alteration, and climate evolution. The mineralogy of the alteration products is a sensitive indicator of formation conditions such as eH, pH, abundance and phase of water, atmospheric chemistry, temperature, and surface pressure. The presence of different types of iron oxides and oxyhydroxides, carbonates, and clays, and their degree of crystallinity are particularly sensitive indicators of formation conditions and can be characterized by VSWIR spectroscopy. Additionally, the mineralogy of unaltered material needs to be determined in order to separate weathering products derived locally under current conditions from material formed under other conditions. Therefore, we also need to know the mafic mineralogy of the source rock (olivine and pyroxene composition and abundance). Contextual information such as the mineralogy of any weathering rinds on rocks and how it differs from that of the soil and the duracrust will be needed to derive an integrated picture of what processes have occurred and when.

The 0.4 to 2.5 μm region contains diagnostic absorption features of minerals, atmospheric gasses, volatiles, and organics. Clark et al. (1990), Swayze (1997), and Swayze et al. (2001) studied the spectral sampling and spectral range needed to resolve absorption bands in spectra and discriminate between mixtures. They found that the ability to identify minerals decreases dramatically at a sampling and spectrometer bandpass (Full-Width at Half-Maximum, FWHM) >20 nm, with detection difficulties beginning at ~15 nm. Modeling, laboratory mixture work, operational experience and field verification with imaging spectroscopy data (e.g., Clark and Roush, 1984; Clark 1983; Swayze 1997; Swayze et al., 2001; Clark 1999; Clark et al. 2001) indicate that important minerals can be detected at abundances of <1% per pixel with a SNR >200:1. However, improved spectral resolution and SNR enable better atmospheric corrections and lower detection limits.

Spectrometers on Mars Rovers: The design and building of in situ spectrometers for Martian rovers must be carefully tailored to the platform and mission. Specifics site geology and mission goals must be considered. A key factor is matching the instrument to the platform and the resources available. Mass, power, data rate, data volume, platform stability, spatial resolution, and pointing requirements all influence the spectrometer design and how it is used.

Spectroscopy on rovers falls into three broad categories. Panoramic imaging spectroscopy produces complete hyperspectral coverage of the location and thus the complete mineralogy of a site. Point spectroscopy can generate hyperspectral coverage, but it is very time consuming. After an initial assessment point spectrometers raster out small areas targeted via multi-spectral imaging and relate the mineralogy of points to the scene via their visible spectral colors. Microscopic spectroscopy looks at mineralogy of rock—basically relating rock texture to composition.

On a rover, the scene changes every time the rover moves. This means that analysis and interpretation of the data must be done in hours to influence the tasks the rover will carry out the next
sol. This type of rapid real time analysis is very different from how most planetary scientists conduct their research. To enable working in this type of environment new analysis tools and approaches need to be developed. Additionally, instrument calibration and performance stability take on a larger importance since artifacts can cause bad decisions to be made.

**Terrestrial Spectroscopy Field Trials:** The Mars Exploration Program is developing technology for future Martian rovers. One area of research is science operations with real instrumentation, including spectrometers. The NASA JPL Field Integrated Design & Operations (FIDO) rover has successfully integrated and validated a point spectroscopy approach using a 1.2-2.4 μm spectroscopy during field trials (Arvidson et al. 2000, Haldeman et al. 2002). In 2001, FIDO field trials were used to model operations of the 2003 Mars Exploration Rovers (MER). Other rovers that use spectrometer data in their field trials include the AMES Marsokhod and K9 rovers (e.g. Stoker et al. 2001).

**Future Directions:** To date most of the research has focused on the 2003 MER whose payload includes the Miniature Thermal Emission Spectrometer (Mini-TES). Mini-TES will be used to determine the mineralogy of rocks that are potential targets of investigation. It will also validate the TES and Themis global remote sensing data sets and interpretations.

The next rover opportunity for will be the 2009 Mars Smart Lander—which calls for a Mobile Science Laboratory. This rover is planned to be nuclear powered and thus operate for substantial periods of time. It will also be the first opportunity to validate the 2005 MRO CRISM imaging spectroscopy data.

Further field trials need to be developed which evaluate instrument types given the differences in resources (power, mass, data rate) between MER and Smart Lander. Additional automation of the analysis and interpretation of spectroscopy data needs to be carried out to sustain long term rover operations affordably.
SPECTRAL FEATURE MAPPING AND ANALYSIS OF MARS GLOBAL SURVEYOR THERMAL EMISSION SPECTROMETER DATA. Roger N. Clark, Todd Hoefen, Michael D. Smith, and John C. Pearl

The Mars Global Surveyor (MGS) spacecraft began orbiting Mars on September 11, 1997. After aerobraking and science phasing periods where the orbit shape and equator timing were adjusted, mapping by science instruments began on March 9, 1999. The Thermal Emission Spectrometer (TES) has obtained 6-50 μm spectra of Mars since the mapping period began and continues to do so to the present. The TES obtains nadir pointed spectra of nominal 5 and 10 cm⁻¹ spectral sampling (143 or 286 spectral channels) from 6.25 to 50 μm (1600 to 200 cm⁻¹) in 2 to 4 seconds. The TES also obtains limb pointed spectra and selected angles in between nadir and limb, as well as space pointed and internal black body pointed (for calibration) spectra. The TES obtains both day and night side data in a 3-pixel cross track and 2-pixel down track array. The pixel size is 3 km across track and 6 km down track. Six-km down-track smearing is caused by orbital motion due to the spacecraft flying backwards from its intended direction and in an orientation where the TES image motion compensation does not work.

Approximately 3 years of MGS TES day-side, nadir-pointed, 10-wavenumber data have been culled from the TES database and projected into image cubes at full TES spatial resolution of ~3 km per pixel to provide near global coverage. Coverage of the poles north and south of 60 degrees latitude has not been included in this analysis because of pervasive clouds in the data set at the polar latitudes. Three years of TES data allowed selection of the best spectra, free of artifacts to be assembled and still have > 80% surface coverage. Multiple observations of the same area on the martian surface were averaged to provide the overall highest quality spectrum at each pixel.

The image cubes were assembled at 20 pixels/degree, or 2.96 km/pixel at the equator. Thus, for coverage from 60 degrees north latitude to 60 degrees south latitude, the hyperspectral image cubes of Mars comprise 7200 pixels in longitude by 2400 pixel in latitude in a simple cylindrical projection, and 143 channels in the spectral dimension.

The hyperspectral image cubes were calibrated to radiance using internal black-body measurements and space measurements. Apparent emissivity was derived for each pixel using temperatures in the TES database. Finally, atmospheric gas absorptions were removed and ancillary data were registered with the images, including albedo and MOLA topographic elevation.

The data cubes have been analyzed for the presence of spectral features due to surface geology. The analysis of this vast data set of tens of millions of spectra is limited by our present knowledge of the spectral properties of materials in the infrared. The results and analysis implications will be discussed.

Spectral features were searched for using least squares feature analysis with reference spectral library features. The search was limited to regions of the TES spectra free of strong gas and dust absorptions and where TES has high signal-to-noise ratio. This effort represents the most extensive and highest resolution search for minerals on Mars to date, to our knowledge.

The search for minerals, however, is limited by current spectral libraries. Spectral features in the infrared are strongly affected by grain size and few minerals have had spectra measured as a function of grain size.

The most spectrally abundant features found in the TES data to date are those due to pyroxenes, olivine, and hematite. In fact, while some other small and weak spectral features can be seen in the data, only spectral features due to pyroxene, olivine, and hematite have been definitively identified and map in large geologic regions on Mars. Searches for outcrops of other minerals, including carbonates, quartz, and mineral signatures of hydrothermal alteration systems and mineral deposits have failed to definitively show in the TES data. Such minerals, if they exist on Mars, are either significantly smaller than a TES pixel, or are buried by dust. More reference spectra in libraries, and as a function of grain size may lead to identification of more minerals.

Olivine shows variable composition in different regions of Mars, and appears stratified in outcrops at certain elevations. The implications of this stratification are under study but may indicate changing volcanic conditions in martian geologic history, or region or both.
In recent years the scientific interest for Mars has grown considerably, spurred mainly by the renewed attention of Space Agencies. In particular the successful NASA missions Mars Pathfinder and Mars Global Surveyor (MGS) have supplied a wealth of new data, but at the same time have opened a large number of new questions concerning both the present and the past of the planet (Mars Pathfinder Team, 1997; MGS/TES Team, 2000). It is worthwhile to note that some of the pending issues are considerably appealing also for the general public. As an example we can consider the consequences that the assessment of past existence of liquid water on the surface of the planet can have for the possibility that life has developed on Mars in the past (McKay, 1991; McKay et al., 1996). It is probable that no definite results can be obtained without a direct analysis of samples retrieved from a carefully chosen landing site, but such an occurrence is not scheduled in the near future. Therefore, for the time being, the information obtained with the observation of the planet by means of orbiting instruments, can play an important role in addressing many important questions concerning the climatic evolution of Mars.

In this respect, the Mars Orbiter Camera on board of MGS has demonstrated, beyond any doubt, the extreme usefulness of the visual inspection at high spatial resolution. Nevertheless a complete picture can be reconstructed only comparing the information retrieved in this way with the results obtainable by means of visible and infrared (IR) spectroscopy. However the interpretation of visible and IR spectra is not straightforward and the amount of retrieved information, as well as its reliability, depends strongly on the possibility to relate the observational data with laboratory spectra of suitable materials, carefully chosen among those thought to be analogues to the Martian ones. Therefore the availability of an adequate spectral library for OMEGA and PFS, the spectrometers on board of the ESA mission Mars Express, planned in 2003 (Chicarro, 1999), is absolutely necessary. In the same way the Arizona State University spectral library has played a major role in the analysis of the spectra obtained by the Thermal Emission Spectrometer (TES) on board of MGS (Christensen et al., 2000).

It is important to realise that the main characteristics of a spectral library has to be tailored following the features of the involved instruments, as well as the peculiarities of the object to be studied. In this presentation the parameters used in defining the structure of the laboratory data set will be described in some detail, together with the requirements needed in order to compare the information contained in the library with spectra available from already existing laboratory data sets. It can be anticipated here that a major constraint is the homogeneity of the collected spectra, involving not only the actual collection of the data, but also the preparation and a thorough characterization of the each sample.

The spectral characteristics of a given material can be retrieved using different techniques: emission, transmission and reflectance and in each case they can be the experimental base for the computation of the optical constants of the examined material (Bohren and Huffman, 1983; Wenzel and Christensen, 1996; Esposito et al., 2000). A spectral library, in order to be used as a reference for the data obtained by OMEGA and PFS, should contain reflection spectra in the range 0.3 - 7 μm and emission spectra in the range 3 - 50 μm, as well as transmission spectra in the whole spectral range, at the appropriate resolution. This would allow using the different spectroscopic techniques for mutual validation and for the derivation of the optical constants in the widest possible range.

The choice of the materials to be examined is a rather complex issue and will be discussed during the presentation. It must be noted, though, that

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the problem is further complicated by the presence of dust on the Martian surface and in the Martian atmosphere and by the fact that the spectral properties of a particulate sample depend on the size of the grains particularly when the particles are much smaller than the radiation wavelength, as in the case of the Martian aerosol (Bohren and Huffman, 1983). This occurrence can be used to retrieve additional information from the observed spectra, but, on the other hand, requires a much longer laboratory work, aimed to differentiate the spectral characteristics in function of the grain size.

It should be clear at this point that the task of preparing an appropriate database is well beyond the capability of a single laboratory. For this reason the outlined program will be accomplished through the joint effort of at least five laboratories. The parallel involvement of different experimenters, using the same procedure, but different equipment should allow for a mutual validation of the results. On the other hand, as it will be discussed in the presentation, the coordination of the experimental work must place additional stress on the concept of data homogeneity especially in connection with the preparation procedure of each particulate sample as well as its chemical, elemental and morphological characterization.

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MAPPING LITHOLOGIC UNITS EXPOSED ON THE SUMMIT OF MAUNA KEA USING AVIRIS HYPERSONTRUAL REFLECTANCE DATA. E. A. Guinness¹, R. E. Arvidson¹, B. L. Jolliff¹, R. V. Morris², and D. W. Ming², ¹Department of Earth and Planetary Sciences, Washington University, 1 Brookings Drive, St. Louis, MO 63130, ²Code SN, NASA-Johnson Space Center, Houston, TX 77058.

Introduction: The Mauna Kea summit region is largely comprised of cinder cones and lava flows that form the cap of the Mauna Kea Volcano. The cones and flows at the summit are part of the Laupahoehoe Volcanic series. The Laupahoehoe volcanism occurred both during and after the late Pleistocene Makanaka glacial episode at the summit [1]. In addition, a few Laupahoehoe cones have been glacially eroded as evidenced by oversteepened slopes, which suggests that they predate the Makanaka glacial period. Two notable examples of possible preglacial cones are Puu Waiau and Puu Poliahu. These two cones are also significantly altered, most likely by hydrothermal activity that has weakly cemented the materials on the cones [1]. Well-crystalline sulfates (alunite and jarosite), phyllosilicates, and zeolites, have been found in samples collected from altered cones at the summit [1-3]. In addition, palagonitic tephra, which have nanophase ferric oxide, allophane, and other poorly crystalline forms of weakly altered basaltic glass (i.e., no phyllosilicates), have been described at several locations on Mauna Kea [e.g., 4, 5]. While several studies have discussed the occurrence of alteration products on Mauna Kea, the distribution of these materials exposed at the summit has not been extensively mapped.

Hyperspectral imaging can provide information for identifying and mapping lithologic units containing alteration minerals, such as are found on Mauna Kea. The Airborne Visible Infrared Imaging Spectrometer (AVIRIS) is a hyperspectral imaging instrument that covers the wavelength range from about 0.4 to 2.5 μm in 224 bands, with a band spacing of 10 nm and average band width of 10 nm [6]. Reflectance spectra in this wavelength range contain electronic transitions and vibrational absorption features that can be used to identify and discriminate ferric oxide, phyllosilicate, and sulfate minerals typically found in alteration zones. AVIRIS data also provides high spatial resolution with a ground instantaneous field of view of 20 m when flown at its nominal altitude of 20 km above sea level. AVIRIS was deployed to Hawaii for the first time in 2000 with AVIRIS data acquired over much of the Hawaiian Islands, including the summit of Mauna Kea.

Methods: The Mauna Kea summit is covered by a 10 x 10 km AVIRIS scene with a pixel size of about 15 x 15 m. The AVIRIS data are corrected for atmospheric scattering and attenuation and converted to ground radiance coefficient values using the ATREM algorithm [7]. ATREM uses a radiative transfer model to compute atmospheric transmittance of gases and scattering from aerosols. The analyses are also restricted to the portion of the scene above the tree line so as to be essentially free of vegetation. Spectrally distinct endmember classes are extracted from the atmospherically corrected AVIRIS reflectance data. The AVIRIS spectra are divided into visible and near infrared (VNIR) and short wave infrared (SWIR) sections so that electronic transition and vibrational absorption features can be analyzed separately. The VNIR wavelength region provides diagnostic absorption features for ferric oxide minerals such as hematite, goethite, and jarosite, whereas the SWIR region contains features due to hydroxyl-bearing minerals, sulfates, and carbonates. Specifically, the wavelength range of 0.41 to 1.06 μm is used in the VNIR analysis and the range of 2.09 to 2.45 μm is used for the SWIR analysis. Maps showing the distribution of each endmember unit are then generated for the VNIR and SWIR data sets using the Spectral Angle Mapper (SAM) method [8]. This method computes the angle between two spectra by treating the spectra as n-dimensional vectors, with n as the number of AVIRIS bands. The angle is determined from the dot product of two vectors where one vector is an endmember spectrum and the other is the spectrum of a given pixel. Small angles mean that the two spectra are similar. The SAM method depends on the shape of the spectra and not on absolute reflectance values, thus minimizing illumination differences. Pixels are assigned to a given endmember unit if the separation angle is less than an assigned threshold.
Results: Atmospherically corrected AVIRIS spectra for visible and near infrared wavelengths of 0.4 to 1.1 μm exhibit electronic transition absorption features related to a suite of ferric oxide units. Spectral features suggest the presence of hematite, palagonite, and possibly jarosite. Three spectrally distinct hematite units are seen in the AVIRIS data in terms of the depth of ferric absorption features with variations likely related to the size of hematite grains. Three units with spectral features related to phyllosilicates were also identified in the AVIRIS data based on metal-OH absorptions in the short wavelength infrared region of 2.0 to 2.5 μm. These three units are characterized by spectral features of kaolinite, montmorillonite, and saponite. Surfaces of relatively fresh, uneroded cinder cones are typically dominated by exposures of the ferric oxide units. These cones exhibit a concentric zoning in the distribution of the hematite units, with the hematite unit having the deepest ferric absorption bands occurring at or near the summit of the cones and units having weaker absorptions being exposed further down the flanks of cones. The palagonite unit is typically exposed at the base of cinder cones and is more widely located on flow surfaces. Surfaces of eroded cinder cones, such as Puu Poliahu and Puu Waiau, have localized exposures of the three phyllosilicate and possible jarosite units. The montmorillonite unit is the most commonly exposed phyllosilicate unit. In some cases there is zoning among the phyllosilicate units with a core of the saponite unit surrounded by montmorillonite. The kaolinite unit is only found in two discrete exposures on Puu Poliahu with one exposure coinciding with a possible jarosite unit. The phyllosilicate units may reflect localized alteration along small fractures or dikes that focused hydrothermal fluids.

STATUS OF REFLECTANCE AND EMISSIVITY MODELS RELEVANT TO MARS STUDIES.
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The status of theoretical models of the interaction of electromagnetic radiation with planetary regoliths relevant to the interpretation of Martian spectroscopic observations is discussed. Most of the problems have to do with particle size effects, because the physics of light scattering is different, depending on whether the particles making up a medium are larger or smaller than the wavelength. The spectral emissivities of media of large and small particles will, in general, be quite different in ways that often are not predictable.

(1) Martian atmospheric dust consists of particles ~ 1-2 μm in size, and powder of similar sized particles probably covers much of the surface. In the visible and near IR the soil particles may be treated as independent scatterers that are large compared to the wavelength. Theory is in fairly good shape in this case.

(2) The major Martian spectral data base is the TES library of IR spectra, which were obtained mainly from powders whose particle sizes are 0.5-1.0 mm, much larger than the wavelengths used by TES. However, the surface and aerosol particles are much smaller than the wavelength.

(3) In going from large to small particles there is a contrast reversal in the strength of emissivity bands. In large particles, strong bands have large spectral contrasts and weak bands have small contrasts. In small particles the opposite is true. Also, the band wavelengths shift. Hence, atmospheric dust and surface sand of the same material may have very different spectra.

(4) A powder composed of large particles can be treated as if the particles scatter radiation independently even though they are touching. However, in a powder of small particles in contact coherent effects are important, and this affects the spectra in ways that are poorly understood.

(5) The peroxide coatings that appear to be present on the surfaces of Martian regolith particles may have created a kind of Martian desert varnish that affects the spectra in unknown ways.

Introduction: The 2003 Mars Exploration Rover science strategy calls on Pancam and Mini-TES to identify promising targets for the rover, which will then traverse to those targets for examination. Team members will select sites using target morphology and color (Pancam), and interpretations of the mineralogy using Mini-TES.

This strategy requires high quality, near real-time interpretations of Mini-TES data. The planetary community has essentially no experience with rapid identification using field images measured similarly to Mini-TES. Department of Defense researchers have instrumentation, data sets, and experience in this area. Here we discuss lessons learned in interpreting field spectra and measurement protocols that improve interpretations. We solicit input for what targets and sites to measure using our hyperspectral field scanners for release to the community.

Instrumentation: The Aerospace Corporation owns the equipment we use. This includes Block Engineering Model 100 (M100) Fourier transform infrared interferometers mounted on three types of van platforms. The M100 measures hyperspectral images using a precisely controlled mirror that raster scans in two dimensions at 25 Hz, and it records the viewing angles with the data. The viewing geometry and scanning system are very similar to the Mini-TES (Table 1).

Extracting signatures: First the data are calibrated to radiance. Fig. 1 shows a calibration curve measured in the field, at 989 cm⁻¹, using blackbodies at 294, 308, and 318 K, and 1st and 2nd order polynomial fits. The calibration works well over the temperature range of the calibration targets, but Fig. 1 illustrates why it is difficult to extrapolate to cold brightness temperatures using only warm calibration targets. X-axis shows raw data, and Y-axis the blackbody radiance values calculated at the measured calibration target temperatures and compensated for the true target emissivity. Radiance units are W/cm²srcm⁻¹ multiplied by 10⁶. (From scene 0209-048.)

Second, the data must be converted to a unit for comparison to laboratory data. Fig. 2 illustrates a conversion to apparent emissivity. When the diffuse downwelling radiance is not known, apparent emissivity uses zero as the zero emissivity reference line (Arrow 2), and is the measured radiance divided by a blackbody fit. When the diffuse downwelling radiance is known, it is used as the zero emissivity reference line (Arrow 1). This is called a special ratio [1], given by (measured-downwelling) / (blackbody fit-downwelling). Fig. 3 shows both results.

Fig. 1: Calibration curve. This illustrates the difficulty in extrapolating to cold brightness temperatures using only warm calibration targets. X-axis shows raw data, and Y-axis the blackbody radiance values calculated at the measured calibration target temperature and compensated for the true target emissivity. Radiance units are W/cm²srcm⁻¹ multiplied by 10⁶. (From scene 0209-048.)

Fig. 2: Field spectra. The upper curve is a blackbody fit to the highest brightness temperature over 820–1278 cm⁻¹; the middle trace was measured of a quartz-rich region, and the lower trace of a diffuse aluminum target that has been adjusted for the laboratory measured reflectance (~90%). Arrow 1 illustrates a ratio compensated for downwelling radiance ("special ratio"), and Arrow 2 shows a simple ratio. We used a second order calibration curve (Fig. 1) to prevent negative radiance values for the cold diffuse downwelling spectrum. (Radiance units: W/cm²srcm⁻¹ × 10⁶). Scene 0424-216)

Table 1: Instrument parameters

<table>
<thead>
<tr>
<th></th>
<th>FOV (mrad)</th>
<th>el (deg)</th>
<th>az (deg)</th>
<th>sampling (cm⁻¹)</th>
<th>range (µm)</th>
<th>height (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mini-TES[2]</td>
<td>20 or 8</td>
<td>-50 to +30</td>
<td>360</td>
<td>10</td>
<td>5–25</td>
<td>~1.4</td>
</tr>
<tr>
<td>M100</td>
<td>8.7</td>
<td>-70 to +90</td>
<td>360</td>
<td>2</td>
<td>7.5–13.5</td>
<td>~2, 2.5, 3</td>
</tr>
</tbody>
</table>

FOV = field of view; el, az = elevation, azimuth range; sampling = spectral sampling interval; range = spectral range; height is above ground.
Conversions for TES use a simple ratio. However, field data have greater atmospheric downwelling radiance contribution than airborne or satellite measurements (because gases absorb where they emit). Our experience is that our airborne hyperspectral data have not required a downwelling radiance compensation for a high quality conversion, but our field spectra do. Similarly for Mars, we should not be lulled into thinking reflected downwelling radiance is unimportant for Mini-TES because of downwelling aerosol radiance and the lack of a diffuse target to measure the downwelling radiance. (Scene 0424-216)

Fig. 3. The “special ratio” and “simple ratio” show the ratios marked by Fig. 2, Arrow 1 and 2, respectively. Most fine spectral details evident are atmospheric features. The special ratio compensates for the downwelling radiance, but the residual ozone doublet shows the compensation here is incomplete, probably because the aluminum target was tilted, not perfectly diffuse, and/or from the calibration extrapolation. Residual downwelling radiance signatures will affect mineralogy interpretations. This will be important for Mini-TES because of downwelling aerosol radiance and the lack of a diffuse target to measure the downwelling radiance. (Scene 0424-216)

Issues for Mini-TES: Our experience with field spectrometers is that the full interpretation chain has many potential sources of error. Difficulties include (1) calibrating to cold brightness temperatures; (2) diffuse, specular, and partial mixing of target and downwelling radiance; (3) determination of diffuse downwelling radiance from direct sky measurements; (4) near real-time interpretations combined with lack of practice data and experience; (5) field signatures are frequently more subtle than laboratory signatures, so practice with field signatures is required to gain the experience to interpret field data accurately; (6) incomplete supporting spectral libraries, particularly of rough, weathered, coated, very fine, and mixed materials.

For Mars, incompletely compensated aerosol dust downwelling radiance can alter interpretations, particularly for silicates. The dust distribution with altitude will affect the magnitude of the contribution. Water ice clouds will also contribute, and the diffuse contribution may be particularly difficult to determine when the cloud coverage varies during direct sky measurements by Mini-TES.

Fig. 4: The “diffuse Al” trace shows a spectrum measured of a diffuse aluminum target, compensated for the true reflectance; the “salt” target is -5 mm rock salt particles; and “sky” shows a point measurement of the sky near zenith. Note that diffuse and line-sight downwelling radiance differ significantly. We measured this scene at a more humid location than in Fig. 1. Negative radiance values illustrate the difficulty in extrapolating from warm calibration targets to very cold brightness temperatures. Here we used a first order fit. (Units: W/cm² sr cm⁻¹ x 10⁶). Scene 0209-048.

Data sets measured similarly to the Mini-TES are critical to have to understand these issues; to develop and test measurement protocols and near real-time and in-depth interpretation methods; and so the instrument team and community can prepare to interpret the Mini-TES data. Lab, airborne/satellite, and single-point field spectra alone are not sufficient because they do not simulate all the critical effects present. Test data sets should include natural scenes to force consideration of unexpected effects, and constructed scenes to extend materials measured (e.g. very fine particles and coatings). Scenes covering the full wavelength range of Mini-TES should also be simulated by seaming with laboratory spectra. They should be degraded to the expected signal-to-noise ratio of the Mini-TES and interpreted both near real-time and more in-depth. The full calibration, conversion, and interpretation chain should be tested near real-time using those data sets and the same measurement protocols as planned for Mini-TES.

Finally, we have found that it is critical to include a known target with good spectral contrast in our field images to test the full chain. Without this reference, it is impossible to evaluate the result. Mini-TES can use targets of opportunity (e.g. airbags) if those targets are measured pre-flight.

MARTIAN ANALOGUE SAMPLE CHARACTERIZATION AND SPECTRAL LIBRARY DEVELOPMENT AT THE JOHNSON SPACE CENTER. Richard V. Morris, Astromaterial Research and Exploration Science Office, NASA Johnson Space Center, Houston, TX 77058.

Introduction. An extensive collection of Martian analogue samples housed at the Johnson Space Center is the focus of ongoing research by the JSC Mars soil genesis group and their collaborators [e.g., 1]. Because the major element composition of Martian meteorites and in situ analyses of Martian soils and rocks indicate that Mars is predominantly an iron-rich basaltic world, the focus of active sample collection and analysis is basaltic materials and their hydrolytic (both aqueous and hydrothermal) and sulfatetic alteration products. Described below are the scope of the JSC Mars analogue sample collection, the characterization process, and plans to incorporate the data into spectral libraries for the Mars 2003 Mars Exploration Rover (MER) and Mars 2005 Mars Reconnaissance Orbiter (MRO) CRISM missions.

Samples and Characterization. The JSC Mars analogue sample collection has 1000-1200 individual samples of rocks, soils, and minerals. Because these samples have been subdivided into 2 to 8 size and/or magnetic separates, the number of samples with distinct physical, chemical, and mineralogical properties is on the order of 3000. Examples of the variation of chemical and mineralogical composition for size and magnetic separates of palagonitic and sulfatetic tephra from Hawaii are given by [1, 2, 3].

Our standard set of characterization analyses includes major elemental analyses, diffuse reflectance spectroscopy between 350 and 2100 nm under desiccating conditions, Mössbauer spectroscopy, X-ray diffraction, and magnetic properties (magnetic susceptibility and saturation magnetization). Most of these analyses have been completed for ~1000 samples. Solution pH and electrical conductivity measurements have been completed for ~300 soil samples. Thermal emission spectra (200-2000 cm-1) have been measured for ~400 samples at Arizona State University. The analytical techniques were selected to both characterize the samples and to maximize overlap with current and future remote sensing and in situ data for Mars.

Samples and Spectral Libraries for Planetary Missions. Part of the JSC Mars analogue sample collection is a set of well-characterized rock slabs. The purpose of these slabs is to validate the calibration and performance of flight instruments. Rock slabs, rather than particulate samples, are used because they present reproducible surfaces for measurement to flight and laboratory instruments. These samples have already been used with CONTOUR and Mars Express OMEGA flight instruments and the mini-TES and Mössbauer MER instruments. The slabs will be used with the other MER analytical instruments (APXS, PANCAM, and MI) and with the CRISM MRO 2005 instrument.

Current plans are to publish the spectral and characterization data for JSC Mars analogue samples on a JSC-based WEB site. For full use with MRO, the JSC Mars analogue samples will require characterization under desiccating conditions in the spectral region between 2 and 5 μm. Work is underway to increase the number of samples in the <5 μm size fraction by size separations of soils and pulverization of rocks. The <5 μm size fraction is corresponds to the size fraction for aeolian dust on Mars [e.g., 4].


Introduction: The Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) on the Mars Reconnaissance Orbiter (MRO) will conduct a comprehensive series of investigations of the Martian surface and atmosphere. The investigations will be accomplished using an instrument design that provides high spatial and spectral resolutions, extended wavelength range, and ability to gimbol through a range of orientations. Baseline investigations include a near-global survey to find high science priority sites, full-resolution measurement of thousands of such sites, and tracking of seasonal variations in atmospheric and surface properties.

Science Overview: The Mars Exploration Payload Analysis Group [1] recommended specific hyper-spectral imaging investigations to characterize Martian geology, climate, and environments of present or past life. CRISM’s three groups of investigations address all of MEPAG’s recommendations. The first two groups correspond to two primary objectives of MRO: to search for evidence of aqueous and/or hydrothermal activity, and to map and characterize the composition, geology, and stratigraphy of surface features. These investigations are implemented by high-resolution hyperspectral mapping of thousands of high priority targets including candidate sedimentary deposits [2], volcanic regions, crustal sections exposed in steep escarpments, and sites which exhibit evidence in Mars Express/Omega data for concentrations of aqueously formed minerals. The third group of investigations addresses the primary MRO objective to characterize seasonal variations in dust and ice aerosols and water content of surface materials, and the secondary objective to provide information on the atmosphere complementary to other MRO instruments. These investigations are implemented using a systematic, global grid of measurements of the emission phase function (EPF) acquired repetitively throughout the Martian year. EPF measurements allow accurate determination of column abundances of water vapor, CO, dust and ice aerosols, and their seasonal variations [3]. At the same time, the grid’s repetitive coverage will track seasonal variations in water content of surface material. Additional, targeted observations of the polar caps will investigate their inventory of water and CO2 ices.

When not taking targeted measurements, CRISM will conduct a ~100 m/pixel, ~59-wavelength survey to search for evidence of aqueous activity that lacks morphologic expression and/or is below the resolution of previous spectral mapping. The survey addresses MRO’s secondary objective to identify new sites with high science potential for future investigation, and will be particularly important for identification of key Noachian deposits. For example, even at low Martian erosion rates [4], morphologic expressions of Noachian hot spring deposits would have been removed in ~109 yrs, so that such deposits may now exist only as mineralized spots in morphologically unremarkable eroded escarpments, crater ejecta, and talus. Much of the survey will be completed before MRO’s highest downlink rates, so that newly discovered sites can be targeted with full-resolution coverage.

Instrument Overview: An overview of the instrument is shown in Figure 1. CRISM’s two major sub-assemblies are the Optical Sensor Unit (OSU) and the Data Processing Unit (DPU). The OSU contains visible (VIS) and infrared (IR) imaging spectrographs that share the same 2.05° field-of-view and cover the wavelength range 400-1050 nm and 1050-4050 at 7 nm/channel. The IR focal plane is cooled with doubly redundant cryogenic coolers. A side-facing radiator cools the spectrometer cavity to decrease instrument background. An onboard integrating sphere provides radiance calibration, and a shutter and dedicated dark pixels on each focal plane provide background measurements interleaved with Mars measurements. Optics and the focal planes are enclosed in a housing that is gimbaled by a high-precision motor/encoder ±60° along-track from nadir. During measurement of a target, along-track scanning takes out most groundtrack speed and allows long integration times and high signal-to-noise ratio (SNR) data to be obtained. At the same time, scanning provides the capability to remeasure a spot repeatedly at multiple emission angles to characterize the EPF. High spatial resolution (~18 m/pixel from 300 km altitude) allows characterization of the surface at the outcrop scale, and wavelength coverage to >4000 nm provides sensitivity to carbonates even at low abundances. The DPU provides lossless or lossy compression of the data stream in real
time. Key design elements are adapted from the CONTOUR and MESSENGER optical instruments.

**Operations Overview:** Figure 2 summarizes CRISM’s three complementary data acquisition strategies, which are built around the three steps needed to characterize high scientific priority, small-scale deposits: find the deposits, separate their signature from that of the atmosphere, and acquire high spectral and spatial resolution measurements with high SNR. Most of the time the OSU views nadir, building up coverage in multispectral survey mode. In the second mode of observing, for a group of ~36 orbits once every ~30° of Ls, EPFs are measured on a 10° longitude x 15° latitude grid. The third mode is targeted observations, approximately 2200 of which will be obtained at key locations. At each site, gimballing is used to take out most along-track motion, so that the field-of-view is slowly scanned over a rectangular swath approximately 11 km wide (when measured from 300 km altitude). Measurements of the swath are bracketed by incoming and outgoing measurements of the EPF of the center-point of the swath at emission angles up to ±60°. Larger high-priority targets will be identified in Mars Express/Omega data and other data sets. The multispectral survey provides redundancy to Omega data in locating targets that have VIS-IR spectral signatures but lack obvious morphologic expressions, and it provides the spatial resolution needed to identify small targets not evident in Omega data.

**Fig. 1.** Preliminary CAD renderings of CRISM’s OSU and DPU.

**Fig. 2.** Schematic depiction of key attributes of CRISM’s measurement plan for the Martian surface and atmosphere.