

Imaging spectroscopy: Earth and planetary remote sensing with the PSI Tetracorder and expert systems: from Rovers to EMIT and Beyond

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35 **Abstract**

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37 A system for rapid analysis of spectroscopy data with emphasis on planetary surfaces, both imaging
38 and single spectrum data is described. The system, called Tetracorder, is commanded by an expert
39 system developed by expert spectroscopists. The Tetracorder and the expert system applies multiple
40 algorithms to analyze a spectrum in segments, leveraging the advantages of each spectral region's
41 sensitivity to detecting different compounds, whether solid, liquid or gas. The algorithms compare
42 measured spectra to the spectral properties of materials in spectral libraries. The libraries include pure
43 minerals, mineral mixtures that include areal mixtures, intimate mixtures, coatings, and molecular
44 mixtures and other compounds such as organics, vegetation, liquids and gases. Absorption bands of a
45 particulate surface change shape with grain size, and shape changes are used in some cases to constrain
46 grain size of each component in the surface. The different algorithm results are compared for each
47 spectral region and specific material composition and average grain size (when possible) are identified.
48 The system is operational analyzing real-time data on a new generation of rover for future planetary
49 missions as well as identifying materials from a spectrometer on the International Space Station. Four
50 abundance models, with increasing sophistication are developed that are computationally fast on
51 imaging spectrometer data are presented, and use Tetracorder identifications to produce maps of
52 mineral abundances. A fifth full radiative model that includes multi-layer surfaces is presented but is
53 computationally intensive. The system is open source and available on Github.

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Introduction

Spectroscopy is a tool that has been used for decades to identify, understand, and quantify solid, liquid or gaseous compounds. Spectroscopy is used in many professions and disciplines ranging from police work to mining and environmental assessment to astronomy for remotely detecting compounds. In the laboratory, spectroscopic measurements are used to detect absorption features caused by specific chemical bonds. Models can be applied to determine the abundance and physical state of the detected absorbing species. Imaging spectroscopy is a tool that can be used to spectrally identify and spatially map compounds having specific chemical bonds (Clark, 1999, 2003 and references therein), whether solid (crystalline or amorphous), liquid or gas.

In this work we describe the software system, called Tetracorder, that is effective at material identification and mapping. Tetracorder employs a set of algorithms within an expert system decision-making framework to identify and map compounds, whether solid, liquid or gas. The expertise in the system has been developed over the last ~ 35 years by a team of expert spectroscopists utilizing their scientific knowledge of spectral identification and material behavior. Tetracorder has approximately 100 person-years in development, testing, and verification. In modern terms of Artificial Intelligence, AI, this might be called Expert Intelligence, or EI. This paper describes the system and innovations developed since publication of the original Tetracorder paper (Clark et al., 2003).

Tetracorder has two modes of data analysis: single spectrum and imaging spectrometer. Single spectrum mode has two modes: 1) command line one spectrum at a time, and 2) follow a growing file of incoming spectra for real time analysis as spectra are received. Tetracorder has been deployed on the Carnegie Mellon University Zoë rover (Wagner et al., 2005, Wettergreen et al., 2005; Wettergreen et al., 2008; Vijayarangan et al., 2018, Clark et al., 2022) analyzing spectra real time as the rover explores autonomously, while making decisions based on Tetracorder identifications. Tetracorder is also being used by the NASA Earth Surface Mineral Dust Source Investigation (EMIT) science team at the Jet Propulsion Laboratory (JPL) on a Beowulf cluster. The EMIT instrument, an imaging spectrometer, is located on the International Space Station and is delivering thousands of scenes per month of the Earth's surface. Each EMIT scene covers about 75 x 75 km with 60 m/pixels and 285 bands from 0.38 to 2.5 μm (Green, 2023). Each scene has the atmospheric absorptions and scattering removed (Thompson et al., 2018; Brodrick et al., 2023), and the solar radiance corrected to derive apparent surface reflectance. The EMIT reflectance image cubes are analyzed by Tetracorder to deliver maps of minerals for use in climate change models to predict the radiative forcing impact of mineral dusts. Tetracorder is also being used by the European Research Council FRontiers in dust minerAloGical coMposition and its Effects upoN climaTe (FRAGMENT) project, which includes field measurements and sampling that can be used to verify EMIT and Tetracorder results. In this paper, we describe Tetracorder 5.27 as deployed on the Zoë rover and for EMIT/JPL in 2022/2023.

An imaging spectrometer data set may include millions of spectra, and Tetracorder can find hundreds of materials in a scene, including minerals, amorphous materials, inclusions, mixtures, and on Earth, vegetation spectral type, water content, chlorophyll red-edge position, photosynthetic and non-photosynthetic vegetation. Ice and snow grain size and melting snow is also identified and mapped.

101 Water is identified and the contaminant levels in water are determined. All these possibilities result in
102 thousands of image files to review, so post Tetracorder analysis summarizes what was found in text
103 files and in derived materials maps as browse products. A standard image stretch is performed so that
104 these products may be included in a mosaic with multiple scenes.

105 106 107 **Tetracorder**

109 Tetracorder is a system for applying multiple algorithms to a single spectrum or a group of spectra
110 (e.g., an imaging spectrometer data set) to identify and map mineralogy, chemistry, and particle grain
111 size. Tetracorder is different from other systems because it applies multiple algorithms to identify
112 materials expressed in the spectra, evaluating the results of those algorithms to make decisions,
113 including identifications, and applying additional algorithms, as needed, to solve specific problems
114 based on results of the previous analysis. The results of these decision processes could be continued
115 with application of additional algorithms and decisions. In theory, there is no limit to the number of
116 algorithm/decision cycles that can be handled by Tetracorder.

118 In traditional remote sensing analyses, an algorithm may be applied to return a score with the result
119 referred to as a “classification.” The algorithm may be applied multiple times, but each classification
120 image is usually not compared with others. Tetracorder applies multiple algorithms to characterize
121 components of a spectrum, and then compares the results to make decisions to derive the best answers.
122 Each spectral range has different sensitivity, thus multiple compounds may be identified from one
123 spectrum.

125 Tetracorder also employs data from other sources, in addition to spectra, e.g., temperature and pressure,
126 if available, to further constrain identifications. In that sense, Tetracorder is an “algorithm to apply
127 algorithms” through commanding by an expert system. Tetracorder benefits from ~35 years of
128 development by a team of expert spectroscopists at the U.S. Geological Survey, and more recently, at
129 the Planetary Science Institute with additional collaborators at other institutions who contributed to the
130 expert system.

132 Tetracorder uses knowledge bases of spectral libraries for comparison to unknown spectral features in
133 measured spectra. The spectra, both spectral library entries and the measured spectra, are split into
134 different wavelength-range intervals, called groups (Table 1) and each group is analyzed independently.
135 Within a group, each measured spectrum has multiple algorithms applied to it when comparing spectral
136 features to a potential match from the spectral library. The routine may be as follows for one measured
137 spectrum and one spectral library entry for one spectral region, for example:

139 spectral feature fit, feature 1,
140 spectral feature fit, feature 2,
141 spectral feature fit, feature 3 etc.,
142 “not” features (features that should not be present).

144 For each of the above features, there can be additional algorithms applied to constrain identifications:
145 Shoulderness constraints,
146 Slope constraints,

147 Threshold constraints,
148 Reflectance times band depth constraints,
149 Diagnostic feature constraints,
150 Optional feature constraints,
151 Must have feature constraints, and
152 Weak feature constraints.

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154 Then after the above are completed, additional algorithms are applied:

155 Weighted band depth calculation,
156 Weighted correlation coefficient calculation (the “fit”),
157 Weighted fit times band depth calculation.
158 Correlation coefficient constraints,
159 Temperature stability constraints,
160 Pressure stability constraints, and
161 Apply special cases as needed.

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163 The result of applying all these algorithms is a fit score. Once all spectral library entries in the expert
164 system are tested against the measured spectrum within one group (a spectral range), where each
165 library entry can have different parameters to all the above algorithms, the fits for all entries are
166 compared and the best match chosen as the answer. Each spectral region (group) analysis can detect
167 different components, including mixtures. If a chosen answer needs additional clarification, the special
168 case test can be invoked, called cases. Cases can trigger additional cases with no limit (except for
169 compile time memory declaration of array sizes).

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171 Tetracorder is one subsystem of the SPECtrum PProcessing system, SPECPR. SPECPR (Clark, 1980,
172 1993) and is a comprehensive spectral analysis system. It includes free-format subroutines for user
173 input, as well as input/output to binary-format SPECPR spectral data files. The U.S. Geological
174 Survey spectral libraries (e.g., Library06: Clark et al., 2003; Library07: Kokaly et al., 2017) are stored
175 in SPECPR format and Tetracorder only reads SPECPR format for reference spectra. Tetracorder uses
176 SPECPR routines to parse the expert system and read reference spectra. SPECPR, Tetracorder source
177 codes, the expert system and its needed spectral libraries are available at

178 <https://github.com/PSI-edu/spectroscopy-tetracorder>

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180 Because of the broad diversity of research by those who have contributed to Tetracorder development,
181 the Tetracorder expert system has been designed to work on surfaces throughout our Solar System (e.g.
182 Clark et al., 2003, 2015, 2016, illustrated in Figure 1), and the same expert system can be used with any
183 spectral range and resolution (Tetracorder version 5.1+). Tetracorder 5+ mapping results are
184 automatically analyzed and color-coded maps are automatically produced (e.g., Figures 1a, 1b).
185 Tetracorder produces maps of hundreds of materials, including chemical substitutions in some
186 minerals. Tetracorder results could be fed to other systems, e.g., real-time robotic systems to guide a
187 robot to resources (In Situ Resource Utilization, ISRU). Indeed, a NASA project, Toolbox for Research
188 and Exploration, TREX (Hendrix et al., 2023 and references therein update these), used Tetracorder for
189 real-time field assessment by a rover (<https://trex.psi.edu/>).

191 Tetracorder solves the material mixture problem by using spectra of measured or computed mixtures,
192 but only for overlapping absorption features that cannot be separated with continuum removal, thus
193 greatly reducing the number of mixtures needed. For example, consider the narrow tremolite
194 absorptions superimposed on the broad pyroxene bands in Figure 2. No reference mixture spectra are
195 needed by Tetracorder, because a short continuum removal adequately isolates the different
196 absorptions. Only if similar width absorptions overlap is a mixture analysis needed. For example, if the
197 pyroxene in Figure 2 contained ice, which has a broad 2- μm absorption, the 2- μm ice band would
198 overlap the 2- μm pyroxene band and a set of mixture spectra would be needed by Tetracorder. The
199 advantage of this strategy is that fewer mixtures are required, and computational time is reduced. Other
200 solutions, e.g., linear equations of an areal mixture problem, involve a matrix inversion, where the
201 compute time for a solution increases as the square of the number of endmembers. By including
202 mixture spectra, areal, intimate, and molecular mixtures are well covered in Tetracorder, as are
203 coatings, and the solution time grows linearly with the number of reference spectra.

204 The rapid response results were demonstrated with Tetracorder during the 2001 World Trade Center
205 disaster and the 2010 Gulf of Mexico oil spill, where results were supplied to first responders within a
206 few weeks, demonstrated that real-time results could soon be possible. Now with EMIT delivering data
207 from the space station, and with rapid correction to surface reflectance using new atmospheric models
208 (Thompson et al., 2018; Brodrick et al., 2023), material maps can be computed by Tetracorder within a
209 few minutes per scene. Correction of EMIT data to surface reflectance currently takes about 1.5 hours
210 on average on the EMIT team Beowulf cluster at JPL using 40 cores from 2 central processing units
211 (cpu). Using the 5.27c1 expert system from github, a Tetracorder run takes about 0.22 hour using one
212 cpu on the JPL computer (not including browse products which are not calculated on the EMIT team
213 computer). EMIT reflectance cubes and Tetracorder products are delivered to the public via the USGS
214 Land Surfaces Data Active Archive Center (LP-DAAC) typically within about one day of receipt of
215 data from the Space Station. Users can run a full Tetracorder analysis on an EMIT reflectance scene on
216 an I7-class cpu laptop (scenes with 1.5+ million spectra) in about 20 minutes, including browse
217 products. Combining rapid production of calibrated surface reflectance (or apparent reflectance), with
218 the atmospheric features removed, enables faster mapping of minerals and other components. As
219 computers become faster, we are now able to generate near real-time results for identifying and
220 mapping many compounds in imaging spectrometer data sets. On an I7 8th generation computer, over
221 2000 spectra per second are analyzed with the Tetracorder 5.27c1 expert system, making real time
222 analysis of spectra from a point spectrometer possible, and this is being done on the Carnegie Mellon
223 Zoë rover and will be discussed further below.

224 Tetracorder has been used to analyze data from all over the Solar System, including mapping ice and
225 other compounds on icy satellite surfaces in the Saturn (e.g., Clark et al., 2012 and references therein)
226 and Jupiter (Carlson et al., 1996) systems, minerals on Mars (e.g., Hoefen et al., 2003; Miliken et al.,
227 2008; Ehlmann et al., 2016 and references therein), and was critical in making the discovery of
228 widespread water on the Moon possible (Clark, 2009; Pieters et al., 2009). Tetracorder has been used

for mapping minerals on Earth (e.g., Swayze et al., 2000, 2002, 2009, 2014; King et al., 1995; Livo et al., 2007). It was used in assessing the environmental damage from the World Trade Center disaster (Clark et al., 2001, 2006), the 2010 Deepwater Horizon oil spill (mapping organics) in the Gulf of Mexico (Clark et al., 2010b), and mapping ecosystems, e.g., mapping vegetation species, bacteria and grizzly bear habitat in Yellowstone (Kokaly et al., 2003, 2007). Derivative software using an early version of the Tetracorder algorithms and expert system coded in IDL has been used to map minerals in a entire country (Kokaly et al., 2013) based on a methodology of Tetracorder before groups and cases were added.

The results from all the above and many more studies (excluding oil spills) have been incorporated into a master expert system, now 5.27c1. That system is now being used to map materials on Mars with the CRISM instrument, the Moon with Moon Mineralogy Mapper, M³, and the Earth – a diversity of environments that required, all with no changes to the expert system. The Clark et al. (2010) oil spill expert system was a separate expert system, and an improved version is under development (Swayze et al. In preparation). The Cassini Visual and Infrared Mapping Spectrometer (VIMS), orbiting Saturn from 2004 to 2017 used a custom expert system designed for cold ice signatures, and this expert system will be brought up to date for the Europa Clipper mission to Jupiter and Jupiter’s moon Europa, scheduled for launch in 2024.

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247 **History of Tetracorder**

The Tetracorder system (Clark et al., 2003), initially developed by a team at the U.S. Geological Survey over ~25 years (~1989 - 2014), is an expert system that can analyze multiple inputs to make identifications and decisions. The main development for Tetracorder is now centered at the Planetary Science Institute (2014 to date). The most recent version (5.x) of Tetracorder (Clark et al., 2015, 2016) employs inputs from other analyses, e.g., temperature and pressure, to further constrain identifications. The system was also modified such that the system automatically adapts to the available data, including spectral range and resolution, and available physical inputs. As a result, the same expert system can be used throughout the solar system in many different environments and with spectrometers that cover different spectral ranges.

Work on early versions of Tetracorder (1990s) concentrated on adding reference spectra and testing different strategies for which continua to use (e.g., Swayze et al., 2003). The main result of that work was a set of spectra and spectral feature definitions that worked between terrestrial atmospheric absorption bands. These workarounds were also valid for spectra from Mars and the Moon or other atmosphere-less bodies. Groups (different spectral wavelength regions) were introduced in 1993 with the mapping of the Summitville, Colorado mine region (King et al., 1995).

Fuzzy logic (Figure 7) was introduced in version 3.7 of the expert system on May 11, 2001. Rather than hard thresholds for parameters, like continuum thresholds, correlation coefficient thresholds and others, fuzzy logic enables a smoother transition from full acceptance and no acceptance.

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Over the summer of 2001, organics were added to the spectral library and to the Tetracorder expert system to aid in discrimination between organics and Mg- and Fe-OH bearing phyllosilicates that have similar position and shape absorption features in the 2.2 to 2.4- μm region. At the time, work was being done to map asbestos-bearing rocks and soils in support of environmental sites (Clark et al., 1998, 2003; Livo et al., 2002; Swayze et al.; 2004a, b). This work led to the ability for a rapid response to the World Trade Center disaster in September 2001 with version 4.0 of the expert system and included mapping asbestiform minerals in the debris (Clark et al., 2001, 2006, Swayze et al., 2006). To map such minerals in the World Trade Center debris, a new spectral “shoulderness” algorithm (Figure 8) was introduced on September 10, 2001, with expert system 4.0a5, just before the World Trade Center disaster on September 11. Testing the new algorithm and expert system was done the evening of September 10, but test results were not examined until September 12 (on September 11, offices were closed). The test results were excellent and used for the 9/11 environmental assessments (Clark et al., 2001, 2006), but the shoulderness algorithm was not well described until the 2010 Deepwater Horizon Gulf of Mexico oil spill in Clark et al. (2010). Shoulderness describes the asymmetric nature of an absorption prior to continuum removal, and the shoulderness value is largely independent of abundance and particle grain size (unless the absorption becomes saturated).

The main work on Tetracorder shifted to the Planetary Science Institute in 2014 with Tetracorder version 5. From 2014 to 2019 work mainly included adding more groups, increasing the spectral range further into the infrared, and including groups that cover spectral regions not well sampled through the Earth’s atmosphere but are spectrally detectable wavelength ranges in the lab and on airless (e.g., satellites, asteroids), or low-pressure atmospheric (e.g., Mars) bodies. The groups and cases in the 2023 expert system 5.27c1, currently on Github, are listed in Table 1.

Table 1. Current and planned groups and cases, Tetracorder Expert System 5.27c1

group 0: catch for other declared groups
group 1: electronic absorptions UV to $\sim 1\text{-}\mu\text{m}$ region
group 2: 2 to 2.5- μm region narrow absorptions (vibrational absorptions)
group 3: vegetation detection
group 4: broad absorptions in the 1.5- μm region
group 5: broad absorptions in the 2- μm region
group 6: 2.5- μm region
group 7: 2.7 to 3- μm OH region
group 8: 2.7 to 2.8- μm OH region narrow bands
group 9: UV (0.1 - 0.3 μm), Future
group 10: 3.5- μm region curved continua
group 11: 3.5- μm region linear continua
group 12: unused, Future
group 13: 1.3 to 1.4- μm OH narrow
group 14: 1.4 to 1.5- μm OH
group 15: 1.5- μm OH
group 16: 1.5 to 1.6- μm OH, Future

309 group 17: 1.7- μm region CH and water, Future
 310 group 18: 1.8- μm region, Future
 311 group 19: 1.9 to 2- μm water and ice
 312 group 20: the search for rare-earth oxides
 313 group 21: the search for rare-earth oxide Neodymium
 314 group 22: the search for rare-earth oxide Samarium
 315 group 23: 3.8- μm region includes OD stretches, Future
 316 group 24: 4- μm region
 317 group 25: 4.1- μm region, Future
 318 group 26: 4.25- μm CO₂ trapped, ice
 319 group 27: 4.5- μm region includes sulfates
 320 group 28: 5- μm region includes silicate overtones, Future
 321 group 29: 6- μm region, includes H-O-H bends, Future
 322 group 30: 7 to 8- μm region, Future
 323 group 31: 8 to 10- μm region, Future
 324 group 32: 10 to 12- μm region, Future
 325 group 33: 12 to 14- μm region, Future
 326 group 34: 14 to 16- μm region, Future
 327 group 35: 16 to 19- μm region, Future
 328 group 36: 19 to 22- μm region, Future
 329 group 37: Experimental: search for methane plume 2.3- μm signatures
 330 group 38: Experimental: search for CO₂ gas, 2- μm signatures
 331
 332 case 1: Vegetation red edge shift
 333 case 2: Vegetation spectral type
 334 case 3: Vegetation 0.9- μm -band depth (water in vegetation)
 335 case 4: Vegetation 1.2- μm -band depth (water in vegetation)
 336 case 5: Vegetation 1.4- μm -band depth (water in vegetation)
 337 case 6: Epidote-Chlorite-Calcite mixture series
 338 case 7: Carbonate 2.3 plus 2.5- μm feature detection
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340 **Tetracorder Algorithms**

341
 342 How Tetracorder operates is dictated by instructions in the expert system, also called the Tetracorder
 343 command file. At its highest level, Tetracorder identifies materials by comparing a remotely sensed
 344 observed spectrum (the unknown) to a large library of spectra of well-characterized materials, but we
 345 do so using several innovations to maximize accuracy and performance. The Clark et al. (2003) study
 346 was based on Tetracorder 3.5. This paper will review the main points of the previous paper for context
 347 and the added innovations since then.
 348

349 While we describe the methodology used now and in the history of Tetracorder, we stress that this is
 350 not the only way Tetracorder can be commanded; it is the way we have developed the system using our
 351 collective decades of experience. Tetracorder could be commanded differently. For example, given
 352 the Spectral Angle Mapper (SAM) algorithm, Tetracorder could be commanded to produce the same
 353 output as SAM in the commercial software ENVI.
 354

We developed the expert system to isolate and analyze spectral features, and to group these analyses for different spectral regions (Table 1). Specifically, we target diagnostic absorption features that are unique to particular materials in shape (variation in intensity with wavelength over a narrow interval) and position. Between diagnostic features are portions of the spectrum that contain little information specific to the material of interest, but being relatively more transparent, are susceptible to absorption by other components in the spectrum of the measured surface. The focus on diagnostic spectral features in analyses of natural scenes is critical because mixtures which obey nonlinear systematics (e.g., coatings, intimate mixtures, solid solutions) are common in the natural environment and frustrate simple matching of spectra (Clark et al., 2003 and references therein).

In Tetracorder, each comparison of an unknown to a reference spectrum is highly tailored to the chemistry of the reference material by focusing on diagnostic spectral features (Figures 3a and 3b). Tetracorder identifies materials by comparing them to a large spectral library and continuum-removing and comparing the diagnostic spectral features between the unknown and library known spectra. Material spectral signatures are most significant over their diagnostic wavelength ranges and a different wavelength range may allow detection of additional materials in a remotely sensed spectrum (Clark et al., 2003). For example, the red spectrum in Figures 3a and 3b shows absorptions at the shorter wavelengths due to hematite and at longer wavelengths due to kaolinite. Tetracorder mitigates false identifications caused by spectrally similar materials by quantitatively comparing the degree of similarity of an unknown to a set of spectrally similar reference spectra. Tetracorder mitigates coincidental false alarms permitted by our specific implementation of our shape-matching algorithm by including ancillary information, including constraints on spectral structure, and physical limits such as pressure and temperature stability (described below). Finally, Tetracorder is not forced to provide a solution; it allows “No Answer” as an answer. The “No Answer” level strategies were guided using information from Swayze et al. (2003) who studied the identification accuracy as functions of sampling interval, bandpass width, and signal-to-noise ratio of spectral features.

Continuum Removal Algorithm. In order to identify a spectral feature by its wavelength position and shape, it must be isolated from other effects, such as reflectance-level changes and slopes due to other absorbing (or emitting) materials. The first step in such isolation is continuum definition and removal (Clark and Roush, 1984). In the Clark et al. (2003) paper, Tetracorder 3.5 only applied linear continua. Tetracorder 5 was improved to use curved, as well as linear continua. Continuum removal examples are shown in Figures 3a, 3b, 4a, and 4b for several spectral features. A continuum is removed by division (Figure 5) in reflectance, transmittance, and emittance spectra because of exponential absorption and scattering processes (Clark and Roush, 1984). Conversely, a continuum should be removed by subtraction with absorbance or absorption coefficient spectra because multiple components are additive.

Straight-line continua can have a disadvantage when the feature depth is weak and superimposed on a larger curved background continuum. Such situations can induce false positives or false negatives (Figure 6). Tetracorder allows a 4-point continuum to be defined (Figures 6, panels C and E), for example the two-point continuum shown in Figures 3 – 5, plus an additional 2 wavelength intervals, one on each side. A cubic spline is fit through the four points and the spectrum is divided by the spline (Figure 6). The disadvantage of the 4-point continuum is that if one continuum interval falls in another absorption band, it can cause wild swings in the fitted spline and induce both false positives and false negatives. In a future version of Tetracorder, we plan on including an upper hull continuum, but this is computationally expensive compared to existing calculations. We have limited the use of curved

continua in Tetracorder 5.27 to spectral features and regions where interference from other absorptions is less likely.

To isolate and identify absorption features, the continuum removal algorithm first removes a continuum from a library reference spectrum and from the observed spectrum using a wavelength interval on each side of the absorption feature that is to be mapped (Figures 3a, 3b, 4a, and 4b). This can be described mathematically by:

$$L_c(\lambda) = L(\lambda) / C_l(\lambda) \quad \text{and} \quad O_c(\lambda) = O(\lambda) / C_o(\lambda), \quad (\text{eqns 1a and 1b})$$

where $L(\lambda)$ is the library spectrum as a function of wavelength, λ , O is the observed spectrum, C_l is the continuum for the library spectrum, C_o is the continuum for the observed spectrum, L_c is the continuum-removed library spectrum, and O_c is the continuum-removed observed spectrum.

The Shape-Matching Algorithm was described in detail by Clark et al., (2003).

The apparent depth of an absorption feature, D , relative to the surrounding continuum in a reflectance or emittance spectrum (Clark and Roush, 1984) is:

$$D = 1 - R_b/R_c \quad (\text{eqn 2})$$

where R_b is the reflectance at the absorption-band center (the minimum in the continuum-removed feature), and R_c is the reflectance value of the continuum at the wavelength of the band center (Figure 5). For an absorption feature, depth, D , is positive. Tetracorder's expert system can also define "emission" features, in which case D is negative. Emission is used loosely here, as any upward-convex feature after continuum removal is considered an "emission" feature. Whether a spectral feature is declared an absorption or emission is dependent on the continuum-removed library reference feature. Identification of a material can use a combination of absorption (positive depth value) and "emission" (negative depth value) features.

The Tetracorder shape matching algorithm is carried out in a two-step process. First, the local spectral slope (the "continuum") is estimated and removed both from the reference and observed (unknown) by fitting the continuum over a diagnostic spectral region (or regions) of these spectra, then dividing these continuum lines out of the observed and reference spectra (equation 1a, 1b).

Because of the near-universal weakness of remotely sensed features relative to those of pure materials, the intensity of the features must also be normalized prior to comparison. The Tetracorder feature-fitting algorithm normalizes the intensity of the reference to that of the unknown by changing the spectral contrast of the continuum-removed reference over the diagnostic range to best match the continuum-removed unknown spectrum over the same range (Figures 4a and 4b). The continuum-removed depth (which we call "spectral contrast") of an absorption feature in a reference library spectrum can be modified by a simple additive constant, k , so that a shape match between the unknown and reference feature can be calculated. We simultaneously perform a comparison between reference and unknown by determining the contrast that maximizes the correlation between reference and unknown. Equation 3 governs this process:

$$L_c' = (L_c + k) / (1.0 + k), \quad (\text{eqn 3})$$

where L_c' is the modified, continuum-removed spectrum that best matches the observed spectrum. If k is less than zero, feature strength (i.e., spectral contrast) increases; if greater than zero, feature strength decreases. Equation 3 can be rewritten in the form:

$$L_c' = a + bL_c, \quad (\text{eqn 4})$$

where

$$\begin{aligned} a &= k / (1.0 + k), \text{ and} \\ b &= 1.0 / (1.0 + k). \end{aligned} \quad (\text{eqn 5})$$

Equation 4 linearizes the spectral feature strength problem, so a direct solution can be found without iteration. In Equation 4 we want to find the a and b that gives a best fit to the observed spectrum O_c . The solution is found using standard linear least squares:

$$\begin{aligned} a &= (\Sigma O_c - b \Sigma L_c) / n, \\ b &= \frac{\Sigma O_c L_c - (\Sigma O_c \Sigma L_c) / n}{\Sigma L_c^2 - (\Sigma L_c)^2 / n}, \end{aligned}$$

and

$$k = (1-b)/b, \text{ also: } k = a/(1-a) \quad (\text{eqn 6}).$$

where n is the number of spectral channels in the fit.

Finally, the correlation coefficient, F , to the fit is derived for that feature:

$$\begin{aligned} b' &= \frac{\Sigma O_c L_c - (\Sigma O_c \Sigma L_c) / n}{\Sigma O_c^2 - (\Sigma O_c)^2 / n}, \\ F &= (b b')^{1/2}. \end{aligned} \quad (\text{eqn 7})$$

The *fit*, F , is a measure of how well the spectral features match. Tetracorder uses the highest fit value to decide which spectral feature is best matched by a given library reference feature, independent of the feature depth, and thus, independent of the abundance of the material. Figures 4a and 4b illustrate graphically and numerically the matches between a remotely sensed spectrum and several Tetracorder reference library mineral spectra.

D, M, O, W Spectral Feature Importance. Feature importance (as judged by the expert spectroscopists) must be assigned to each library spectral feature to be matched by Tetracorder. Not all features are equally important in spectrally identifying a material.

496
497 D = A Diagnostic feature that must be present. If there are multiple, defined diagnostic features, only
498 one of those diagnostic features must be present. The fit, depth, and fit*depth must be above
499 thresholds.
500
501 M = A “Must have diagnostic feature,” unconditionally. If only one diagnostic feature is defined,
502 there is no difference between D and M designation. But if there is more than one diagnostic feature
503 defined, the M designation requires that feature to be present even if there are other diagnostic, D,
504 features detected. The fit, depth, and fit*depth must be above thresholds.
505
506 O = An Optionally present feature. If an optional feature is not detected in the unknown’s spectrum,
507 the reference spectrum’s fit and depth are set to zero but the material might still be identified by the
508 presence of other absorption features, though the weighted fit may lower the score enough to cause that
509 material to be rejected. Use of optional features should be used sparingly. Swayze et al. (2003) showed
510 that in some cases, including optional features may negatively impact identification when those
511 optional features are weak relative to the background noise in an unknown’s spectrum.
512
513 W = A weak feature must be present, but the feature’s calculated area is set to zero so it has no effect
514 on the fit, unless there is no detection. Noise can mask a weak band’s presence reducing detection even
515 when a strong diagnostic band is present, so it is used only when necessary.
516
517 There is a speed advantage to listing diagnostic features first because if diagnostic features (D or M)
518 are not detected, there is no point in computing O and W features.
519
520 D vs M details. The D is a diagnostic feature. When there are multiple diagnostic features defined,
521 only one is needed to be enabled for a detection. In the case of azurite which has two important
522 features, both are needed, but the band between 0.45 and 1.3 μm is more important than the feature
523 near 2.3 μm , so it is marked M and listed first in the expert system entry for that mineral.
524
525 If one diagnostic (D) feature is disabled because of poor calibration over its spectral region, a second, if
526 present, (or third) diagnostic (D) feature will still allow detection. This approach is different than if all
527 diagnostic features are enabled, because in this case if one feature is not present (i.e., feature strength is
528 zero or fit too low) then the material will not be found. On other words, all enabled diagnostic features
529 must be present to allow identification.
530
531 The must be present (M) feature importance solves the problem of a disabled diagnostic (D) feature,
532 requiring all M-declared features to be enabled and present. If one M feature is disabled, the material
533 identification is disabled. This strategy was required for group 1 azurite, for example. The EMIT
534 spectral range, after deleting intervals where the corrections for terrestrial atmospheric water
535 absorptions were unstable, several minerals had features defined as diagnostic but were disabled for
536 EMIT resulting in false identifications. Changing those required diagnostic to the must have (M)
537 category solved the identification problem. For example, consider a mixture of chlorite + muscovite,
538 vs goethite + muscovite. While the muscovite 2.2 and 2.3- μm features are diagnostic of muscovite,
539 what the muscovite is mixed with is dependent on the absorptions in the 1- μm region. Those 1- μm
540 absorptions need to be marked must have (M) features because if there were no 1- μm features present,
541 the mixture could be erroneously identified.
542

Weighted Results Algorithm. Tetracorder uses the relative areas (including the depths and widths) of continuum-removed-reference spectral features to compute a weighted *fit* that is used in the decision process. The continuum removal and feature *fits* to multiple features in a spectrum are illustrated in Figures 3a, 3b, 4a, and 4b. Three parameters for each spectrum are computed (equation 8): weighted *fit*, F_w , weighted *depth*, D_w , and weighted *fit times depth* ($fit*depth$), FD_w . They are computed by weighting the relative areas of the absorption features of the reference library spectrum:

$$\begin{aligned} F_w &= \sum c_i F_i, \\ D_w &= \sum c_i D_i, \quad \text{and} \\ FD_w &= \sum c_i F_i D_i, \end{aligned} \quad (\text{eqn 8})$$

where “i” is the feature number, c_i is the relative fractional area of library reference features between each feature and its continuum:

$$\sum c_i = 1.0. \quad (\text{eqn 9})$$

F_i , D_i are the *fits* (the correlation coefficients) and *depths* of the corresponding features. The feature *depths* and relative feature areas are calculated from the fitted library reference features. The relative feature area is found by integration of the continuum-removed feature (the area between the continuum-removed feature curve and 1.0) divided by the sum of the areas of all features analyzed for each reference material.

Not-Feature Algorithm

A “not” feature is a feature that should not be present to identify a particular material. For example, both muscovite and illite have a ~2.2- μm absorption feature that is very close to the same position, width and shape as an absorption feature in a montmorillonite spectrum, but both muscovite and illite also have a 2.3- μm feature while montmorillonite does not (Figure 3b). In the identification of montmorillonite, the 2.2- μm absorption feature is diagnostic but there also must not be a 2.3- μm muscovite/illite feature. Therefore, in the expert system’s feature definitions for montmorillonite entries, a pointer to the muscovite/illite 2.3- μm absorption feature is defined and the presence of that feature relative to the strength of the 2.2 feature depth is defined. If a 2.3- μm muscovite/illite feature is found above that relative depth and above the fit threshold, montmorillonite cannot be identified in the spectrum.

Continuum Thresholds

Continuum thresholds are used where a pure material has a limited observed reflectance. For example, green vegetation with significant water content has low reflectance in the 2 to 2.5- μm region, and relatively low reflectance in the blue/ultraviolet. If continuum thresholds are defined, and the observed continua fall outside those thresholds, that material identification is rejected.

Continuum thresholds are also set for minimum reflectance values below which noise dominates. These values are best set for the performance of individual spectrometers. For that case, the continuum

589 thresholds are made variables in the expert system and those variables can be simply modified in one
590 location to customize specific spectrometers.

591

592 Fore example:

593 ct n1 n2 where ct means the minimum and maximum center continuum thresholds,

594 lct n1 n2 where lct means the minimum and maximum left continuum thresholds,

595 rct n1 n2 where rct means the minimum and maximum right continuum thresholds,

596 and where n1 and n2 are reflectance levels.

597

598 **Spectral Constraint Algorithms and Fuzzy Logic**

599

600 **Fuzzy Logic Algorithm**

601

602 Fuzzy logic modifies the fit values so that it is not a simple on or off hard limit. The fuzzy logic
603 algorithm is described in Figure 7. Fuzzy logic can include either 2 or 4 parameters (Figure 7). With
604 two values, it is a lower limit, with 4 it is a lower and upper limit. Fuzzy logic is a way to degrade a fit
605 value as the probability of a spectral parameter indicating the match to a specific material is less likely.
606 There is no hard rule; these levels are set through experience of the experts programming the expert
607 system after running tests with multiple spectra and imaging spectrometer data sets covering different
608 geologic environments.

609

610

611 **Continuum Ratio Algorithms with Fuzzy Logic**

612

613 lct/rct> n1 n2 where n1 n2 are positive real numbers

614 rct/lct> n1 n2 where n1 n2 are positive real numbers

615

616 **Shoulderness Algorithms with Fuzzy Logic**

617

618 Shoulderness (Figure 8) describes the continuum level relative to the spectral feature band bottom.
619 There are 4 potential conditions, two each for right shoulderness (rcbbbc), and two for left shoulderness
620 (lcbbrc). The Tetracorder keywords are:

621

622 rcbbbc> n1 n2 where n1 n2 are the fuzzy logic values,

623 rcbbbc< n1 n2 where n1 n2 are the fuzzy logic values,

624 lcbbrc> n1 n2 where n1 n2 are the fuzzy logic values, and

625 lcbbrc< n1 n2 where n1 n2 are the fuzzy logic values.

626

627 **Reflectance times Band Depth with Fuzzy Logic**

628

629 A potential spectral match can be constrained by reflectance times band depth, r*bd, with fuzzy logic.

630

631 r*bd> n1 n2 where n1 n2 are the fuzzy logic values.

632

633 **Feature Ratio Constraints with Fuzzy Logic**

634

635 Spectral feature band depth ratios can be constrained, Tetracorder keyword = fratio.

constraint: fratio: $a / b = n1 \ n2 \ m1 \ m2$ where a, b = spectral feature number

Fit Constraints Algorithms with Fuzzy Logic

There are nine constraints on the output fit, depth and fit*depth images, each with fuzzy logic:

constraint: FIT> $n1 \ n2$ fit threshold, apply to fit value,
constraint: FITALL> $n1 \ n2$ fit threshold, apply to fit, depth, fit*depth values,
constraint: DEPTH> $n1 \ n2$ depth threshold, apply to depth value,
constraint: DEPTHALL> $n1 \ n2$ depth threshold, apply to fit, depth, fit*depth values,
constraint: DEPTH-FIT> $n1 \ n2$ fit threshold, apply to depth value,
constraint: FD> $n1 \ n2$ fit*depth threshold, apply to fit*depth value,
constraint: FDALL> $n1 \ n2$ fit*depth threshold, apply to fit, depth, fit*depth values,
constraint: FD-FIT> $n1 \ n2$ fit threshold, apply to fit*depth value, and
constraint: FD-DEPTH> $n1 \ n2$ depth threshold, apply to fit*depth value.

If the parameter, e.g. band depth, fit, or fit*depth value falls outside the allowed range the indicated parameters are set to zero. If it is within the $n1$ to $n2$ range, it is decreased by linear interpolation as indicated in Figure 7. For example, if the correlation coefficient, the fit, is 0.8 and FITALL> $n1$ and $n2$ values are 0.7 and 0.9, this falls mid-way between 0.7 and 0.9, and the fuzzy logic multiplier would be 0.5. Then the fit, depth, and fit*depth values would each be multiplied by 0.5. These modified values would next be used in comparison with those from other materials to determine the best match.

Physical Constraints Algorithm with Fuzzy Logic

The temperature and pressure range over which a material is stable, or metastable can be constrained. For example, liquid water is stable over the temperature range 0 to 100° C at Earth's atmospheric pressure. On Mars liquid water is not stable due to the low atmospheric pressure. Therefore, we constrain liquid water with the following fuzzy logic limits, ($n1, n2, m1, m2$ defined in Figure 7):

Temperature: C $n1 \ n2 \ m1 \ m2$
Pressure: bar $n1 \ n2 \ m1 \ m2$

For example:

Temperature: C -10 -5 99 105
Pressure: bar 0.10 0.20 98 99.

Setting broad limits beyond the actual stability field is done to reflect uncertainty in the estimated temperature. If we had precise temperature and pressure for every pixel in a scene, the values could be more restrictive. But even with precise temperature, there could be sub-pixel effects. For example, a patch of snow could be sub pixel, with the other materials in the pixel warmer and above the freezing point. Including some additional range helps to account for these problems. This model is simple but effective. Temperature can be specified in Centigrade or Kelvin.

683 To be more precise, a phase diagram needs to be encoded. This simplistic method currently in place
684 adequately (and correctly) rejects liquid water on Mars, the Moon, and other airless bodies. It does not
685 do as well for discriminating between liquid water and ice in a terrestrial scene with mountains and
686 valleys where temperatures can cover a large range and where there is no temperature information with
687 the imaging spectrometer data.

688
689 Not all imaging spectroscopy data has temperatures and pressures measured. The user determines at
690 run time the plausible ranges of temperature and pressure for the data set. For example, the Moon may
691 have temperatures in the 200 to 400 Kelvin range, and pressure essentially zero. A typical terrestrial
692 scene with desert and mountains could be in the range -20 to 40 C. With such large ranges of plausible
693 temperatures, liquid versus solid water could not be determined by temperature, but pressure
694 constraints could restrict the solution, with the Moon rejecting liquid water. Some minerals shift
695 absorption band positions with temperature, and the temperature constraints can be used to restrict
696 solutions. For example, ice measured at 80 Kelvin is plausible to Saturn's rings and satellites, but not
697 for terrestrial snowpacks. The temperature constraints help determine solutions that are plausible for
698 the physical environment.

699

700

701 **Normalized Vegetation Red Edge Shift, NVRES**

702

703 The wings of absorption bands change with a variety of conditions. For example, see Figure 2, top, and
704 notice that the width of absorptions change with particle size, which reflects changing scattering and
705 mean optical path length through the material. Now look at only the right half of the absorptions in
706 Figure 2, top. The absorption's edge position from the absorption minimum to the continuum changes
707 with particle size.

708

709 The position of an absorption edge, e.g., the chlorophyll absorption near 0.7 μm can also shift with
710 chlorophyll content, vegetation type, and health (e.g., Clark, 1999, Clark et al., 2003 and references
711 therein).

712

713 In vegetation, the chlorophyll absorption edge is near 0.7 μm (Figure 9a, 9b) and because there are
714 other absorptions at shorter wavelengths, the short wavelength side of the absorption is not seen well.
715 Therefore, the red-edge position is used. The Tetracorder NVRES algorithm normalizes the depth from
716 0.75 to 0.68 μm with the reference spectrum, ratios to the reference spectrum, and uses the shape-
717 matching algorithm described above to determine the magnitude of the shift relative to the reference
718 spectrum using the ratio, and reference ratios stored in the spectral library. In order not to be confused
719 by mineral absorptions, the red-edge position is only determined after a chlorophyll absorption has
720 been identified successfully, and then a special case is triggered to run the NVRES algorithm. In the
721 current expert system, a lawn-grass spectrum is used that has the strongest chlorophyll absorption in the
722 reference library and the longest wavelength for the red-edge position.

723

724

725 **Example Tetracorder Output and Expert System Entry**

726

727 Example Tetracorder output is shown in Figures 10, 11a – 11g. A single mineral detection is shown in
728 Figure 10. Figures 11a – 11d show mineral products, coded by color, and Figures 11e – 11g show

729 vegetation products. The vegetation products in Figures 11e – 11g are only calculated as special cases
730 after chlorophyll has been detected. The red edge position is shown in Figure 11g.
731

732 An example Tetracorder expert system entry is shown in Table 2. An entry starts with a group or case
733 number. Table 1 shows an entry for Group 1. The second line turns on or off the entry. If you want to
734 experiment with effectiveness of an entry, and turn it off, it is simple to change to “use= no” instead of
735 deleting all the lines for that entry. The “udata” line tells what the analysis should cover, and in this
736 case, the data should be in reflectance. Future uses for this variable could be emittance and data
737 converted on the fly to what is needed, e.g., convert emittance data to reflectance if the library entry is
738 in reflectance. But Tetracorder 5.27 currently has all udata in reflectance.
739

740 The convolve line is a placeholder for the future to run spectral library convolutions during analysis.
741 Early experiments showed we need the convolved libraries for post Tetracorder analysis and
742 comparisons in scientific papers, so this convolution is currently not done. The placeholder remains in
743 case a future spectrometer has varying wavelengths within a scene (e.g., large spectral smile) where
744 such convolutions would become necessary.
745

746 Preratio and preprocess lines are used in some cases, for example, in the vegetation red-edge position
747 calculations. In such calculations, the unknown is divided by a reference spectrum in the preprocess
748 step and the shape and magnitude of features in the ratio are analyzed.
749

750 The algorithm keyword selects the algorithm to be applied, and tricorder-primary applies equations 1 –
751 9. ID= needs to be a unique identifier. It can be the same as the output base file name.
752

753 The “define library records” defines which library spectra to use. Tetracorder 5.27 can use up to three
754 reference library spectra for different spectral features, and would be coded as spectrum a, b, or c. For
755 example, one reference spectrum could be from a Visible-Near-IR spectrometer, (a), and another from
756 an FTIR spectrometer in the further infrared (b). Then the “a” or “b” selects which reference spectrum
757 to use for each feature. The spectral ID is the specpr format convolved library reference file and the
758 record number where the spectrum is found. Spectral libraries use the fixed record length specpr
759 format, but different length spectra can span across different numbers of records. The scripts that build
760 the convolved library pad the records to keep all spectra up to a certain number of channels with the
761 same record number. The SMALL keyword is for spectra up to 2171 channels. Next is an information
762 title.
763

764 The “define features” section contains the feature definitions and constraints on those features. The
765 “define constraints” are constraints applied to the weighted fit, weighted depth and weighted fit times
766 depth results. The “define output” section defines which files to output in imaging mode, the integer
767 bits per channel (8 or 16), and how to scale the floating-point results to the integer image data. In
768 single spectrum mode, the “define output” section is not used and the floating-point results are
769 reported.
770

771 Finally, the “define actions” block describes what analyses or other tasks to do next if this material
772 passes all the tests and is identified as the best answer for this group. The sound1 action announces the
773 answer in single spectrum mode. The idea for sound is when operating a spectrometer in the field,
774 Tetracorder can announce the results so that the operator does not have to look at a computer screen
775 that can be difficult to see in bright sun.

776

777 **Table 2. Example Tetracorder 5.27 Expert System Entry**

778

779 group 1

780 use= yes \# yes or no, if no, skip this entry.

781 udata: reflectance

782 convolve: no

783 preratio: none

784 preprocess: none

785 algorithm: tricorder-primary

786 ID=hematite.fine.gr.gds76

787

788 define library records

789 a SMALL: [sprlb06] 744 d \# file ID, rec no. 1 to 2171 channels

790 endlibraryrecords

791 \#=-=-=-=-=-=-=-=-=- TITLE=Hematite.02+Quartz.98 GDS76 W1R1Ha

792 [DELETPTS]

793 Fe3+ hematite fine grain + qtz GDS76 \# output title

794

795 define features

796 f1a DLw 0.4400 0.4550 0.6117 0.6315 ct [CTHRESH4] rct/lct> 0.9 1.1

797 f2a OLw 0.7375 0.7645 1.0500 1.0700 ct [CTHRESH4] rct/lct> 0.4 0.6

798 endfeatures

799

800 define constraints

801 constraint: FD-FIT>[GLBLFDFIT] DEPTH-FIT>[GLBLDPFIT]

802 constraint: FITALL>[GLBLFITALL]

803 endconstraint

804

805 define output

806 output=fit depth fd

807 fe3+_hematite.fine.gr.gds76 \# Output base file name

808 8 DN 255 = 0.5000

809 compress= zip

810 endoutput

811

812 define actions

813 action: sound1

814 action: none

815 endaction

816

817 In the define features section, features to be analyzed begin with “f” followed by a feature number.

818 Next is D, O, W, or M for diagnostic, optional, weak, or must have, as defined above.

819 Next is L or C for linear or curved continua. The “w” means the following continuum

820 points are in wavelength (same units as the wavelength file).

821 After the continuum wavelengths are feature constraints.

Post-Tetracorder analysis of imaging data and browse products

Work on post-Tetracorder analyses has been improved significantly starting in 2015 and continues to date. The problem with imaging spectroscopy is the potentially overwhelming number of identified products. For each Tetracorder reference material, three image products are produced: a band depth image, a correlation coefficient image (called the fit), and a fit*depth image. Each of these products are weighted by the area of the spectral features used for the identification. With hundreds of reference spectra, the end-user can be overwhelmed by the many hundreds of output image products. Previous to circa 2014, each of the output images needed to be brought into an image processing program and stretched to see what was found. This step took days of intense effort. To alleviate this problem, browse products that pre-stretch the fit*depth images are automatically created. The stretch uses the same equations across different scenes, so that results from multiple scenes could be mosaicked together.

Tetracorder expert system 5.27c1 contains 639 reference spectra over 23 active groups and 7 cases (Table 1). With 639 reference spectra, Tetracorder generates 639 times 3, or 1917 output image files (*.fit, *.depth, and .fd for fit * depth). Each of these files are linear 8-bits/pixel images (Tetracorder also can output 16-bit files, but we have found 8-bit to be adequate). Except for deep absorption bands, an output data number, DN, level of 255 corresponds to band depth or fit * depth of 0.5. This gives a band depth resolution of 0.00196. These are settings in the expert system setup command file and can be changed if the need arises, as described above.

With so many image files to evaluate, several quick-look reference files are created. A file called “results” lists how many pixels were identified for each material. A geospatial cluster analysis is done and a file named “results.cluster.sorted” is generated that puts the top scores for each group listed first, with both quantitative cluster values and a qualitative descriptor to indicate the most significant matches that likely are real detections, not noise. Next, for each fit * depth file, the linear data is tone mapped with the variable gamma equation similar to the tone curve employed in consumer digital cameras:

$$x' = x * 7.5 * 0.08^{\sqrt{x/400}} \quad (\text{eqn 10})$$

where x' is image brightness on a 0 to 255.0 scale, and x is a 32-bit floating point number for the calculation, which is then converted to an 8-bit integer for the output image. As seen by eqn 10 and Table 3, the tone mapped values boost faint signals at the expense of compressing the brightest signals. The constants were determined empirically by running equations with different constants and finding ones with good representation of mapped results through visual judgment for the browse products. This equation is a little less aggressive than what is performed on consumer digital camera images in terms of boosting the low end and compressing the high end.

865 **Table 3 Tone map values from Equation 10**

x	x'
1	7
10	50
50	154
100	212
150	240
200	251
255	255

866

867 The tone-mapped fit * depth image is written as a gif-format image, thus producing another 639 image
868 files with the 5.27c1 expert system. This approach still generates a lot of files to evaluate, and locating
869 mapped pixels on a black background often does not show context, thus another set of browse images
870 is produced: the mapped pixels for each identification converts the gif image to red and overlays it on a
871 gray-scale background (another 639 images). Sometimes it is hard to see the red pixels on the gray
872 background, so another set is made by putting the red on gray image alongside the gray scale gif image,
873 converting the set to RGB and outputting a jpeg format image (Figure 10), another set of 639 images.

874

875 Many reference materials are not found in a given image cube, so many images of these reference
876 materials are zero (non-detect) resulting in completely black images. Having many images with no
877 detections also takes time to review, so another set of images that only include some detections, like
878 shown in Figure 10, are copied into another set of directories, results.dual.group.*.notzero. These
879 directories contain only images of detected reference materials.

880

881 The final set of browse products are summary products, where multiple materials are colored
882 differently and put on images beside a visible color RGB image. These images are located in
883 directories labeled: color.results, color.results+labels, and color.results+labels-jpegs. These images are
884 png format except for the jpeg-specific images that are smaller and therefore easier to email. Examples
885 are shown in Figures 11a-g and Figures 12a – 12d, 13a – 13d, and 14. The colored materials maps are
886 also suitable as figures in scientific reports.

887

888

889

890 **Real-Time Single Spectrum Mode**

891

892 Tetracorder has two modes. The first, discussed above, analyzes an imaging spectrometer data cube,
893 called “Cube Mode.” The second mode analyzes individual spectra, called “Single Spectrum Mode”
894 (referred to here as SSM). SSM can have 5 output modes shown in Table 4.

895

896 **Table 4. Tetracorder Single Spectrum Output Options**

Option	Action
0	(default) one-line answers only
1	abbreviated answers only
2	weighted fit + answer
3	for full diagnostic output: (individual fits, weighted fits and answer)
4	one-line answers to screen, and full diagnostic output to results file

897

898 Options 0 and 1 provide quick results for the final answer with option 1 showing more information
899 about the reference spectrum best match over option 0.

900

901 Option 2 shows the weighted fit values for each reference material plus the option 0 output.

902

903 Option 3 provides the full diagnostic output, with fit, and depth values for each spectral feature for each
904 reference spectrum, then the weighted result of all reference spectra and rejection decisions. Use this
905 output (or number 4) to understand how Tetracorder makes decisions.

906

907 Option 4 is option 3 written to the file called “results,” and the option 0 results are written to the
908 terminal window. Use this output (or number 3) for understanding how Tetracorder makes decisions.

909

910 In addition to the above options, single spectrum mode can operate on a spectrum one at a time, or
911 watch a growing file as new spectra are added. With the growing file option, option 4 is the preferred
912 mode because the use of other options writes so much information to the terminal that it goes by too
913 fast to read with about 1900 lines of diagnostic output. Option 4 provides the basic answers (about 16
914 to 40 lines depending on the spectrometer spectral range), and the full diagnostic output written to the
915 results file. Example output is shown in the SSERVI TREX section below.

916

917 **EMIT**

918

919 The NASA Earth Surface Mineral Dust Source Investigation (EMIT), located on the International
920 Space Station (ISS) is an imaging spectrometer covering the 0.38 to 2.5- μm region in 285 bands with
921 spectral resolution of 0.008 to 0.009 μm Full Width at Half Maximum (FWHM). There are 1280 pixels
922 cross track, approximately 60 x 60 meters per pixel, giving a width of about 77 km. The exact width
923 and pixel footprint is dependent on the exact height of the ISS. Each scene has the atmospheric
924 absorptions and scattering removed (Thompson et al., 2018; Brodrick et al., 2023), and the solar
925 radiance corrected to derive apparent surface reflectance. The surface reflectance image cubes are
926 analyzed by Tetracorder to deliver maps of minerals for use in climate change models to predict the
927 radiative forcing impact of mineral dusts. But Tetracorder computes more than the small subset of 10
928 minerals studied by the EMIT science team, including hundreds of minerals, vegetation (spectral type,
929 water content, red-edge position of the chlorophyll absorption at $\sim 0.7 \mu\text{m}$, and non-photosynthetic
930 vegetation), water, snow and melting snow, man-made materials, and some environmental materials.
931 Example standard products are shown in Figures 12 – 14.

932 Example EMIT mineral maps are shown in Figures 12a, 12b, 12c, and 12d. Each color on these maps
933 may represents multiple Tetracorder identifications that could be further split if the science need arises.
934 For example, examine the green coded illite/muscovite in Figure 12c. The muscovite absorption near
935 2.2 μm shifts with aluminum substitution in the octahedral layer of the muscovite structure. This
936 changing composition is shown in Figure 12d where low to high octahedral layer aluminum content is
937 coded in different colors.

938 Vegetation, water, contaminants in water and snow and melting snow are assembled into a colored
939 materials map, an example of which shown in Figure 13a. The colors in this browse product are
940 combinations from multiple Tetracorder entries and could be split further if needed.

941 Vegetation spectral type for the same scene as in Figure 13a is shown in Figure 13b. Only empirically
942 determined spectral type rather than specific vegetation species is possible to map in the general case
943 because the chlorophyll changes as a function of growing season, plus soil and water characteristics,
944 adding complexity to species identification. The vegetation red-edge position is shown in Figure 13c
945 and the water content in the vegetation is shown in Figure 13d.

946 Vegetation, water, ice and snow and melting snow for a different EMIT scene are shown in Figure 14.
947 Here we see that at high elevations the snow is solid, but at lower elevations, it is melting. Repeat
948 imaging with time could show the evolution of the snowpack with changing seasons.

949

950 **SSERVI TREX**

951

952 Tetracorder has been installed on the Carnegie Mellon University Zoë rover (Clark et al., 2022) as part
953 of the NASA Solar System Exploration Research Virtual Institute (SSERVI, <https://sservi.nasa.gov/>),
954 Toolbox for Research and Exploration (TREX), a multi-institutional collaboration led out of the
955 Planetary Science Institute (Hendrix et al., 2023 and references therein). Zoë is a solar-powered rover

capable of performing autonomous science operations (Wagner, et al., 2005, Wettergreen et al., 2005; Wettergreen et al., 2008; Vijayarangan et al., 2018). It carries an Analytical Spectral Devices ASD FieldSpec spectrometer, mounted on a pan-tilt unit, and can observe spectra at any point around the rover. The rover (Figures 15), and its data flow (Figure 16) includes and an ASD-spectrometer covering 0.35 – 2.5 μm to provide real-time data as the rover drives autonomously. The rover also runs a second instance of Tetracorder to analyze FTIR data in the 2.5 to 5- μm range.

Zoë uses the Robot Operating System (ROS) from the Stanford Artificial Intelligence Laboratory, <https://www.ros.org>. ROS uses a message-passing system for communication between the different components in the system that enables each component to operate independently without having to know who or how many consumers are using the data produced by the components.

Tetracorder analyzes the spectra real time with single spectrum mode and is described in Clark et al. (2023). Tetracorder output of a single spectrum analysis is in tabular form, and example analysis is presented in Figure 17 in graphic form to illustrate the features that Tetracorder analyzed. Another program monitors the Tetracorder tabular output and uses the identified minerals to assess the geologic origin of the area, updates a geologic-origin map and uses the information to plan a new route autonomously to explore the area (Candela et al., 2017, 2020; Noe Dobrea et al., 2022, 2023a, 2023b).

Field tests were conducted in fall 2021 and fall 2022 on the Colorado Plateau (Clark et al., 2022, Noe Dobrea et al., 2022, 2023a, Clark et al., 2023). In 2022, additional spectrometers were employed as contact instruments, including an ASD spectrometer with a contact probe, and a contact FTIR instrument covering 2.5 to 15 μm . The rover collected data from these instruments and sent them, along with imaging data to a remote server via satellite communication. This strategy simulated a rover on a remote body (e.g., the Moon, Mars, asteroid), or a remote location on Earth that may be hazardous for humans (e.g., an environmental disaster or volcano emitting toxic gases). The remote server ran three instances of Tetracorder for the three spectrometers giving a near real-time readout of what materials the spectra indicated were present. By near real-time we mean limited by communication delays, and the three second wait loop for checking for new spectra to arrive. The science team, at remote locations, could monitor the incoming images, spectra, and Tetracorder results real time (within data rate limitations; images sometimes took a while to download).

Example Tetracorder output from two spectrometers deployed in the field are compared to XRD analyses of the same rock in Table 5, and the spectra are shown in Figure 17. The Tetracorder expert system in use included identifications from 0.35 to about 4.5 μm . The results in Figure 17 and Table 5 illustrate that different methods and wavelength ranges are sensitive to differing minerals and abundances. The XRD analysis found quartz, feldspar, and calcite. Nano-phase hematite is X-ray amorphous and undetectable by XRD. Reflectance spectroscopy is more sensitive to phyllosilicates than XRD, thus the illite/muscovite that was easily detected from the 2.2-2.3- μm absorptions in the reflectance spectra was too low in abundance for XRD detection. But XRD has good sensitivity to quartz and feldspar, both of which are relatively transparent in the 0.4 to 4- μm region. The weakness of the calcite absorptions near 3.5 and 4 μm indicate low abundance of carbonate, that is too low to show absorptions in the 2.3- μm region, especially with the strong phyllosilicate bands that are present. This example illustrates the power of extended spectral range beyond the 2.5 μm limit, common in terrestrial remote sensing studies.

1002 Tetracorder reported absorptions due to hydroxyl in the 1.4- μm region and water in the 1.9- μm region.
1003 These absorptions may be diagnostic of mineralogy, but the Tetracorder 5.27 expert system needs
1004 additional reference spectra added before unique mineralogy can be identified. Until those additions
1005 are made, these 1.9- μm absorptions are only identified by their band positions.
1006
1007 Historically, the 2- μm water absorption has received little attention as a feature to identify mineralogy
1008 because the Earth's atmospheric water causes too much interference. However, the 1.4 and 1.9- μm
1009 absorptions could be useful for studying airless bodies or planets with thin, dry atmospheres (e.g.,
1010 Mars). Even terrestrial studies could be enhanced if this spectral range were acquired by *in situ*
1011 instruments with a local light source, thus minimizing atmospheric path lengths. Different mineral
1012 groups have varied hydrogen bonding, that shifts the position and width of the water absorptions
1013 (Figure 18). In addition to the changing wavelength position and width of the absorptions plotted in
1014 Figure 18, the band shapes, including asymmetry and shoulders from overlapping water absorptions
1015 further distinguish the absorptions from different minerals, improving specific mineral identification.
1016 Tetracorder reports the position of detected absorptions in the 1.9- μm region (e.g., Table 5), and
1017 indicates the mineral that is best matched, although the output is not always a unique identification
1018 (e.g., Figure 19). With more reference spectra coded into the expert system, identification accuracy
1019 might be improved, but this possibility needs additional study.
1020

1021 **Table 5. Tetracorder and XRD results for sample T8 Spot 1.**

1022

1023

XRD: Xrd_2022_1019_022200_s_t08_spot-ka_tfb

1024

1025

Quartz90 %

1026

2:1 clay mineral-

1027

Kaolinite-

1028

Felspar5

1029

Calcite5

1030

Hematite-

1031

100 %

1032

1033

Tetracorder single spectrum mode, ASD contact instrument:

1034

Spectrum: sps0051312ASD2_20221019_1500_REFL_T8_Spot1

1035

Grp/CseMaterialFitDepthF*D

1036

grp 11um region67MATCHES: fe3+_hematite.nano.BR34b2b0.72670.07570.0699

1037

grp 22-2.5um149MATCHES: micagrp_illite.gds40.96810.06080.0599

1038

grp 3veg detectnone

1039

grp 41.5um broad322MATCHES: fe2+_wollastonite_hs348.3b0.74710.03970.0297

1040

grp 52um broadnone

1041

grp131.3-1.4 nrw421MATCHES: oh_1.406_silica-opal0.95190.06480.0617

1042

grp141.4-1.5 nrw445MATCHES: ohb_1.416_mica-roscoelite0.99220.05560.0552

1043

grp151.5um OH472MATCHES: ohc_1.451_hydroxide-gibbsite0.80910.04280.0346

1044

grp191.9-2um H2O489MATCHES: water_1.910_halloysite0.99440.20680.2056

1045

grp20rare-earthnone

1046

grp21Neodymiumnone

1047

grp22Samariumnone

1048

1049

Tetracorder single spectrum mode, FTIR instrument:

1050

Spectrum: sps0053252FTIR_20221019_134900_T8_Spot1_10_19_2022

1051

Grp/CseMaterialFitDepthF*D

1052

grp 62.5um region343MATCHES: adularia_2.5um0.79070.02660.0210

1053

grp 72.5-3um354MATCHES: grossular_3.17um0.73080.09290.0679

1054

grp 83.2um region358MATCHES: oh2.76um_ref_illite_gds40.77691.03900.8072

1055

grp103.5um curveC367MATCHES: carbonate_trace-b_3.4um.curv0.95420.17030.1625

1056

grp113.5um linear386MATCHES: carbonate_trace-b_3.4um_linc0.94860.15930.1511

1057

grp244-um region530MATCHES: carbonate_calcite_4um_linc0.97860.28720.2810

1058

grp264.25um CO2539MATCHES: trapped-co2-4.26um_ref-cordierite0.58990.01410.0092

1059

grp274.5um regionnone

1060

1061 Notes:

- 1062 Group 4 fe2+_wollastonite is a shape match for a broad feature, not a specific mineral ID.
- 1063 It is likely that the Fe²⁺ feature is from the illite / muscovite.
- 1064 Group 13, 14,15, 19 are feature position matches, not specific mineral IDs.
- 1065 Group 6 adularia_2.5um is a shape match, not a specific mineral ID.
- 1066 Group 8 oh2.76um is a feature position match, not a specific mineral ID.
- 1067 The features are marked on spectra in Figure Z1.
- 1068 The Fit is the correlation coefficient to the least-squares fir to the reference spectral feature(s)
- 1069 Depth is the fitted depth, and F*D is the weighted fits times depths of all the features used in the
- 1070 identification.

1071 **Abundances**

1072

1073 Deriving abundances from remotely obtained reflectance spectra has been a difficult problem, due to
1074 heterogenous particle sizes and non-linear spectral mixing, requiring inversion of radiative transfer
1075 models using an iterative solution. The optical constants of all components in the surface are needed
1076 for the general case. Particle sizes and the size distribution also needs to be known to iteratively solve
1077 the radiative transfer models to derive abundances. Because of the non-linear iterative nature of the
1078 radiative transfer model inversions, it is not feasible to apply this full solution to imaging spectroscopy
1079 data that often includes millions of spectra. Therefore, various studies have used simpler solutions, for
1080 example using linear mixture models that assume pure materials in spatially separate areas (i.e., the
1081 “checkerboard” model). But there are other models, and here we describe four models that are
1082 operational in the Tetracorder system and can be applied to imaging spectroscopy data. These models
1083 were developed as part of the EMIT and FRAGMENT projects and are currently limited to the EMIT
1084 10 minerals: hematite, goethite, calcite, chlorite, dolomite, gypsum, kaolinite, illite/muscovite,
1085 montmorillonite, and vermiculite. Other minerals can be added.

1086

1087 **Model 1:** Relative linear band depth as a proxy for abundance, popularly called “spectral abundance.”
1088 The measured band depth is compared to the band depth in the reference library and the library
1089 sample’s known abundance. This model is a reasonable approximation if the albedo and
1090 particle sizes of the remote surface are similar to the reference spectrum. Figure 20 shows
1091 observed band depth for hematite at varying abundances and albedos.

1092

1093 Note: Models 2-4 use solutions for Mean Optical Path Length, MOPL, derived by Clark and Roush
1094 (1984). Absorption strength is a direct measure of the MOPL but requires accurate optical constants.

1095

1096 **Model 2:** Absolute Abundance in a non-scattering 2-way slab model (Figure 21a). This model
1097 requires optical constants for calculating the diagnostic absorption band centers and the
1098 continuum wavelengths. Results are in mass per unit area in the optical surface, e.g., grams
1099 per sq meter. The major remaining unknown is how deep is the actual optical layer and how it
1100 varies from mineral to mineral.

1101

1102 **Model 3:** Mass in the optical layer assuming isotropic random walk by photons (Figure 21b). Hapke
1103 (1981) argued that after the first scatter, photon direction within a particulate surface is
1104 randomized so an isotropic scattering assumption is a good approximation. Results are in mass
1105 per unit area in the optical surface, e.g., grams / sq meter. The major remaining unknown is the
1106 optical layer thickness and how it varies from mineral to mineral. This model requires optical
1107 constants for calculating the diagnostic absorption band centers and continuum wavelengths.

1108

1109 **Model 4:** Relative Abundance in the optical layer assuming isotropic random walk by photons with
1110 estimates of particle sizes of quartz and feldspar, which are typically dominant in arid regions of
1111 the Earth. This model solves the problem of depth of the optical layer in Model 3. Results are
1112 fractional mass abundance on a 0 to 1 scale. This model requires optical constants for
1113 calculating the diagnostic absorption band centers and each continuum, and the average particle
1114 size of quartz and feldspar.

1115

1116 **Model 5:** Full radiative transfer model with layers. This model is too computationally intensive for
1117 inversion of a full radiative transfer scene but can be used on individual spectra.

1118
 1119
 1120 **Model 1 Relative Linear Band depth as a Proxy for Abundance.** The model scales band depth to
 1121 band depth of reference mineral and assumes linear scaling of this scaled band depth = relative
 1122 fractional abundance, F_A :

$$1123$$

$$1124 F_A = R_{AB} * BD_O / BD_R, \quad (eqn 11)$$

$$1125$$

1126 where:

1127 R_{AB} = Reference material abundance in the reference spectrum,
 1128 BD_O = Band depth in the observed spectrum (the unknown), and
 1129 BD_R = Band depth in the reference spectrum.

1130
 1131 The band depth, BD_O , can be from a Tetracorder analysis.

1132
 1133 **Model 2 Slab Layer Mass.** The Mean Optical Path Length, MOPL, derives directly from Beers Law,
 1134 after Clark and Roush (1984, their equation 11):

$$1135$$

$$1136 R = e^{(-k*x)}, \quad (eqn 12)$$

$$1137$$

1138 where

1139 k = absorption coefficient (usually expressed in inverse centimeters).
 1140 x = path length through the material
 1141 = Mean Optical Path Length in a scattering medium, MOPL.

$$1142$$

$$1143 -\ln(R) = kx, \text{ and} \quad (eqn 13)$$

$$1144$$

1145 Extending equation 13 using Clark and Roush (1984, their equation 30), multiple components would
 1146 have:

$$1147$$

$$1148 -\ln(R) = k_1x_1 + k_2x_2 + K_3x_3 + \dots \quad (eqn 14)$$

$$1149$$

1150 Unfortunately, R is influenced by more than just a single material we are interested in. But we can
 1151 work around this problem by using continuum-removed band depths of diagnostic spectral features.

1152
 1153 Clark and Roush (1984, their equation 32) showed the band depth, BD , relative to the continuum is

$$1154$$

$$1155 BD = (R_c - R_b)/R_c = 1 - R_b/R_c, \quad (eqn 15)$$

$$1156$$

1157 where

1158 R_c = reflectance of the continuum = $\exp(-k_c * x_c)$,
 1159 R_b = reflectance at the band center = $\exp(-k_b * x_b)$,
 1160 k_c = absorption coefficient of the continuum,
 1161 x_c = mean optical path length of the continuum,
 1162 k_b = absorption coefficient at the band center, and
 1163 x_b = mean optical path length at the band center.

1164

1165 Therefore,
1166
1167 $x = \ln(1-BD) / (-\Delta k),$ (eqn 16)
1168

1169 where $\Delta k = k_b - k_c =$ delta absorption coefficient (Figure 22).
1170

1171 Depth probed for model 2, independent of other components, Figure 21a, is then
1172

1173 $T_{\text{slab}} = x/2.$ (eqn 17)
1174

1175 For 3 optical depths:
1176

1177 Model 2 Mass = $3 * T_{\text{slab}} * (100^2) * \text{density},$ (eqn 18)
1178

1179 where density is in gm/cc and mass = grams per sq meter in optical layer.
1180

1181 Model 1 is used by the EMIT team for initial abundance delivery.
1182

1183 **Model 3 Random Walk Mass** is similar to model 2 but includes scattering in a random walk (Figure
1184 21b). Again, the MOPL is a direct calculation from equation 16. If we can constrain the grain size,
1185 e.g., derived from the shape of absorption bands (Clark, 1999, Clark et al., 2003 and references
1186 therein), we can compute the number of grains encountered in the random walk process using Clark
1187 and Roush (1984, their equations 16 and 19):
1188

1189 $m = \ln(R) / \ln(1/(1+2kD)),$ (eqn 19)
1190

1191 where $m =$ number of scatters, $k =$ absorption coefficient, and $D =$ distance between scatters.
1192 In model 3, $D =$ grain diameter. The light penetration depth is then
1193

1194 $T = (\pi/4) * D * (m/2)^{1/2},$ (eqn 20)
1195

1196 and for three optical depths with density in gm/cc and the result in grams per sq meter in the optical
1197 layer is:
1198

1199 Model 3 Mass = $3 * T * (100^2) * \text{density}.$ (eqn 21)
1200
1201

1202 **Model 4 Relative Abundances.** This model is designed to derive the fractional abundances of the
1203 EMIT 10 minerals. EMIT's goal is to derive mineralogy in the arid regions of the Earth to feed into
1204 climate change models for dust radiative properties. Terrestrial arid dust-generating regions commonly
1205 have a high component of quartz plus feldspar of larger grain sizes. There are usually no spectral
1206 features from quartz or feldspar in the visible-near-infrared spectral range making it difficult to identify
1207 and quantify their abundance directly from EMIT data. Instead, we use an estimate of the quartz plus
1208 feldspar particle (hereafter grain) size, and assuming that quartz plus feldspar, which are relatively
1209 transparent in the visible to 2.5- μm spectral range, is a significant mass fraction of the soil/rock surface.
1210 We can use quartz plus feldspar grain diameter as a proxy for distance between scatterings from other
1211 mineral grains. For model 4, equation 20 becomes:

1212
 1213 $T = (\pi/4) * D_q / n * (m/2)^{1/2},$ (eqn 22)
 1214

1215 where D_q is the quartz plus feldspar grain diameter and n = average number of mineral grains (e.g.,
 1216 hematite) per quartz/feldspar grain. The value of “ n ” needs to be derived with a model checked against
 1217 observations or derived empirically for a given region. The D in equation 19 remains the grain
 1218 diameter of the mineral whose mass is to be determined.

1219
 1220 Using equation 22 in a model 3 mass calculation, the mass of quartz plus feldspar is derived using the
 1221 value of m from equation 19 and D_q .

1222
 1223 The relative abundance for component i of j total components is:

1224
 1225 $M_{R,i} = M_i / (\sum_i^j (M_i)),$ (eqn 23a)
 1226

1227 where Relative Mass is $M_{R,i}$ of i^{th} component absolute mass M_i .

1228 The Tetracorder reference material parameters for computing the band depths for a given set of
 1229 reference spectra are stored in ascii files that get parsed by the abundance programs. An example set
 1230 for hematite includes 13 reference spectra covering four grain size ranges and is shown in Appendix 1,
 1231 Table A1. The full tables are available on github in each tetracorder.cmds directory.

1232
 1233 **Layered Regoliths and Contaminants.** A major physical characteristic observed on planetary
 1234 surfaces, including in the Saturn system, Mars and the Moon, yet so far ignored by the remote sensing
 1235 community is the changing grain size with depth in the regolith. The reason for ignoring this factor is
 1236 mainly the lack of development of radiative transfer algorithms to handle layered media. Layered
 1237 regoliths are directly imaged on the Earth, and also in rover tracks on the Moon (Figure 23) and Mars.
 1238 For example, rover tracks on the Moon and Mars show darker regolith below a lighter surface. The
 1239 lunar and Martian surfaces commonly are coated by finer grains (dust). This condition is also observed
 1240 in the Saturn system as expressed by variations in band depths of the different intrinsic strength ice
 1241 absorptions. An example model with grains increasing with depth is shown in Figure 24 with
 1242 measured band depths in Table 6.

1243
 1244 **Model 5: Layered Media and Abundances with Full Radiative Transfer Model.** Planetary surfaces
 1245 can have different compositions and/or grain size at the surface, compared to deeper down (e.g., Figure
 1246 23). Radiative transfer models need to include these changes with depth. Clark and Roush (1984)
 1247 gave equations for penetration depths into a surface, and these equations have been added to the Clark
 1248 *et al.* (2012) radiative transfer model that is based on Hapke (1980, 2012) with extensions for sub-
 1249 micron particles and diffraction Clark *et al.* (2012).

1250
 1251 This full radiative transfer model has been used in multiple studies, for example, Clark *et al.* (2012,
 1252 2019) where it was used to model the ice in the Saturn system including complex darkening by
 1253 contaminants. The mean penetration depth into a regolith is mainly a function of absorption
 1254 coefficient, not wavelength (Clark and Roush, 1984). Using equations 18 to 24 from Clark and Roush,
 1255 it was a simple extension to derive transmission, absorption, and reflections between multiple layers.
 1256 An example 2-layer radiative transfer model is shown in Figure 24.

1257

1258 The radiative transfer code is based on the Hapke model (1980, 2012):

1259

$$1260 \quad r(w, \lambda, \mu_o, \mu, g) = (w/4\pi)[\mu_o/(\mu_o + \mu)]\{[1 + B(g)]P(g) + H(\mu_o)H(\mu) - 1\} \quad (\text{eqn 24})$$

1261

1262 where r is the reflectance (radiance factor) at wavelength λ , μ_o is the cosine of the angle of incident
1263 light, μ is the cosine of the angle of emitted light, g is the phase angle, w is the average single scattering
1264 albedo, $B(g)$ is a backscatter function, $P(g)$ is the average single particle phase function, and H is the
1265 Chandrasekhar (1960) H-function for isotropic scatterers. When $r > 0.9$, Hapke's approximation of the
1266 H-function shows considerable error and equation 24 deviates from measurements (Hapke, 1981, Clark
1267 1999). Because of this deviation, a table interpolation subroutine using "exact" values from
1268 Chandrasekhar (1960) is used. The table interpolation is computationally faster than the Hapke
1269 approximation and more accurate.

1270

1271 We extended the single scattering albedo calculation from Hapke (1980, 2012) to include diffraction
1272 effects when particles much smaller than the wavelengths are present (Clark et al., 2012). We use the
1273 scattering efficiency from Hapke (1993, p. 94), and adapt his equation (5.25):

1274

$$1275 \quad Q_s = Q_d + Q_s' \quad (\text{eqn 25})$$

1276

1277 where Q_d is the scattering due to diffraction, and Q_s' is the scattering from the particles not including
1278 diffraction (Q_s' computed using the standard Hapke model). For small particles, we implement
1279 equations (5.13) and (5.14) from Hapke (1993) for Q_A (absorption) and Q_s (scattering). The resulting
1280 single-layer model reproduces the spectral shapes of dark surfaces seen in the Visible and Infrared
1281 Mapping Spectrometer (VIMS) data for the Saturn system. The model computes both Rayleigh
1282 scattering and Rayleigh absorption (Clark et al., 2012).

1283

1284 The layered spectra and model shown in Figures 24 and 25 illustrates the basics for interpreting real
1285 planetary regoliths. Previously published results of relatively pure icy surfaces in the Saturn system
1286 never matched the intensity and shape of the 3 to 5- μm region and the depths of the 1.04, 1.25, 1.5 and
1287 2- μm ice bands at the same time (e.g., Ciarniello *et al.*, 2017). When the longer wavelengths were
1288 matched, the shorter wavelength absorptions, especially the 1.04 and 1.25- μm ice bands were too weak.
1289 However, the multiple layer regolith model (Figure 24, solid red line) solves the absorption-band-depth
1290 problem because where the absorption coefficients are smaller, light penetrates deeper. Where larger
1291 grains are encountered, there are deeper absorptions in the spectrum. Table 6 shows the quantitative
1292 band depths where in the 2-layer model the 1.04/1.5- μm band depth ratio has been increased by over a
1293 factor of two over non layered models. As contaminant levels increase, e.g., as observed on Saturn's
1294 moon Phoebe, penetration depths (and layered-regolith effects) decrease, and non-layered radiative
1295 transfer models are adequate.

1296

1297 The multi-layer radiative transfer model has been coded and is operational since 2019. This improved
1298 model will lead to better accuracy in deriving material abundance as a function of depth, especially for
1299 ices that are more transparent. Given the above considerations, multi-stream calculation is performed
1300 between multiple layers, as illustrated in Figure 25. Through testing with ice optical constants, it has
1301 been determined that calculation to 4th order scattering between layers is sufficient, even for
1302 transparent-ice materials. At very low absorption coefficients (e.g., pure ice at 0.5 μm) with no
1303 contaminants in the surface, calculation to 6th order is needed.

1304

Table 6. Multi-Layer Model

Model, g.d. = grain diameter	Band Depth				Depth Ratio
	1.04 μm	1.25 μm	1.5 μm	2.0 μm	1.04 / 1.5 μm
H ₂ O ice 2 layer g.d.= top: 28, 11 microns, bottom: 3.5, 2.1 mm	0.2014	0.3266	0.5713	0.4450	0.3526
H₂O ice 2-layer fine on coarse lab data	0.2178	0.3484	0.5462	0.4031	0.3988
H ₂ O ice 1 layer g.d.= 4 microns	0.0717	0.0190	0.3132	0.4142	0.2289
H ₂ O ice 1 layer g.d.= 1.73 mm	0.1989	0.3815	0.9903	0.9821	0.2008

Measured band depths for the spectra in Figure 24. Note the band depth ratio of the 1.04 / 2.0 μm band. Only a multi-layer surface can create observed band depth ratios that are high while not saturating the 1.5 and 2- μm band depths. This effect is observed on icy surfaces in the Saturn and Jupiter systems and is indicative of increasing grain size with depth.

Abundance Examples

EMIT data over Morocco were analyzed with the first four abundance models. This area has been studied by the FRAGMENT project (González-Romero et al., 2023). An EMIT subscene was extracted from EMIT scene emit20230206t101334_o03707_s000_l2a_rfl_b0106_v01 and mapped with Tetracorder (Figures 26 and 27). The EMIT 10 minerals include 17 categories to cover mineralogy and grain size ranges. There is one category each for calcite, chlorite, dolomite, illite+muscovite, kaolinite, montmorillonite and vermiculite (7 categories, each one grain size). There are 4 categories for goethite (nano, fine, medium and coarse grained), 2 for gypsum (fine and coarse grained), and 4 for hematite (nano, fine, medium, and coarse grained). For the results in Figures 28-31, n=5 and the quartz-feldspar grain diameter was set to 100 microns.

Results for determining hematite abundance in the Morocco scene for the 4 models are shown in Figure 28. Models 1 and 4 show similar patterns but different magnitude abundances. In this case, model 1 shows higher abundances of hematite than model 4. Models 1 and 4 can't be compared with the mass results from models 2 and 3 because the former are in % abundance while the later are in gm/m^2 . Models 2 and 3 show the same pattern, but different abundances, with model 2 returning higher values. The average abundances by mass for the Morocco scene are shown in Table 7. Because model 4 is based on the masses in model 3 with additional information to derive quartz + feldspar abundance, if model 4 agrees with field data, then model 3 should be in similar agreement. However, there are no lab studies that we know of to date that derive what the optical layer is for a scene like the one used, nor absolute abundances of the individual components present, so it is difficult to verify model 4 results in more detail.

Models 1 to 4 show the same basic patterns because they originate from the same band depth images. Models 1 and 4 are compared for the other EMIT 10 minerals in Figures 29a and 29b. The quartz derivation from model 4 is shown in Figure 30.

Table 7:
Abundance Models 2 and 3 Results for Morocco Study Area
Abundance in the Optical Layer for 3 Optical Depths,
Tetracorder 5.27d1

Mineral	Model 2	Model 3
	gm / sq meter	gm / sq meter
calcite	220.0	122.0
chlorite	25.62	46.80
dolomite	116.1	287.0
goethite-nano	1.92	1.01
goethite-fine	0.64	2.60
goethite-med	0.62	3.63
goethite-large	0.68	5.97
gypsum-fine	22.31	27.03
gypsum-coarse	13.33	145.3
hematite-nano	4.89	1.90
hematite-fine	0.56	2.88
hematite-med	0.56	4.04
hematite-large	0.78	7.60
illite+muscovite	34.76	23.16
kaolinite	16.38	15.38
montmorillonite	24.79	17.98
Vermiculite	0.0	0.0

1341

1342

1343 The FRAGMENT study of the Morocco field site has characterized the mineralogy and grain size
1344 information (González-Romero et al., 2023). The abundances for model 4 are compared to the average
1345 field data in Table 8. Examination of the 10 EMIT minerals shown in Figures 28, 29a, 29b show large
1346 variations in local mineral abundances. While the average abundances in Table 8 are mostly consistent.

1347

1348 The iron oxide Field Sample results in Table 8 are from X-Ray Diffraction, XRD. XRD is not very
1349 sensitive with sub-micron iron oxide grains, which are the dominant grain sizes in the Morocco scene
1350 according to spectroscopy. The Table 8 XRD derived iron oxide abundances from field samples are
1351 lower than the Model 4 derived abundances. Therefore, we compared wet chemistry from González-
1352 Romero et al., (2023) derived iron oxide abundances to Model 4 derived abundances and plot the
1353 results in Figure 31 with good agreement.

1354

1355 A more in-depth comparison with field-derived abundances is needed and will be conducted when the
1356 Morocco data become available for individual sites located in the EMIT scene.

1357

1358

Table 8: Model 4 Abundances Compared to Field Data

Mineral	Model 4 Fractional Abundance			González-Romero et al. (2023) Field Sample Fractional Abundance	
	max	mean	standard deviation	mean	std dev
calcite	0.554	0.100	0.176	0.138	0.082
dolomite	0.000	0.000	-	0.025	0.016
chlorite	0.664	0.0002	0.009	0.008	0.006
gypsum-fine	0.000	0.000	0.000	0.001	0.003
gypsum-coarse	0.654	0.000	0.002		
goethite-nano	0.000	0.000	0.000	0.004	0.003
goethite-fine	0.228	0.008	0.012		
goethite-med	0.372	0.000	0.002		
goethite-large	0.000	0.000	0.000	0.004	0.004
hematite-nano	0.020	0.015	0.004		
hematite-fine	0.016	0.000	0.000		
hematite-med	0.000	0.000	0.000		
hematite-large	0.000	0.000	0.000		
illite+muscovite	0.286	0.091	0.056	0.067	0.045
kaolinite	0.143	0.0004	0.007	0.047	0.043
montmorillonite	0.107	0.013	0.023	0.001	0.002
quartz+feldspar	0.980	0.772	0.147	0.69	0.15
vermiculite	0.0000	0.0000	0.0000	-	-

1360 The Model 4 results are for the area in the white box in Figure 26 using Tetracorder 5.27d1. The Model
1361 4 standard deviations represent the scene variability, not the error in the abundance of a pixel. Field
1362 results are averages for X-Ray Diffraction analyses from the entire field study area as reported in
1363 González-Romero et al. (2023), their Table 2 for crust, paved sediment and dune samples, and includes
1364 areas not imaged by EMIT in the Figures 26 and 27 boxed area. The field and EMIT results are in
1365 approximate agreement, usually within the standard deviations of the measurements and models, except
1366 the field goethite and hematite values are lower, as expected from XRD results of fine particles.
1367 The maximum values found by model 4 are from a few small locations and indicate a local spot may
1368 have large variability from the mean.

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Known issues

A known issues file is maintained with each tetracorder.cmds github directory containing the expert system. The file is called “AAAAA.KNOWN-ISSUES.txt” and should be reviewed before interpreting any results from the Tetracorder system.

The Tetracorder expert system has been developed for researcher’s projects and field study sites. As the diversity of sites has grown over the decades, new geologic environments have shown weaknesses in the spectral libraries and/or the expert system. Thus, any results from the Tetracorder expert system still need to be checked for accuracy. The calibration to reflectance of the input spectra also needs to be checked. Calibration errors can impact identification accuracy. With EMIT now collecting imaging spectroscopy data over the Earth, the diversity of environments that may be studied with Tetracorder or other systems has never been greater. Thus, diligence is needed to confirm results and deficiencies, and if known additions or fixes to the expert system and spectral libraries are identified, they should be reported to the authors. Deficiencies can then be added to the known issues file, and noted when improvements have been implemented.

While analyzing the EMIT data for this manuscript, we encountered two anomalies that illustrate why checking results are important. Initial testing of the Morocco scene was made with Tetracorder expert system 5.27c1, and a large amount of gypsum and jarosite was “mapped” that did not agree with the analyses of the field samples. The expert system’s 0.35 to 2.5- μ m spectral range was developed mainly with AVIRIS data and the system used a combination of radiative transfer models plus known spectral reflectance areas to correct errors in the radiative transfer model (Clark et al., 2003c). That calibration method was known not to work on a global scale, so the EMIT data had some additional channels deleted around the 1.4- and 1.9- μ m atmospheric water bands for the Tetracorder analysis. The resulting loss of diagnostic mineral absorptions in the EMIT data near the atmospheric water bands resulted in gypsum being misidentified as present. A mitigation strategy was implemented in 5.27d1 and tested on multiple AVIRIS and EMIT scenes.

The areas of misidentification of jarosite in the Morocco EMIT data was found to be a nano-hematite plus fine-grained goethite mixture. Tetracorder 5.27c1 and earlier expert systems had no nano-hematite + goethite reference spectra, leading to the misidentification. A mixture spectrum was added to expert system 5.27d1. While this new reference spectrum reduced the misidentification, as we see in Figure 26, jarosite still shows over significant area, some of which may be other grain sizes of hematite-goethite mixtures. More goethite-hematite mixtures of specific grain sizes and proportions are needed to solve this problem.

Discussion and conclusions

Tetracorder is an open-source operational system with proven results for a wide variety of applications, including geologic mapping on the Earth and other planets and moons, mapping of ecosystems on the Earth and conducting environmental assessments. The breadth of environments where Tetracorder has been applied on the Earth and throughout the Solar System has contributed greatly to the development of the expert system and helped to make it widely applicable to diverse environments. However, it is

1419 still an evolving system with improvements to be made as Tetracorder is applied to new areas with
1420 different geology and ecosystem environments than previously studied.

1421
1422 While experience and testing in multiple environments has helped develop the Tetracorder system and
1423 proven it is robust in those environments, we have not tested all possible environments. A new
1424 environment may show deficiencies in either needed reference spectra, or the strategy to identify a
1425 specific chemistry, for example, due to different instrument characteristics (spectral range, spectral
1426 resolution, signal-to-noise ratio). Thus, there remains a need to check results for consistency and
1427 accuracy. Users are requested to report known deficiencies to the authors so that the deficiency may be
1428 repaired or mitigated.

1429
1430 The abundance models all need refinement. While the equations used for the abundance models are
1431 well established, one of the main issues is accuracy of the input optical constants. Available optical
1432 constants need to be reviewed and where differences are found in the literature, new measurements
1433 need to be made. As grain size gets small, into the tens of nanometers and smaller, the surface-to-
1434 volume ratio of each particle is increasing, and chemical bonds at and near the surface have different
1435 bonding, e.g., electric fields are different. Thus, optical constants are expected to change with particle
1436 size in the sub-micron range. Optical constants are needed as a function of grain size for micron and
1437 sub-micron particles.

1438
1439 Model 4 has a free parameter, the value of n , which is the number of other mineral grains per large
1440 quartz+feldspar grain. The value of n needs to be studied empirically, by a model, or ideally, both.

1441 1442 1443 **Acknowledgments**

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Appendix A

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Table A1. Hematite Reference spectra and abundance parameters.

1463

1464	Nano Hematite (grain size= 50 nanometers):					
1465	#	DN	BD	Band		convolved
1466	# file	scale	factor	depth	title	reference spectrum
1467	group.1um/fe3+_hematite.nano.BR34b2.depth.gz	0.5	0.01	0.2727	Nanohematite BR93-34B2	splib06 3468
1468	Fine grained Hematite (grain size =1 micron):					
1469	#	DN	BD	Band		convolved
1470	# file	scale	factor	depth	title	reference spectrum
1471	group.1um/fe3+_hematite.fine.gr.fe2602.depth.gz	0.5	1.0	0.3957	Hematite FE2602	splib06 2100
1472	group.1um/fe3+_hematite.fine.gr.ws161.depth.gz	0.5	0.79	0.4596	Hematite WS161	splib06 2208
1473	group.1um/fe3+_hematite.fine.gr.gds76.depth.gz	0.5	0.020	0.2876	Hematite.02+Quartz.98 GDS76 W	splib06 5790
1474	group.1um/fe2+fe3+mix_with_hematite_br5b.depth.gz	0.5	0.17	0.1597	Magnetite_skarn BR93-5B	splib06 5934
1475	group.1um/fe2+fe3+_hematite_weathering.depth.gz	0.5	0.01	0.1239	Basalt_weathered BR93-43	splib06 5460
1476	group.1um/fe3+_hematite.thincoat.depth.gz	0.5	0.05	0.5045	Hematite_Thin_Film GDS27	splib06 6198
1477						
1478	Medium grained Hematite (grain size =2 microns):					
1479	#	DN	BD	Band		convolved
1480	# file	scale	factor	depth	title	reference spectrum
1481	group.1um/fe3+_hematite.med.gr.gds27.depth.gz	0.5	1.00	0.5700	Hematite GDS27	splib06 2106
1482	group.1um/fe3+_hematite.med.gr.br25b.depth.gz	0.5	0.050	0.4408	Hematite_Coatd_Qtz BR93-25B	splib06 6174
1483						
1484	Large grained Hematite (grain size =5 microns):					
1485	#	DN	BD	Band		convolved
1486	# file	scale	factor	depth	title	reference spectrum
1487	group.1um/fe3+_hematite.lg.gr.br25a.depth.gz	0.5	0.01	0.4556	Hematite_Coatd_Qtzt BR93-25A	splib06 6186
1488	group.1um/fe3+_hematite.lg.gr.br25c.depth.gz	0.5	0.69	0.5660	Hematite_Coatd_Qtzt BR93-25C	splib06 6192
1489	group.1um/fe3+_hematite.lg.gr.br34c.depth.gz	0.5	0.63	0.5146	Hematite_Coatd_Qtz BR93-34C	splib06 6180
1490	group.1um/fe3+_maghemite.depth.gz	0.5	0.85	0.7649	Maghemite GDS81 Syn (M-3)	splib06 2928
1491						
1492						
1493						

1494 Table A2. Delta-Absorption Coefficients and Parameters for Models 2-4

1495					
1496	Mineral	Del K	Density	Reflectance	Grain Diameter
1497		absorption	grams / cc	Wavelength	(μm)
1498		coefficient		(μm)	
1499		cm-1			
1500	calcite	10.51	2.71	2.18	9
1501	chlorite	76.96	2.8	2.14	11
1502	dolomite	10.51	2.84	2.17	90
1503					
1504	goethite-fine	5120	3.8	0.76	1
1505	goethite-med	5120	3.8	0.76	2
1506	goethite-large	5120	3.8	0.76	5
1507					
1508	gypsum	50	2.36	2.09	75
1509					
1510	hematite-nano	1304	5.3	0.75	0.05
1511	hematite-fine	6400	5.3	0.75	1
1512	hematite-med	6400	5.3	0.75	2
1513	hematite-large	6400	5.3	0.75	5
1514					
1515	illite+muscovite	91.2	2.78	2.14	2
1516	kaolinite	181.0	2.6	2.11	2
1517					
1518	montmorillonite	100	2.35	2.12	2
1519	vermiculite	100	2.5	2.15	10

1520
1521 Values are subject to refinement as new information is obtained.

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Appendix B

FRAGMENT Morocco field site mineralogy and EMIT Model 4 abundances comparison

Analysis of FRAGMENT field samples from González-Romero et al. (2023):

Site #/ Sample	Micro- cline	Albite	Calcite	Dolomite	Smectite/ Montmorillonite	Mica/ Illite
Name	Quartz	Anorthite	Calcite	Dolomite	Palygorskite	Illite
105	0.663	0.117	0.067	0.884	0.006	0.001
106	0.348	0.015	0.032	0.177	0.011	0.003
107	0.772	0.069	0.073	0.045	0.0034	0.000
108	0.600	0.037	0.055	0.108	0.0099	0.0019
109	0.546	0.047	0.039	0.072	0.018	0.000
110	0.293	0.066	0.058	0.056	0.018	0.002

Sample	Kaolinite	Chlorite	Halite	Gypsum	Hematite	Goethite
105	0.009	0.010	0.000	0.000	0.005	0.004
106	0.094	0.058	0.000	0.001	0.005	0.011
107	0.013	0.004	0.000	0.000	0.000	0.0019
108	0.034	0.0098	0.081	0.0021	0.0013	0.0019
109	0.033	0.0061	0.162	0.020	0.000	0.0013
110	0.011	0.005	0.460	0.008	0.002	0.001

Morocco EMIT scene: 800 x 700 pixel crop

Model 4 mineral abundances for 3x3 pixel box, upper left x, y to lower right x, y:

NOTES: pixel coordinates are rotated 180 degrees from the images in Figures AM1 - AM6.

It is difficult to spectrally detect small amounts of calcite or dolomite in the presence of a few percent illite/muscovite. Similarly with chlorite. The OH absorptions are stronger than the carbonate absorptions in the 2.2 to 2.4- μ m region.

Model 4 abundances with quartz+feldspar grain diameter = 100 microns, n=5.

Site # 105: pixels 17 432 to 19 434

Mineral	min	max	mean	std_dev	FRAGMENT field mineralogy
calcite	0.0000	0.0000	0.0000	0.0000	0.084
chlorite	0.2794	0.3063	0.2873	0.0086	0.010
dolomite	0.0000	0.0000	0.0000	0.0000	0.006
goethite-fine	0.0208	0.0217	0.0214	0.0003	0.004
goethite-large	0.0000	0.0000	0.0000	0.0000	0.
goethite-med	0.0000	0.0000	0.0000	0.0000	0.
goethite-nano	0.0000	0.0000	0.0000	0.0000	0.
gypsum-coarse	0.0000	0.0000	0.0000	0.0000	0.
gypsum-fine	0.0000	0.0000	0.0000	0.0000	0.000
hematite-fine	0.0000	0.0000	0.0000	0.0000	0.
hematite-large	0.0000	0.0000	0.0000	0.0000	0.
hematite-med	0.0000	0.0000	0.0000	0.0000	0.
hematite-nano	0.0129	0.0134	0.0132	0.0002	0.005
illite+muscovite	0.0000	0.0000	0.0000	0.0000	0.034
kaolinite	0.0000	0.0000	0.0000	0.0000	0.009
montmorillonite	0.0000	0.0000	0.0000	0.0000	0.001
quartz-feldspar	0.6600	0.6855	0.6780	0.0082	0.847
vermiculite	0.0000	0.0000	0.0000	0.0000	0.

(includes palygorskite)
q+f = 0.663 + 0.117+0.067

Comment: The ~1% chlorite masks the calcite absorption.

Site # 106: pixels 56 412 to 58 414

Mineral	min	max	mean	std_dev	FRAGMENT field mineralogy
calcite	0.0000	0.0000	0.0000	0.0000	0.177
chlorite	0.0000	0.0000	0.0000	0.0000	0.058
dolomite	0.0000	0.0000	0.0000	0.0000	0.011
goethite-fine	0.0184	0.0253	0.0206	0.0032	0.011
goethite-large	0.0000	0.0000	0.0000	0.0000	0.
goethite-med	0.0000	0.0000	0.0000	0.0000	0.
goethite-nano	0.0000	0.0000	0.0000	0.0000	0.
gypsum-coarse	0.0000	0.0000	0.0000	0.0000	0.
gypsum-fine	0.0000	0.0000	0.0000	0.0000	0.001

1604	hematite-fine	0.0000	0.0000	0.0000	0.0000	0.
1605	hematite-large	0.0000	0.0000	0.0000	0.0000	0.
1606	hematite-med	0.0000	0.0000	0.0000	0.0000	0.
1607	hematite-nano	0.0000	0.0116	0.0076	0.0057	0.005
1608	illite-muscovite	0.1473	0.2114	0.1697	0.0312	0.246
1609	kaolinite	0.0978	0.1403	0.1127	0.0207	0.094
1610	montmorillonite	0.0000	0.0000	0.0000	0.0000	0.003 (includes palygorskite)
1611	quartz-feldspar	0.6234	0.7246	0.6893	0.0493	0.395 q+f = 0.348 + 0.015+0.032
1612	vermiculite	0.0000	0.0000	0.0000	0.0000	0.000

1613 Comment: The high illite/muscovite absorptions masks calcite/dolomite detection.

1615

1616 Site # 107: pixels 87 411 to 89 413

1618	Mineral	min	max	mean	std_dev	FRAGMENT	field mineralogy
1620	calcite	0.0000	0.0000	0.0000	0.0000	0.045	
1621	chlorite	0.0000	0.0000	0.0000	0.0000	0.004	
1622	dolomite	0.0000	0.0000	0.0000	0.0000	0.0034	
1623	goethite-fine	0.0244	0.0247	0.0245	0.0001	0.0019	
1624	goethite-large	0.0000	0.0000	0.0000	0.0000	0.	
1625	goethite-med	0.0000	0.0000	0.0000	0.0000	0.	
1626	goethite-nano	0.0000	0.0000	0.0000	0.0000	0.	
1627	gypsum-coarse	0.0000	0.0000	0.0000	0.0000	0.	
1628	gypsum-fine	0.0000	0.0000	0.0000	0.0000	0.000	
1629	hematite-fine	0.0000	0.0000	0.0000	0.0000	0.	
1630	hematite-large	0.0000	0.0000	0.0000	0.0000	0.	
1631	hematite-med	0.0000	0.0000	0.0000	0.0000	0.	
1632	hematite-nano	0.0151	0.0153	0.0151	0.0001	0.000	
1633	illite-muscovite	0.1308	0.1362	0.1343	0.0018	0.017	
1634	kaolinite	0.0000	0.0000	0.0000	0.0000	0.013	
1635	montmorillonite	0.0000	0.0000	0.0000	0.0000	0.000	
1636	quartz-feldspar	0.8244	0.8292	0.8261	0.0016	0.912	q+f 0.770 + 0.069+0.073
1637	vermiculite	0.0000	0.0000	0.0000	0.0000	0.	

1638 Comment: The high illite/muscovite absorptions masks calcite/dolomite detection.

1640

1641 Site # 108: pixels 399 352 to 401 354

1643	Mineral	min	max	mean	std_dev	FRAGMENT	field mineralogy
1645	calcite	0.0000	0.0000	0.0000	0.0000	0.110	
1646	chlorite	0.0000	0.0000	0.0000	0.0000	0.0098	
1647	dolomite	0.0000	0.0000	0.0000	0.0000	0.099	
1648	goethite-fine	0.0250	0.0254	0.0252	0.0001	0.0019	
1649	goethite-large	0.0000	0.0000	0.0000	0.0000	0.	
1650	goethite-med	0.0000	0.0000	0.0000	0.0000	0.	
1651	goethite-nano	0.0000	0.0000	0.0000	0.0000	0.	
1652	gypsum-coarse	0.0000	0.0000	0.0000	0.0000	0.	
1653	gypsum-fine	0.0000	0.0000	0.0000	0.0000	0.0021	Halite= 0.081
1654	hematite-fine	0.0000	0.0000	0.0000	0.0000	0.	
1655	hematite-large	0.0000	0.0000	0.0000	0.0000	0.	
1656	hematite-med	0.0000	0.0000	0.0000	0.0000	0.	
1657	hematite-nano	0.0155	0.0157	0.0156	0.0001	0.0013	Total Fe = 0.028
1658	illite-muscovite	0.1191	0.1260	0.1224	0.0022	0.057	
1659	kaolinite	0.0000	0.0000	0.0000	0.0000	0.034	
1660	montmorillonite	0.0000	0.0000	0.0000	0.0000	0.0019	
1661	quartz-feldspar	0.8335	0.8397	0.8368	0.0020	0.692	q+f= 0.60 + 0.037+0.055
1662	(halite+quartz+feldspar	0.8335	0.8397	0.8368	0.0020	0.773	h+q+f= 0.081 + 0.60 + 0.037+0.055
1663	vermiculite	0.0000	0.0000	0.0000	0.0000	0.	

1664 Comment: The high illite/muscovite absorptions masks calcite/dolomite detection.

1665 Comment: Salt grains are transparent like quartz or feldspar so will have s similar
1668 scattering contribution as quartz or feldspar. This combination
1669 is included for comparison.

1670

1671

1672 Site # 109: pixels 418 162 to 420 164

1674	Mineral	min	max	mean	std_dev	FRAGMENT	field mineralogy
1676	calcite	0.0000	0.0000	0.0000	0.0000	0.072	
1677	chlorite	0.0000	0.0000	0.0000	0.0000	0.0061	
1678	dolomite	0.0000	0.0000	0.0000	0.0000	0.018	
1679	goethite-fine	0.0000	0.0248	0.0137	0.0130	0.0013	
1680	goethite-large	0.0000	0.0000	0.0000	0.0000	0.	
1681	goethite-med	0.0000	0.0000	0.0000	0.0000	0.	
1682	goethite-nano	0.0000	0.0000	0.0000	0.0000	0.	

1683	gypsum-coarse	0.0000	0.0000	0.0000	0.0000	0.	
1684	gypsum-fine	0.0000	0.0000	0.0000	0.0000	0.020	Halite = 0.16
1685	hematite-fine	0.0000	0.0000	0.0000	0.0000	0.	
1686	hematite-large	0.0000	0.0000	0.0000	0.0000	0.	
1687	hematite-med	0.0000	0.0000	0.0000	0.0000	0.	
1688	hematite-nano	0.0151	0.0165	0.0158	0.0007	0.000	Total Fe = 0.028
1689	illite+muscovite	0.1134	0.1351	0.1244	0.0094	0.054	
1690	kaolinite	0.0000	0.0000	0.0000	0.0000	0.033	
1691	montmorillonite	0.0000	0.0000	0.0000	0.0000	0.000	
1692	quartz-feldspar	0.8254	0.8701	0.8461	0.0216	0.636	q+f = 0.55 + 0.047 + 0.039
1693	(halite+quartz+feldspar	0.8254	0.8701	0.8461	0.0216	0.796	h+q+f = 0.16 + .55 + 0.047 + 0.039)
1694	vermiculite	0.0000	0.0000	0.0000	0.0000	0.	

1695 Comment: The high illite/muscovite absorptions masks calcite/dolomite detection.

1696 Comment: Salt grains are transparent like quartz or feldspar so will have s similar
1699 scattering contribution as quartz or feldspar. This combination
1700 is included for comparison.

1701

1702

1703 Site # 110: pixels 326 194 328 196

1705	Mineral	min	max	mean	std_dev	FRAGMENT	field mineralogy
1707	calcite	0.0000	0.4132	0.0912	0.1810	0.056	
1708	chlorite	0.0000	0.0000	0.0000	0.0000	0.005	
1709	dolomite	0.0000	0.0000	0.0000	0.0000	0.018	
1710	goethite-fine	0.0000	0.0250	0.0169	0.0106	0.001	
1711	goethite-large	0.0000	0.0000	0.0000	0.0000	0.	
1712	goethite-med	0.0000	0.0000	0.0000	0.0000	0.	
1713	goethite-nano	0.0000	0.0000	0.0000	0.0000	0.	
1714	gypsum-coarse	0.0000	0.0000	0.0000	0.0000	0.	
1715	gypsum-fine	0.0000	0.0000	0.0000	0.0000	0.008	Halite: 0.46
1716	hematite-fine	0.0000	0.0000	0.0000	0.0000	0.	
1717	hematite-large	0.0000	0.0000	0.0000	0.0000	0.	
1718	hematite-med	0.0000	0.0000	0.0000	0.0000	0.	
1719	hematite-nano	0.0086	0.0166	0.0141	0.0032	0.002	
1720	illite+muscovite	0.0000	0.1319	0.0964	0.0552	0.017	
1721	kaolinite	0.0000	0.0000	0.0000	0.0000	0.011	
1722	montmorillonite	0.0000	0.0548	0.0121	0.0240	0.002	
1723	quartz-feldspar	0.5096	0.8726	0.7693	0.1466	0.417	q+f = 0.293 + 0.066 + 0.058
1724	(halite+quartz+feldspar	0.5096	0.8726	0.7693	0.1466	0.877	h+q+f = 0.46 + 0.293 + 0.066 + 0.058)
1725	vermiculite	0.0000	0.0000	0.0000	0.0000	0.	

1726 Comment: Here is a case where the calcite absorption was strong enough to be
1728 detected in the presence of illite/muscovite.

1729 Comment: Salt grains are transparent like quartz or feldspar so will have s similar
1731 scattering contribution as quartz or feldspar. This combination
1732 is included for comparison.

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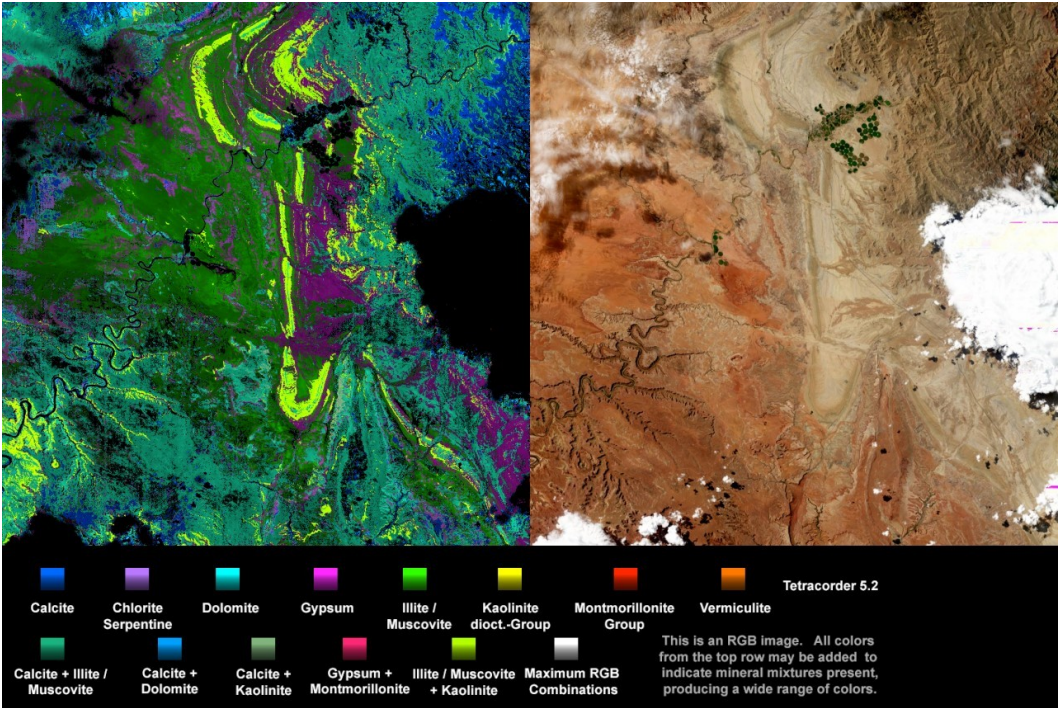
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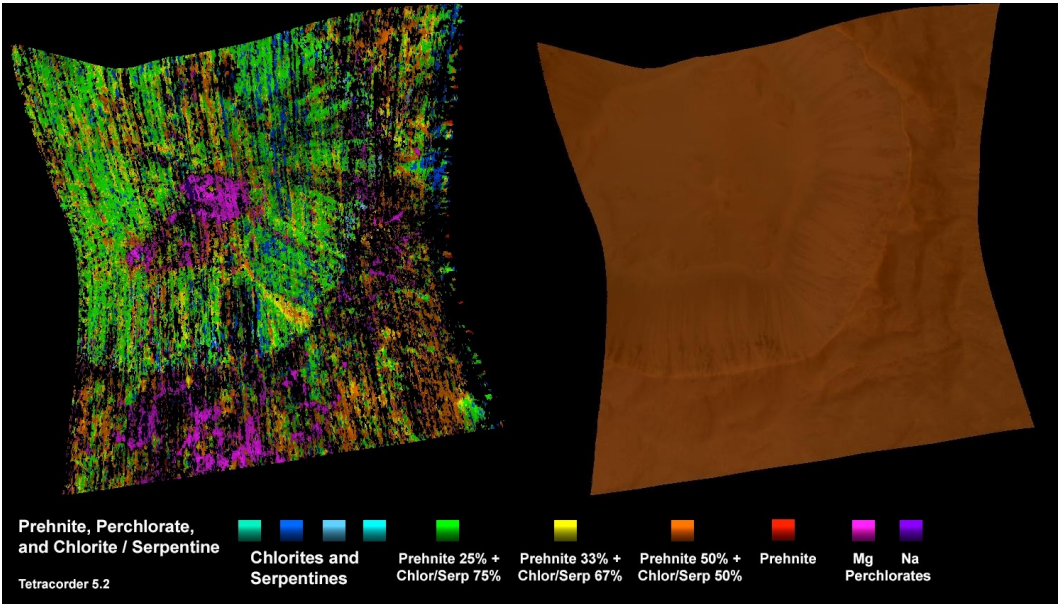
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1984 **Figures**
1985
1986 a)



1987 b)



1989 **Figure 1. Tetracorder mineral map expert system standard products.** (a) EMIT image cube of
1990 Utah, USA. Arches National Park is in the lower right corner. Results here show minerals detected
1991 using absorption features in the near-infrared region. (b) Mars Reconnaissance Orbiter, Compact
1992 Reconnaissance Imaging Spectrometer for Mars (CRISM) scene FRT000148C1_07_IF164J_MTR3 for
1993 a crater at 7.7°S, 84.5°E. The Tetracorder expert system was the same for this wavelength region as the
1994 Tetracorder EMIT results in (a).

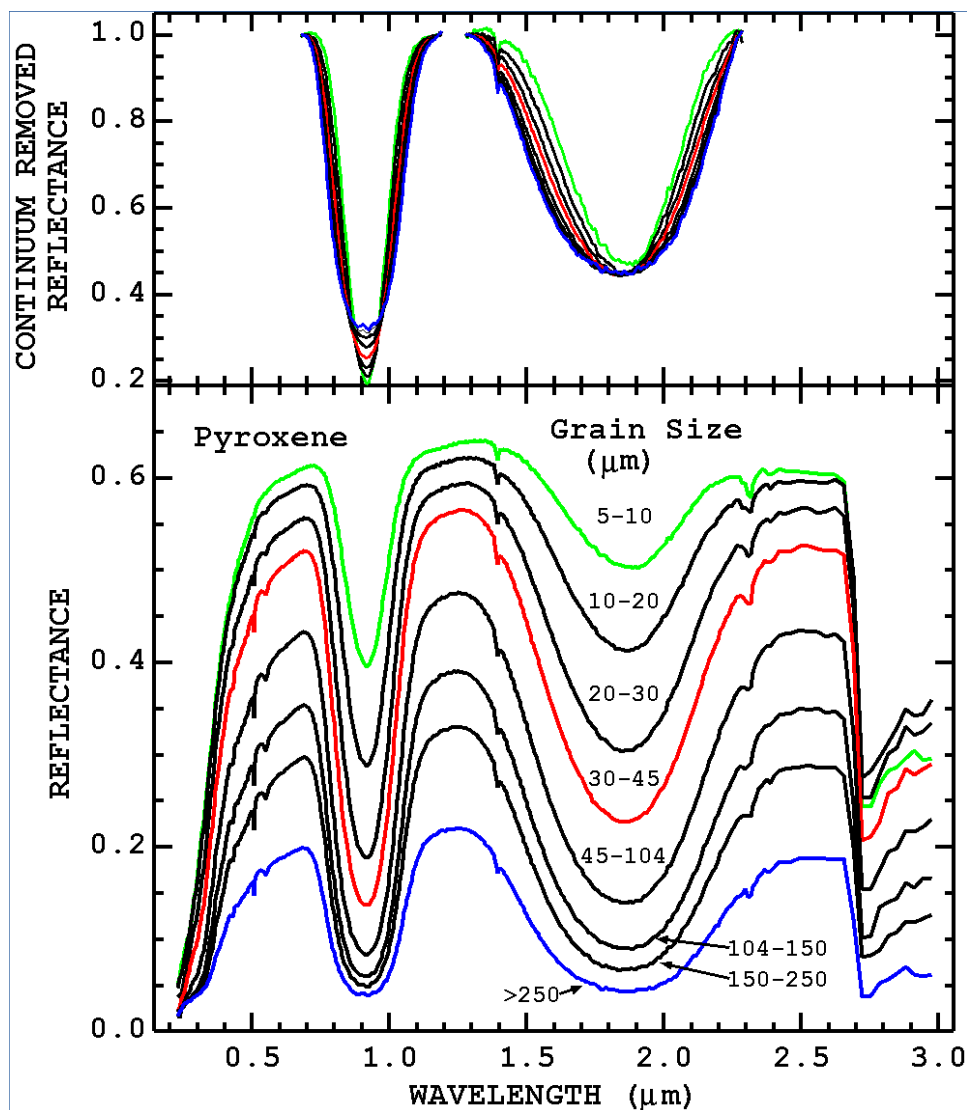
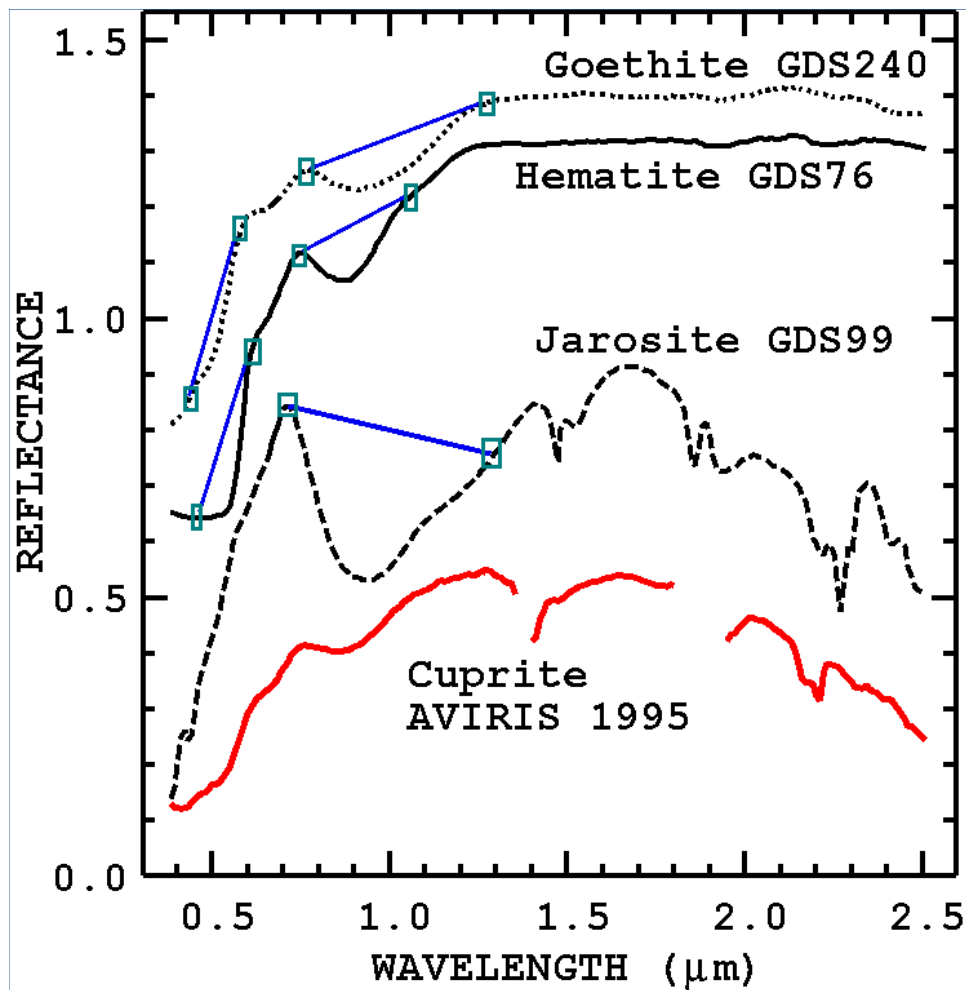
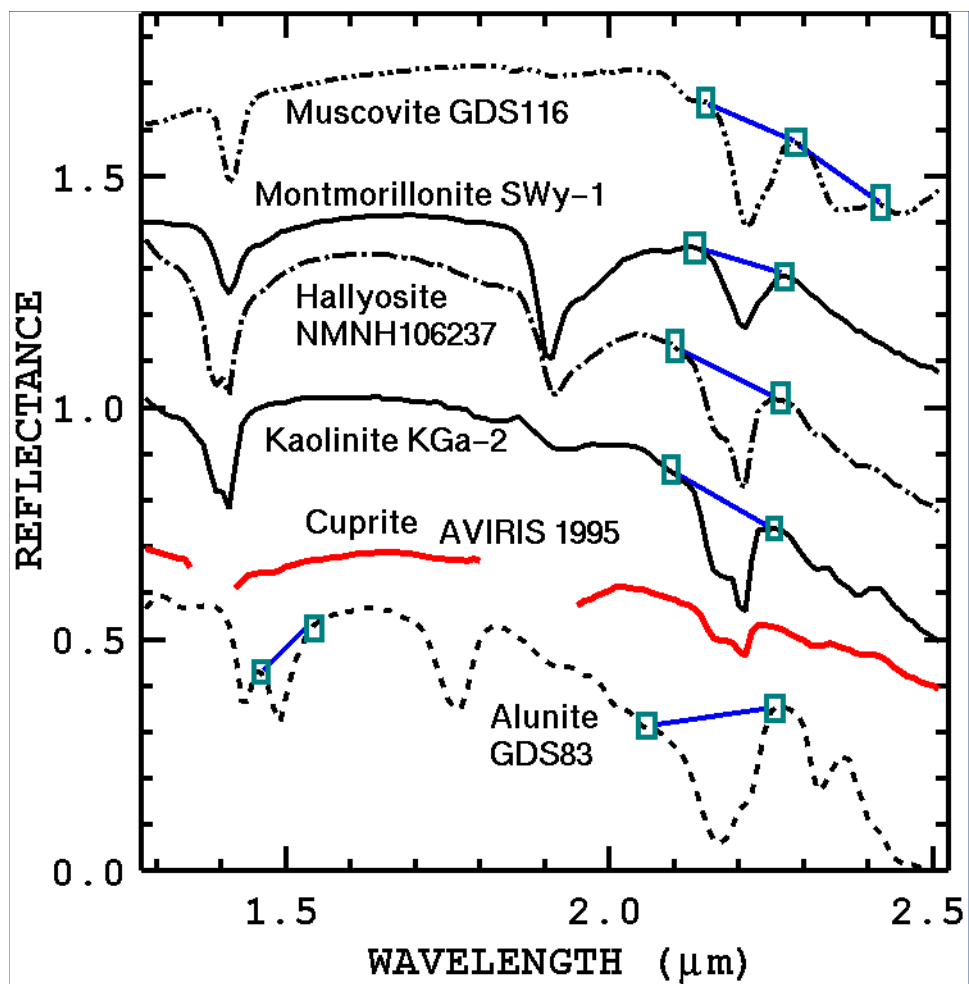


Figure 2. Effects of mixtures and grain size on band shape. Pyroxene reflectance spectra as a function of grain size. As the grain size becomes larger, more light is absorbed, the reflectance decreases, and the absorption feature bottoms flatten. Note the trace tremolite contamination causing the narrow absorption features near 1.4 and 2.3 μm . The broader pyroxene absorptions are the continuum background to the narrow tremolite features. This example shows how the components in a mixture can be readily identified even though no unmixing analysis is done. The component features are “spectrally separated” in wavelength position and width, as well as shape. Continuum-removed feature fits (top) show the similarity in shape of features at different grain sizes. The small change in shape can be used to determine grain size from the spectra, independent of abundance. Data from Clark et al., 2003a, USGS spectral library 06.



2010
 2011 Figure 3a. Continuum removal process employed by the Tetracorder spectral feature shape matching
 2012 algorithm. Three reference spectra are shown: goethite, jarosite and hematite. Each spectral feature
 2013 has its own continuum end-points (illustrated by the boxes). The continuum is removed from both the
 2014 observed and reference spectra. For example, the hematite 0.9- μm feature continuum is removed from
 2015 the Cuprite unknown spectrum, then the goethite continuum is removed, and so on. This allows a
 2016 specific comparison between each spectral library feature and the unknown. The spectra are offset for
 2017 clarity. From Clark et al., 2003, a public domain image.



2018 Figure 3b. Spectral features as on Figure 3a except for comparison with vibrational absorptions near
 2019 2.2 μm . Note that alunite also has a diagnostic absorption near 1.5 μm . The spectra are offset for
 2020 clarity. From Clark et al., 2003, a public domain image.

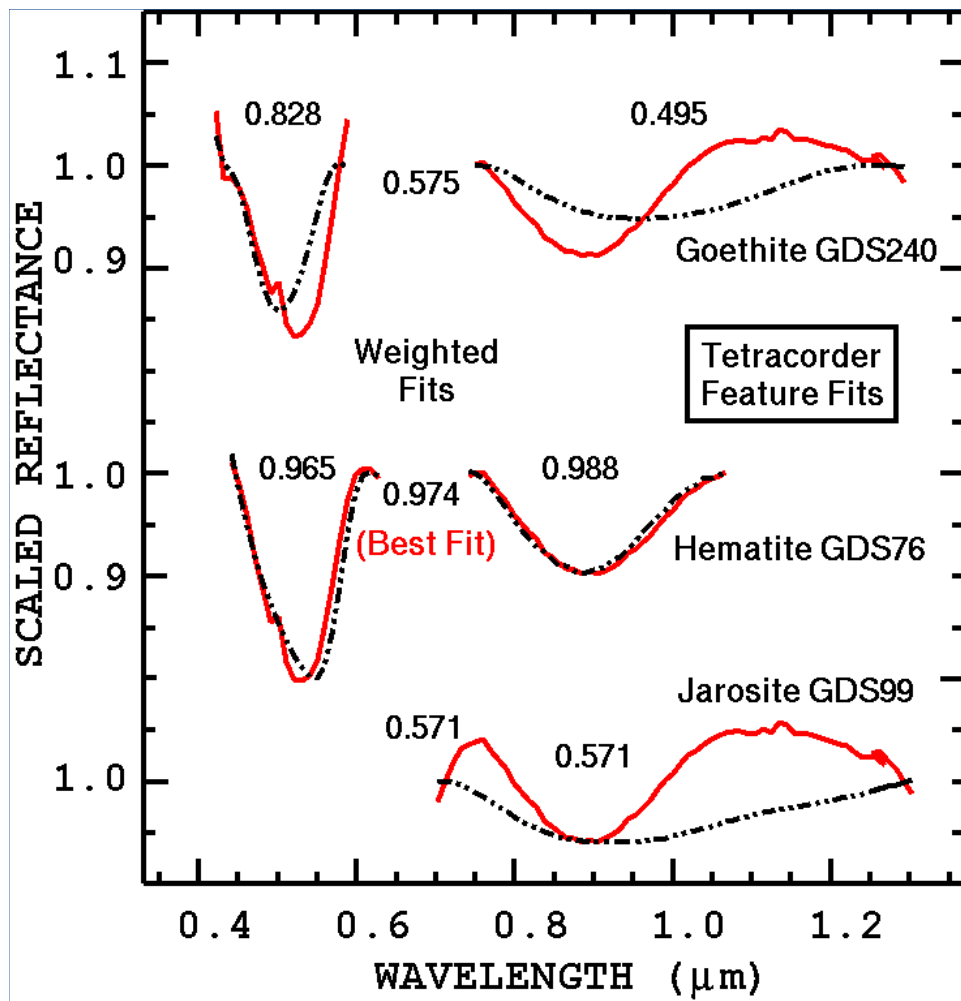
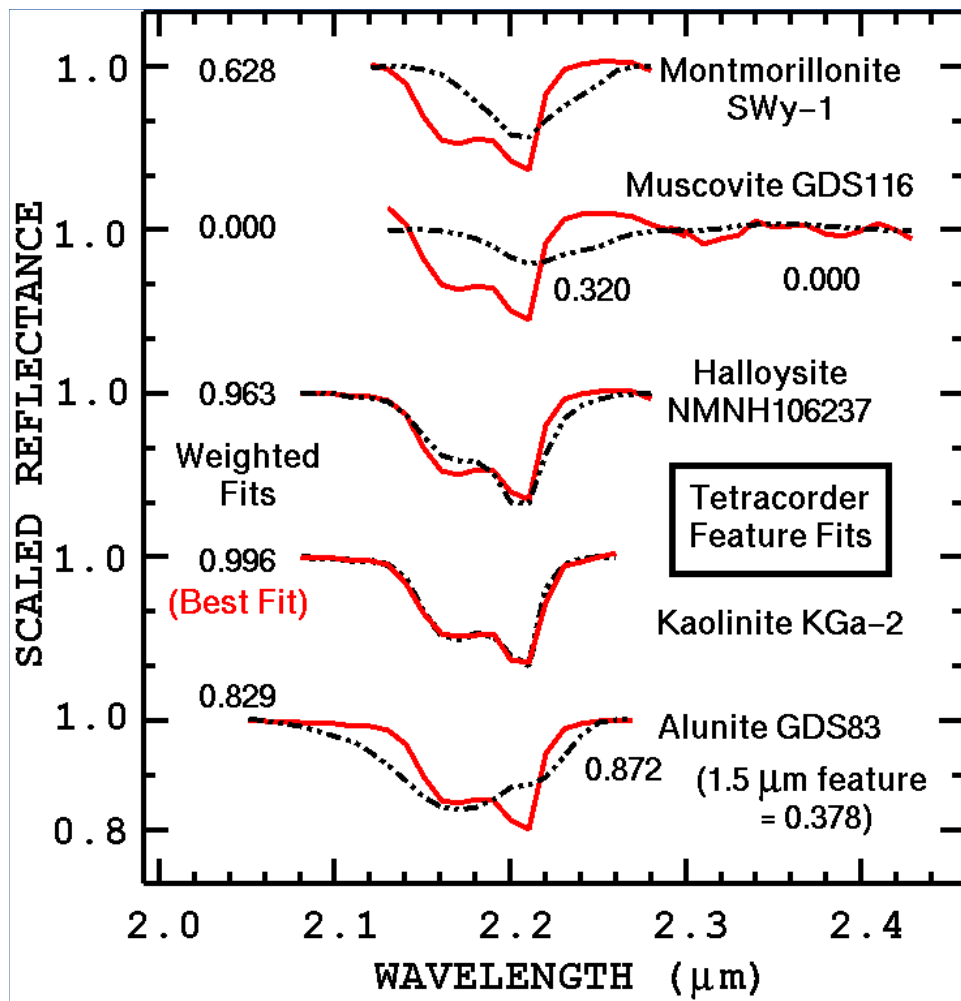


Figure 4a. The continuum removed spectra from Figure 3a are fit to each other using a modified least squares calculation. The library reference feature strength is increased or decreased to best match the observed feature. Tetracorder compares the least-squares fits to many features from many library reference spectra to determine which one matches best. The solid red line in each case is the unknown and the dash double dotted black line is the library reference feature. For each feature, the least squares correlation coefficients (the *fits*) are given, and along a vertical central column, the weighted fits are shown. The best match to the Cuprite spectrum is hematite. Hematite has two features used in the identification: the 0.9 μm feature gives a fit of 0.988, and the 0.5 μm feature gives a fit of 0.965. The area-weighted fit is 0.974. From Clark et al., 2003, a public domain image.



2032 Figure 4b. The continuum removed spectra from Figure 3b are fit together using a modified least
 2033 squares calculation. Kaolinite is the best match to the Cuprite spectrum. The muscovite spectrum has
 2034 two features, one near 2.2 and the other near 2.3 μm . No 2.3- μm muscovite feature could be detected
 2035 in the Cuprite spectrum, so the weighted fit is zero (left hand column). Note the very similar fits
 2036 between kaolinite (0.996) and halloysite (0.963), yet the halloysite profile clearly does not match as
 2037 well as the kaolinite profile. This illustrates that small differences in fit numbers are significant.
 2038 Alunite has two diagnostic spectral features, but the 1.5- μm feature is not shown. From Clark et al.,
 2039 2003, a public domain image.

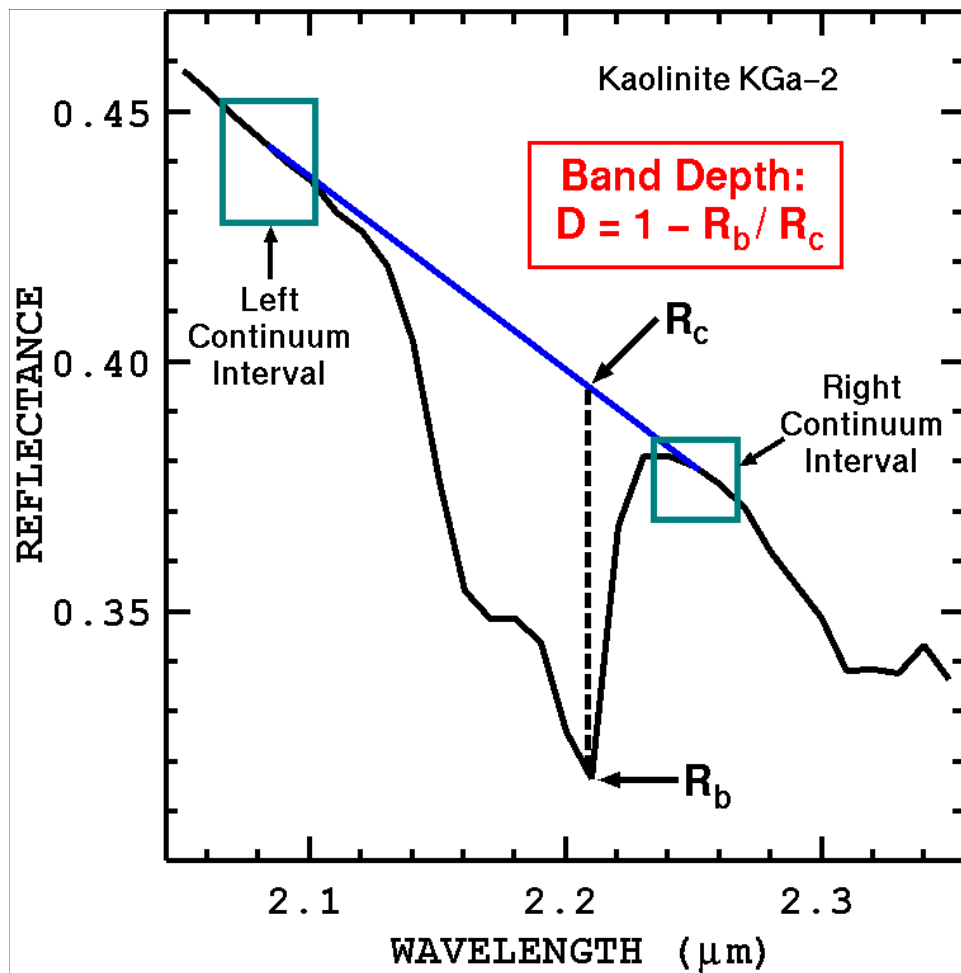
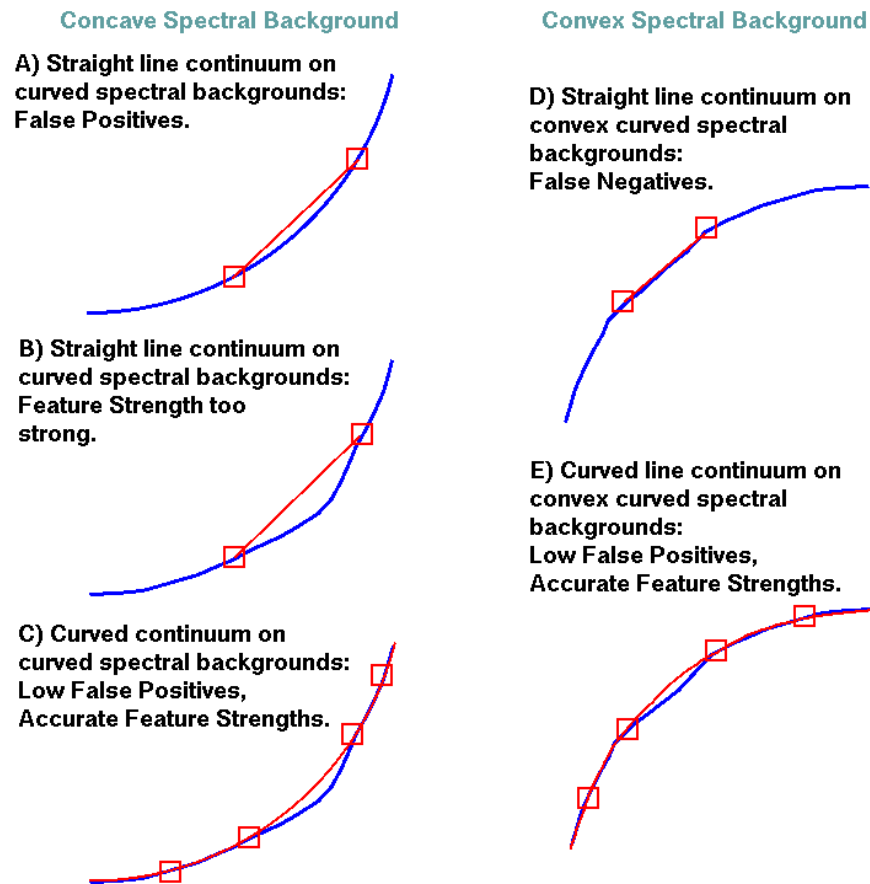


Figure 5. Characteristics of an absorption feature. A continuum interval is chosen on each side of the feature to reduce noise. The continuum intervals in this example are about 30nm wide. A straight-line continuum is fit between the end points. The reflectance at the band center (R_b) and the corresponding continuum reflectance at the band center (R_c) are found to compute the band depth, D . The continuum is removed by division from both the library reference spectrum and from the unknown's spectrum.

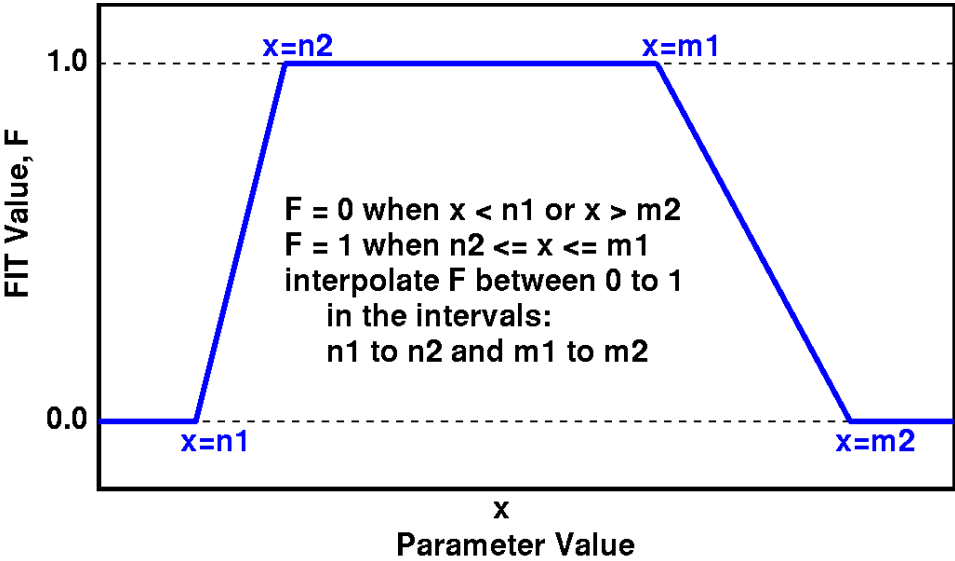
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2052 Figure 6. Curved versus straight line continua. For weak spectral features on a curved continuum
2053 background, straight line continua can lead to false positives (A), errors in band depth (B) and false
2054 negatives (D). Curved continua (C, E) solve these problems but requires additional continuum
2055 intervals (4 endpoints instead of 2). The disadvantage of more continuum endpoints is that if one falls
2056 in another absorption band, it can distort off the cubic spline, creating false positives and false
2057 negatives. Tetracorder allows for both linear and curved continua to be used.

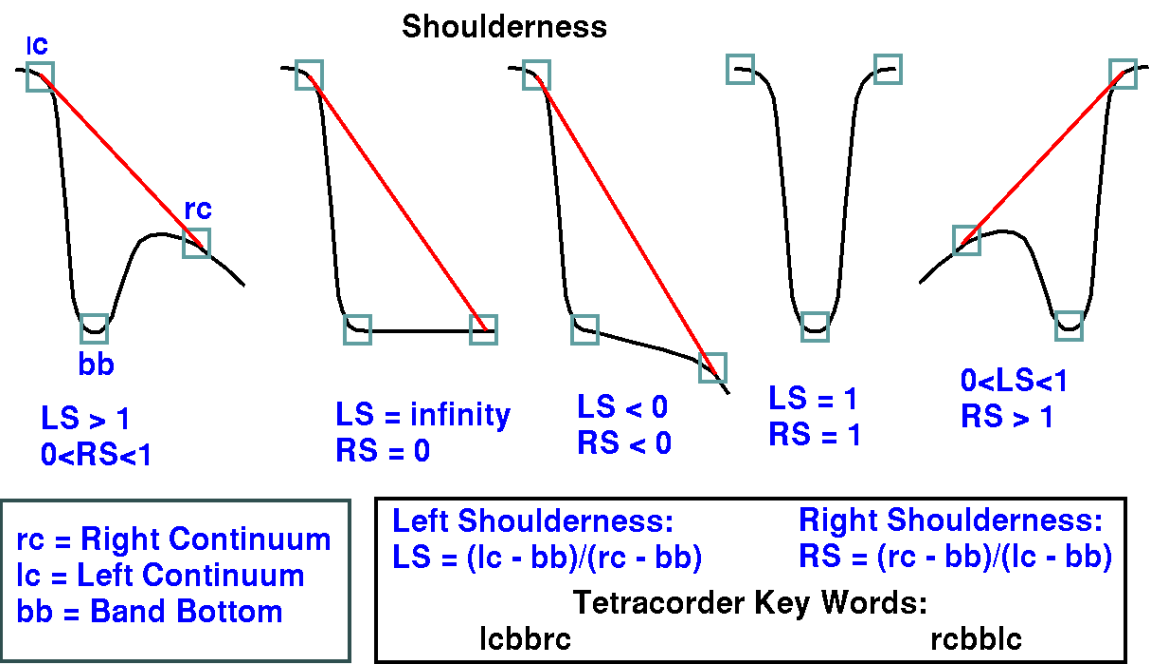
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2062 Figure 7. Fuzzy logic. The correlation coefficient (the fit) value is multiplied by the fuzzy logic value.
2063 When a parameter value is less than n1 or greater than m2, the fuzzy logic value is set to zero and the
2064 fit will be zero. If the parameter value is between n2 and m1, the fuzzy logic value is set to 1.0 and the
2065 fit is unchanged. If between n1 and n2 or m1 and m2, the fuzzy logic value is interpolated between 0
2066 and 1, decreasing the fit value.

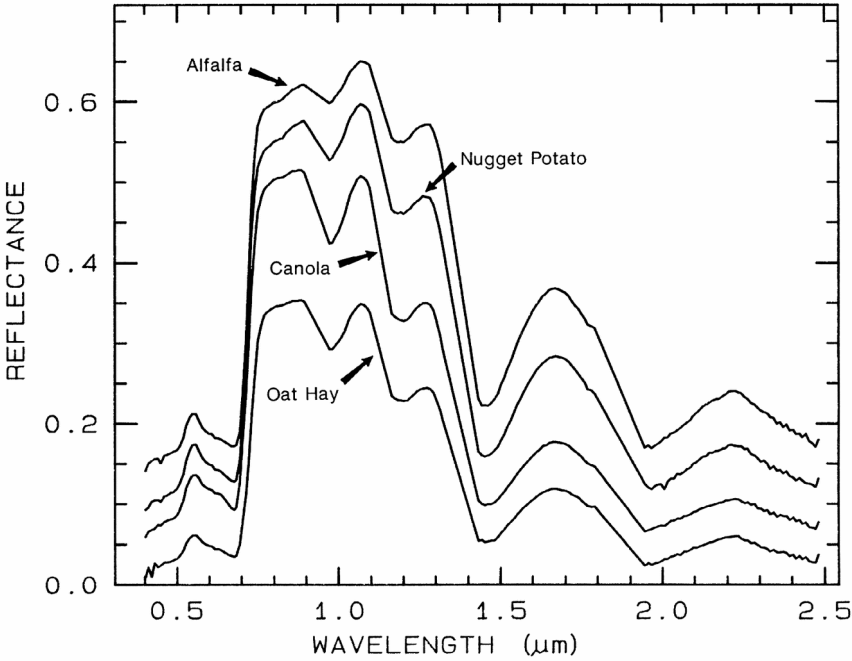
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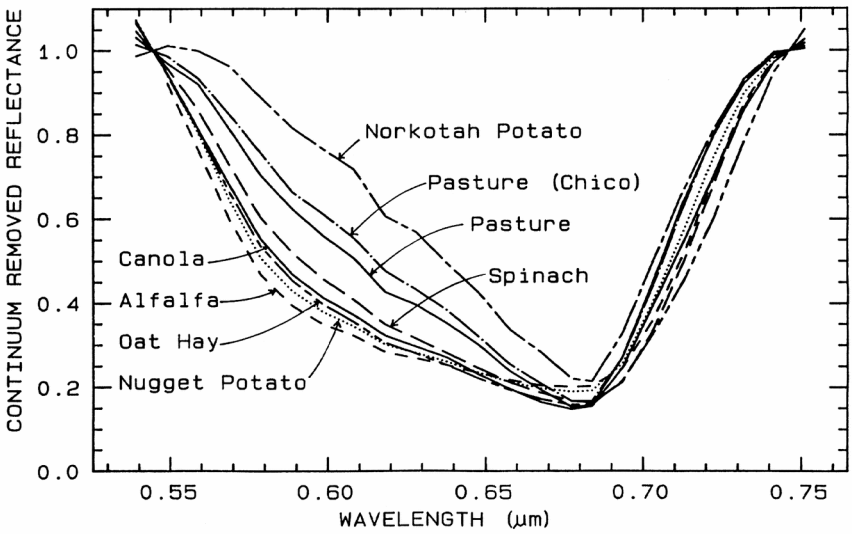
2071 Figure 8. Shoulderness definitions. The red line represents the straight-line continuum between
2072 lc and rc.

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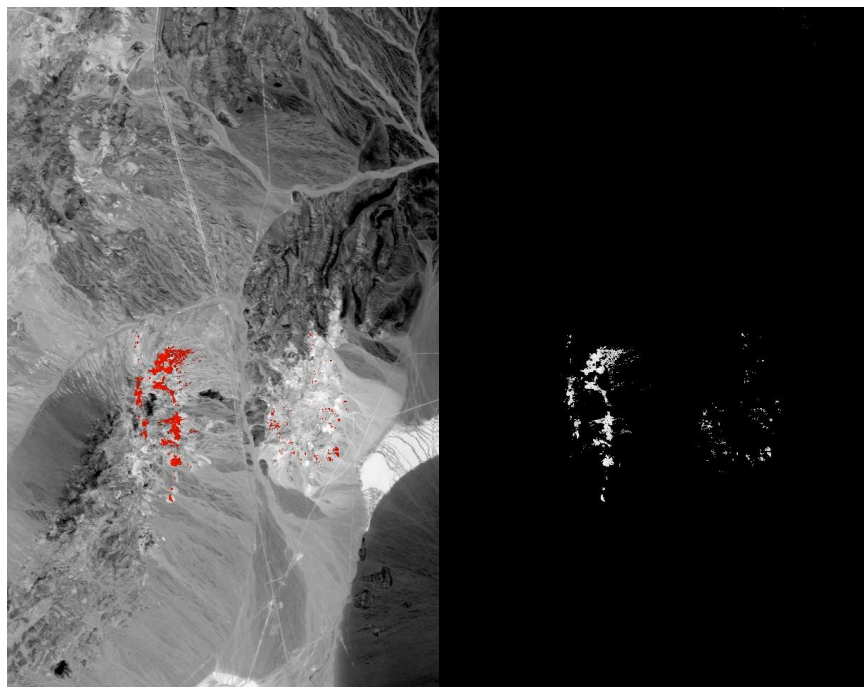


2076 Figure 9a. Vegetation spectra. From Clark, 1999.
2077



2079 Figure 9b. Vegetation spectra showing shape changes with vegetation type, and the red edge position
2080 shifts (the edge from ~ 0.68 to ~ 0.75 μm). The ~ 0.55 to 0.65 - μm shape changes could also be used.
2081 From Clark, 1999.
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2088 Figure 10. Tetracorder browse product for K-alunite. This browse image includes multiple K-bearing
2089 alunites into one image. On the left, the pixels containing K-alunite are shown in red on a gray scale
2090 background, and on the right, white on a black background. This is an auto-generated Tetracorder
2091 product. These images are found in the results.dual.group.* directories.
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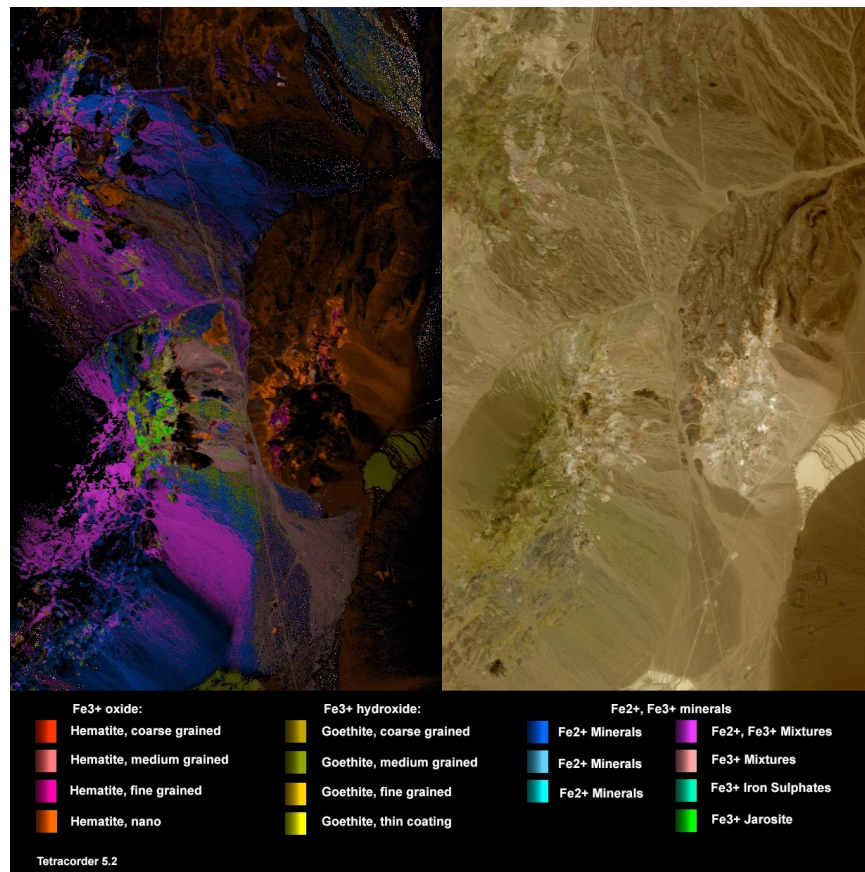
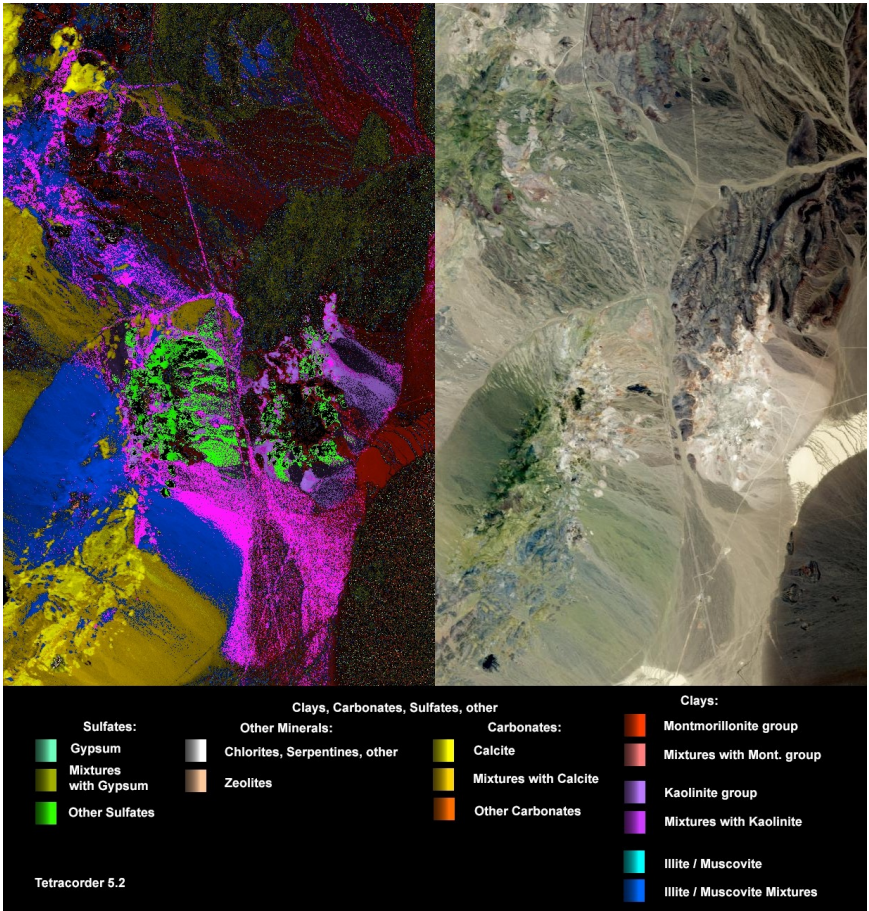
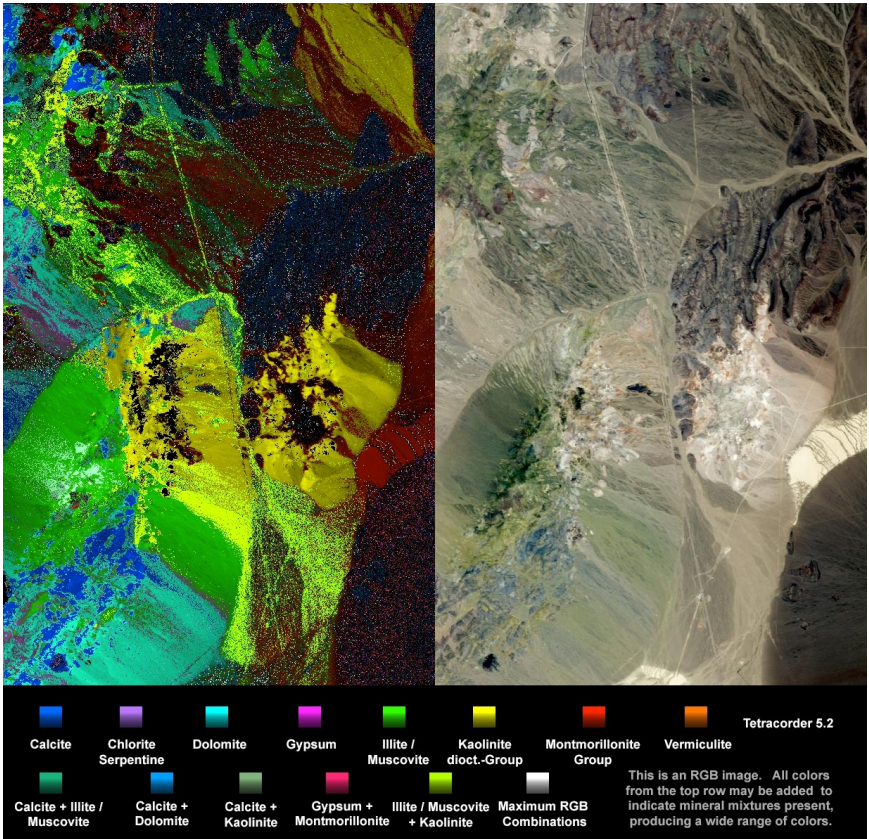


Figure 11a. Group 1 minerals mapped. This is a Tetracorder 5.27 standard product, expert system 5.27d1. The image on the right is an approximate true color image using red, green and blue channels from the spectrometer data. It is approximate because only a single channel for each color is used instead of a spectral profile of human eye response. The user can define the channels used for each sensor. The channels used for this 1995 AVIRIS data are 30, 20 and 10 for red, green, and blue, respectively.



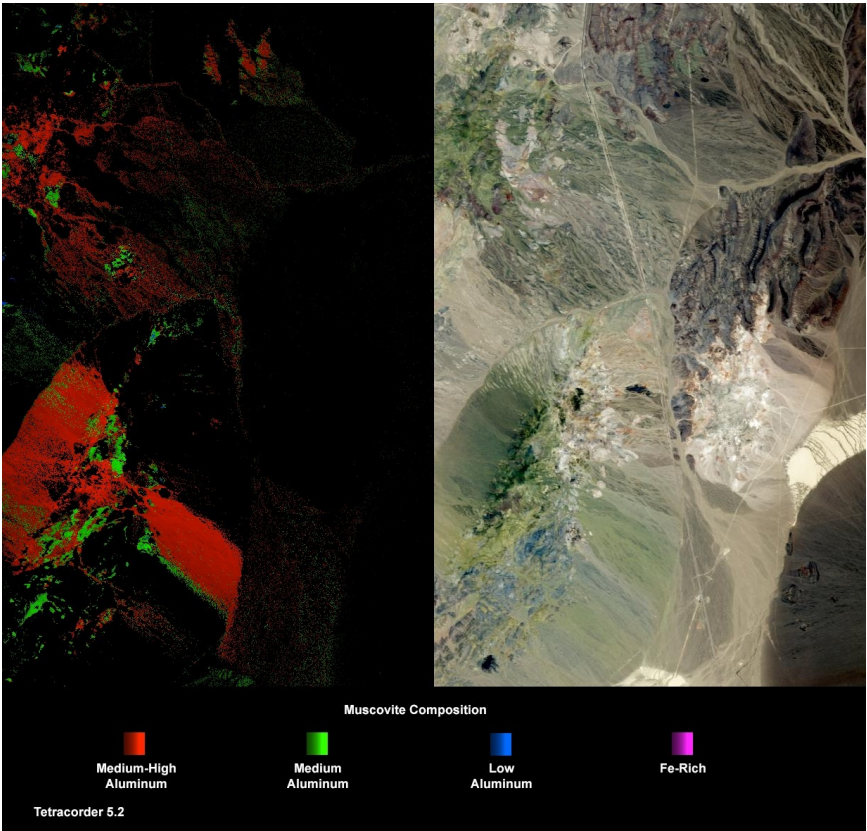
2106 Figure 11b. Group 2 minerals mapped. This is a Tetracorder standard product.
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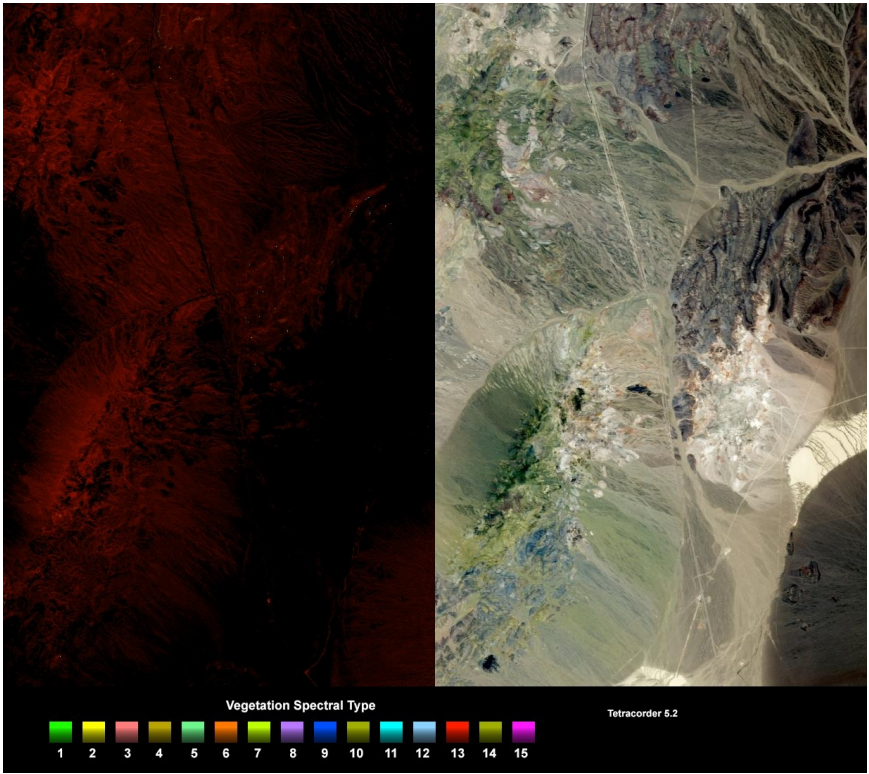
2110 Figure 11c. EMIT 8, custom RGB color composite product. This is a Tetracorder standard product.

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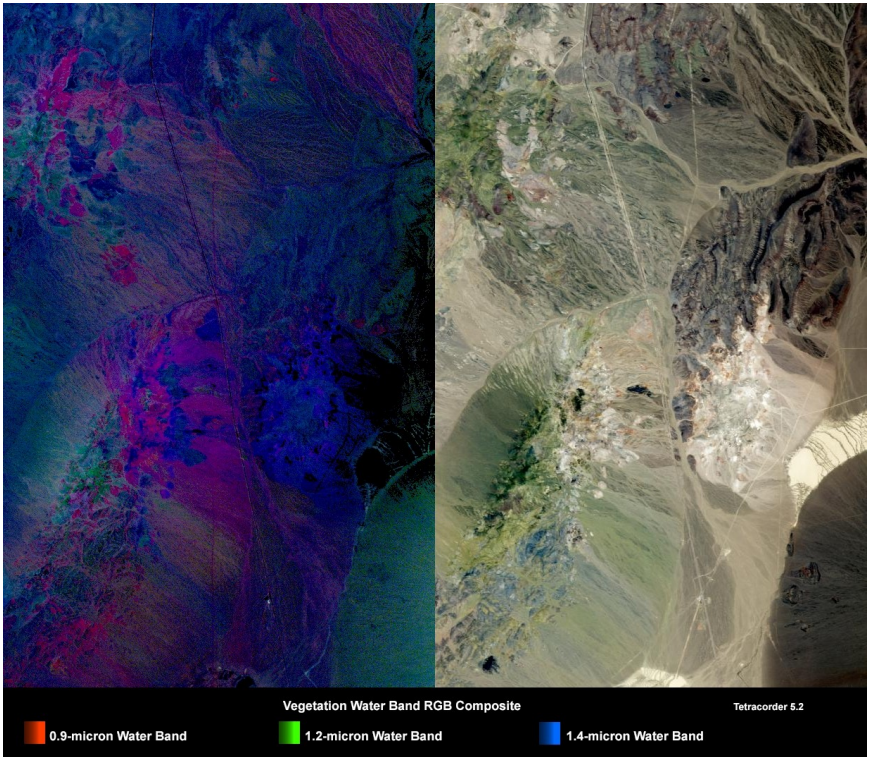


2116 Figure 11d. Muscovite aluminum content in the muscovite octahedral sites illustrates specialty product
2117 useful for specific applications. Constructing additional products like this is copying and modifying a
2118 simple script to put in the materials desired and their colors. This is a Tetracorder standard product.
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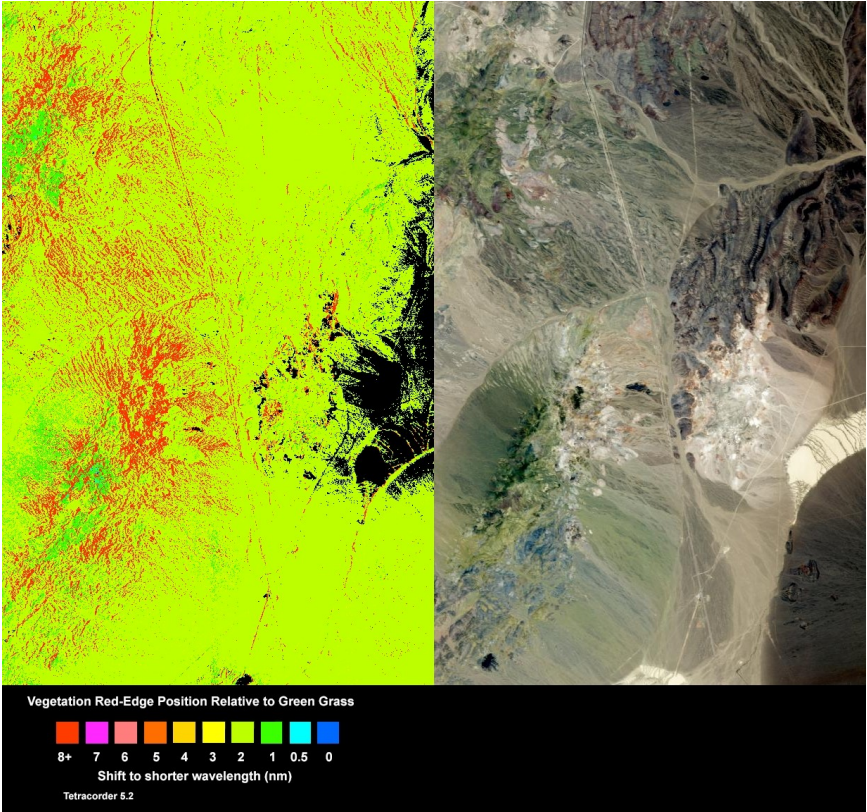


2124 Figure 11e. Detected vegetation spectral type. This is a Tetracorder standard product.
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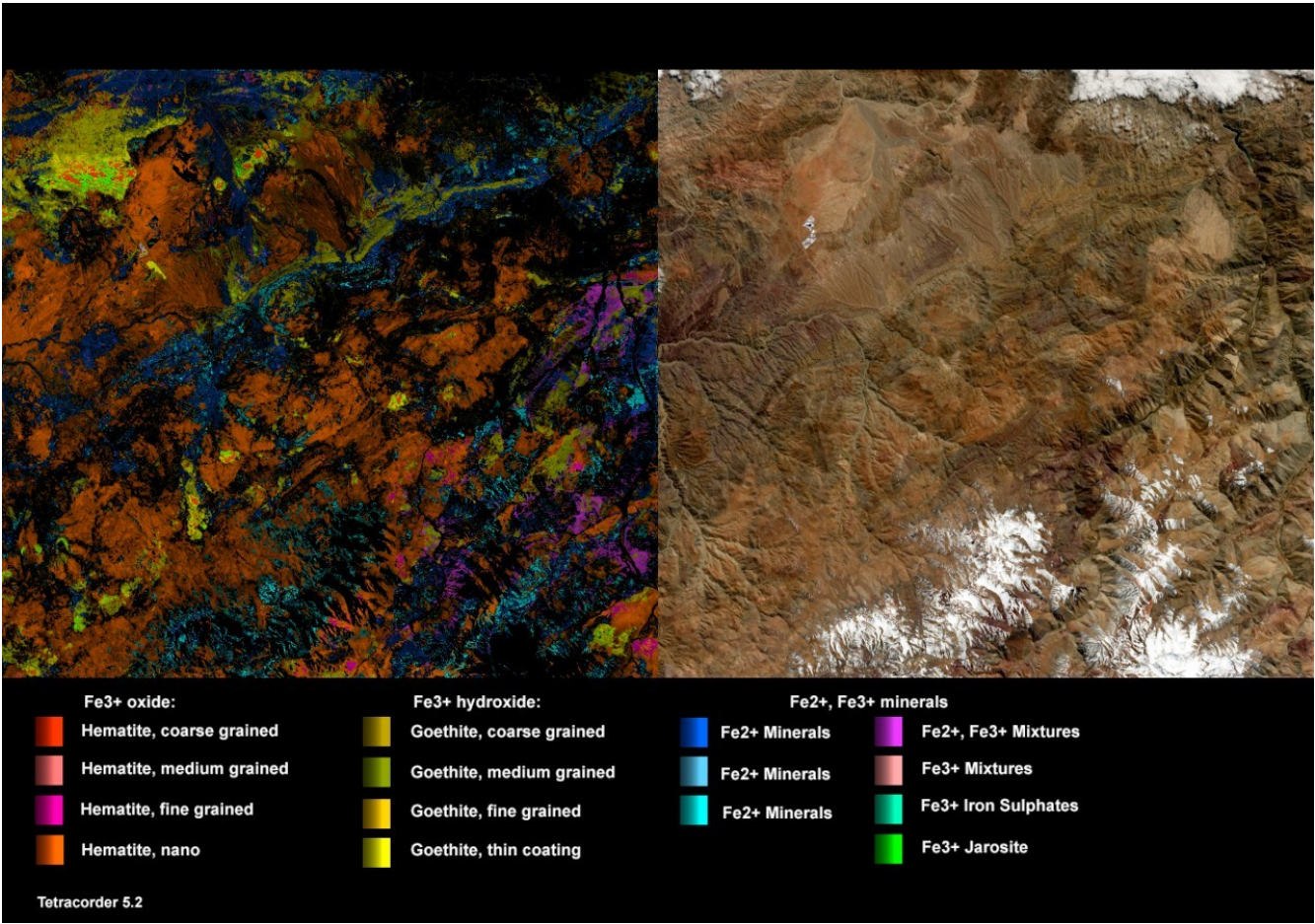


2129 Figure 11f. Vegetation water content. The water image on the left is an RGB color composite. This is
2130 a Tetraorder standard product.
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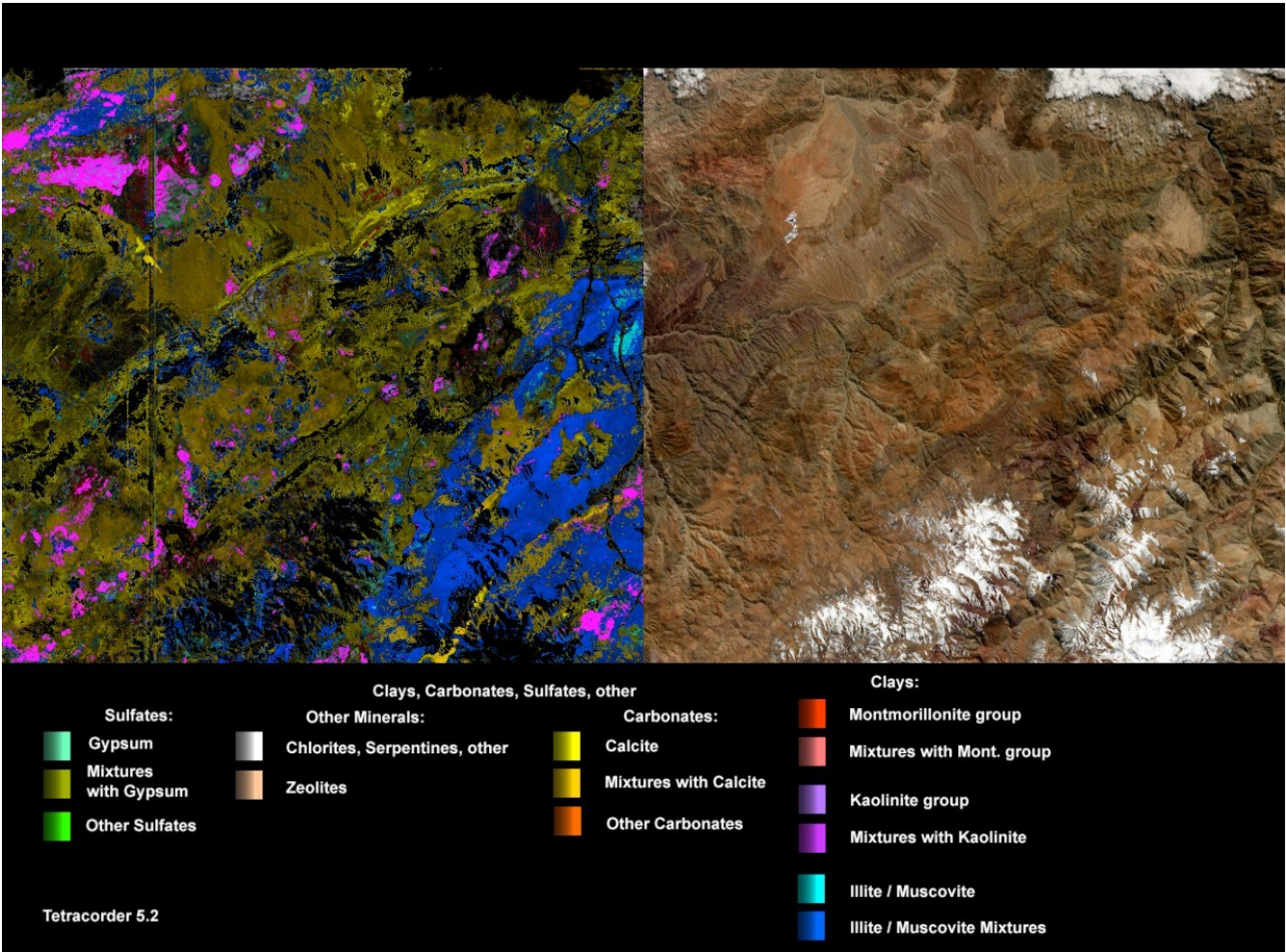
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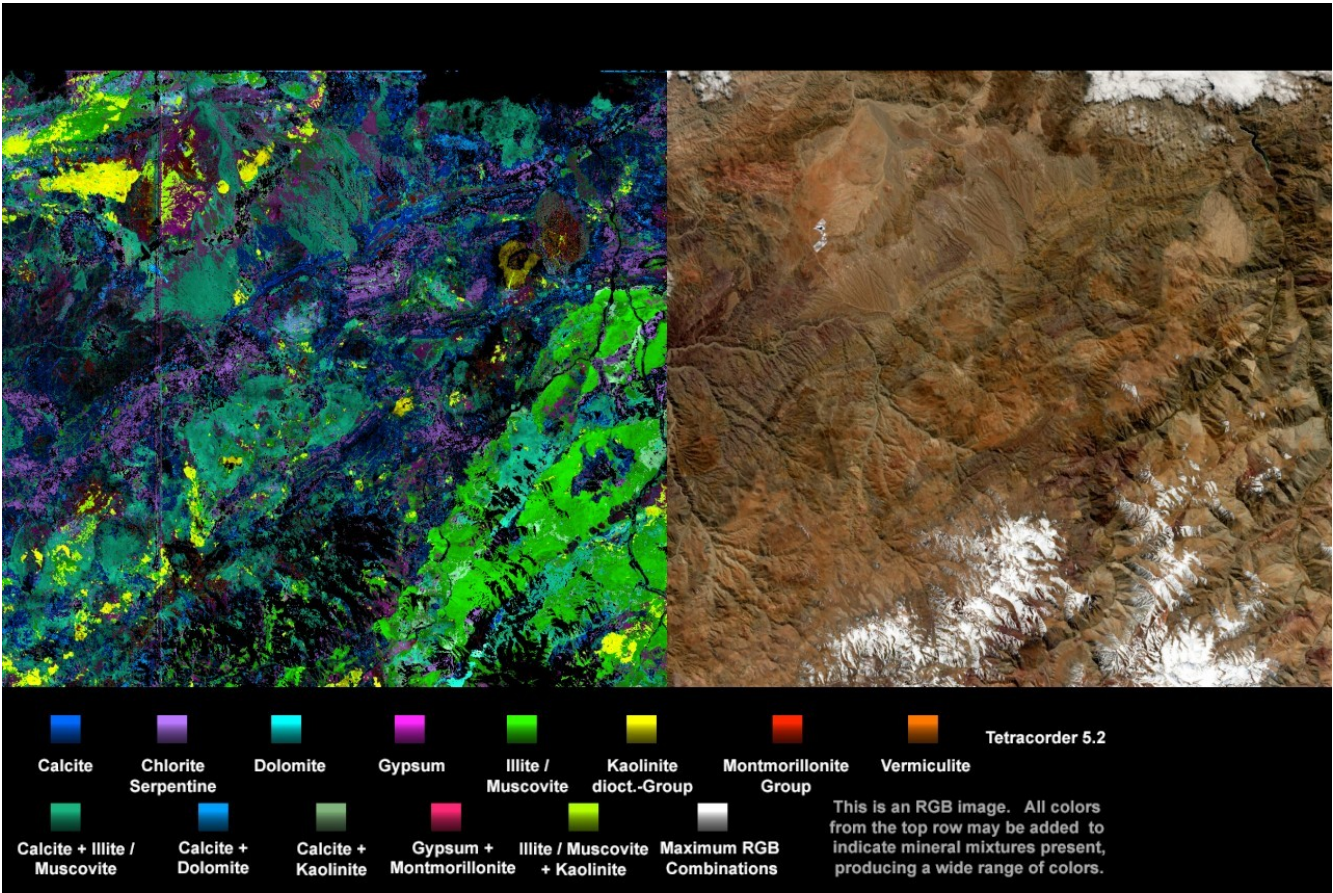
2136 Figure 11g. Vegetation red-edge position. This is a Tetracorder standard product.
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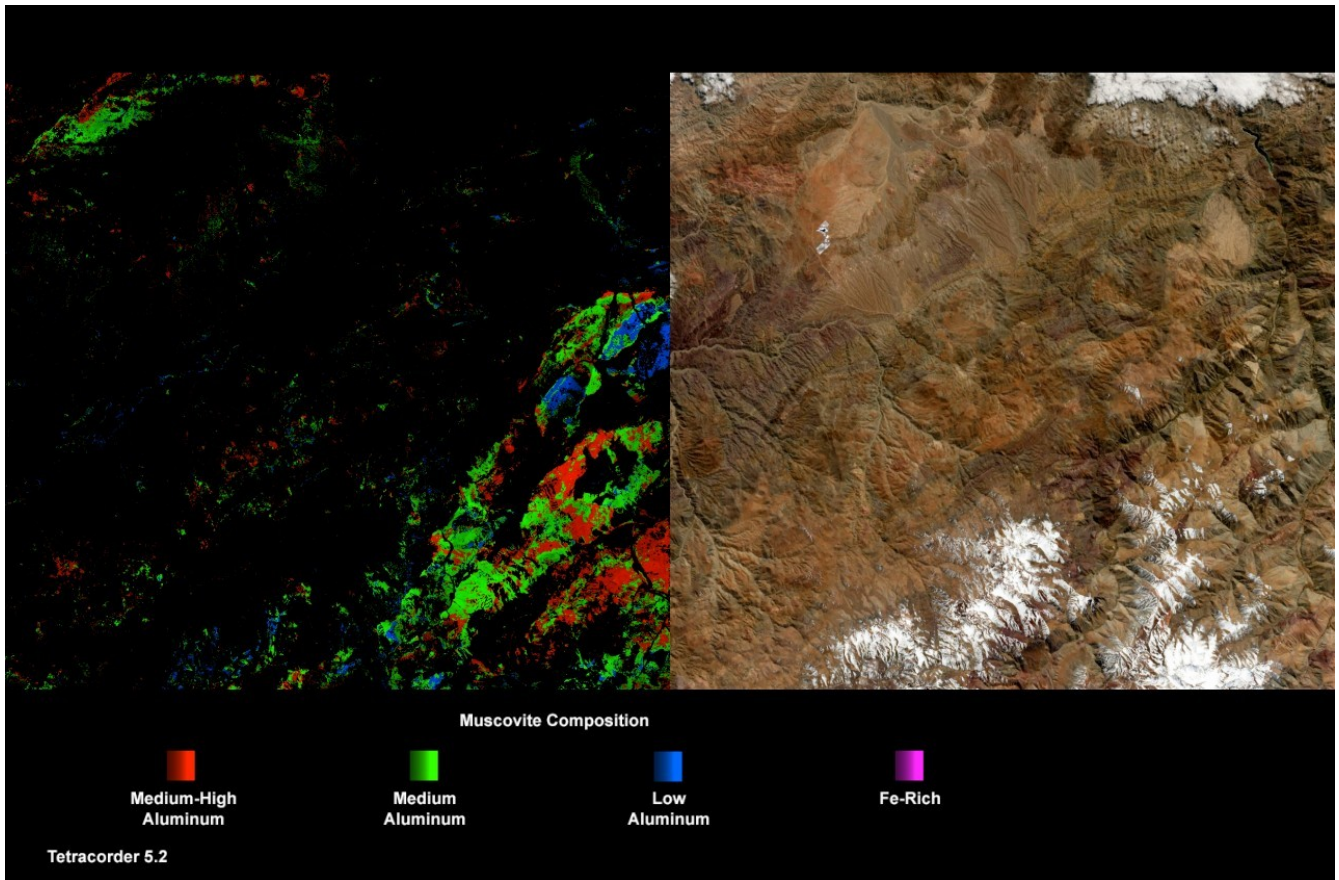
2141 Figure 12a. EMIT scene emit20220831t171631_o24311_s000_l2a_rfl_b0106_v01 Tetracorder
2142 standard product for Fe²⁺ and Fe³⁺ bearing mineral electronic absorptions in the visible to very-near
2143 infrared spectral range. The EMIT swath with is approximately 77 km, in this non-ortho-corrected
2144 scene over Chile. This is a Tetracorder standard product.
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2148 Figure 12b. EMIT scene emit20220831t171631_o24311_s000_l2a_rfl_b0106_v01 Tetracorder
2149 standard product for vibrational absorptions in the near-infrared region. The EMIT swath with is
2150 approximately 77 km, in this non-ortho-corrected scene over Chile. This is a Tetracorder standard
2151 product.
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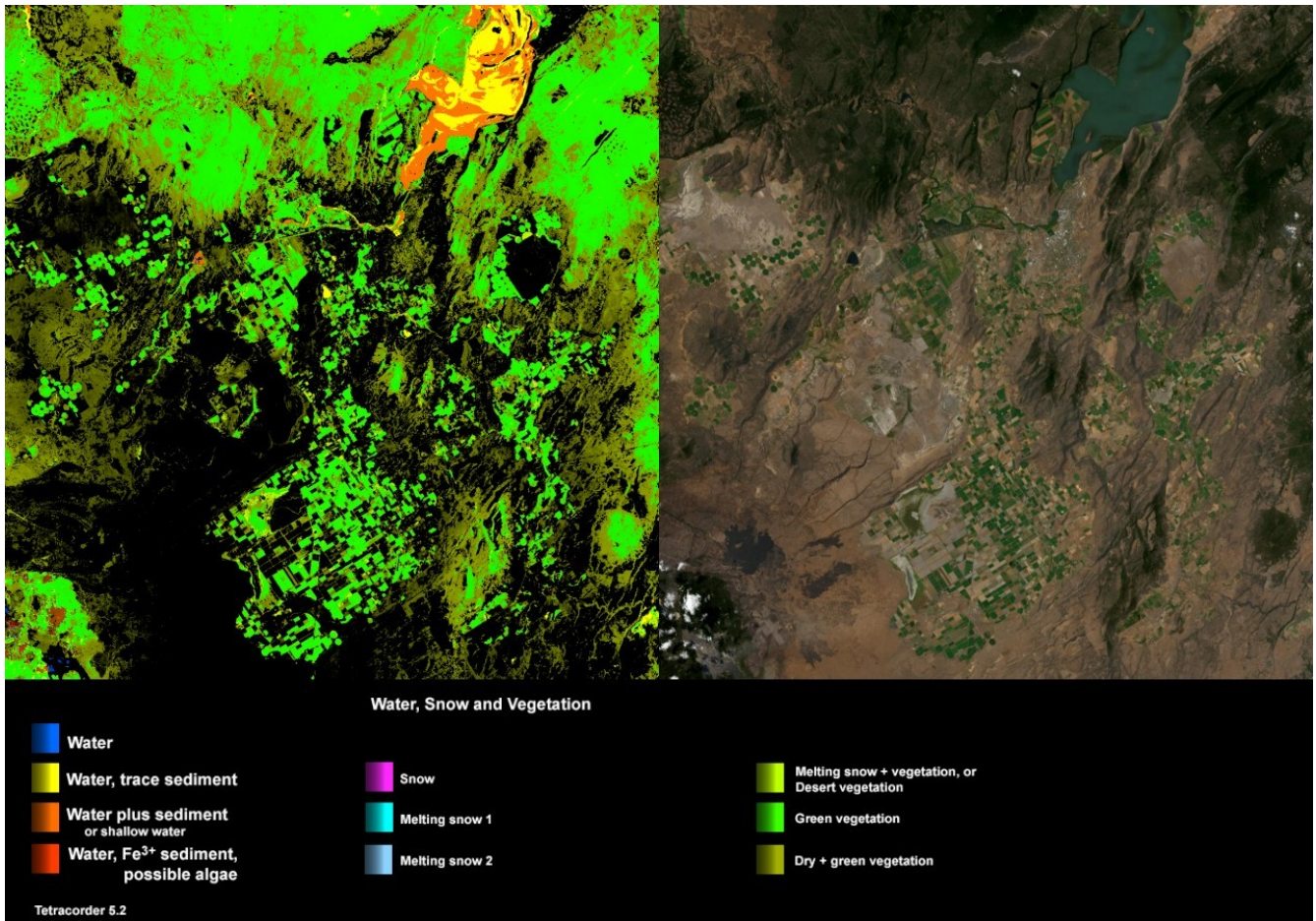


2155 Figure 12c. EMIT scene emit20220831t171631_o24311_s000_l2a_rfl_b0106_v01 Tetracorder
2156 standard product for the EMIT 8 minerals (excluding hematite and goethite): calcite,
2157 chlorite/serpentine, dolomite, gypsum, illite/muscovite, kaolinite-dioctahedral group, montmorillonite
2158 group, and vermiculite. The EMIT swath with is approximately 77 km, in this non-ortho-corrected
2159 scene over Chile. This is a Tetracorder standard product.
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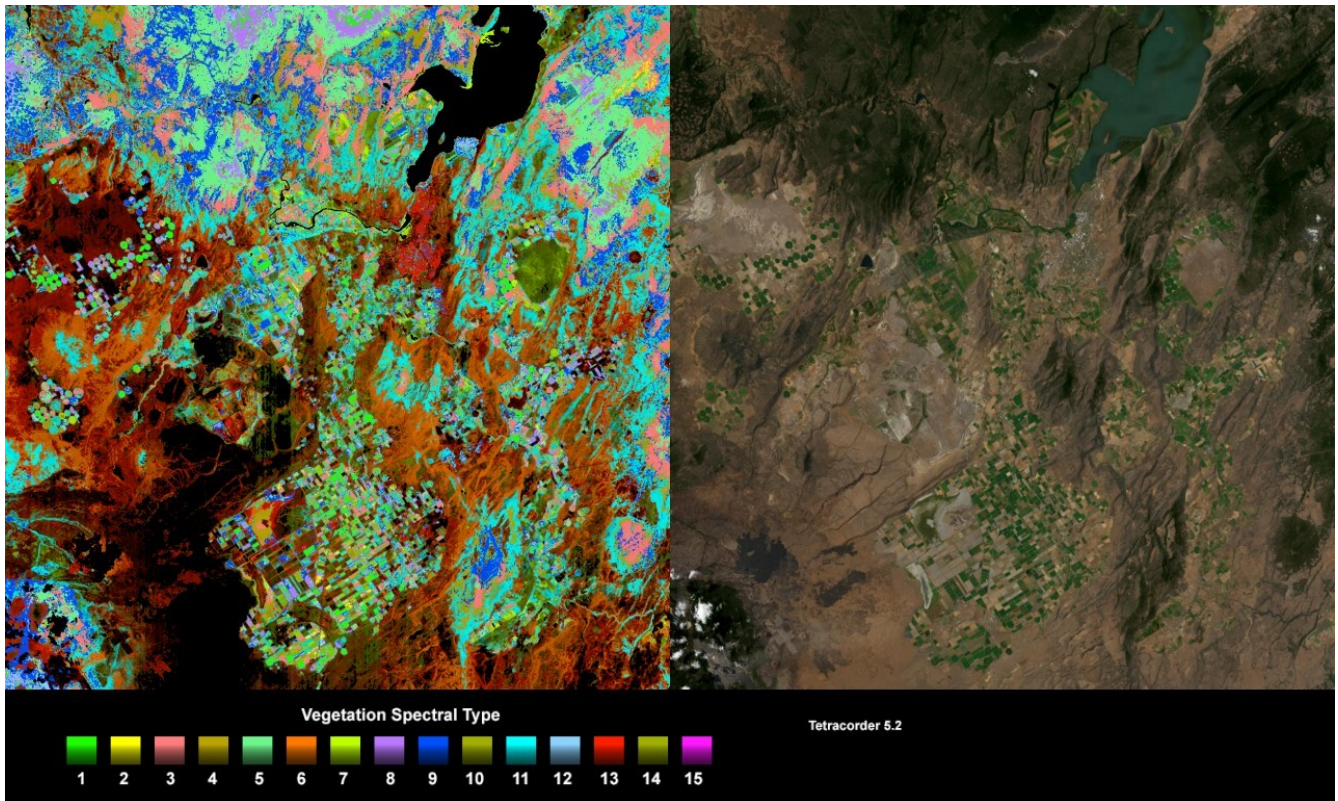


2163 Figure 12d. EMIT scene emit20220831t171631_o24311_s000_l2a_rfl_b0106_v01 Tetracorder
 2164 standard product for aluminum content in the octahedral layer in muscovite/illite. The EMIT swath
 2165 with is approximately 77 km, in this non-ortho-corrected scene over Chile. This is a Tetracorder
 2166 standard product.
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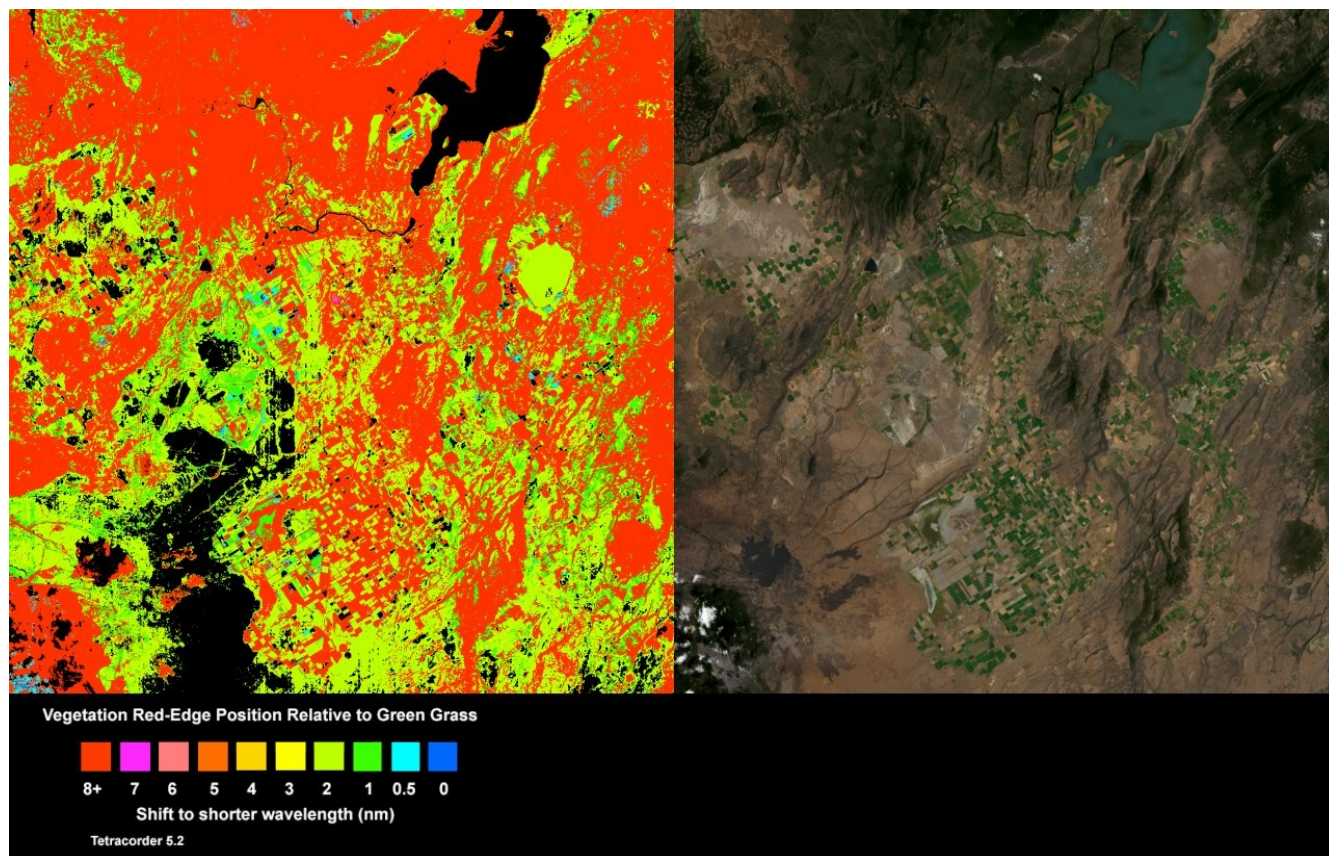


2171 Figure 13a. EMIT scene emit20220814t223444_o22615_s000_l2a_rfl_b0106_v01 Tetracorder
2172 standard product showing vegetation, snow and and melting snow, and water sediments and another
2173 contaminants. Each of these are combinations of images showing finer detail. The EMIT swath with is
2174 approximately 77 km, in this non-ortho-corrected scene on the U. S. California-Nevada border. North
2175 is to the upper right. This is a Tetracorder standard product.
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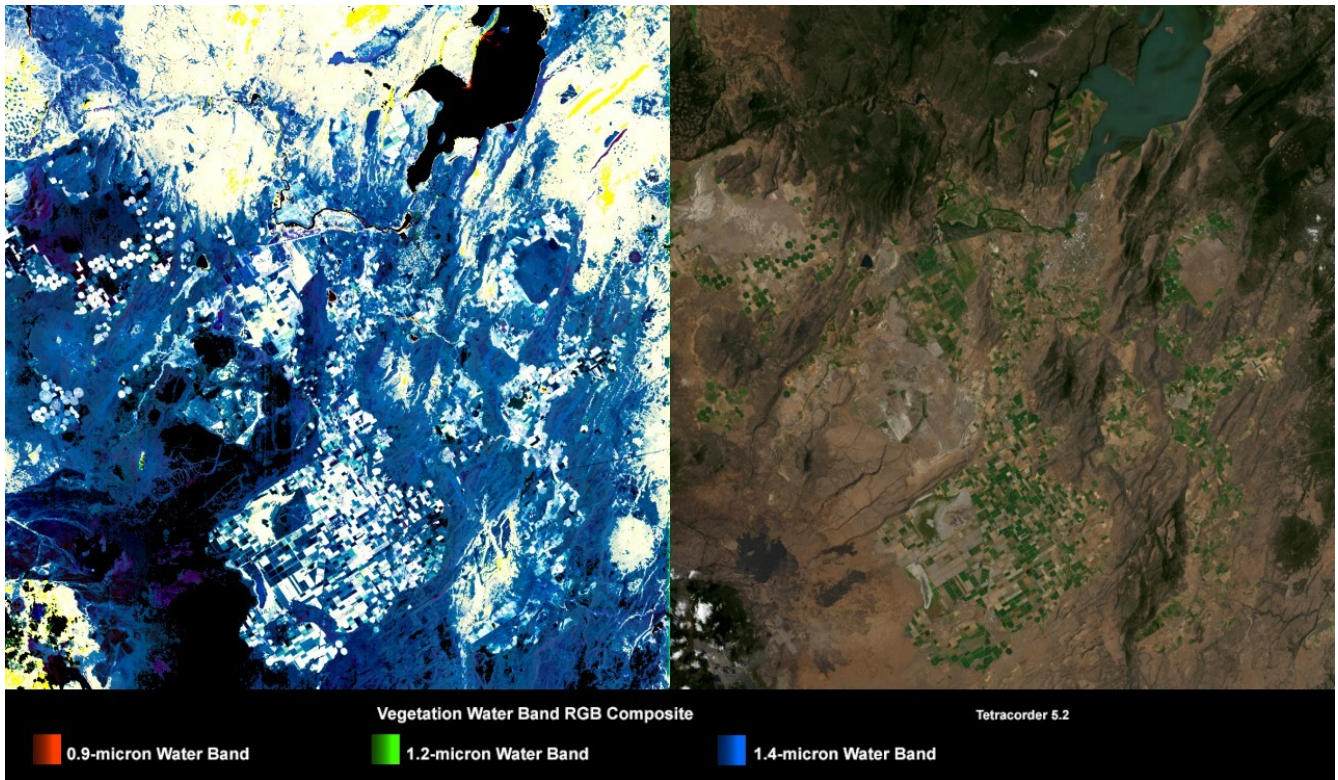


2181 Figure 13b. EMIT scene emit20220814t223444_o22615_s000_l2a_rfl_b0106_v01 Tetracorder
 2182 standard product showing vegetation spectral type. The spectral type was determined using the shape
 2183 of the chlorophyll absorption like that shown in Figure 9b. The EMIT swath width is approximately 77
 2184 km, in this non-ortho-corrected scene on the U. S. California-Nevada border. North is to the upper
 2185 right. This is a Tetracorder standard product.
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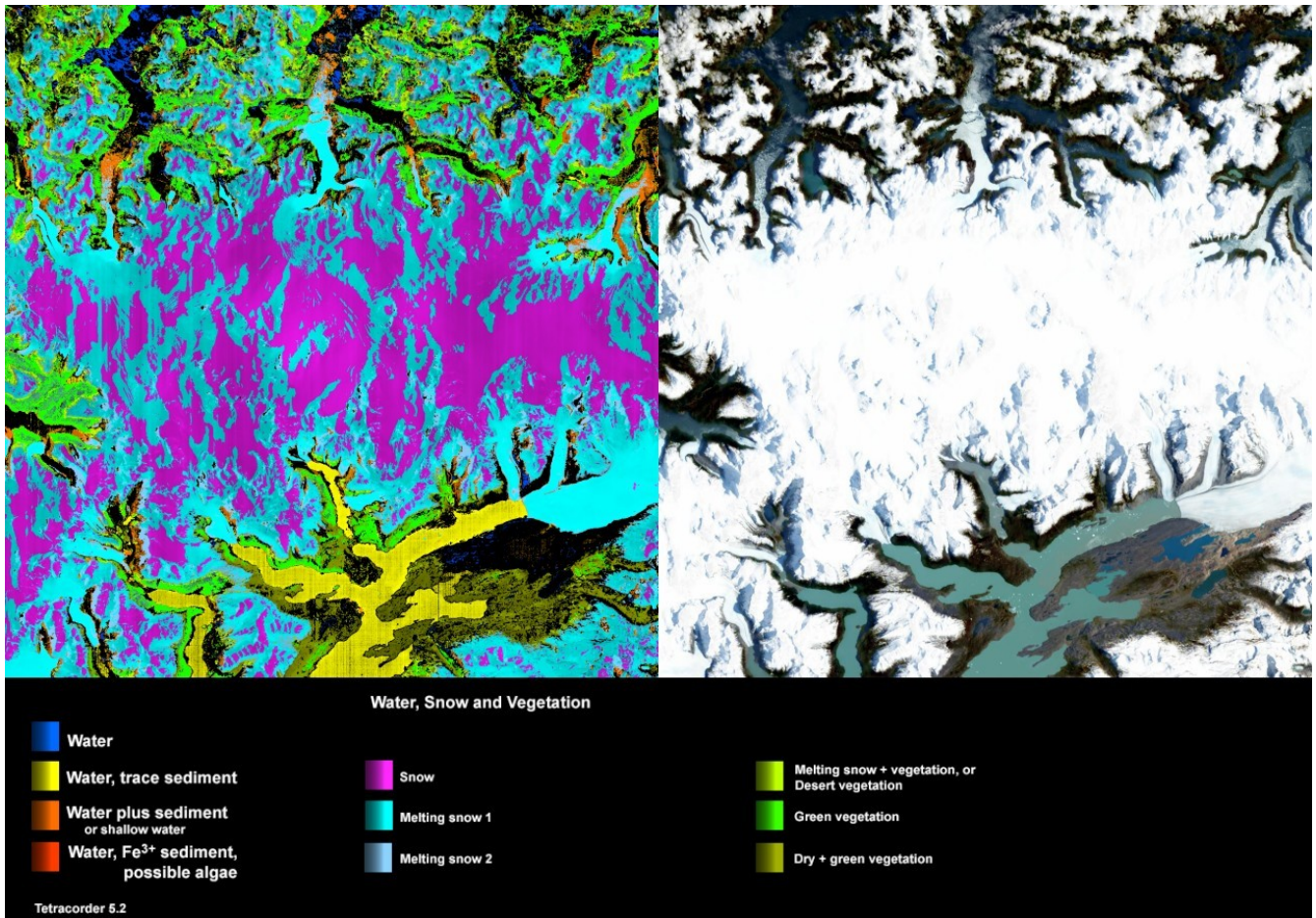


2191 Figure 13c. EMIT scene emit20220814t223444_o22615_s000_l2a_rfl_b0106_v01 Tetracorder
2192 standard product showing the chlorophyll absorption edge position near $0.7\text{ }\mu\text{m}$ relative to the position
2193 of a green lawn grass. The EMIT swath width is approximately 77 km, in this non-ortho-corrected scene
2194 on the U. S. California-Nevada border. North is to the upper right. This is a Tetracorder standard
2195 product.
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2200 Figure 13d. EMIT scene emit20220814t223444_o22615_s000_l2a_rfl_b0106_v01 Tetracorder
 2201 standard product showing relative strengths of the water absorptions in vegetation in the RGB
 2202 composite image. Blue areas have relatively weak 0.9 and 1.2- μm water absorptions thus less water.
 2203 White areas have three absorptions strong, thus higher water content. The EMIT swath with is
 2204 approximately 77 km, in this non-ortho-corrected scene on the U. S. California-Nevada border. North
 2205 is to the upper right. This is a Tetracorder standard product.
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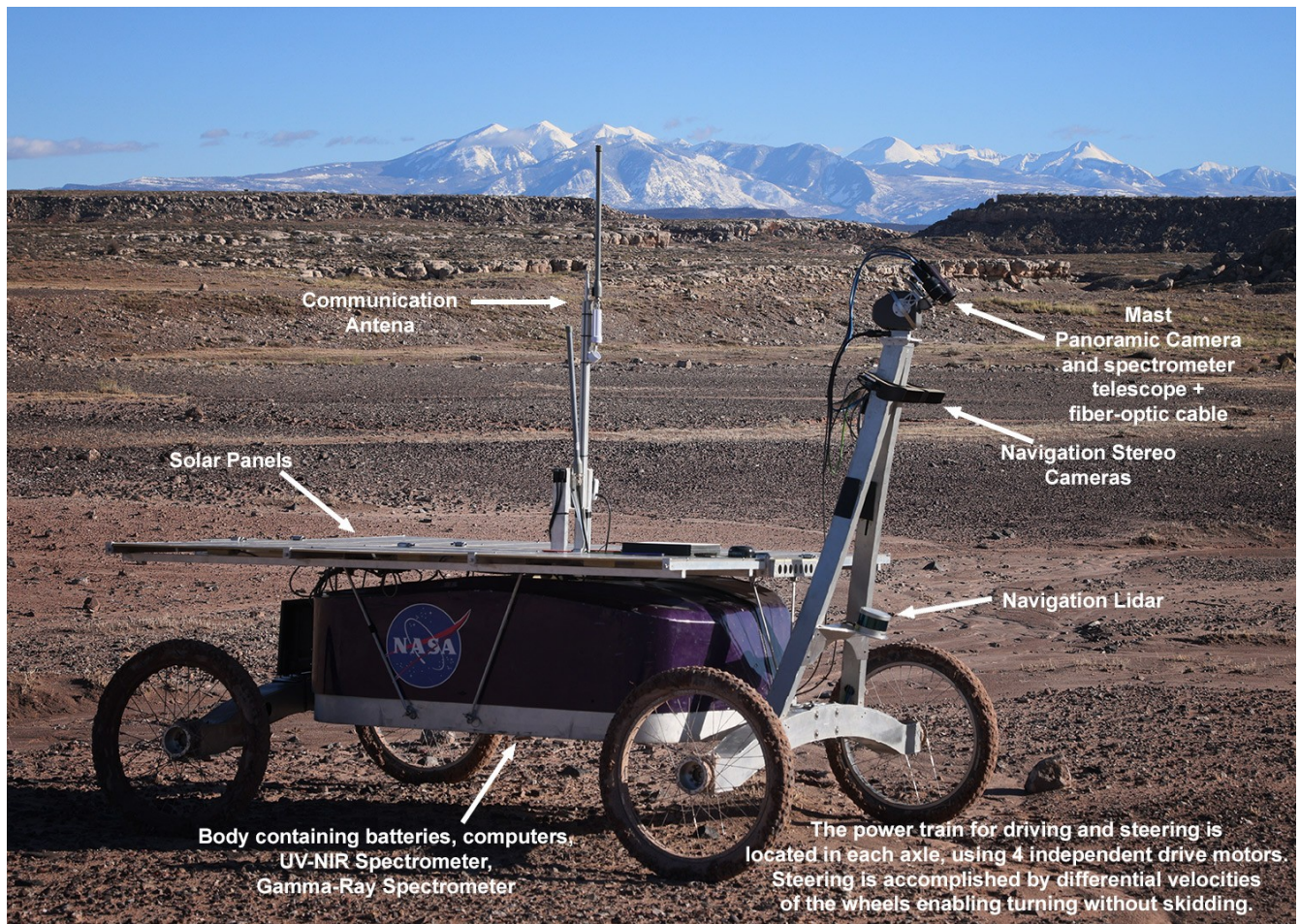
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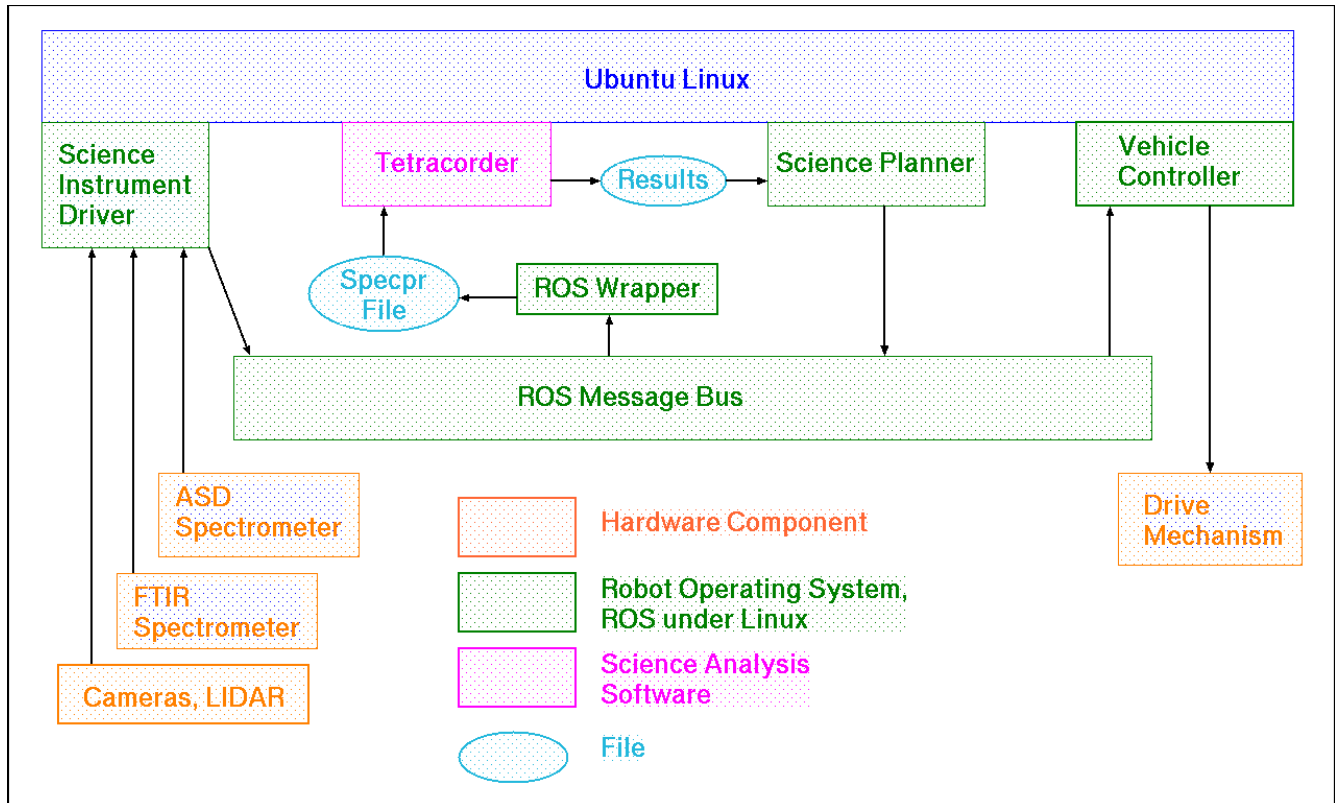
2212 Figure 14. EMIT scene emit20220912t154138_o25510_s001_l2a_rfl_b0106_v01 Tetracorder
2213 standard product showing a mountain snow scene in the Chile-Argentina border. The snow shows no
2214 detectable melting at higher elevations (magenta), but melting at lower elevations (cyan, light blue).
2215 Also shown are sediments in water from the snow melt. The EMIT swath width is approximately 77
2216 km. This is a Tetracorder standard product.

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2225 Figure 15. Zoë rover in the field. For scale, the height of the Mast is about 3 meters. Tetracorder runs
2226 on a Ubuntu Linux computer in the body of the rover, analyzing data real time from an Analytical
2227 Spectral Devices, ASD, spectrometer covering 0.35 to 2.5 μm . The spectrometer is located in the body
2228 under the solar panels and receives light via a fiber optic feed from a telescope mounted at the top of
2229 the mast. Here the telescope and mast camera are point down in front of the rover to analyze data as
2230 the rover autonomously drives forward. The view is to the southeast toward the La Sal Mountains near
2231 Moab Utah.
2232



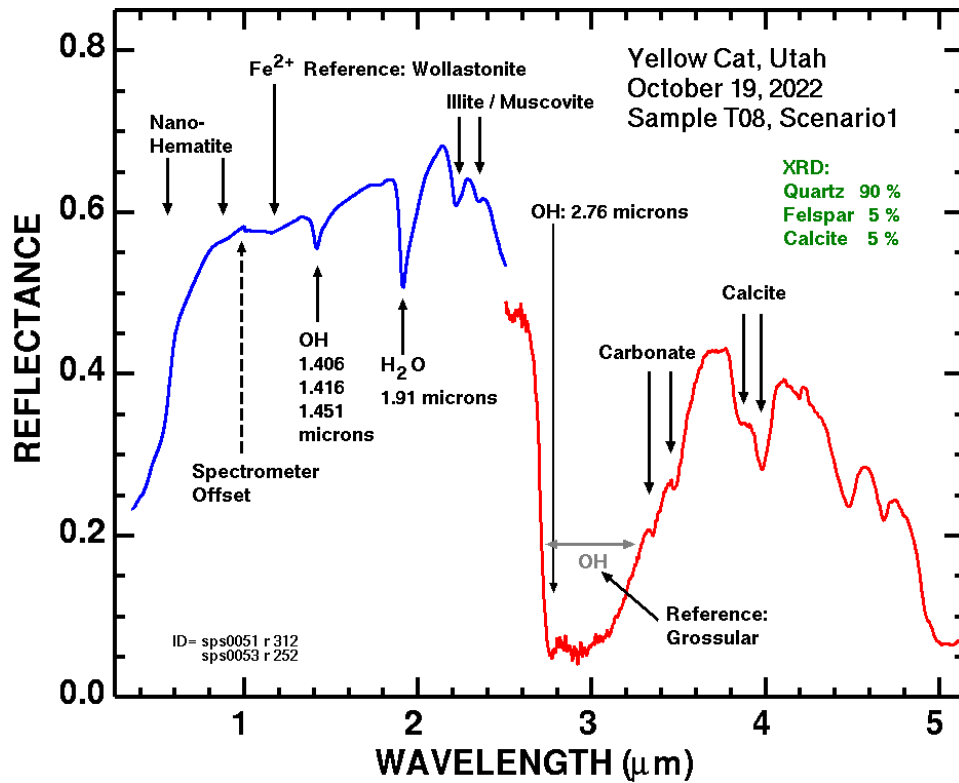
2235 Figure 16. A simplified version of the data flow and how Tetracorder is integrated into the system.
 2236 Data from the ASD spectrometer is collected and pushed to the ROS message bus. Tetracorder is
 2237 started using a ROS wrapper program and spectra are fed by updating a specpr file. Tetracorder is run
 2238 using the 'single spectrum' mode for this operation, following the growing specpr file. After processing
 2239 the spectra, Tetracorder writes the results to a results file which is then read by the Science Planner
 2240 which analyzes the detections and generates guidance plans. The Vehicle Controller picks up the
 2241 plans generated by the Science Planner and gives instructions to the drive mechanism to visit the next
 2242 location.

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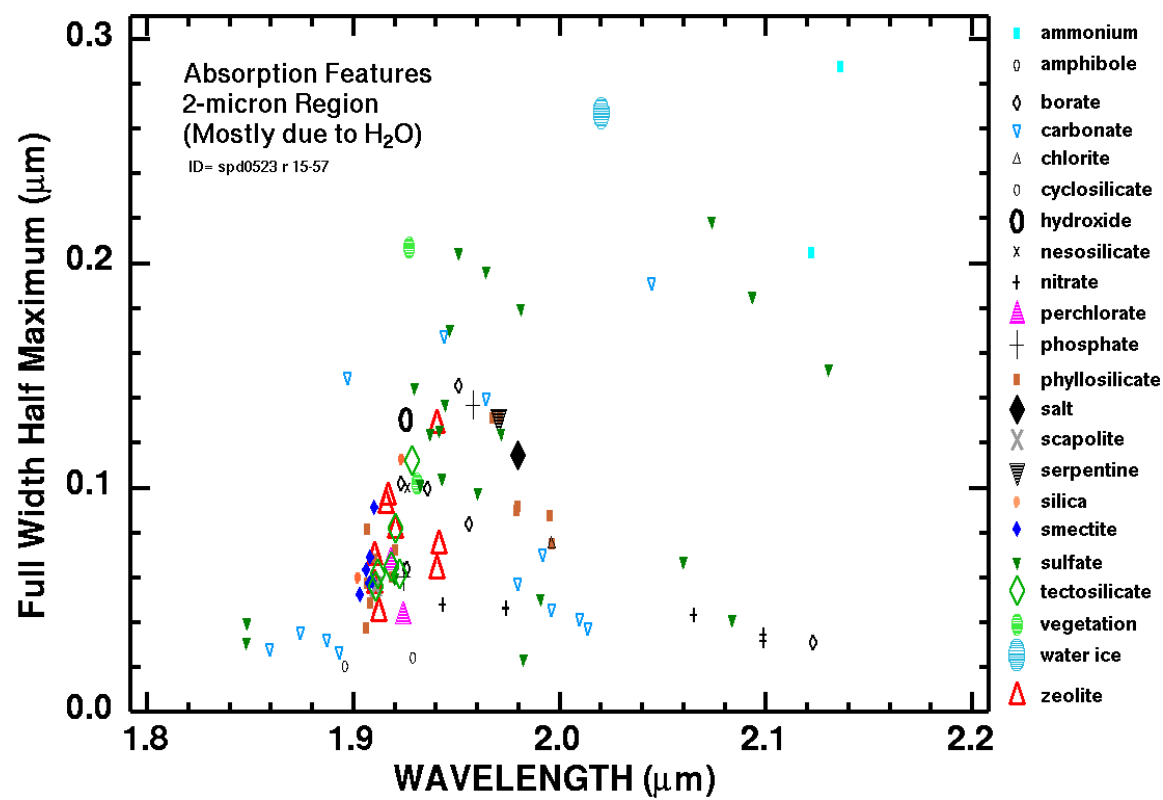
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2251 Figure 17. Spectra and XRD results obtained by the Zoë rover contact instruments during the Yellow
2252 Cat, Utah October 2022 field campaign. The labeled spectral features are the Tetracorder
2253 identifications. XRD results were not obtained real time for the rover to use. The blue spectrum is
2254 from an ASD spectrometer, and the red spectrum is from an FTIR spectrometer, both contact
2255 instruments. Flagged features (arrows) are Tetracorder identifications. The Fe²⁺ Wollastonite is an
2256 identification of and Fe²⁺ absorption and not necessarily diagnostic of Wollastonite, only that
2257 Wollastonite was the reference spectrum. Features with no arrows were not evaluated by Tetracorder.
2258 Note that the carbonate features near 3.4 μm, could be misidentified as organics if there are no
2259 carbonate reference spectra for this wavelength region in the Tetracorder expert system.

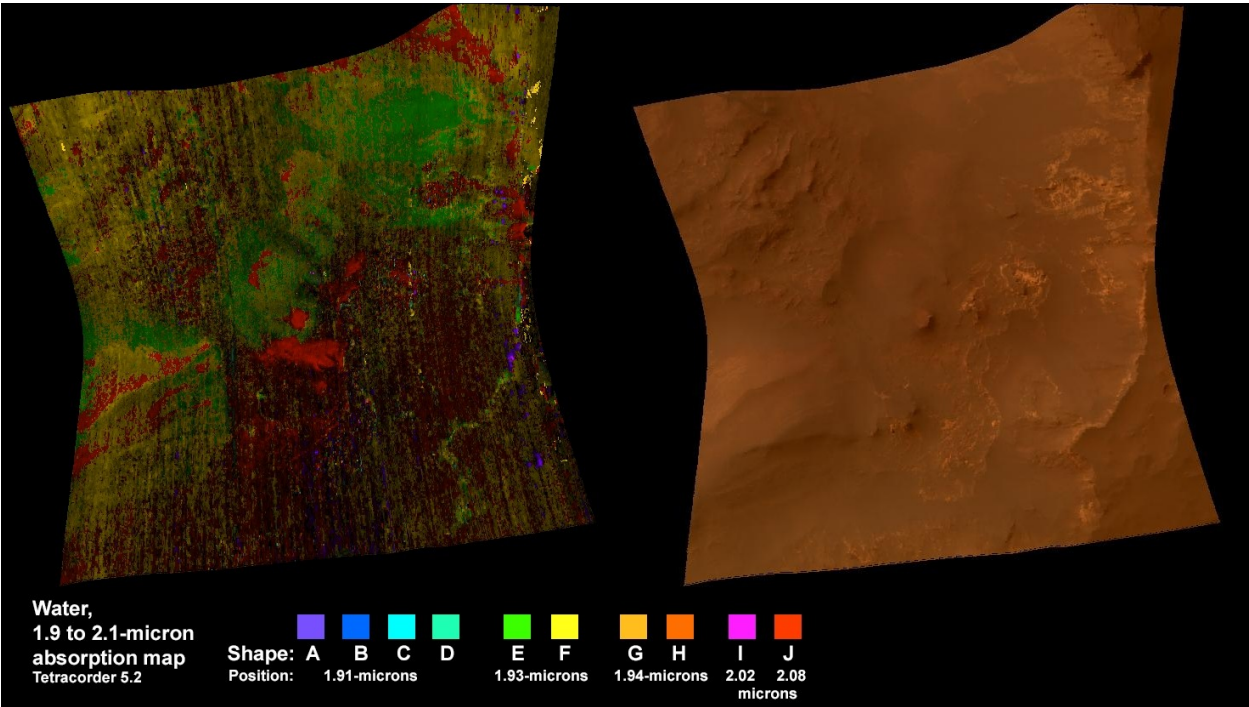
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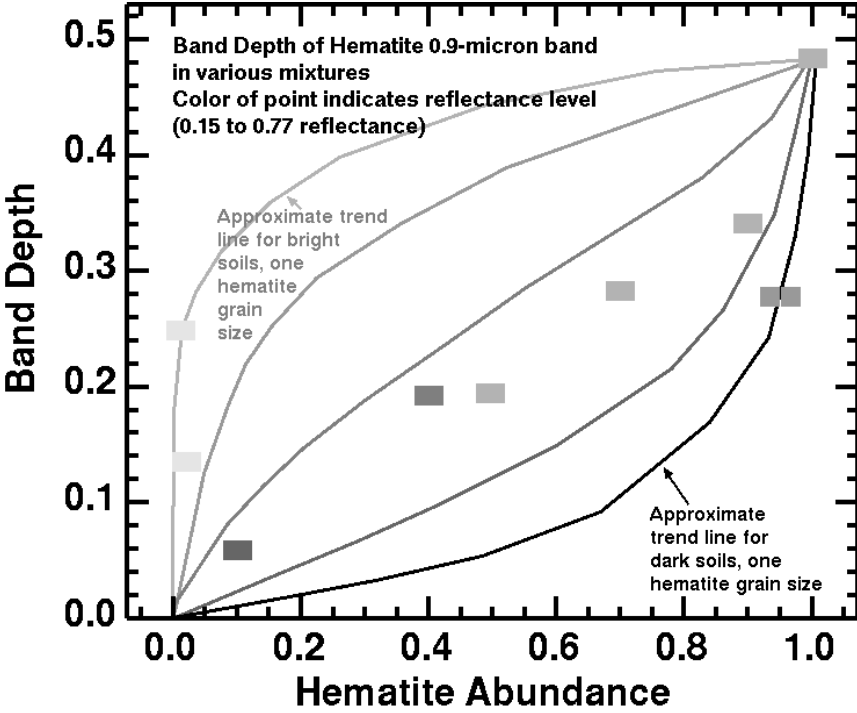


2265 Figure 18. Water absorption positions and widths derived from the USGS spectral library 06 (Clark et
2266 al., 2007) for materials measured in a dry environment.

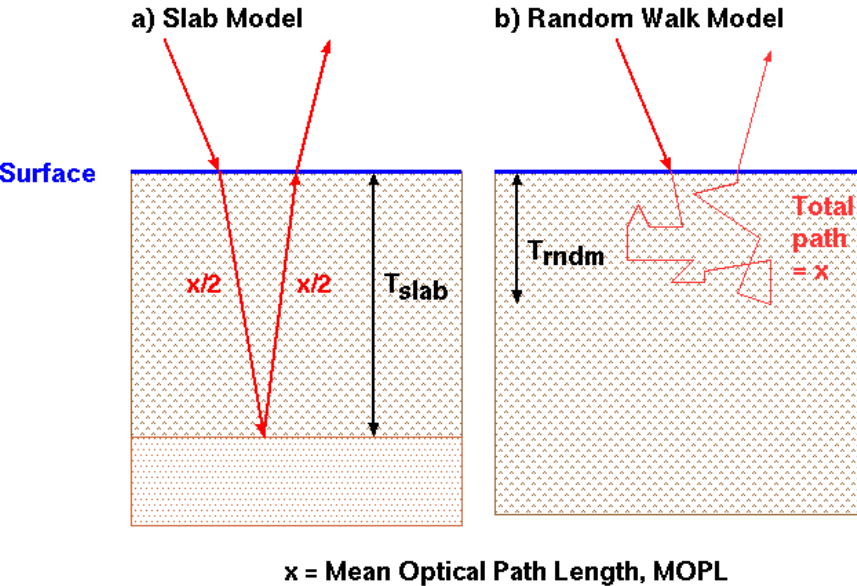
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2272 Figure 19. Tetracorder standard product showing the 1.9-μm water band position for Mars
2273 Reconnaissance Orbiter, Compact Reconnaissance Imaging Spectrometer for Mars (CRISM) image
2274 cube FRT0000B385_07_IF164J_MTR3. Red indicates a very long 1.9-μm band position typical of
2275 sulfates. Absorptions indicate the sulfate kieserite is present. Green and yellow, indicating absorptions
2276 in the 1.93-μm region are less diagnostic, consistent with phyllosilicates or other sulfates. Some
2277 montmorillonite mapped in the green area near the upper right corner based on detection of a 2.2-μm
2278 feature.

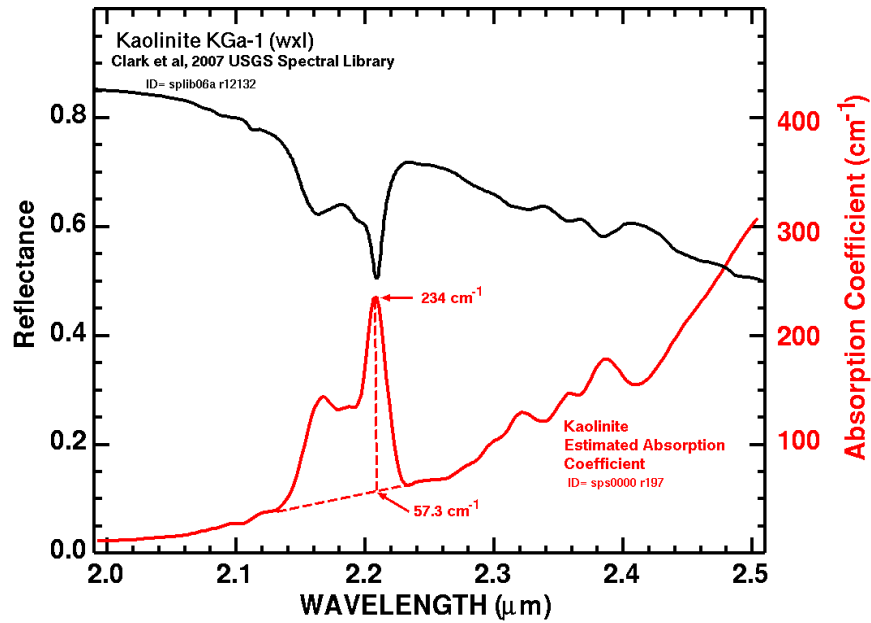


2280 Figure 20. Band depth of the Hematite 0.9- μ m band as a function of abundance and continuum
2281 reflectance (lightness of the gray rectangles). The relationship can be considered piece wise linear as
2282 long as one stays within the bounds where linearity is valid. The trend lines are derived from models.
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2288 Figure 21. a) The non-scattering slab model used the derived MOPL from optical constants and is used
 2289 in Model 2. b) The random walk model uses the derived MOPL from optical constants and is used in
 2290 Models 3 and 4.

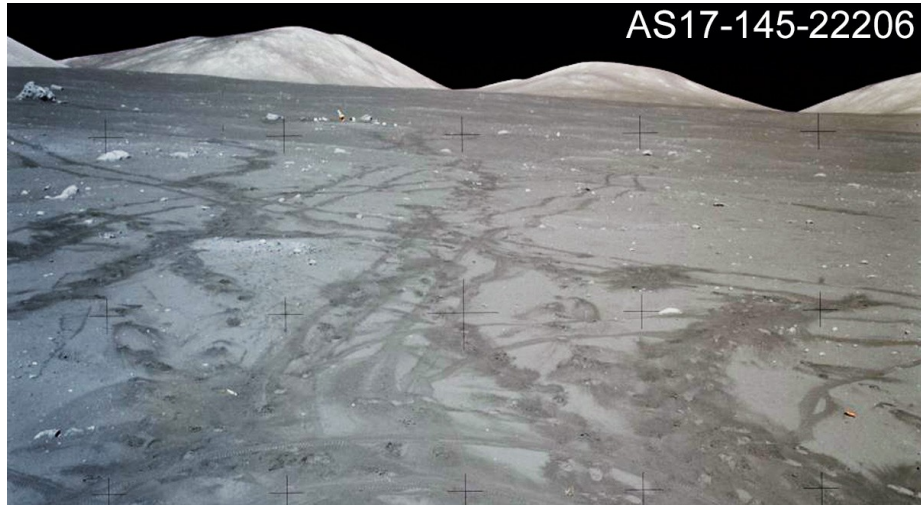
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 2292



2293 Figure 22. Reflectance and estimated absorption coefficients for kaolinite in the USGS spectral library
 2294 6 (Clark et al., 2007). The delta absorption coefficient, $\Delta k = k_b - k_c = 234 - 57.3 = 176.7 \text{ cm}^{-1}$. From the
 2295 observed band depth in the reflectance spectrum, the MOPL = 24 μm .

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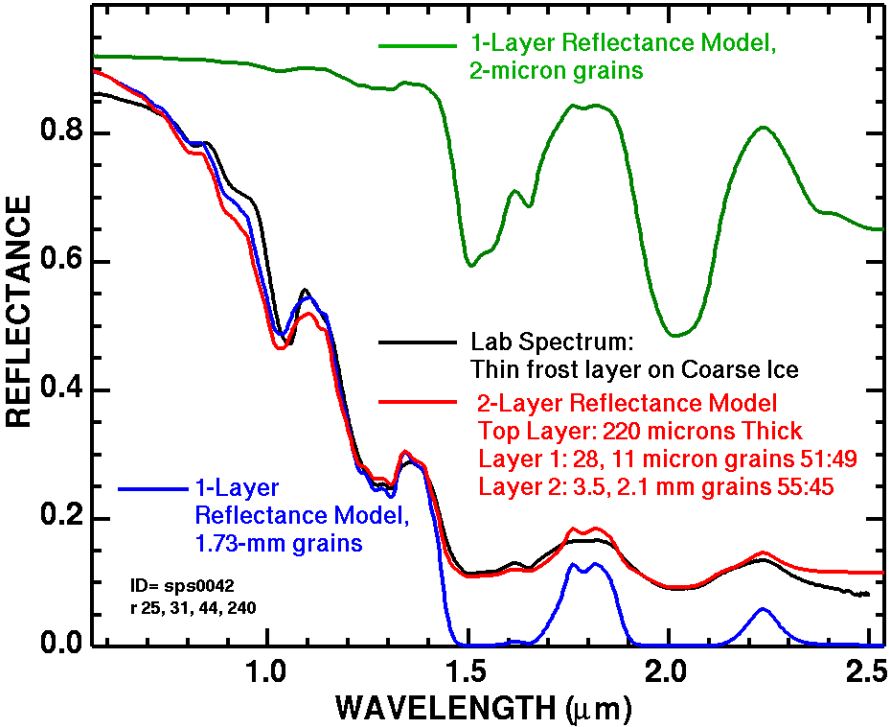
2301 Figure 23. Image of the lunar surface with rover tracks showing the disturbed soil is darker and
2302 different in color than the surface, indicating changes in grain size and/or composition
2303 with depth. Contrast has been increased from the original to show the tracks better. AS17-145-22206
2304 Apollo 17, 1972 Hasselblad image taken post Extravehicular Activity EVA 3. The original film
2305 magazine was labeled D.

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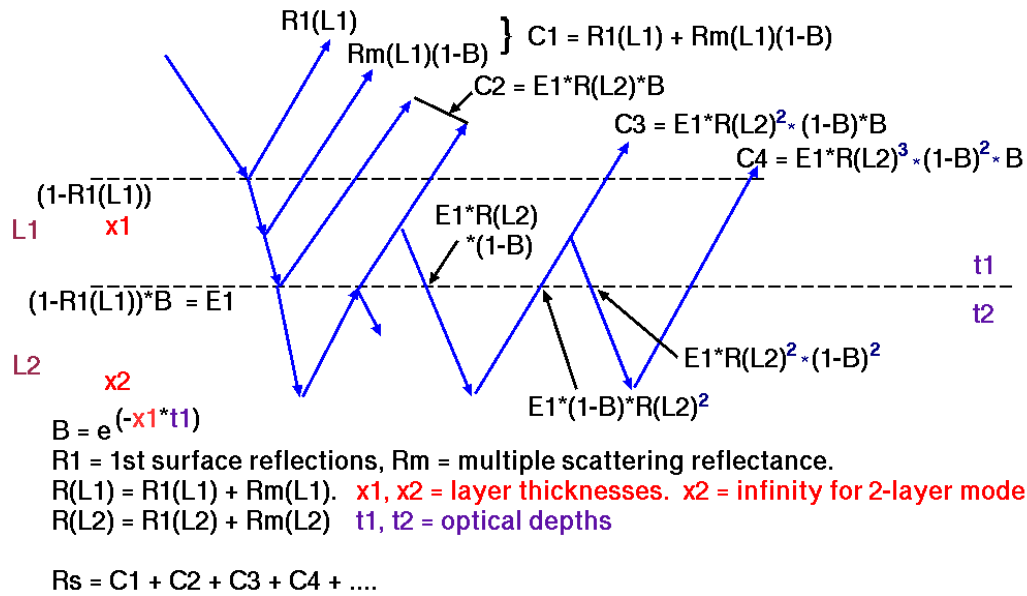
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2312 Figure 24. Model spectra of a layered surface with larger grain sizes deeper down (red line) results in
2313 increasing band depths in spectral regions with lower absorption coefficients and matches the
2314 lab data (black line). Such layered media enhances weak bands, like the 1.04- μm absorption, exactly as
2315 observed in the Saturn system. Non-layered models (green and blue curves) cannot match
2316 the observed lab spectrum (black curve), but the layered model (red curve) shows a close
2317 match. Non layered models can only match band depths for some absorptions whereas the
2318 layered model closely matches all. This new model is derived from the Clark et al. (2012)
2319 radiative transfer algorithms plus Clark and Roush (1984) equations 18 to 24. See Table 6
2320 for derived band depths.

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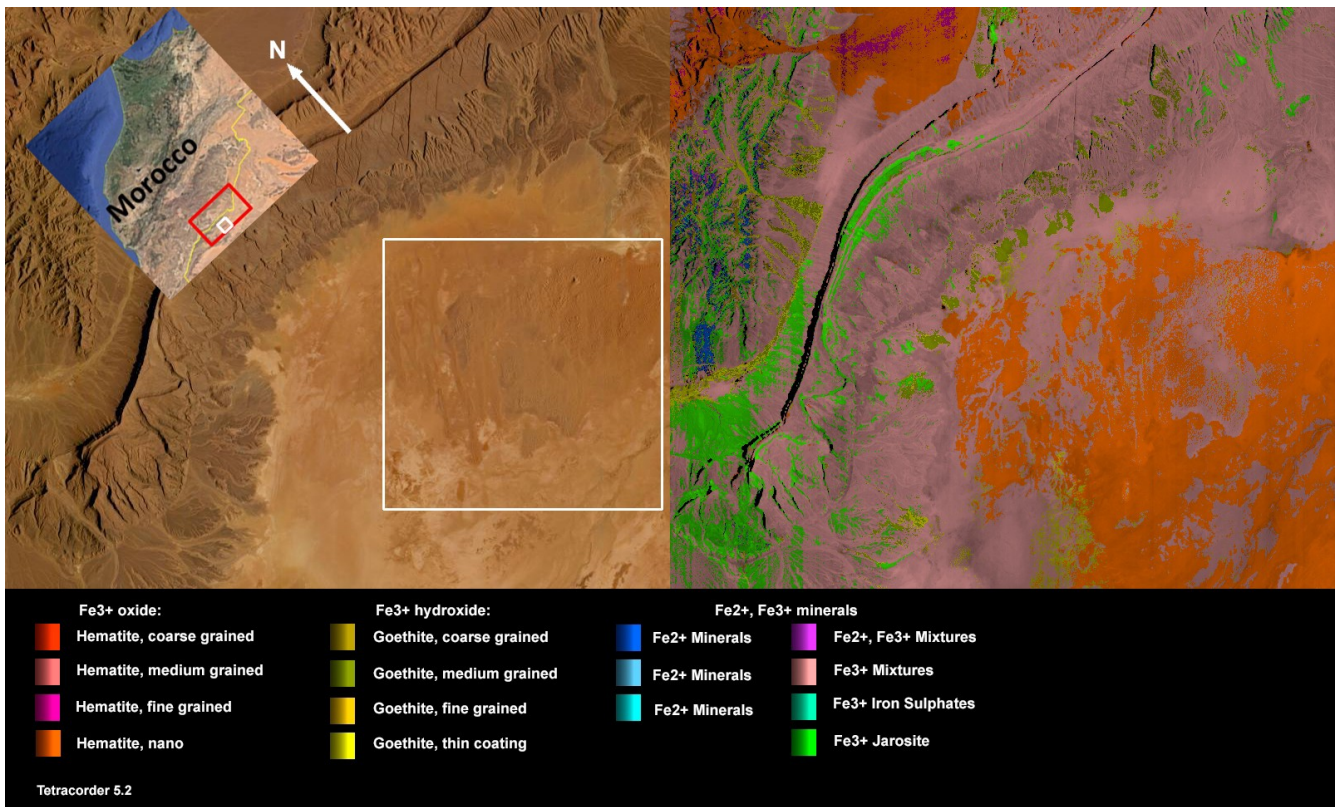
2327 Figure 25. Example of multi-stream equations for reflectance, R_s , from a multi-layer surface. The
 2328 multi-stream model is coded and operational for up to 3-layer models.

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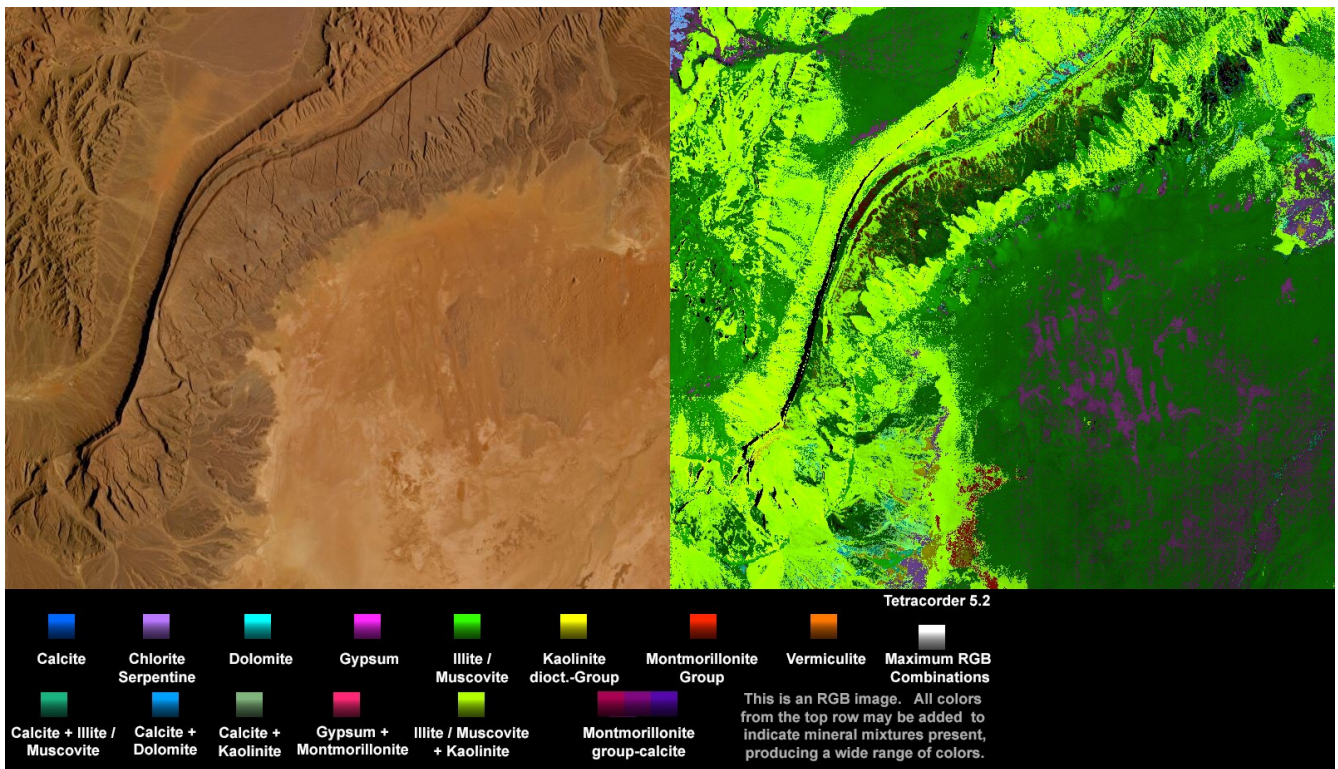
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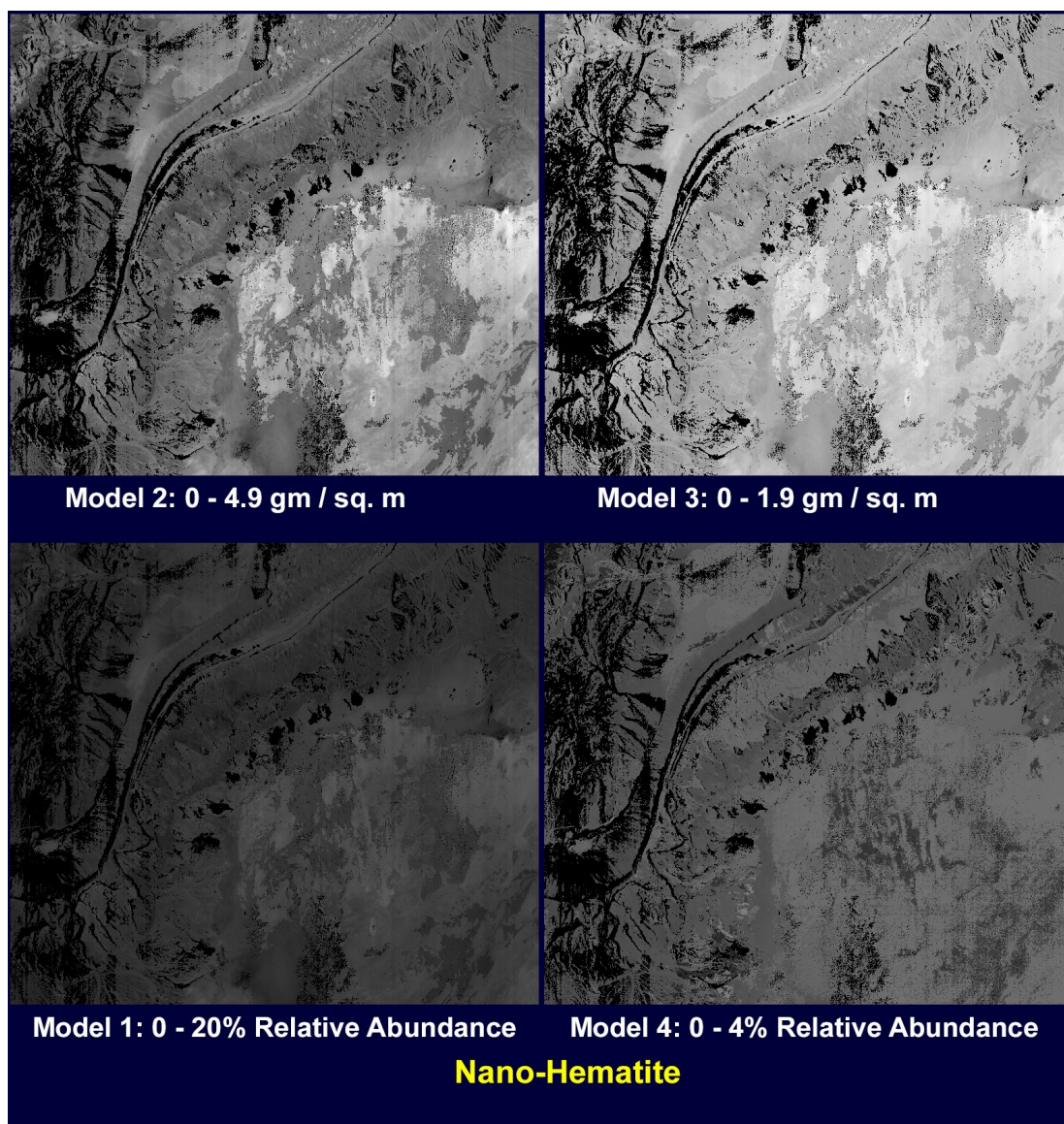
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2333 Figure 26. Tetracorder 5.27d1 results for a portion of the FRAGMENT study area in Morocco. The
 2334 scene is a crop from EMIT cube emit20230206t101334_o03707_s000_l2a_rfl_b0106_v01. The
 2335 salmon color is mainly areas containing hematite-goethite mixtures. The green areas, jarosite, is a
 2336 misidentification caused by a deficiency in the spectral libraries used: the green areas appear to be
 2337 hematite-goethite mixtures with grain sizes not represented in the libraries. The white box is the area
 2338 where abundances were derived and reported in Table 8.
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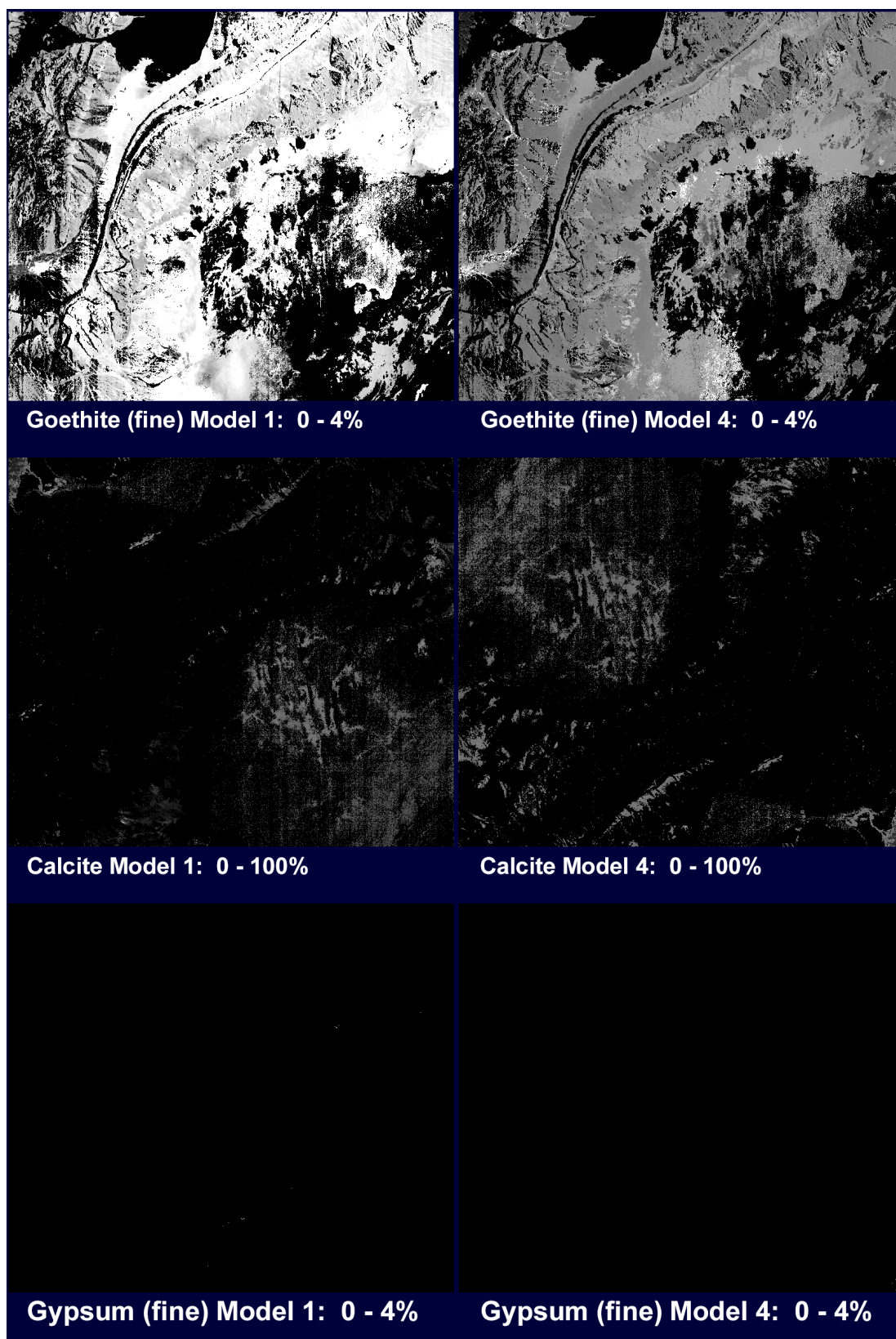
2340 Figure 27. Tetracorder 5.27d1 results of the EMIT 8 minerals for a portion of the FRAGMENT study
 2341 area in Morocco. The purple areas in the lower right are calcite-montmorillonie group mixtures.
 2342 The scene is a crop from EMIT cube emit20230206t101334_o03707_s000_l2a_rfl_b0106_v01.



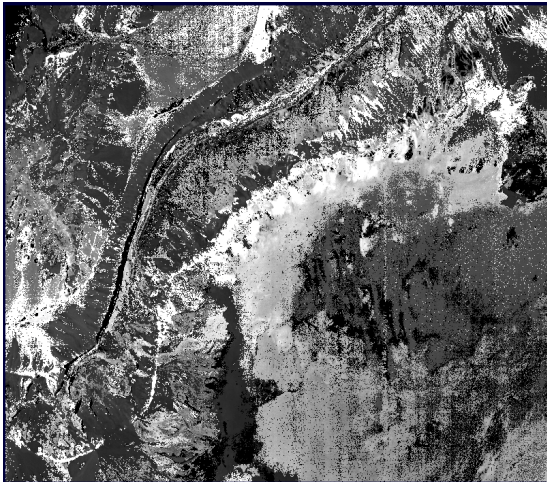
2344 Figure 28. Tetracorder 5.27d1 results for nano-hematite and 4 abundance models for the image area
2345 shown in Figures 26 and 27.

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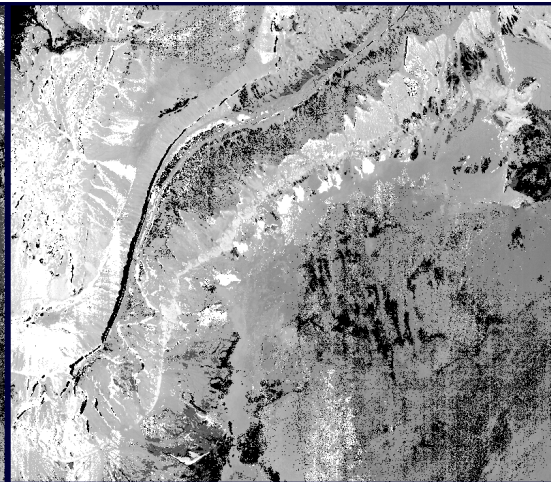
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2348 Figure 29a. Tetracorder 5.27d1 results for 2 abundance models for goethite, calcite and gypsum for the
 2349 image area shown in Figures 26 and 27.



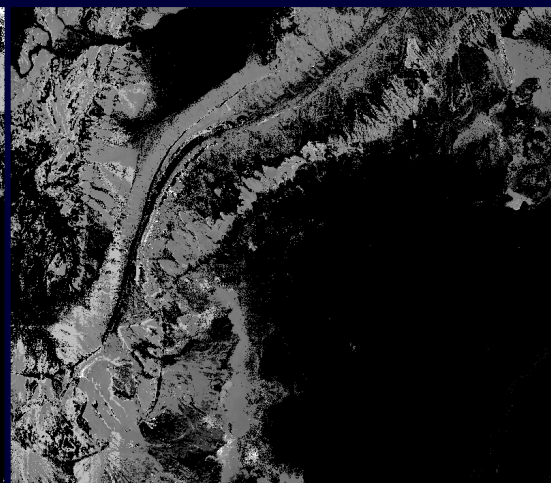
Illite / Muscovite Model 1: 0 - 20%



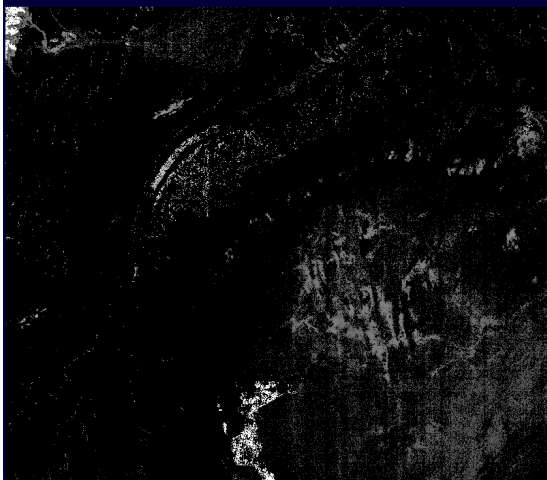
Illite / Muscovite Model 4: 0 - 20%



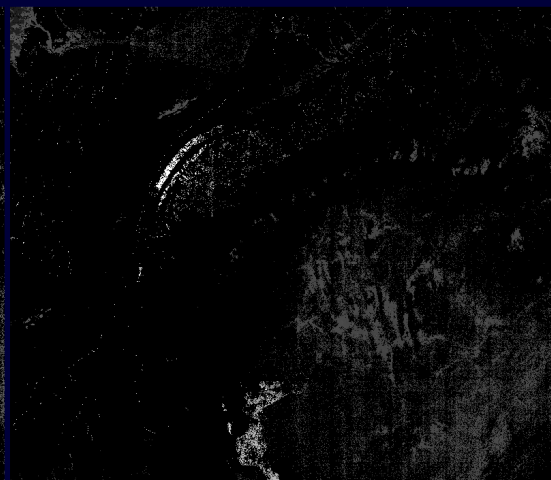
Kaolinite Model 1: 0 - 20%



Kaolinite Model 4: 0 - 20%



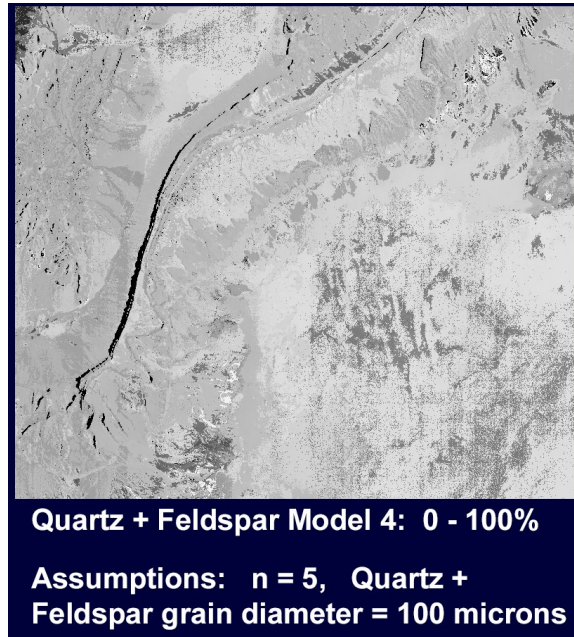
Montmorillonite Model 1: 0 - 20%



Montmorillonite Model 4: 0 - 20%

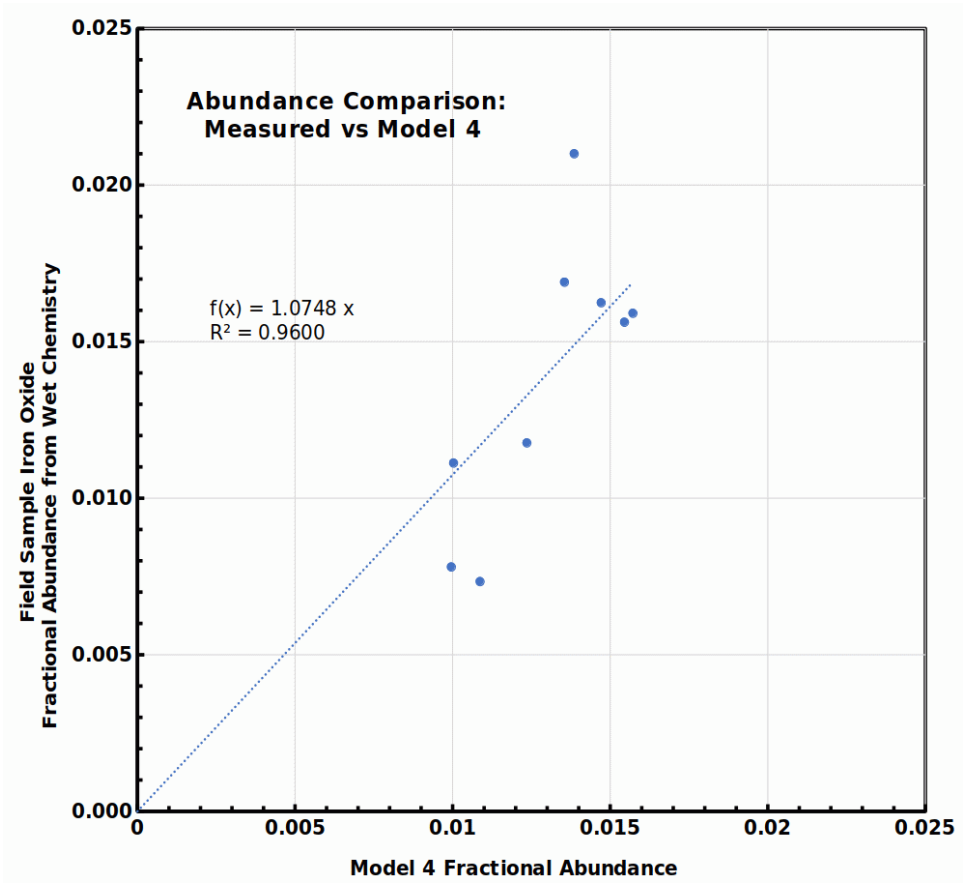
2351 Figure 29b. Tetracorder 5.27d1 results for 2 abundance models for illite/muscovite, kaolinite and
2352 montmorillonite for the image area shown in Figures 26 and 27.

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2361 Figure 30. Tetracorder 5.27d1 Model 4 abundance results for quartz +feldspar for the image area
2362 shown in Figures 26 and 27.

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2366 Figure 31. Comparison of wet chemistry data from González-Romero et al., 2023 converted to iron
2367 oxide abundance is compared to Model 4 abundance.

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