Mineral Detection Algorithm

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Version 1.0
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1. Algorithm Description

1.1. Overview

Tetracorder is a well-validated mineral detection system that uses diagnostic spectral absorption features with modified least squares regression against reference library spectra to identify unknown materials, focusing on robust detection of geologic and biologic materials (Clark et al., 2003). Applications have included studying sources of heavy metal pollution from mining (Dalton et al., 2005; Swayze et al., 2000), tracking the extent and severity of oil spills (Clark et al., 2010), and characterizing mineralogy of hydrothermal alteration zones (Berger et al., 2003; Swayze et al., 2014). Tetracorder is also the basis for characterizing the mineralogy of dust source regions for the EMIT mission (Clark et al., 2020). Compared to band ratios, Tetracorder's shape matching algorithm reduces the need for subjective interpretation in order to carry out precise material identification.

Spectroscopic principles
Tetracorder identifies materials by comparing the shape of spectral features in its reference libraries to the shape of features in unknown spectra. The shape-matching algorithm uses a weighted least-squares goodness of fit test to correlate the observed spectrum against a series of well-characterized library spectra (Clark et al., 2003). This procedure is carried out independently for different wavelength regions which have different chemical processes underlying their spectral features. Absorption features in the visible and near infrared (~0.4 to 1.0 μm) are mainly due to electronic processes. Chemical differences in materials, such as the presence of Fe^{2+} versus Fe^{3+}, manifest as differences in the shape and position of absorption features. In the near infrared and longer wavelength regions, absorption features are based on OH stretching vibrations and their overtones and combinations. The outputs of Tetracorder indicate the material that is spectrally dominant in different spectral regions. Note that some minerals common in nature such as quartz and low-iron feldspars have no diagnostic absorptions in the Vis-NIR range (0.4 to 2.5 μm).

Performance
Results of mineral maps produced with Tetracorder can be evaluated for accuracy through human verification of the analyzed spectra, field checking of mineral maps, and laboratory analysis of collected samples from mapped areas. See (Clark et al., 2003) for a detailed discussion about the verification of Tetracorder version 3.5 including comparison of Tetracorder results with laboratory analysis of more than 100 samples across multiple locations and "virtual" sampling of data set by extracting spectra and comparing to known mineral standards and interpretation by expert spectroscopists.

1.2. Theoretical Background

This section summarizes the implementation of Tetracorder algorithms, which were first described in (Clark et al., 2003). Subsequent updates and new features are detailed in comments in the source code as well as publications and reports including (Dalton et al., 2004) and (Clark et al., 2010).

Diagnostic spectral features

Of importance for understanding the implementation of the algorithm is the use of diagnostic spectral features, which are used to identify the best fitting reference material separately in several different wavelength regions (Figure 1.1). Only portions of the spectrum known to be diagnostic of reference materials are used, which means Tetracorder has the ability to detect mixtures of materials that are spectrally active in different wavelength regions (e.g. a mixture of iron oxides and clay minerals). Each unknown spectrum is classified as the reference material whose correlation has the highest fit to the features of the normalized continuum-removed spectrum from the reference library, or no identification is made if features do not meet the defined constraints for any material. The focus on diagnostic features in analysis of natural scenes is critical because mixtures that obey nonlinear systematics (e.g. coatings, intimate mixtures, and solutions) are common in the natural environment and frustrate simple matching over large spectral ranges.

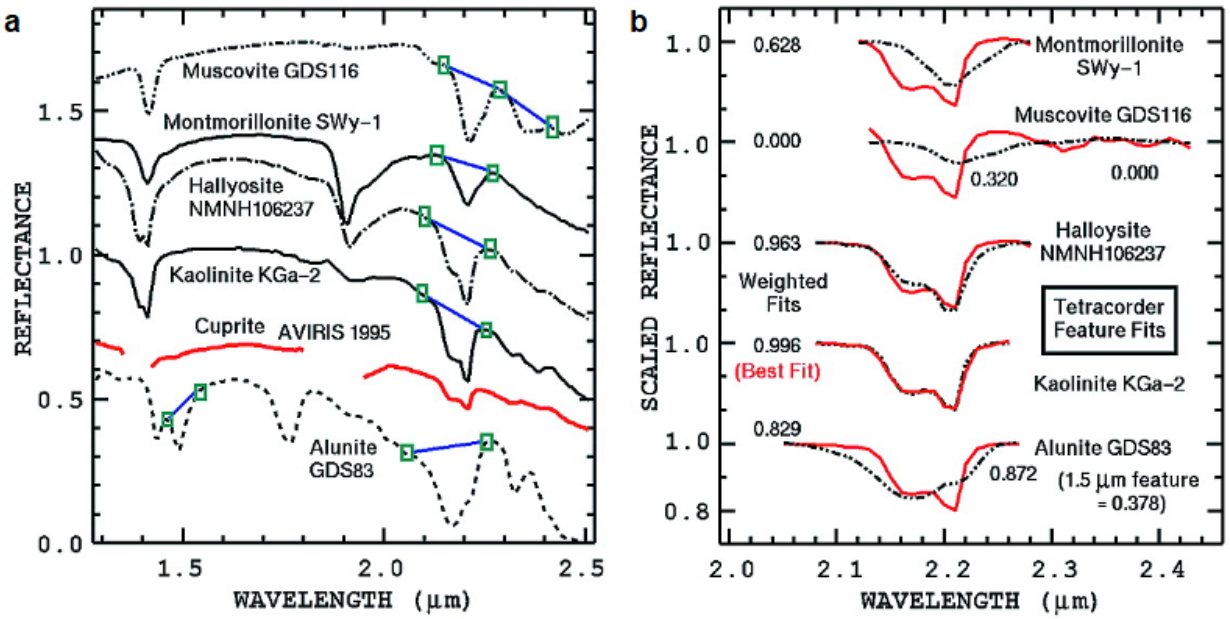

Figure 1.1. Depiction of spectral feature fitting from Clark et al. (2003). a) Reflectance spectra of five reference materials with continuum interval regions indicated by green boxes and an unknown spectra in red. Gaps indicate deleted channels. b) Comparison of least squares fits between continuum removed normalized reflectance of the unknown (red) and the same five reference materials. Reflectance values are offset for readability.

Calculated values

Tetracorder calculates three output layers comparing the measured reflectance spectra to each endmember material in the expert system: fit, depth, and fit times depth (fd). These calculations are carried out using

mathematical functions in the program Specpr, which is a dependency of Tetracorder. Pixels in each of the three output layers only have positive values for the best-fitting endmember in each wavelength region.

Fit is the primary basis for material identification. It is calculated as the least-squares correlation coefficient between continuum-removed normalized reflectance of the reference and unknown spectra over the range of wavelengths in each diagnostic feature. This value quantifies how well a feature in the unknown spectrum matches a reference feature, independent of a material's abundance. Features are defined by continuum endpoints on either side of an absorption or emission feature (Figure 1.1a; Appendix C). For certain materials where diagnostic features are located near atmospheric water absorptions (e.g. the right side of a jarosite feature near 1.4 μm or the left side of the alunite feature close to 1.9 μm), endpoints are carefully selected to avoid those regions. In cases where multiple strong diagnostic features exist, a weighted fit is calculated using the relative size of features, which is determined from integrating the area of continuum-removed features in reference spectra (Figure 1.1b). Unknown spectra are identified as the material with the highest fit value in each wavelength region. Fit ranges from 0 to 1 with 0 being a poor fit and 1 being an excellent match between the feature shapes in the library spectra and in the unknown spectrum. Values are reported as 8 bit scaled integers (ranging from 0 to 255). Note that an unknown spectrum may have excellent fits (> 0.95) to many reference materials, however identification is based only on the highest fit value. This criterion means detections rely on every feature definition and constraint within each expert system group, and that detections can be highly sensitive to minor changes.

Absorption feature **depth** is the difference between the minimum reflectance of the continuum-removed normalized feature and the corresponding reflectance of the continuum at the same wavelength. Absorption depth varies based on intrinsic absorption strength, grain size, abundance of the material, as well as the properties of all other materials present in the sampled environment. Holding grain size constant, feature depth may be proportional to the abundance of a material. In general, larger grain sizes increase absorption depth, but for some materials with intense absorptions, e.g. hematite and goethite absorptions near 0.9 μm, grain size differences may also affect the shape of the feature and can therefore be used to determine grain size. Absorption depth is used in EMIT's Level 2B product to calculate spectral abundance for a subset of Tetracorder endmembers (Clark et al., 2020). These calculations also depend on measurements relating band depth to mineral abundance in a comparable manner across endmembers. Direct comparison is limited because spectral features of remotely measured materials will generally be weaker than those of features in reference spectra.

Fit times depth (fd) is the product of fit and depth. Although fd values are not directly comparable across endmembers, they can be useful for visualization and qualitative assessment of detection patterns.

Wavelength regions

Tetracorder's expert system file is structured into groups of endmember materials that have overlapping spectral features, so that spectrally similar materials compete for the best fit within their own group. For example materials with strong electronic absorptions near 1μm are categorized as Group 1, and materials with strong vibrational absorptions near 2μm are categorized as Group 2. Materials such as snow, water, and vegetation that have features dominating the entire spectrum can interfere with mineral identification;

these materials comprise Group 0 and are included as potential endmembers with all other groups. See Appendix B for more details.

Mixtures
Tetracorder routinely detects the presence of multiple materials in an unknown spectrum, without performing unmixing analysis, by identifying diagnostic features of different materials in different spectral regions. For example, a mixture of iron oxides and clays should have both electronic absorptions in the visible to 1.3 μm wavelength range as well as vibrational overtone features in the 1.4 to 2.5 μm range. Detection of more than one material can only occur for materials without overlapping spectral features (i.e. materials in different groups in the expert system), except for those mixtures with reference spectra used in the expert system. Mixtures in the reference library are either modeled or measured, and are categorized as intimate mixtures (e.g. soils), areal mixtures, and/or coatings.

Other constraints
Additional criteria are used to mitigate coincidental ambiguities that arise from using continuum removal and normalization to calculate fits. These constraints complement and supersede the goodness of fit comparison. They include overall goodness of fit thresholds, minimum/maximum reflectance levels for continuum endpoints, continuum slope thresholds, and the presence or absence of key ancillary spectral features to distinguish among materials with nearly identical feature shapes. See Appendix C for more details.

1.3 Target minerals

This section summarizes implementation of Tetracorder for Carbon Mapper applications.

The expert system file (version 5.27a1) evaluates unknown spectra against 560 potential endmember materials. For material mapping on Earth and the minerals of interest for Carbon Mapper (Figure 1.2; Table 1.1), relevant endmembers are in Group 1 and Group 2 wavelength regions. As described above, Tetracorder calculates 3 output layers for each endmember in the expert system. Depending on the application, inference may be based on looking at detections of single endmembers or groups of related endmembers. For example, spatial relationships among materials may indicate patterns associated with hydrothermal alteration (Swayze et al., 2014) or weathering processes that produce acid mine drainage (Swayze et al., 2000). For potentially harmful materials, detections of a single endmember may identify the location or extent of a contaminated area (Kokaly, Couvillion, et al., 2013; Swayze et al., 2009).

Output layers for Carbon Mapper minerals of interest are based on aggregating endmembers corresponding to each mineral, similar to the methodology used to create the EMIT Level 2b product (Clark et al., 2020). For each mineral, there are 3 levels of aggregation: mineral endmembers only, mineral endmembers and mixture endmembers in which the target mineral is dominant, and aggregations of all endmembers that include the target mineral (e.g. even in trace amounts of a mixture). Endmember aggregations implemented in version 1 are listed in Appendix A. See Appendix E for aggregations that have been defined for other applications.

Detections in each wavelength region are carried out separately. Because nontronite and epidote have diagnostic features in both Group 1 and Group 2 wavelength regions, they may be identified in one or both regions when present, depending on the influence of other co-occurring materials.

Table 1.1 Target minerals of interest for Carbon Mapper Land and Ocean applications.

Group 1 µm Minerals	**Group 2 µm Minerals**
Epidote, Goethite, Hematite, Nontronite, Pyrite	Alunite, Buddingtonite, Calcite, Chlorite, Dickite, Dolomite, Epidote, Halloysite, Illite, Jarosite, Kaolinite, Montmorillonite, Muscovite, Nontronite, Pyrophyllite

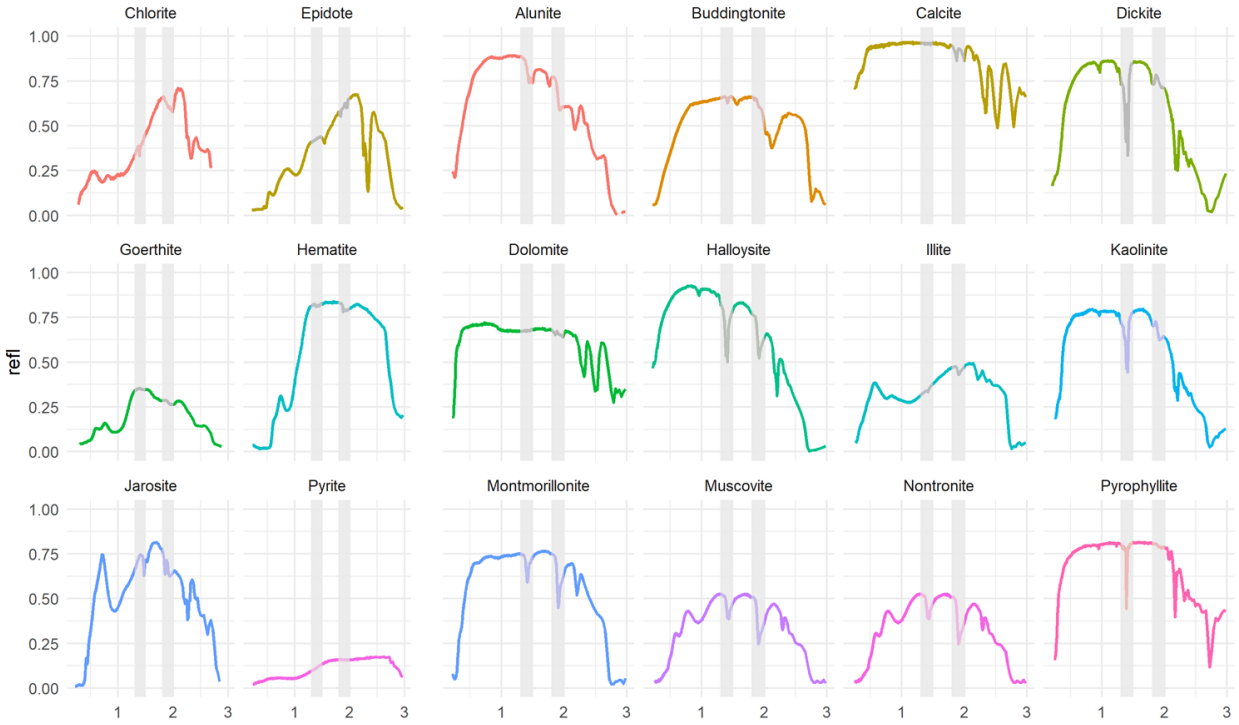

Figure 1.2. Spectra of representative mineral endmembers. Gray bars indicate deleted channels associated with atmospheric water absorptions.

1.4 Assumptions and Limitations

General limitations

Applications of Tetracorder require careful interpretation and expert spectroscopic knowledge to verify and validate the results for a given situation. Tetracorder reports the best match in each wavelength region, but it is left to the analyst to understand the significance and robustness of any such identification. Misidentification can arise due to errors in calibration to reflectance, inherent spectral ambiguity, or because of minerals or other materials in the environment that are not covered by the expert system.

Influence of vegetation or water

Tetracorder aims to identify the uppermost material of exposed mineral substrates, meaning algorithm performance may be degraded for areas influenced by vegetation or water coverage. Tetracorder will try to detect minerals if vegetation is sparse enough, but in areas with thick vegetation mineral identification becomes difficult. Mineral detection is also difficult on wet surfaces due to the suppression of photon path length into the ground from near infrared absorption (e.g. as in (Kokaly, King, et al., 2013)).

Spectral uniqueness

Very different materials may have spectrally similar absorption features that may be confused because of imperfect data calibration, low signal to noise ratio, and/or fundamental limits on the spectral uniqueness of different materials. Refer to the Known Issues file[1] for a short description of specific known limitations of the current expert system regarding shallow water, organic materials, desert vegetation, and minerals with particularly difficult detections. Deficiencies of the expert system version 3.5 originally described in Clark et al. (2003) include: 1) calcite-epidote-chlorite-mixtures, 2) shallow water/suspended sediment, 3) halloysite versus kaolinite with another clay absorption, 4) talc-hectorite-saponite, 5) wet or desert vegetation mapping as melting snow plus vegetation, 6) influence of clouds or cloud shadows, 7) reflectance calibration or shifts in wavelength calibration, 8) non-diagnostic features for many Fe2+ bearing minerals, 9) alunite formation temperatures, 10) staurolite similarity to vegetation plus water, 11) false positives of pyrophyllite in areas of hydrothermal alteration. Deficiency 1 was subsequently addressed in (Dalton et al., 2004) and with updates to the expert system. The suggestion for handling deficiency 8 is to aggregate all Fe2+ mineral detections into a layer of generic Fe2+ bearing minerals rather than specific mineral identifications.

Deleted channels/spectral resolution

For each instrument configuration, the user specifies which bands to exclude from analysis (see Section 3.1 for implementation details). Endmember materials may be affected or excluded from the analysis if deleted bands overlap the continuum regions for features of that endmember. If a mandatory ("M") feature is affected, or if all diagnostic ("D") features are affected, then a material will be disabled. In cases where one or more features are disabled but the material remains enabled, detections for that material's group may be compromised depending on the diagnostic importance of the disabled feature. Using the selected default ranges for deleted channels (0–0.400 µm, 1.300–1.500 µm, 1.800–2.000 µm), melting snow/slush endmembers in Group 0 are disabled due to a mandatory diagnostic feature with an endpoint between 1.315–1.345 µm. Disabled features and materials are listed in the output of each Tetracorder run in the file `00_info/disabled-materials.txt`. Note that this file uses material IDs, which differ from the names of many materials in output file names.

2. User Guide

This section provides a high-level overview of how to implement version 1 of the Carbon Mapper Land and Oceans mineral detection algorithm, which corresponds to version 5.27a of Tetracorder. Technical details follow in Section 3.

[1] https://github.com/PSI-edu/spectroscopy-tetracorder/blob/main/tetracorder.cmds/tetracorder5.27a.cmds/AAAAA.KNOWN-ISSUES.txt

A note on formatting:
In this document, lines of code start with $ and are formatted in Courier New font, such as:

```
$ sh convolve_libraries.sh [HDR_FILE] [SL1_DIR] [TET_CMD_BASE] [SENSOR_ID]
[SENSOR_YR] [SENSOR_LET] [SETUP_DIR] [DEL_RANGES]
```

Square brackets indicate placeholders for arguments and variable names in code and text. In sections of text, names of files and directories are enclosed in backticks such as `cmd.lib.setup.t5.27a1` and are relative to a top level directory containing folders `sl1` and `tetracorder.cmds` unless otherwise specified.

2.1. Key dependencies and input data requirements

Tetracorder runs on Linux/Unix operating systems. The program is written in Fortran, Ratfor, and C and must be compiled prior to use. The source code for Teteacorder version 5.27a is available on GitHub: https://github.com/PSI-edu/spectroscopy-tetracorder. Bash scripts were written to install and run Tetracorder with less user interaction, a streamlined number of files, and modified post-Tetracorder processing, however the operational structure of the program was retained. Input files must be ENVI rasters with band interleave format and BIL must be capitalized in the ENVI hdr file. The full path to the compiled program needs to be specified on line 21 in the file `tetracorder.cmds/tetracorder5.27a.cmds/cmd.runtet`; the default path is `/usr/local/bin/tetracorder5.27`.

Reference Spectral Libraries
Reference library spectra are stored as binary data in Specpr format and are contained in the folder `sl1`. Spectral Library 06 is file `sl1/usgs/library06.conv/splib06b` and Research Library 06 is file `sl1/usgs/rlib06/sprlb06b`. A list of materials in each library can be found in the corresponding files with the suffix ".list-h.1". Note that the expert system only uses a subset of materials in each of these libraries.

2.2. Convolve reference libraries

For each instrument configuration, use the script `convolve_libraries.sh` to prepare the reference libraries and the other necessary files to support a Tetracorder analysis. These files only need to be prepared once for each configuration of the instrument supplying the data. See section 3.1 for details.

```
$ sh convolve_libraries.sh [HDR_FILE] [SL1_DIR] [T1_DIR] [SENSOR_ID]
[SENSOR_YR] [SENSOR_LET] [SETUP_DIR] [DEL_RANGES]
```

For example:

```
$ sh convolve_libraries.sh example/input/ang20200712t201415_corr_v2y1_img.hdr
sl1 t1 anextgen 2020 a
```

Note that the code will check if convolved libraries already exist for the provided combination of [SENSOR_ID], [SENSOR_YR], and [SENSOR_LET].

2.3. Run Tetracorder

Once the reference libraries are convolved, use the script `run_tetracorder.sh` to run Tetracorder on an image, using the appropriate dataset keyword to use the convolved libraries and associated files matching the instrument as configured to collect that image. See section 3.2 for details.

```
$ sh run_tetracorder.sh [TET_OUT_DIR] [REFL_FILE] [DATASET] [T1_DIR] [SCALE]
[SETUP_DIR] [TMP_DIR]
```

For example:

```
$ sh run_tetracorder.sh example/output/
example/input/ang20200712t201415_corr_v2y1_img avirisng_2020a t1 1
tetracorder5.27a.cmds /home/scratch
```

3. Technical Details

This document is based on using Tetracorder version 5.27 with expert system file Tetracorder commands in the directory `tetracorder.cmds/tetracorder5.27a.cmds`.

3.1 Library configuration

Purpose
The script `convolve_libraries.sh` creates convolved versions of Tetracorder's two reference spectral libraries (USGS Spectral Library 06 and Research Library 06) and several other necessary files for carrying out a Tetracorder mapping analysis, using the metadata ENVI .hdr file for the image to be analyzed. This step only needs to be completed once for a given instrument configuration. The convolved libraries are saved within the `sl1` directory. The .hdr file should contain the wavelengths and full width half max for each band.

Library code names
Convolved libraries have 8 character names with 3 characters to identify the library ("s06" or "r06") plus unique 5 letter codes to identify each instrument configuration (e.g. "av95a" or "emita"). The 5 character codes are constructed from inputs to `convolve_libraries.sh`: the first 2 characters of [SENSOR_ID] plus the last 2 characters of [SENSOR_YR] plus the [SENSOR_LET]. See Appendix D for examples.

3.1.1 Inputs

There are six required inputs and two optional inputs to run `convolve_libraries.sh`:

```
$ sh convolve_libraries.sh [HDR_FILE] [SL1_DIR] [T1_DIR] [SENSOR_ID]
[SENSOR_YR] [SENSOR_LET] [SETUP_DIR] [DEL_RANGES]
```

Table 3.1. Input arguments to `convolve_libraries.sh`.

Input	Description	Example
HDR_FILE	Path to ENVI .hdr file with wavelengths and resolution in nanometers.	example/input/ang20200712t201415_corr_v2y1_img.hdr
SL1_DIR	Path to spectral libraries directory (folder where usgs/library06 and usgs/rlib06 subfolders are)	sl1
T1_DIR	Path to base Tetracorder directory (folder where tetracorder.cmds subfolder is)	t1
SENSOR_ID	Sensor name. First two letters will be used for library code name.	anextgen
SENSOR_YR	Sensor configuration year. Last two digits will be used for library code name	2020
SENSOR_LET	Letter code for sensor configuration version.	a
SETUP_DIR (optional)	Setup directory for version of tetracorder cmds (which folder in `t1/tetracoder.cmds/` to use)	tetracorder5.27a.cmds (default)
DEL_RANGES (optional)	Comma separated list with ranges of wavelengths to exclude from analysis	0-400, 1300-1500, 1800-2000 (default)

3.1.2. What the code does:

Library convolution is carried out through functions in Specpr and produces output in Specpr formatted files. This section describes the code carried out in each of the labeled sections of `convolve_libraries.sh`.

Setup

The library convolution code requires single column ascii files with the target wavelengths and resolution (full width half-max) of the sensor, in microns. These files must have no tabs or carriage returns immediately after the numbers (a space then a carriage return is OK). `convolve_libraries.sh` uses the "wavelength" and "fwhm" sections of the input HDR_FILE to create `sl1/usgs/library06.conv/waves.txt` and `sl1/usgs/library06.conv/resol.txt`. Values in the HDR_FILE are divided by 1000 to convert from nm to microns.

The variable N_CHANS is defined as the length of `sl1/usgs/library06.conv/waves.txt`, then variables for the names of the two spectral libraries are defined. Then, the file `sl1/usgs/library06.conv/splib06b.list-h.1` is edited by replacing the first line with a copy of the second line. The first record (originally "Acmite NMNH133746 Pyroxene") does not convolve correctly so it is replaced with a duplicate of the second record listed. Neither spectra is used in the expert system and therefore this adjustment does not affect results.

Spectral library 06 convolutions

This section first runs `sl1/usgs/library06.conv/make.new.convol.library.start.file`, which itself runs `sl1/usgs/library06.conv/make.new.restart.file`. This step makes new copies of the files `sl1/usgs/library06.conv/restartfiles/r.s06NNNNN`, and `sl1/usgs/library06.conv/startfiles/s06av95a.start`, then updates each with the new instrument code in the new filename. To view the contents of the new library start file file use the Specpr function `spprint` (Figure 3.1).

Next the Specpr function `spsetwave` is used to set pointers for wavelength and resolution in records 6, 12, and 18 (Figure 3.2). Then `sl1/usgs/library06.conv/mak.convol.library` is run to do the convolution calculations. First a Specpr convolution command file is created (eg. `sl1/usgs/library06.conv/ conv.s06an20a.cmds`) from running `sl1/usgs/library06.conv/mak.convolve.1.cmds` and inputs from the file `sl1/usgs/library06.conv/ splib06b.list-h.1`. Then the newly created command file is used to create the convolved library. This step may take one or two minutes. The convolved library should be approximately 12.33 MB. The first spectrum in the convolved library file needs to begin at record 30 (Figure 3.3).

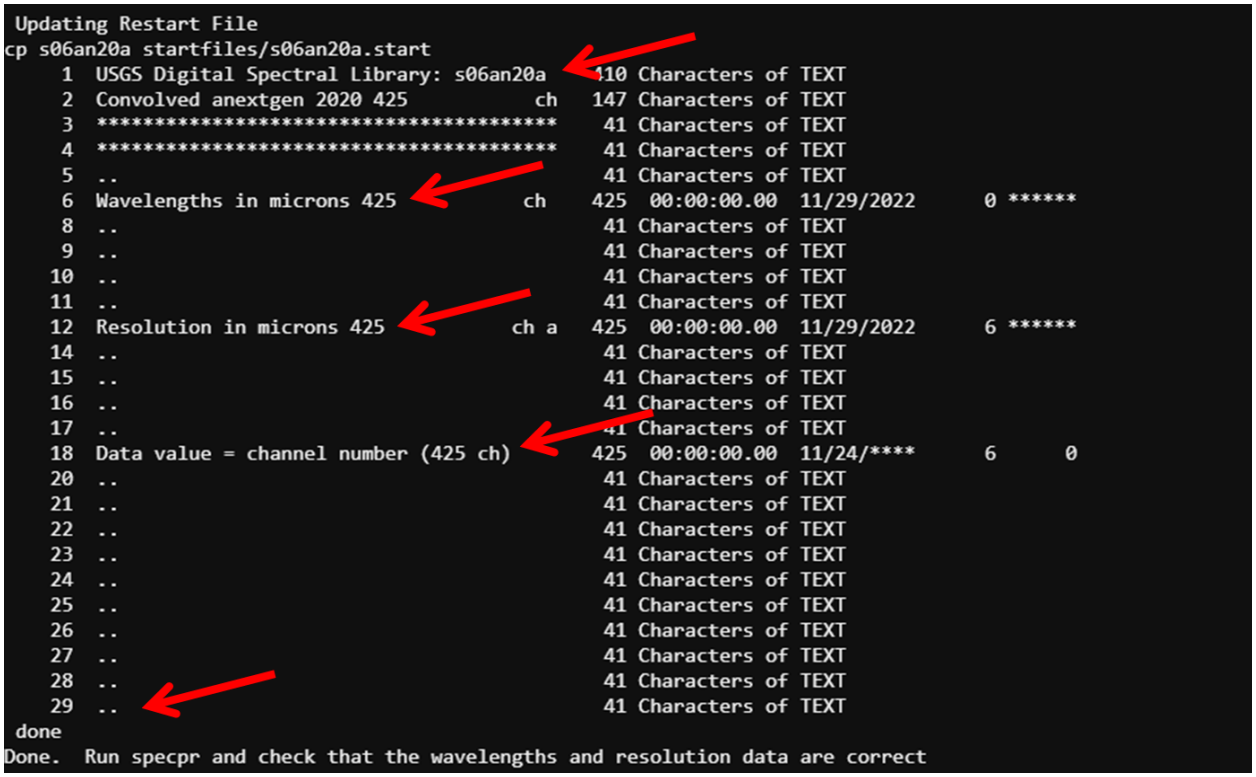

Figure 3.1 Example output of `./make.new.convol.library.start.file` showing the new convolved library start file for library "s06an20a" created from the first step of Spectral Library 06 convolutions. The start file should have 29 records with the new library name in record 1, Wavelengths in record 6, Resolution in record 12, and Data value in record 18.

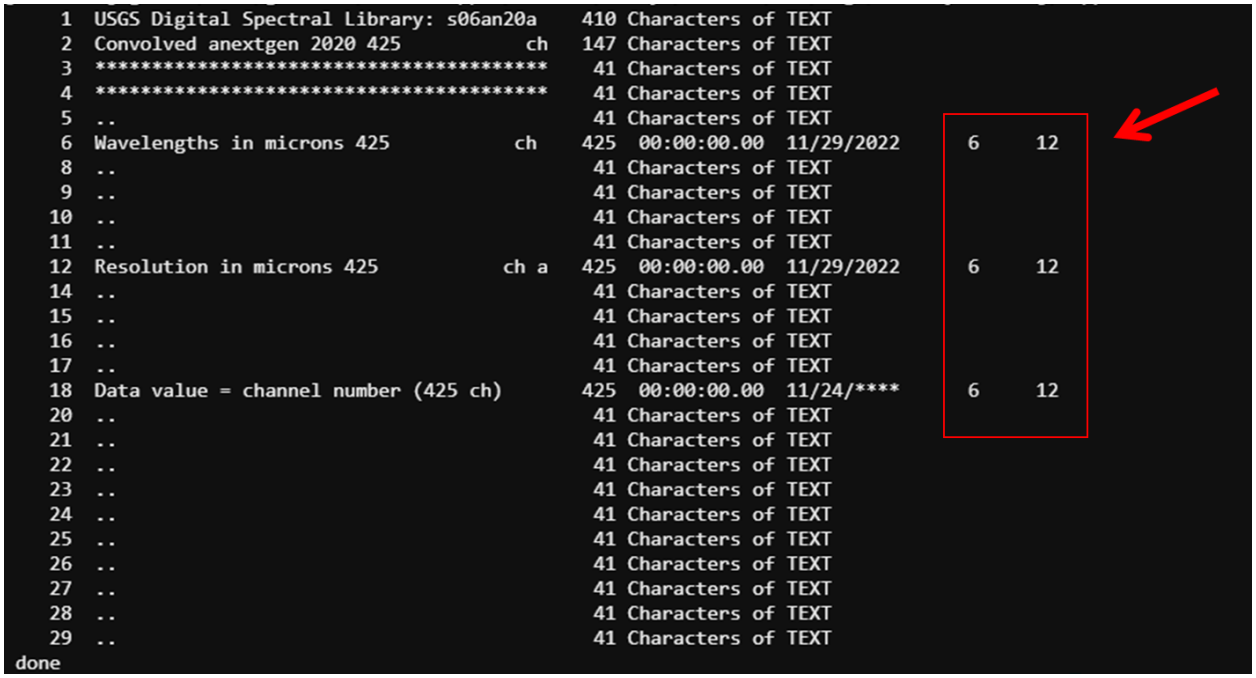

Figure 3.2. Example of new convolved library start file after running `spsetwave` functions. The pointers to wavelength and resolution in records 6, 12, and 18 should all be set to 6 and 12.

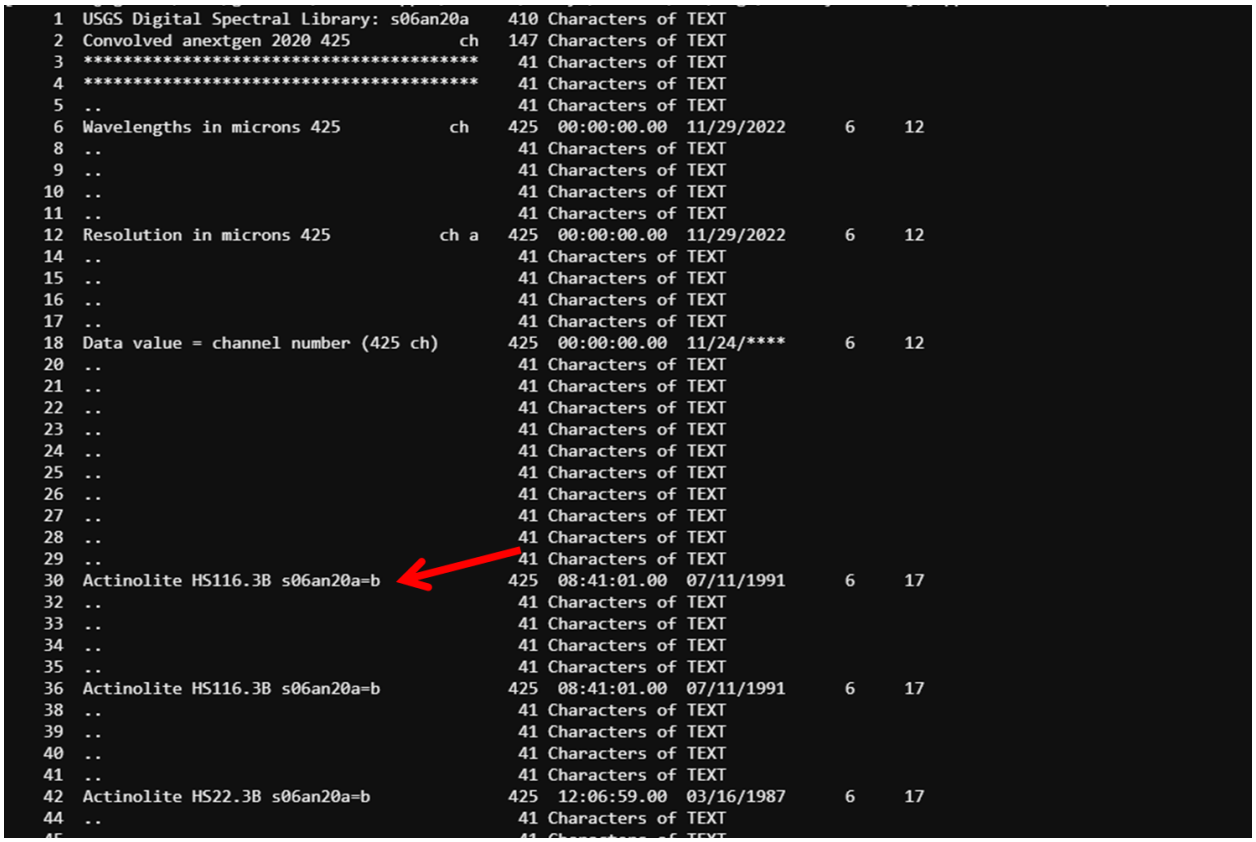

Figure 3.3. Newly convolved library s06an20a showing the first reference spectrum in record 30.

Research Library 06 Convolutions

A similar procedure is then carried out to convolve spectra in Research Library 06. Files created from Spectral Library 06 convolution are used as templates, with necessary modifications to replace references to Spectral Library 06 (eg. replacing "splib06b" with "sprl06b"). Specpr functions (`spsettitle`, `spsetwave`) are used to make replacements in the start file and `sed` commands are used to make replacements in the restart file.

Other necessary files

Next a file is created in the `tetracorder.cmds/tetracorder5.27a.cmds/DATASETS` folder to link the sensor identifier to the appropriate restart file. Then the new restart file from the spectral libraries directory (`sl1`) is copied to the `tetracorder.cmds/tetracorder5.27a.cmds/restart_files` directory. Note that the restart filenames start with "r.s06" in the `sl1` directory (e.g. "r.s06an20a") but they begins with "r-" in the tetracorder directory (eg. `r-an20a`). The latter is the name that should be referenced in the file created in the `tetracorder.cmds/tetracorder5.27a.cmds/DATASETS` folder (Figure 3.4). Then three replacements are made in the restart file to specify the appropriate restart file path, research library name, and spectral library name.

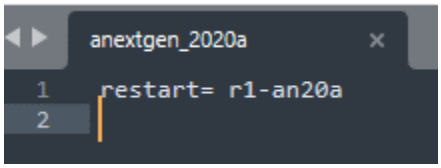

Fig 3.4. Example dataset keyword file for DATASET "anextgen_2020a" which corresponds to convolved reference libraries ending in "an20a".

Make deleted.channels file

Tetracorder also requires information specifying which band numbers of the input image to exclude from analysis (e.g. atmospheric water absorption bands), which can either be contained in the file `tetracorder.cmds/tetracorder5.27a.cmds/DELETED.channels/ DELETED.channels.txt` or a separate file in the DELETED.channels folder. The default ranges are <400 nm, 1300–1500 nm, and 1800–2000 nm. Deleted channel ranges can affect results because materials in the expert system may be disabled if bands from the region of the diagnostic features overlap the deleted regions, depending on the classification of the feature.

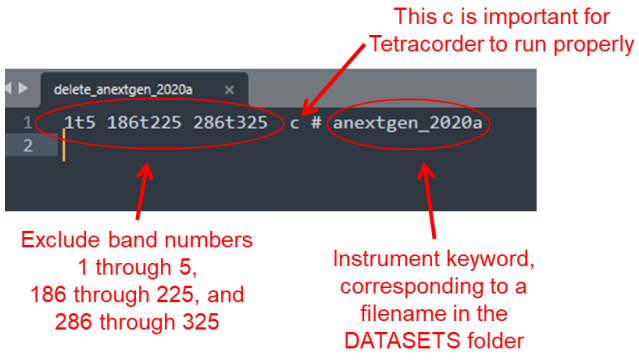

Fig 3.5. Example deleted channels file, indicating band numbers to exclude and the instrument keyword.

3.1.3 Outputs:

Table 3.2. Main outputs of `convolve_libraries.sh`. File paths reflect default [SETUP_DIR].

Output	**Description**
sl1/usgs/library06.conv/[S_LIBNAME]	Convolved USGS spectral library 06. [S_LIBNAME] is “s06” + a 5 character code (first 2 characters of [SENSOR_ID] + last 2 characters of [SENSOR_YR] + [SENSOR_LET])
sl1/usgs/rlib/[R_LIBNAME]	Convolved research library with additional spectra used in expert system. [R_LIBNAME] is “r06” + a 5 character code (first 2 characters of [SENSOR_ID] + last 2 characters of [SENSOR_YR] + [SENSOR_LET])
tetracorder.cmds/tetracorder5.27a.cmds/DATASETS/[SENSOR_ID]_[SENSOR_YR][SENSOR_LET]	File in DATASETS named with keyword for running Tetracorder with the convolved libraries of interest. This is one line of text starting “restart=r1-”
tetracorder.cmds/tetracorder5.27a.cmds/DELETED.channels/[SENSOR_ID]_[SENSOR_YR][SENSOR_LET]	File in DELETED.channels folder specifying the band numbers corresponding to the wavelengths supplied as deleted channels. Ranges are specified as e.g. 1t11 for bands 1 through 11
tetracorder.cmds/tetracorder5.27a.cmds/restart_files/r1-[(5 character sensor code)]	Restart file in t1 directory for new instrument configuration, named as `r1-` + the 5 character instrument code e.g. `r1-an20a`.
sl1/usgs/library06.conv/waves.txt	Wavelengths (in microns) of image to analyze. Must be a single column ascii file without any tabs, and the same length as resol.txt.
sl1/usgs/library06.conv/resol.txt	Full width half max (in microns) of image to analyze. Must be a single column ascii file without any tabs, and the same length as waves.txt.
sl1/usgs/library06.conv/conv.[S_LIBNAME].cmds	Specpr command file for s06 library convolutions
sl1/usgs/rlib06/conv.[R_LIBNAME].cmds	Specpr command file for r06 library convolutions

3.2 Run Tetracorder

The script `run_tetracorder.sh` carries out a Tetracorder mapping analysis for a reflectance image file. Each mapping run requires its own new output directory, which will contain all the newly generated files.

3.2.1 Inputs

There are four required inputs and three optional inputs to run `run_tetracorder.sh`:

```
$ sh run_tetracorder.sh [TET_OUT_DIR] [REFL_FILE] [DATASET] [T1_DIR] [SCALE]
[TMP_DIR] [SETUP_DIR]
```

Table 3.3. Input arguments to `run_tetracorder.sh`.

Input	**Description**	**Example**
TET_OUT_DIR	Output sub directory name. Must not already exist.	example/output
REFL_FILE	Path to input ENVI BIL format image to analyze	example/input/ang20200712t201415_corr_v2y1_img
DATASET	Instrument code to indicate which set of convolved libraries to use. Must correspond to a file name in DATASETS directory	anextgen_2020a
TI_DIR	Path to base Tetracorder directory	t1
SCALE (optional)	(Optional) Multiplier to scale image data to reflectance. Must be between 0.000001 and 100000000.0.	1 (default)
TMP_DIR (optional)	Path to temporary directory for copying image and spectral libraries. The full path to the image (TMP_DIR + base name of REFL_FILE) cannot be longer than 73 characters.	/tmp (default)
SETUP_DIR (optional)	Setup directory for version of tetracorder cmds (which folder in `t1/tetracoder.cmds/` to use)	tetracorder5.27a.cmds (default)

Table 3.4. Description of important files for tetracorder analysis. File paths are all within the directory `tetracorder.cmds/tetracorder5.27a.cmds`.

Filename or path	**Description**
cmd.lib.setup.t5.27a1	This is the expert system file.
cmd-setup-tetrun	Script to make sub-directories and install all needed tetracorder command files to perform a standard mapping run. Line 20 specifies the full path to the setup directory (set as `[T1_DIR]/tetracorder.cmds/[SETUP_DIR]`). Line 25 specifies the name of the expert system file. Lines 172-177 set default temperature and pressure ranges.
cmd.runtet	Script to run Tetracorder for a standard mapping run. Line 21 specifies the location of the compiled tetracorder program (default `/usr/local/bin/tetracorder5.27` requires root access).

	Line 167 runs Tetracorder. Line 176 creates the disabled materials file. Lines 204-226 compress the Tetracorder output files. Also includes code to run many Davinci scripts to summarize and plot results. These are not implemented reliably and outputs are not used.
TETNCPU.txt	Number of CPUs to use. Set to 24.
restart_files/r1-[(5 character sensor code)]	Restart file for instrument configuration, named as `r1-` + the 5 character instrument code e.g. `r1-an20a`. The DATASET input used with `run_tetracorder.sh` determines which restart file is copied and used in the analysis. See section 3.2.2 “Prepare for Tetracorder” and Figure 3.4 for more details.

3.2.2. What the code does:

This section describes the code carried out in each of the labeled sections of `run_tetracorder.sh`:

Prepare for Tetracorder
The image [REFL_FILE] and associated hdr file are copied to the temporary directory. This step iss implemented to handle the 73 character limitation for the image file path.

The source file path to the base Tetracorder directory [T1_DIR] and the version of the [SETUP_DIR] are used to define paths to the setup file `cmd-setup-tetrun`. The directory `[T1_DIR]/tetracorder.cmds/[SETUP_DIR]` also needs to contain the files listed in Table 3.4 that are used within `run_tetracorder.sh`: the expert system file, an instrument-specific file in the DATASETS folder, an instrument-specific file in DELETED.channels, and a file the restart_files folder corresponding to the information in the DATASETS file.

The appropriate convolved libraries (eg. r06an20a and s06an20a) are copied from directories within [SL1_DIR] to the temporary directory, and these paths are defined in the appropriate restart file (Figure 3.6). This step is implemented because the full file path to convolved libraries has a character limit.

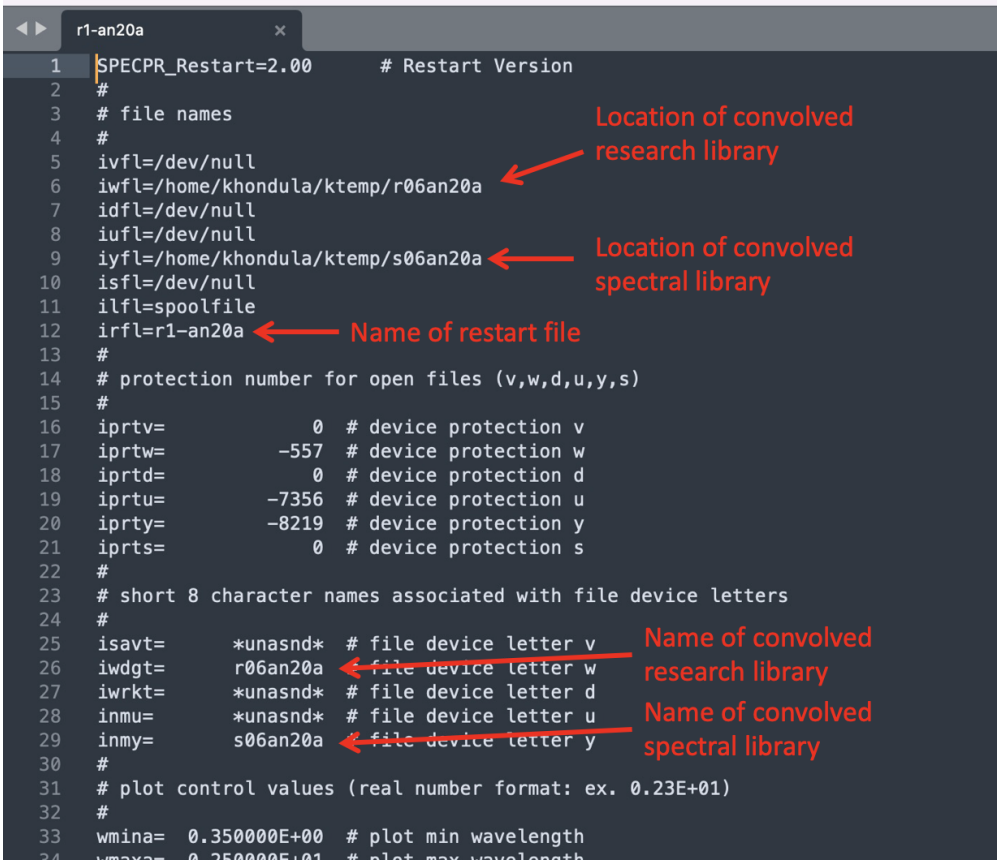

Fig 3.6. Example restart file: `tetracorder.cmds/tetracorder5.27a.cmds/restart_files/r1-an20a`, indicating instrument-specific modifications. Not shown: line 62 should contain the appropriate number of bands.

Setup and run Tetracorder

Next the script `tetracorder.cmds/ tetracorder5.27a.cmds/cmd-setup-tetrun` is run with supplied arguments as inputs. This will create a new directory [TET_OUT_DIR] and populate it with files for running Tetracorder and create numerous subfolders for outputs. Arguments to `cmd-setup-tetrun` that are assumed fixed are 1) running Tetracorder in "cube" rather than "single spectrum" mode, and 2) temperature and pressure ranges (-20 to 80 C, 0.5 to 1.5 bar). These ranges were chosen to match those used by the EMIT mission. Default ranges if none are supplied are 0 to 9999 K and 0 to 999 bar. Adjusting temperature and pressure ranges will disable endmembers with temperature or pressure constraints outside of the supplied ranges (e.g. snow and ice).

Then `cmd.runtet` is run from within the newly created [TET_OUT_DIR]. This is when the main image processing occurs. The example image runs in approximately 2.5 hours on ASU's Agave computer cluster. To run, Tetracorder uses the text restart file `[TET_OUT_DIR]/r1` and two command scripts: `[TET_OUT_DIR]/cmds.start.t5.27a`, which has settings that may change for each image run such as image name, and `[TET_OUT_DIR]/cmd.lib.setup.t5.27a1`, which contains the expert system (~26,000 lines) and is generally only modified by an expert spectroscopist.

Post Tetracorder

After Tetracorder finishes, output files are aggregated and organized into numbered folders. First, the output hdr files are edited to remove unnecessary spaces and to add spatial reference information from the original reflectance image. Fit, depth, and fd layers for all Group 1 and Group 2 endmembers (direct output from Tetracorder) are retained in folders `01_tetfits`, `01_tetdepths`, and `01_tetfds`.

Then mineral maps are created by aggregating the appropriate endmember fit maps for each of the target minerals, using three different criteria for aggregation (Table 3.5). Mineral endmembers for each of the target minerals are aggregated into geotiff files in folder `02_minerals_only` (Figure 4.1b, 4.1d). Mineral endmembers plus mixtures in which the target mineral is dominant are aggregated into geotiff files in folder `03_mineral_mix` (Figure 4.1c, 4.1e). Group 2 mixtures without a dominant target mineral (e.g. 50% Alunite and 50% Muscovite) are aggregated into separate geotiffs “group2_amix” for non-dominant areal mixtures and “group2_imix” for non-dominant intimate mixtures. All Group 1 mixtures included have a dominant target mineral. Finally, all mineral endmembers that include each target mineral (even in trace amounts) are aggregated into separate geotiffs in the folder `04_minerals_all`. This level of aggregation represents all detections of each target mineral (Figure 4.2). For the aggregations in `02_minerals_only` and `03_mineral_mix`, each pixel is only included in a maximum of one output layer per group. For aggregations in `04_minerals_all`, pixels classified as mixtures may be included in multiple output layers depending on how many target minerals are represented in the best-fitting endmember (Figure 4.2). Because epidote and nontronite have diagnostic features in both wavelength regions they may be identified in one or both regions when present, depending on the influence of other co-occurring materials. See Appendix A for the list of endmembers used for each aggregation level. Selected additional files produced from Tetracorder are retained in `00_info` for diagnostics and troubleshooting (Table 3.6) and unused output files (e.g. for visualizing outputs with legacy Davinci code) produced from Tetracorder are removed. Only the files in numbered folders are retained.

3.2.3 Outputs:

The output from Tetracorder is a large set of files with a highly nuanced naming and folder structure that comprise the results of the algorithm, as well as many placeholders for unimplemented optional outputs of programs e.g. for summarizing and plotting results. The unused outputs from Tetracorder are removed in the post Tetracorder section of `run_tetracorder.sh` and retained output files are copied into numbered folders `example/output/01_tetfits`, `example/output/01_tetdepths`, and `example/output/tetfds`.

The Tetracorder outputs used for the mineral output maps are a subset of fit files (and associated .hdr files) in the output directory folders group.1um/ and group.2um/. The endmembers aggregated for each target mineral are aggregated from the .fit files, as described in Section 3.2.2 “Post Tetracorder” and Appendix A.

Table 3.5. Main output folders in `example/output`. Each folder contains separate sub-folders for target minerals in Group 1 and Group 2.

Output folder	**Description**
00_info	Diagnostic information and metadata. See below for details

01_tetfits 01_tetdepths 01_tetfds	Individual endmember fits, depths, and fds (reorganized direct output from Tetracorder algorithm). Pixels with positive values indicate detection.
02_minerals_only	Aggregations of all mineral endmembers for a target mineral.
03_minerals_mix	Aggregations of mineral endmembers plus mixture endmembers where the target mineral is the most abundant out of the minerals of interest. Areal and intimate mixtures without dominant minerals are provided as separate layers (e.g. 50/50 mixtures; only relevant for Group 2). This is the highest level of aggregation that allows for composite maps.
04_minerals_all	Aggregations of all endmembers containing the target mineral at any level. Note that endmembers may be used in multiple aggregations.

Table 3.6. Description of files in `00_info`.

File	**Description**
cmd.runtet.out	Output of cmd.runtet. Includes duration of analysis and outputs from post-Tetracorder results.
disabled-materials.txt	Copied lines from tetracorder.out file indicating which features and materials are affected by deleted channels.
cubepath.txt	Original path to image.
tetracorder.out	Output log from Tetracorder.

4. Example data set

An AVIRIS NG reflectance image collected in 2020 over the Cuprite mining district of Nevada is used here as an example dataset. This region is a classic and well-studied hydrothermal system often used as a NASA-JPL test site and has been sampled extensively (Clark et al., 2003; Swayze et al., 2014; Thompson et al., 2020). The example image file (flightline ang20200712t201415) is 4.24 GB and can be downloaded from the AVIRIS-NG FTP site here: https://avng.jpl.nasa.gov/avng/y20_data/ang20200712t201415.tar.gz. Related files and metadata and are available on the data portal: https://avirisng.jpl.nasa.gov/dataportal/. Example outputs are available on Zenodo at: https://doi.org/10.5281/zenodo.7383236.

Mineral detections are depicted in Figure 4.1 along with a true color image of the input data. Output layers with only mineral endmembers (Figure 4.1b, 4.1d) exclude mixtures and are a subset of output layers shown in Figure 4.1c and Figure 4.1d. Endmembers without dominant minerals (e.g. 50/50 mixtures) are aggregated into separate layers “group2_amix” for areal mixtures and “group2_imix” for intimate mixtures. Selected output layers aggregating all endmembers for a given target mineral are

depicted in Figure 4.2. In these layers, pixels classified as mixtures that include multiple target minerals will appear as detections (i.e. have positive fit values) in multiple output layers. Comparisons of mineral aggregation levels are shown in greater detail in Figures 4.3–4.7. Refer to Appendix A for the complete list of endmembers included in each aggregation level for each of the target minerals.

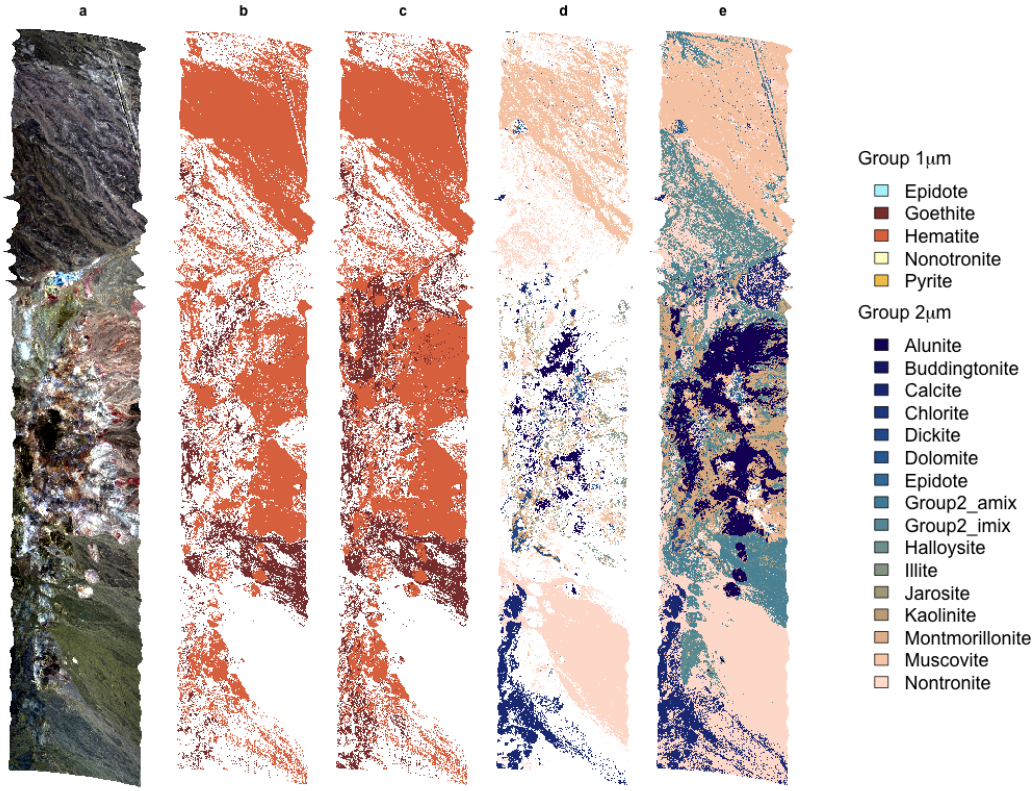

Figure 4.1. Example data set and results. From left to right: a) true color, b) Group 1µm minerals, c) Group 1µm minerals and mixtures, d) Group 2 µm minerals, e) Group 2 µm minerals and mixtures.

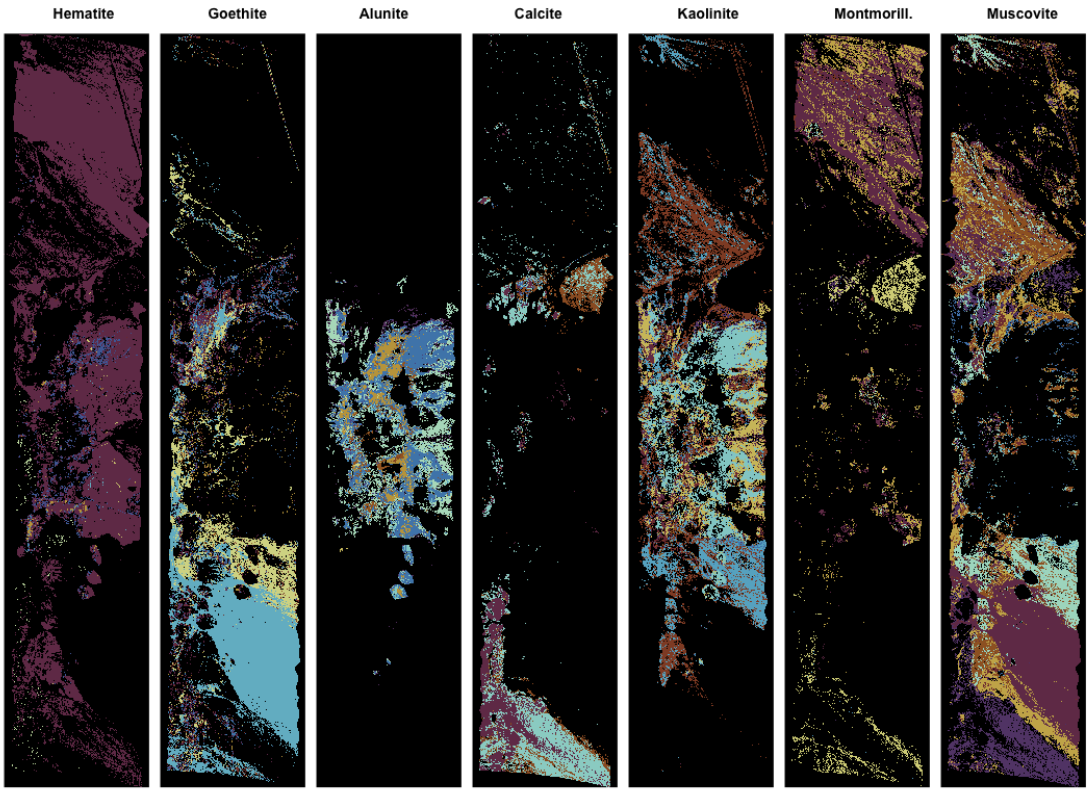

Figure 4.2 Detections for all endmembers of selected target minerals. Colors correspond to different endmembers within each image, see Appendix A for full list.

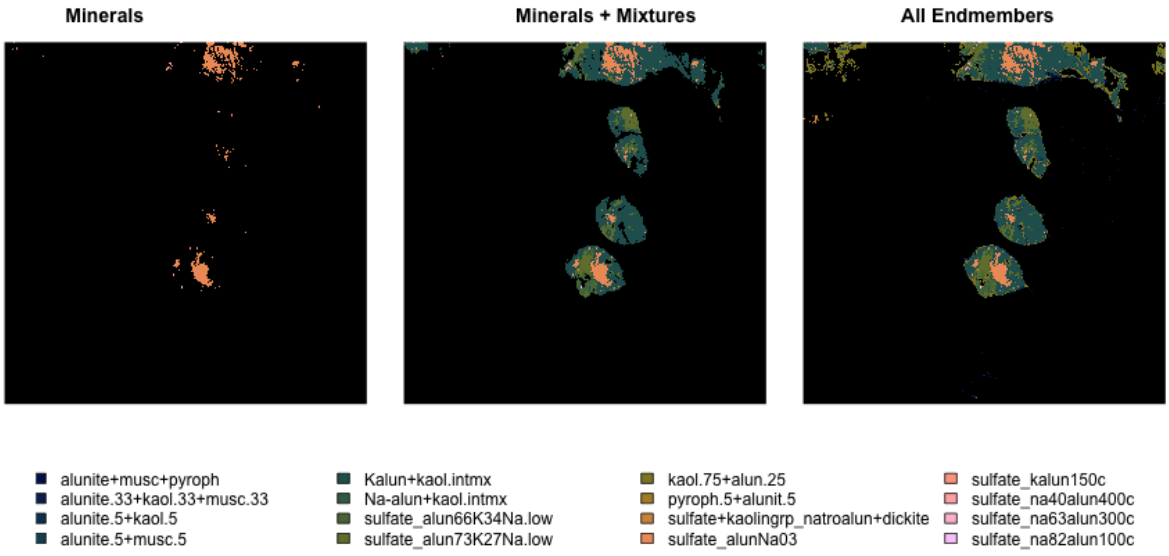

Figure 4.3 Comparison of aggregation levels for alunite endmembers (group 2) in the Alunite Hill area.

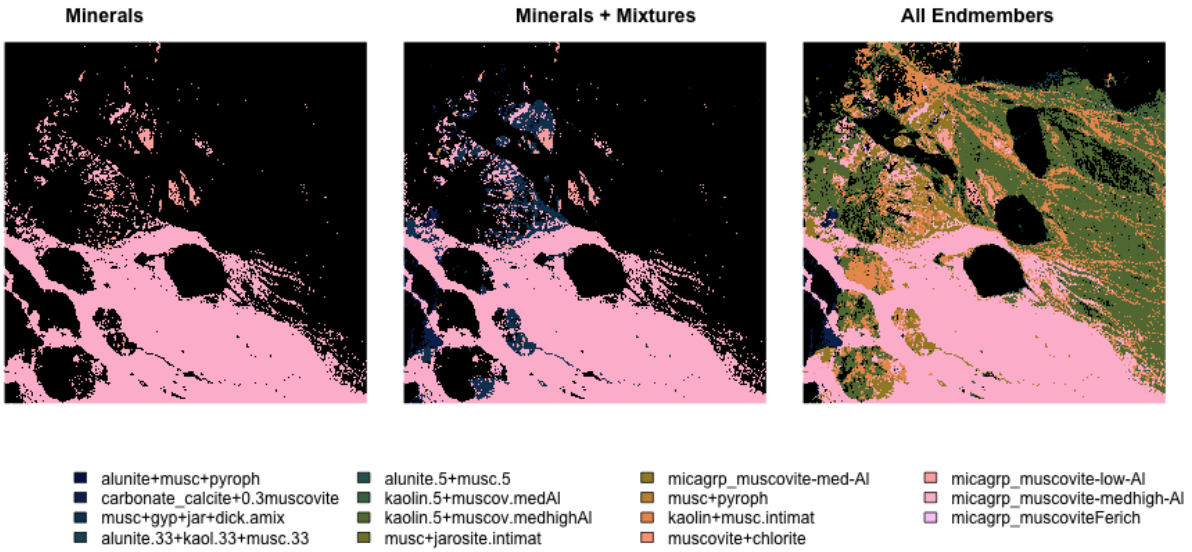

Figure 4.4 Comparison of aggregation levels for muscovite endmembers (group 2) in the Alunite Hill area.

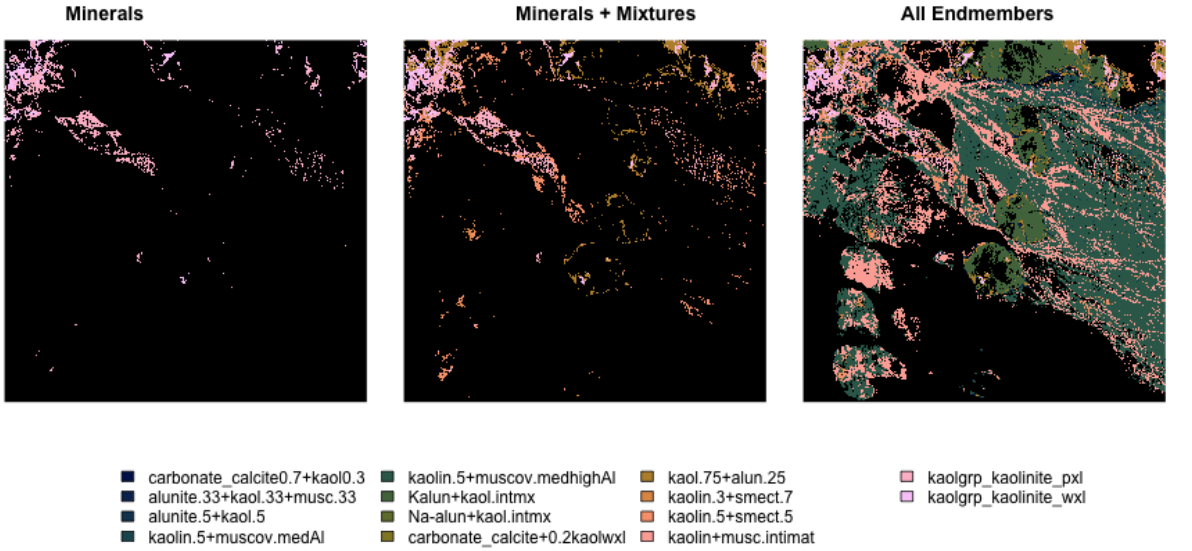

Figure 4.5 Comparison of aggregation levels for kaolinite endmembers (group 2) in the Alunite Hill area.

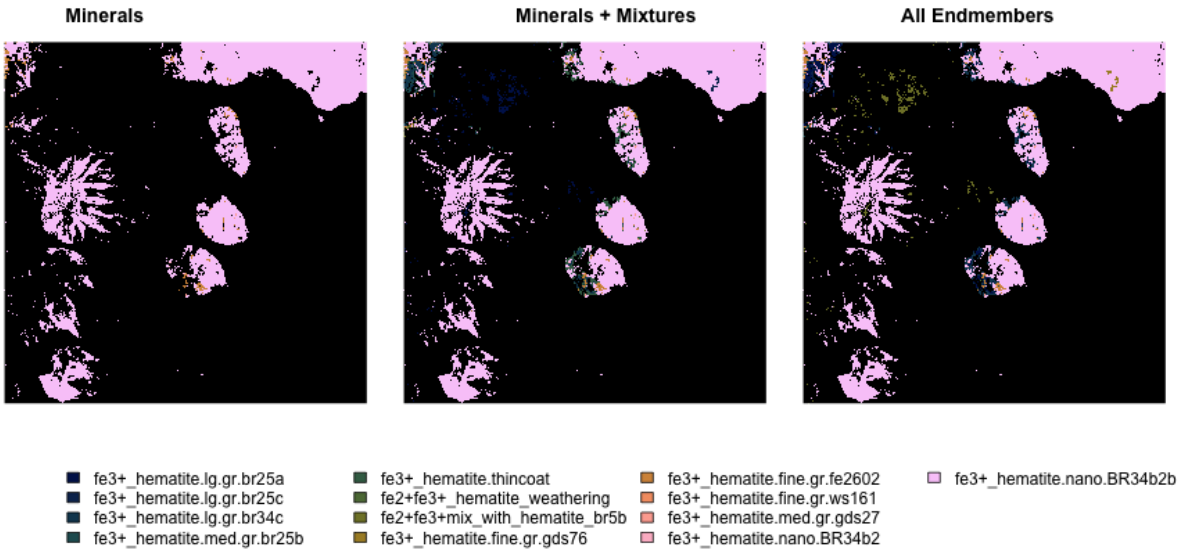

Figure 4.6 Comparison of aggregation levels for hematite endmembers (group 1) in Alunite Hill area.

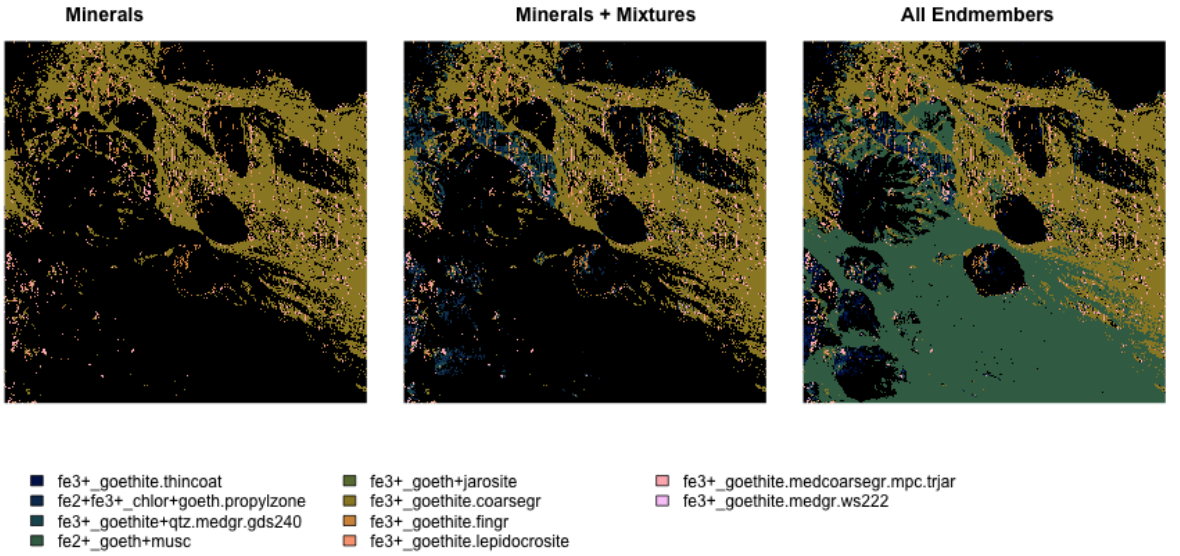

Figure 4.7. Comparison of aggregation levels for goethite endmembers (group 1) in Alunite Hill area.

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Appendix A. Endmembers used for each mineral

This section provides a summary and details of which endmembers are aggregated for each target mineral using each of the three criteria (mineral endmembers, mineral endmembers + mixtures where target mineral is dominant, and all endmembers with target mineral). Tables A1 and A2 summarize the number of endmembers aggregated for each group at each level, and the endmember file names are listed in Table A3 for minerals, A4 for mixtures, and A5 for all endmembers.

Table A1. Group 1 minerals, formulae, and number of endmembers included in each output level: minerals only (N_{min}), minerals and mixtures (N_{mix}), and total (N_{tot}).

Mineral	**Formulae**	**N_{min}**	**N_{mix}**	**N_{tot}**
Epidote	$Ca_2(Al,Fe^{3+})_3(SiO_4)_3(OH)$	2	2	2
Goethite	alpha-FeO(OH)	5	8	10
Hematite	alpha-Fe_2O_3	7	13	14
Nontronite	$Na0.33(Fe^{3+})_2(Si,Al)_4O_{10}*nH_20$	1	1	1
Pyrite[2]	FeS_2; $CuFeS_2$	2	2	2

Table A2. Group 2 minerals, formulae, and number of endmembers included in each output level: minerals only (N_{min}), minerals and mixtures (N_{mix}), and total (N_{tot}). Note that Group 2 Mixtures output also includes separate layers for Non-dominant areal mixtures (N endmembers) and Non-dominant intimate mixtures (N endmembers).

Mineral	**Formulae**	**N_{min}**	**N_{mix}**	**N_{tot}**
Alunite	$(Na,K)Al_3(SO_4)_2(OH)_6$	12	18	26
Buddingtonite	(NH4)AlSi3O8*0.5H20	1	1	2
Calcite	$CaCO_3$	1	6	13
Chlorite	$(Mg,Fe)_3(Si_3,Al)_4O_{10}(OH)_2$-$(Mg,Fe)_3(OH)_6$ $(Mg,Fe^{2+})_5Al(Si_3Al)O_{10}(OH)_8$	8	12	13
Dickite	$Al_2Si_2O_5(OH)_4$	1	2	5
Dolomite	$CaMg(CO_3)_2$	1	1	7
Epidote	$Ca_2(Al,Fe^{3+})_3(SiO_4)_3(OH)$	1	1	1
Halloysite	$Al_2Si_2O_5(OH)_4$	1	1	1

[2] The Pyrite library reference spectra are 1) an intimate mixture of weathered pyrite from mine tailings (from Spectral Library soils chapter), and 2) the Chalcopyrite mineral endmember.

Illite	$(K,H_3O)(Al,Mg,Fe)_2(Si,Al)_4O_{10}[(OH)_2,H_2O]$	4	4	5
Jarosite	$(NH_4)(Fe^{3+})_3(SO_4)_2(OH)_6$ $(Na)(Fe^{3+})_3(SO_4)_2(OH)_6$ $(K,H_3O)(Fe^{3+})_3(SO_4)_2(OH)_6$	4	6	11
Kaolinite	$Al_2Si_2O_5(OH)_4$	2	6	15
Montmorillonite	$(Na,Ca)0.33(Al,Mg)_2Si_4O_{10}(OH)_2*nH_20$	8	14	20
Muscovite	$KAl_2Si_3O_{10}(OH)_2$	4	10	20
Nontronite	$Na0.33(Fe^{3+})_2(Si,Al)_4O_{10}*nH_20$	1	1	1
Pyrophyllite	$Al_2Si_4O_{10}(OH)_2$	1	2	8

Table A3. Mineral only endmembers aggregated for each target mineral for outputs in `02_minerals_only`. Filenames for endmembers in Spectral Library 06 refer to .asc files in chapter subfolders of `sl/usgs/library06/ASCII`.

Target	Grp	tetracorder_file	Chap	filename
Alunite	2	sulfate_alunNa03	M	alunite_gds84.1187
Alunite	2	sulfate_alunNa56450c	M	alunite_res10.1624
Alunite	2	sulfate_alunNa78.450c	M	alunite_res12.1663
Alunite	2	sulfate_kalun150c	M	alunite_gds97.1347
Alunite	2	sulfate_kalun250c	M	alunite_gds96.1308
Alunite	2	sulfate_kalun450c	M	alunite_res2.1468
Alunite	2	sulfate_na40alun400c	M	alunite_res9.1585
Alunite	2	sulfate_na63alun300c	M	alunite_gds83.1079
Alunite	2	sulfate_na82alun100c	M	alunite_gds82.1063
Alunite	2	sulfate_naalun150c	M	alunite_gds95.1269
Alunite	2	sulfate_naalun300c	M	alunite_res4.1546
Alunite	2	sulfate_naalun450c	M	alunite_res3.1507
Buddingtonite	2	feldspar_buddingtonite_ammonium	M	buddingtonite_gds85.3924
Calcite	2	carbonate_calcite	M	calcite_ws272.4159
Chlorite	2	chlorite	M	chlorite_smr13.4908
Chlorite	2	chlorite_clinochlore	M	clinochlore_gds158.5327
Chlorite	2	chlorite_clinochlore.fe.gds157	M	clinochlore_gds157.5542
Chlorite	2	chlorite_clinochlore.fe.sc-cca-1	M	clinochlore_sc-cca-1.5725
Chlorite	2	chlorite_clinochlore.nmnh83369	M	clinochlore_nmnh83369.5457
Chlorite	2	chlorite_cookeite-car-1.a	M	cookeite_car1.6074

Chlorite	2	chlorite_cookeite-car-1.c	M	cookeite_car1.6228
Chlorite	2	chlorite_thuringite	M	thuringite_smr15.21810
Dickite	2	kaolgrp_dickite	M	dickite_nmnh106242.6820
Dolomite	2	carbonate_dolomite	M	dolomite_hs102.7116
Epidote	1	epidote	M	epidote_gds26.7546
Epidote	2	epidote	M	epidote_gds26.7546
Epidote	1	fe2+generic_br33a_bioqtzmonz_epidote	M	epidote_br93-33a.7490
Goethite	1	fe3+_goethite.coarsegr	M	goethite_ws222.8459
Goethite	1	fe3+_goethite.fingr	M	goethite_mpcma2b.8351
Goethite	1	fe3+_goethite.lepidocrosite	M	lepidochros_gds80.12600
Goethite	1	fe3+_goethite.medcoarsegr.mpc.trjar	M	goethite_mpcma2c.8365
Goethite	1	fe3+_goethite.medgr.ws222	M	goethite_ws222.8447
Halloysite	2	kaolgrp_halloysite	M	halloysite_nmnh106237.8999
Hematite	1	fe3+_hematite.fine.gr.fe2602	M	hematite_fe2602.9271
Hematite	1	fe3+_hematite.fine.gr.ws161	M	hematite_ws161.9776
Hematite	1	fe3+_hematite.med.gr.gds27	M	hematite_gds27.9282
Hematite	1	fe3+_hematite.nano.BR34b2	M	nanohematite_br93-34b2.15589
Hematite	1	fe3+_hematite.nano.BR34b2b	-	*research library*
Hematite	1	fe3+_maghemite	M	maghemite_gds81.13124
Hematite	1	fe3+_hematite.fine.gr.gds76	M	hema_qtz_gds76.25384
Illite	2	micagrp_illite	M	illite_imt1.11041
Illite	2	micagrp_illite.gds4	M	illite_gds4.10903
Illite	2	micagrp_illite.roscoelite	M	roscoelite_en124.19682
Illite	2	smectite_ammonillsmec	M	ammoniumillsmec_gds87.1757
Jarosite	2	sulfate_ammonjarosite	M	amojarosite_scrnhj.1851
Jarosite	2	sulfate_jarosite-K	M	jarosite_gds99.11469
Jarosite	2	sulfate_jarosite-lowT	M	jarosite_sj1.11629
Jarosite	2	sulfate_jarosite-Na	M	jarosite_gds24.11320
Kaolinite	2	kaolgrp_kaolinite_pxl	M	kaolinite_kga2.12190
Kaolinite	2	kaolgrp_kaolinite_wxl	M	kaolinite_cm9.11962
Montmorillonite	2	organic_benzene+montswy	A	montmorillonite_benzene.28220
Montmorillonite	2	organic_tce+montswy	A	montmorillonite_tce.28232
Montmorillonite	2	organic_toluene+montswy	A	montmorillonite_toluene.28244
Montmorillonite	2	organic_trichlor+montswy	A	montmorillonite_trichlor.28256
Montmorillonite	2	organic_unleaded.gas+montswy	A	montmorillonite_unleaded_gas.28268

Montmorillonite	2	smectite_montmorillonite_ca_swelling	-	*research library*
Montmorillonite	2	smectite_montmorillonite_fe_swelling	-	*research library*
Montmorillonite	2	smectite_montmorillonite_na_highswelling	M	montmorillonite_swy1.14688
Muscovite	2	micagrp_muscovite-low-Al	M	muscovite_cu93-1.14848
Muscovite	2	micagrp_muscovite-medhigh-Al	M	muscovite_gds113.15059
Muscovite	2	micagrp_muscoviteFerich	M	muscovite_gds116.15173
Muscovite	2	prehnite+muscovite	M	mizzonite_bm931-12.14023
Nontronite	1	fe3+_smectite_nontronite	M	nontronite_ng1.15991
Nontronite	2	smectite_nontronite_swelling	M	nontronite_ng1.15991
Pyrite	1	sulfide_pyrite	S	pyrite_lv95-6a.26297
Pyrite	1	sulfide_copper_chalcopyrite	M	pyrite_s29-4.18629
Pyrophyllite	2	pyrophyllite	M	pyrophyllite_pys1a.18885

Table A4. Mixture endmembers aggregated along with mineral endmembers in Table A3 for outputs in `03_minerals_mix`. Mixture type, dominant target mineral, and descriptions are taken from endmember metadata files in `sl/usgs/library06/DESCRIP` for mixtures in Spectral Library 06, and inferred from expert system entries for mixtures in Research Library 06. The 11 areal mixtures with no dominant target mineral are aggregated as `03_minerals_mix/group2um/group2_amix.tif` and the 9 intimate mixtures with no dominant target mineral are aggregated as `03_minerals_mix/group2um/group2_imix.tif`.

Grp	tetracorder_file	Mixture Type	Dominant Target Mineral	Description
2	alunite.33+kaol.33+musc.33	Areal	none	Alun. 33% +Kaol 33% + Musc 33%
2	alunite.5+kaol.5	Areal	none	Alun. 50%, Kaol 50%
2	alunite.5+musc.5	Areal	none	50% Alun 50% Muscovite
2	alunite+musc+pyroph	Areal	Muscovite	40% Muscovite 30% Alunite 30% Pyroph
2	alunite+pyrophyl	Intimate	none	Alunite, Pyrophyllite
2	calcite.25+dolom.25+Na-mont.5	Areal	Montmorillonite	50% Montmorillonite 25% calcite 25% dolomite
2	calcite+0.2Na-mont	Intimate	Calcite	80% Calcite
2	calcite+0.5Ca-mont	Areal	none	50% Calcite and 50% Ca-Montmorillonite
2	carbonate_calcite.25+dolom.25+Ca-mont.5	Areal	Montmorillonite	50% Montmorillonite 25% calcite 25% dolomite
2	carbonate_calcite+0.2Ca-mont	Areal	Calcite	80% Calcite
2	carbonate_calcite+0.2kaolwxl	Intimate	Calcite	80% Calcite + 20% kaolinite
2	carbonate_calcite+0.3muscovite	Areal	Muscovite	Calcite + 33% Muscovite 77%
2	carbonate_calcite+dolomite.5	Areal	none	Calcite 50% dolomite 50%

2	carbonate_calcite0.7+kaol0.3	Areal	Calcite	70% Calcite + 30% kaolinite
2	carbonate_dolo+.5ca-mont	Areal	none	50% Dolomite 50% Montmorillonite
2	carbonate_dolomite.5+Na-mont.5	Areal	none	50% Dolomite 50% Montmorillonite
2	carbonate_smectite_calcite.33+Ca-mont.67	Areal	Montmorillonite	67% Montmorillonite 33% Calcite
2	chlorite-skarn	Intimate	Chlorite	Major: Lizardite, Trace: Chlorite (clinochlore), Antigorite, and Orthochrysotile
2	dick+musc+gyp+jar.amix	Areal	Dickite	40% Dickite, 30% Muscovite, 20% Gypsum, 10% Jarosite
1	fe2+_goeth+musc	Intimate	Muscovite	Quartz (major), muscovite (minor), clinochlore (trace)
1	fe2+fe3+_chlor+goeth.propylzone	Intimate	Goethite	Goethite coated Chlorite Phyllite
1	fe2+fe3+_hematite_weathering	Intimate	Calcite	Major: Calcite, Minor: Anorthite, Augite, Hematite, Trace: Montmorillonite
1	fe2+fe3+mix_with_hematite_br5b	Intimate	Hematite	Major: Phlogopite, Minor: Magnetite and magnesioferrite, Trace: Albite
1	fe3+_goethite.thincoat	Coating	Goethite	Goethite_Thin_Film
1	fe3+_goethite+qtz.medgr.gds240	Intimate	Goethite	98% Quartz 2% Goethite
1	fe3+_hematite.fine.gr.gds76	Intimate	Hematite	98% Quartz 2% Hematite
1	fe3+_hematite.lg.gr.br25a	Coating	Hematite	Hematite coating on muscovite bearing quartzite
1	fe3+_hematite.lg.gr.br25c	Coating	Hematite	Hematite coating on muscovite bearing quartzite
1	fe3+_hematite.lg.gr.br34c	Coating	Hematite	Strong coating of hematite on a muscovite bearing quartzite
1	fe3+_hematite.med.gr.br25b	Coating	Hematite	Hematite coating on muscovite bearing quartzite
1	fe3+_hematite.thincoat	Coating	Hematite	Hematite_Thin_Film
2	feldspar_buddington.namont	Intimate	none	Buddingtonite (Feldspar group)+ Na-Mont
2	feldspar_buddington.namont2	Intimate	none	Buddingtonite (Feldspar group)+ Na-Mont
2	Kalun+kaol.intmx	Intimate	Alunite	Major: Alunite, minor: kaolinite
2	kaol.75+alun.25	Intimate	Kaolinite	Kaolinite 75% + Alunite 25%
2	kaol.75+pyroph.25	Areal	Kaolinite	Kaolinite 75% Pyroph 25%
2	kaolin.3+smect.7	Intimate	Kaolinite	30% kaolinite 70% smectite

2	kaolin.5+muscov.medAl	Areal	none	50% kaolinite 50% muscovite
2	kaolin.5+muscov.medhighAl	Areal	none	50% kaolinite 50% muscovite
2	kaolin.5+smect.5	Intimate	Kaolinite	50% kaolinite 50% smectite
2	kaolin+musc.intimat	Intimate	none	Kaolinite, Muscovite
2	micagrp_muscovite-med-Al	Intimate	Muscovite	Quartz (major), muscovite
2	musc+gyp+jar+dick.amix	Areal	Muscovite	40% Muscovite, 30% Gypsum, 20% Dickite, 10% Jarosite
2	musc+jarosite.intimat	Intimate	Jarosite	Muscovite phyllite + jarosite coating
2	musc+pyroph	Intimate	Muscovite	Quartz, minor muscovite, minor pyrophyllite
2	muscovite+chlorite	Intimate	none	Chlorite, Muscovite
2	Na-alun+kaol.intmx	Intimate	Alunite	quartz (major) + natro-alunite (major) + kaolinite (minor) + hematite (trace)
2	organic_drygrass+.17Na-mont	Areal	Montmorillonite	Dry grass and 17% montmorillonite
2	prehnite+.50chlorite	Areal	Chlorite	Prehnite+.50Chlorite AMIX
2	prehnite+.67chlorite	Areal	Chlorite	Prehnite+.67Chlorite AMIX
2	prehnite+.75chlorite	Areal	Chlorite	Prehnite+.75Chlorite AMIX
2	pyroph.5+alunit.5	Intimate	none	50% Pyrophyllite 50% Alunite
2	pyroph.5+mont0.5	Areal	none	50% Pyrophyllite 50% Montmorillonite
2	pyroph+tr.musc	Intimate	Pyrophyllite	Quartz, minor pyrophyllite, trace muscovite
2	smectite_beidellite_gds123	Intimate	Montmorillonite	Beidellite+Montmor GDS123
2	smectite_beidellite_gds124	Intimate	Montmorillonite	Beidellite+Montmor GDS124
2	sulfate_alun35K65Na.low	Intimate	Alunite	Fine grained and coarse grained Alunite
2	sulfate_alun66K34Na.low	Intimate	Alunite	Two alunite phases
2	sulfate_alun73K27Na.low	Intimate	Alunite	Two alunite phases
2	sulfate_ammonalunite	Intimate	Alunite	Ammonioalunite + Jarosite
2	sulfate-mix_gyp+jar+musc.amix	Areal	Jarosite	50% gypsum, 30% jarosite, 20% muscovite
2	sulfate-mix_gyp+jar+musc+dick.amix	Areal	none	40% Gypsum, 20% Muscovite, 20% Dickite, 20% Jarosite
2	sulfate-mix_gypsum+jar+illite.intmix	Intimate	none	Albite (major), quartz (minor), gypsum (minor), natrojarosite (minor), illite (minor), muscovite (minor), pyrite (trace), dolomite (trace)

2	sulfate+kaolingrp_natroalun+dickite	Intimate	none	Quartz (major), natroalunite (minor), dickite (minor), and gypsum (trace)
2	talc+calcite.parkcity	Areal	Calcite	Major - Calcite, Talc
2	talc+carbonate.parkcity	Intimate	none	Major - Dolomite, Calcite

Table A5. List of all endmembers aggregated for each target mineral for outputs in `04_minerals_all`

Target Mineral	Group	tetracorder_file
Alunite	group.2um	alunite+musc+pyroph
Alunite	group.2um	alunite.33+kaol.33+musc.33
Alunite	group.2um	alunite.5+kaol.5
Alunite	group.2um	alunite.5+musc.5
Alunite	group.2um	Kalun+kaol.intmx
Alunite	group.2um	Na-alun+kaol.intmx
Alunite	group.2um	sulfate_alun35K65Na.low
Alunite	group.2um	sulfate_alun66K34Na.low
Alunite	group.2um	sulfate_alun73K27Na.low
Alunite	group.2um	sulfate_ammonalunite
Alunite	group.2um	kaol.75+alun.25
Alunite	group.2um	alunite+pyrophyl
Alunite	group.2um	pyroph.5+alunit.5
Alunite	group.2um	sulfate+kaolingrp_natroalun+dickite
Alunite	group.2um	sulfate_alunNa03
Alunite	group.2um	sulfate_alunNa56450c
Alunite	group.2um	sulfate_alunNa78.450c
Alunite	group.2um	sulfate_kalun150c
Alunite	group.2um	sulfate_kalun250c
Alunite	group.2um	sulfate_kalun450c
Alunite	group.2um	sulfate_na40alun400c
Alunite	group.2um	sulfate_na63alun300c
Alunite	group.2um	sulfate_na82alun100c
Alunite	group.2um	sulfate_naalun150c
Alunite	group.2um	sulfate_naalun300c
Alunite	group.2um	sulfate_naalun450c
Buddingtonite	group.2um	feldspar_buddington.namont
Buddingtonite	group.2um	feldspar_buddington.namont2
Buddingtonite	group.2um	feldspar_buddingtonite_ammonium
Calcite	group.2um	carbonate_calcite+0.2Ca-mont

Calcite	group.2um	carbonate_calcite0.7+kaol0.3
Calcite	group.2um	talc+calcite.parkcity
Calcite	group.2um	calcite.25+dolom.25+Na-mont.5
Calcite	group.2um	carbonate_calcite.25+dolom.25+Ca-mont.5
Calcite	group.2um	carbonate_smectite_calcite.33+Ca-mont.67
Calcite	group.2um	carbonate_calcite+0.3muscovite
Calcite	group.2um	calcite+0.5Ca-mont
Calcite	group.2um	carbonate_calcite+dolomite.5
Calcite	group.2um	calcite+0.2Na-mont
Calcite	group.2um	carbonate_calcite+0.2kaolwxl
Calcite	group.2um	talc+carbonate.parkcity
Calcite	group.2um	carbonate_calcite
Chlorite	group.2um	prehnite+.50chlorite
Chlorite	group.2um	prehnite+.67chlorite
Chlorite	group.2um	prehnite+.75chlorite
Chlorite	group.2um	chlorite-skarn
Chlorite	group.2um	muscovite+chlorite
Chlorite	group.2um	chlorite
Chlorite	group.2um	chlorite_clinochlore
Chlorite	group.2um	chlorite_clinochlore.fe.gds157
Chlorite	group.2um	chlorite_clinochlore.fe.sc-cca-1
Chlorite	group.2um	chlorite_clinochlore.nmnh83369
Chlorite	group.2um	chlorite_cookeite-car-1.a
Chlorite	group.2um	chlorite_cookeite-car-1.c
Chlorite	group.2um	chlorite_thuringite
Dickite	group.2um	dick+musc+gyp+jar.amix
Dickite	group.2um	musc+gyp+jar+dick.amix
Dickite	group.2um	sulfate-mix_gyp+jar+musc+dick.amix
Dickite	group.2um	sulfate+kaolingrp_natroalun+dickite
Dickite	group.2um	kaolgrp_dickite
Dolomite	group.2um	calcite.25+dolom.25+Na-mont.5
Dolomite	group.2um	carbonate_calcite.25+dolom.25+Ca-mont.5
Dolomite	group.2um	carbonate_calcite+dolomite.5
Dolomite	group.2um	carbonate_dolo+.5ca-mont
Dolomite	group.2um	carbonate_dolomite.5+Na-mont.5
Dolomite	group.2um	talc+carbonate.parkcity
Dolomite	group.2um	carbonate_dolomite
Epidote	group.1um	epidote

Epidote	group.2um	epidote
Epidote	group.1um	fe2+generic_br33a_bioqtzmonz_epidote
Goethite	group.1um	fe3+_goethite.thincoat
Goethite	group.1um	fe2+fe3+_chlor+goeth.propylzone
Goethite	group.1um	fe3+_goethite+qtz.medgr.gds240
Goethite	group.1um	fe2+_goeth+musc
Goethite	group.1um	fe3+_goeth+jarosite[3]
Goethite	group.1um	fe3+_goethite.coarsegr
Goethite	group.1um	fe3+_goethite.fingr
Goethite	group.1um	fe3+_goethite.lepidocrosite
Goethite	group.1um	fe3+_goethite.medcoarsegr.mpc.trjar
Goethite	group.1um	fe3+_goethite.medgr.ws222
Halloysite	group.2um	kaolgrp_halloysite
Hematite	group.1um	fe3+_hematite.lg.gr.br25a
Hematite	group.1um	fe3+_hematite.lg.gr.br25c
Hematite	group.1um	fe3+_hematite.lg.gr.br34c
Hematite	group.1um	fe3+_hematite.med.gr.br25b
Hematite	group.1um	fe3+_hematite.thincoat
Hematite	group.1um	fe2+fe3+_hematite_weathering
Hematite	group.1um	fe2+fe3+mix_with_hematite_br5b
Hematite	group.1um	fe3+_hematite.fine.gr.gds76
Hematite	group.1um	fe3+_hematite.fine.gr.fe2602
Hematite	group.1um	fe3+_hematite.fine.gr.ws161
Hematite	group.1um	fe3+_hematite.med.gr.gds27
Hematite	group.1um	fe3+_hematite.nano.BR34b2
Hematite	group.1um	fe3+_hematite.nano.BR34b2b
Hematite	group.1um	fe3+_maghemite
Illite	group.2um	sulfate-mix_gypsum+jar+illite.intmix
Illite	group.2um	micagrp_illite
Illite	group.2um	micagrp_illite.gds4
Illite	group.2um	micagrp_illite.roscoelite
Illite	group.2um	smectite_ammonillsmec
Jarosite	group.2um	dick+musc+gyp+jar.amix
Jarosite	group.2um	sulfate-mix_gyp+jar+musc.amix
Jarosite	group.2um	musc+gyp+jar+dick.amix
Jarosite	group.2um	sulfate-mix_gyp+jar+musc+dick.amix
Jarosite	group.2um	sulfate_ammonalunite

[3] Intimate and areal mixture: 50% area Jarosite, 50% area Intimate mixture 98% quartz 2% Goethite

Jarosite	group.2um	musc+jarosite.intimat
Jarosite	group.2um	sulfate-mix_gypsum+jar+illite.intmix
Jarosite	group.2um	sulfate_ammonjarosite
Jarosite	group.2um	sulfate_jarosite-K
Jarosite	group.2um	sulfate_jarosite-lowT
Jarosite	group.2um	sulfate_jarosite-Na
Kaolinite	group.2um	carbonate_calcite0.7+kaol0.3
Kaolinite	group.2um	kaol.75+pyroph.25
Kaolinite	group.2um	alunite.33+kaol.33+musc.33
Kaolinite	group.2um	alunite.5+kaol.5
Kaolinite	group.2um	kaolin.5+muscov.medAl
Kaolinite	group.2um	kaolin.5+muscov.medhighAl
Kaolinite	group.2um	Kalun+kaol.intmx
Kaolinite	group.2um	Na-alun+kaol.intmx
Kaolinite	group.2um	carbonate_calcite+0.2kaolwxl
Kaolinite	group.2um	kaol.75+alun.25
Kaolinite	group.2um	kaolin.3+smect.7
Kaolinite	group.2um	kaolin.5+smect.5
Kaolinite	group.2um	kaolin+musc.intimat
Kaolinite	group.2um	kaolgrp_kaolinite_pxl
Kaolinite	group.2um	kaolgrp_kaolinite_wxl
Montmorillonite	group.2um	carbonate_calcite+0.2Ca-mont
Montmorillonite	group.2um	calcite.25+dolom.25+Na-mont.5
Montmorillonite	group.2um	carbonate_calcite.25+dolom.25+Ca-mont.5
Montmorillonite	group.2um	carbonate_smectite_calcite.33+Ca-mont.67
Montmorillonite	group.2um	organic_drygrass+.17Na-mont
Montmorillonite	group.2um	calcite+0.5Ca-mont
Montmorillonite	group.2um	carbonate_dolo+.5ca-mont
Montmorillonite	group.2um	carbonate_dolomite.5+Na-mont.5
Montmorillonite	group.2um	pyroph.5+mont0.5
Montmorillonite	group.2um	calcite+0.2Na-mont
Montmorillonite	group.2um	smectite_beidellite_gds123
Montmorillonite	group.2um	smectite_beidellite_gds124
Montmorillonite	group.2um	organic_benzene+montswy
Montmorillonite	group.2um	organic_tce+montswy
Montmorillonite	group.2um	organic_toluene+montswy
Montmorillonite	group.2um	organic_trichlor+montswy
Montmorillonite	group.2um	organic_unleaded.gas+montswy

Montmorillonite	group.2um	smectite_montmorillonite_ca_swelling
Montmorillonite	group.2um	smectite_montmorillonite_fe_swelling
Montmorillonite	group.2um	smectite_montmorillonite_na_highswelling
Muscovite	group.2um	dick+musc+gyp+jar.amix
Muscovite	group.2um	sulfate-mix_gyp+jar+musc.amix
Muscovite	group.2um	alunite+musc+pyroph
Muscovite	group.2um	carbonate_calcite+0.3muscovite
Muscovite	group.2um	musc+gyp+jar+dick.amix
Muscovite	group.2um	alunite.33+kaol.33+musc.33
Muscovite	group.2um	alunite.5+musc.5
Muscovite	group.2um	kaolin.5+muscov.medAl
Muscovite	group.2um	kaolin.5+muscov.medhighAl
Muscovite	group.2um	sulfate-mix_gyp+jar+musc+dick.amix
Muscovite	group.2um	musc+jarosite.intimat
Muscovite	group.2um	micagrp_muscovite-med-Al
Muscovite	group.2um	musc+pyroph
Muscovite	group.2um	kaolin+musc.intimat
Muscovite	group.2um	muscovite+chlorite
Muscovite	group.2um	pyroph+tr.musc
Muscovite	group.2um	micagrp_muscovite-low-Al
Muscovite	group.2um	micagrp_muscovite-medhigh-Al
Muscovite	group.2um	micagrp_muscoviteFerich
Muscovite	group.2um	prehnite+muscovite
Nontronite	group.1um	fe3+_smectite_nontronite
Nontronite	group.2um	smectite_nontronite_swelling
Pyrite	group.1um	sulfide_copper_chalcopyrite
Pyrite	group.1um	sulfide_pyrite
Pyrophyllite	group.2um	kaol.75+pyroph.25
Pyrophyllite	group.2um	alunite+musc+pyroph
Pyrophyllite	group.2um	pyroph.5+mont0.5
Pyrophyllite	group.2um	musc+pyroph
Pyrophyllite	group.2um	alunite+pyrophyl
Pyrophyllite	group.2um	pyroph.5+alunit.5
Pyrophyllite	group.2um	pyroph+tr.musc
Pyrophyllite	group.2um	pyrophyllite

Appendix B. Wavelength regions

Table B1. Wavelength region groups as defined in Tetracorder version 5.27. Mineral mapping on Earth using airborne VNIR imagery primarily relies on endmembers in Groups 0, 1, and 2. Output directory names refer to outputs directly from Tetracorder; only outputs from Groups 1 and 2 are retained and used for aggregated outputs described in this document. Adapted from `group.names.txt`[4]. *Group 0 outputs are included in all other output folders unless otherwise specified on line 660 of the expert system file.

Group	Output directory	Group Name	Description
0	*see above	catchall	catch for other declared groups
1	group.1um	1um region	electronic absorptions 1-micron region
2	group.2um	2-2.5um	2 to 2.5-micron region narrow
3	group.veg	veg detect	vegetation detection
4	group.1.5um-broad	1.5um broad	broad absorptions in the 1.5-micron region
5	group.2um-broad	2um broad	broad absorptions in the 2-micron region
6	group.2.5um	2.5um region	2.5-micron region
7	group.3um	2.5-3um	2.7 to 3-micron OH region
8	group.2.8um	3.2um region	3.2-micron region empty at the moment
9	group.zz	UV	Placeholder for future UV
10	group.3.5um_curve	3.5um curveC	testing 3.5 um curved continua
11	group.3.5um	3.5um linear	3.5-micron region linear continua
12	group.4um	4um region	4-micron region
13	group.1.3-1.4um	1.3-1.4 nrw	1.3-1.4 micron OH narrow
14	group.1.4um	1.4-1.5 nrw	1.4-1.5 micron OH
15	group.1.5um	1.5um OH	1.5 micron OH
17	group.1.7um	1.7um region	Placeholder for future 1.7 microns CH and water
19	group.1.9um	1.9-2um H2O	1.9-2 micron water and ice
20	group.ree	rare-earth	the search for rare-earth oxides
21	group.ree_neod	Neodymium	the search for rare-earth oxide Neodymium
22	group.ree_samar	Samarium	the search for rare-earth oxide Samarium

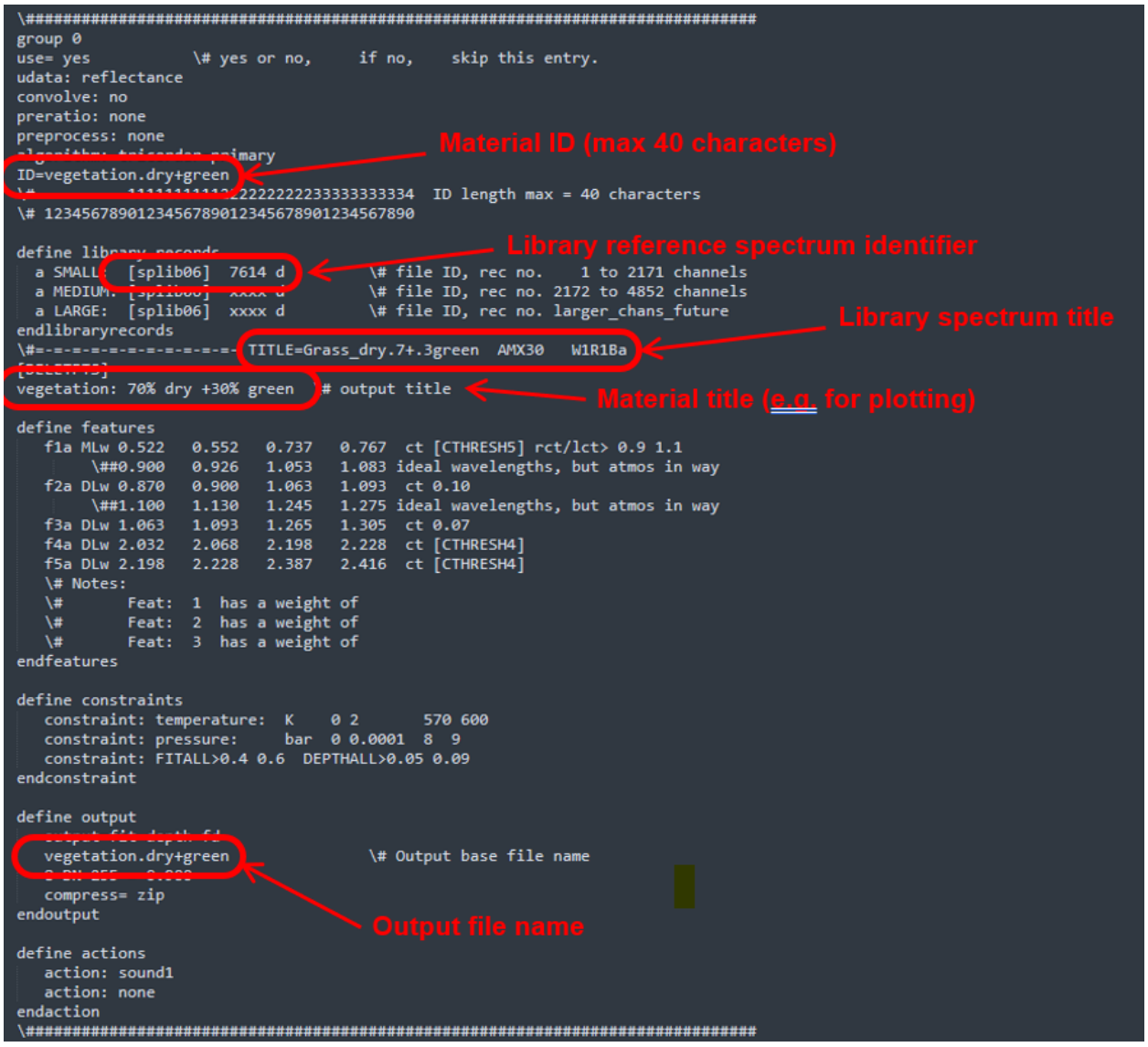
[4] https://github.com/PSI-edu/spectroscopy-tetracorder/blob/main/tetracorder.cmds/tetracorder5.27a.cmds/group.names.txt

Table B2. Group 0 endmember names, filenames in Tetracorder output, associated spectra file names, and spectral library chapter (V = vegetation, L = liquids, A = artificial). Group 0 spectra are all from USGS Spectral Library 06 and files are in `sl1/usgs/library06/ASCII`.

Endmember spectrum name	Tetracorder output file	Library spectrum file	Chapter
vegetation.green	vegetation1	firtree_ih91-2.29889	V
vegetation: 70% dry +30% green	vegetation.dry+green	grass_dry+green_series.31008	V
snow H2O ice	snow.and.ice	h2o_ice_gds136.26841	L
melting Snow 1a	snow.melting.1a	melting_snow_1-16.26997	L
melting snow 3	snow.melting.3	melting_snow_1-16.27044	L
melting snow 8	snow.melting.8	melting_snow_1-16.27137	L
melting snow (slush) 9	snow.slush.9	melting_snow_1-16.27185	L
melting snow (slush) 16	snow.slush.16	melting_snow_1-16.26925	L
5 melting snow 1a + veg 0.5	snow.melting1a+0.5veg	melting_snow_veg_1-16.27021	L
5 melting snow 9 + veg 0.5	snow.melting9+0.5veg	melting_snow_veg_1-16.27209	L
5 melting snow 16 + veg 0.5	snow.melting16+0.5veg	melting_snow_veg_1-16.26974	L
water high chlorophyll	water.high.chlorophyll	seawater_coast_sw1.27251	L
water low chlorophyll	water.low.chlorophyll	seawater_open_ocean_sw2.27262	L
red coated algea water	water.red.algae	red_coated_algea.27230	L
water + mont. (1.67g/liter)	water+mont16.5gpl	water_mont_mix_a.27324	L
water + mont. (0.5g/liter)	water+mont5.01gpl	water_mont_mix_a.27348	L
water + mont. (5.01g/liter)	water+mont1.67gpl	water_mont_mix_a.27299	L
water + mont. (16.5g/liter)	water+mont0.5gpl	water_mont_mix_a.27273	L
dry long grass AV87-2	organic_dry_long_grass-thick	dry_longgrass_av87-2.29812	V
white PVC pipe	organic_white_pvc_pipe	pipe_gds338.28978	A
organic, green plastic tarp	organic_green_plastic_tarp	tarp_gds339.29036	A

Appendix C. Expert system entries

Spectral features, constraints, and all other endmember-specific information are specified in the expert system command file (`tetracorder.cmds/tetracorder5.27a.cmds/cmd.lib.setup.t5.27a1`). This section provides details and an annotated example of an expert system entry.




```
\#############################################################################
group 0
use= yes           \# yes or no,     if no,    skip this entry.
udata: reflectance
convolve: no
preratio: none
preprocess: none
ID=vegetation.dry+green
\#         1111111111222222222233333333334  ID length max = 40 characters
\# 12345678901234567890123456789012345678901234567890

define library records
  a SMALL:  [splib06]  7614 d          \# file ID, rec no.    1 to 2171 channels
  a MEDIUM: [splib06]  xxxx d          \# file ID, rec no. 2172 to 4852 channels
  a LARGE:  [splib06]  xxxx d          \# file ID, rec no. larger_chans_future
endlibraryrecords
\#=-=-=-=-=-=-=-=-=-=-=- TITLE=Grass_dry.7+.3green  AMX30   W1R1Ba
vegetation: 70% dry +30% green   # output title

define features
   f1a MLw 0.522   0.552   0.737   0.767  ct [CTHRESH5] rct/lct> 0.9 1.1
        \##0.900   0.926   1.053   1.083 ideal wavelengths, but atmos in way
   f2a DLw 0.870   0.900   1.063   1.093  ct 0.10
        \##1.100   1.130   1.245   1.275 ideal wavelengths, but atmos in way
   f3a DLw 1.063   1.093   1.265   1.305  ct 0.07
   f4a DLw 2.032   2.068   2.198   2.228  ct [CTHRESH4]
   f5a DLw 2.198   2.228   2.387   2.416  ct [CTHRESH4]
   \# Notes:
   \#       Feat:  1  has a weight of
   \#       Feat:  2  has a weight of
   \#       Feat:  3  has a weight of
endfeatures

define constraints
   constraint: temperature:  K    0 2       570 600
   constraint: pressure:     bar  0 0.0001  8  9
   constraint: FITALL>0.4 0.6  DEPTHALL>0.05 0.09
endconstraint

define output
   vegetation.dry+green              \# Output base file name
   compress= zip
endoutput

define actions
   action: sound1
   action: none
endaction
\#############################################################################
```

Figure C1. Identifiers in an example expert system entry.

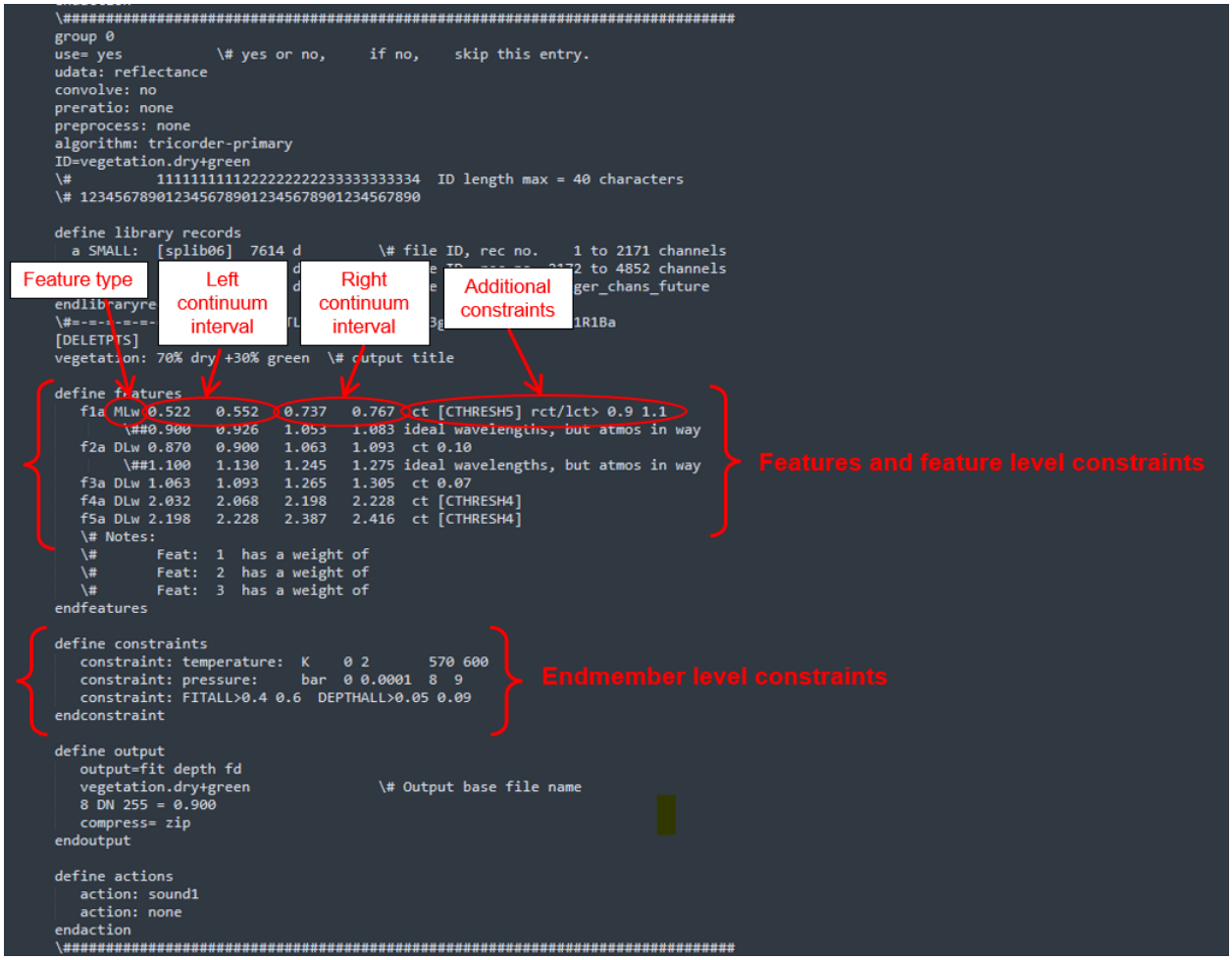


Figure C2. Features and constraints in example expert system entry. This example contains 1 mandatory ("M") feature and 4 additional diagnostic features. Each feature is defined by 4 wavelengths: the first 2 identify the continuum interval on the left side of the feature and the next 2 identify the continuum interval on the right side of the feature. Additional feature-level constraints follow.

Table C1. Description of spectral feature types in expert system file.

Code	Type	Description
D	Diagnostic	Must be present. fit, depth, fit*depth must be above thresholds. If a diagnostic feature is enabled but not present in the measured spectrum, the feature strength will be zero or too low and the material will not be detected. When there are multiple diagnostic features defined, only one feature needs to be enabled for the material to be enabled.
M	Must have	Unconditionally diagnostic. If this feature is disabled the material is disabled. Added in 5.27a1 to handle problems associated with disabled diagnostic features.

O	Optionally present	If an optional feature is not detected, its fit and depth are set to zero and the material may be identified by the presence of other absorption features
W	Weak	Must be present, but the area of the feature is set to zero for calculations. Only used when necessary because noise can mask the presence of a weak band.

In addition to diagnostic spectral features, expert system entries may contain other constraints required for positive detections. Many constraints use fuzzy logic to calculate a multiplier between 0 and 1 as described in the expert system file comments (lines 324–353) and (Clark et al., 2010).

Table C2. Description of ancillary constraints; adapted from expert system file comments (lines 315–425).

Type	**Description**	**Examples**
Continuum thresholding	Feature level constraint. Minimum or maximum values for the reflectance values of the whole continuum, left interval, or right interval. Variables CTHRESH1, CTHRESH2, CTHRESH4, CTHRESH5 are set on lines 420–423 of the expert system file.	ct [CTHRESH5] ct 0.10 lct 0.0 0.08 rct 0 .04
Continuum slope or shape	Feature level constraint. Minimum or maximum values for slope or shape of continuum. Shape refers to the spectral "shoulderness" of features before continuum removal as described in (Clark et al., 2010).	rct/lct> 0.9 1.1 lct/rct> 0.9 1.1 rcbblc< 0.9 0.8 rcbblc< 0.3 0.4 r*bd> [RBD10]
Feature ratios	Minimum or maximum ratio between fit or depth among diagnostic features.	
NOT features	Presence or absence of ancillary features, as determined by depth and fit thresholds for specified features.	[NOTGREENVEG] 1 0.50a 0.5 [NOTjarosite] 2 0.03a 0.6
Fit or depth thresholding	Endmember level constraint. If a calculated value falls below this value then the material is not identified. Default values for fit, depth, and fit times depth are set in lines 199-202 of the expert system file. There is a separate default value for group 2.	FIT> 0.2 0.4 DEPTH> 0.004 0.006 FITALL>0.4 0.6
Temperature or pressure	Endmember level constraint. Minimum or maximum temperature or pressure thresholds for a material.	temperature: C -6 -3 3 6

Table C2. Reference spectra used to define NOT features.

Feature	**Library**	**Reference spectrum**
NOTDRYVEG	splib06	Dry_Long_Grass AV87-2
NOTGREENVEG	splib06	Fir_Tree IH91-2
NOTMONTSWY	sprlb06	Montmorillonite SWy-1
NOTMONTAZ	sprlb06	Montmorillonite SAz-1
NOTMUSCOVITE1	splib06	Muscovite GDS113 Ruby
NOTMUSCOVITE2	splib06	Muscovite CU91-250A med Al
NOTNAALUNITE1	splib06	Alunite GDS95 Na Syn (150C)
NOTKALUNITE1	splib06	Alunite GDS97 K Syn (150C)
NOTKALUNITE2	splib06	Alunite GDS96 K Syn (250C)
NOTbroadFe2	splib06	Chlorite+Muscovite CU93-65A
NOTepidote	splib06	Epidote GDS26.a 75-200um
NOTgypsum	sprlb06	Gypsum HS333.3B (Selenite)
NOTjarosite	splib06	Jarosite GDS99 K 200C Syn
NOTCH1	splib06	Plastic_PVC GDS338 White
NOTDOLOMITE	sprlb06	Dolomite HS102.3B

Appendix D. Convolved Library Codes

This section describes the naming convention for convolved spectral libraries. It is adapted from the `sl1/usgs/library06.conv` folder readme file[5].
Convolved spectral libraries are named using 8 character codes conforming to the standard: **annccyyd**.

Table D1. Standard for naming convolved reference libraries.

	Description
a	s for spectral library or r for research library
nn	Library version number (06)
cc	Output convolved spectrometer model/type
yy	Year or other code
d	Output spectrometer version within year yy

Table D2. Spectrometer model/type codes for existing convolved libraries available in PSI GitHub repository (https://github.com/PSI-edu/spectroscopy-tetracorder).

Code	**Description**
as	aster
av	aviris
an	Aviris-ng next gen
cr	crism
hd	Hydice
hy	HyMap
mi	MIVIS
mm	Moon Minerology Mapper (2008)
nm	nims
pb	probe
pf	Mars pathfinder

[5] https://github.com/PSI-edu/spectroscopy-tetracorder/blob/main/sl1/usgs/library06.conv/AAAAAA.README.txt

tm	LandsatTM
vm	vims
ag	Agilent hand held FTIR 1.5-15 micron spectrometer
gn	Generic 20, 30, 40 etc. nm bandpass
pr	PRISMA 2021 ESA Earth orbiter (238 channels)
nc	Nicolet, followed by wavenumber resolution, eg. nc04 is 4 cm^-1
fs00	ASD field spectrometer 2151
fs71	ASD field spectrometer 717 ch
fs35	Field spectrometer 358 ch
bk1x	USGS beckman
gr	Gregg Swayze's resolution study
ag21	Agilent hand held FTIR 2.5-15 micron spectrometer

Table D3. Example names of convolved libraries available in PSI GitHub repository (https://github.com/PSI-edu/spectroscopy-tetracorder).

Name	**Description**
s06av95a	Aviris 1995
s06vm07a	Cassini VIMS 2007 wavelengths
s06mm09c	Moon Mineralogy Mapper 2009
s06crj3a	CRISM 2012 J_MTR3 merged V+IR
lab3800a	Lab 3800 channels 1-6 microns
s06ag21a	Agilent hand held FTIR 2.5-15 micron

Appendix E. Additional aggregations

Table E1. Endmember aggregations used for EMIT minerals

Group	file	BD	Depth
calcite.group2	group.2um/carbonate_calcite.depth	0.995	0.2112
calcite.group2	group.2um/talc+calcite.parkcity.depth	0.5	0.3022
calcite.group2	group.2um/talc+carbonate.parkcity.depth	0.33	0.2187
calcite.group2	group.2um/carbonate_calcite+0.2Ca-mont.depth	0.796	0.1068
calcite.group2	group.2um/carbonate_calcite+dolomite.5.depth	0.497	0.2741
calcite.group2	group.2um/calcite.25+dolom.25+Na-mont.5.depth	0.249	0.1105
calcite.group2	group.2um/carbonate_calcite.25+dolom.25+Ca-mont.5.depth	0.249	0.1274
calcite.group2	group.2um/calcite+0.2Na-mont.depth	0.796	0.0939
calcite.group2	group.2um/calcite+0.5Ca-mont.depth	0.497	0.1711
calcite.group2	group.2um/carbonate_calcite+0.3muscovite.depth	0.667	0.2254
calcite.group2	group.2um/carbonate_smectite_calcite.33+Ca-mont.67.depth	0.328	0.1186
calcite.group2	group.2um/carbonate_calcite+0.2kaolwxl.depth	0.796	0.1504
calcite.group2	group.2um/carbonate_calcite0.7+kaol0.3.depth	0.696	0.2145
chlorite.group2	group.2um/chlorite.depth	1	0.3724
chlorite.group2	group.2um/chlorite-skarn.depth	0.61	0.238
chlorite.group2	group.2um/muscovite+chlorite.depth	0.03	0.1594
chlorite.group2	group.2um/chlorite_clinochlore.depth	0.998	0.2887
chlorite.group2	group.2um/chlorite_clinochlore.nmnh83369.depth	1	0.2428
chlorite.group2	group.2um/chlorite_clinochlore.fe.gds157.depth	1	0.2204
chlorite.group2	group.2um/chlorite_clinochlore.fe.sc-cca-1.depth	1	0.2009
chlorite.group2	group.2um/chlorite_cookeite-car-1.a.depth	0.94	0.2283
chlorite.group2	group.2um/chlorite_cookeite-car-1.c.depth	0.81	0.0794
chlorite.group2	group.2um/chlorite_thuringite.depth	1	0.3134
chlorite.group2	group.2um/prehnite+.50chlorite.depth	0.5	0.3015
chlorite.group2	group.2um/prehnite+.67chlorite.depth	0.67	0.307
chlorite.group2	group.2um/prehnite+.75chlorite.depth	0.75	0.3112
dolomite.group2	group.2um/carbonate_dolomite.depth	0.996	0.2903
dolomite.group2	group.2um/talc+carbonate.parkcity.depth	0.33	0.2187
dolomite.group2	group.2um/carbonate_calcite+dolomite.5.depth	0.498	0.2741
dolomite.group2	group.2um/carbonate_dolo+.5ca-mont.depth	0.5	0.1314
dolomite.group2	group.2um/calcite.25+dolom.25+Na-mont.5.depth	0.249	0.1105
dolomite.group2	group.2um/carbonate_calcite.25+dolom.25+Ca-mont.5.depth	0.249	0.1274
dolomite.group2	group.2um/carbonate_dolomite.5+Na-mont.5.depth	0.498	0.1027

goethite-fine.group1	group.1um/fe3+_goethite.fingr.depth	0.2	0.3065
goethite-fine.group1	group.1um/fe3+_goethite.lepidocrosite.depth	1	0.5526
goethite-fine.group1	group.1um/fe3+_goethite.thincoat.depth	0.1	0.5296
goethite-fine.group1	group.1um/fe3+_goeth+jarosite.depth	0.02	0.2184
goethite-fine.group1	group.1um/fe2+_goeth+musc.depth	0.04	0.1954
goethite-large.group1	group.1um/fe3+_goethite.coarsegr.depth	1	0.4869
goethite-med.group1	group.1um/fe3+_goethite.medgr.ws222.depth	1	0.4443
goethite-med.group1	group.1um/fe3+_goethite.medcoarsegr.mpc.trjar.depth	0.37	0.2699
goethite-med.group1	group.1um/fe2+fe3+_chlor+goeth.propylzone.depth	0.02	0.143
goethite-med.group1	group.1um/fe3+_goethite+qtz.medgr.gds240.depth	0.02	0.1069
hematite-fine.group1	group.1um/fe3+_hematite.fine.gr.fe2602.depth	1	0.3957
hematite-fine.group1	group.1um/fe3+_hematite.fine.gr.ws161.depth	0.79	0.4521
hematite-fine.group1	group.1um/fe3+_hematite.fine.gr.gds76.depth	0.02	0.3144
hematite-fine.group1	group.1um/fe2+fe3+mix_with_hematite_br5b.depth	0.17	0.1475
hematite-fine.group1	group.1um/fe2+fe3+_hematite_weathering.depth	0.01	0.1239
hematite-fine.group1	group.1um/fe3+_hematite.thincoat.depth	0.05	0.5045
hematite-large.group1	group.1um/fe3+_hematite.lg.gr.br25a.depth	0.01	0.4218
hematite-large.group1	group.1um/fe3+_hematite.lg.gr.br25c.depth	0.69	0.5286
hematite-large.group1	group.1um/fe3+_hematite.lg.gr.br34c.depth	0.63	0.4616
hematite-large.group1	group.1um/fe3+_maghemite.depth	0.85	0.7649
hematite-med.group1	group.1um/fe3+_hematite.med.gr.gds27.depth	1	0.5523
hematite-med.group1	group.1um/fe3+_hematite.med.gr.br25b.depth	0.05	0.4408
hematite-nano.group1	group.1um/fe3+_hematite.nano.BR34b2.depth	0.01	0.2727
hematite-nano.group1	group.1um/fe3+_hematite.nano.BR34b2b.depth	0.01	0.2727
illite.group2	group.2um/micagrp_illite.depth	0.99	0.1127
illite.group2	group.2um/micagrp_illite.gds4.depth	0.76	0.2103
illite.group2	group.2um/sulfate-mix_gypsum+jar+illite.intmix.depth	0.33	0.1323
illite.group2	group.2um/smectite_ammonillsmec.depth	0.5	0.1899
illite.group2	group.2um/micagrp_illite.roscoelite.depth	0.15	0.1342
illite+muscovite.group2	group.2um/micagrp_muscovite-med-Al.depth	0.59	0.1989
illite+muscovite.group2	group.2um/micagrp_muscovite-medhigh-Al.depth	1	0.2769
illite+muscovite.group2	group.2um/micagrp_muscovite-low-Al.depth	0.22	0.1694
illite+muscovite.group2	group.2um/micagrp_muscoviteFerich.depth	1	0.2646
illite+muscovite.group2	group.2um/pyroph+tr.musc.depth	0.04	0.3864
illite+muscovite.group2	group.2um/musc+pyroph.depth	0.15	0.3067
illite+muscovite.group2	group.2um/alunite+musc+pyroph.depth	0.4	0.1982
illite+muscovite.group2	group.2um/kaolin.5+muscov.medAl.depth	0.295	0.3232
illite+muscovite.group2	group.2um/kaolin.5+muscov.medhighAl.depth	0.5	0.3501

illite+muscovite.group2	group.2um/kaolin+musc.intimat.depth	0.1	0.2215
illite+muscovite.group2	group.2um/musc+jarosite.intimat.depth	0.27	0.2172
illite+muscovite.group2	group.2um/sulfate-mix_gyp+jar+musc.amix.depth	0.2	0.1942
illite+muscovite.group2	group.2um/sulfate-mix_gyp+jar+musc+dick.amix.depth	0.2	0.2619
illite+muscovite.group2	group.2um/musc+gyp+jar+dick.amix.depth	0.4	0.2561
illite+muscovite.group2	group.2um/dick+musc+gyp+jar.amix.depth	0.3	0.2901
illite+muscovite.group2	group.2um/alunite.5+musc.5.depth	0.295	0.3901
illite+muscovite.group2	group.2um/alunite.33+kaol.33+musc.33.depth	0.195	0.3265
illite+muscovite.group2	group.2um/muscovite+chlorite.depth	0.53	0.1594
illite+muscovite.group2	group.2um/carbonate_calcite+0.3muscovite.depth	0.33	0.2254
illite+muscovite.group2	group.2um/prehnite+muscovite.depth	0.1	0.1756
kaolinte.group2	group.2um/kaolgrp_kaolinite_wxl.depth	0.97	0.3651
kaolinte.group2	group.2um/kaolgrp_kaolinite_pxl.depth	1	0.3106
kaolinte.group2	group.2um/kaolgrp_halloysite.depth	0.99	0.4099
kaolinte.group2	group.2um/kaolgrp_dickite.depth	1	0.5162
kaolinte.group2	group.2um/kaolin.5+smect.5.depth	0.5	0.2144
kaolinte.group2	group.2um/kaolin.3+smect.7.depth	0.3	0.2053
kaolinte.group2	group.2um/kaol.75+pyroph.25.depth	0.73	0.3122
kaolinte.group2	group.2um/alunite.5+kaol.5.depth	0.475	0.3502
kaolinte.group2	group.2um/kaol.75+alun.25.depth	0.73	0.3792
kaolinte.group2	group.2um/Kalun+kaol.intmx.depth	0.4	0.4078
kaolinte.group2	group.2um/Na-alun+kaol.intmx.depth	0.32	0.2589
kaolinte.group2	group.2um/kaolin.5+muscov.medAl.depth	0.485	0.3232
kaolinte.group2	group.2um/kaolin.5+muscov.medhighAl.depth	0.485	0.3501
kaolinte.group2	group.2um/kaolin+musc.intimat.depth	0.485	0.2215
kaolinte.group2	group.2um/alunite.33+kaol.33+musc.33.depth	0.313	0.3265
kaolinte.group2	group.2um/carbonate_calcite+0.2kaolwxl.depth	0.19	0.1504
kaolinte.group2	group.2um/carbonate_calcite0.7+kaol0.3.depth	0.19	0.2145
kaolinte.group2	group.2um/sulfate+kaolingrp_natroalun+dickite.depth	0.485	0.2929
montmorillonite.group2	group.2um/smectite_montmorillonite_na_highswelling.depth	0.84	0.2017
montmorillonite.group2	group.2um/smectite_montmorillonite_fe_swelling.depth	0.83	0.0695
montmorillonite.group2	group.2um/smectite_montmorillonite_ca_swelling.depth	0.99	0.2169
montmorillonite.group2	group.2um/pyroph.5+mont0.5.depth	0.42	0.1429
montmorillonite.group2	group.2um/feldspar_buddington.namont.depth	0.1	0.0502
montmorillonite.group2	group.2um/feldspar_buddington.namont2.depth	0.1	0.0502
montmorillonite.group2	group.2um/carbonate_calcite+0.2Ca-mont.depth	0.17	0.1068
montmorillonite.group2	group.2um/carbonate_dolo+.5ca-mont.depth	0.42	0.1314
montmorillonite.group2	group.2um/calcite.25+dolom.25+Na-mont.5.depth	0.42	0.1105

montmorillonite.group2	group.2um/carbonate_calcite.25+dolom.25+Ca-mont.5.depth	0.42	0.1274
montmorillonite.group2	group.2um/calcite+0.2Na-mont.depth	0.17	0.0939
montmorillonite.group2	group.2um/calcite+0.5Ca-mont.depth	0.42	0.1711
montmorillonite.group2	group.2um/organic_drygrass+.17Na-mont.depth	0.14	0.0321
montmorillonite.group2	group.2um/carbonate_dolomite.5+Na-mont.5.depth	0.42	0.1027
montmorillonite.group2	group.2um/carbonate_smectite_calcite.33+Ca-mont.67.depth	0.66	0.1186
montmorillonite.group2	group.2um/organic_benzene+montswy.depth	0.756	0.1302
montmorillonite.group2	group.2um/organic_trichlor+montswy.depth	0.756	0.6991
montmorillonite.group2	group.2um/organic_toluene+montswy.depth	0.798	0.1571
montmorillonite.group2	group.2um/organic_unleaded.gas+montswy.depth	0.756	0.1002
montmorillonite.group2	group.2um/organic_tce+montswy.depth	0.756	0.2067

Table E2. Endmember aggregations used to visualize Tetracorder outputs.

Grouping	**Endmembers**
group.1um/fe2+generic.all	group.1um/fe2+generic_nrw.cummingtonite.fd group.1um/fe2+generic_nrw.actinolite.fd group.1um/fe2+generic_nrw.hs-actinolite.fd group.1um/fe2+generic_med.jadeite.fd group.1um/fe2+generic_brd.br5a_actinolite.fd group.1um/fe2+generic_brd.br22c_actinolite.fd group.1um/fe2+generic_brd.br36a_chlorite.fd group.1um/fe2+generic_basalt_br46b.fd group.1um/fe2+generic_broad_br60b.fd group.1um/fe2+generic_vbroad_br20.fd
(fine grained hematite) group.1um/fe3+_hematite.fine.gr.all	group.1um/fe3+_hematite.fine.gr.fe2602.fd group.1um/fe3+_hematite.fine.gr.gds76.fd group.1um/fe3+_hematite.fine.gr.ws161.fd
(med grained hematite) group.1um/fe3+_hematite.med.gr.all	group.1um/fe3+_hematite.med.gr.gds27.fd group.1um/fe3+_hematite.med.gr.br25b.fd
(large grained hematite) group.1um/fe3+_hematite.lg.gr.all	group.1um/fe3+_hematite.lg.gr.br25a.fd group.1um/fe3+_hematite.lg.gr.br25c.fd group.1um/fe3+_hematite.lg.gr.br34c.fd
(all hematites, sum) group.1um/fe3+_hematite.all	group.1um/fe3+_hematite.fine.gr.fe2602.fd group.1um/fe3+_hematite.fine.gr.gds76.fd group.1um/fe3+_hematite.fine.gr.ws161.fd group.1um/fe3+_hematite.med.gr.gds27.fd group.1um/fe3+_hematite.med.gr.br25b.fd group.1um/fe3+_hematite.lg.gr.br25a.fd group.1um/fe3+_hematite.lg.gr.br25c.fd group.1um/fe3+_hematite.lg.gr.br34c.fd
(AMD oxides) group.1um/fe3+mix_AMD.assemb1+2.fd	group.1um/fe3+mix_AMD.assemb1.fd group.1um/fe3+mix_AMD.assemb2.fd

(med grained goethite) group.1um/fe3+_goethite.medgr	group.1um/fe3+_goethite.medgr.ws222.fd group.1um/fe3+_goethite+qtz.medgr.gds240.fd
(coarse grained goethite) group.1um/fe3+_goethite.coarsegr.ALL	group.1um/fe3+_goethite.coarsegr.fd group.1um/fe3+_goethite.medcoarsegr.mpc.trjar.fd
Fe2+, generic all	group.1um/fe2+generic.all
Fe2+ pyroxene	group.1um/fe2+_pyroxene.hypersthene
Fe2+ siderite	group.1um/fe2+generic_carbonate_siderite1
Fe2+ Fe3+ mix	group.1um/fe2+fe3+_hematite_weathering group.1um/fe2+_goeth+musc
Fe3+ mix AMD	group.1um/fe3+mix_AMD.assemb1+2
Fe3+ sulphate copiapite	group.1um/fe3+fe2+_sulfate_copiapite
Fe3+ sulphate jarosite	group.1um/fe3+_sulfate_jarosite_br34a2
Fe3+ hydroxide, FeOOH (goethite coarse/med/fine/thin coat)	group.1um/fe3+_goethite.coarsegr.ALL group.1um/fe3+_goethite.medgr group.1um/fe3+_goethite.fingr group.1um/fe3+_goethite.thincoat
Fe3+ oxide (hematite coarse/med/fine/nano)	group.1um/fe3+_hematite.lg.gr.all group.1um/fe3+_hematite.med.gr.all group.1um/fe3+_hematite.fine.gr.all group.1um/fe3+_hematite.nano.BR34b2 group.1um/fe3+_hematite.nano.BR34b2b
group.2um/alunite+pyroph.added	group.2um/alunite+pyrophyl.fd group.2um/pyroph.5+alunit.5.fd
group.2um/sulfate_alunite_k.all	group.2um/sulfate_kalun150c.fd group.2um/sulfate_kalun250c.fd group.2um/sulfate_kalun450c.fd group.2um/sulfate_alunNa03.fd
group.2um/sulfate_alunite_na.all	group.2um/sulfate_naalun150c.fd group.2um/sulfate_naalun300c.fd group.2um/sulfate_naalun450c.fd group.2um/sulfate_na82alun100c.fd
sulfate_alunite_int-comp.all	group.2um/sulfate_na63alun300c.fd group.2um/sulfate_na40alun400c.fd group.2um/sulfate_alunNa56450c.fd group.2um/sulfate_alunNa78.450c.fd group.2um/sulfate_alun35K65Na.low.fd group.2um/sulfate_alun73K27Na.low.fd group.2um/sulfate_alun66K34Na.low.fd
group.2um/kaolinite+muscovite.added	group.2um/kaolin+musc.intimat.fd group.2um/kaolin.5+muscov.medAl.fd

	group.2um/kaolin.5+muscov.medhighAl.fd
group.2um/pyroph+musc.added	group.2um/musc+pyroph.fd group.2um/pyroph+tr.musc.fd
group.2um/talc.all.fd	group.2um/talc.crsgrnd.fd group.2um/talc.fngrnd.fd group.2um/tremolite.or.talc.fd group.2um/saponite.or.talc.fd group.2um/talc+carbonate.parkcity.fd group.2um/talc+calcite.parkcity.fd
group.2um/kaolinite.3+.5+smectite.5+.7.added	group.2um/kaolin.3+smect.7.fd group.2um/kaolin.5+smect.5.fd
group.2um/alunite+kaolinite.muscovite.added	group.2um/alunite.33+kaol.33+musc.33.fd group.2um/alunite.5+musc.5.fd group.2um/alunite.5+kaol.5.fd
montmorillonite group 2.2um	group.2um/smectite_beidellite_gds123 group.2um/smectite_beidellite_gds124 group.2um/smectite_montmorillonite_na_highswelling
montmorillonite group 2.3um	group.2um/smectite_nontronite_swelling group.2um/smectite_montmorillonite_fe_swelling
phyllosilicates	group.2um/micagrp_biotite group.2um/palygorskite group.2um/micagrp_muscovite-low-Al group.2um/micagrp_muscovite-med-Al group.2um/micagrp_muscovite-medhigh-Al group.2um/micagrp_illite group.2um/micagrp_paragonite
Si-OH hydrated silica	group.2um/sioh_chalcedony group.2um/sioh_hydrated_basaltic_glass
kaolinite group	group.2um/kaolgrp_halloysite group.2um/kaolgrp_kaolinite_pxl group.2um/kaolgrp_kaolinite_wxl
kaolin+alunite	group.2um/alunite.5+kaol.5 group.2um/alunite+kaolinite.muscovite.added group.2um/Kalun+kaol.intmx group.2um/kaol.75+alun.25 group.2um/Na-alun+kaol.intmx group.2um/alunite.33+kaol.33+musc.33
K-alunite	group.2um/sulfate_alun35K65Na.low group.2um/sulfate_alun66K34Na.low group.2um/sulfate_alun73K27Na.low group.2um/sulfate_kalun150c group.2um/sulfate_kalun250c group.2um/sulfate_kalun450c

Na-alunite	group.2um/sulfate_alunNa03 group.2um/sulfate_alunNa56450c group.2um/sulfate_alunNa78.450c group.2um/sulfate_na40alun400c group.2um/sulfate_na63alun300c group.2um/sulfate_na82alun100c group.2um/sulfate_naalun150c group.2um/sulfate_naalun300c group.2um/sulfate_naalun450c group.2um/sulfate_ammonalunite
Alunite+other	group.2um/alunite.5+musc.5 group.2um/alunite+kaolinite.muscovite.added group.2um/alunite+musc+pyroph group.2um/alunite+pyrophyl group.2um/Kalun+kaol.intmx
kaolin+other	group.2um/carbonate_calcite0.7+kaol0.3 group.2um/kaol.75+pyroph.25 group.2um/kaolin.3+smect.7 group.2um/kaolin.5+muscov.medAl group.2um/kaolin.5+muscov.medhighAl group.2um/kaolin.5+smect.5 group.2um/kaolinite.3+.5+smectite.5+.7.added group.2um/kaolinite+muscovite.added group.2um/kaolin+musc.intimat
jarosite	group.2um/sulfate_jarosite-K group.2um/sulfate_jarosite-lowT group.2um/sulfate_jarosite-Na
sulfates: kiess szomol gypsum	group.2um/sulfate_kieserite group.2um/sulfate_szomolnokite group.2um/sulfate_szomolnokite_heated group.2um/sulfate_gypsum
perchlorate, 2.4 features	group.2um/perchlorate_mg group.2um/perchlorate_na group.2um/portlandite