THE EFFECT OF REFERENCE MINERAL LIBRARY SELECTION ON ESTIMATING MINERAL ABUNDANCES FROM INFRARED EMISSION SPECTRA USING SPECTRAL MIXTURE ANALYSIS.

Paras Angell and Hema Werner
School of Earth and Space Exploration, Arizona State University, Tempe, AZ-85287. Paras.Angell@asu.edu

Introduction: Minerals have characteristic vibrational modes that give rise to diagnostic absorption features in their infrared spectra [1]. Thermal infrared emission spectroscopy is a non-invasive diagnostic tool for studying vibrational modes in minerals and rocks [1,2]. Study of infrared emission spectra of rocks on Earth aids in the analysis of remote sensing infrared spectra of planetary surfaces such as Mars and the Moon [3, 4].

Multispectral remote sensing spectra are interpreted by comparing them to spectra of known reference minerals [3]. Spectral Mixture Analysis (SMA) uses linear best-fit matches of the experimental spectra to reference spectra to estimate the percent abundance of end-member minerals present in the sample spectrum [5,6]. The goal of this study is to perform a detailed comparison of Spectral Mixture Analysis results using different reference mineral libraries. This could have implications for compiling reference mineral libraries for analyzing infrared remote sensing data from planetary surfaces.

Experimental Methods: Infrared emission spectra from a suite of naturally weathered rock specimens collected from the Granite Wash Mountains and South Mountains of Arizona were studied [7]. Thermal infrared emission spectra were recorded in the mid infrared spectral range between 200 cm^{-1} to 2000 cm^{-1} (25 µm to 5 µm) with the Nicolet iS50 spectrometer located in the Mars Space Flight Facility at Arizona State University [1]. The spectra are plotted as emissivity vs wavenumber in cm^{-1} (Figure 1).

SMA uses a linear mixing algorithm to build a composite model spectrum from a library of reference mineral spectra to yield a model spectrum that is a best fit to the experimental spectrum [6]. Linear best-fit matches of the data are used to estimate the percent abundance of end-member minerals present in the sample spectrum [6].

Results:

Infrared Emission Spectroscopy Figure 1 shows mid-infrared emission spectra of naturally weathered rock specimens of different compositions. The spectra show diagnostic absorption features of silicate minerals. Absorption features between 1000 cm^{-1} and 1250 cm^{-1} correspond to Si-O stretching modes. Features between 400 cm^{-1} and 800 cm^{-1} correspond to Si-O-Si bending modes [1].

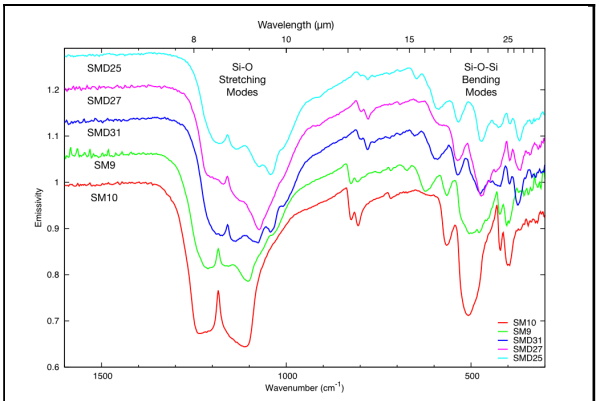

Figure 1. Infrared emission spectra of a suite of naturally weathered rock specimens showing diagnostic absorption features of silicate minerals. The spectra are offset along the vertical axis for clarity.

Spectral Mixture Analysis SMA was performed on the infrared emission spectra in the range of 400 cm^{-1} to 1600 cm^{-1} using four different spectral mineral reference libraries. These libraries are labeled as GenLib, IgLib, MetaLib, which are part of the ASU Spectral Library [5], and CustLib3, which is a customized subset of GenLib.

The results of mineral abundances (% compositions) estimated by SMA with the four different libraries are shown in Table 1 for rock sample SM9 and Table 2 for SMD25. Grouped SMA shows the abundance of mineral groups in the sample.

A comparison of SMA was performed with four different libraries on a suite of more that 20 naturally weathered rock samples. The RMS error of the best fit model spectra ranges from 0.7% to 3% across different libraries.

Table 1. Mineral abundances obtained from Spectral Mixture Analysis (SMA) using different mineral spectral reference libraries. (speclib.mars.asu.edu)

Name of Sample	General Library (73 minerals)	Igneous Library (37 minerals)	Metamorphic Library (45 minerals)	Custom Library 3 (27 minerals)
SM9	Chert 34% Quartz 21% Albite 20% Anorthoclase 11% Orthoclase 6% RMS error 0.961%	Quartz 46% Anorthoclase 21% Albite 17% K-rich Glass 12% RMS error 1.036%	Quartz 50% Microcline 23% Albite 22% RMS error 1.114%	Quartz 46% Anorthoclase 21% Albite 17% K-rich Glass 12% RMS error 1.036%
SM9 Grouped	Quartz 56% Plagioclase 20% Alkali Feldspar 17% Other 7%	Quartz 46% Alkali Feldspar 21% Plagioclase 17% Glass 12% Other 4%	Quartz 50% Alkali Feldspar 23% Plagioclase 22% Other 4%	Quartz 46% Alkali Feldspar 21% Plagioclase 17% Glass 12% Other 4%

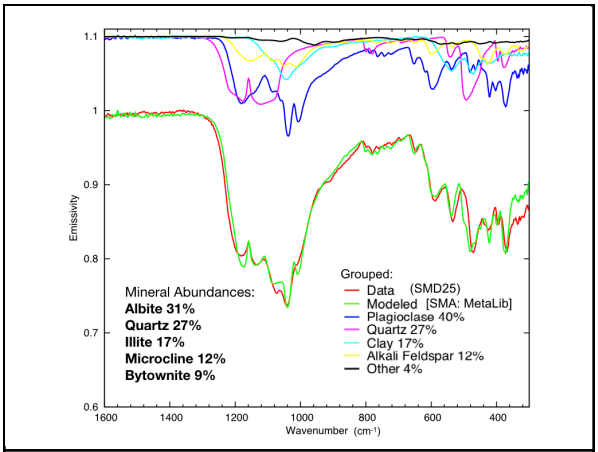

Figure 2. Spectral mixture analysis of the infrared spectrum of SMD25 rock sample using a metamorphic reference library. SMA yields abundances of 31% albite, 27% quartz, 17% illite, 12% microcline, and 9% bytownite. RMS error is 0.881%.

Figures 2 and 3 show the results of SMA performed on rock sample SMD25 using the metaphoric library (MetaLib) and the custom library (CustLib3). We find that using different libraries identifies different minerals and their quantities. However, although the use of distinct libraries results in differing mineral identifications, the minerals identified belong to the same mineral groups, as shown by the grouped SMA results in figures 2 and 3. The primary mineral groups identified in this suite of rocks are quartz, alkali feldspar, and plagioclase feldspar, in addition to clays.

Table 2. Mineral abundances obtained from SMA using different mineral spectral reference libraries.

Name of Sample	General Library (73 minerals)	Igneous Library (37 minerals)	Metamorphic Library (45 minerals)	Custom Library 3 (27 minerals)
SMD25	Chert 30% Albite 22% Illite 10% Anorthoclase 8% Hematite 8% Oligoclase 7% RMS error 0.805%	Albite 25% Quartz 20% Anorthoclase 19% Apatite 8% K-rich Glass 7% Forsterite 5% MgHornblende 5% RMS error 0.906%	Albite 31% Quartz 27% Illite 17% Microcline 12% Bytownite 9% RMS error 0.946%	Quartz 24% Albite 21% Anorthoclase 19% Bytownite 8% Montmorillonite 6% RMS error 0.881%
SMD25 Grouped	Quartz 30% Plagioclase 29% Clay 10% Alkali Feldspar 8% Iron Oxide 8% Phosphate 6% Other 8%	Plagioclase 25% Quartz 20% Alkali Feldspar 19% Phosphate 8% Glass 7% Iron Oxide 6% Olivine 5% Amphibole 5% Other 4%	Plagioclase 40% Quartz 27% Clay 17% Alkali Feldspar 12% Other 4%	Plagioclase 29% Quartz 24% Alkali Feldspar 19% Clay 16% Other 11%

Table 3. Selection of minerals in CustLib 3

Group	Minerals - End Members
Quartz	Quartz, Chert
Plagioclase	Andesine, Oligoclase, Albite, Bytownite, Labradorite, Anorthite
Alkali Feldspar	Anorthoclase, Orthoclase
Amphibole	MgHornblende, FeHornblende, Hornblende
Iron Oxide	Hematite, HematiteGTSH4, GeothiteGTS4, Magnetite
Clay	Nontronite, Montmorillonite, Illite, Saponite
Mica	Muscovite, Biotite
Pyroxene	Spodumene
Epidote	Epidote
Phosphate	Apatite
Glass	K-rich Glass

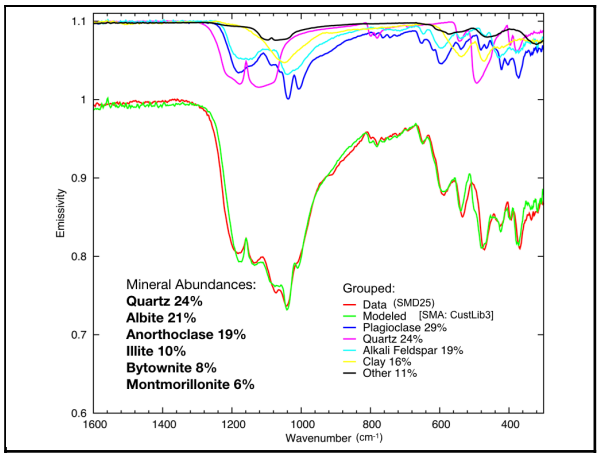

Figure 3. Spectral mixture analysis of the infrared spectrum of SMD25 rock sample using a custom reference library (CustLib3). The red line is the experimental spectrum. The green line is the best fit model spectrum. Spectra of reference minerals are shown on top of the plot. SMA yields mineral abundances of 24% quartz, 21% albite, 19% anorthoclase, 8% bytownite, and 6% montmorillonite. RMS error is 0.881%.

Discussion: SMA is a versatile tool for estimating mineral composition of rocks from infrared emission spectra in the lab and from remote sensing data. This study demonstrates that using different reference mineral libraries can identify different minerals and their estimated abundances. However, in a given sample the minerals indicated with different libraries belong to the same mineral groups.

One of the limitations of SMA in the study of data from planetary surfaces is that the number of end members in a spectral library must be less than the number of spectral data points recorded. SMA also does not account for non-linear mixing of minerals.

Future Work: Future work includes an XRD study of the composition of select powdered rock samples to correlate with estimated SMA mineral abundances. Other possible work includes training a machine learning model with a variety of spectral libraries to identify minerals from remote sensing spectral data.

Acknowledgements: We are grateful to Prof. Steve Reynolds and Prof. Phil Christensen for helpful discussions.

References: [1] Christensen, P. R., et al. (2000). JGR, 105, 9735-9739.
[2] Michalski, J. R., et al., (2004). JGR, 109, E03007.
[3]. Ruff, S. W., et al., (2006). JGR Planets. 111.E12.
[4] Nash, D. B. (1993). JGR, 98 (E12) 23535-23552.
[5] Ruff, S. W., et al., (1997). JGR, 102, 14899-14913.
[6] Ramsey, M. S., and Christensen, P. R. (1998). JGR, 103, B1, 577-596. [7] Angell, P., et al., (2020). AGU Fall Meeting Abst. EP036-0016.