THE U. S. GEOLOGICAL SURVEY, DIGITAL SPECTRAL LIBRARY AND ANALYSIS SOFTWARE

ROGER N. CLARK, GREGG A. SWAYZE, TRUDE V.V. KING,
BARRY MIDDLEBROOK, WENDY M. CALVIN, and NOEL GORELICK
U.S. Geological Survey, MS 964
Box 25046 Federal Center
Denver, CO 80225-0046
(303) 236-1332

ABSTRACT

The U. S. Geological Survey, Denver Spectroscopy Laboratory has developed a digital spectral library, library management software, and spectral analysis software. The software and library will be ready for general release in the summer of 1990. The library will include approximately 410 spectra measured from 0.2 to 3.0 μm with sample documentation. The library search software will enable a user to search on documentation parameters as well as spectral features. The analysis system includes general spectral analysis routines, plotting packages, radiative transfer software for computing intimate mixtures, routines to derive optical constants from reflectance spectra, tools to analyze spectral features, and the capability to access imaging spectrometer data cubes for spectral analysis. The laboratory spectral library will also be convolved to flight instrument spectral resolution and spectral sampling. Users may build customized libraries for their own instruments/flight conditions using software tools and command files. Absorption coefficients will be derived from all spectra so that the radiative transfer routines can be used to compute mineral mixtures.

INTRODUCTION

Imaging spectroscopy instruments such as AVIRIS have narrow band widths in many contiguous spectral channels that permit accurate definition of absorption features from a variety of materials. Identification of materials from such data requires a knowledge base: a spectral library of minerals, vegetation, man-made materials, and other subjects in the scene. Acquiring spectral measurements and sample characterizations for this library has taken several years. The first release will contain approximately 410 spectra and software to manage the library and provide scientific analysis capability.

THE SPECTRAL LIBRARY

The spectral library contains spectra of approximately 180 minerals (Table 1). In some cases, several spectra were measured to

span a solid solution series and/or a grain size series.

All spectra were run on a modified Beckman 5270 spectrometer (Clark *et al.*, 1990) from 0.2 to 3.0 μm and corrected to absolute reflectance. (Any use of trade names is for descriptive purposes only and does not imply endorsement by the U.S. Geological Survey.) Each sample has a documentation entry to describe the mineral, its composition, formula, and pointers to corresponding spectra in the library (an example is shown in Table 2). Each spectrum has a pointer to the documentation, so that all related data are properly cross-referenced.

The sample documentation includes extensive analyses such as X-ray diffraction, electron microprobe, X-ray fluorescence, and petrographic microscope examination. Not all analyses have been completed for all samples, but all samples have at least one analysis. These analyses are expensive and time consuming and limited funding has precluded complete analysis of all samples for this release of the library. Sample analysis will continue and the sample documentation will be updated in future releases of the library.

The intent of the spectral library is to serve as a knowledge base for spectral analysis. Comparison of spectral data is best done when the spectral resolutions of the knowledge base and the spectra undergoing analysis are identical. The spectral analysis software has tools for convolving the spectral library to the resolution and sampling interval of any instrument. The native (laboratory) spectral library is also convolved to nominal AVIRIS, HIRIS, GERIS, and TM resolution and sampling (e.g. Figure 1) for the terrestrial instruments, and to NIMS and VIMS for the planetary imaging spectrometer instruments. The convolution to any other instrument (laboratory, or flight) is a simple matter of changing pointers in a command file to the custom resolution and sampling data sets and running the command file with the spectral analysis system.

The spectral feature analysis tools and search facilities included with the library allow users to find entires based on selected parameters, such as those in the sample documentation as well as spectral features. For example, one might search for all minerals with an SiO_2 content of 10 to 30% and containing a 2.2-μm feature.

For computing intimate mineral mixtures (e.g. rock or soil) radiative transfer algorithms using the Hapke reflectance model (Hapke, 1981) are available. To compute mixture or pure end-member spectra, a set of optical constants is required as a function of wavelength. The algorithms use the model at the optical constant level so spectra can be calculated as a function of grain size, abundance in the mixture, and viewing geometry. Grain size distributions can also be simulated by computing a mixture of the same mineral (or even several minerals) at several grain sizes. A future release of the library will include optical constants for the spectra in the library. Optical constant libraries will also be computed for the same flight instrument spectral resolutions and wavelengths as the convolutions to the native spectral library. We anticipate the optical constant libraries to be completed this fall.

Table 1

Minerals in the Spectral Library, Version 1

1 Acmite	1 Clinozoisite	4 Illite	3 Pyrophyllite
5 Actinolite	1 Cobaltite	1 Ilmenite	9 Pyroxene
1 Adularia	3 Cookeite	1 Jadeite	1 Pyrrotite
3 Albite	1 Copiapite	3 Jarosite	4 Quartz
1 Allanite	1 Coquimbite	7 Kaolinite	1 Rectorite
5 Almandine	1 Cordierite	1 Kerogen	2 Rhodochrosite
2 Alunite	1 Corrensite	1 Kyanite	3 Rhodonite
1 Amphibole	1 Corundum	2 Labradorite	2 Richterite
1 Analcime	1 Covellite	1 Laumonite	2 Riebeckite
2 Andalusite	1 Cronstedtite	1 Lazurite	3 Ripidolite
1 Andesine	1 Cuprite	3 Lepidolite	1 Roscoelite
5 Andradite	2 Datolite	1 Limonite	2 Rutile
1 Anhydrite	1 Diaspore	4 Lizardite	1 Samarium Oxide
2 Annite	7 Diopside	1 Magnesite	2 Sanidine
3 Anorthite	1 Dolomite	2 Magnetite	2 Saponite
2 Anorthoclase	1 Dumortierite	1 Malachite	9 Scapolite
1 Anthophyllite	3 Elbaite	1 Manganite	1 Scolecite
7 Antigorite	1 Endellite	3 Marialite	4 Sepiolite
1 Apatite	2 Enstatite	2 Mascagnite	2 Serpentine
1 Arsenopyrite	4 Epidote	4 Meionite	1 Siderite
1 Attapulgite	1 Erionite	1 Mesolite	1 Sillimanite
1 Augite	1 Europium Oxide	5 Microcline	1 Smaragdite
1 Axinite	1 Fassaite	1 Monazite	4 Spessartine
1 Barite	1 Ferric Oxide	1 Monticellite	7 Sphalerite
2 Beryl	1 Fibroferrite	15 Montmorillonite	1 Sphene
1 Biotite	2 Forsterite	1 Mordenite	1 Spodumene
1 Bronzite	8 Galena	2 Muscovite	1 Staurolite
1 Brookite	3 Gibbsite	2 Natrolite	1 Stilbite
1 Brucite	1 Glauconite	1 Neodymium Oxide	1 Strontianite
1 Buddingtonite	1 Glaucophane	1 Nepheline	1 Sylvite
1 Bytownite	4 Goethite	1 Nephrite	4 Talc
2 Calcite	1 Granite	3 Nontronite	1 Tephroite
1 Carbon	3 Grossular	2 Oligoclase	4 Thuringite
1 Carphosiderite	2 Grossularite	16 Olivine	18 Topaz
1 Cassiterite	1 Gypsum	4 Orthoclase	1 Tosudite
1 Celsian	1 Halite	2 Paragonite	1 Tourmaline
1 Chabazite	5 Halloysite	2 Pectolite	2 Tremolite
2 Chalcopyrite	2 Hectorite	1 Perthite	1 Uralite
7 Chlorite	1 Hedenbergite	5 Phlogopite	1 Uvarovite
1 Chromite	9 Hematite	1 Pigeonite	6 Vermiculite
1 Chrysoberyl	1 Heulandite	1 Praseodymium Ox.	1 Witherite
1 Chrysocolla	1 Holmquisite	3 Prochlorite	1 Wollastonite
1 Chrysotile	3 Hornblende	1 Psilomelane	1 Zincite
1 Cinnabar	1 Hydrogrossular	5 Pyrite	1 Zircon
1 Clinochlore	1 Hypersthene	2 Pyrope	1 Zoisite
1 Clinoptilolite	1 Idocrase		

Total: 414 spectra of 182 different minerals.

Table 2

Sample Documentation Example

```
TITLE: Kaolinite CM9 DESCRIPT

DOCUMENTATION_FORMAT: MINERAL

SAMPLE_ID: CM9

MINERAL_TYPE: Phyllosilicate

MINERAL: Kaolinite, a clay mineral of the Kaolinite-Serpentine group.

FORMULA: Al2Si2O5(OH)4

FORMULA_NROFF: Al2Si2O5(OH)4

COLLECTION_LOCALITY: Mesa Alta, New Mexico

ORIGINAL_DONOR: Clay Mineral Standard from Wards Natural Science Inc.

CURRENT_SAMPLE_LOCATION: USGS Denver Spectroscopy Lab

ULTIMATE_SAMPLE_LOCATION: USGS Denver Spectroscopy Lab

SAMPLE_DESCRIPTION:

A spectrum for this sample was published by:
Clark, R.N., T.V.V. King, M. Klejwa, G. Swayze, and N. Vergo, 1990, High
spectral resolution reflectance spectroscopy of minerals:
J. Geophys Res., in press, 96pp,
who noted that it was spectrally pure.

END_SAMPLE_DESCRIPTION.

XRD_ANALYSIS:

Analysis by Norma Vergo indicates the sample is well ordered kaolinite.
The <2μm cut is kaolinite + small amount of quartz.

END_XRD_ANALYSIS.

COMPOSITIONAL_ANALYSIS_TYPE: XRF          # XRF, EM(WDS), ICP(Trace), WChem

COMPOSITION:      SiO2:   47.1  wt%    NROFF: SiO2
COMPOSITION:      TiO2:    0.46 wt%    NROFF: TiO2
COMPOSITION:     Al2O3:   37.4  wt%    NROFF: Al2O3
COMPOSITION:     Cr2O3:         wt%    NROFF: Cr2O3
COMPOSITION:      V2O3:         wt%    NROFF: V2O3
```

continued...

Table 2 Continued

```
COMPOSITION:      Fe2O3:     0.47 wt%    NROFF: Fe2O3
COMPOSITION:        FeO:          wt%    NROFF: FeO
COMPOSITION:        NiO:          wt%    NROFF: NiO
COMPOSITION:        MnO:    <0.02 wt%    NROFF: MnO
COMPOSITION:        MgO:     0.16 wt%    NROFF: MgO
COMPOSITION:        SrO:          wt%    NROFF: SrO
COMPOSITION:        ZnO:          wt%    NROFF: ZnO
COMPOSITION:        BaO:          wt%    NROFF: BaO
COMPOSITION:        CaO:     0.05 wt%    NROFF: CaO
COMPOSITION:       Li2O:          wt%    NROFF: Li2O
COMPOSITION:       Na2O:    <0.15 wt%    NROFF: Na2O
COMPOSITION:        K2O:     0.08 wt%    NROFF: K2O
COMPOSITION:       P2O5:    <0.05 wt%    NROFF: P2O5
COMPOSITION:         Cl:          wt%    NROFF: Cl
COMPOSITION:          F:          wt%    NROFF: F
COMPOSITION:          S:          wt%    NROFF: S
COMPOSITION:        SO3:          wt%    NROFF: SO3
COMPOSITION:        CO2:          wt%    NROFF: CO2
COMPOSITION:       H2O+:          wt%    NROFF: H2O+
COMPOSITION:       H2O-:          wt%    NROFF: H2O-
COMPOSITION:        H2O:          wt%    NROFF: H2O
COMPOSITION:        LOI:    14.1  wt%    NROFF: LIO
COMPOSITION: ----------------------
COMPOSITION:      Total:  100.04 wt%
COMPOSITION:  O=Cl,F,S:          wt%  #correction for Cl, F, S
COMPOSITION: New Total:          wt%

COMPOSITION_TRACE:

COMPOSITION_DISCUSSION:

XRF Analysis by Branch of Analytical Chemistry, USGS, Denver.

END_COMPOSITION_DISCUSSION.

MICROSCOPIC_EXAMINATION:

END_MICROSCOPIC_EXAMINATION.

DOCUMENTED_BY: wcalvin@speclab (Wendy M. Calvin)

LIB_SPECTRA_HED:  where          Wave Range  Av_Rs_Pwr  Comment

LIB_SPECTRA:  splib00_ r____     0.2-3.0μm      200     g.s.=
```

Notes: The last line contains the file identification and record number for the spectral data entry and is blank until the final assembly of the library.

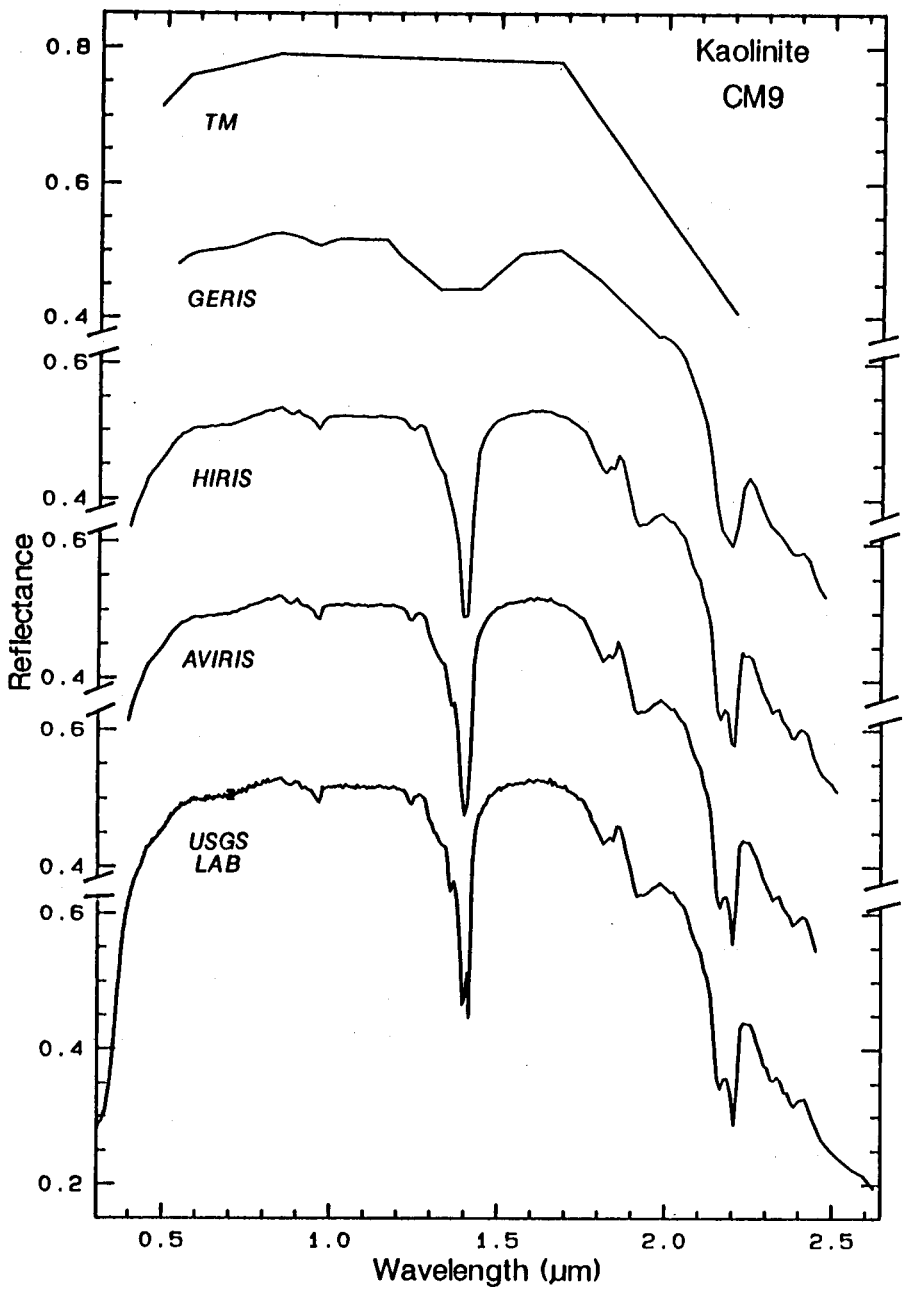

Figure 1. Sample spectra for kaolinite sample CM9 is shown at the native spectral library resolution (labeled USGS Lab), and for AVIRIS, HIRIS, GERIS, and TM.

SPECTRAL ANALYSIS SOFTWARE

With the spectral library, version 3.0 the SPECtrum Processing Routines (SPECPR), an integrated program for analysis of spectral data is available. Specpr is an interactive system for detailed processing of a few to many (meaning thousands) spectra and permits the user to be intimately involved with each spectrum and analysis step. Specpr is also a general x-y paired data processing system, where x and y can be many things (like reflectance versus wavelength, band intensity versus grain size, water content versus time, etc.). Specpr also has facilities for managing the spectral library. It is currently in use by several research groups around the country and an earlier version (version 1.0) was described in Clark (1980).

Specpr version 3.0 includes access to imaging spectrometer data sets in BIL, BIP and BSQ formats. It has routines for manipulating spectra (addition, subtraction, multiplication, division, logs, trigonometric functions, powers, etc.), plotting spectra on graphics terminals, and analyzing absorption bands for depth, position, shape, asymmetry. Specpr also has many special functions such as smoothing, spectral feature analysis, Planck black body generation, continuum removal, and many more.

HARDWARE REQUIREMENTS

The software consists of 50,000 lines of code and runs on Unix computers. The programs currently run on HP Unix machines, Sun Microsystems workstations, and DEC VAXes under Berkeley 4.3 Unix, Ultrix, and Wolongong's Eunice (Unix under VMS). To install the software, about 25 megabytes of disk space are required. The executable programs total about 3 megabytes.

The graphics requirement for the system needs either an HP-compatible graphics terminal (or a PC running an HP-graphics terminal emulator), or a Tektronix Plot-10 compatible graphics terminal. However, some interactive graphics routines are not supported on Tektronix Plot-10 terminals simply because those terminals do not have the needed graphics capability. X-Windows support is currently under development and will be available by the fall of 1990.

The spectral libraries will require about 50 megabytes of disk space, not including the optical constant libraries (which will require another 50 megabytes). Selected libraries, such as the AVIRIS library will be on the order of 5 megabytes, and each can be loaded separately.

AVAILABILITY

The software and spectral libraries will be published as USGS Open File Reports. They will be submitted for review in July and will be available for public release as soon as the review cycle is complete.

Contact any of the authors at the above address, or send electronic mail to:

rclark%speclab.uucp@csm9a.mines.colorado.edu # Internet
STAR::"rclark%speclab.uucp@csm9a.mines.colorado.edu" # SPAN

or

r.clark on NASAMAIL

for information on how to acquire the software and libraries.

FUTURE PLANS

The senior author (RNC) is a team member on the EOS HIRIS flight investigation team and is developing spectral libraries for the team. He is also a team member on Mars Observer Thermal Emission spectrometer, Mars 94 VIMS, and CRAF VIMS. To satisfy the requirements of all these missions, the mineral spectral library will be extended to cover the spectral range 0.2 to 200 μm and include many more minerals. For the HIRIS team, spectral libraries will be developed for all disciplines represented by team members.

REFERENCES

Clark, R.N., 1980. A Large Scale Interactive One Dimensional Array Processing System, *Pub. Astron. Soc. Pac.*, **92**, 221-224.

Clark, R.N., T.V.V. King, M. Klejwa, G. Swayze, and N. Vergo, 1990. High Spectral Resolution Reflectance Spectroscopy of Minerals: *J. Geophys Res.* in press.

Hapke, B., 1981. Bidirectional reflectance spectroscopy 1. Theory, *J. Geophys. Res.* **86**, 3039-3054.