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Availability of a library of infrared (2.1–25.0 μm) mineral spectra

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ABSTRACT

All previously published libraries of infrared mineral spectra are in the form of transmittance. Reflectance spectra are, however, more useful for remote sensing and some potential laboratory applications, such as the use of an infrared microscope for mineral identification on polished sections. This note points out that construction of a new library of infrared (2.1–25.0 μm) mineral spectra is in progress. Both transmittance and reflectance measurements of a selection of 63 different, well-characterized minerals have been published to date. These data are available in both hard copy and digital form.

INTRODUCTION

In a thorough review of the use of infrared spectroscopy in mineralogy, Estep-Barnes (1977) listed libraries of infrared mineral spectra published prior to 1975. Only Ferraro (1982) has been published subsequently. All of these mineral libraries are based on transmittance spectra, as are the mineralogical applications discussed by Estep-Barnes (1977). In part, this former reliance on transmittance was the result of early instrumental limitations (i.e., the relatively low sensitivity of previous detectors). In addition, transmittance measurements are more easily interpreted because absorbance is a simple function of the absorption coefficient (Salisbury et al., 1987a).

The introduction of more sensitive detectors and the common availability of interferometer spectrometers, having higher energy throughput than grating instruments, have made reflectance measurements possible. In fact, infrared microscopes have recently been developed that offer the potential for spectral reflectance measurements and mineral identification at a scale as small as 10 μm. At a much larger scale, broad-band infrared spectroscopic measurements from aircraft (Kahle and Goetz, 1983) show the potential for compositional remote sensing using emittance rather than reflectance.

Both reflectance and emittance spectra are a complex function of the absorption coefficient and the refractive index (Hapke, 1981; Salisbury et al., 1987a). One result is that spectral features that are seen in reflectance or emittance differ from those in transmittance, and this difference increases with increased scattering (Salisbury et al., 1987a). As a result of this scattering effect, a rough or particulate surface may exhibit a spectrum that is significantly changed from that of a polished surface of the same material. Some spectral changes due to scattering in a fine (0–74 μm) particulate material may have beneficial mineralogic applications. For example, absorption bands due to water, hydroxyl, carbonate, and sulfate or hydrocarbon are enhanced in spectra of a fine particulate material (Salisbury et al., 1987a), making it possible to detect a very small amount of these constituents (Salisbury and Walter, unpublished manuscript).

To broaden the range of spectral data that are available for a variety of potential applications, we have published the first edition of a library of infrared mineral spectra containing both transmittance and reflectance spectra (Salisbury et al. 1987b). In this library, reflectance spectra typically are presented for three different mineral states: a smooth surface of a solid sample, a 74- to 250-μm particle-size range, and a 0- to 74-μm particle-size range.

It is the purpose of this note to inform the mineralogical community about the availability of this mineral library in both hard copy and digital form and to briefly describe this ongoing effort.

SAMPLE ACQUISITION AND PREPARATION

Most samples were acquired, often as single crystals, from the Smithsonian National Museum of Natural History. A few samples were obtained from a U.S. Geological Survey collection in Denver or from individual donors.

Samples were crushed in a steel percussion mortar. Any magnetic particles resulting from this treatment were removed with a hand magnet. Crushed samples were handpicked when impurities were present. They were then ultrasonically cleaned and subjected, when necessary, to an acid wash to improve purity. Samples were ground in a sintered sapphire mortar under either acetone or (more

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commonly) alcohol, which facilitated grinding, avoided disordering of the sheet silicates, and prevented the finest particles from drifting away as aerosols.

Particulate samples were dry-sieved to two different particle-size ranges (74–250 μm and 0–74 μm), and the coarser particle-size range was subsequently washed in acetone or alcohol to remove clinging fines. Clay samples were disaggregated ultrasonically, and the <2-μm size fraction was concentrated with a centrifuge.

SAMPLE CHARACTERIZATION

Mineral specimens were initially examined as hand samples and as grain mounts under a petrographic microscope. This examination, combined with X-ray diffraction and microprobe analysis, generally served to identify those samples that were pure mineral phases and to establish their chemical and mineral compositions. Impure samples were discarded.

MINERALS MEASURED

The first edition of this mineral library measured 78 samples of 63 different minerals, which are listed in Table 1.

TABLE 1. Minerals measured

- Acmite
- Albite
- NH_4-alunite
- K-alunite
- Na-alunite
- Andalusite
- Andradite
- Anorthite
- Antigorite
- Augite
- Beryl
- Bustamite
- Calcite
- Mg-rich clinochlore
- Fe-rich clinochlore
- Cordierite
- Diopside
- Enstatite
- Epidote
- Grossular
- Gypsum
- Hedenbergite
- Hemimorphite
- Hornblende
- Hyperthsene
- Illite
- Illite/smectite
- Kaolinite
- Kyanite
- Labradorite
- Microcline
- Montmorillonite
- Muscovite
- Nontronite
- Olivine (FO11)
- Olivine (FO18)
- Olivine (FO29)
- Olivine (FO41)
- Olivine (FO51)
- Olivine (FO60)
- Olivine (FO66)
- Olivine (FO88)
- Olivine (FO91)
- Olivine (FO92)
- Orthoclase
- Pectolite
- Phlogopite
- Pyrophyllite
- Quartz
- Rhodonite
- Richterite
- Riebeckite
- Sanidine
- Saponite
- Sepiolite
- Smectite
- Spessartine
- Spodumene
- Talc
- Tourmaline
- Tremolite
- Vermiculite
- Wollastonite

SPECTRAL MEASUREMENTS

Spectra were acquired at 4 cm^{-1} resolution (data points every 2 cm^{-1}) by using a Nicolet[1] 5 DXB interferometer spectrometer with a triglycine sulfate (TGS) detector. Spectral data were recorded from 4808.8 to 192.9 cm^{-1} (2.08 to 51.8 μm), but are displayed in hard copy over a nominal range of 4600 to 400 cm^{-1} (2.17 to 25.0 μm) because both ends of the spectral range tend to be noisy.

Transmittance was measured by passing the focused beam (6-mm diameter) of the interferometer through a KBr disk (commonly referred to as a pellet) containing sample material made in the manner of Stimson and O'Donnell (1952). Reflectance spectra were recorded by using a Spectra Tech "Collector" diffuse reflectance attachment that uses two 90° off-axis ellipsoids that act as 6× beam condensers. Consequently, the focused beam diameter is reduced to 1 mm, and illumination and reflection take place over a solid angle that closely approaches π steradians. Thus, our bidirectional reflectance measurements actually record biconical reflectance over a large solid angle.

DATA AVAILABILITY

Spectral data are initially stored in digital form on 8-inch floppy disks in Nicolet DX format. Digital data have also been transferred to a VAX 11/780 where they are stored as *x,y* values in ASCII format (VMS operating system). For information on how these data can be obtained, write or call the senior author at (703) 648-6382. Hard copy of these data are published as a U.S. Geological Survey Open-File Report (Salisbury et al., 1987b).

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REFERENCES CITED

Estep-Barnes, P.A. (1977) Infrared spectroscopy. In J. Zussman, Ed., Physical methods in determinative mineralogy (2nd edition), p. 529–603. Academic Press, New York.

Ferraro, J.R. (1982) The Sadtler infrared spectra handbook of mineral and clays. Sadtler Research Laboratories, 3316 Spring Garden St., Philadelphia, Pennsylvania 19104, 476 p. (proprietary).

Hapke, B. (1981) Bidirectional reflectance spectroscopy: 1, Theory. Journal of Geophysical Research, 86, 3039–3054.

Kahle, A.B., and Goetz, A.F.H. (1983) Mineralogic information from a new airborne thermal infrared multispectral scanner. Science, 222, 24–27.

Salisbury, J.W., Hapke, B., and Eastes, J.W. (1987a) Usefulness of weak bands in mid-infrared remote sensing of particulate planetary surfaces. Journal of Geophysical Research, 92, 703–710.

Salisbury, J.W., Walter, L.S., and Vergo, N. (1987b) Mid-infrared (2.1–25 μm) spectra of minerals (1st edition). U.S. Geological Survey Open-File Report 87-263, 356 p.

Stimson, M.M., and O'Donnell, M.J. (1952) The infrared and ultraviolet spectra of cystine and isocystine in the solid state. Journal of the American Chemical Society, 74, 1805–1808.

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[1] Use of trade names is for identification purposes only and does not constitute an endorsement by the U.S. Geological Survey or NASA.