The reflectance spectra of minerals are studied as a function of spectral resolution in the range from 0.2 to 3.0 μm. Selected absorption bands were studied at resolving powers (λ/Δλ) as high as 2240. At resolving powers of approximately 1000, many OH-bearing minerals show diagnostic sharp absorptions at the resolution limit. At low resolution, some minerals may not be distinguishable, but as the resolution is increased, most can be easily identified. As the resolution is increased, many minerals show fine structure, particularly in the OH-stretching overtone region near 1.4 μm. The fine structure can enhance the ability to discriminate between minerals, and in some cases the fine structure can be used to determine elemental composition. For example, in amphiboles and talcs, four absorption bands are observed in the samples analyzed in this study that are due to hydroxyl linked to Mg\(_{3+}\), Mg\(_{2}\)Fe, MgFe\(_{2}\), and Fe\(_3\) sites. The band intensities have been shown by other investigators to give the Fe:Fe+:Mg ratio from transmission spectra. This study shows that the same equations can be used to obtain the ratio from reflectance spectra of unprepared samples. High-resolution reflectance spectroscopy of minerals may prove to be a very important tool in the laboratory, in the field using field-portable spectrometers, from aircraft, and from satellites looking at Earth or other planetary surfaces.

INTRODUCTION

In the region of solar reflected light (0.3–3 μm), many minerals show diagnostic absorption bands due to vibrational overtones, electronic transitions, charge transfer, and conduction processes. See Hunt [1977] for an excellent review of the causes of absorption features. The spectral properties of minerals have been well studied [e.g., Hunt and Salisbury, 1970, 1971, Hunt et al., 1971a, b, 1972, 1973; Hunt, 1977, and references therein], and in recent years the nonlinear effects of mineral mixtures have been studied [e.g., Clark, 1983; Singer, 1981; Johnson et al., 1983; Clark and Lucey, 1984, and references therein].

Early reflectance spectroscopy studies typically used commercial instrumentation such as those by Cary and Beckman. (Any use of trade names is for descriptive purposes only and does not imply endorsement by the U.S. Geological Survey.) These instruments were called "ratio recording" but never actually performed a ratio. While the method for obtaining reflectance was clever, there are drawbacks for modern spectroscopic studies. Such instruments used a servo loop with the reference signal fed to a servo motor controlling the slit. That resulted in a constant reference signal so the signal from the sample was proportional to the instrument happened to select at the time and rarely reported resolution in their published results. Thus intercomparison of data sets between machines or even with the same machine could be difficult.

Modern remote sensing instrumentation makes use of detector arrays and fixed slits (for a given spectral run), so the resolution is well defined [e.g., Vane and Goetz, 1985]. These new data are also digital so that sophisticated spectral modeling may be performed to identify the minerals present on the surface and derive estimates as to their abundances [e.g., Hapke, 1981; Johnson et al., 1983; Clark and Roush, 1984, and references therein]. These new analysis techniques require a digital data base of the optical properties of minerals. Probably the largest such data base was published by Hunt, Salisbury, and colleagues (see references) and is hereafter referred to as the HS spectral data base (the HS stands for Hunt and Salisbury). The HS spectral data base is often used by remote sensing investigators to examine the spectral properties of rocks and minerals. However, the data base consists only of the published reflectance spectra in the journals. Clearly, a modern digital spectral data base is needed for analyses of modern remote sensing data. The spectral resolution and wavelength accuracy should be documented and the data should be obtained digitally to high precision and corrected to absolute reflectance (the HS spectral data base was relative to MgO).

We have begun building a spectral data base that meets the above requirements. R. N. Clark is a member of the High Resolution Imaging Spectrometer (HIRIS) flight team on the Earth Observation System, as well as NASA Mars Observer team, and a Comet Rendezvous and Asteroid Fly-by team, each of which requires a spectral data base to analyze spectroscopic data. It is anticipated that spectra from this
and other studies will be part of the spectral library for those and other missions.

The samples used in this study included those used in the HS spectral database; the HS samples are located at the Geological Survey (USGS) spectroscopy laboratory in Denver. Additional samples from Wards Scientific Company, the Source Clays Minerals Repository at the University of Missouri, the National Museum of Natural History, and from individual investigators were also used. The total inventory contains over 3000 samples at present. The samples reported here are listed in Table 1.

Early in the development of the spectral data base, it became apparent that many minerals had absorptions containing previously unreported fine structure. It was decided to examine systematically absorptions at higher resolution to determine if important diagnostic features could be found. This paper presents the first results of the study; it will be shown that features not previously reported in the literature can be useful for distinguishing mineral types, sometimes between minerals that previous data indicated could not be distinguished. Also derived is an optimum resolution curve as a function of wavelength for maximum detection capability, while minimizing total data volume. This function is preliminary, however, because additional measurements may indicate that higher resolution is necessary in some spectral regions.

The phrase high spectral resolution must be understood in context. The resolution used in this study is not high by all standards, but it is when compared to reflectance spectra that have been published in the geologic communities. The highest resolution reported here is similar to that achievable (~4 cm⁻¹) in reflectance with standard commercial Fourier Transform Infra-Red (FTIR) spectrometers.

INSTRUMENTATION AND SOFTWARE

The spectrometer used in this study was a custom-modified Beckman 5270 double-grating, double-beam instrument. Ordinarily, the commercial Beckman 5270 uses the servo slit method to derive reflectance, with the output sent to a strip chart. The Beckman was modified so all functions (e.g., servo mechanism, slit width, wavelength drive, and signals from the phototube and lead sulphide detectors) were interfaced to IBM-PC computer with a Tecmar analog to digital board that includes 24-bit digital I/O, 12-bit digital to analog (D to A) converters, 12-bit analog to digital (A to D) and 16-bit counter/timers. The digital I/O was used to interface directly to the wavelength stepper motor drive electronics. The signal from the reference to the slit servo was disconnected, and a D to A voltage from the computer was used to control the slit. The signals from the detectors were connected to a voltage to frequency converter, and a 16-bit counter was used to integrate the signal over precise time intervals. Additional signals were interfaced via the digital I/O lines to provide information on when dark, sample, or reference levels were being measured.

To control the spectrometer, a 1500-line compiled BASIC (necessary for speed) program was written. Wavelength positioning is checked by digitizing voltages applied to potentiometers on the grating worm drive and main grating rotation shaft. These position indicators give a coarse absolute position accurate to ±0.004 μm and the worm drive position accurate to ±0.0002 μm within a 0.064-μm segment. The coarse position is used to determine in which segment the fine position is located. Wavelength stepping is done by sending TTL pulses to the stepper motor drive board. The hardware setup is shown schematically in Figure 1.

The spectrometer controlling software asks the user to input a title and additional text, wavelength region to measure, resolution, and desired signal-to-noise ratio. The spectrometer steps to the beginning wavelength under computer control, sets the slit to the proper band pass, checks signal levels, changes gain if necessary, and begins integrating. Because the Beckman is a double-beam instrument, the computer alternately measures the dark, reference, second dark, and sample signal levels. This cycle repeats at a 5-Hz rate, with each signal level integrated for 33 ms. The detector gains are controlled by a 3-bit programmable gain stage that has gains of 1, 3, 10, 30, 100, 300, 1000, and 3000. After one sampling interval, the computer computes reflectance levels by subtracting dark levels and ratioing to the reference. Each integration interval is called a cycle and takes 0.2 s including computations. An older version of the system used the original Beckman 30-Hz rate, with the integration time on each signal level of 4 ms, and eight integration intervals were used, taking 0.33 s per cycle. The change to the slower rate allows the v-f converters to operate more efficiently and allows for higher gains with the new indium antimonide detector (the detector + preamp time constant would limit preamp gains with a 4-ms chop). After more than one cycle, the standard deviation of the mean is computed on the reference signal level. The reference signal level is used to keep the total scan time independent of sample reflectance, which makes it easier to plan spectrometer time. The integration cycle continues until the desired signal to noise, or a given maximum cycle, selected by the user, is reached. At that point the gratings are stepped to the next wavelength and the next integration is started.

As each integration is completed by the IBM computer, the reflectance data, including signal levels, resolution, standard deviation, and wavelength, are transmitted via an RS232 interface to a Hewlett Packard (HP) 9000 computer (see Figure 1). The IBM will also transmit signal overflow and underflow messages and other spectrometer status messages to the HP as they occur. The HP is a multiuser minicomputer, and the programs resident on the HP capture the incoming spectrometer data, allowing anyone logged on to monitor spectrometer data and functions real time. This aspect proved very important for this project, because many integrations were run over a weekend or overnight, and the data and spectrometer could be monitored from the home of the user.

The spectral data received by the HP computer are translated to the format of the spectrum processing routines (SPECPR). The SPECPR program is described by Clark [1980] but has been substantially improved to handle the larger data sets now being obtained. A paper describing the new spectrum processing system is in preparation. Because SPECPR processes data as one-dimensional arrays, it is advantageous to disk space and I/O times to include the wavelengths of each spectrum only once. If the wavelengths of each spectrum were included with the reflectance data, the disk space would nearly double. For this reason, a standard slit program was defined, and the user can increase the resolution by factors of 0.25, 0.5, 1.0, 1.5, 2, 3, 4, 8, and 16 times. The sampling wavelengths are generated from the
TABLE 1. Sample Mineralogy and Spectral Purity

<table>
<thead>
<tr>
<th>Sample</th>
<th>Mineralogy</th>
<th>Spectral Purity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actinolite HS22.3B</td>
<td>No XRD; EM, indicates stoichiometric actinolite</td>
<td>SP</td>
</tr>
<tr>
<td>Actinolite HS116.3B</td>
<td>XRD, actinolite + chlorite; M, ~1% opaque, chlorite ~5 vol % as inclusions</td>
<td>SP, no chlorite bands detected</td>
</tr>
<tr>
<td>Alunite HS295.3B</td>
<td>XRD, alunite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Analcime GDS1</td>
<td>XRD, analcime pure</td>
<td>SP</td>
</tr>
<tr>
<td>Antigorite NMNH96917</td>
<td>XRD, antigorite + medium amount of hornblende + others; M, 6-8 vol % hornblende</td>
<td>SP</td>
</tr>
<tr>
<td>Attapulgite CM46</td>
<td>XRD, attapulgite, medium amount of quartz, trace amount of smectite</td>
<td>SP, no smectite bands detected</td>
</tr>
<tr>
<td>Beryl GDS9</td>
<td>XRD, beryl + trace other</td>
<td>SP</td>
</tr>
<tr>
<td>Biotite HS28.3B</td>
<td>XRD, biotite + trace other</td>
<td>SP</td>
</tr>
<tr>
<td>Brucite HS247.3B</td>
<td>XRD, brucite + medium amount dolomite + small amount of other; HCl treatment shows ~8% carbonate.</td>
<td>SP</td>
</tr>
<tr>
<td>Calcite HS48.3B</td>
<td>XRD, calcite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Calcite WS272</td>
<td>XRD, calcite + small amount other</td>
<td>SP</td>
</tr>
<tr>
<td>Chrysotile HS23.1B</td>
<td>no XRD; SEM analysis indicates pure chrysotile</td>
<td>SP</td>
</tr>
<tr>
<td>Clinoptilolite GDS2</td>
<td>XRD, clinoptilolite + medium amount other</td>
<td>SP</td>
</tr>
<tr>
<td>Cookeite SC Car-1</td>
<td>XRD, cookeite + medium amount quartz</td>
<td>SP, spectral purity unknown</td>
</tr>
<tr>
<td>Corrensite SC CorWa-1</td>
<td>XRD, corrensite + albite + quartz; &lt;2 μm cut corrensite + quartz; M, albite ~8 vol %, quartz ~4%; corrensite coats albite and quartz grains</td>
<td>spectral purity unknown</td>
</tr>
<tr>
<td>Datolite HS442.3B</td>
<td>XRD, datolite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Dolomite HS102.3B</td>
<td>XRD, dolomite + trace calcite</td>
<td>SP</td>
</tr>
<tr>
<td>Epidote HS332.3B</td>
<td>XRD, epidote + large amount quartz + small amount other; M, ~2% magnetite on epidote, ~15% quartz, ~3% plagioclase, no carbonate</td>
<td>SP</td>
</tr>
<tr>
<td>Gypsum HS333.3B</td>
<td>XRD, gypsum pure</td>
<td>SP</td>
</tr>
<tr>
<td>Halloysite CM13</td>
<td>XRD, halloysite + quartz, &lt;2 μm 7-Å halloysite + smectite + trace 10-Å halloysite</td>
<td>SP</td>
</tr>
<tr>
<td>Halloysite</td>
<td>XRD, pure 7-Å halloysite</td>
<td>SP</td>
</tr>
<tr>
<td>NMNH106236</td>
<td>XRD, hectorite + medium quartz + large calcite + small % dolomite; &lt;2 μm cut hectorite + trace calcite; M, &lt;3% quartz, &lt;1% magnetite; HCl and Na-acetate buffer treatment indicates 50 wt % carbonate; XRF indicates 50 wt % calcite</td>
<td>a portion of the 2.5-μm band could be due to calcite, otherwise spectrally pure sample darker than normal from carbonaceous impurities, otherwise spectrally pure</td>
</tr>
<tr>
<td>Hecterite SC SHCa-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Illite GDS4</td>
<td>XRD, illite/smectite: 80% illite layers, R3 ordered; trace feldspar; &lt;2 μm illite + illite/smectite carbonaceous impurities lower albedo</td>
<td></td>
</tr>
<tr>
<td>(Marblehead, Wisconsin)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Illite SC IMt-1</td>
<td>XRD, illite + quartz; &lt;2 μm cut 95% illite/smectite</td>
<td>SP</td>
</tr>
<tr>
<td>Jarosite NMNH95074-1</td>
<td>XRD, natrojarosite + quartz</td>
<td>SP</td>
</tr>
<tr>
<td>Kaolinite CM9</td>
<td>XRD, well-ordered kaolinite; &lt;2 μm cut kaolinite + small amount of quartz</td>
<td>SP</td>
</tr>
<tr>
<td>Kaolinite SC KGa-1</td>
<td>XRD, kaolinite + trace anatase; &lt;2 μm cut pure kaolinite</td>
<td>SP</td>
</tr>
<tr>
<td>Kaolinite SC KGa-2</td>
<td>XRD, kaolinite + trace anatase</td>
<td>SP</td>
</tr>
<tr>
<td>Lizardite NMNH4678</td>
<td>XRD, lizardite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Montmorillonite CM20</td>
<td>XRD, smectite + trace quartz; &lt;2 μm cut pure smectite; M, no visible quartz, ~1% limonite individual grains</td>
<td>SP</td>
</tr>
<tr>
<td>Montmorillonite CM26</td>
<td>XRD, smectite + large quartz; &lt;2 μm cut pure smectite; M, trace limonite, no visible quartz, slight HCl fizz</td>
<td>SP</td>
</tr>
<tr>
<td>Montmorillonite CM27</td>
<td>XRD, bentonite + quartz + feldspar + bassanite; &lt;2 μm cut pure smectite + quartz; M, trace limonite, no visible quartz, slight HCl fizz</td>
<td>SP</td>
</tr>
<tr>
<td>Montmorillonite SC</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SAz-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Montmorillonite SC</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SCA-2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Montmorillonite SC</td>
<td></td>
<td></td>
</tr>
<tr>
<td>STx-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Sample</td>
<td>Mineralogy</td>
<td>Spectral Purity</td>
</tr>
<tr>
<td>--------------------</td>
<td>-----------------------------------------------------------------------------</td>
<td>-----------------</td>
</tr>
<tr>
<td>Montmorillonite SC</td>
<td>XRD, smectite + quartz + feldspar; &lt;2 µm cut smectite + quartz; M, trace magnetite or biotite, no HCl fizz, no visible quartz or feldspar</td>
<td>SP</td>
</tr>
<tr>
<td>SWy-1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Muscovite HS146.3B</td>
<td>XRD, muscovite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Natrolite HS168.3B</td>
<td>XRD, natrolite + large amount of analcime + small amount of clinoptilolite + large amount other</td>
<td>SP</td>
</tr>
<tr>
<td>Natrolite HS169.3B</td>
<td>XRD, natrolite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Nontronite SC NG-1</td>
<td>XRD, nontronite + quartz + other; &lt;2 µm cut nontronite + trace quartz; M, 50% quartz, 1-2% opaque, no HCl fizz</td>
<td>SP</td>
</tr>
<tr>
<td>Nontronite SC SWa-1</td>
<td>XRD, Fe-smectite + small quartz; &lt;2 µm cut pure smectite</td>
<td>SP</td>
</tr>
<tr>
<td>Phlogopite HS23.3B</td>
<td>XRD, phlogopite pure</td>
<td>SP</td>
</tr>
<tr>
<td>Pyrophyllite GDS</td>
<td>XRD, pyrophyllite + small amount other</td>
<td>SP</td>
</tr>
<tr>
<td>Rectorite SC RAr-1</td>
<td>XRD, rectorite + chlorite + muscovite; &lt;2 µm cut rectorite + trace chlorite + trace muscovite M, 10-15% quartz, 2% chlorite, 2% opaque, no HCl fizz</td>
<td>mostly pure, 2.18-µm band is unique; no chlorite or muscovite bands</td>
</tr>
<tr>
<td>Saponite SapCa-1</td>
<td>XRD, saponite + quartz + calcite + other; &lt;2 µm cut saponite + other; HCl treatment indicates 21 wt % calcite</td>
<td>SP, no calcite bands, calcite affects continuum only; Na-acetate buffer purification</td>
</tr>
<tr>
<td>Scapolite HS351.3B</td>
<td>XRD, scapolite + large amount feldspar; M, ~2% pyrrhotite; slight HCl fizz</td>
<td>SP</td>
</tr>
<tr>
<td>Sepiolite SC SepNev-1</td>
<td>XRD, sepiolite + small amount of dolomite; HCl treatment indicates 40 wt % carbonate</td>
<td>SP, no calcite bands, calcite affects continuum only; confirmed by Na-acetate purification</td>
</tr>
<tr>
<td>Sepiolite SC SepSP-1</td>
<td>XRD, sepiolite + calcite; HCl treatment indicates 30 wt % carbonate</td>
<td>SP</td>
</tr>
<tr>
<td>Talc HS21.3B</td>
<td>XRD, talc + medium amount chlorite; M, ~2% chlorite, &lt;1% magnetite</td>
<td>SP</td>
</tr>
<tr>
<td>Talc WS327.3B</td>
<td>XRD, talc + large amount of chlorite; M, ~10% chlorite</td>
<td>SP</td>
</tr>
<tr>
<td>Talc HS659</td>
<td>no XRD; EM, indicates stoichiometric talc</td>
<td>SP</td>
</tr>
<tr>
<td>Topaz HS184.2B</td>
<td>XRD, topaz + large amount of albite; M, 50% albite, no HCl fizz</td>
<td>SP</td>
</tr>
<tr>
<td>Tourmaline HS282.2B</td>
<td>XRD, tourmaline + medium amount mica + small quartz</td>
<td>SP</td>
</tr>
<tr>
<td>Tremolite HS18.3</td>
<td>XRD, tremolite + medium amount quartz + small amount mica + large amount others; M, ~1% magnetite, no other minerals visible</td>
<td>SP</td>
</tr>
<tr>
<td>Vermiculite SC VTx-1</td>
<td>XRD, pure vermiculite</td>
<td>SP</td>
</tr>
<tr>
<td>Zoisite HS347.3B</td>
<td>XRD, zoisite + medium amount quartz + small amount other(s); M, ~40% quartz</td>
<td>SP</td>
</tr>
</tbody>
</table>


slit program starting at 4.0 µm, so if the user requests a wavelength range from 1.000 to 2.036 µm one time and 1.128 to 2.031 µm another, the wavelengths sampled would be exactly the same in the overlap region. To limit further the number of possible wavelength sets and to help alignment of the data arrays, the data are blocked in 256-channel segments. Thus, in the previous example the channels in the overlap region occur at the same array locations, so if a ratio
were desired, it is a simple division of the array elements. This alignment necessitates that some channels be marked deleted where no data are obtained. The SPECPR program automatically handles management of deleted points. This method results in a small total number of wavelength sets that can be generated. This sampling methodology also assures that all spectra are sampled at the same wavelengths so comparison of absorption features is easier. The standard slit program, called 1X resolution, was a compromise between the desire to maintain resolving power (Δλ/λ) at 200 and the energy available at the detector. Figure 2 shows the 1X slit program. The resolution decreases at the extremes of the detector ranges (near 0.2 μm, beyond 2.6 μm, and at the lead sulphide-phototube crossover at 0.85 μm).

At resolutions higher than the standard 1X the slit must be decreased to a narrower width. Because the Beckman is a dual-grating, dual-slit monochromer, each time the slit width is decreased by a factor of 2 (resolution increased by 2), the energy throughput is decreased by a factor of 4; thus integration times must be increased by a factor of 16 per channel to achieve the same signal to noise as at the lower resolution. When the resolution is increased by a factor of 2, the number of channels to be obtained increases by 2. Thus, for a 2X resolution increase it takes 32 times longer to obtain a full spectrum. A 4X resolution takes 1024 times longer, and an 8X resolution takes 32,768 times longer than a 1X spectrum. Because of these long times, the high-resolution spectra were obtained only over short spectral regions that showed absorption bands at the 1X resolution. In some cases, only a very small quantity of sample was obtainable, and a very small spot had to be measured (an example was the lizardite where a spot about 2 mm in diameter was measured). Measuring small spots requires an aperture to be placed at a focal point in the spectrometer, with the resulting loss of light. On a 1X resolution sample of normal size (a rectangular spot 10 by 15 mm), the minimum integration time was typically set at 3 s per channel, while on the 8X resolution, small spot lizardite measurement, the integration took 4.7 hours per channel and was measured over several days. A liquid nitrogen dewar containing silicon and indium antimonide detectors is nearly complete and will provide better sensitivity and shorter integration times than with the present detectors, as well as coverage to 4 μm.

The sample holders used for the particulate measurements are described by Hunt [1980]. These sample holders are attached to an integrating sphere, but the light actually measured is not directional-hemispherical because of the
lower-than-unity reflectance of the holder walls. The average phase angle measured was 30°.

The spectrometer measures the reflectance $r_m$ according to

$$r_m = \frac{I_s + I_{ds} - I_e}{I_s + I_{de} - I_e}$$

(1)

where $I_s$ is the intensity at the sample, $I_{ds}$ is the dark at the sample, $I_s$ is the intensity of the Halon in the reference beam, $I_{de}$ is the dark in the reference beam, and $I_e$ is the electronic dark and is measured when the chopper blocks the light beam. The dark measurement is done with a black hole, $I_{bl}$:

$$I_{bl} = \frac{I_{ds} - I_e}{I_r + I_{de} - I_e}$$

(2)

The black hole measurement is discussed further by R. N. Clark et al. (Experimental verification of the Hapke reflectance theory, 1, Computation of reflectance as a function of grain size and wavelength based on optical constants, submitted to Journal of Geophysical Research, 1989). The reference Halon is measured along a different optical path than the sample, so errors in a double-beam instrument must be calibrated out. It is a simple procedure to measure a Halon sample relative to Halon in the reference holder to provide the beam inequality correction:

$$r_H = \frac{I_H + I_{ds} - I_e}{I_r + I_{de} - I_e}$$

(3)

where $I_H$ is the intensity of the Halon measured in the sample holder. The dark subtracted, reference beam corrected, absolute reflectance is then

$$r = \frac{r_m - I_{bl}}{R_H - I_{bl}}$$

(4)

where $R_H$ is the absolute reflectance of Halon and is discussed in the next section. Conveniently, the dark in the reference beam and the beam inequality are canceled out by measuring the Halon in the sample holder. The dark measurement $I_{bl}$ has a typical level of about 0.005-0.01 reflectance units, so when the reflectance is very low, the dark is a substantial portion of the signal; however, for most of the samples in this study the dark is insignificant except in the UV.

Each spectrum obtained consisted of the reflectance and standard deviation of the mean (error bar). Because many hundreds of points were sampled, plotting of error bars would produce messy plots, so the error bars were plotted only when they were large enough that the bar would be distinguishable from the line representing the spectrum. The Beckman had two grating-order separating filters that crossed at 2.3 μm and resulted in a low signal; thus the error bars are often seen on the spectra at that wavelength. Otherwise, at most wavelengths the error bars were too small to be noticeable on the data plotted in this paper.

### Reflectance of Halon to 3.0 μm

The reflectance standard used in this study is Halon, whose absolute reflectance has been measured by Weidner and Hsia [1981] from 0.2 to 2.5 μm. In the present study, the spectral range 0.2-3.0 μm was measured, so the Halon reflectance had to be extended. The reflectance of Halon relative to sulfur and ground aluminum was measured. The sulfur was an ultrapure sample that was baked in a vacuum oven overnight and removed just before measurement. The aluminum was freshly ground and cleaned with methanol just before measurement. The dry atmosphere of Denver apparently added no noticeable water to the samples (or exactly the same spectrally) because the Halon/sulfur and Halon/ground aluminum ratios were identical within the error bars. We assumed that the reflectance of the sulfur and aluminum was flat in the 2.5-3.0 μm region, so the relative reflectance data were scaled to that of the absolute reflectance of Halon given by Weidner and Hsia [1981] in the 2.0- to 2.5-μm region. The scaled Halon/sulfur and Halon/ground aluminum data were then assumed to equal the absolute reflectance in the 2.5- to 3.0-μm region. The spectral response of Halon derived here agrees with that of Nash [1986] and is listed in Table 2 at the 1X resolution and shown in Figure 3. Because of the low signals given by the lead

<table>
<thead>
<tr>
<th>Micrometers</th>
<th>Reflectance</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.400</td>
<td>0.9620</td>
</tr>
<tr>
<td>2.418</td>
<td>0.9620</td>
</tr>
<tr>
<td>2.440</td>
<td>0.9613</td>
</tr>
<tr>
<td>2.466</td>
<td>0.9605</td>
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<tr>
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</table>
used a Siemens D-500 X-ray diffractometer with CuKα radiation to achieve random orientation. There were several minerals analyzed using both SEM and XRD. The XRD analysis (except chrysotile which was analyzed by scanning electron microscope (SEM); halloysite was analyzed using both SEM and XRD). The XRD analysis (compared to the JCPDS file cards). These patterns were modeled by calculating allowed d-spacings from input unit cell dimensions using the Appleman and Evans [1973] computer program written by R. C. Reynolds (Dartmouth College).

Additional tests were done to characterize the clay minerals. The <2-μm fraction was oriented on a glass slide using a Millipore filter setup [Drever, 1973]. These slides were then analyzed in the air-dried and glycol-solvated states. The mixed-layer clay minerals were modeled using methods outlined by Reynolds [1980] and using the NewMod computer program written by R. C. Reynolds (Dartmouth College).

XRD results are listed in Table 1. The analysis of the <74-μm size fraction is listed first. If additional analyses were done, they are subsequently listed. Mineralogical abundances were estimated by peak height and are designated by large, medium, and small amounts.

Additional analysis done on some samples includes X-ray fluorescence (XRF) and/or electron microprobe (M), and visible-light microscopic examination. Samples that were contaminated with carbonate were further analyzed to determine its content, and in some cases the carbonate was removed with a Na-acetate buffer treatment [Jackson, 1979] to assess the spectral contamination of the carbonate. The mineralogical results are summarized in Table 1.

To determine if any of the contaminant minerals were causing a spectral impurity, the spectra were cross-correlated to see if any of the observed absorption bands were due to the contaminant. This process involved the intercomparison of the spectra of the minerals indicated to be contaminants from XRD, examination under a microscope to estimate the contaminant abundances, and an assessment of the possible level of contamination. The high-resolution spectra aided considerably in this assessment.

In determining the spectral purity of each mineral, the spectral features were analyzed for feature position, width, shape, and depth. To analyze a feature, a continuum was removed in the manner described by Clark [1981] and Clark and Roush [1984]. Once a continuum was removed, the band minima were found, the full width at half maxima determined, and the asymmetry computed using an interactive band analysis program that is part of the specpr program.

For example, in Table 1, the XRD analysis indicates that the sepiolite sample SepSp-1 contains calcite. However, the 2.3-μm band in sepiolite is about 3 times narrower in width than in calcite, is shifted to a shorter wavelength, and has fine (doublet) structure not displayed in calcite. The band in sepiolite near 2.53 μm is weak but is also narrower than in calcite. With this sample, one could only conclude that calcite could possibly be depressing the continuum somewhat; however, the absorptions and their fine structure are due to sepiolite. The narrow absorptions and their purity are the most important aspects of this study, not the general continuum level and slope. The absorption band spectral purity in sepiolite is further strengthened by analysis of a second sepiolite sample (SepNev-1) that is contaminated with dolomite: there are no band shifts similar to the band shift from calcite to dolomite. In these cases, the spectral purity was checked by dissolving the carbonate (using the Na-acetate buffer treatment) and measuring the spectra of purified samples. No change in the band positions or shape was found, so the spectra are considered spectrally pure.

Specific discussions on spectral purity will be discussed with the spectrum of each mineral, as appropriate. As noted in Table 1, some of the weakest bands in spectra of some minerals could be due to contaminants, but even if they were, they are negligible for most applications. Overall, the samples are good spectral standards for the study of narrow absorption features in the 0.2- to 3.0-μm region. The presence of mineral contaminants only decreases the apparent band strengths and not their position or structure for the cases presented here.

MINERAL AND SPECTRAL PURITY

The purity of each sample was determined by X-ray diffraction (XRD) analysis (except chrysotile which was analyzed by scanning electron microscope (SEM); halloysite was analyzed using both SEM and XRD). The XRD analysis used a Siemens D-500 X-ray diffractometer with CuKα radiation. Samples were mounted using a side pack sample holder to achieve random orientation. There were several samples that were reported to be nonmineralic using optical methods but that had "extra" peaks in the X-ray patterns (compared to the JCPDS file cards). These patterns were modeled by calculating allowed d-spacings from input unit cell dimensions using the Appleman and Evans [1973] cell refinement program. The differences between the JCPDS and modeled patterns typically could be attributed to differences in ionic substitutions.

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Spectral Features

This study represents a survey of narrow absorption features in minerals. Because spectra of all minerals can not be shown in one paper, a representative fraction is presented. This study is intended to be a beginning for other in-depth studies. For example, King and Clark [1989] studied high-resolution spectra of serpentines and chlorites, and Swayze and Clark [1990] analyzed spectra of scapolites.

In order to reduce the quantity of minerals to survey for...
high-resolution spectral properties, the (analog) spectra in
the published HS spectral data base were surveyed, and the
minerals which had sharp absorptions were measured digi-
tally on the new spectrometer. The spectra published by
Hunt and colleagues include most common minerals and
most of those important to remote sensing studies. A few
additional minerals that were not published in the HS
spectral data base were also included, such as spectra of
samples from the Source Clay Minerals Repository (Univer-
sity of Missouri). These samples represent a uniform collec-
tion [Van Olphan and Fripat, 1979] from which other inves-
tigators may obtain additional material. The sample orig-
nes are listed in Table 1 and the 0.2- to 3.0-µm spectra at the
standard 1X resolution are shown in Figures 4a–4g.

Absorption Features

Very broad absorption bands in the visible and near-IR are
typically caused by electronic transitions such as ligand field
and metal-metal charge transfers (e.g., see Hunt [1977] for a
general review of absorption processes). The absorptions
due to OH−, H2O, and CO −2, seen in the 0.9- to 2.5-µm
region, are due to overtones and combinations of the funda-
mentals that occur at longer wavelengths.

Each higher overtone or combination absorption band has
an intrinsic strength about 30–100 times weaker than the next
lower overtone/combination or fundamental bands. How-
ever, in reflectance, photons will penetrate more material
when the absorption coefficient is lower, tending to enhance
the observed band strength [e.g., Clark, 1981; Clark and
Roush, 1984]. Because of band saturation effects, there are
scattering conditions that will show the combinations and
overtones with stronger apparent band depths than the
fundamentals [e.g., Clark, 1981; Clark and Lucey, 1984].

In the following discussions, band positions are cited in
two forms: wavelength and wave number. In the mid-IR, the
convention of wave number (cm −1) is used and the wave-
length (µm) is given in parentheses. In the near-IR, the
wavelength is used following the convention used in terres-
trial and planetary remote sensing and laboratory studies,
and wave number is given in parentheses. Band positions of
fundamentals will always be given in wave number followed
by wavelength in parentheses.

The fundamental band width, defined in this paper as the
full width at half maximum (FWHM). The FWHM indicates
how accurately a band position can be determined and how
small a shift might be detected. For example, an OH stretch
absorption band near 3600 cm −1 (2.7 µm) can have a width
as small as about 10 cm −1 (0.008 µm) and very small shifts
(e.g., 2 cm −1) are detectable. On the other hand, if the width
was much larger (e.g., 100 cm −1), then small shift would not
be detectable.

The ability to resolve an absorption band is sometimes
given in resolving power: the wavelength λ divided by the
spectrometer resolution Δλ. For example, at a wavelength of
2.2 µm and an absorption with a width of 0.0044, the
resolving power (λ/Δλ) is 500. As stated earlier, the standard
(1X) resolving power in this study is near 200, and selected
absorption bands were studied at powers up to 2240.

Water and Hydroxyl in Minerals

The water molecule has three infrared-active-fundamental
absorptions. The free molecule has a symmetric OH stretch
\( \nu_1 \) at 3651.7 cm −1 (2.738 µm), an asymmetric OH stretch \( \nu_3 \)
at 3753.8 cm −1 (2.6625 µm), and an H-O-H bend \( \nu_2 \) at 1395
cm −1 (6.269 µm). In H2O gas, these absorptions show
numerous closely spaced bands due to combinations with
rotational modes, and in the near-IR, combination bands
show rotational fine structure at the milliangstrom scale. In
liquid water there is no rotational fine structure, and the

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Fig. 4a. Reflectance spectra at the standard 1X resolution from
0.2 to 3.0µm for talc, tremolite, actinolite, topaz, brucite, and
datolite. The organization of the spectra is a compromise between
grouping similar minerals together and trying to preserve space by
grouping minerals with similar spectral features together.
bands shift to $\nu_1 = 3219 \text{ cm}^{-1} (3.106 \mu \text{m})$, $\nu_3 = 3445 \text{ cm}^{-1} (2.903 \mu \text{m})$, and $\nu_2 = 1645 \text{ cm}^{-1} (6.079 \mu \text{m})$. In ice the bands shift further to $\nu_1 = 3221 \text{ cm}^{-1} (3.105 \mu \text{m})$, $\nu_3 = 3400 \text{ cm}^{-1} (2.941 \mu \text{m})$, and $\nu_2 = 1650 \text{ cm}^{-1} (6.06 \mu \text{m})$. The large shifts in the band positions are due to hydrogen bonding. The lack of rotational fine structure in the liquid and solid phases is due to the inability of the molecule to rotate.

In the near-IR the isolated water molecule has absorptions at $\sim 1.875 \mu \text{m} (\nu_2 + \nu_3; 5333 \text{ cm}^{-1})$, $1.454 \mu \text{m} (2\nu_2 + \nu_3; 6878 \text{ cm}^{-1})$, $1.379 \mu \text{m} (\nu_1 + \nu_2 + \nu_3; 8811 \text{ cm}^{-1})$, and $0.942 (2\nu_1 + \nu_2; 10600 \text{ cm}^{-1})$ [Hunt and Salisbury, 1970]. In minerals, water has combination and overtone bands close to these positions. Water can be
physically adsorbed on the surfaces of mineral grains, or it can occupy specific lattice sites (e.g., beryl), or it can be an integral part of the crystal structure (e.g., gypsum). The water bands may be sharp, as in the well-ordered sites in beryl, or broad due to multiple or poorly ordered sites, as in montmorillonite. The presence of a 1.9-μm band indicates molecular water in the sample, whereas the absence of a 1.9-μm band but the presence of a 1.4-μm band indicates that only OH is present.

Hydroxyl is often a part of the crystal structure of a mineral. There is only one vibration of OH$^-$ and it is infrared active. Hunt and Salisbury [1970] cited a position of "somewhere near 3600 cm$^{-1}$" for the OH stretch, with the exact position depending on the lattice site. There is a
general impression that the OH stretch is always close to 3600 cm⁻¹ (2.78 μm). The first overtone generally occurs near 1.4 μm (2 νOH; 7100 cm⁻¹), and the second occurs near 0.95 μm (3 νOH; 10500 cm⁻¹). These positions seem to be commonly cited values [e.g., Adams, 1975; Hunt, 1977, 1979; Hunt et al., 1971a, b; Goetz et al., 1983, and references therein]. However, Ryskin [1974] states that the lower limit to the OH stretching fundamentals is as low as ~2900 cm⁻¹ (3.45 μm) and the overtone positions would vary similarly.

In the layer silicates the range of the OH stretching vibration is 3400–3750 cm⁻¹ (2.94–2.67 μm) according to Farmer [1974]. The frequency of the OH vibration is related to the site that it occupies. For example, in common chain, ribbon, and ring silicates the absorption band position is related to the electronegativity difference between Mg and another cation when the cation substitutes into the Mg site [Strens, 1974]. Ionic size, formal charge, and mass have little effect on the position, except possibly for Cu²⁺, but the Cu-OH bond is the (more ionic) bond of a Jahn-Teller distorted octahedron [Strens, 1974]. Ionic substitutions in other sites are also known to cause shifts in the OH band position. Shifts as small as 2 cm⁻¹ have been shown to be diagnostic [e.g., Strens, 1974].

In the case of hydroxyl there is no H-O-H bend as in the water molecule, so the lack of an absorption band at 1.9 μm (H-O-H bend plus OH stretch) indicates the absence of
TABLE 3. OH Librations

<table>
<thead>
<tr>
<th>Species</th>
<th>Wave Number, cm^{-1}</th>
<th>Wavelength, μm</th>
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<tbody>
<tr>
<td>Al_2OH</td>
<td>915-1020</td>
<td>11-9.8</td>
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<tr>
<td>Fe_2+AlOH</td>
<td>~890</td>
<td>11.3</td>
</tr>
<tr>
<td>MgAlOH</td>
<td>~840</td>
<td>11.9</td>
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<td>Fe_3+OH</td>
<td>818</td>
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<td>Fe_2+Fe_3+OH</td>
<td>~800</td>
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</tr>
<tr>
<td>MgFe_2+3OH</td>
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<td>12.5</td>
</tr>
<tr>
<td>MgOH</td>
<td>600-670</td>
<td>17-15</td>
</tr>
</tbody>
</table>

After Farmer [1974].

In carbonates, the observed absorptions are due to the planar CO_3^{2-} ion. There are four vibrational modes in the free CO_3^{2-}: the symmetric stretch, ν_1: 1063 cm^{-1} (9.407 μm); the out-of-plane bend, ν_3: 879 cm^{-1} (11.4 μm); the asymmetric stretch, ν_2: 1415 cm^{-1} (7.067 μm); and the in-plane bend, ν_4: 680 cm^{-1} (14.7 μm). The ν_1 is not infrared active in minerals. There are actually six modes in the CO_3^{2-} ion, but two are degenerate with the ν_3 and ν_4 modes. In carbonate minerals the ν_3 and ν_4 bands often appear as a doublet. The doubling has been explained in terms of the lifting of the degeneracy [e.g., White, 1974] due to mineral structure and anion site.

Combination and overtone bands of the CO_3 fundamentals occur in the near IR. The two stronger ones are ν_1 + 2ν_3 at 2.50-2.55 μm (4000-3900 cm^{-1}) and 3ν_3 at 2.35-2.35 μm (4150-4520 cm^{-1}, e.g., Figures 4d and 8g). Three weaker bands occur near 2.12-2.16 μm (ν_1 + ν_3 or 2ν_1 + 2ν_3; 4720-4630 cm^{-1}), 1.97-2.00 μm (2ν_1 + 2ν_3; 5080-5000 cm^{-1}), and 1.85-1.87 μm (ν_1 + 3ν_3; 5400-5550 cm^{-1}; e.g., Figure 4d) [e.g., Hunt and Salisbury, 1971]. The band positions in carbonates vary with composition [Hunt and Salisbury, 1971; Gaffey, 1984]. An example of such a band shift is seen in Figure 8g from calcite to dolomite.

Scapolite consists of a solid solution between Na and Ca end-members marialite and meionite. Near-IR spectra of OH-bearing scapolites have a weak band at 1.41 μm (7092 cm^{-1}) due to the first overtone of the OH stretch (Figure 4e). This OH stretch may be attributed to an OH^- ion located in the anion site coordinated by alkali cations or to an O-H bond in protonated tetrahedral oxgens. Some mizzonitic and meionitic scapolites contain HCO_3^- and HSO_4^- [Swazy and Clark, 1990], and these scapolites have an additional sharp feature at 1.47 μm (6803 cm^{-1}). This band is the first overtone of an OH stretch associated with the hydroxyl bond in HSO_4^- (Figure 8g).

Sulfate- and Chlorine-containing scapolites are relatively featureless in the 1.4- and 2.3-μm region, provided that they do not contain OH, or else they will have the 1.41 μm band. Carbonate containing scapolites have relatively weak second-order overtones and combinations attributed to the symmetric and asymmetric stretches of the CO_3^{2-} ion in the anion site. The presence of small quantities of HCO_3^- and HSO_4^- produce a band quadruplet centered at 2.36 μm.
Phlogopite

possibly another at 1.396/am (Figure 6b). The fact that these Mg-OH combination band.

The 2.322- and 2.379-/am features (Figure 8e) show two OH fundamentals near 3640 and 3510 cm - (2.75

(7184 cm -1) in tremolite, 1.404/am (7123 cm -) in topaz, and

1.471/am (6798 cm -1) in datolite. Biotite (Figure 4b) clearly

1.77-/am absorption (5650 cm -) to a combination comprised of the second overtone of the Al-OH bend, pAOH, whose fundamental occurs near 1050 cm -1 (9.5 /am), plus the OH stretch (pOH). When the computation gives reasonable agreement with the observed 1.77-/am position, the assignment is not consistent with all Al-OH-bearing minerals; only sulfates show a band in this region.

Hunt et al. also assigned the 2.17-/mu (4610 cm -1) absorption to the OH stretch plus the Al-OH bend and the 1.0-/mu (10,000 cm -1) band to the third overtone of the OH stretch. However, the 1.0-/mu band is too wide for a stretch overtone. It has the shape and width appropriate to be a combination of 2 pOH + 2 pAOH.

It appears that confusion still exists as to the correct assignments in alunite near-infrared spectrum and, by analogy, to other sulfates. Further work is needed.

Talc

The spectrum of Talc (Figure 4a) shows a single sharp band at 1.4 /mu at the standard 1X resolution (0.005 /mu) and two broad and weak features near 1.43 and 1.55 /mu (7000 and 6450 cm -1). The 1.55-/mu band is probably due to a small amount of adsorbed water. As the resolution is increased, the sharp 1.4-/mu band may be resolved into a doublet, or even a triplet (Figure 5a) located at 1.3913, 1.3978, and 1.4059 /mu (7188, 7154, and 7113 cm -1) if there is a small amount of iron present. Similarly, the 2.3-/mu (4350 cm -1) band resolves into a doublet located at 2.29 and 2.31 /mu (4370 and 4330 cm -1), with a third band seen as a shoulder at 2.325 /mu (4300 cm -1; Figure 5b). Clearly, an increase in resolution over the 0.01 /mu (10 nm) commonly used in remote sensing studies will show potentially useful detail.

The XRD analysis of talc sample HS21.3B indicates chlorite contamination. Examination under a microscope indicates less than 1% contamination in the HS21.3B. The chlorites measured by King and Clark [1989] have broader 1.4-/mu absorption bands located at different positions than in the talc. There is no detectable chlorite spectral contamination in the 1.4-/mu (7100 cm -1) region. Chlorites often have only a weak 1.4-/mu band because it is suppressed by strong (broad) iron absorption. At 2.3 /mu there are no detectable chlorite bands in the HS21.3B spectrum. A second talc (WS659) is pure, but a third talc (HS327.3B) was found to contain 10 wt % chlorite; and there appears to be

Alunite (Figure 4d) has two widely separated OH stretching frequencies at 3486 cm -1 (2.87 /mu) and 3513 cm -1 (2.85

/mm) [Salisbury et al., 1987]. Although the fundamentals are not fully resolved in Figure 4d, a characteristic doublet shows in the 1.4-/mu overtone (7100 cm -1) region. XRD analysis indicates sample HS295 to be pure alunite.

Absorptions in the spectrum of alunite from 1.7 to 2.6 /mu (5900–3800 cm -1) are combinations with bending (librational) and translational modes with the OH stretches. These bands do not show the fine structure of the 1.4-/mu complex because the libration and translation bands have a greater width than the OH stretches. Hunt et al. [1971b] assigned the 1.77-/mu absorption (5650 cm -1) to a combination comprised of the second overtone of the Al-OH bend, pAOH, whose fundamental occurs near 1050 cm -1 (9.5 /mu), plus the OH stretch (pOH). When the computation gives reasonable agreement with the observed 1.77-/mu position, the assignment is not consistent with all Al-OH-bearing minerals; only sulfates show a band in this region.

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It appears that confusion still exists as to the correct assignments in alunite near-infrared spectrum and, by analogy, to other sulfates. Further work is needed.

Jarosite, Tourmaline, Zoisite, and Epidote

which swamps the weaker carbonate features. Absorptions at 2.334 and 2.354 /mu (4284 and 4248 cm -1) are attributed to combinations of OH stretches with a O-H...O bend from HCO3-(Figure 8e). Those at 2.389 and 2.412 /mu (4186 and 4146 cm -1) are attributed to combinations of OH stretches with a O-H...O bend from HSOd-. It should be noted that scapolites containing HCO3- and HSOd- are rather rare, and the origin of these ions is not well understood at this time.

Vibrational absorptions by other species such as sulfates, borates, and phosphates have not been reported in the near-IR because their fundamentals all lie beyond about 1100 cm -1 (9 /mu). An absorption in the 1- to 2.5-/mu (10,000–4000 cm -1) region would involve at least the fourth overtone and would be extremely weak [e.g., Hunt et al., 1971b].

Talc

The spectrum of Talc (Figure 4a) shows a single sharp band at 1.4 /mu at the standard 1X resolution (0.005 /mu) and two broad and weak features near 1.43 and 1.55 /mu (7000 and 6450 cm -1). The 1.55-/mu band is probably due to a small amount of adsorbed water. As the resolution is increased, the sharp 1.4-/mu band may be resolved into a doublet, or even a triplet (Figure 5a) located at 1.3913, 1.3978, and 1.4059 /mu (7188, 7154, and 7113 cm -1) if there is a small amount of iron present. Similarly, the 2.3-/mu (4350 cm -1) band resolves into a doublet located at 2.29 and 2.31 /mu (4370 and 4330 cm -1), with a third band seen as a shoulder at 2.325 /mu (4300 cm -1; Figure 5b). Clearly, an increase in resolution over the 0.01 /mu (10 nm) commonly used in remote sensing studies will show potentially useful detail.

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chlorite contaminating the 2.30- and 2.36-μm (4350 and 4340 cm⁻¹) regions. The full spectrum of HS327 is not shown, but the spectrally pure 1.4-μm region is shown in Figure 5a to illustrate the spectrum of a high-iron talc. Chlorites also have a single strong band near 2.25 μm but not a doublet like that in HS21.3B (Figure 8e). Strong iron bands occur in chlorite near 0.7, 0.9, and 1.1 μm but no such bands are seen in the spectra for sample HS21.3B (Figure 4a), further indicating that it is spectrally pure. The iron band near 1 μm in HS21.3B is not characteristic of chlorite bands and must be due to the small amount of iron in the talc.

Figures 6a–6h show high-resolution spectral details of absorptions in the 1.4- to 1.7-μm (7100–5900 cm⁻¹) region. Figures 6a–6h are organized in approximately increasing shift to longer wavelengths of the OH stretch overtones. Figure 7 shows the high-resolution spectral details in the 1.6- to 1.9-μm (6200–5300 cm⁻¹) region for selected minerals. Figures 8e–8g show the high-resolution spectral details in the 2.0- to 3.0-μm (5000–3300 cm⁻¹) region.

Tremolite, Actinolite, and Talc

An noted earlier, there are four bands in the OH stretching region of some minerals due to OH linked to Mg3, Mg2Fe, MgFe2, and Fe3. Tremolite, actinolite and talc (Figure 6a) all have an absorption near 1.392 μm (7184 cm⁻¹). The 1.392-μm (7184 cm⁻¹) band is due to Mg3, Tremolite, the Mg end-member in the tremolite-ferroactinolite solid solution series, shows no OH bands involving Fe. The band near 1.398 μm (7153 cm⁻¹) is due to Mg3FeOH and the bands near 1.404 μm (7120 cm⁻¹) to MgFe2OH. These samples do not contain enough iron to show the Fe3-related band, except extremely weakly; it occurs near 1.412 μm (7082 cm⁻¹).

The spectral purity of the tremolite and actinolite samples was assessed by the same method as the talc previously discussed. The XRD analysis of actinolite HS116.3B indicates that chlorite is present, but no chlorite bands were detected in the spectrum. The XRD analysis of tremolite HS18.3B indicates that mica is present, but no mica bands can be detected in the spectrum.

Chrysotile, Lizardite, and Antigorite

The isochemical series chrysotile, lizardite and antigorite is shown in Figure 6a. Chrysotile has a cylindrical crystal lattice, lizardite has a rectilinear lattice, and antigorite has a corrugated rectilinear lattice. The fine structure seen at high resolution shows that these minerals can be distinguished from each other. They are more difficult to differentiate solely on spectral features in the 2.3-μm (4350 m⁻¹) region (Figure 8f). See King and Clark (1989) for a detailed discussion of the high-resolution spectra of these minerals.

Saponite, Sepiolite, and Hectorite

High-resolution saponite and sepiolite spectra are shown in Figures 6b, 6c, and 8f. At a low resolution (~0.01 μm), the
Fig. 6a. High-resolution spectral details in the 1.36- to 1.45-μm spectral region. Absorption bands with relatively sharp absorption features just short of 1.4 μm for talc, tremolite, actinolite, chrysotile, lizardite, and antigorite.

Fig. 6b. Same as Figure 6a, except for saponite, sepiolite, hectorite, pyrophyllite, brucite, vermiculite, zoisite, and phlogopite.
Fig. 6c. Absorption bands that are relatively broad and centered just beyond 1.4 μm for saponite, sepiolite, nontronite, natrolite, analcime, clinoptilolite, and vermiculite.

Fig. 6d. Same as Figure 6c, except for muscovite, Cookeite, topaz, halloysite, and kaolinite.
1.4-μm region is indistinguishable from minerals like montmorillonite because the sharp band near 1.39 μm (7190 cm⁻¹) is not resolved. The 2.3-μm (4350 cm⁻¹) band resolves as a doublet in both saponite and sepiolite at high resolution (Figure 8f). Hectorite, sepiolite, and saponite are difficult to distinguish based on the 2.3-μm bands alone (Figure 8f), unless a careful comparison is made at high resolution. In hectorite, the 2.3-μm band is slightly narrower, and the weak band at 2.39 μm (4180 cm⁻¹) is also narrower than the corresponding band in saponite. The 2.39-μm band is barely a shoulder in sepiolite.

In the 1.4-μm spectral region at high resolution, it is easier to distinguish between saponite, sepiolite, and hectorite than in the 2.3-μm region. The OH overtone occurs at 1.3904 μm (7192 cm⁻¹) in hectorite, 1.3867 μm (7211 cm⁻¹) in sepiolite, and 1.3910 μm (7189 cm⁻¹) in saponite (Figure 6b). The saponite band is also considerably wider than the sepiolite band.

The spectral purity of the sepiolite data was discussed in the first part of this section. The analyses of the hectorite and saponite are similar: the absorptions are narrower and at different positions than bands in the carbonates with the exception of the 2.5-μm band in hectorite. That band could be partially due to carbonate, but it appears more like a liquid water absorption and no absorption with a position and width characteristic of the carbonate 2.32- or 2.34-μm band is seen. This argues against significant carbonate spec-
Fig. 6g. Absorption bands near 1.45 μm that are relatively sharp.

Fig. 6h. Absorption bands in the 1.35- to 1.7-μm spectral region.

Central contamination. In any event, the narrow bands in saponite, sepiolite, and hectorite at 1.4 and 2.3 μm indicate that these minerals are spectrally pure.

Pyrophyllite

Pyrophyllite (Figures 4b, 6b, and 8a) shows numerous sharp bands throughout the near IR. These bands remain single sharp bands at high resolution, occasionally with a shoulder that cannot be resolved. The pyrophyllite bands make excellent wavelength standards for reflectance spectroscopy with bands located at 0.951 μm (10500 cm⁻¹), 1.235 μm (8110 cm⁻¹), 1.335 μm (7491 cm⁻¹), 1.393 μm (7177 cm⁻¹), 2.06 μm (shoulder, 4850 cm⁻¹), 2.086 μm (4794 cm⁻¹), 2.166 μm (4617 cm⁻¹), 2.314 μm (4232 cm⁻¹), and 2.504 μm (3994 cm⁻¹). The sample PYSIA has been distributed to several investigators as a wavelength standard. The wavelength accuracy of the spectrometer has been checked by measurement of this mineral on a Fourier Transform instrument of J. W. Salisbury (USGS, Reston, Virginia) and the FTIR at the USGS Denver spectroscopy laboratory.

Zeolites: Natrolite, Analcime, and Clinoptilolite

Zeolite spectra (natrolite, analcime, and clinoptilolite) are shown in Figures 4f, 6c, 6g, 7, and 8g. The absorptions in these minerals are due to water molecules trapped in cavities of the zeolite crystal lattice and do not show fine structure. XRD analysis indicates sample HS169.3B (Figure 4f) is a pure natrolite. The water content can radically change the fine detail in the spectra. When the water content is very high, the bands are saturated and become broader, washing out the separate bands. Sample HS169.3B has a lower water content than HS168.3B so the absorptions are more easily distinguished.

The band near 2.2 μm (4550 cm⁻¹) in natrolite (Figure 8g) could be confused with some clays, whereas the band near 2.5 μm (4000 cm⁻¹; Figure 8g) in analcime and clinoptilolite could be confused with a carbonate band. A mixture of two minerals, one a zeolite and the other a mineral with a band near 2.35 μm (4250 cm⁻¹) might appear similar to the
carbonate bands in some remote sensing studies (remote spectral work through the Earth's atmosphere is usually limited to about 2.5 \( \mu m \) because of atmospheric water absorptions).

**Brucite**

Brucite (Figure 8g) is another mineral whose absorptions could be confused with those of carbonates at low spectral resolution, although brucite is not geologically as common as carbonates. However, if the spectral resolution is maintained near 0.005 \( \mu m \), the possibility of confusion is reduced. The XRD analysis of brucite (sample HS247.3B) indicates the presence of dolomite, and the 2.3- and 2.5-\( \mu m \) (4350 and 4000 cm\(^{-1}\)) bands in brucite are similar in position to those in dolomite, but they do not have the same structure. Microscopic examination and dissolution of dolomite grains with HCl indicate about 8\% dolomite contamination in the sample. The brucite absorptions are very strong (reflectance continuum level \( \sim 20\% \), 2.5-\( \mu m \) band depth \( \sim 70\% \)) compared to dolomite (reflectance continuum level \( \sim 60\% \), 2.5-\( \mu m \) band depth \( \sim 40\% \)). Radiative transfer models [e.g., Hapke, 1981] indicate that the brucite 2.3- and 2.5-\( \mu m \) bands are 1-2 orders of magnitude stronger than the corresponding dolomite bands. Thus any dolomite spectral contamination of the brucite is much less than 1\%. The brucite HS247.3B sample is spectrally pure.

**Kaolinite and Halloysite**

Kaolinite (Figures 4c and 8b) shows a well-known doublet absorption near 2.2 \( \mu m \). Halloysite also shows a similar doublet (Figures 4c and 8b). Both these minerals show a doublet at 1.4 \( \mu m \) (7100 cm\(^{-1}\); Figure 6d) at high resolution. A well-ordered kaolinite (KGa-1) shows as a triplet at both
1.4 and 2.2 μm (7100 and 4550 cm\(^{-1}\); Figures 6d and 8b), although the third band is a weak feature between two strong bands. Halloysite does not show a similar triplet. The two doublet absorption bands (ignoring the weak third band) in kaolinite consist of a broad absorption with a sharper band at slightly longer wavelength: 1.395 and 1.415 μm (7168 and 7067 cm\(^{-1}\)) for the OH stretch overtones and 2.163 and 2.2085 μm (4623 and 4528 cm\(^{-1}\)) for the Al-OH bend plus OH stretch combinations. In halloysite the absorption bands near 2.2 μm occur at nearly the same location as in kaolinite: 2.16 and 2.207 μm (4630 and 4531 cm\(^{-1}\)). The position of the longer band varies from 2.2077 to 2.2063 μm in the samples that we have measured, but the 2.16-μm band is too broad to

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**Fig. 8c.** Absorption features in montmorillonite near 2.2 μm.
have its band center accurately defined enough to see small shifts. Near 1.4 \( \mu \text{m} \) the broad component of the doublet absorption is shifted to around 1.390 \( \mu \text{m} \) (7190 cm\(^{-1}\)) or slightly shorter to 1.388 \( \mu \text{m} \) (7205 cm\(^{-1}\)) in some halloysite samples (Figure 6d) as compared to kaolinite. The other absorption shifts shortward to between 1.414 and 1.413 \( \mu \text{m} \) (7072 and 7077 cm\(^{-1}\)). Both of these halloysite absorptions are broader than the corresponding kaolinite bands.

There is still confusion about the crystal structure of halloysites. It appears that the crystals have a hollow prismatic morphology and a monoclinic two-layered unit cell with an unusual stacking sequence and a range of order-disorder similar to that found in kaolinite [Swindale, 1975]. Sometimes the crystals appear as curled plates. The observed variation in the halloysite band positions and widths may reflect the degree of disorder. The degree of disorder in kaolinites has been shown to cause band shifts in kaolinite. See Crowley and Vergo [1987] for additional discussion.

Halloysite also has a 1.9-\( \mu \text{m} \) (5260 cm\(^{-1}\)) band due to molecular water. At low resolution (e.g., 0.01 \( \mu \text{m} \)) a physical mixture of montmorillonite and kaolinite shows spectral properties indistinguishable from halloysite (Figure 9).

**Illite, Muscovite, and Montmorillonite**

Illite (Figures 4b, 6e, 8b, and 10), muscovite (Figures 4b, 6d, 8b, 10), and montmorillonite (Figures 4g, 6f, 8c, and 10)
Fig. 8f. Absorption features showing less complexity than in Figure 8e and just long of 2.3 μm.

Fig. 8g. Spectra with absorption features beyond 2.3 μm.
have similar absorption bands that do not show fine structure. Illite and muscovite have additional absorption bands near 2.35 and 2.45 μm as opposed to montmorillonite (Figure 10). The 2.45-μm (4080 cm⁻¹) absorption in illite is poorly defined, and the shorter band is located at 2.34 μm (4270 cm⁻¹). Thus, if these two bands can be detected, it is possible to distinguish the three minerals from each other (Figure 10). For example, montmorillonite has no 2.34- or 2.35-μm absorptions, illite has a band at 2.34 μm, and muscovite has one at 2.35 μm. A resolution of about 0.005 μm (or better) is required to distinguish illite from muscovite. All too often in remote sensing, the 2.2-μm band is weak, and the other absorption bands are below the detection limits. In that case, the three minerals can not be reliably distinguished.

**Attapulgite and Montmorillonite**

The mineral attapulgite has a spectrum that, at low resolution (Figure 4e) is similar to montmorillonite. However, at high resolution the 1.4-μm (7100 cm⁻¹) absorption (Figure 6g) and the 2.22-μm (4500 cm⁻¹) absorption (Figure 8b) are significantly narrower than in montmorillonite (Figures 6f and 8c). At high resolution the attapulgite absorptions are unique. However, at resolutions coarser than about 0.01 μm the spectra of montmorillonite and attapulgite are indistinguishable.

The XRD analysis of attapulgite sample CM46 indicates a trace amount of smectite. The attapulgite OH stretch overtone is at 1.414 μm (7072 cm⁻¹) and is quite narrow. The corresponding montmorillonite absorption band is at 1.411 μm (7087 cm⁻¹) and many times broader. Similarly, the attapulgite Al-OH bend plus OH stretch combination occurs at 2.22 μm (4500 cm⁻¹), whereas in the closest matching montmorillonite spectrum (sample SAz-1) the absorption occurs at 2.215 μm (4515 cm⁻¹) and has a width 3 times greater than attapulgite. No montmorillonite absorption bands can be detected in the attapulgite spectrum.

**Rectorite**

The spectrum of rectorite has absorptions at shorter wavelengths and with narrower band widths than observed in spectra of montmorillonite, muscovite or illite. The XRD analysis of sample RA-1 indicates the presence of chlorite and muscovite, but no absorptions associated with these minerals are seen in the rectorite spectrum. At resolutions coarser than 0.01 μm the rectorite bands might be confused with those of montmorillonite.

**Datolite**

The spectrum of Datolite shows a single absorption at 1.47 μm (6800 cm⁻¹) due to the OH stretch overtone (Figure 6g) and from 2.1 to 2.5 μm (4800–4000 cm⁻¹; Figures 4a and 8a) a very complex structure involving at least 13 bands. These bands are combination bands involving the OH stretch and B-OH librational and translational modes. The XRD analysis indicates that the datolite sample is pure.

**Jarosite and Alunite**

Jarosite and alunite (Figure 6g) have an overtone OH stretch near 1.475 μm. In jarosite the OH stretch fundamentals occur at 3430, 3355, and 3260 cm⁻¹ (2.915, 2.981, 3.067 μm) [Ross, 1974]. The 3355-cm⁻¹ band appears the strongest, and OH librations occur at 790 and 512 cm⁻¹ (12.6 and 19.5 μm). The 2.27 μm (4400 cm⁻¹) band in jarosite (Figure 8d) is due to a combination OH stretch and Fe-OH bend. In jarosite (Figure 8d) and alunite (Figure 8f) the bands do not show as much fine structure as does scapolite. Sulphate-bearing minerals also have an absorption near 1.7 or 1.8 μm, as discussed in the alunite section. The cause needs further study.
### Table 4. Band Positions in the OH Stretching and Overtone Region

<table>
<thead>
<tr>
<th>Band</th>
<th>Cause</th>
<th>Fundamental Position</th>
<th>Overtone Position</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Wave Number, cm⁻¹</td>
<td>Wavelength, μm</td>
</tr>
<tr>
<td>A</td>
<td>Mg₂ +</td>
<td>3678</td>
<td>2.719</td>
</tr>
<tr>
<td>B</td>
<td>Mg₂Fe</td>
<td>3663</td>
<td>2.730</td>
</tr>
<tr>
<td>C</td>
<td>MgFe₂</td>
<td>3646</td>
<td>2.743</td>
</tr>
<tr>
<td>D</td>
<td>Fe³</td>
<td>3624</td>
<td>2.759</td>
</tr>
</tbody>
</table>

*aDerived from Strens [1974].

**Nontronite**

Nontronite has a strong OH stretch fundamental at 3564 cm⁻¹ (2.806 μm) and a weaker fundamental at ~3620 cm⁻¹ (2.76 μm [e.g., Farmer, 1974]). These two stretches are responsible for the doublet overtone at 1.415 and 1.435 μm (7067 and 6969 cm⁻¹; Figure 6g). An Fe-OH bend occurs at 818 cm⁻¹ (12.2 μm [e.g., Farmer, 1974]) giving a combination OH stretch plus Fe-OH bend at 2.29 μm (4370 cm⁻¹; Figure 8d).

**Applications**

We have seen that much of the fine structure observed in mid-IR transmission studies of minerals also shows in reflectance spectra of powdered samples. This fine structure could potentially be used to provide mineralogical information on unprepared samples in the laboratory or in situ by portable field spectrometers. As an example, we will discuss the potential of determining the iron and magnesium in talcs, amphiboles, and minerals with brucite-like crystal structure.

**Iron and Magnesium Minerals**

As discussed in the previous sections, the OH stretching region of amphiboles and minerals with brucite-like structure has four absorption bands. These were labeled A–D [Burns and Strens, 1966; Burns and Greaves, 1971; Farmer, 1974; Strens, 1974] and are shown in Table 4. Burns and Greaves [1971] found nine absorptions due to Mg, Fe²⁺, and Fe³⁺, but those due to Fe³⁺ are much weaker. In the following analysis, Fe³⁺ is ignored because there is so little of it in our samples.

The strength of an absorption is related to the amount of absorber species in the light path. One measure of an absorption is to integrate the area between the absorption curve and a local continuum. Burns and Greaves [1971] showed that if the integrated intensities of the four OH fundamental absorption bands, A–D, are normalized to unity, giving A ′, B ′, C ′, and D ′, then the M(1) and M(3) site populations in per formula unit (pfu) can be determined. The following equations were simplified from Burns and Greaves [1971]:

\[ \text{Fe}^{2+} \text{ in } (\text{M}(1)\text{M}(3)\text{M}(1)) = B' + 2C' + 3D' \]  

and

\[ \text{Mg}^{2+} \text{ in } (\text{M}(3)\text{M}(3)\text{M}(1)) = 3A' + 2B' + C' \]

where absorption band A ′ is due to Mg₃OH, B ′ to Mg₂FeOH, C ′ to Mg Fe₂OH, and D ′ to Fe₃OH. The equation should be applicable to both the fundamental OH absorptions as well as overtones.

When analyzing the overtone absorptions in the 1.4-μm region in reflectance, the observed band depths are strongly influenced by the grain size of the mineral and the amount of contaminants. However, the normalization of the integrated band intensities compensates for most effects due to the change in band depths with grain size. It also compensates for contaminants, as long as the contaminants are spectrally neutral in the overtone region. The normalization alone would not be adequate for relatively large grain sizes which cause the bands to saturate in reflectance. However, band saturation in reflectance is easily identifiable and the correction is discussed below.

Combining (5) and (6), the iron to iron plus magnesium ratio can be found from either normalized or unnormalized integrated band intensities:

\[ \text{Fe} \left( \frac{\text{M}(1) + \text{M}(3)}{\text{Fe} + \text{Mg}} \right) = \frac{\left( B + 2C + 3D \right)}{A + B + C + D} \]

Applying (7) to the talcs, tremolite, and actinolite spectra (Figure 6a), the iron contents were derived by reflectance spectroscopy and compared to electron microprobe analyses (Table 5). The iron derived by reflectance spectroscopy is overestimated. This is because in reflectance, scattering controls the band depth and where the absorption coefficient is lower, photons penetrate through more material. As a result, weak bands become enhanced relative to stronger bands when compared with transmission spectra [e.g., Clark and Roush, 1984; Clark and Lucey, 1984; Clark, 1981].

The reflectance must be converted to some form of transmittance before applying equations (4)–(7). This was done by using the Hapke reflectance theory [Hapke, 1981] to invert the spectrum to absorption coefficient [e.g., Clark and Roush, 1984]. The absorption coefficient can be closely estimated from the reflectance spectrum by using an approximate index of refraction for the material, an approximate grain size, the reflectance, and the radiative transfer model. The grain size can be estimated from the depth of several absorption features in the reflectance spectrum given reference spectra of samples whose grain sizes are known. With this method, the reflectance spectrum itself contains all the information to invert the bands to absorption coefficient for analysis. It is practical to use such methods on spectra of remotely obtained surfaces.

The absorption coefficient of each sample was derived from the observed reflectance spectrum by comparison with...
the radiative transfer model reflectance. The index and grain size are treated as knowns in the model. A simple iterative procedure that started with a guess of an absorption coefficient, allowed the reflectance to be computed and compared with the observed reflectance. If the computed and observed spectra did not match within a small tolerance, the guess absorption coefficient was adjusted. A few iterations converged on the absorption coefficient that made the model match the observations.

To compare the Fe:Fe+Mg ratio from different methods, derived absorption coefficients from the reflectance spectra for each sample and the analysis from overtone bands was checked against transmission spectra of the fundamental using actinolite HS116. The transmission spectrum was provided by Salisbury et al. [1987]. The 1.4-μm absorption coefficient spectrum gives a Fe:Fe+Mg ratio of 0.166, while the 2.7-μm transmittance spectrum gave 0.146, reasonably close agreement. In reflectance, the 2.7-μm absorption band gives a Fe:Fe+Mg ratio of 0.26, while the 1.4-μm absorption gives 0.231. The increased values from reflectance are a result of the greater relative intensity of the weak bands.

The Fe:Fe+Mg ratio from spectroscopy agrees quite well with the oxide weight percent values from electron microprobe but are consistently higher than the pfu values for which the formulas were derived. Because single crystals were probed to determine composition, the ratios should be sufficiently accurate for this study. The composition of each sample is the average of several grains, and each grain appeared consistent. Spectral contamination is also insignificant except for talc HS327.3B which contains about 10% chlorite. The chlorite bands are at slightly different positions, which tend to weaken the band depths. It should be noted that mineral mixtures should not cause a problem unless the other minerals have sharp absorptions in this region. For example, metamorphic calcic amphiboles may contain anthophyllite and/or cummingtonite exsolution/intergrowths, so each will contribute sharp OH overtones (possibly with small offsets). Such a mixture might be difficult to interpret, whether in reflectance or transmittance.

The above example showed the absorptions in a binary case (Mg and Fe), but for more complex situations than simple binary, individual bands become weaker and additional bands appear. In three-component mixtures, 10 bands appear, while in four-component mixtures, 20 bands appear. With the increase in absorption bands, the overlap can sometimes smear the fine structure and produce a single broad band (e.g., Strens, 1974).

The equations in this example can be used for other binary cases besides Mg and Fe. Other cations besides Fe can substitute for Mg and produce OH absorption bands. Slight shifts in the band positions are observed with different cations. For example, equation (5) was tested on synthetic

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**TABLE 5. Comparison of Spectroscopic and Electron Microprobe Analyses**

<table>
<thead>
<tr>
<th>Sample</th>
<th>Reflectancea</th>
<th>Absorption Coefficientb</th>
<th>pfu²</th>
<th>Oxide, wt %</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tremolite HS18</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.008</td>
<td>0.014</td>
</tr>
<tr>
<td>Talc WS659</td>
<td>0.018</td>
<td>0.008</td>
<td>0.003</td>
<td>0.007</td>
</tr>
<tr>
<td>Talc HS21</td>
<td>0.133</td>
<td>0.063</td>
<td>0.017</td>
<td>0.028</td>
</tr>
<tr>
<td>Talc HS327</td>
<td>0.166</td>
<td>0.114</td>
<td>0.049</td>
<td>0.083</td>
</tr>
<tr>
<td>Actinolite HS116</td>
<td>0.231</td>
<td>0.116</td>
<td>0.099</td>
<td>0.164</td>
</tr>
<tr>
<td>Actinolite HS22</td>
<td>0.256</td>
<td>0.220</td>
<td>0.124</td>
<td>0.201</td>
</tr>
</tbody>
</table>

aRatio determined using reflectance spectra.
bRatio determined using absorption coefficient data derived from reflectance data.
²Per formula unit cation numbers.

---

1. Fe/(Fe + Mg) ratios.
2. Cper formula unit cation numbers.
3. *Ratio determined using absorption coefficient data derived from reflectance spectra.*
5. *Per formula unit cation numbers.*
library. These spectra, covering the 0.2- to 3.0-/\(\mu m\) band positions in Figures 10 and 11), will be combined with 2.2- to 2.3-/\(\mu m\) range, to distinguish montmorillonite from muscovite (compare the observed is shown in Figure 11. If the band position occurs at the higher-wavelength end of the range, it is more difficult to distinguish from illite and muscovite.

Montmorillonites

Examination of high-resolution spectra of the 2.2-/\(\mu m\) band in montmorillonites shows that the band position varies from about 2.204 to 2.214 /\(\mu m\). This shift in the OH-stretching frequency has been attributed to interaction with interlayer cation field [e.g., Ryskin, 1974], although this interpretation has been disputed [Farmer, 1974]. Six montmorillonites that have no contamination were measured to examine the band position as a function of composition (Figures 4g and 8c). There is an apparent trend (at least among these samples) that montmorillonite is more difficult to distinguish from muscovite.

Optimum Resolution Function

The design of imaging and field spectrometers should take into consideration the spectral properties of minerals. Imaging spectrometers will return literally millions of spectra in a grid of points on a planetary surface [e.g., Vane and Goetz, 1985]. Because of the large data volumes and intense compute requirements needed to analyze a single spectrum, the number of sampled points in the spectrum must be kept to a minimum. However, at least in some applications, it is desirable to have high enough spectral resolution to conduct mineralogical investigations that might approach what is possible in the laboratory. Calibration of atmospheric absorptions will always be a problem on Earth, but not all planetary surfaces have dense atmospheres.

In accordance with existing and planned imaging spectrometers, the resolution in this study is defined to be equal to the instrument sampling interval. Currently, the band width of most of these instruments is close to the sampling interval. We assume that a minimum of two samples are required per FWHM of a mineral absorption feature to adequately resolve the feature. Then the optimum resolution function that maintains high resolution where minerals have fine structure, while decreasing resolution where minerals do not have fine structure, would accomplish the sampling strategy stated above.

The spectra presented in this study, as well as others measured on the USGS spectrometer, were analyzed for the band position, width, depth, and asymmetry. A representative number of the half widths at half maximum (HWHM) of these absorptions are plotted as a function of band position in Figure 12. The HWHM value gives the representative number of the half widths at half maximum (HWHM) of these absorptions are plotted as a function of band position in Figure 12. The HWHM value gives the optimum resolution function. The curvature of the spline was restricted so that the resolution does not change dramatically from channel to channel.

The narrowest features observed have a FWHM of only 0.0019 /\(\mu m\) in the 1.4-/\(\mu m\) spectral region. The resolving power of the spectrometer is similar for both the 1.4- and 2.2-/\(\mu m\) regions, yet the fine structure observed at 1.4 /\(\mu m\) is near 0.001 /\(\mu m\) (for a required resolving power near 1000), while the finest features near 2.2-2.4 /\(\mu m\) have fine structure of 0.007 /\(\mu m\) (required resolving power of only 328). The fact

Digital Spectral Library: Call for Samples

The spectral data obtained in this study and by other USGS investigators are being installed into a digital spectral library. These spectra, covering the 0.2- to 3.0-/\(\mu m\) (50,000-3300 cm\(^{-1}\)) range, will be combined with 2.2- to 25-/\(\mu m\) (4500-400 cm\(^{-1}\)) data from Salisbury et al. [1987] and 1.3- to 200-/\(\mu m\) (7700-50 cm\(^{-1}\)) data also being measured in the Denver spectroscopy lab to form an unprecedented 0.2- to 200-/\(\mu m\) data set. Further, the resolution is well defined and greater than that for existing and proposed imaging spectrometers, so the library data may be convolved to the exact sampling interval and resolution of those instruments. The mineral samples are being analyzed by X-ray diffraction, X-ray fluorescence, electron microprobe, and atomic absorption for major and trace elements and mineral purity. Our knowledge of spectroscopy is also being used to test for mineral purity.

The authors request that other investigators, who have well-characterized pure mineral samples and are interested in the digital spectral library, contact the authors to discuss the possibility of incorporating data on the samples into the data base.

Mg-Ni t alc transmission spectra [from Farmer, 1974] with excellent results.

Absorption bands in reflectance spectroscopy are sensitive to cation substitution, and the positions and strengths can be used to determine mineral composition. Reflectance spectroscopy has the advantage over transmission methods because there is no sample preparation.

Chemical changes recognized by high-resolution spectroscopy promises to be a useful tool in mapping subtle chemical variations which can be correlated with ore deposits. King and Clark [1989] discuss examples where the Fe:Fe+Mg ratio can be an important indicator in ore deposits. Recognition of the relationships between zones in an ore body can result in a better refinement of targets for exploration.
that bands at 2.2-2.4 μm have less fine structure is supported by infrared studies that show the OH fundamentals are sharper than the metal-OH bending absorption bands [Farmer, 1974, and references therein]. Thus one would expect combination bands involving the bending modes to be broader and have less fine structure. High-resolution data have not yet been obtained in the 2.6- to 3.0-μm region (because of low light levels on the USGS spectrometer), but it is likely that there is another cluster of sharp features in the 2.6- to 3-μm where the OH stretch fundamentals occur.

Spectrometers are typically designed with relatively constant resolution over a wide wavelength range. If one was designed with a resolution of 0.001 μm from 0.3 to 2.5 μm there would be 2200 points per spectrum (if the sampling interval equals the resolution), too much data for imaging spectroscopy instrumentation and available computers to process. However, such a data volume is not overwhelming in a laboratory environment. The regions of the spectrum that require high resolution are quite small. The derived resolution function requires 725 channels to cover 0.2-3.0 μm, or 648 channels to cover 0.3-2.5 μm. For terrestrial studies, the 1.4-μm region is not observable through the atmosphere, so high resolution in that spectral region is not warranted.

Conclusions

This study has shown that (high resolution) reflectance spectroscopy can be a more diagnostic mineralogical identification tool than previously believed. Minerals within solid-solution series and isoschemical end-members can be distinguished from each other. For minerals that have very sharp absorption features, impurities or substitutions might distort the lattice crystal enough to cause observable band shifts. With appropriately designed spectrometers and a digital spectral data base, high-resolution spectra can be used as an analytical tool in the laboratory, in the field, from aircraft, and from space. The resolution required for future imaging spectrometers should be evaluated carefully using this new information.

Acknowledgments.

We dedicate this paper to Norma Vergo, an excellent scientist, who passed away on January 28, 1990. We would like to thank Ardith J. Bartel (USGS) for XRF analysis of many samples and Barbara Lockett and Karen Hester (USGS) for mounting samples for the electron microprobe. We thank the Smithsonian Institution for donating samples and Dave Sherman for assisting with the band assignments. Thanks to Roger Burns and an anonymous reviewer for making suggestions to improve the manuscript. This research is supported by the USGS Development of Assessment Techniques program and by NASA Interagency agreement W15805.

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(Received April 30, 1987; revised October 18, 1989; accepted November 2, 1989.)