Hyperspectral Remote Sensing

UNIT-1

Dr. J. SARAVANAVEL
Assistant Professor
Department of Remote Sensing
Bharathidasan University
Tiurchirappalli, Tamil Nadu
Email : saravanavel@bdu.ac.in

- Since the beginning of time, light was thought to be pure and singular.

- In 1666, Isaac Newton, separate the light into the color spectrum using prism

- For longtime, thought that the light to be a bullet-like particle that traveled in a straight beam

- The scientist like Christian Huygens and Thomas Young prove that the motion of light followed wave patterns (Young, 1804).

-

- At about the same time in the 1800s, William Herschel observed that the different Colors actually varied in temperature. Blues and greens were cooler, while reds were warmer. In fact, he further discovered that the energy present outside the red spectrum was warmer yet, and this region became known as infrared.

- This was the first documented reference that the visible light spectrum was related to frequency and wavelength.

- These discoveries of the interrelations among color, frequency, and wavelength laid the framework for hyperspectral remote sensing because these fundamental principles can be used to characterize the reflection of light against objects.

Definitions

The term "multi" is derived from the Latin word for "many" and "hyper" is the Greek word for "over," "above," or an "exaggerated amount." These, combined with "spectral," which relates to colors, are combined to form "multispectral" and "hyperspectral," which figuratively mean "many colors."

Differs from conventional remote sensing in that it covers many narrowly defined spectral channels, *where as*, conventional remote sensing looks at several broadly defined spectral regions.

Hyperspectral remote sensing is the science of acquiring digital imagery of earth materials in many narrow contiguous spectral bands.

The simultaneous acquisition of images of the same area in many (usually 100 or more), narrow, contiguous, spectralbands. The preferred term is “imaging spectroscopy”.

Hyperspectral sensing (imaging spectrometry) takes remote sensing from the era of "picturing" into the era of "measurement".

Ultraspectral ("beyond hyperspectral") is used to describe datasets containing thousands of bands.

Although no such sensor has been designed with this complexity, it is regarded as the future of imaging spectroscopy.

Photon

A photon is a discrete particle of electromagnetic energy having no mass, no electric charge, and an indefinite life. The existence of photons was first based on the interpretation of experimental results and presented in a scientific paper by Albert Einstein in 1905.

The energy E of any photon is related to its frequency as follows, where h is Planck's constant (6.626068×10^{-34} m^2 kg/s) and υ is the frequency:

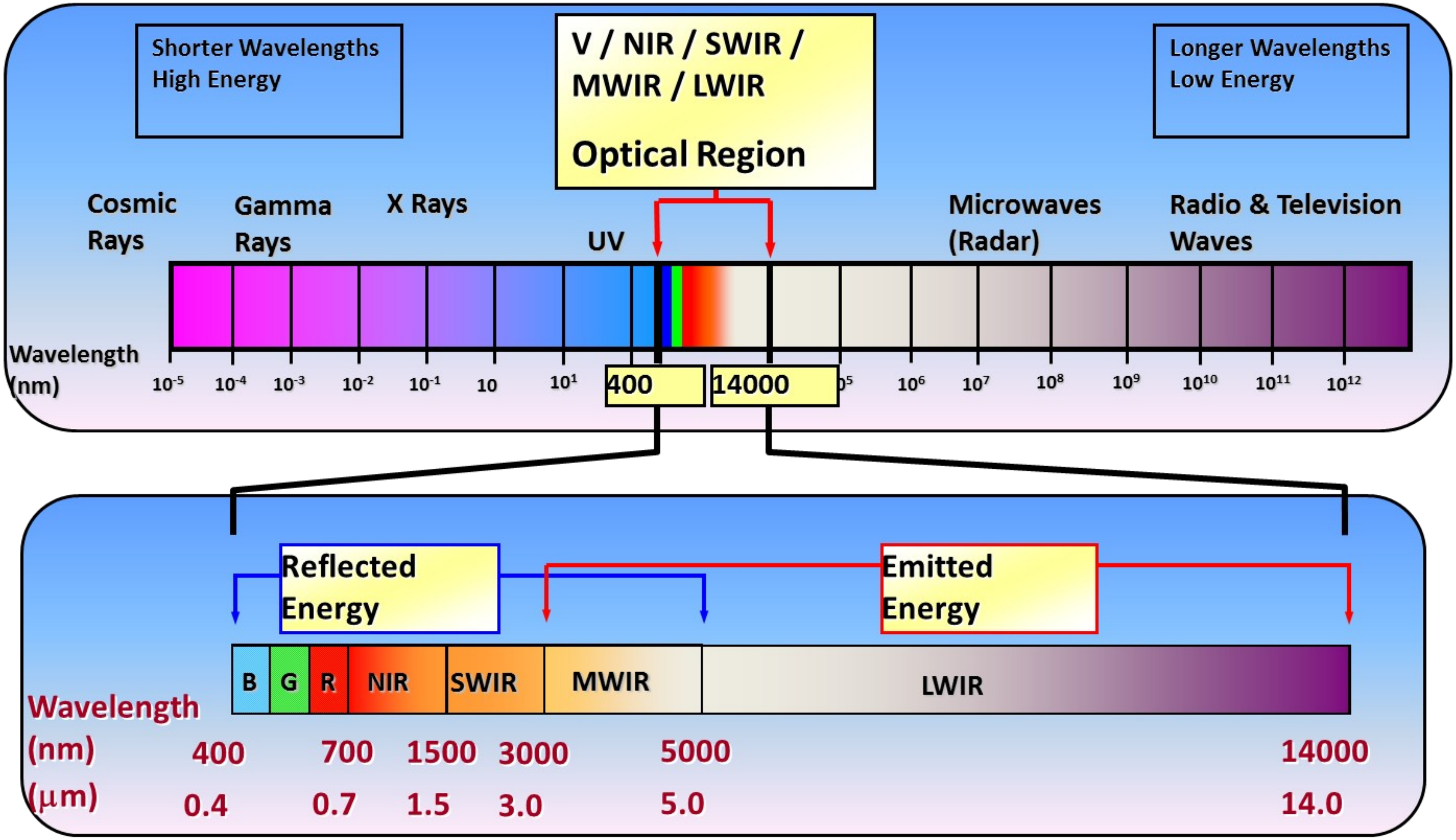
$$E = h\upsilon$$

Speed of light is 'c' and is related to the frequency 'v' and the wavelength 'λ' in any part of the electromagnetic spectrum

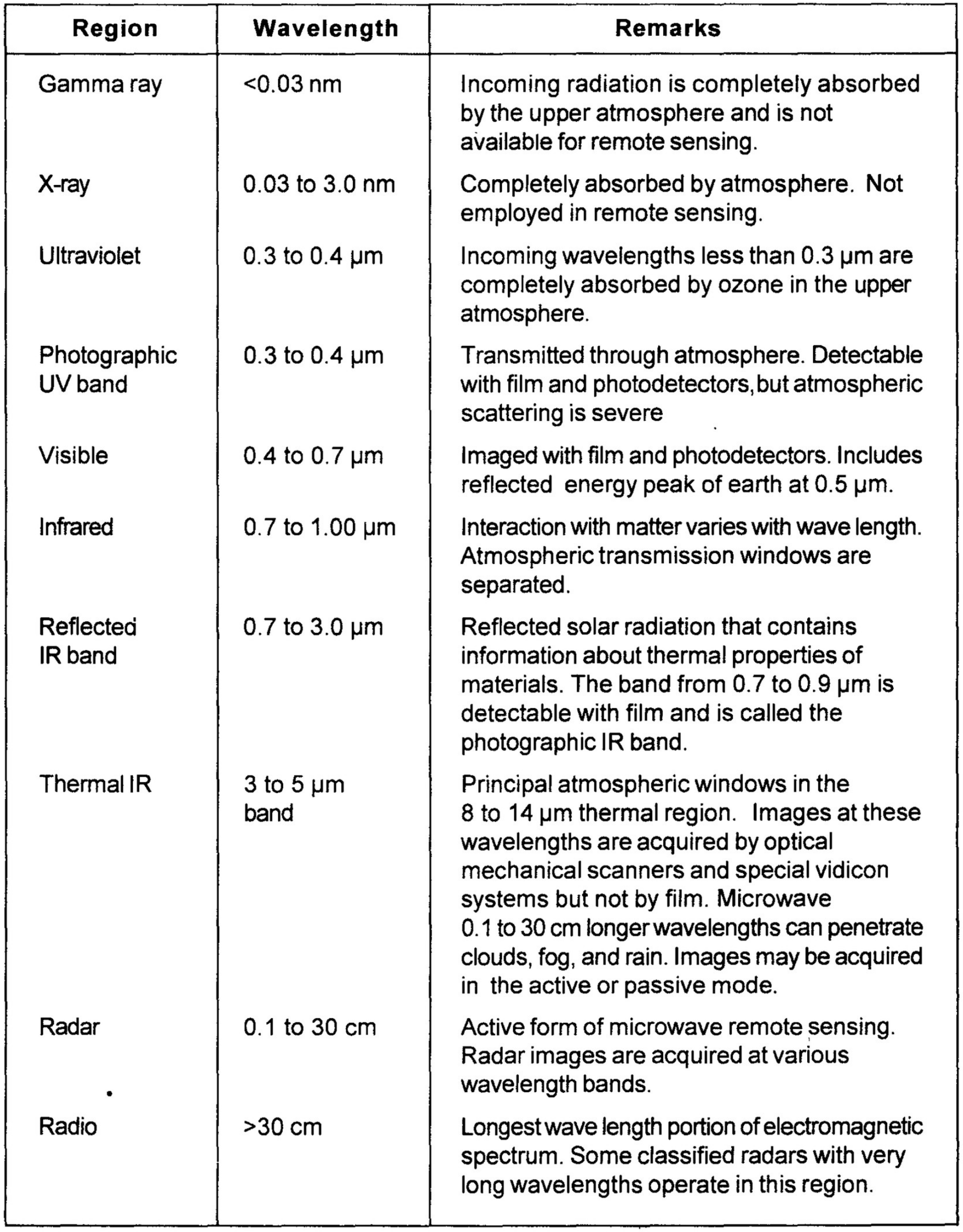
$$c = \nu\lambda$$

Electromagnetic Spectrum

Each photon of the electromagnetic spectrum has a wavelength determined by its energy level. Light and other forms of electromagnetic radiation commonly are described in terms of their wavelengths.



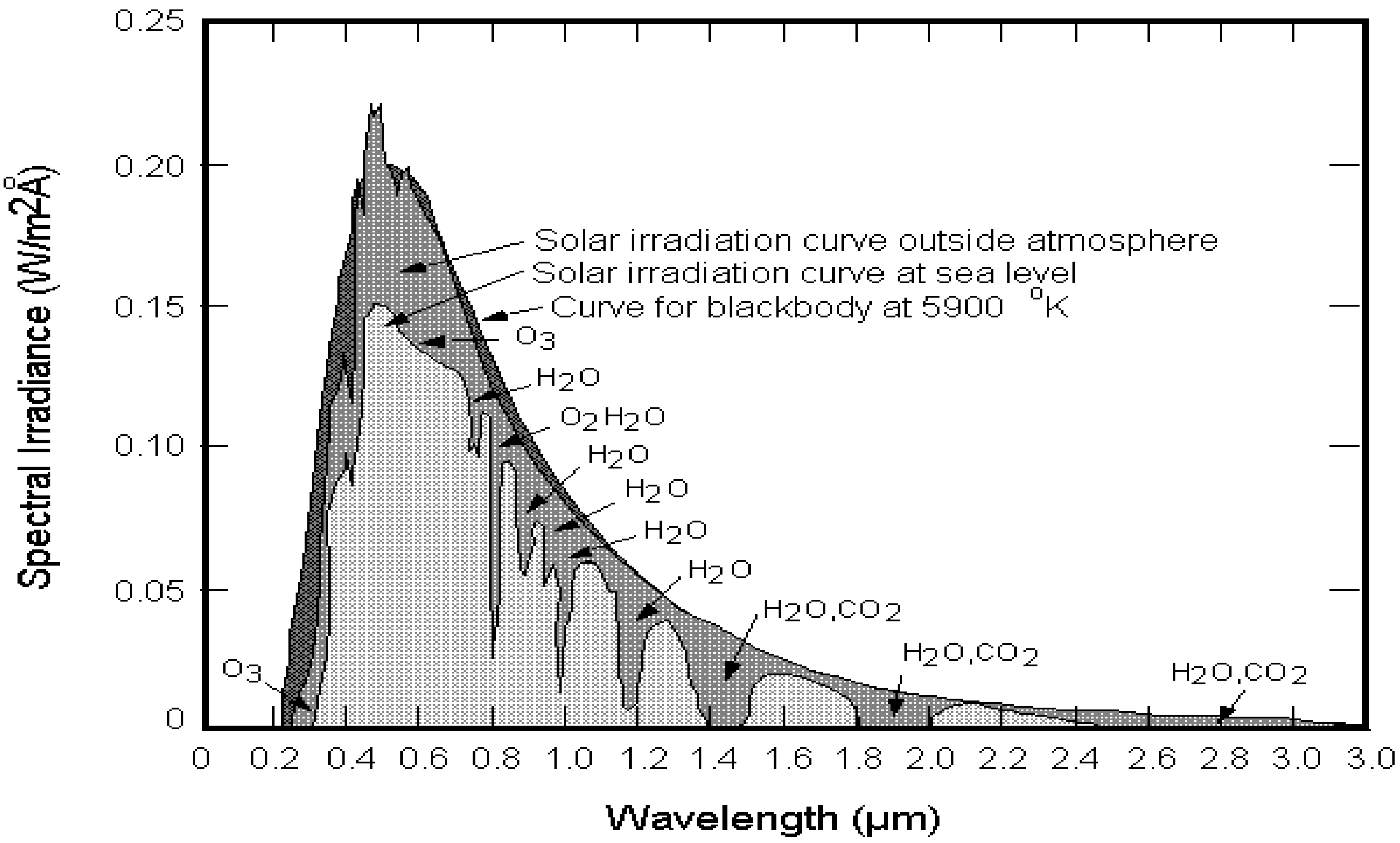
Electromagnetic spectral regions (Sabines, 1987)



Region	Wavelength	Remarks
Gamma ray	<0.03 nm	Incoming radiation is completely absorbed by the upper atmosphere and is not available for remote sensing.
X-ray	0.03 to 3.0 nm	Completely absorbed by atmosphere. Not employed in remote sensing.
Ultraviolet	0.3 to 0.4 μm	Incoming wavelengths less than 0.3 μm are completely absorbed by ozone in the upper atmosphere.
Photographic UV band	0.3 to 0.4 μm	Transmitted through atmosphere. Detectable with film and photodetectors, but atmospheric scattering is severe
Visible	0.4 to 0.7 μm	Imaged with film and photodetectors. Includes reflected energy peak of earth at 0.5 μm.
Infrared	0.7 to 1.00 μm	Interaction with matter varies with wave length. Atmospheric transmission windows are separated.
Reflected IR band	0.7 to 3.0 μm	Reflected solar radiation that contains information about thermal properties of materials. The band from 0.7 to 0.9 μm is detectable with film and is called the photographic IR band.
Thermal IR	3 to 5 μm band	Principal atmospheric windows in the 8 to 14 μm thermal region. Images at these wavelengths are acquired by optical mechanical scanners and special vidicon systems but not by film. Microwave 0.1 to 30 cm longer wavelengths can penetrate clouds, fog, and rain. Images may be acquired in the active or passive mode.
Radar	0.1 to 30 cm	Active form of microwave remote sensing. Radar images are acquired at various wavelength bands.
Radio	>30 cm	Longest wave length portion of electromagnetic spectrum. Some classified radars with very long wavelengths operate in this region.

Electromagnetic Energy

Atmospheric Absorption



Atmospheric Transmittance: Windows for Remote Sensing

Any effort to measure the spectral properties of a material through a planetary atmosphere, must consider where the atmosphere absorbs.

The drop toward the ultraviolet is due to scattering and strong ozone absorption at wavelengths short of 0.35 µm. Ozone also displays an absorption at 9.6 µm. Oxygen absorbs at 0.76 µm in a narrow feature. CO2 absorbs at 2.01, 2.06, and a weak doublet near 1.6 µm. Water causes most of the rest of the absorption throughout the spectrum

However, these spectral regions can be used in the laboratory where the atmospheric path lengths are thousands of times smaller, or when measuring spectra of other planets from orbiting spacecraft

Table 4.1 Principal Molecular Absorption Lines in the Earth Atmosphere

Wavelength (μm)	Molecule	Wavelength (μm)	Molecule
0.26	O_3	3.9	N_2O
0.60	O_3	4.3	CO_2
0.69	O_2	4.5	N_2O
0.72	H_2O	4.8	O_3
0.76	O_2	4.9	CO_2
0.82	H_2O	6.0	H_2O
0.93	H_2O	6.6	H_2O
1.12	H_2O	7.7	N_2O
1.25	O_2	7.7	CH_4
1.37	H_2O	9.4	CO_2
1.85	H_2O	9.6	O3
1.95	CO_2	10.4	CO_2
2.0	CO_2	13.7	O_3
2.1	CO_2	14.3	O_3
2.6	H_2O	15	CO_2
2.7	CO_2		

Source: Rees, W.G., *Physical Principles of Remote Sensing*, 2nd ed., Cambridge University Press, 2001. With permission.

Emission and Reflection

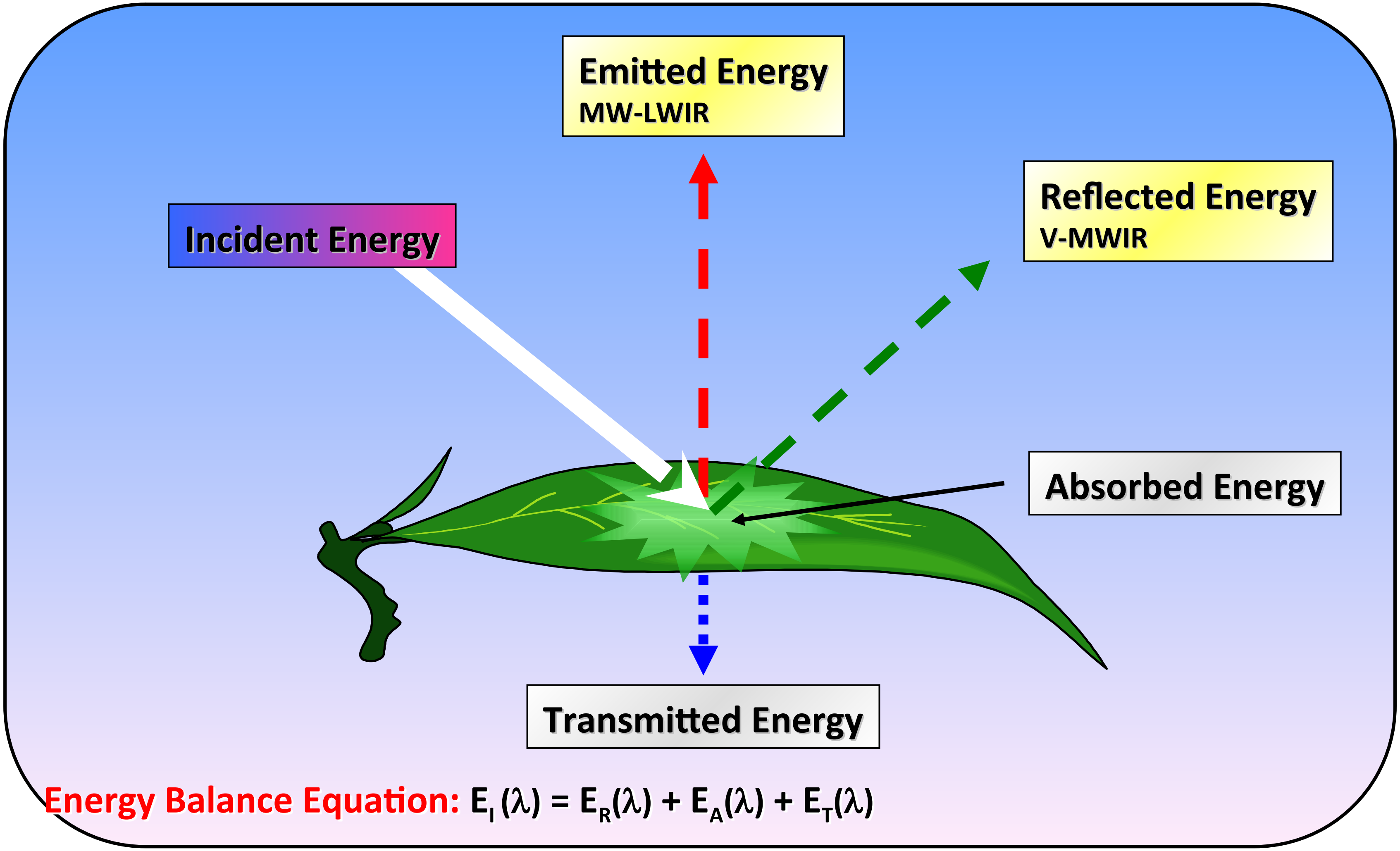
Photons can be absorbed, reflected, or transmitted. In the realm of thermodynamics, radiated heat creates photons.

Radiation heat transfer is the exchange of thermal radiation energy between two or more bodies. Thermal radiation is defined as electromagnetic radiation in the wavelength range of 0.1 to 100 microns.

Radiation heat transfer must account for both incoming and outgoing thermal radiation and can be expressed as:

$$1 = \varepsilon_{\text{reflected}} + \varepsilon_{\text{absorbed}} + \varepsilon_{\text{transmitted}}$$

Interaction of energy and objects



Energy Balance Equation: $E_I(\lambda) = E_R(\lambda) + E_A(\lambda) + E_T(\lambda)$

Because most solid bodies are opaque to thermal radiation, transmission can be ignored.

$$1 = \varepsilon_{\text{reflected}} + \varepsilon_{\text{absorbed}}$$

To account for emissive radiation, a comparison is made to a perfect blackbody, which is a theoretical object that absorbs 100% of the incident radiation, reflects none, and appears perfectly black.

The ratio of the actual emissive radiation *E* to the emissive power of a blackbody is defined as the surface emissivity ε.

$$\varepsilon = E/E_{\text{blackbody}}$$

Reflectance is the percentage of incident light that is reflected by a material.

Reflectance is the ratio of reflected energy to incident energy.

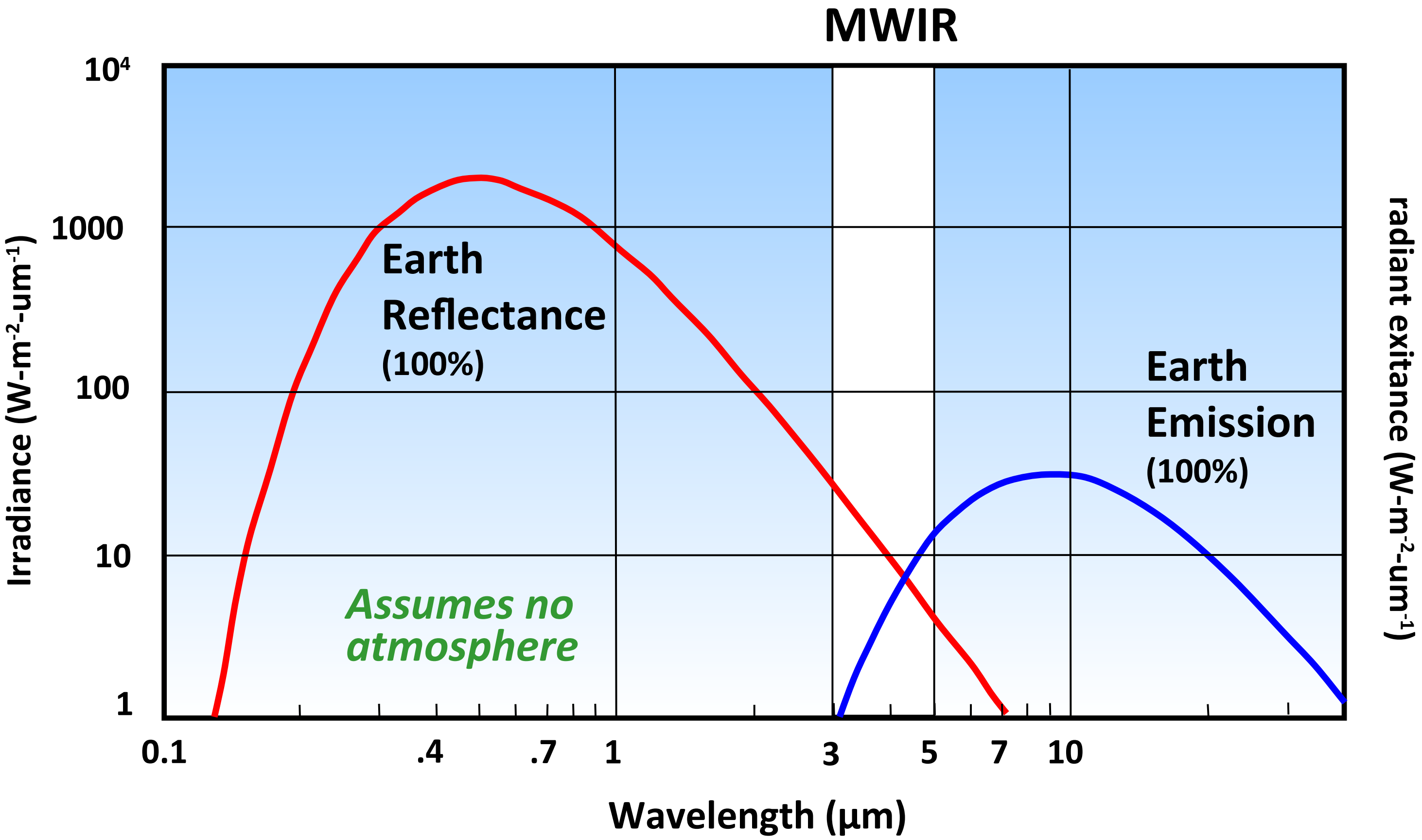
- *Varies with wavelength*
- *Function of the molecular properties of the material*

In climatology and remote sensing, reflectivity is commonly referred to as "albedo," the Latin term for white

Reflectivity R can be expressed as:

$$R = 1 - \varepsilon$$

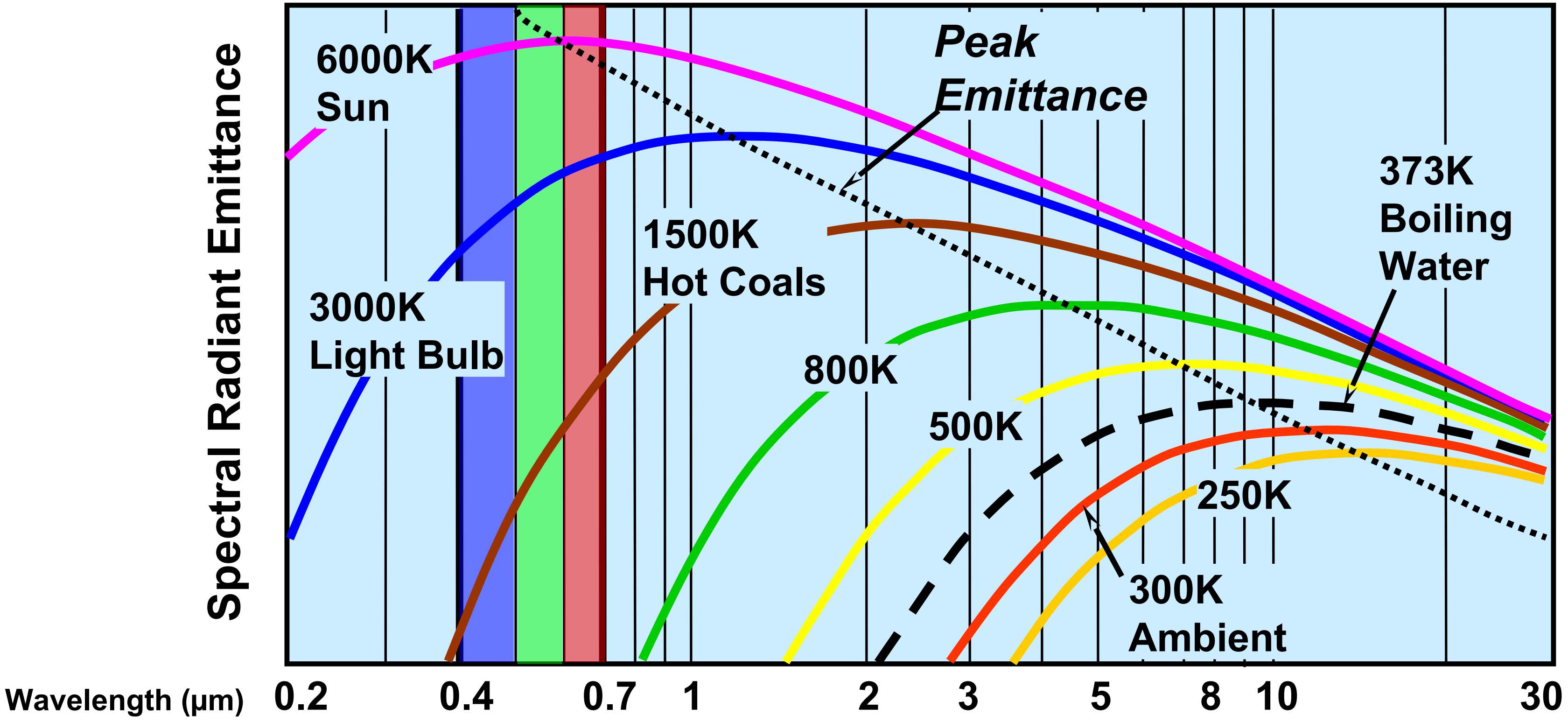
Reflected vs. Emitted Energy



Emissive Energy

Basic Concepts

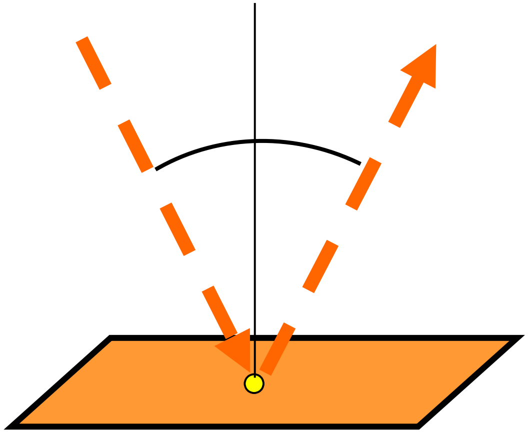
- Blackbody – A theoretical material that absorbs and radiates 100% of the energy incident upon it. BB curve is a function of temperature and wavelength.
- Planck's Law – gives shape of blackbody curve at a specific temperature.
- Wien's Displacement Law – determines wavelength of peak emittance.



Reflected Energy

- The manner in which a material reflects energy is primarily a function of the optical properties and surface roughness of the feature.
- Most objects are diffuse reflectors

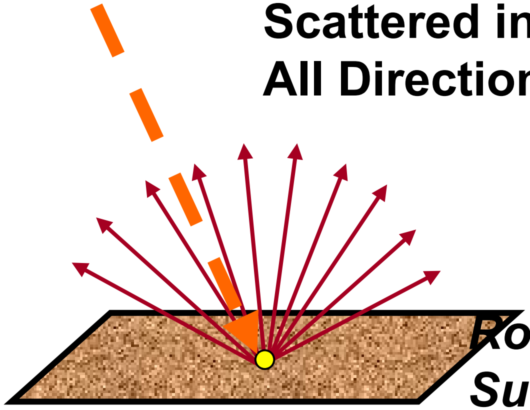
Angle of Incidence = Angle of Reflectance



Smooth Surface

Specular Reflectance

Energy Scattered in All Directions



Rough Surface (Microscopic)

Diffuse Reflectance

Emissivity and reflectivity are two of the fundamental physics principles that govern hyperpsectral remote sensing.

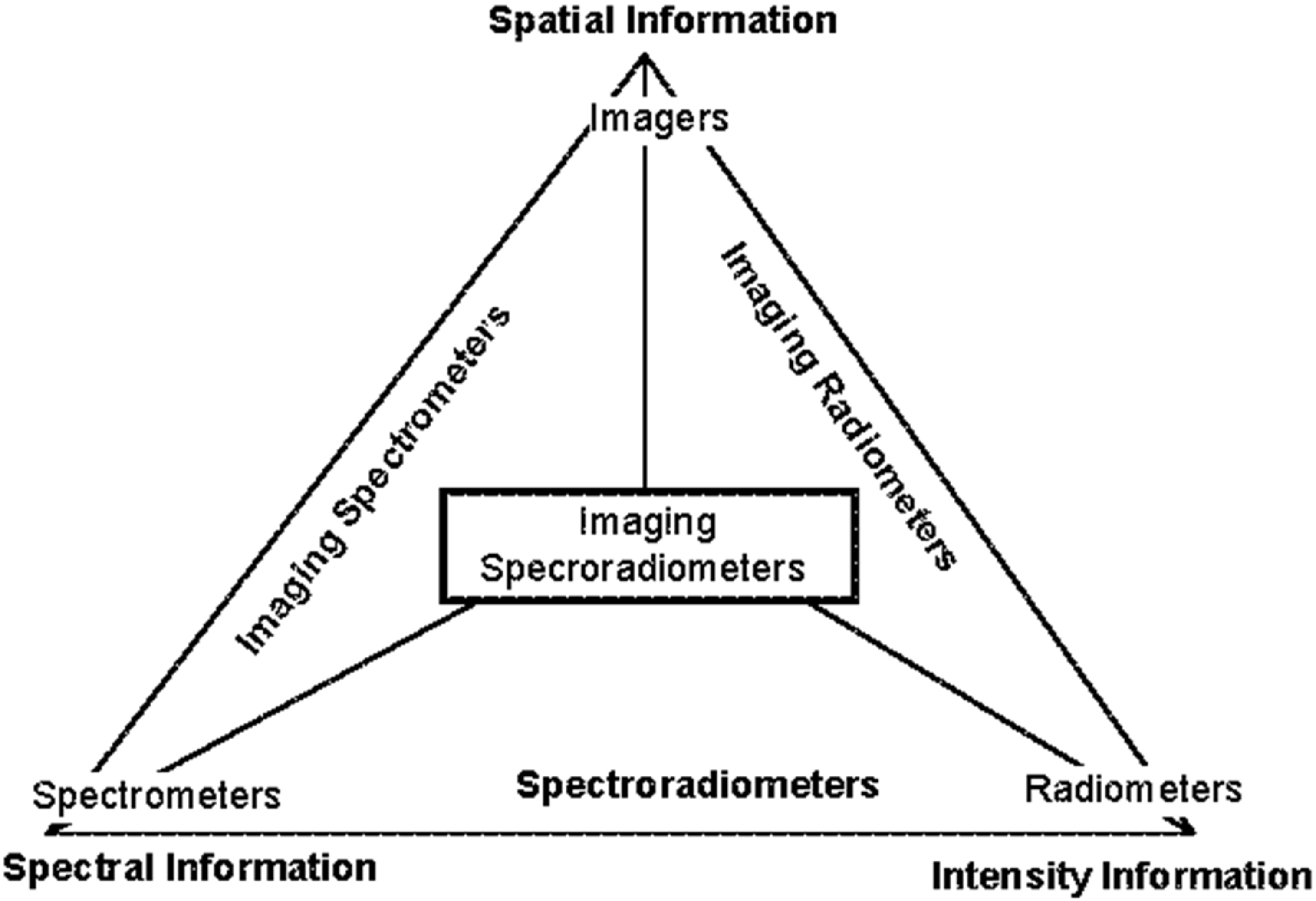
The portion of the electromagnetic spectrum sought for exploitation from a hyperspectral sensor—visible, near infrared, shortwave infrared, midwave infrared, or longwave infrared

Principles of Spectral Radiometry

Radiometry is the physical measurement of electromagnetic radiation within the ultraviolet, visible, and infrared wavelengths.

A radiometer is a device used to measure the radiant flux or power in electromagnetic radiation.

The most important characteristics of a radiometer are spectral range (wavelengths measured), spectral sensitivity (sensitivity vs. wavelengths measured), field of view (18 degrees or limited to a certain narrow field), and directional response



Spatial Information

Imagers

Imaging Spectrometers

Imaging Radiometers

Imaging
Specroradiometers

Spectrometers

Spectroradiometers

Radiometers

Spectral Information

Intensity Information

Radiance, Irradiance, and Flux

Radiance and spectral radiance are radiometric measures that describe the amount of light that passes through or is emitted from a particular area and falls within a given solid angle in a specified direction

These measures are used to characterize both emission from diffuse sources and reflection from diffuse surfaces. The SI unit of radiance is watts per steradian per square meter ($W \cdot sr^{-1} \cdot m^{-2}$).

Radiance characterizes total emission or reflection, while spectral radiance characterizes the light at a single wavelength or frequency.

The radiance is equal to the sum (or integral) of all the spectral radiances from a surface.

The SI units for spectral radiance are W·sr–1·m–3 when measured per unit wavelength, and $W \cdot sr^{-1} \cdot m^{-2} \cdot Hz^{-1}$ when measured per unit frequency interval.

Radiance is useful because it indicates how much of the power emitted by an emitting or reflecting surface will be received by an optical system looking at the surface from some angle of view

“Irradiance,” “radiant emittance,” and “radiant existence” are radiometry terms for the power of electromagnetic radiation at a surface per unit area.

The term “irradiance” is used when the electromagnetic radiation is incident on the surface.

The SI units for all of these quantities are watts per square meter (W/m2). These quantities are sometimes called “intensity,”

All of these quantities characterize the total amount of radiation present, at all frequencies. Each frequency is also commonly considered in the spectrum separately.

When this is done for a radiation incident on a surface, it is called “spectral irradiance” and has SI units W/m3, or Commonly $\mathrm{W \cdot m^{-2} \cdot nm^{-1}}$.

Radiant flux or radiant power is the measure of the total power of electromagnetic radiation (including visible light). The power can be the total emitted from a source or the total landing on a particular surface.

Radiance vs. Reflectance

Radiance is the variable directly measured by remote sensing instruments.

Radiance is the amount of light the instrument detects from the object being observed.

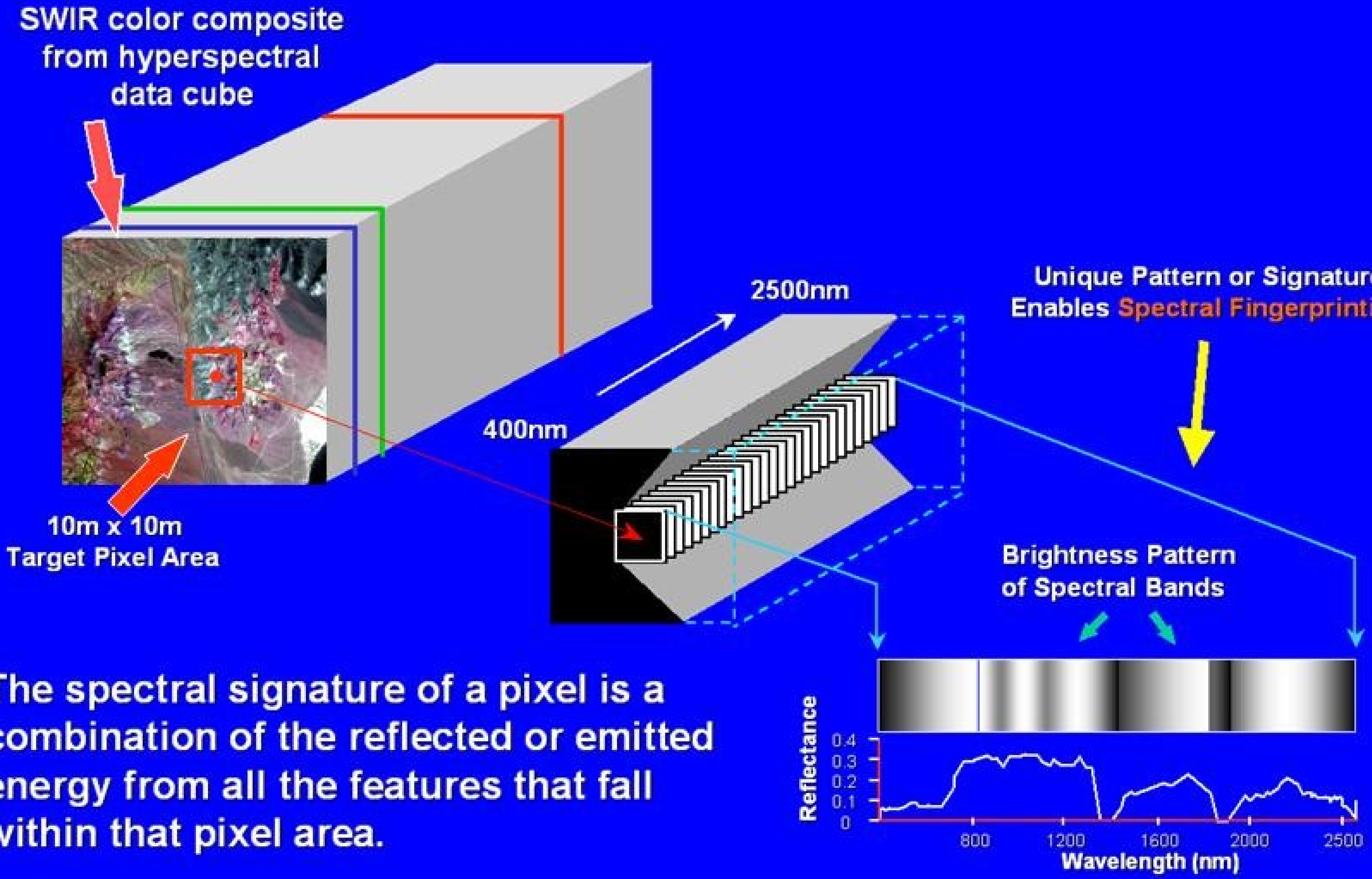
When looking through an atmosphere, some light scattered by the atmosphere will be seen by the instrument and included in the observed radiance of the target.

An atmosphere will also absorb light, which will decrease the observed radiance.

Reflectance is the ratio of the amount of light leaving a target to the amount of light striking the target. If all of the light leaving the target is intercepted for the measurement of reflectance, the result is called "hemispherical reflectance."

Radiance, on the other hand, depends on the illumination (both its intensity and direction), the orientation and position of the target, and the path of the light through the atmosphere.

Spectral Signature Development



SWIR color composite from hyperspectral data cube

10m x 10m Target Pixel Area

2500nm

400nm

Unique Pattern or Signature Enables Spectral Fingerprinting

Brightness Pattern of Spectral Bands

The spectral signature of a pixel is a combination of the reflected or emitted energy from all the features that fall within that pixel area.

NASA AVIRIS Cuprite, NV, HSI Data, (1995)

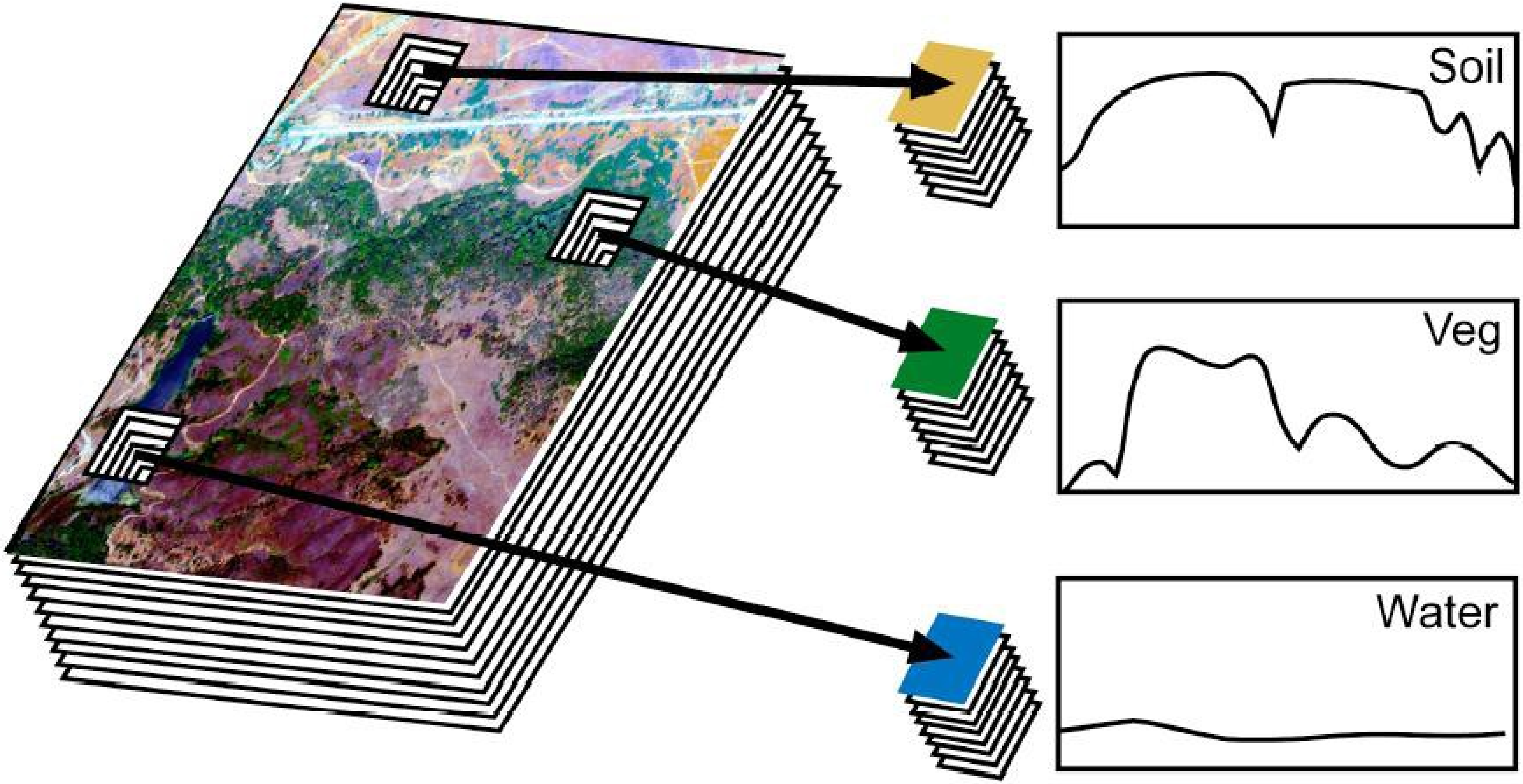
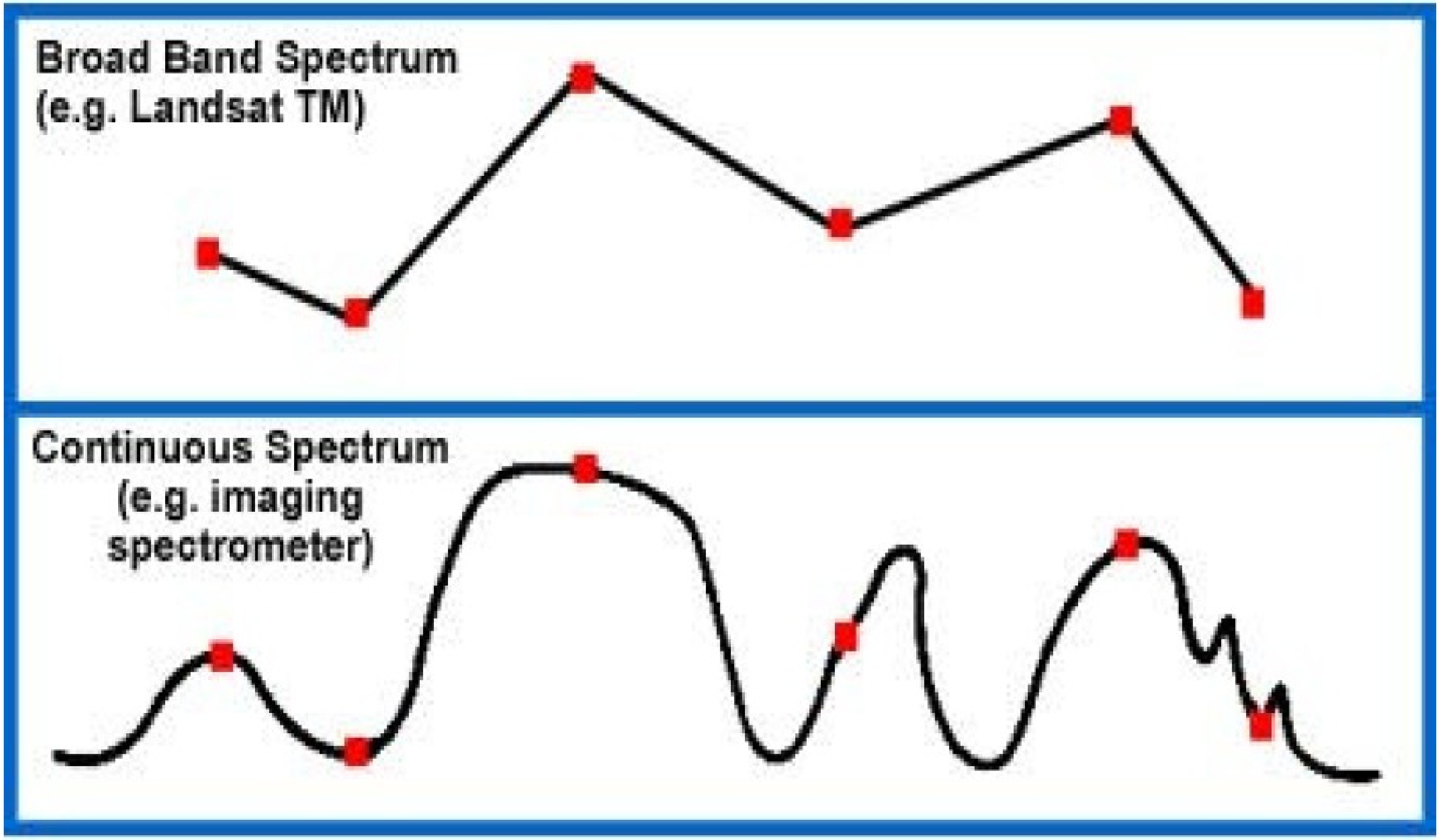
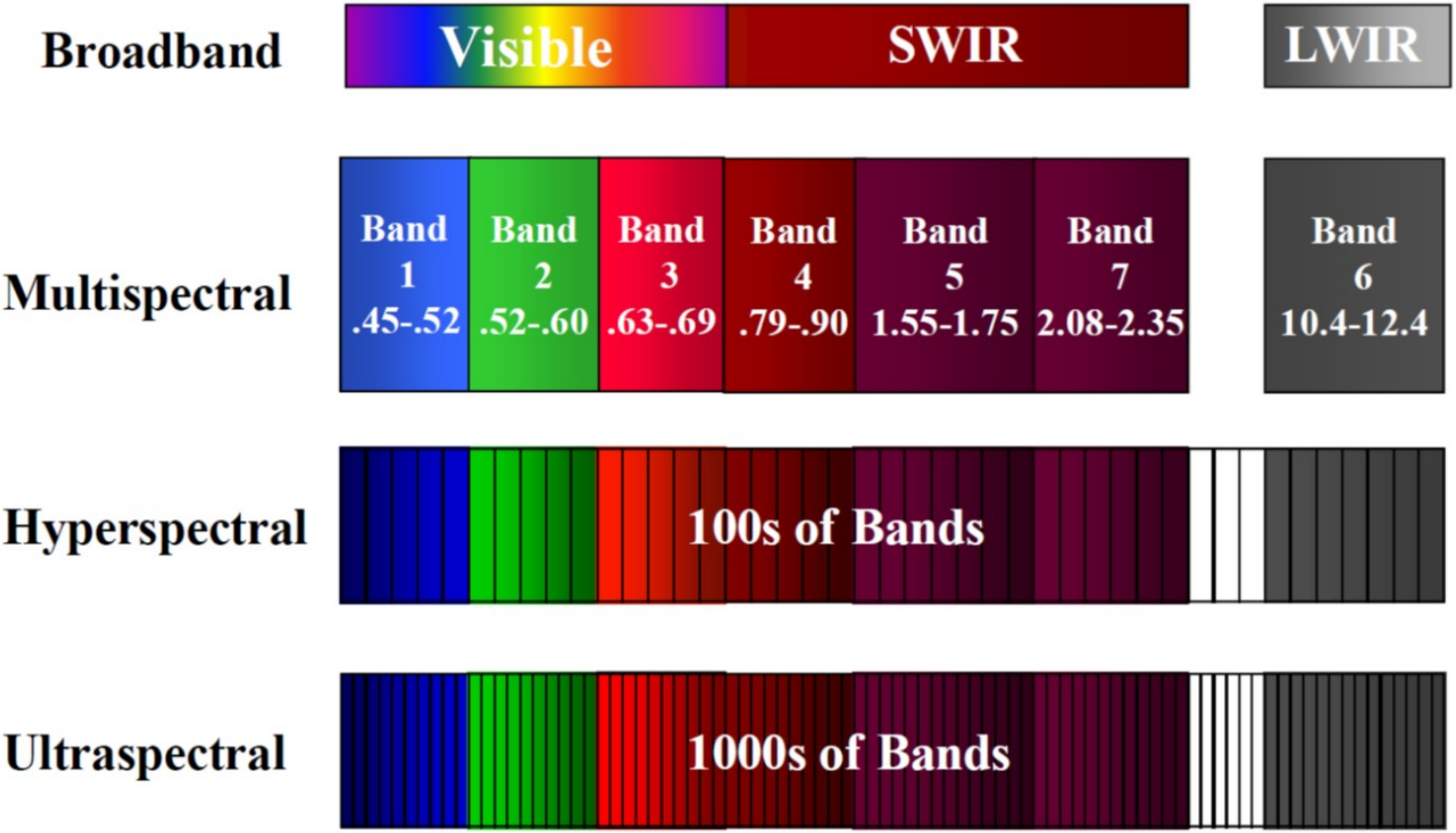


Figure 3. The concept of hyperspectral imagery. Image measurements are made at many narrow contiguous wavelength bands, resulting in a complete spectrum for each pixel.

Spectral comparison between hyperspectral and broad-band data



Multi Spectral vs Hyperspectral



Broadband

Visible

SWIR

LWIR

Multispectral

Band 1 .45-.52

Band 2 .52-.60

Band 3 .63-.69

Band 4 .79-.90

Band 5 1.55-1.75

Band 7 2.08-2.35

Band 6 10.4-12.4

Hyperspectral

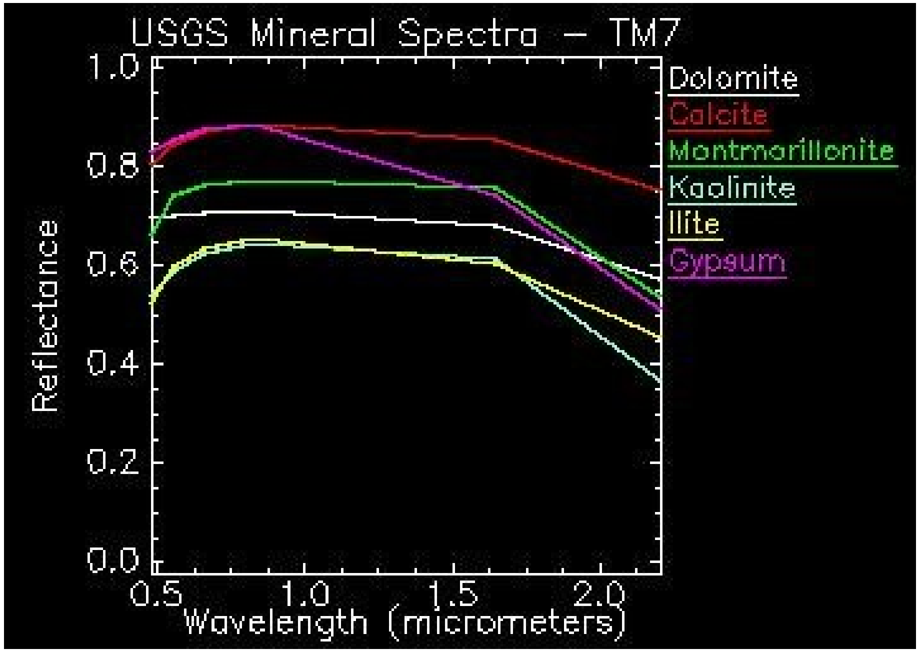
100s of Bands

Ultraspectral

1000s of Bands

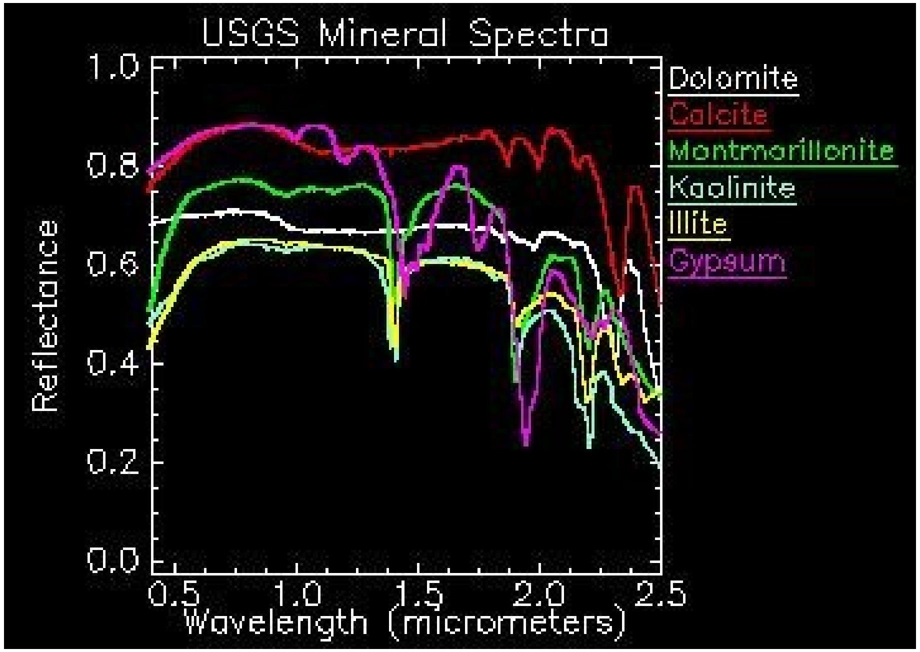
Multispectral - Hyperspectral Signature Comparison

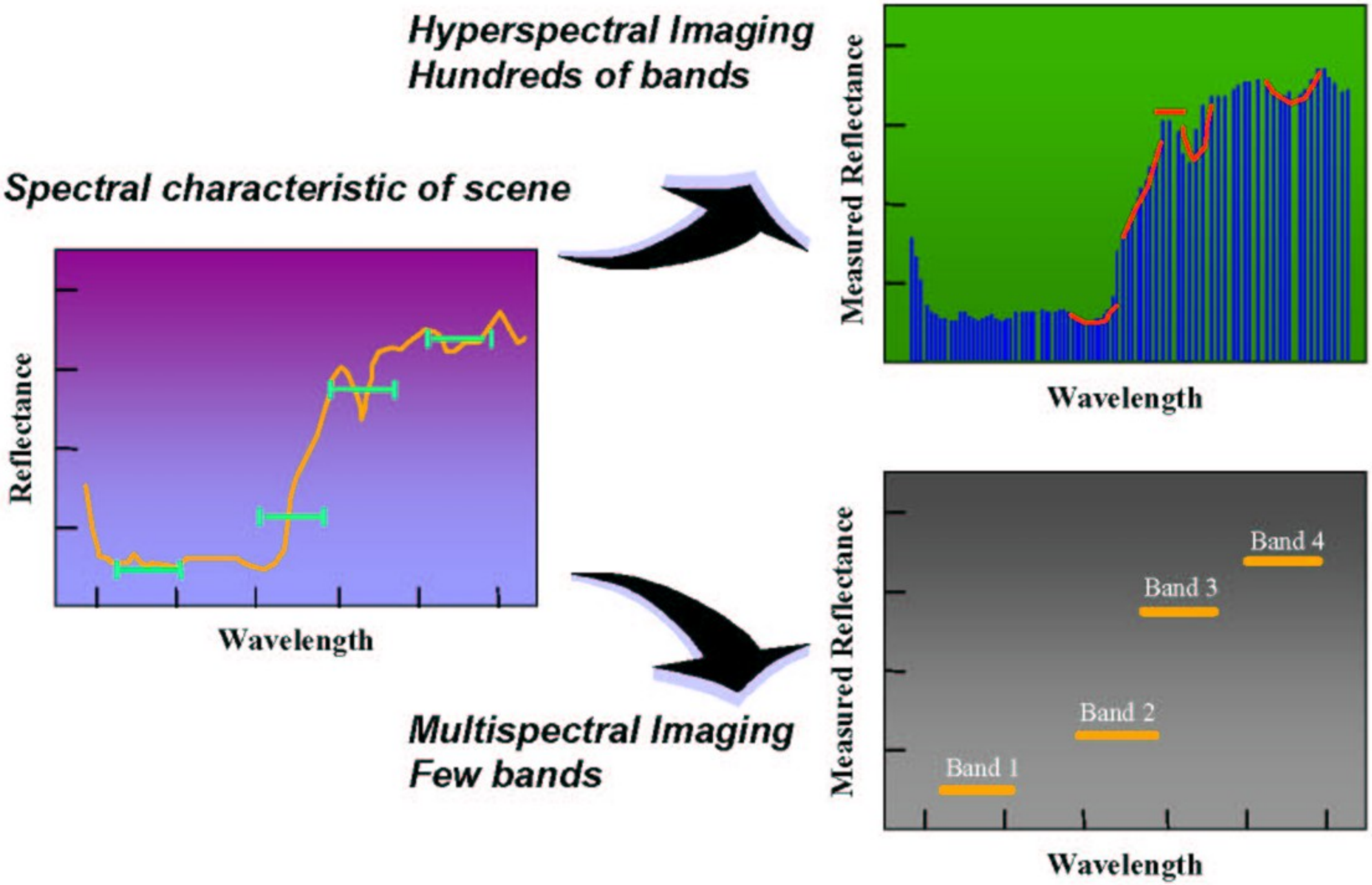
Multispectral



Resampled to Landsat TM7 Bands

Hyperspectral





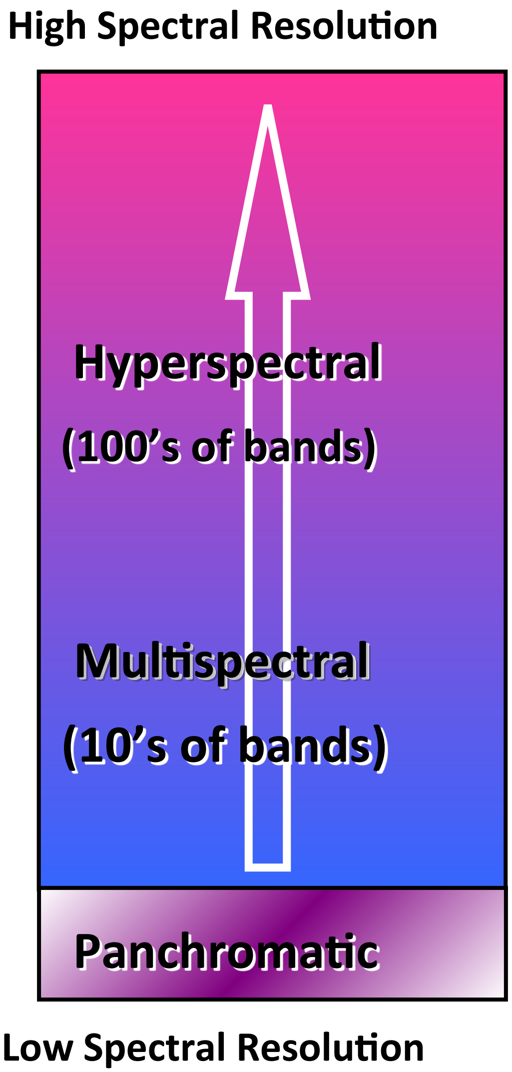
Spectral characteristic of scene

Hyperspectral Imaging
Hundreds of bands

Multispectral Imaging
Few bands

Levels of Spectral Information

Multi Spectral vs Hyperspectral



High Spectral Resolution

Hyperspectral

(100's of bands)

Multispectral

(10's of bands)

Panchromatic

Low Spectral Resolution

Quantification: Determines the abundance of materials.

Characterization: Determines variability of identified material (e.g. wet/dry sand, soil particle size effects).

Identification: Determines the unique identity of the foregoing generic categories (i.e. material identification).

Discrimination: Determines generic categories of the foregoing classes.

Classification: Separates materials into spectrally similar groups.

Detection: Determines the presence of materials, objects, activities, or events.

Multispectral vs. hyperspectral remote sensing

Multispectral	**Hyperspectral**
separated spectral bands	no spectral gaps
wider bandwidths	narrow bandwidths (10nm)
coarse representation of the spectral signature	complete representation of the spectral signature
not able to discern small differences between reflectance spectra	ability to detect subtle spectral features
smaller data volumes	large data volumes
fewer problems with calibration	radiometric and spectral calibration are time-consuming
multi-decadal history of continuous image acquisition	currently no functioning sensors in orbit

Limitations and Issues of Hyperspectral Data

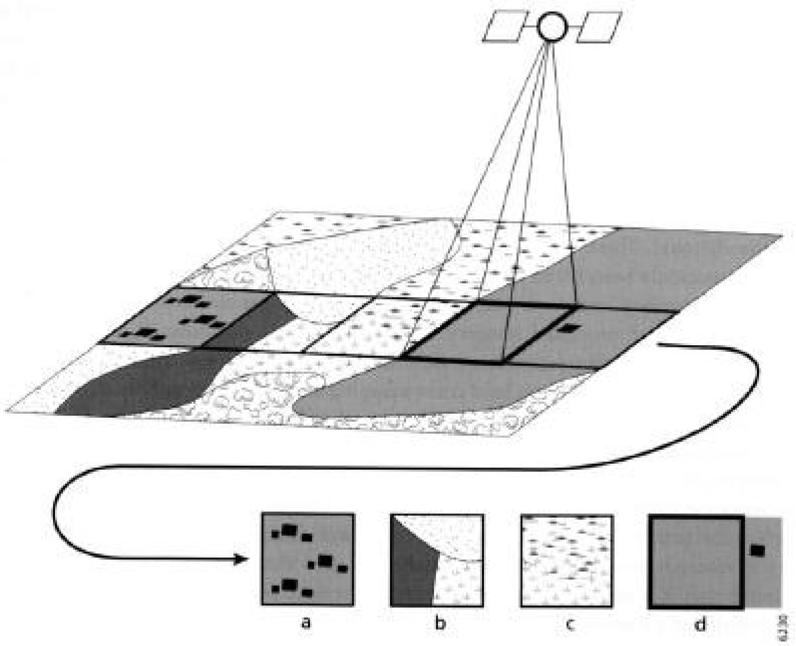
Very sensitive to noise

Difficult to interpret the spectral signatures of an “impure” pixel

It need for calibration

- Because of the high spectral resolution of hyperspectral imaging, fine atmospheric absorption features will be detected, which may be confused with the ground material being imaged

Mixed Pixel Problem



- **Presence of small or sub pixel targets**
- **Presence of boundaries of discrete parcels**
- **Gradual transition between land cover classes**
- **Contribution of areas outside the area represented by a pixel**

The spectral reflectance of a mixed pixel is generally the weighted average of the spectral response of the classes within it

Data volume

- storage and transmission of hyperspectral data are one of the issues (AVIRIS=40*TM)

Redundancy

- overlap of information content over several bands (not all data is needed to characterize a pixel properly)

Hyperspectral data characteristics

- Hyperspectral datasets generally contain at least 16 contiguous bands of high spectral resolution over a region of the electromagnetic spectrum.

- Advancements in solid-state technology in recent years have made possible collection of multispectral data in as many as 200 or more (~288) spectral bands.

- Most are able to collect images starting at about 400 nm which is the edge of the blue visible part of the spectrum.

Typically these systems can measure energy to 1100 or even 2500 nm.

Hyperspectral sensors or imaging spectrometers measure earth materials and produce complete spectral signatures with no wavelength omissions.

Such instruments are flown aboard space and air-based platforms.

To understand the Hyper spectral Remote Sensing, it is necessary to have a basic knowledge of spectroscopy in the 0.4 to 2.5µm region covered by the sensors.

Spectroscopy is the study of light as a function of wavelength that has been emitted, reflected or scattered from a solid, liquid, or gas

Absorption and Scattering. As photons enter a mineral, some are reflected from grain surfaces, some pass through the grain, and some are absorbed.

Those photons that are reflected from grain surfaces or refracted through a particle are said to be scattered. Scattered photons may encounter another grain or be scattered away from the surface so they may be detected and measured.

Photons may also originate from a surface, a process called emission. All natural surfaces emit photons when they are above absolute zero

Photons are absorbed in minerals by several processes. The variety of absorption processes and their wavelength dependence allows us to derive information about the chemistry of a mineral from its reflected or emitted light.

The human eye is a crude reflectance spectrometer: we can look at a surface and see color. Our eyes and brain are processing the wavelength-dependent scattering of visible-light photons to reveal something about what we are observing, like the red color of hematite or the green color of olivine.

A modern spectrometer, however, can measure finer details over a broader wavelength range and with greater precision. Thus, a spectrometer can measure absorptions due to more processes than can be seen with the eye.

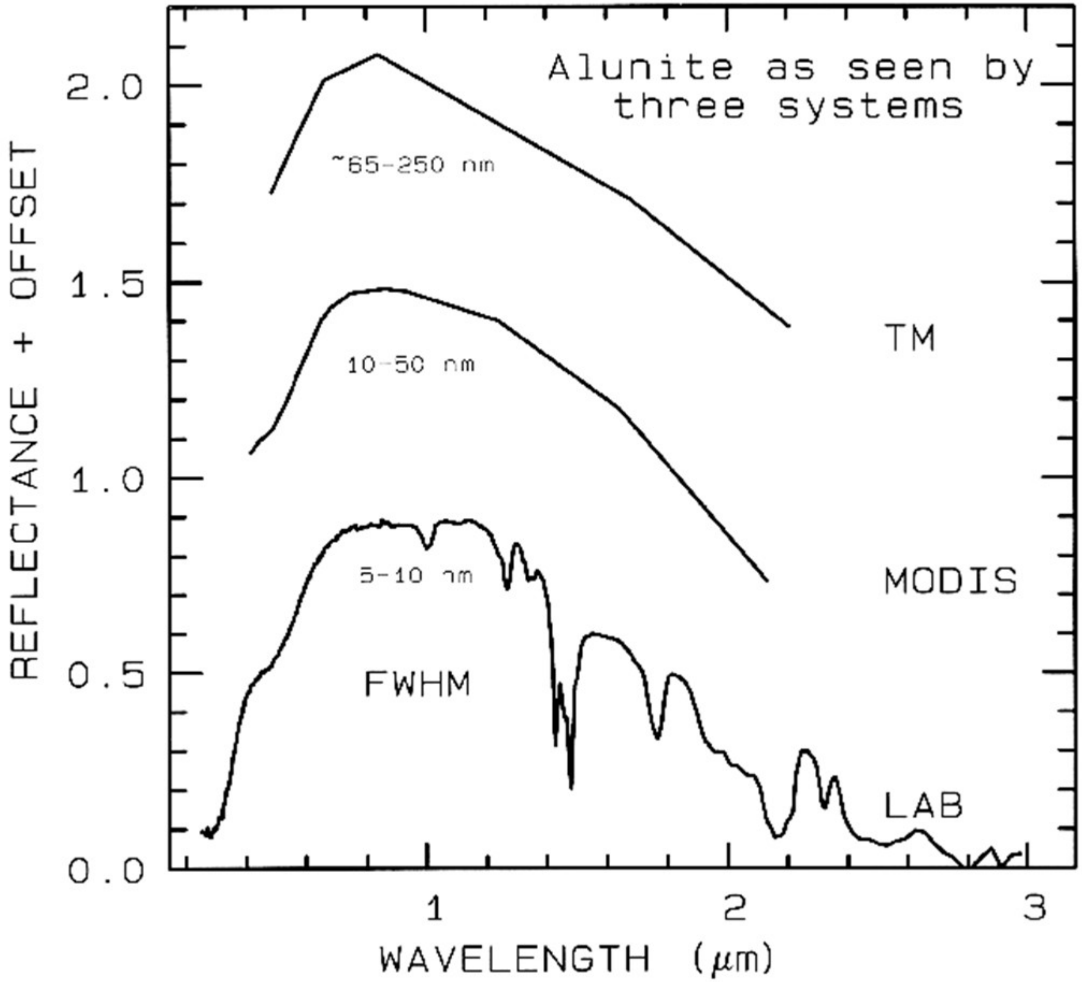
Spectroscopy Terms There are 4 general parameters that describe the capability of a spectrometer:

1) spectral range,
2) spectral bandwidth,
3) spectral sampling, and
4) signal-to-noise ratio (S/N).

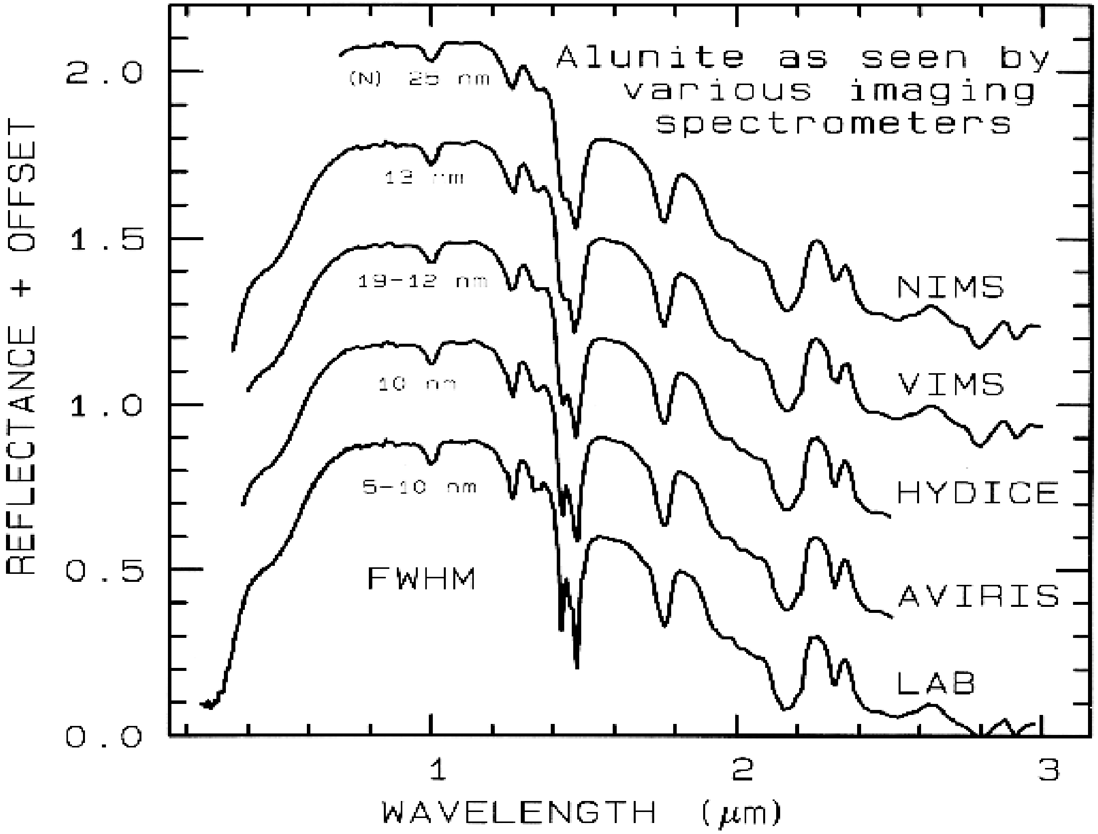
There are general **spectral ranges** that are in common use, each to first order controlled by detector technology: a) ultraviolet (UV): 0.001 to 0.4 μm, b) visible: 0.4 to 0.7 μm, c) near-infrared (NIR): 0.7 to 3.0 μm, d) the mid-infrared (MIR): 3.0 to 30 μm, and d) the far infrared (FIR): 30 μm to 1 mm

Spectral bandwidth is the width of an individual spectral channel in the spectrometer. The narrower the spectral bandwidth, the narrower the absorption feature the spectrometer will accurately measure, if enough adjacent spectral samples are obtained

Some systems have a few broad channels, not contiguously spaced and, thus, are not considered spectrometers. Examples include the Landsat Thematic Mapper (TM) system and the MODerate Resolution Imaging Spectroradiometer (MODIS), which can't resolve narrow absorption features



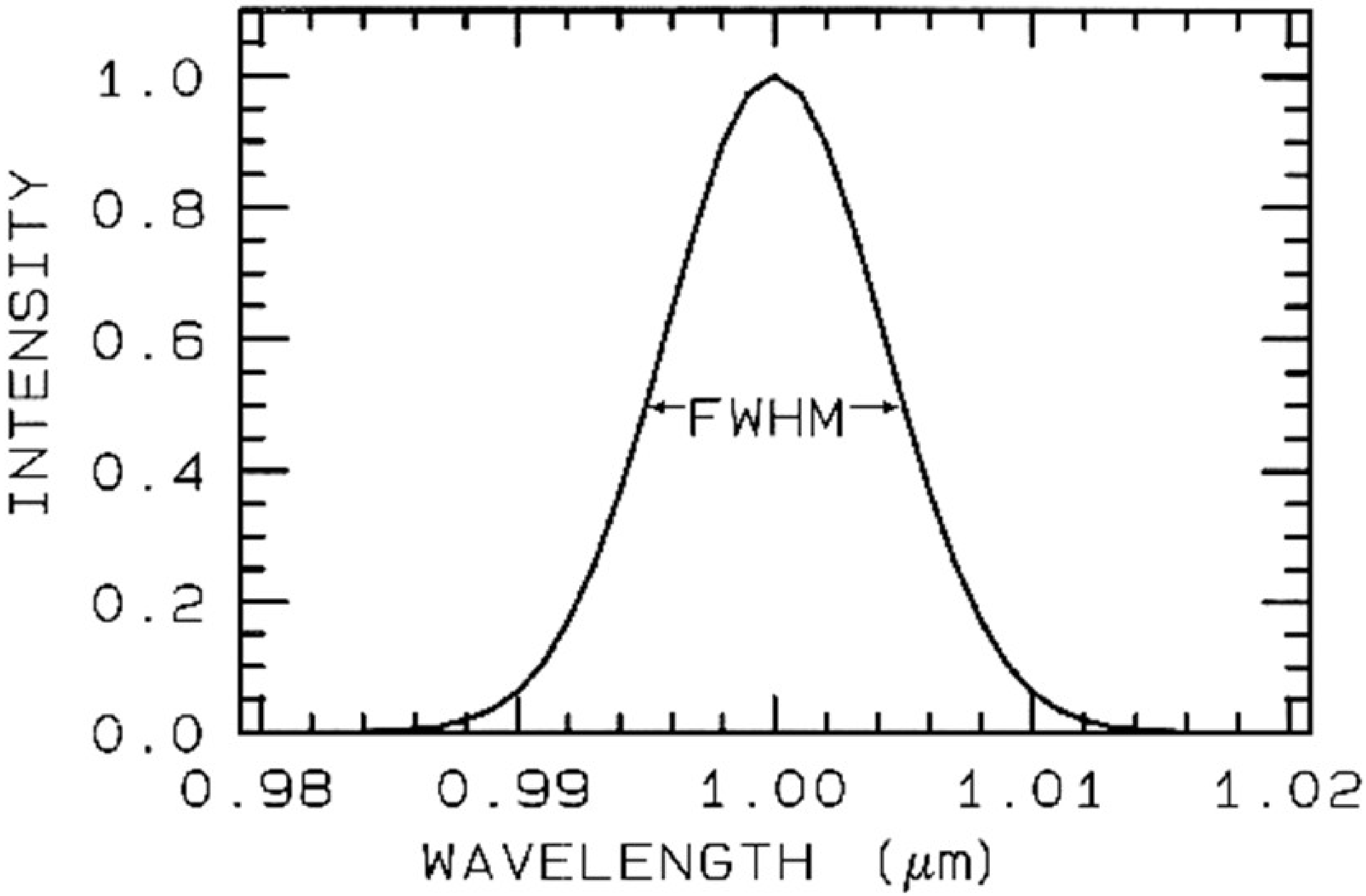
Like the NASA JPL Airborne Visual and Infra-Red Imaging Spectrometer (AVIRIS) system, VIMS, NIMS, HYDICE have many narrow bandwidths, contiguously spaced. Bandwidths and sampling greater than 25 nm rapidly lose the ability to resolve important mineral absorption features



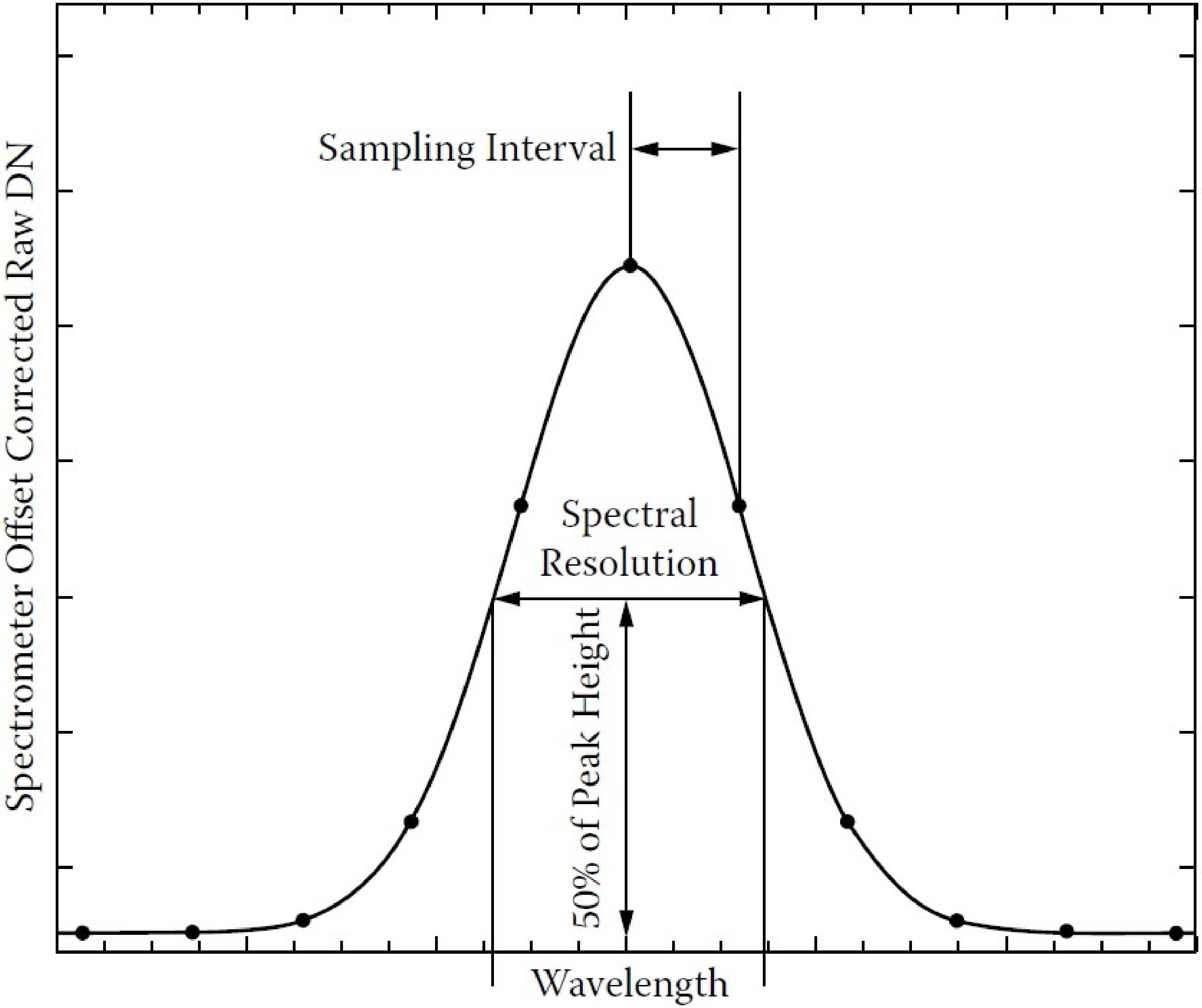
The shape of the bandpass profile is also important. Ideally each spectrometer channel rejects all light except that from within a given narrow wavelength range, but occasionally, due to optical effects, light may leak in from out of the bandpass (e.g. scattering within the optical system, or inadequate blocking filters).

The most common bandpass in spectrometers is a Gaussian profile. While specific spectrometer designs may have well-defined theoretical bandpass profiles, aberrations in the optical system usually smears the profile closer to a Gaussian shape.

The width of the bandpass is usually defined as the width in wavelength at the 50% response level of the function, as shown in Fig, called the Full Width at Half Maximum (FWHM).



A Gaussian profile with a Full Width at Half Maximum (FWHM) of 10 nm is shown. This profile is typical of spectrometers such as AVIRIS which has 224 such profiles spaced at about 10 nm



Full width at half maximum (FWHM).

Spectral sampling is the distance in wavelength between the spectral bandpass profiles for each channel in the spectrometer as a function of wavelength. Spectral sampling is often confused with bandpass, with the two lumped together and called resolution

The **signal-to-noise ratio (S/N)** required to solve a particular problem will depend on the strength of the spectral features under study.

The S/N is dependent on the detector sensitivity, the spectral bandwidth, and intensity of the light reflected or emitted from the surface being measured.

A few spectral features are quite strong and a signal to noise of only about 10 will be adequate to identify them, while others are weak, and a S/N of several hundred (and higher) are often needed (Swayze *et al.*, 1997).

Imaging Spectroscopy

Today, spectrometers are in use in the laboratory, in the field, in aircraft (looking both down at the Earth, and up into space), and on satellites.

Reflectance and emittance spectroscopy of natural surfaces are sensitive to specific chemical bonds in materials, whether solid, liquid or gas

Spectroscopy's historical disadvantage is that it is too sensitive to small changes in the chemistry and/or structure of a material. The variations in material composition often causes shifts in the position and shape of absorption bands in the spectrum.

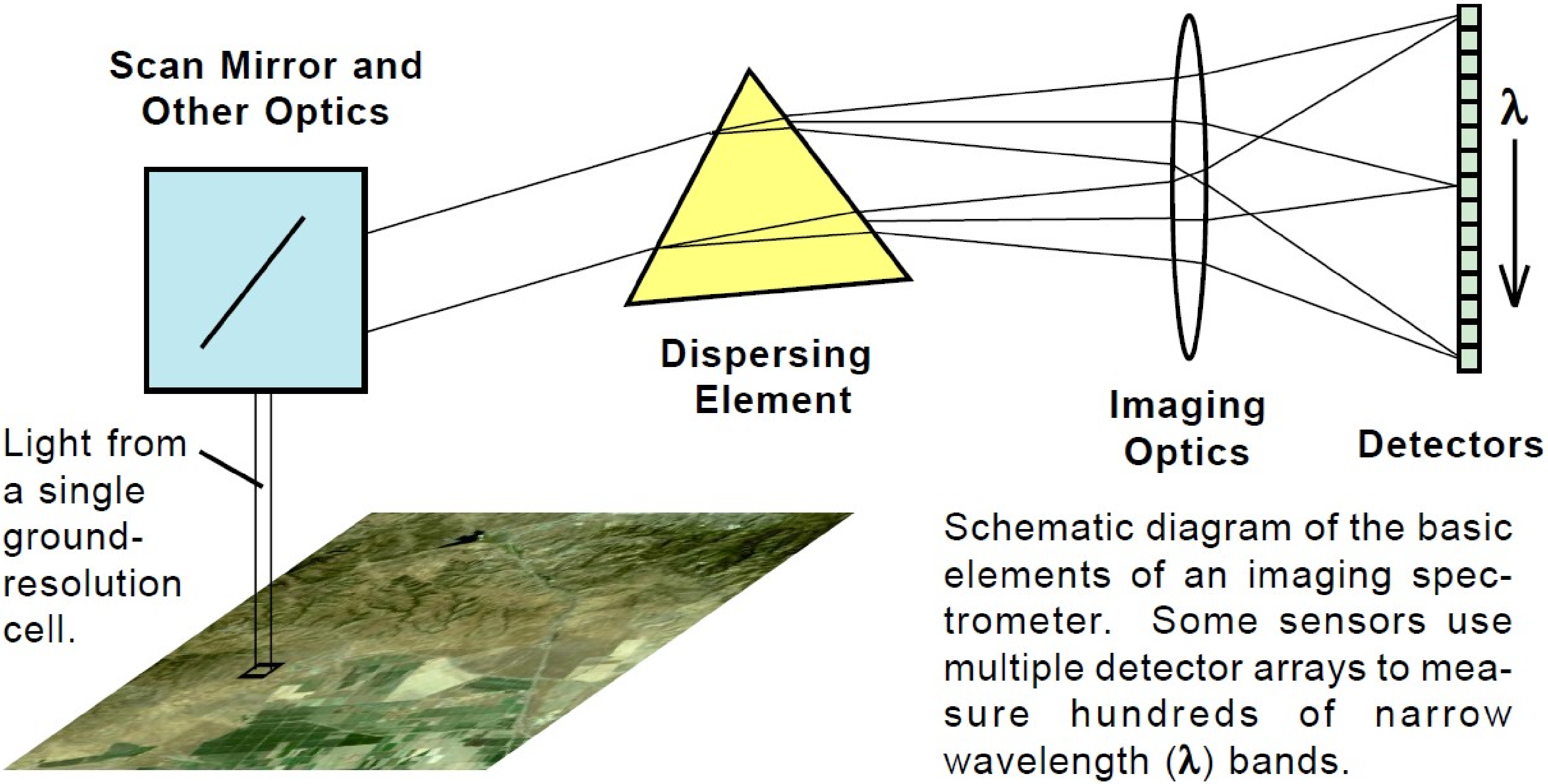
Thus, with the vast variety of chemistry typically encountered in the real world, spectral signatures can be quite complex and sometimes unintelligible.

However, that is now changing with increased knowledge of the natural variation in spectral features and the causes of the shifts. As a result, the previous disadvantage is turning into a huge advantage, allowing us to probe ever more detail about the chemistry of our natural environment.

With the advances in computer and detector technology, the new field of imaging spectroscopy is developing.

Imaging spectroscopy is a new technique for obtaining a spectrum in each position of a large array of spatial positions so that any one spectral wavelength can be used to make a recognizable image.

By analyzing the spectral features, and thus specific chemical bonds in materials, one can map where those bonds occur, and thus map materials. Such mapping is best done, in this author's opinion, by spectral feature analysis.



Schematic diagram of the basic elements of an imaging spectrometer. Some sensors use multiple detector arrays to measure hundreds of narrow wavelength (λ) bands.

Imaging spectroscopy has many names in the remote sensing community, including imaging spectrometry, hyperspectral, and ultraspectral imaging.

Imaging spectroscopy for remote sensing involves the acquisition of image data in many contiguous spectral bands with an ultimate goal of producing lboratory quality reflectance spectra for each pixel in an image (Goetz,1992)

Spectroscopy is the study of electromagnetic radiation. Spectrometry is derived from spectro-photometry, the measure of photons as a function of wavelength.

THE REFLECTION AND ABSORPTION PROCESSES

When a stream of photons encounter a medium with a change in the index of refraction some are reflected and some are refracted into the medium

All materials have a complex index of refraction

$$m = n - jK$$

where m is the complex index of refraction, n is the real part of the index, $j = (-1)^{1/2}$, and K is the imaginary part of the index of refraction, sometimes called extinction coefficient

When photons enter an absorbing medium, they are absorbed according to Beers Law:

$$I = I_o e^{-kx}, \text{ (eqn 1b)}$$

where I is the observed intensity, I_o is the original light intensity, k is an absorption coefficient and x is the distance traveled through the medium

As distance increases through a medium, more photons will be intercepted

The rate of interception of photons is higher with shorter wave length

The absorption coefficient is related to the complex index of refraction by the equation:

$$k = 4 \pi K/\square, \text{ (eqn 1c)}$$

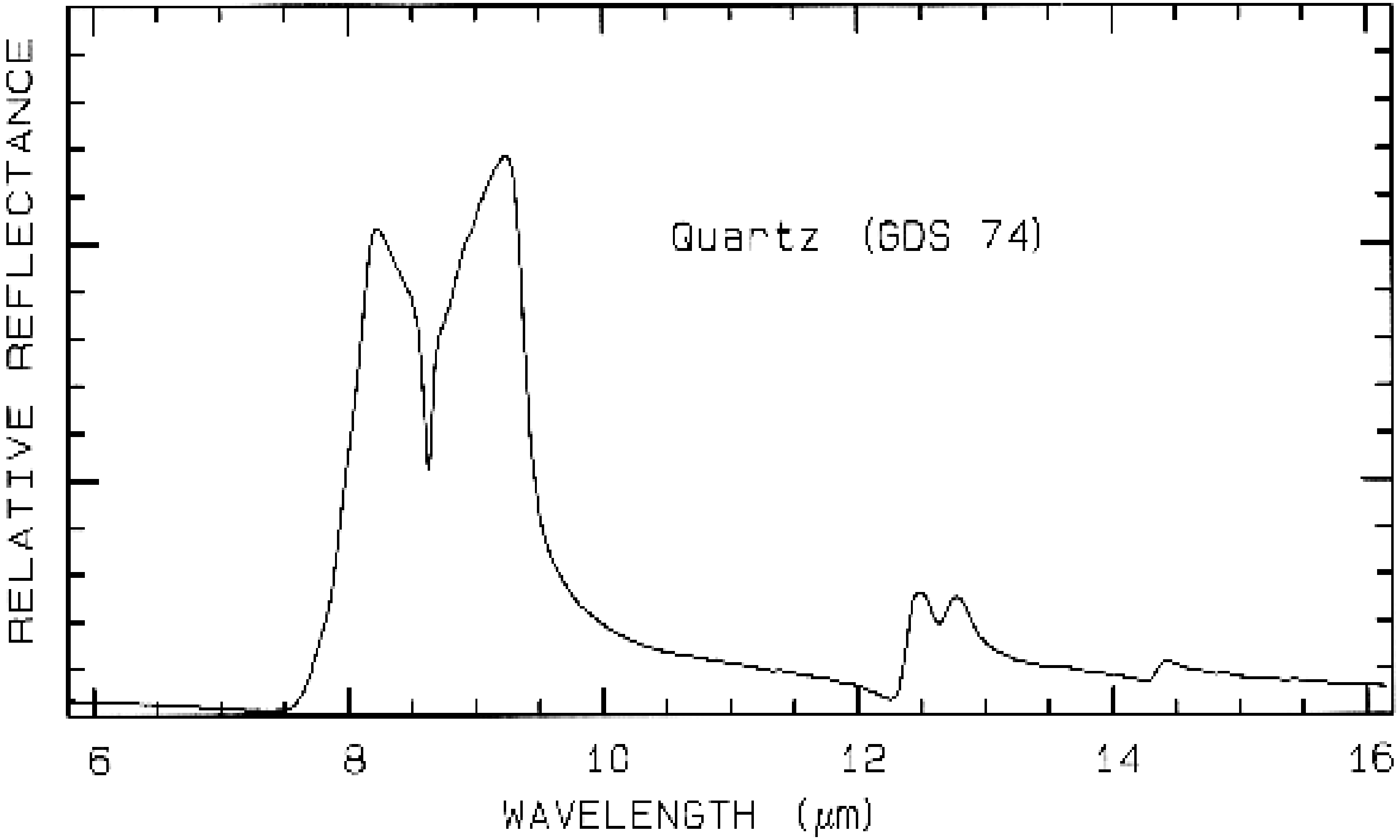
where '▯' is the wavelength of light.

The reflection of light, R, normally incident onto a plane surface is described by the Fresnel equation

$$R = [(n - 1)^2 + K^2] / [(n + 1)^2 + K^2]. \text{ (eqn 1d)}$$

At angles other than normal, the reflectance is a complex trigonometric function involving the polarization direction of the incident beam .

R = Reflection of light normally incident onto plane surface



The reflection from quartz grains as measured on a laboratory spectrometer

The absorption coefficient (k = 4 π K/) determine how far into a material light of a particular wave length can penetrate before it is absorbed . In a material with low a low absorption coefficient, light is only poorly absorbed

The absorption coefficient as a function of wavelength is a fundamental parameter describing the interaction of photons with a material.

So is the index of refraction, but it generally varies less than the absorption coefficient as a function of wavelength, especially at visible and near-infrared wavelengths

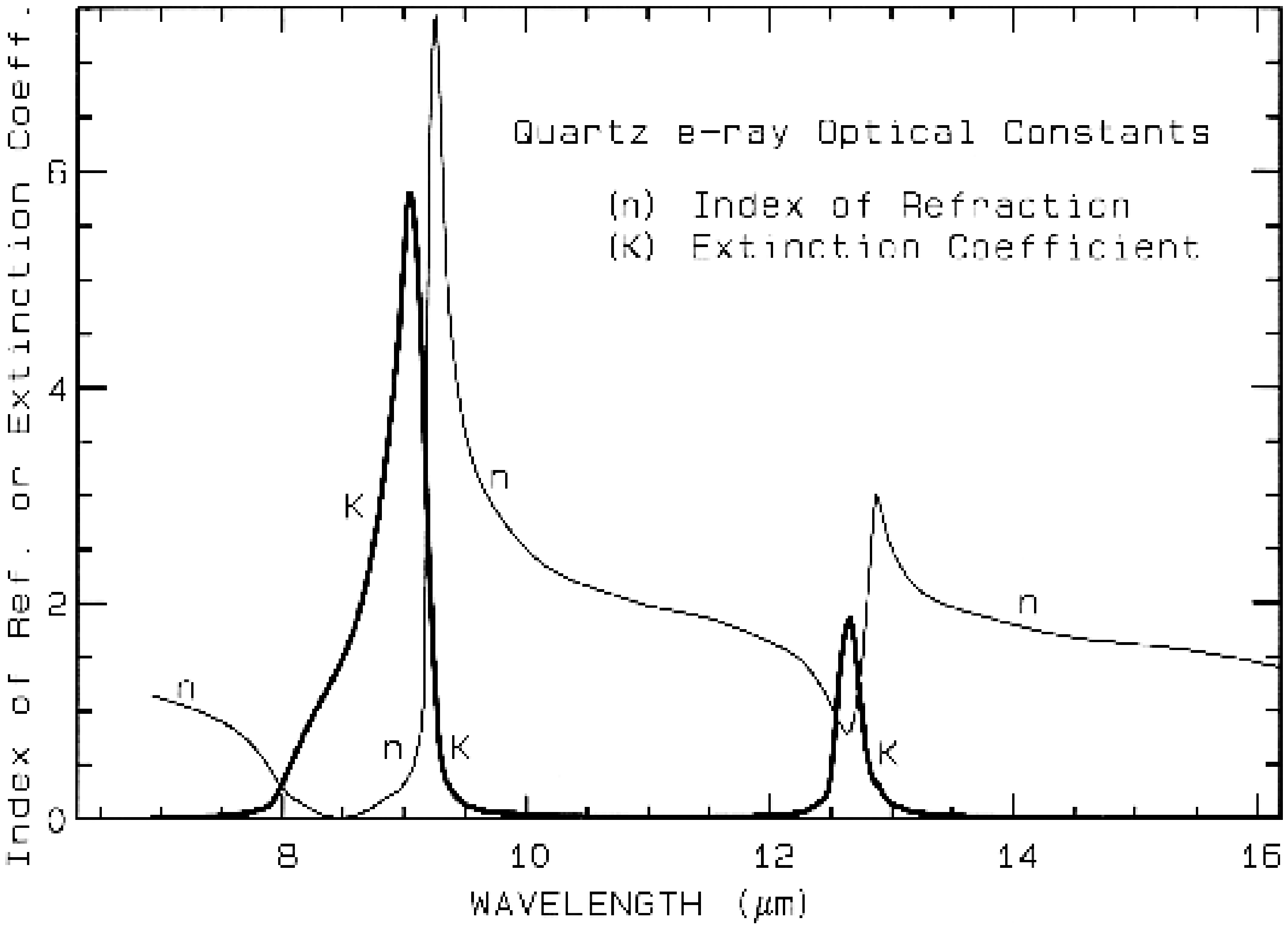
At fundamental absorption bands, both n and K vary strongly with wavelength, though K still varies over more orders of magnitude than n.

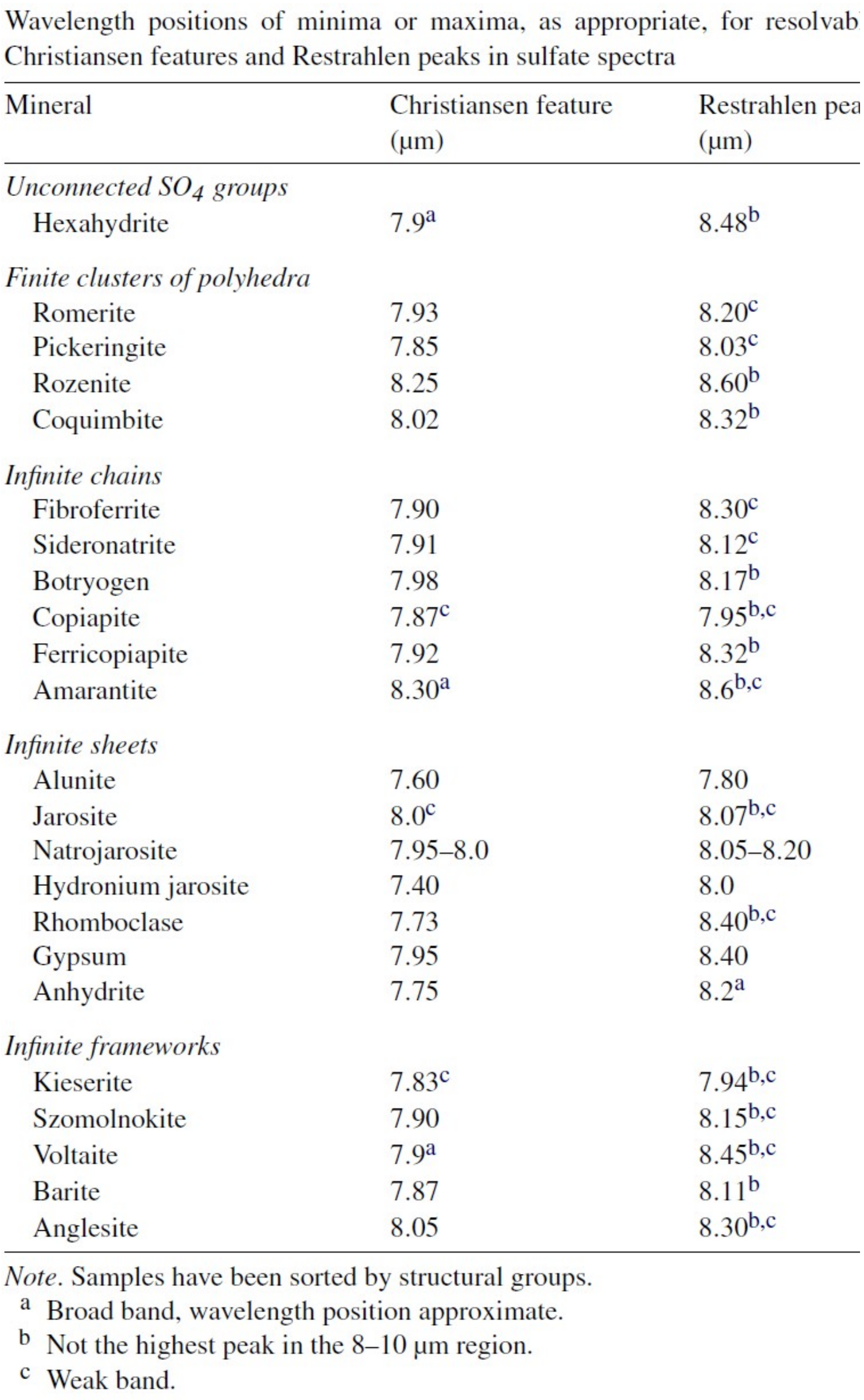
The complex interaction of light with matter involves reflection and refraction from index of refraction boundaries, a process we call scattering, and absorption by the medium as light passes through the medium. The amount of scattering versus absorption controls the amount of photons we receive from a surface.

The complex index of refraction important properties of materials. As one moves to longer wavelengths, the index of refraction decreases to a minimum just before a sharp rise (e.g. at 8.5 and 12.6 µm). The minimum is often near or even below n = 1. The wavelength where n = 1 is called the Christensen frequency and usually results in a minimum in reflected light because of the small (to zero) difference in the index of refraction compared to the surrounding medium (e.g. air or vacuum).

The location of the observed reflectance minimum is also controlled by the extinction coefficient according to equation 1d.

This maximum is called the restrahlen band: the location of fundamental vibrational stretching modes in the near and mid-infrared. The combination of n and K at these wavelengths often results in high reflectance.


Quartz e-ray Optical Constants
(n) Index of Refraction
(K) Extinction Coefficient
Index of Ref. or Extinction Coeff.
0
2
4
6
8
10
12
14
16
WAVELENGTH (μm)
n
K
n
K
n
K
n
n



Wavelength positions of minima or maxima, as appropriate, for resolvab
Christiansen features and Restrahlen peaks in sulfate spectra

Mineral	Christiansen feature (μm)	Restrahlen pea (μm)
Unconnected SO_4 groups		
Hexahydrite	7.9[a]	8.48[b]
Finite clusters of polyhedra		
Romerite	7.93	8.20[c]
Pickeringite	7.85	8.03[c]
Rozenite	8.25	8.60[b]
Coquimbite	8.02	8.32[b]
Infinite chains		
Fibroferrite	7.90	8.30[c]
Sideronatrite	7.91	8.12[c]
Botryogen	7.98	8.17[b]
Copiapite	7.87[c]	7.95[b,c]
Ferricopiapite	7.92	8.32[b]
Amarantite	8.30[a]	8.6[b,c]
Infinite sheets		
Alunite	7.60	7.80
Jarosite	8.0[c]	8.07[b,c]
Natrojarosite	7.95–8.0	8.05–8.20
Hydronium jarosite	7.40	8.0
Rhomboclase	7.73	8.40[b,c]
Gypsum	7.95	8.40
Anhydrite	7.75	8.2[a]
Infinite frameworks		
Kieserite	7.83[c]	7.94[b,c]
Szomolnokite	7.90	8.15[b,c]
Voltaite	7.9[a]	8.45[b,c]
Barite	7.87	8.11[b]
Anglesite	8.05	8.30[b,c]

Note. Samples have been sorted by structural groups.

[a] Broad band, wavelength position approximate.

[b] Not the highest peak in the 8–10 μm region.

[c] Weak band.

So the Christensen frequency and Restrahlen peak are the characteristic features of individual group of minerals and hence their fundamental absorption wave length

The complex interaction of light with matter involves reflection and refraction from index of refraction boundaries, a process we call scattering, and absorption by the medium as light passes through the medium. The amount of scattering versus absorption controls the amount of photons we receive from a surface.

CAUSES OF ABSORPTION

Isolated atoms or ions have discrete energy states. A change of the energy state is referred to as transition. If a photon of a specific wavelength is absorbed or emitted, the energy state is changed.

Absorption results in a higher energy state and emission in a lower energy state.

Since an absorbed photon of a specific wavelength is usually not emitted at the same wavelength, absorption bands can be generated.

Absorption bands within the visible and reflected infrared light are related to electronic and vibrational processes within the crystal lattice.

Electronic transition processes require more energy; hence they occur mainly at shorter wavelengths within the VIS and NIR spectrum, and give rise to broad absorption features.

Vibrational processes take place within the infrared spectra (NIR, SWIR and thermal) and result typically in small and sharp absorption bands.

The position and shape (depth, width and asymmetry) of an absorption feature are controlled primarily by the kind of absorbing ion or molecule and its position within the crystal lattice (e.g. octahedral, tetrahedral site). But also the kind of chemical bond and the elements involved in the bond influence the position and shape of the absorption feature.

Electronic processes

In minerals, electronic transition processes yielding absorption features are related to crystal field effects, conduction bands, charge transfer transition and colour centres. Which processes take effect depends on the chemical bond and the involved elements.

Crystal field effects: The most common electronic process revealed in the spectra of minerals is due to unfilled electron shells of transition elements (Ni, Cr, Co, Fe, etc.). Iron is the most common transition element in minerals.

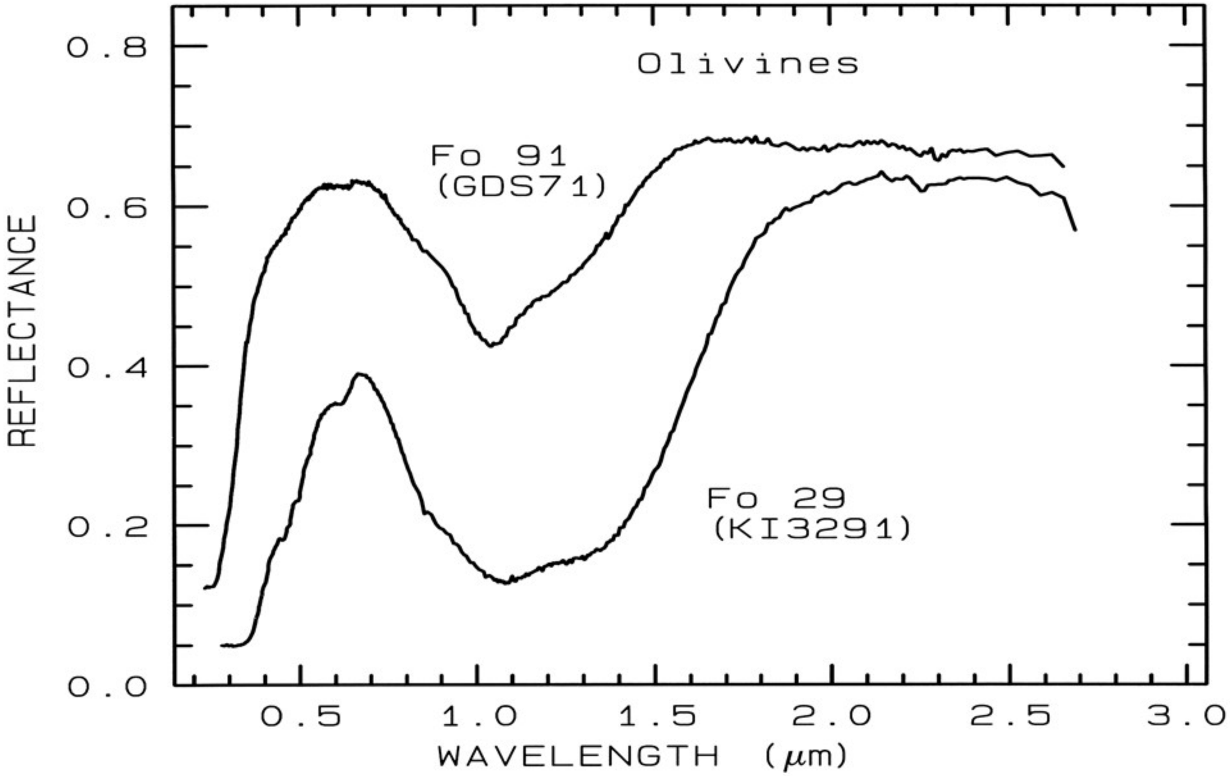
For all transition elements, d orbitals have identical energies in an isolated ion, but the energy levels split when the atom is located in a crystal field (e.g. see Burns, 1970, 1993).

This splitting of the orbital energy states enables an electron to be moved from a lower level into a higher one by absorption of a photon having an energy matching the energy difference between the states.

The energy levels are determined by the valence state of the atom (e.g. Fe^{2+}, Fe^{3+}), its coordination number, and the symmetry of the site it occupies.

The levels are also influenced by the type of ligands formed, the extent of distortion of the site, and the value of the metal-ligand interatomic distance (e.g. Burns, 1993).

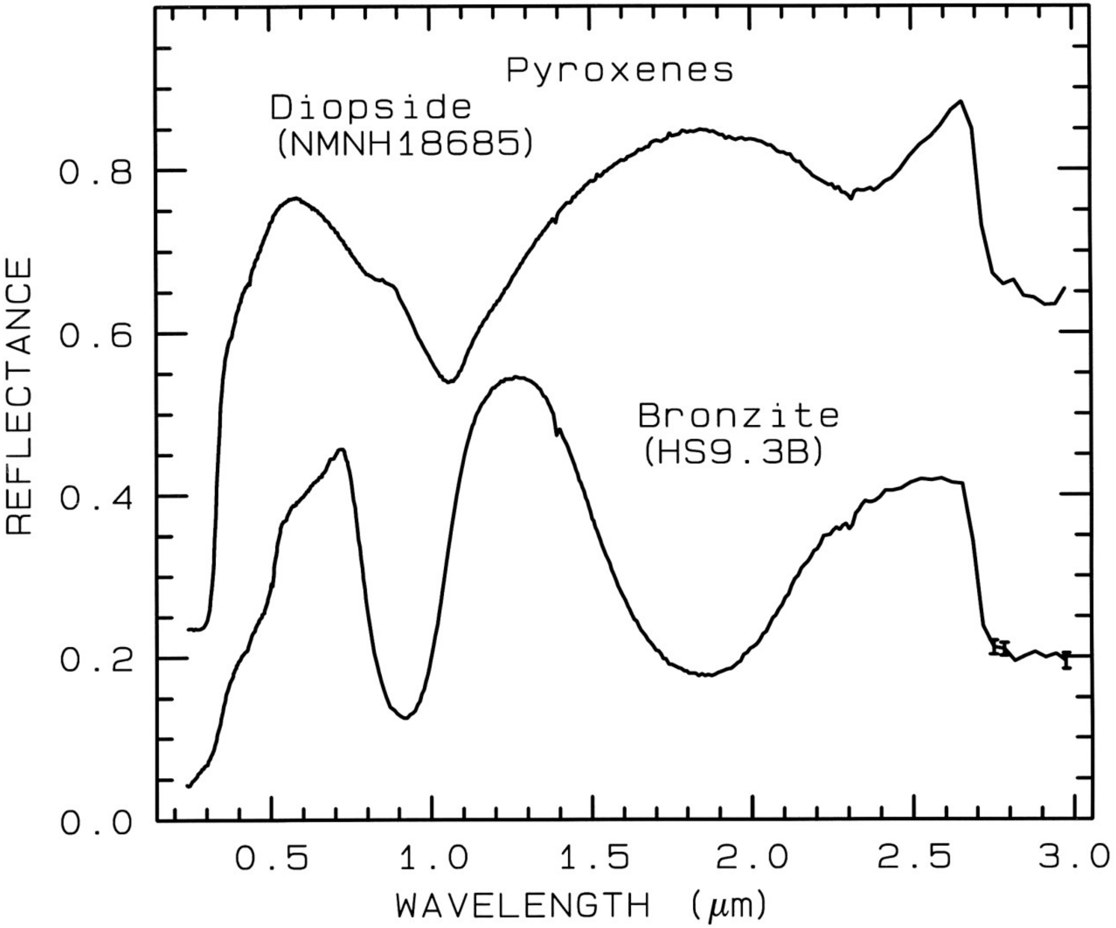
The crystal field varies with crystal structure from mineral to mineral, thus the amount of splitting varies and the same ion (like Fe^{2+}) produces obviously different absorptions, making specific mineral identification possible from spectroscopy



Reflectance spectra of two olivines showing the change in band position and shape with composition. The 1-μm absorption band is due to a crystal field absorption of Fe^{2+}.

The Fo 29 sample has an FeO content of 53.65%, while the Fo 91 sample has an FeO content of 7.93%.

The mean grain size is 30 and 25 μm respectively. The 1-μm band position varies from about 1.08 μm at Fo 10 to 1.05 μm at Fo 90 (King and Ridley, 1987).



Reflectance spectra of two pyroxenes showing the change in Fe^{2+} - absorption band position and shape with composition (from Clark *et al.*, 1993b).

Diopside is $CaMgSi_2O_6$, but some Fe^{2+} substitutes for Mg.

Bronziteis $(Mg,Fe)SiO_3$ with mostly Mg.

The 1-µm versus the 2-µm band position of a pyroxene describes the pyroxene composition

Charge Transfer Absorptions

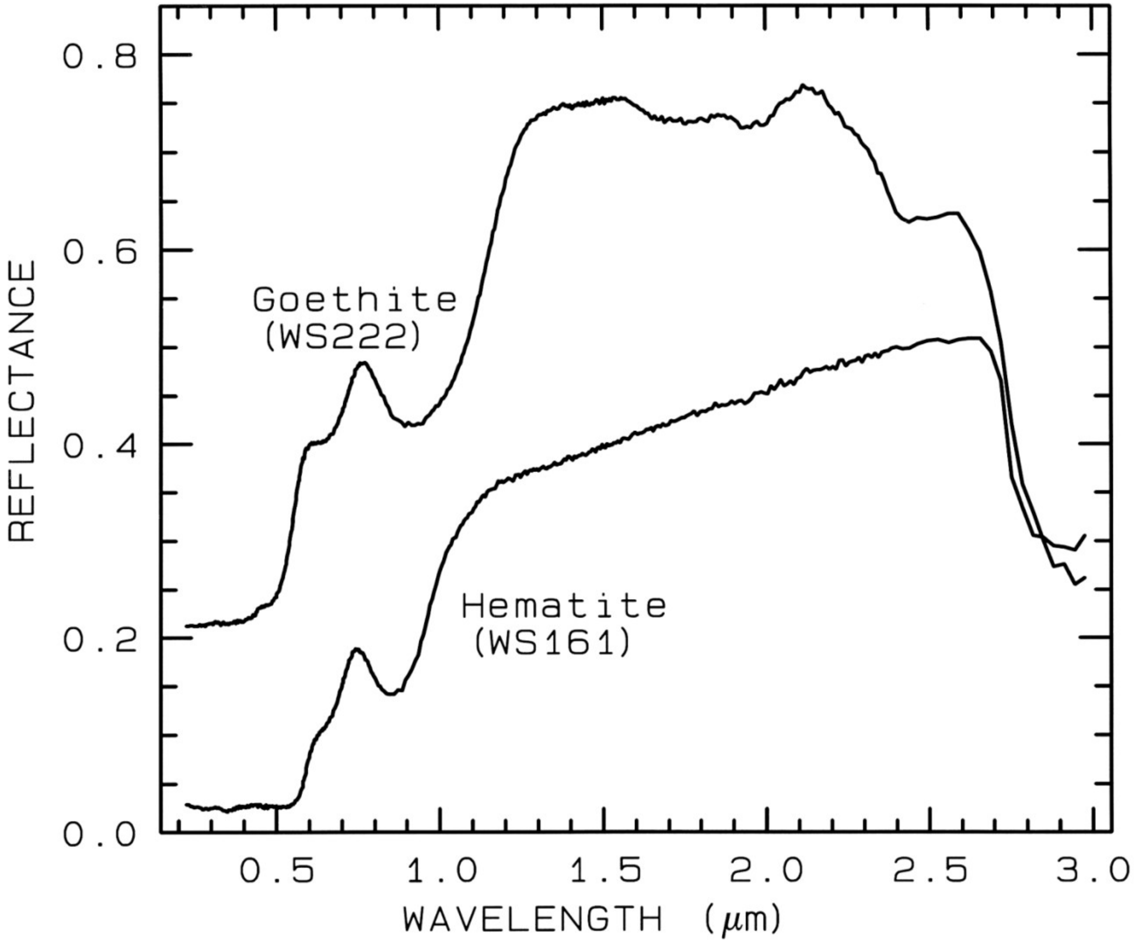
Absorption bands can also be caused by charge transfers, or inter-element transitions where the absorption of a photon causes an electron to move between ions or between ions and ligands.

The transition can also occur between the same metal in different valence states, such as between Fe^{2+} and Fe^{3+}.

In general, absorption bands caused by charge transfers are diagnostic of mineralogy.

Their strengths are typically hundreds to thousands of times stronger than crystal field transitions.

The band centers usually occur in the ultraviolet with the wings of the absorption extending into the visible. Charge transfer absorptions are the main cause of the red color of iron oxides and hydroxides.



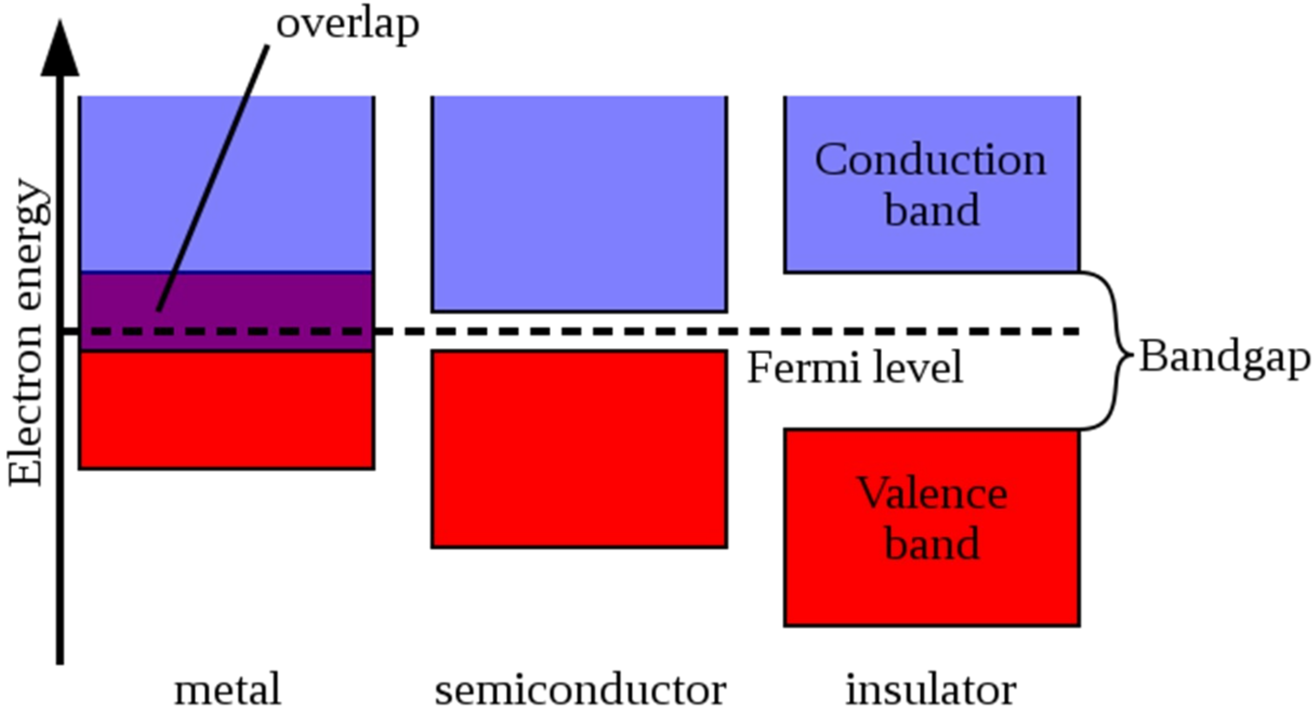
Reflectance spectra of the iron oxide hematite (Fe2O3) and iron hydroxide goethite (FeOOH, from Clark et al., 1993b). The intense charge-transfer band in the UV (< 0.4 µm) is "saturated" in reflectance, so only first surface (specular) reflection is seen in these spectra. The 0.9-µm and 0.86-µm absorption features are due to Laporte-forbidden transitions (e.g. Morris et al, 1985; Sherman, 1990 and references therein). The absorption at 2.7-3 µm is due to trace water in the samples., and in the case of goethite, the OH. The goethite spectrum is offset upward 0.2 units.

Conduction Bands. In some minerals, there are two energy levels in which electrons may reside: a higher level called the "conduction band," where electrons move freely throughout the lattice, and a lower energy region called the "valence band," where electrons are attached to individual atoms.

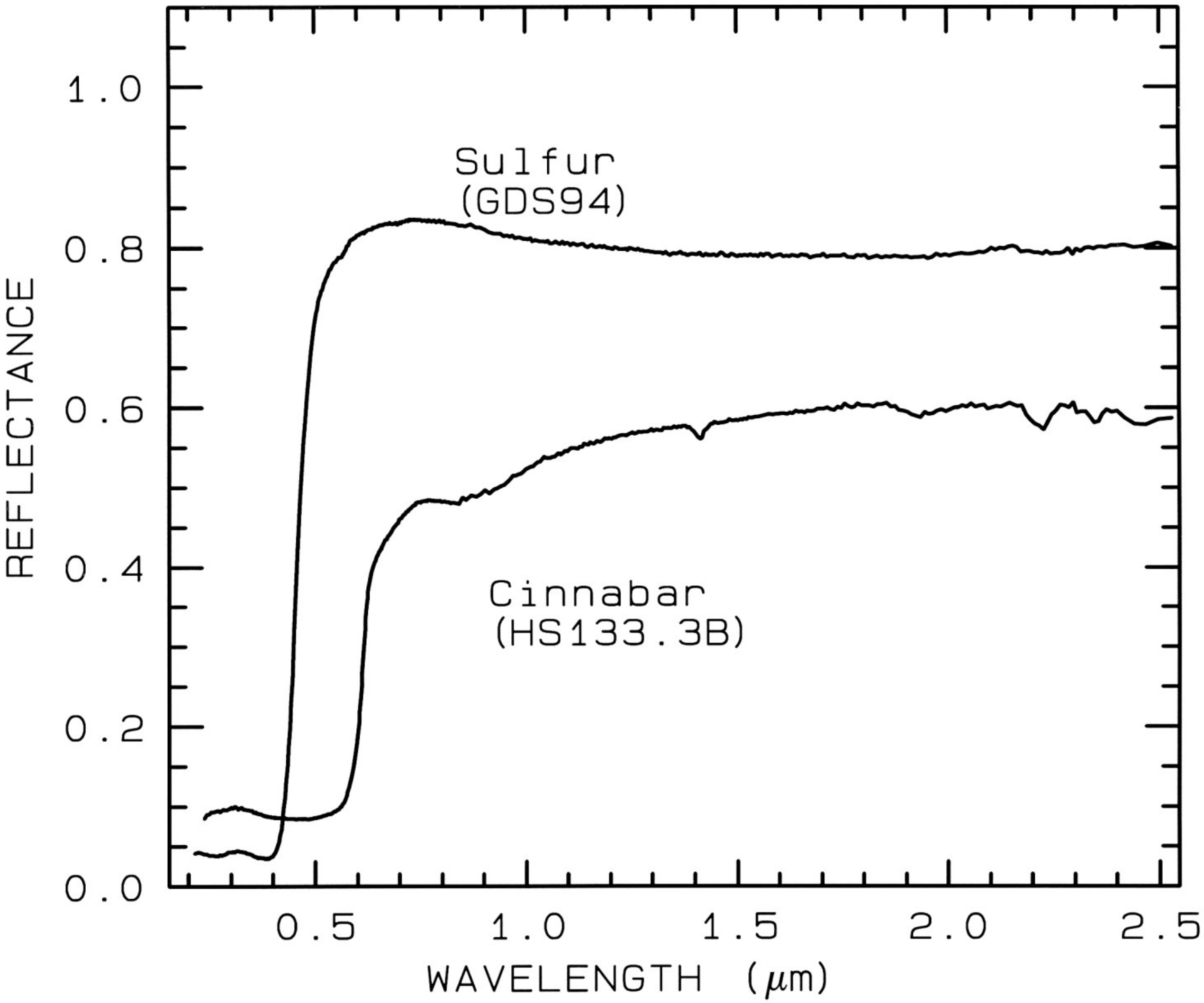
The difference between the energy levels is called the band gap. The band gap is typically small or non-existent in metals, and very large in dielectrics.

In semiconductors, the band gap corresponds to the energy of visible to near-infrared wavelength photons and the spectrum in these cases is approximately a step function.

The yellow color of sulfur is caused by such a band gap. The minerals cinnabar (HgS) and Sulfur (S) have spectra showing the band gap in the visible



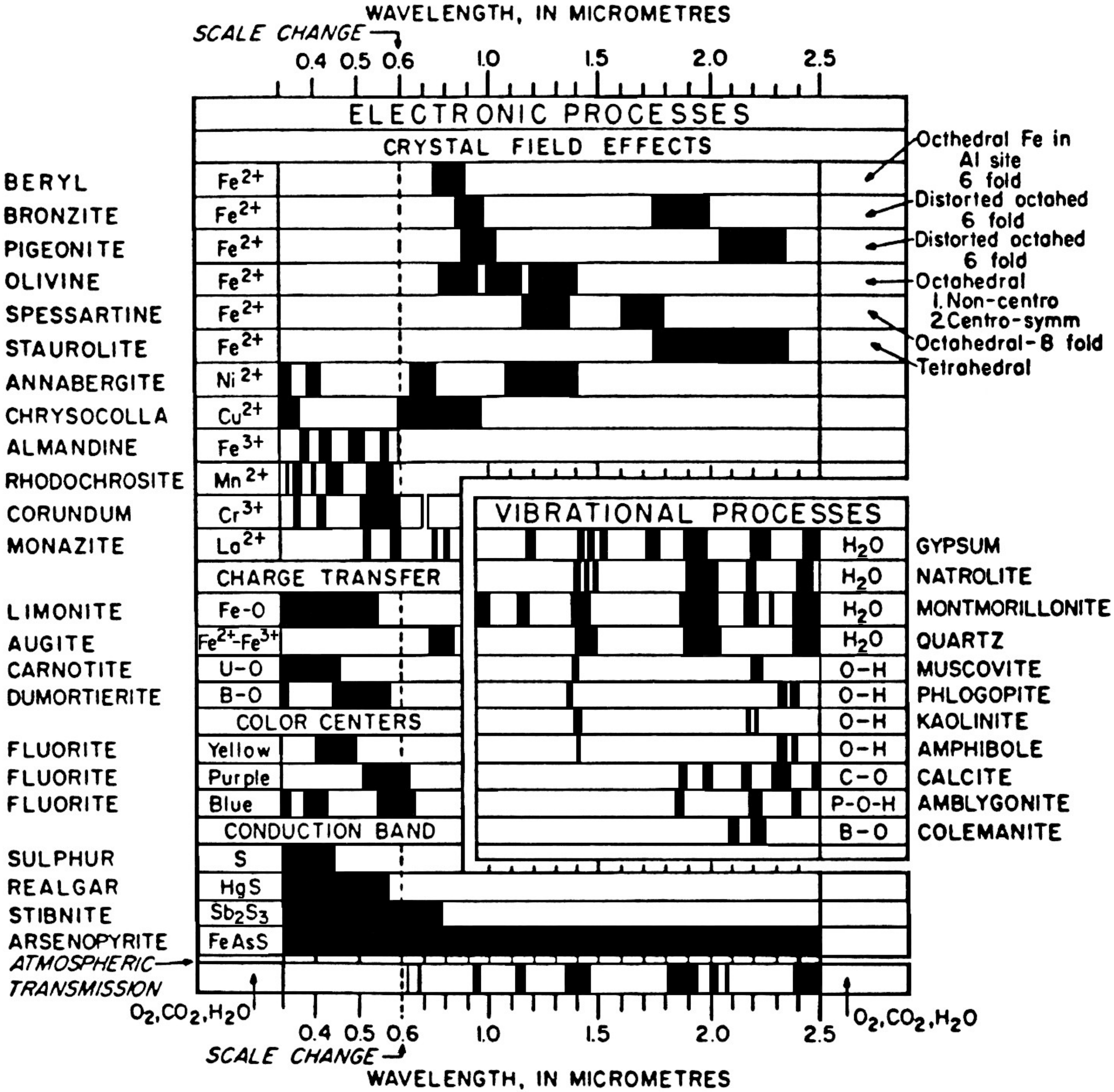
Absorption occurs when photons have sufficient energy to excite electrons across the forbidden band. Many sulphides show absorption features related to conduction bands.



Reflectance spectra of Sulfur, S, (top) and cinnabar, HgS, (bottom) showing conduction bands in the visible (from Clark *et al*., 1993b).

Color Centers. A few minerals show color due to absorption by "color centers." A color center is caused by irradiation (e.g. by solar UV radiation) of an imperfect crystal.

Crystals in nature have lattice defects that disturb the periodicity of the crystal. For example, defects might be caused by impurities. These defects can produce discrete energy levels and electrons can become bound to them. The movement of an electron into the defect requires photon energy. The yellow, purple and blue colors of fluorite are caused by color centers. See Hunt (1977) and references therein for more details.


WAVELENGTH, IN MICROMETRES
SCALE CHANGE
0.4 0.5 0.6 1.0 1.5 2.0 2.5
ELECTRONIC PROCESSES
CRYSTAL FIELD EFFECTS
BERYL Fe^{2+}
BRONZITE Fe^{2+}
PIGEONITE Fe^{2+}
OLIVINE Fe^{2+}
SPESSARTINE Fe^{2+}
STAUROLITE Fe^{2+}
ANNABERGITE Ni^{2+}
CHRYSOCOLLA Cu^{2+}
ALMANDINE Fe^{3+}
RHODOCHROSITE Mn^{2+}
CORUNDUM Cr^{3+}
MONAZITE La^{2+}
Octhedral Fe in Al site 6 fold
Distorted octahed 6 fold
Distorted octahed 6 fold
Octahedral
1. Non-centro
2. Centro-symm
Octahedral - 8 fold
Tetrahedral
CHARGE TRANSFER
LIMONITE Fe-O
AUGITE Fe^{2+}-Fe^{3+}
CARNOTITE U-O
DUMORTIERITE B-O
COLOR CENTERS
FLUORITE Yellow
FLUORITE Purple
FLUORITE Blue
CONDUCTION BAND
SULPHUR S
REALGAR HgS
STIBNITE Sb_2S_3
ARSENOPYRITE FeAsS
VIBRATIONAL PROCESSES
H_2O GYPSUM
H_2O NATROLITE
H_2O MONTMORILLONITE
H_2O QUARTZ
O-H MUSCOVITE
O-H PHLOGOPITE
O-H KAOLINITE
O-H AMPHIBOLE
C-O CALCITE
P-O-H AMBLYGONITE
B-O COLEMANITE
ATMOSPHERIC TRANSMISSION
O_2, CO_2, H_2O
O_2, CO_2, H_2O
0.4 0.5 0.6 1.0 1.5 2.0 2.5
SCALE CHANGE
WAVELENGTH, IN MICROMETRES

Vibrational Processes

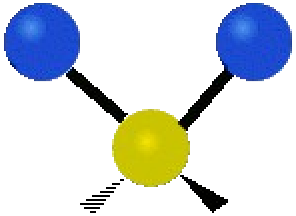
When light at the same wavelength as a molecule (or part of a molecule) strikes the molecule, it causes the molecule (or part of the molecule) to vibrate. This leads to light absorption. In general these absorptions are very narrow, although their widths and depths vary. Most of these absorptions can be detected with hyperspectral sensors.

The bonds in a molecule or crystal lattice are like springs with attached weights: the whole system can vibrate. The frequency of vibration depends on the strength of each spring (the bond in a molecule) and their masses (the mass of each element in a molecule).

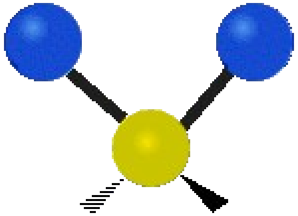
For a molecule with N atoms, there are 3N-6 normal modes of vibrations called fundamentals. Each vibration can also occur at roughly multiples of the original fundamental frequency. The additional vibrations are called overtones when they involve multiples of a single fundamental mode, and combinations when they involve different modes of vibrations.

Vibrational Processes

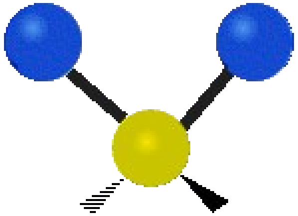
Symmetrical stretching



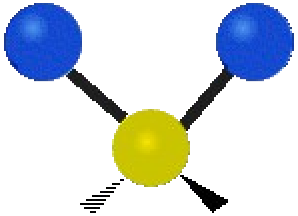
Antisymmetrical stretching



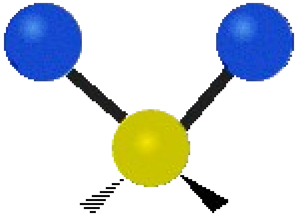
Scissoring



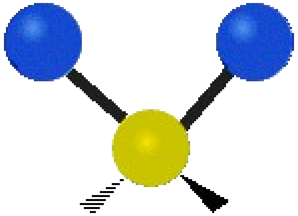
Rocking

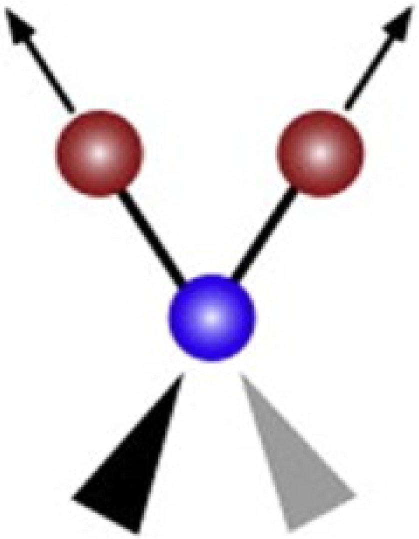


Wagging

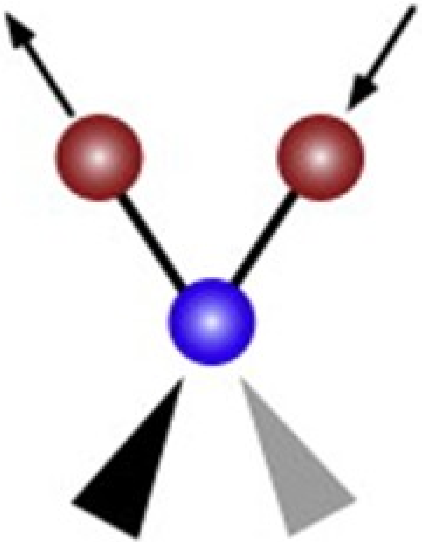


Twisting

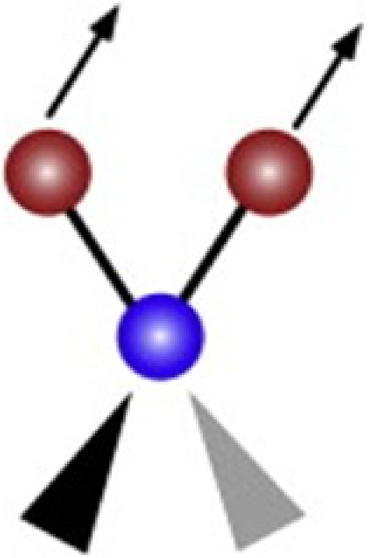




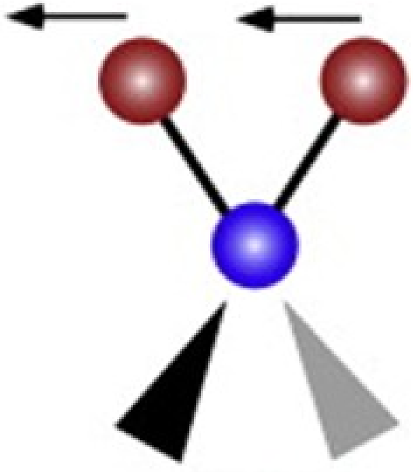
Symmetric stretching



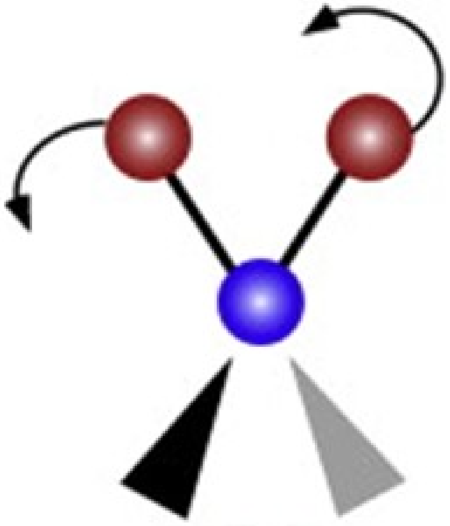
Asymmetric stretching



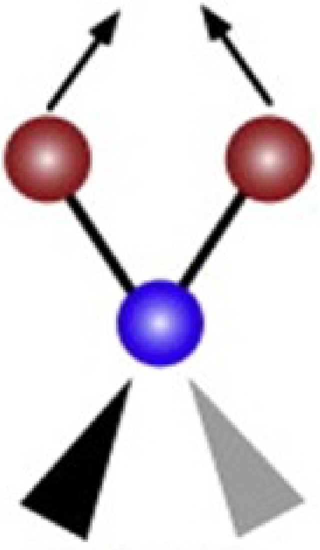
Wagging



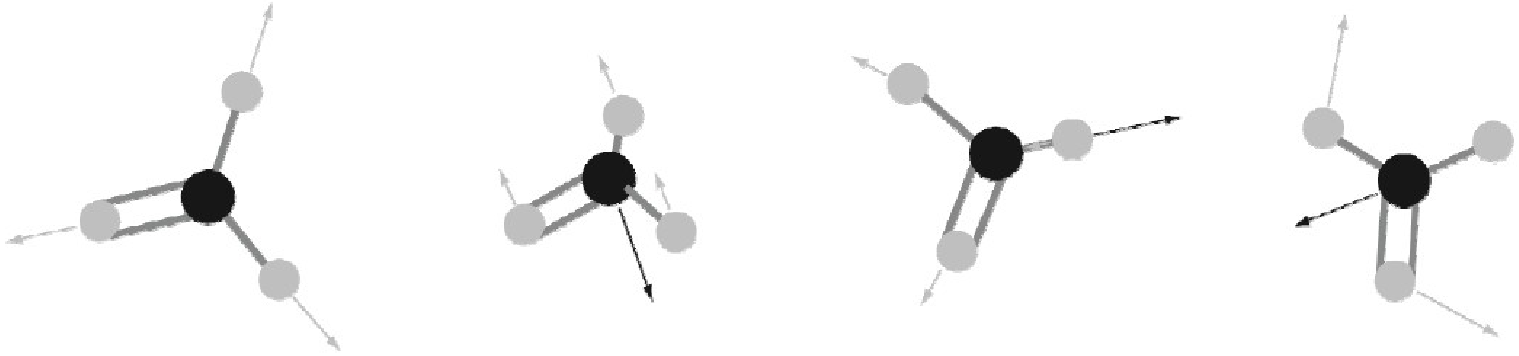
Rocking



Twisting

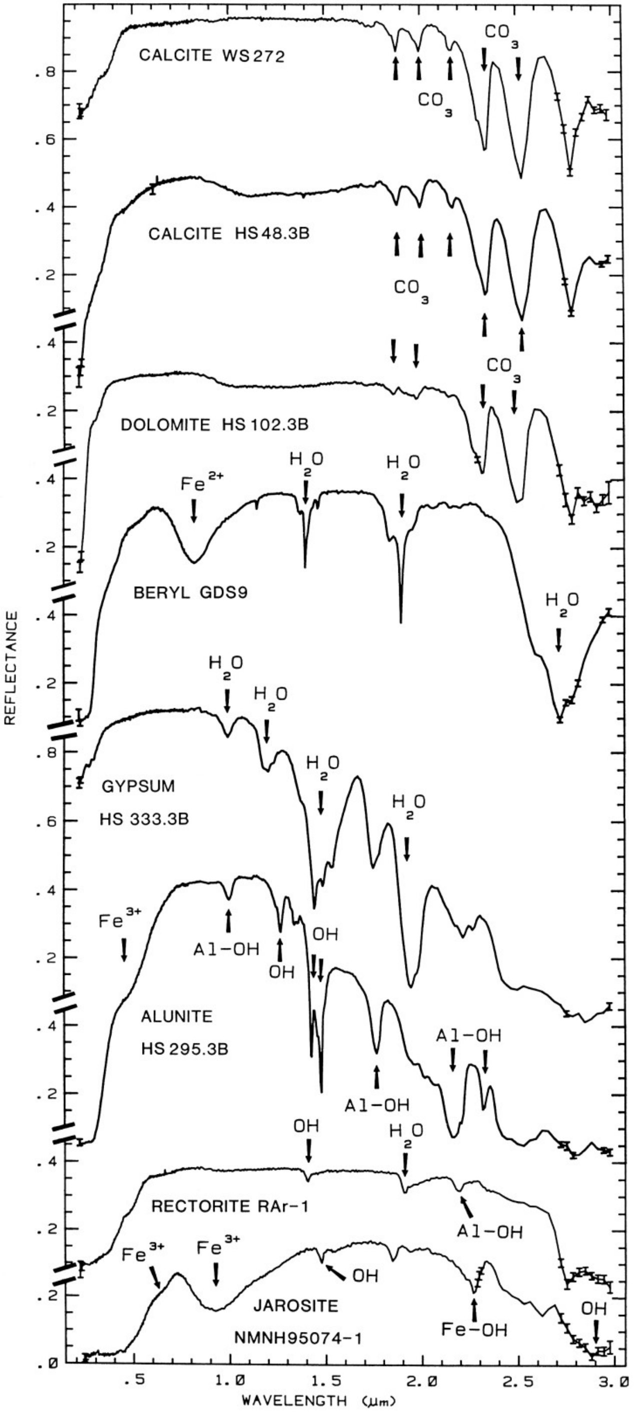


Scissoring



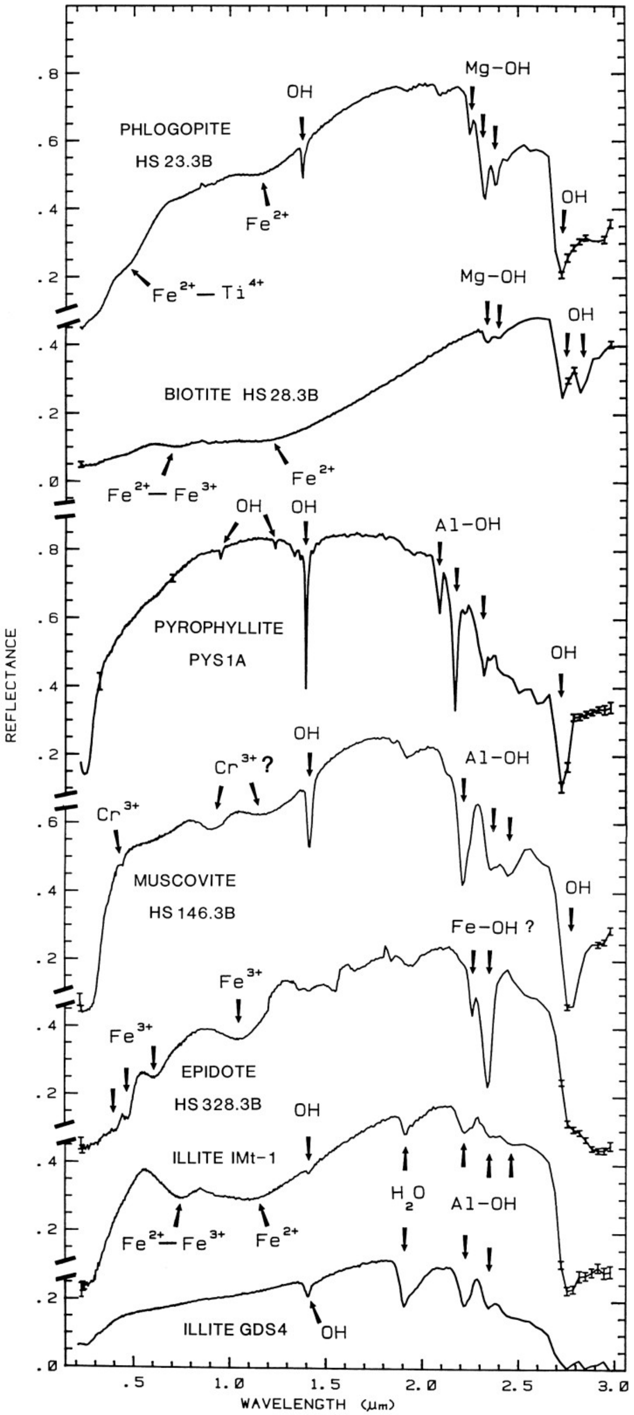
ν_1 symmetric stretch | ν_2 out-of-plane bend | ν_3 asymmetric stretch | ν_4 in-plane bend

Fig 3 Fundamental vibration modes with motion vectors of a free carbonate ion (CO_3^{2+}) (after www1).

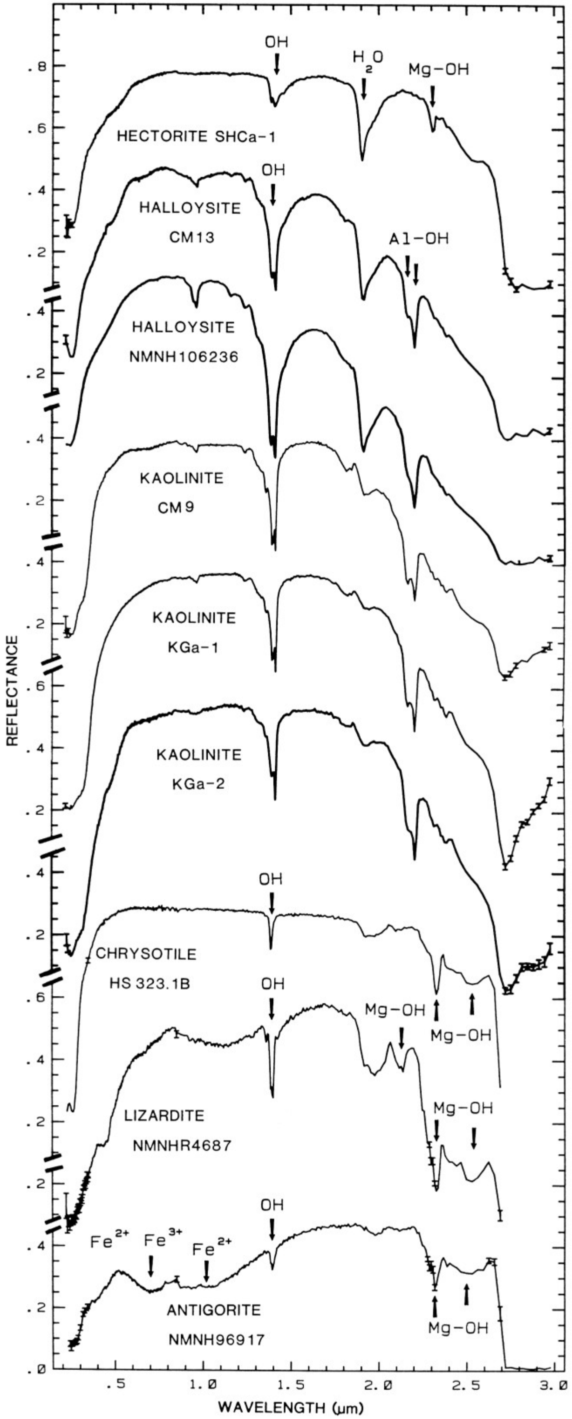


A vibrational absorption will be seen in the infrared spectrum only if the molecule responsible shows a dipole moment (it is said to be infrared active).

Reflectance spectra of calcite, dolomite, beryl, gypsum, alunite, rectorite, and jarosite showing vibrational bands due to OH, CO3 and H2O, from Clark et al., 1990a)



Reflectance spectra of phlogopite, biotite, pyrophyllite, muscovite, epidote, and illite showing vibrational bands due to OH and H2O, from Clark et al., 1990a).

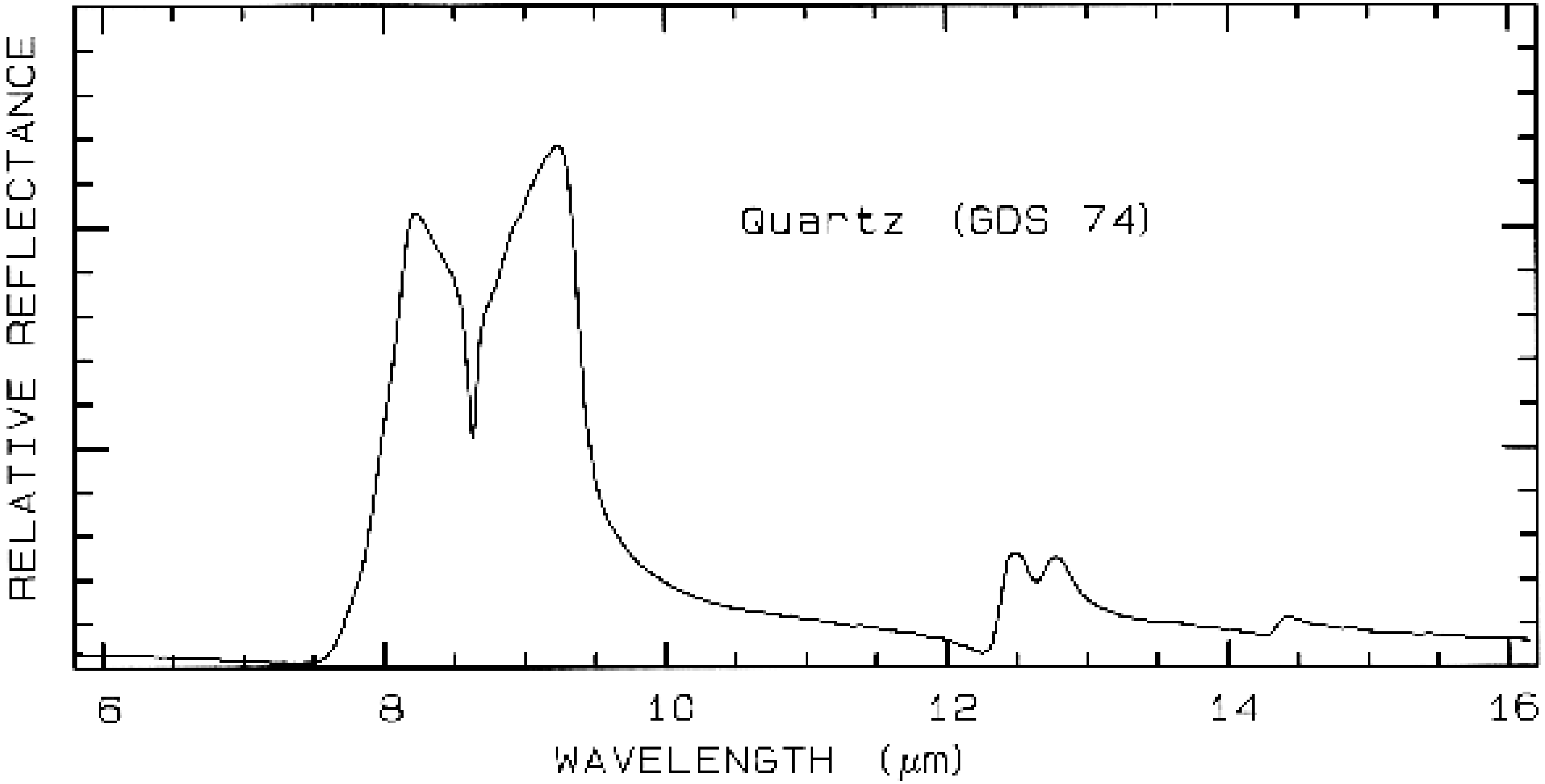


Reflectance spectra of hectorite, halloysite, kaolinite, chrysotile, lizardite, and antigorite showing vibrational bands due to OH

Mid-infrared reflectance spectra of quartz. The strong 9-µm Si-O-Si asymmetric stretch fundamental is obvious from the reflection maximum.

The O-Si-O bending mode occurs near 25 µm and is the second strongest absorption.

The absorption between 12 and 13 µm is the Si-O-Si symmetric stretch fundamental.



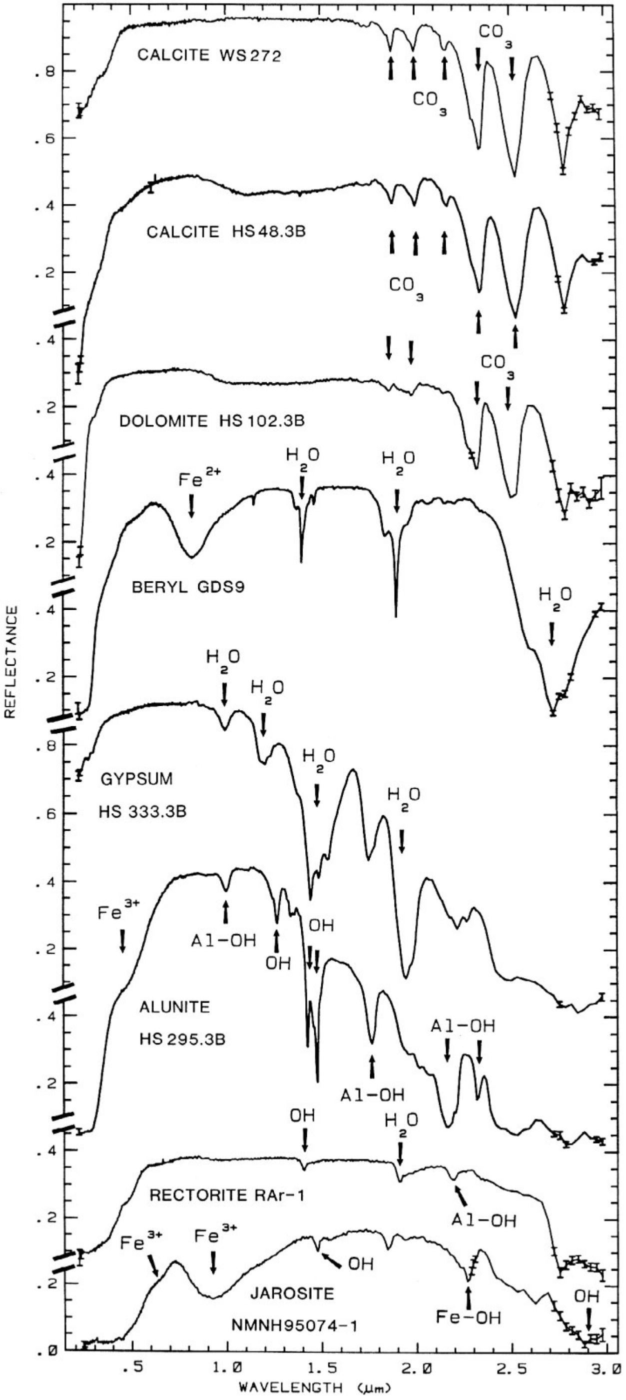
Water and Hydroxyl. Water and OH (hydroxyl) produce particularly diagnostic absorptions in minerals. The water molecule (H_2O) has N=3, so there are 3N-6=3 fundamental vibrations.

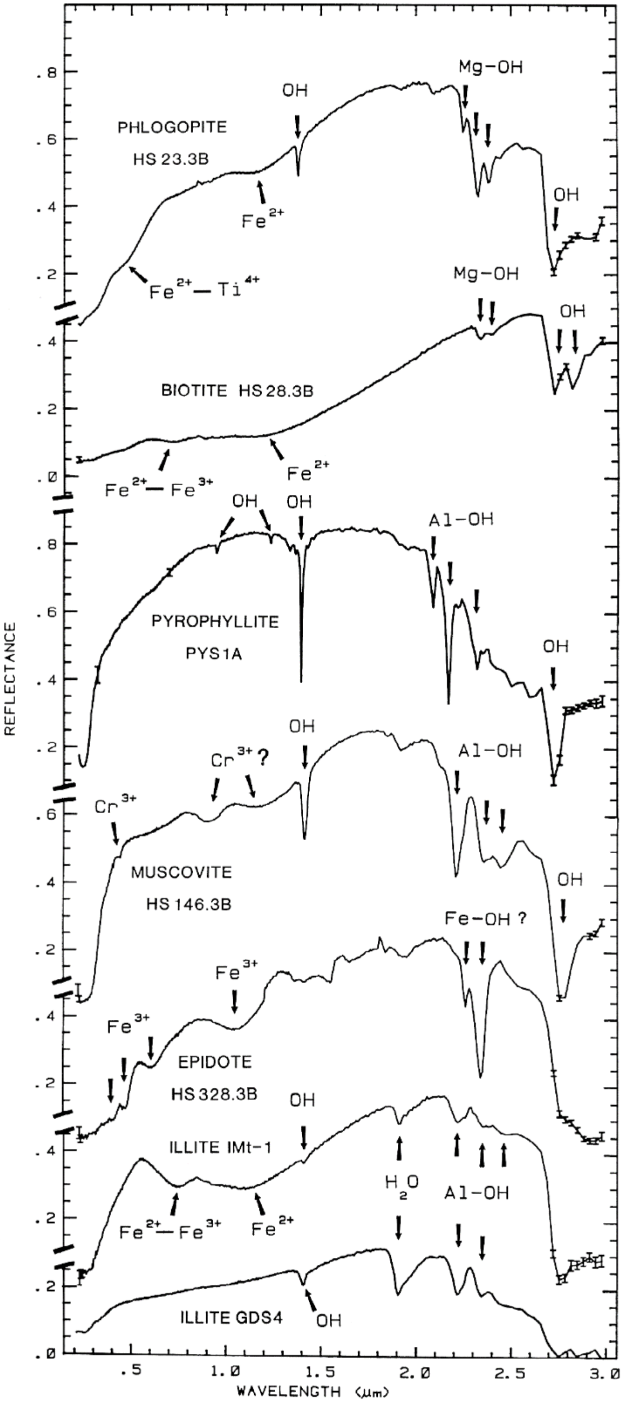
In the isolated molecule (vapor phase) they occur at 2.738 µm (v_1, symmetric OH stretch), 6.270 µm (v_2, H-O-H bend), and 2.663 µm (v_3, asymmetric OH stretch).

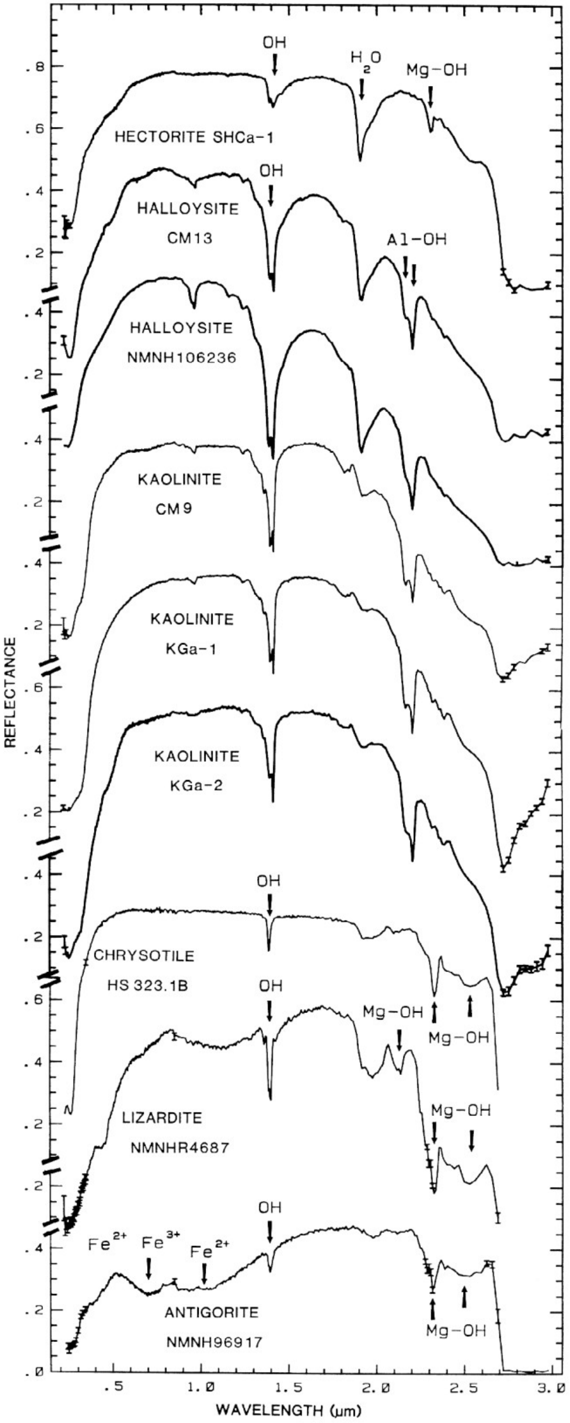
In liquid water, the frequencies shift due to hydrogen bonding: v_1=3.106 µm, v_2=6.079 µm, and v_3=2.903 µm.

The overtones of water are seen in reflectance spectra of H_2O-bearing minerals.

The first overtones of the OH stretches occur at about 1.4 µm and the combinations of the H-O-H bend with the OH stretches are found near 1.9 µm.


CALCITE WS272
CO_3
CO_3
CALCITE HS48.3B
CO_3
CO_3
DOLOMITE HS102.3B
Fe^{2+}
H_2O
H_2O
BERYL GDS9
H_2O
H_2O
H_2O
GYPSUM
HS 333.3B
H_2O
H_2O
Fe^{3+}
Al-OH
OH
OH
ALUNITE
HS295.3B
Al-OH
Al-OH
OH
H_2O
RECTORITE RAr-1
Al-OH
Fe^{3+}
Fe^{3+}
OH
JAROSITE
NMNH95074-1
Fe-OH
OH
REFLECTANCE
WAVELENGTH (μm)
.5
1.0
1.5
2.0
2.5
3.0


PHLOGOPITE
HS 23.3B
OH
Mg-OH
Fe^{2+}
Fe^{2+}—Ti^{4+}
OH
Mg-OH
OH
BIOTITE HS28.3B
Fe^{2+}—Fe^{3+}
Fe^{2+}
OH
OH
Al-OH
PYROPHYLLITE
PYS1A
OH
OH
Cr^{3+}?
Cr^{3+}
Al-OH
MUSCOVITE
HS146.3B
OH
Fe^{3+}
Fe-OH ?
Fe^{3+}
EPIDOTE
HS328.3B
OH
ILLITE IMt-1
H_2O
Al-OH
Fe^{2+}—Fe^{3+}
Fe^{2+}
ILLITE GDS4
OH
REFLECTANCE
WAVELENGTH (μm)
.5
1.0
1.5
2.0
2.5
3.0


OH
H_2O
Mg-OH
HECTORITE SHCa-1
HALLOYSITE
CM13
OH
Al-OH
HALLOYSITE
NMNH106236
KAOLINITE
CM9
KAOLINITE
KGa-1
KAOLINITE
KGa-2
OH
CHRYSOTILE
HS 323.1B
Mg-OH
OH
Mg-OH
Mg-OH
LIZARDITE
NMNHR4687
Mg-OH
OH
Fe^{2+}
Fe^{3+}
Fe^{2+}
ANTIGORITE
NMNH96917
Mg-OH
REFLECTANCE
WAVELENGTH (μm)
.5
1.0
1.5
2.0
2.5
3.0

Thus, a mineral whose spectrum has a 1.9-µm absorption band contains water (e.g. hectorite and halloysite), but a spectrum that has a 1.4-µm band but no 1.9-µm band indicates that only hydroxyl is present (e.g. kaolinite has only a small amount of water because of the weak 1.9-µm absorption but a large amount of OH).

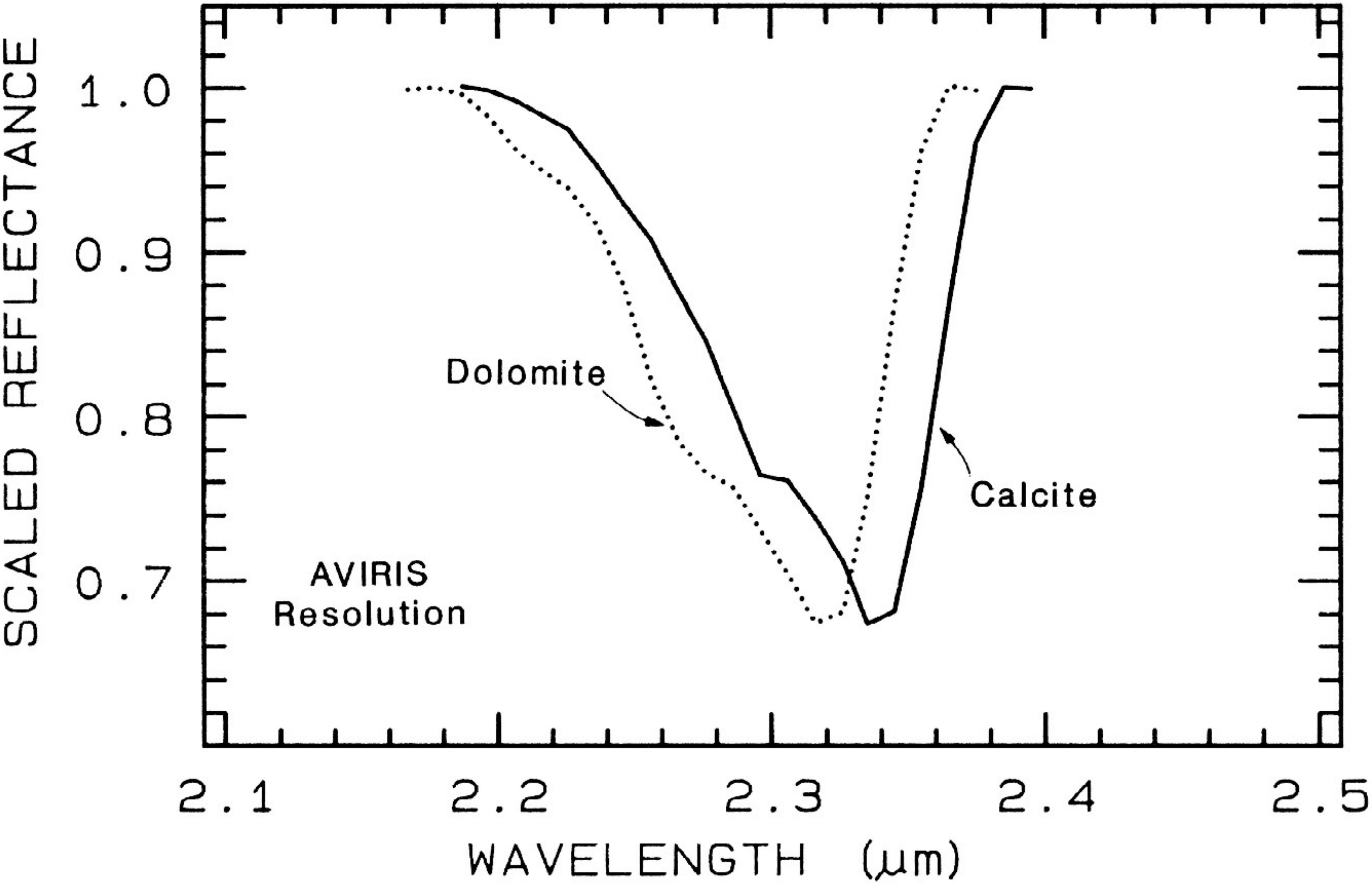
The hydroxyl ion has only one stretching mode and its wavelength position is dependent on the ion to which it is attached. In spectra of OH-bearing minerals, the absorption is typically near 2.7 to 2.8 µm, but can occur anywhere in the range from about 2.67 µm to 3.45 µm (e.g. see Clark *et al*., 1990 and references therein).

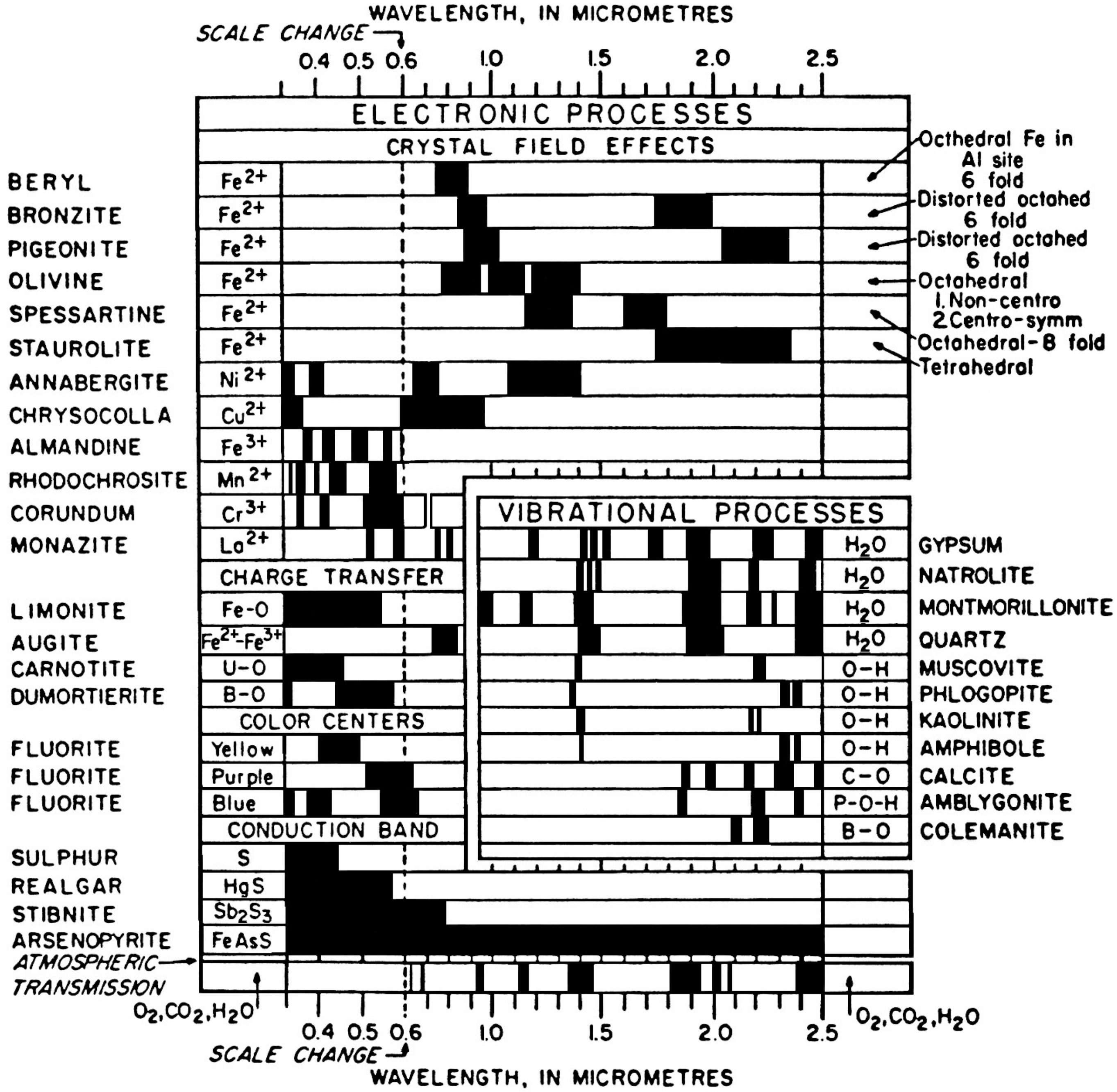
The OH commonly occurs in multiple crystallographic sites of a specific mineral and is typically attached to metal ions. Thus, there may be more than one OH feature. The metal-OH bend occurs near 10 µm (usually superimposed on the stronger Si-O fundamental in silicates). The combination metal-OH bend plus OH stretch occurs near 2.2 to 2.3 µm and is very diagnostic of mineralogy (e.g. see Clark *et al*., 1990 and references therein).

Carbonates. Carbonates also show diagnostic vibrational absorption bands.

The observed absorptions are due to the planar CO_3^{-2} ion. There are four vibrational modes in the free CO_3^{-2} ion: the symmetric stretch, v_1: 1063 cm^{-1} (9.407 µm); the out-of-plane bend, v_2: 879 cm^{-1} (11.4 µm); the asymmetric stretch, v_3: 1415 cm^{-1} (7.067 µm); and the in-plane bend, v_4: 680 cm-1 (14.7 µm)

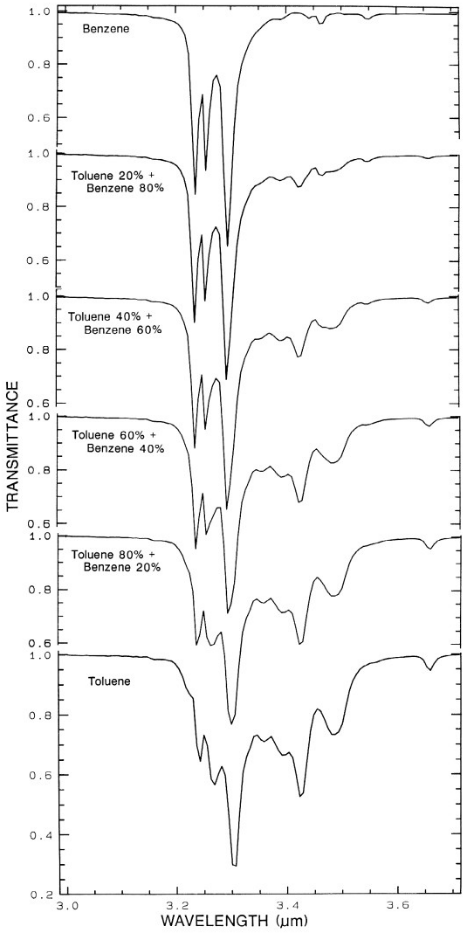
Combination and overtone bands of the CO_3 fundamentals occur in the near IR. The two strongest are $v_1 + 2v_3$ at 2.50-2.55µm (4000-3900 cm^{-1}), and $3v_3$ at 2.30-2.35 µm (4350-4250 cm^{-1}; e.g. Figure 10a). Three weaker bands occur near 2.12-2.16 µm ($v_1 + 2v_3 + v_4$ or $3v_1 + 2v_4$; 4720-4630 cm^{-1}), 1.97-2.00 µm ($2v_1 + 2v_3$; 5080-5000 cm^{-1}), and 1.85-1.87 µm ($v_1 + 3v_3$; 5400-5350 cm^{-1}; (e.g. Hunt and Salisbury, 1971). The band positions in carbonates vary with composition (Hunt and Salisbury, 1971; Gaffey, 1986, Gaffey *et al.*, 1993). An example of such a band shift in absorption position from calcite to dolomite.


SCALED REFLECTANCE
1.0
0.9
0.8
0.7
2.1
2.2
2.3
2.4
2.5
WAVELENGTH (μm)
Dolomite
Calcite
AVIRIS
Resolution

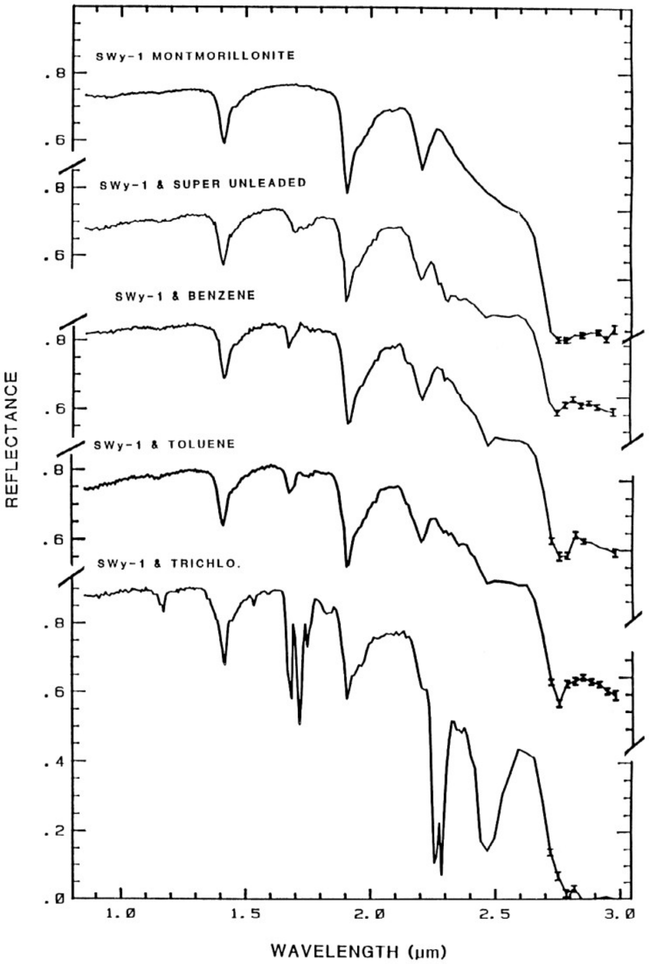

WAVELENGTH, IN MICROMETRES
SCALE CHANGE
0.4 0.5 0.6 1.0 1.5 2.0 2.5
ELECTRONIC PROCESSES
CRYSTAL FIELD EFFECTS
BERYL Fe^{2+}
BRONZITE Fe^{2+}
PIGEONITE Fe^{2+}
OLIVINE Fe^{2+}
SPESSARTINE Fe^{2+}
STAUROLITE Fe^{2+}
ANNABERGITE Ni^{2+}
CHRYSOCOLLA Cu^{2+}
ALMANDINE Fe^{3+}
RHODOCHROSITE Mn^{2+}
CORUNDUM Cr^{3+}
MONAZITE La^{2+}
Octhedral Fe in Al site 6 fold
Distorted octahed 6 fold
Distorted octahed 6 fold
Octahedral
1. Non-centro
2. Centro-symm
Octahedral - 8 fold
Tetrahedral
CHARGE TRANSFER
LIMONITE Fe-O
AUGITE Fe^{2+}-Fe^{3+}
CARNOTITE U-O
DUMORTIERITE B-O
COLOR CENTERS
FLUORITE Yellow
FLUORITE Purple
FLUORITE Blue
CONDUCTION BAND
SULPHUR S
REALGAR HgS
STIBNITE Sb_2S_3
ARSENOPYRITE FeAsS
VIBRATIONAL PROCESSES
H_2O GYPSUM
H_2O NATROLITE
H_2O MONTMORILLONITE
H_2O QUARTZ
O-H MUSCOVITE
O-H PHLOGOPITE
O-H KAOLINITE
O-H AMPHIBOLE
C-O CALCITE
P-O-H AMBLYGONITE
B-O COLEMANITE
ATMOSPHERIC TRANSMISSION
O_2,CO_2,H_2O
O_2,CO_2,H_2O
0.4 0.5 0.6 1.0 1.5 2.0 2.5
SCALE CHANGE
WAVELENGTH, IN MICROMETRES

SPECTRA OF MISCELLANEOUS MINERALS AND MATERIALS

Organics. Organic materials are found all over the Earth, and in the solar system. The C-H stretch fundamental occurs near 3.4 µm, the first overtone is near 1.7 µm, and a combination band near 2.3 µm. The combinations near 2.3 µm can sometimes be confused with OH and carbonate absorptions in minerals especially at low spectral resolution.



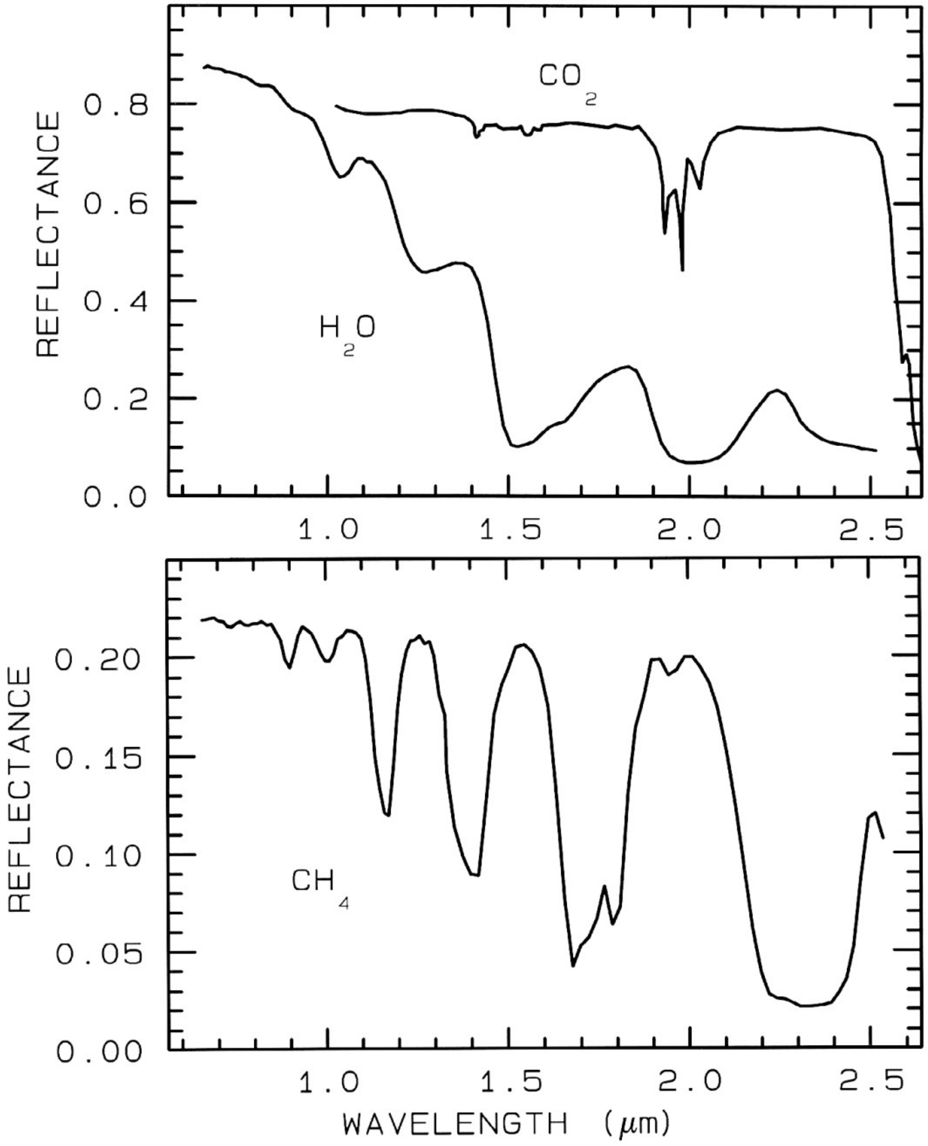
Transmittance spectra of organics and mixtures showing the complex absorptions in the CH-stretch fundamental spectral region



Reflectance spectra of montmorillonite, and montmorillonite mixed with super unleaded gasoline, benzene, toluene, and trichlorethylene. Montmorillonite has an absorption feature at 2.2 µm, whereas the organics have a CH combination band near 2.3 µm. The first overtone of the CH stretch can be seen at 1.7 microns, and the second overtone near 1.15 µm. From King and Clark (1989b).

Ices

Just like water in minerals shows diagnostic absorption bands, ice (crystalline H_2O) which is formally a mineral, also shows strong absorption bands. Spectra of solid H_2O, CO_2, and CH_4 in Figure. The spectral features in Figure are all due to vibrational combinations and overtones. Note the H_2O spectra show broad absorptions compared to the others. The reason is that while ice is normally a hexagonal structure, the hydrogen bonds are orientationally disordered (e.g. Hobbs, 1974), and the disorder broadens the absorptions.



Reflectance spectra of solid carbon dioxide, CO2, methane, CH4, and water, H2O, from Clark et al. (1986).

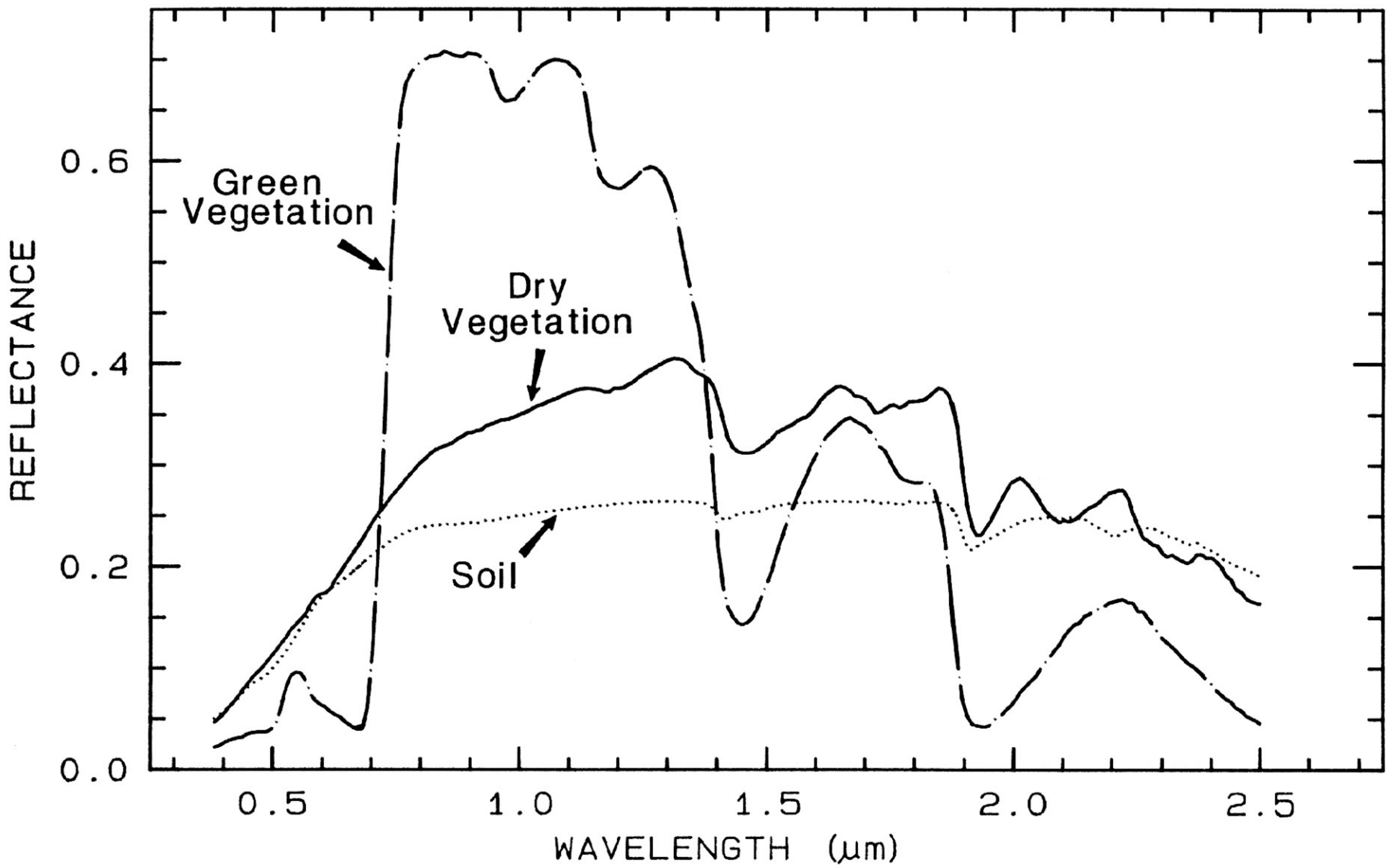
Vegetation

Spectra of vegetation come in two general forms: green and wet (photosynthetic), and dry non-photosynthetic but there is a seemingly continuous range between these two end members.

The spectra of these two forms are compared to a soil spectrum in Figure. Because all plants are made of the same basic components, their spectra appear generally similar.

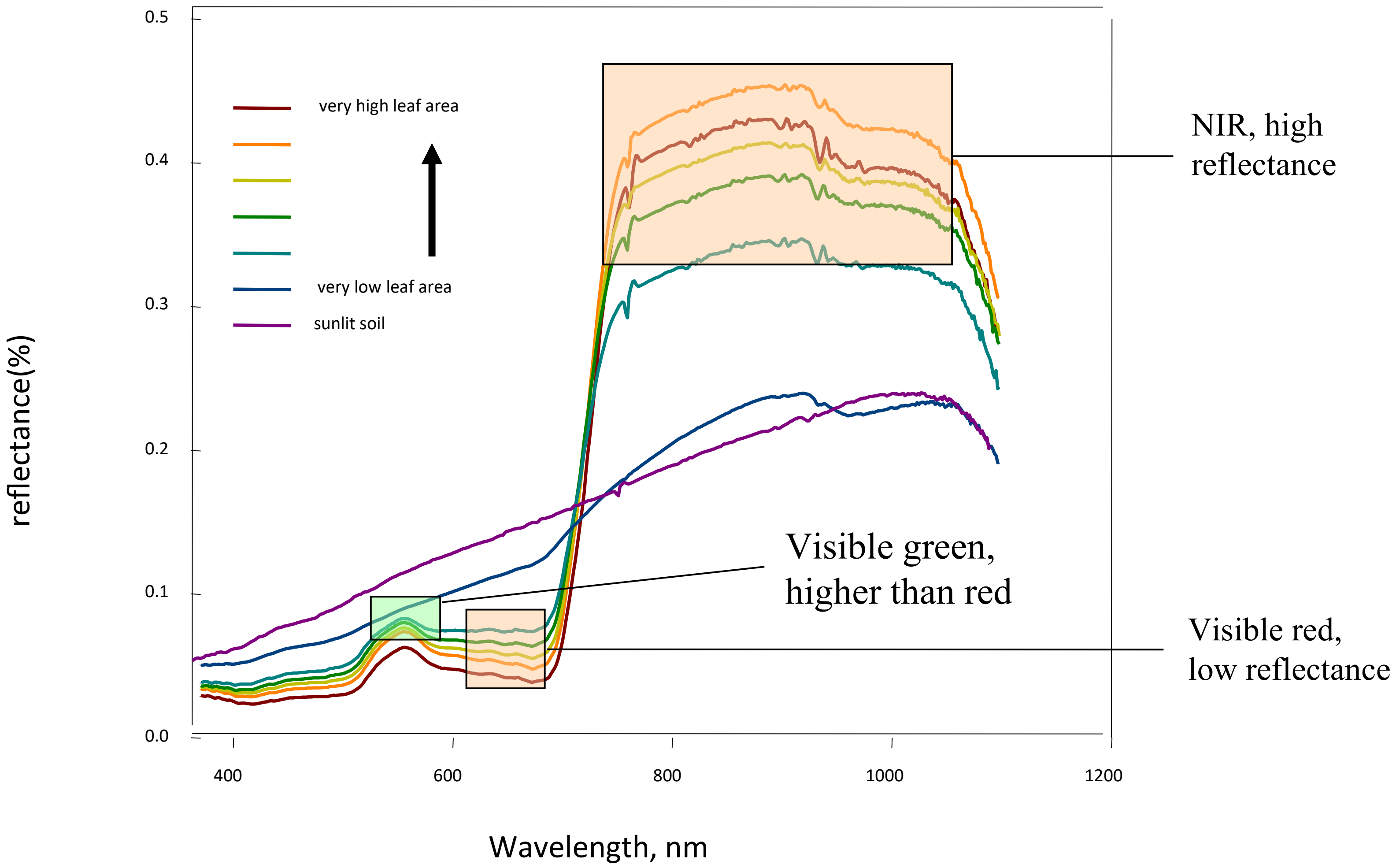
The near-infrared spectra of green vegetation are dominated by liquid water vibrational absorptions.

The water bands are shifted to slightly shorter wavelengths than in liquid water, due to hydrogen bonding. The absorption in the visible is due to chlorophyll. The dry non-photosynthetic vegetation spectrum shows absorptions due to cellulose, lignin, and nitrogen. Some of these absorptions can be confused with mineral absorptions, unless a careful spectral analysis is done



Reflectance spectra of photosynthetic (green) vegetation, non-photosynthetic (dry) vegetation, and a soil. The green vegetation has absorptions short of 1 μm due to chlorophyll. Those at wavelengths greater than 0.9 μm are dominated by liquid water. The dry vegetation shows absorptions dominated by cellulose, but also lignin and nitrogen. These absorptions must also be present in the green vegetation, but can be detected only weakly in the presence the stronger water bands.

Spectral information: vegetation

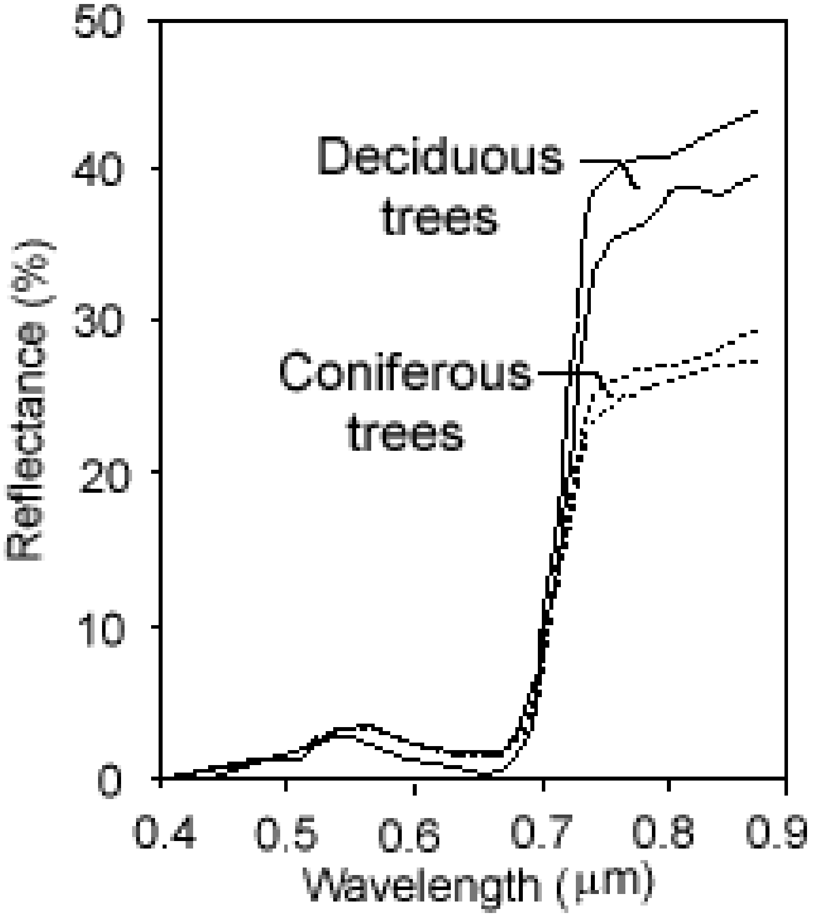


NIR, high reflectance

Visible green, higher than red

Visible red, low reflectance

Vegetation characteristics



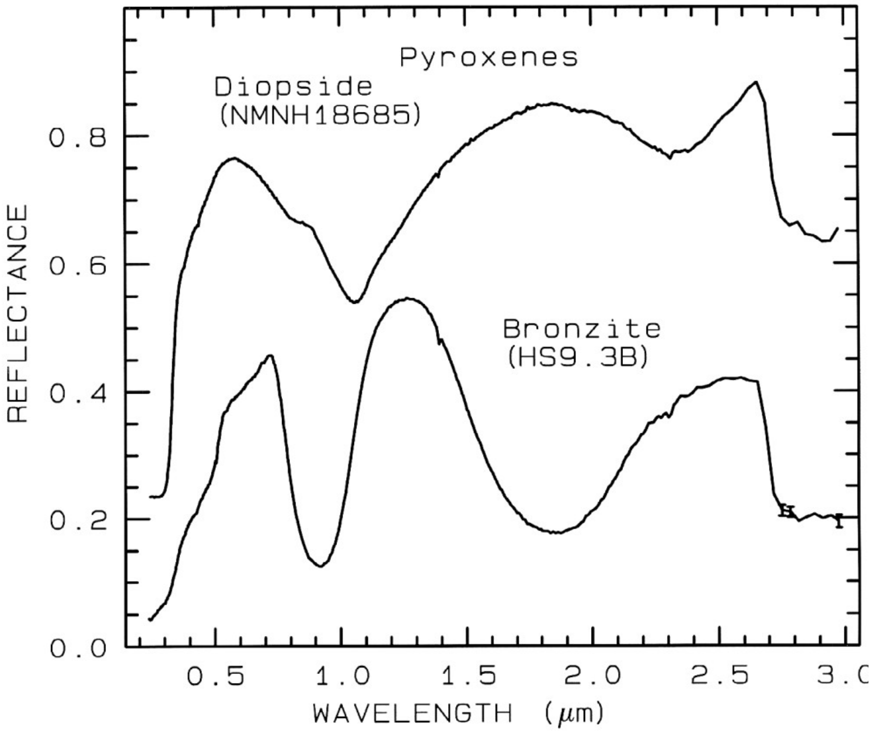
- high reflectivity in NIR
- - distinguish between vegetation types on basis of spectral reflection curves

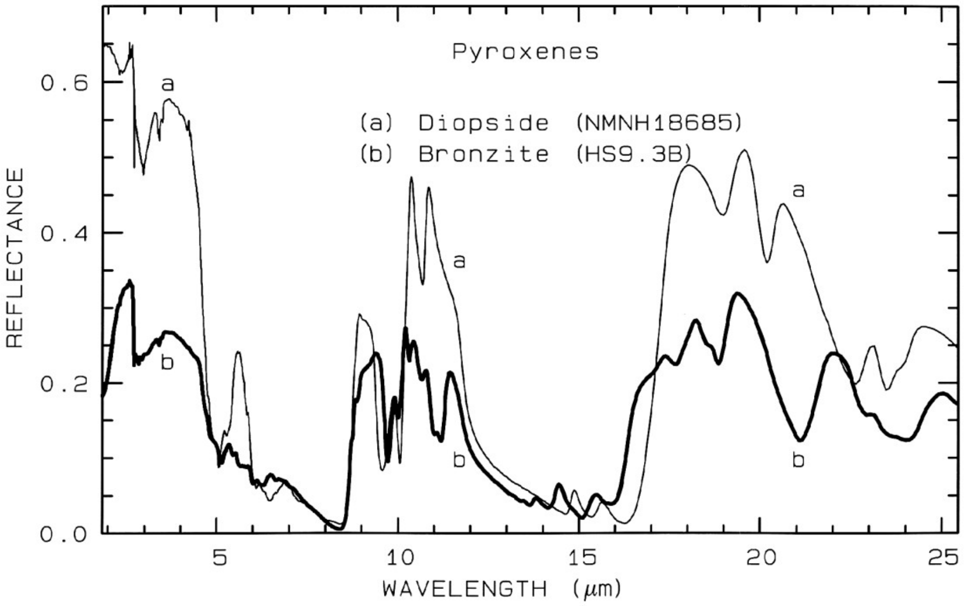
THE SENSITIVITY OF ABSORPTION BANDS TO CRYSTAL STRUCTURE AND CHEMISTRY

In many cases spectroscopy is very sensitive to subtle changes in crystal structure or chemistry. This has resulted in confusion in the past over cause and effect. More recently, this sensitivity has been recognized as a powerful means of studying the structure and composition of minerals

Because spectroscopy is sensitive to so many processes, the spectra can be very complex and there is still much to learn. However, it is because of this sensitivity that spectroscopy has great potential as a diagnostic tool. In fact for some materials, spectroscopy is an excellent tool not only for detecting certain chemistries, but also at abundance levels unmatched by other tools.

Pyroxenes. The iron bands near 1 and 2 µm shift with pyroxene composition





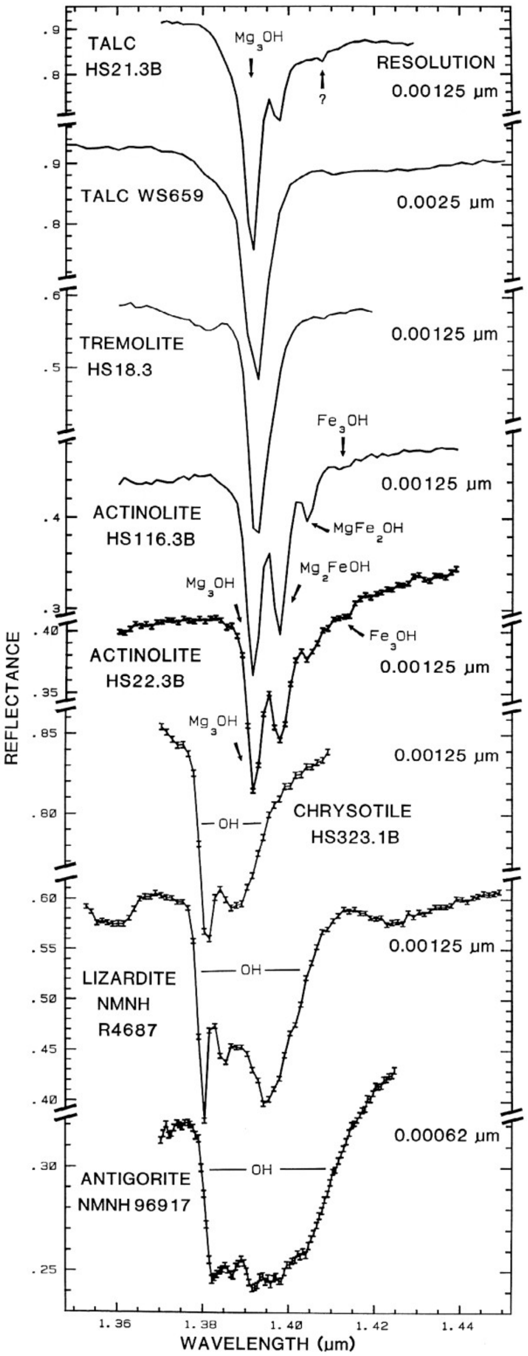
The change in Fe^{2+} -absorption band position and shape with composition

OH Examples. The sharper OH-related absorption bands allow smaller band shifts to be measured. These bands can be so sensitive that it is possible to distinguish between the isochemical end-members of the Mg-rich serpentine group, chrysotile, antigorite, and lizardite (King and Clark, 1989a, and Figure).

Mustard (1992) calibrated changes in the 1.4-µm and 2.3-µm absorptions in the tremolite-actinolite solid solution series; example spectra of the 1.4-µm absorptions are shown in Figure.

High spectral resolution reflectance spectra of the first overtone of OH in talc, tremolite, actinolite, crysotile, lizardite, and antigorite. The three sharp absorption bands in talc, tremolite and actinolite are caused by Mg and Fe ions associated with the hydroxyls, causing small band shifts. The Fe:Fe+Mg ratio can be estimated. In chrysotile, lizardite and antigorite, the absorptions change with small structural differences even though the composition is constant

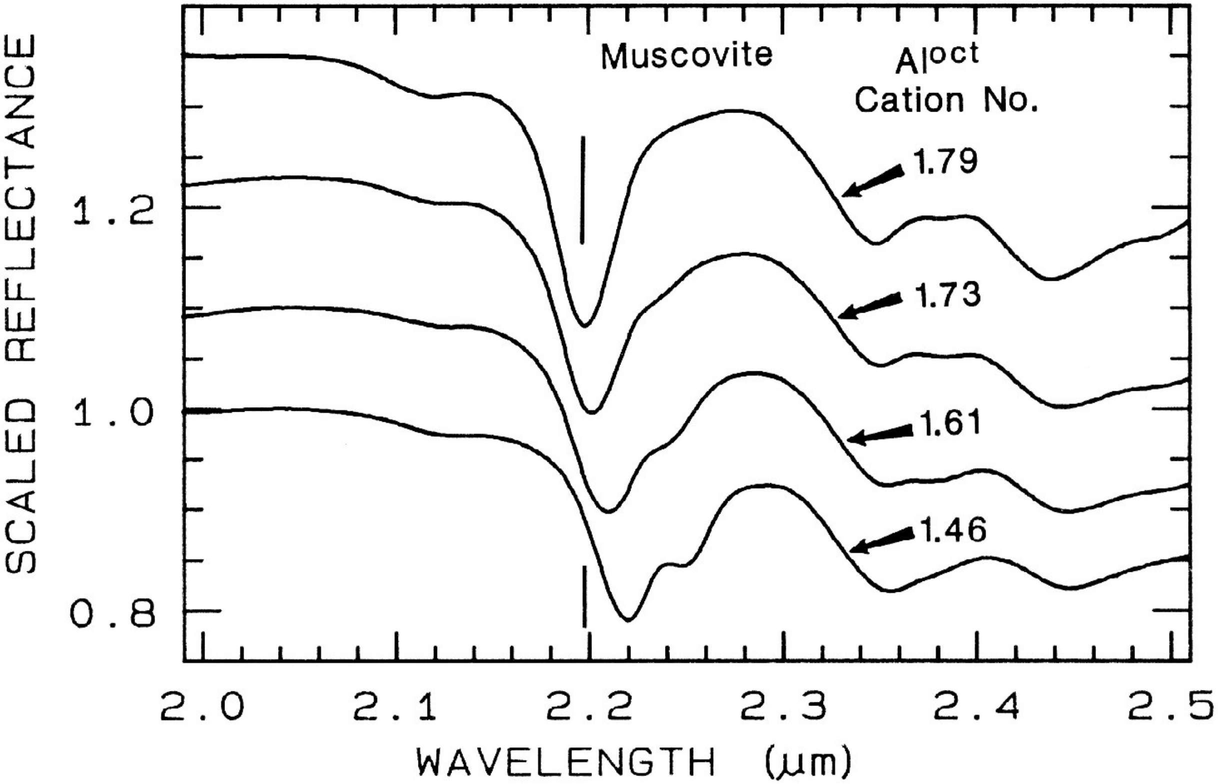
The strong and sharp OH features have proven particularly diagnostic of clay mineralogy



Al in Muscovite

More recently, subtle shifts have been found in muscovite series with aluminum composition. As elements substitute for aluminum in the crystal structure, the crystal becomes slightly distorted relative to no substitutions.

This causes slight changes in Al-O-H bond lengths and thus shifts absorption band position. In this case, the shift of the 2.2-µm absorption appears continuous with composition.



Reflectance spectra of muscovite showing band shifts due to changing aluminum composition

Reflectance spectroscopy can be used without sample preparation, and it is non-destructive. This makes mapping of exposed minerals from aircraft possible, including detailed clay mineralogy (e.g. Clark *et al*., 1993a).

Visual and near-infrared spectroscopy, on the other hand, is insensitive to some minerals which do not have absorptions in this wavelength region. For example, quartz has no diagnostic spectral features in the visible and near-infrared.

Quartz must be detected at its fundamental Si-O stretching region near 10 µm.

FACTROS AFFECTING SPECTRA

THE SCATTERING PROCESS

Scattering is the process that makes reflectance spectroscopy possible: photons enter a surface, are scattered one or more times, and while some are absorbed, others are scattered from the surface so that we may see and detect them.

Scattering can also be thought of as scrambling information. The information is made more complex, and because scattering is a non-linear process, recovery of quantitative information is more difficult.

Reflectance of a particulate surface, however, is much more complex and the optical path of photons is a random walk. At each grain the photons encounter, a certain percentage are absorbed. If the grain is bright, like a quartz grain at visible wavelengths, most photons are scattered and the random walk process can go on for hundreds of encounters.

If the grains are dark, like magnetite, the majority of photons will be absorbed at each encounter and essentially all photons will be absorbed in only a few encounters

The stronger absorption will penetrate less into the surface, encountering fewer grains because the photons are absorbed.

At the wavelengths of the weaker absorption, less photons are absorbed with each encounter with a grain, so the random walk process goes further, increasing the average photon path length.

The greater path length will result in more absorption, thus strengthening the weak absorption in a reflectance spectrum.

Mixtures

The real world is a complex mixture of materials, at any scale we view it. In general, there are 4 types of mixtures

1) Linear Mixture. The materials in the field of view of the detector are optically separated, so the reflectance at each wavelength is the fraction of each materials. This is also called areal mixture.

2) Intimate Mixture. An intimate mixture occurs when different materials are in intimate contact in a scattering surface, such as the mineral grains in a soil or rock. Depending on the optical properties of each component, the resulting signal is a highly non-linear combination of the end-member spectra.

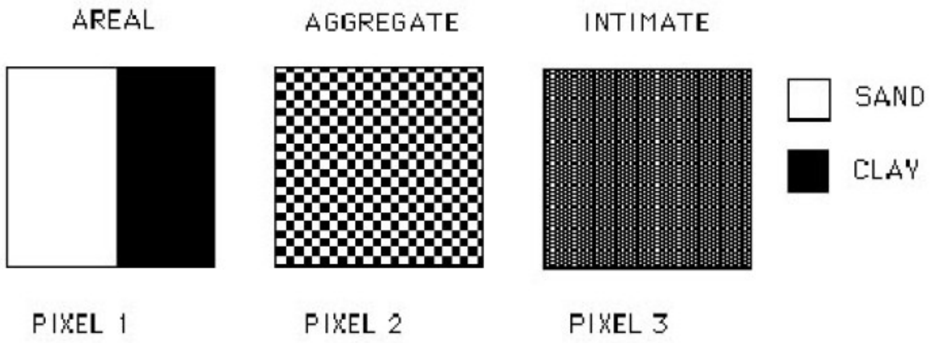
3) Coatings. Coatings occur when one material coats another. Each coating is a scattering/transmitting layer whose optical thickness varies with material properties and wavelength.

4) Molecular Mixtures. Molecular mixtures occur on a molecular level, such as two liquids, or a liquid and a solid mixed together. Examples: water adsorbed onto a mineral; gasoline spilled onto a soil. The close contact of the mixture components can cause band shifts in the adsorbate, such as the interlayer water in montmorillonite, or the water in plants.

Spectral Mixtures

- Areal
- Aggregate
- Intimate

TYPES OF MIXTURES

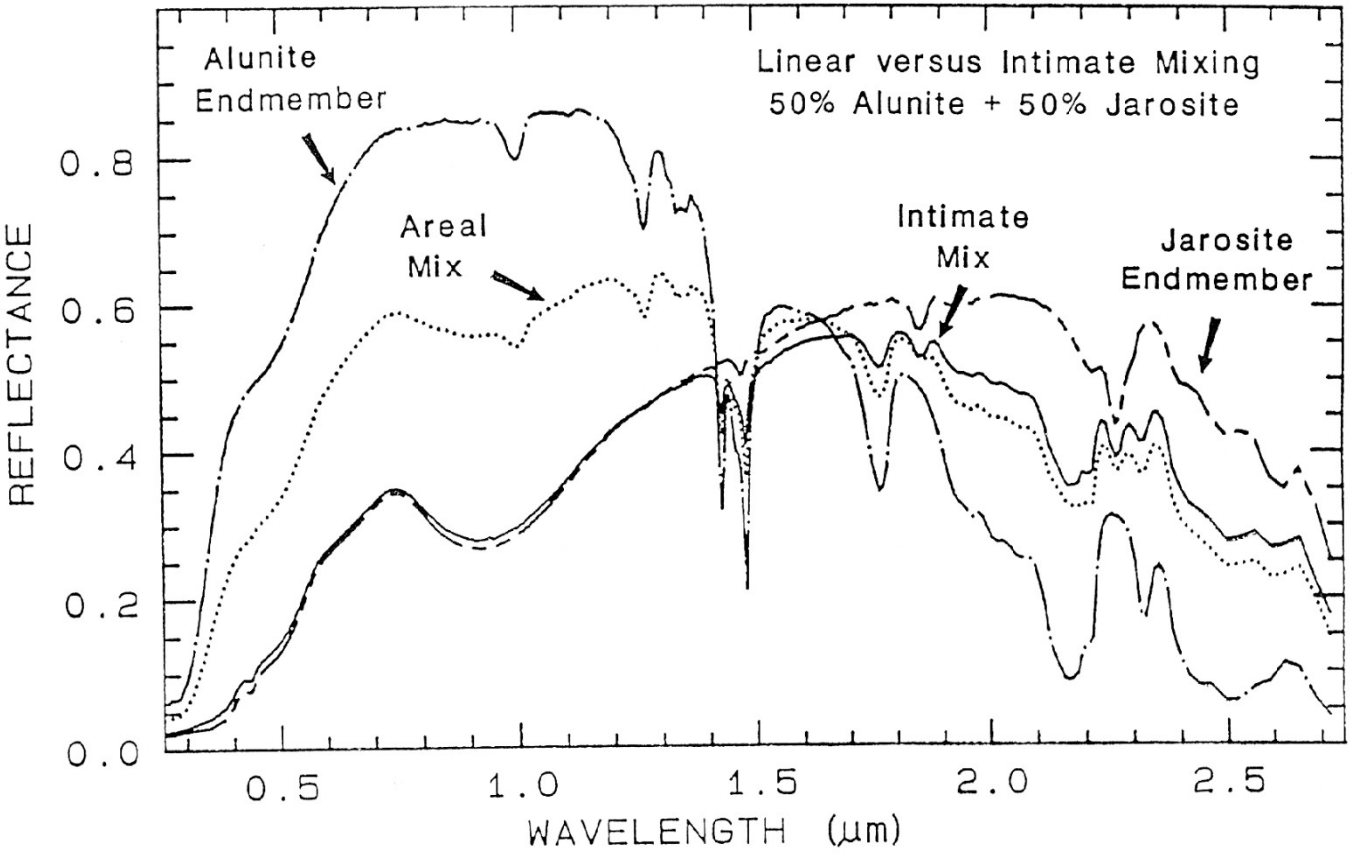


50/50 MIXTURES OF SAND AND CLAY

An example mixture comparison for alunite and jarosite. Note in the intimate mixture how the jarosite dominates in the 0.4 to 1.3-µm region.

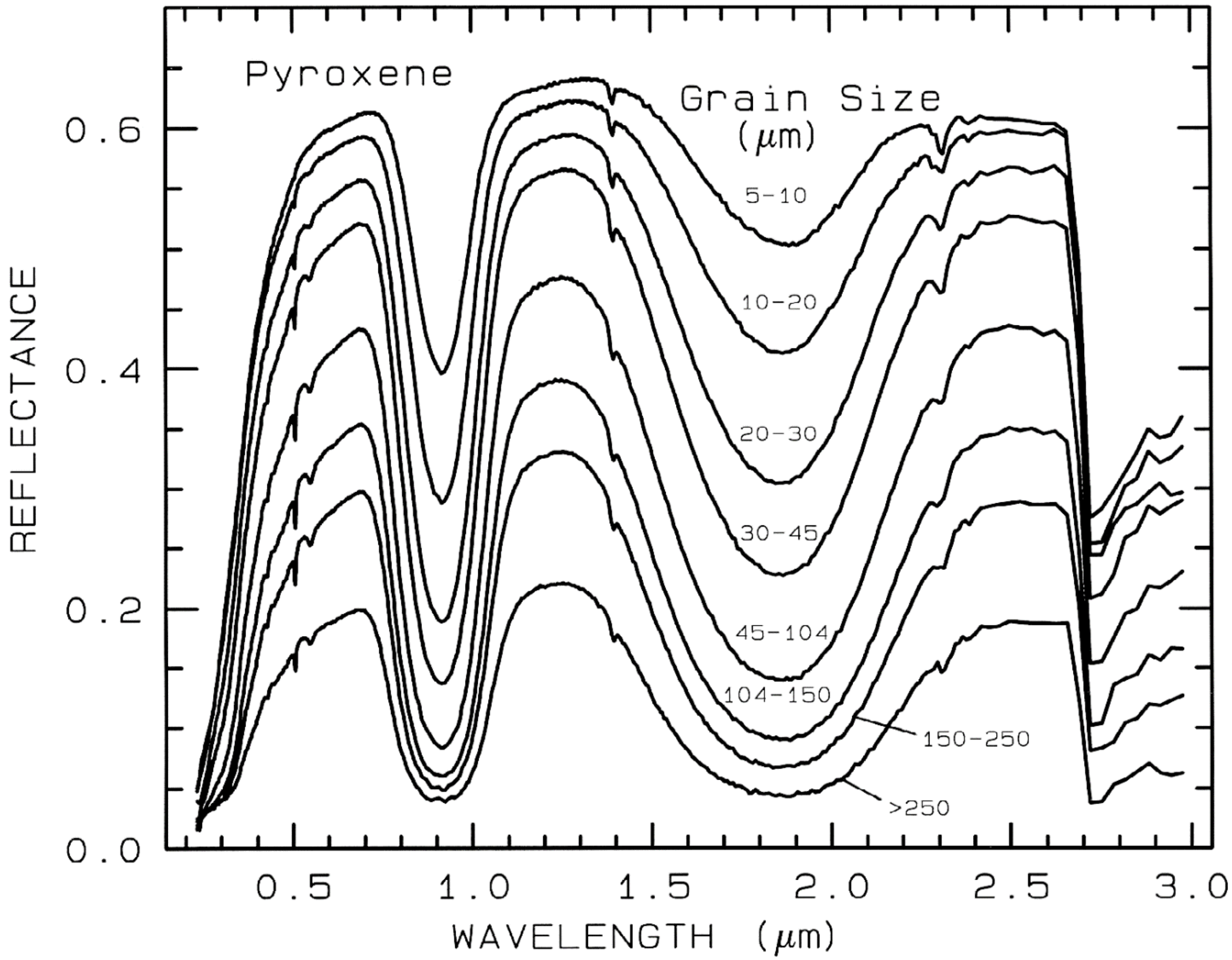
The reason is because in an intimate mixture, the darker material dominates because photons are absorbed when they encounter a dark grain.

In the areal mixture, the brighter material dominates. because the jarosite is finer grained than the alunite and tends to coat the larger alunite grains.



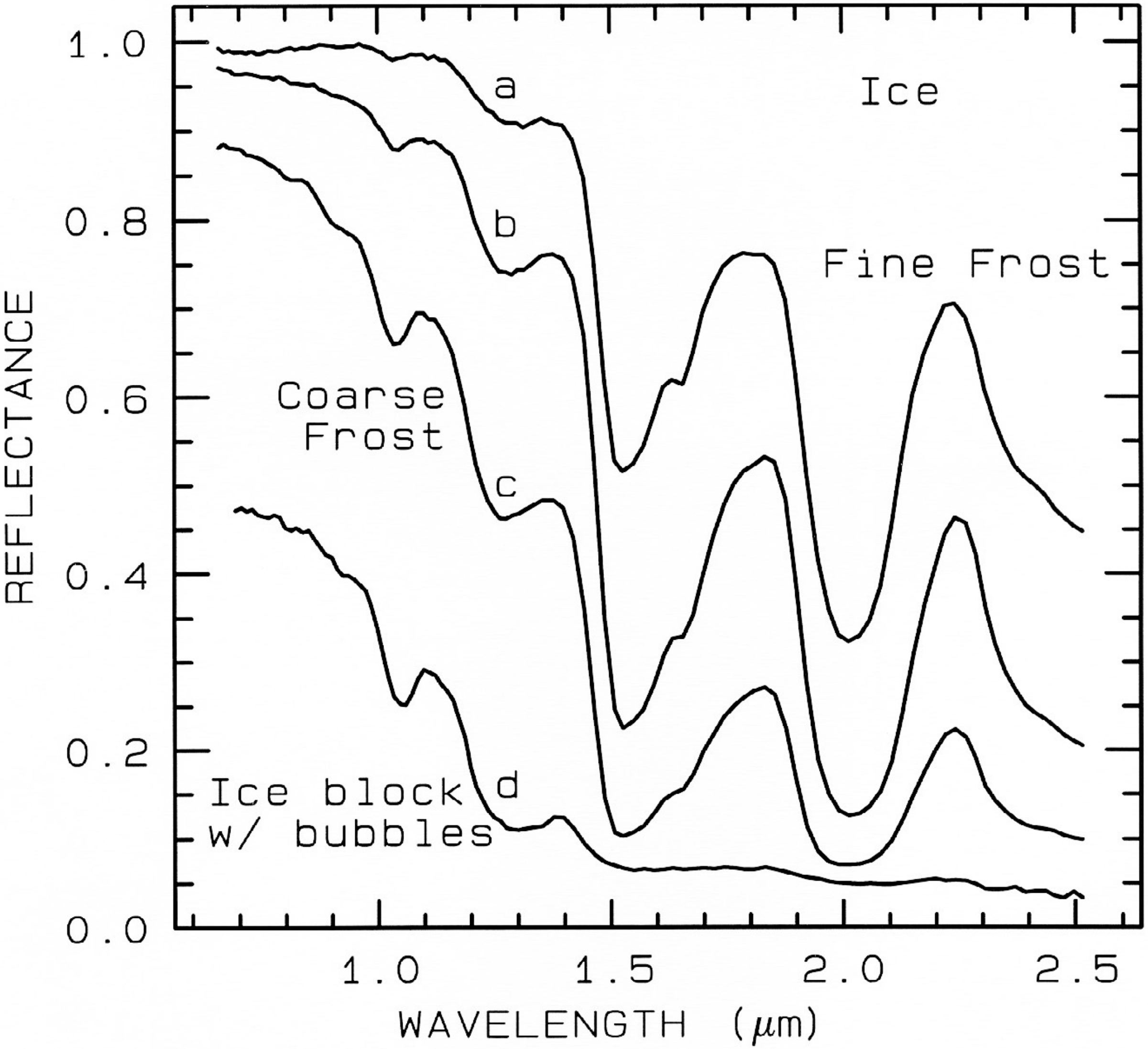
Grain Size Effects

The amount of light scattered and absorbed by a grain is dependent on grain size (e.g. Hapke, 1993; Clark and Roush, 1984). A larger grain has a greater internal path where photons may be absorbed according to Beers Law. In a smaller grain there are proportionally more surface reflections compared to internal photon path lengths. The reflectance decreases as the grain size increases.



Absorption band contrast varies with particle size but does not affect positions of absorption features

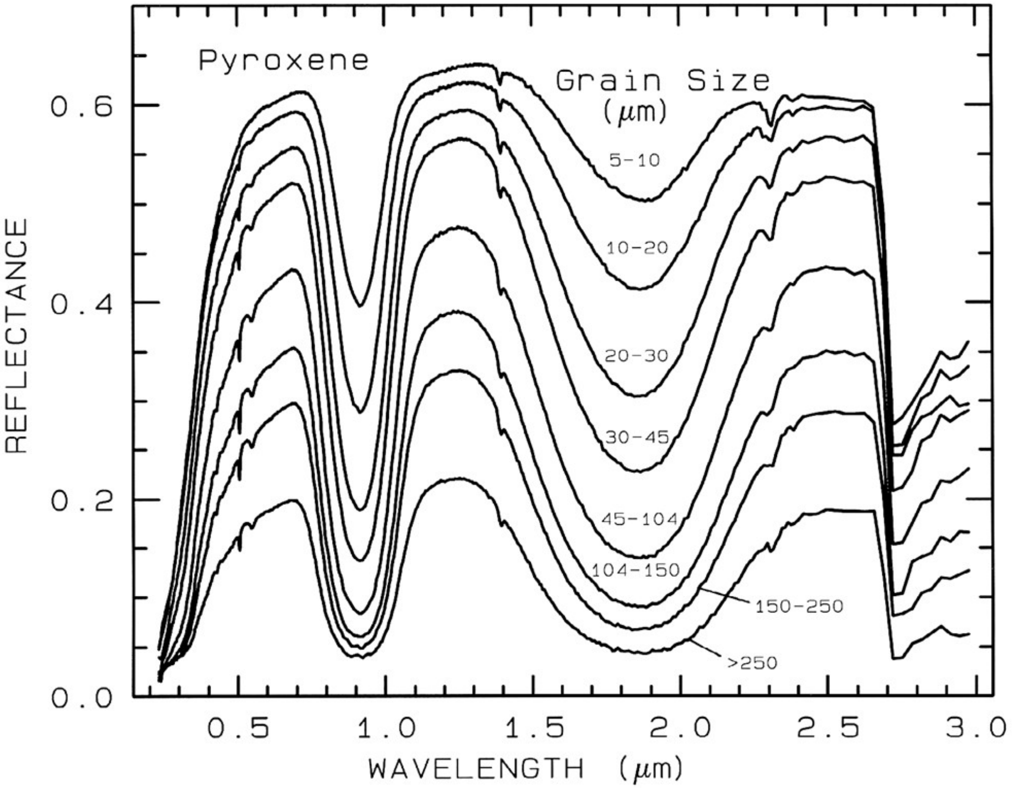
The near-infrared spectral reflectance of A) a fine grained (~50 µm) water frost, B) medium grained (~200 µm) frost, C) coarse grained (400-2000 µm) frost and D) an ice block containing abundant microbubbles. The larger the effective grain size, the greater the mean photon path that photons travel in the ice, and the deeper the absorptions become. Curve D is very low in reflectance because of the large path length in ice

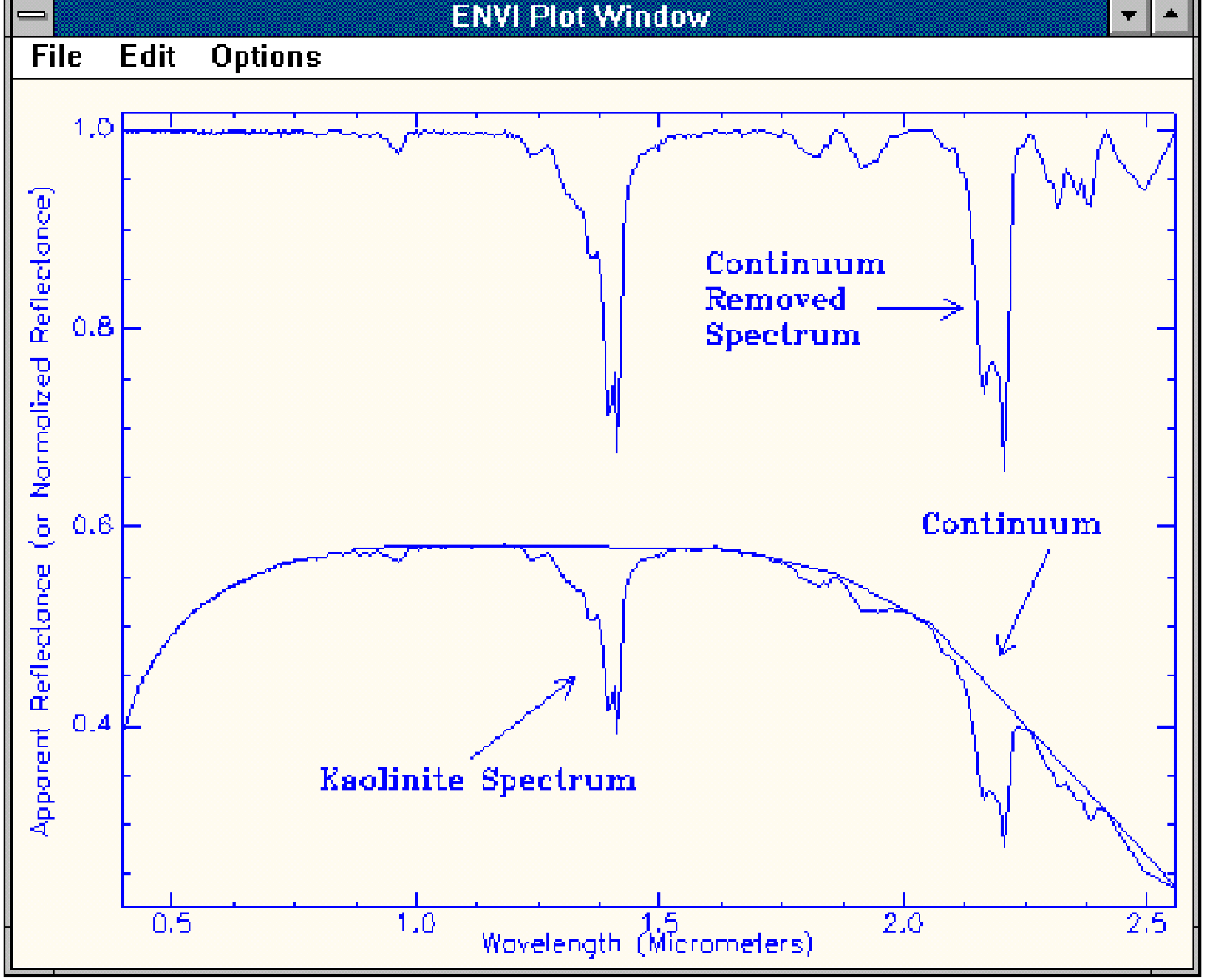


The Continuum and Band Depth

Absorptions in a spectrum have two components: continuum and individual features.
The continuum is the "background absorption" onto which other absorption features are superimposed (Clark and Roush, 1984). It may be due to the wing of a larger absorption feature.

For example, in the pyroxene spectra, the weak feature at 2.3 µm is due to a trace amount of tremolite in the sample and the absorption is superimposed on the broader 2-µm pyroxene band. The broader pyroxene absorption is the continuum to the narrow 2.3-µm feature.



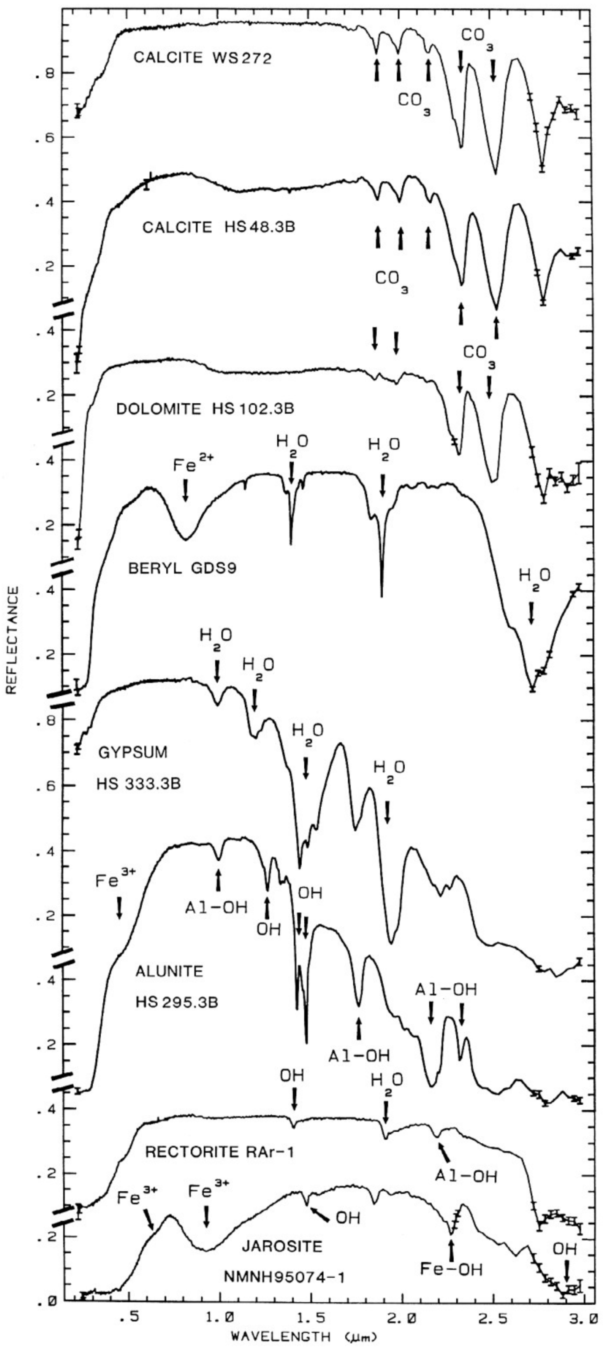


Spectra are normalized to a common reference using a continuum formed by defining high points of the spectrum (local maxima) and fitting straight line segments between these points. The continuum is removed by dividing it into the original spectrum.

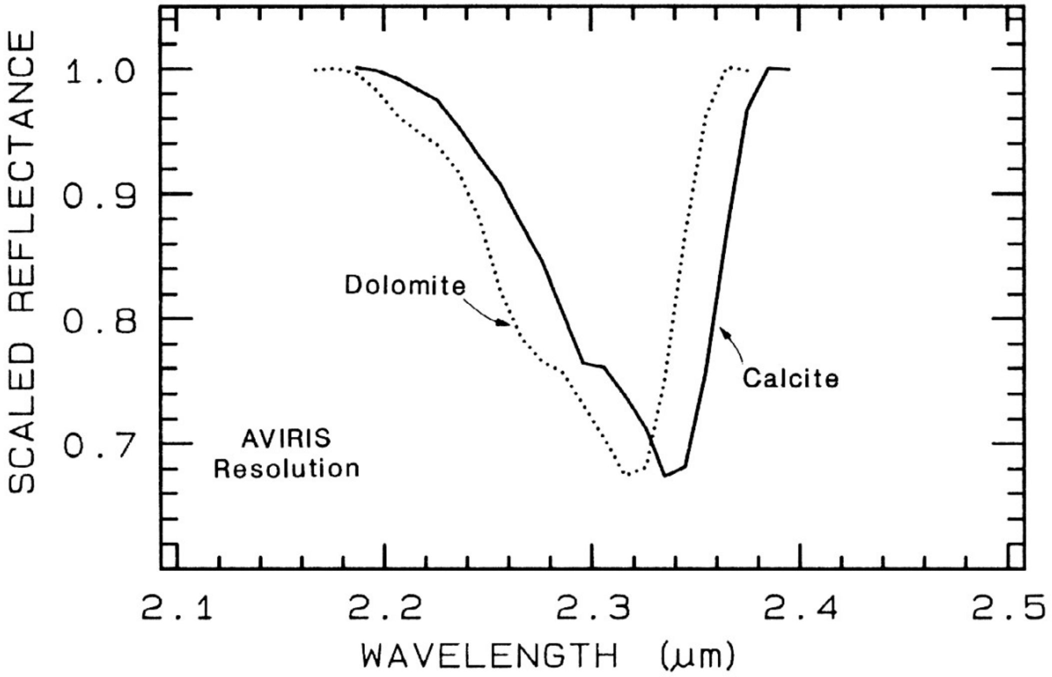
Source: ENVI Manual

A fitted continuum (bottom) and a continuum-removed (top) spectrum for the mineral kaolinite

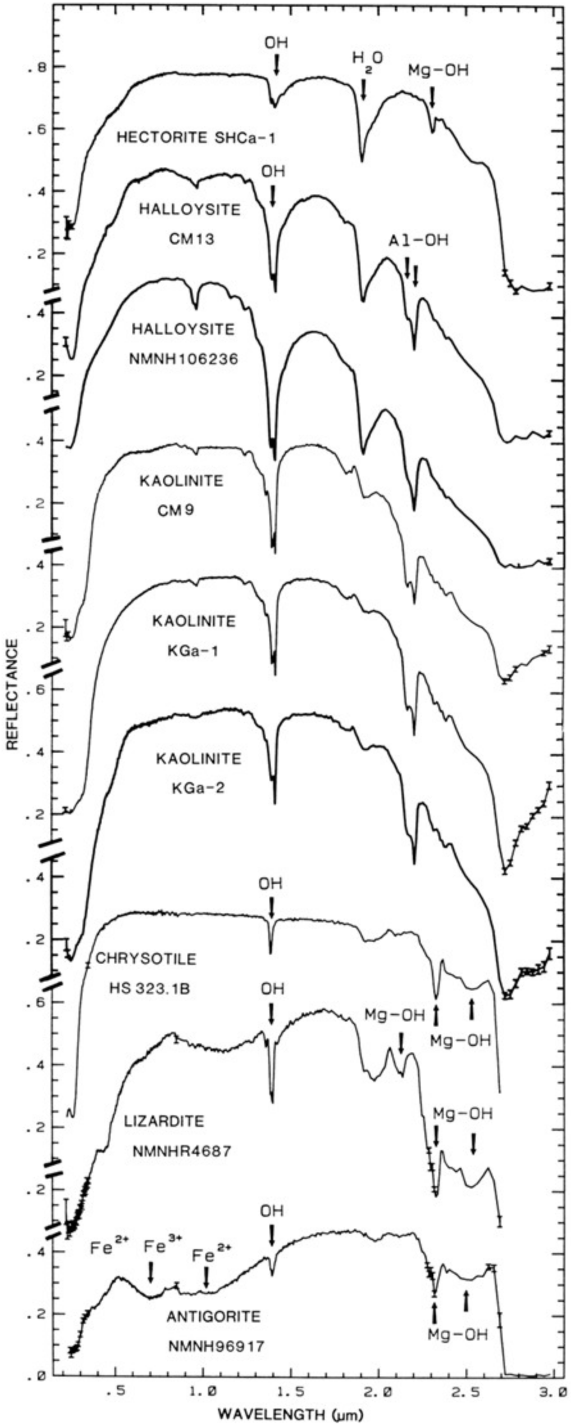
Continuum-Removed Spectral Feature Comparison.



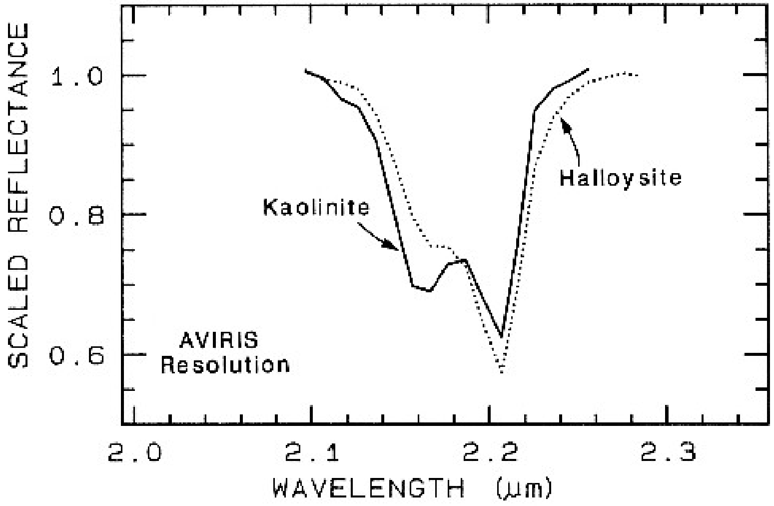
The continuum-removal process isolates spectral features and puts them on a level. Continuum removal was applied to the selected absorption features. Continuum removal normalizes reflectance spectra in order to allow comparison of individual absorption features from a common baseline



For example, compare the spectra of calcite ($CaCO_3$) and dolomite ($CaMg(CO_3)_2$. If we isolate the spectral features, remove the continuum, and scale the band depth (or band area) to be equal, we can see subtle band shifts and shapes.



Compare a harder case: halloysite and kaolinite. You might note that halloysite has a different absorption feature at 1.9 µm. However, if you were obtaining the spectrum through the Earth's atmosphere, you would have virtually no data in that wavelength region because atmospheric water absorbs too much of the signal. The diagnostic feature is the 2.2-µm band. The continua removed 2.2-µm features for halloysite and kaolinite, where we can see significant differences between the spectra of the two minerals.



Comparison of kaolinite and halloysite spectral features. Both mineral spectra have the same band position at 2.2 µm. However, the kaolinite spectrum shows a stronger feature at 2.16 µm than in the halloysite spectrum

Viewing Geometry

We have seen tremendous variation in the spectral properties of minerals and materials in general, due to composition, grain size, and mixture types. So far viewing geometry has not been discussed.

Viewing geometry, including the angle of incidence, angle of reflection, and the phase angle: the angle between the incident light and observer (the angle of reflection), all affect the intensity of light received.

Varying the viewing geometry results in changes in shadowing and the proportions of first surface to multiple scattering (e.g. Hapke, 1993; Nelson, 1986; Mustard and Pieters, 1989), which can affect band depths a small amount except in rare cases (like extreme specular reflection off a mirror or lake surface). While measuring precise light levels are important for things like radiation balance studies, they are of lesser importance in spectral analysis