

Soil Spectroscopy: Principle and Applications



THE REMOTE SENSING
LABORATORIES



Prof. Eyal Ben Dor
Department of Geography and Human Environment

Brno Czech Republic, June 25-26



european
social fund in the
czech republic



EUROPEAN UNION



MINISTRY OF EDUCATION,
YOUTH AND SPORTS



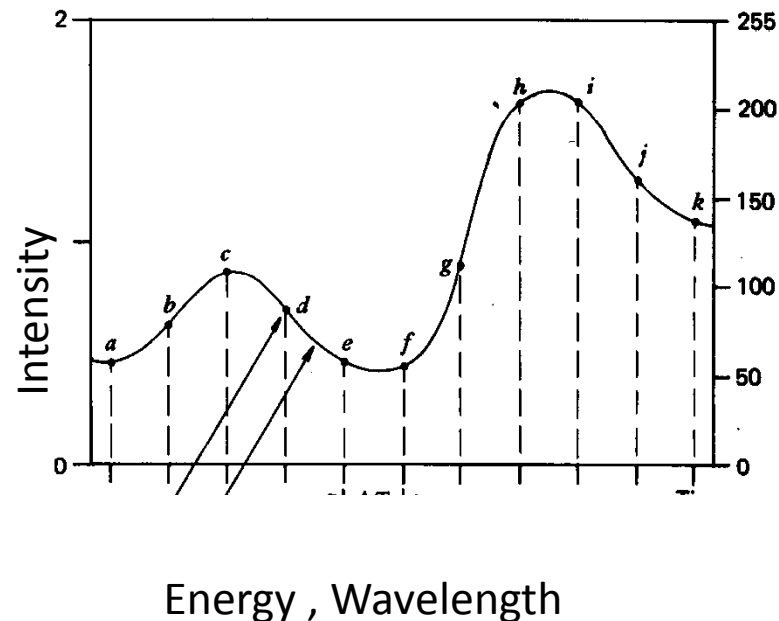
OP Education
for Competitiveness

INVESTMENTS IN EDUCATION DEVELOPMENT

Absorption Mechanism and Spectral Features in Soil

Lesson 3

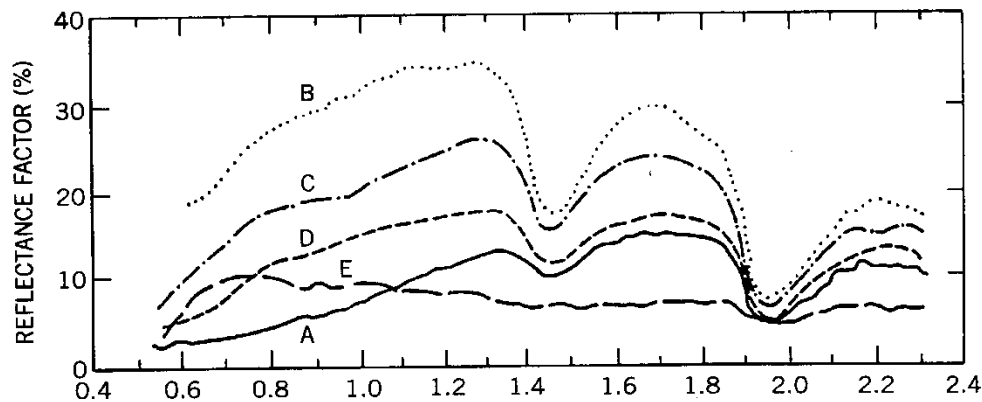
Reflectance Spectrum



A curve describing the relative intensity of the incident and reflected EM as a function of its energy

Chemical Chromophore: A substance that changes the EM in specific wavelength

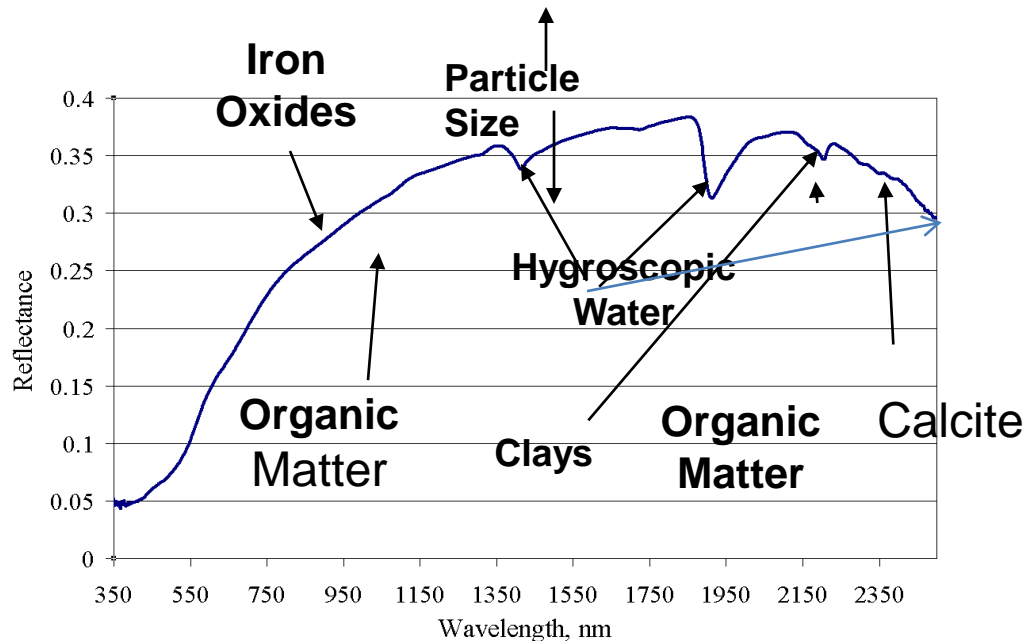
Physical Chromophore: A substance that changes the EM in all wavelength



5 spectral types
in USA

1984

Stoner, E.R. and M.F., Baumgardner, 1981. Characteristic variations in reflectance of surface soils. *Soil Science Society of American Journal* 45: 1161-1165



Main Soil
Chromophores

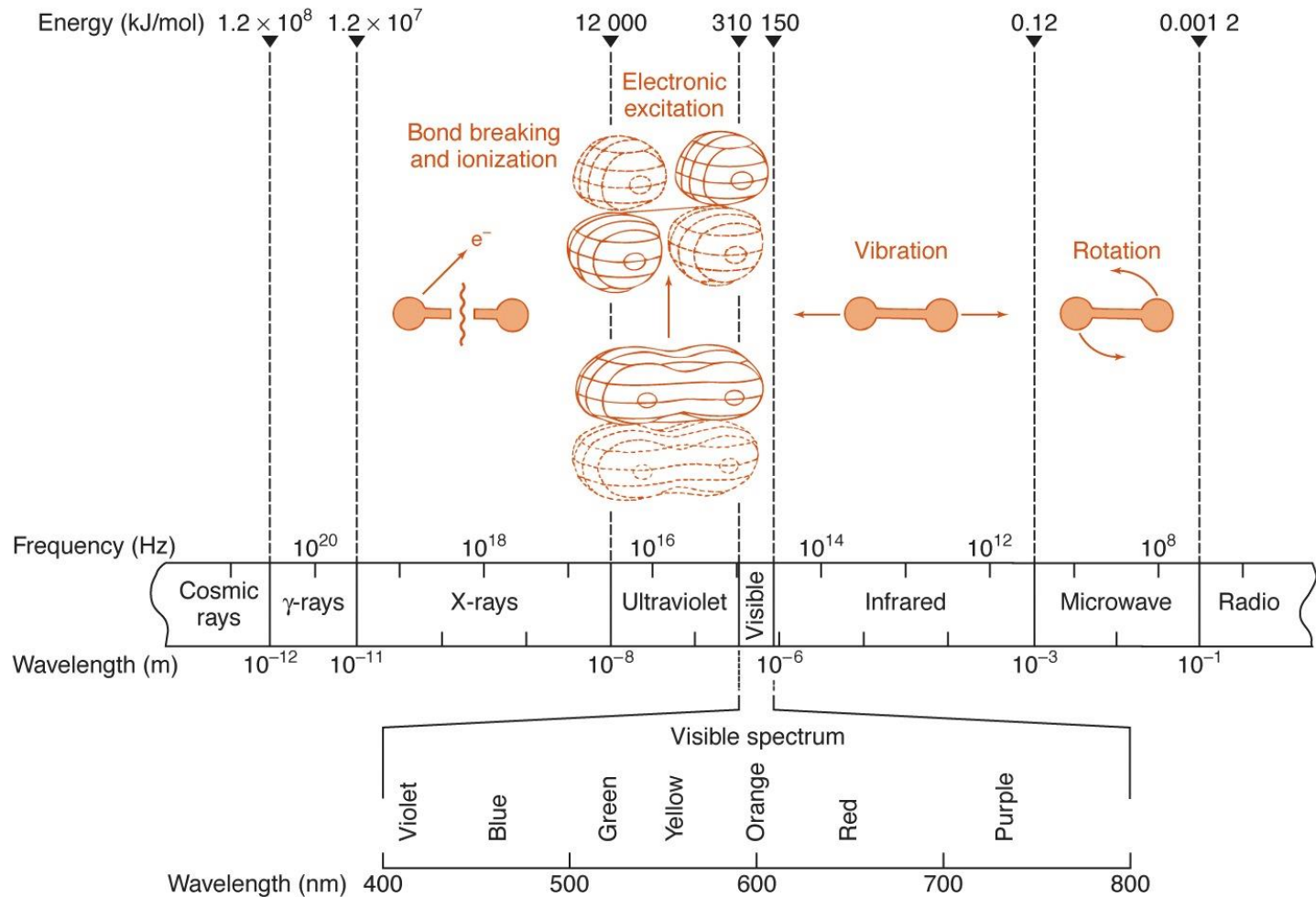
1994

Ben-Dor E., and A. Banin 1995b, Near infrared analysis (NIRA) as a Simultaneously method to evaluate spectral featureless constituents in soils., *Soil Science* 159:259-269

The importance of Spectral Information

- 1) Precise recognition of the targets
- 2) Quantitative analysis
- 3) Ability to go beyond the pixel size (sub pixel analysis)
if HSR data is collected

EM Spectrum and Matter's Interaction



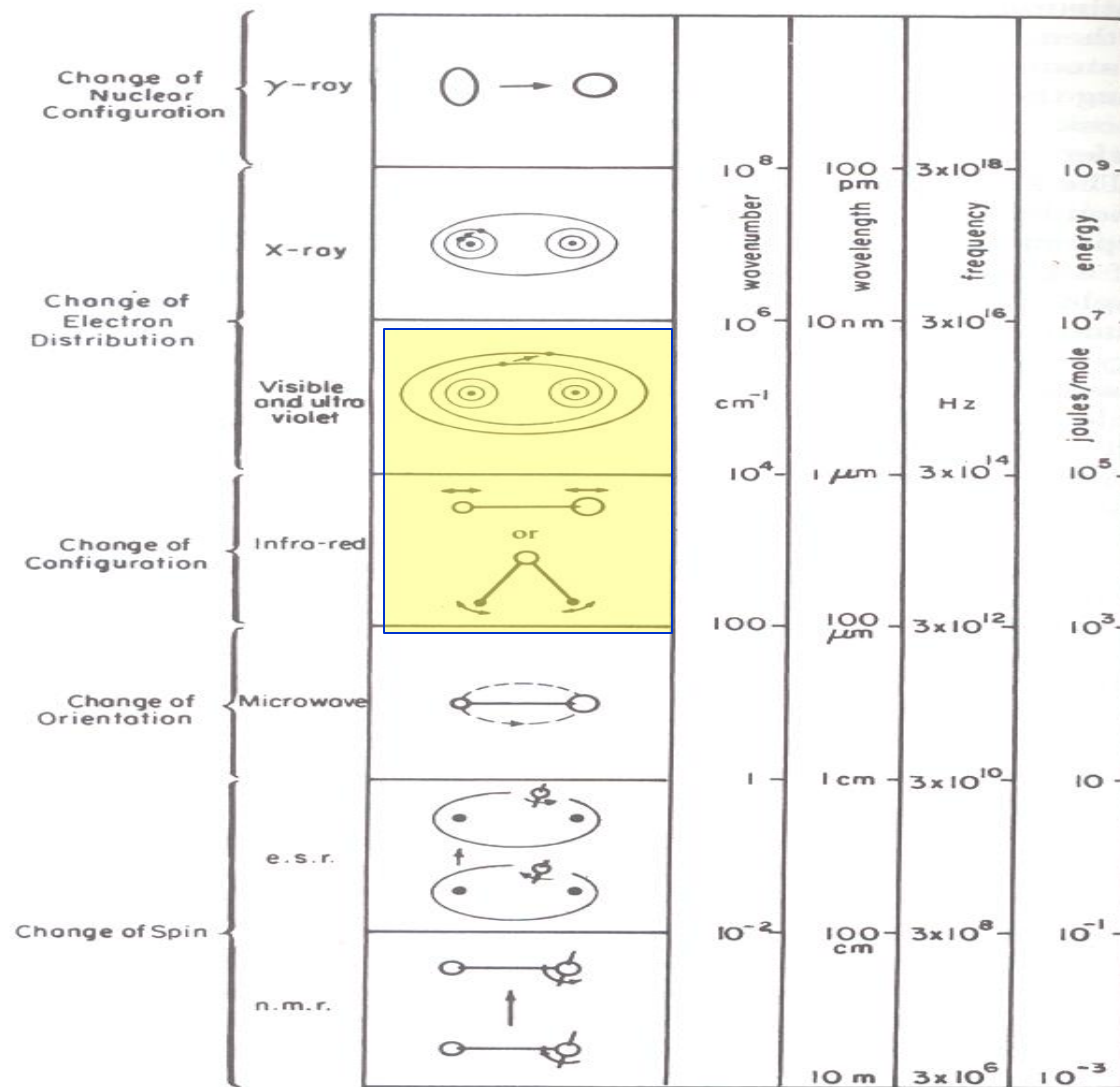


Figure 3.3 The electromagnetic spectrum and the possible types of interactions between photons and a molecule or atom (Banwell, 1983).

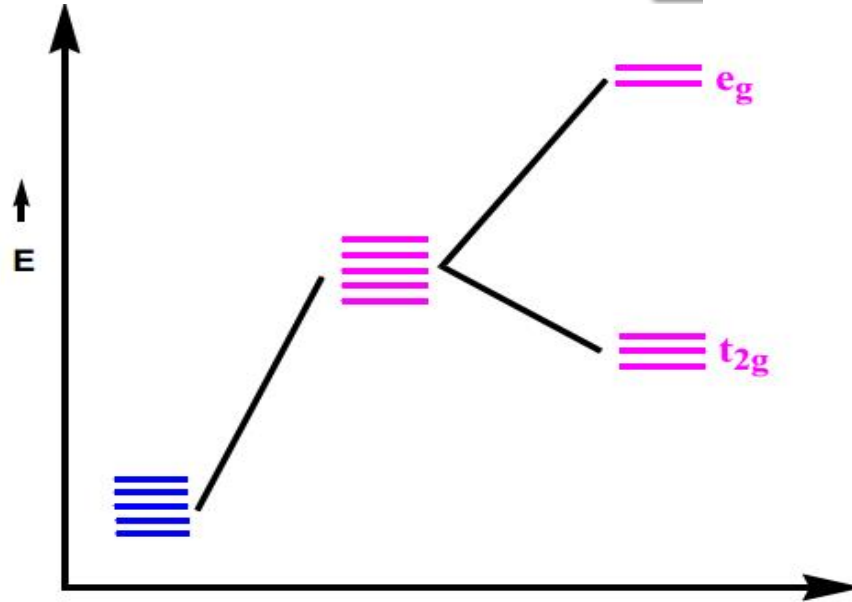
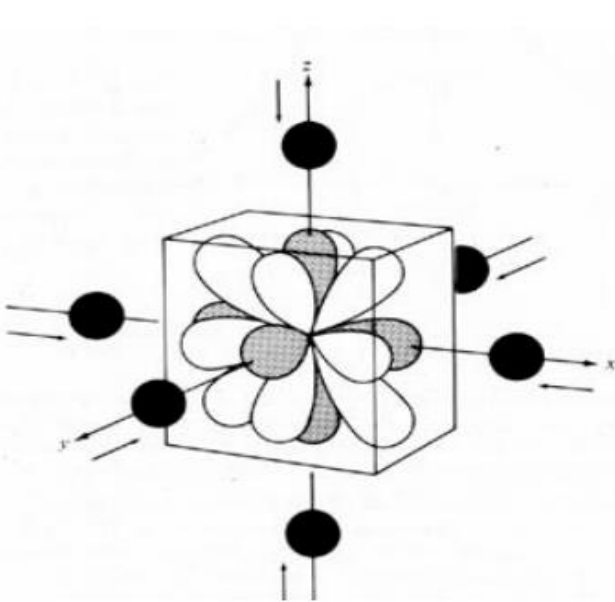
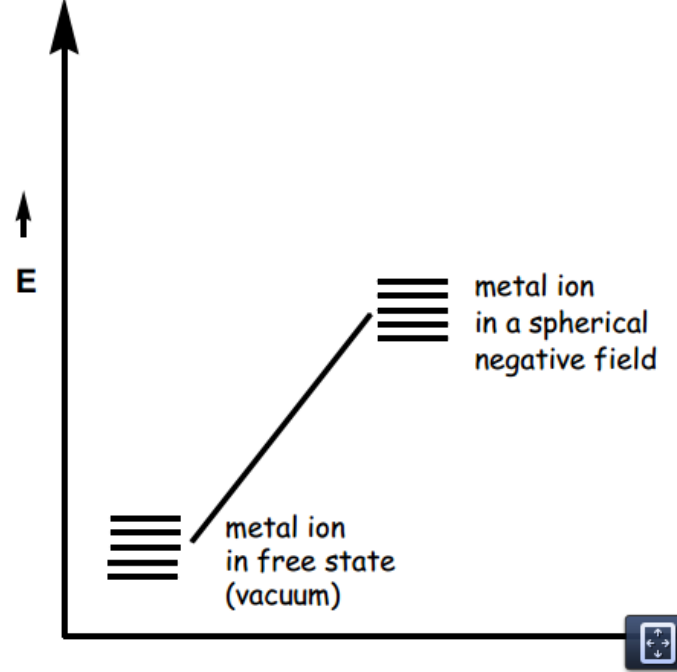
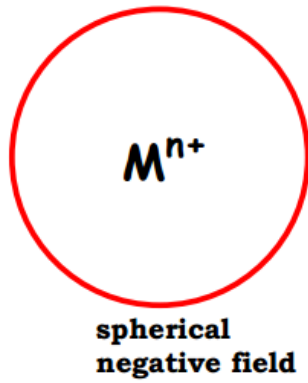
VIS –NIR

ELECTRONIC PROCESSES

- **Crystal field effects**
- **Charge transfer**
- **Semiconductor**
- **Color centers**

CRYSTAL FIELD EFFECTS

- **Energy levels of an ion**
 - **Split and displaced in crystal field**
 - **Determined by**
 - **Valence state**
 - **Coordination number and symmetry**
- **Reflectance spectrum**
 - **Determined primarily by mineralogy not cation**
 - **Depth of feature grain-size dependent**

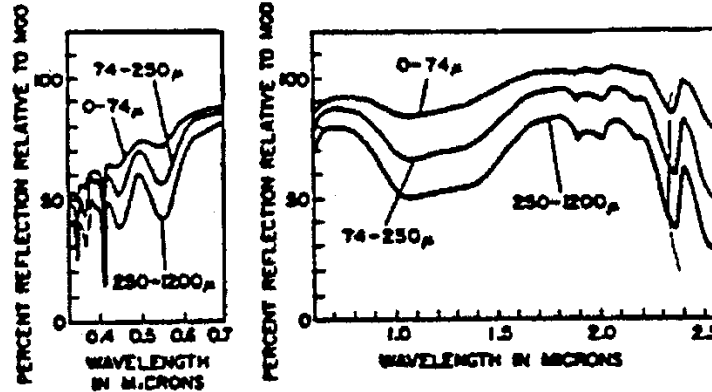


CRYSTAL FIELD EFFECTS

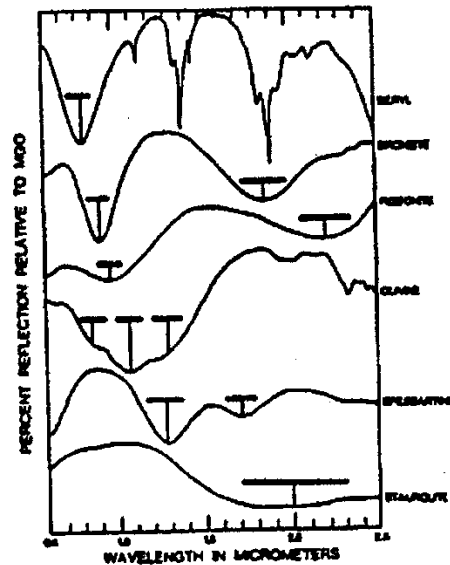
Iron most important

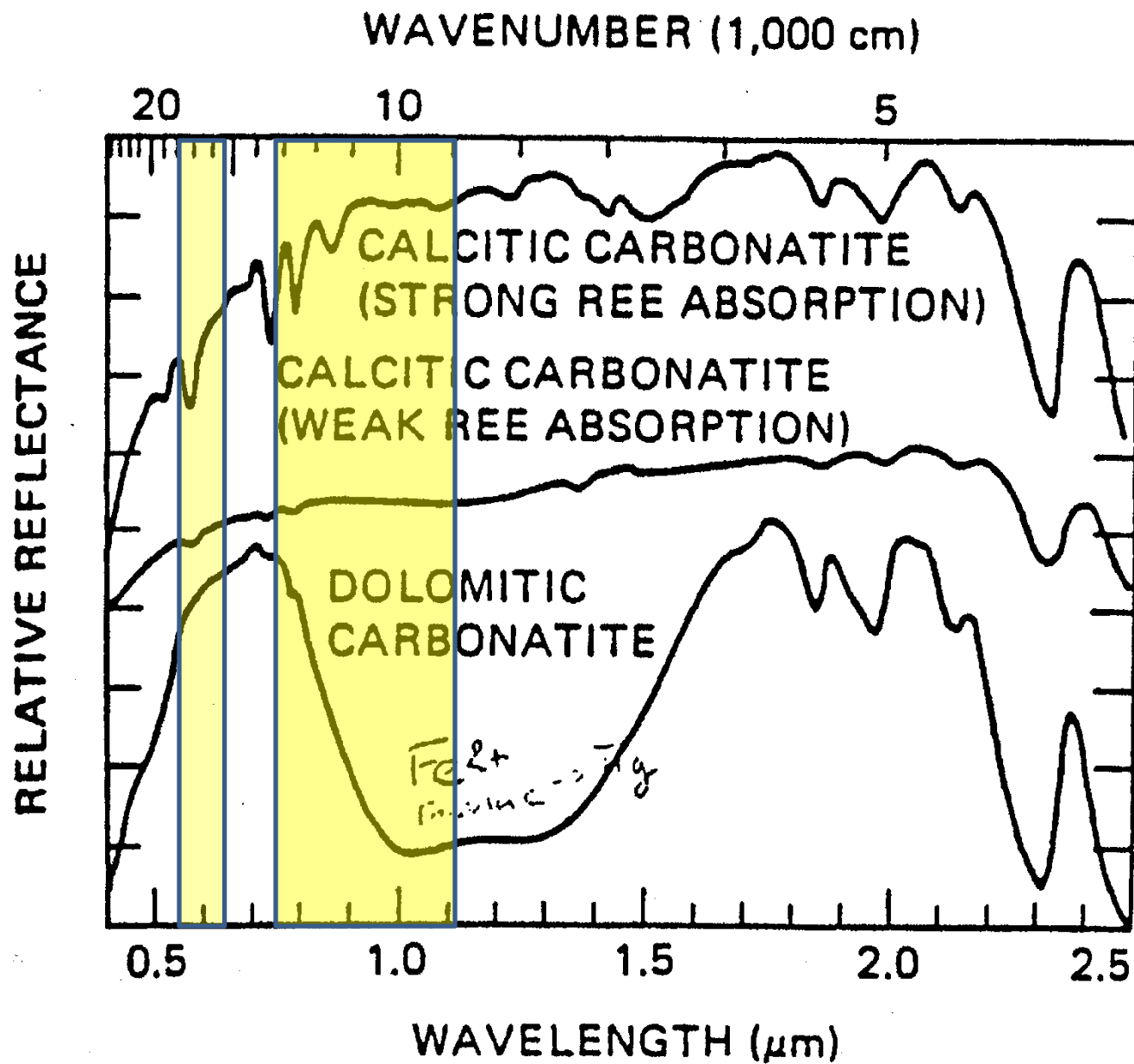
- **Most abundant**
- **Fe^{2+} , Fe^{3+} can substitute**
 - **Mg^{2+}**
 - **Al^{3+}**

**RHODOCHROSITE 67
CATAMARCA PROVINCE, ARGENTINA**

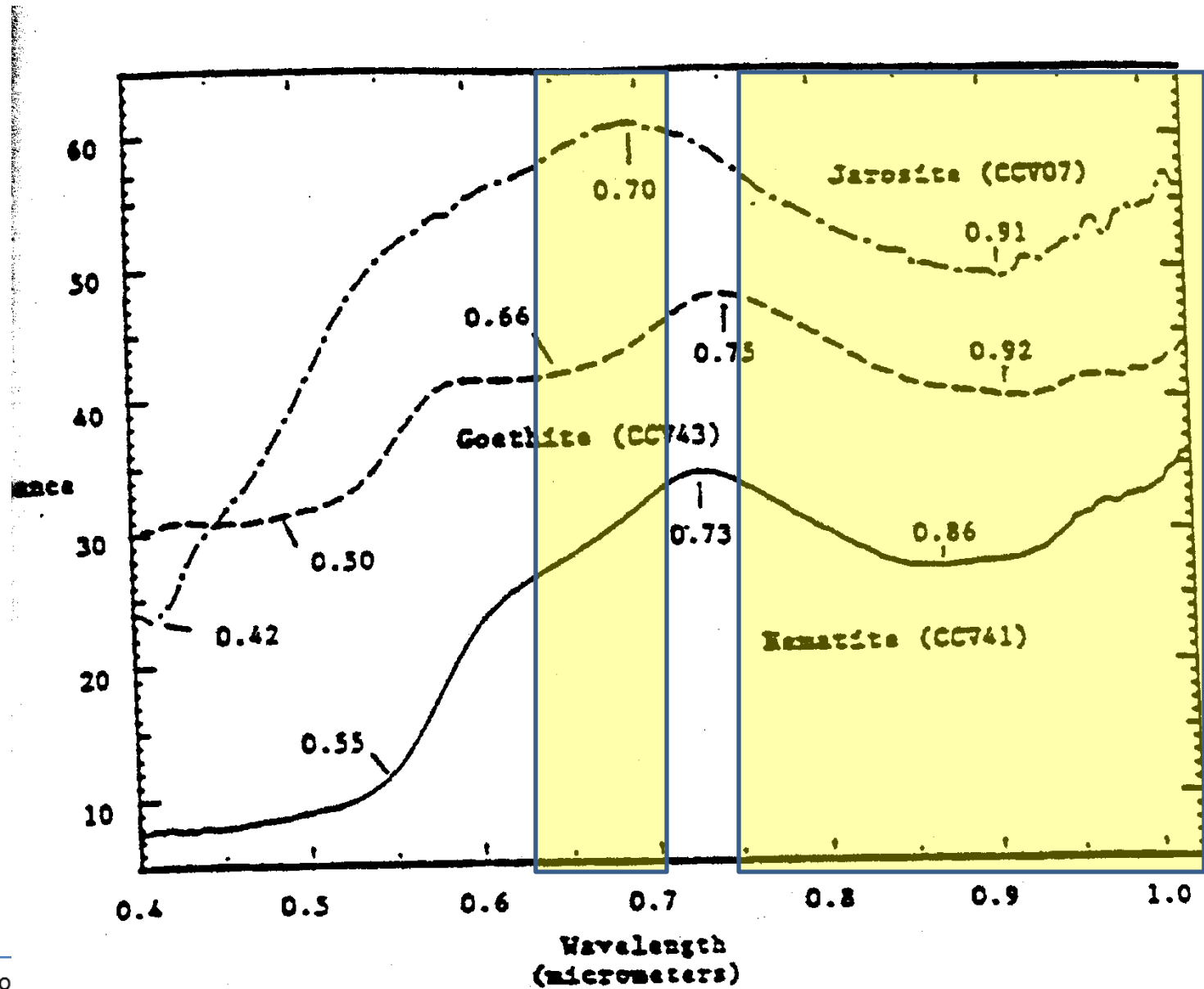


Crystal Field absorption





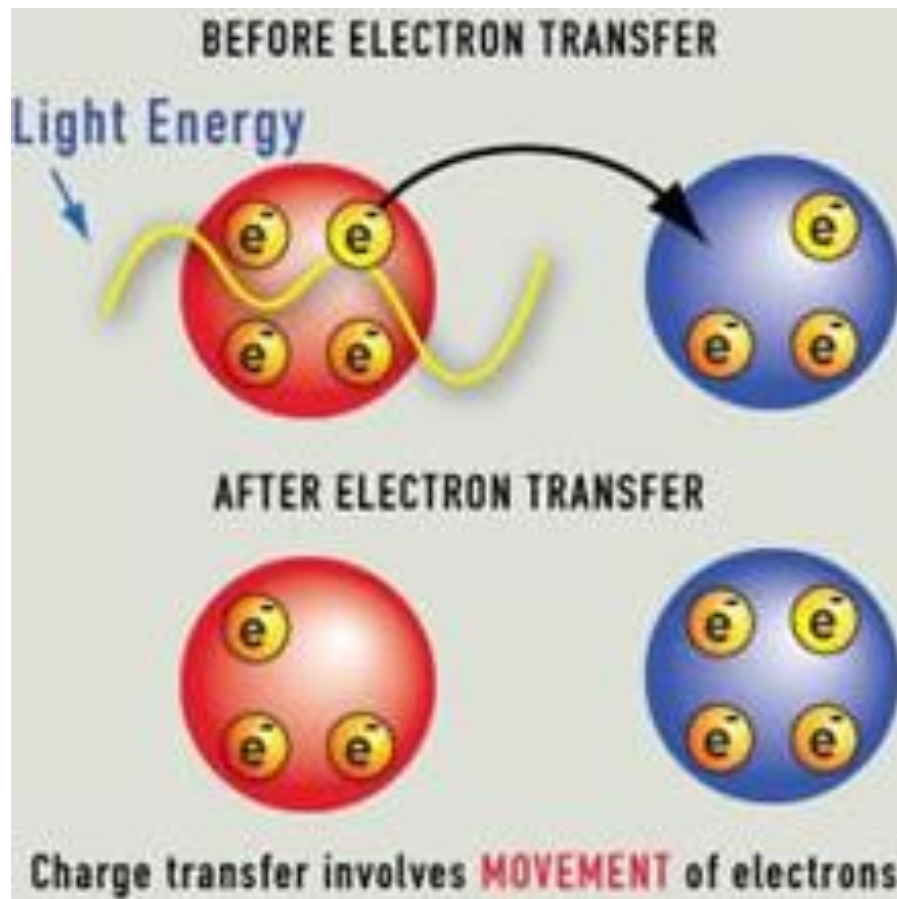
Fe bearing minerals

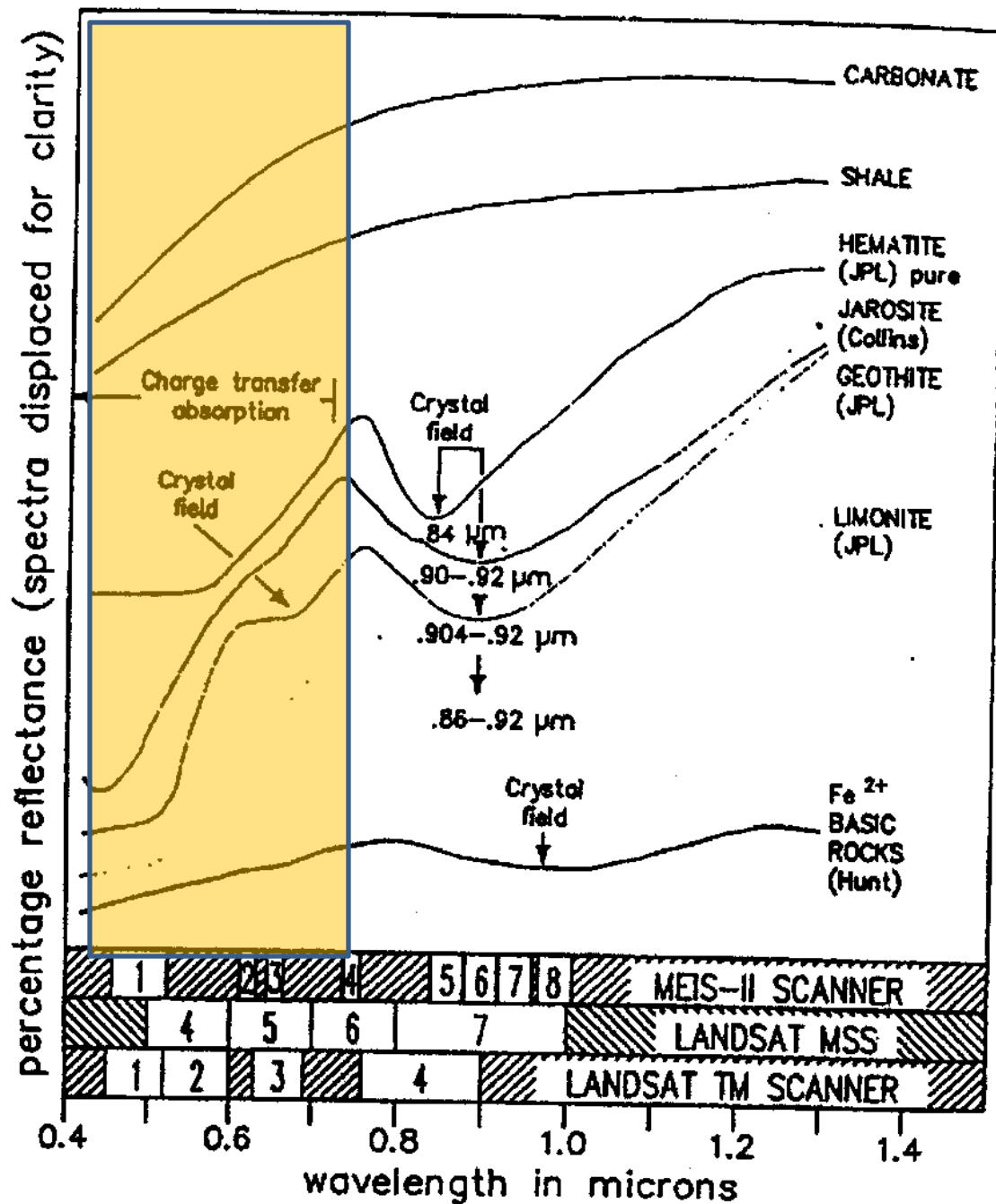


CHARGE TRANSFER

Electrons transfer from one atom to another

Fe-O transfer responsible for reflectance falloff towards UV



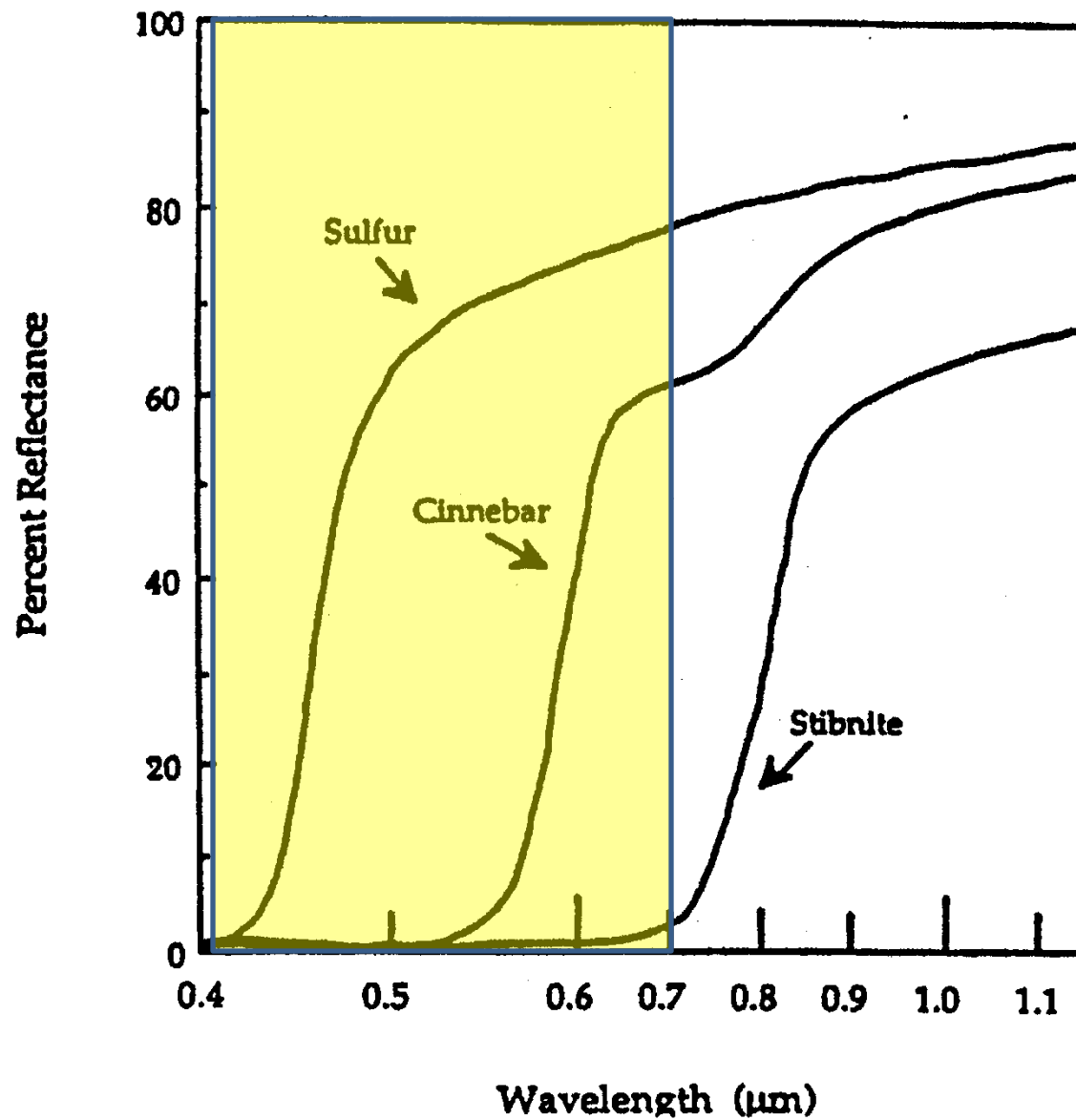


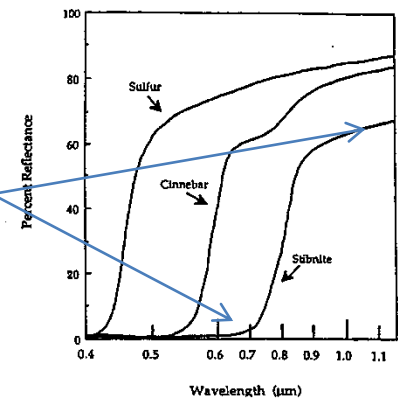
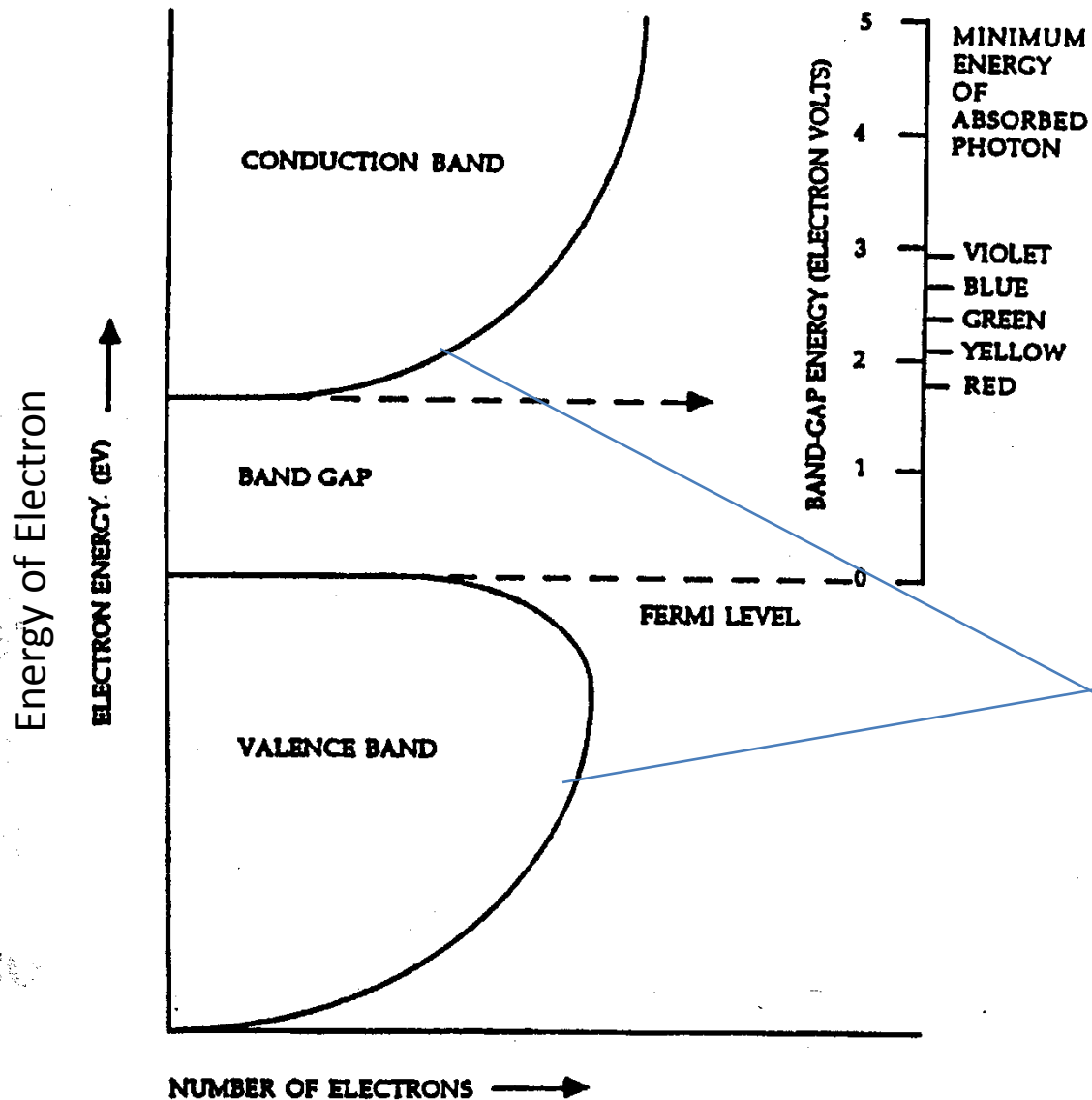
SEMICONDUCTORS

Detectors

Absorption edge in reflectance spectrum

- Created by width of forbidden energy band gap
- Incoming photons must have enough energy to promote valence band electrons into conduction band
- Reflectance increases dramatically at wavelength corresponding to band gap energy

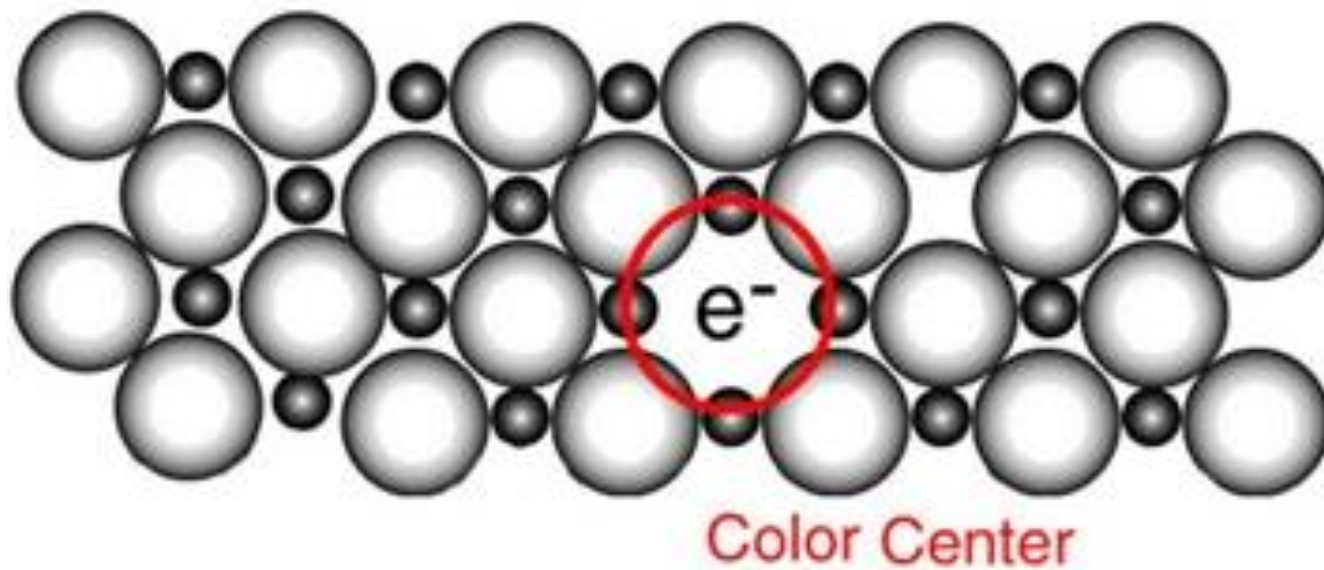




COLOR CENTERS

Rare Ore Minerals

- **Electron trapped in a structural defect such as a missing ion**
- **In fluorite (CaF_2) a color center is formed when an F ion is missing and replaced by an electron**
- **Transition states created cause red-green absorption, hence purple color**



VIBRATIONAL PROCESSES

Fundamental vibrations

**For solids, generally occur beyond $2.5\ \mu\text{m}$
Si-O, Al-O occur in $10\ \mu\text{m}$ region, no effect
in VNIR or SWIR**

**OH, H₂O, CO₃ occur in $2.6\text{-}6\ \mu\text{m}$ region,
overtones and combinations found in VNIR,
SWIR**

$3N-6$ possible degrees of freedom

**H₂O has 3 fundamental vibrations at 2.66 ,
 2.74 , $6.08\ \mu\text{m}$**

OVERTONES AND COMBINATIONS

Overtones

- Multiples of the fundamental frequency
- $2\nu_1, 3\nu_2, \dots$

Combinations

- Sums and differences of fundamental or overtone frequencies
- $\nu_1 + \nu_2, 2\nu_1 + \nu_3, \nu_1 + \nu_2 + \nu_3, \dots$

Frequencies not wavelengths added

- $\nu \cdot \lambda = c, \nu = \frac{c}{\lambda}$

- Frequency units in cm^{-1}
- $2.5 \mu\text{m} = 4000 \text{ cm}^{-1}$

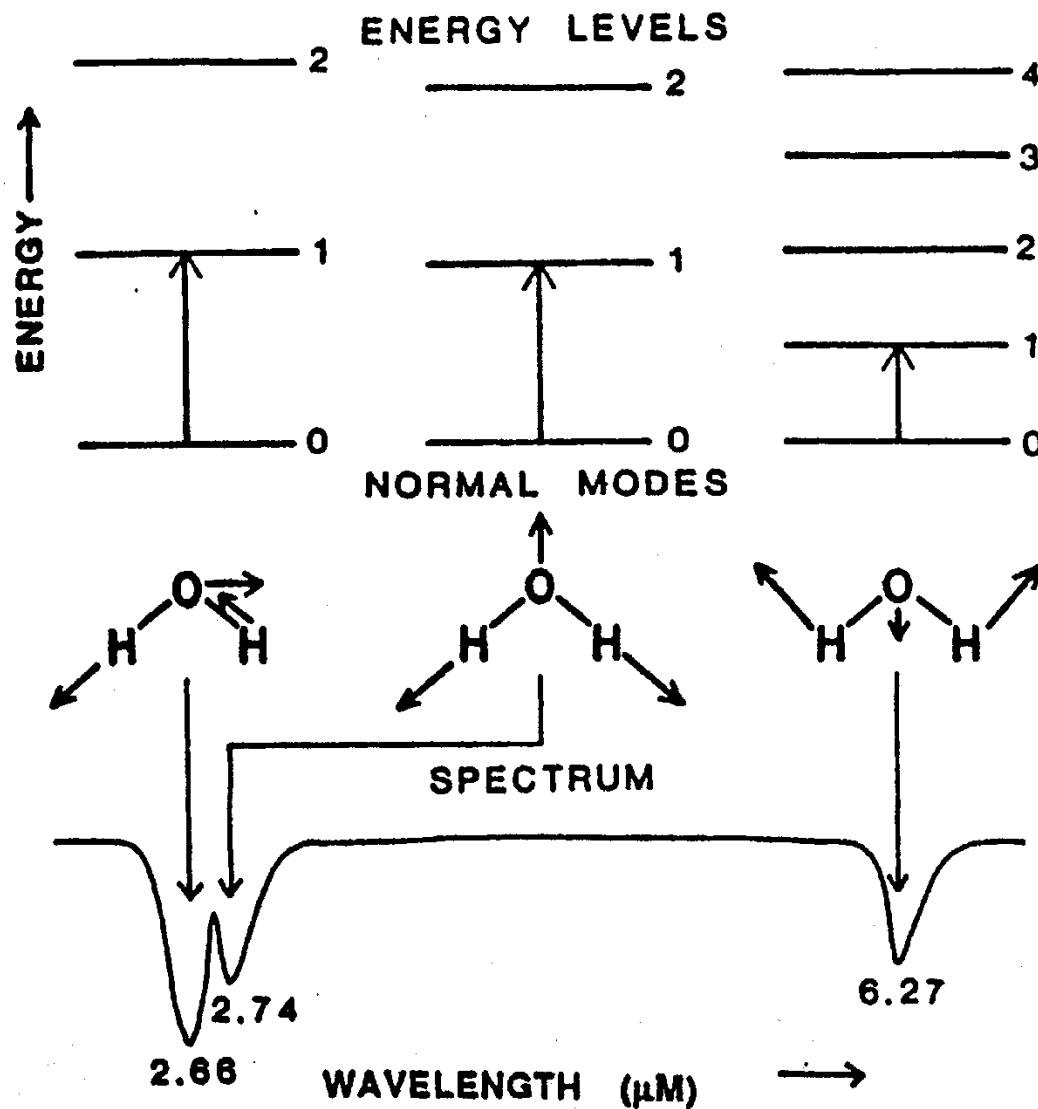
WATER VAPOR

Absorption fundamentals

- $\nu_1 = 3657.05 \text{ cm}^{-1} = 2.734 \text{ }\mu\text{m}$ symmetric stretch
- $\nu_2 = 1594.75 \text{ cm}^{-1} = 6.271 \text{ }\mu\text{m}$ bend
- $\nu_3 = 3755.93 \text{ cm}^{-1} = 2.662 \text{ }\mu\text{m}$ asymmetric stretch

Important water vapor absorptions

- $\nu_2 + \nu_3 = 1.865 \text{ }\mu\text{m}$
- $\nu_1 + \nu_3 = 1.379 \text{ }\mu\text{m}$
- $\nu_1 + \nu_2 + \nu_3 = 1.135 \text{ }\mu\text{m}$
- $2\nu_1 + \nu_3 = 0.942 \text{ }\mu\text{m}$



LIQUID WATER

Absorption fundamentals

- $\nu_1 = 3219.57 = 3.106 \mu\text{m}$
- $\nu_2 = 1644.74 = 6.08 \mu\text{m}$
- $\nu_3 = 3444.71 = 2.903 \mu\text{m}$

HYDROXYL [OH]

- **Absorption fundamental**
 - **2.77 μm stretch**
 - **Exact location depends on site on which it is located**
- **Overtone**
 - **$2\nu \sim 1.4 \mu\text{m}$**
 - **Most common feature in terrestrial material spectra**
- **Combinations**
 - **Al or Mg - OH bending modes**
 - **Features in 2.2 & 2.3 μm region**

SPECTRAL PROPERTIES

SOME COMMON ABSORPTION FEATURE

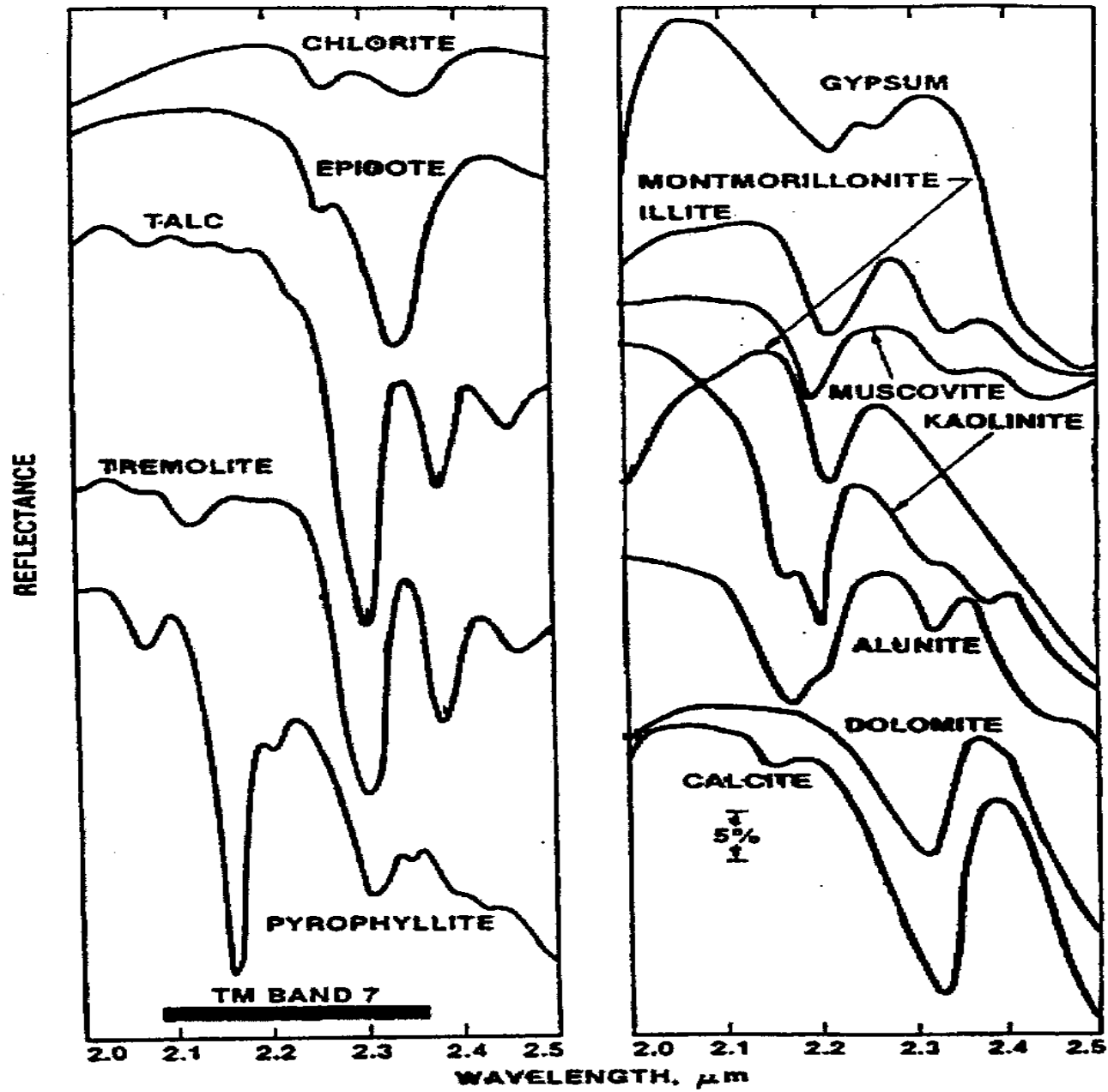
All Mechanisms

FEATURE

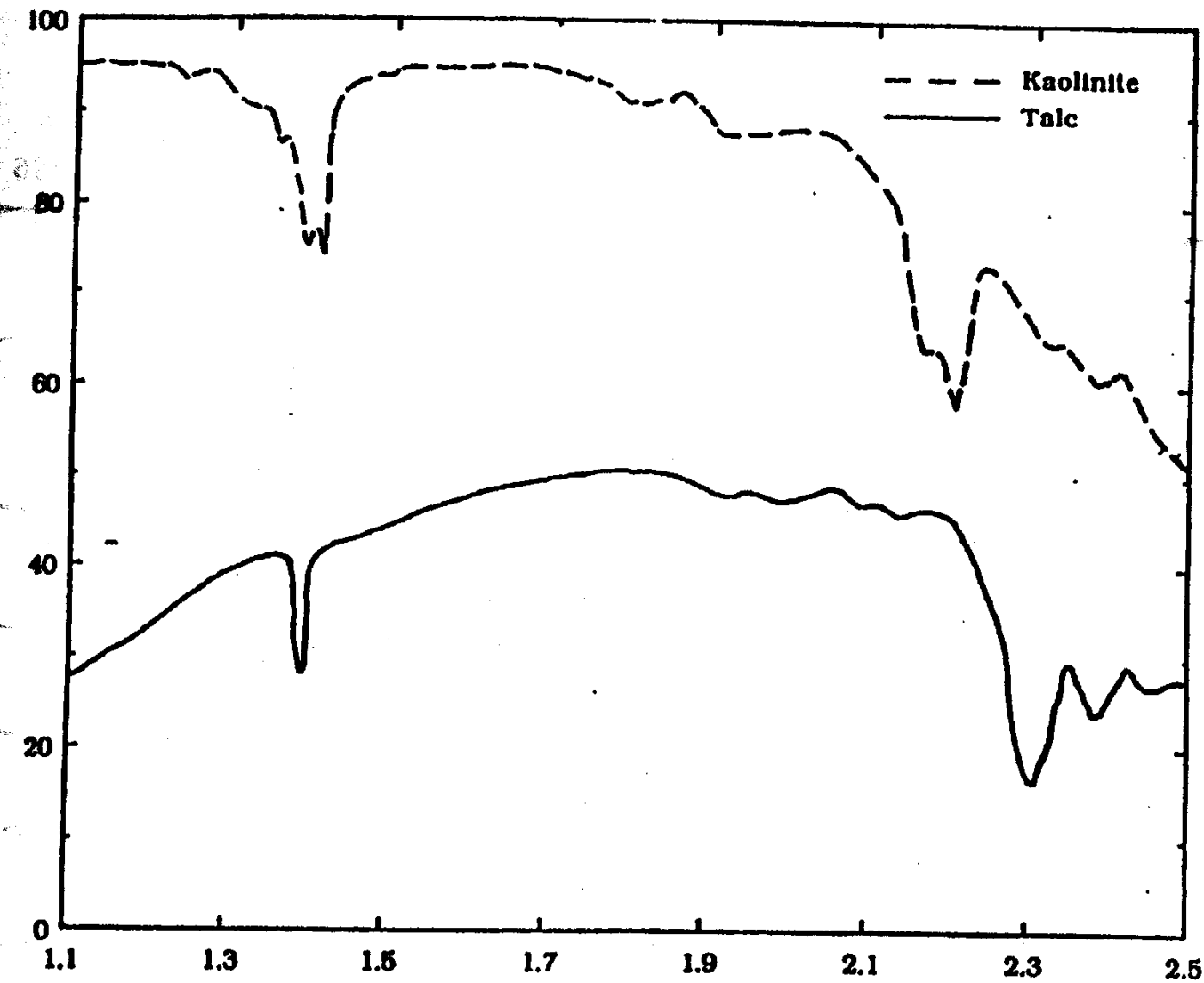
POSITION

Fe³⁺	0.4 - 0.6 μm, 0.66 μm, 0.85 - 0.95 μm
Al - OH	2.15 - 2.22 μm
Mg - OH	2.30 - 2.39 μm
Fe - OH	2.24 - 2.27 μm
Si - OH	2.25 μm (broad)
H₂O	1.9 μm
CO₃	2.30 - 2.35 μm
NH₄	2.0 - 2.13 μm

F.A.Ki



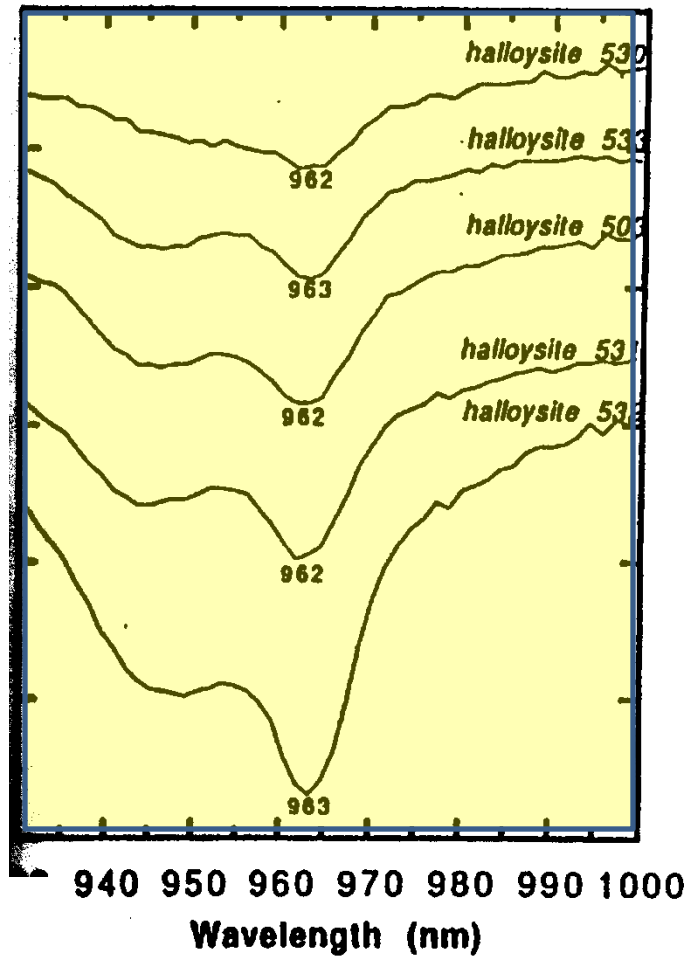
Vibrations



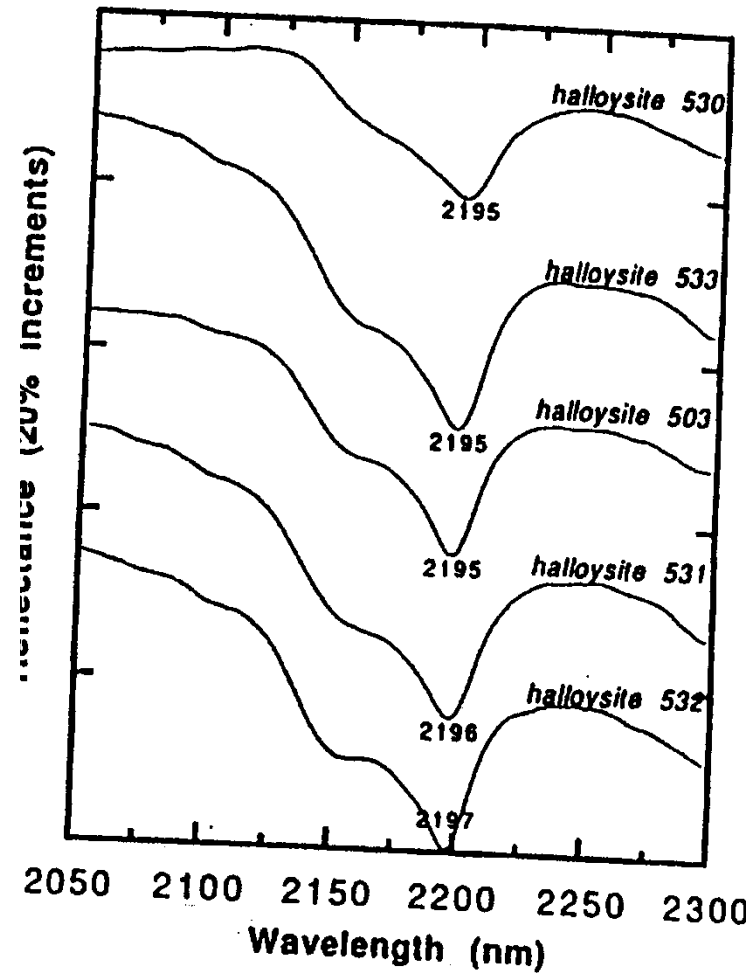
Vibrations

Wavelength (μm)

Second Overtone



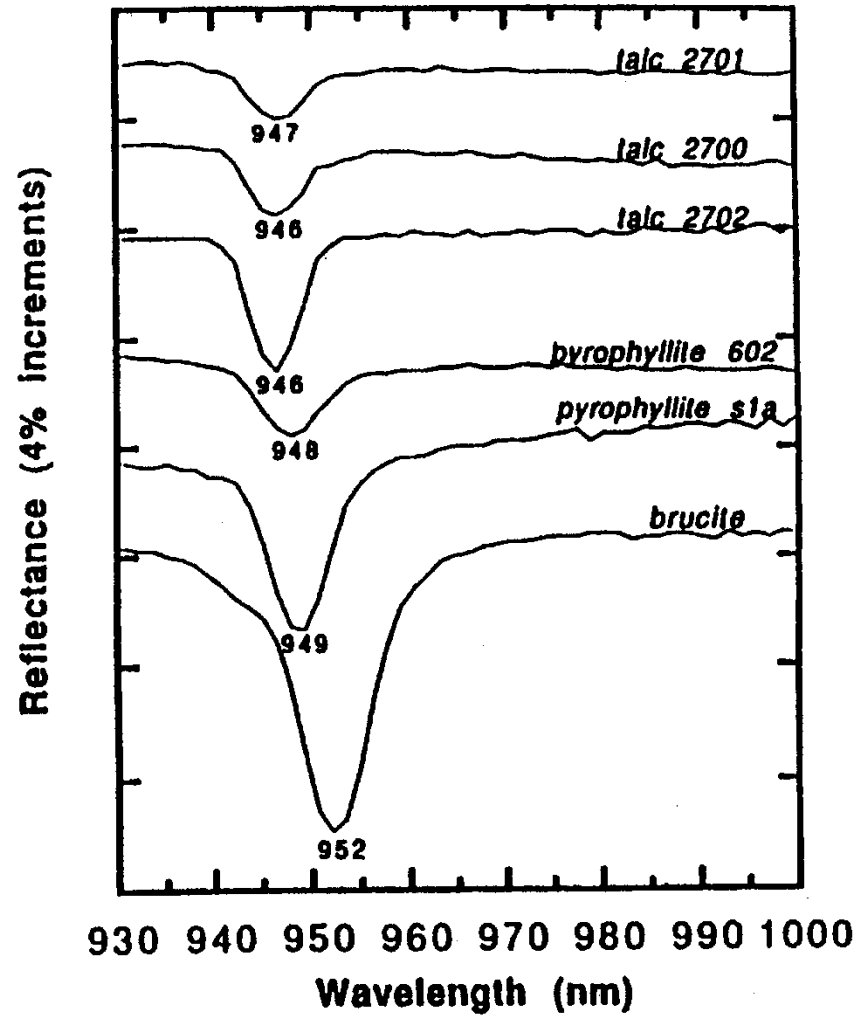
Overtone Combination



Only in pure and well crystalized mineral

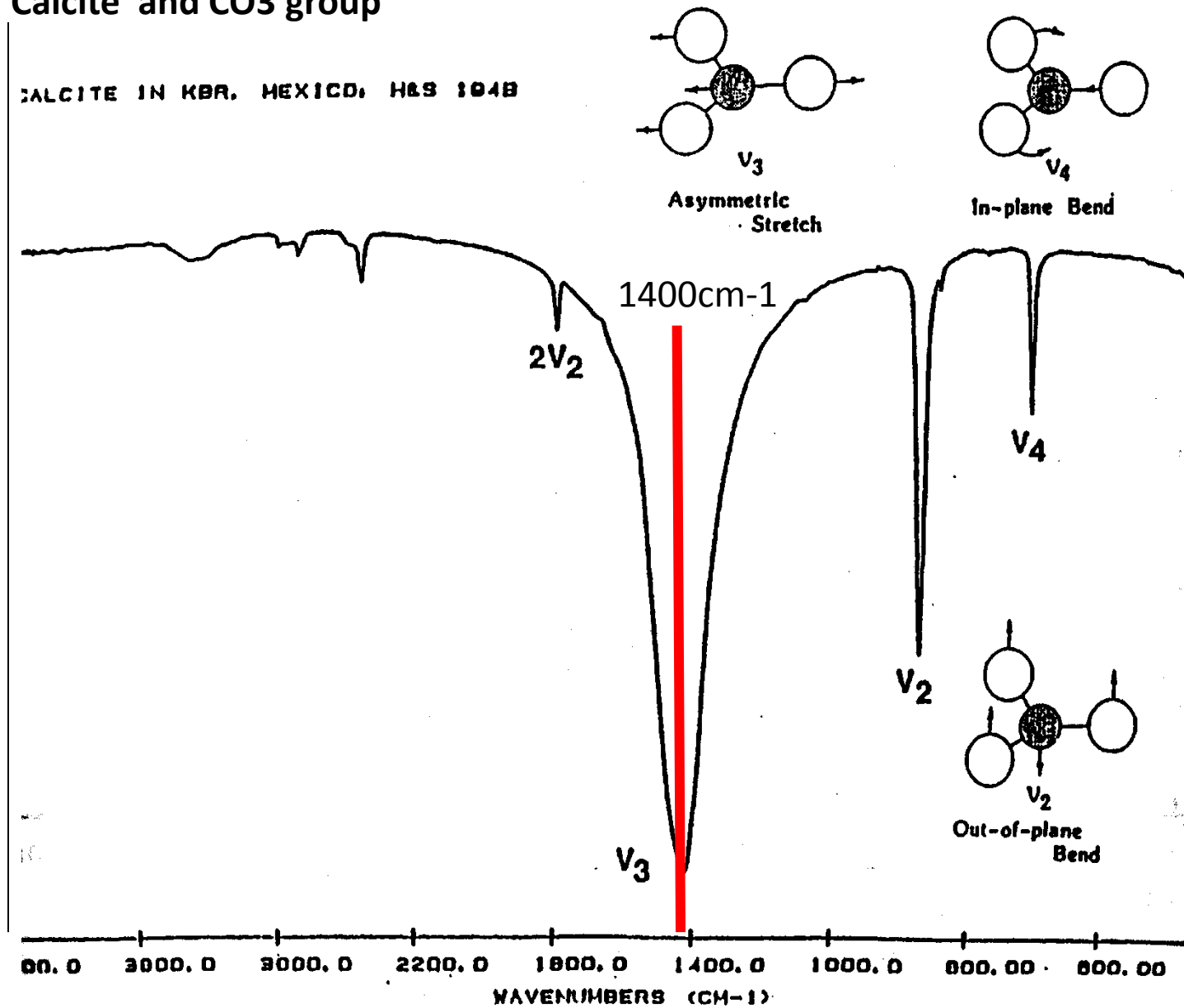
More example of the second overtone

Second Overtone



Calcite and CO3 group

CALCITE IN KBR. MEXICO, H&S 1948



Overtone Calculation

Example for CaCO₃

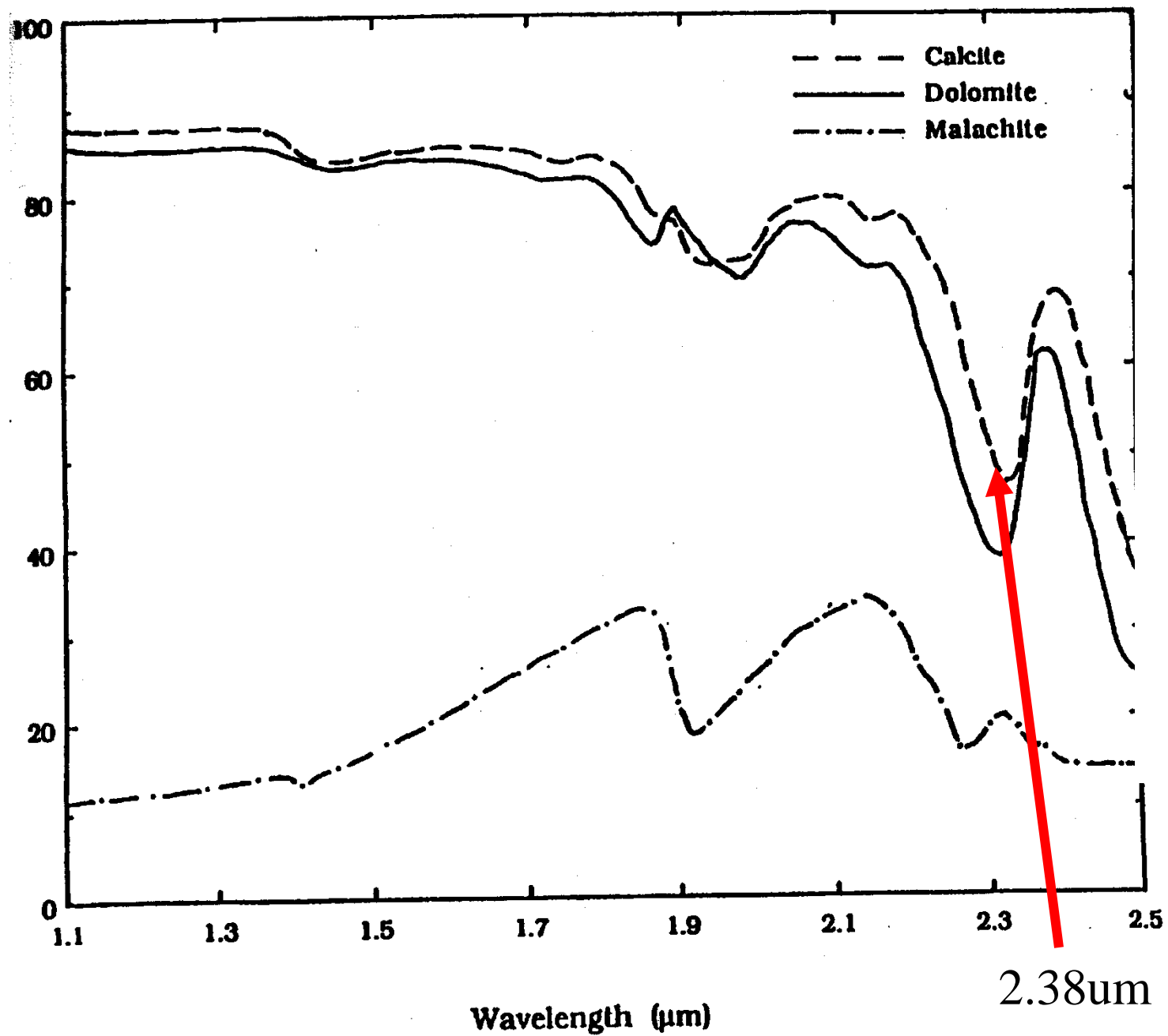
Always in Wavenumber!! (*as we work with energy*)

$$E_1 + E_2 = hc/\lambda + hc/\lambda$$

$$1/\lambda + 1/\lambda + 1/\lambda$$

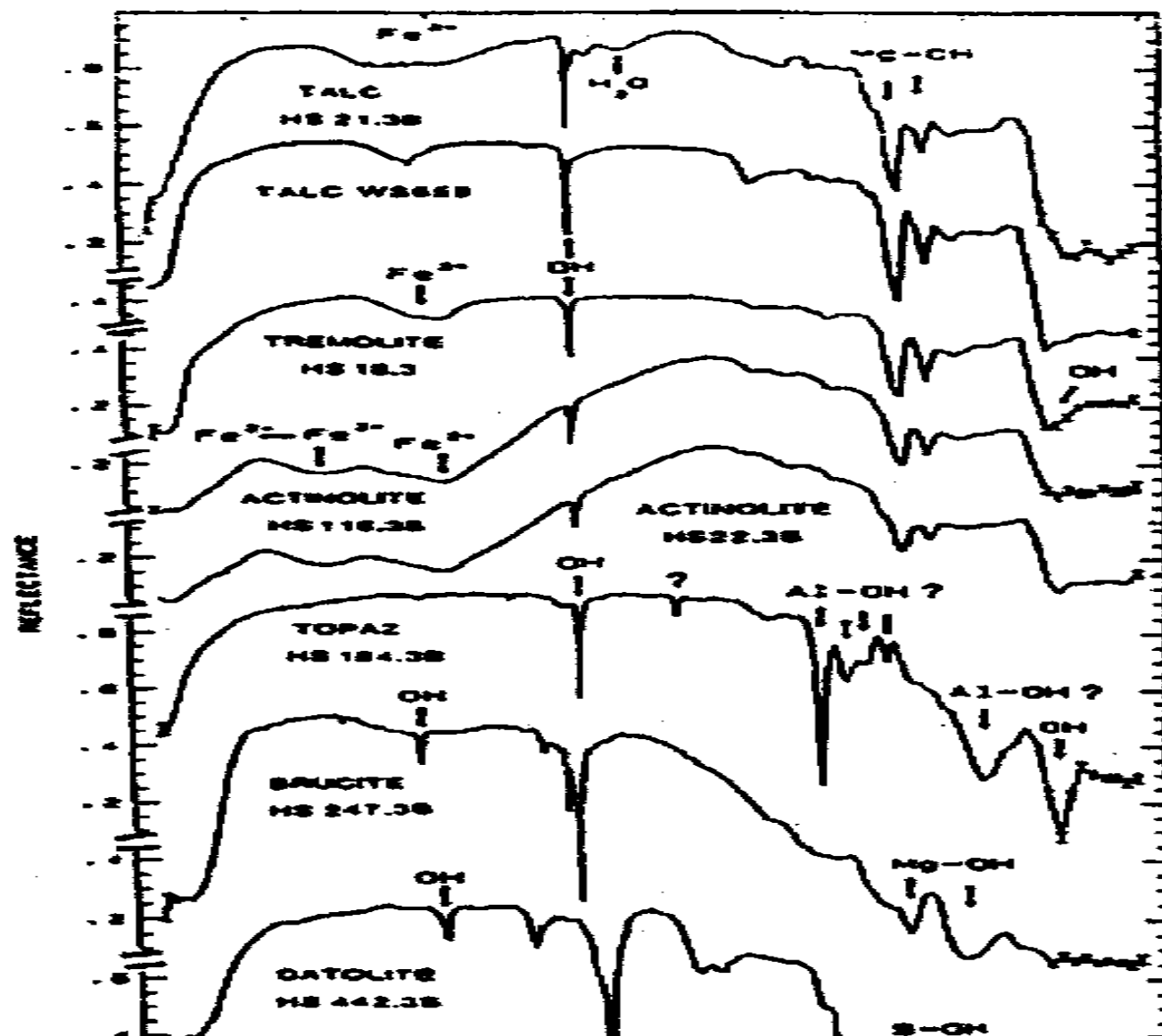
$$3 \nu_1$$

$$3 * 1400 = 4200 \text{ cm}^{-1} = \underline{\underline{2.38 \text{ } \mu\text{m}}}$$



2.38 μm





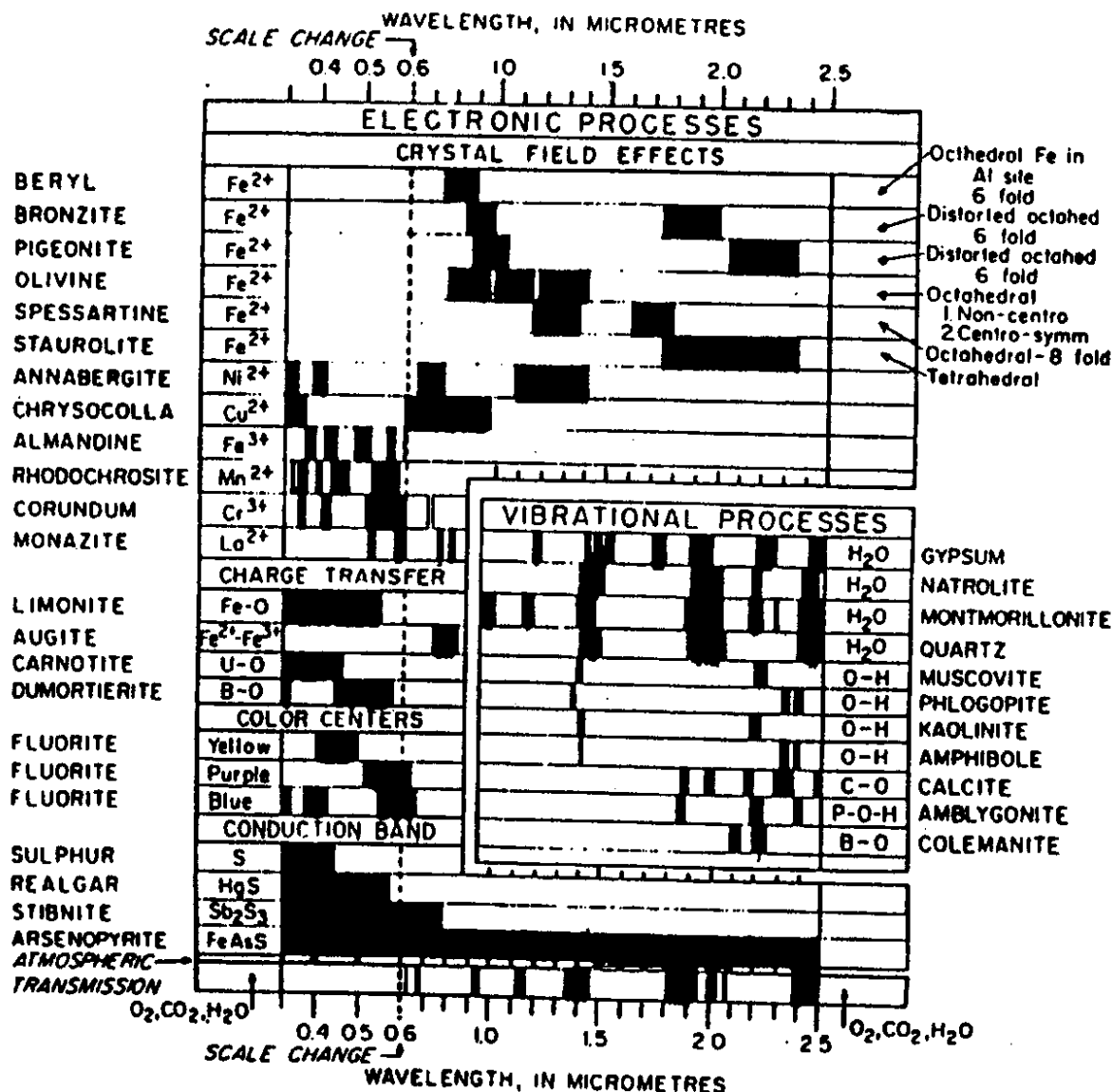
Hunts' Library

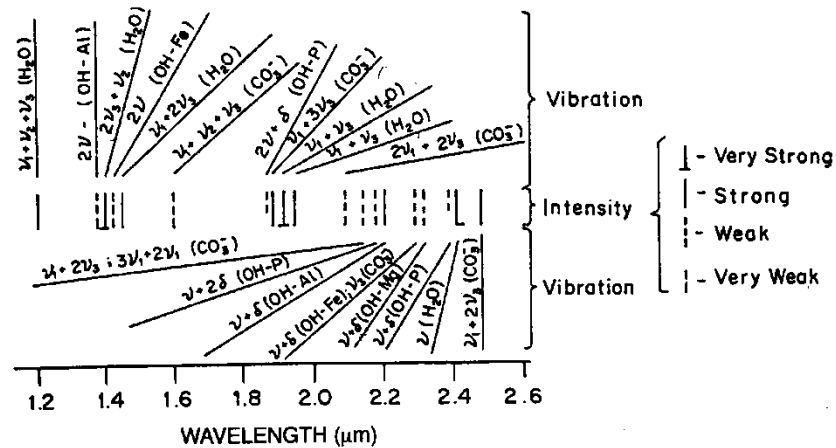
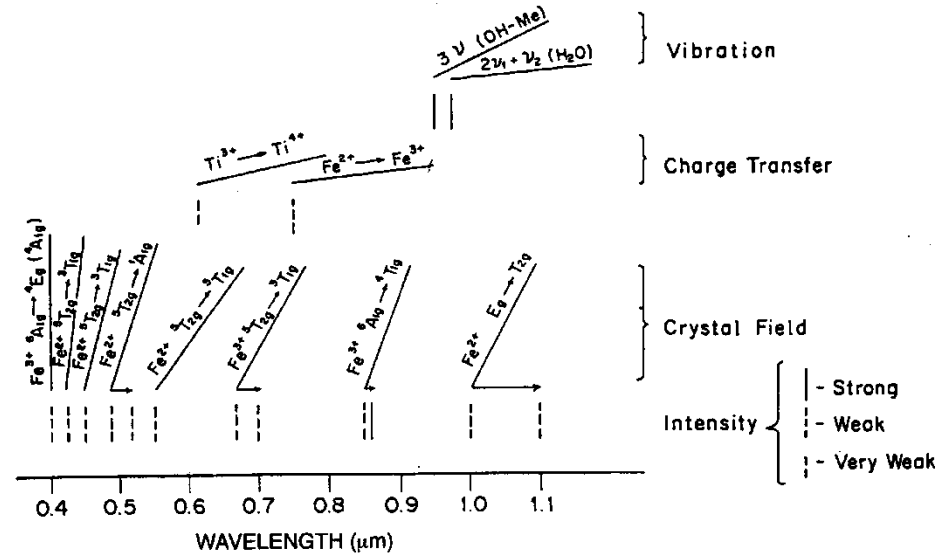


Reference

- Hunt, G.R., and J.W., Salisbury, 1970, Visible and near infrared spectra of minerals and rocks: I: Silicate minerals. *Modern Geology*, 1:283-300.
- Hunt, G.R., Salisbury J.W. and A., Lenhoff., 1971a. Visible and near-infrared spectra of minerals and rocks: III Oxides and hydroxides. *Modern Geology* 2:195-205.
- Hunt G.R., Salisbury J.W., and C.J., Lenhoff., 1971b Visible and near-infrared spectra of minerals and rocks: Sulfides and sulfates. *Modern Geology* 3:1-14.
- Hunt G.R., Salisbury J.W., and C.J., Lenhoff, 1971c Visible and near-infrared spectra of minerals and rocks: Halides, phosphates, arsenates, vandates and borates. *Modern Geology* 3:121-132.
- Hunt G.R. and J.W. Salisbury, 1971d Visible and near infrared spectra of minerals and rocks: Carbonates. *Modern Geology* 2:23-30.
- Hunt G.R., and J.W., Salisbury, 1976 Visible and near infrared spectra of minerals and rocks: XI Sedimentary rocks. *Modern Geology* 5:211-217.
- Hunt G.R., 1980 Spectroscopic Properties of Rock and Minerals In: *Handbook of Physical Properties Rocks* (Stewart C.R. Ed.) CRC Press. pp.295.
- Ben-Dor E., J.A. Irons and A. Epema, 1998, Soil Spectroscopy. In: ***Manual of Remote Sensing, Third Edition***, A. Rencz (ed.) J. Wiley & Sons Inc. New-York, Chichester, Weinheim, Brisbane, Singapore, Toronto. pp.111-189
-
- Clark R. 1998 Spectroscopy of Rocks and Minerals, and Principle of Spectroscopy In: ***Manual of Remote Sensing, Third Edition***, A. Rencz (ed.) J. Wiley & Sons Inc. New-York, Chichester, Weinheim, Brisbane, Singapore, Toronto. pp.3-110.
- Ben Dor et al . 1998 Spectroscopy of Soil In: ***Manual of Remote Sensing, Third Edition***, A. Rencz (ed.) J. Wiley & Sons Inc. New-York, Chichester, Weinheim, Brisbane, Singapore, Toronto. pp.110- 155.

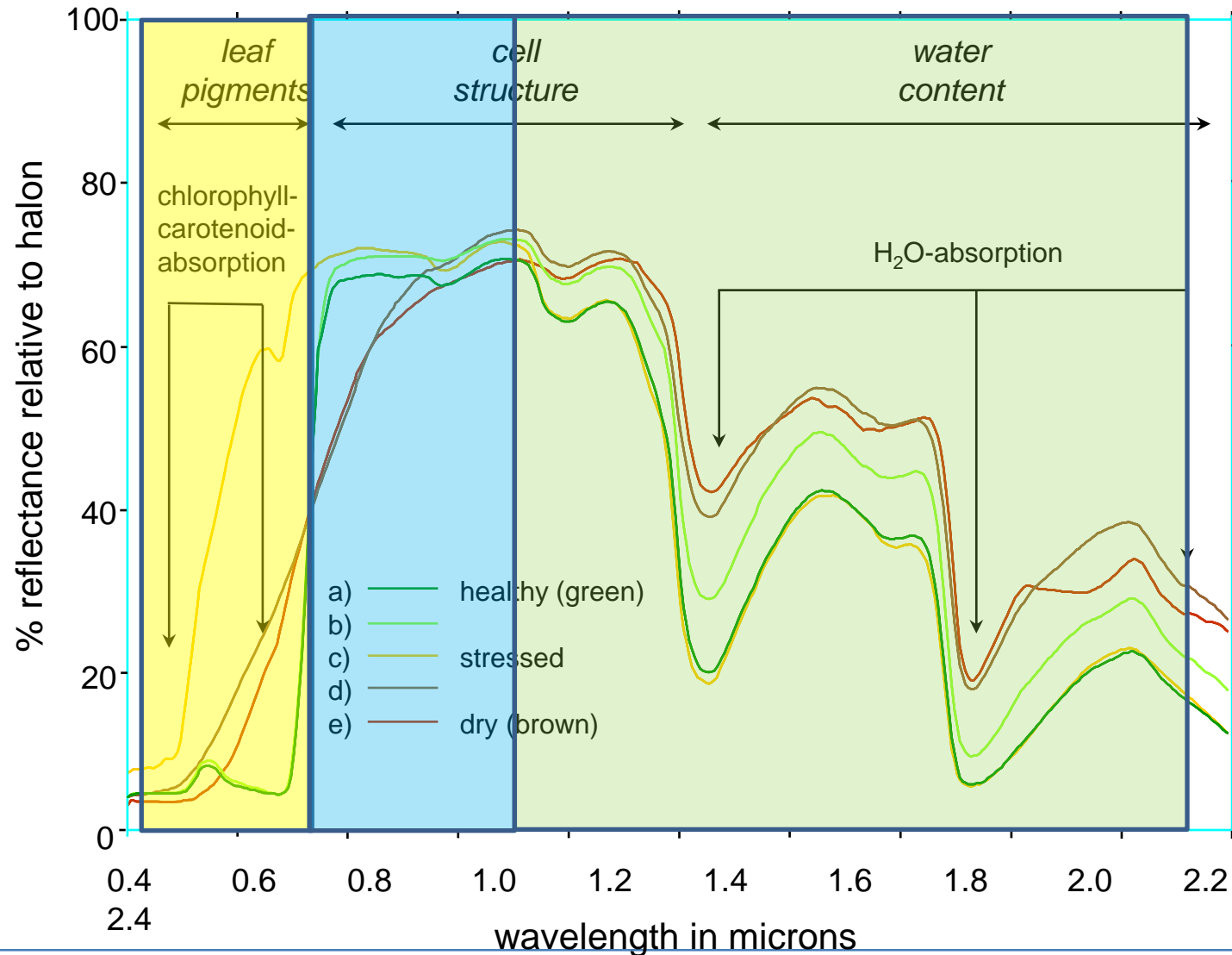
MINERAL SPECTRAL ABSORPTION BANDS





From Ben Dor et al, Manual of Remote Sensing

Spectral Characteristics of Vegetation



SELECTED DIGITAL SPECTRAL DATA BASES

- **JPL Publication 92-2 - Laboratory reflectance spectra of 160 minerals, 0.4 to 2.5 micrometers**
- **Contact:**

**Dr. Simon Hook
JPL, MS 183-501
4800 Oak Grove Drive
Pasadena, CA 91109
Phone: 818-354-0974
Fax: 818-354-0966**

**E-mail: Simon.J.Hook@jpl.nasa.gov
Web: <http://speclib.jpl.nasa.gov/>**

SELECTED DIGITAL SPECTRAL DATA BASES

CSIRO Spectral Library

Contact:

Dr. Jon Huntington

CSIRO, Division of Exploration Geoscience

P.O. Box 136

North Ryde

N.S.W. Australia 2113

Phone: (02) 9490-8839

FAX: (02) 9490-8921

E-mail: jon.huntington@dem.csiro.au

Web: <http://www.syd.dem.csiro.au/research/MMTG/>

SELECTED DIGITAL SPECTRAL DATA BASES

USGS (Denver) Spectral Library

Contact:

Dr. Roger Clark

U.S.G.S.

P.O. Box 25046, MS 964

Denver, CO 80225-0046

Phone: 303-236-1332

Fax: 303-236-1425

E-mail: rclark@speclab.cr.usgs.gov

Web: <http://speclab.cr.usgs.gov/>

THE IGCP-264 SPECTRAL PROPERTIES DATABASE

EDITORS: Fred A. Kruse and Phoebe L. Hauff**

**CENTER FOR THE STUDY OF EARTH FROM SPACE (CSES)
Cooperative Institute for Research in Environmental Sciences (CIRES)**

**UNIVERSITY OF COLORADO
Boulder, Colorado 80309-0449**

JULY 1992

DOCUMENTATION AND REFERENCES FOR PROGRAM DSPECT

John C. Price
Agricultural Research Service, USDA
Beltsville, MD 20705

Copy to E. BEN-DOR
TEL-AVIV UNIVERSITY

Technical information

This program displays spectra from a library of 3417, and user spectra, and finds closest matches within the library for spectra spanning the full range (0.4 - 2.5 micrometers). It must be emphasized that the library spectra are APPROXIMATE, being based on a formalism which has been described in (Price, 1994). The program was written to to evaluate the validity of the approximation and to improve it. Some header information is truncated. Because of outdoor spectra the water vapor regions (1.35-1.47, 1.81-2.02) should not be used.

Matching Spectra

The program uses root mean square difference, integrated over wavelength, as a measure of difference. Water vapor absorption regions are displayed, but are ignored in finding closest matches.

Output files - LIST.DSP(listing) and DSPECT.DSP(spectra).

Absolute versus relative spectra

You may display or match by absolute reflectance value or by shape, where matching by shape implies that spectra 2,3,4 are each multiplied by a constant to minimize rms difference. The latter is recommended because instrument calibration and surface moisture can affect the amplitude of measured spectra. See Price, J. C., 1994, How Unique are Spectral Signatures?, Rem. Sens. of Environ., 48:181-186

Format for user spectra

You may replace file INPUT.DSP with your own spectra, as long as the format remains the same. Up to five user spectra are stored in a buffer which scrolls when additional spectra are entered. See Price, 1995, Table 1.

Please report problems or errors to the author.

John C. Price
RSRL - Bldg. 7
BARC - West
Beltsville, MD 20705

JPRICE@ASRR.ARSUSDA.GOV

May 1980

Atlas of Soil Reflectance Properties

E. R. Stoner, M. F. Baumgardner, L. L. Biehl and B. F. Robinson
Department of Agronomy and the
Laboratory for Application of Remote Sensing,
Purdue University

with support of the
Johnson Space Center, National Aeronautics and Space Administration
and the Soil Conservation Service, U.S. Department of Agriculture

