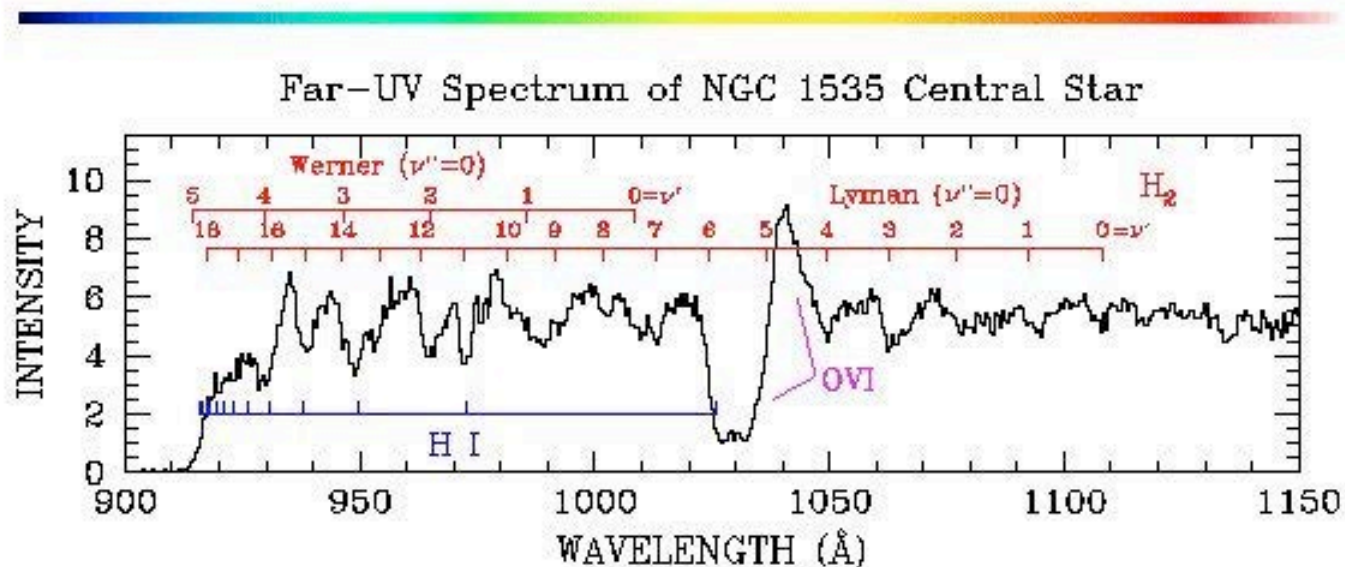


Spectroscopy: The Study of Squiggly Lines

[\[Astronomical Distances\]](#) [\[Basics of Light\]](#) [\[Tools for Light Analysis\]](#)
[\[Measuring Light\]](#) [\[Electromagnetic Spectrum\]](#) [\[Fun with Units\]](#)
[\[Atmospheric Transmission\]](#) [\[Space Links\]](#)

What are Those Squiggly Lines?

Using Light to Learn About the Universe



Spectroscopy in Curiosity's site selection

Eberswalde
Crater

Holden
Crater

Gale
Crater

Mawrth
Vallis



Morphologic

Evidence for water

Spectral

Interaction of Radiant Energy and Matter

What causes absorption features in spectra?

- 1) Rotational absorption (gases)**
- 2) Electronic absorption**
- 3) Vibrational absorption**

Rotational Processes

Photons striking *free* molecules can cause them to rotate. The rotational states are quantized, so there are discrete photon energies that, when absorbed, cause the molecules to spin.

Rotational interactions are low-energy interactions and the absorption features are at long infrared wavelengths.

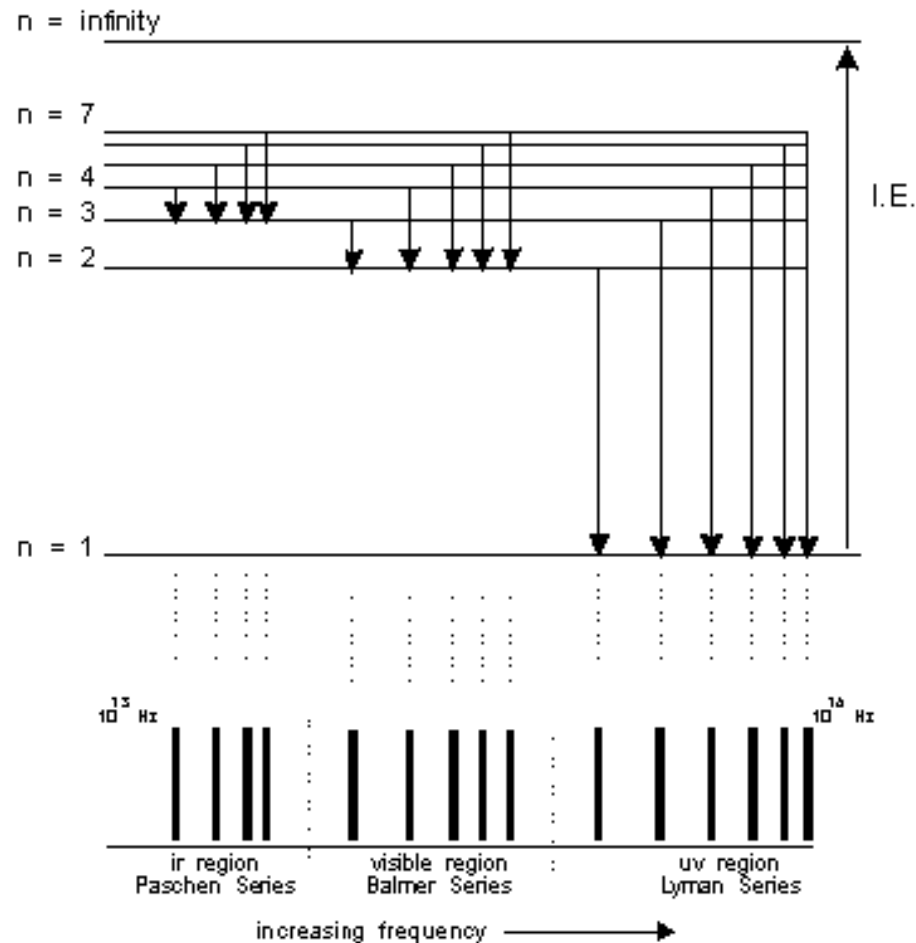
Not important in remote sensing of solid materials

Electronic Processes

Isolated atoms and ions have discrete energy states. Absorption of photons of a specific wavelength causes a change from one energy state to a higher one.

In solids, four types:

- Crystal Field Effects
- Charge Transfer Absorptions
- Conduction Bands
- Color Centers

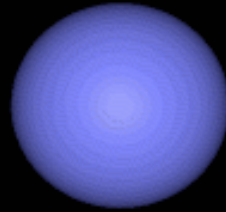


Electronic Processes

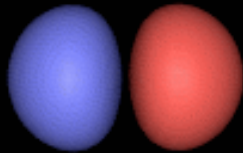
Crystal Field Effects

The electronic energy levels of an isolated ion are usually split and displaced when located in a solid. Unfilled d orbitals are split by interaction with surrounding ions and assume new energy values. These new energy values (transitions between them and consequently their spectra) are primarily determined by the valence state of the ion (Fe^{2+} , Fe^{3+}), coordination number, and site symmetry.

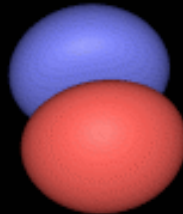
Electron Orbits



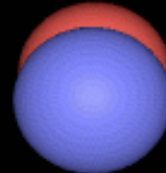
s



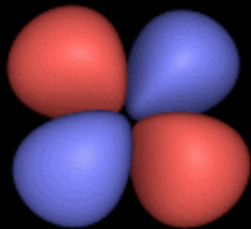
p_x



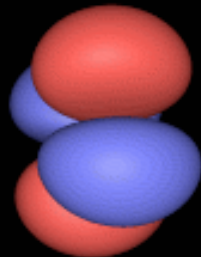
p_y



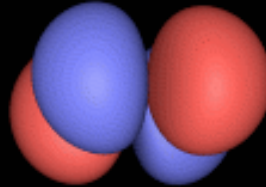
p_z



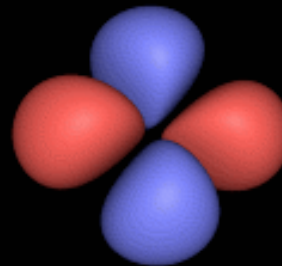
d_{xy}



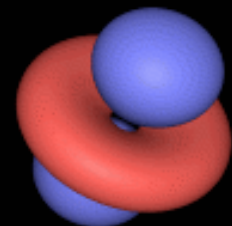
d_{xz}



d_{yz}



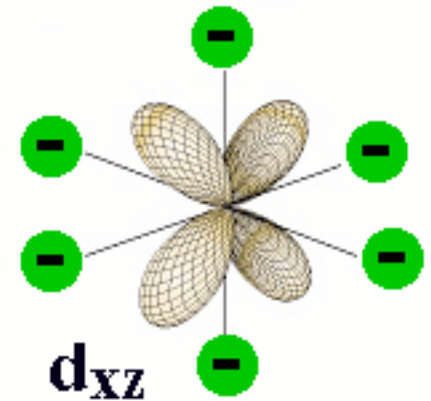
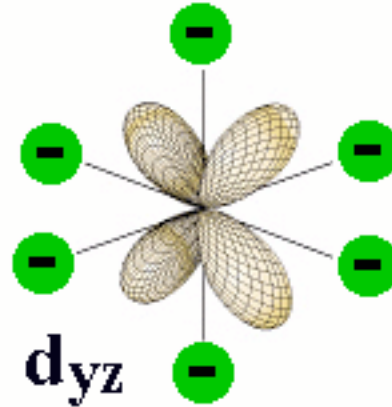
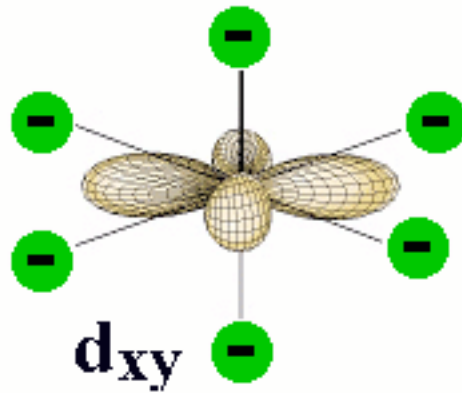
d_{x² - y²}



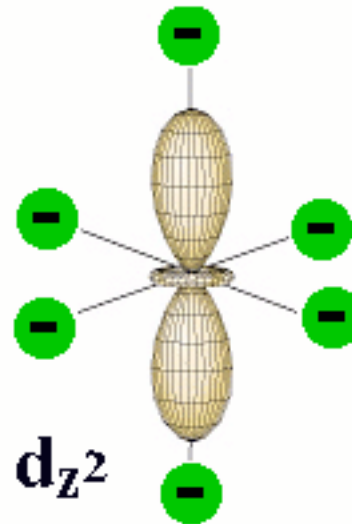
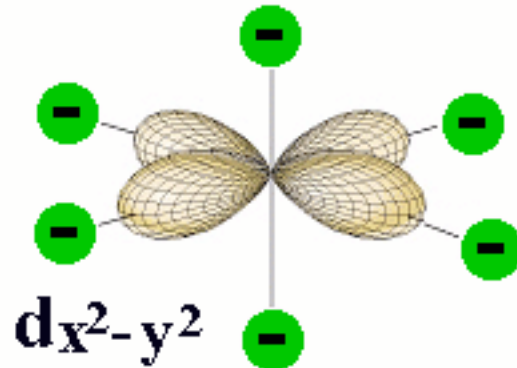
d_{z²}

Energy Level Splitting in Solids: Part 1

**Lower
Energy
Levels**

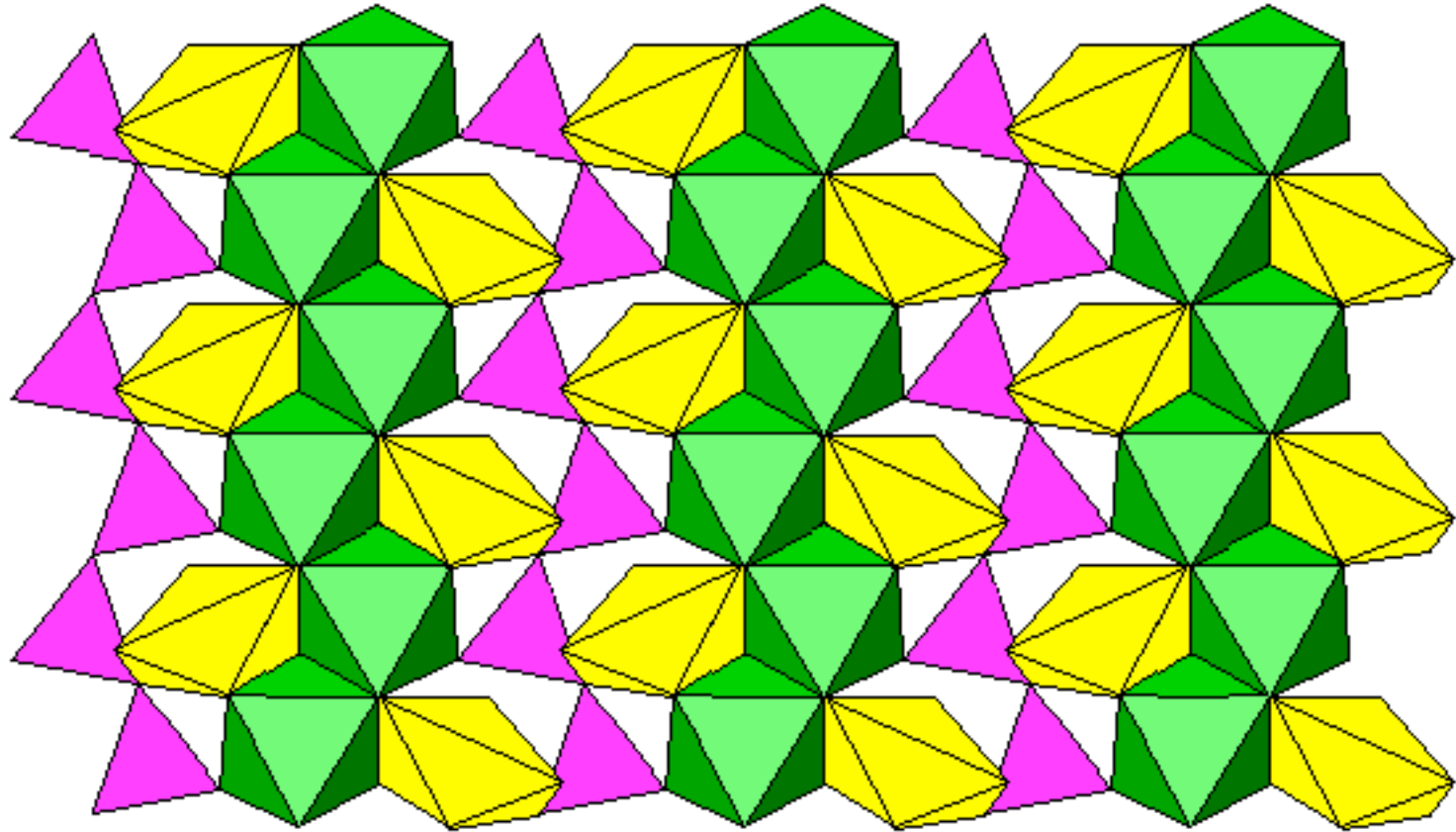


**Higher
Energy
Levels**



In a free atom these have equal energy, but not in a crystal...

Energy Level Splitting in Solids: Part 2



Distortion of some “sites” in a crystal → further energy splitting
→ *diagnostic of mineralogy*

Unfilled *d* orbitals: the transition metals

Periodic Table of the Elements

1 1 H Hydrogen 1.00784	2 4 He Helium 4.002602											13 5 B Boron 10.811	14 6 C Carbon 12.0107	15 7 N Nitrogen 14.00644	16 8 O Oxygen 15.9994	17 9 F Fluorine 18.9984032	18 10 Ne Neon 20.1797			
3 3 Li Lithium 6.941	4 4 Be Beryllium 9.012182											13 13 Al Aluminum 26.981538	14 14 Si Silicon 28.0855	15 15 P Phosphorus 30.973761	16 16 S Sulfur 32.066	17 17 Cl Chlorine 35.453	18 18 Ar Argon 39.948			
11 3 Na Sodium 22.989770	12 2 Mg Magnesium 24.3050	3 21 Sc Scandium 44.955910	4 22 Ti Titanium 47.867	5 23 V Vanadium 50.9415	6 24 Cr Chromium 51.9961	7 25 Mn Manganese 54.938049	8 26 Fe Iron 55.845	9 27 Co Cobalt 58.933200	10 28 Ni Nickel 58.6934	11 29 Cu Copper 63.546	12 30 Zn Zinc 65.409	13 31 Ga Gallium 69.723	14 32 Ge Germanium 72.64	15 33 As Arsenic 74.92160	16 34 Se Selenium 78.96	17 35 Br Bromine 79.904	18 36 Kr Krypton 83.798			
19 5 K Potassium 39.0983	20 2 Ca Calcium 40.078	39 4 Y Yttrium 88.90585	40 4 Zr Zirconium 91.224	41 4 Nb Niobium 92.90638	42 4 Mo Molybdenum 95.94	43 4 Tc Technetium (98)	44 4 Ru Ruthenium 101.07	45 4 Rh Rhodium 102.90550	46 4 Pd Palladium 106.42	47 4 Ag Silver 107.8682	48 4 Cd Cadmium 112.411	49 4 In Indium 114.818	50 4 Sn Tin 118.710	51 4 Sb Antimony 121.760	52 4 Te Tellurium 127.60	53 4 I Iodine 126.90447	54 4 Xe Xenon 131.293			
37 5 Rb Rubidium 85.4678	38 2 Sr Strontium 87.62	57 to 71										81 4 Tl Thallium 204.3853	82 4 Pb Lead 207.2	83 4 Bi Bismuth 208.98038	84 4 Po Polonium (209)	85 4 At Astatine (210)	86 4 Rn Radon (222)			
55 6 Cs Cesium 132.90545	56 2 Ba Barium 137.327	89 to 103										113 4 Uut Ununtrium (284)	114 4 Uuq Ununquadium (288)	115 4 Uup Ununpentium (288)	116 4 Uuh Ununhexium (292)	117 4 Uus Ununseptium	118 4 Uuo Ununoctium			
87 7 Fr Francium (223)	88 2 Ra Radium (226)											104 4 Rf Rutherfordium (261)	105 4 Db Dubnium (262)	106 4 Sg Seaborgium (266)	107 4 Bh Bohrium (264)	108 4 Hs Hassium (269)	109 4 Mt Meitnerium (268)	110 4 Ds Darmstadtium (271)	111 4 Rg Roentgenium (272)	112 4 Uub Ununbium (285)

Atomic masses in parentheses are those of the most stable or common isotope.

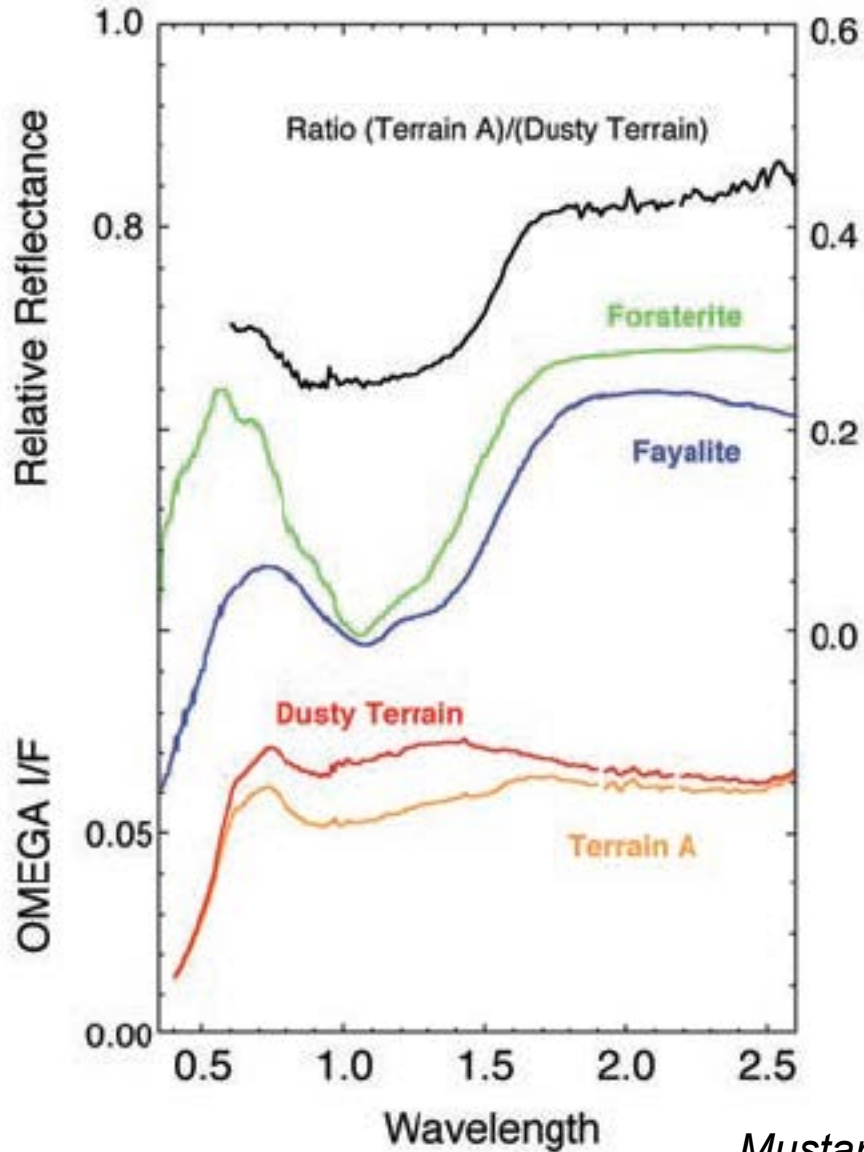
Design Copyright © 1997 Michael Dayah (michael@dayah.com) <http://www.dayah.com/periodic/>

Note: The subgroup numbers 1-18 were adopted in 1984 by the International Union of Pure and Applied Chemistry. The names of elements 112-118 are the Latin equivalents of those numbers.

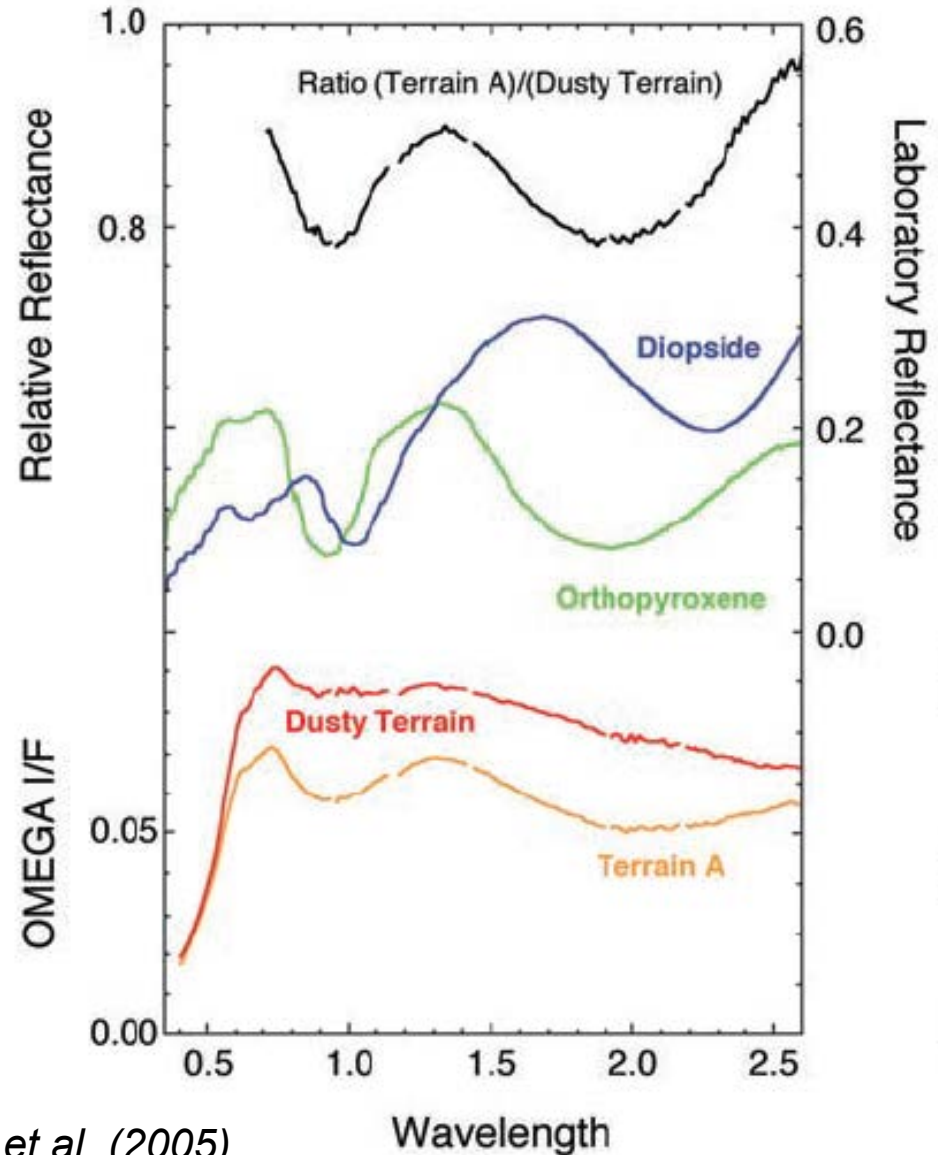
57 2 La Lanthanum 138.9055	58 2 Ce Cerium 140.116	59 2 Pr Praseodymium 140.90765	60 2 Nd Neodymium 144.24	61 2 Pm Promethium (145)	62 2 Sm Samarium 150.36	63 2 Eu Europium 151.964	64 2 Gd Gadolinium 157.25	65 2 Tb Terbium 158.92534	66 2 Dy Dysprosium 162.500	67 2 Ho Holmium 164.93032	68 2 Er Erbium 167.259	69 2 Tm Thulium 168.93421	70 2 Yb Ytterbium 173.04	71 2 Lu Lutetium 174.967
89 2 Ac Actinium (227)	90 2 Th Thorium 232.0381	91 2 Pa Protactinium 231.03688	92 2 U Uranium 238.02891	93 2 Np Neptunium (237)	94 2 Pu Plutonium (244)	95 2 Am Americium (243)	96 2 Cm Curium (247)	97 2 Bk Berkelium (247)	98 2 Cf Californium (251)	99 2 Es Einsteinium (252)	100 2 Fm Fermium (257)	101 2 Md Mendelevium (258)	102 2 No Nobelium (259)	103 2 Lr Lawrencium (262)

Iron is the most geologically abundant transition metal

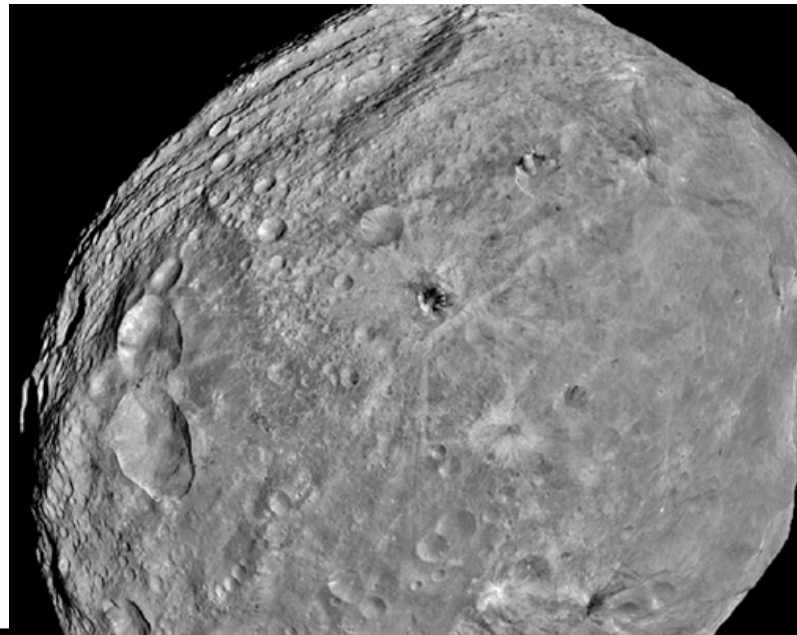
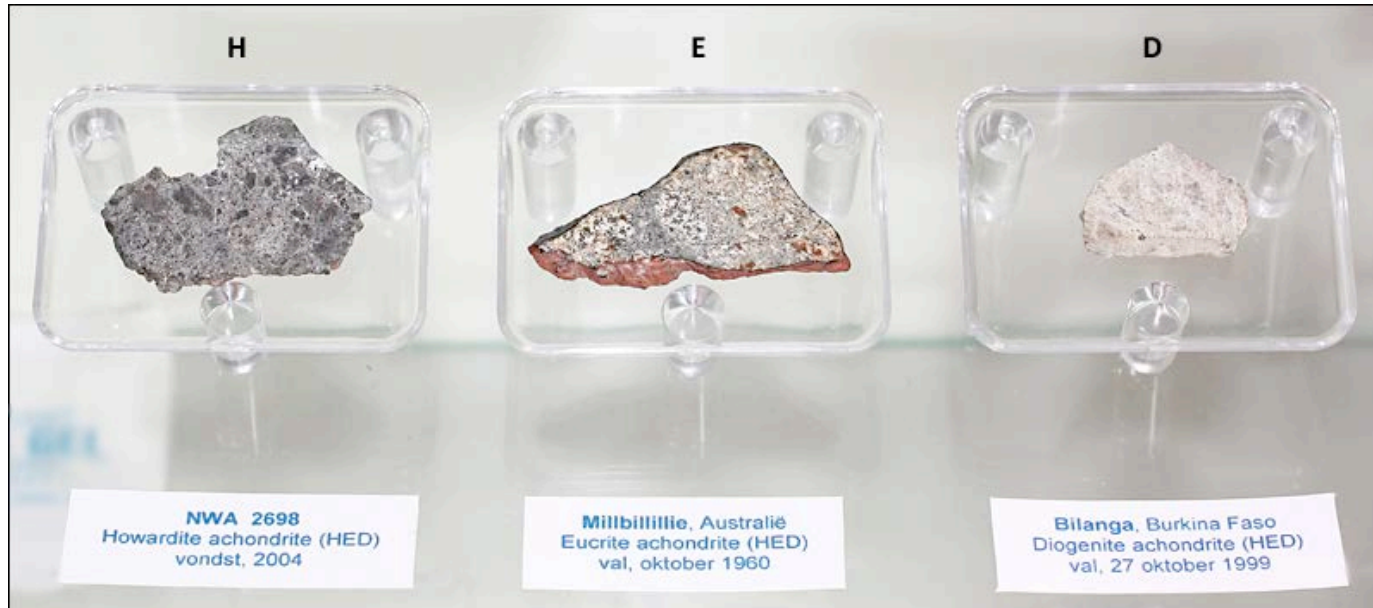
Fe electronic transitions in olivine, pyroxene



Mustard et al. (2005)



Spectroscopy: linking meteorites to asteroids



Electronic Processes

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. The transition can also occur between the same metal in different valence states, such as between Fe^{2+} and Fe^{3+} . Absorptions are typically strong. A common example is Fe-O band in the uv, causing iron oxides to be red.

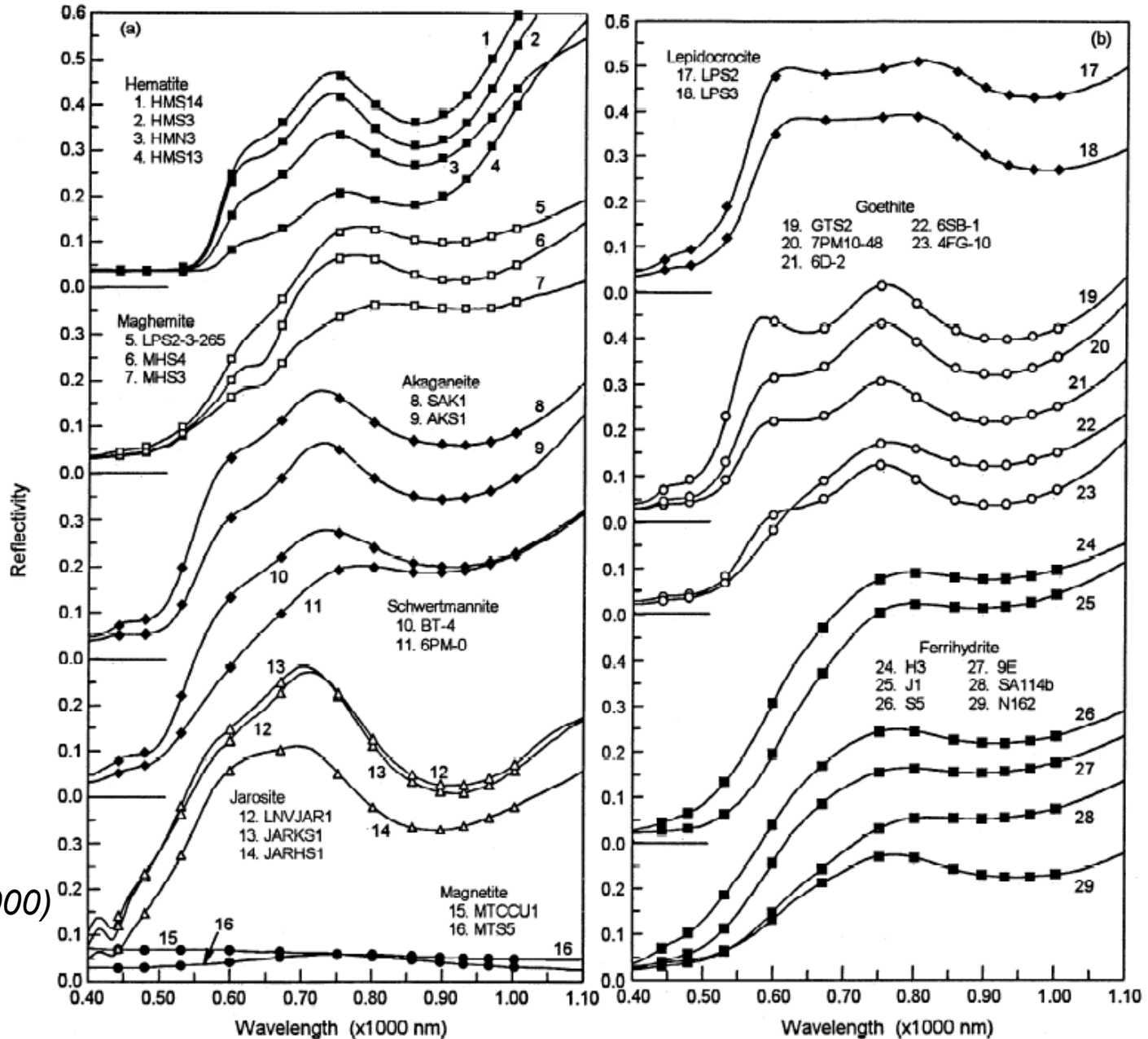


<http://en.wikipedia.org/wiki/Image:Hematite.jpg>



<http://www.galleries.com/minerals/silicate/olivine/olivine.jpg>

Electron charge transfer: why Mars is red!



Morris et al. (2000)

Electronic Processes

Conduction Bands

In metals and 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 yellow color of gold and sulfur is caused by conduction-band absorption.

Gold



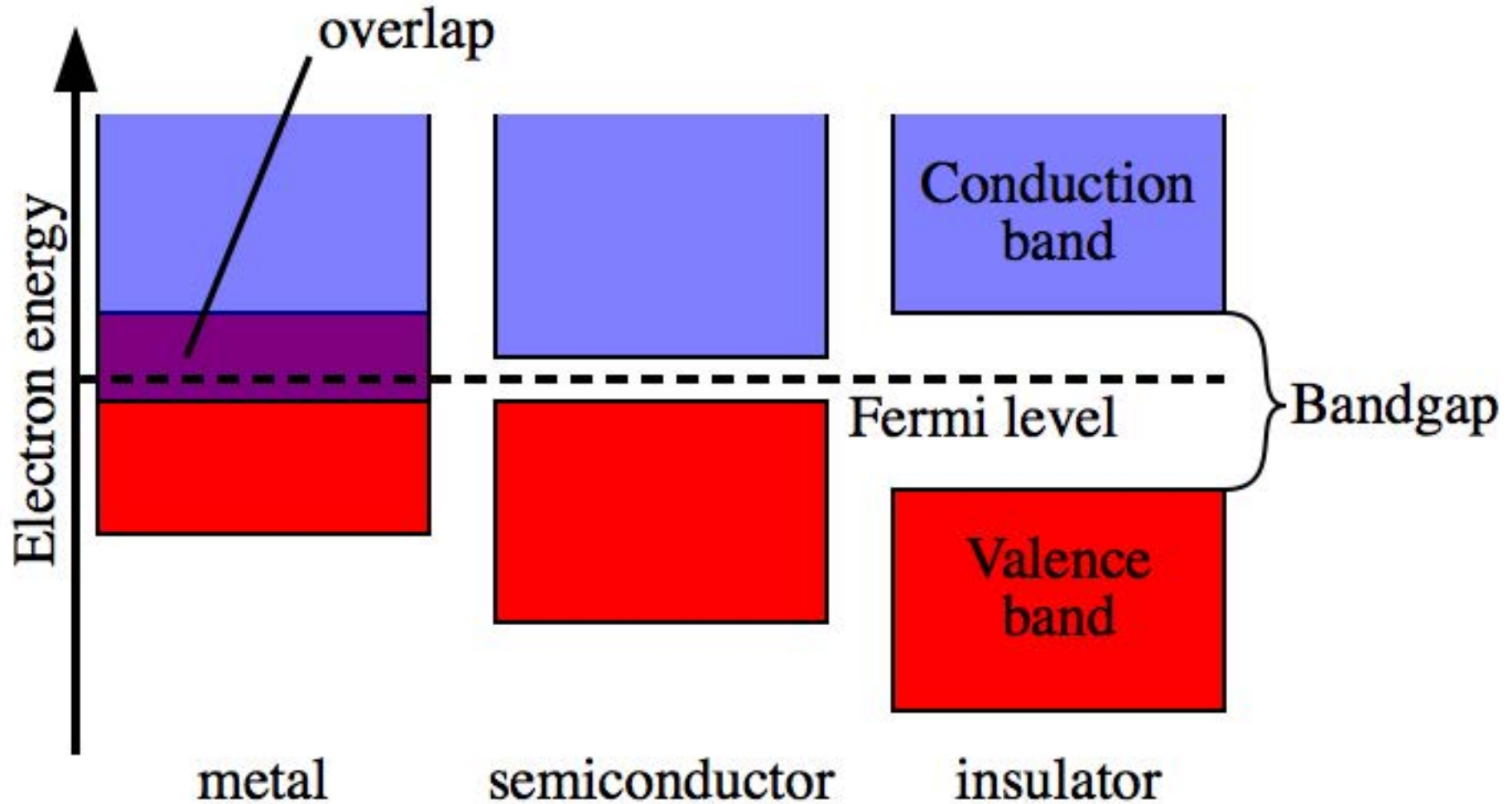
www.egyptcollections.com

Sulfur

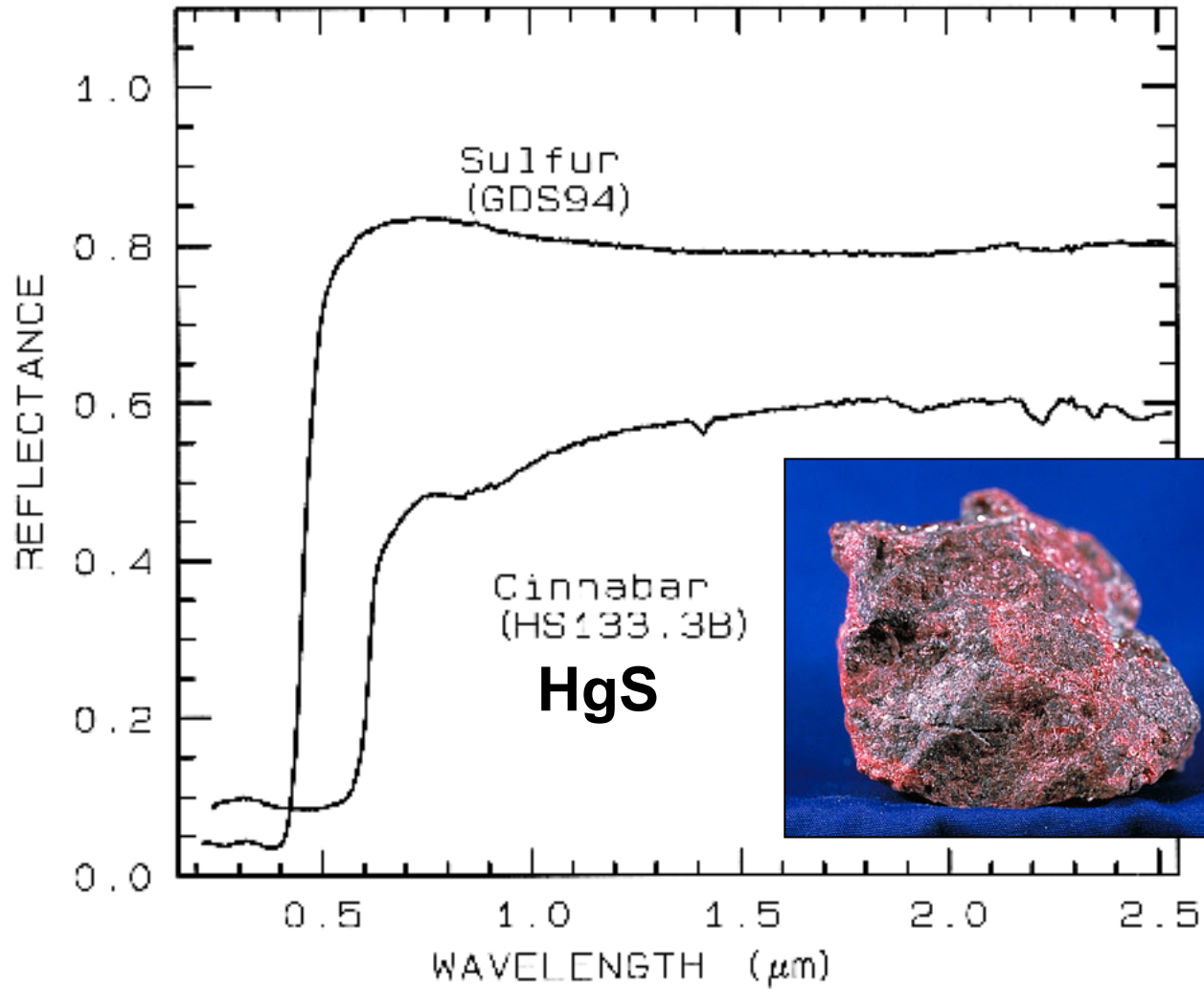


web.syr.edu/~iotz/Gallery.htm

Semiconductor physics



Conduction band processes

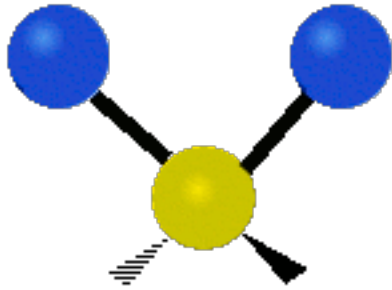


<http://www.mii.org/Minerals/Minpics1/Cinnabar.jpg>

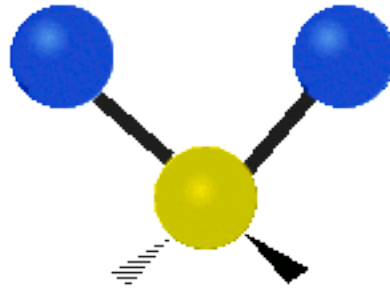
Yellow color of sulfur (e.g., on Io) due to band gap transitions

Molecular vibrations

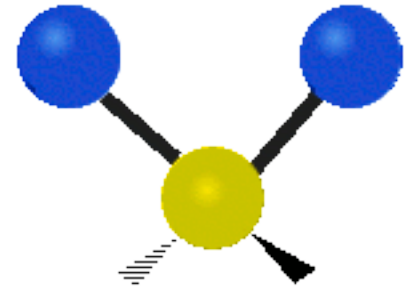
Symmetric stretch



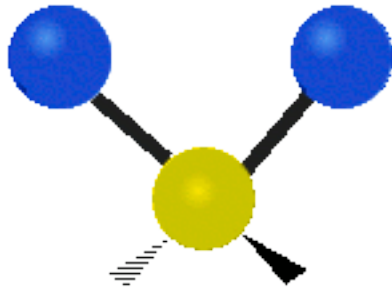
Asymmetric stretch



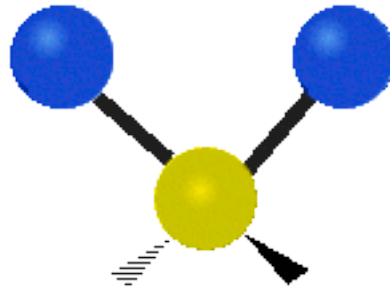
Scissor/bend



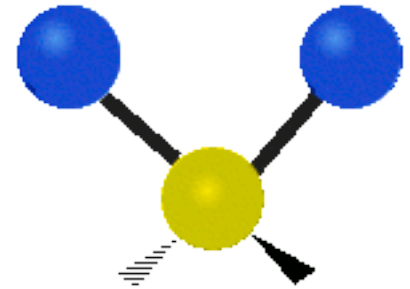
Rocking



Wagging

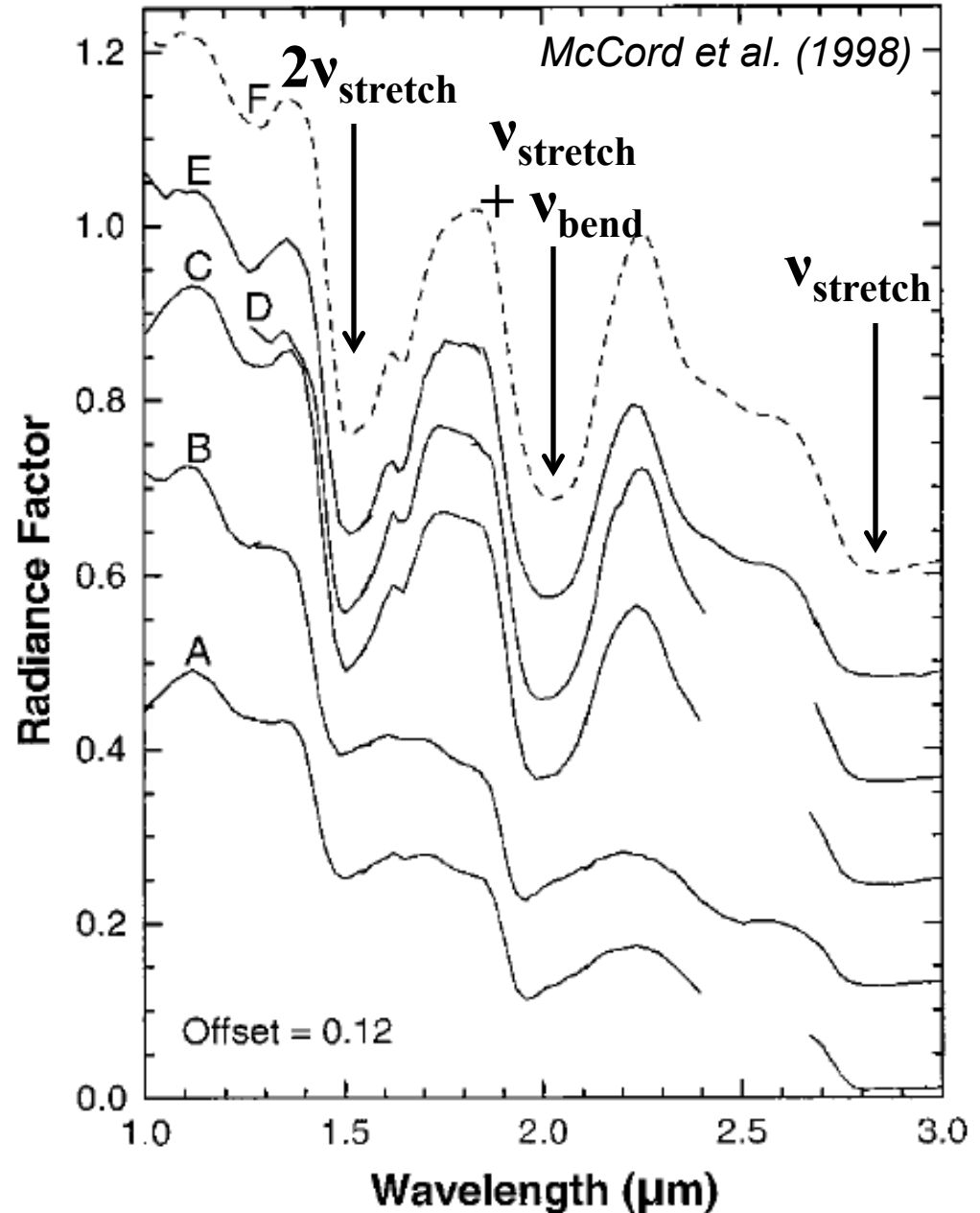


Twist

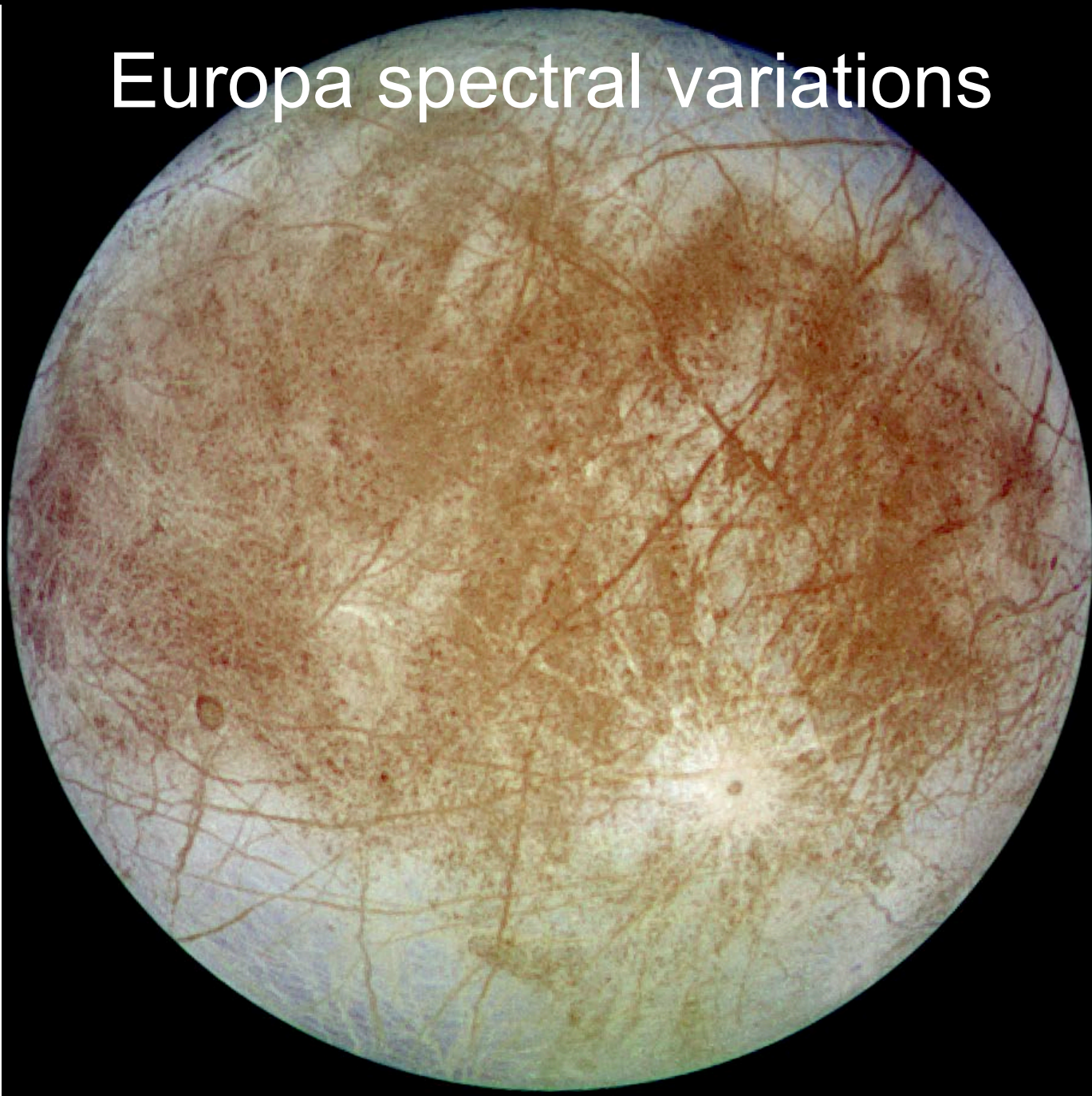


Water vibrations: ice vs. hydrated minerals

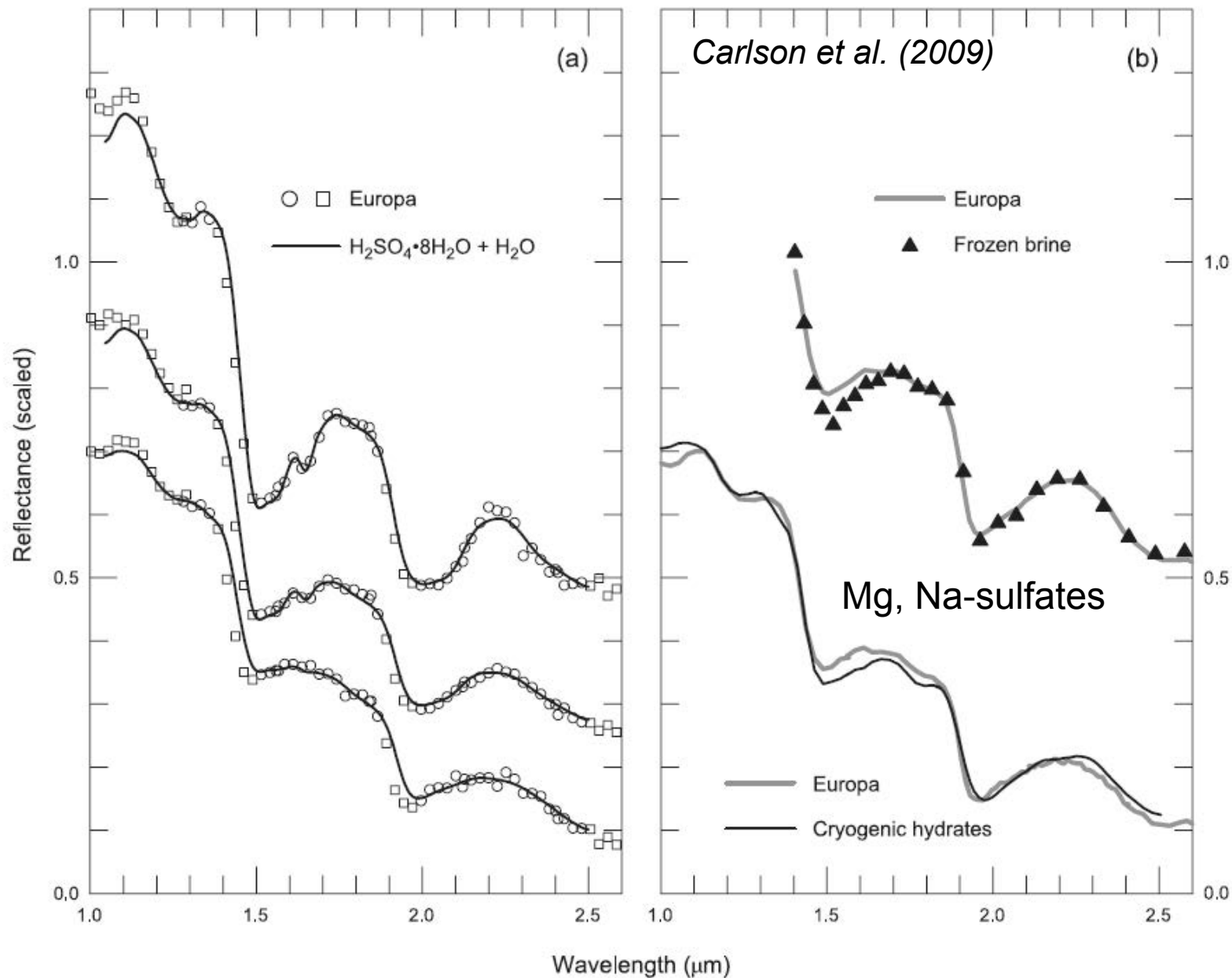
A – D are Europa,
E is Ganymede,
F is model ice spectrum



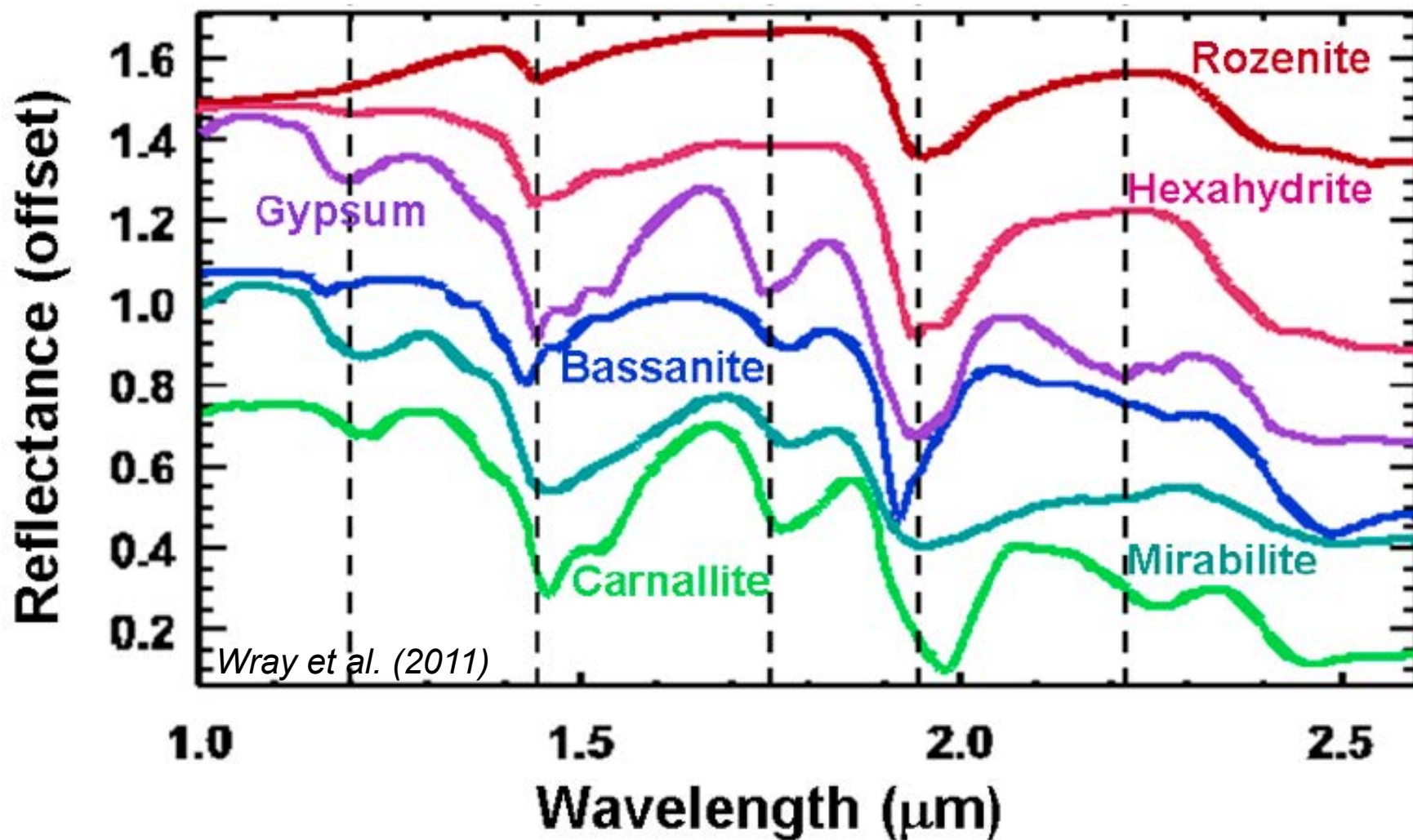
Europa spectral variations



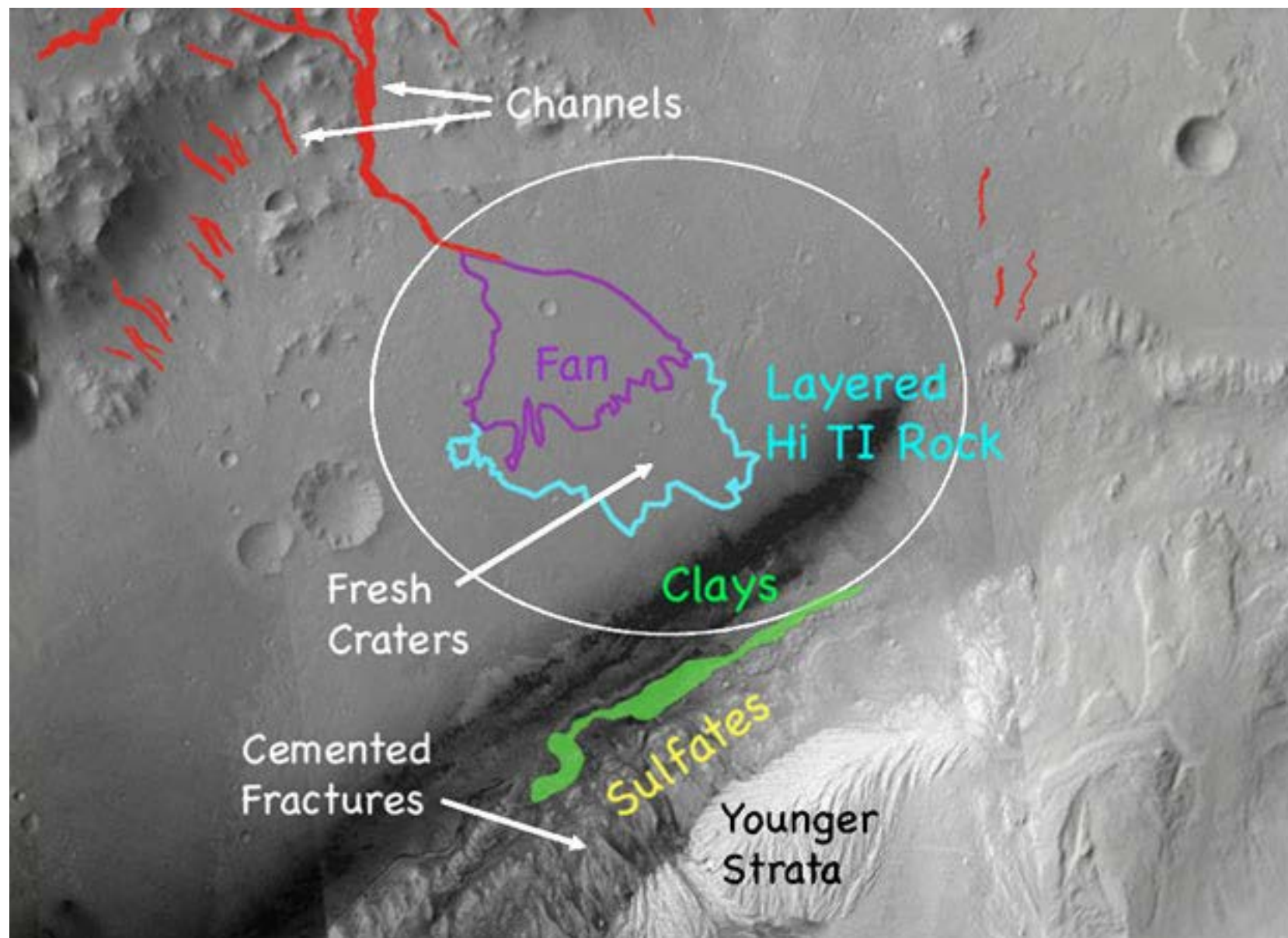
Europa's hydrates: acid or salts?



Hydrated salt spectra

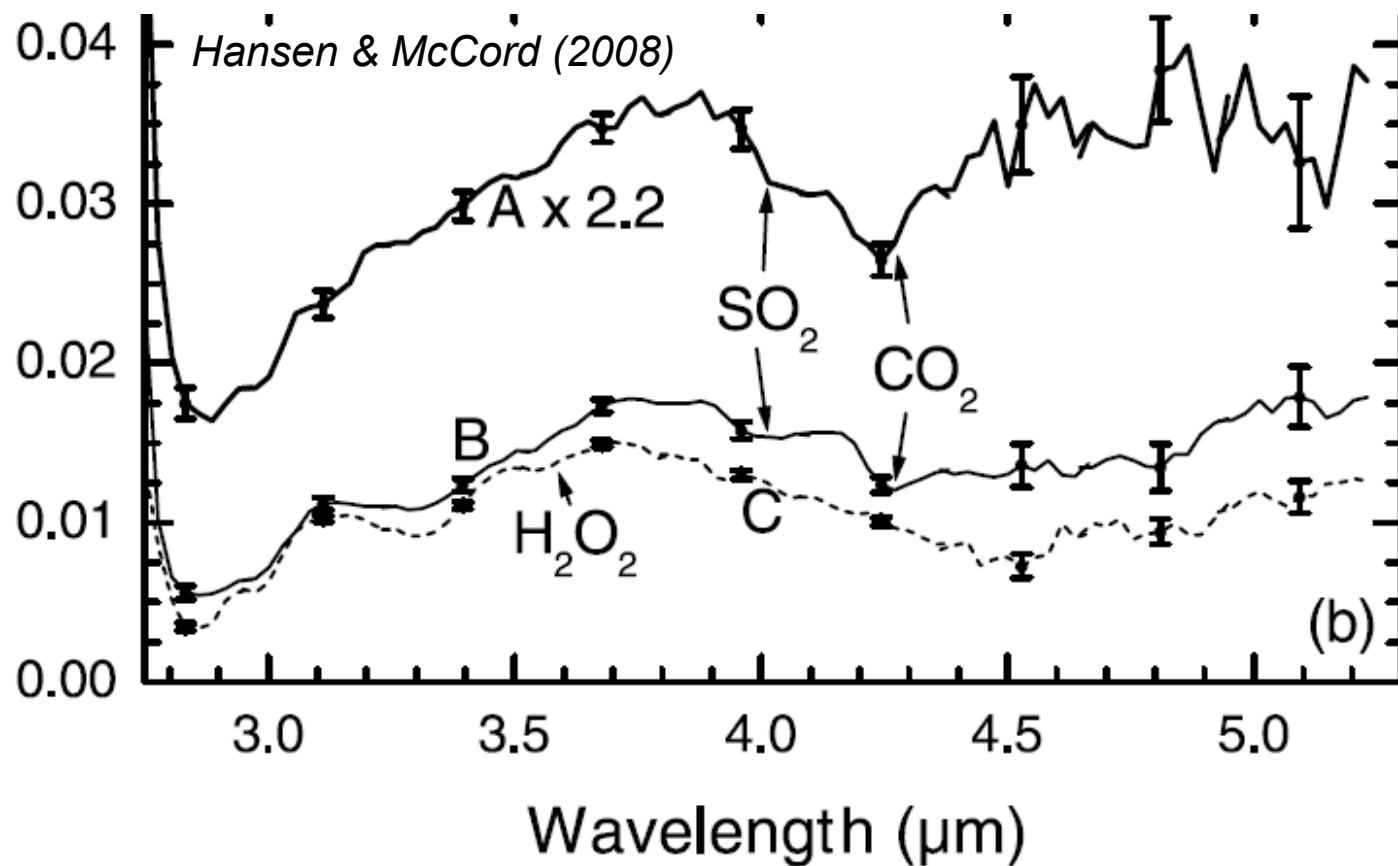


Spectroscopy-guided roving

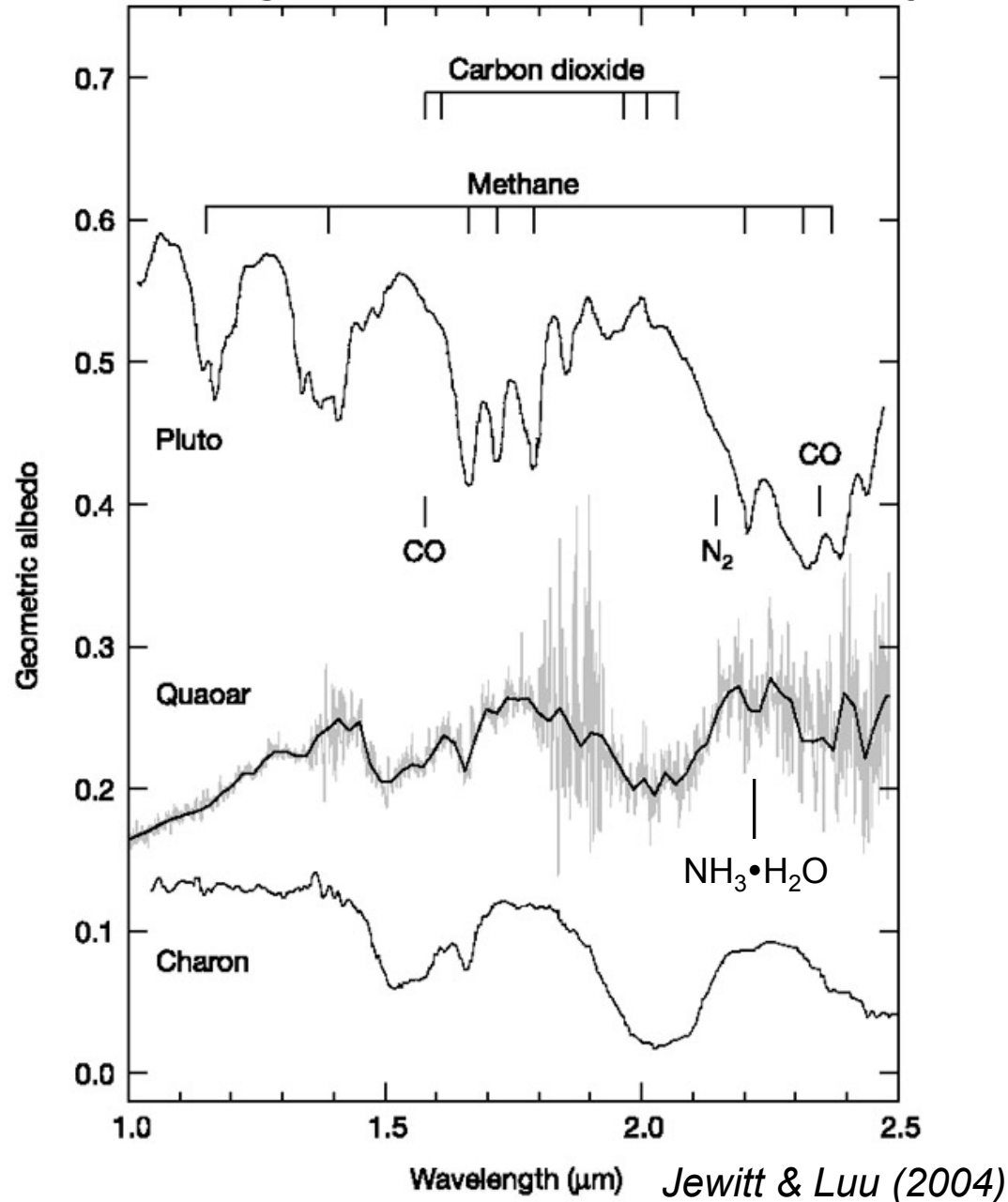


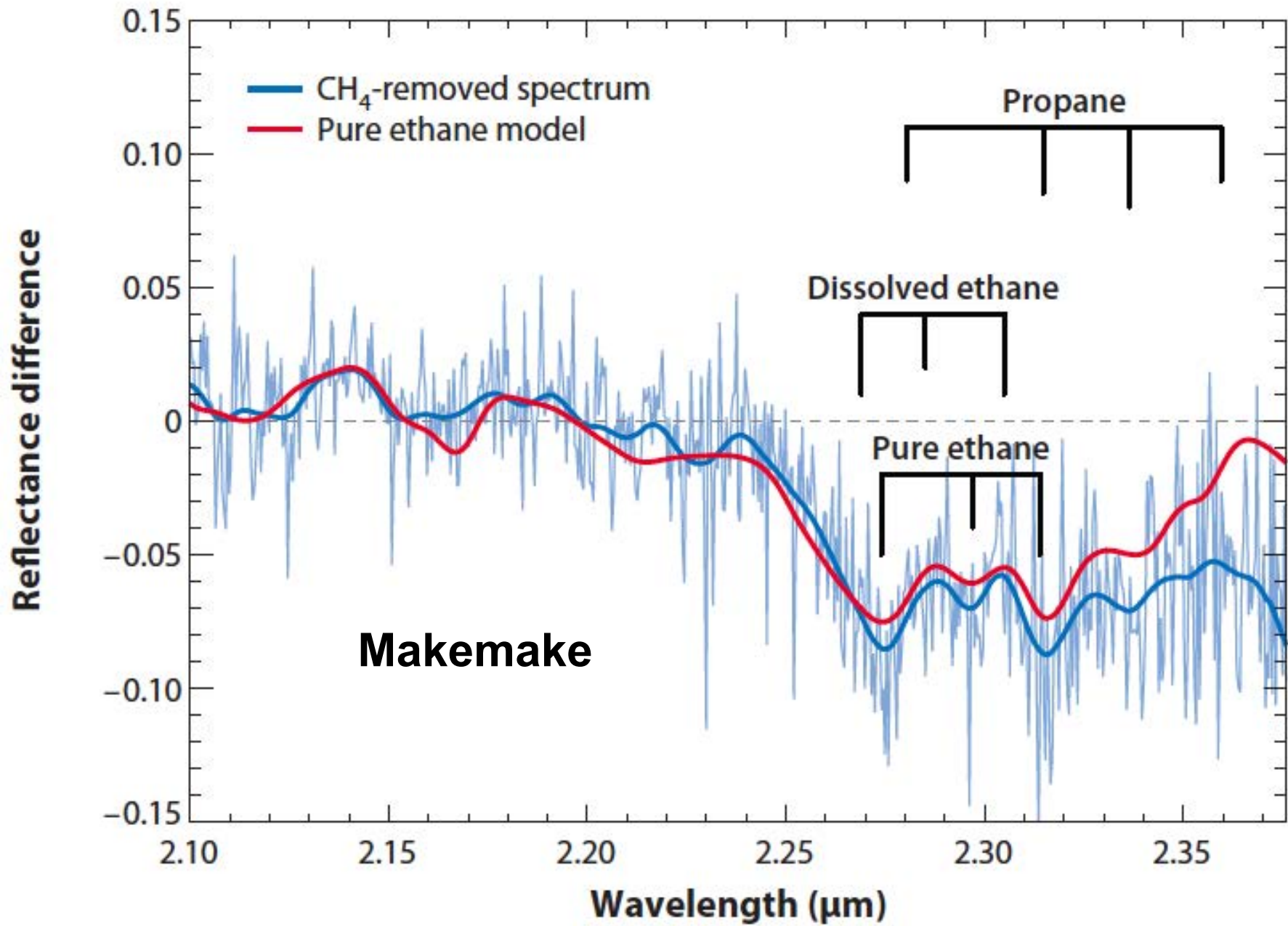
Peroxide, CO₂ and more on Europa

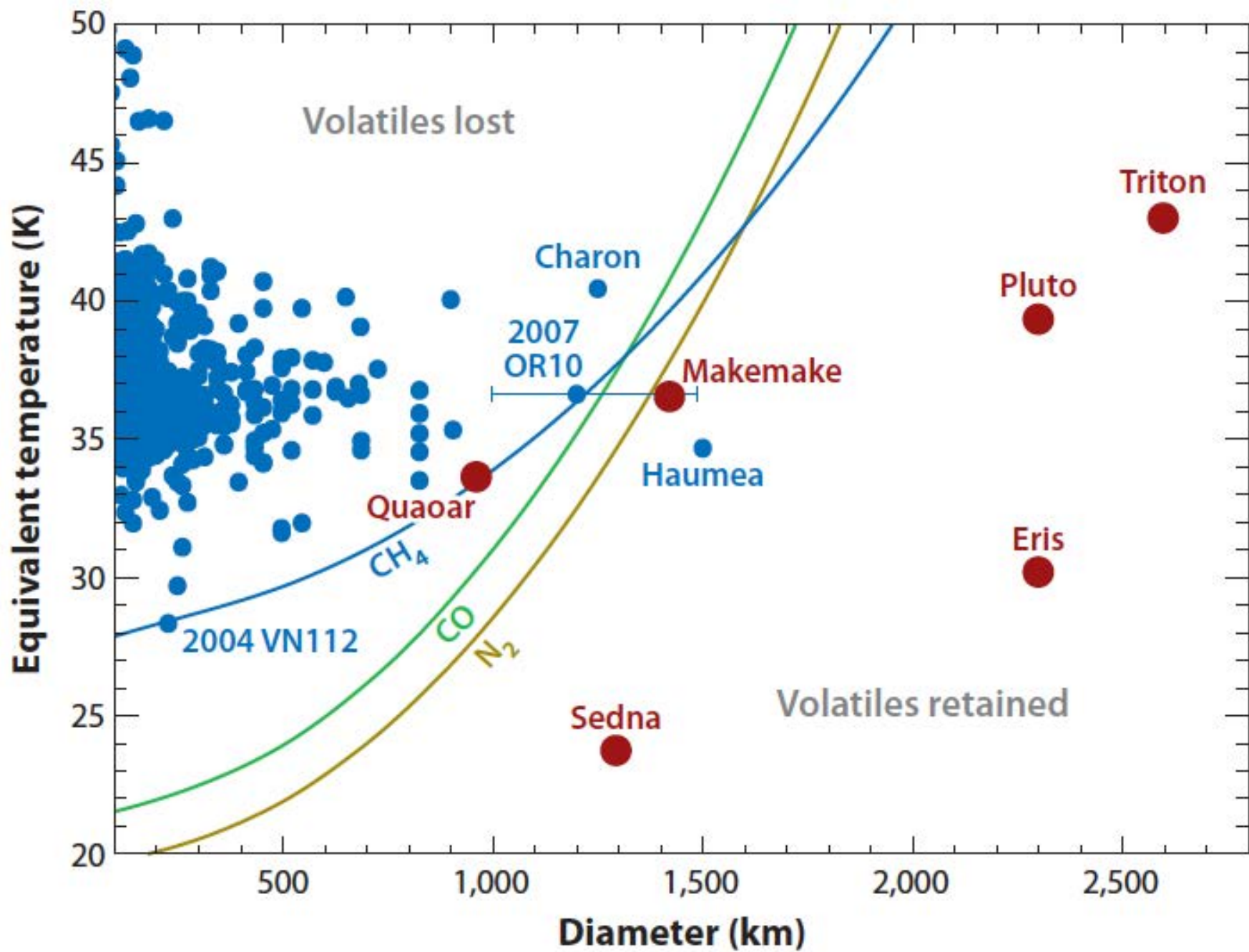
(and Ganymede, Callisto)



Kuiper belt objects: spectrally diverse







Brown (2012)

Organic molecules

Identified on Callisto, Ganymede, Iapetus, Phoebe, ...

