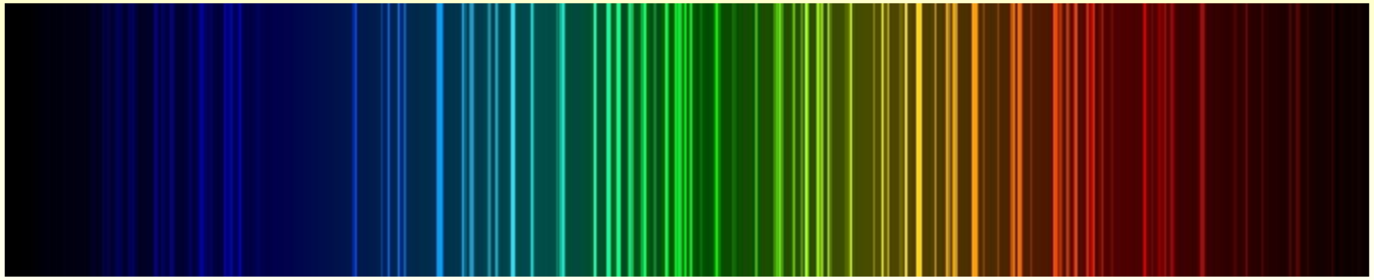
ESPECTROSCOPÍA
una potente herramienta para conocer el universo

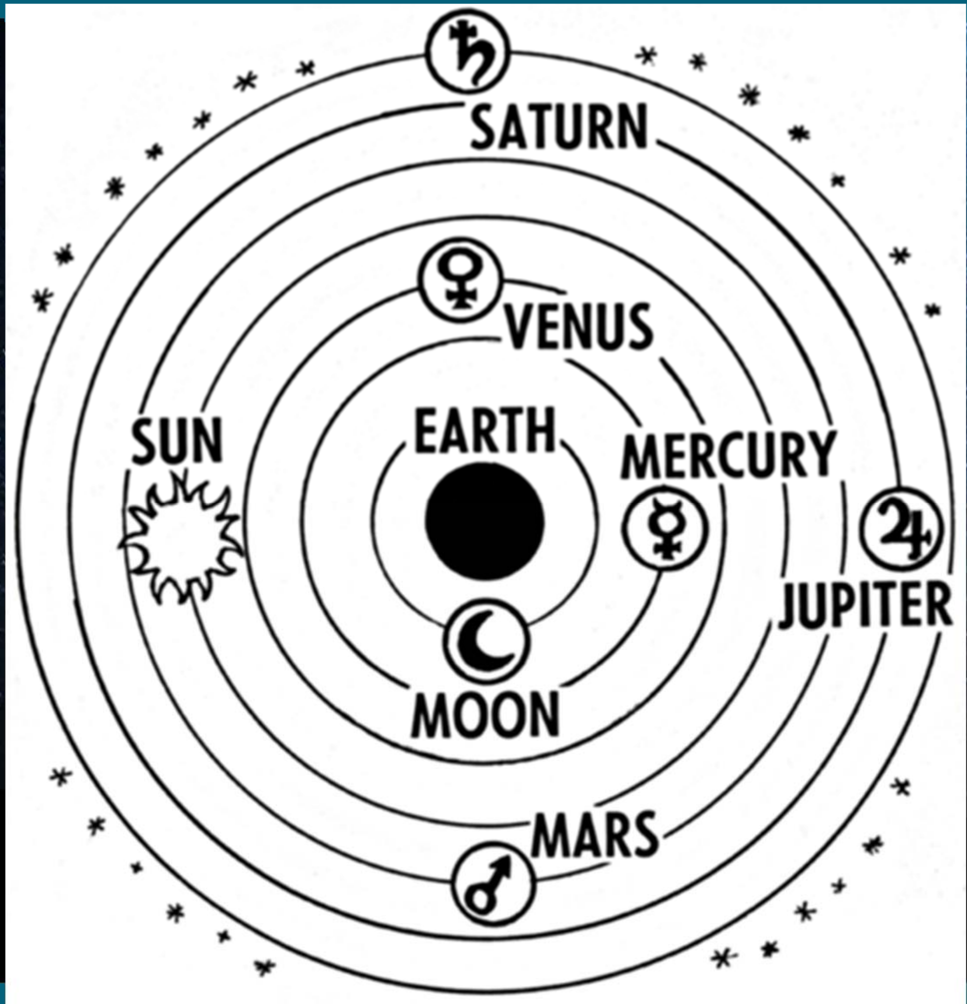


José Mª Fernández

Instituto de Estructura de la Materia, CSIC

www.iem.csic.es/fismol/fdm/

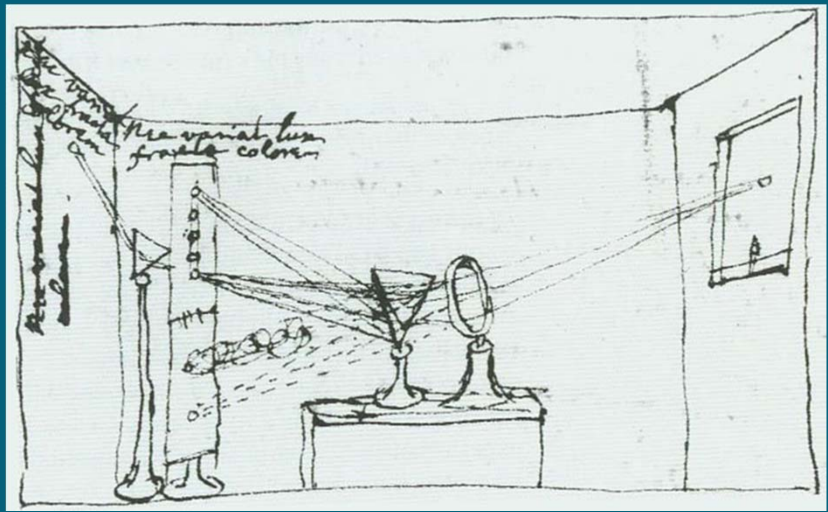
Introducción. Estrellas y planetas



"We will never know how to study by any means the chemical composition (of stars), or their mineralogical structure"

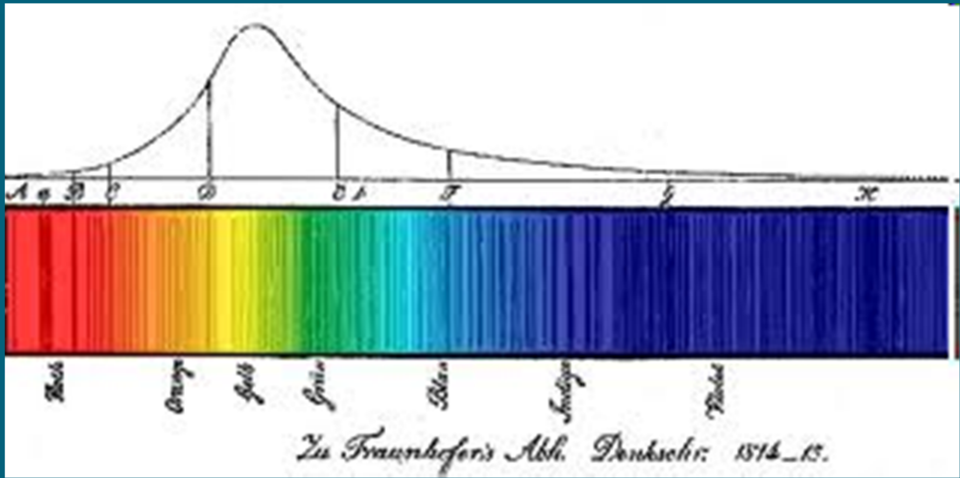
(Auguste Compte, 1835)

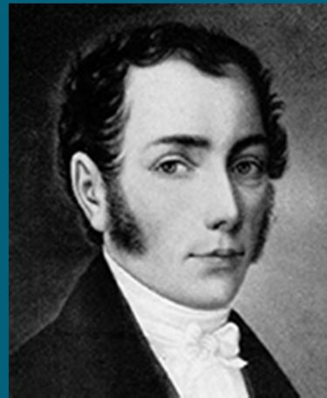
Newton: espectro de la luz blanca



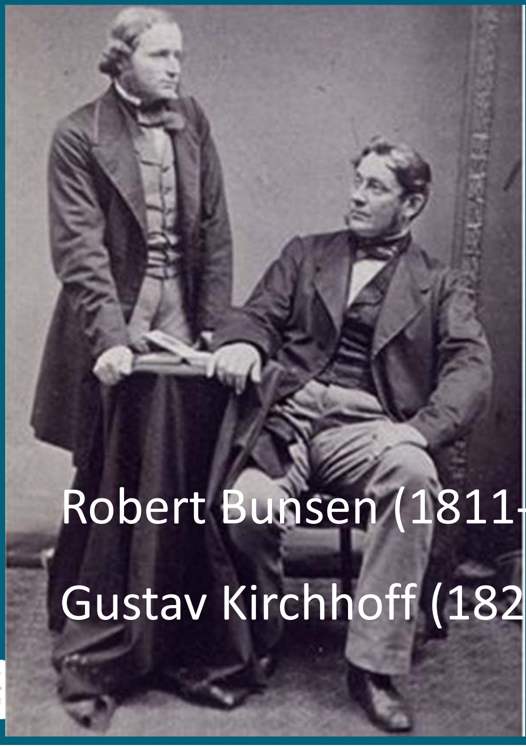
espectro.
(Del lat. *spectrum*).
1. m. fantasma (‖ imagen de una persona muerta).
2. m. *Fís.* Distribución de la intensidad de una radiación en función de una magnitud característica, como la longitud de onda, la energía, la frecuencia o la masa.

Fraunhofer, Bunsen, Kirchhoff



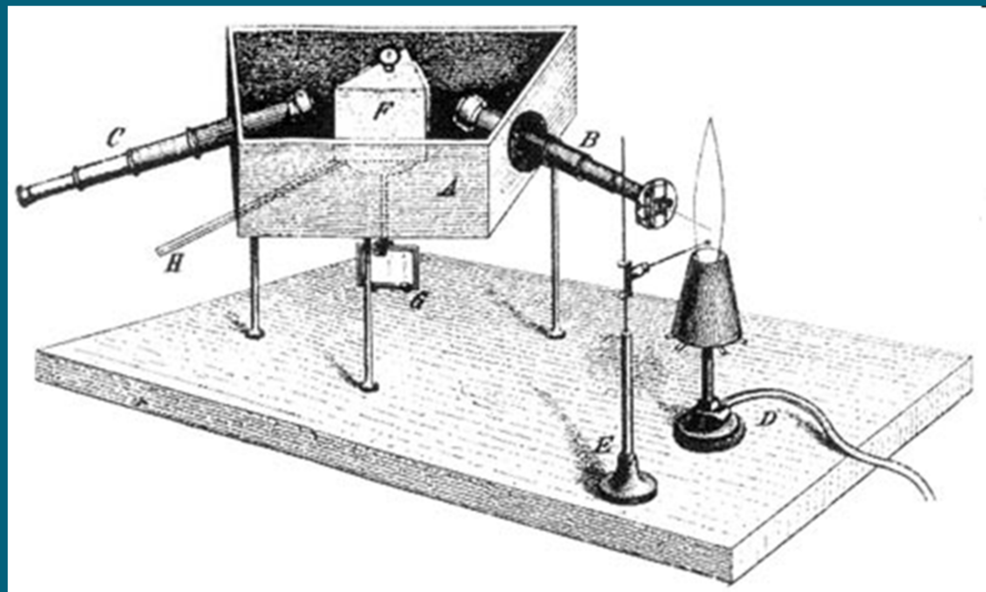


Joseph von Fraunhofer (1787-1826)



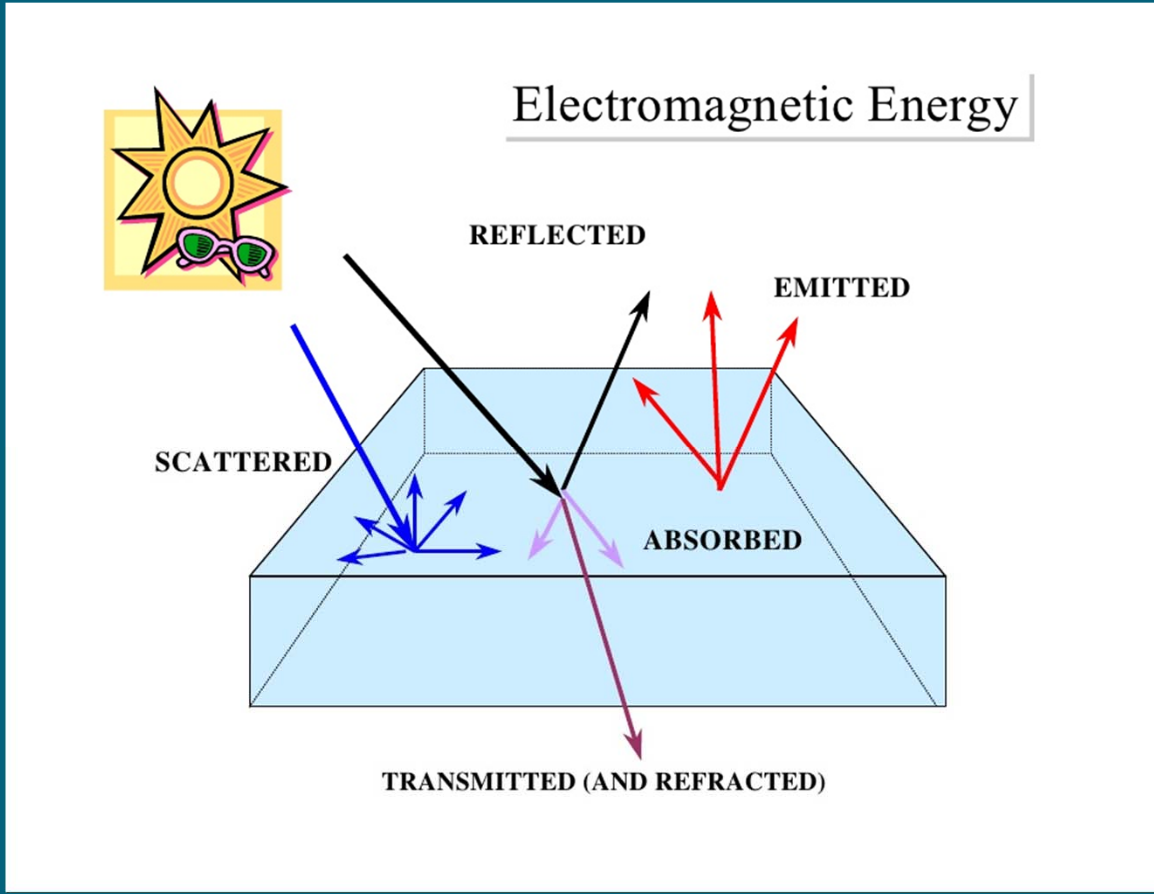
Robert Bunsen (1811-1899)

Gustav Kirchhoff (1824-1887)

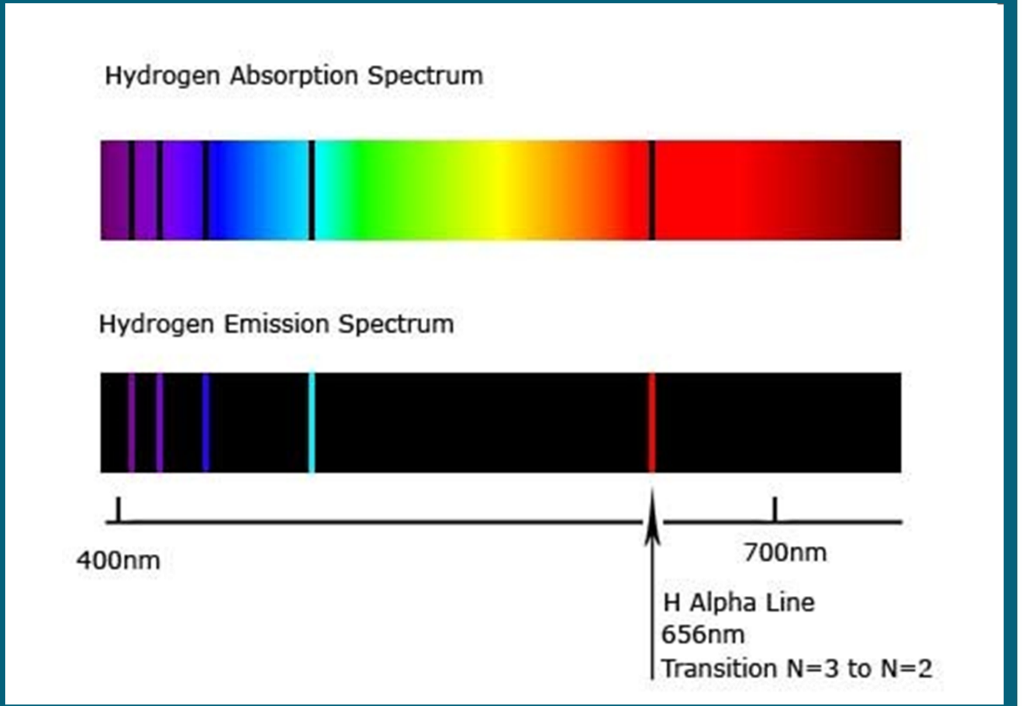


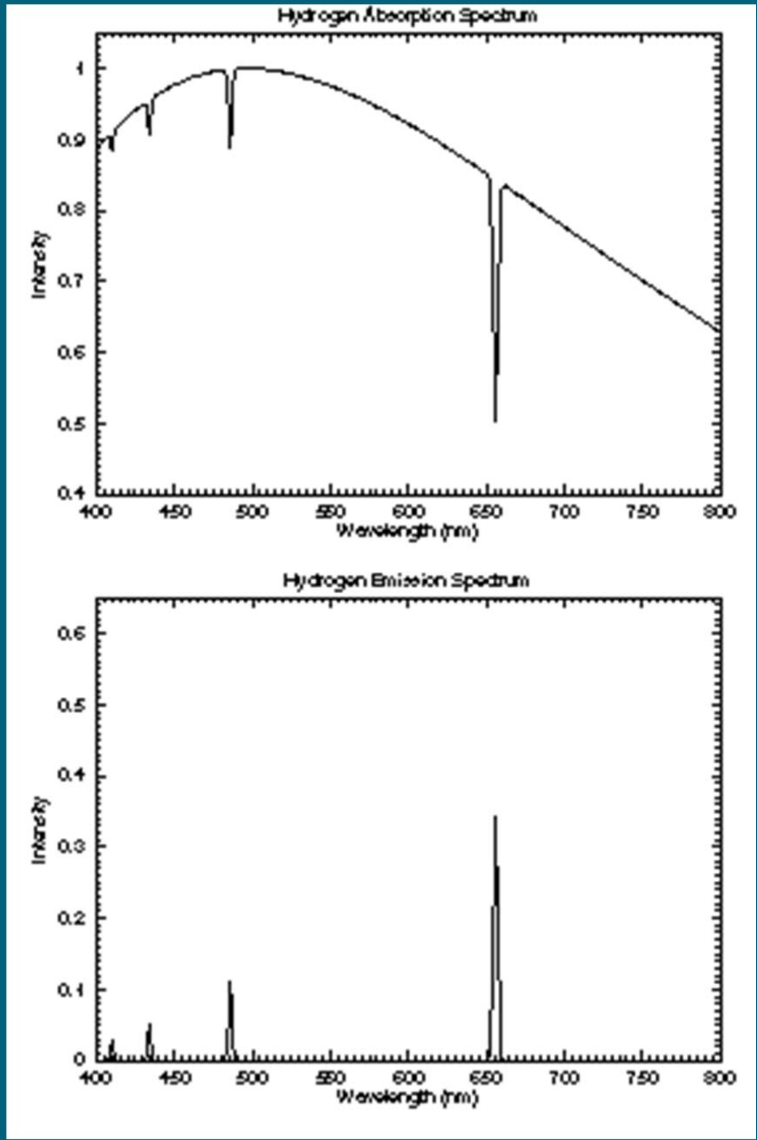
Interacción luz-materia

- dispersión
- reflexión
- transmisión (refracción)
- absorción
- (re)-emisión



Espectros de absorción y emisión

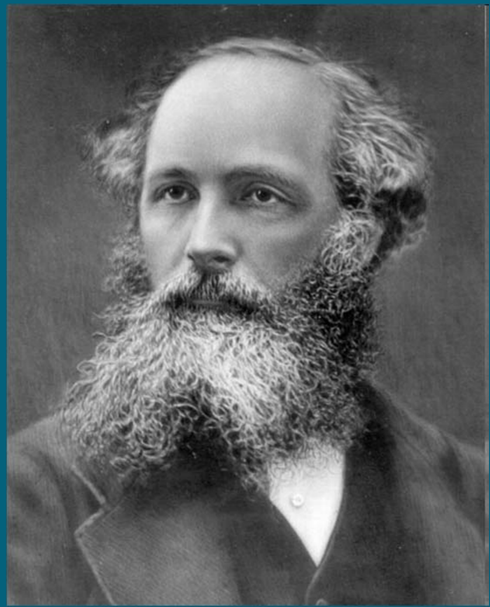




Herschel, Maxwell, Hertz

Wilhelm Herschel
(1738-1822)

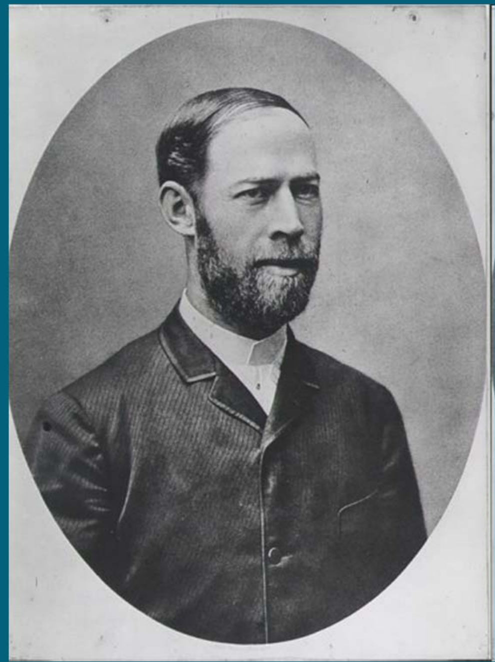
Radiación infrarroja



James Maxwell
(1831-1879)

Ecuaciones del campo electromagnético:

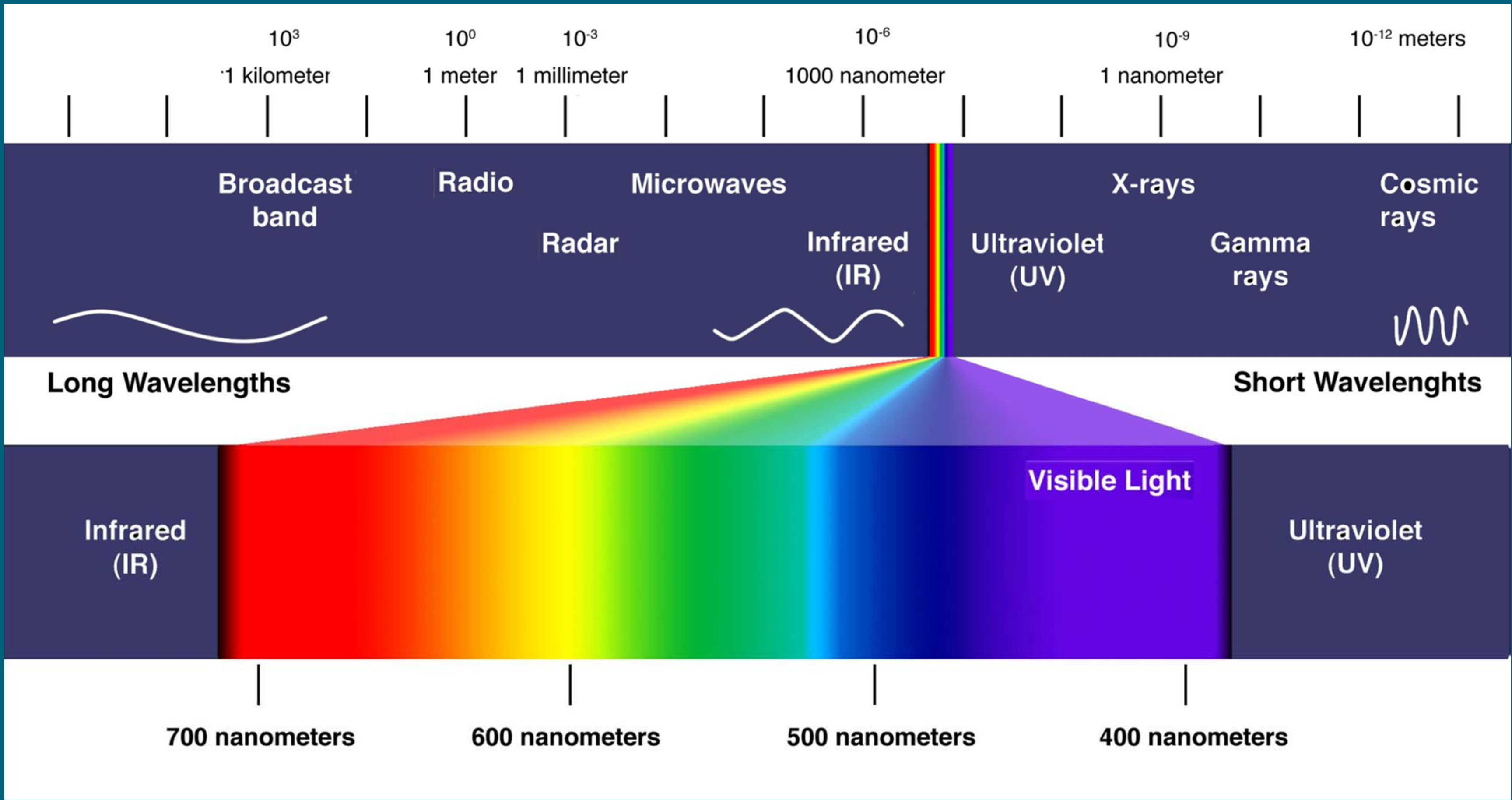
$$c = 1/\sqrt{\varepsilon_0 \mu_0}$$



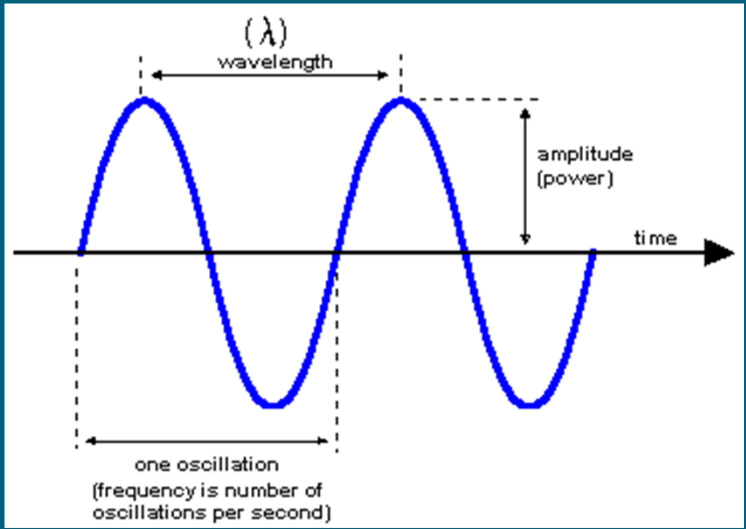
Heinrich Hertz
(1857-1894)

Propagación ondas electromagnéticas

Espectro electromagnético



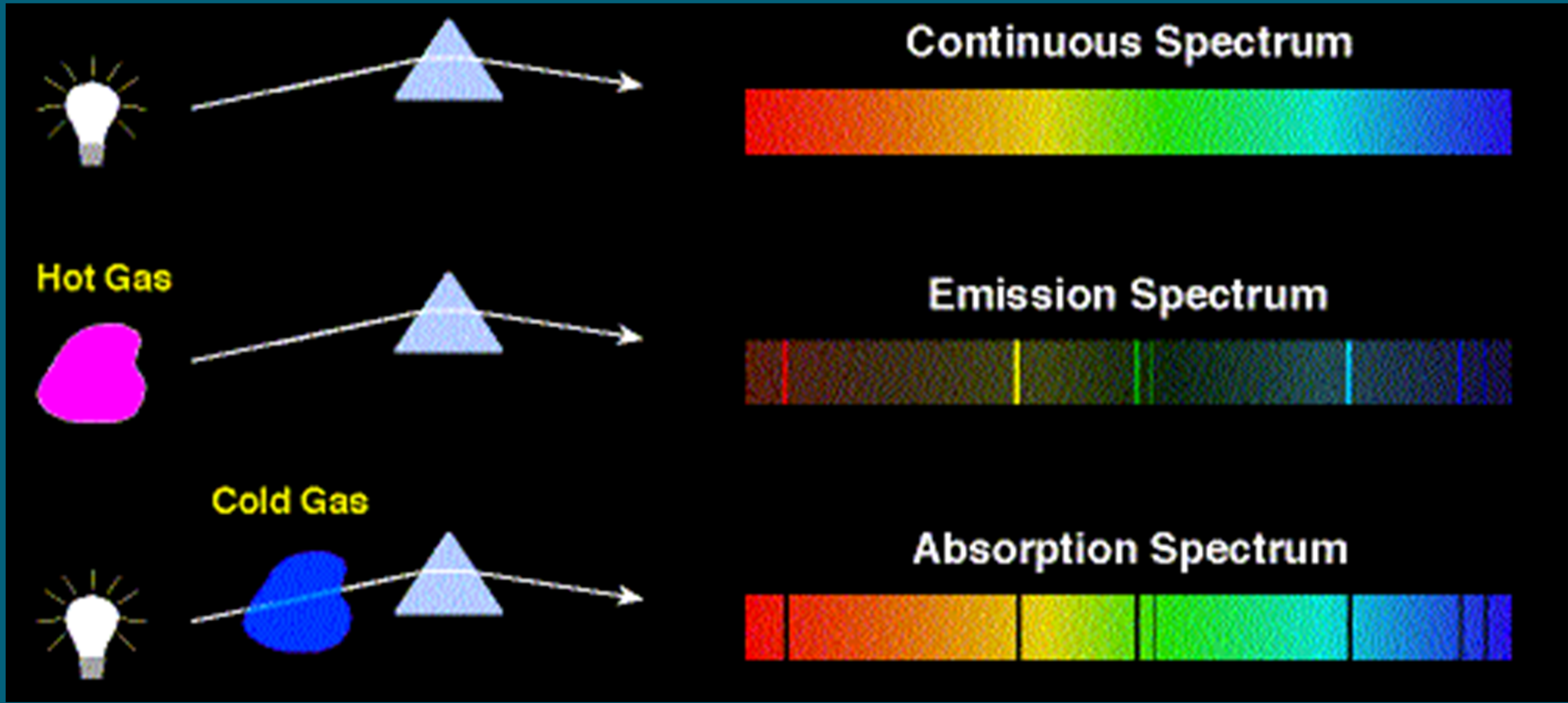
Frecuencia, longitud de onda, número de ondas



- Longitud de onda λ [μm, nm]
- Periodo T [s]
- Frecuencia ν=1/T [MHz, GHz]
- Número de ondas $\kappa=1/\lambda$ [cm^{-1}]

$$c = \frac{\lambda}{T} = \lambda\nu = \frac{\nu}{\kappa}$$

Espectros continuos vs discretos

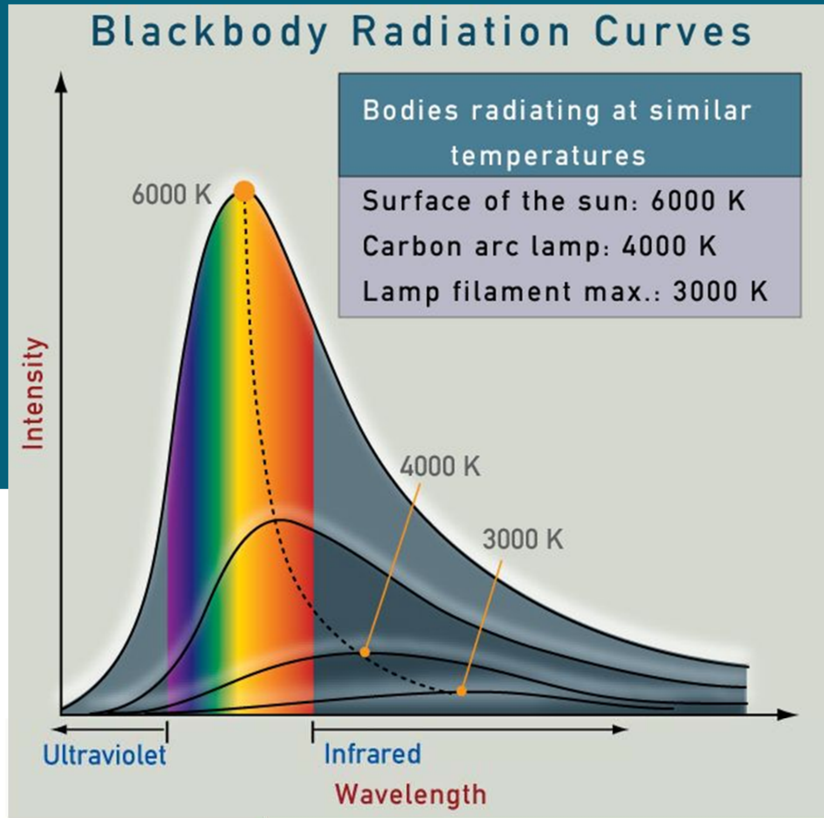


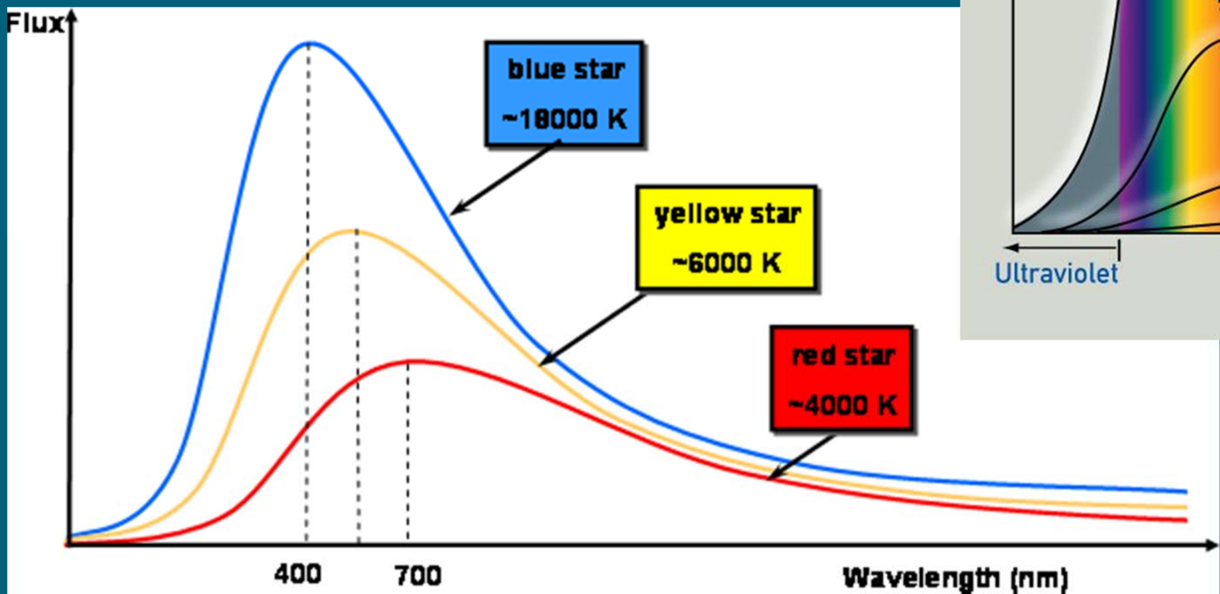
- Espectros discretos <-> estados ligados de átomos y moléculas
- Espectros continuos <-> radiación térmica, estados no-ligados

Emisión del cuerpo negro

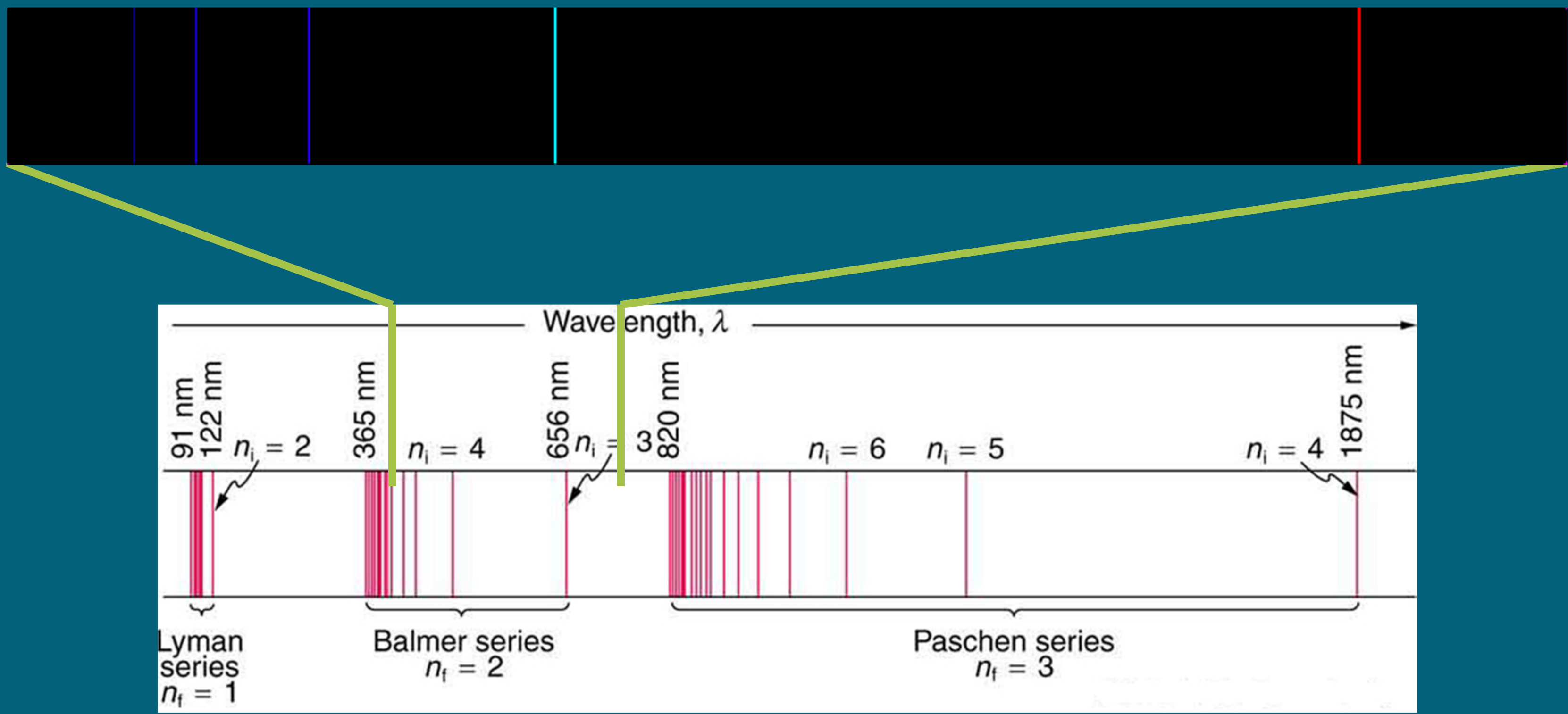
- $E = \sigma\, T^4$ (Stefan-Boltzmann)

  $\sigma = 5{,}67 \times 10^{-8}\ \mathrm{Wm^{-2}K^{-2}}$
- λ_{max}= 2900 µm K / T (Wien)
- $E = h\nu$ (Planck)





Espectro de H atómico



$$\frac{1}{\lambda} = R_H\left(\frac{1}{n^2} - \frac{1}{m^2}\right)$$

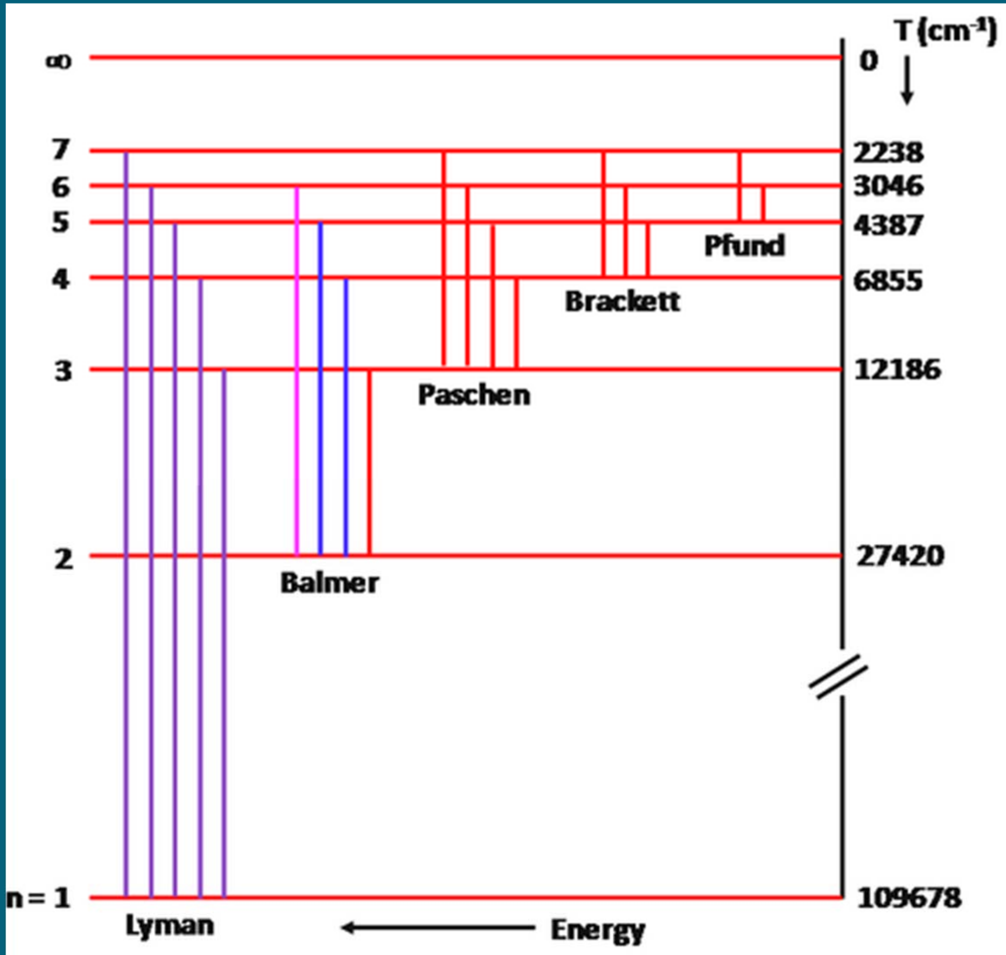
Rydberg $R_H = 109677{,}581\ \mathrm{cm}^{-1}$

Modelo atómico de Bohr

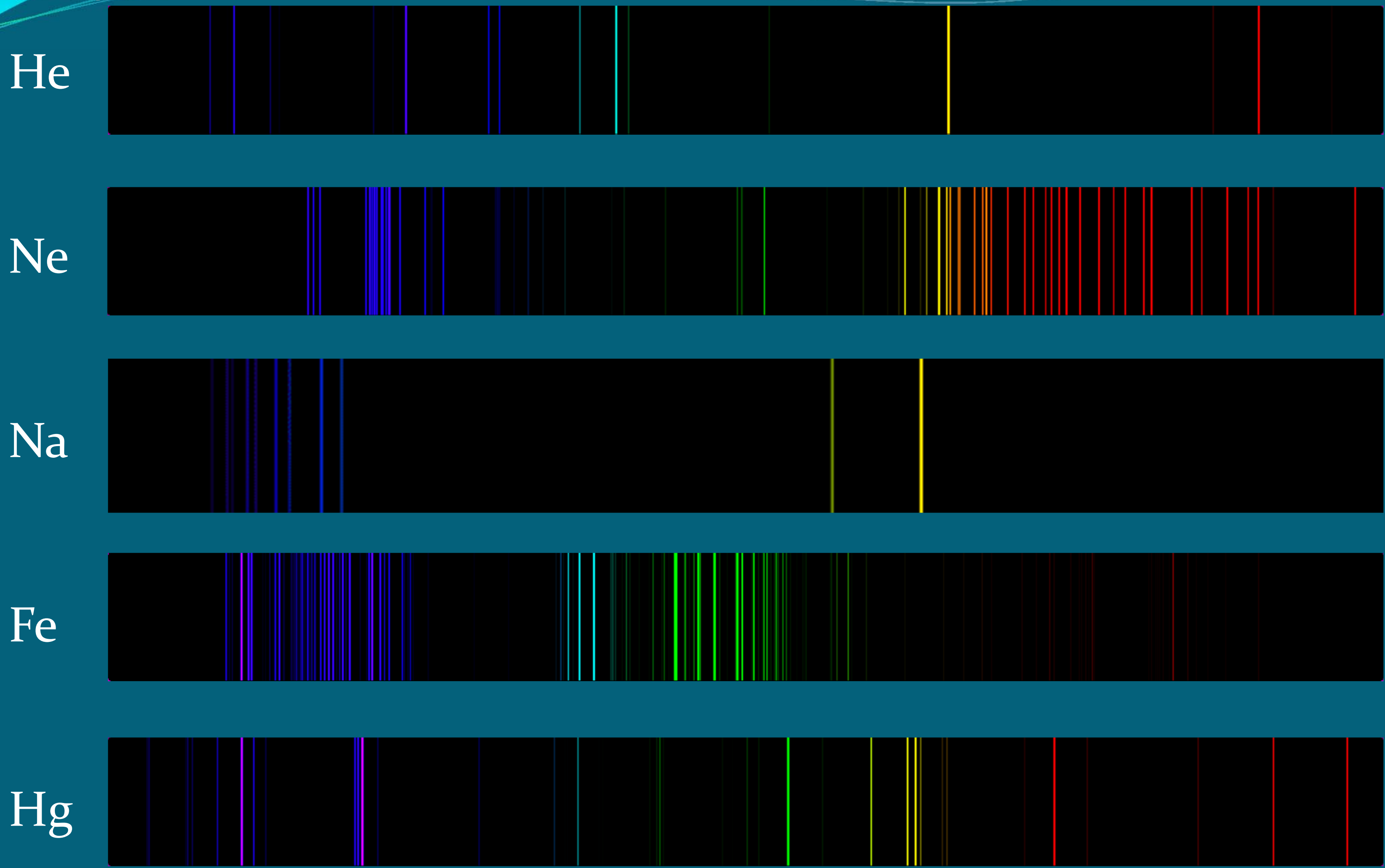
- Electrón en órbitas circulares estacionarias
- Impulso angular múltiplo de h/2π
- $E_n = - R/n^2$
- Tránsitos entre estados

absorción/emisión de luz

$$\nu = (E_j - E_i)/h$$

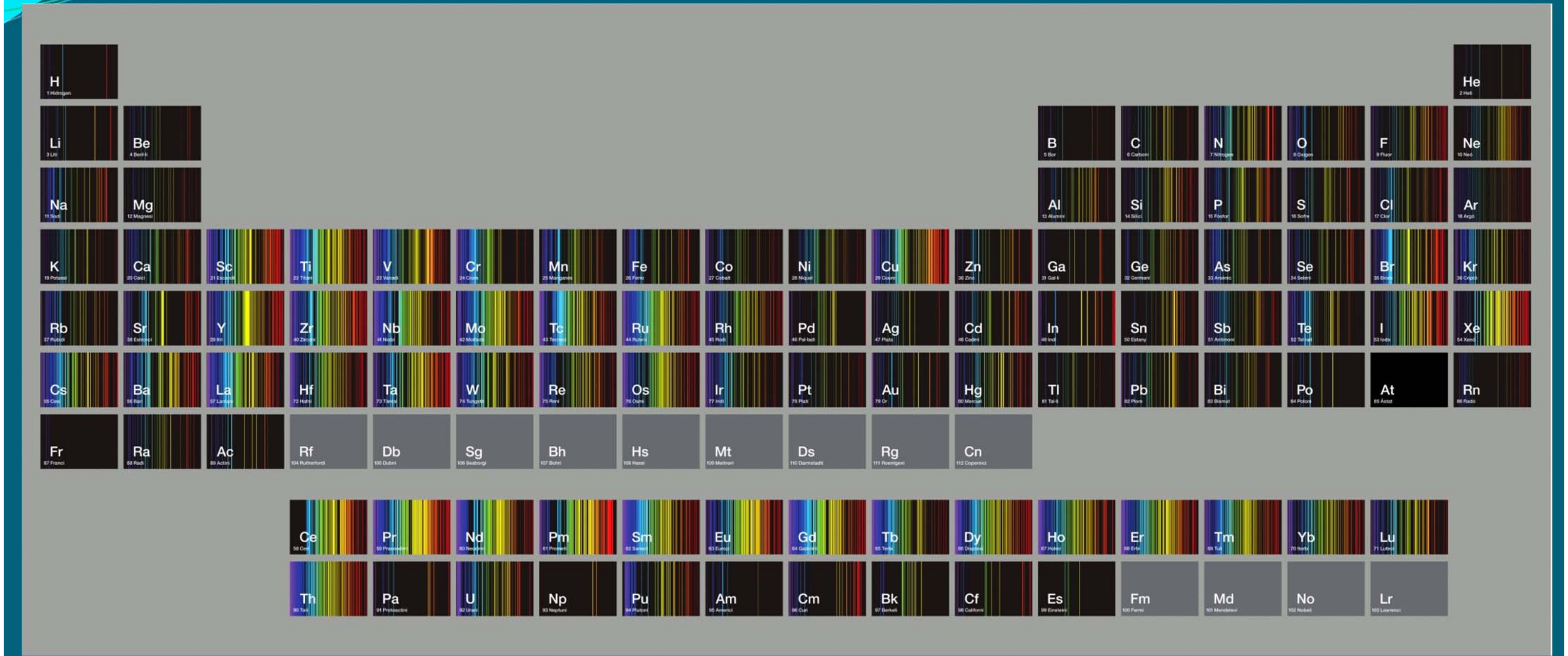


Espectros atómicos I



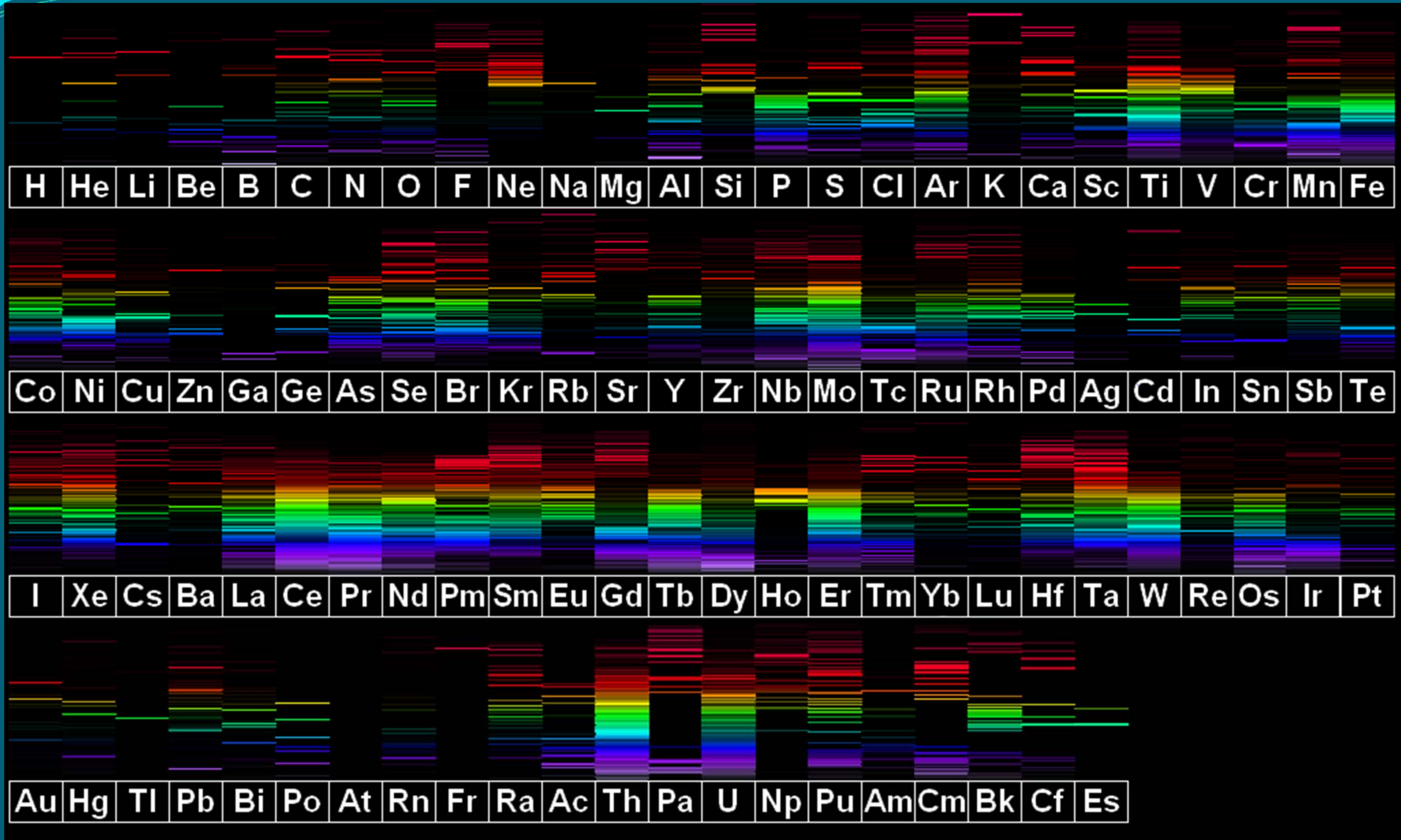
http://www.astronomy.ohio-state.edu/~pogge/Ast350/Labs/Lamps/

Espectros atómicos II



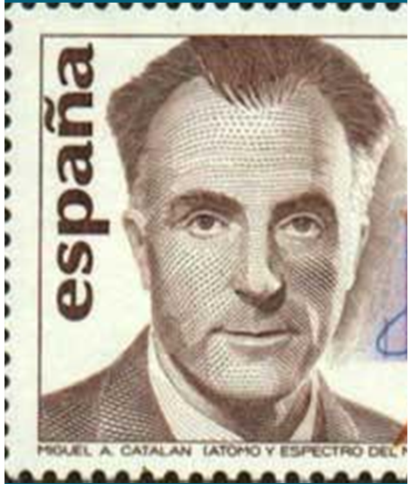
Eugenia Balcells, Homenaje a los elementos (2010)

Espectros atómicos III



Rochester Institute of Technology (http://spiff.rit.edu/classes/phys230/lectures/spectrographs/)

Miguel A. Catalán y los multipletes

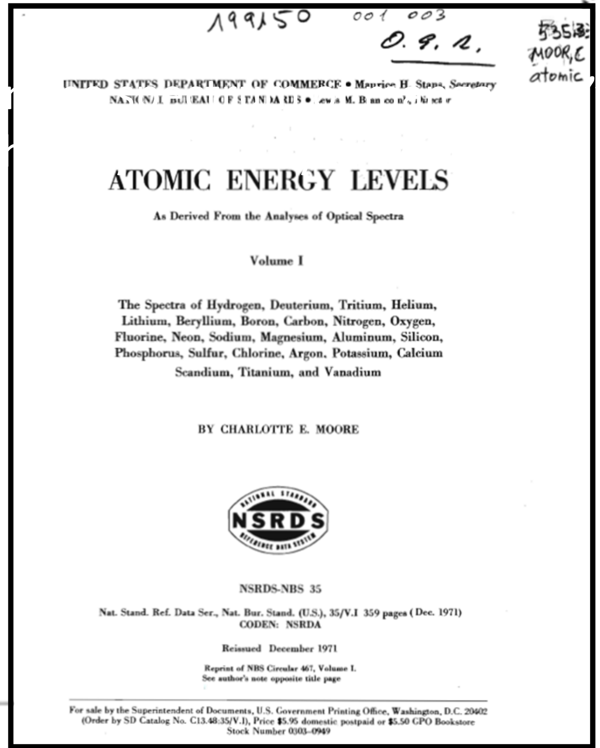


Miguel A. Catalán (1...

TABLE 25. THE PERIODIC SYSTEM*

1	1s	H 1, He 2
2	2s	Li 3, Be 4
	2p	B 5, C 6, N 7, O 8, F 9, Ne 10
3	3s	Na 11, Mg 12
	3p	Al 13, Si 14, P 15, S 16, Cl 17, A 18
4	4s	K 19, Ca 20
	3d	Sc 21, Ti 22, V 23, Cr 24, Mn 25, Fe 26, Co 27, Ni 28, Cu 29, Zn 30
	4p	Ga 31, Ge 32, As 33, Se 34, Br 35, Kr 36
5	5s	Rb 37, Sr 38
	4d	Y 39, Zr 40, Cb 41, Mo 42, Tc 43, Ru 44, Rh 45, Pd 46, Ag 47, Cd 48
	5p	In 49, Sn 50, Sb 51, Te 52, I 53, Xe 54
6	6s	Cs 55, Ba 56
	4f	La 57, Ce 58, Pr 59, Nd 60, Pm 61, Sm 62, Eu 63, Gd 64, Tb 65, Dy 66, Ho 67, Er 68, Tm 69, Yb 70
	5d	Lu 71, Hf 72, Ta 73, W 74, Re 75, Os 76, Ir 77, Pt 78, Au 79, Hg 80
	6p	Tl 81, Pb 82, Bi 83, Po 84, At 85, Rn 86
7	7s	Fr 87, Ra 88
	5f	Ac 89, Th 90, Pa 91, U 92, Np 93, Pu 94, Am 95, Cm 96, 97, 98, 99, 100, 101, 102
	6d	103 -- -- -- -- -- -- -- -- --

*This arrangement is by Catalán. The electrons indicated in column two that are connected by braces have approximately the same binding energy. Consequently, for some elements one type of electron is preferred over another in the normal configuration, as for example, Cr, Cb, Pd, La, Ac, Th.



UNITED STATES DEPARTMENT OF COMMERCE • Maurice H. Stans, Secretary
NATIONAL BUREAU OF STANDARDS • Lewis M. Branscomb, Director

ATOMIC ENERGY LEVELS

As Derived From the Analyses of Optical Spectra

Volume I

The Spectra of Hydrogen, Deuterium, Tritium, Helium, Lithium, Beryllium, Boron, Carbon, Nitrogen, Oxygen, Fluorine, Neon, Sodium, Magnesium, Aluminum, Silicon, Phosphorus, Sulfur, Chlorine, Argon, Potassium, Calcium Scandium, Titanium, and Vanadium

BY CHARLOTTE E. MOORE

NSRDS

NSRDS-NBS 35

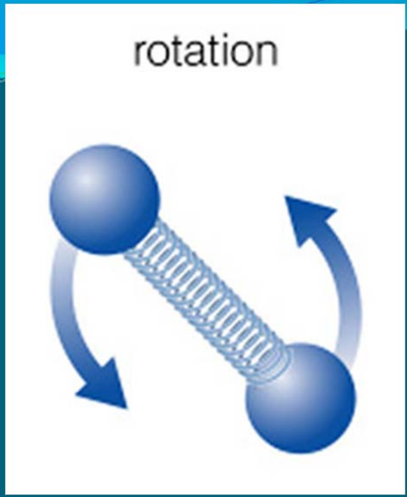
Nat. Stand. Ref. Data Ser., Nat. Bur. Stand. (U.S.), 35/V.I 359 pages (Dec. 1971)
CODEN: NSRDA

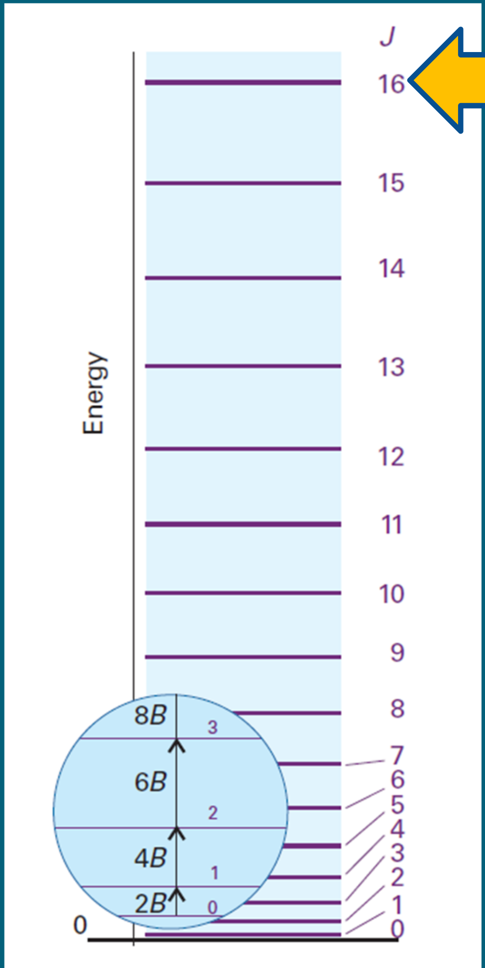
Reissued December 1971

Reprint of NBS Circular 467, Volume I.
See author's note opposite title page

For sale by the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402 (Order by SD Catalog No. C13.48:35/V.I), Price $5.95 domestic postpaid or $5.50 GPO Bookstore
Stock Number 0303-0949

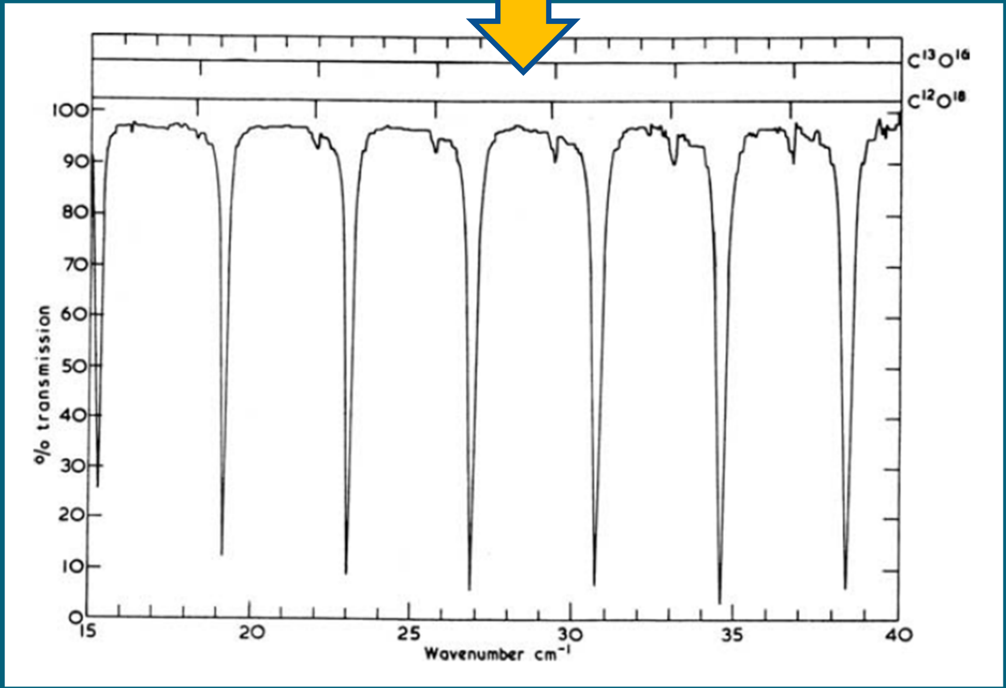
Espectros moleculares I



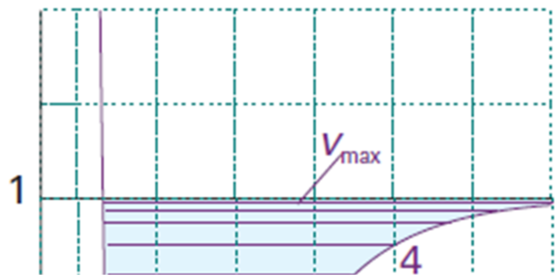


$$E(J) = B\,J(J+1)$$

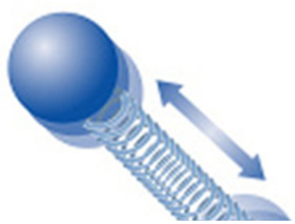
$$\nu = 2B(J+1)$$

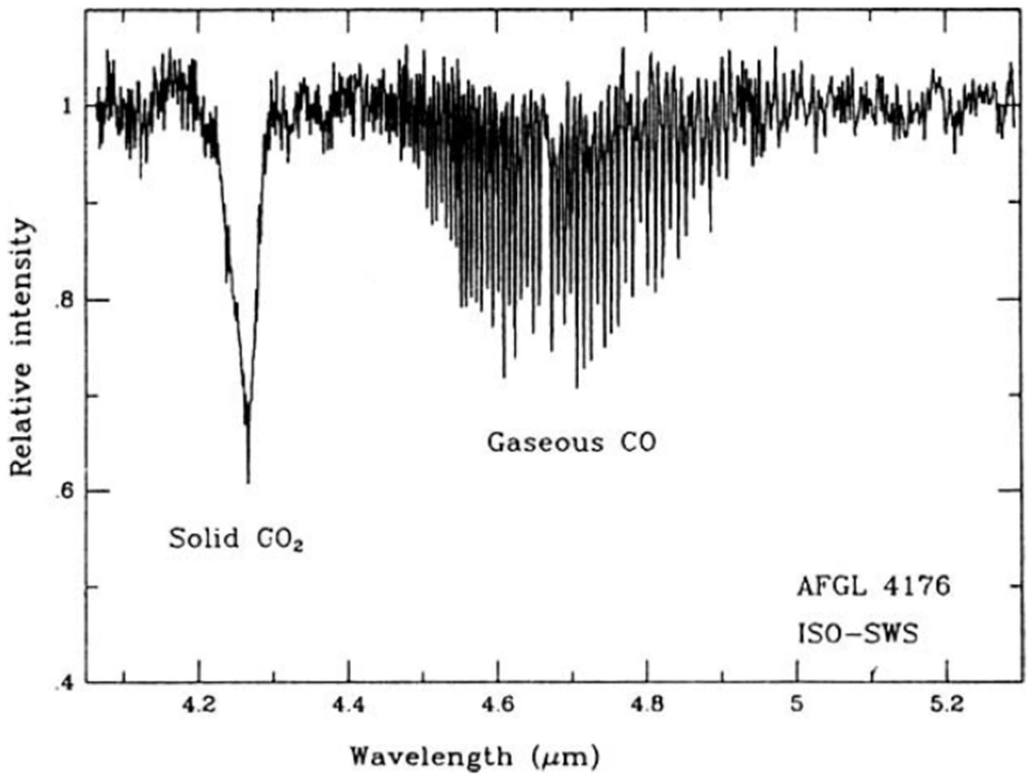


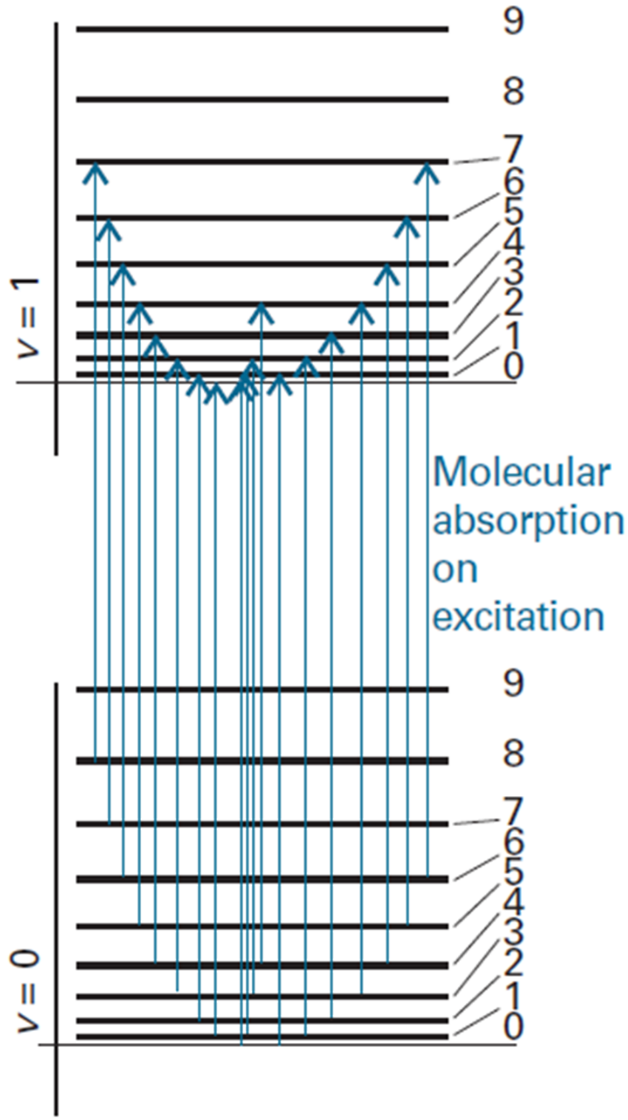
Espectros moleculares II



vibration







Intensidad, población, temperatura

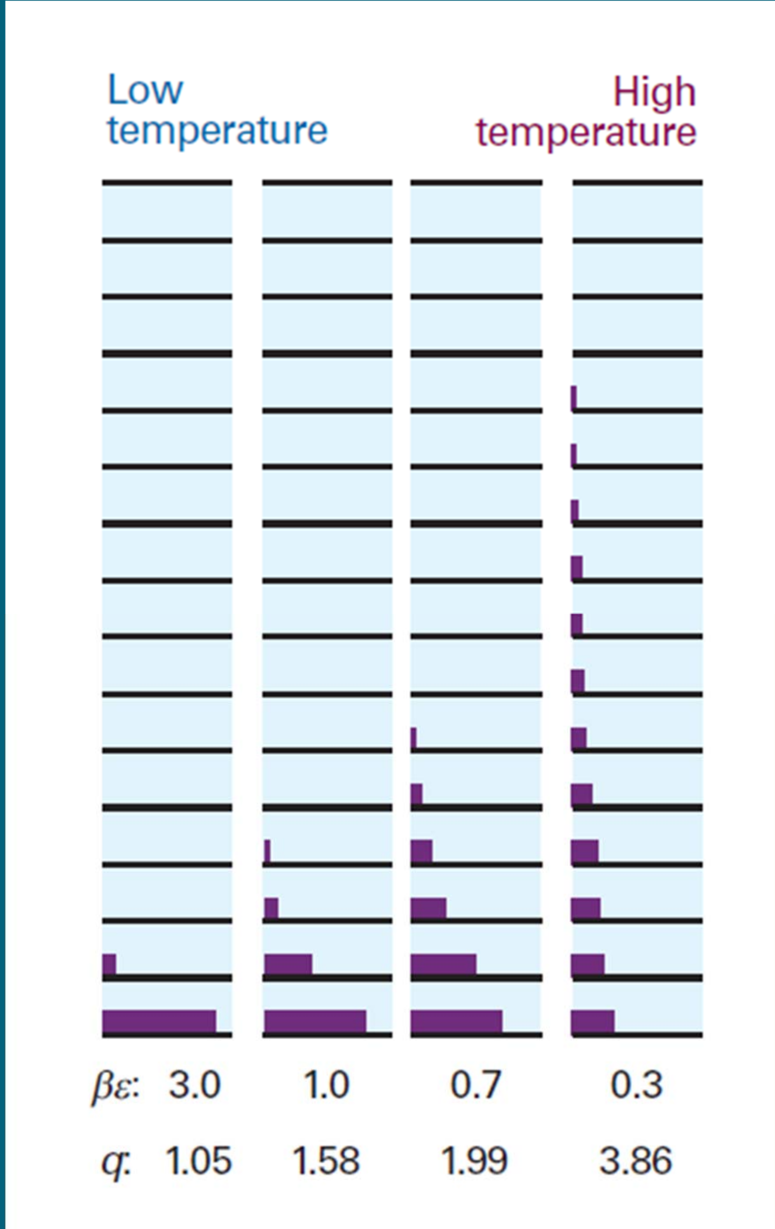
- Intensidad de la línea (absorción neta) entre los niveles i <-> j

$$I_{ij} = (n_i - n_j)B\rho$$

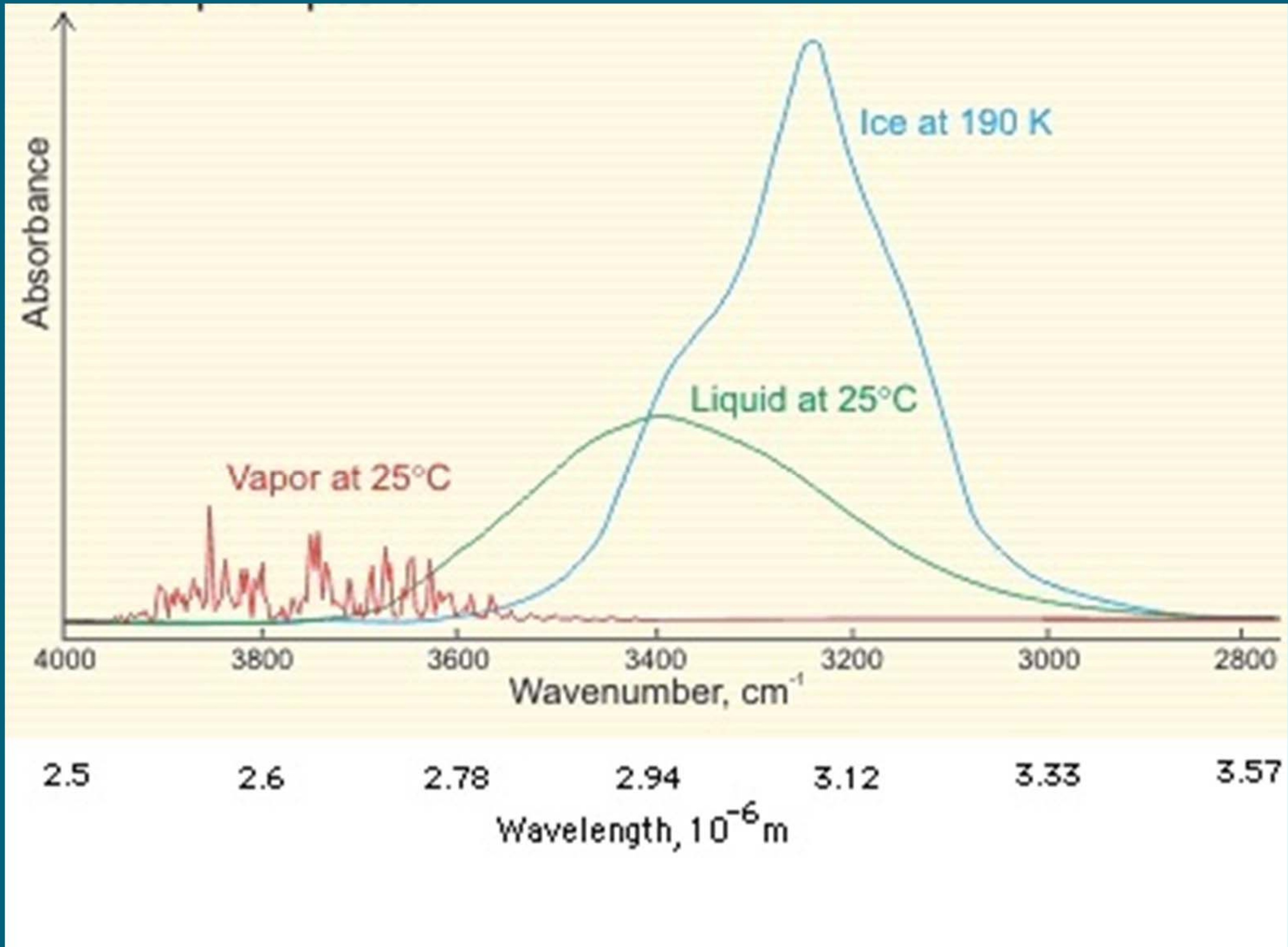
- Distribución Boltzmann de poblaciones

$$P_i = \frac{n_i}{N} = \frac{\exp(-\beta\varepsilon_i)}{\sum_i \exp(-\beta\varepsilon_i)}$$

$$\beta = 1/(k_B T)$$



Espectros de fases condensadas

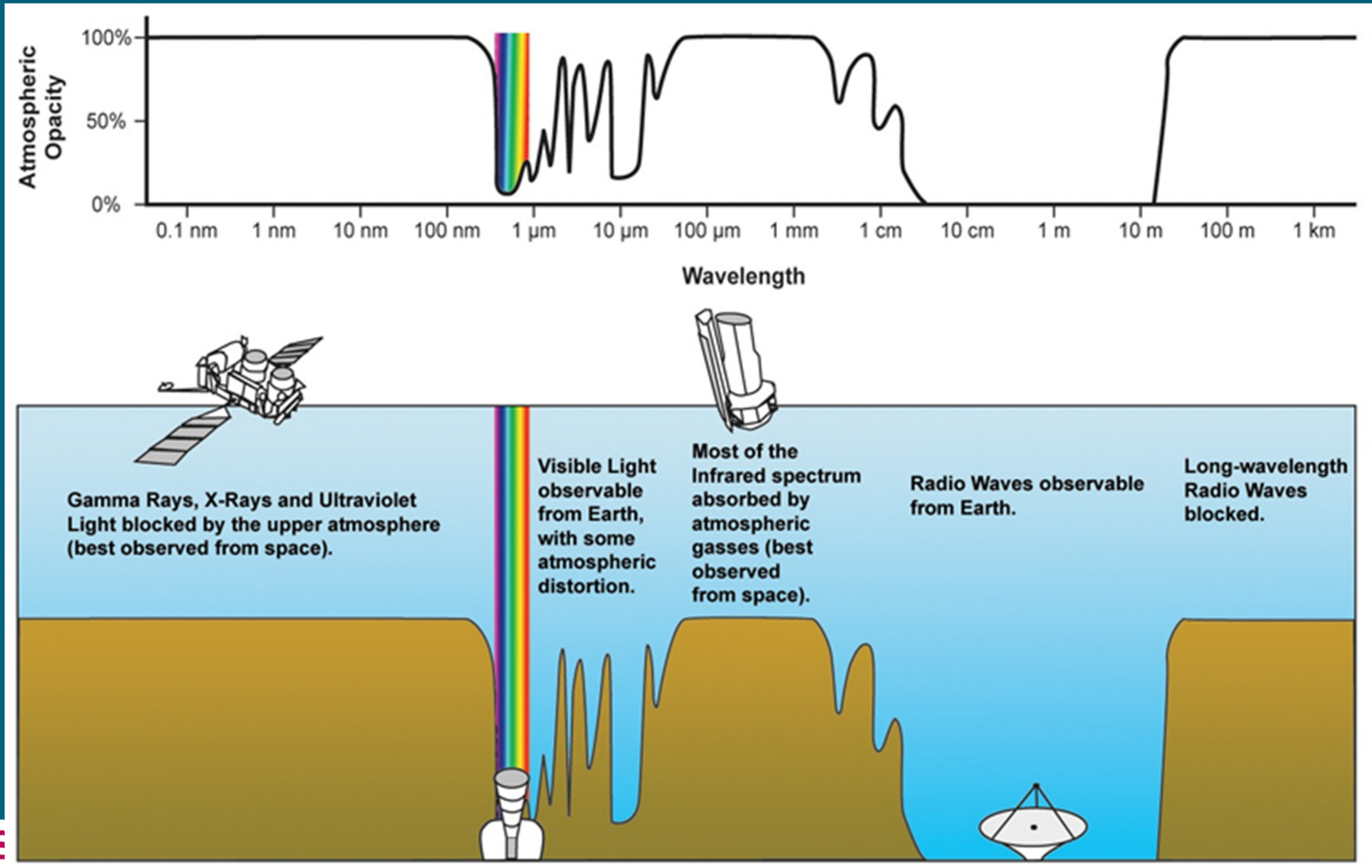


Aplicaciones de la Espectroscopía

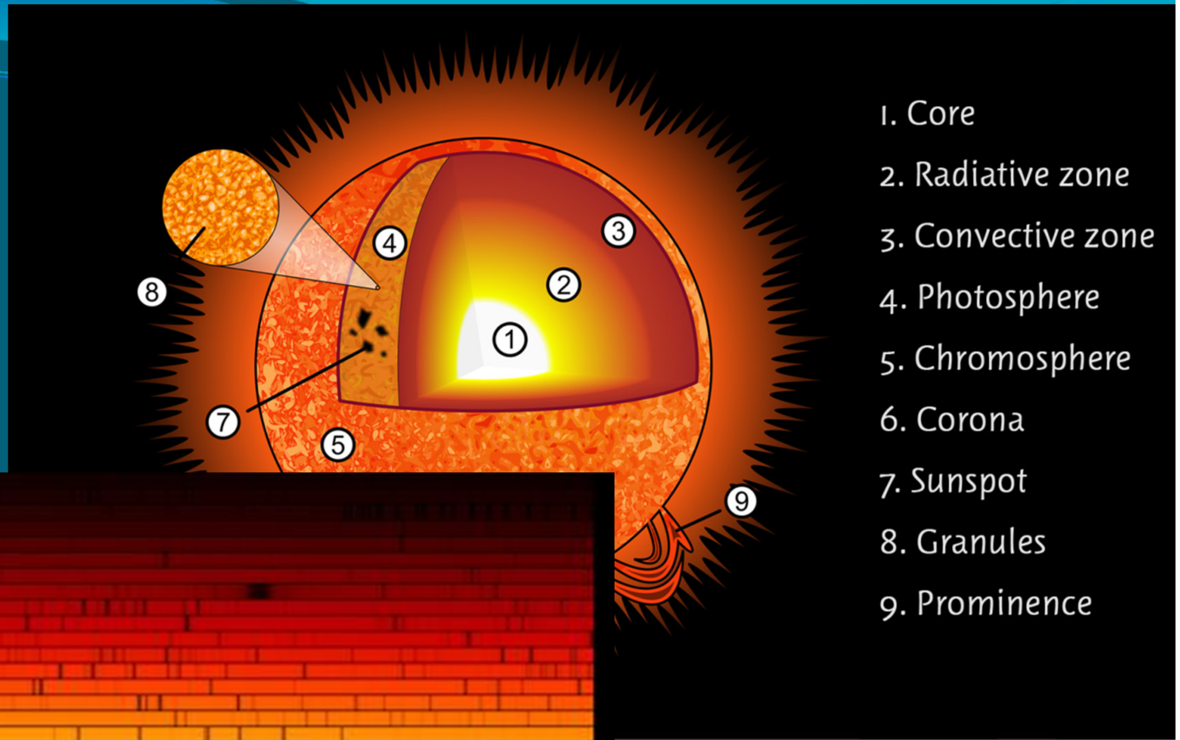
- Desarrollo Mecánica Cuántica (estructura atómica)
- Estructura molecular
- Análisis químico:
  - elemental (átomos)
  - composición molecular
- Detección remota (atmósfera, entornos hostiles)
- Metrología
- Astrofísica

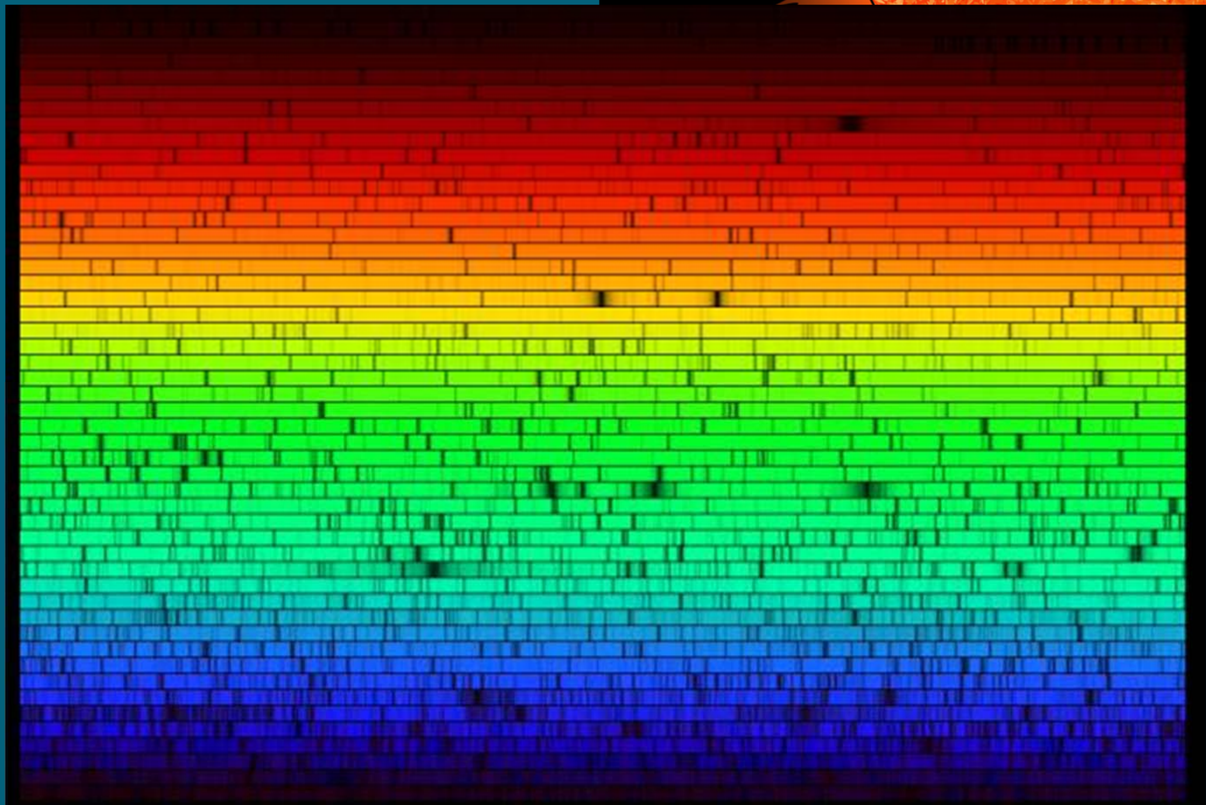
Regiones espectrales. Ventanas atmosféricas

- diferente información
- diferente tecnología (fuentes, espectrómetros, detectores, telescopios)



Espectro del sol





NOAO/AURA/NSF

Espectro solar II
Rayos X

- Átomos altamente ionizados
- Corona solar

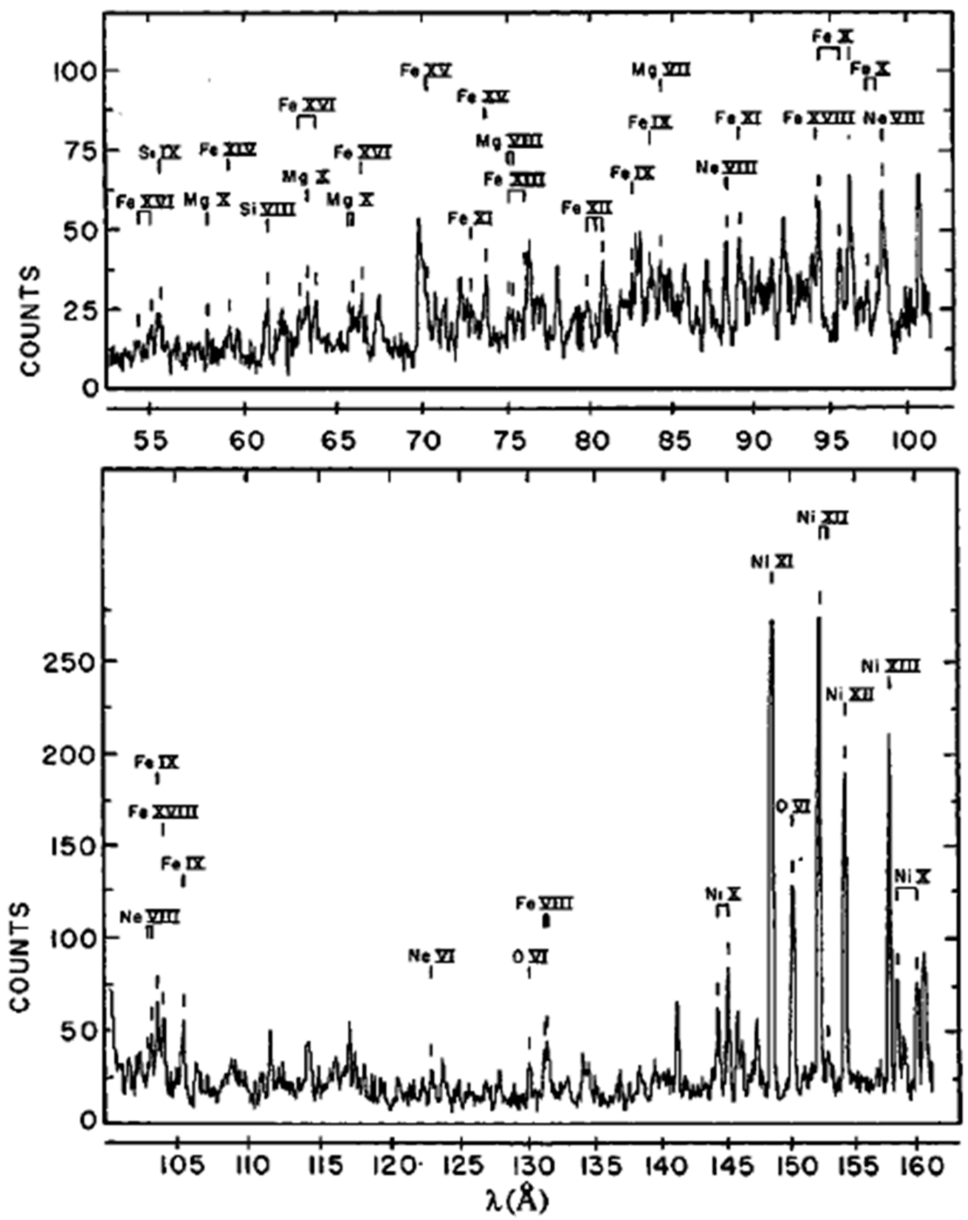
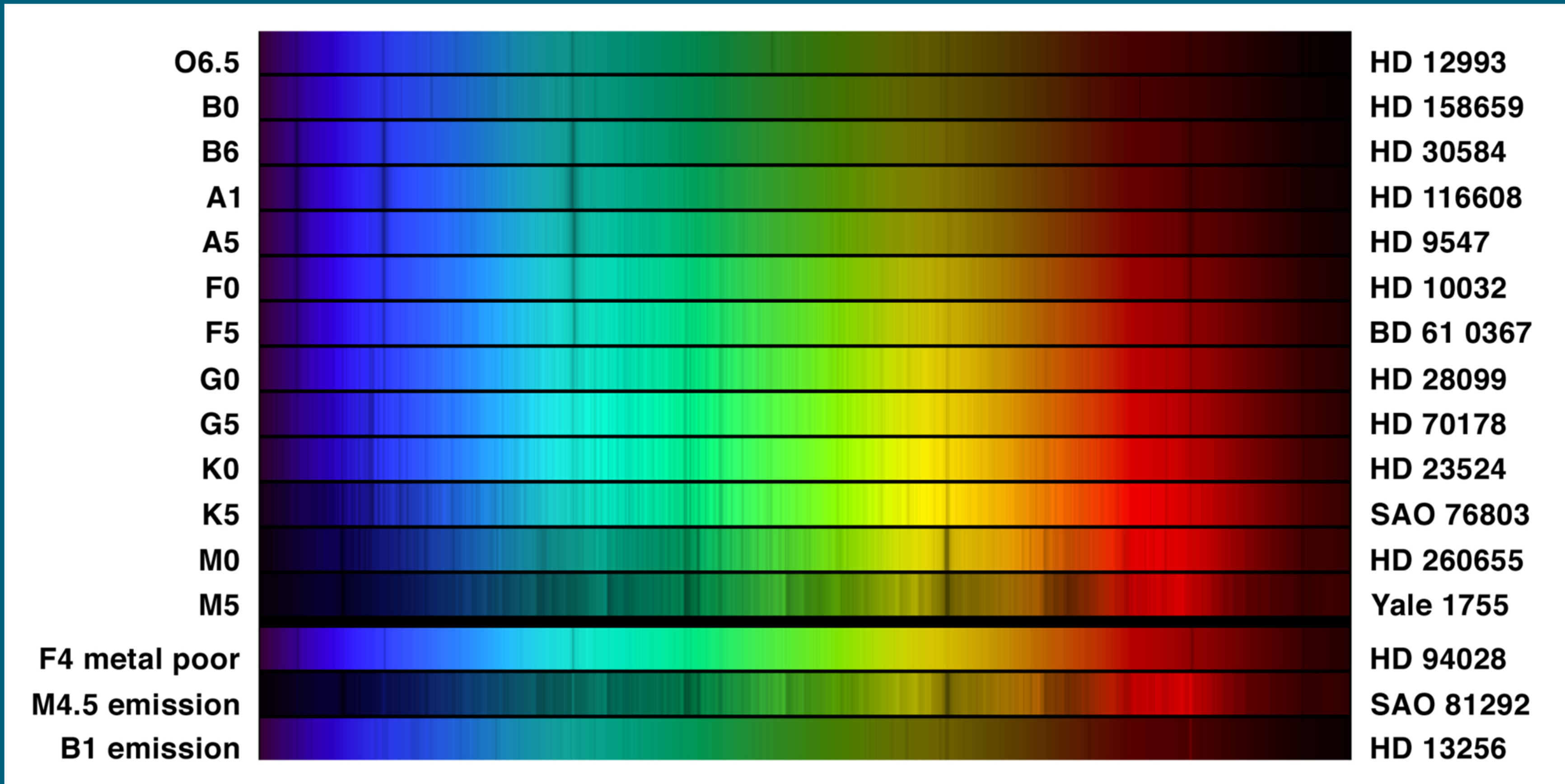


Fig. 8.2. X-ray spectrum of the entire solar disk recorded using a rocket-based experiment. [Adapted from M. Malinovsky and L. Heroux, *Astrophys. J.* **181**, 1009 (1973).]

Otras estrellas

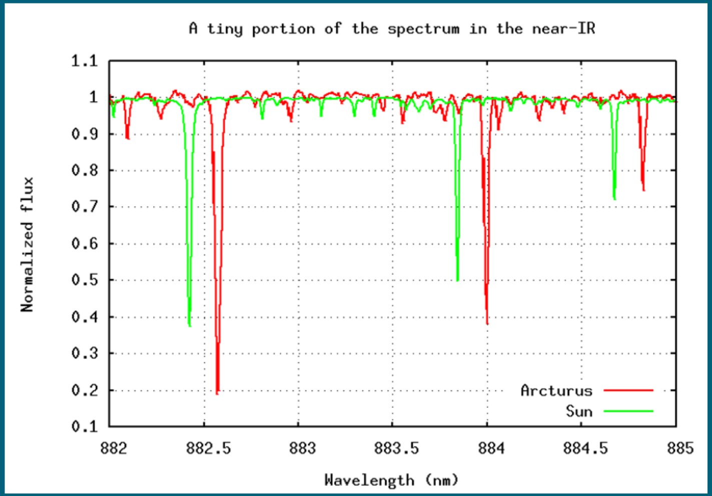


NOAO/AURA/NSF

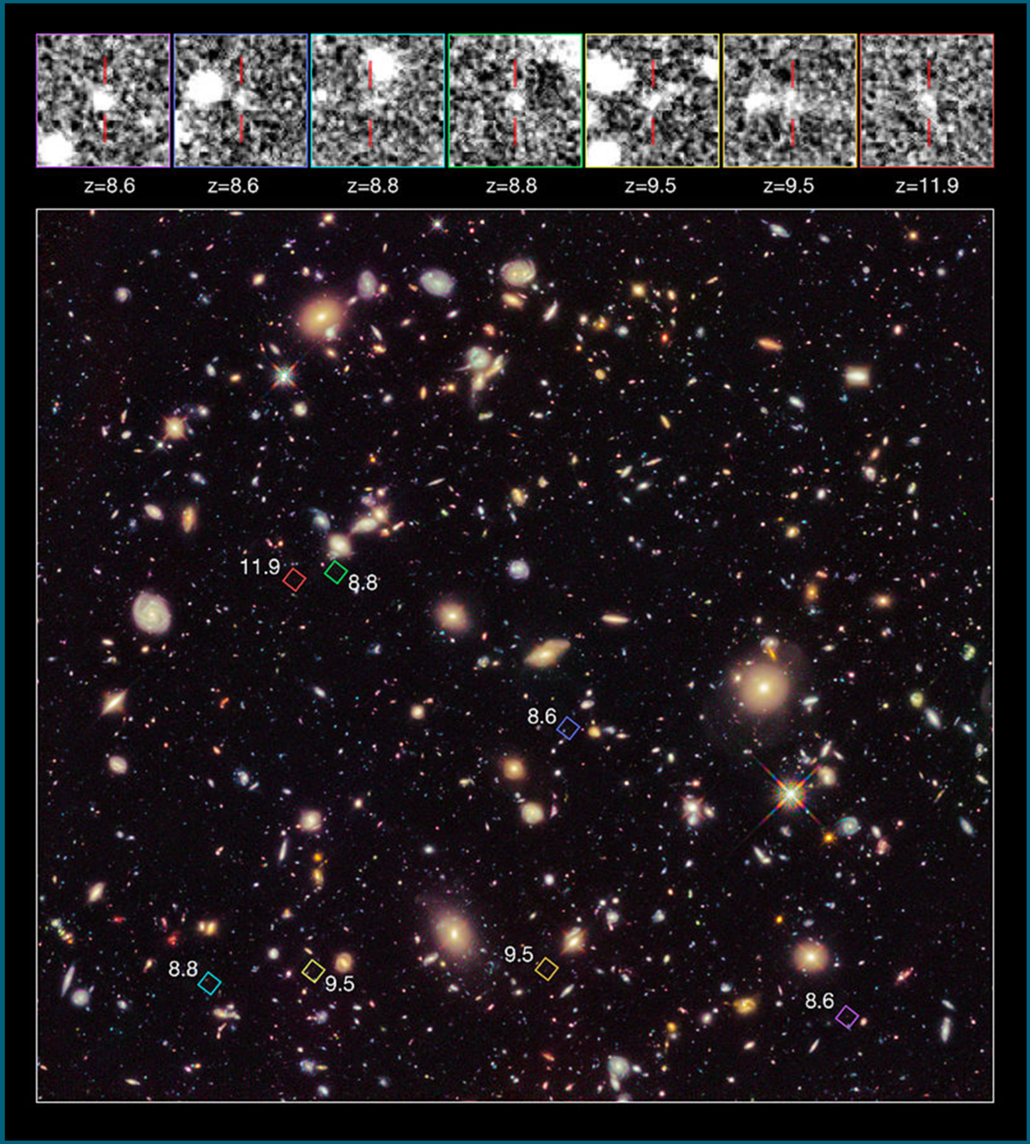
Corrimiento al rojo

Efecto Doppler

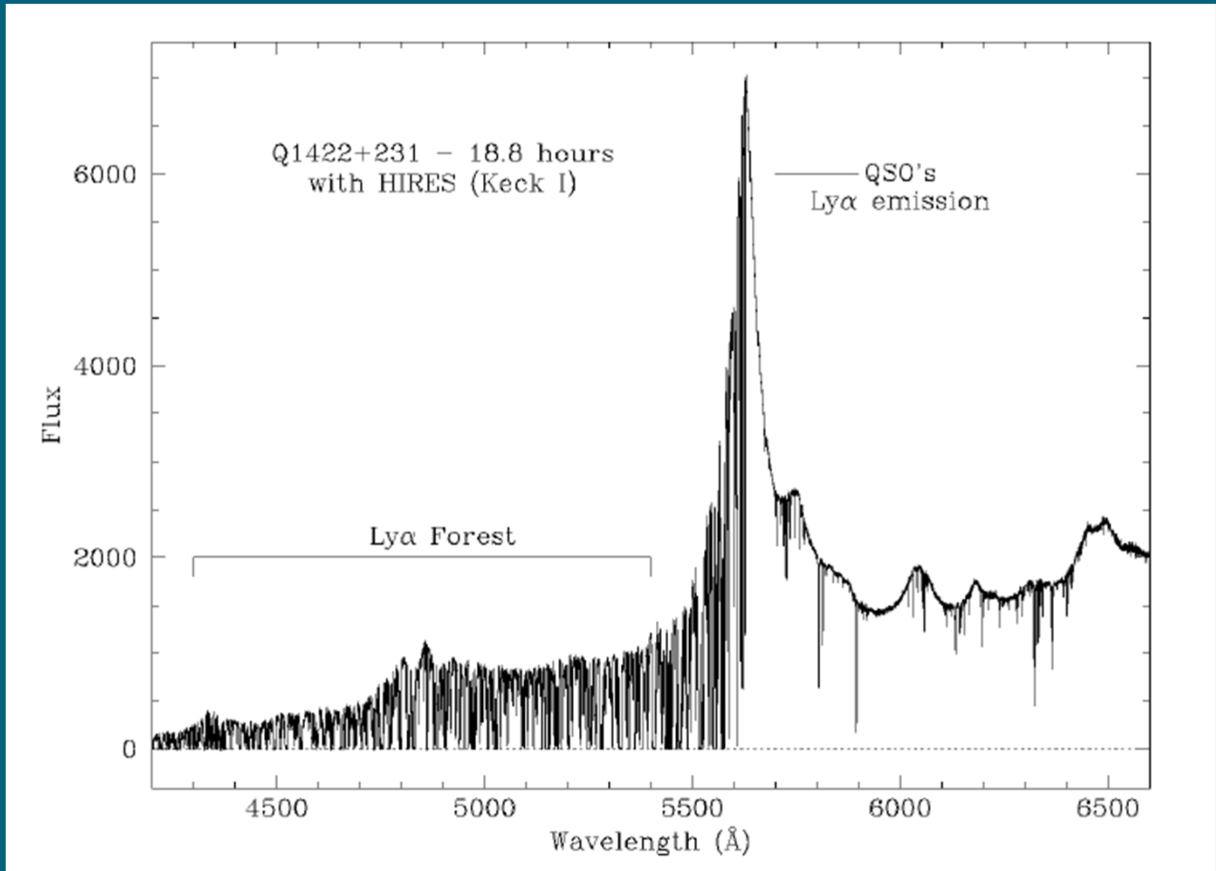
- $z = (\lambda_{obs} - \lambda_0)/\lambda_0$
- $1 + z = \frac{1+v_R/c}{\sqrt{1-v^2/c^2}}$
- $z \approx v_R/c \quad (\text{para } v \ll c)$



Hubble Ultra Deep Field (2012)



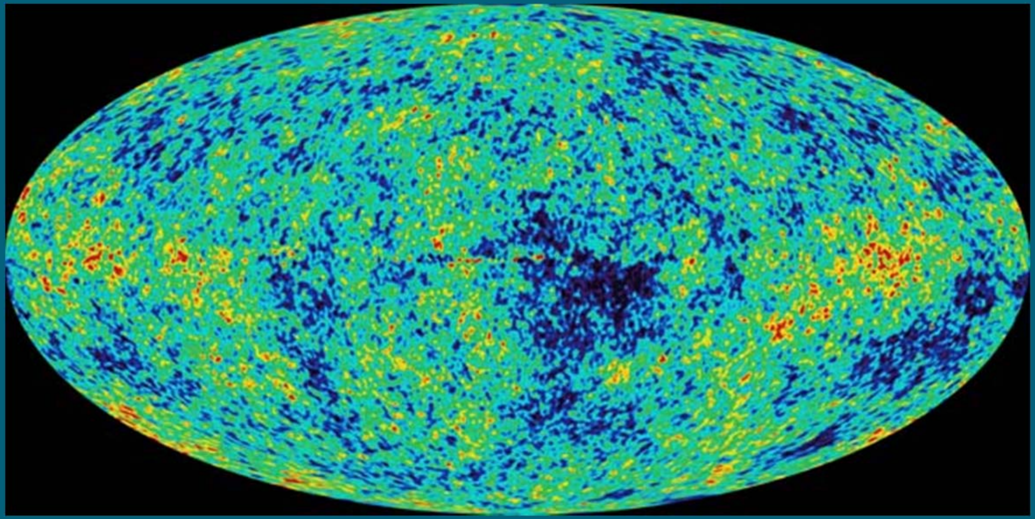
Galaxias



Spectrum of QSO Q1422+231 redshift z=3,625
High Resolution Echelle Spectrograph on the Keck telescope in Hawaii

Fondo cósmico de microondas

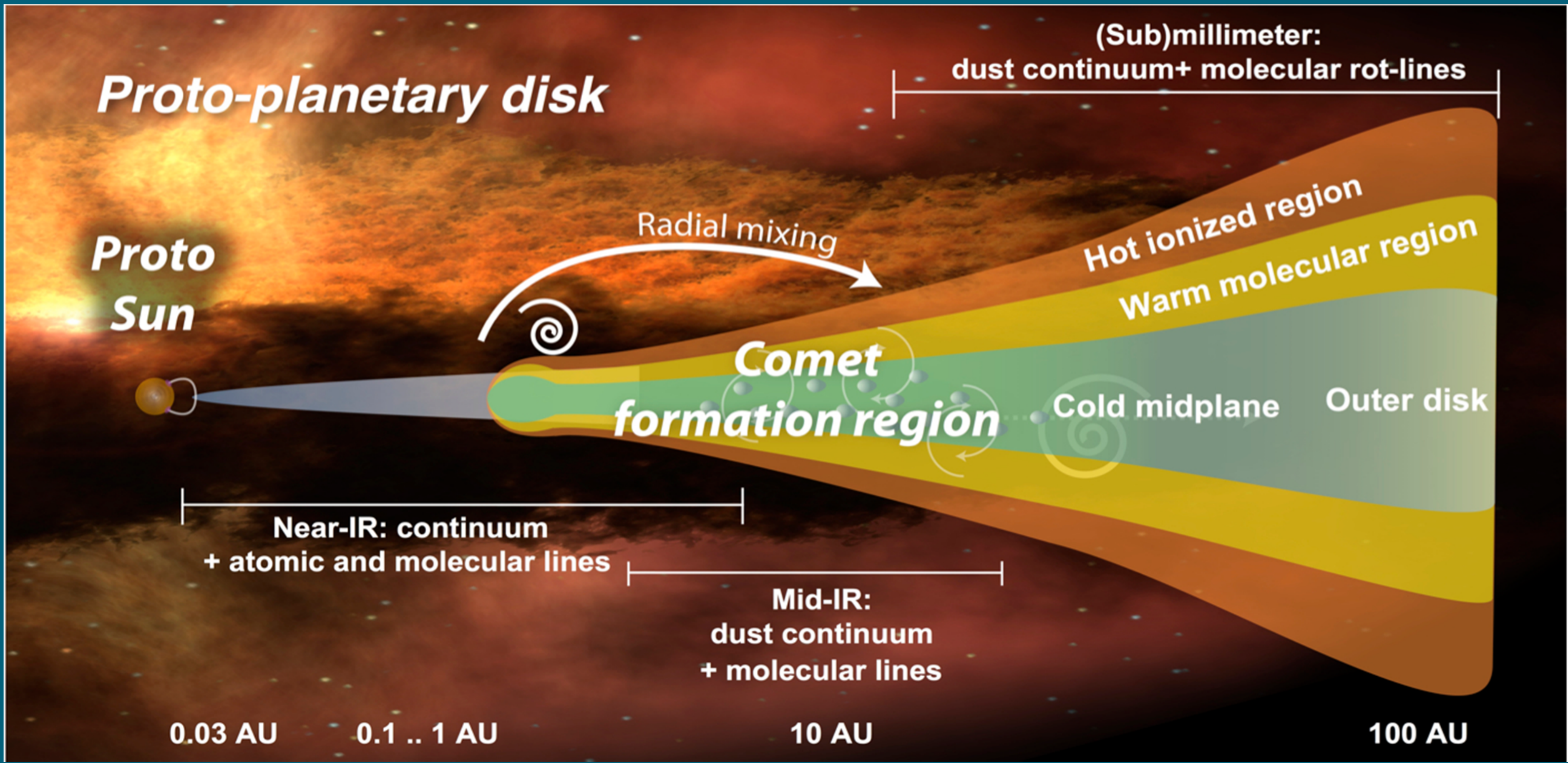
- Señal de microondas en todas direcciones del universo
- A. Penzias y R.W. Wilson 1965 (Nobel 1978)
- Cuerpo negro a T=2,7 K (max 160 GHz)
- Uniforme (fluctuaciones ~1/100.000)
- Se considera un resto del Big-bang



Wilkinson Microwave Anisotropy Probe (WMAP)
Space based microwave telescope

Medio interestelar I

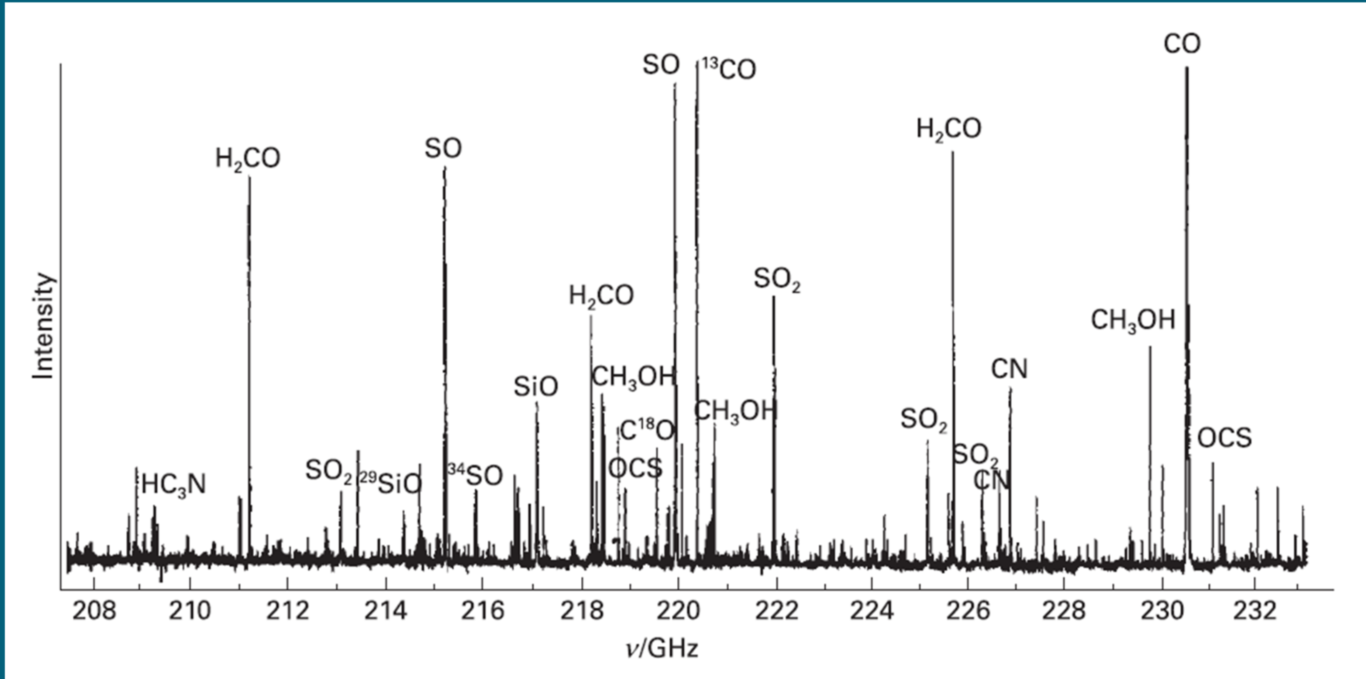
- Gas ionizado (HII), átomos (HI), moléculas (H_2), partículas de polvo
- Rangos T de 10 K a miles K
- Nubes moleculares (10-20 K): formación de estrellas y sistemas planetarios



Medio interestelar II

Los “pilares de la creación”
Nebulosa del Águila
Hubble Space Telescope (2014)

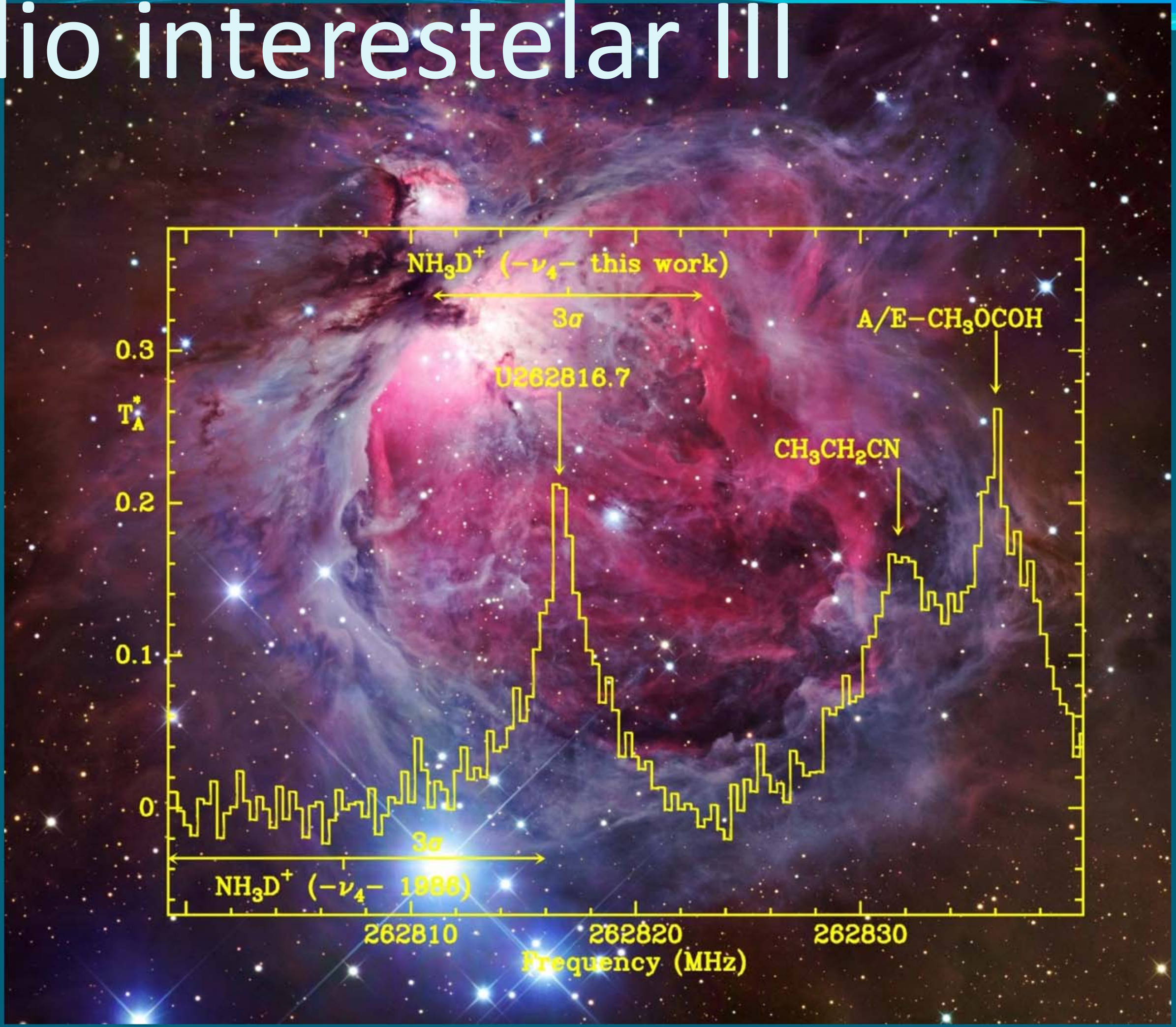
Medio interestelar II



Rotational spectrum of the Orion nebula, showing spectral fingerprints of diatomic and polyatomic molecules present in the interstellar cloud.

G.A. Blake et al., Astrophys. J. 315, 621 (1987).

Medio interestelar III



J. Cernicharo et al., Astrophys. J. Lett. 771, L10 (2013).

J. L. Domenech et al., Astrophys. J. Lett. 771, L11 (2013).

Medio interestelar IV

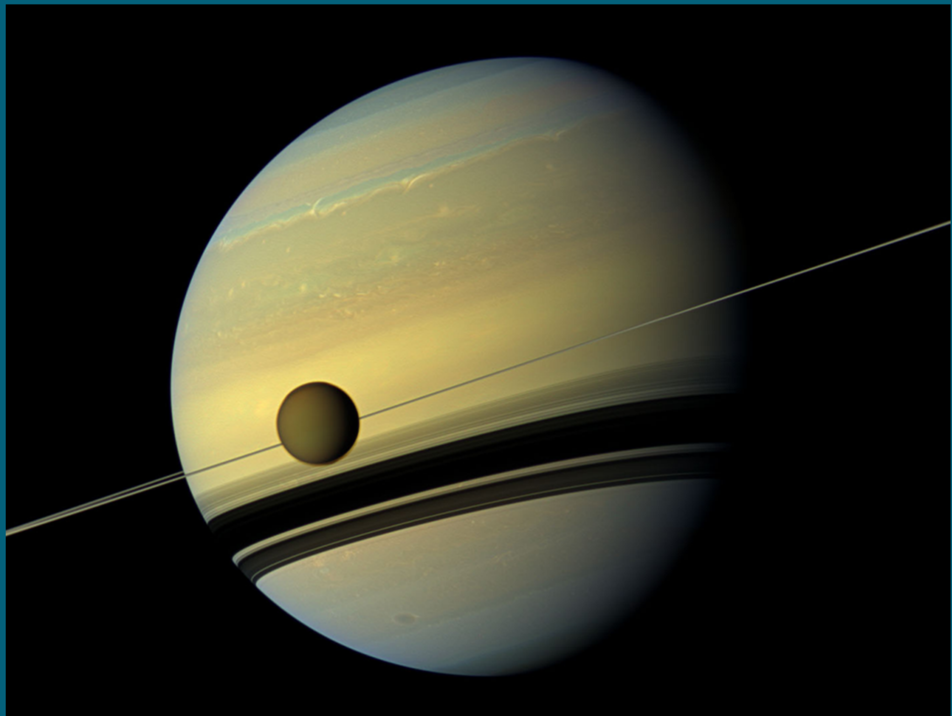
- ~200 moléculas se han detectado en el medio interestelar o circumestelar
- 60 moléculas extragalácticas

Molecules in the Interstellar Medium or Circumstellar Shells (as of 11/2016)						
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	8 atoms
H2	C3 *	c-C3H	C5 *	C5H	C6H	CH3C3N
AlF	C2H	l-C3H	C4H	l-H2C4	CH2CHCN	HC(O)OCH3
AlCl	C2O	C3N	C4Si	C2H4*	CH3C2H	CH3COOH
C2**	C2S	C3O	l-C3H2	CH3CN	HC5N	C7H
CH	CH2	C3S	c-C3H2	CH3NC	CH3CHO	C6H2
CH+	HCN	C2H2*	H2CCN	CH3OH	CH3NH2	CH2OHCHO
CN	HCO	NH3	CH4 *	CH3SH	c-C2H4O	l-HC6H *
CO	HCO+	HCCN	HC3N	HC3NH+	H2CCHOH	CH2CCHCN
CO+	HCS+	HCNH+	HC2NC	HC2CHO	C6H–	H2NCH2CN
CP	HOC+	HNCO	HCOOH	NH2CHO	CH3NCO	CH3CHNH
SiC	H2O	HNCS	H2CNH	C5N		
HCl	H2S	HOCO+	H2C2O	l-HC4H *		
KCl	HNC	H2CO	H2NCN	l-HC4N		
NH	HNO	H2CN	HNC3	c-H2C3O		
NO	MgCN	H2CS	SiH4 *	C5N–		
NS	MgNC	H3O+	H2COH+	HNCHCN		
NaCl	N2H+	c-SiC3	C4H–			
OH	N2O	CH3 *	HC(O)CN			
PN	NaCN	C3N–	HNCNH			
SO	OCS	PH3	CH3O			
SO+	SO2	HCNO	NH4+			
SiN	c-SiC2	HOCN	NCCNH+			
SiO	CO2 *	HSCN				

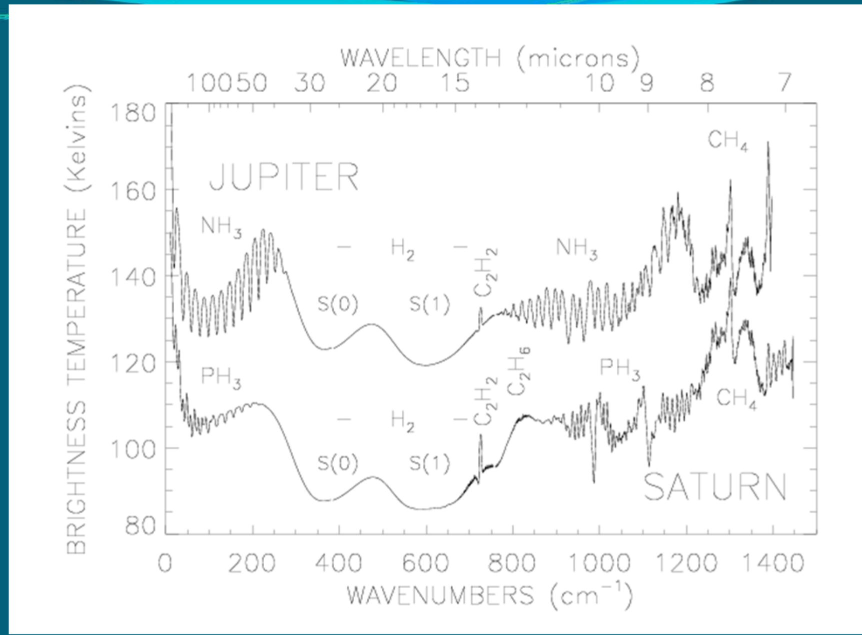
Extragalactic Molecules (as of 04/2016)					
2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms
OH	H2O	H2CO	c-C3H2	CH3OH	CH3CCH
CO	HCN	NH3	HC3N	CH3CN	CH3NH2
H2 *	HCO+	HNCO	CH2NH	HC4H *	CH3CHO
CH	C2H	C2H2 *	NH2CN	HC(O)NH2	
CS	HNC	HOCO+	l-C3H2		
CH+ **	N2H+	c-C3H	H2CCN		
CN	OCS	H3O+	H2CCO		
SO	HCO	l-C3H	C4H		
SiO	H2S				
CO+	SO2				
NO	HOC+				
NS	C2S				
NH	H2O+				

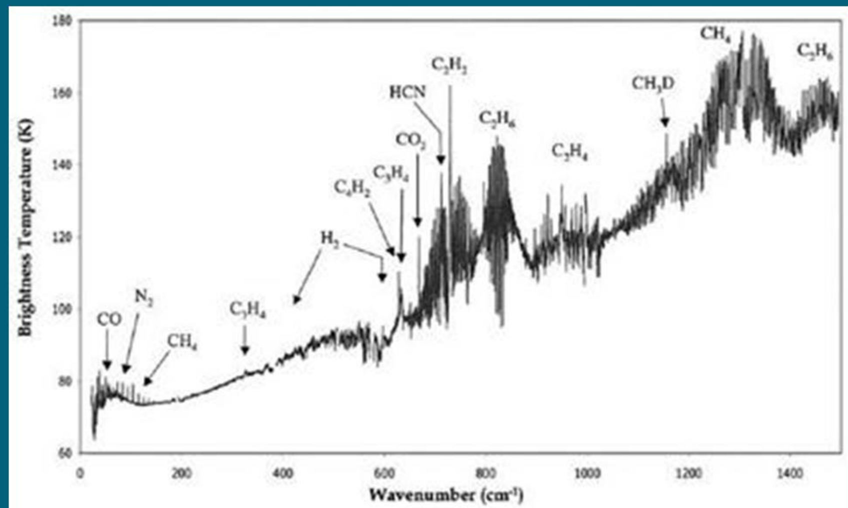
Universidad de Colonia (Alemania)
https://www.astro.uni-koeln.de/cdms/molecules

Sistema solar



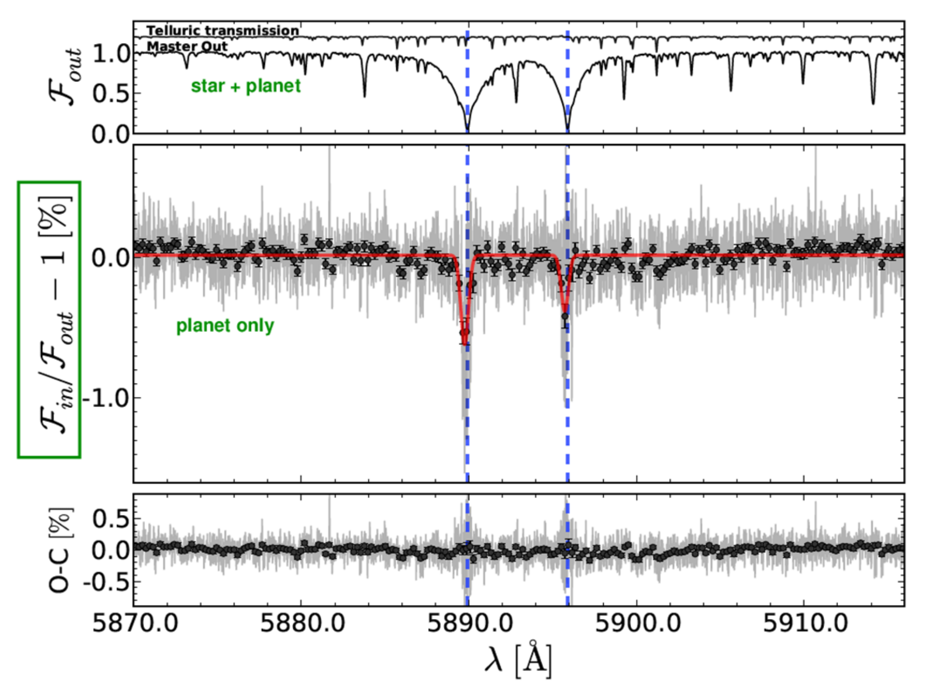
Saturno y Titán
(Cassini-Huygens)





Exoplanetas

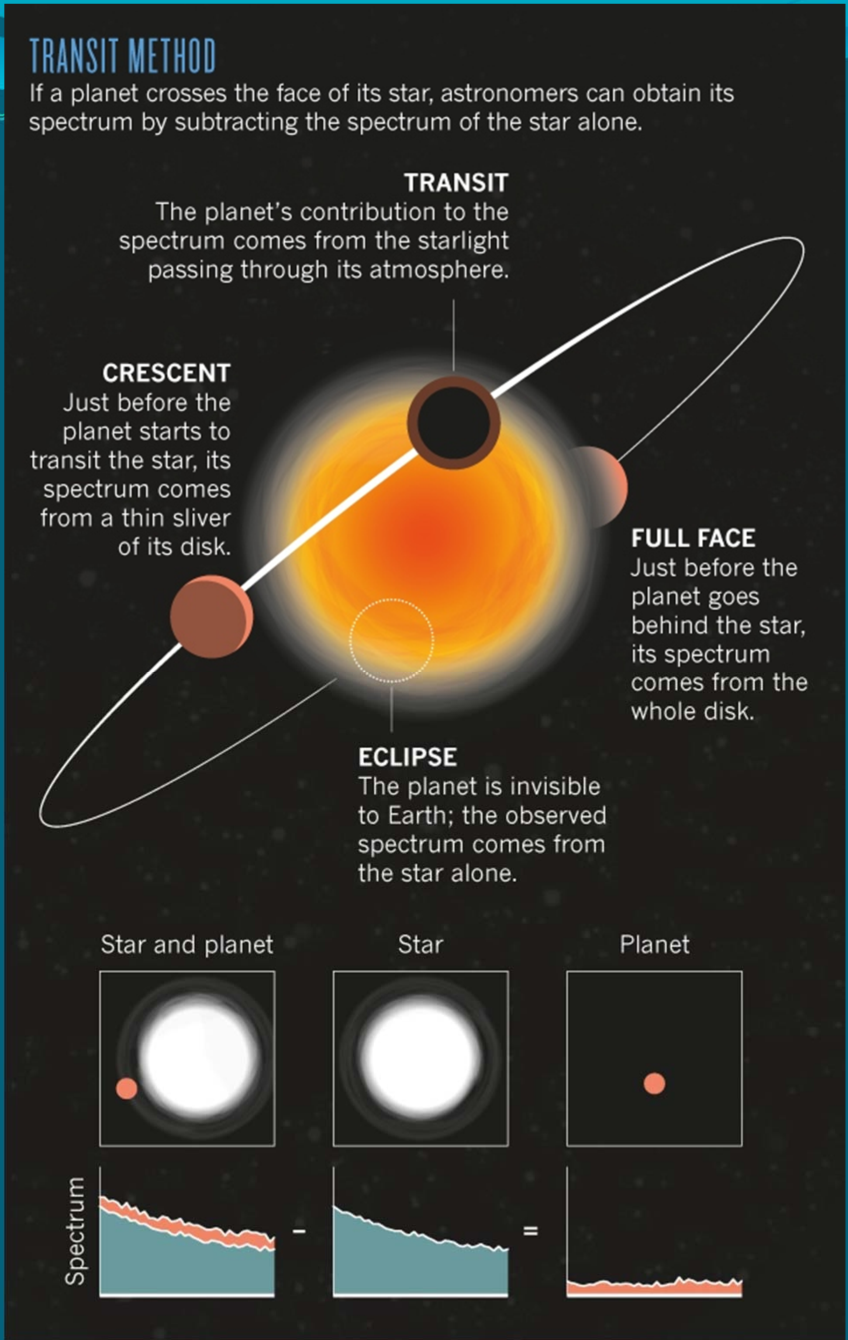
- Primera detección 1992
- Hasta hoy >3600 (>2200 Kepler)



Spectrally resolved detection of sodium in the atmosphere of HD189733b with the HARPS spectrograph

Wyttenbach et al. A&A 577, A62 (2015)

DOI: 10.1051/0004-6361/201525729



Resumen y conclusiones

- [Casi] Toda la información de objetos astronómicos más allá del Sistema Solar nos llega a través de la luz
- Analizando esa luz mediante instrumentos con alta resolución espectral podemos conocer muchas propiedades de esos objetos, como:
  - composición química
  - abundancia relativa (concentración)
  - temperatura
  - movimiento respecto a la Tierra
  - presión (densidad de partículas)
  - campo magnético
  - rastro de vida ??
- Para interpretar los espectros astronómicos se necesita conocimiento previo de la Física atómica y molecular mediante experimentos de laboratorio.


¡Gracias por vuestra atención!