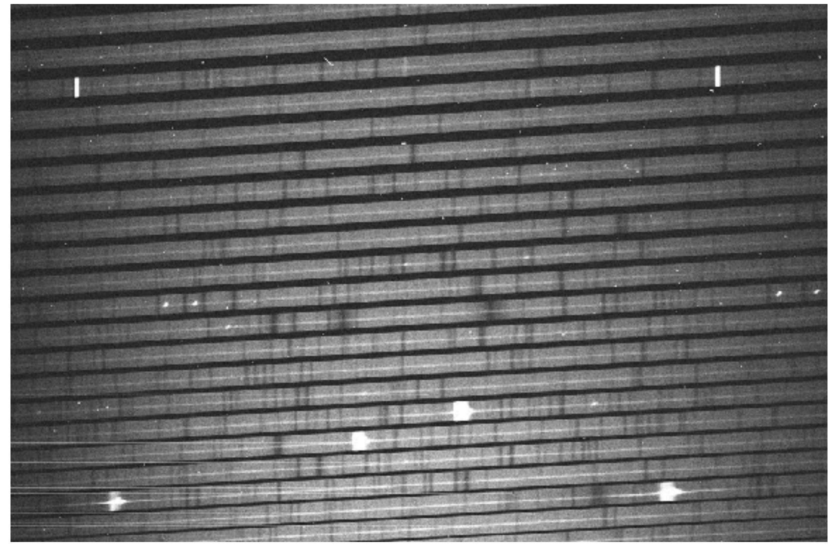
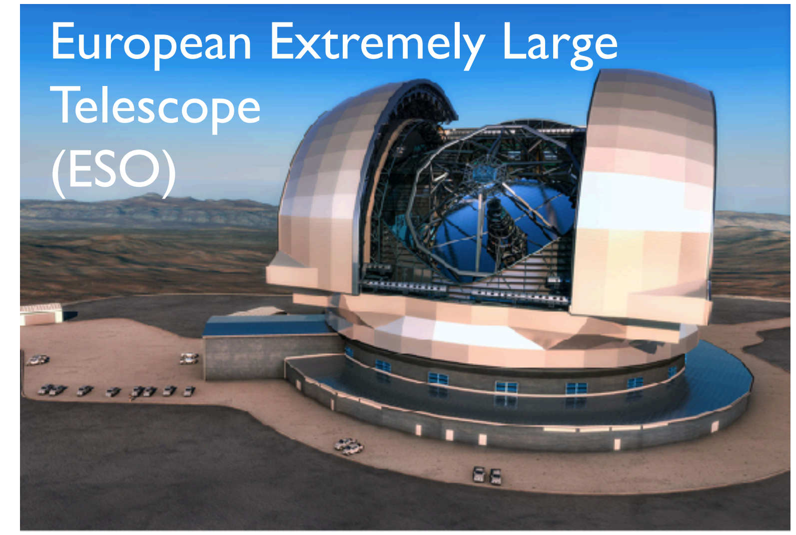
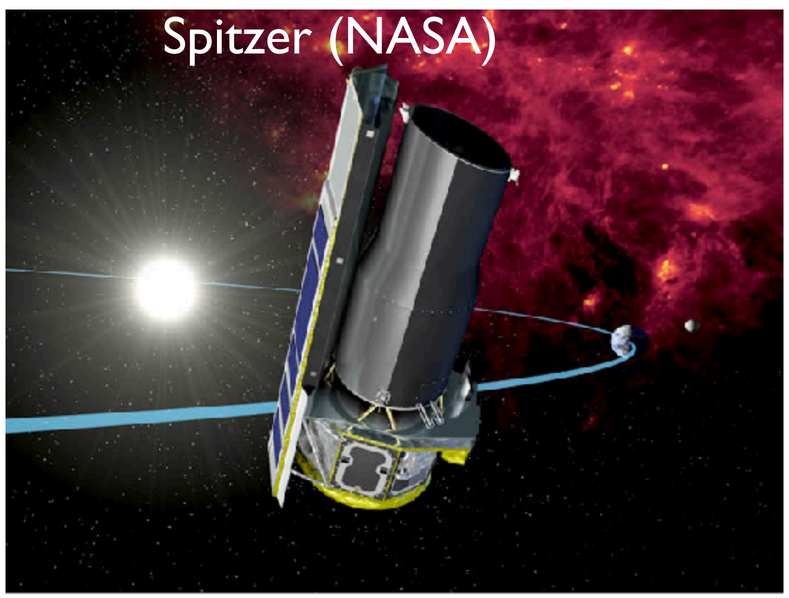
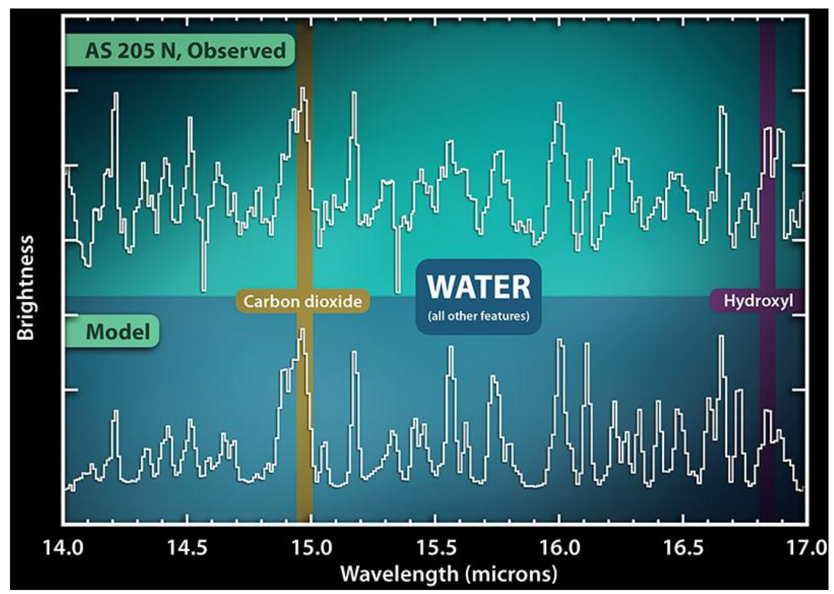
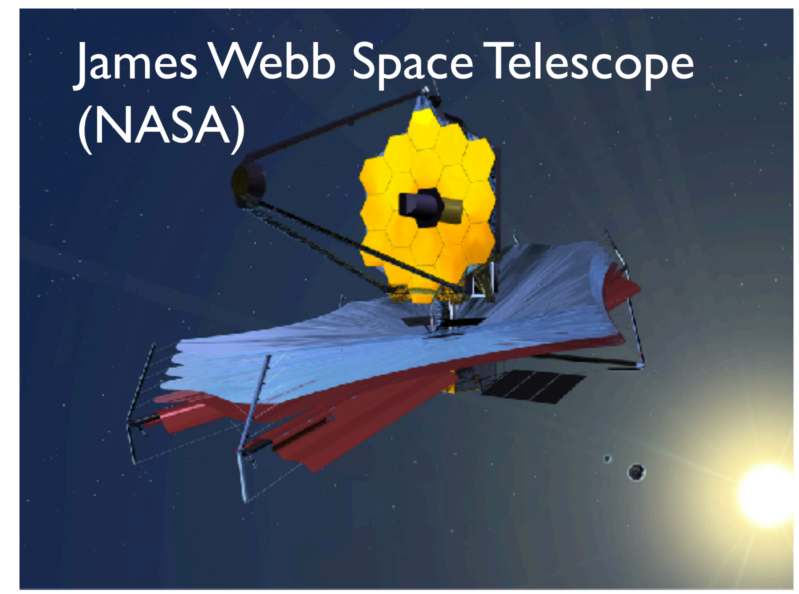
Lecture 3: Different ways to detect molecules

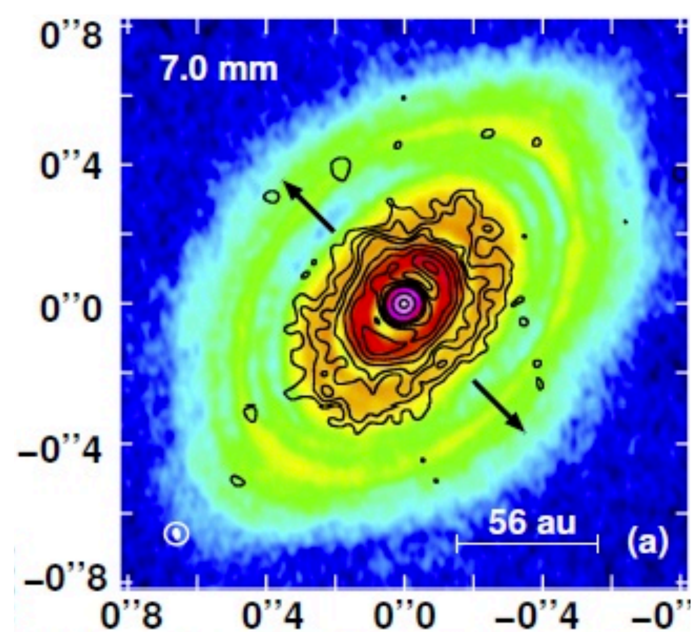












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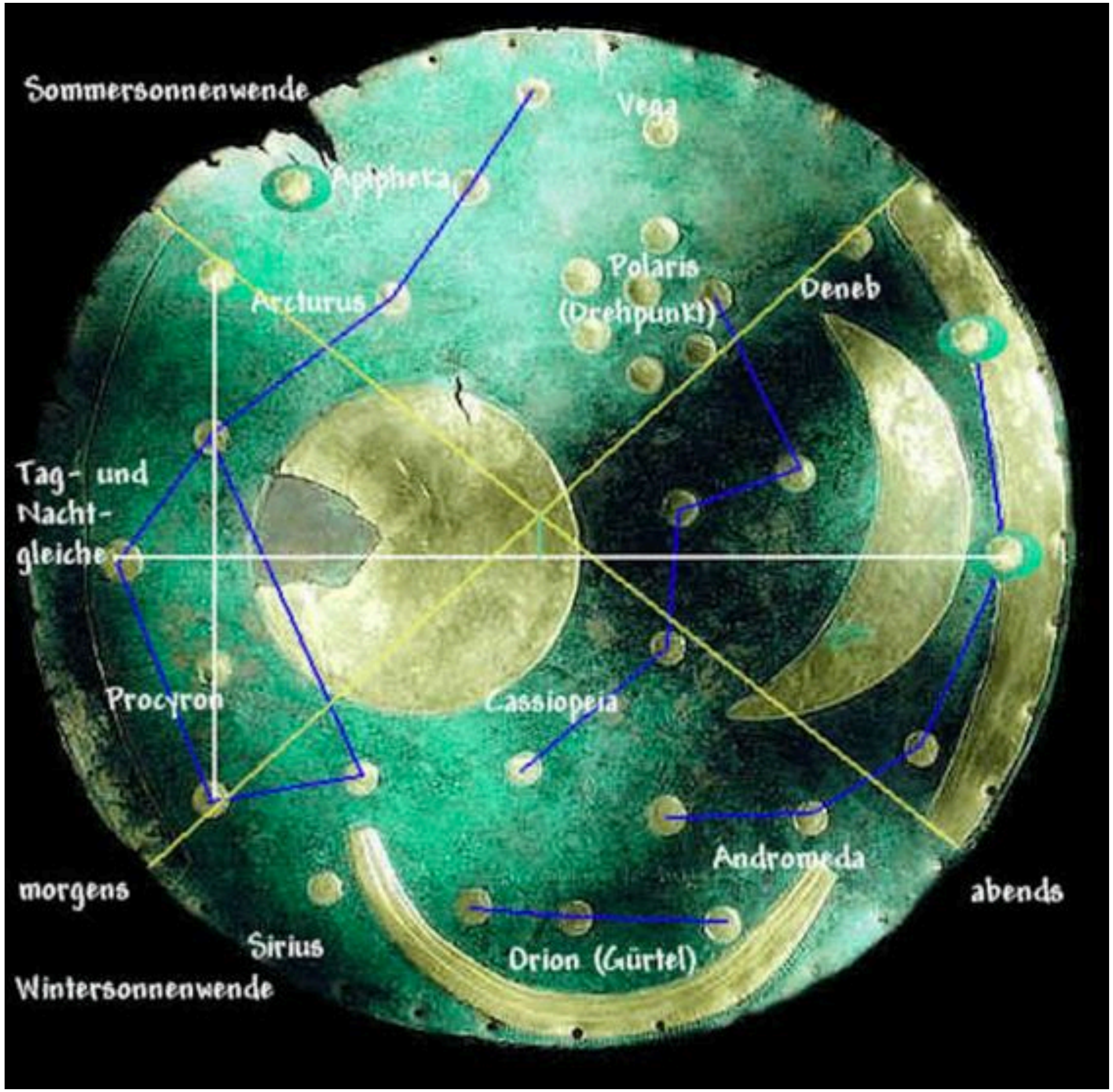
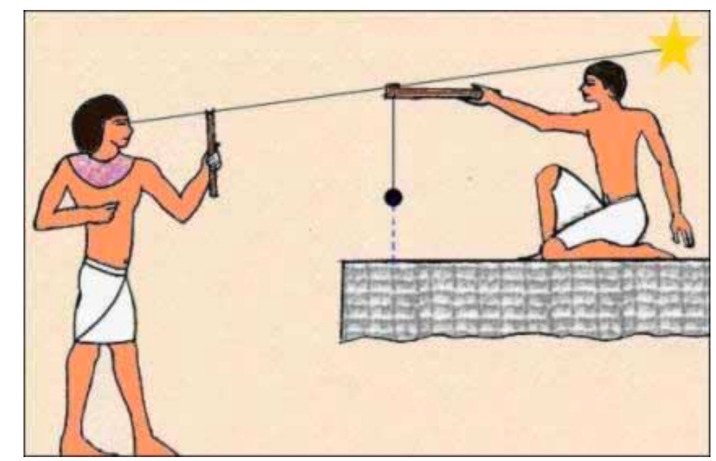
Astronomical observations: an old story



- Nebra sky disk, Bronze/Iron Age, 3 600 years old
- Sun, Moon, constellations, angles between solstices

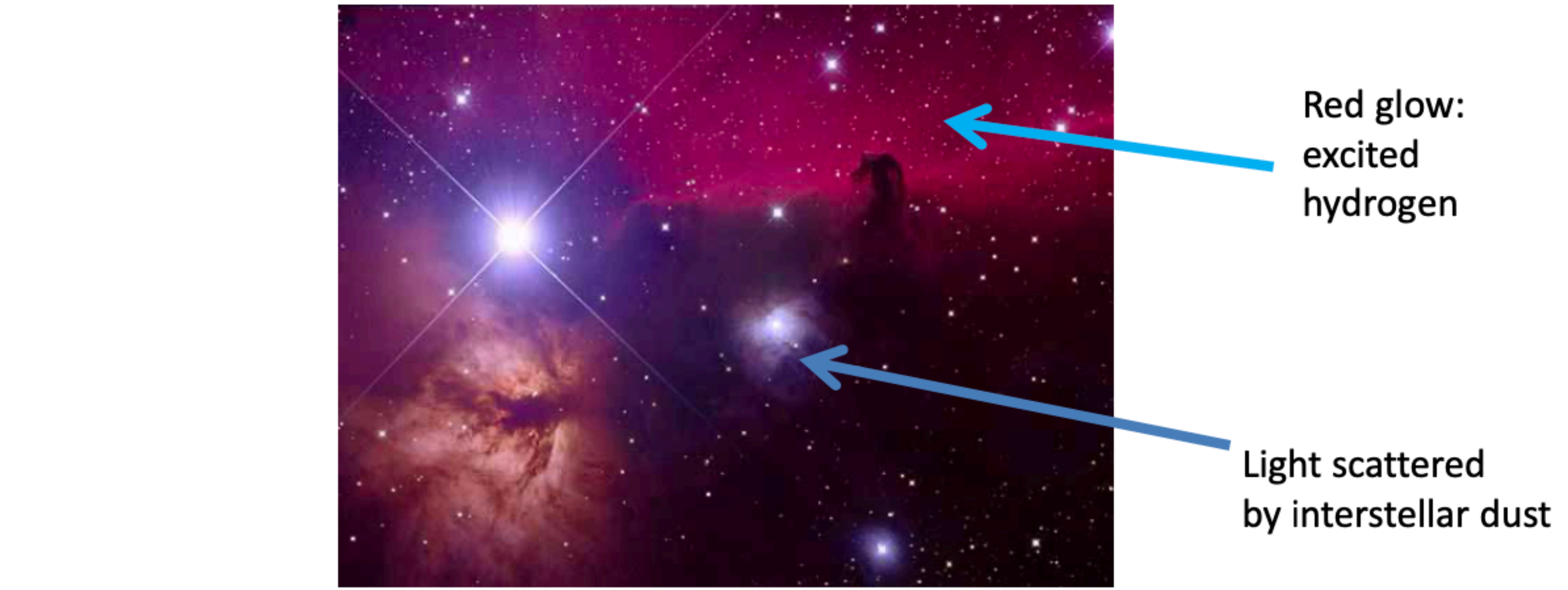
First astronomical observations

- **Calendar and religion**
- **Ancient Egypt (3000 BC):** Sirius risings
- **Sumer & Babylonia (1200 BC):** first stellar catalog, Venus risings, 18-year lunar eclipse cycle
- **Ancient Greece (~200 BC):** Earth size, axial tilt, stellar catalog (Almagest), stellar magnitudes, planetary orbits
- **Ancient China:** records of supernovae & comets
- **Medieval Middle East:** stellar catalogs, SN 1006, Magellanic Clouds
- **Renaissance Europe:** stellar catalog by Tycho Brahe completed by Kepler (1627), Kepler laws (1609-1619), Copernican revolution (1543)



Why observations are so important?

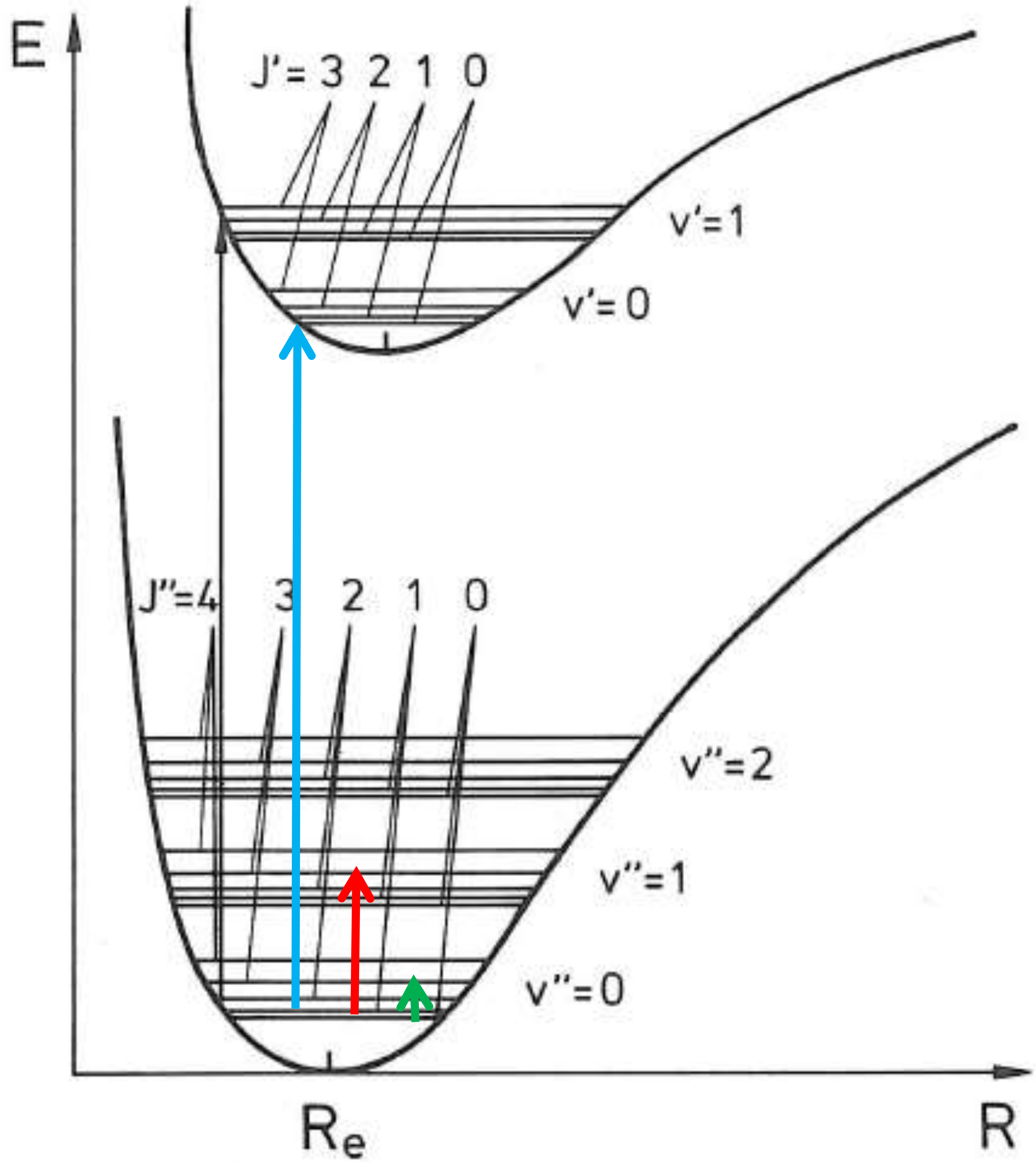
Almost all of the information we have about the Universe comes from the study of electromagnetic radiation (light)



Modern telescopes permit us to take detailed images of interstellar objects. These images contain a lot of information for the trained eye.

"A picture maybe be worth a thousands words, but a spectrum is worth a thousands pictures"

Overview of molecular energy levels



Electronic Transitions:

ΔE = 1-15 eV

Visible-UV

Vibrational Transitions:

ΔE = 0.1-1 eV

Infrared

Rotational Transitions:

ΔE = 0.01-0.1 eV

(sub)-Millimeter

Transition Intensities: Einstein Coefficients

Equilibrium:
absorbed photons = emitted photons

$$\left[B_{21}\rho(\nu) + A_{21}\right]\ N_2 = B_{12}\ N_1\ \rho(\nu) \qquad (1)$$

Solving for ρ(v):

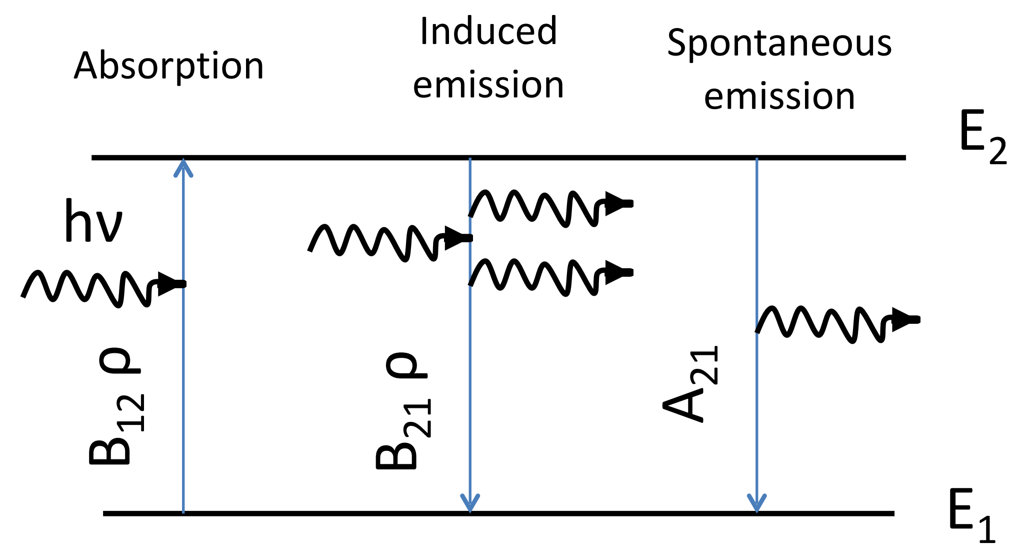
$$\rho(\nu) = \frac{A_{21}\ N_2}{B_{12}\ N_1\ -\ B_{21}\ \ N_2} \qquad (2)$$

Using Boltzmann distribution:

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} e^{-\frac{h\nu}{kT}} \quad \longrightarrow \quad N_1 = N_2 \frac{g_1}{g_2} e^{\frac{h\nu}{kT}} \qquad (3)$$

Insert (3) into (2):

$$\rho(\nu) = \frac{A_{21}\ N_2}{B_{12}\ N_2 \frac{g_1}{g_2} e^{\frac{h\nu}{kT}} - B_{21}\ \ N_2} = \frac{\frac{A_{21}}{B_{21}}}{\frac{g_1}{g_2}\ \frac{B_{12}}{B_{21}}\ e^{\frac{h\nu}{kT}} - 1} \qquad (4)$$

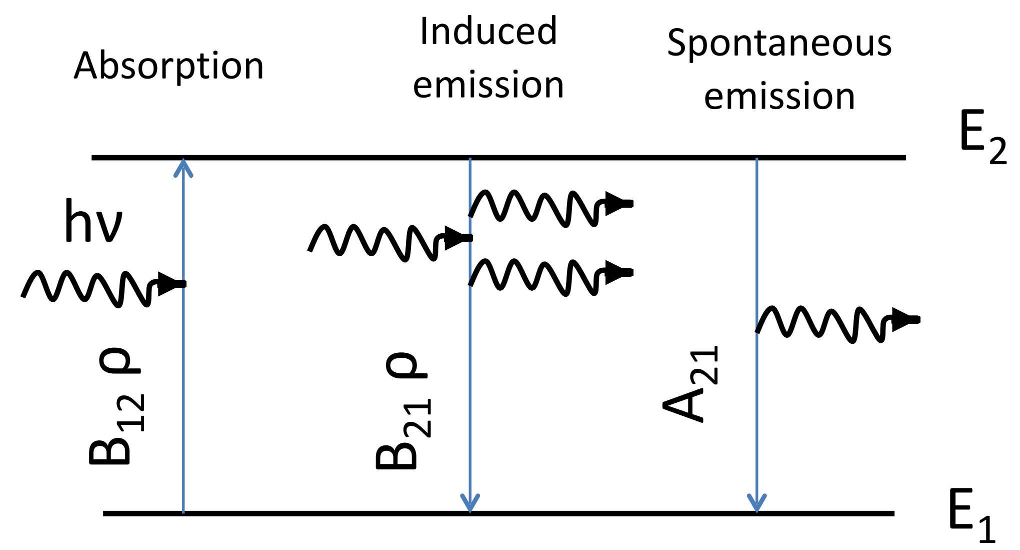


ρ: energy density of the radiation field

N_2, N_1: number of atoms in
lower, upper state, respcetively

Transition Intensities: Einstein Coefficients

$$\rho(\nu) = \frac{\frac{A_{21}}{B_{21}}}{\frac{g_1}{g_2}\frac{B_{12}}{B_{21}} e^{\frac{h\nu}{kT}} - 1} \quad (4)$$



ρ: energy density of the radiation field

Planck's thermal radiation law

$$\rho(\nu) = \frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} \quad (5)$$

Equating (4) and (5):

$$\frac{8\pi\nu^2}{c^3}\frac{h\nu}{e^{\frac{h\nu}{kT}} - 1} = \frac{\frac{A_{21}}{B_{21}}}{\frac{g_1}{g_2}\frac{B_{12}}{B_{21}} e^{\frac{h\nu}{kT}} - 1} \quad (6)$$

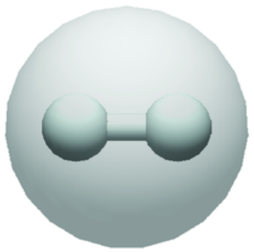
$$B_{12} = \frac{g_2}{g_1}B_{21} \qquad A_{21} = \frac{8\pi h\nu^3}{c^3}B_{21} \quad (7)$$

Lifetimes and Einstein A:

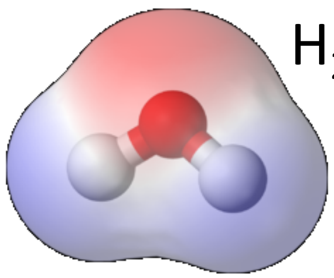
The lifetime T of an initial state i
Is given by the sum of the Einstein
coefficients summed over all final states

$$T = \frac{1}{\sum_f A_{if}}$$

What makes transitions strong: accelerated charges



H_2



H_2O

Transition frequency

Transition dipole moment

$$A_{21} = \frac{2\omega_{21}^3}{3\varepsilon_0 hc^3} \mu_{21}^2$$

In general, the dipole moment is defined as the summation of the product of the charges q_j times the position vector r_j for all charged particles j:

$$\mu = \Sigma_j q_j r_j$$

Vibrations: change in dipole moment with vibr. coordinate required $d\mu/dR \neq 0$
Rotations: rotating polar molecule (perm. dipole moment) looks like oscillating dipole

Electric Dipole transitions: $\mu_{21} \approx e\, a_0 \longrightarrow A_{21} \approx e^2 a_0^2$

Dipole moments are measured in Debye, molecules with permanent dipole moments typically have 1-3D

Electric Quadrupole transitions are weaker by a factor $(e\, a_0 \lambda)^2/(e\, a_0)^4 \approx 10^8$

Magnetic dipole transitions scale with the Bohr magneton $(eh/4\pi mc)$,
They are weaker by $\alpha^2 \approx 10^5$

Molecular transitions: Einstein coeff A_{ji} and oscillator strength f_{ji}

Type of transition	$f_{\rm ul}$	$A_{\rm ul}(\rm s^{-1})$	Example	λ	$A_{\rm ul}(\rm s^{-1})$
Electric dipole					
UV	1	10^9	Lyα	1216 Å	2.40×10^8
Optical	1	10^7	Hα	6563 Å	6.00×10^6
Vibrational	10^{-5}	10^2	CO	4.67 μm	34.00
Rotational	10^{-6}	3×10^{-6}	CS[b]	6.1 mm	1.70×10^{-6}

- Oscillator strength ~ probability of absorption or emission
- Lifetime of molecule in an excited state: $t_{\rm ex} \propto 1/A_{ul}$

Transition frequency

Transition dipole moment

$$A_{21} = \frac{2\omega_{21}^3}{3\varepsilon_0 hc^3} \mu_{21}^2$$

CO_2: 0 D

CO: 0.112 D

H2O: 1.85 D

HCN: 2.98 D

Tielens' book (2005)

Resources: HITRAN database

The HITRAN Database

HITRAN is an acronym for **hi**gh-resolution **tran**smission molecular absorption database. HITRAN is a compilation of spectroscopic parameters that a variety of computer codes use to predict and simulate the transmission and emission of light in the atmosphere. The database is a long-running project started by the Air Force Cambridge Research Laboratories (AFCRL) in the late 1960's in response to the need for detailed knowledge of the infrared properties of the atmosphere.

For additional background, see Interview.

The HIT
and its a
HITEM
spectros
paramet
develop
Molecul
Harvard
for Astr
continue
Laurenc

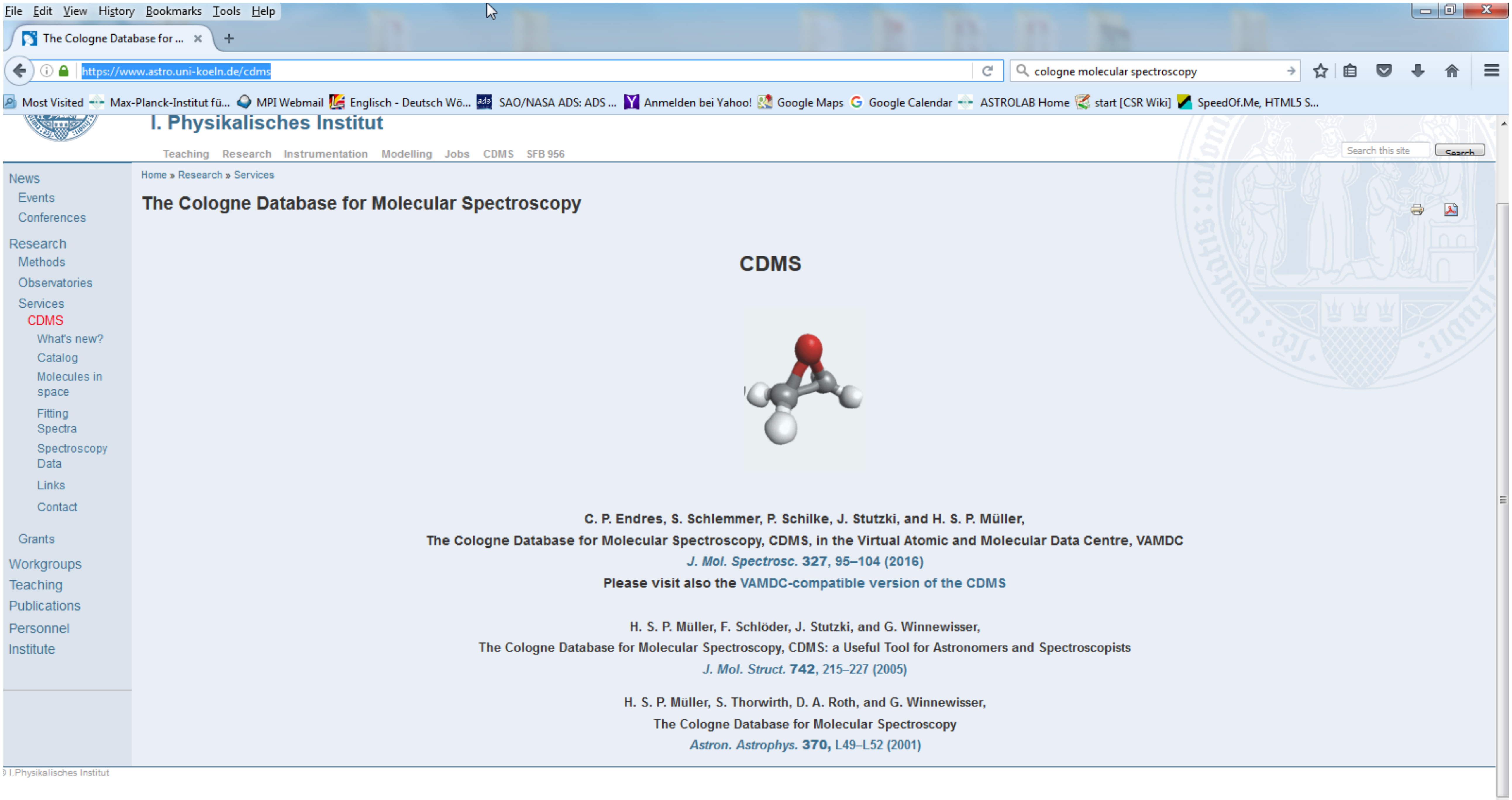
HITRAN Facts

The HITRAN2012 Database contains 7,400,447 spectral lines for 47 different molecules, incorporating 120 isotopologues. Included in these 47 species are the oxygen atom (singlet) and the NO^+ ion. Files for three of the molecules ($ClONO_2$, SF_6, and CF_4) are stored separately in the **/HITRAN2012/Supplemental/** folder.

- See a list of molecules and their associated isotopologues that are currently included in the HITRAN database.
- You can see their allowable vibrational modes.
- See a list of molecules represented by infrared absorption cross-sections that are currently included in the HITRAN compilation.
- The uncertainty indices used in HITRAN are defined in this table.
- Database formats are shown for the most recent HITRAN compilations.
- It is helpful to view the tree structure of the HITRAN compilation.

http://www.cfa.harvard.edu/hitran/

Resources: Cologne Database for Molecular Spectroscopy



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The Cologne Database for ...

https://www.astro.uni-koeln.de/cdms

cologne molecular spectroscopy

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The Cologne Database for Molecular Spectroscopy

CDMS

C. P. Endres, S. Schlemmer, P. Schilke, J. Stutzki, and H. S. P. Müller,
The Cologne Database for Molecular Spectroscopy, CDMS, in the Virtual Atomic and Molecular Data Centre, VAMDC
J. Mol. Spectrosc. **327**, 95–104 (2016)
Please visit also the VAMDC-compatible version of the CDMS

H. S. P. Müller, F. Schlöder, J. Stutzki, and G. Winnewisser,
The Cologne Database for Molecular Spectroscopy, CDMS: a Useful Tool for Astronomers and Spectroscopists
J. Mol. Struct. **742**, 215–227 (2005)

H. S. P. Müller, S. Thorwirth, D. A. Roth, and G. Winnewisser,
The Cologne Database for Molecular Spectroscopy
Astron. Astrophys. **370,** L49–L52 (2001)

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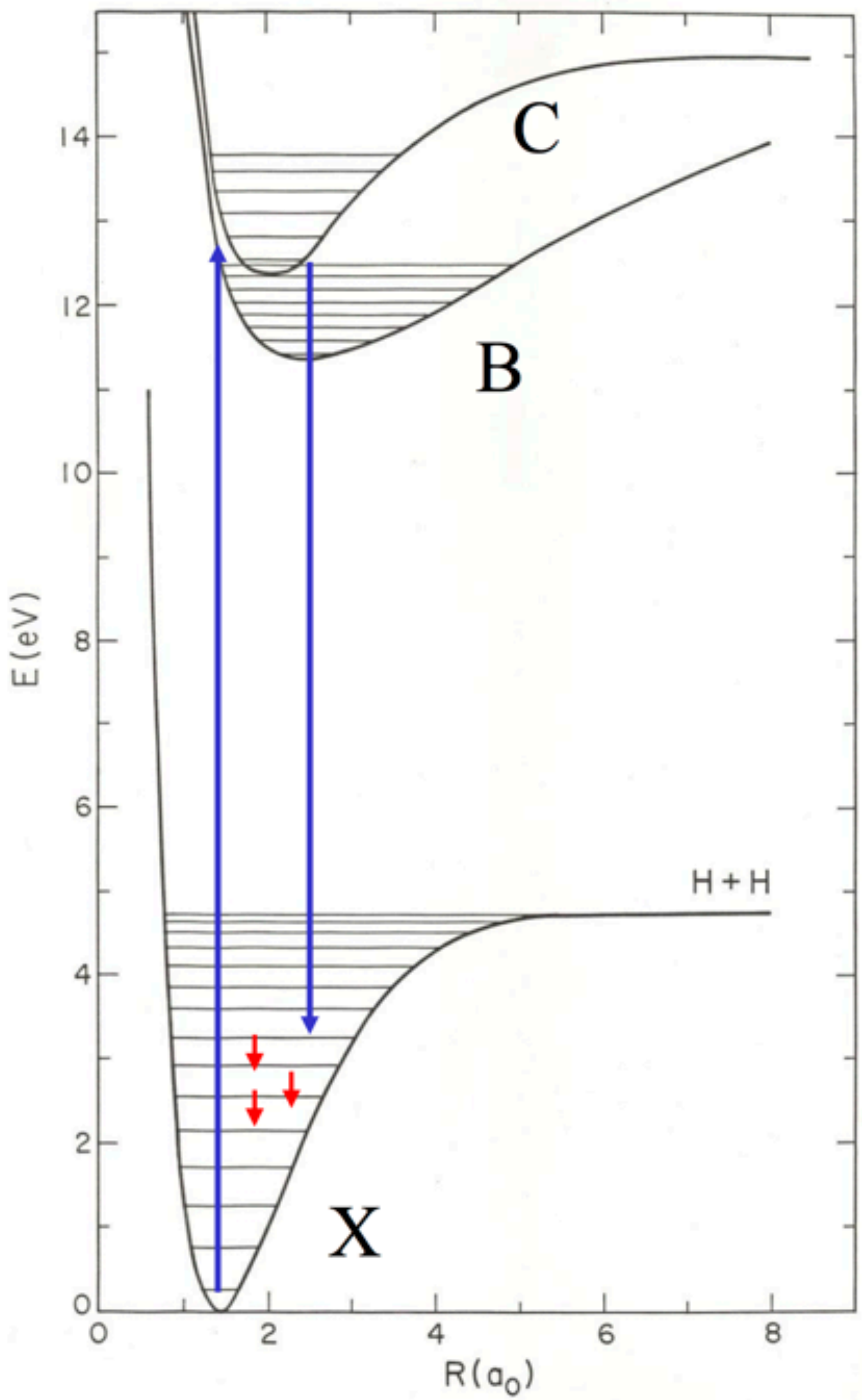
https://www.astro.uni-koeln.de/cdms

Electronic transitions (UV-optical)



- H_2
- B-X: Lyman system (<1125 Å)
- C-X: Werner system (<1051Å)

TABLE VI

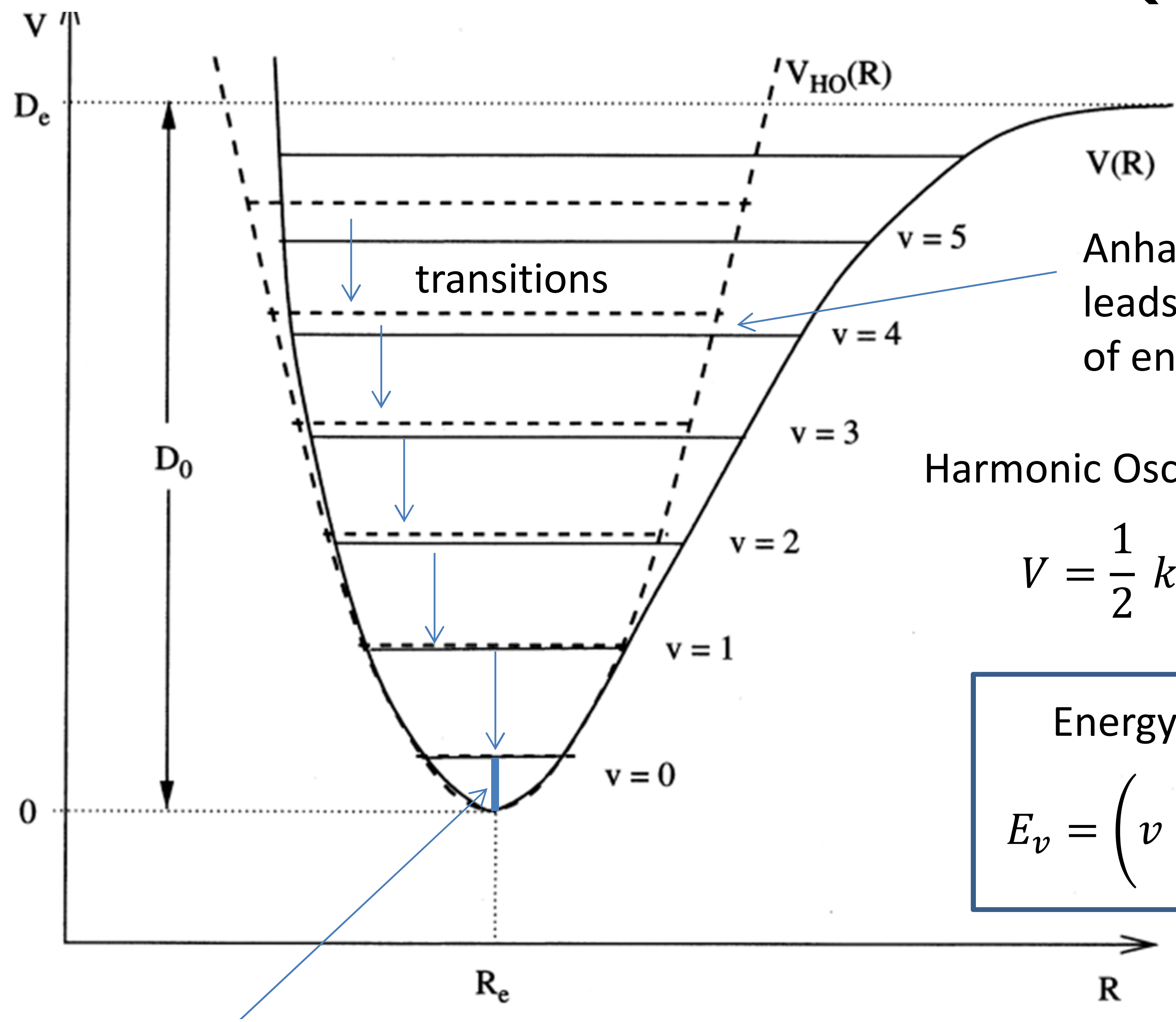
Experimentally Determined Level Energies (in cm^{-1}) of the $B^1\Sigma_u^+$ state of H_2.

J	v→ 0	1	2	3	4	5	6	7	8	J
0	90203.57	91521.85	92803.36	94050.06	95263.10	96443.05	97590.62	98706.05	99790.03	0
1	90242.31	91558.72	92838.58	94083.82	95295.52	96474.28	97620.65	98734.91	99818.04	1
2	90319.68	91632.27	92908.87	94151.23	95360.28	96536.65	97680.70	98792.66	99874.00	2
3	90434.64	91741.63	93013.39	94251.53	95456.72	96629.48	97770.12	98878.80	99957.45	3
4	90586.45	91886.11	93151.69	94384.26	95584.40	96752.39	97888.61	98993.04	100068.31	4
5	90773.35	92064.30	93322.33	94548.15	95742.11	96904.42	98035.08	99134.38	100206.19	5
6	90993.98	92274.93	93524.30	94742.33	95929.00	97084.53	98208.99	99302.17	100388.07	6
7	91246.40	92516.21	93755.85	94965.09	96143.77	97291.67	98408.80	99495.34	100548.50	7
8	91528.60	92786.55	94015.61	95215.21	96384.90	97524.27	98633.59	99712.47	100760.11	8
9	91838.29	93083.69	94301.73	95490.96	96650.90	97781.22	98881.74	99952.54	100992.78	9
10	92173.45	93406.01	94612.13	95790.48	96940.15	98060.87	99152.03	100213.92	101245.97	10
11	92531.77	93751.14	94945.16	96112.22	97251.11	98361.57	99442.98	100495.22	101518.54	11
12	92910.96	94117.35	95298.96	96454.23	97581.94	98681.67	99752.72	100795.13	101808.88	12
13	93309.09	94502.22	95671.37	96814.75	97930.88	99019.44	100080.06	101112.19	102115.93	13
14	93723.93	94904.24	96060.90	97192.01	98296.54	99373.79	100423.18	101444.52	102438.00	14
15	94153.74	95321.28	96465.24	97584.15	98676.88	99742.40	100750.65	101790.99	102773.67	15
16	94596.58	95751.75	96883.26	97990.09	99070.66	100124.44	101151.09	102150.27	103122.05	16
17	95050.72	96193.55	97312.98	98407.46	99475.81	100517.76	101532.81	102520.48	103481.28	17
18	95515.10	96645.84	97753.08	98835.23	99891.63	100921.36	101924.52	102900.75	103850.02	18
19	95987.60	97106.72	98201.88	99271.62	100315.98	101333.72	102324.79	103289.47	104227.17	19
20	96467.66	97575.20	98658.14	99716.26	100748.14	101753.99	102733.02	103685.63	104611.89	20
21	96953.68	98049.54	99120.77	100166.56	101186.89	102180.36	103147.44	104088.13	105002.60	21
22	97445.25	98529.56	99589.24	100622.68	101630.35	102612.08	103567.11	104496.16	105398.51	22
23	97940.86	99013.66	100061.55	101083.24	102079.50	103047.95	103991.36	104908.33	105798.36	23
24	98440.03	99501.62	100537.42	101547.10	102530.74	103487.59	104418.73	105323.53	106202.13	24
25	98942.08	99991.84	101016.05	102014.24	102985.88	103930.39	104848.88	105742.07		25
26	99446.41	100484.65	101496.33	102482.40	103441.76	104374.35	105281.27	106161.39		26
27	99952.29	100978.83	101979.46	102951.68	103900.43	104820.11	105714.67			27
28	100458.92	101473.77	102461.84	103423.40	104358.40	105266.91	106149.66			28

Abgrall et al. (1993)

Courtesy of E. van Dishoeck (2011)

Vibrational transitions (IR)



$$V = \frac{1}{2} k (R - R_e)^2$$

Energy levels

$$E_v = \left(v + \frac{1}{2}\right) \hbar \omega$$

- Zero-point $E_{vib} = 1/2\hbar\omega$, scales as mass$^{-1/2}$
- Equidistant separation of levels: only harmonic approximation
- Many degrees of freedom

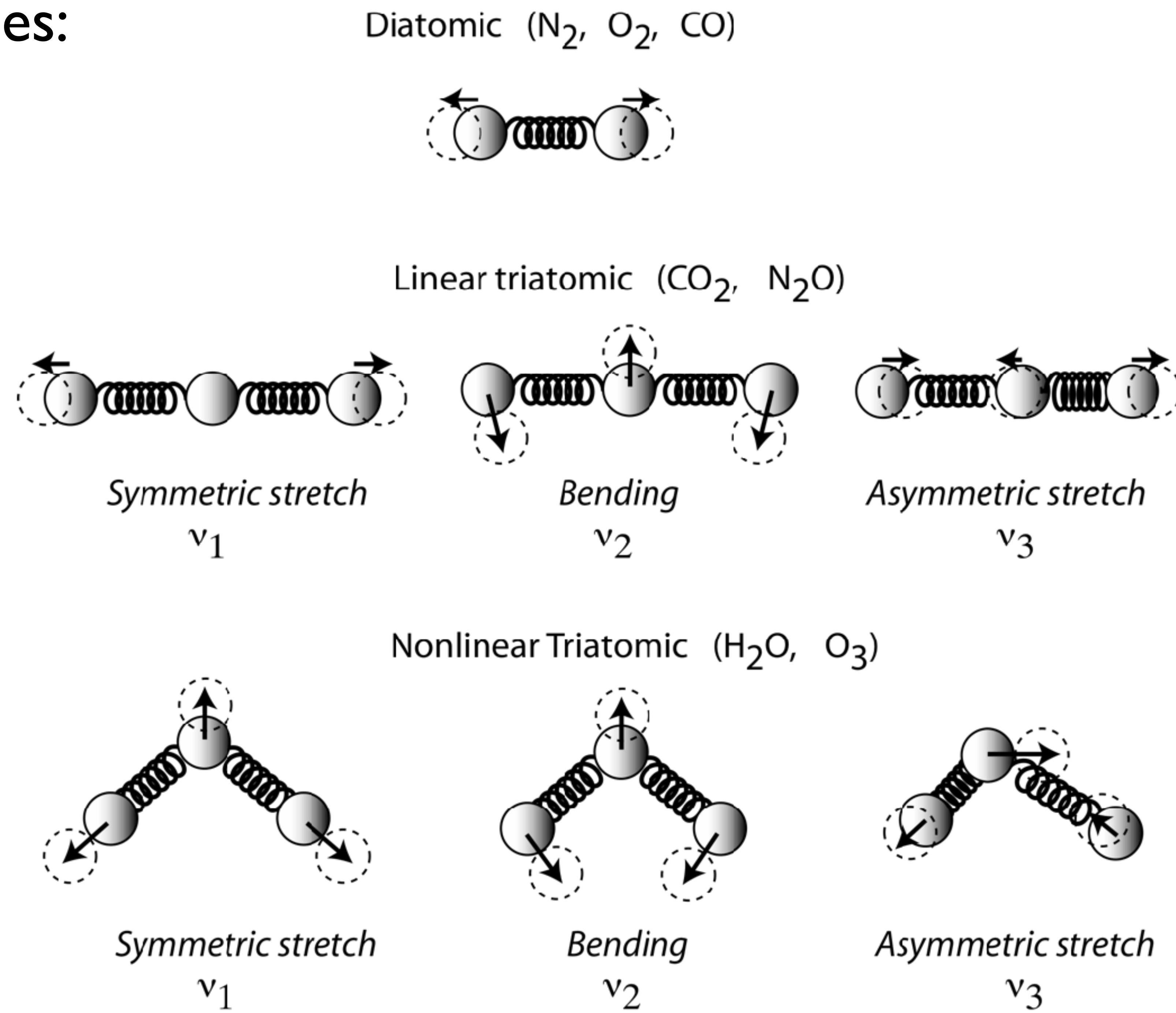
Vibration modes of simple molecules

Fundamental or normal modes:

ν_1 Symmetric stretch

ν_2 Bend

ν_3 Asymmetric stretch



Overtones, combinations and differences of fundamental vibrations (e.g., $2v_1$, v_1+v_3 etc.)

A non-linear molecule of N atoms: 3N-6 normal modes (linear has 3N-5)

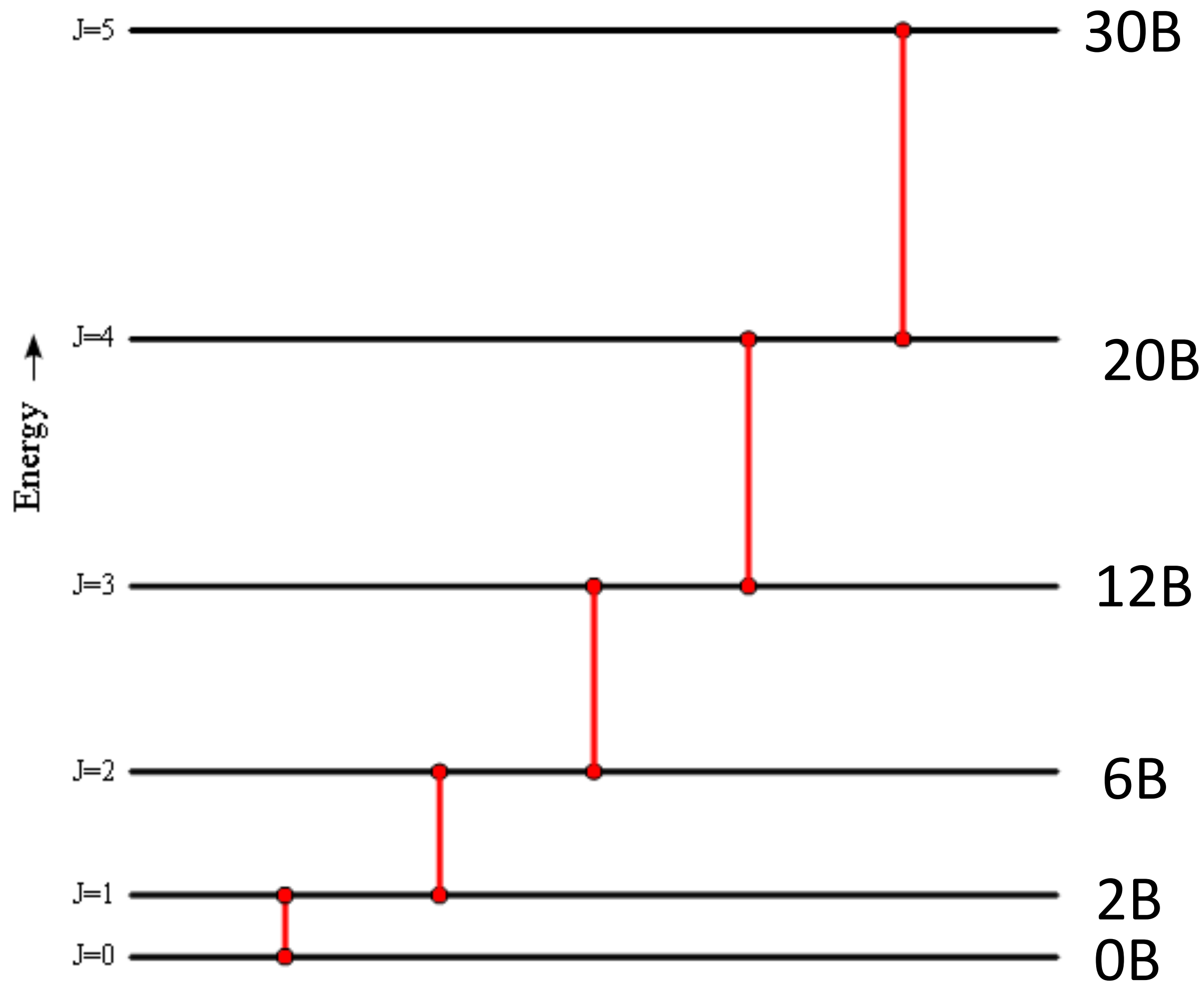
Vibrational modes: hydrocarbons

Group	Mode	Frequency (cm^{-1})	
CH stretch			
	≡C–H	3280–3340	
	=C–H	3000–3100	
	CO–CH_3	2900–3000	ketones
	C–CH_3	2865–2885	symmetric
		2950–2975	asymmetric
	O–CH_3	2815–2835	symmetric
		2955–2995	asymmetric
	N–CH_3	2780–2805	aliphatic amines
	N–CH_3	2810–2820	aromatic amines
	CH_2	2840–2870	symmetric
		2915–2940	asymmetric
	CH	2880–2900	
C≡C stretch			
	C≡C	2100–2140	terminal group
	C–C≡C–C	2190–2260	
C=C stretch	C–C≡C–C–C≡C–	2040–2200	
	–HC=C=CH_2	1945–1980	
	–HC=C=CH–	1915–1930	
CH bend			
	CH_3	1370–1390	symmetric
		1440–1465	asymmetric
	CH_2	1440–1480	
	CH	1340	

NASA Ames database: http://www.astrochem.org/pahdb/

Tielens' book (2005)

Rotational transitions (IR-radio)



Energy levels

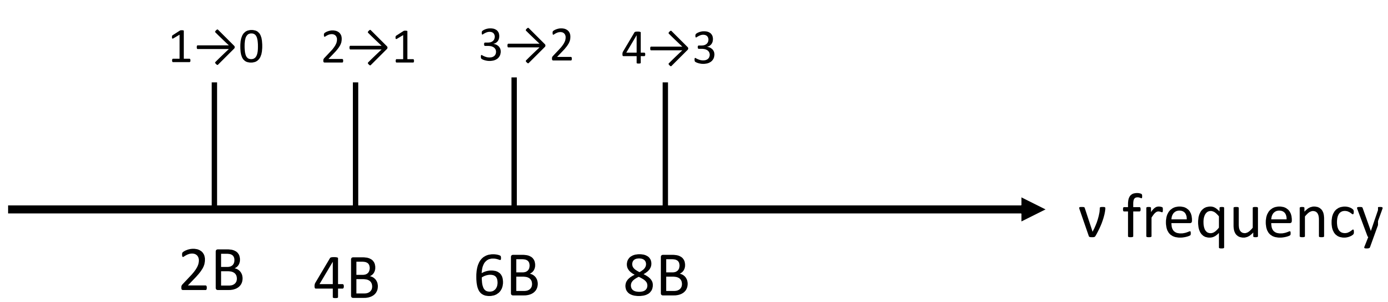
$$E_r = B\,J(J+1)$$

Selection rule:

$$\Delta J = \pm 1$$

Transitions:

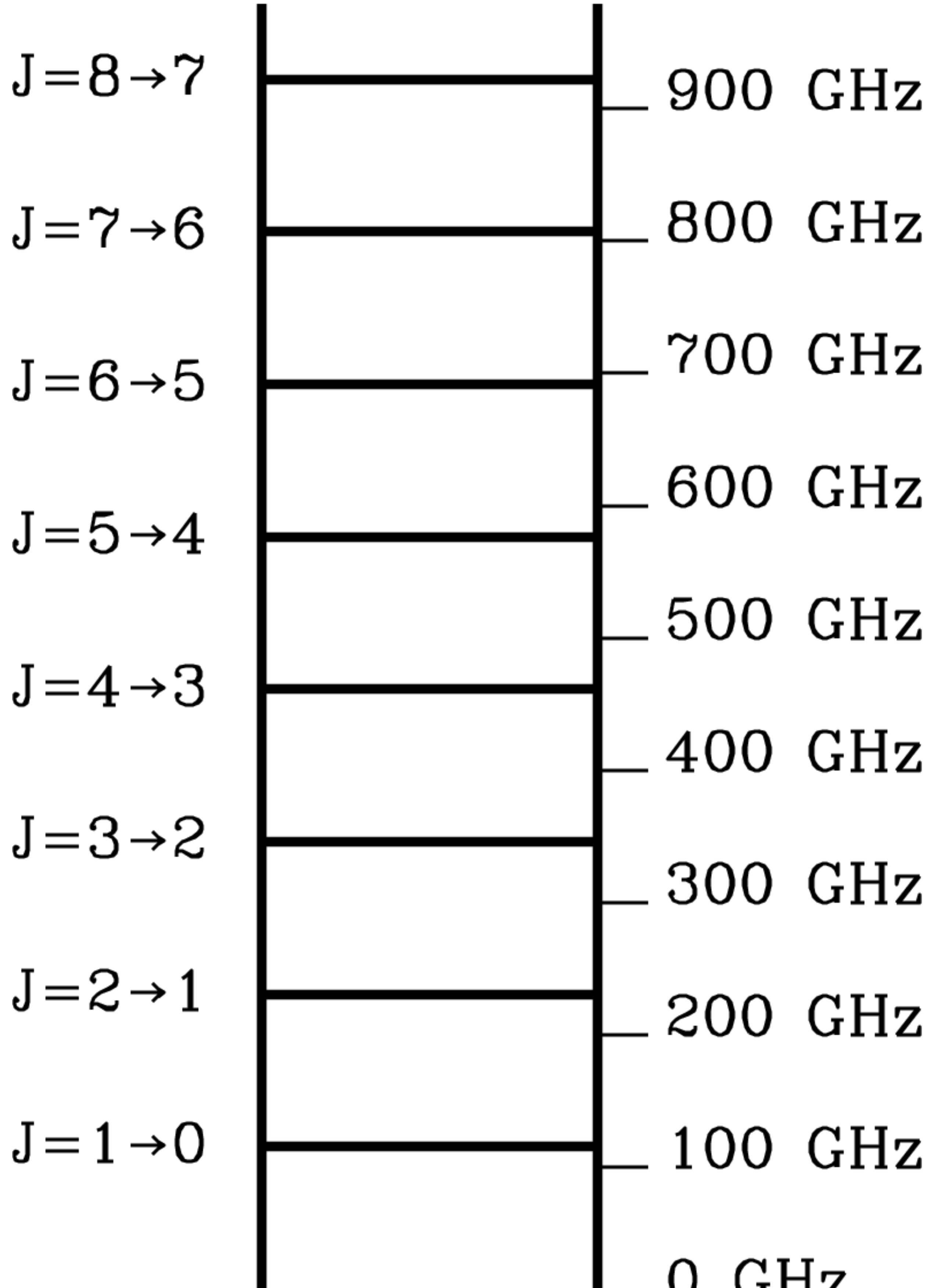
$$E_r(J+1) - E_r(J)$$
$$= B\,[(J+1)(J+2) - J(J+1)]$$



$$\Delta E = 2B[J+1]$$

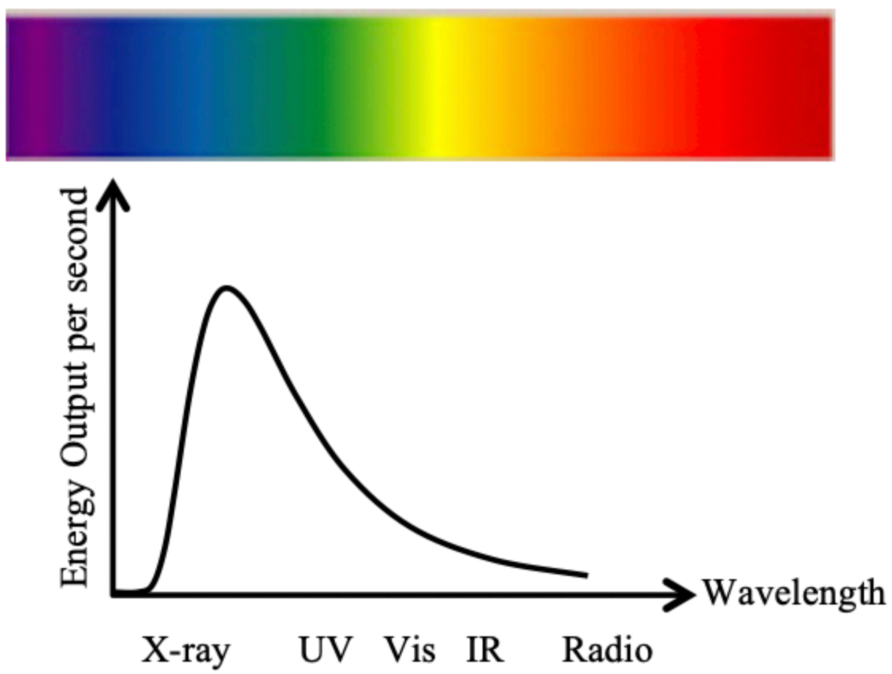
- Rigid rotors: B ~ $\hbar^2/2I$, where I - moment of inertia (depends on mass)
- Equidistant separation of line frequencies

CO rotational ladder

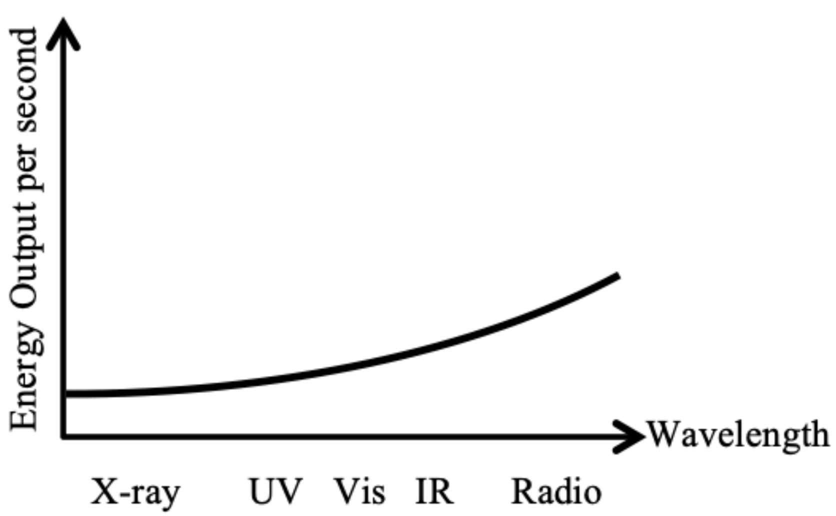


Types of spectra

Continuous

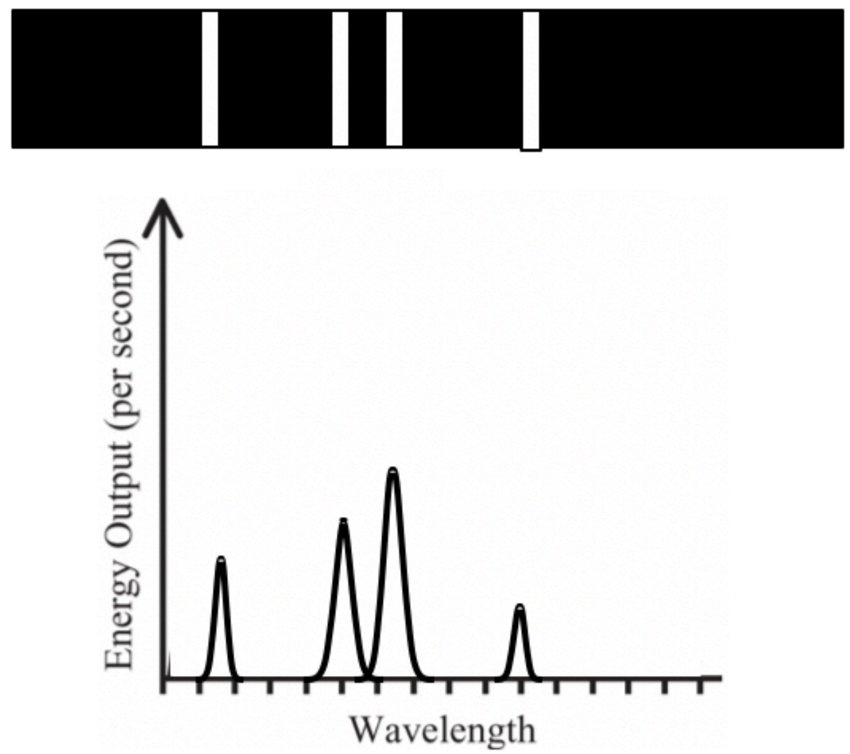


thermal (blackbody)



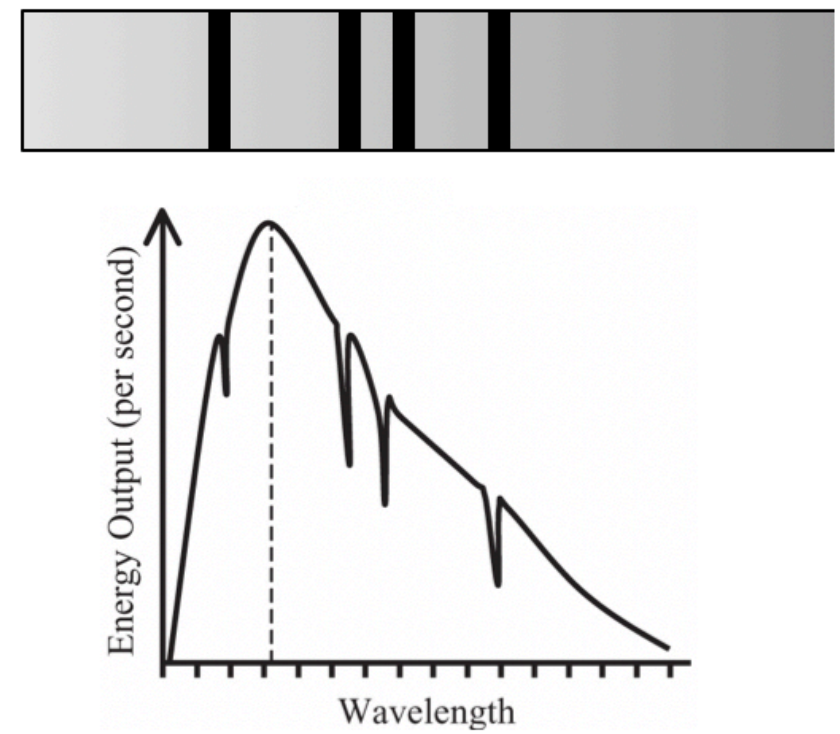
synchrotron

Emission



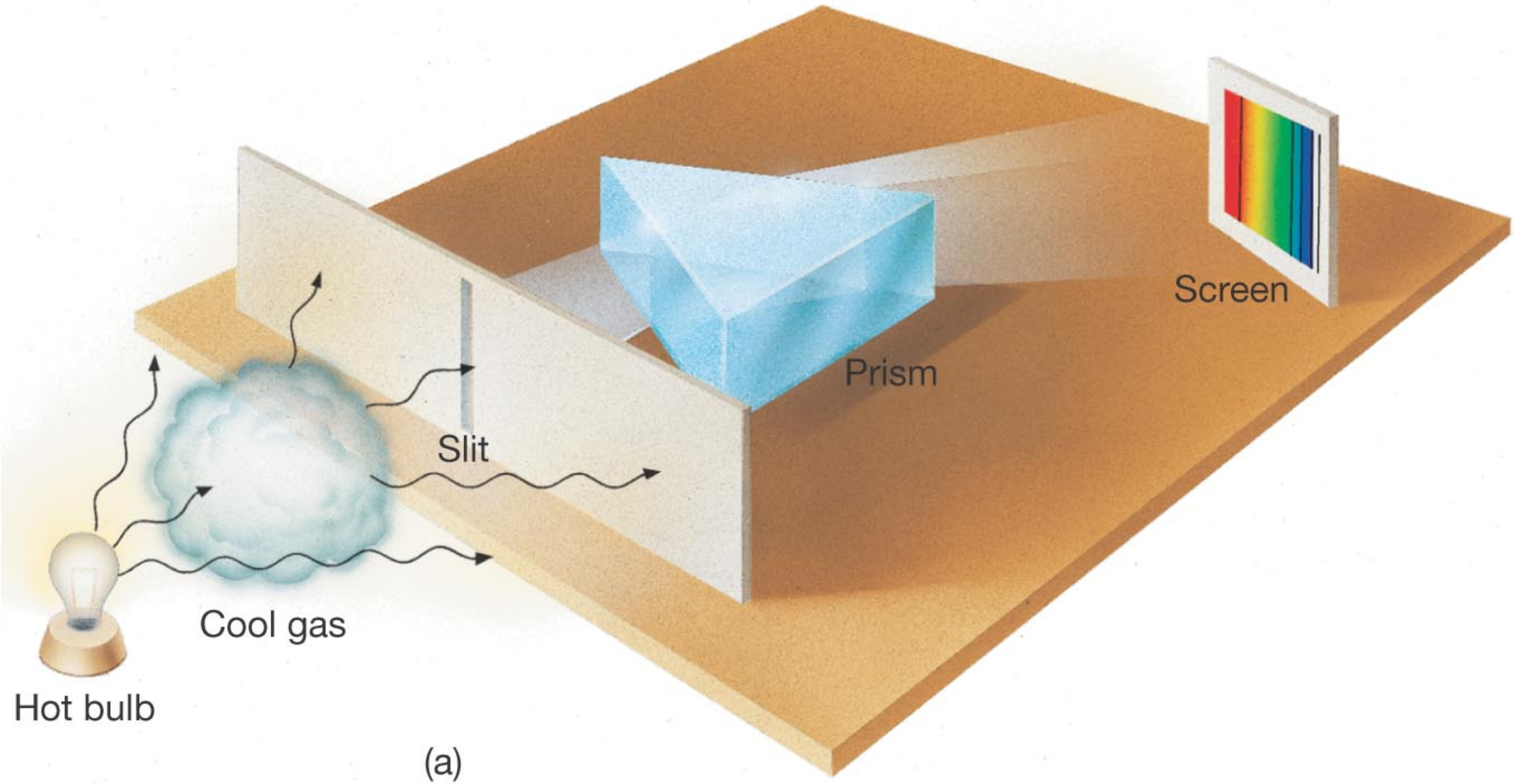
produced by atoms and molecules

Absorption



produced by atoms and molecules

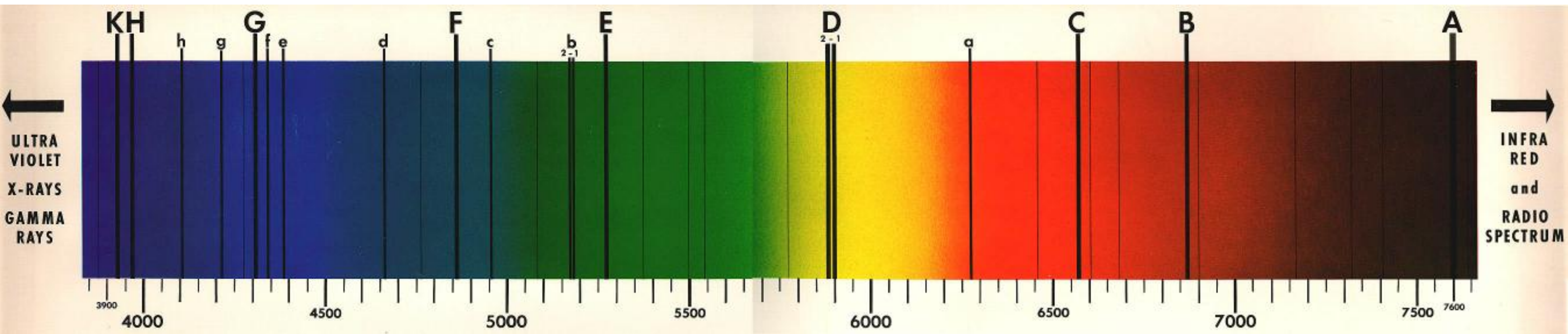
Absorption lines



- Cool gas in front of warm continuum
- Slit + diffraction grating/prism + detector
- Specific frequencies determined by gas composition

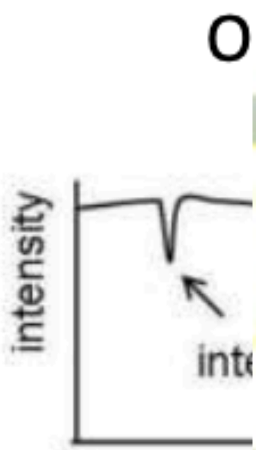
Absorption lines

- 1802, William Hyde Wollaston ⇒ dark features in the solar spectrum
- 1814, Joseph von Fraunhofer ⇒ systematic measurements, 574 lines
- 1860, Gustav Kirchhoff and Robert Bunsen ⇒ first identification (Na)



Designation	Element	Wavelength (nm)	Designation	Element	Wavelength (nm)
A	O_2	759.370	d	Fe	466.814
B	O_2	686.719	e	Fe	438.355
C	Hα	656.281	G'	Hγ	434.047
a	O_2	627.661	G	Fe	430.790
D_1	Na	589.592	G	Ca	430.774
D_2	Na	588.995	h	Hδ	410.175

Absorption spectroscopy



Star

In other words:
(consider use density)

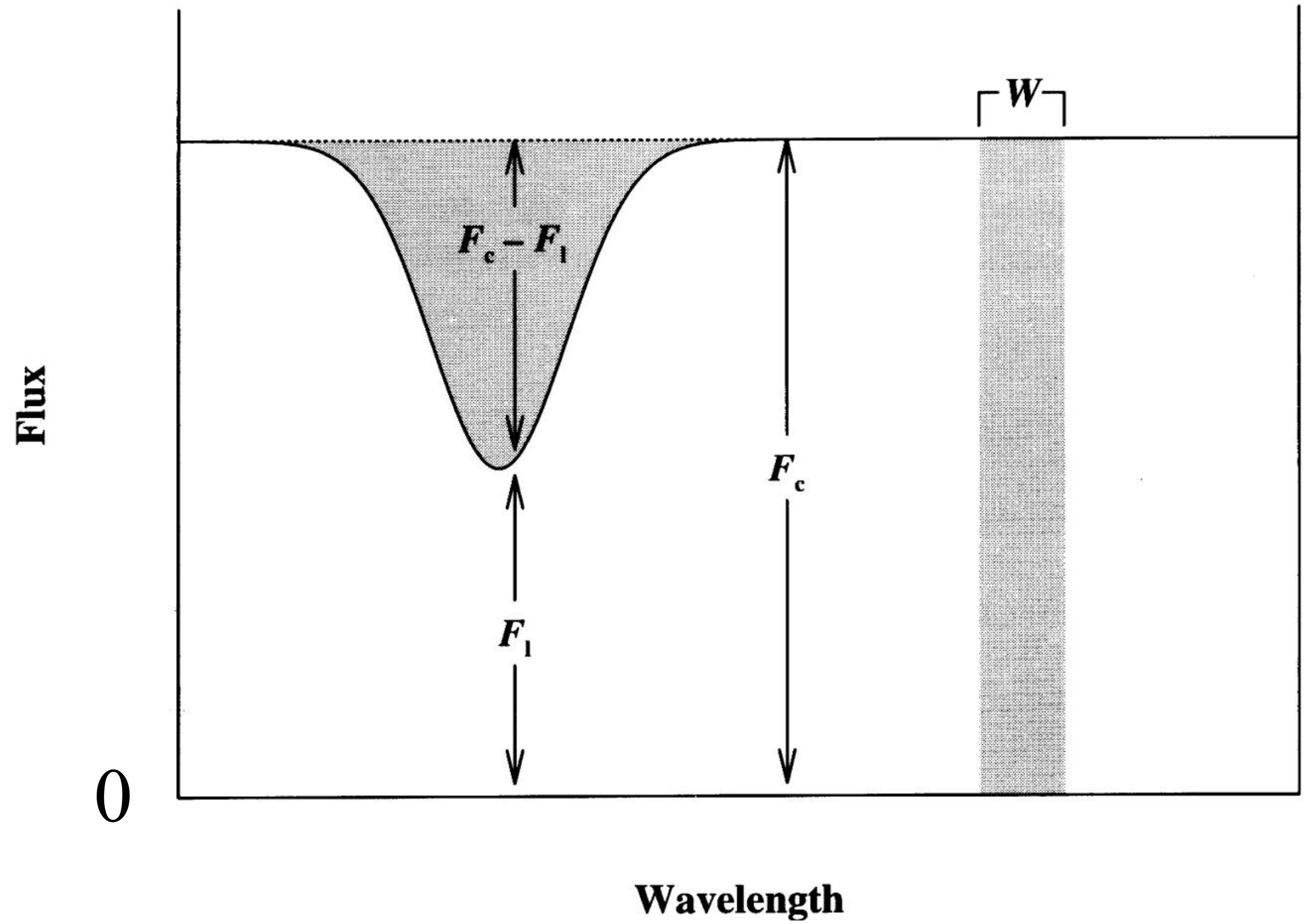
$$T = \frac{I(f)}{I_0} = e^{-n\,\sigma\,x}$$

transmission

n : gas density [cm^{-3}]
σ: cross section [area, cm^2]
x: path length

Absorption spectroscopy

- Optical spectroscopy has limited resolution: equivalent width **W**



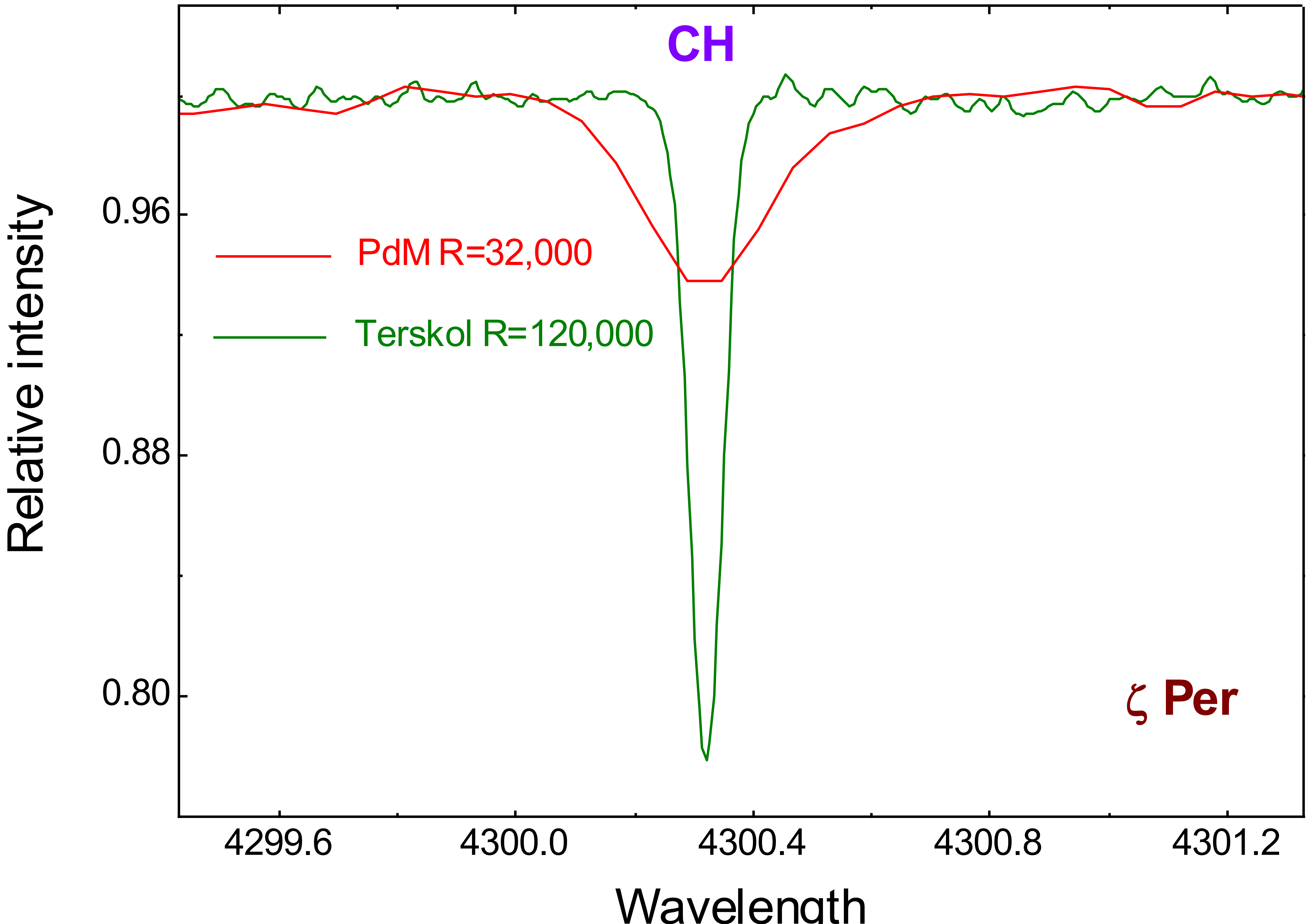
- Equivalent width:

$$\boldsymbol{W_\nu} = \int_{-\infty}^{\infty} \left[\frac{I_\nu(0) - I_\nu}{I_\nu(0)} \right] \mathrm{d}\nu \quad \mathrm{Hz}$$

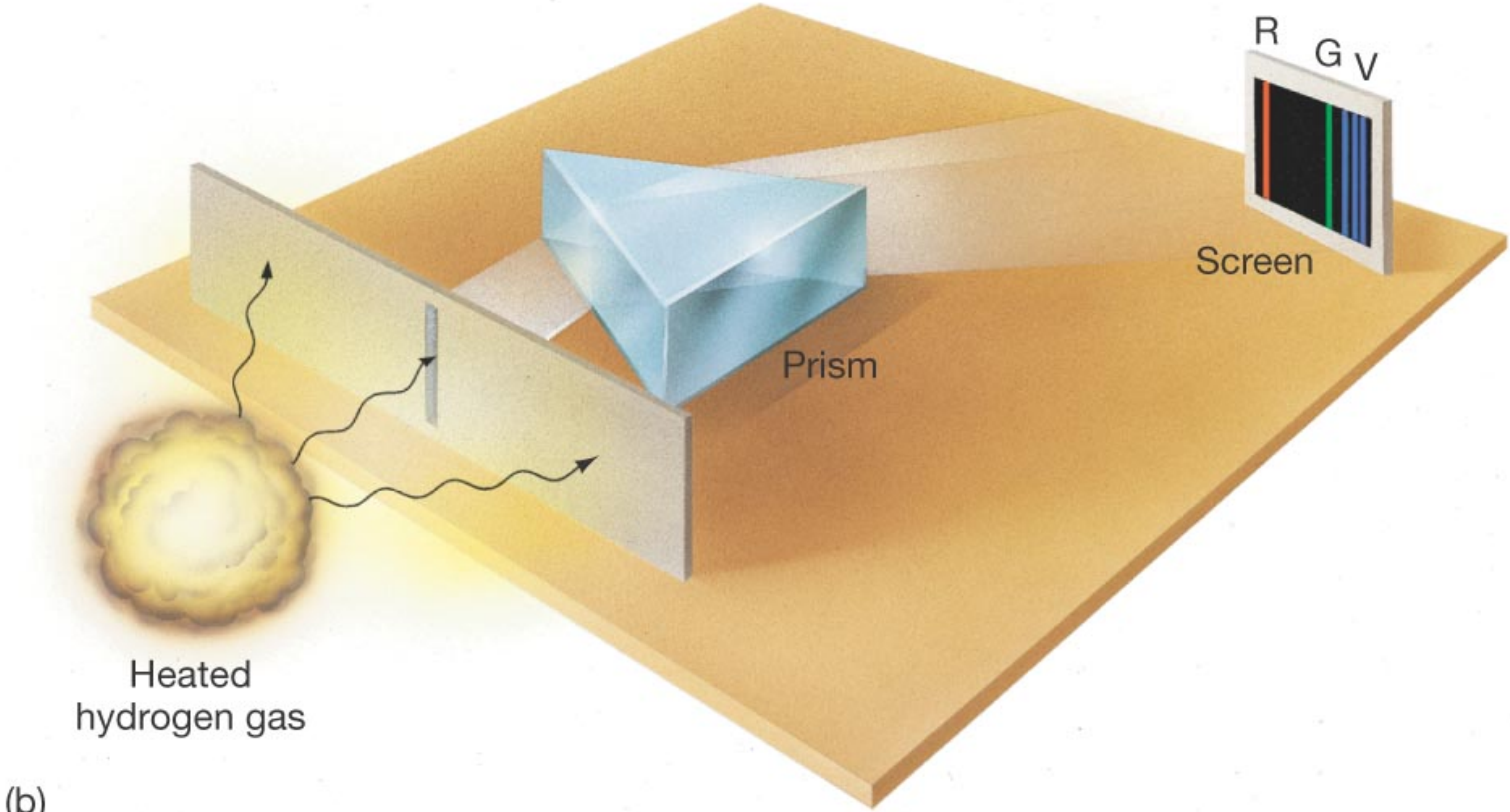
Absorption spectroscopy

- If line is not fully saturated:
- W_v ~ oscillator strength f x amount of molecules N
- Oscillator strengths for molecules could be hard to compute
- Direct measure of the column density (amount of matter on the line of sight): $N \propto W_v / f$

CH absorption towards ζ Per

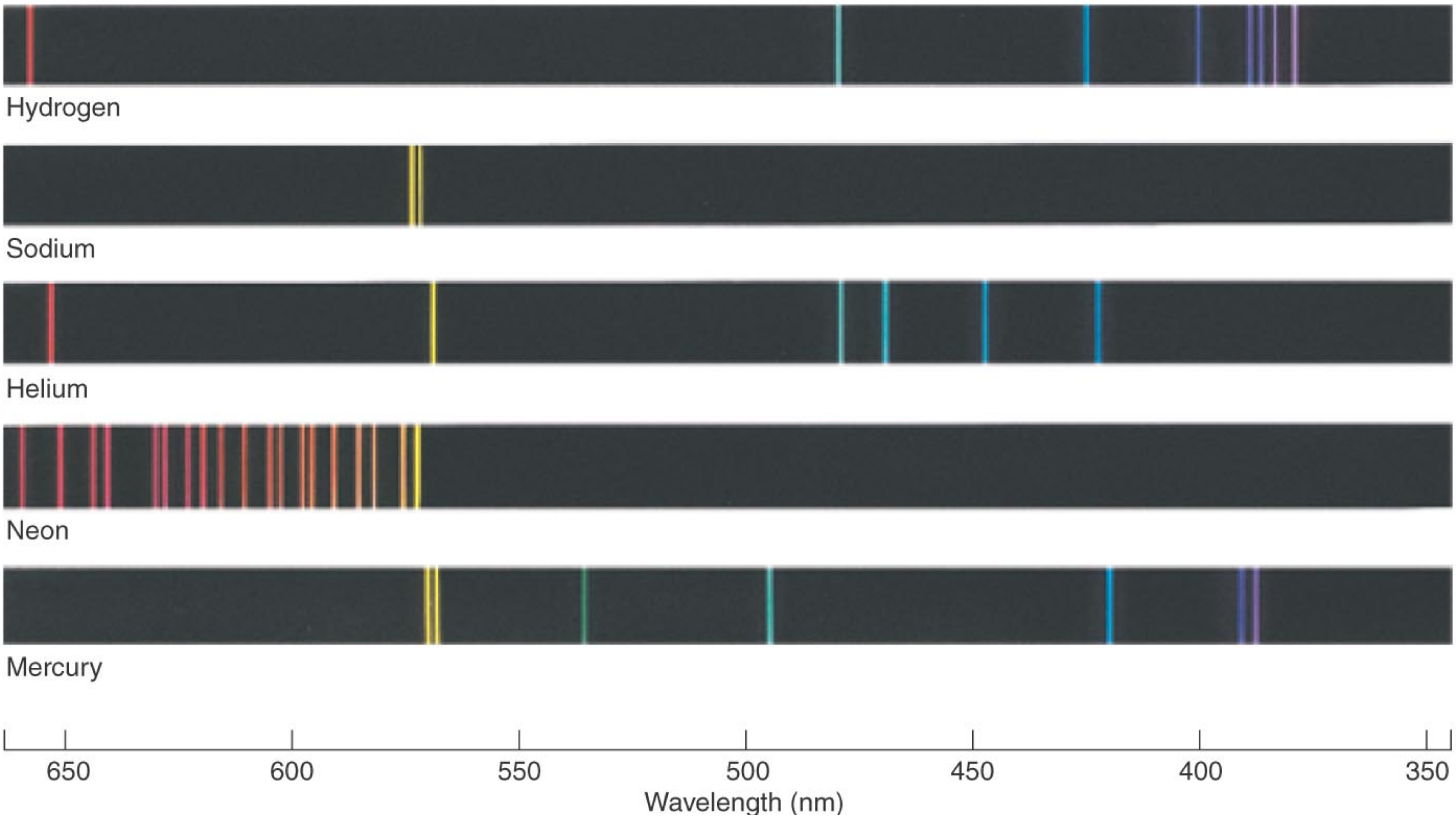


Emission lines



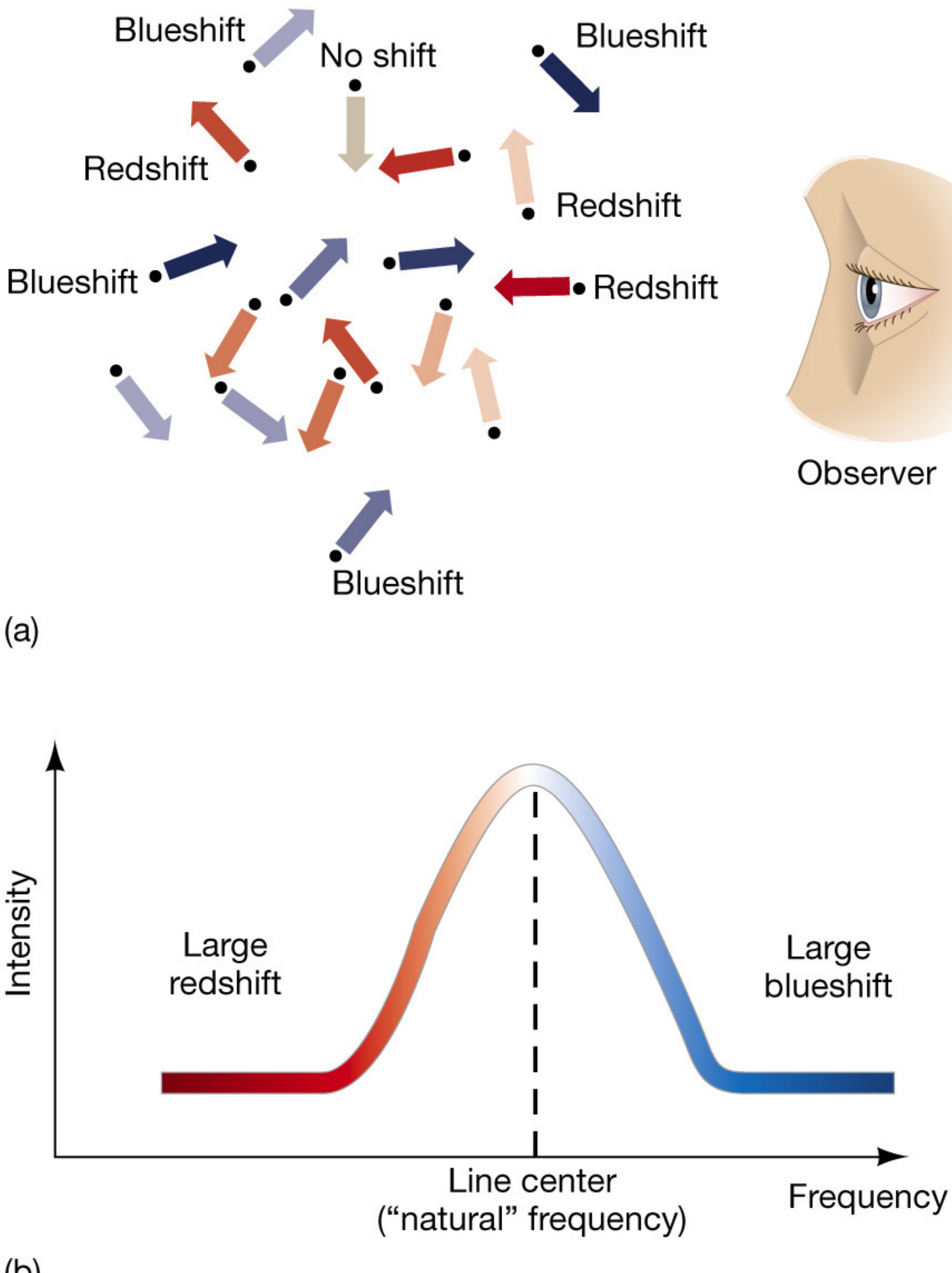
- Warm gas
- Harder to analyze compared to absorption spectra

Emission lines



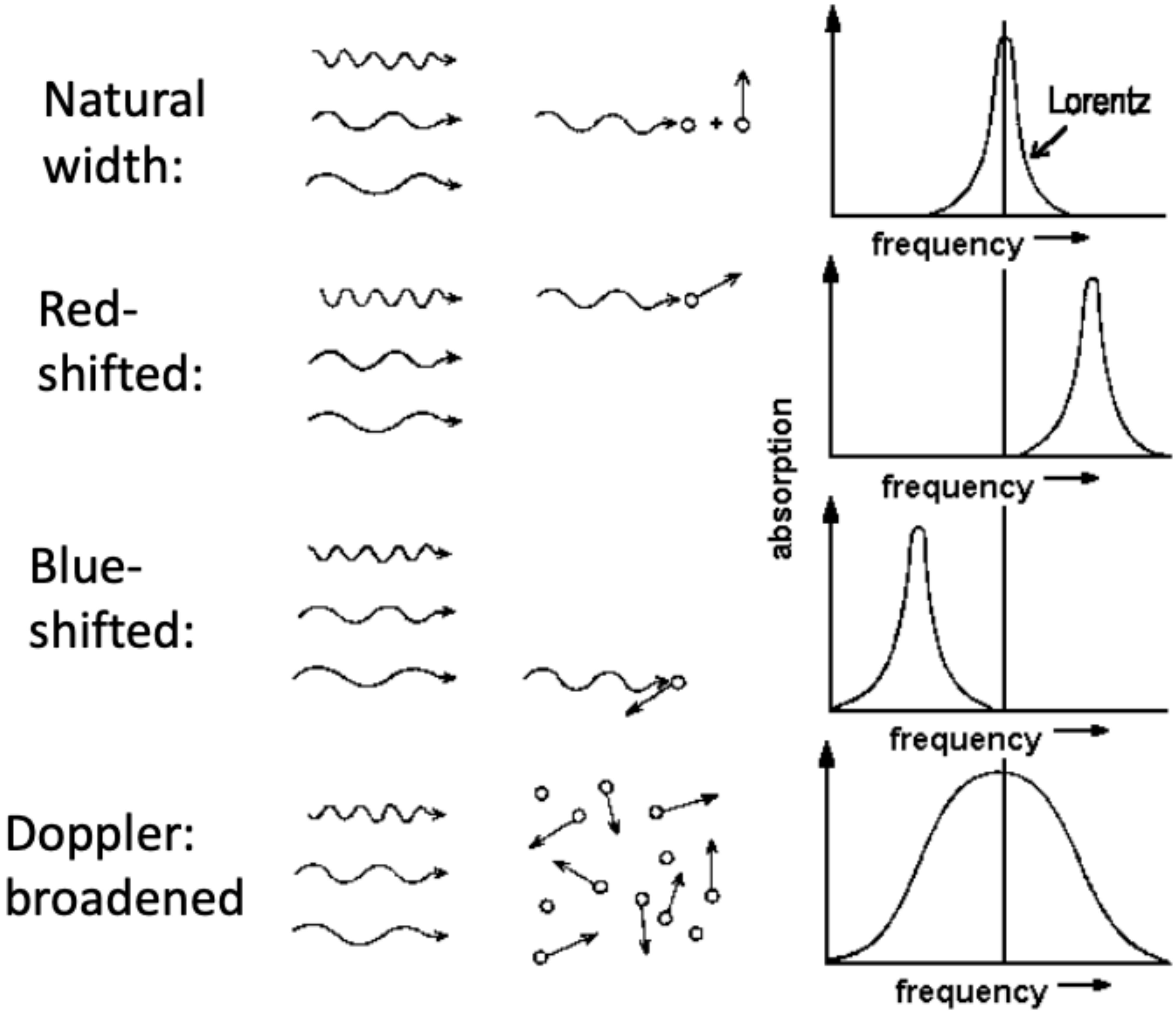
• Lines are „fingerprints“ => identification when line frequencies are computed or measured in laboratory

Emission line profiles

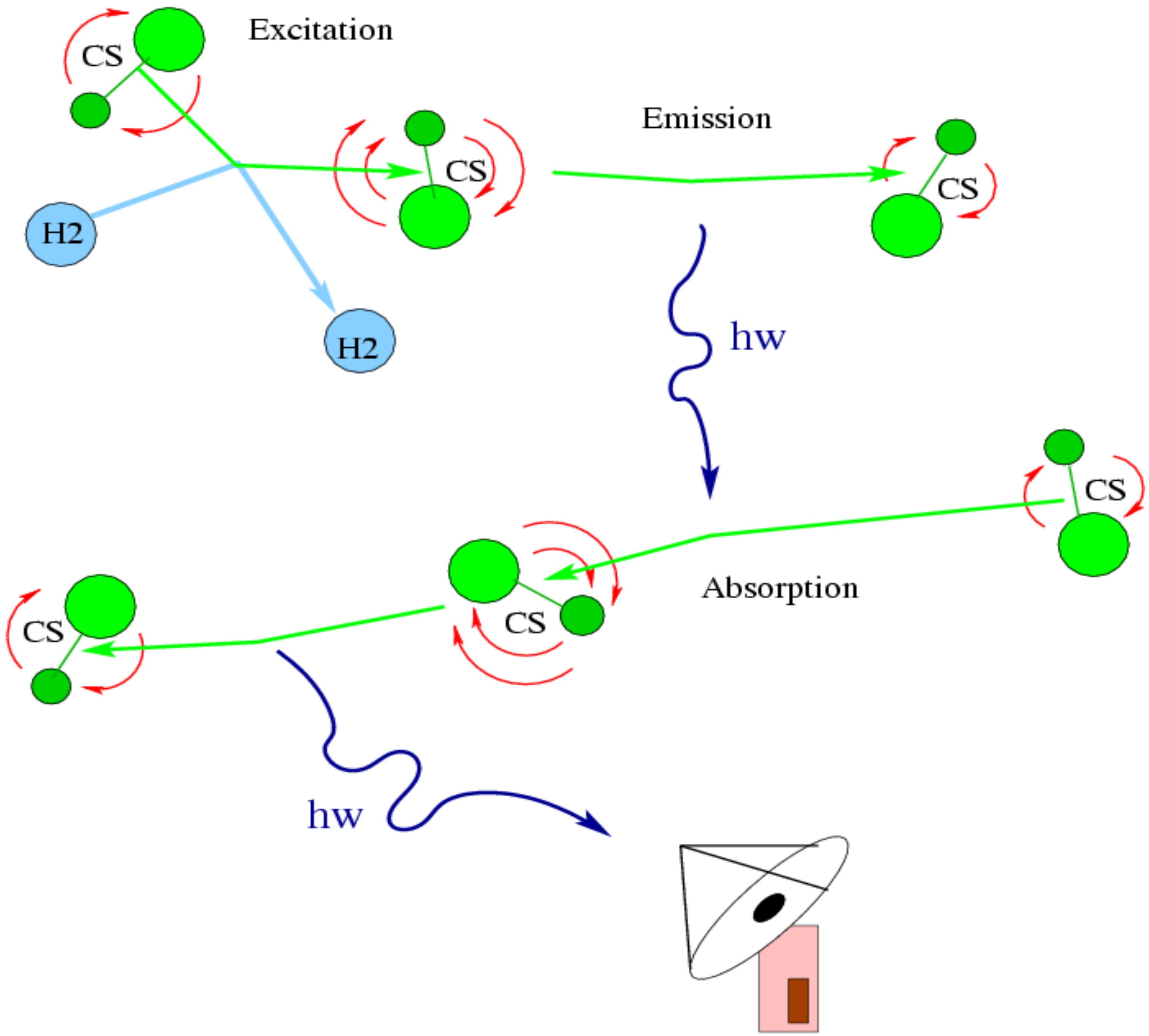


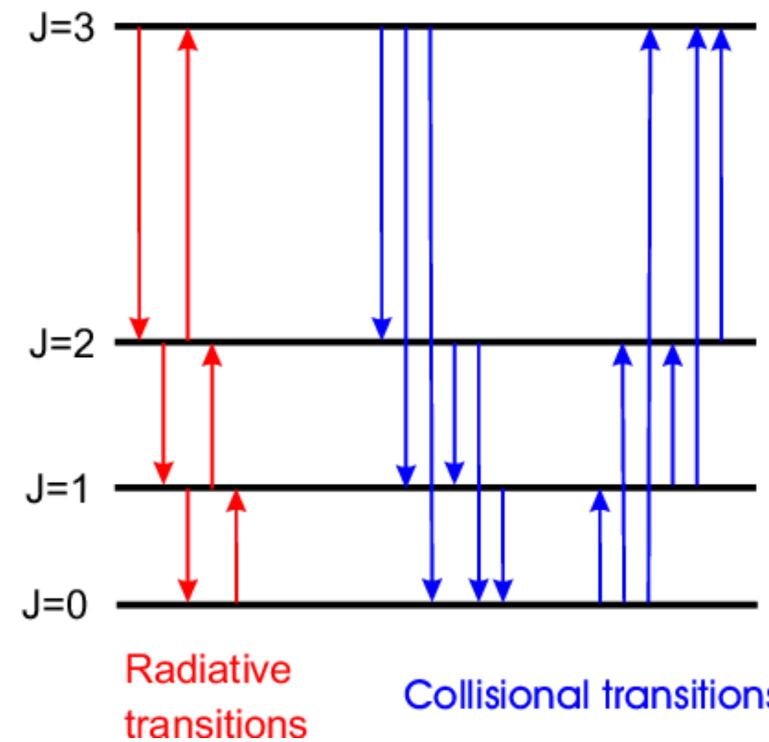
- Line shape and width (FWHM):
  – Natural
  – Thermal
  – Kinematics
  – Pressure, etc

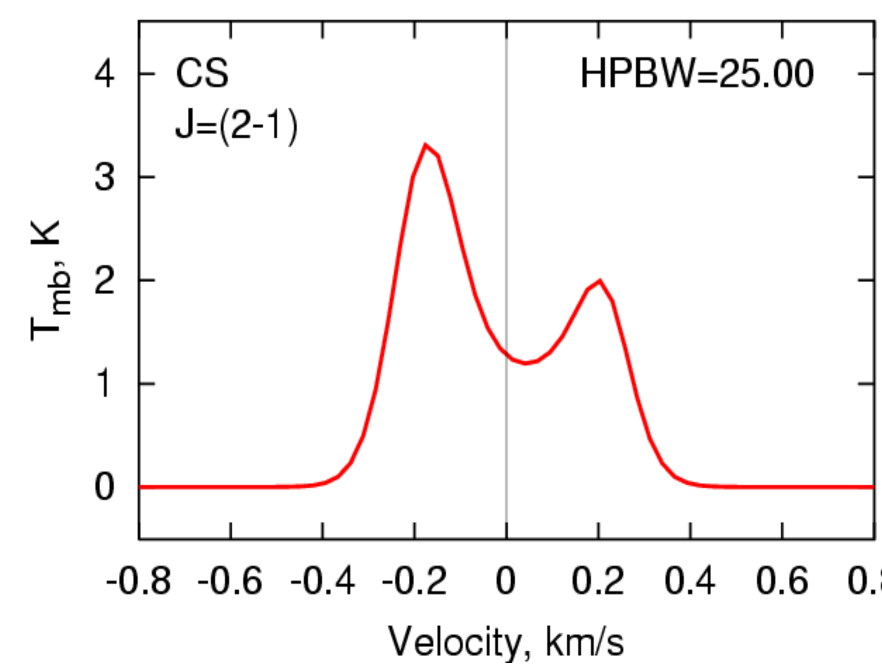
Line profiles



Emission line spectra







Depends on physical conditions and distribution of molecules

Molecular lines: population of energy levels

- Statistical equilibrium of level populations:

$$n_l \left[\sum_{k<l} A_{lk} + \sum_{k\neq l} (B_{lk} J_\nu + C_{lk})\right] =$$

$$\sum_{k>l} n_k A_{kl} + \sum_{k\neq l} n_k (B_{kl} J_\nu + C_{kl}).$$

A_{lk} - spontaneous emission

B_{lk} - stimulated emission (absorption)

C_{lk} - collisional excitation (de-excitation)

J_ν - local mean intensity

n_j - level population of the level j

- **Critical density for line excitation:** $n_{cr} = A_{ul} / C_{ul}$

Critical densities: examples

- Line data from LAMDA database (Schöier et al. 2005)
- CS J=1-0 line at 48.991 GHz:
  - 10 K: $A_{10} = 1.75\ 10^{-6}\ s^{-1}$, $C_{10} = 3.49\ 10^{-11}\ cm^3\ s^{-1}$: $n_{cr} = 5.0\ 10^4\ cm^{-3}$
  - 300 K: $A_{10} = 1.75\ 10^{-6}\ s^{-1}$, $C_{10} = 2.97\ 10^{-11}\ cm^3\ s^{-1}$: $n_{cr} = 5.9\ 10^4\ cm^{-3}$
- CS J=7-6 line at 342.883 GHz:
  - 10 K: $A_{76} = 8.40\ 10^{-4}\ s^{-1}$, $C_{76} = 5.82\ 10^{-11}\ cm^3\ s^{-1}$: $n_{cr} = 1.4\ 10^7\ cm^{-3}$

- **Presence of high-lying rotational lines indicate high density**

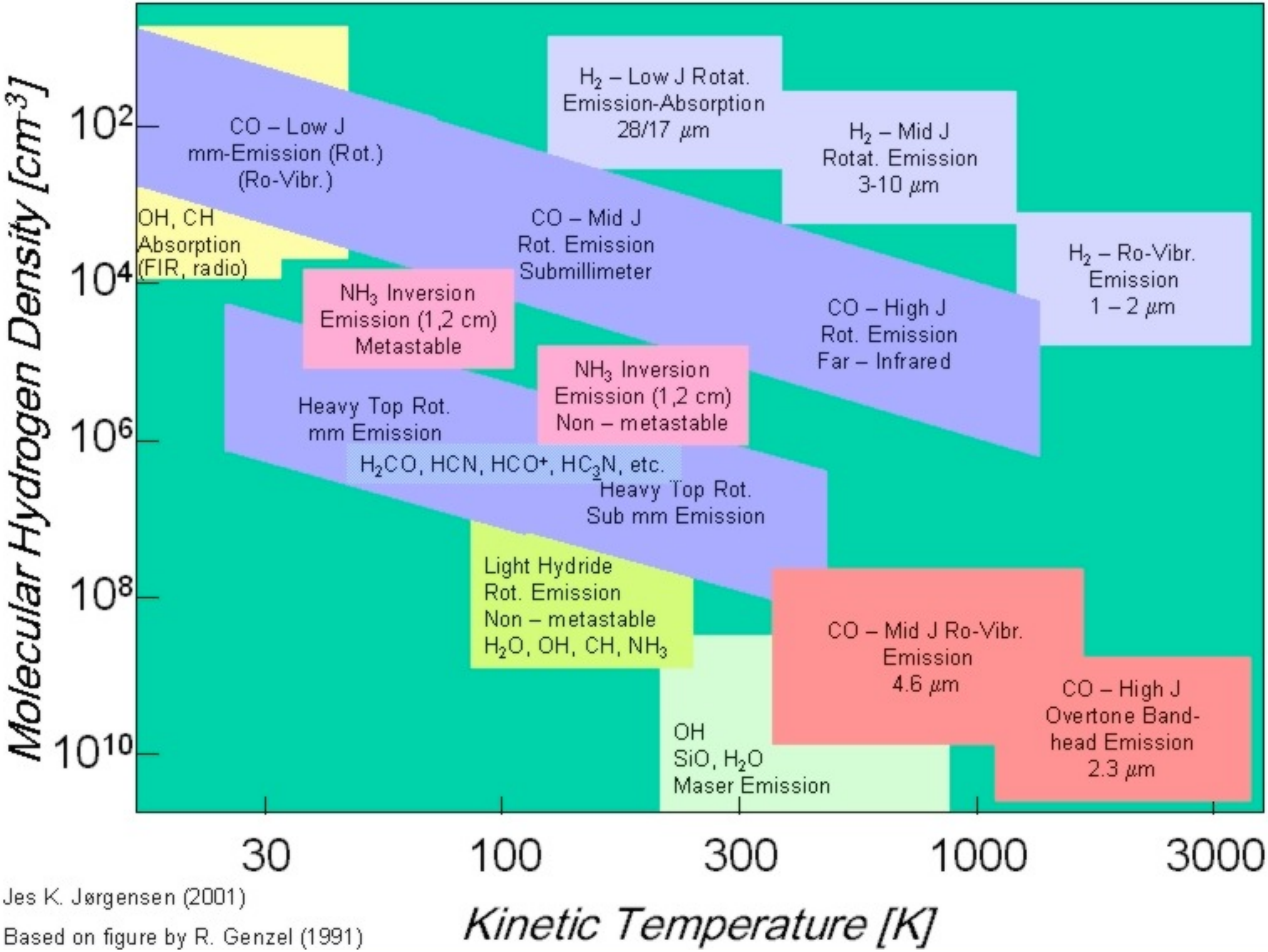
Emission lines: diagnostics

- Solving statistical equilibrium equations is numerically challenging
- Local Thermodynamic Equilibrium ($T_{ex} = T_{kin}$) is often assumed
- Level population follows Boltzmann's distribution:

$$\frac{n_u}{n_l} = \frac{g_u}{gl} \exp[-E_{ul}/kT_{kin}] = \frac{g_u}{gl} \exp[-E_{ul}/kT_{ex}]$$

- Excitation vs kinetic temperature (general rule):
  - High densities ***($n \gg n_{cr}$): $T_{ex} \sim T_{kin}$***
  - Low densities ***($n \ll n_{cr}$): $T_{ex} < T_{kin}$***

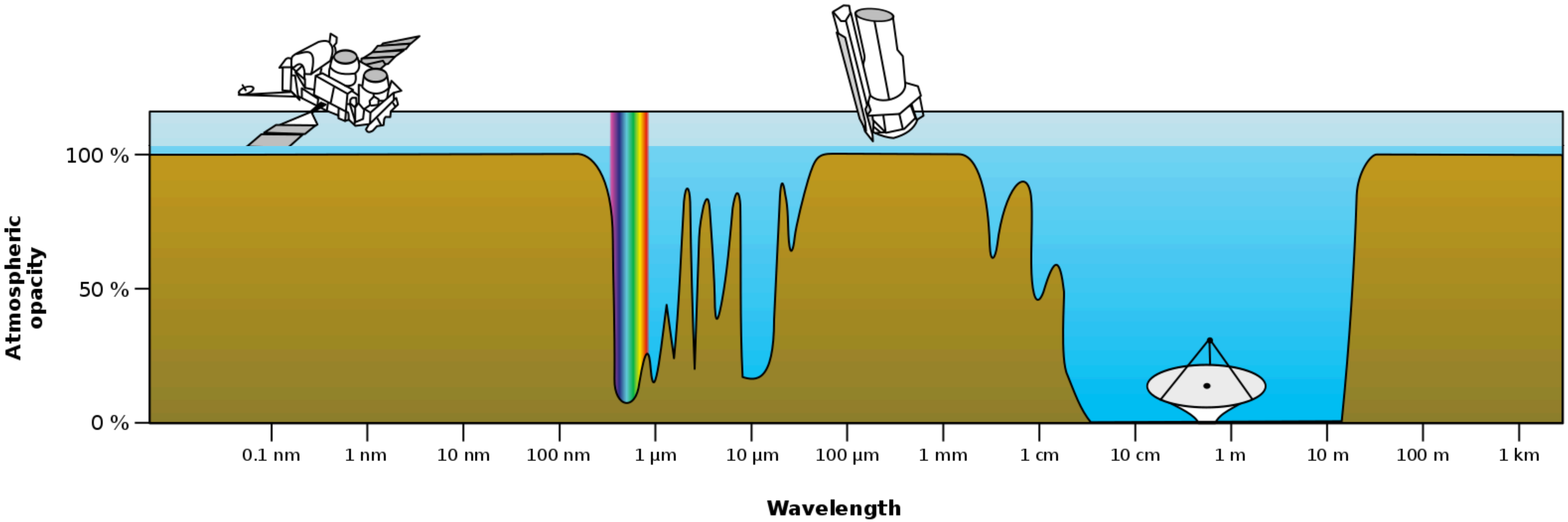
Molecules as probes of physical conditions



Jes K. Jørgensen (2001)

Based on figure by R. Genzel (1991)

Opaqueness of the Earth atmosphere



- Blocked: X-ray & UV (<300nm)
- Mid-IR/sub-mm (20µm–0.3mm)
- Long radio wavelengths (>10m)

Telescopes and Detectors: key properties

- Collecting area (diameter D) => angular resolution
- D and focal length => field of view
- Spectral coverage
- Spectral resolution: $R = \nu/\Delta\nu$:

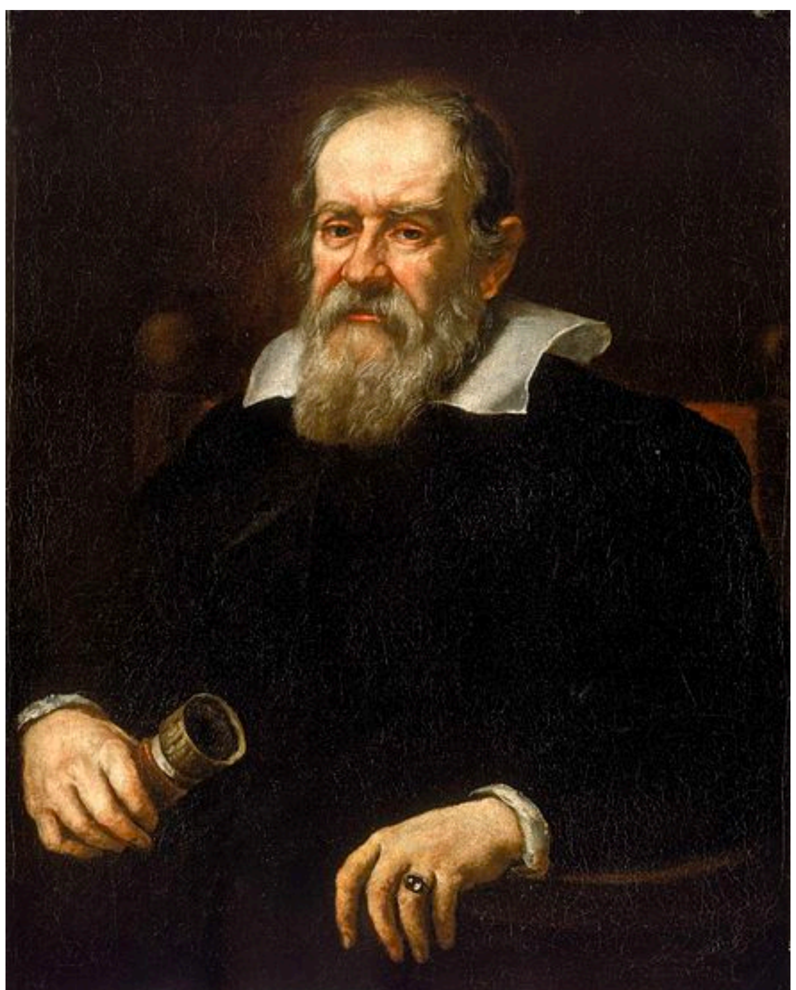
  - UV-optical: $R = 10^5$

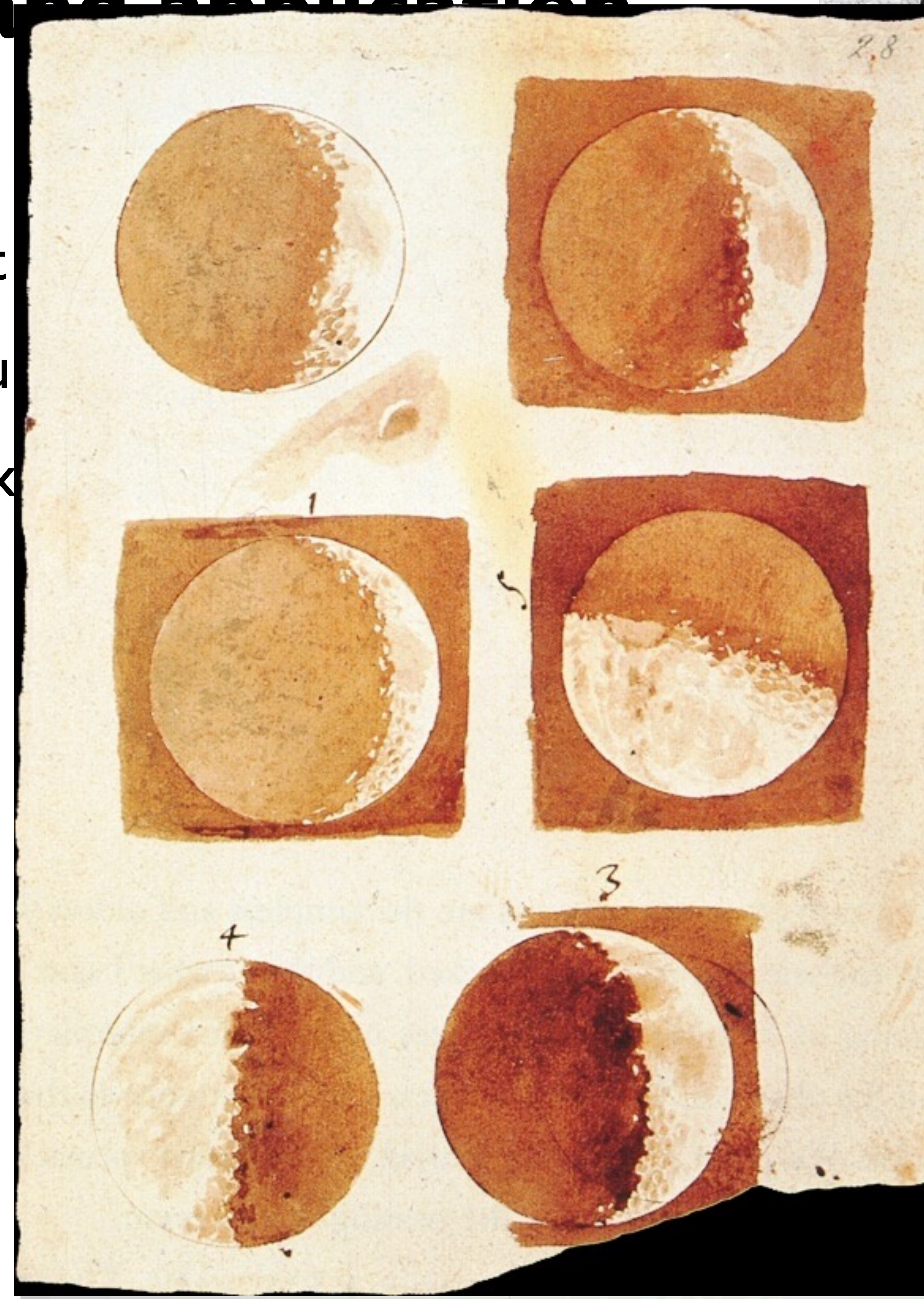
  - IR: $R \sim 10^3$–10^4

  - Radio: $R = 10^6$
- Sensitivity (QE) and noise
- Stability, response
- Pixel size, exposure, etc.

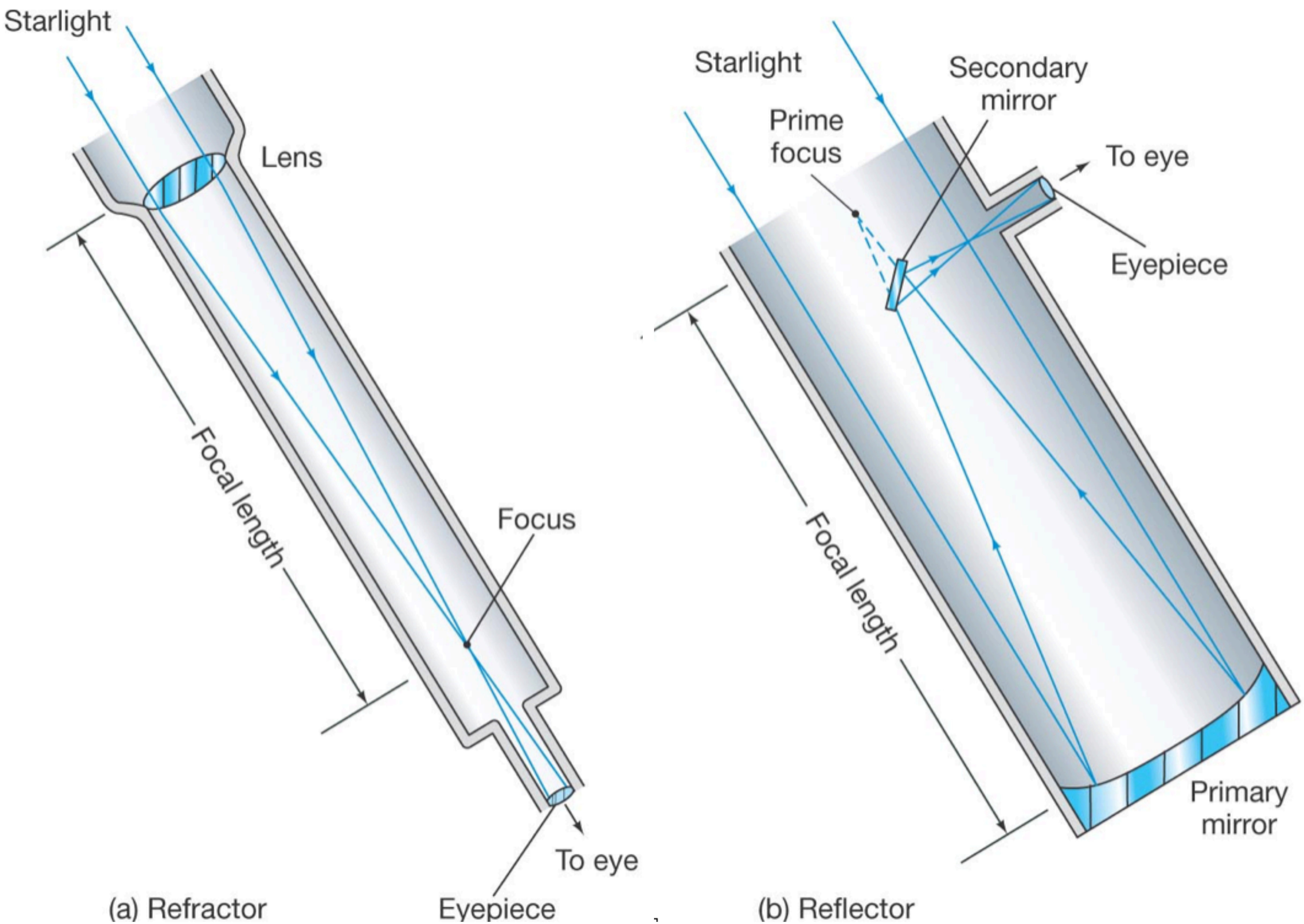
First telescope and application

- Patent by a Dutch eyeglass
- Galileo Galilei (1609): first
- Moon craters, rings of Satu
- Kepler (1611): two convex

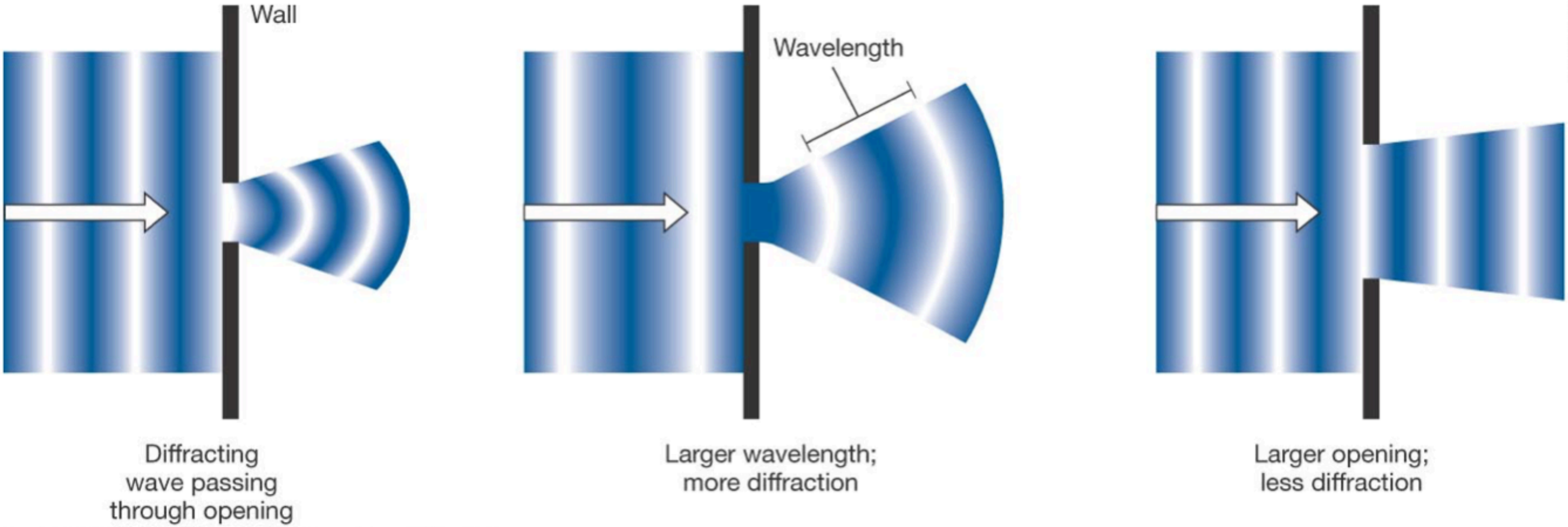




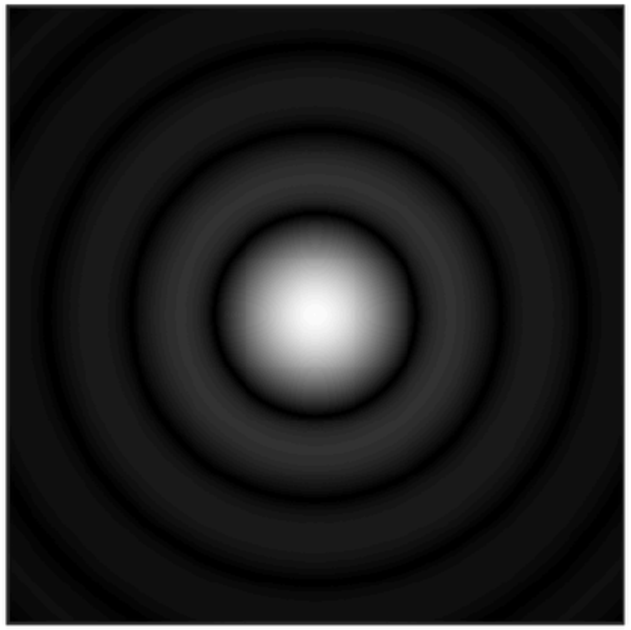
Refractors and reflectors



Diffraction limit



- Accurate observations by Francesco Grimaldi (1660)
- Bending of EM waves through boundaries of aperture
- Airy disk: smallest resolution element
- Atmospheric conditions ("seeing")

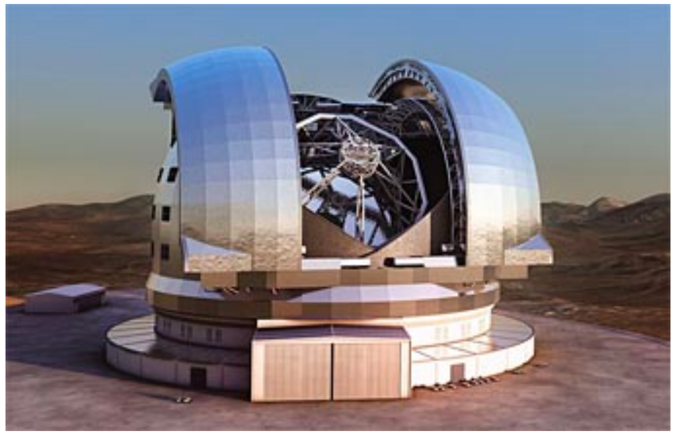


Properties of telescopes

- First and foremost: collecting area $S = \pi * D^2/4$:
  - 10 m dish: 79 m^2
  - 30 m dish: 707 m^2
  - 100 m dish: 7854 m^2

- Angular resolution $\theta'' \sim 2.1 \times 10^5\ \lambda/D$:
  - 100 nm (1000 Å): $\theta \sim 0.02''$ for D = 1m
  - 1mm (230 GHz): $\theta \sim 210''$ for D = 1m
  - 1mm (230 GHz): $\theta \sim 2.10''$ for D = 100 m

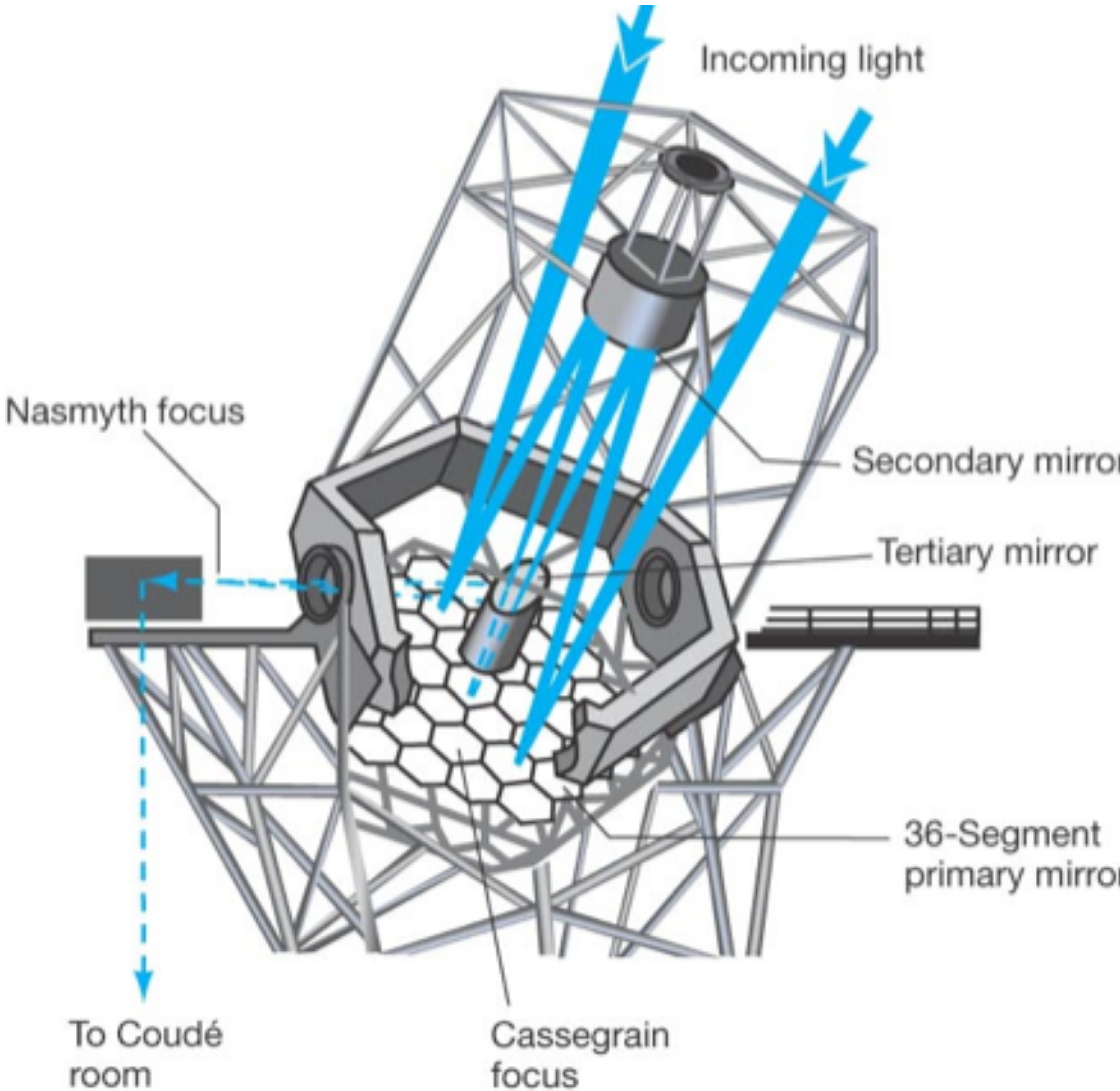
Properties of telescopes



- Reflectors with parabolic-like mirrors
- Various designs to redirect light to detectors
- UV-near-IR:
  - Mirrors made of low thermal expansion glass (Zerodur)
  - Metal coating (Al, Ag, Au, Cu)

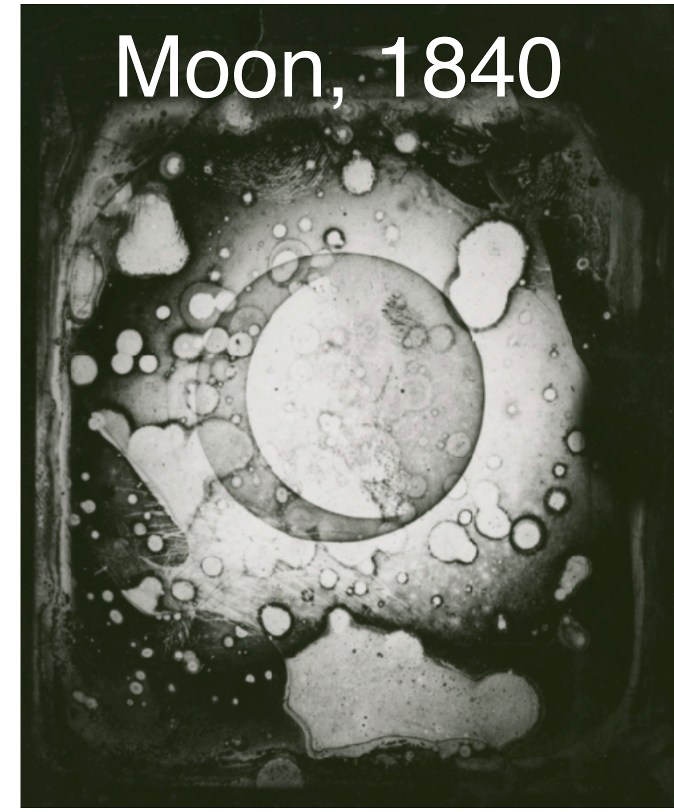
- IR: optical telescopes with special mirrors (Be, SiC)
- (Sub)-millimeter antennas:
  - Parabolic metallic antenna (Heinrich Herz, 1887)
  - Small feed antenna at the focus

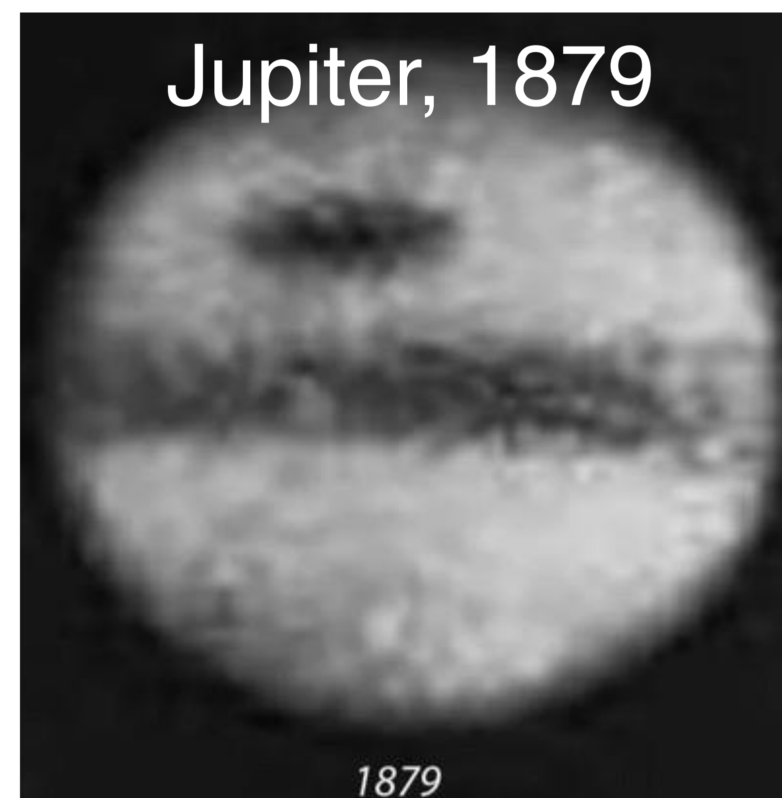
Example: Keck 10m telescope



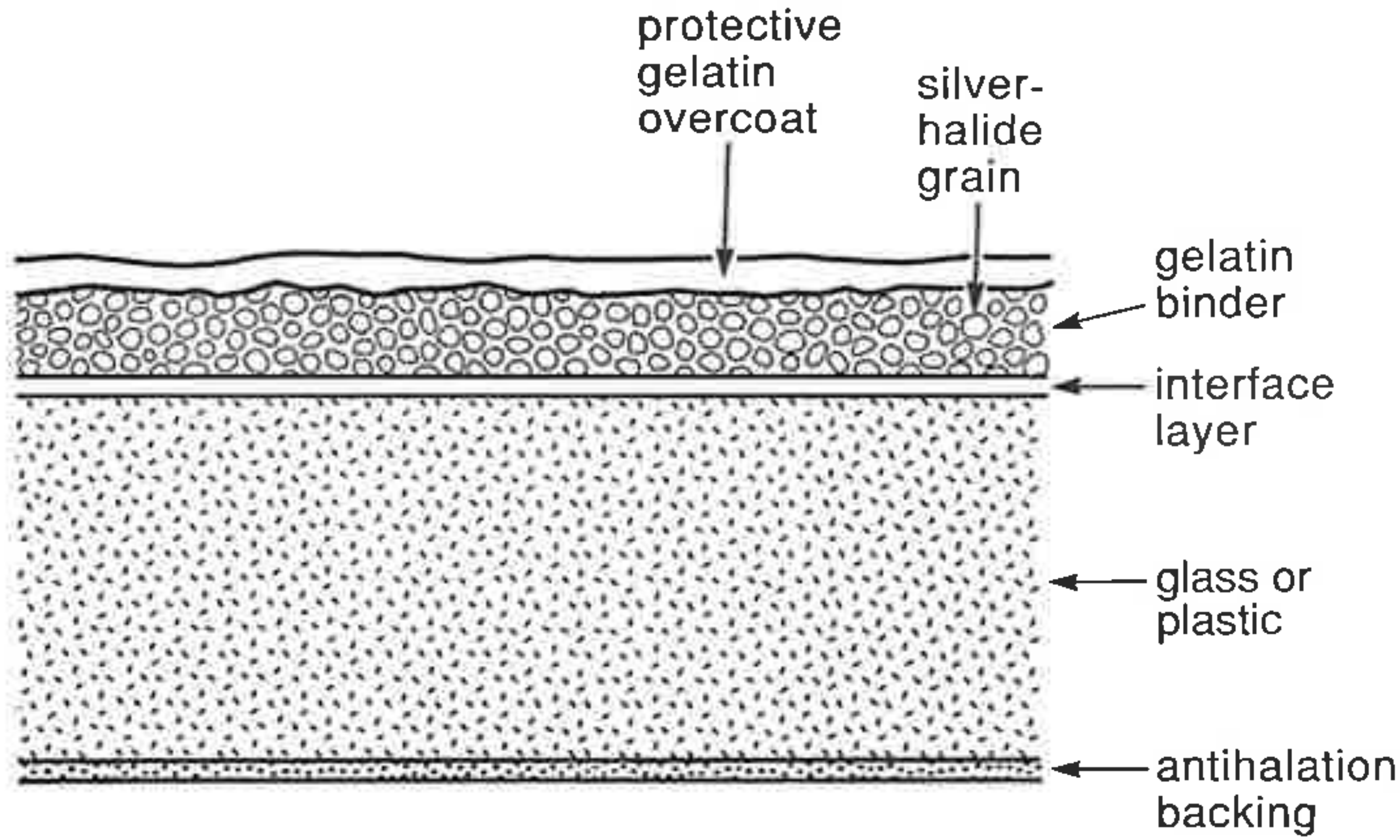
Photographic plates

- First 2D detectors
- 1840: J.W. Draper, photo of the Moon
- 1858: W. De La Rue, sunspots
- Early 1900s: E. Hubble, galaxies, expansion of the Universe
- Dominated astronomy for ~ 100 years





Photographic plates



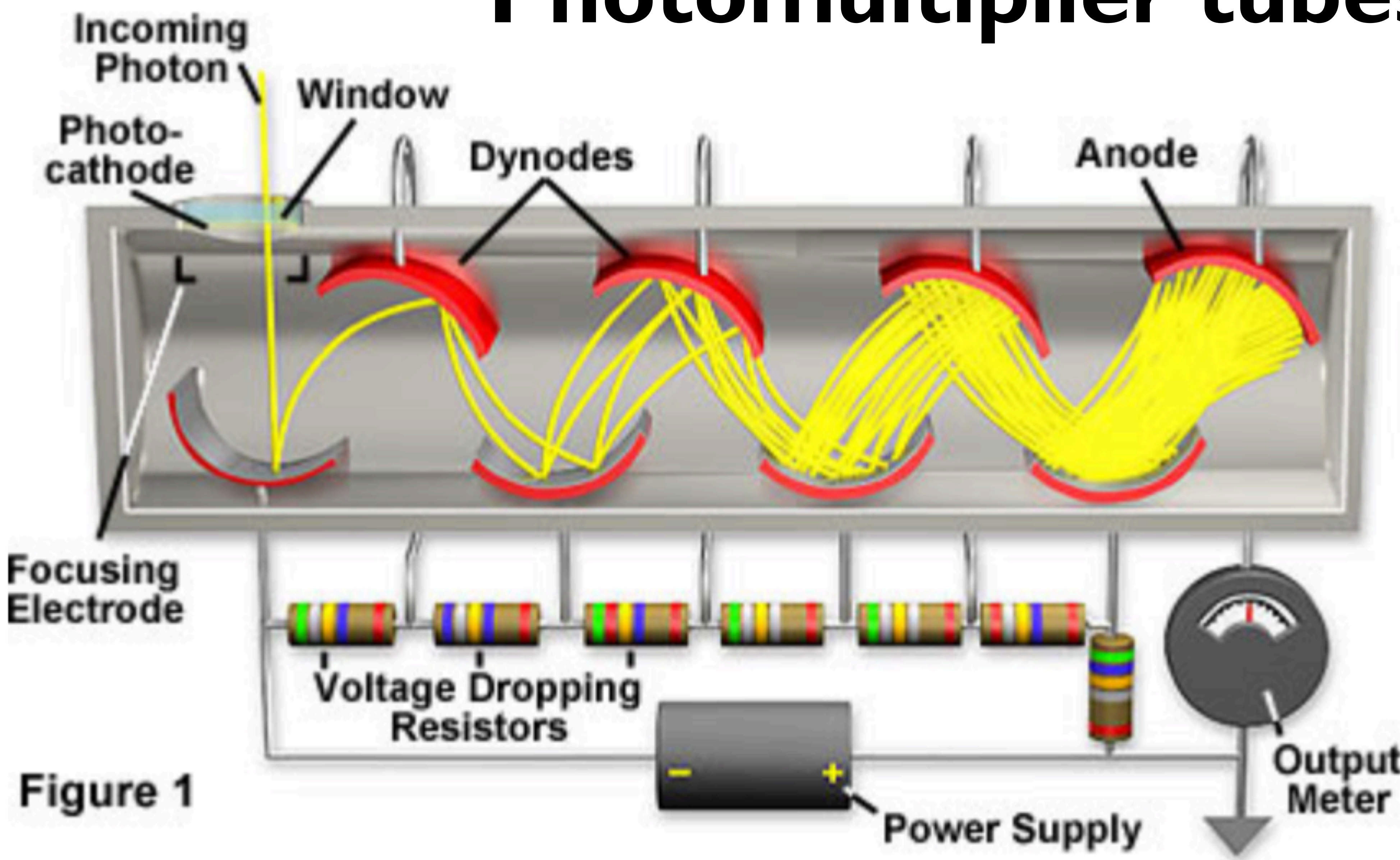
- Emulsion: gelatine + silver-halide grains
- Exposition: Ag+ => Ag, Ag- => Ag_2 =>…)
- Alkaline solution: Silver halide grains => Silver metal
- Acidic stop bath

Photographic plates

- Very low QE (1-4%), non-linear response
- Very small "pixels" (grains of silver compounds)
- Hard to digitize
- Unique photo plate libraries (variability, stellar motions):

  e.g. Harvard College Obs (>130 years, >500,000 plates)

Photomultiplier tubes

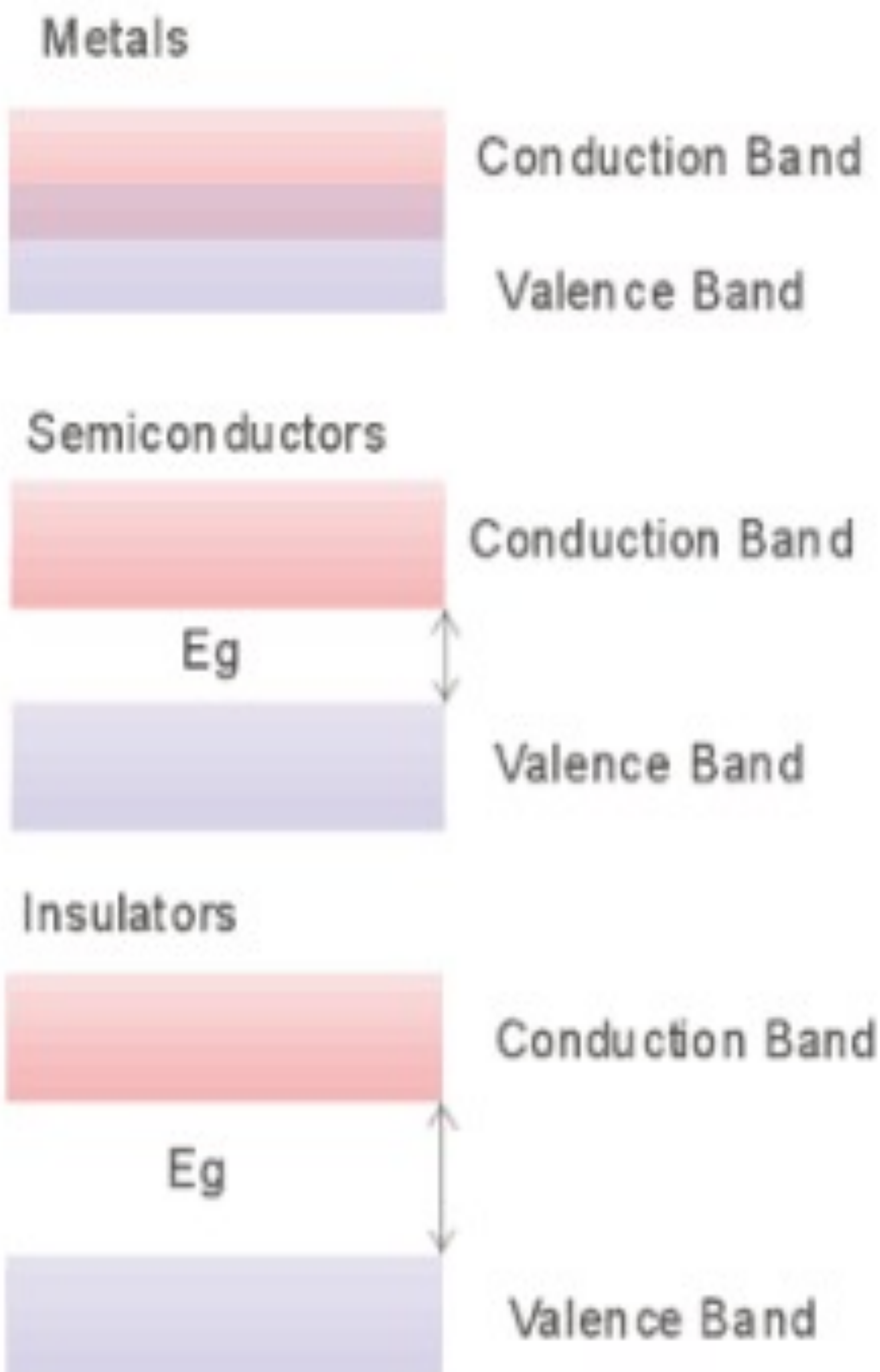


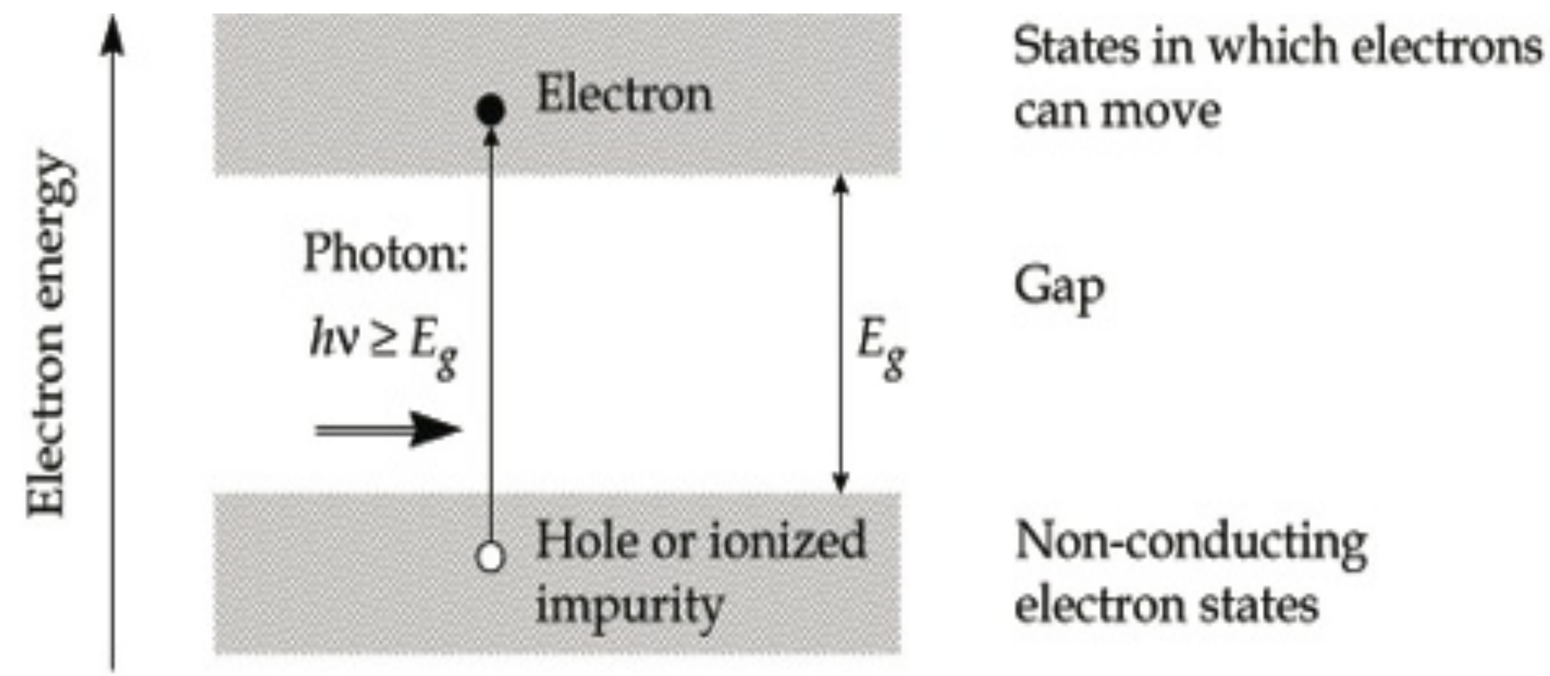
- Photon counting devices (>1934)
- Each photon produces e- cascade (from 1 to 10^8 e-)
- Efficient at UV, 300–1200 nm
- Moderate QE (10-20%), linear response
- Easily coupled to digital outputs

Photomultiplier tubes

- Must be operated at high voltages (>2000 V)
- High light levels can destroy the tube
- Not very efficient in optical region
- Single channel devices
- Used to measure sky objects' fluxes

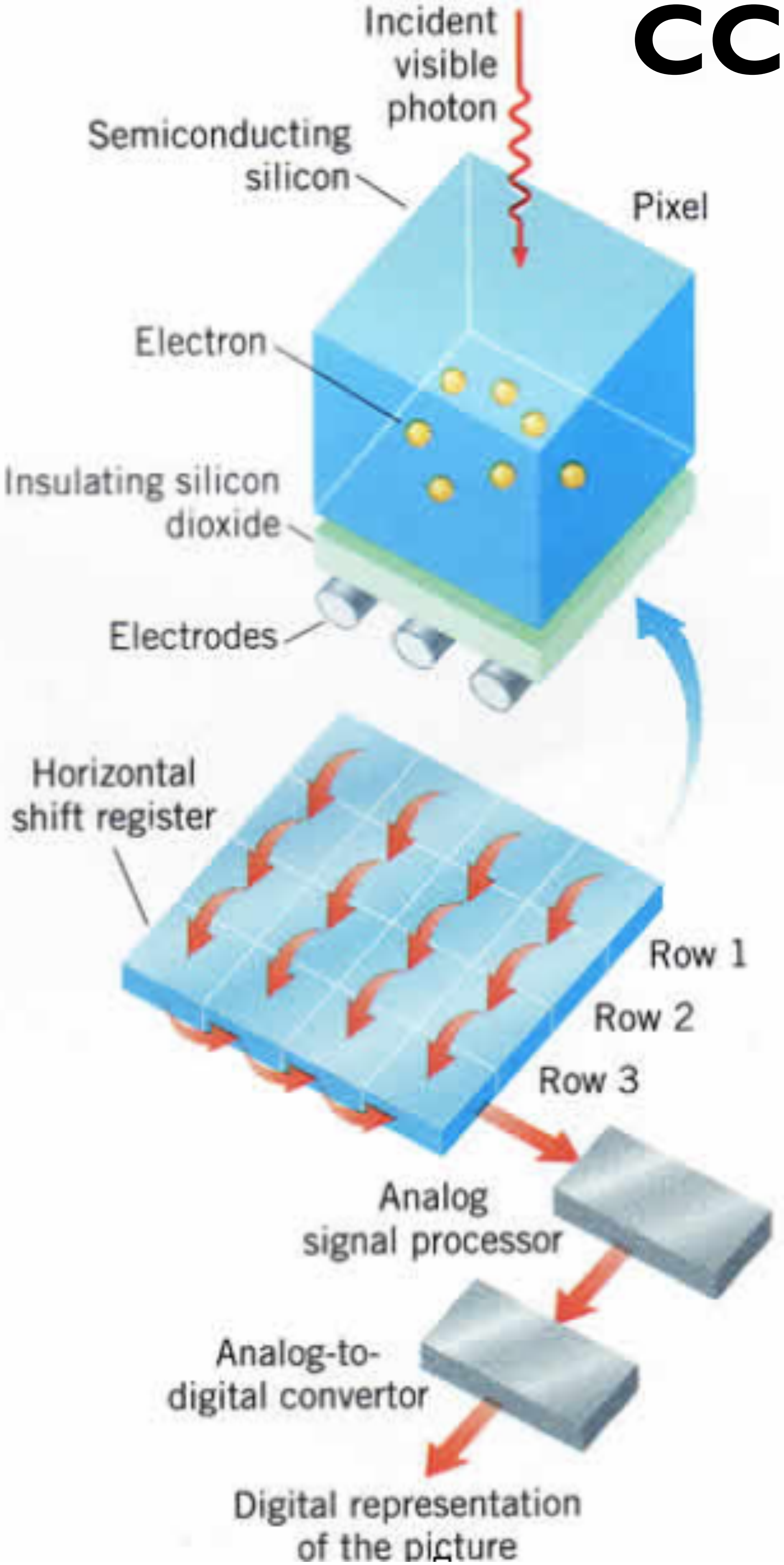
Semiconductors





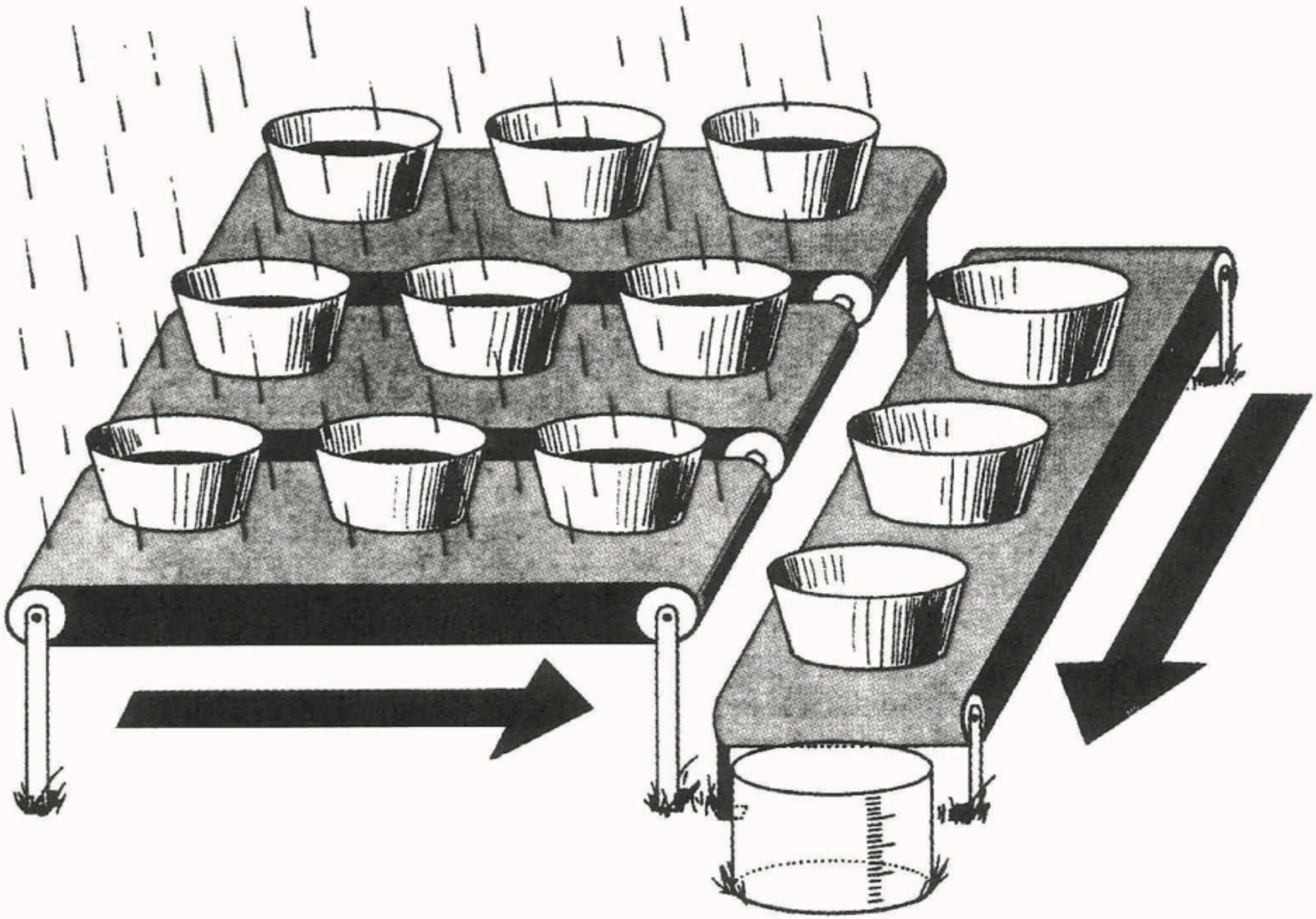
- Transition from bound to unbound e-
- Band gaps: ~0.2 - a few eV
- Made of Si, InSb, $Hg_xCd_{1-x}Te$, GaAr,..
- Easily coupled to digital outputs

CCD (Charge-Coupled Device)

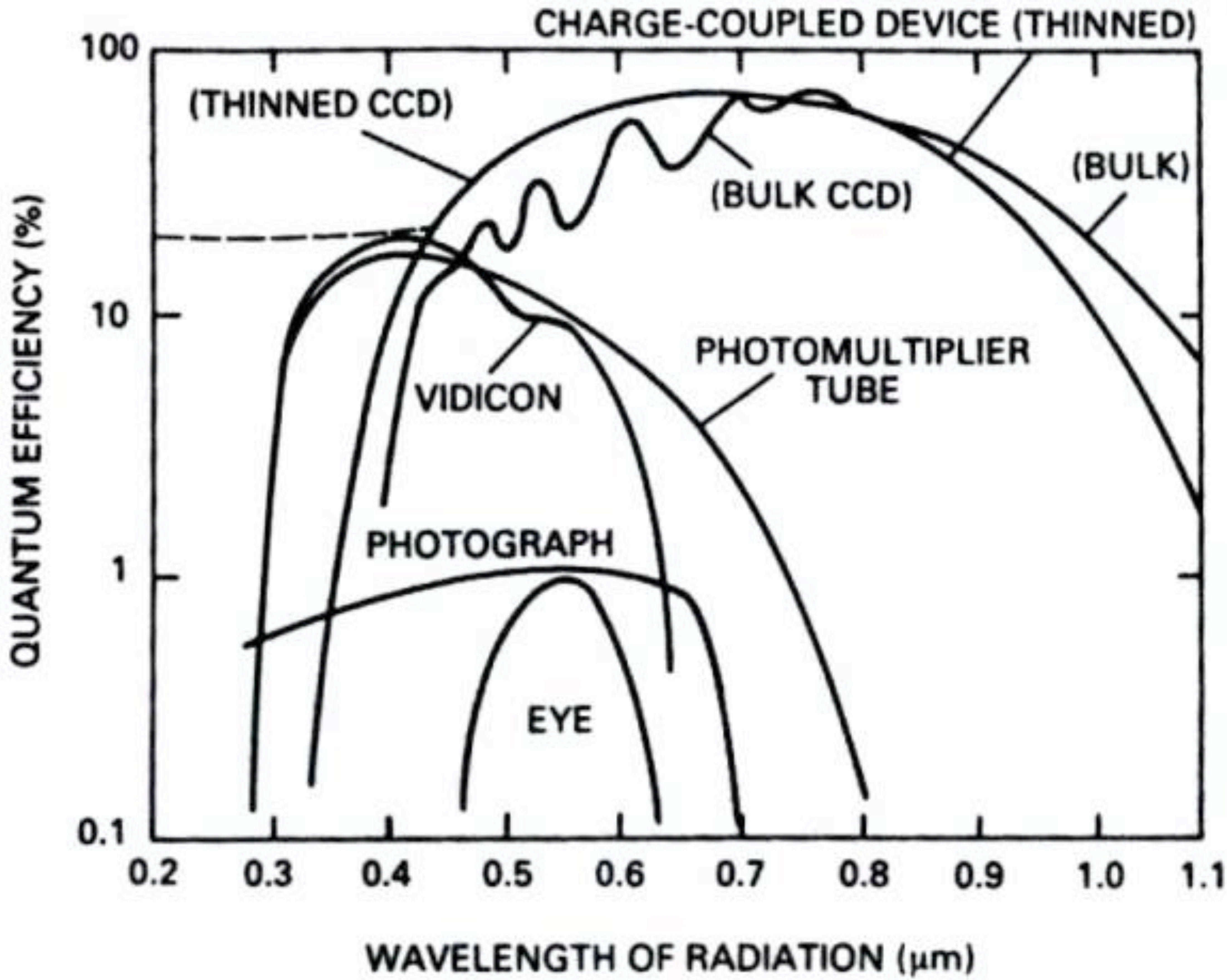


- Invented 1969 in AT&T Bell Labs by Boyle & Smith (Nobel prize 2009)
- 2D pixel arrays
- Photoactive + transmission layer
- Read out charges in a staged fashion
- Truly digital
- Very high QE up to >95%

Light Bucket Analogy



Quantum Efficiency of detectors



UV-optical detections

• Selection rules are not as restrictive (e.g. H_2 and N_2 do not usually emit at IR and radio)

• Strength:

- CCD => high quality spectra

• Weakness:

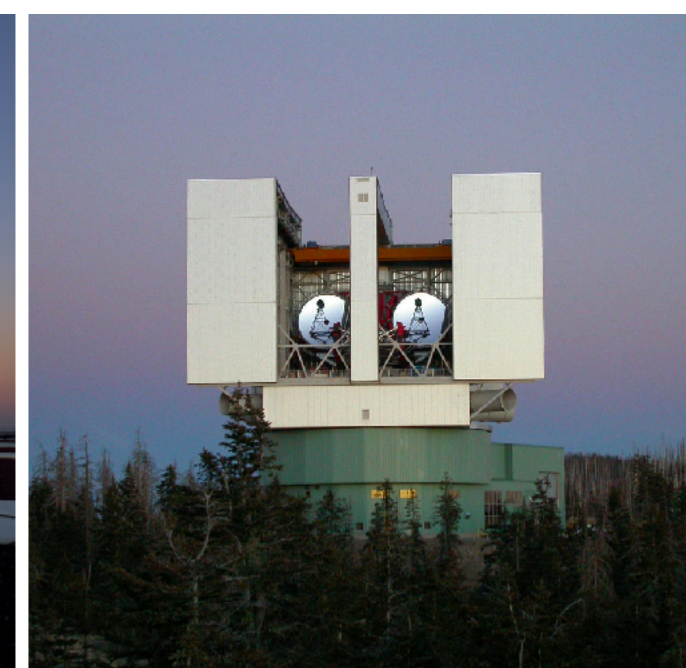
- Some molecules do not have intense electronic transitions
- Dissociative excited states lead to broad features
- FUV is only accessible from space

UV-optical telescopes

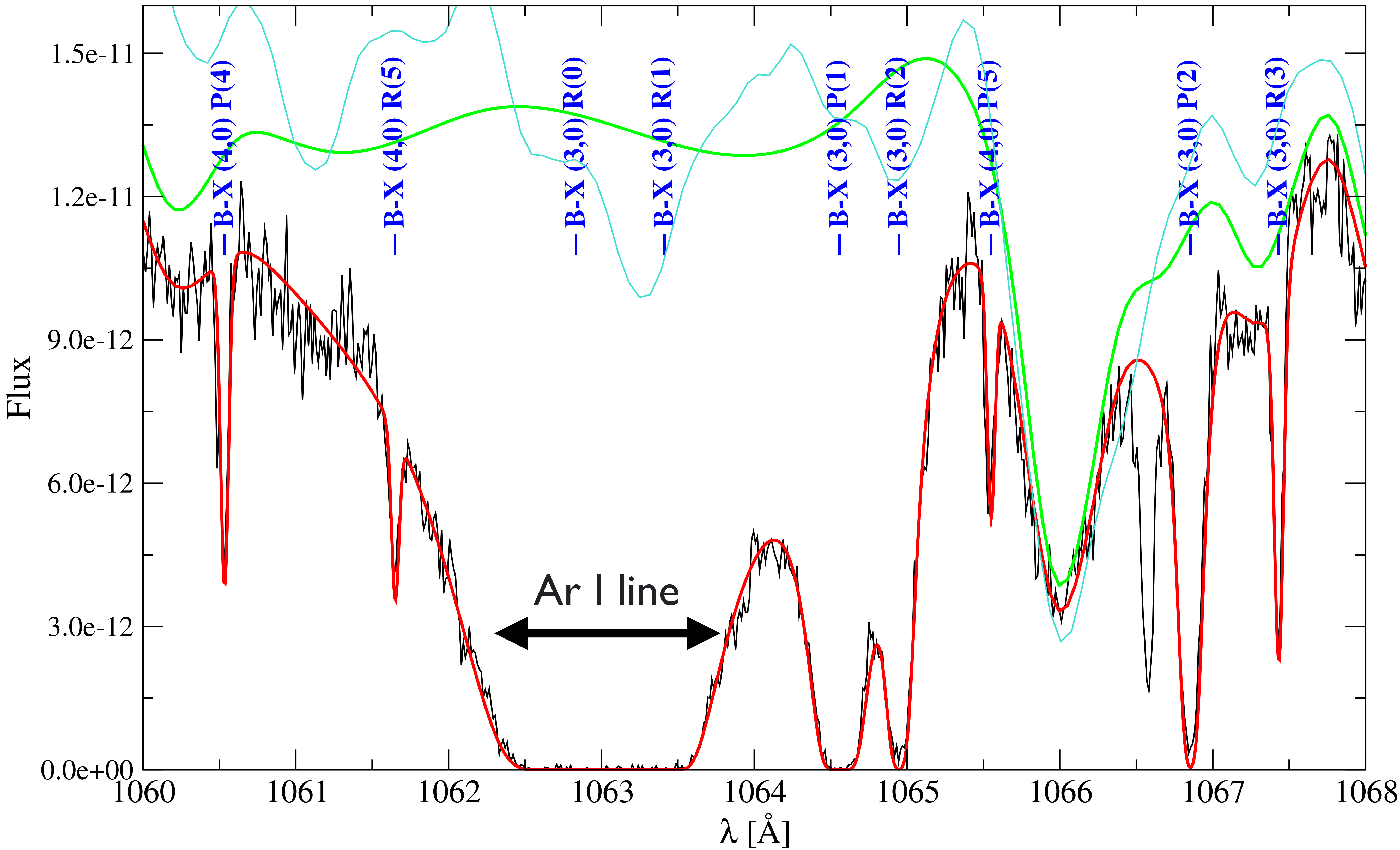
- **Ground-based**: Very Large Telescope (8.2 m), Keck (10 m), Gemini (8.2 m), Large Binocular Telescope (10 m), Subaru (8 m), Palomar (5 m),...
- **Space**: Hubble (2.4 m), Copernicus (0.5 m), FUSE (0.7 m),...

- Resolution: <0.1"





H_2 absorption lines in diffuse ISM



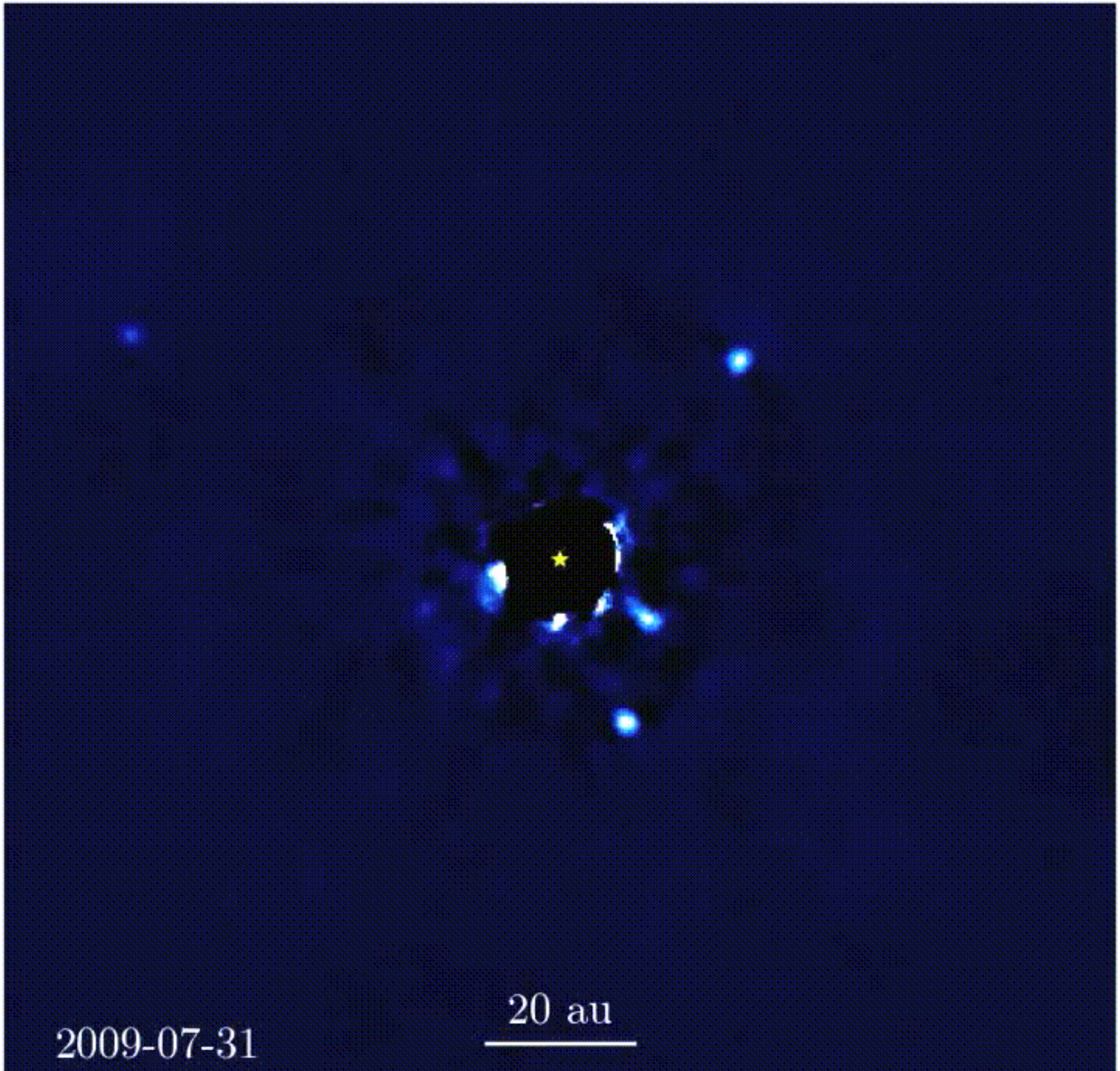
Hubble: H_2 in translucent cloud HD 147888

Gnacinski (2013), A&A

Pillars of Creation

HST (1995): gas and dust in Eagle nebula (Serpens)

Exoplanets around HR 8799 (Keck 10m)



Infrared detections

- Polyatomic molecules and ices
- Intense vibrational transitions: H_2CO, OH, benzene, C_3, C_5

- Strength:
  - Numerous (ro-)vibrational lines => identification
  - High sensitivity

- Weakness:
  - Atmosphere is largely opaque
  - Limited space missions
  - A less precise identification than via radio (resolution)

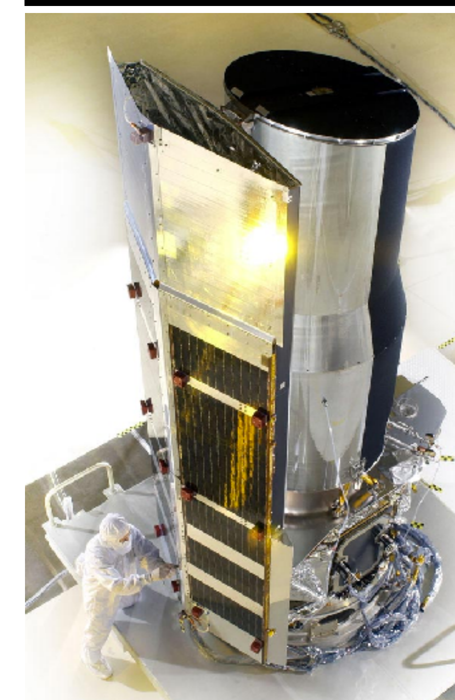
IR telescopes

- **IRAS** (1983): 0.6 m, 12–100 µm => first sky survey, warm dust (β Pictoris disk)

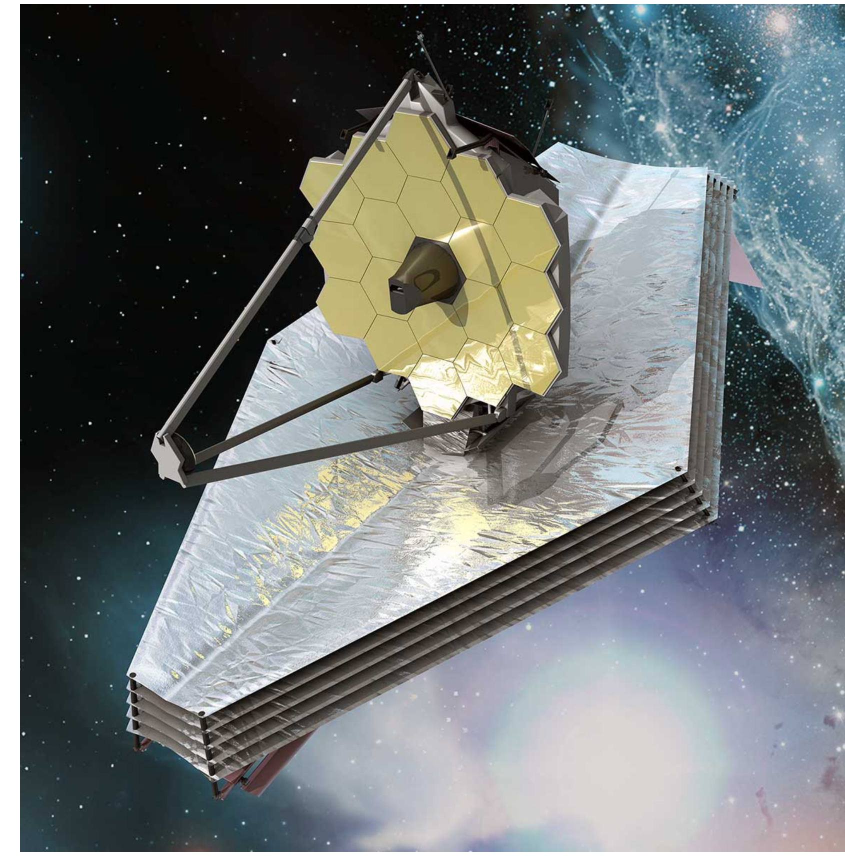
- **Infrared Space Observatory** (1995–1998): 0.6 m, 2.5–240 µm => H_2O, HF, star formation

- **Spitzer Space Telescope** (2003–2009): 0.85 m, 3–180 µm = > high-sensitivity imaging, molecules and ices, exoplanets, first stars, galaxies

- **Herschel Space Observatory** (2009–2012): 2.4 m, 60–670 µm = > high-sensitivity imaging, molecules (HD, O_2) and ices, star formation, starburst galaxies

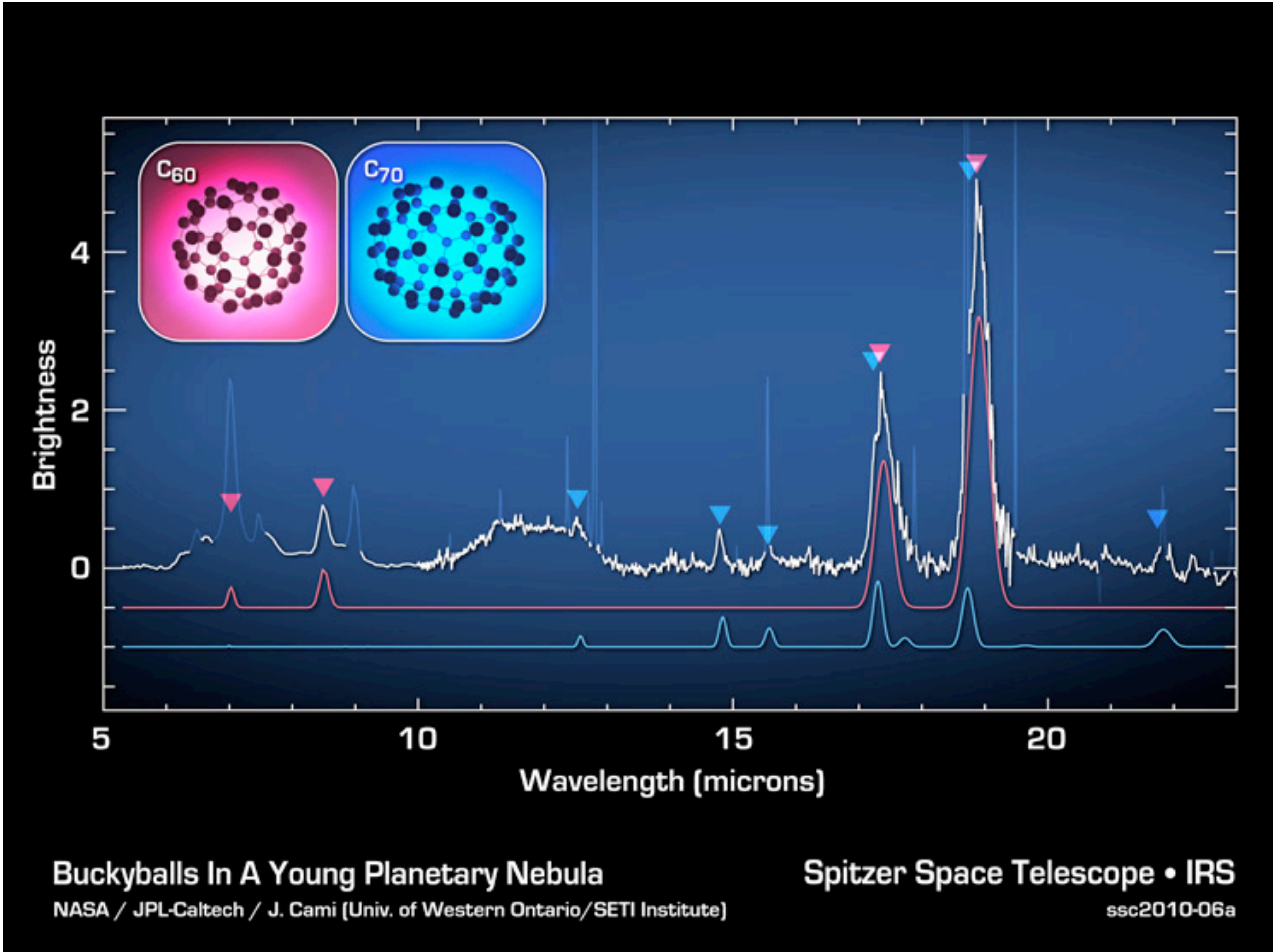


James Webb Space Telescope

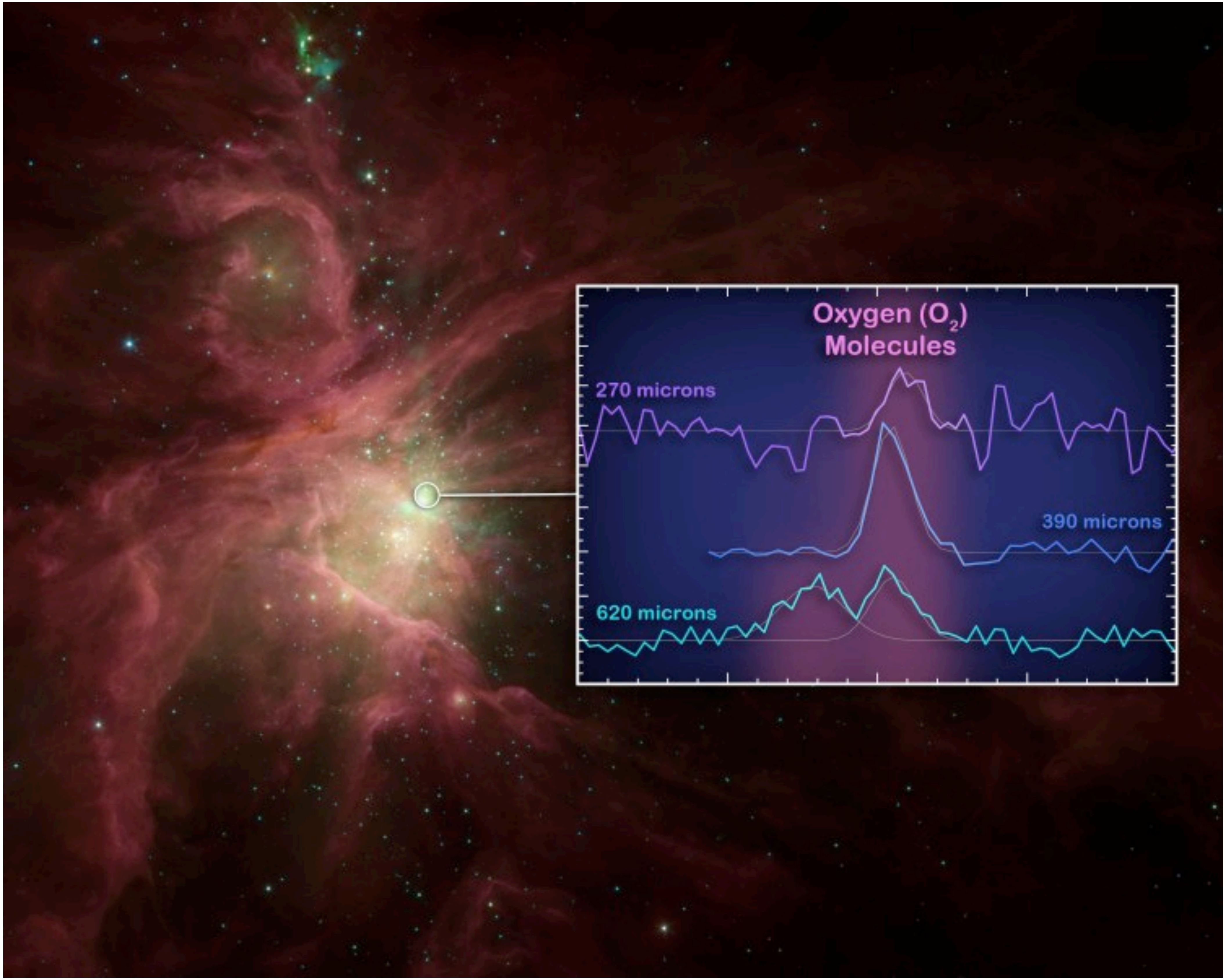


- JWST (launched on Christmas of 2021)
- 6.5 m 18-segment mirror (Gold-plated Be)
- L2 orbit (Passive Cooling to 45 K)
- Life >10 years
- Four cryogenic science instruments:
  - Near-Infrared Camera (NIRCam): 2.2'x4.4', 0.6-5 μm
  - Near-IR Spectrometer (NIRSpec): 3.4'x3.4', 1-5 μm; R=100, 1000, 2700
  - Mid-Infrared Instrument (MIRI): 5-27 μm, imager, coronograph, medium resolution spectrograph (MRS), 3.7'x3.7' – 7.7'x7.7'
  - Fine Guidance Sensor: stabilisation of the line-of-sight

Detection of fullerenes (C_{60} & C_{70})



O_2 in Orion, 487–1121 GHz, Herschel



Goldsmith et al. (2011)

Pillars of Creation

Gas and dust in Eagle nebula (Serpens)

Radio observations

- Unambiguous detection of molecular species

- Line strengths scale with square of the dipole moment

- Strength:
  - Observation of several lines at expected frequencies
  - High sensitivity

- Weakness:
  - Bias towards polar molecules
  - Symmetric species cannot be observed

History of radio telescopes

• 1929: Karl Jansky (Bell Telephone Labs): Milky

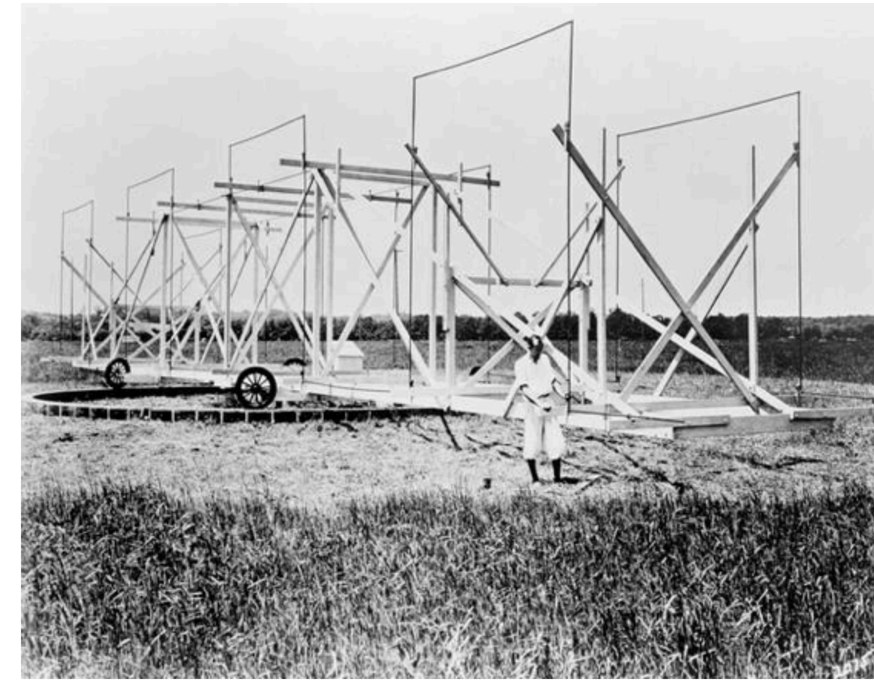
Way radio emission (20.5 MHz)

•1930s: Grote Reber, first radio astronomer,

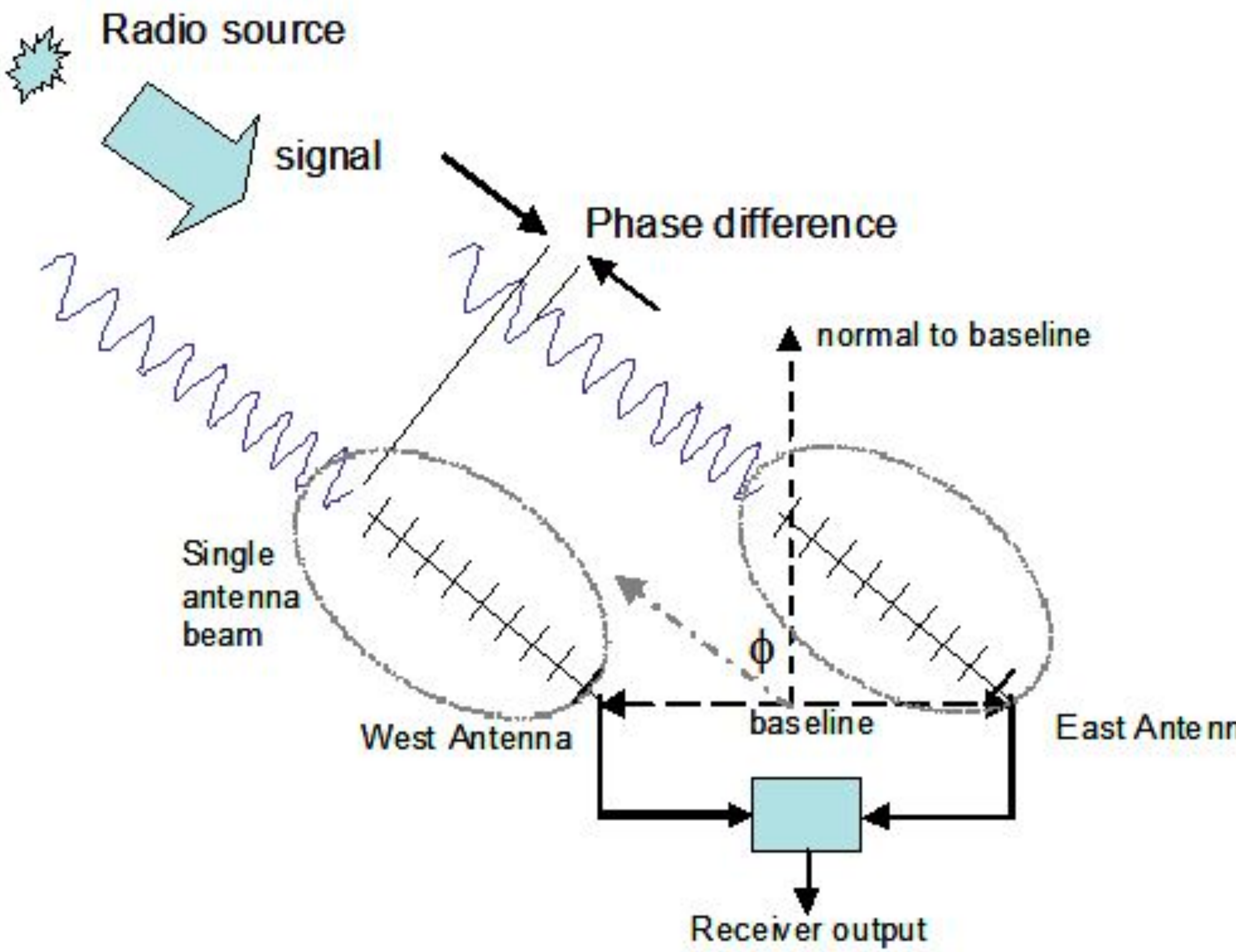
first parabolic antenna: Cyg A, Cas A

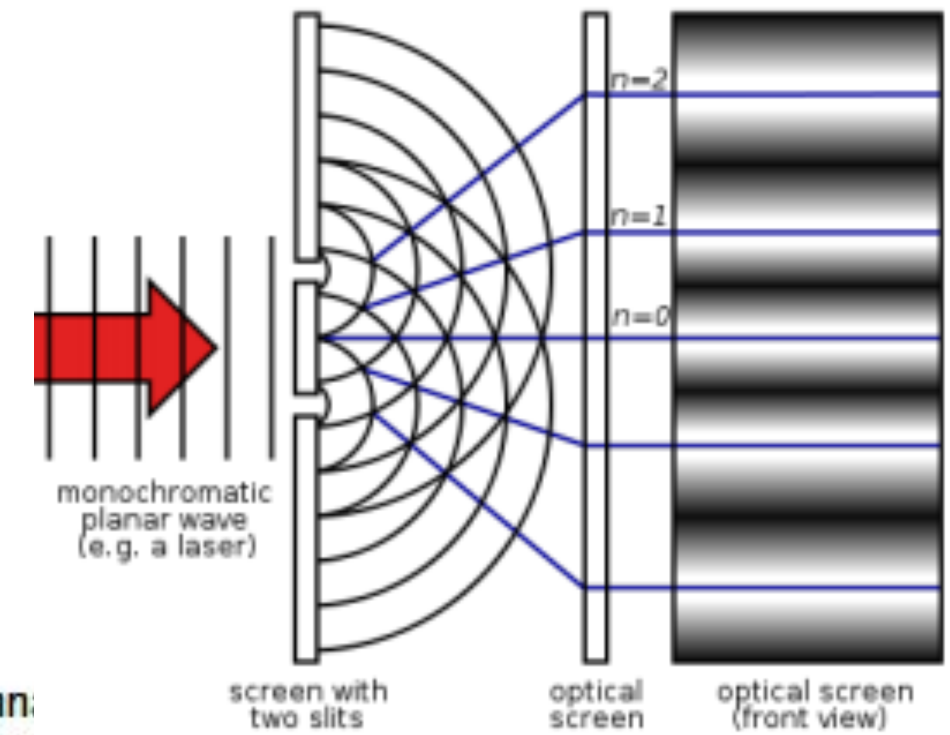
• 1940s: WWII, radar: 21 cm H line (Jan Oort)

• 1960s: Single-dish & Interferometers



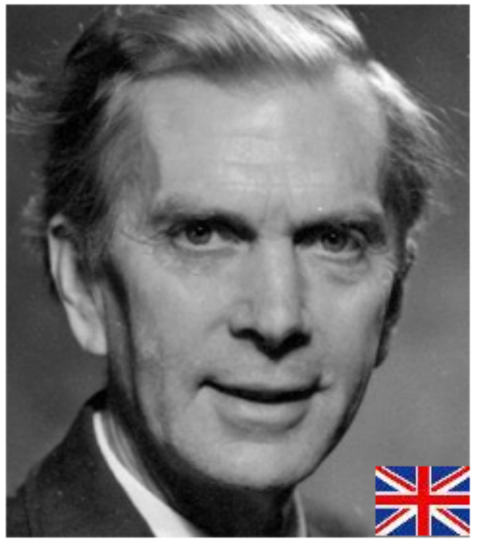
Radio interferometry





- Antenna pairs (one baseline): interference
- Combination of signals from N antennas: N(N-1)/2 baselines
- Angular resolution is determined by largest baselines!

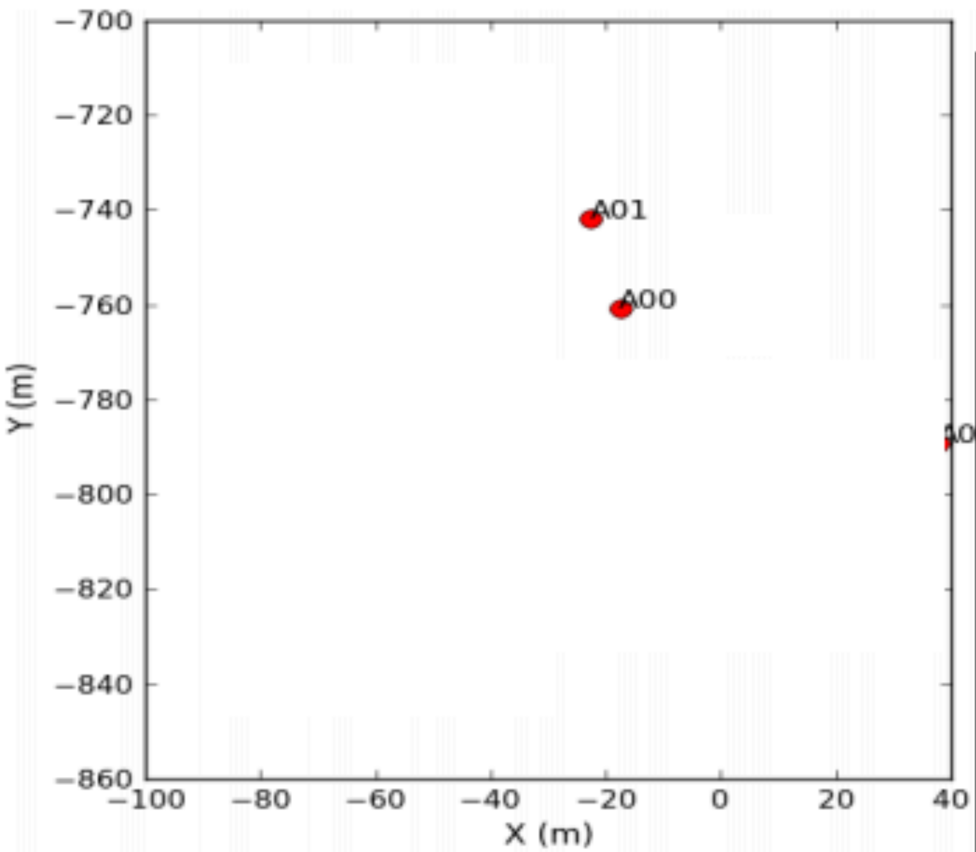
Aperture synthesis

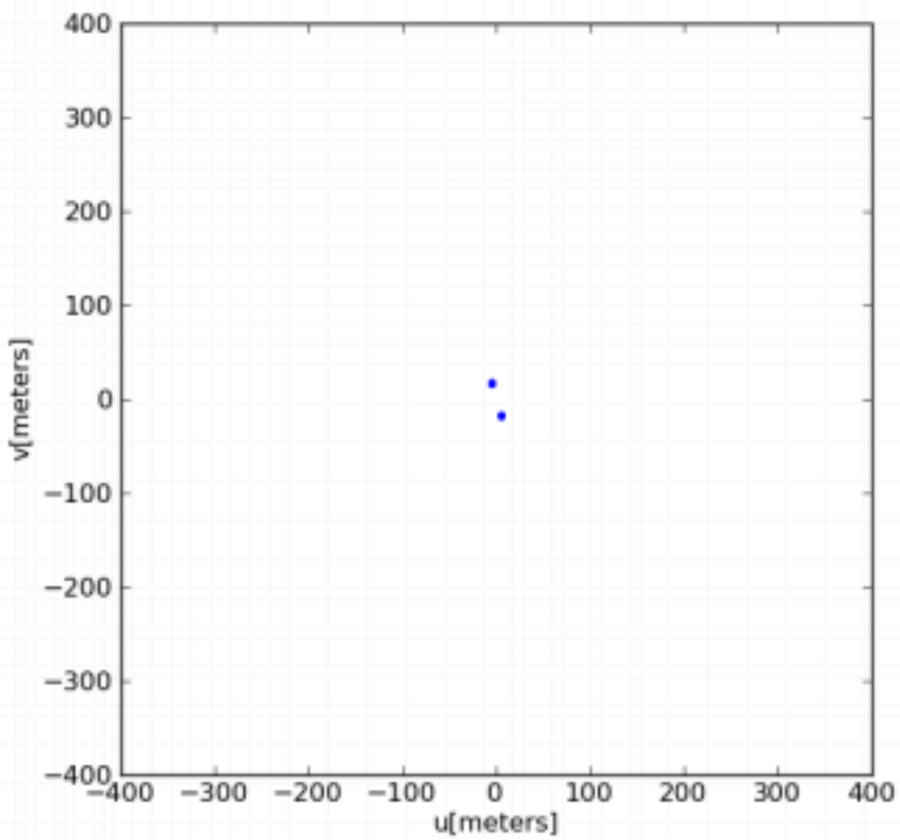


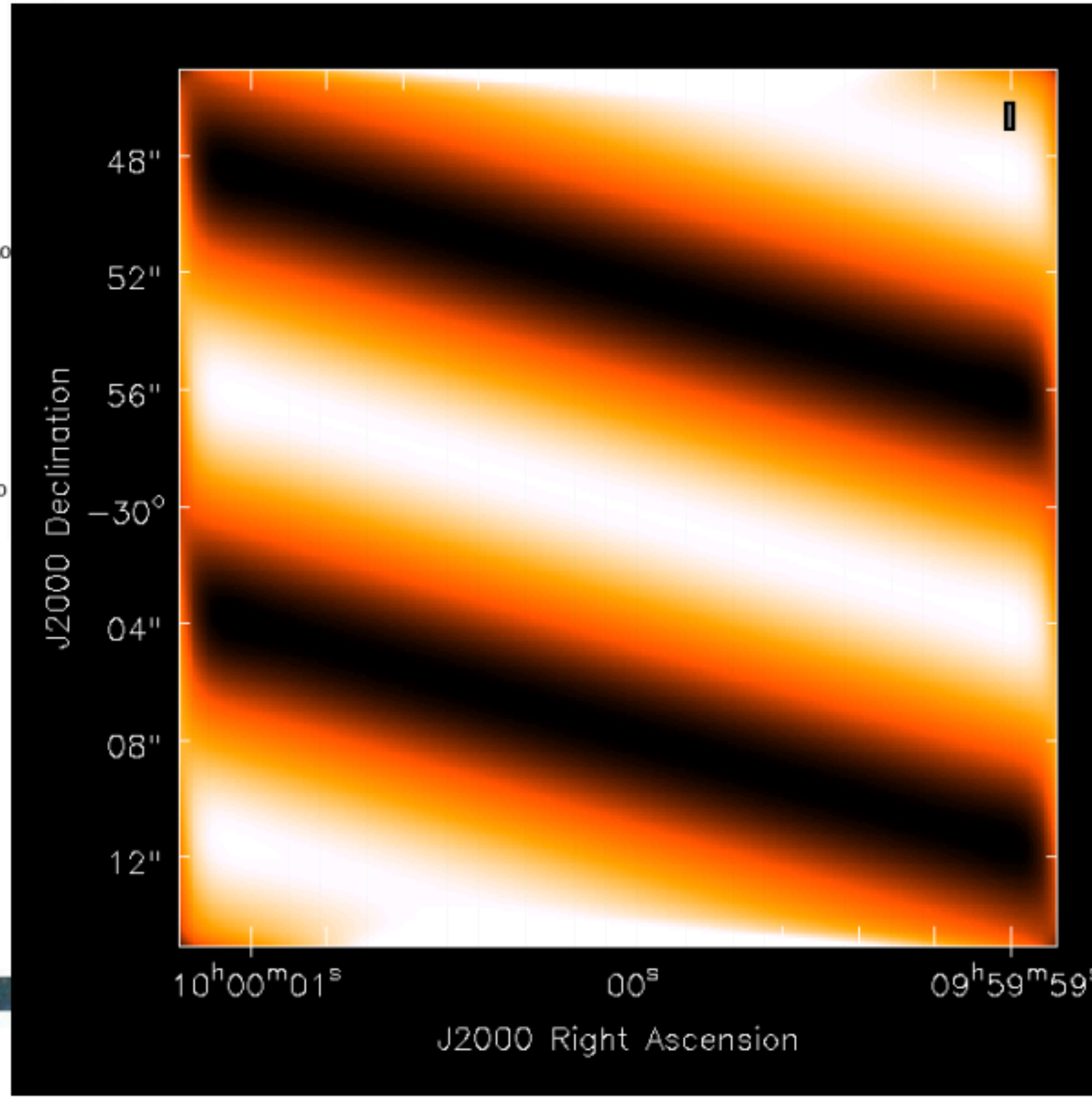
Sir Martin Ryle
1918-1984

- Sir Martin Ryle, 1974 Nobel Prize in Physics
- Sample V(u,v) at many (u,v) points using distributed aperture antennas to synthesize a large aperture antenna of size (u_{max},v_{max})
- One pair of antennas = one baseline, two V(u,v) samples
- Use Earth rotation to fill in (u,v) plane over time
- Reconfigure N antennas for more samples

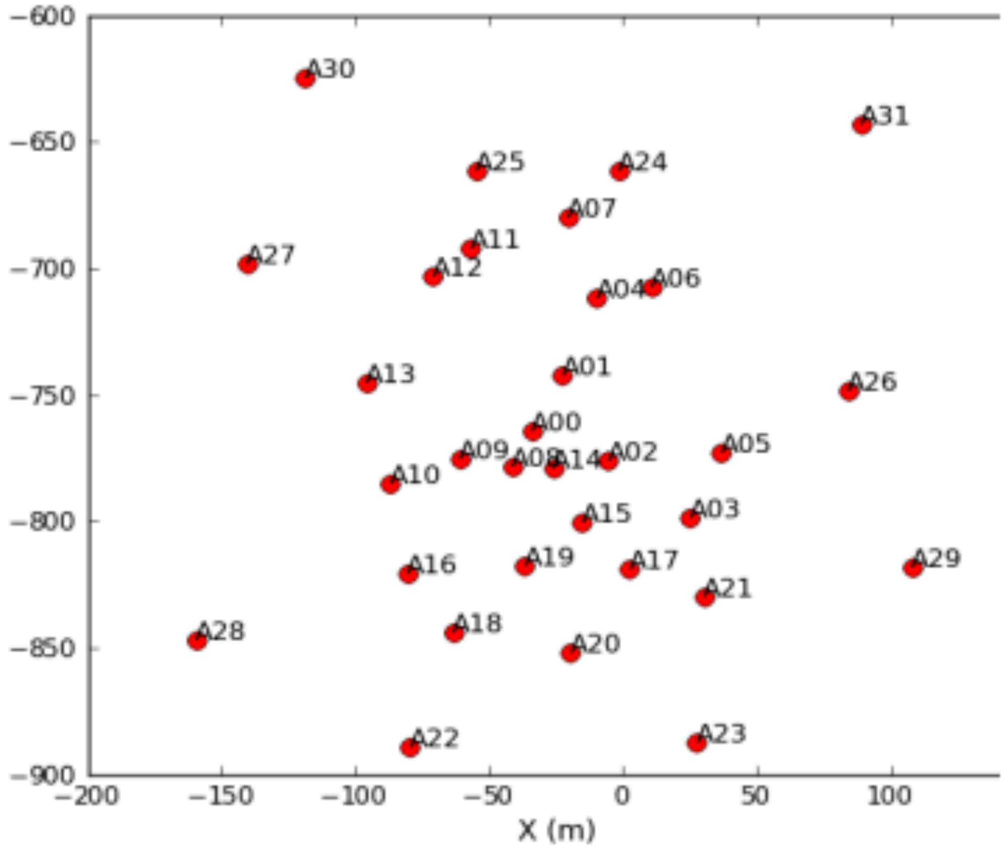
Example: Fringe pattern with 2 Antennas (1 baseline)

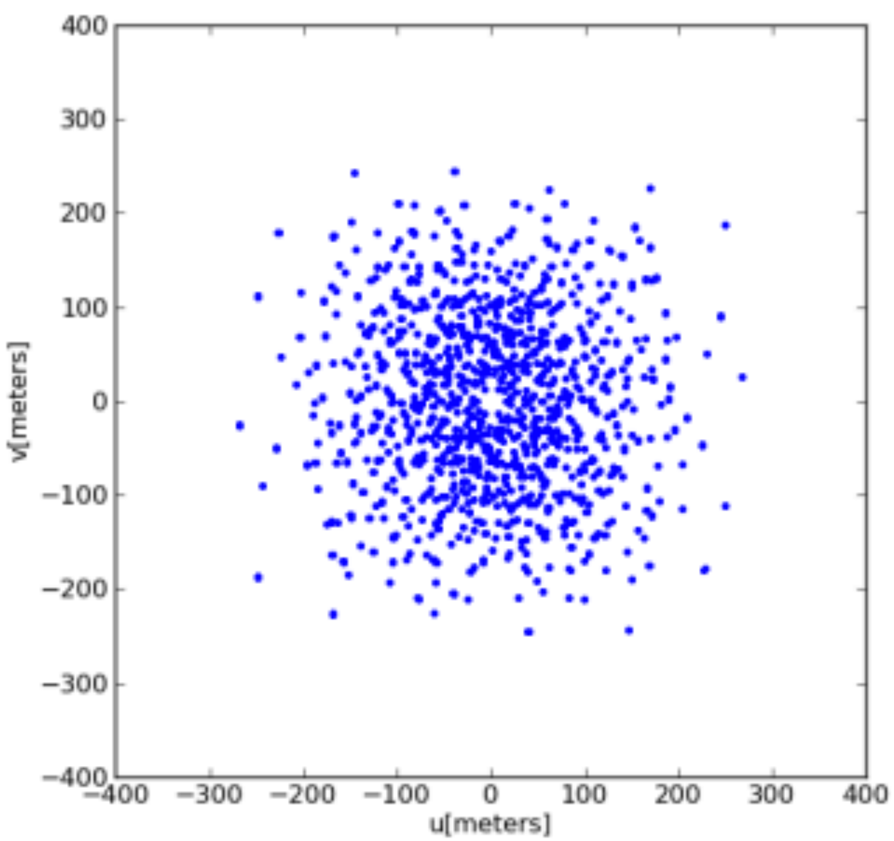


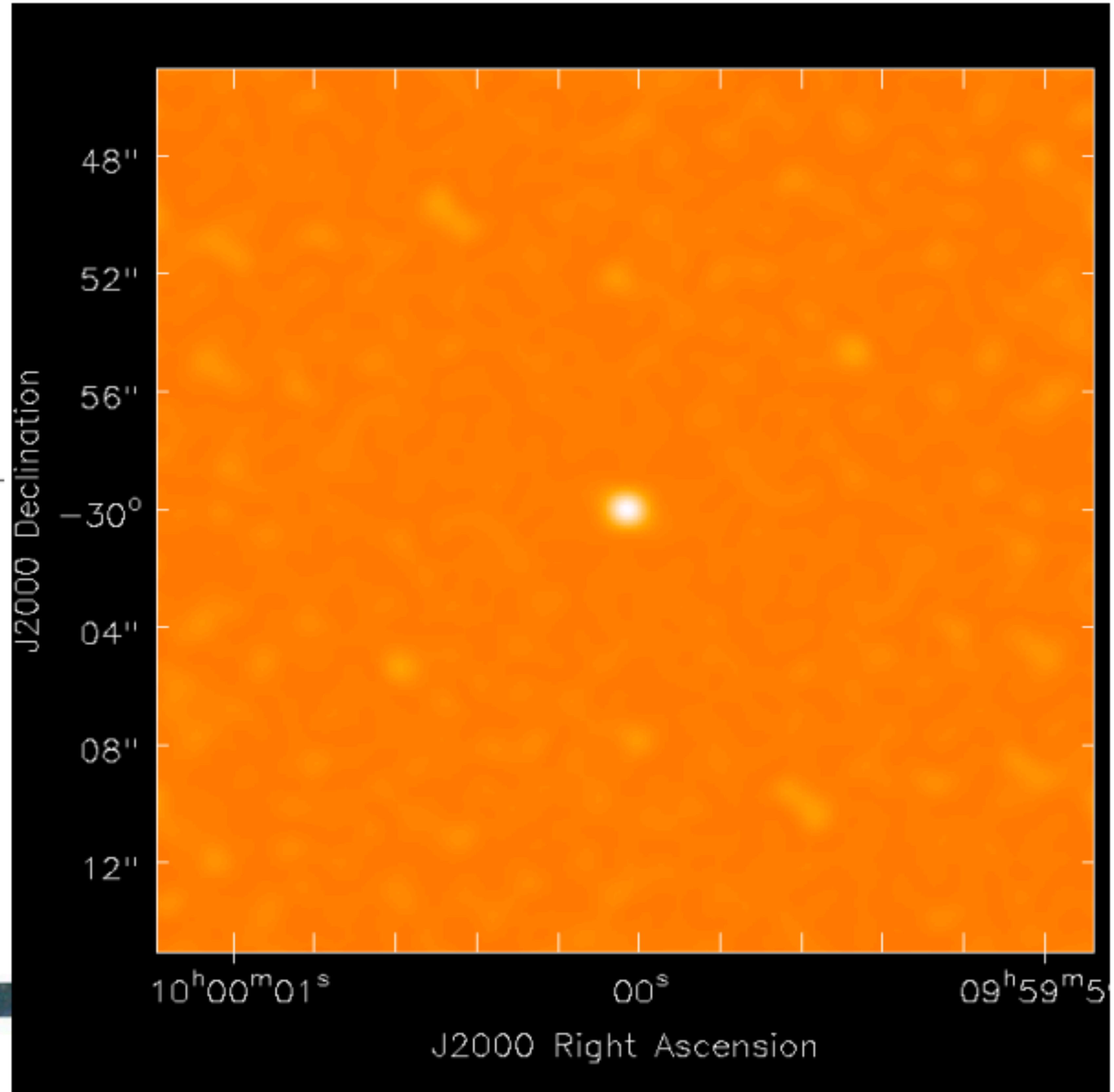




32 Antennas – Instantaneous







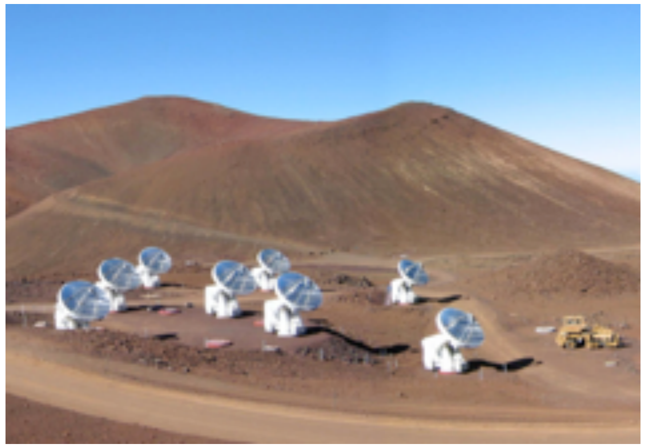
(Sub-)millimeter telescopes

- **Single-dish**: IRAM 30m, GBT 100m, APEX 12m, Effelsberg 100m, Nobeyama 45m, …

Typical beam sizes 12–30"

- **Interferometers**:

NOEMA 12 x 15m, SMA 8 x 6m, eVLA 27 x 25m, ALMA 50 x 12m + 16 x 7m



Typical beam sizes:

100 GHz: 0.1-5"

230 GHz: 0.03-1"

ALMA interferometer

- 50 12-m + 12 7-m antennas at 5,000 m (Chile)
- ~5000 m^2 area
- Frequencies: 86–950 GHz (250 μm–1 mm)
- Resolution: 0.01" @ 950 GHz

IR vs (sub-)mm telescopes

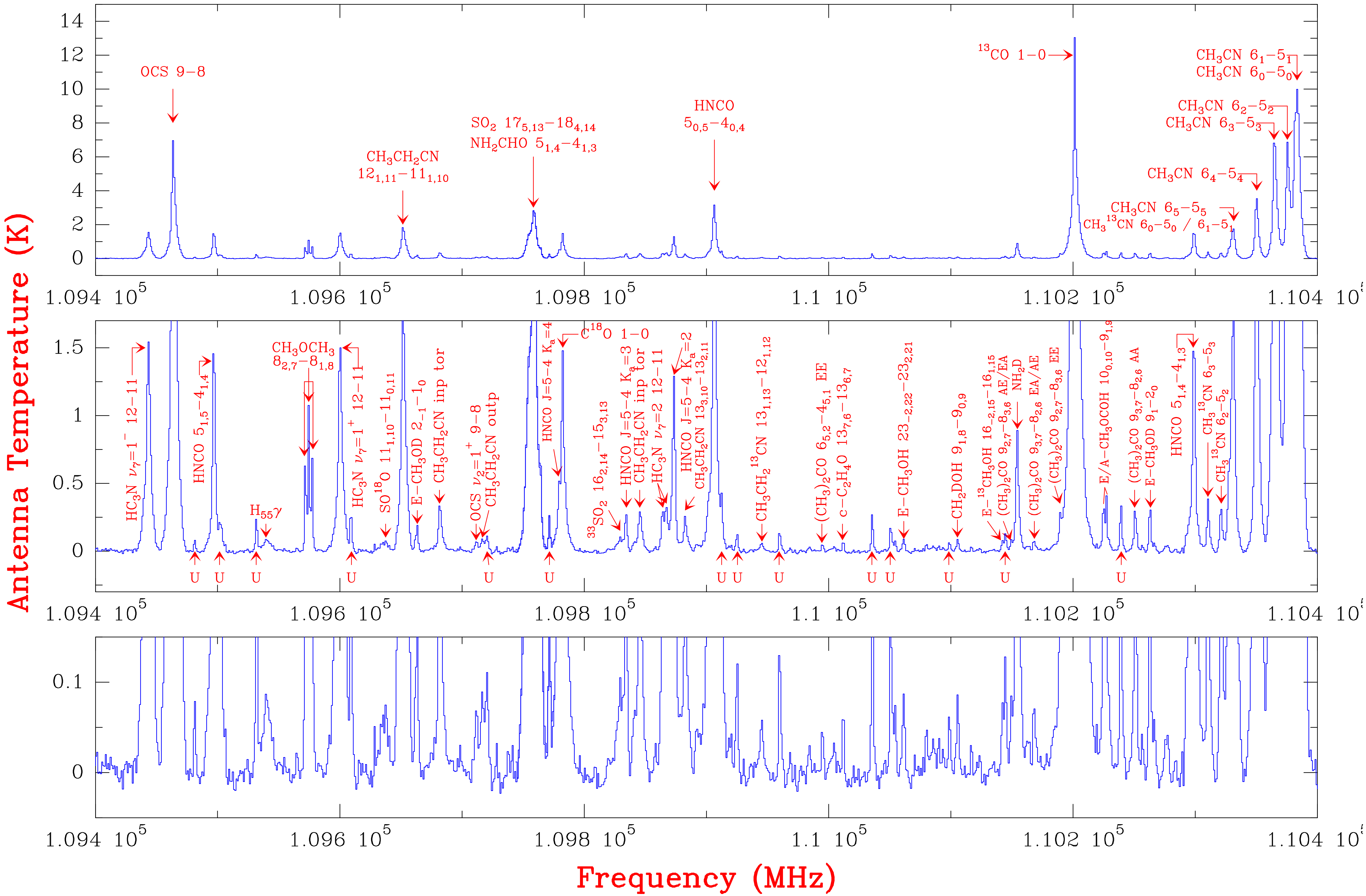
Submillimeter:

- High spectral resolution ($R>10^6$, <0.1 km/s)
- Gas-phase molecules: abundances > 10^{-11}
- Mapping of emission
- Ground-based (<1 THz), long lifetime

Infrared:

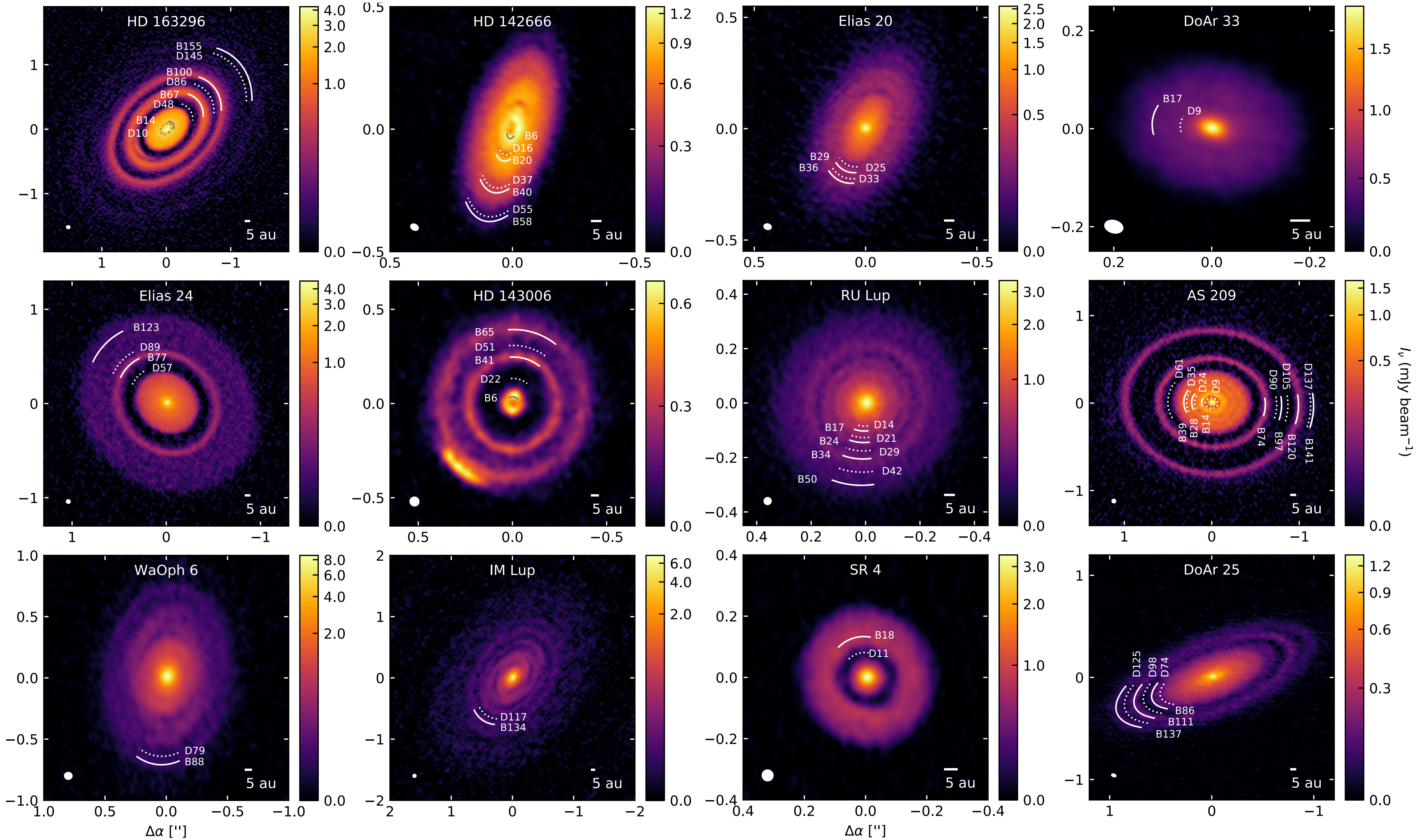
- Moderate spectral resolution ($R\sim10^3$–10^4)
- Gases and ices: abundances >10^{-8}
- Probe major reservoirs of C, N and O
- Molecules without permanent dipole moments (H_2, C_2H_2, CH_4, CO_2, ...)
- Absorption & emission
- Often in space => must be cryogenically cooled => short lifetime

Orion KL Survey, 3 mm, IRAM 30-m



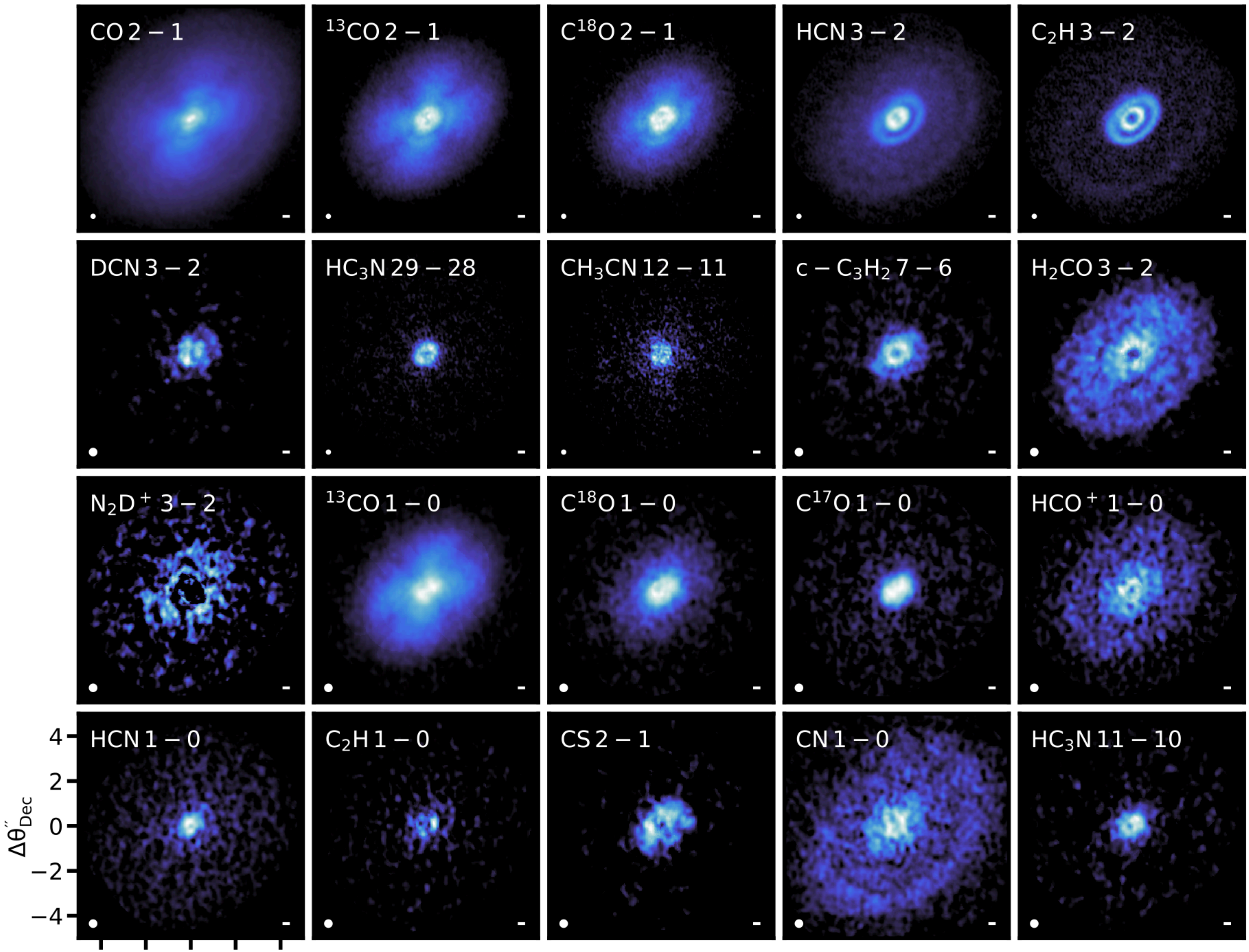
Tercero et al. (2010)

Protoplanetary Disks with ALMA: thermal dust emission at 1.25 mm



S. Andrews ea (2018)

Protoplanetary Disks with ALMA: molecular lines



Comparison of observational facilities

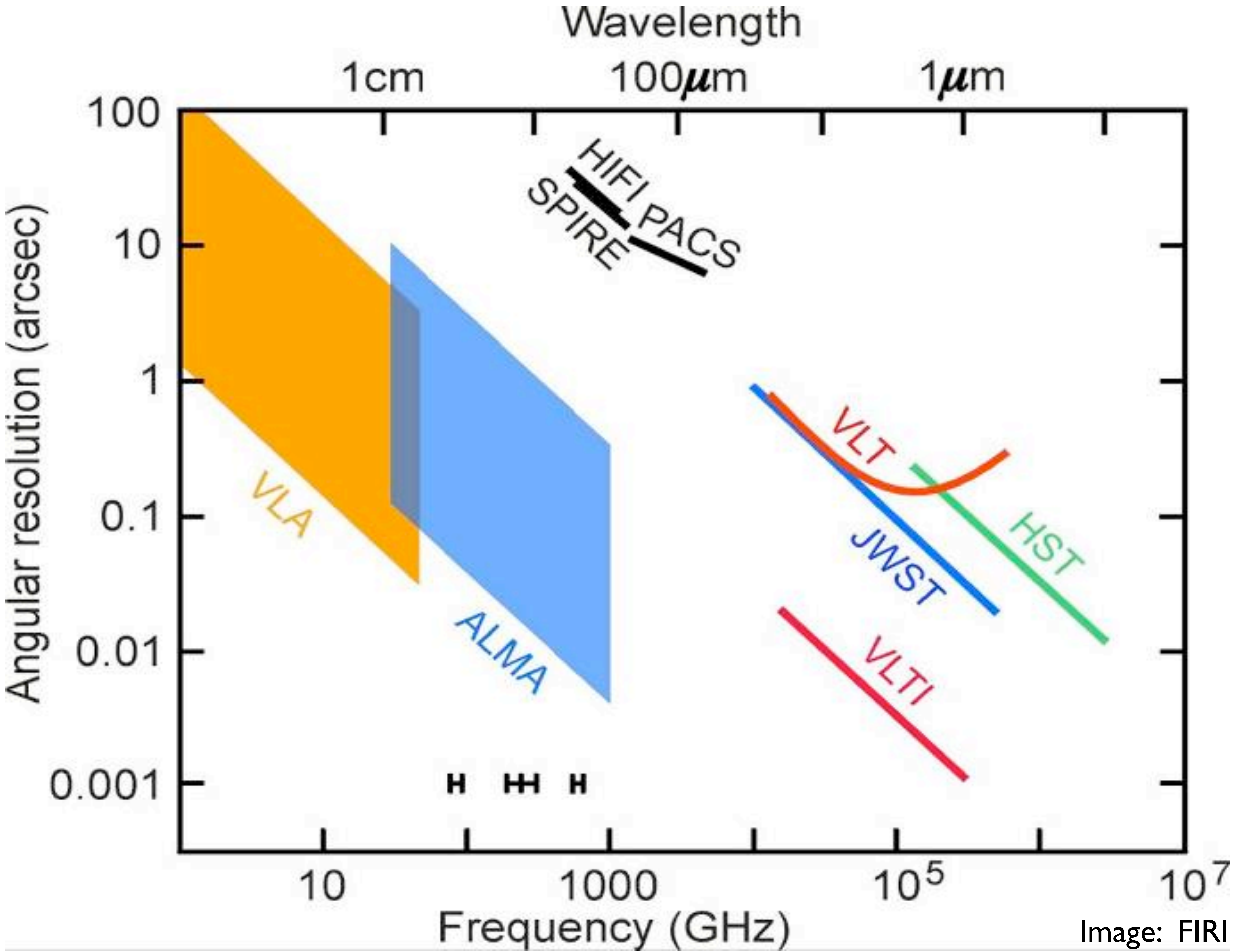


Image: FIRI team

Suggested literature

- A. G.G.M. Tielens, "The Physics and Chemistry of the ISM" (2007), Cambridge Uni. Press

- G. Rieke, "Detection of light" (2003), Cambridge Uni. Press

- T. Wilson et al., "Tools of Radioastronomy" (2009), Springer

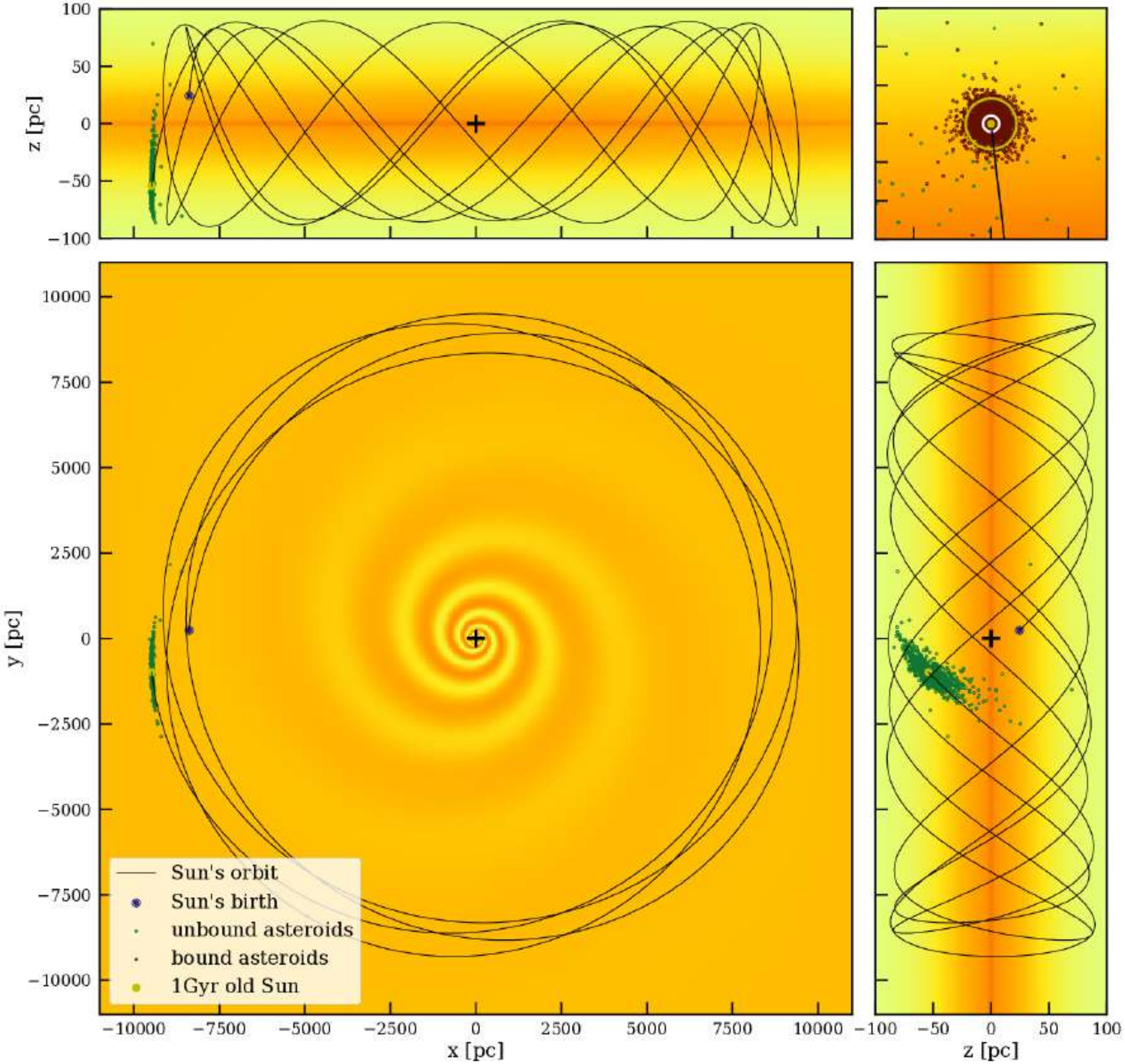
- F. R. Chromey, " To Measure the Sky: An Introduction to Observational Astronomy" (2010), Cambridge Uni. Press

- E. C. Sutton, "Observational Astronomy: Techniques and Instrumentation" (2011), Cambridge Uni. Press

Heidelberg Joint Astronomical Colloquium

Winter Semester 2022 — Tuesday November 8th, 16:00

Main Lecture Theatre, Philosophenweg 12



Simon Portegies Zwart

(Sterrewacht Leiden):

How the Sun and its siblings were born as a Family but drifted apart

The figure shows a face-on view of the Galaxy with the Sun's orbit and the cloud of asteroids following in its wake

Those unable to attend the colloquium in person are invited to participate online through Zoom.
More information is given on HePhySTO: https://www.physik.uni-heidelberg.de/hephysto/