Molecules in Stars and Planets

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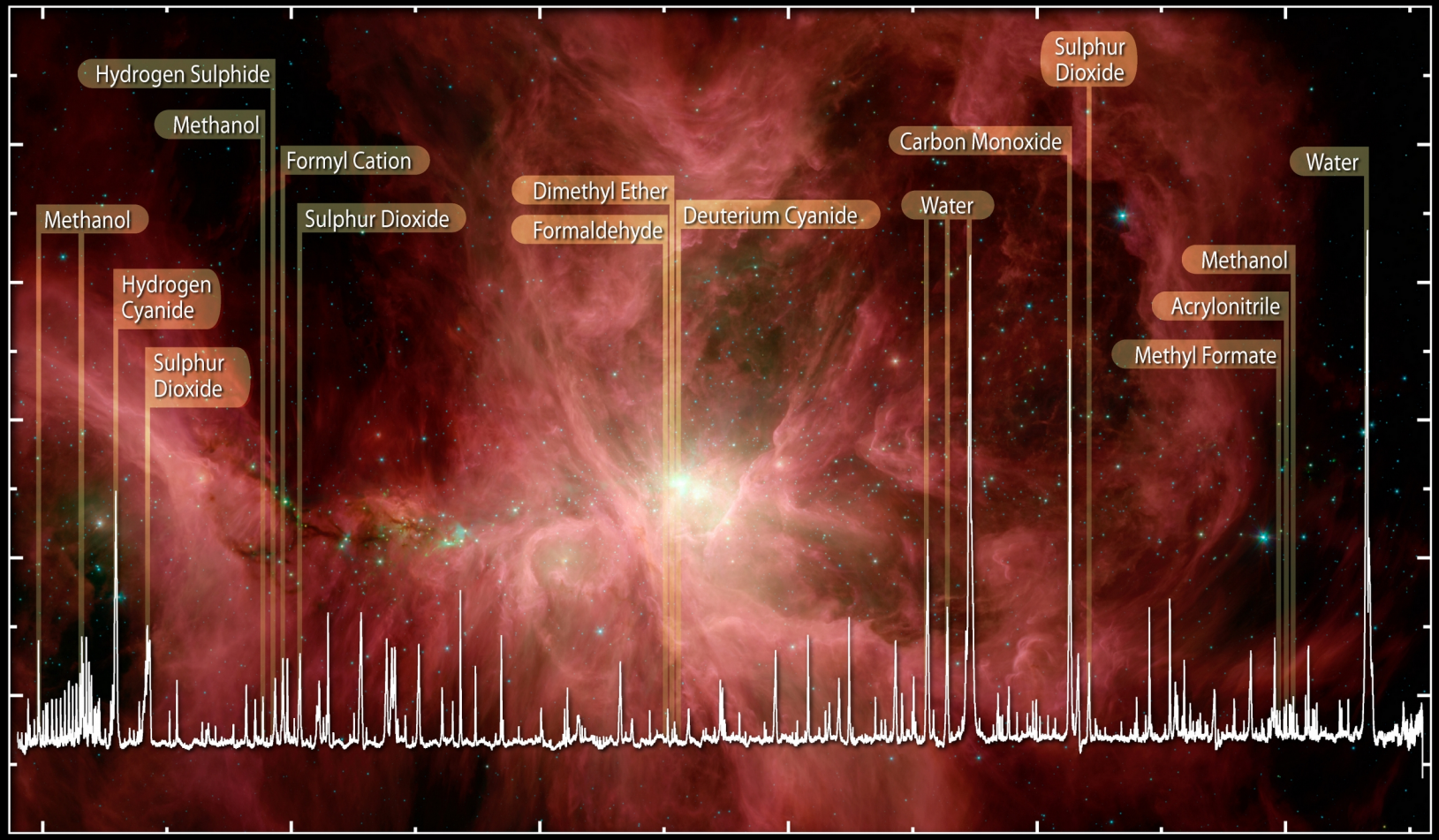

HIFI Spectrum of Water and Organics in the Orion Nebula

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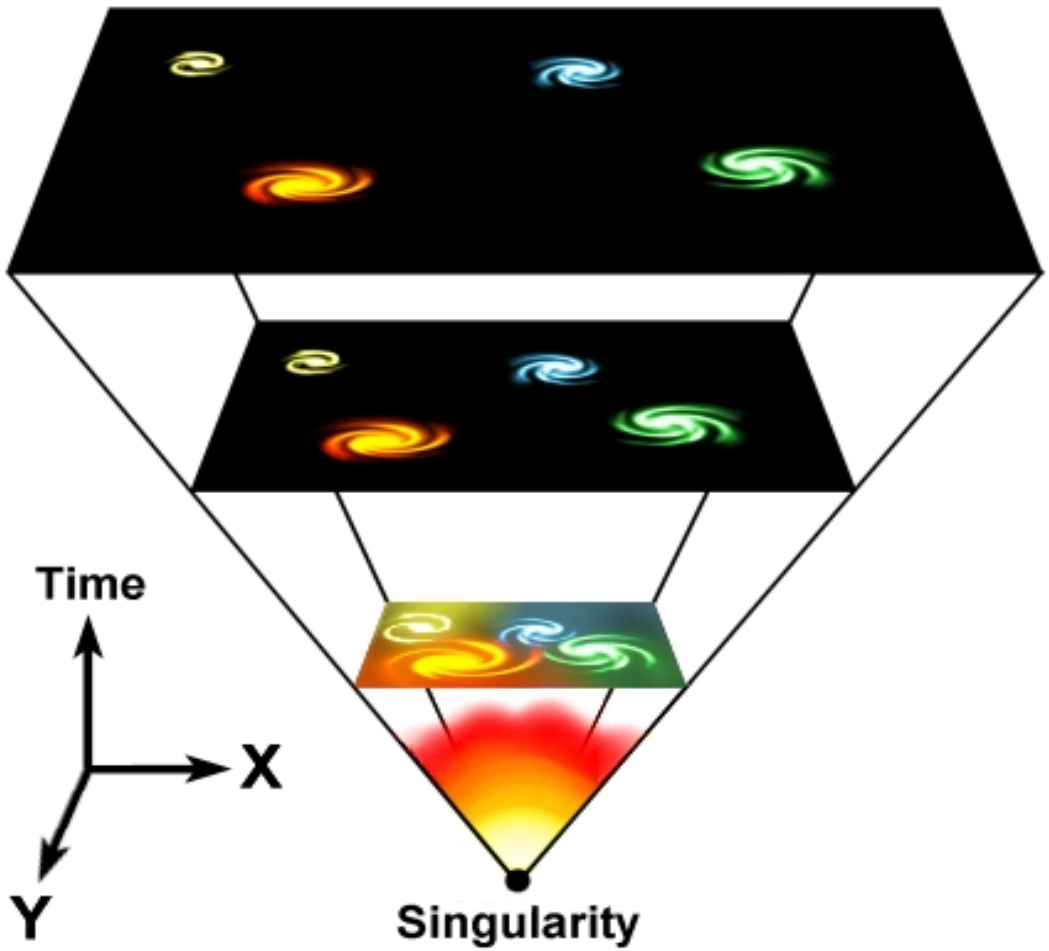
E. Bergin

The light elements H, D, He and Li were formed after the Big Bang



After 5 minutes, density and temperature were too low for nuclear fusion to continue

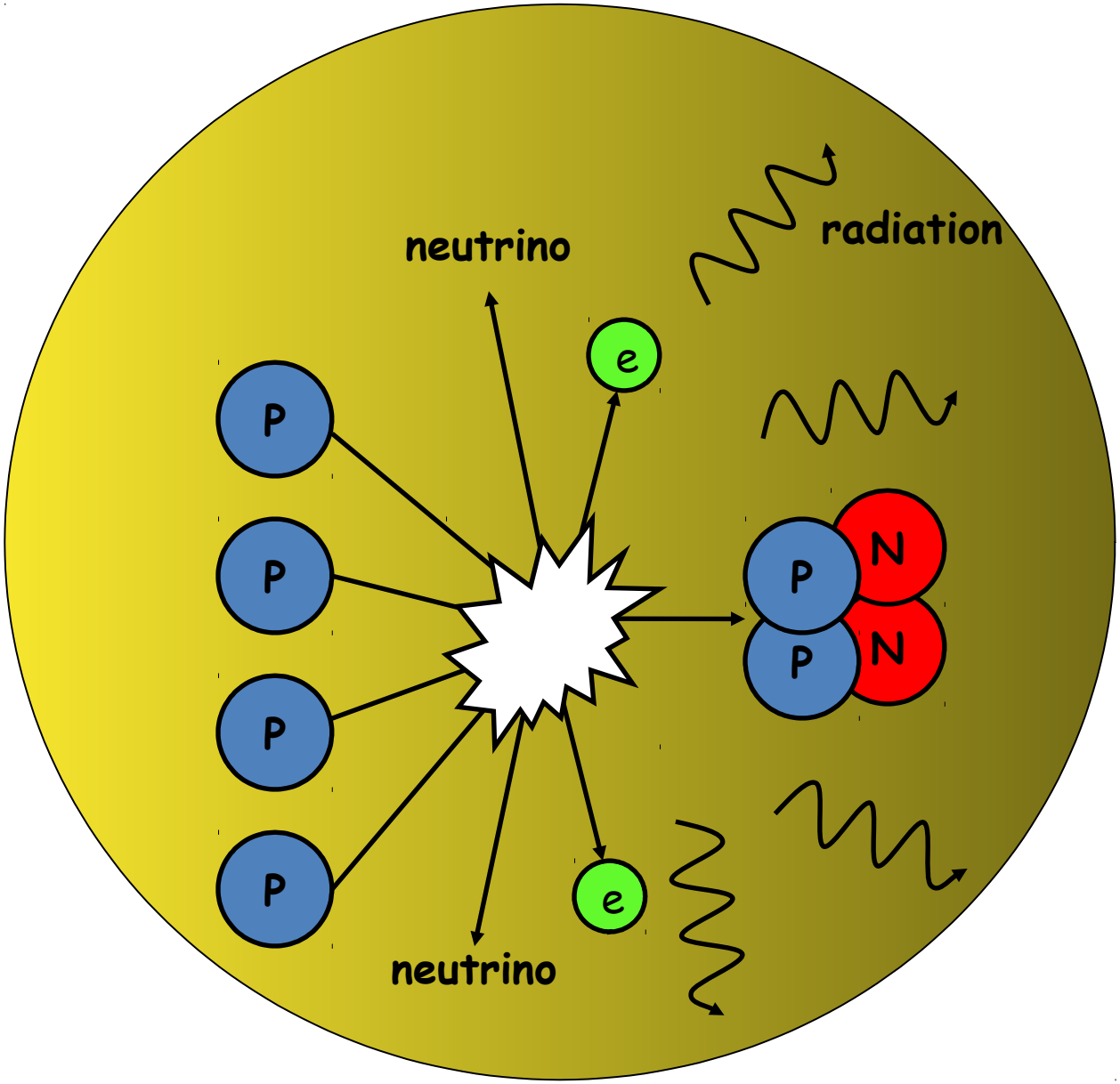
After a few 100000 yr, the first chemical reactions started

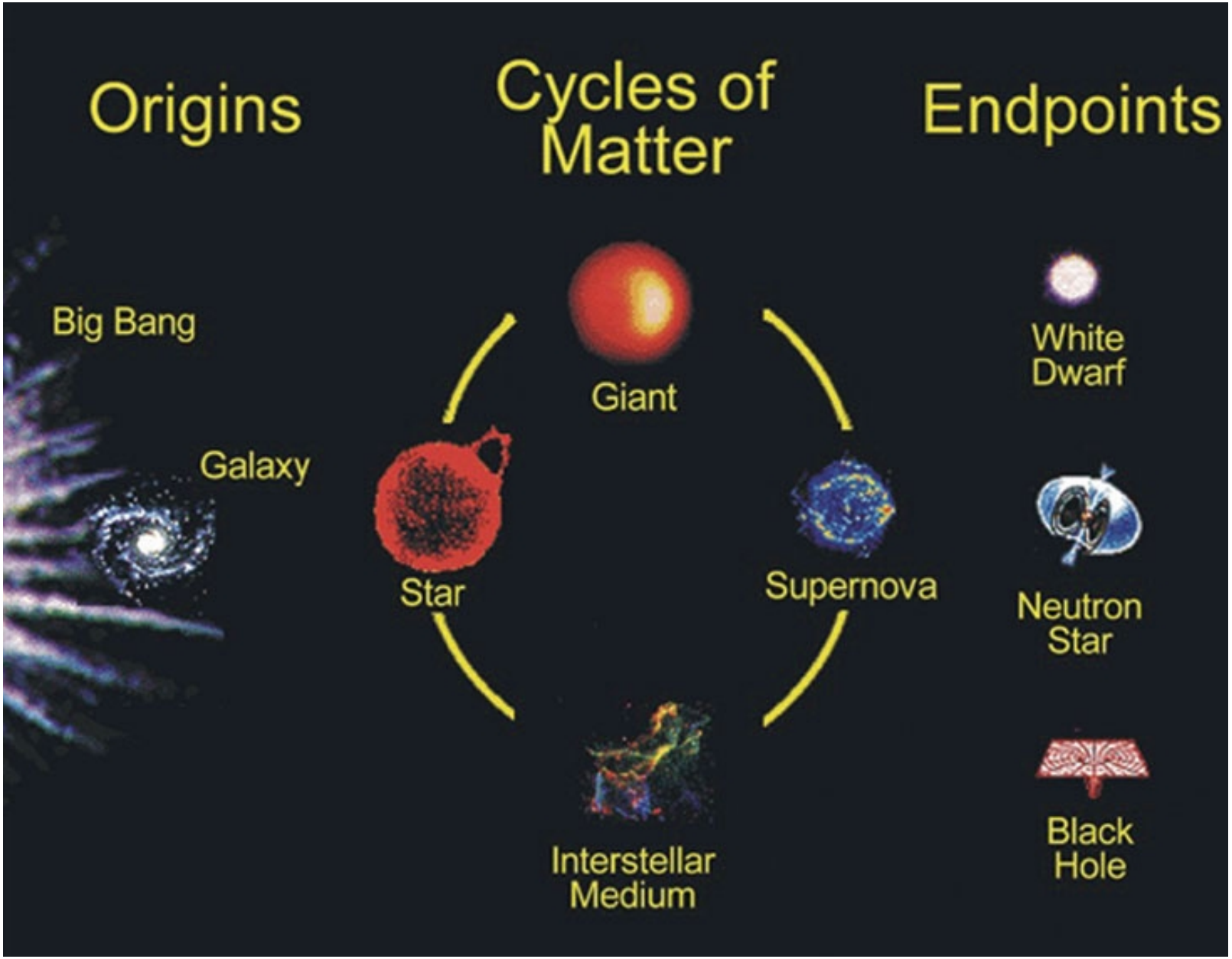
$$H^- + H \longrightarrow H_2 + \text{electron}$$

$$H_2^+ + H \longrightarrow H_2 + H^+$$

leading to formation of the simplest molecule, H_2

Stellar Nuclear Synthesis




Origins
Cycles of Matter
Endpoints
Big Bang
Galaxy
Giant
Star
Supernova
Interstellar Medium
White Dwarf
Neutron Star
Black Hole

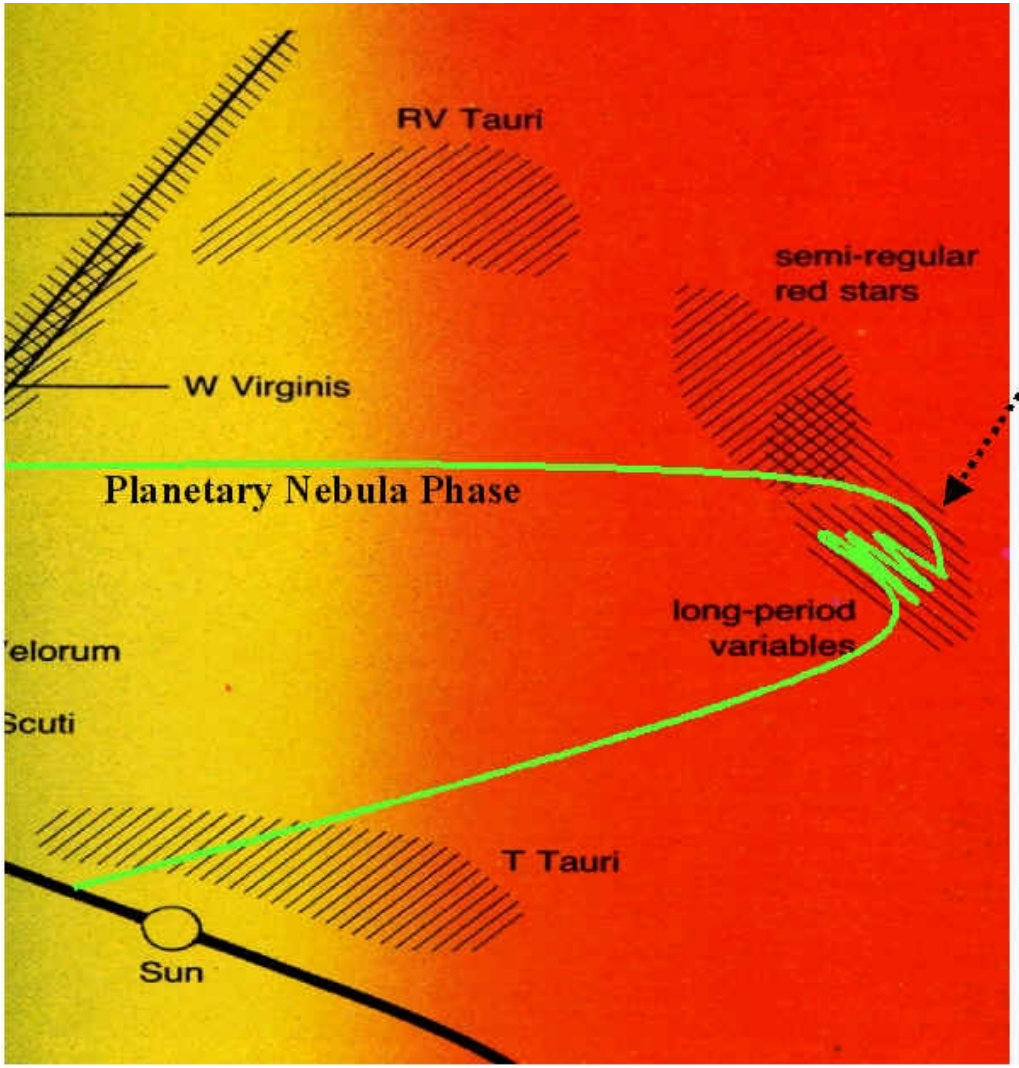
Heavy elements (> Fe) are synthesized through neutron capture

$$(Z, A) + n \longrightarrow (Z,A+1) + \gamma$$

followed by β - decay

$$(Z,A+1) \longrightarrow (Z+1,A+1) + e^- + \nu_e$$

Sources of neutrons: red giants or supernovae



Death of a Star, Birth of the Elements

C and S Stars: Thermal Pulse Phase

1) $He \longrightarrow {}^{12}C$

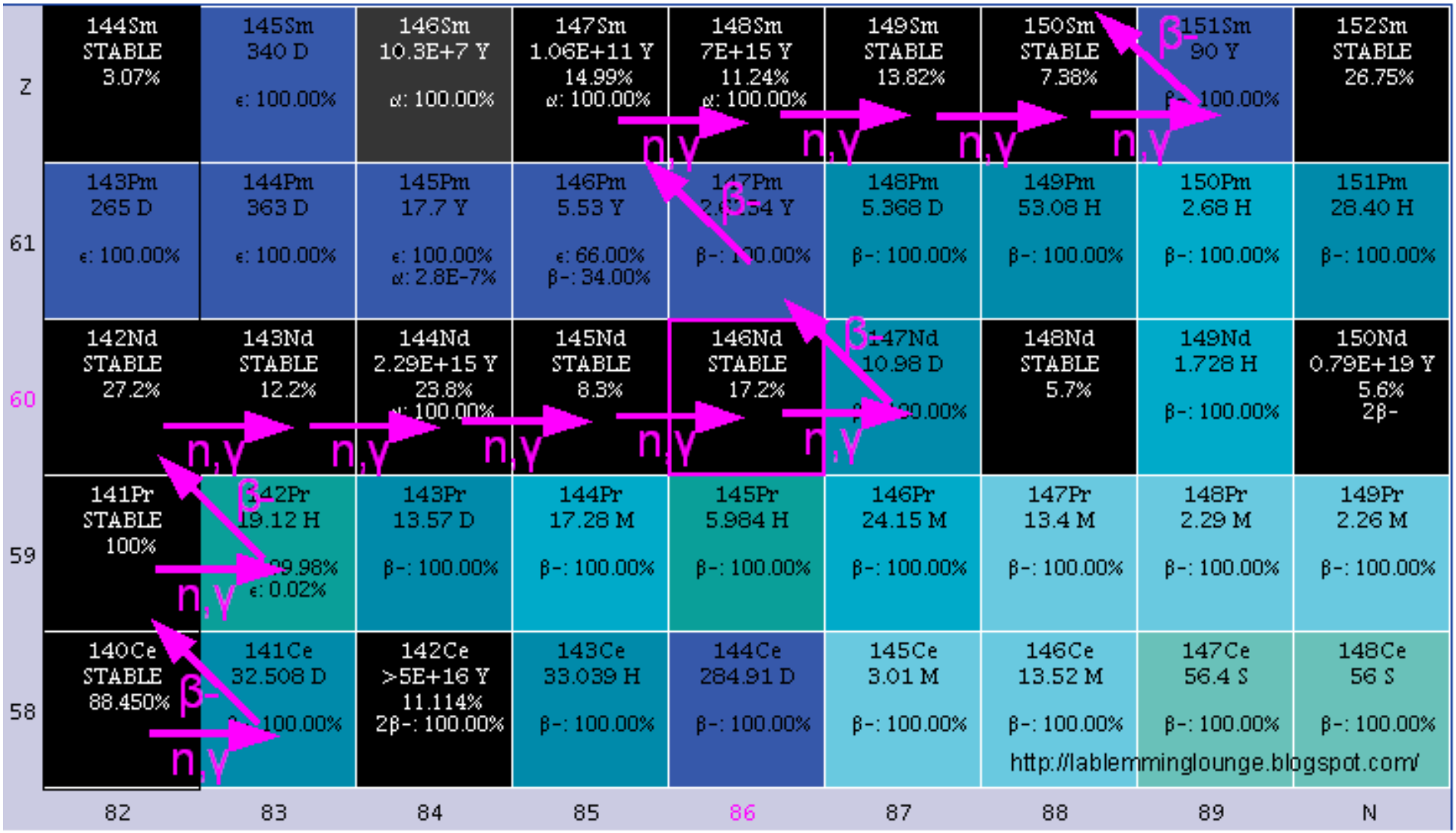
2) ${}^{12}C \longrightarrow {}^{13}C$

3) ${}^{13}C + He \longrightarrow {}^{16}O + n$

$^{22}Ne + He \longrightarrow {}^{25}Mg + n$

Total lifetime in TP: ~100,000 years
Total TP: ~15-20
Slow Neutron Capture Synthesis
of heavy elements: >Fe
Between TP: Dredge Up Period

Synthesis of Neodimium isotopes



Is Neodimium used in any real world application ?

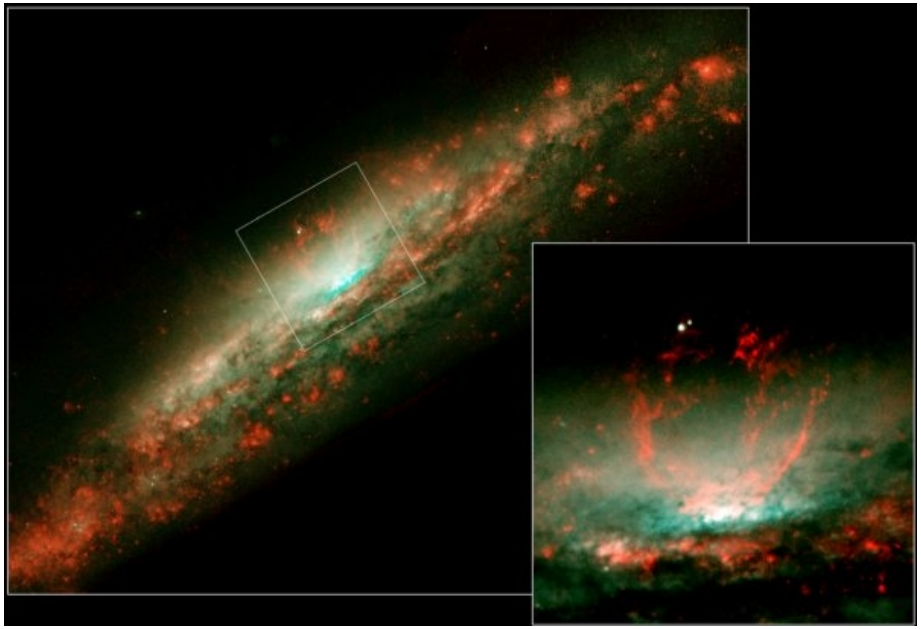
Yes ! Green laser pointer !

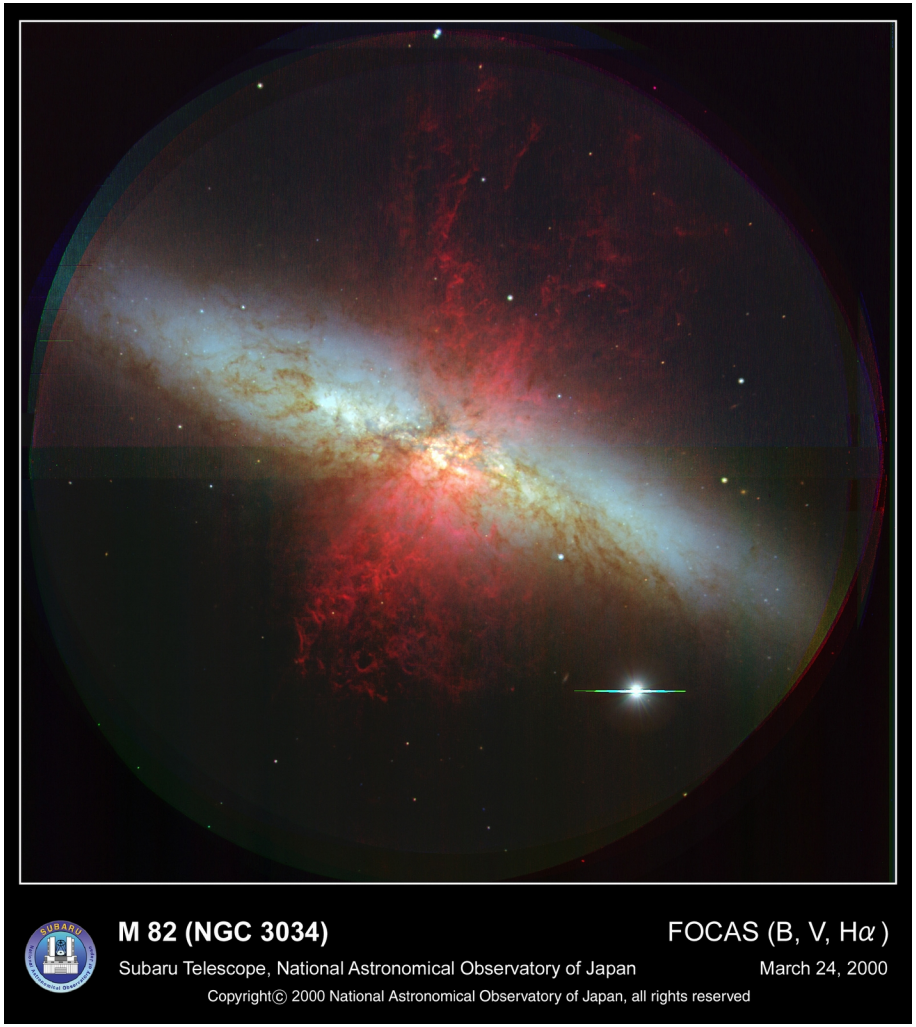
Nd:YAG laser in atmospheric research (LIDAR)

Gas phases:

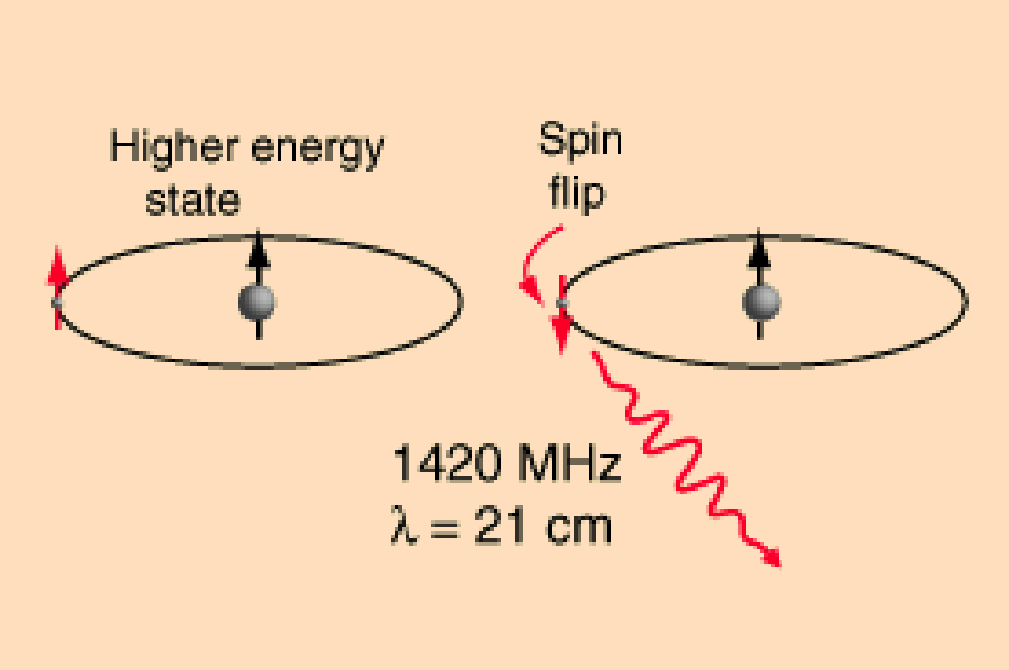
Phase	n [cm^{-3}]	T [K]	f_V [%]	f_m [%]	h [pc]	Tracer
molecular	$10^2 \cdots 10^5$	$10 \cdots 50$	< 1	~20	~70	CO
cold neutral	$40 \cdots 80$	$50 \cdots 200$	$2 \cdots 4$	~40	~140	HI (absorpt.)
warm neutral	$0.1 \cdots 0.6$	$5500 \cdots 8500$	~30	~30	~400	HI (emission)
warm ionized	~0.2	~8000	~20	~10	~900	Hα radio
hot ionized	$10^{-3} \cdots 10^{-2}$	$10^5 \cdots 10^7$	~50	~1	≥ 1000	[OVI] X-rays

Galactic wind observed in H-alpha

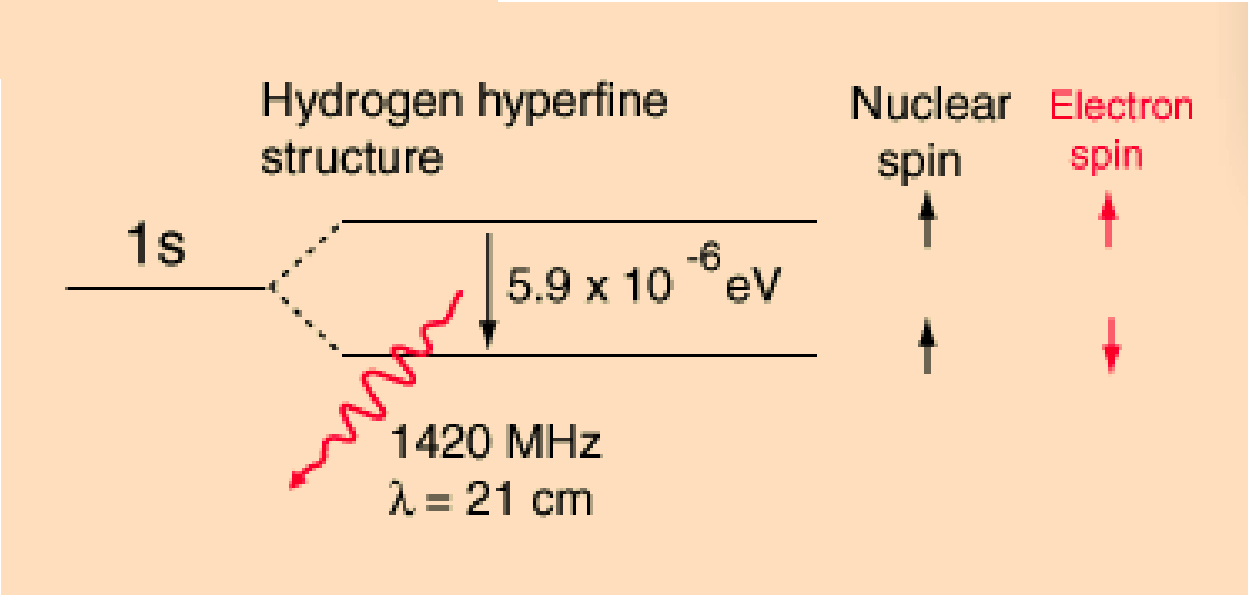




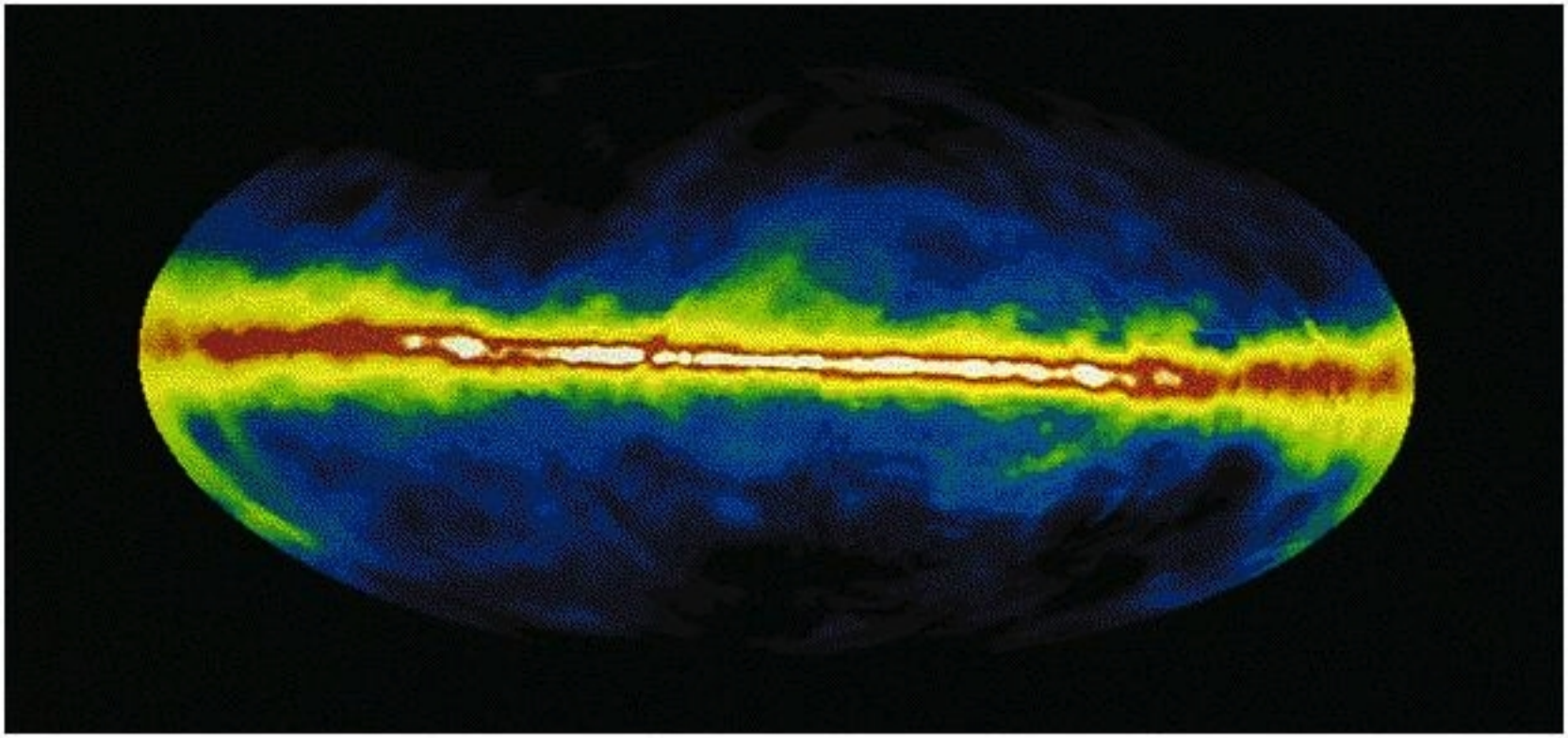
Observing cold neutral hydrogen HI



Interaction between electron spin and nuclear spin



21-cm emission from the entire Milky Way



Some important atomic lines

	Transition	λ [μm]	ν [GHz]	T_{cool} [K]	n_{crit} [cm^{-3}]	Layer
[CI]	$^3P_1 \rightarrow {}^3P_0$	610	492	$\sim$ 24		
	$^3P_2 \rightarrow {}^3P_1$	371	809	$\sim$ 39	$3\cdot10^3$	surface
[CII]	$^2P_{1/2} \rightarrow {}^2P_{3/2}$	158	1899	$\sim$ 92	$3\cdot10^3$	surface
[OI]	$^3P_2 \rightarrow {}^3P_1$	185	1620	$\sim$ 98		
	$^3P_1 \rightarrow {}^3P_2$	63	4757	$\sim$ 228	> 10^5	intermed.
CO	J= 1 $\rightarrow$ 0	2600	115	> 5.3	$3\cdot10^3$	core

Discovery of molecules

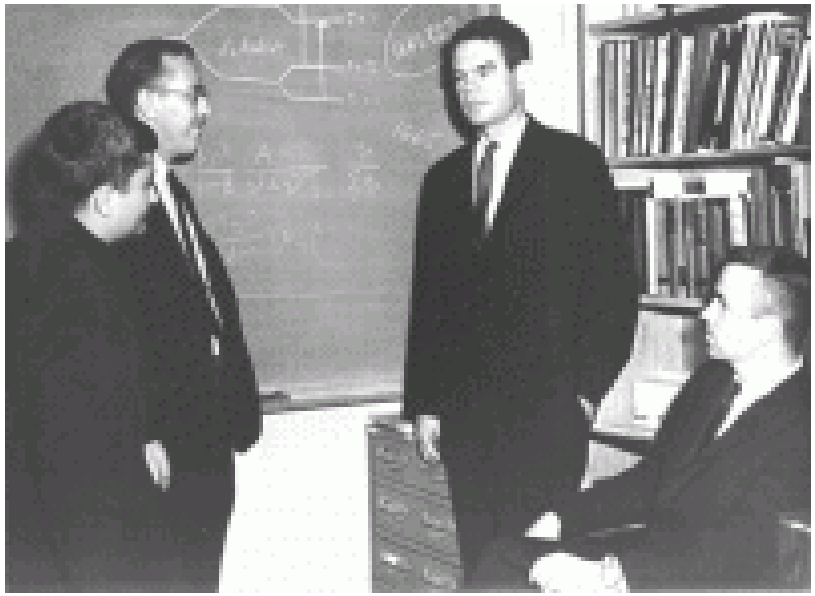
Before 1937: Scientists thought that the ISM was composed by atoms

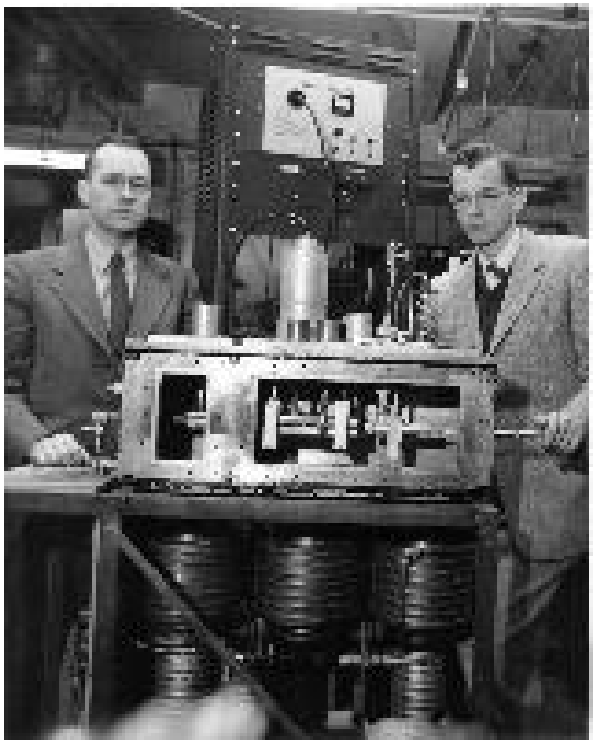
1937-1941: The first three diatomic molecules (CH,CN,CH^+) are detected (optical lines).

CN radical was later found to be a very powerful probe of the temperature of the Cosmic Background Radiation.

- - - - THE BIRTH OF RADIOASTRONOMY - - - -

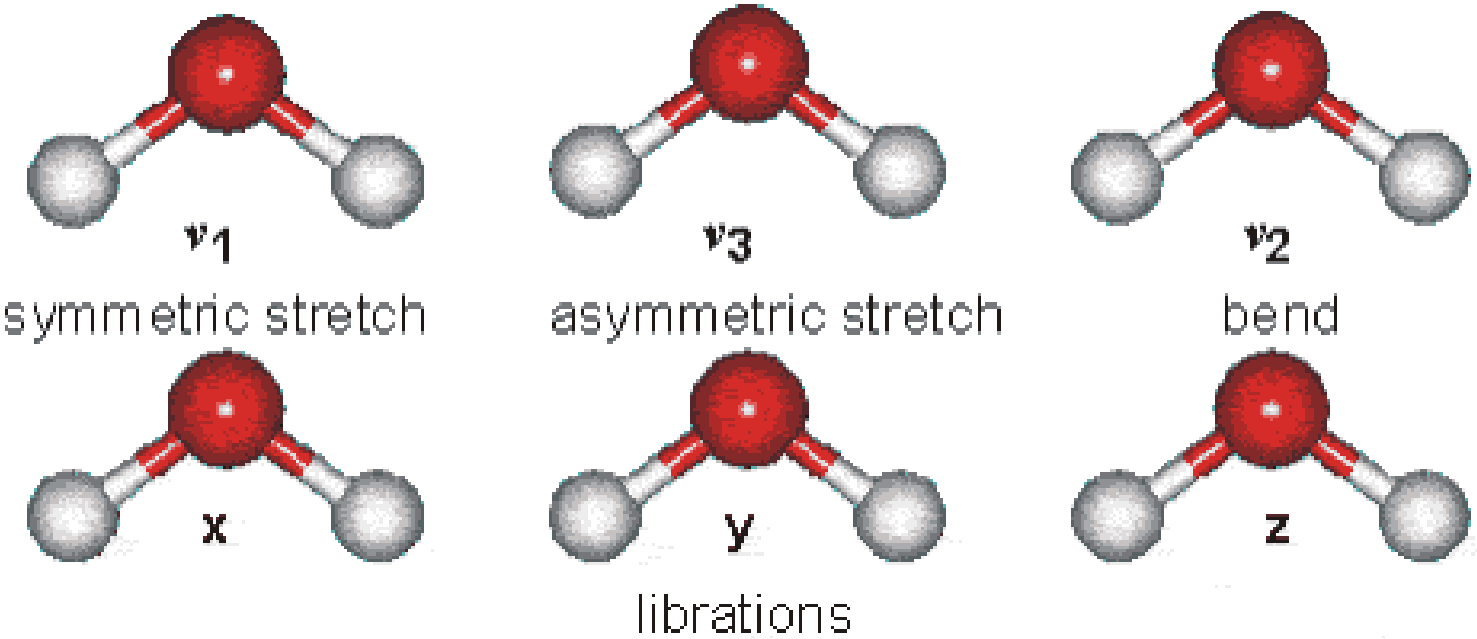
1963: Weinreb and collaborators detected OH in the Galactic Center.

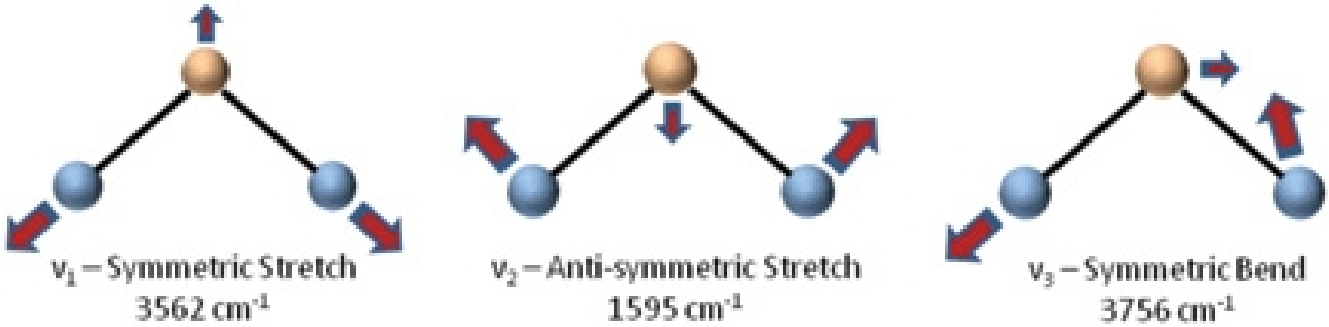




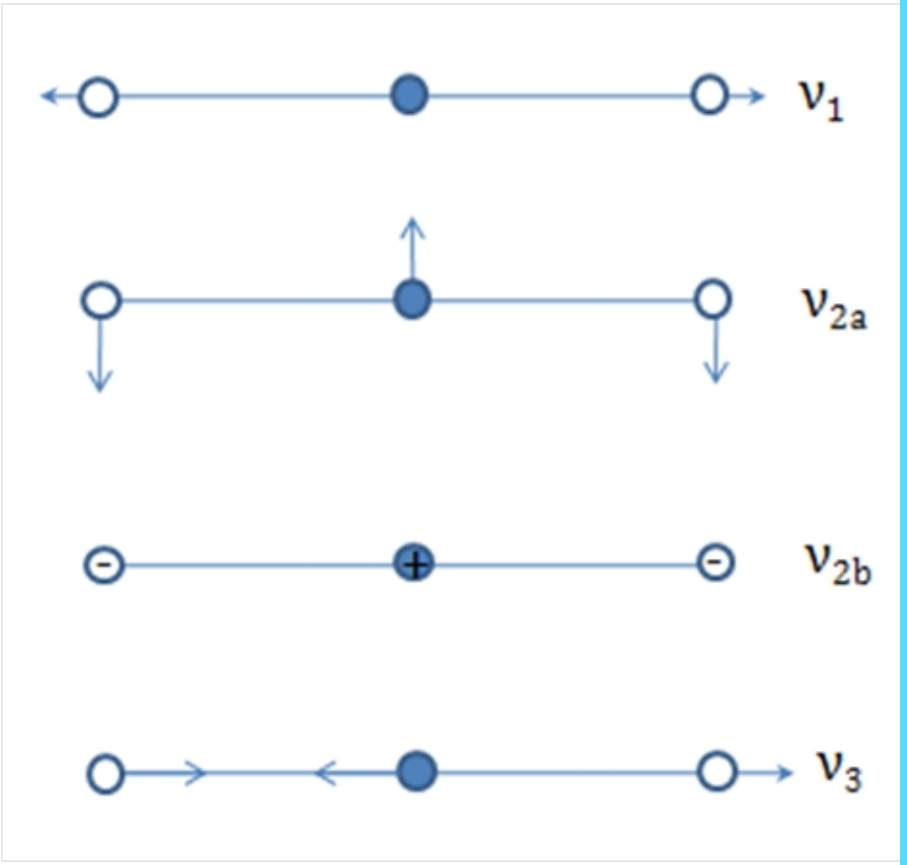
1968: Charles Townes and collaborators detected H_2O & NH_3.

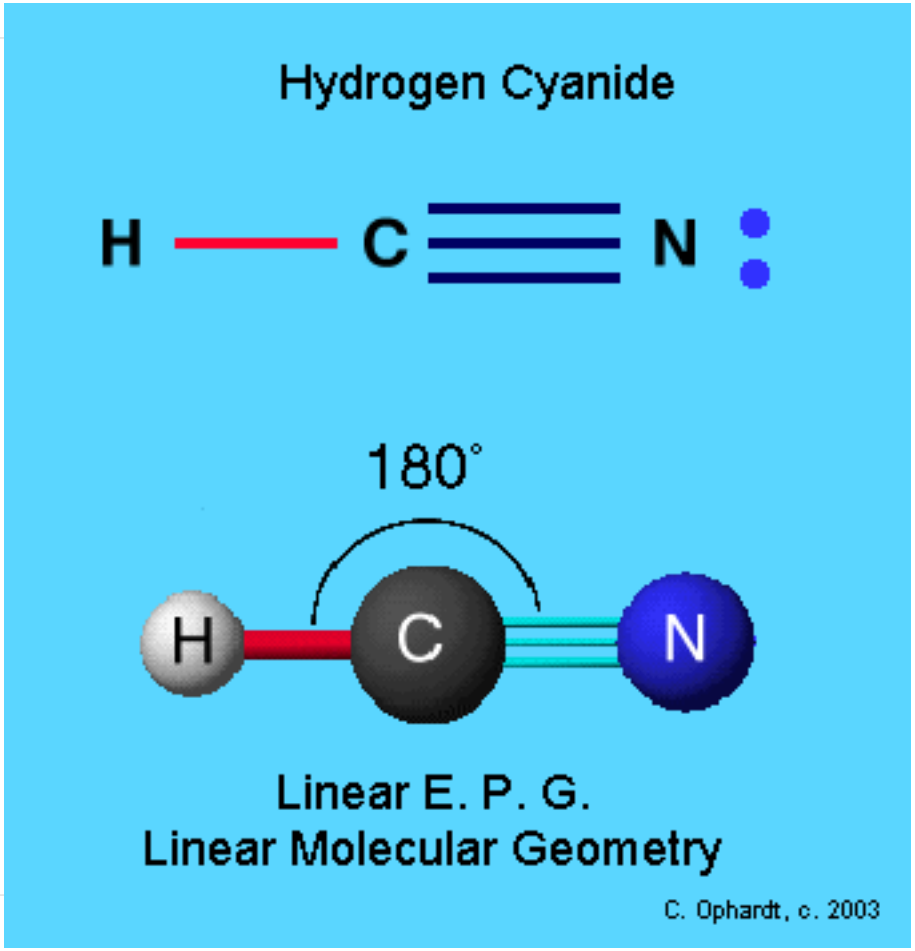
Vibration mode of water molecule H_2O





HCN and its vibration modes



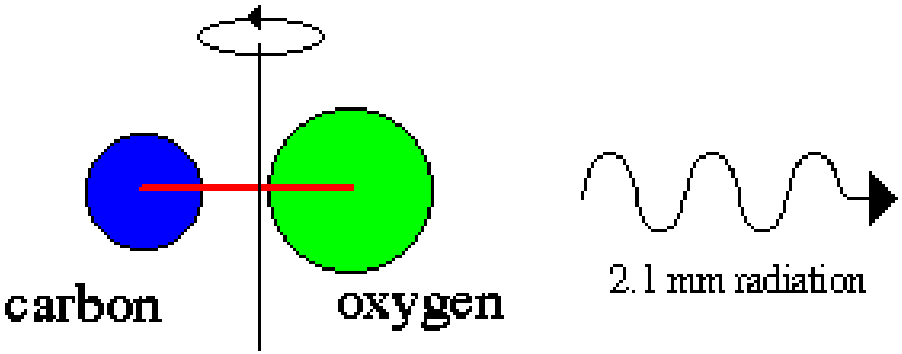


Rotation of molecules

Radiation from Interstellar Molecules

Interstellar molecules (such as H_2, CO, CN,) emit radiation by rotation rather than direct transition of their electrons

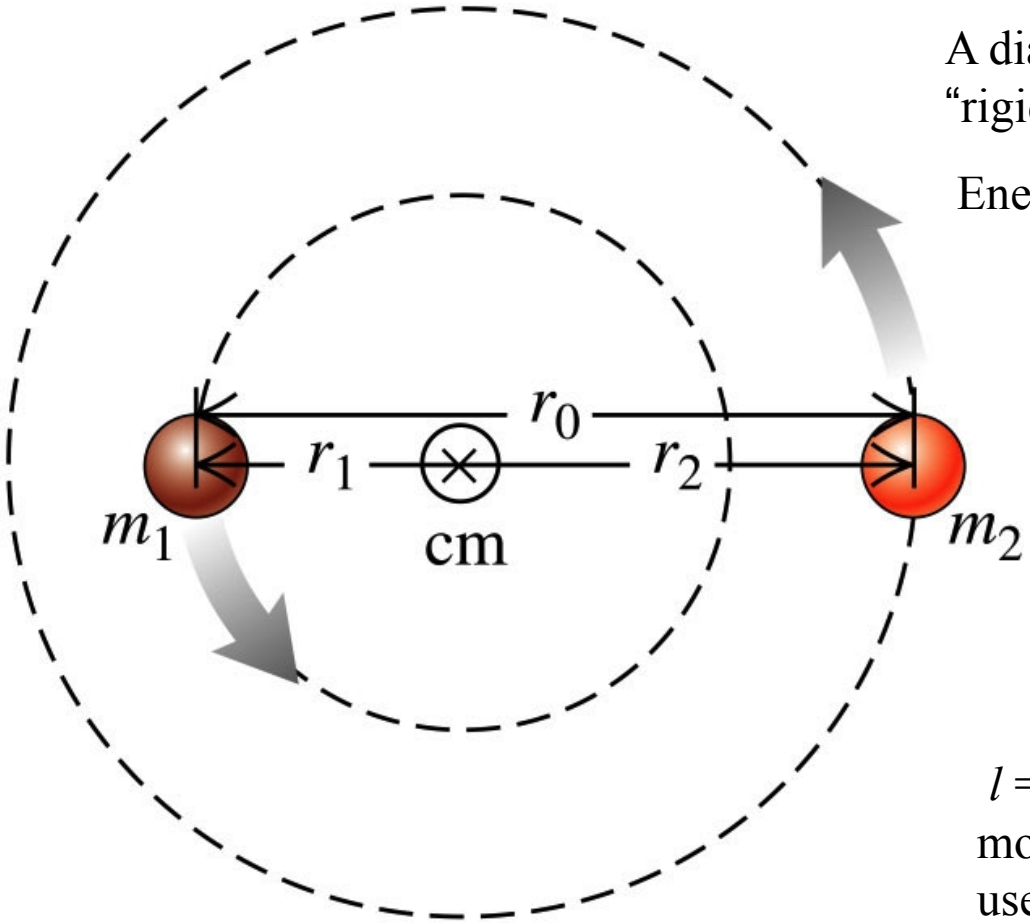
carbon monoxide molecule



Radio waves in the centimeter, millimeter and sub-millimeter region

The radiation emitted tends to be in the microwave region of the spectrum.

Diatomic molecules



A diatomic molecule modeled as a "rigid rotor"

Energy is rotational KE

$$E = \frac{L^2}{2I}$$

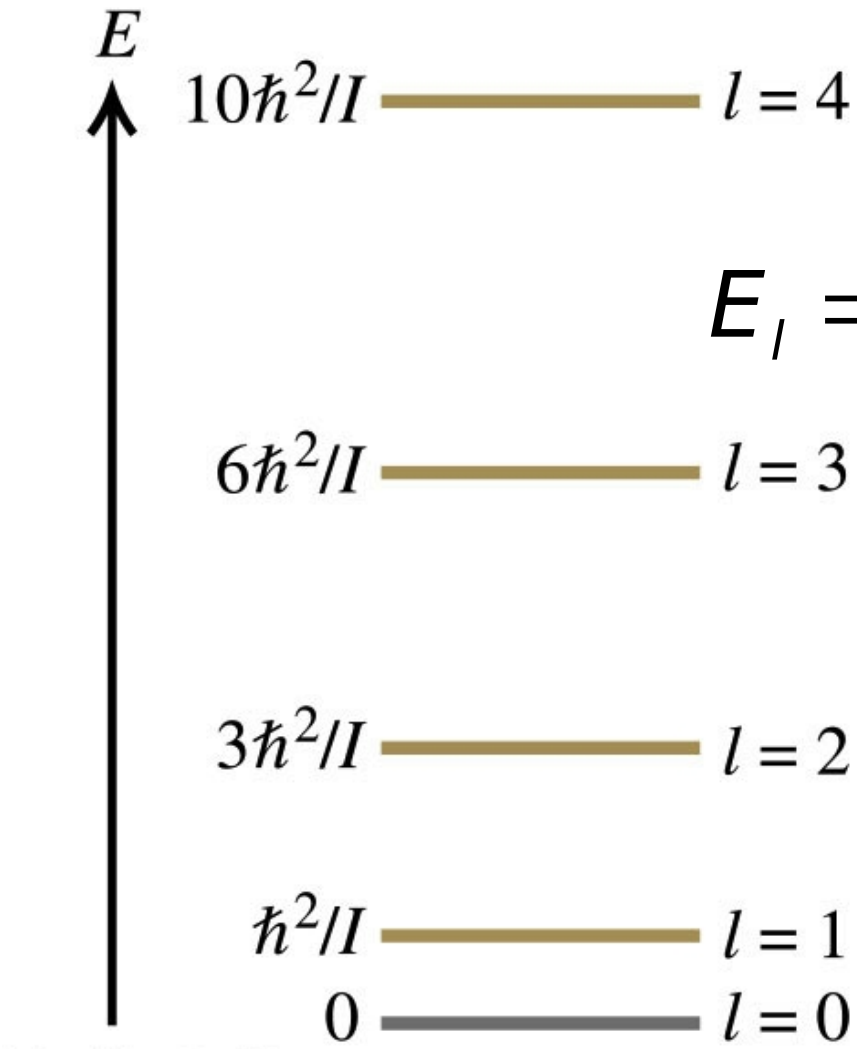
$$L = \sqrt{l(l+1)}\hbar$$

l = (rotational) angular momentum quantum #. Our book uses J

Rotational energy levels of a diatomic molecule:

$$E_l = l(l+1)\frac{\hbar^2}{2I} \quad (l = 0, 1, 2, \ldots)$$

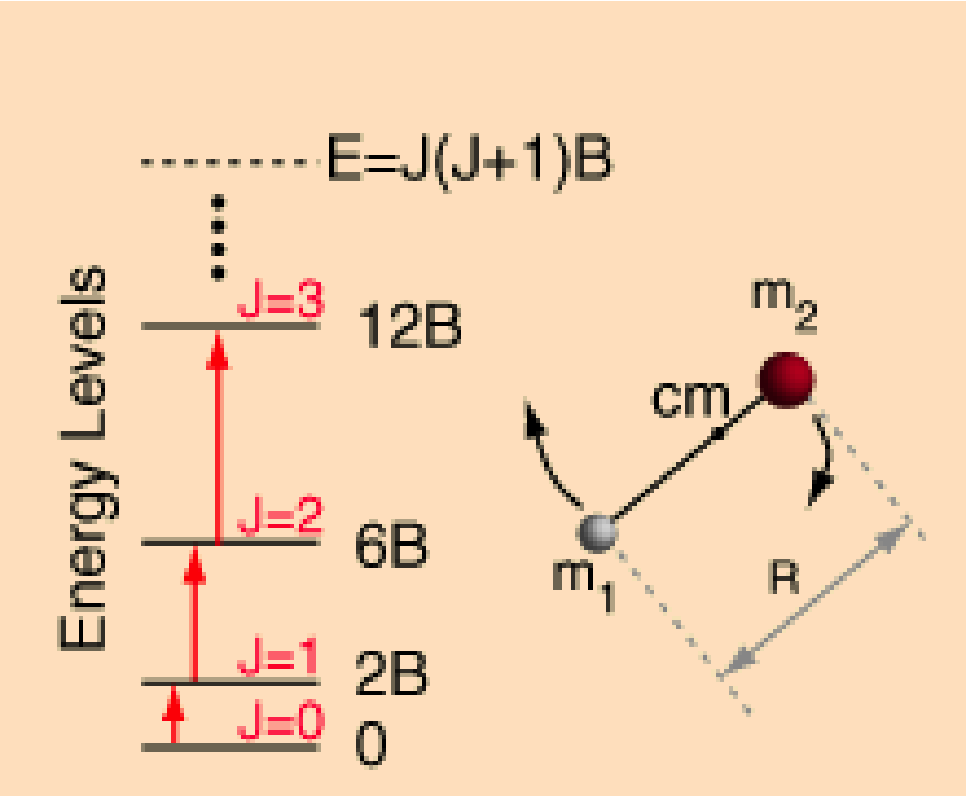
Rotational energy levels for a diatomic molecule

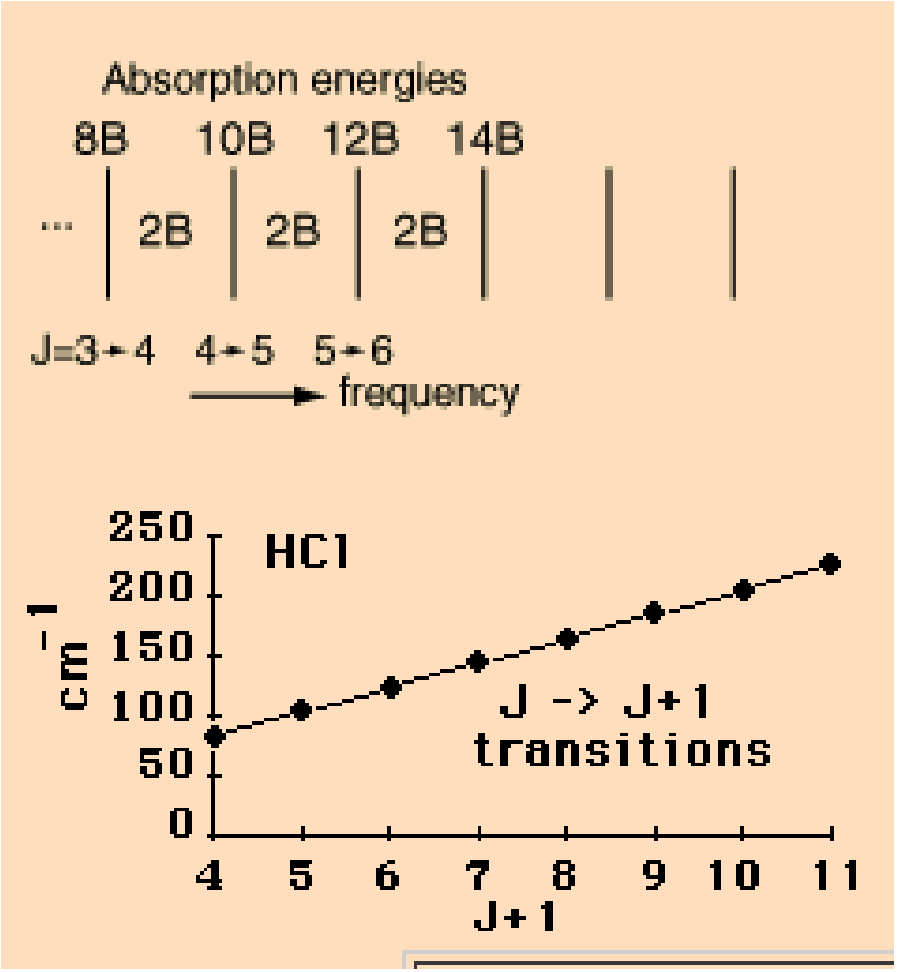


$$E_l = l(l+1)\frac{\hbar^2}{2I} \quad (l = 0,1,2,\ldots)$$

$$B = \frac{\hbar^2}{2I}$$

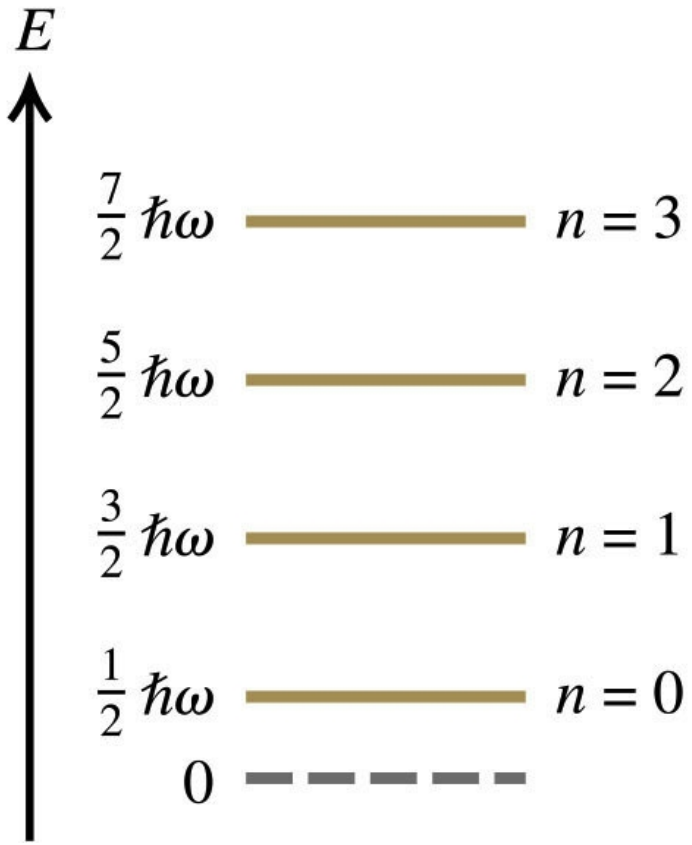
$$\Delta J = \pm 1$$

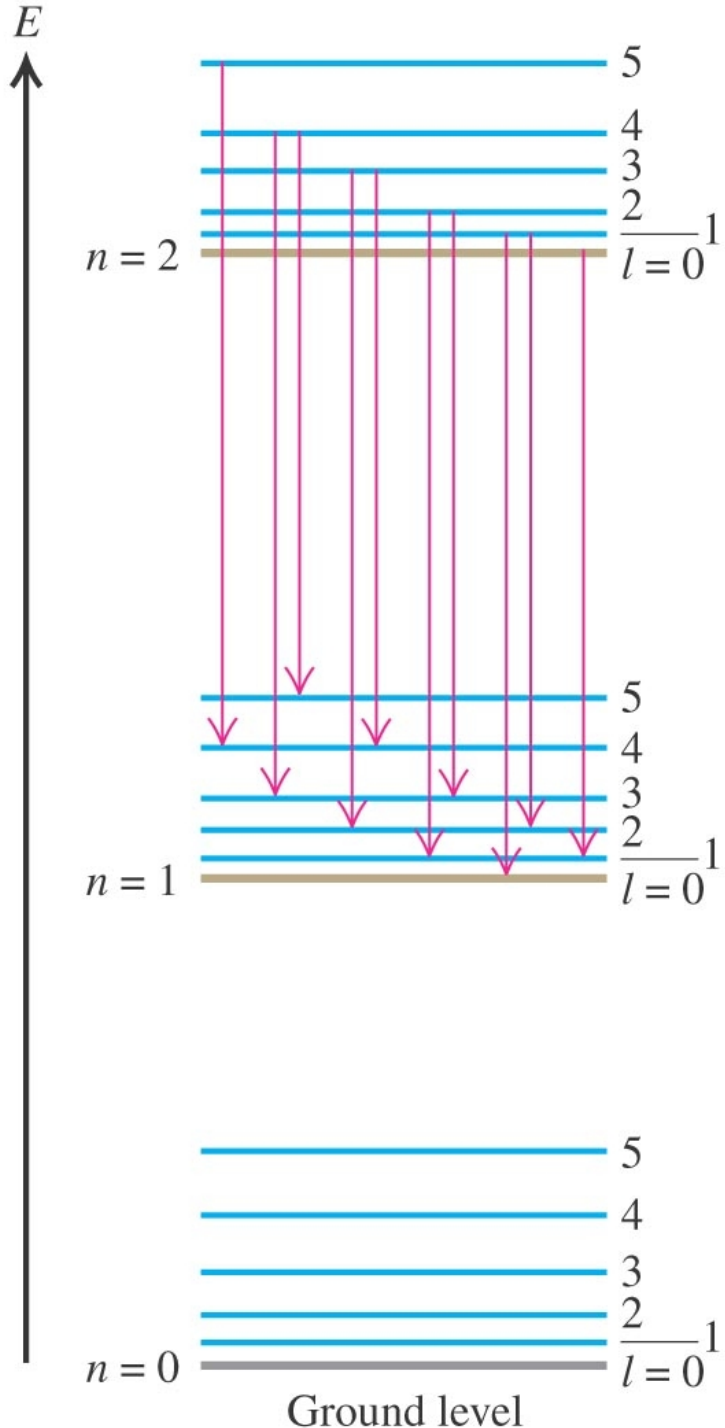




Vibrational levels for a diatomic molecule (harmonic oscillator):

- Equally spaced





Vibrational and rotational energy levels

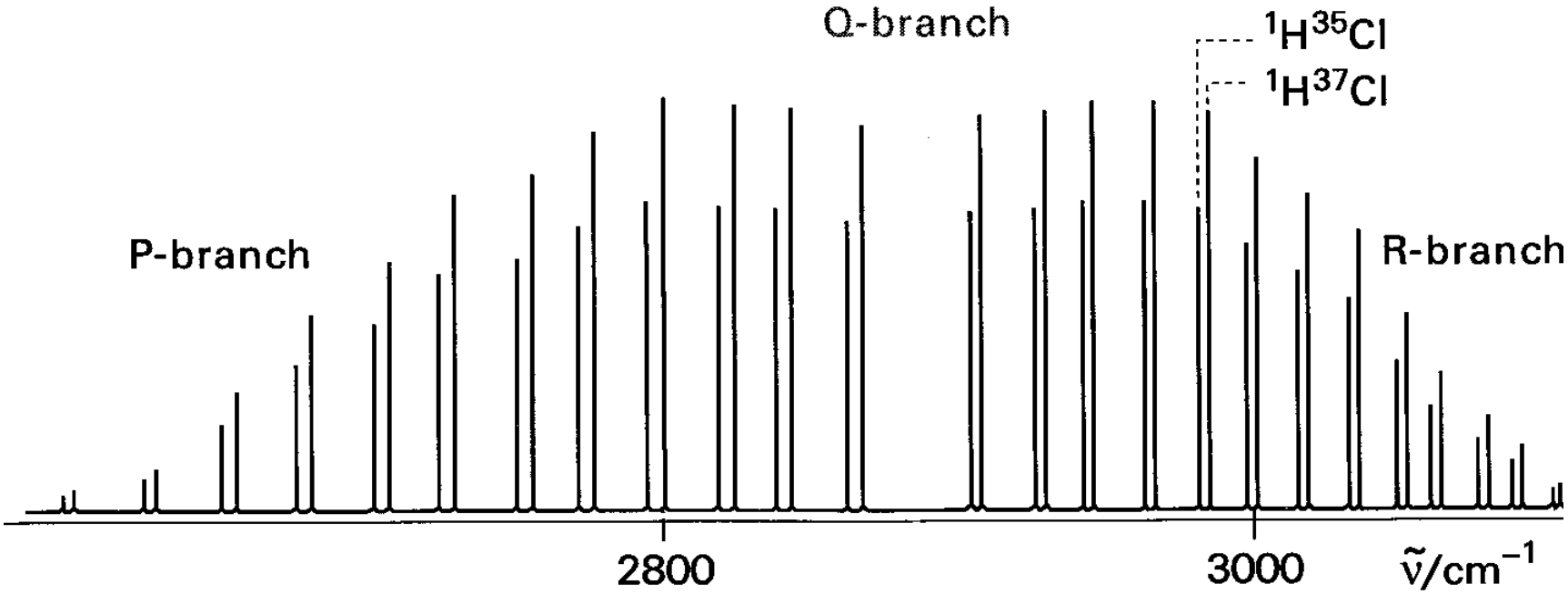
$$E_{nl} = l(l+1)\frac{\hbar^2}{2I} + (n+\frac{1}{2})\hbar\omega$$

$$\Delta l = \pm 1$$

If vibrational level changes,

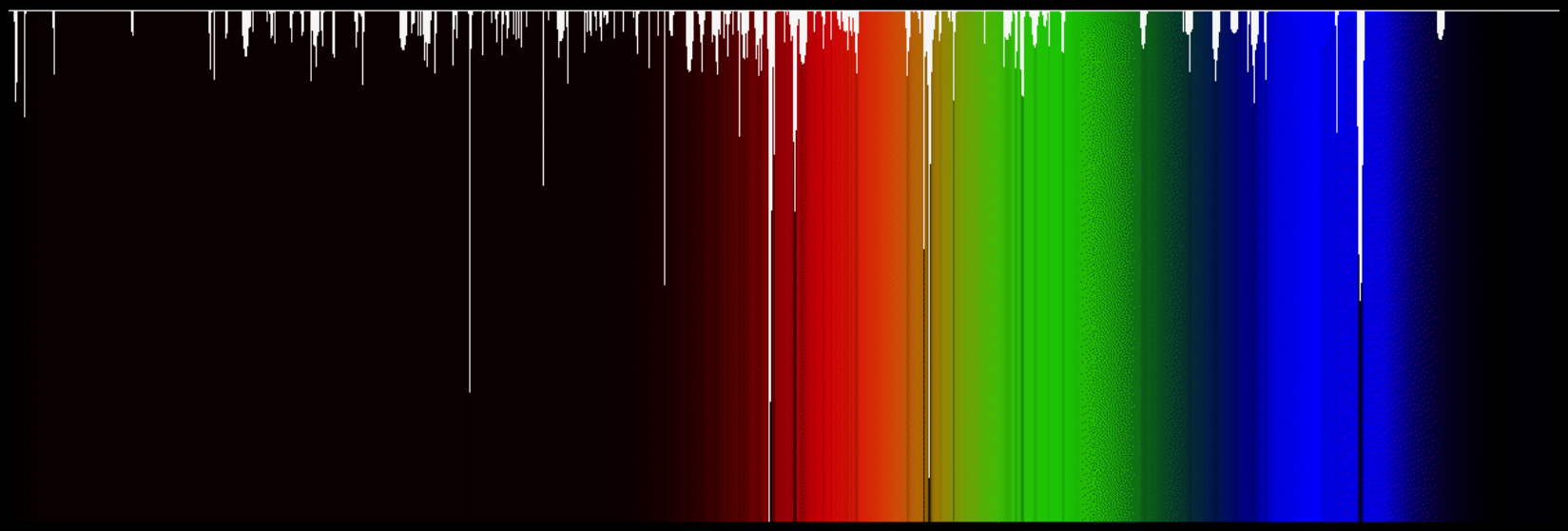
- n must increase by 1 if a photon is absorbed
- n must decrease by 1 if a photon is emitted

High resolution spectrum of HCl



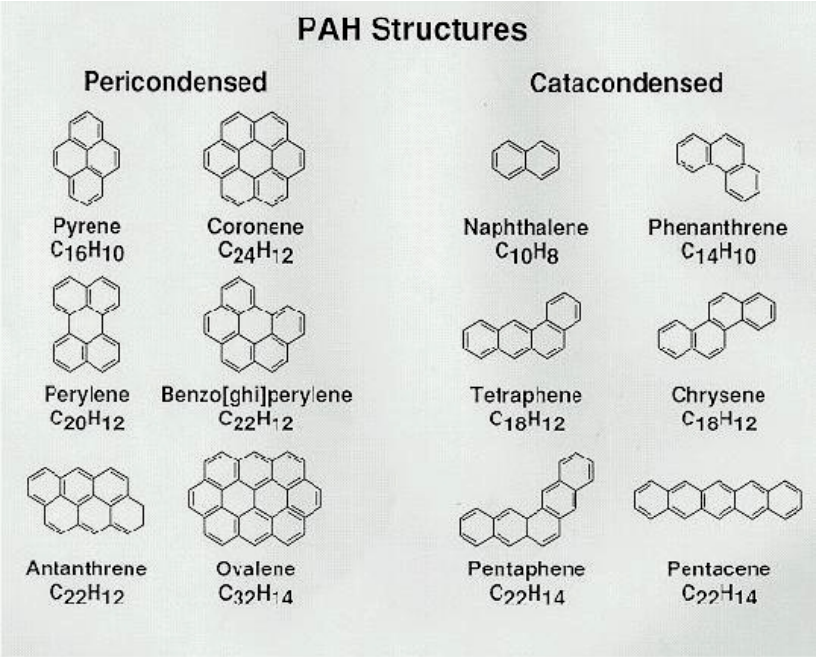
- Above the “gap”; $\Delta J = +1$
- Below the “gap”: $\Delta J = -1$
- Intensities mirror populations of starting levels

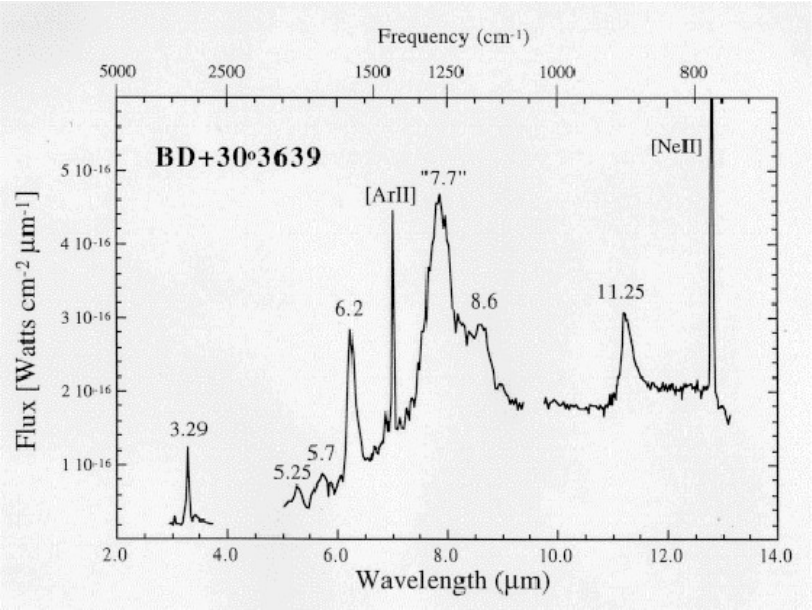
The Diffuse Interstellar Bands

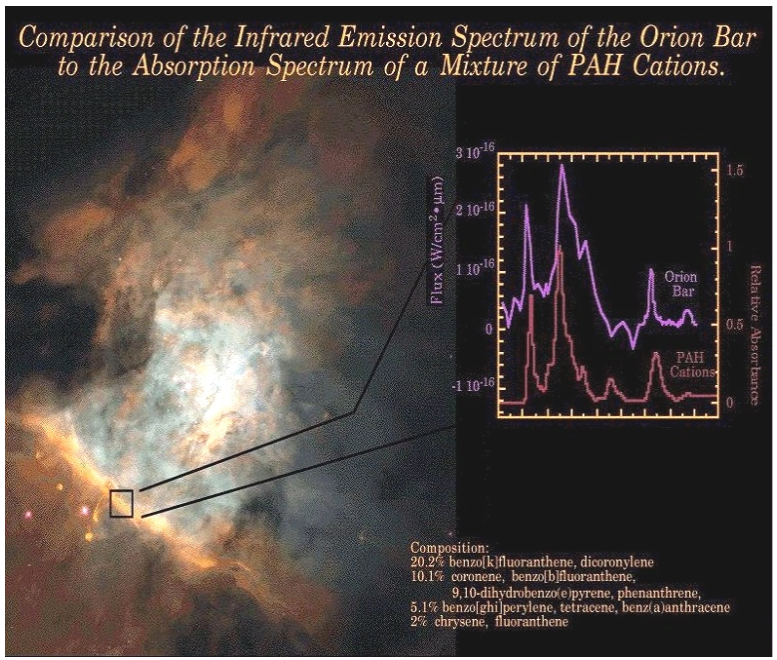


Courtesy: P. Jenniskens, F.-X. Desert

Polyaromatic hydro carbons







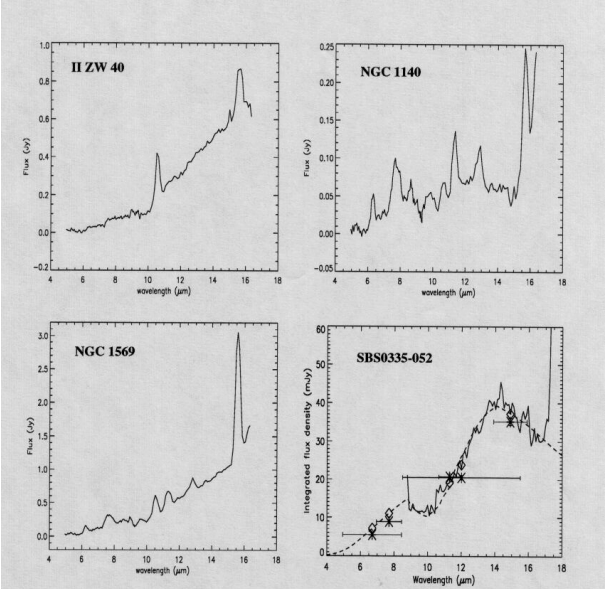


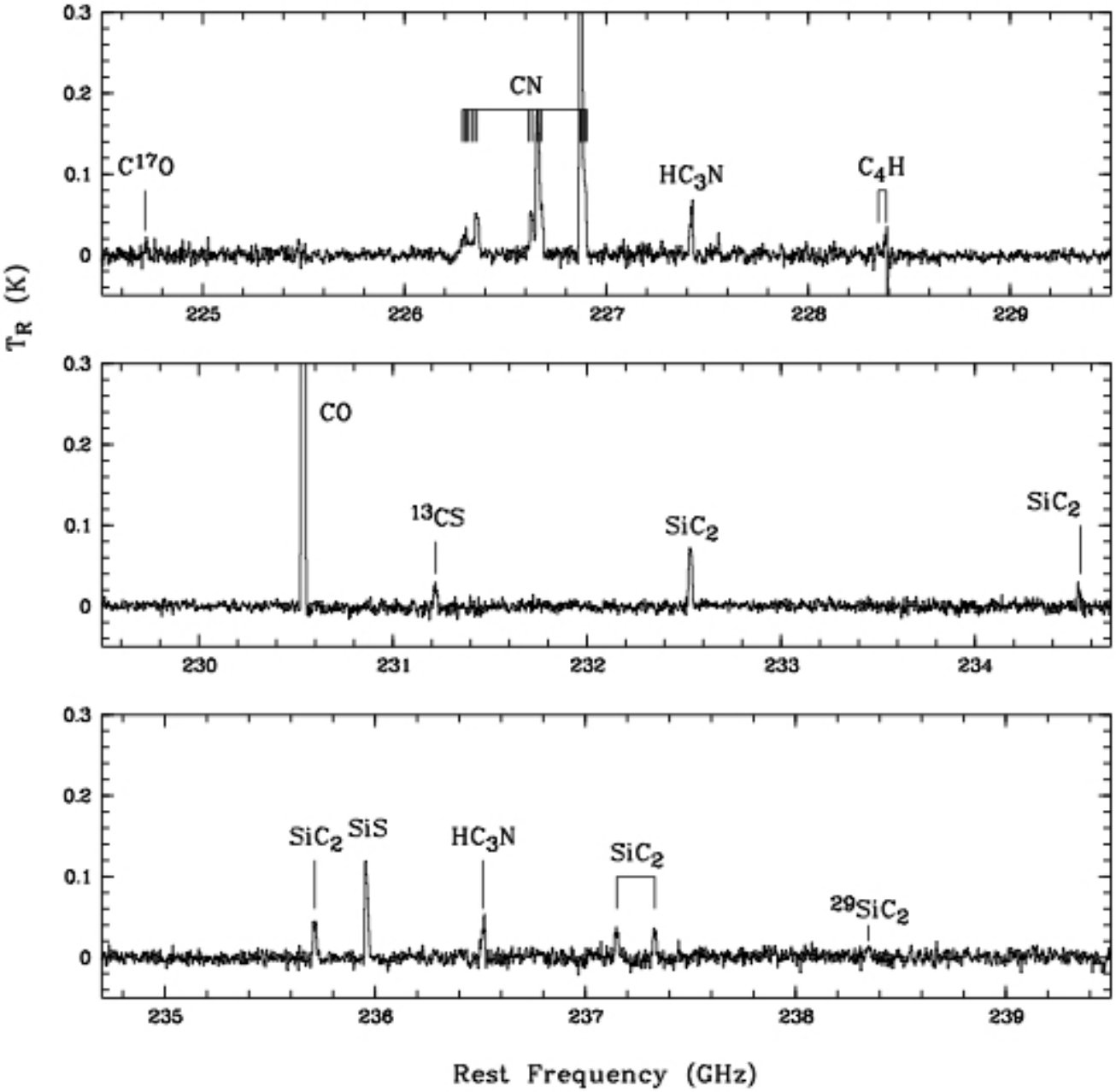
Fig. 2. ISOCAM MIR spectra of dwarf galaxies: IIZw40, NGC 1569, NGC 1140 and SBS0335-052. The horizontal lines in SBS0335-052 are broad band measurements; the dashed line is a blackbody with $A_v \sim 20$ [14]. Note the absorption attributed to amorphous silicates at ~ 9 and 18 μm.

Sub-millimeter Telescope Observatory

IRAM 30m Telescope

ALMA radio interferometer

Very Large Array (VLA) Radio Interferometer



Zhang, Kwok and Dinh-V-Trung

Table 2

List of Detected Interstellar Molecules with Two to Seven Atoms, Categorized by Number of Atoms, and Vertically Ordered by Detection Year

2 Atoms		3 Atoms		4 Atoms	5 Atoms	6 Atoms	7 Atoms
CH	CP	H_2O	N_2O	NH_3	HC_3N	CH_3OH	CH_3CHO
CN	NH	HCO^+	MgCN	H_2CO	HCOOH	CH_3CN	CH_3CCH
CH^+	SiN	HCN	$H3^+$	HNCO	CH_2NH	NH_2CHO	CH_3NH_2
OH	SO^+	OCS	SiCN	H_2CS	NH_2CN	CH_3SH	CH_2CHCN
CO	CO^+	HNC	AlNC	C_2H_2	H_2CCO	C_2H_4	HC_5N
H_2	HF	H_2S	SiNC	C_3N	C_4H	C_5H	C_6H
SiO	N_2	N_2H^+	HCP	HNCS	SiH_4	CH_3NC	c-C_2H_4O
CS	CF^+	C_2H	CCP	$HOCO^+$	c-C_3H_2	HC_2CHO	CH_2CHOH
SO	PO	SO_2	AlOH	C_3O	CH_2CN	H_2C_6	C_6H^-
SiS	O_2	HCO	H_2O^+	l-C_3H	C_5	C_5S	CH_3NCO
NS	AlO	HNO	H_2Cl^+	$HCNH^+$	SiC_4	HC_3NH^+	HC_5O
C_2	CN^-	HCS^+	KCN	H_3O^+	H_2CCC	C_5N	
NO	OH^+	HOC^+	FeCN	C_3S	CH_4	HC_4H	
HCl	SH^+	SiC_2	HO_2	c-C_3H	HCCNC	HC_4N	
NaCl	HCl^+	C_2S	TiO_2	HC_2N	HNCCC	c-H_2C_3O	
AlCl	SH	C_3	CCN	H_2CN	H_2COH^+	CH_2CNH	
KCl	TiO	CO_2	SiCSi	SiC_3	C_4H^-	C_5N^-	
AlF	ArH^+	CH_2	S_2H	CH_3	CNCHO	HNCHCN	
PN	NS^+	C_2O	HCS	C_3N^-	HNCNH	SiH_3CN	
SiC		MgNC	HSC	PH_3	CH_3O		
		NH_2	NCO	HCNO	NH_3D^+		
		NaCN		HOCN	H_2NCO^+		
				HSCN	$NCCNH^+$		
				HOOH	CH_3Cl		
				l-C_3H^+			
				HMgNC			
				HCCO			
				CNCN			

Note. Column headers and molecule formulas are in-document hyperlinks in most PDF viewers.

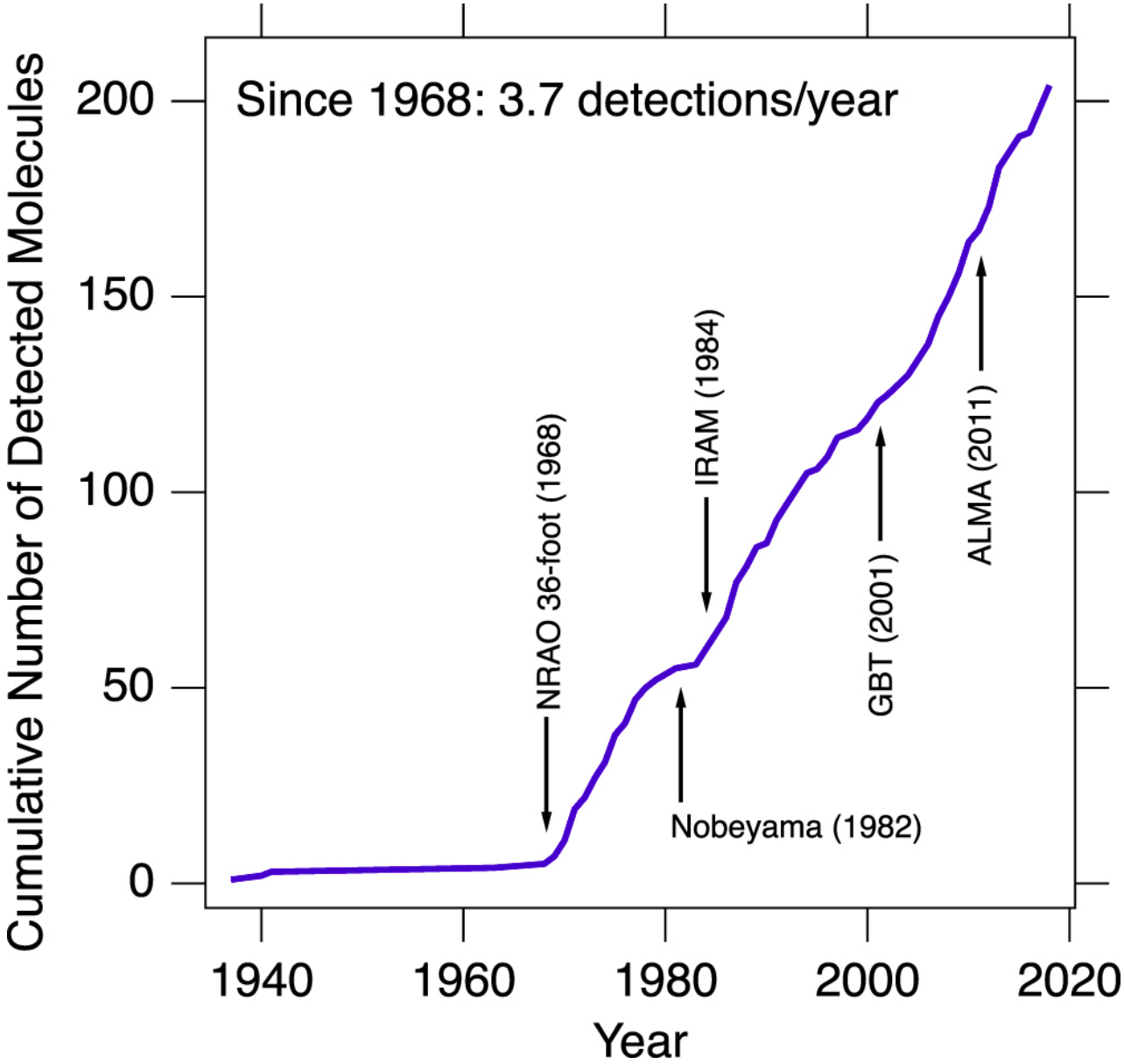
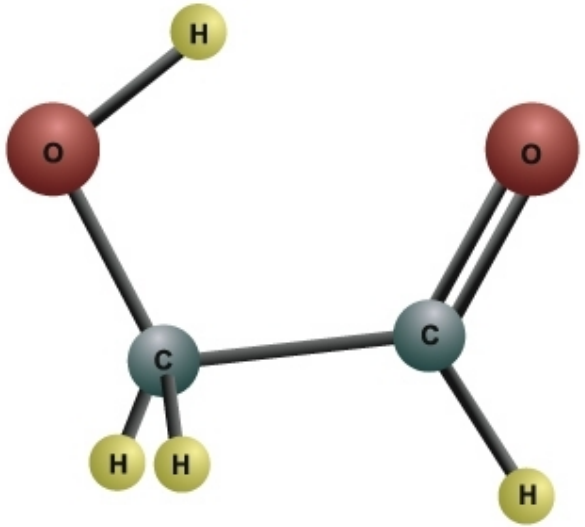

Since 1968: 3.7 detections/year
Cumulative Number of Detected Molecules
200
150
100
50
0
1940
1960
1980
2000
2020
Year
NRAO 36-foot (1968)
IRAM (1984)
Nobeyama (1982)
GBT (2001)
ALMA (2011)

Table 4.1 *Generic gas phase reactions and their rates*

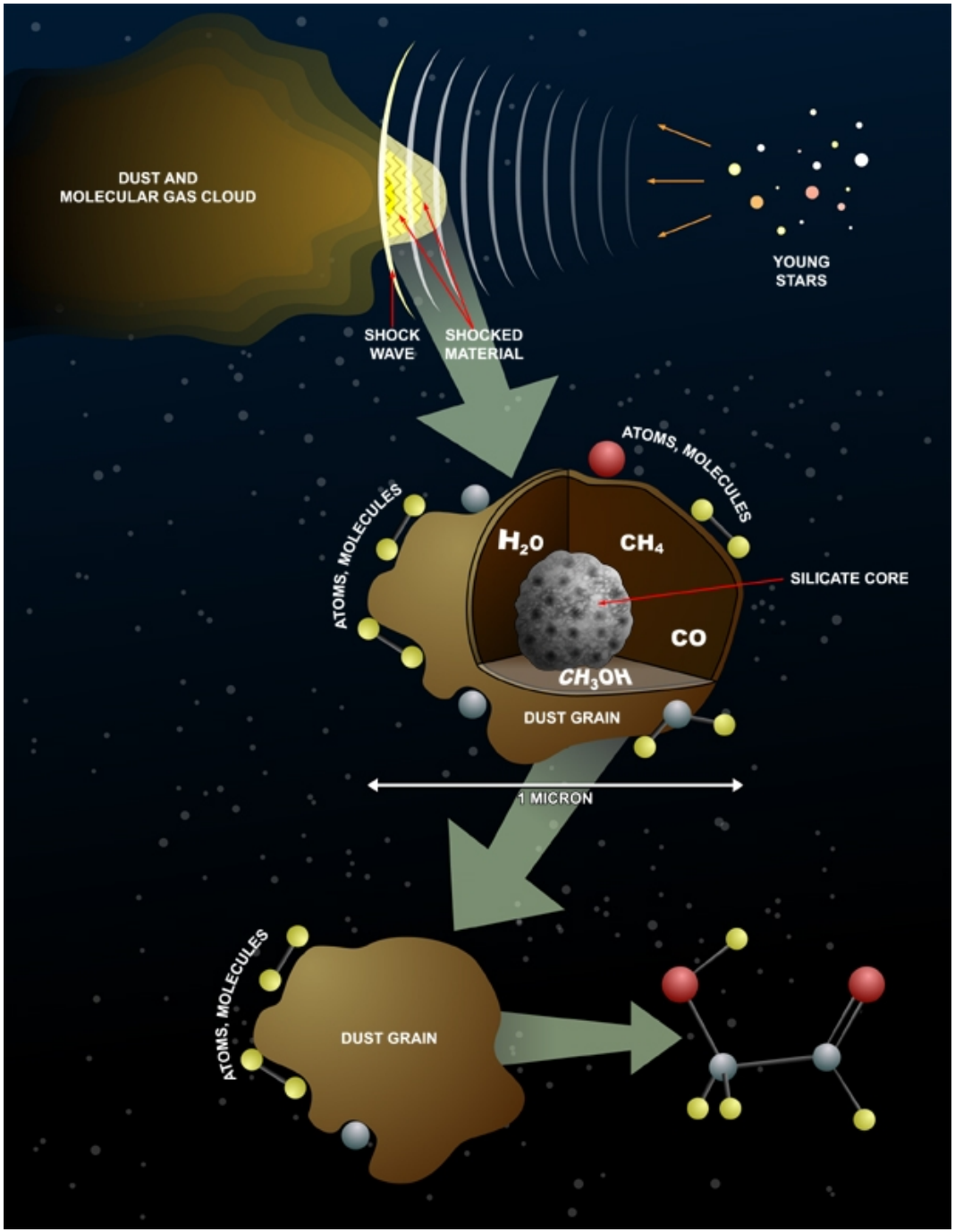
	reaction	rate	unit	note
Photodissociation	$AB + h\nu \rightarrow A + B$	10^{-9}	s^{-1}	(*a*)
Neutral–neutral	$A + B \rightarrow C + D$	4×10^{-11}	$cm^3\,s^{-1}$	(*b*)
Ion–molecule	$A^+ + B \rightarrow C^+ + D$	2×10^{-9}	$cm^3\,s^{-1}$	(*c*)
Charge-transfer	$A^+ + B \rightarrow A + B^+$	10^{-9}	$cm^3\,s^{-1}$	(*c*)
Radiative association	$A + B \rightarrow AB + h\nu$			(*d*)
Dissociative recombination	$A^+ + e \rightarrow C + D$	10^{-7}	$cm^3\,s^{-1}$	
Collisional association	$A + B + M \rightarrow AB + M$	10^{-32}	$cm^6\,s^{-1}$	(*c*)
Associative detachment	$A^- + B \rightarrow AB + e$	10^{-9}	$cm^3\,s^{-1}$	(*c*)

(*a*) Rate in the unshielded radiation field.
(*b*) Rate in the exothermic direction and assuming no activation barrier (i.e., radical–radical reaction).
(*c*) Rate in the exothermic direction.
(*d*) Rate highly reaction specific.

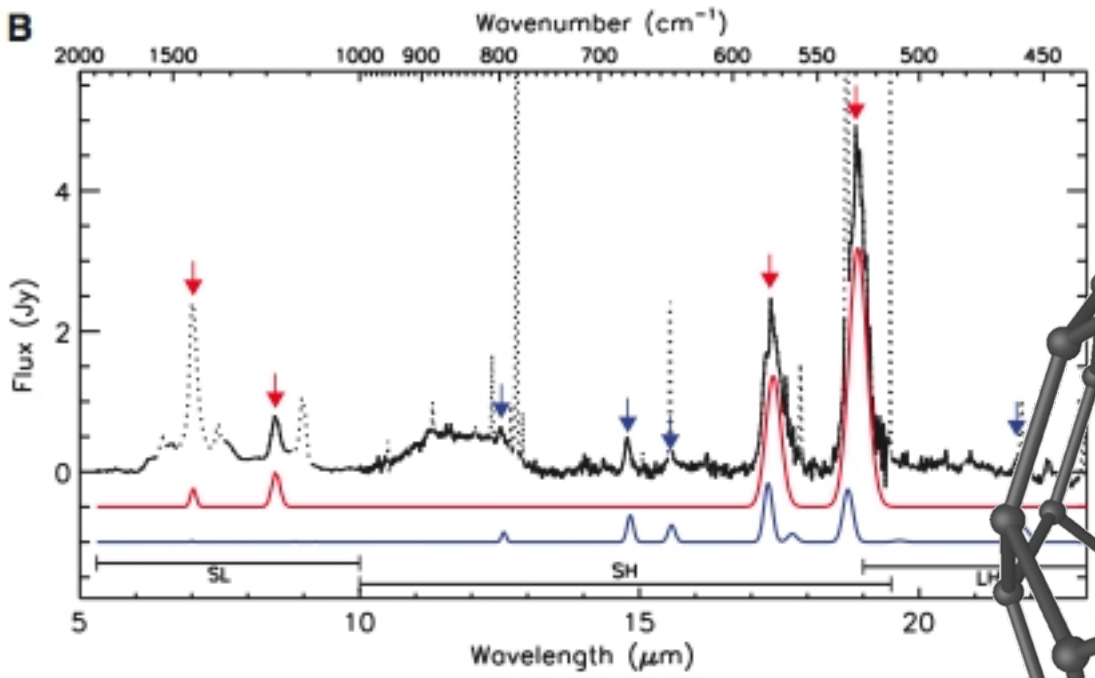
Surface chemistry

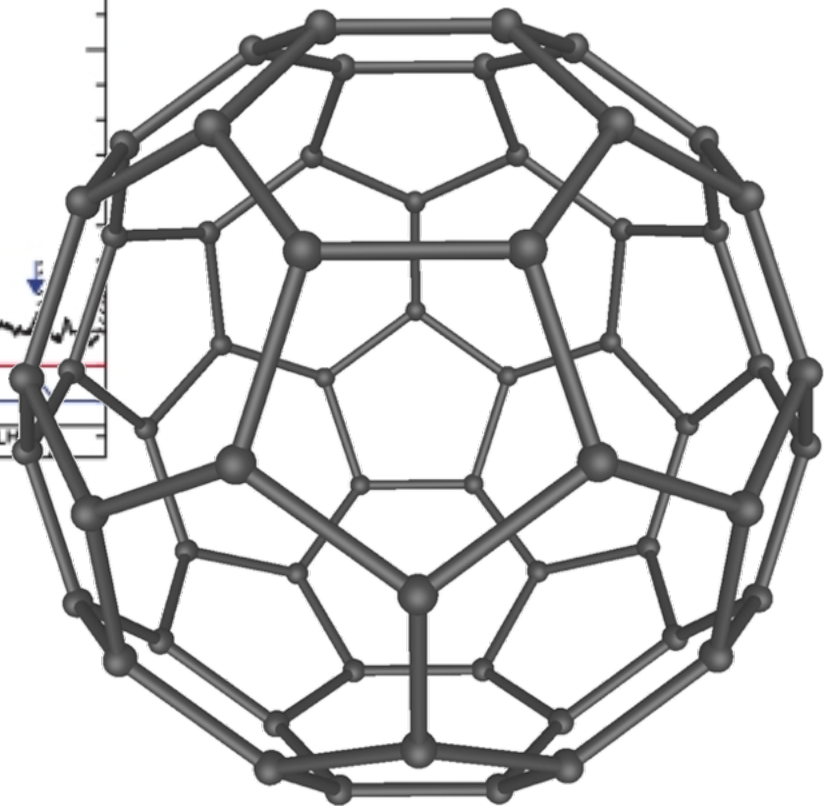


GLYCOLALDEHYDE

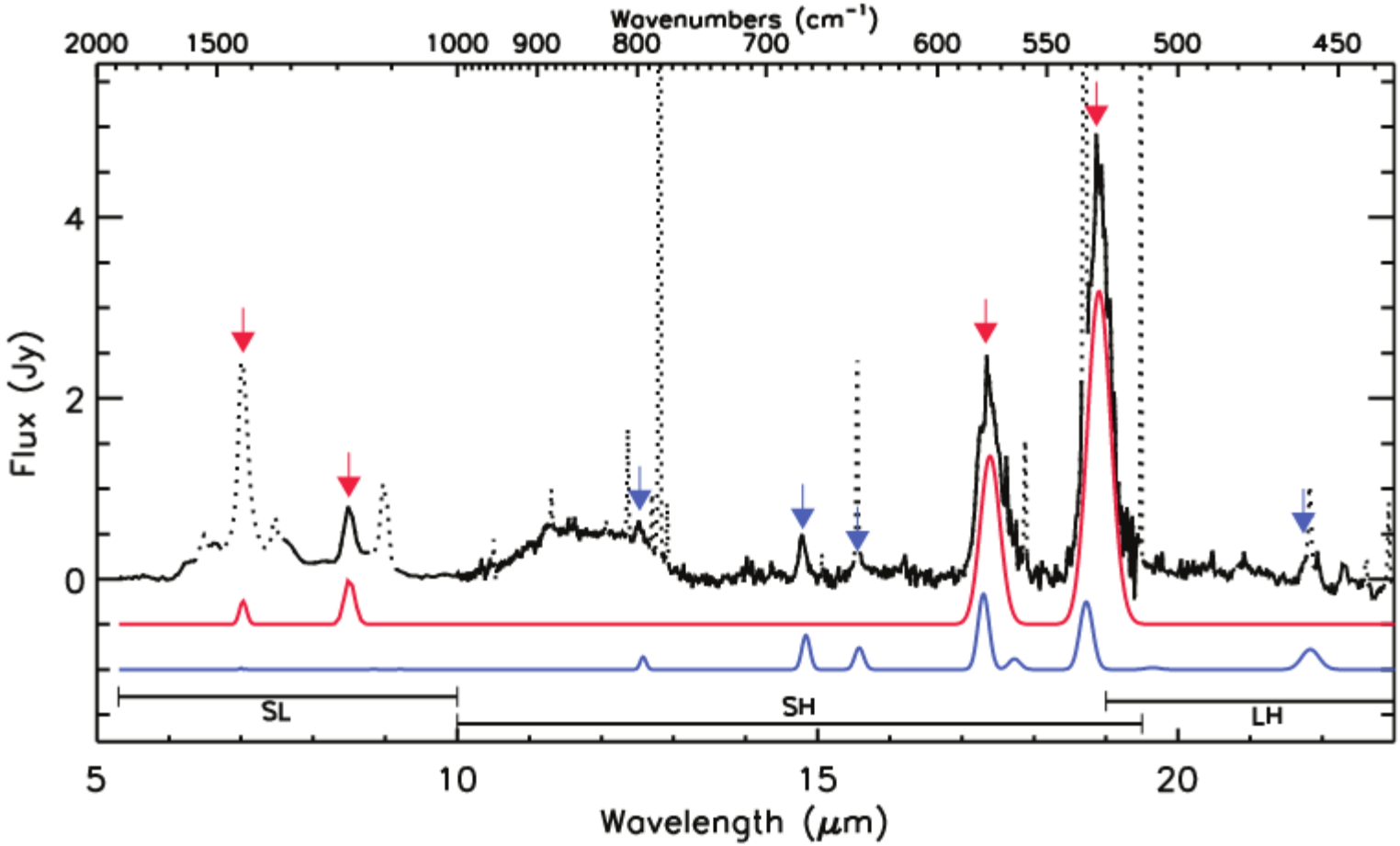


Complex molecules such as C60 can form around stars





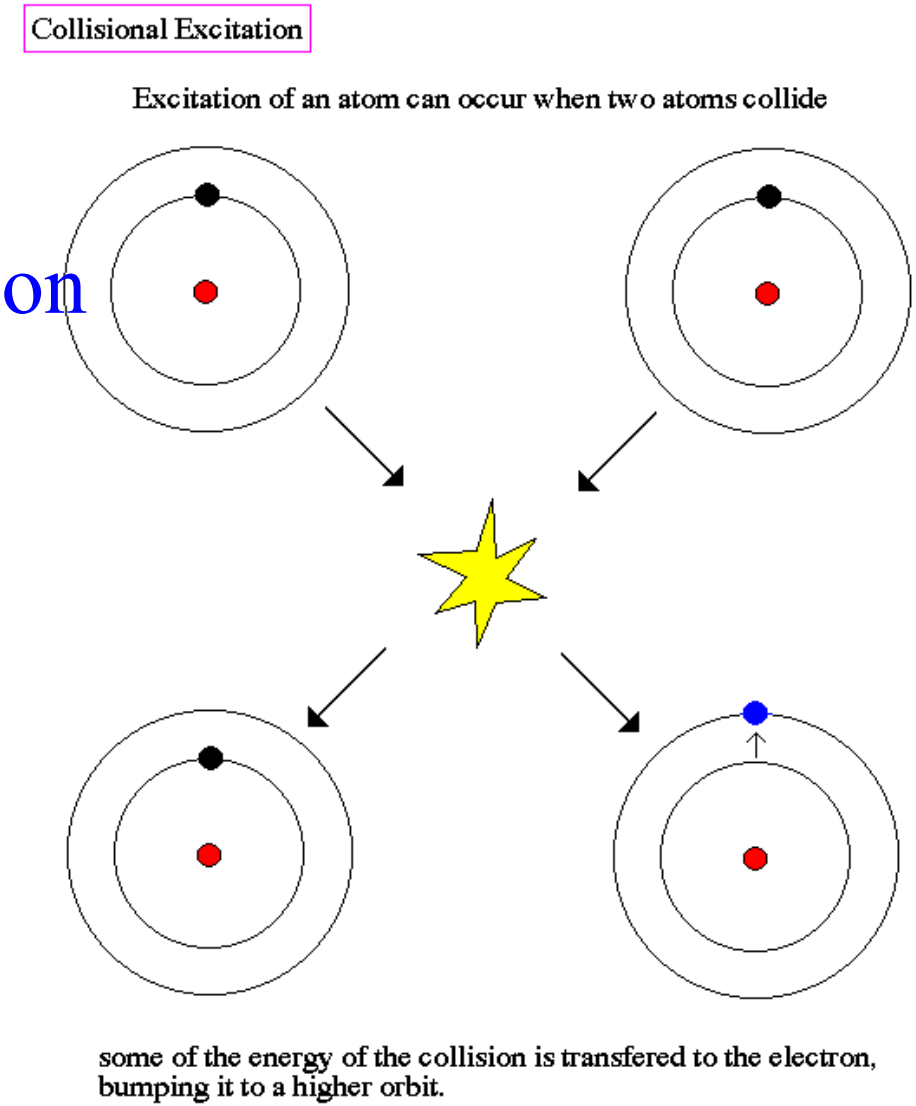
Fullerene C_{60}



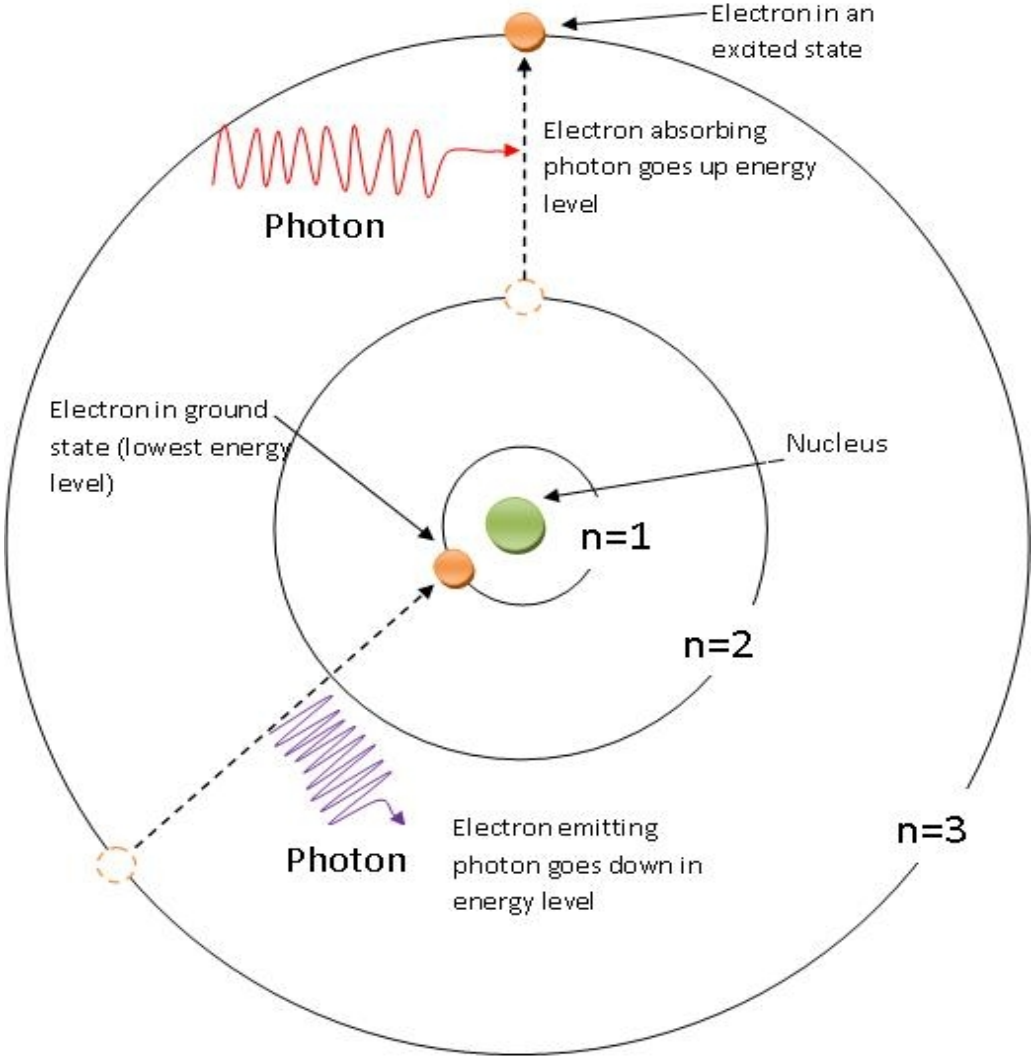
First detection of C_{60} and C_{70} in Spitzer observations of the young PN Tc1
(Cami et al., 2010, Science, 329, 1180)

Excitation of atoms and molecules

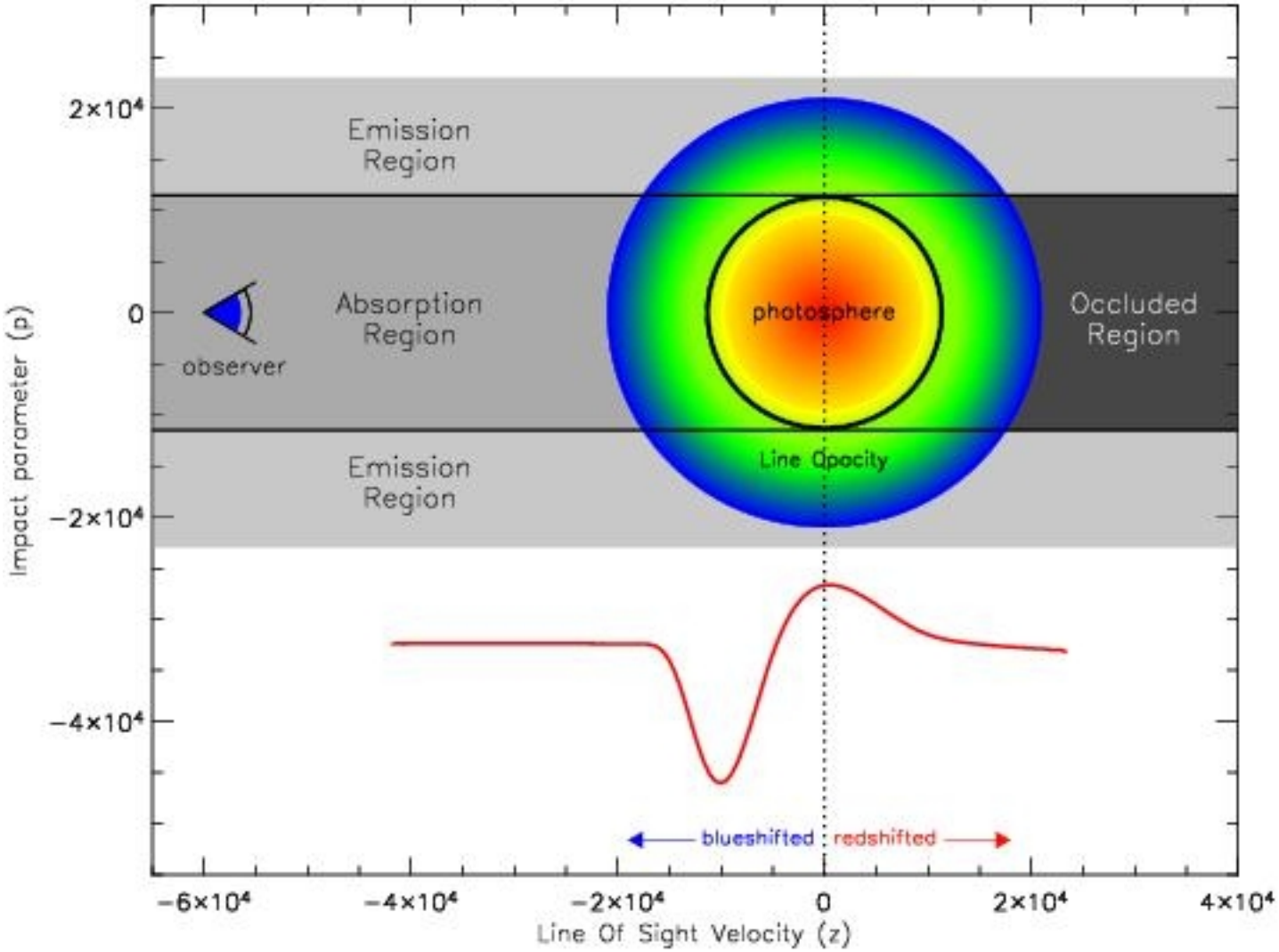
- Collision
- Absorption of radiation



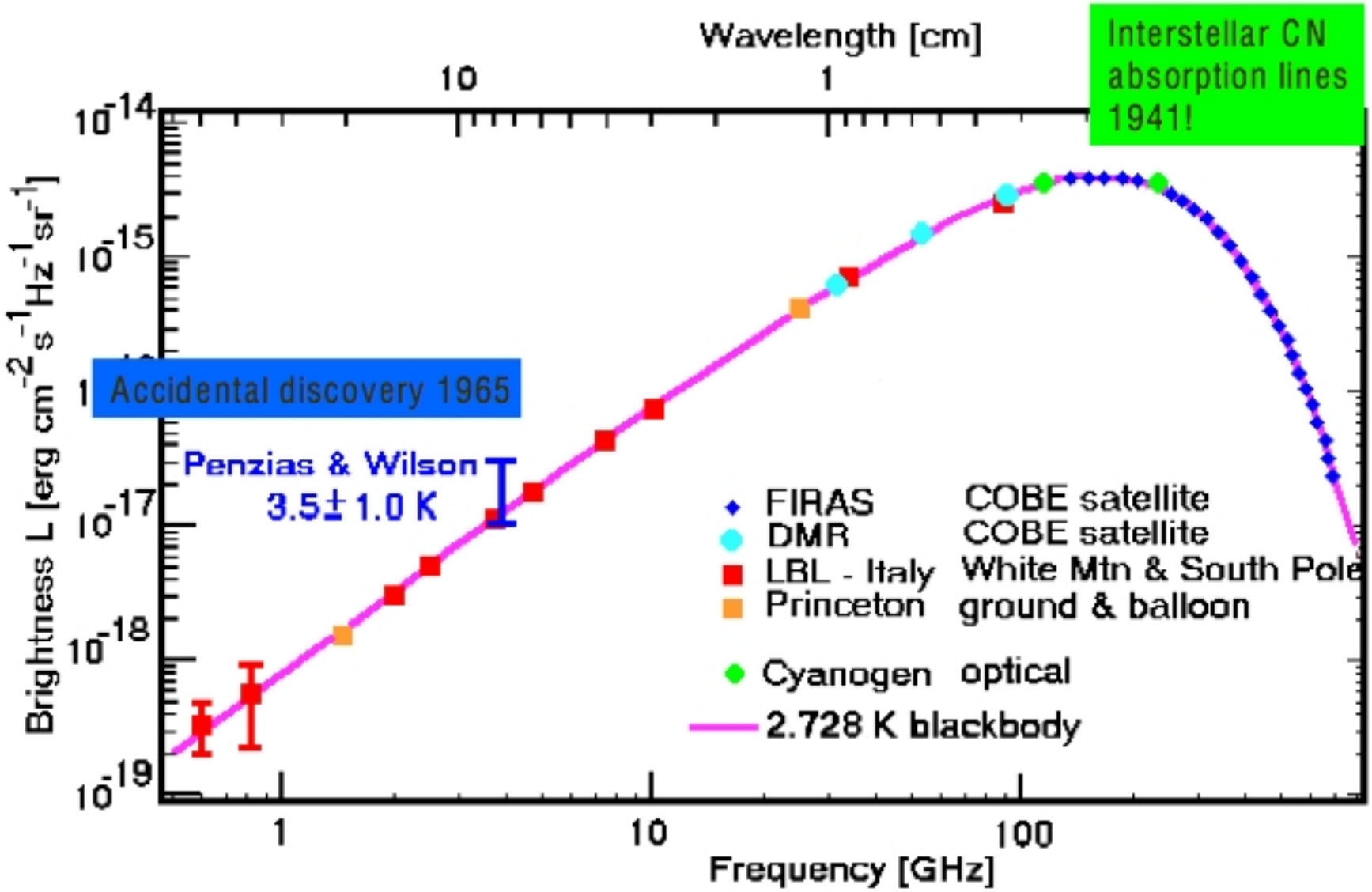
Radiative excitation

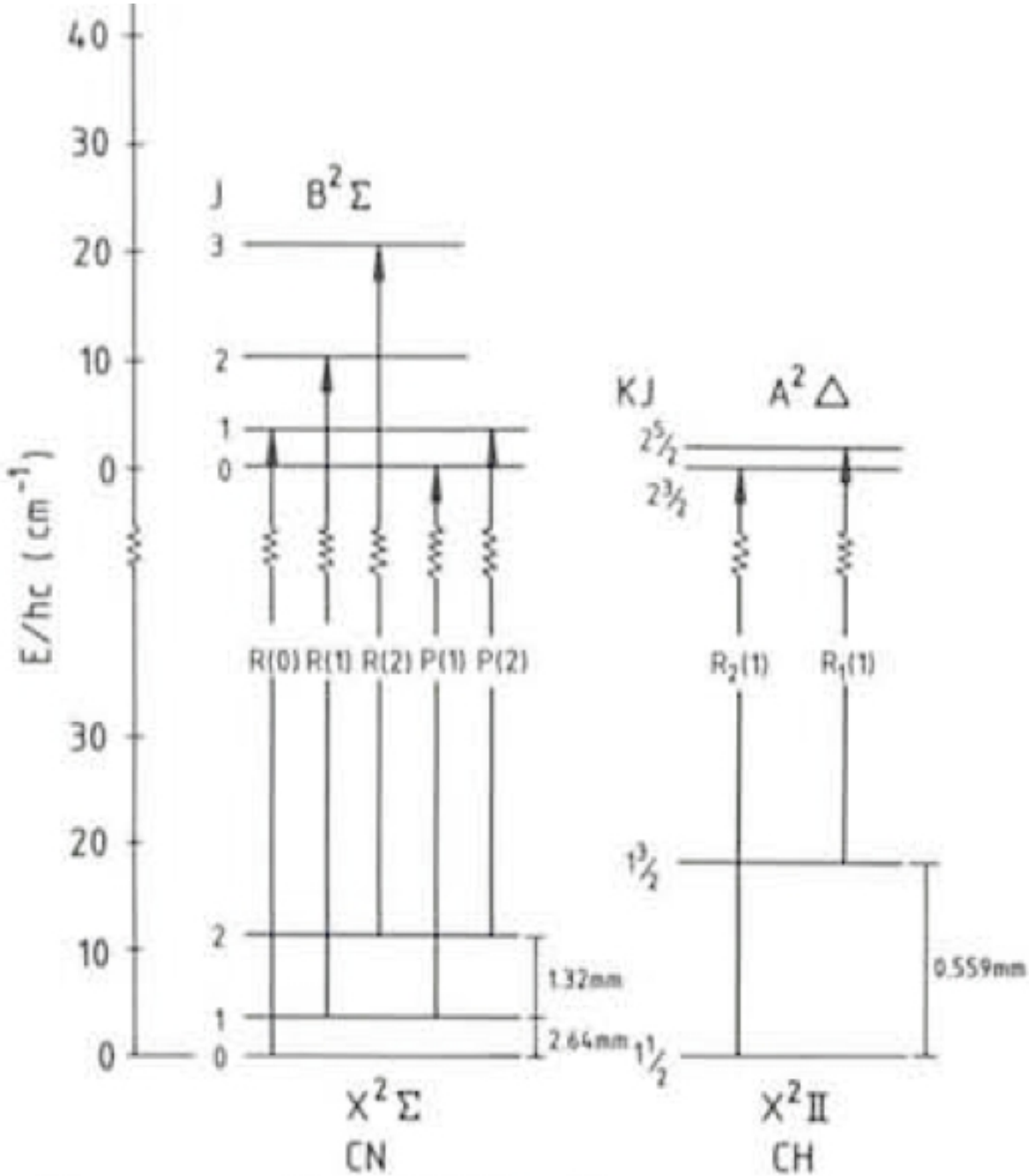


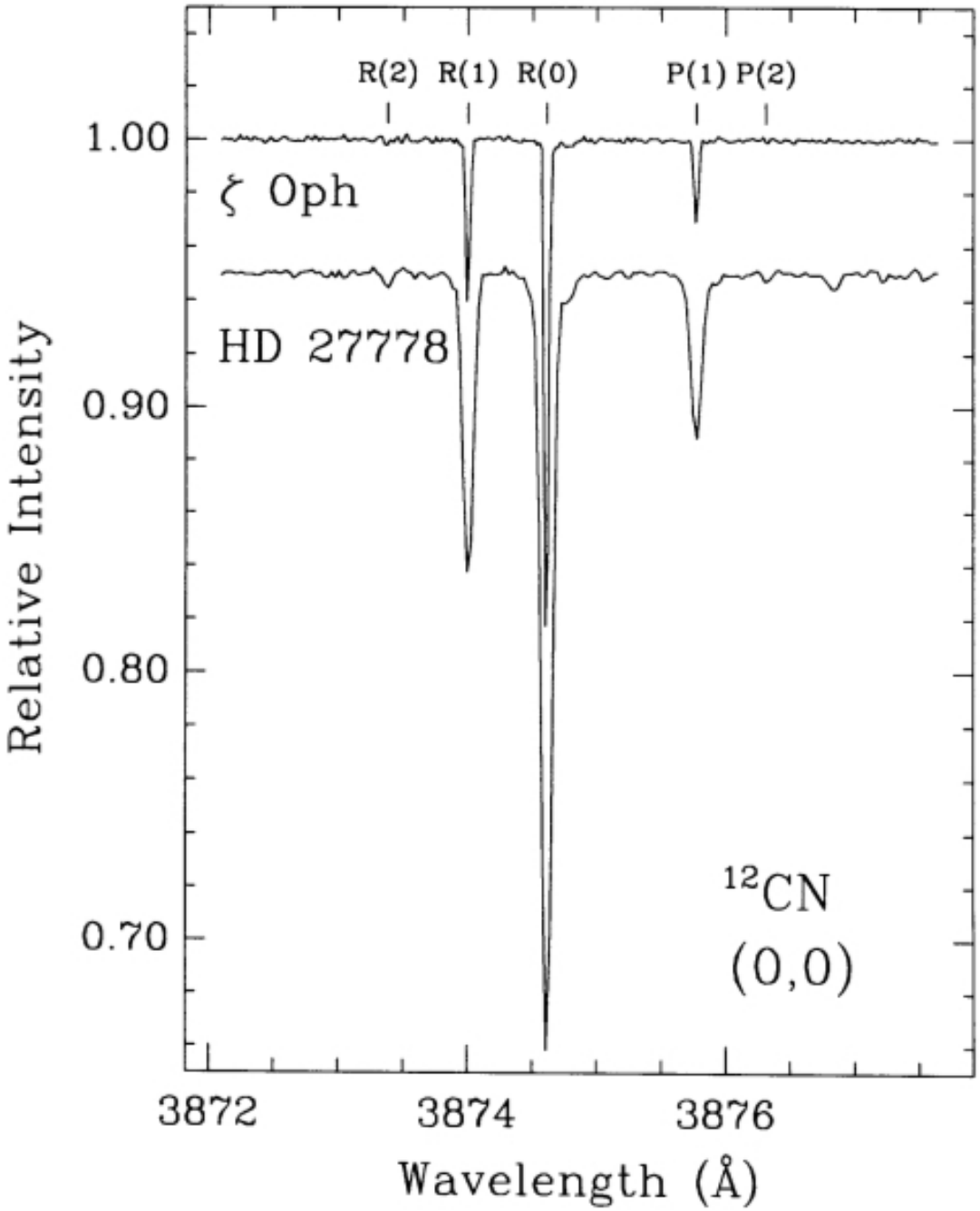
Spectral line formation



CN absorption lines and the determination of CMB brightness temperature

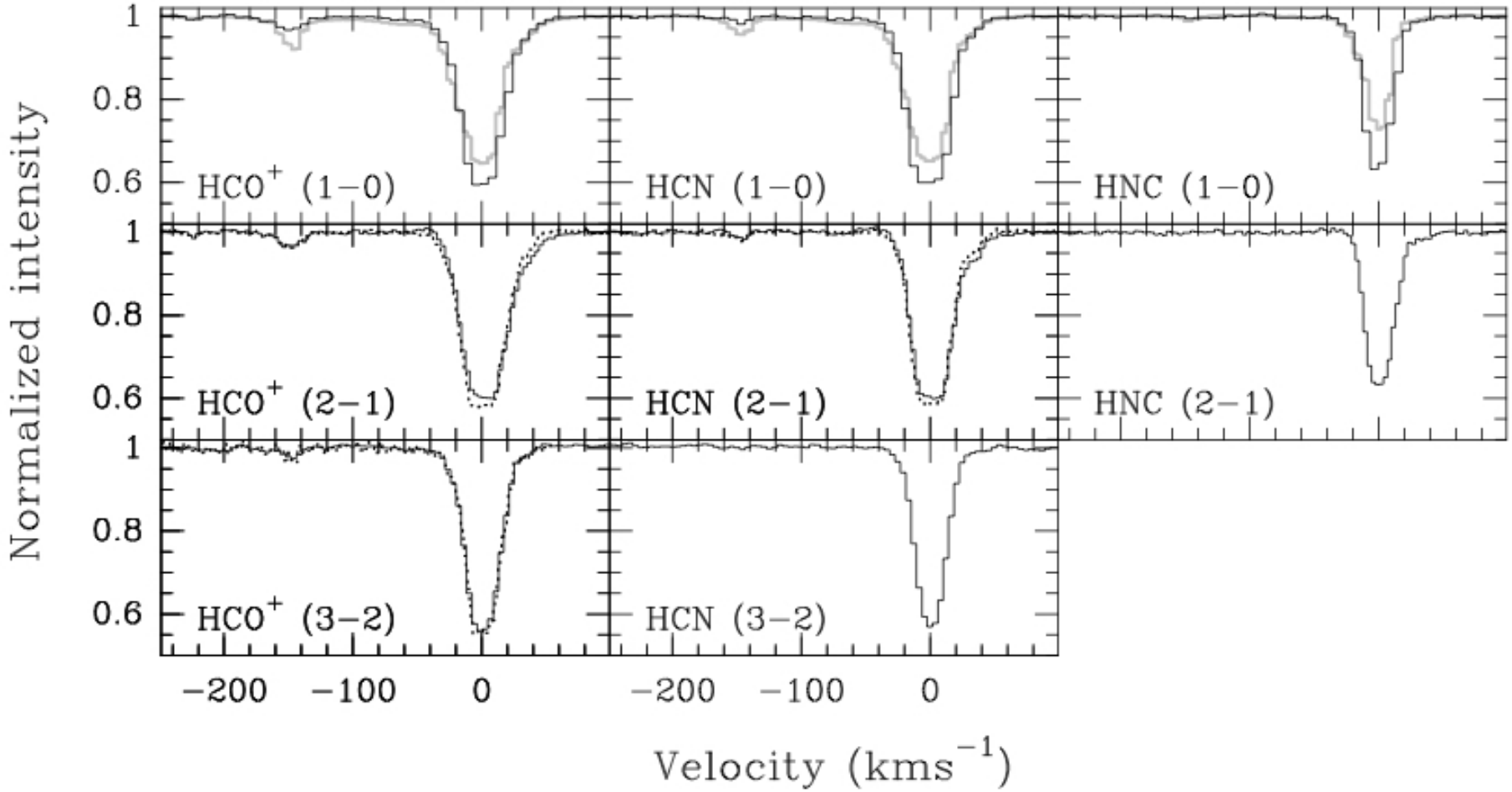


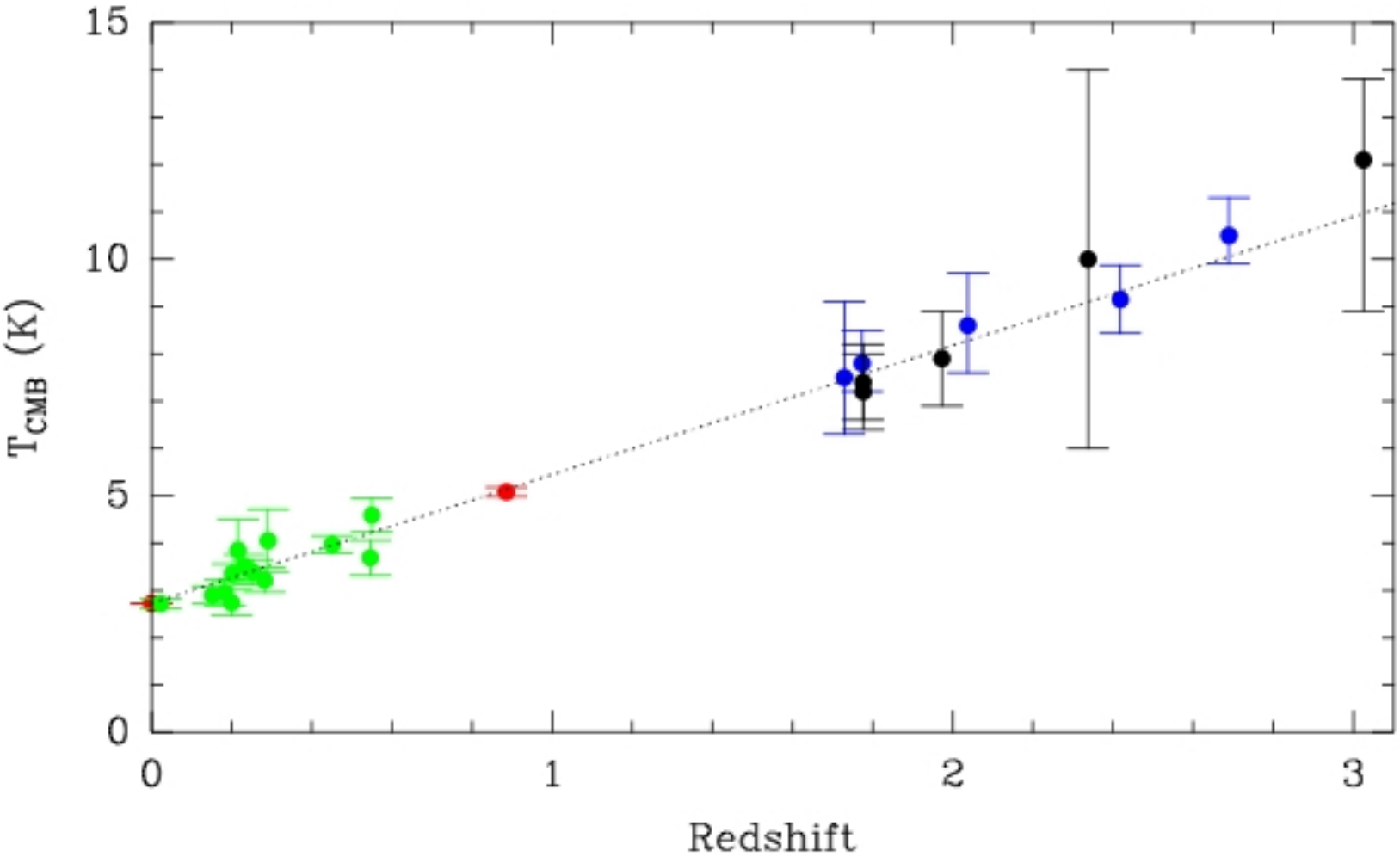

E/hc (cm⁻¹)
40
30
20
10
0
J
B²Σ
3
2
1
0
R(0) R(1) R(2) P(1) P(2)
30
20
10
0
2
1
0
1.32mm
2.64mm
X²Σ
CN
KJ
A²Δ
2 5/2
2 3/2
R₂(1)
R₁(1)
1 3/2
1 1/2
0.559mm
X²Π
CH


R(2) R(1) R(0) P(1) P(2)
1.00
0.90
0.80
0.70
ζ Oph
HD 27778
Relative Intensity
^{12}CN
(0,0)
3872
3874
3876
Wavelength (Å)

T_{ex} = 2.729 K !!!

Absorption lines seen toward Lensed Quasar at z=0.89

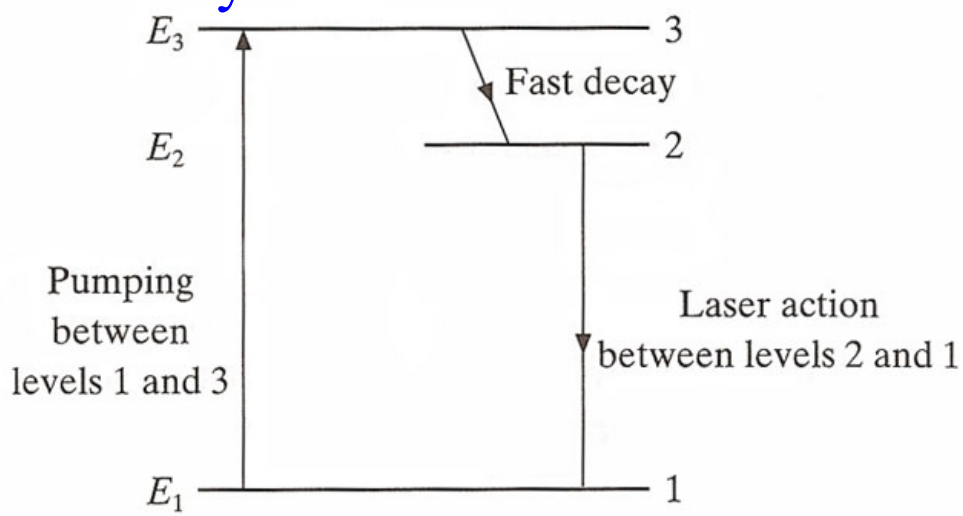



15
10
5
0
0
1
2
3
T_{CMB} (K)
Redshift

Creating a Population Inversion

- Under normal conditions of thermal equilibrium, the number of particles in lower energy levels is always greater than the number in higher energy levels. This leads to radiation being absorbed rather than amplified.

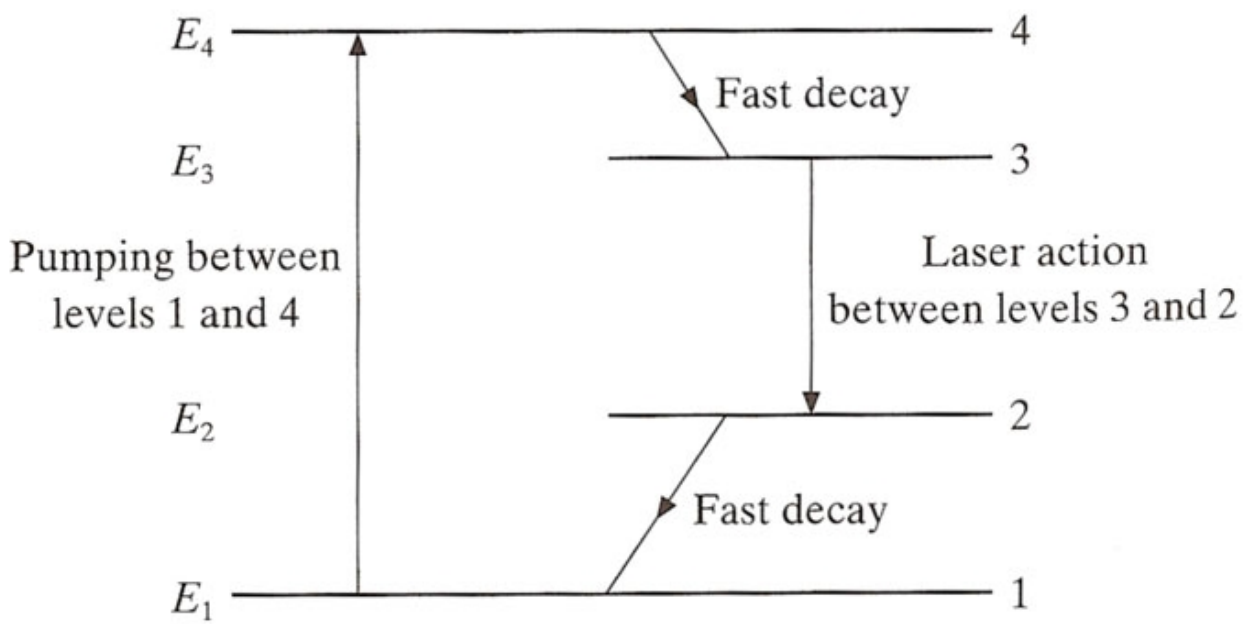
- One requirement in creating an inversion is "pumping", either collisionally or radiatively.



Principle of the three-level laser.

Creating a Population Inversion

- Three-level pumping is difficult. It takes a LOT to get more than half of the atoms/molecules in level 2.
- The easier solution is four-level pumping.

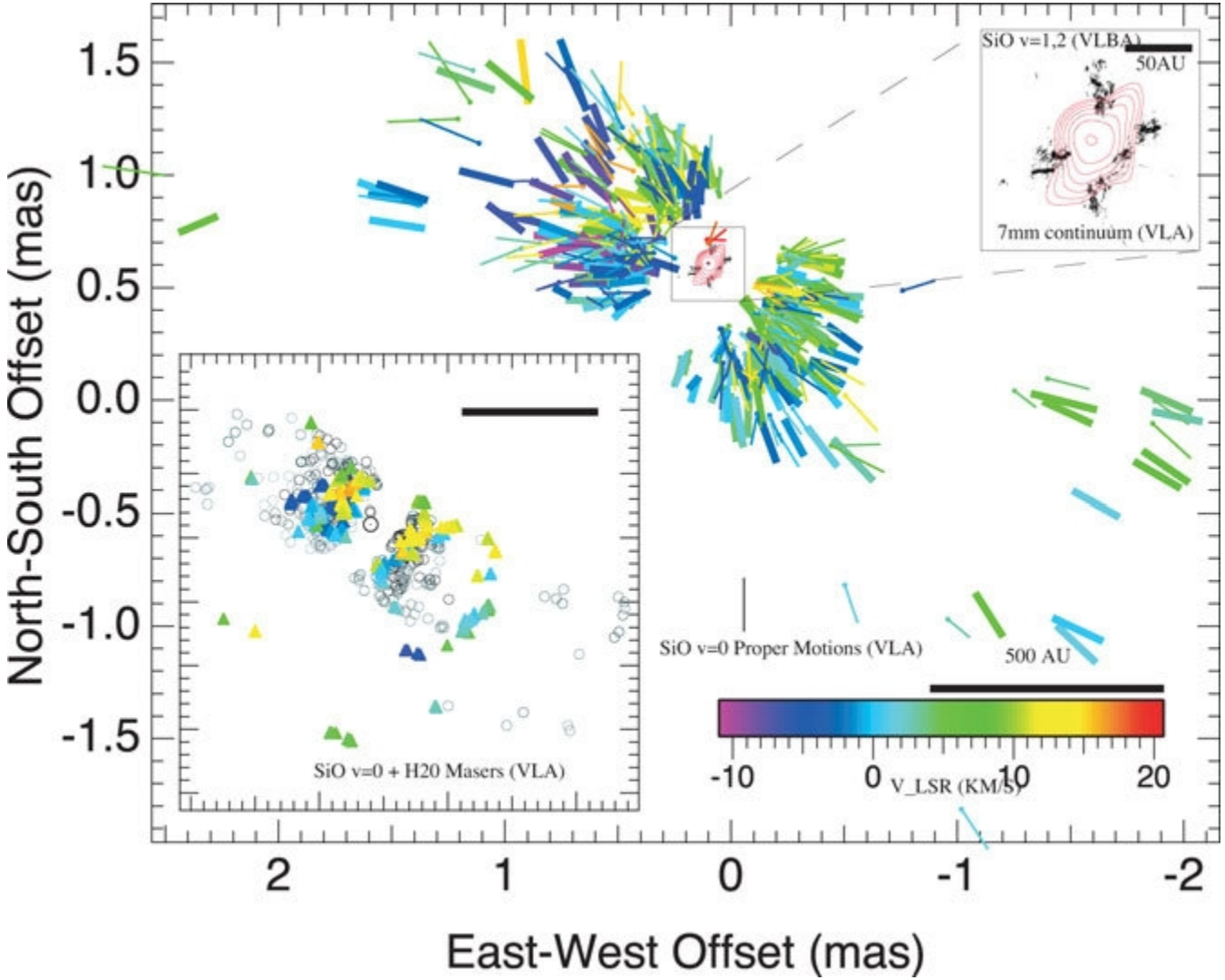


Principle of the four-level laser.

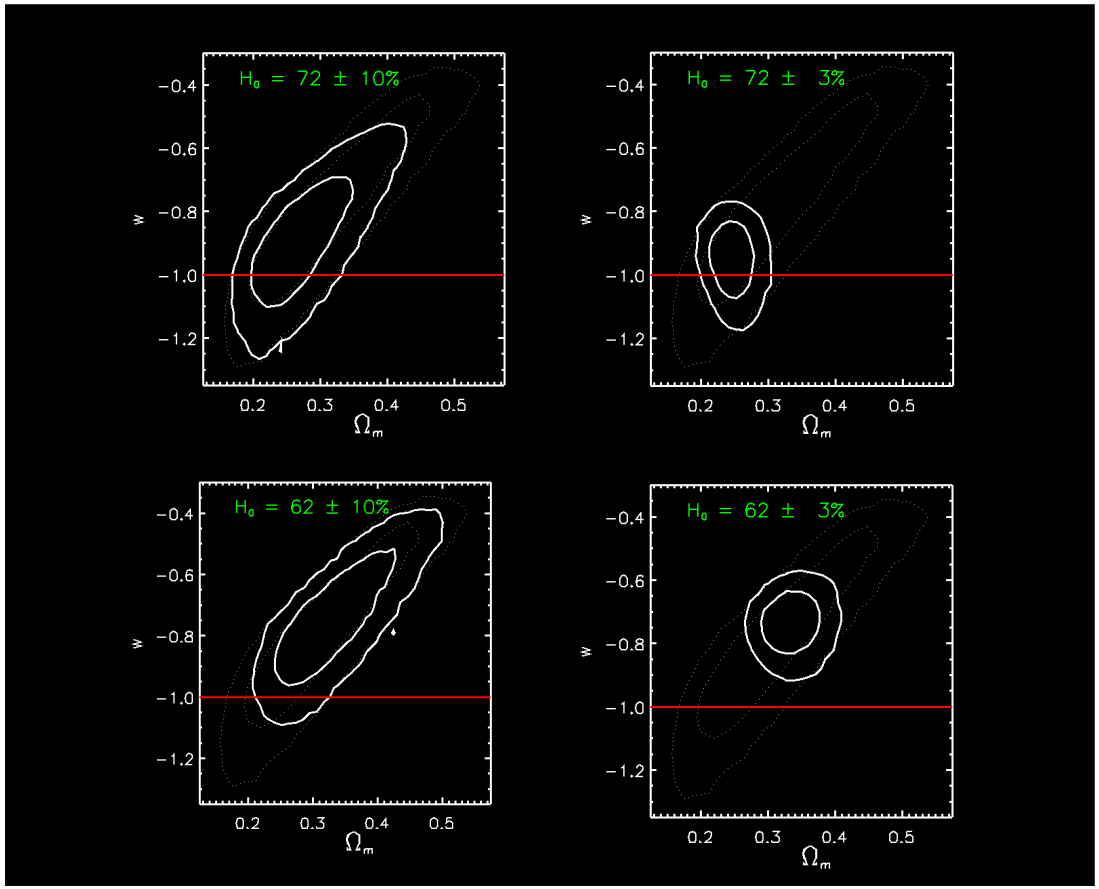
Molecules Known to Exhibit Maser Emission

- OH (hydroxyl)
- H_2O
- SiO
- CH
- H_2CO
- CH_3OH (methanol)
- NH_3
- HC_3N
- HCN

Proper motion of SiO masers in Orion KL young stellar object



The Impact of an H_0 Prior on CMB Models



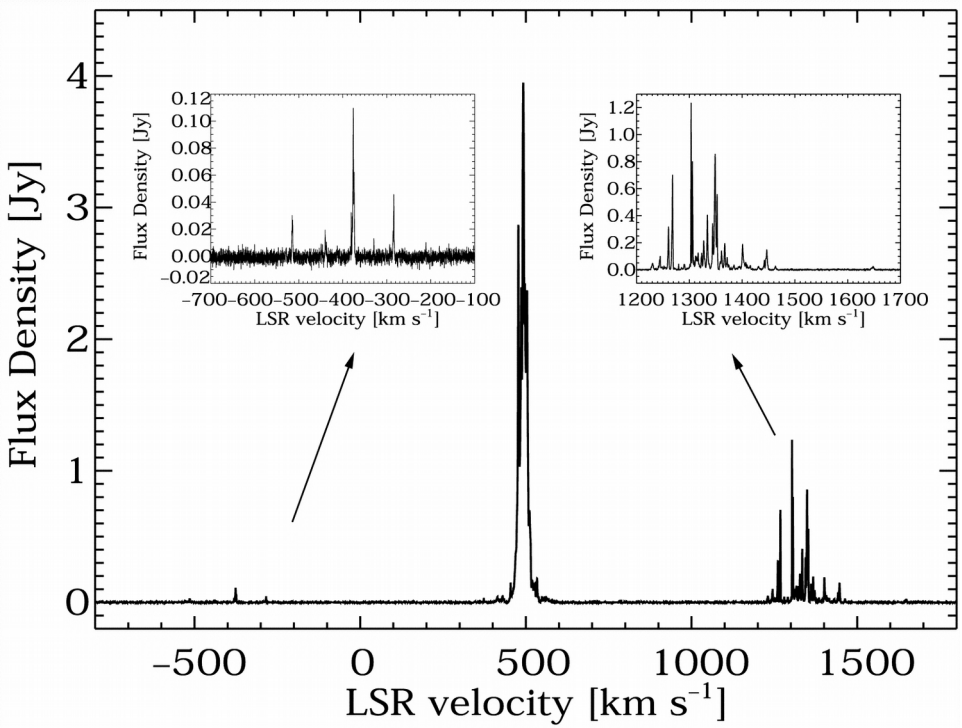
$H_0 = 72 \pm 3_r \pm 7_s$ km s^{-1} Mpc^{-1}

Freedman et al. 2001

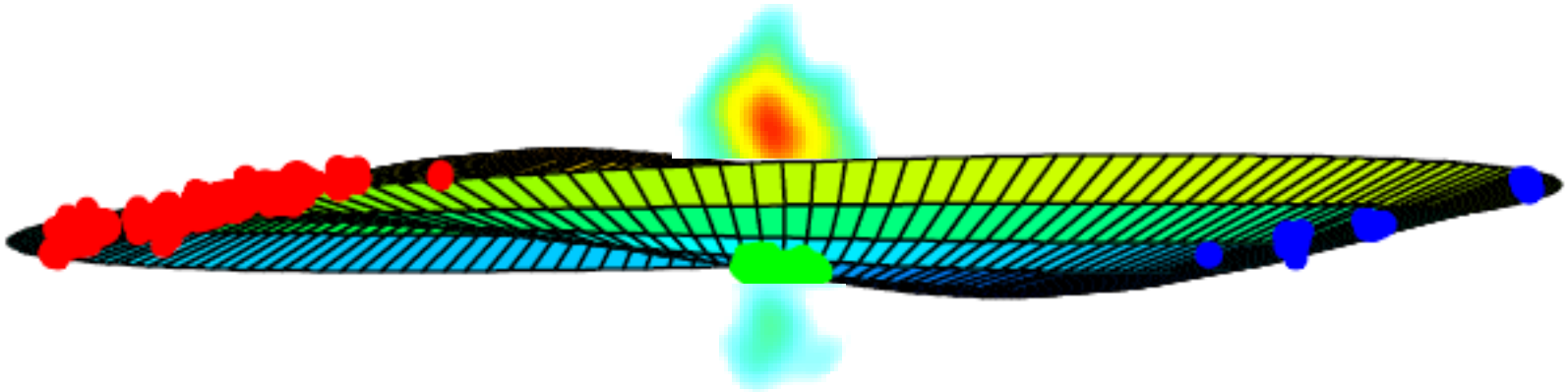
$H_0 = 62 \pm 1_r \pm 5_s$ km s^{-1} Mpc^{-1}

Sandage et al. 2006

WMAP Likelihood Surfaces



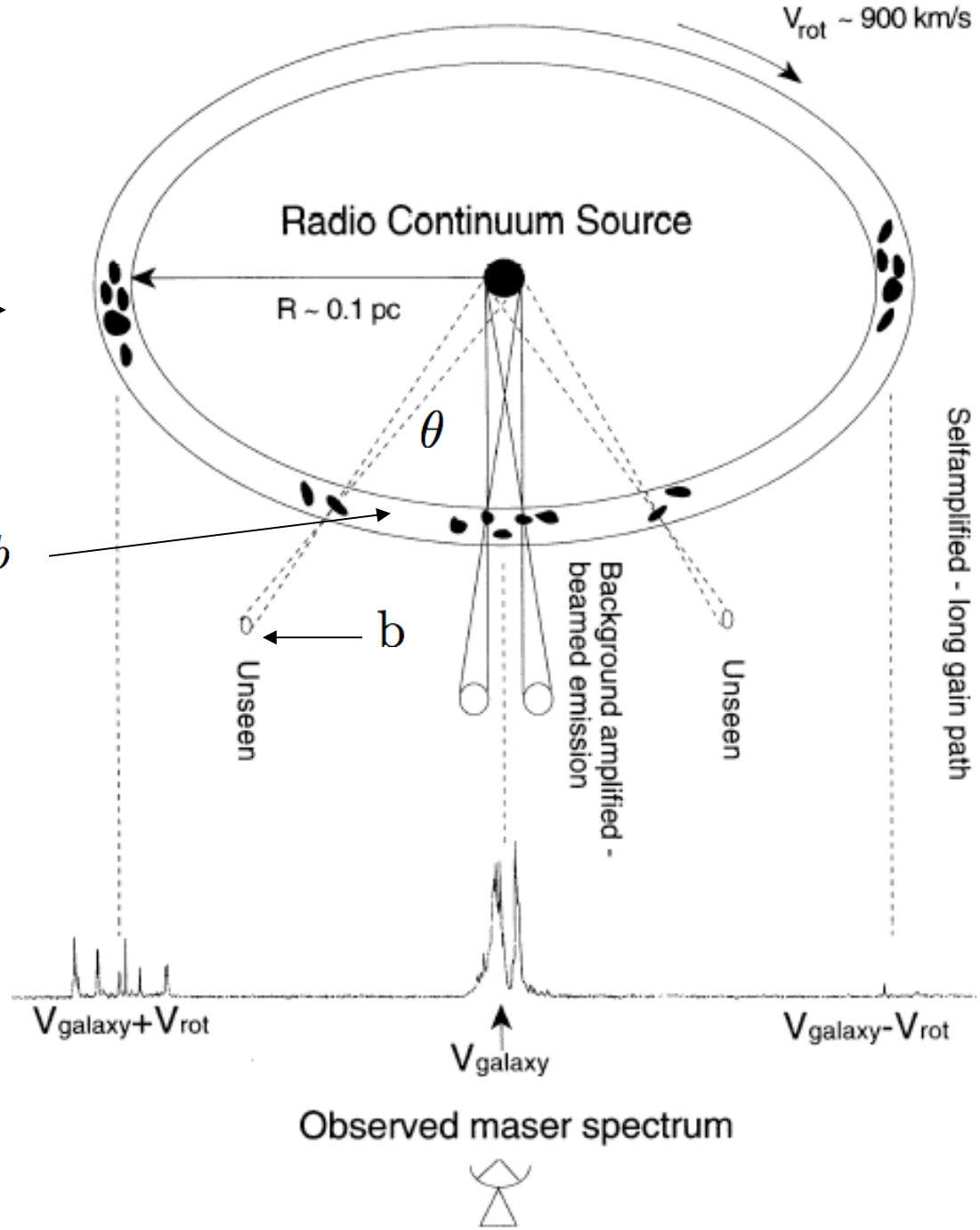
The Archetype: NGC 4258



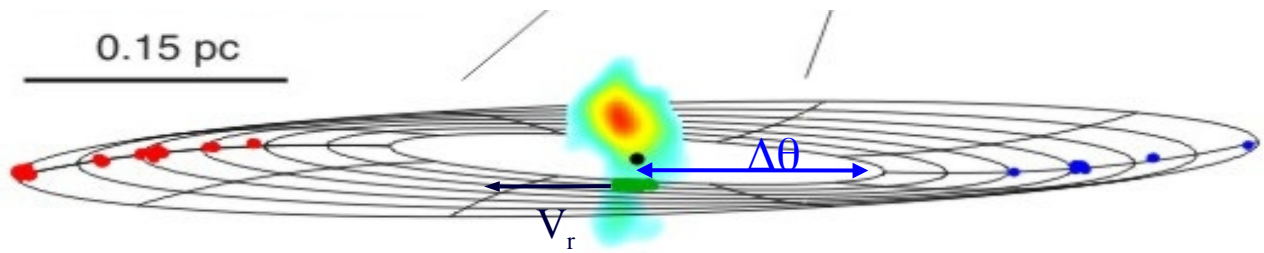
$$V_z = \sqrt{\frac{GM}{R}} \sin\theta$$

$$V_z = \sqrt{\frac{GM}{R}}$$

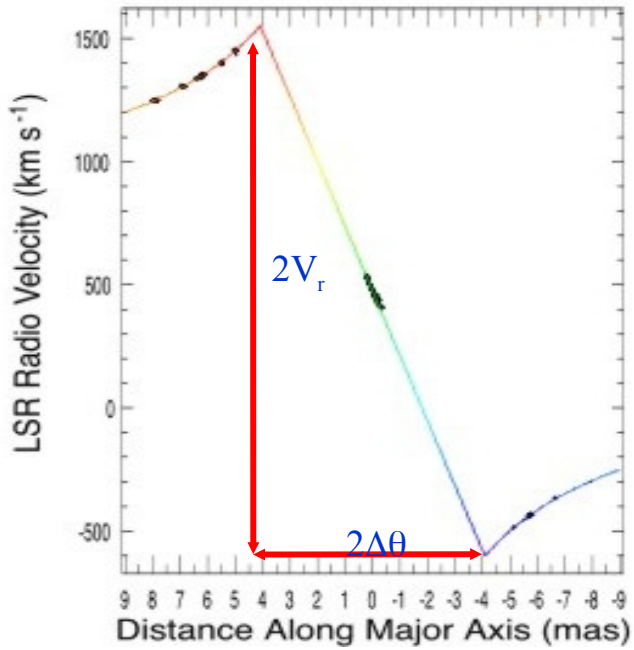
$$V_z = \sqrt{\frac{GM}{R}}\,\frac{b}{R} = \sqrt{\frac{GM}{R^3}}\; b$$



Measuring Distances to H_2O Megamasers



NGC 4258



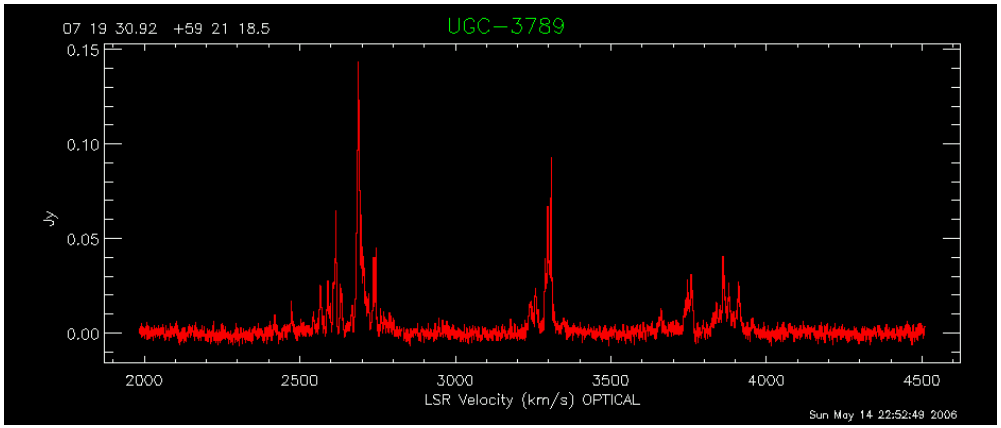
$D = r/\Delta\theta$

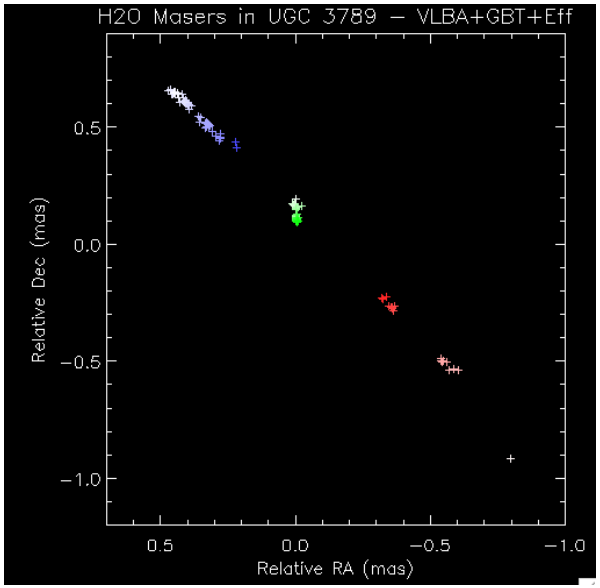
$a = V_r^2/r$

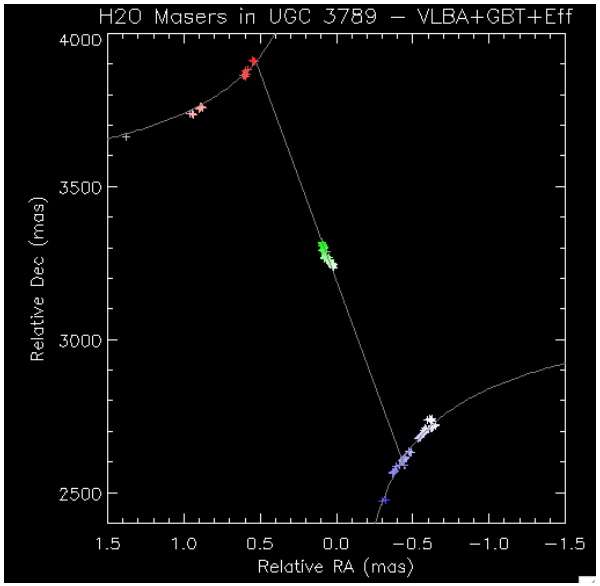
$D = V_r^2/a\Delta\theta$

$D = 7.2 \pm 0.5$ Mpc

UGC 3789



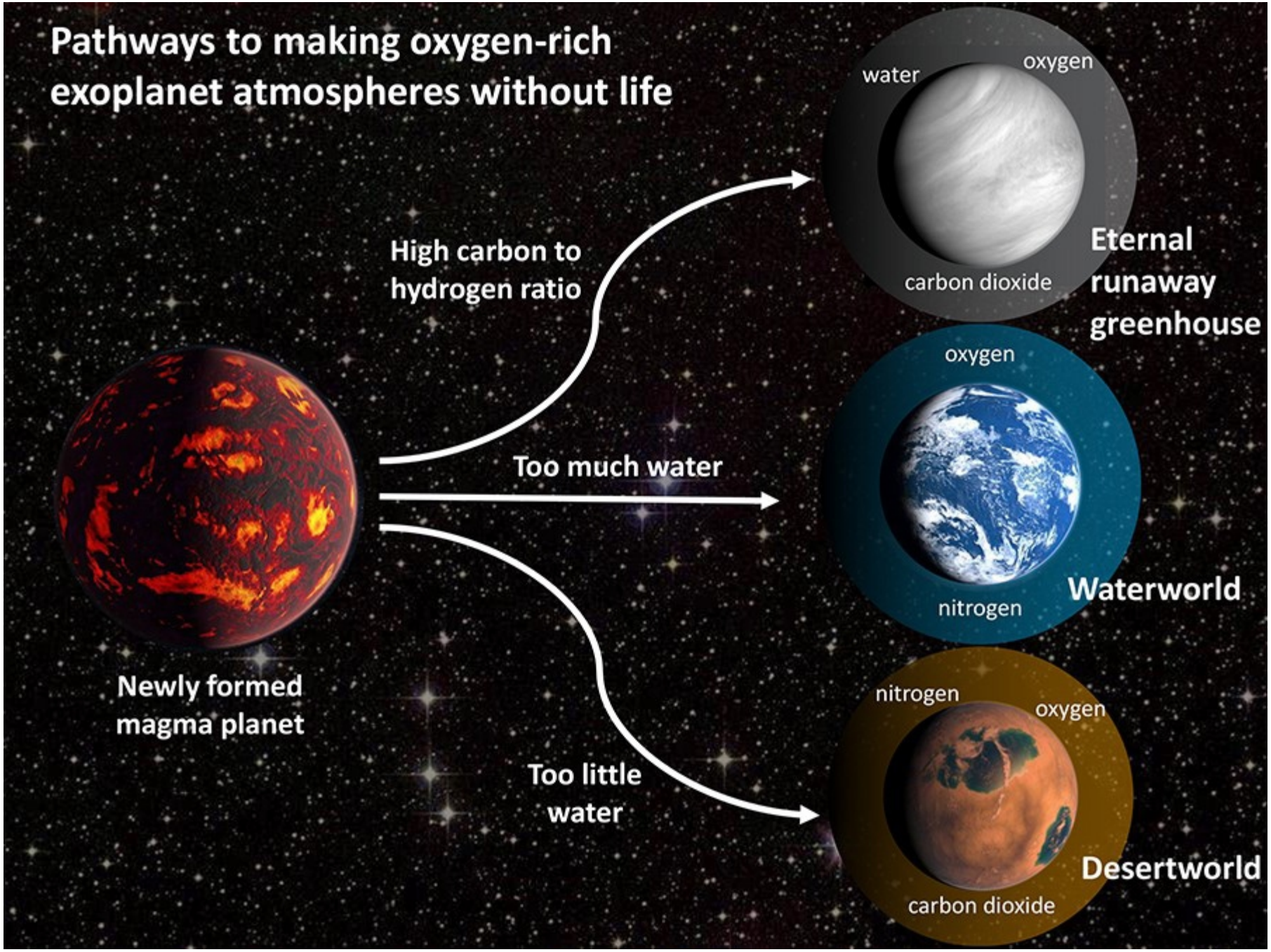


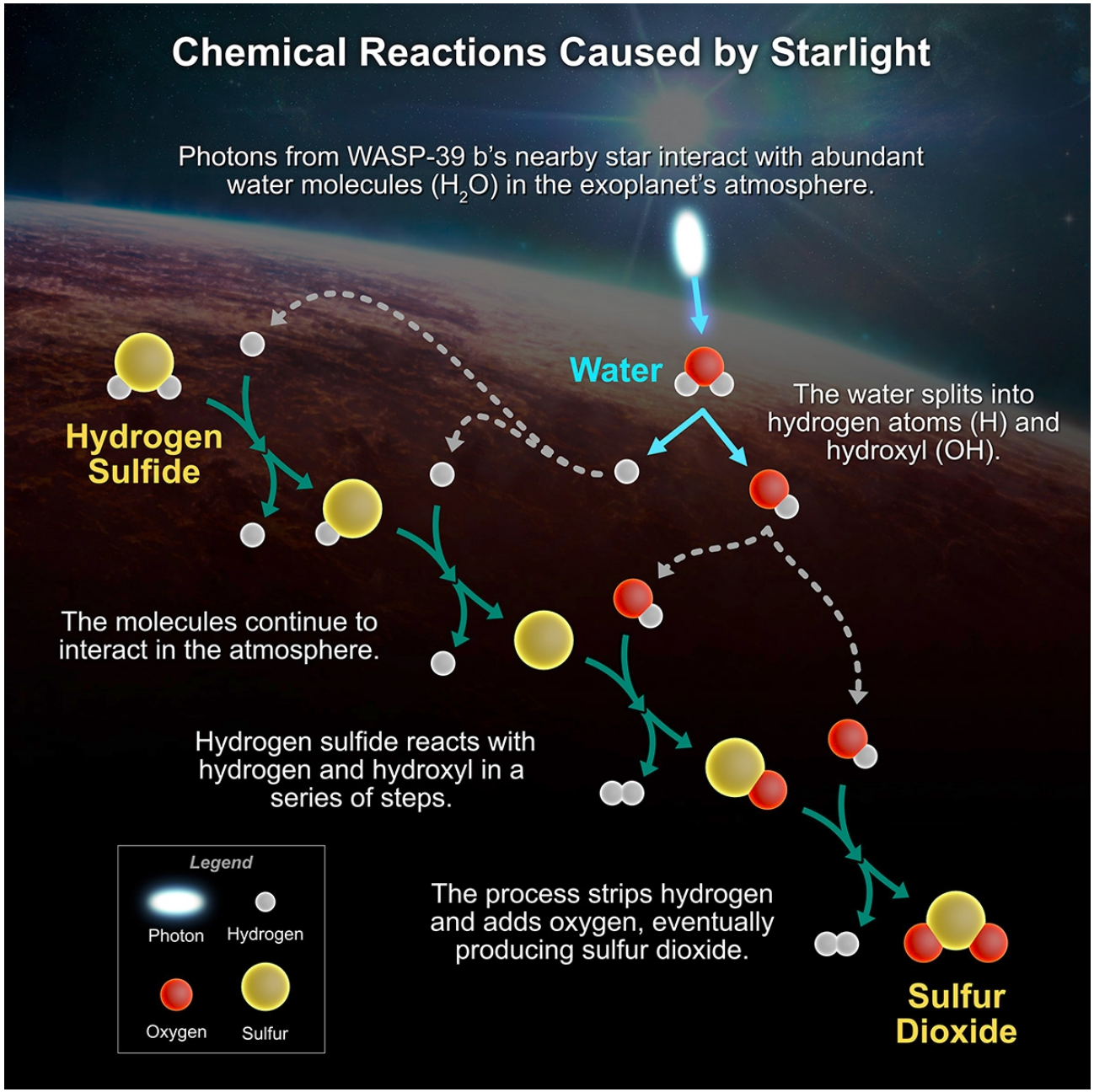


Properties of UGC 3789 Maser Disk

R ~ 0.09 - 0.20 pc (0.40 - 0.87 mas)
V ~ 750 - 450 km/s
M_{bh} ~ 1.2 x 10^7 M_{sun}
a ~ 3.6 km s^{-1} yr^{-1} (mean value)

D ~ 51 Mpc (15%)
H_0 ~ 65 km s^{-1} Mpc^{-1}

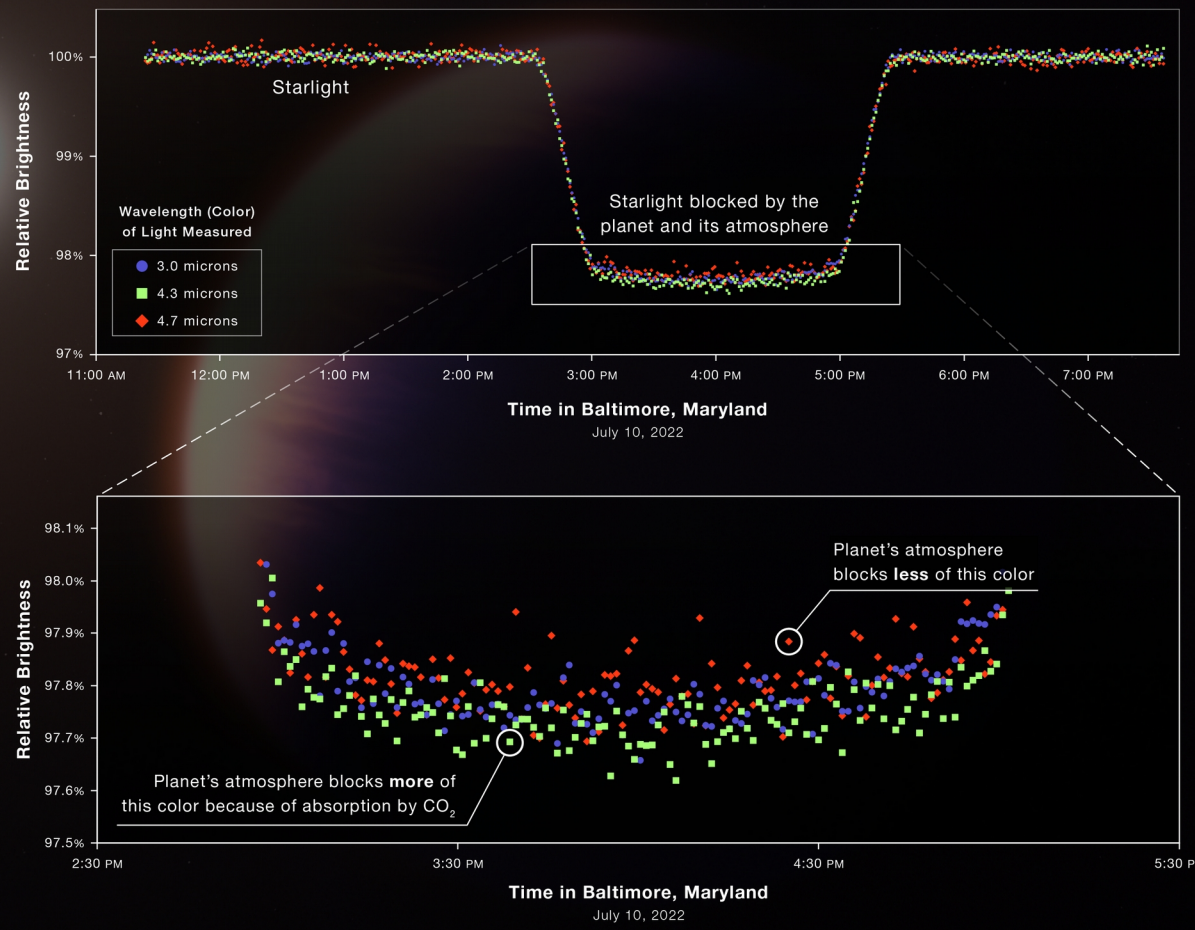

Pathways to making oxygen-rich exoplanet atmospheres without life
High carbon to hydrogen ratio
Too much water
Too little water
Newly formed magma planet
water
oxygen
carbon dioxide
Eternal runaway greenhouse
oxygen
nitrogen
Waterworld
nitrogen
oxygen
carbon dioxide
Desertworld


Chemical Reactions Caused by Starlight
Photons from WASP-39 b's nearby star interact with abundant water molecules (H_2O) in the exoplanet's atmosphere.
Water
The water splits into hydrogen atoms (H) and hydroxyl (OH).
Hydrogen Sulfide
The molecules continue to interact in the atmosphere.
Hydrogen sulfide reacts with hydrogen and hydroxyl in a series of steps.
Legend
Photon
Hydrogen
Oxygen
Sulfur
The process strips hydrogen and adds oxygen, eventually producing sulfur dioxide.
Sulfur Dioxide

HOT GAS GIANT EXOPLANET WASP-39 b

TRANSIT LIGHT CURVE

NIRSpec | Bright Object Time-Series Spectroscopy

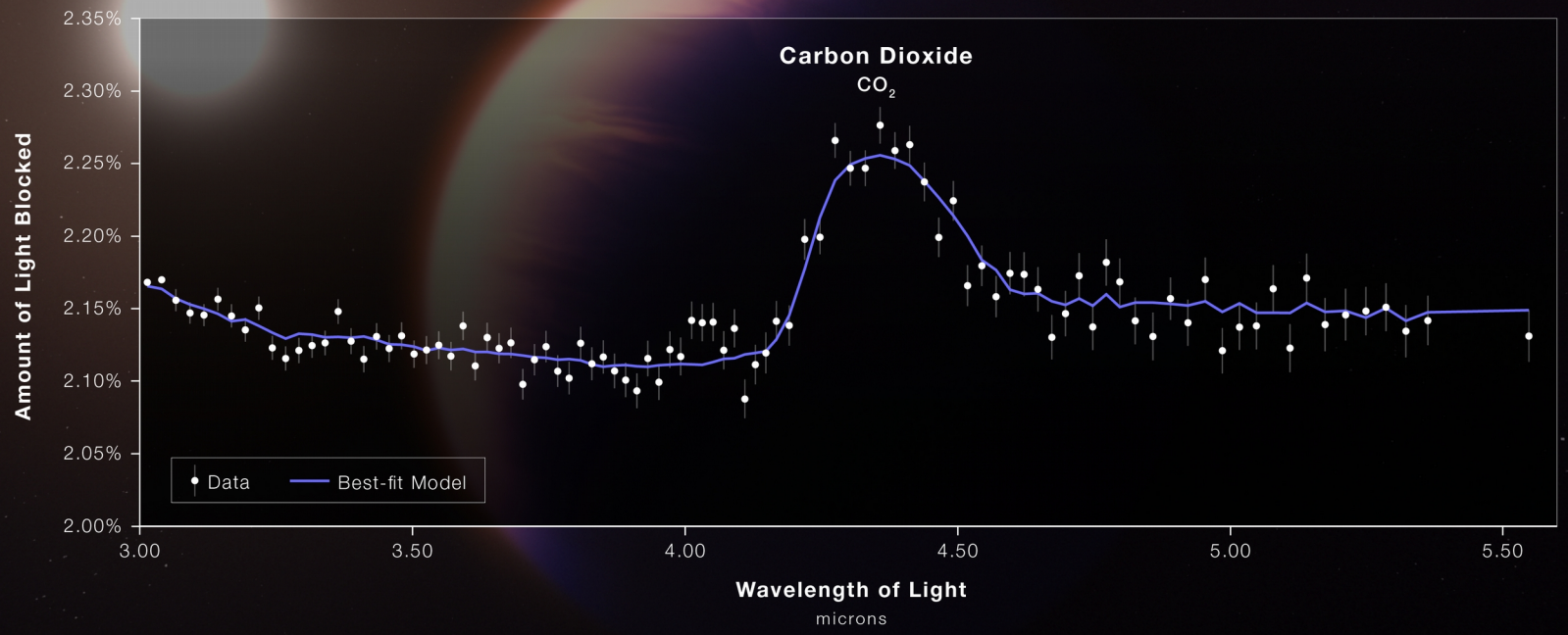


WEBB SPACE TELESCOPE

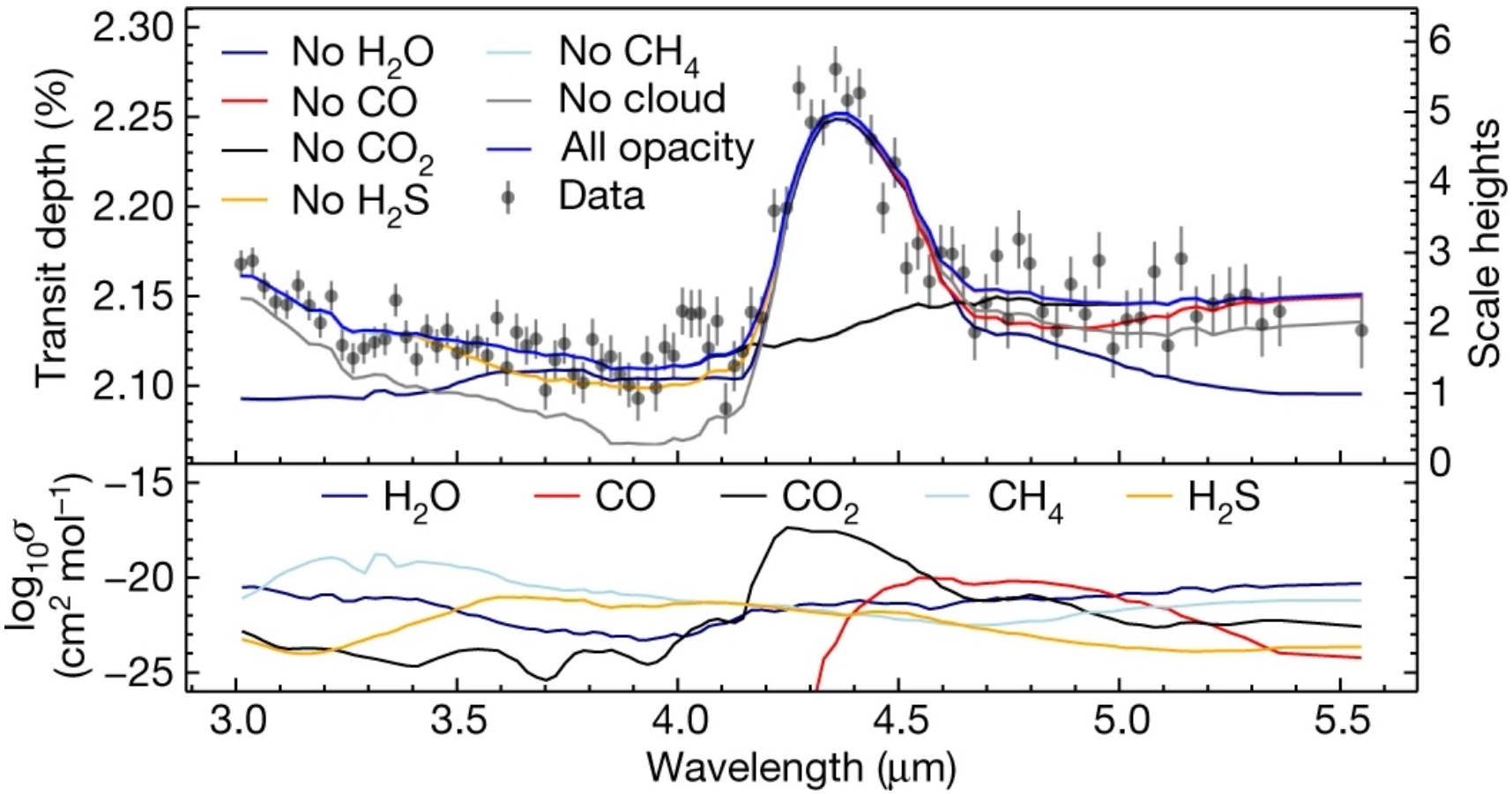
HOT GAS GIANT EXOPLANET WASP-39 b

ATMOSPHERE COMPOSITION

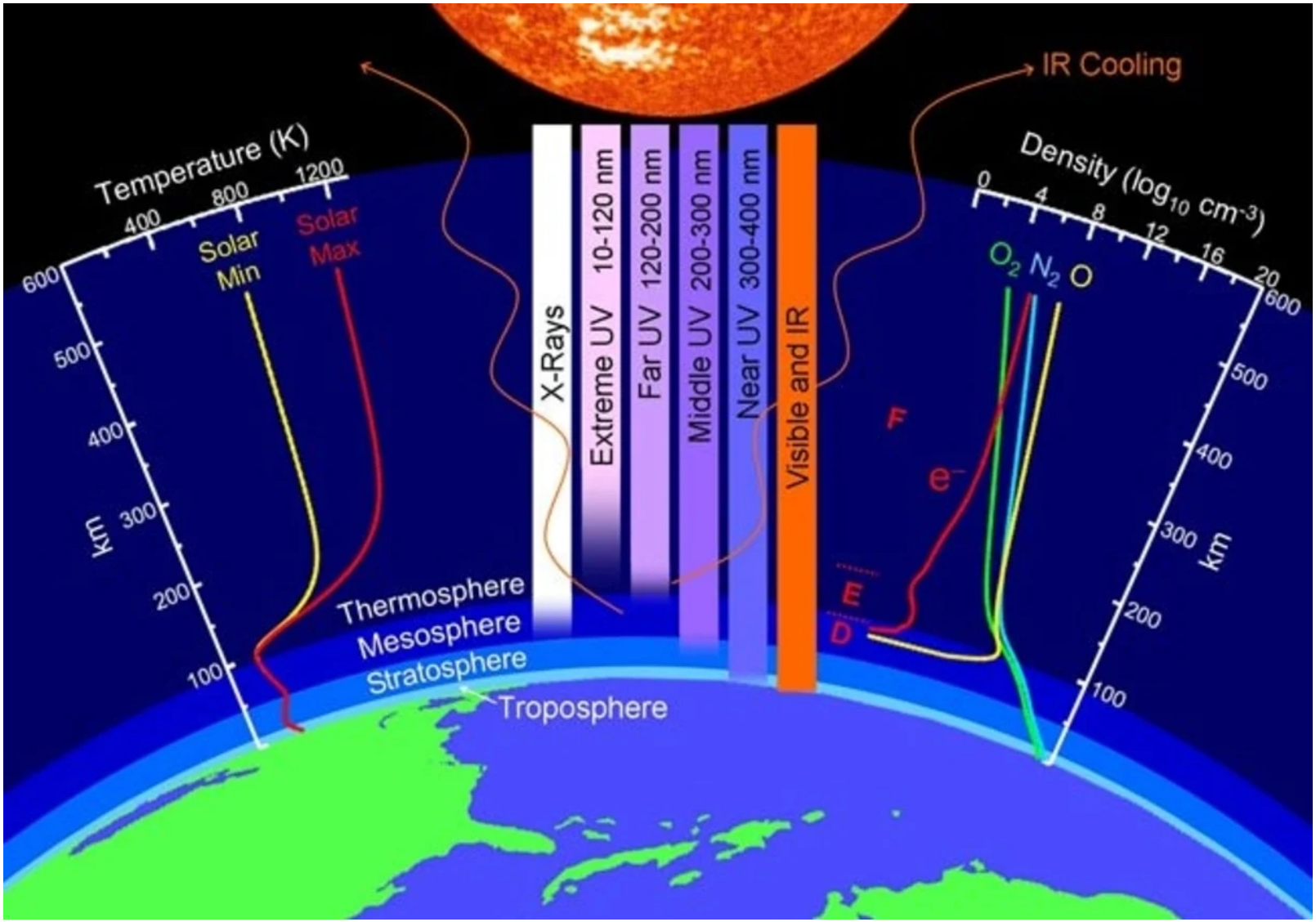
NIRSpec | Bright Object Time-Series Spectroscopy



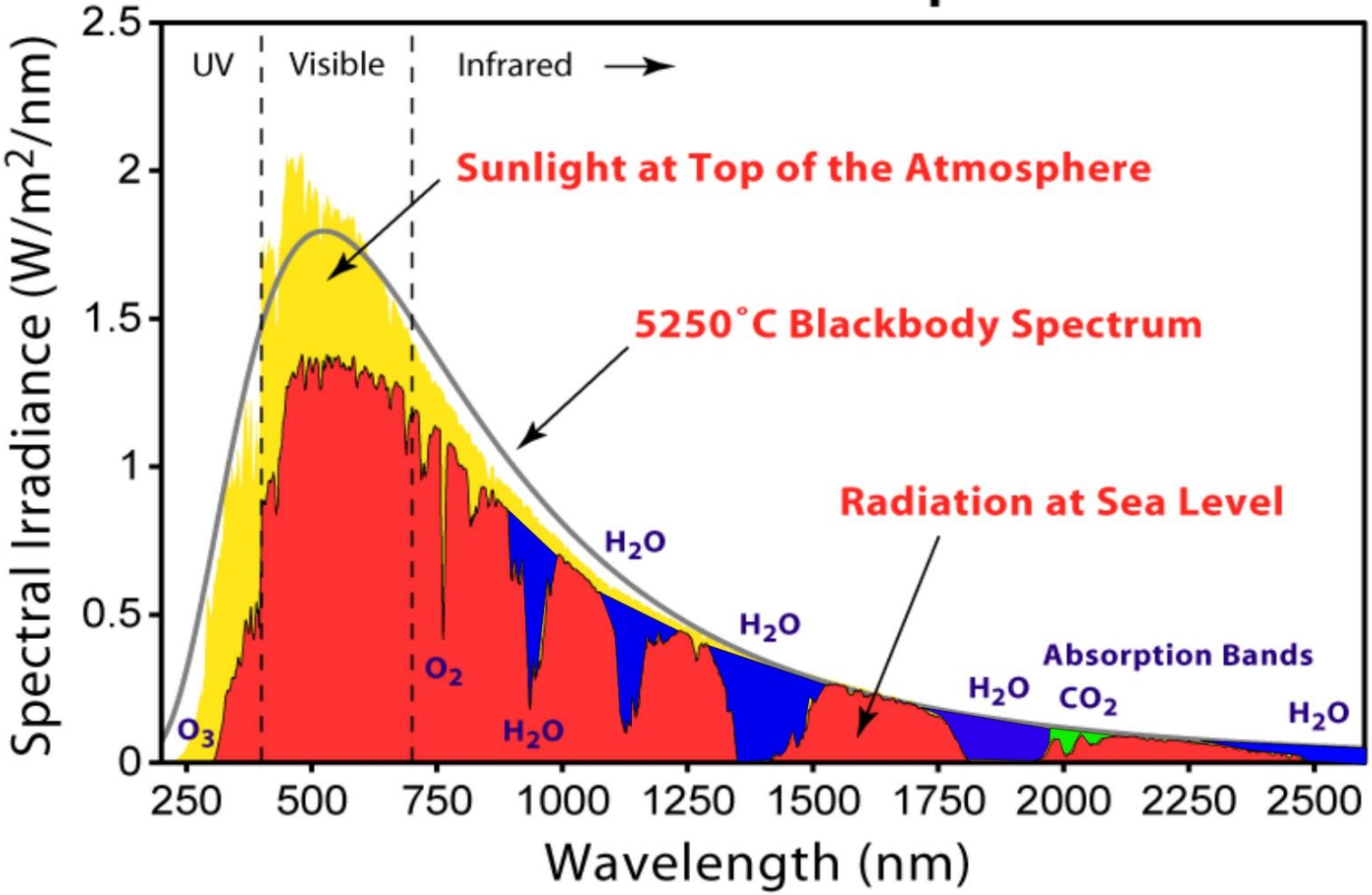
WEBB SPACE TELESCOPE

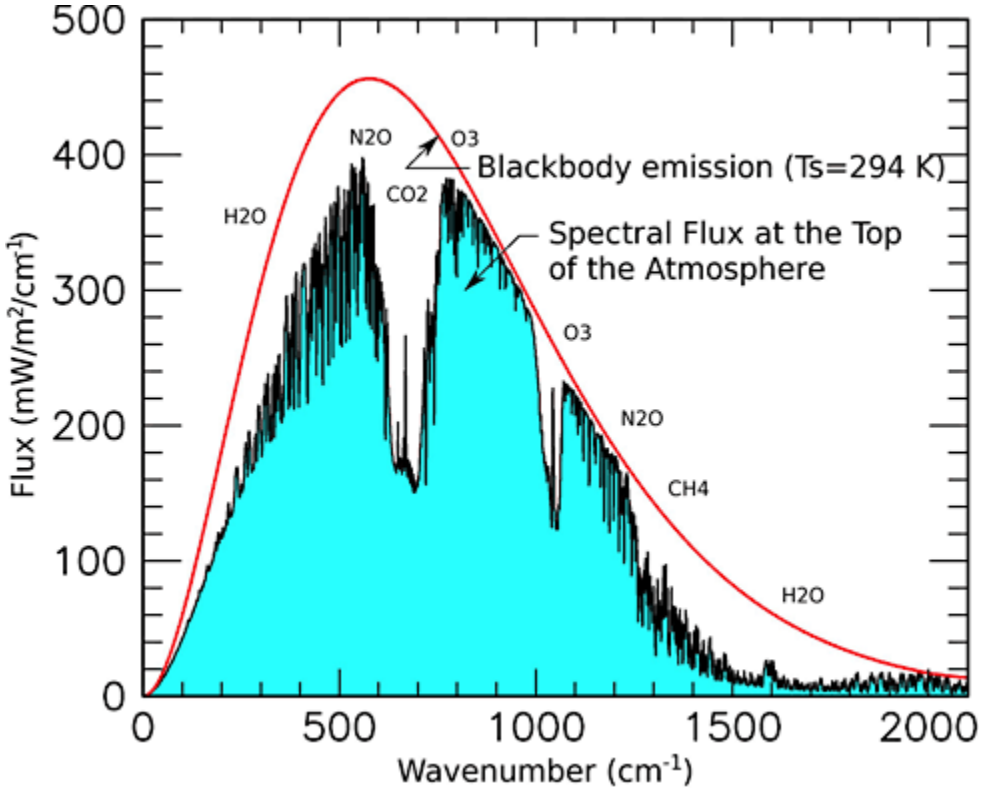

No H_2O
No CO
No CO_2
No H_2S
No CH_4
No cloud
All opacity
Data
Transit depth (%)
Scale heights
H_2O
CO
CO_2
CH_4
H_2S
$\log_{10}\sigma$ (cm^2 mol^{-1})
Wavelength (μm)

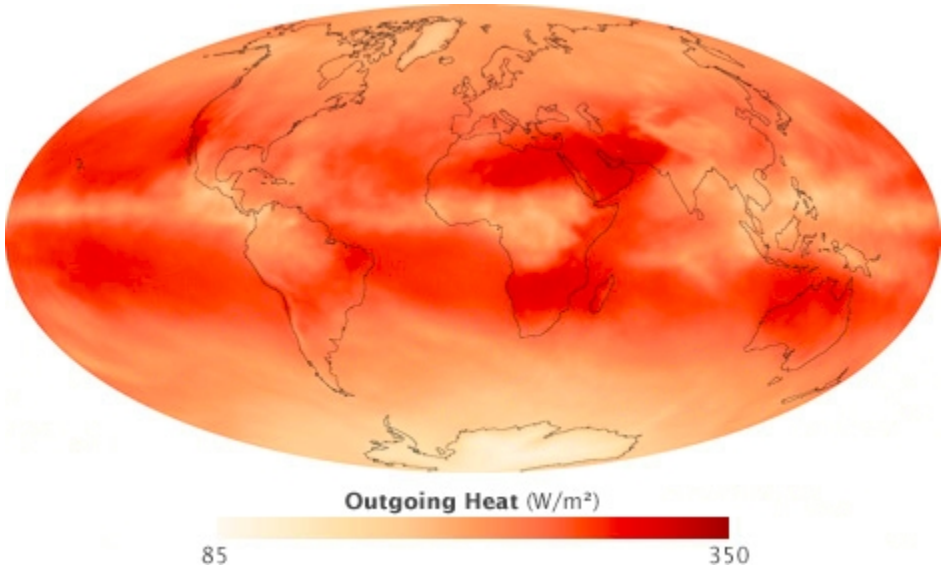
The Earth's Atmosphere



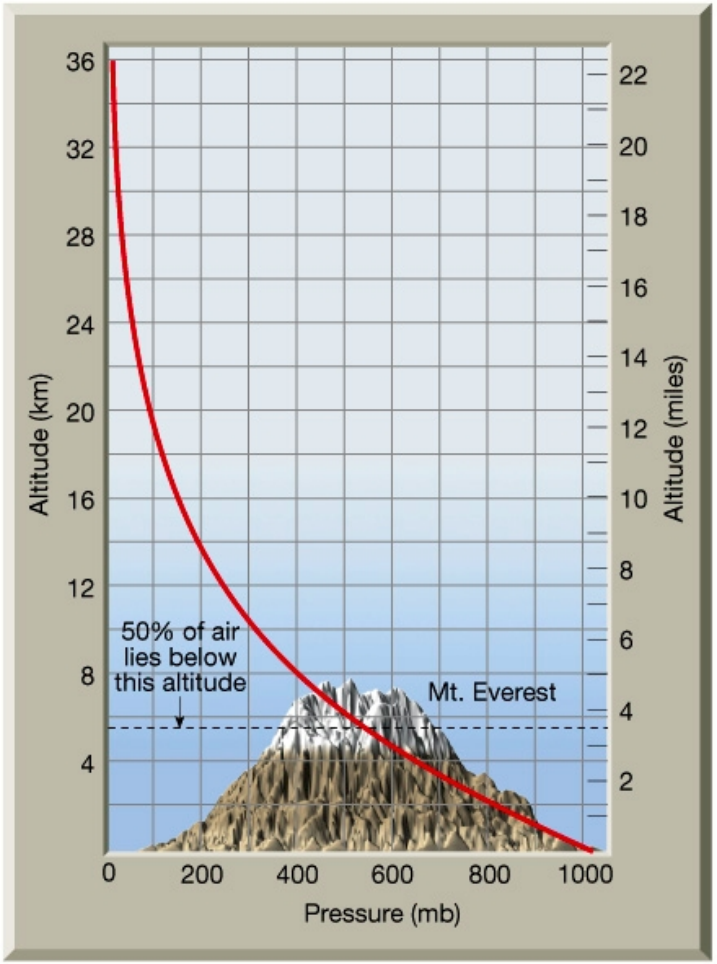
Solar Radiation Spectrum

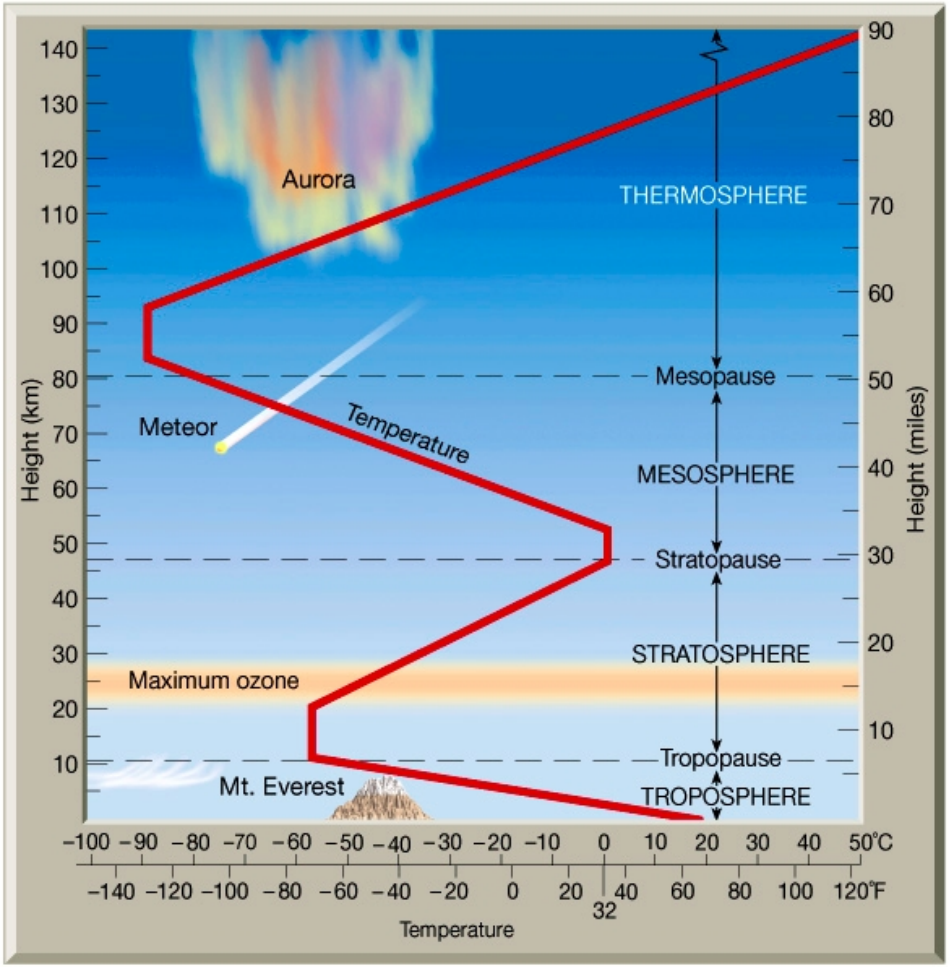
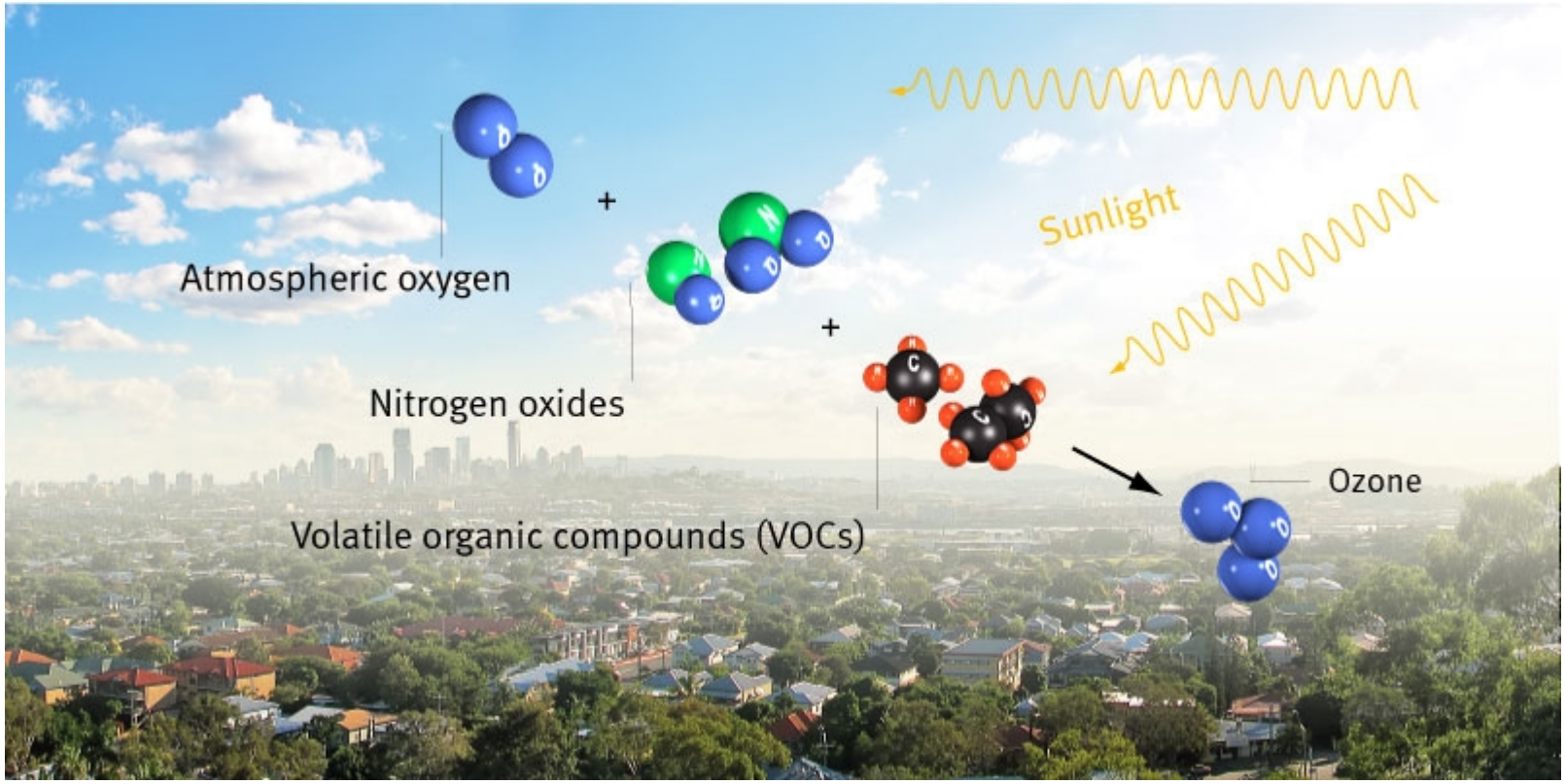



500
400
300
200
100
0
0
500
1000
1500
2000
Flux (mW/m²/cm⁻¹)
Wavenumber (cm⁻¹)
N2O
O3
CO2
H2O
Blackbody emission (Ts=294 K)
Spectral Flux at the Top of the Atmosphere
O3
N2O
CH4
H2O


Outgoing Heat (W/m²)
85
350

Structure of Earth's atmosphere





Atmospheric photochemistry