Spectroscopy for Photon-dominated regions* (PDR)

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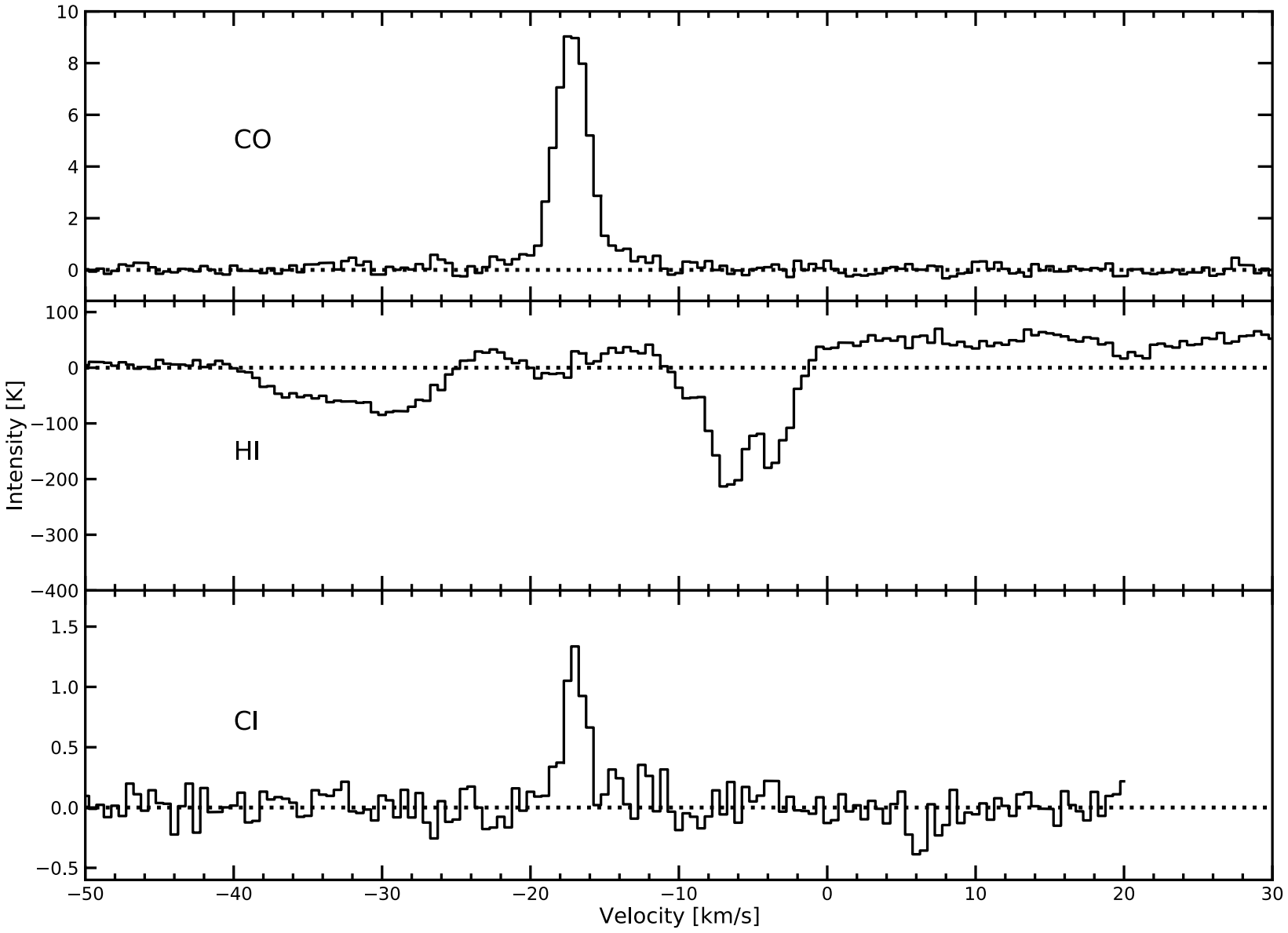
* Photo Dissociation Regions

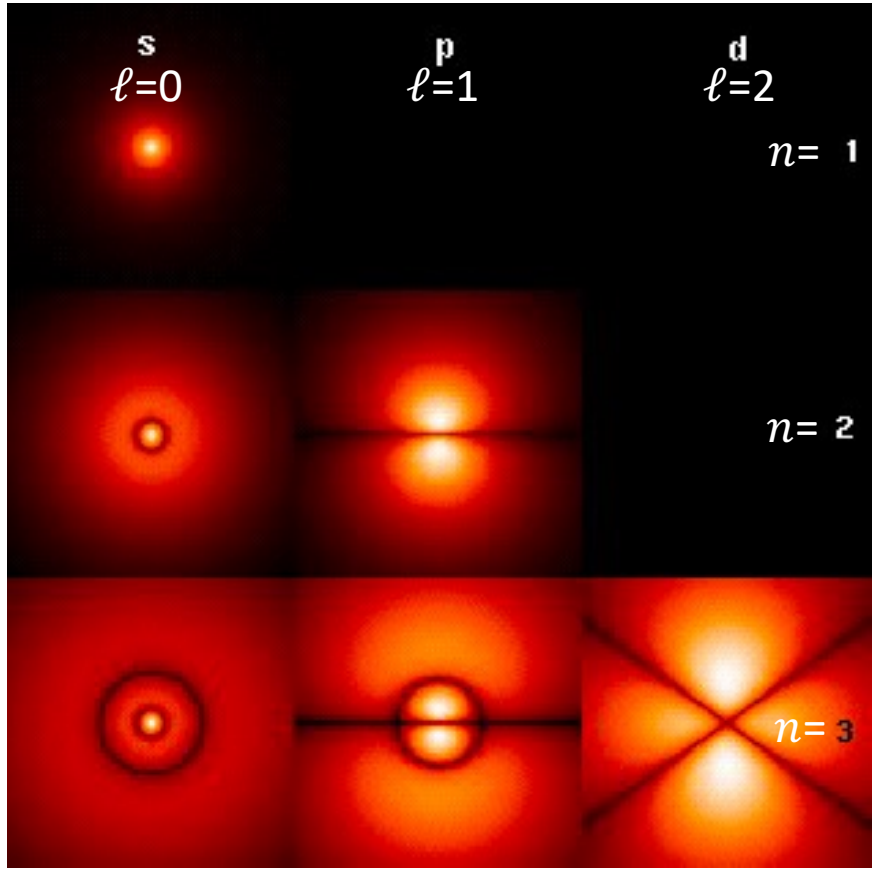


Astrophysics = Astronomy + Physics

Recall of Basic Atomic Physics: Quantum numbers

Describing the distribution of electrons in the atom.
Three basic quantum numbers

- n : principle (main) quantum number (n=1,2,3,…)
- ℓ : orbital quantum number (ℓ = 0,..,n-1)
- m_ℓ: magnetic quantum number
  (projection of ℓ on the z-axis) (m_ℓ=$-\ell$, … , ℓ)



Recall of Basic Atomic Physics: Atomic Hydrogen

For Hydrogen: one proton and one electron

$$\Delta E = E_n - E_{n'} = -13.6\text{ev} \times \left(\frac{1}{n^2} - \frac{1}{n'^2}\right)$$

- n'=1 : Lyman series (UV)
- **n'=2 : Balmer series (optical)**
- n'=3 : Paschen series (near-IR)
- n'=4: Brackett series (mid-IR)
- …

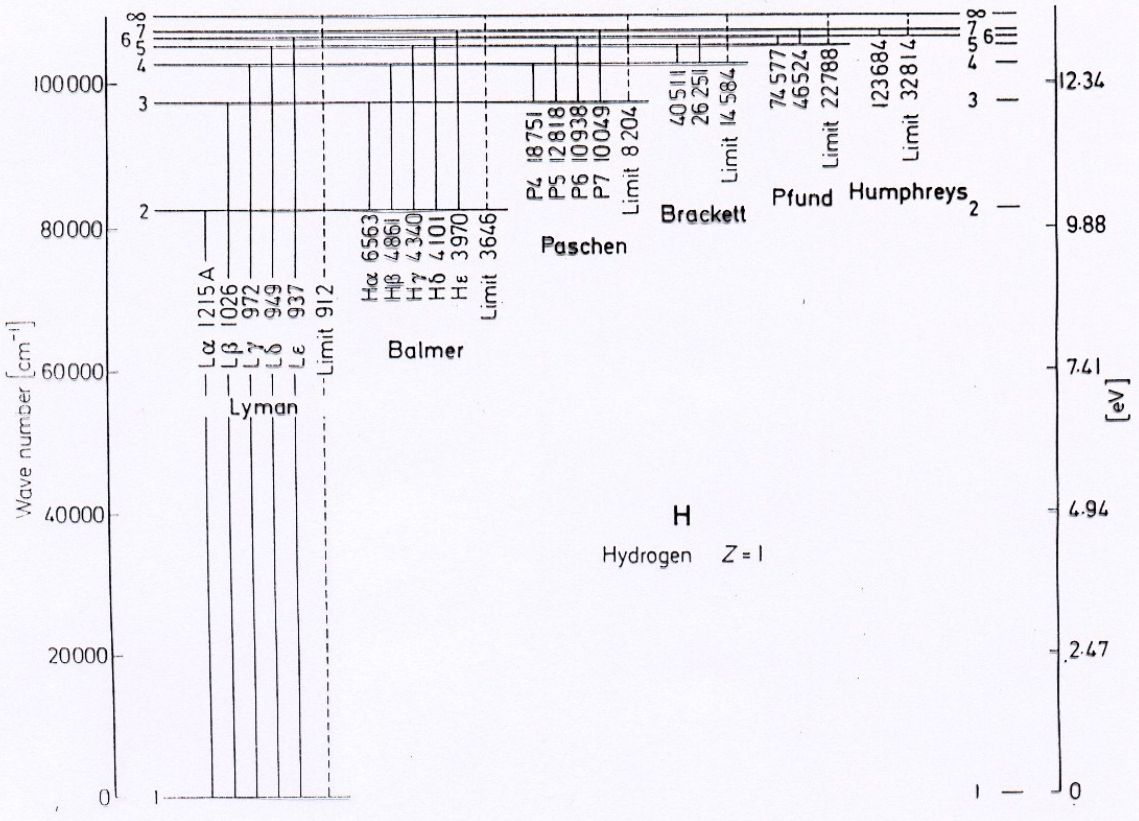
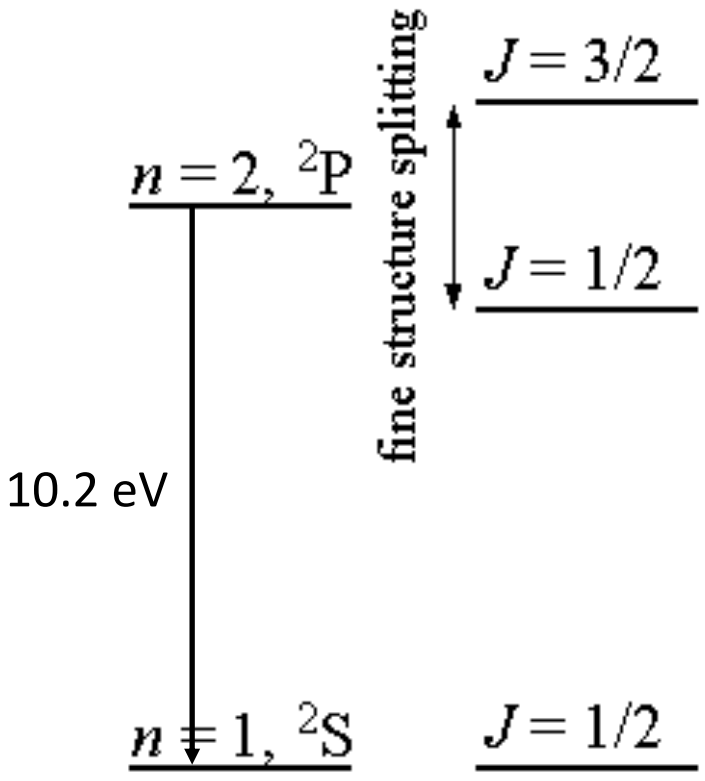


Fig. 13. Grotrian diagrams for H, He I, He II, C II, C III, C IV, O I, O II, O III, N II, Mg I, Mg II, Ca I, Ca II, Fe I, and Fe II. (After MOORE and MERRILL, 1968)

Recall of Basic Atomic Physics: Fine Structure

- **Spin of electron (s=1/2)**
- Total angular momentum $\vec{j} = \vec{\ell} + \vec{s}$
  $(j = |\ell - s|, \ldots, |\ell + s|)$
- Example: atomic Hydrogen:
  - n=1→ ℓ=0 → j=1/2
    → no fine structure line
  - n=2→ ℓ=0,1 → j=1/2,3/2
    → fine structure line

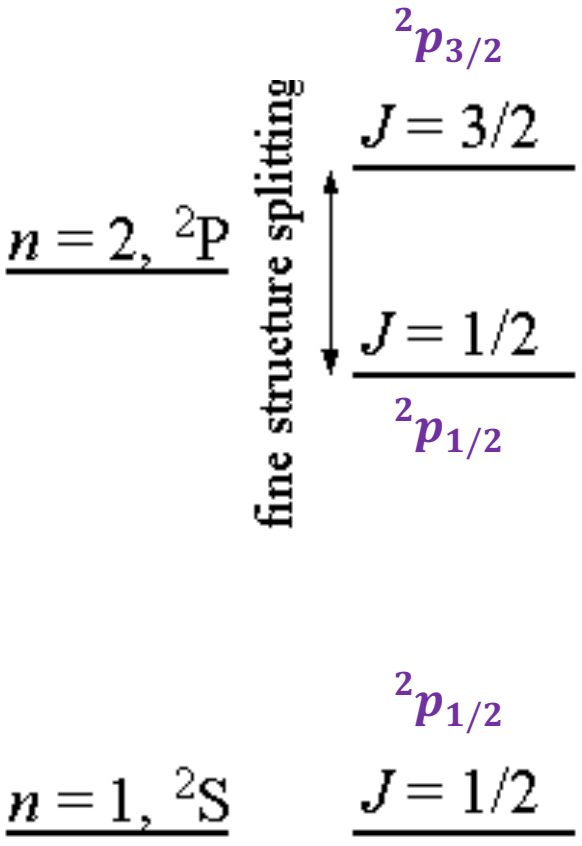


$\Delta E \approx 4.5\times10^{-5}\,\mathrm{eV}$
$\nu \approx 10.9\ \mathrm{GHz}$
$\lambda \approx 2.8\ \mathrm{cm}$
(radio)

Recall of Basic Atomic Physics: Notation

$$\boxed{{}^{2s+1}\ell_j}$$

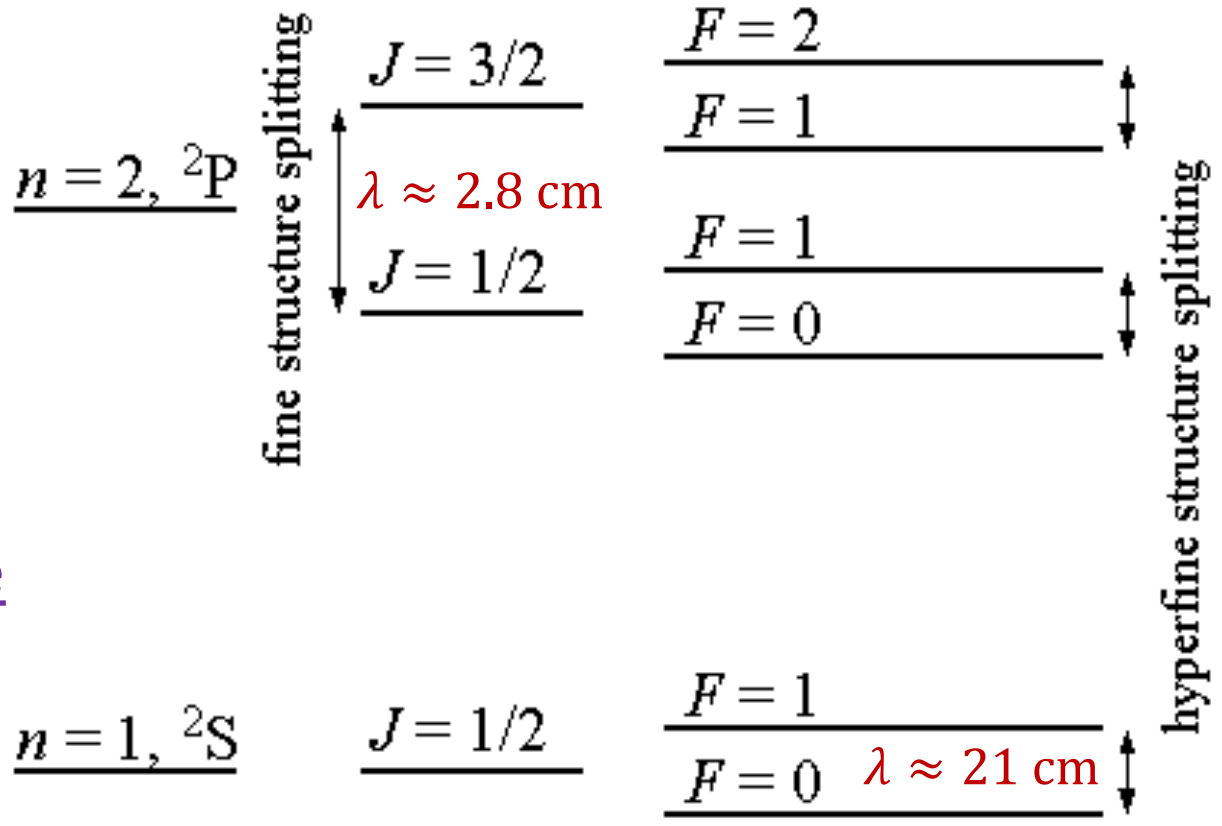
ℓ=0: s
ℓ=1: p
ℓ=2: d
ℓ=3: f
ℓ=4: g
ℓ=5: h



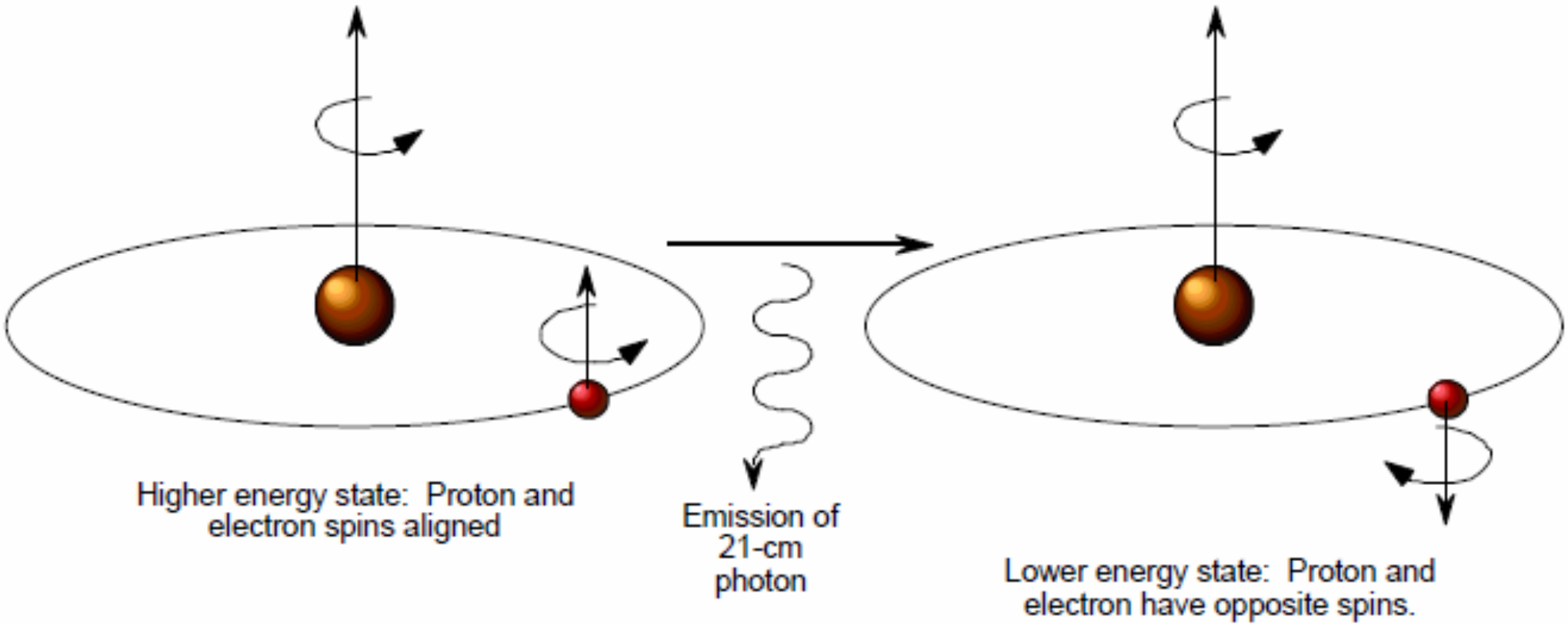
Recall of Basic Atomic Physics: HyperFine Structure

- Spin of electron (s=1/2)
- **Spin of nucleus (i=1/2)**
- Total angular momentum $\vec{f} = \vec{j} + \vec{i}$
  $(j = |j - i|, \dots, |j + i|)$
- Example: atomic Hydrogen:
  - n=1 → ℓ=0 → j=1/2
    → no fine structure line
    - j=1/2 → f=0, 1 → hyperfine structure
  - n=2 → ℓ=0,1 → j=1/2,3/2
    → fine structure line
    - j=1/2 → f=0,1
    - j=3/2 → f=1,2

hyperfine structure



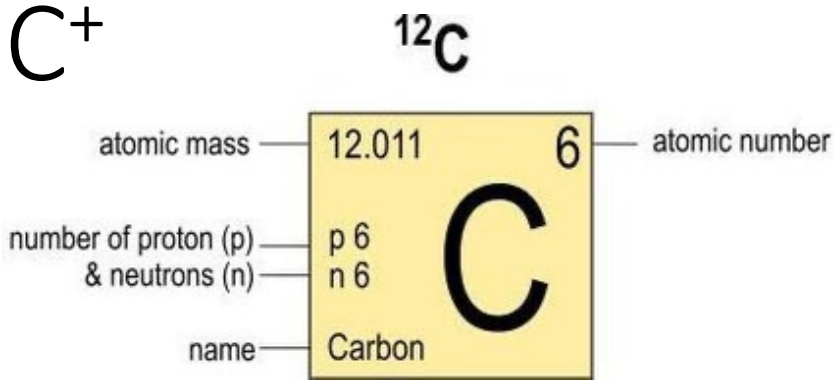
Formation of the 21-cm Line of Neutral Hydrogen



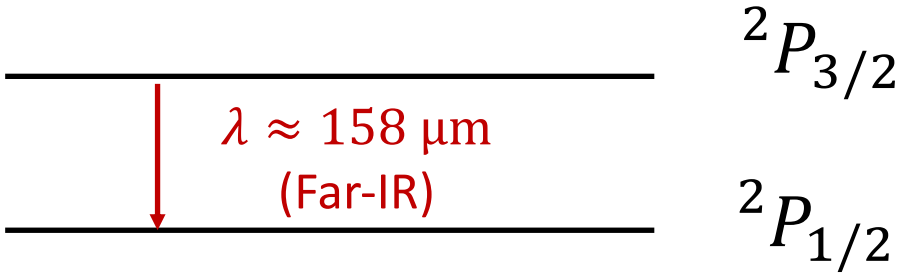
Recall of Basic Atomic Physics: Atoms (multiple electrons system)

- Approximation
  - Total orbital: $\vec{L} = \sum \vec{\ell}_i$
    (ℓ_i is the individual orbital quantum number)
  - Total spin: $\vec{S} = \sum \vec{s}_i$
  - (s_i is the individual spin number)
  - Total angular momentum: $\vec{J} = \vec{L} + \vec{S}$
- Spectroscopy notation: $^{2S+1}L_J$

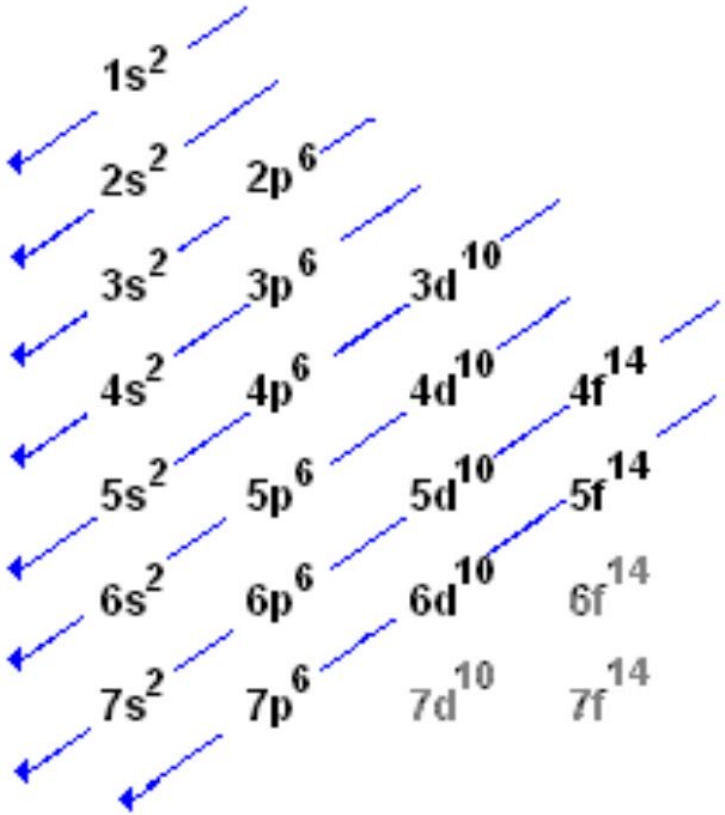
Recall of Basic Atomic Physics: $^{12}C^{+}$



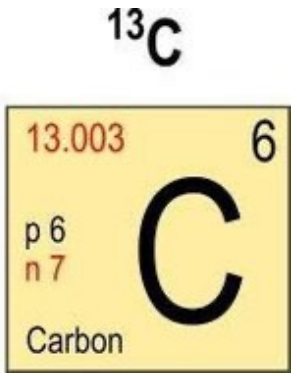
- Writing down the electron configuration $1s^2 2s^2 2p^1$
- Only thirdshell is open (because the p shell can occupy upto 6 electrons)
- L = 1, S=1/2 → J = 1/2 and 3/2



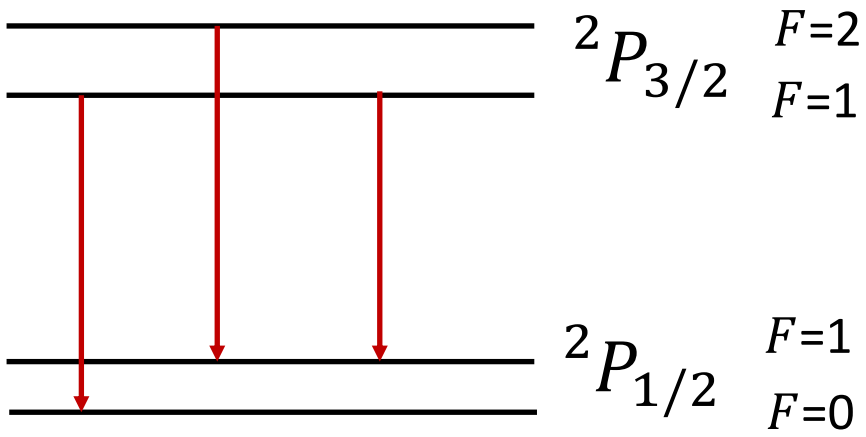
- Nuclear spin of ^{12}C: I = 0
  → no hyperfine structure lines



Recall of Basic Atomic Physics: $^{13}C^{+}$



- Writing down the electron configuration $1s^2 2s^2 2p^1$
- Only thirdshell is open (because the p shell can occupy upto 6 electrons)
- L = 1, S=1/2 → J = 1/2 and 3/2
- Nuclear spin of ^{13}C: I = 1/2 → hyperfine structure lines



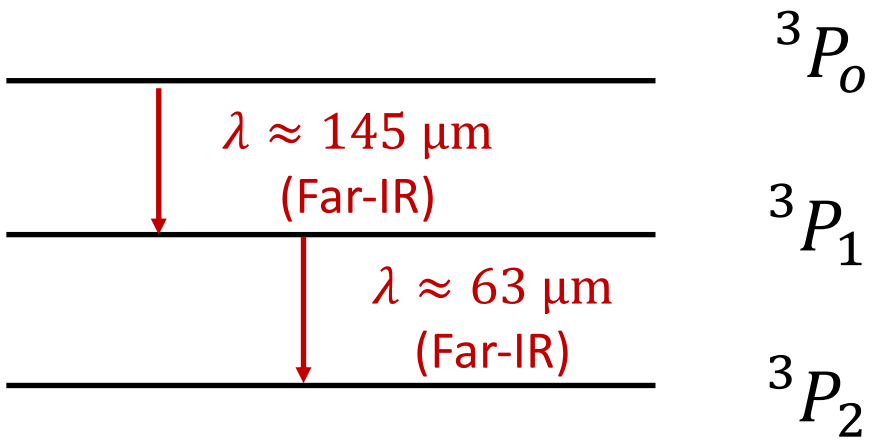
Line	Statistical g_u	Weight g_l	Frequency ν (GHz)
[^{12}CII] $^2P_{3/2}-^2P_{1/2}$	4	2	1900.5369
[^{13}CII] F=2→1	5	3	1900.4661
[^{13}CII] F=1→0	3	1	1900.9500
[^{13}CII] F=1→1	3	3	1900.1360

Recall of Basic Atomic Physics: ^{16}o

- Writing down the electron configuration $1s^2 2s^2 2p^4$
- Only thirdshell is open (because the p shell can occupy upto 6 electrons)
- Each electron has s=1/2 (m_s=1/2, -1/2), ℓ=1 ($m_l = -1,0,1$)

→ All 6^4 possible combinations.

→ Pauli principle: 3 possibilities



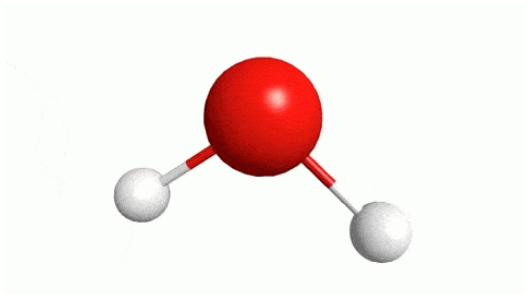
- Nuclear spin of ^{16}O: I =0
  → No hyperfine structure lines
- Nuclear spin of ^{17}O: I =5/2
  → hyperfine structure lines

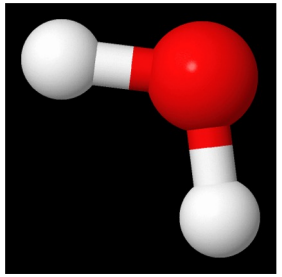
Recall of Basic Molecule: H_2 and CO

Quantum number v **Quantum number J**

- Electronic Excitation > Vibrational Excitation > Rotational Excitation

(High excited energy)





- H_2: homogenous molecule → no electric dipole moment → rotationally excited at higher temperature → trace warm gas.
  E.g.,H2 v=0, J=3->1 (or H2 S(1)), T_{ex} = 500K.
- CO: electric dipole moment → rotationally excited at lower temperature → trace cooler gas.
  E.g., CO J=1->J=0 (or CO(1-0)), T_{ex}= 5.5K

Some Fundamental Unit conversions

1. Emissivity [erg s^{-1} cm^{-3} Hz^{-1} sr^{-1}]: $j = \frac{h\nu}{4\pi} A \times n$
2. Specific intensity [erg s^{-1} cm^{-2} Hz^{-1} sr^{-1}]: $I = \int_{\text{cloud depth}} j \times dl$
   - **Meaning: power per unit area per one direction per one channel**
3. Flux [erg s^{-1} cm^{-2} sr^{-1}]: $F = \Delta\nu \times I$
   - **Meaning: power in all channels**
   - $\Delta\nu$ is the resolution of the spectrograph (instrument)

Some Fundamental Unit conversions

4. The power resolution is $R = \frac{\lambda}{\Delta\lambda}$

- $\frac{\lambda}{\Delta\lambda} = \frac{\nu}{\Delta\nu} \Longrightarrow \Delta\nu = \nu \times \frac{\Delta\lambda}{\lambda} = \nu \times \frac{1}{R}$
- $\nu = c/\nu \Longrightarrow \Delta\nu = c \times \frac{\Delta\lambda}{\lambda^2}$

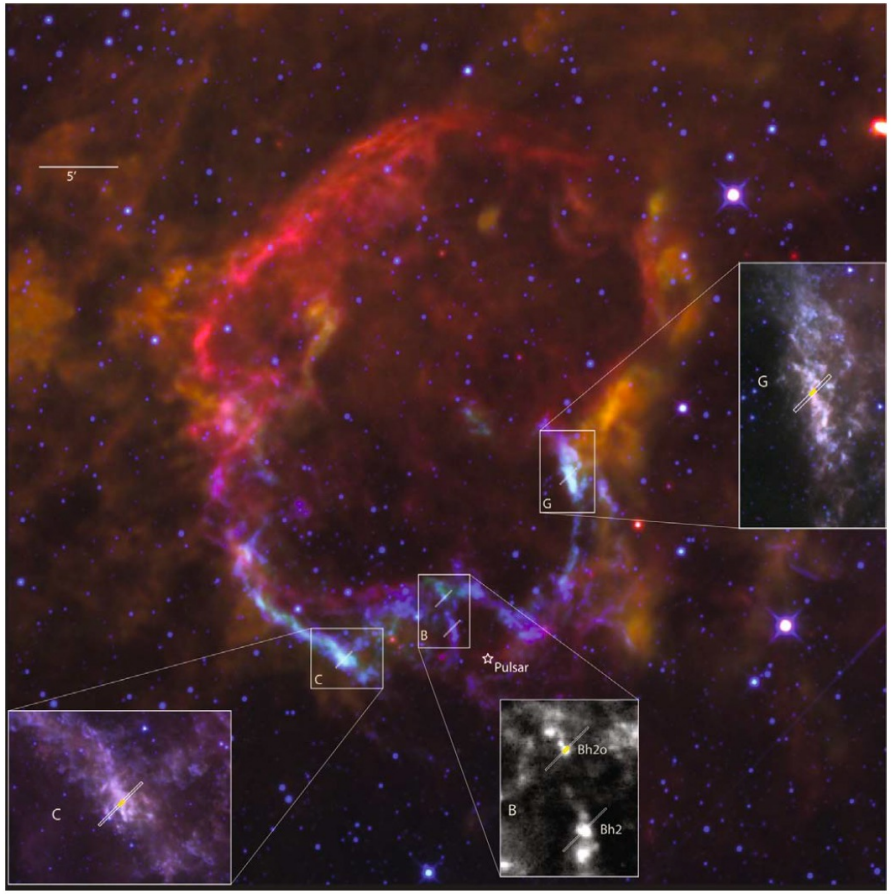
❑ **<u>IF the unit is per wavenumber (cm^{-1}):</u>**

- $\Delta\nu = \text{wavenumber/R} = \Delta\nu \frac{1}{\lambda \times R}$

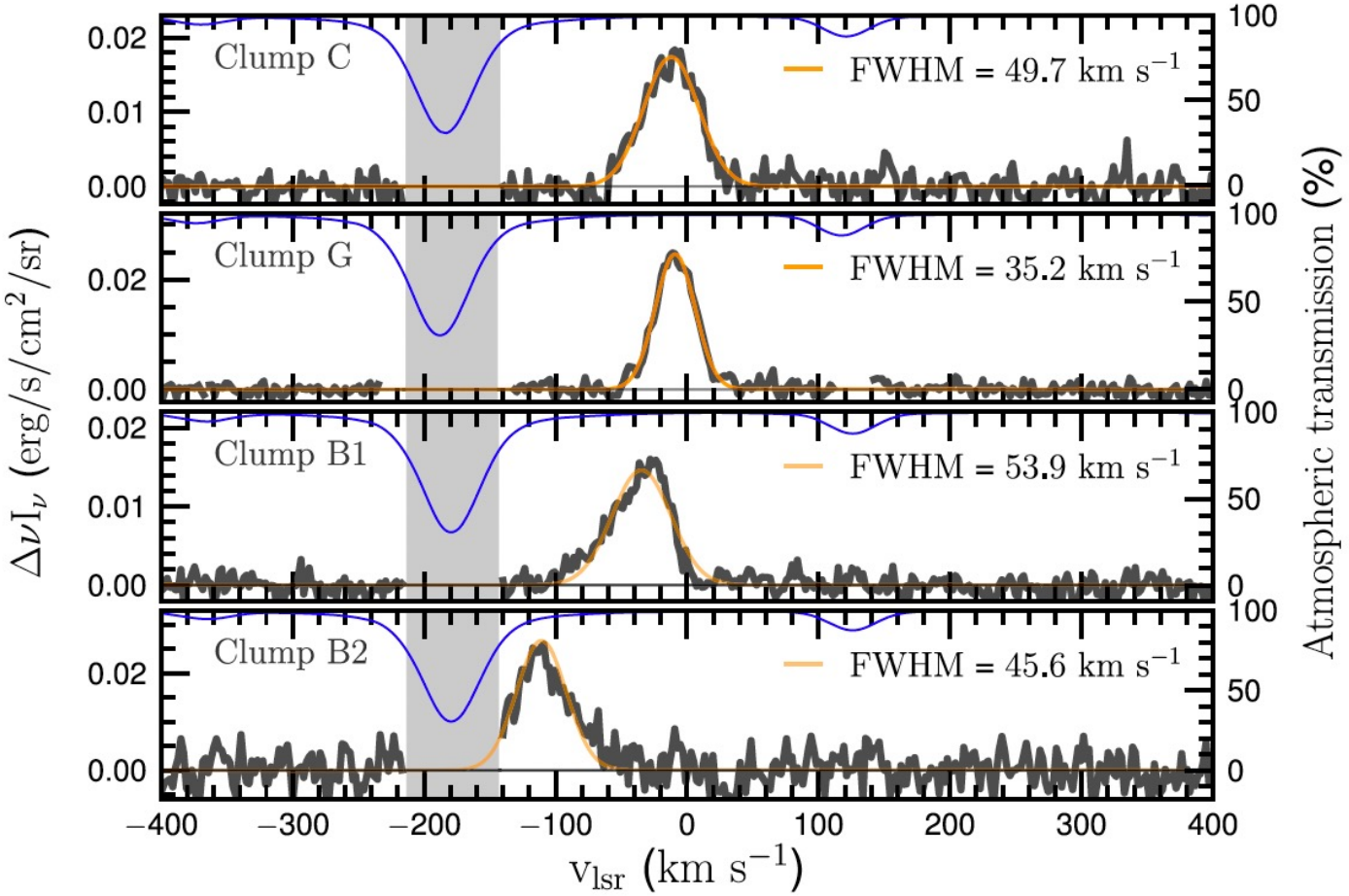
Name	Wavelength Range Resolving Power R =λ/Δλ
EXES	4.5 – 28.3 μm R = 1,000 – 10^5
FIFI-LS	51 – 200 μm R = 600 – 2,000
FORCAST	5 – 40 μm R = 100 – 300
GREAT	63 – 612 μm R = 10^6 – 10^8
HAWC+	50 – 240 μm Δλ = 9 – 43 μm
FPI+	0.36 – 1.10 μm R = 0.9 – 29.0

SOFIA instrument

Example: Supernova Remnant IC 443



Reach, Tram et al. 2019



Some Fundamental Unit conversions

5. Spectrum resolution

- $R = \frac{\lambda}{\Delta\lambda}$
- **Doppler effect:**
  - ❖ Observed frequency: $\nu = (1 + \frac{\Delta \mathrm{v}}{\mathrm{c}})\, \nu_0$
  - ❖ Change in frequency: $\Delta\nu = \nu - \nu_0 = \frac{\Delta \mathrm{v}}{\mathrm{c}} \times \nu_0$

    ==> $\Delta \mathrm{v} = \frac{c}{R}$

Some Fundamental Unit conversions

Name	Wavelength Range Resolving Power R =λ/Δλ
EXES	4.5 – 28.3 μm R = 1,000 – 10^5
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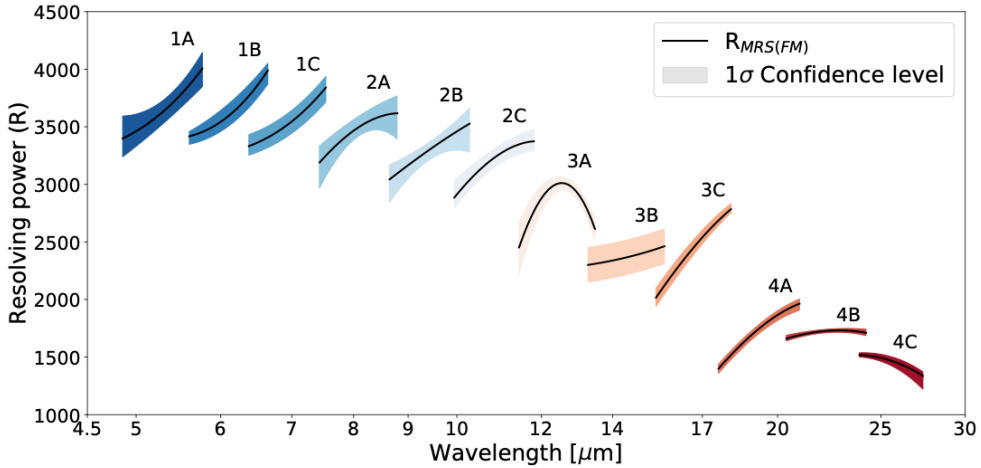
SOFIA instrument

Table 1
Observed Spectral Lines

Species	Transition	λ (μm)[a]	Beam (″)[b]	R ($\lambda/\Delta\lambda$)[b]
ISO:				
[O I]	$^3P_2 \rightarrow {}^3P_1$	63.18372	87.2	223
[N II]	$^3P_2 \rightarrow {}^3P_1$	121.8981	78.2	209
[O I]	$^3P_1 \rightarrow {}^3P_0$	145.52547	70.0	249
[C II]	$^2P_{\frac{3}{2}} \rightarrow {}^2P_{\frac{1}{2}}$	157.7409	70.1	270
SPIFI:				
[N II]	$^3P_1 \rightarrow {}^3P_0$	205.1782	54	4250

ISO/LWS (Oberst et al. 2011)



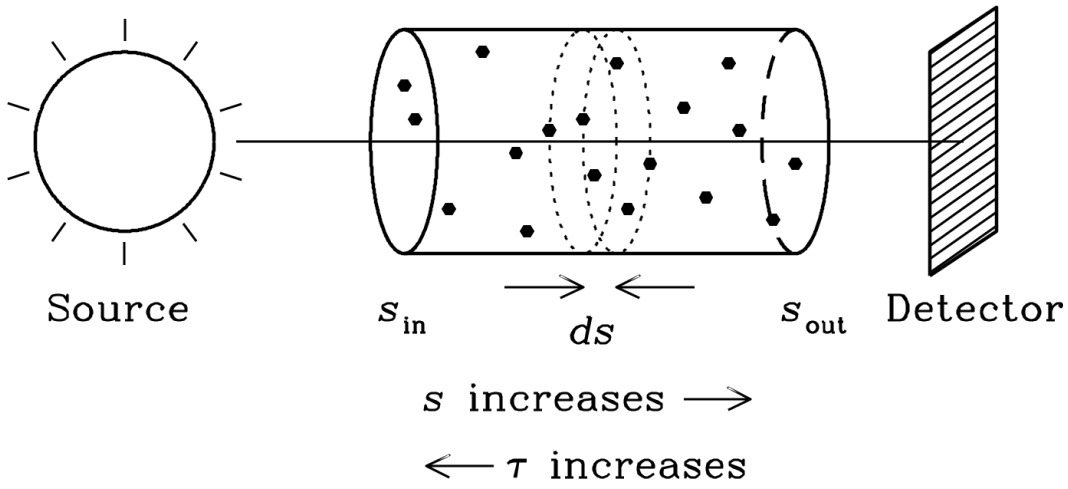
JWST/MIRI

Spectral resolution in velocity for

1. SOFIA/GREAT,
2. ISO/LWS of [OI] and [CII],
3. JWST/MIRI at 5 and 14um

Physical Properties

❖ General idea: we need to follow the path of radiation



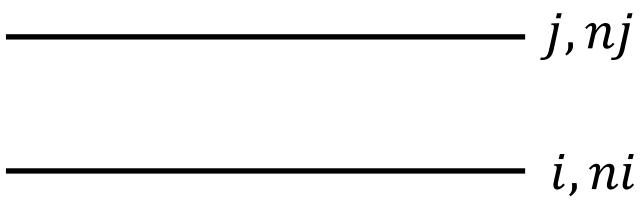
$$\frac{dI_\nu}{ds} = \epsilon_\nu - \kappa_\nu I_\nu$$

$$\frac{dI_\nu}{d\tau} = S_\nu - I_\nu$$

$S_\nu = \frac{\epsilon_\nu}{\kappa_\nu}$: Source Function

$d\tau = \kappa_\nu ds$: optical depth

❖ Consider a transition from $j \longrightarrow i$



Local Thermal Equilibrium (LTE)

- The source function $S_\nu = \frac{\epsilon_\nu}{\kappa_\nu} \equiv$ Planck function $(B_\nu(T_{\mathrm{ex}}))$
- ϵ_ν, κ_ν and T_{ex} are constants along the ligh-of-sight (LOS)
- Population is followed the Boltzmann distribution $(n_i \sim e^{-hEi/T_{\mathrm{ex}}})$

Specific intensity
$(\mathrm{ergs}^{-1}\mathrm{cm}^{-2}\mathrm{Hz}^{-1}\mathrm{sr}^{-1})$

$$I_\nu = [B_\nu(T_{\mathrm{ex}}) - B_\nu(T_{\mathrm{bg}})](1 - e^{-\tau_\nu})$$

⬇

Radiation Temperature
(K)

$$T_R = f \times [J_\nu(T_{\mathrm{ex}}) - J_\nu(T_{\mathrm{bg}})](1 - e^{-\tau_\nu})$$

f: filling factor

$$J_\nu(T) = \frac{h\nu/k_B}{e^{h\nu/k_B T} - 1}$$

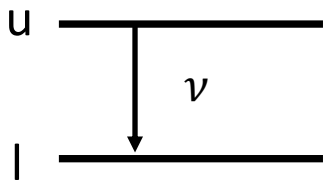
Physical Properties: method 1 -- background

Line Column Density

Consts. Param.? Obs.

- Finite optical depth:

$$N_{\mathrm{tot}} = \frac{8\pi k B \nu^2}{hc^3 A_{ul}} \frac{Q_{\mathrm{rot}}(T_{\mathrm{ex}})}{g_u} \frac{\tau}{1-e^{-\tau}} e^{-E_u/T_{\mathrm{ex}}} \int \frac{T_{\mathrm{mb}} dv}{\mathrm{K\ cms^{-1}}}$$



Gas Column Density

- Assuming the abundance ($X=N_{line}/N_{gas}$) → $N_{gas} = X \times N_{tot}$

Requirement

- Two transitions: one optically thin and one optically thick

Weaknesses

- Constraining only the column density of the "thin" transition line
- Dependence on the abundance assumption

Physical Properties: method 1 -- practical

- As an example, making use of ^{12}CO(1-0) and ^{13}CO(1-0)
- Assuming the beam filling factor of 1, In LTE

$$T_R = [J_\nu(T_{\rm ex}) - J_\nu(T_{\rm bg})](1 - e^{-\tau_\nu})$$

$$J_\nu(T) = \frac{h\nu/k_B}{e^{h\nu/k_B T} - 1}$$

- Assuming ^{12}CO(1-0) is very optically thick ($\tau \to \infty$)

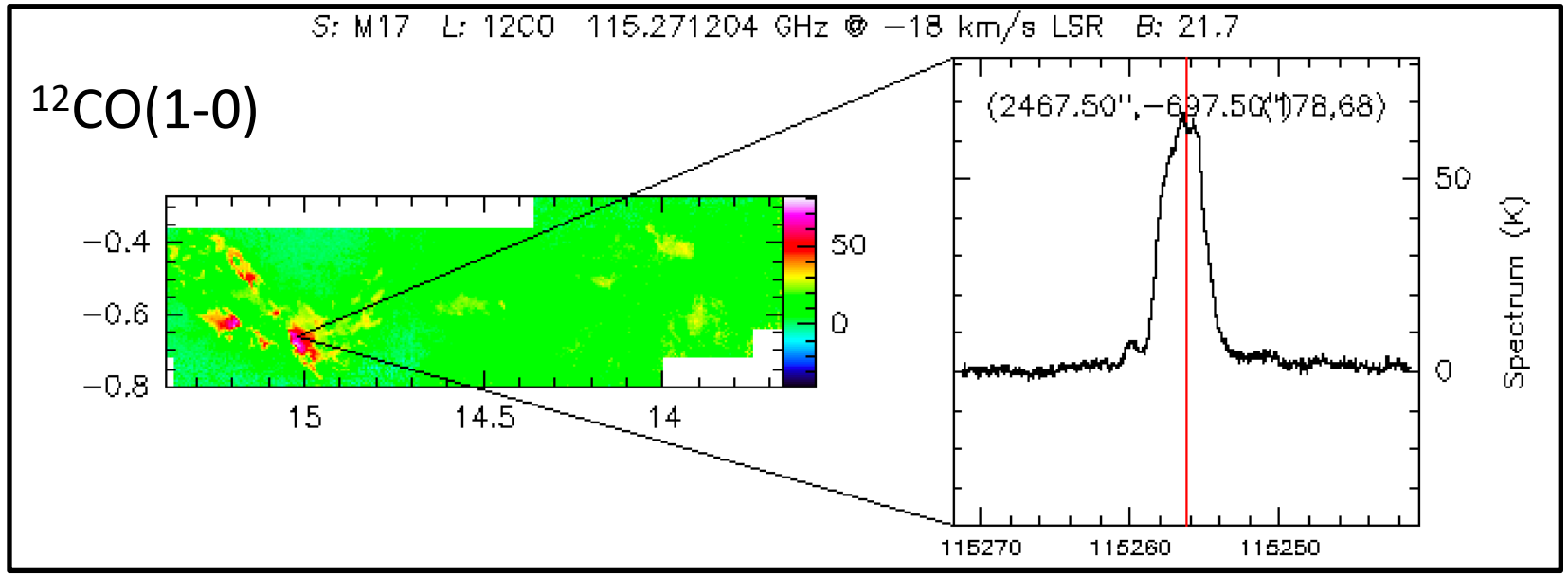
Obs. → $T_R = [J_\nu(T_{\rm ex}) - J_\nu(T_{\rm bg})]$ → $T_{\rm ex}$

- Assuming ^{12}CO(1-0) and ^{13}CO(1-0) sharing the same $T_{\rm ex}$

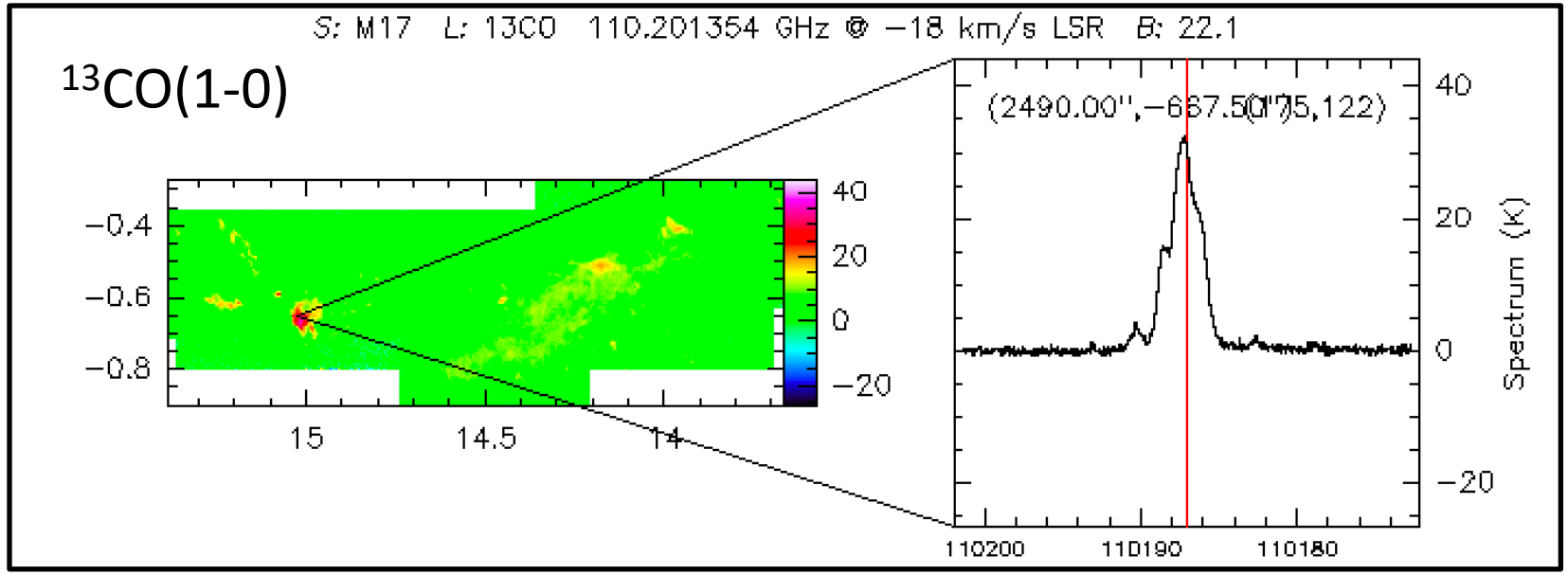
Obs. → $T_R = [J_\nu(T_{\rm ex}) - J_\nu(T_{\rm bg})](1 - e^{-\tau_\nu})$ → $\tau_{^{13}\rm CO}$

- Estimating the $N(^{13}\rm CO)$

Physical Properties: method 1 -- practical



$T_{R,12CO}$ = 65 K



$T_{R,13CO}$ = 35 K

Physical Properties: method 2 -- background

Requirement

- Two transitions of the same atomic/molecular line: ν_1 and ν_2

Line Column Density

- Line Ratio: both lines are optically thin ($\tau_\nu \ll 1$)

$$R^{\text{thin}}_{\nu 1/\nu 2} = \frac{[J_{\nu 1}(T_{\text{ex}}) - J_{\nu 1}(T_{\text{bg}})]\tau_1}{[J_{\nu 2}(T_{\text{ex}}) - J_{\nu 2}(T_{\text{bg}})]\tau_2}$$

Dependence only on T_{ex}

- Line Ratio: both lines are optically thick ($\tau_\nu \gg 1$)

$$R^{\text{thick}}_{\nu 1/\nu 2} = \frac{[J_{\nu 1}(T_{\text{ex}}) - J_{\nu 1}(T_{\text{bg}})]}{[J_{\nu 2}(T_{\text{ex}}) - J_{\nu 2}(T_{\text{bg}})]}$$

Dependence only on T_{ex}

- Line Ratio: One optically thin and one optically thick

$$R_{\nu 1/\nu 2} = \frac{[J_{\nu 1}(T_{\text{ex}}) - J_{\nu 1}(T_{\text{bg}})]\tau_1}{[J_{\nu 2}(T_{\text{ex}}) - J_{\nu 2}(T_{\text{bg}})]}$$

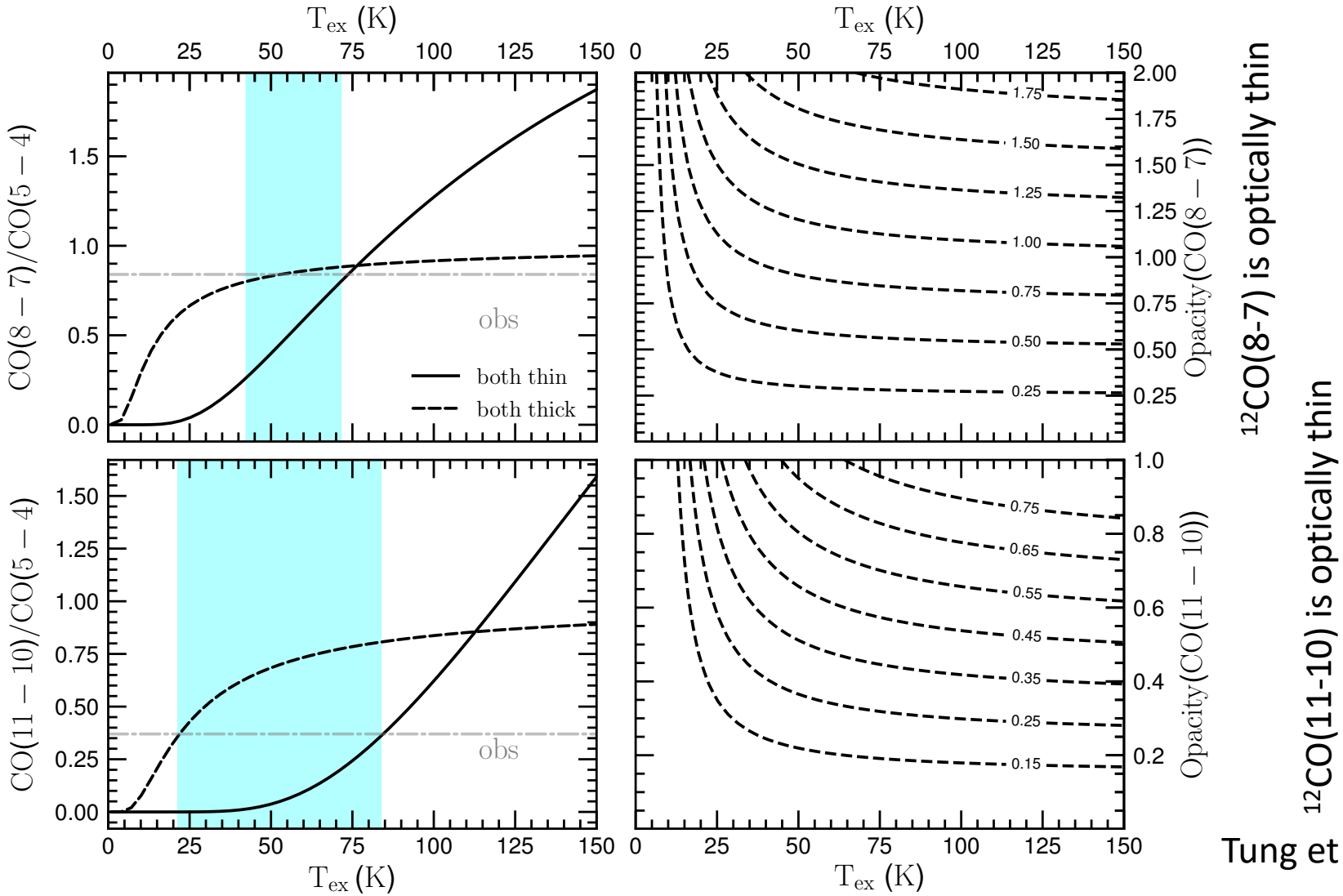
Dependence on both T_{ex} and τ

Weakness

- Need multiple lines of the same atom/molecule

Physical Properties: method 2 -- practical

- As an example, considering multiple lines of ^{12}CO



^{12}CO(8-7) is optically thin

^{12}CO(11-10) is optically thin

Tung et al., subm

Physical Properties: method 3 -- background

Requirement

- Isotopic Transitions of atomic/molecular lines: ν_1 and ν_2

Line Column Density

$$N_{\mathrm{tot}} = f(T_{\mathrm{ex}}) \frac{\tau}{1-e^{-\tau}} \int \frac{T_{\mathrm{mb}} dv}{\mathrm{K\,cms^{-1}}}$$

- Integrated Intensity Ratio:

$$R_{\nu 1/\nu 2} = \frac{\int T_{\mathrm{mb}\,1} dv}{\int T_{\mathrm{mb}\,2} dv} \approx \frac{1-e^{-\tau_1}}{1-e^{-\tau_2}}$$

Abundance ratio: $[N_1]/[N_2] \cong \tau_1/\tau_2$

$$R_{\nu 1/\nu 2} = \frac{1-e^{-\tau_1}}{1-e^{-\varphi\tau_1}}$$

φ: relative abundance ratio of two isotopologues

- Radiation temperature

$$T_R = \eta \times [J_{\nu 1}(T_{\mathrm{ex}}) - J_{\nu 1}(T_{\mathrm{bg}})](1-e^{-\tau_1})$$

Trick

If possible: Use method 1 or 2 to first determine T_{ex}

Weakness

Physical Properties: method 3 -- practical

For instance, we have: $^{12}C^{18}O$(1-0), $^{12}C^{17}O$(1-0), $^{13}C^{18}O$(1-0)

- Isotopic Transitions of atomic/molecular lines: ν_1 and ν_2
- Integrated Intensity Ratio

$$\frac{\int T_{\mathrm{mb},^{12}C^{18}O}\,dv}{\int T_{\mathrm{mb},^{12}C^{17}O}\,dv} \equiv R_1 \cong \frac{1-e^{-\tau_{^{12}C^{18}O}}}{1-e^{-\tau_{^{12}C^{18}O}/A}}$$

$$\frac{\int T_{\mathrm{mb},^{12}C^{18}O}\,dv}{\int T_{\mathrm{mb},^{13}C^{18}O}\,dv} \equiv R_2 \cong \frac{1-e^{-\tau_{^{12}C^{18}O}}}{1-e^{-\tau_{^{12}C^{18}O}/B}}$$

$$\frac{\int T_{\mathrm{mb},^{12}C^{17}O}\,dv}{\int T_{\mathrm{mb},^{13}C^{18}O}\,dv} \equiv R_3 \cong \frac{1-e^{-\tau_{^{12}C^{18}O}/A}}{1-e^{-\tau_{^{12}C^{18}O}/B}}$$

$A = [^{18}O]/[^{17}O]$
$B = [^{13}C]/[^{12}C]$

Reccommendation
Use MCMC to solve this set of equations

See Giannetti et al. 2014

- Radiation temperature

$$T_{\mathrm{mb},^{12}C^{18}O} = \eta \times [J_{\nu 1}(T_{\mathrm{ex}}) - J_{\nu 1}(T_{\mathrm{bg}})](1-e^{-\tau_{^{12}C^{18}O}})$$
$$T_{\mathrm{mb},^{12}C^{17}O} = \eta \times [J_{\nu 1}(T_{\mathrm{ex}}) - J_{\nu 1}(T_{\mathrm{bg}})](1-e^{-\tau_{^{12}C^{18}O}/A})$$

Physical Properties: method 4 -- background

Requirement

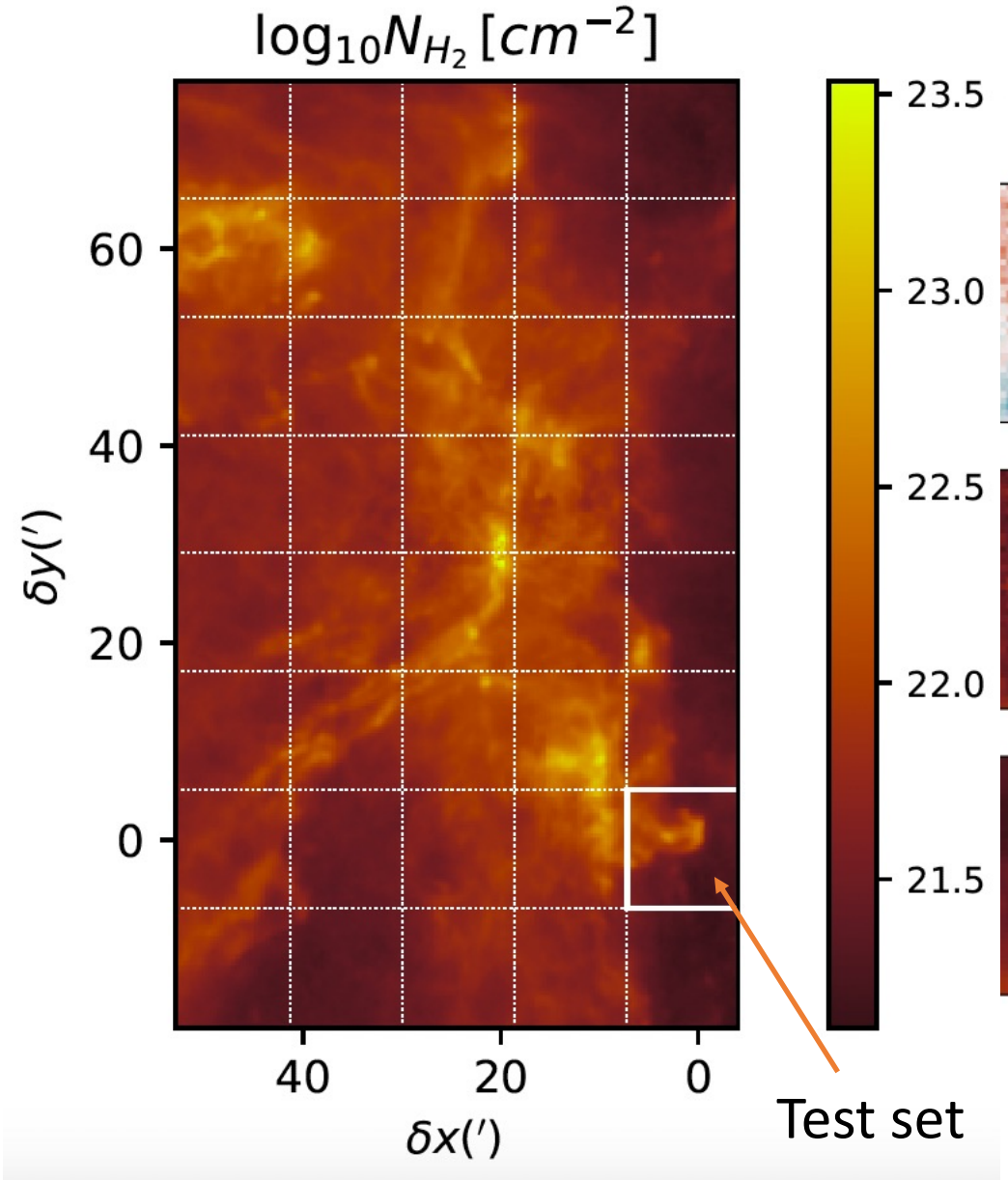
- Continuum Spectral Energy Distribution (SED, dust)
- Line emission (gas)

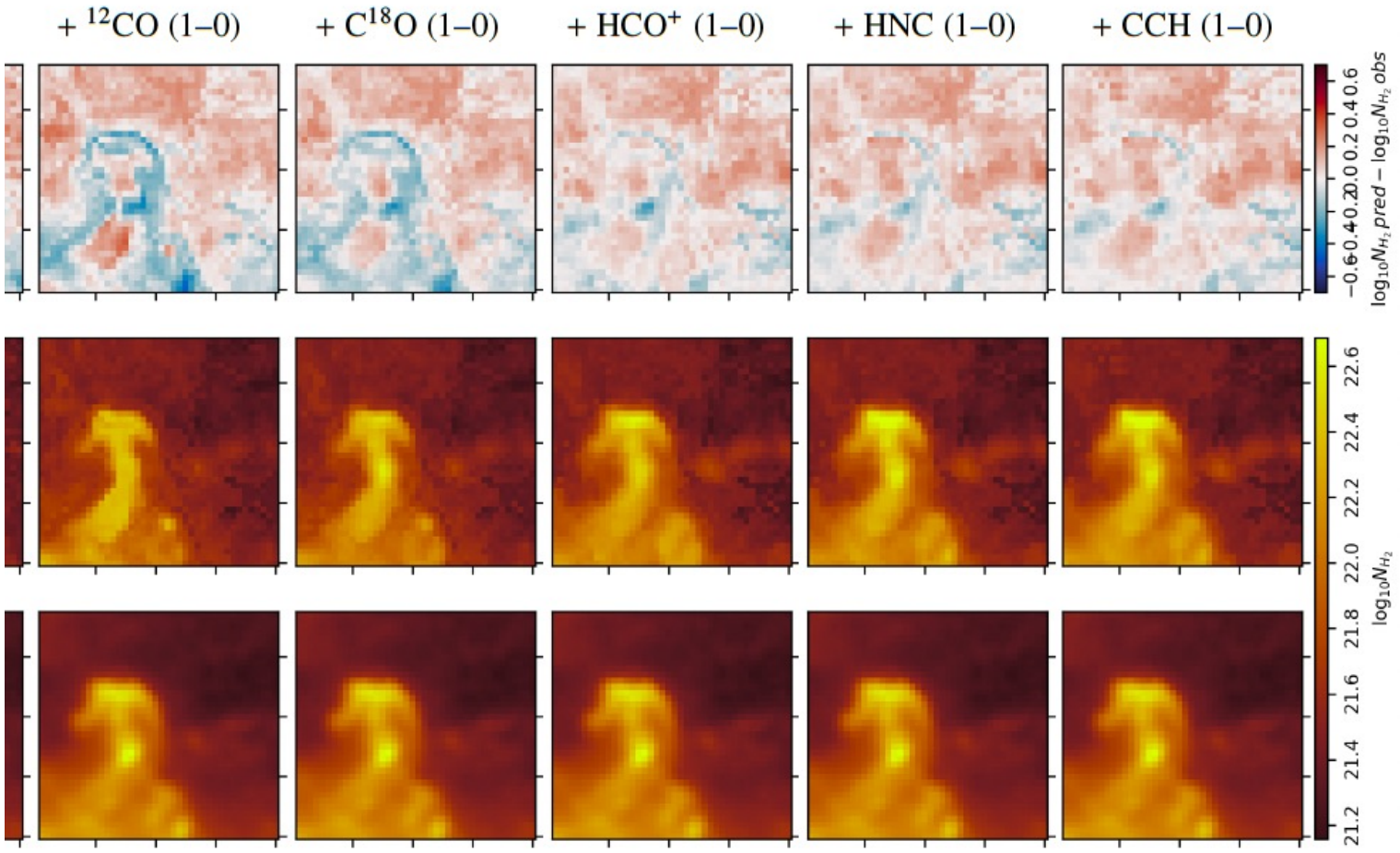
Procedure

- Fit modified black-body radiatio to dust SED → N_{H2}^{d}
- Solving for this relation $N_{\mathrm{H2}}^{d} = f(T_{mb,\,i}, Wi) + e$
  - ❖ $T_{mb,i}$ = peak temperature of line *i*
  - ❖ W_i=*intergrated intensity of line i*
- Use Machine Learning to find $f(T_{mb,\,i}, Wi)$

Non-linear function (unknown)

Physical Properties: method 4 -- practical





Gratier et al. 2021

Non-Local Thermal Equilibrium (non-LTE): background

- ~~The source function $S_\nu = \frac{\epsilon_\nu}{\kappa_\nu} \equiv$ Planck function ($B_\nu(T_{ex})$)~~
- ~~Population is followed the Boltzmann distribution ($n_i \sim e^{-hEi/T_{ex}}$)~~

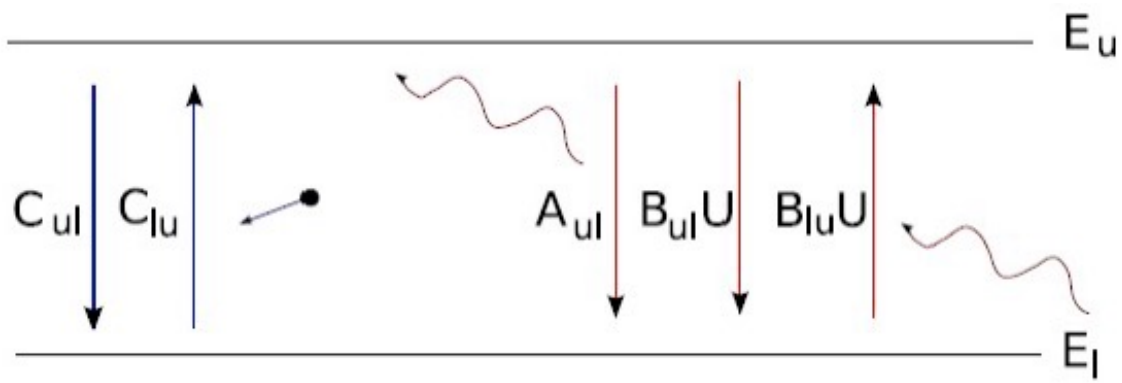
$$\boxed{\frac{dI_\nu}{ds} = \epsilon_\nu - \kappa_\nu I_\nu}$$

emissivity: $\epsilon_{\nu_{ji}} = \frac{h\nu_{ji}}{4\pi} n_j A_{ji} \phi(\nu)$

absoprtion: $\kappa_{\nu_{ji}} = \frac{h\nu_{ji}}{4\pi} n_i B_{ji} (g_j n_i / g_i n_j - 1) \phi(\nu)$

$\Rightarrow$ need to know n_j and n_i

Non-Local Thermal Equilibrium (non-LTE): background



$$\frac{dn_i}{dt} = \sum_{j>i} [n_j A_{ji} + (n_j B_{ji} - n_i B_{ij}) J_{ji}]$$

$$- \sum_{j<i} [n_i A_{ji} + (n_i B_{ij} - n_j B_{ji}) J_{ji})]$$

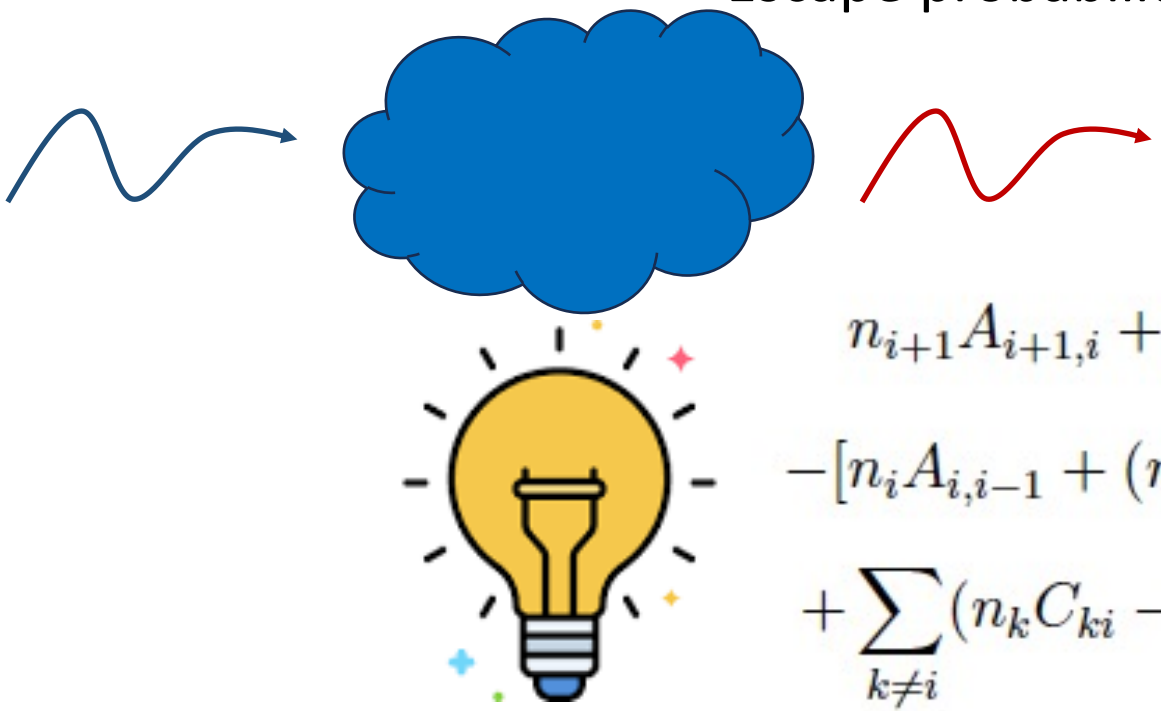
$$+ \sum_{j \neq i} [n_j C_{ji} - n_i C_{ij}] \quad = 0$$

To solve J_{ji}, we need to know n_j and n_i
To solve n_j and n_i, we need to know J_{ji}

Non-Local Thermal Equilibrium (non-LTE): background

- Escape probability approximation

Escape probability β

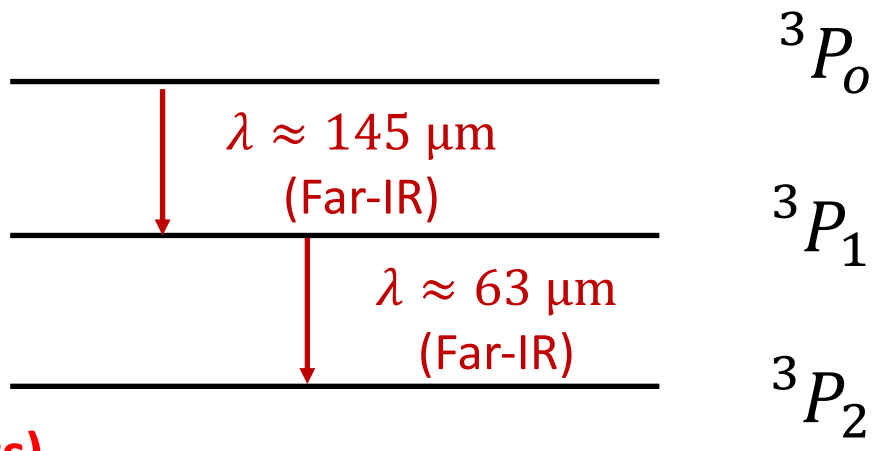


$$J_{ji} = S_{ji}(1 - \beta_{ji}) + \beta_{ji} I_{c,\nu}$$

$$n_{i+1}A_{i+1,i} + (n_{i+1}B_{i+1,i} - n_i B_{i,i+1})(S_{i+1,i}(1 - \beta_{i+1,i}) + \beta_{i+1,i} I_{c,\nu})$$
$$-[n_i A_{i,i-1} + (n_i B_{i,i-1} - n_{i-1} B_{i-1,i})(S_{i,i-1}(1 - \beta_{i,i-1}) + \beta_{i,i-1} I_{c,\nu})]$$
$$+ \sum_{k \neq i} (n_k C_{ki} - n_i C_{ik}) = 0$$

- RADEX as a simple tool (Van de Tak et al. 2007)

Non-Local Thermal Equilibrium (non-LTE): practical

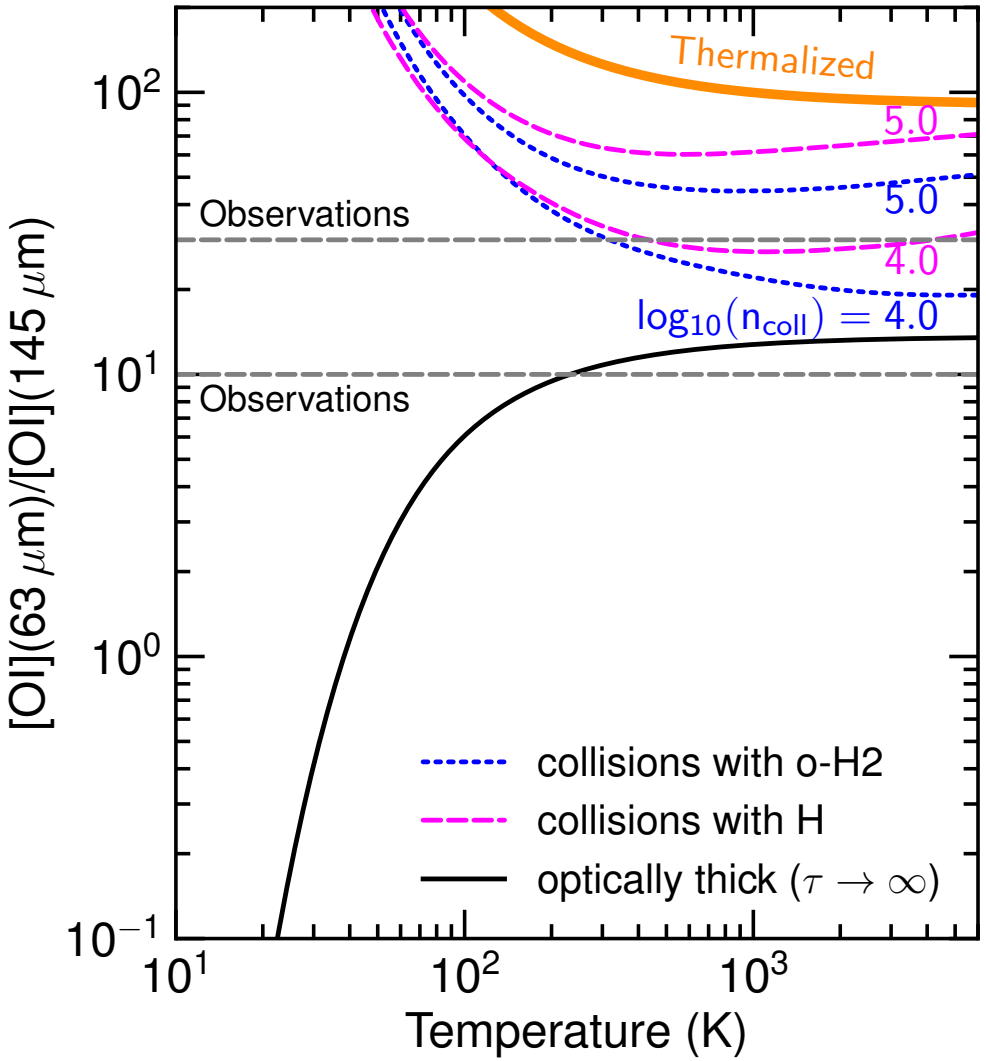


- Oxygen: 3 levels system
- Statistical equlibrium:
  (ignoring the absorption and stimulated coefficients)

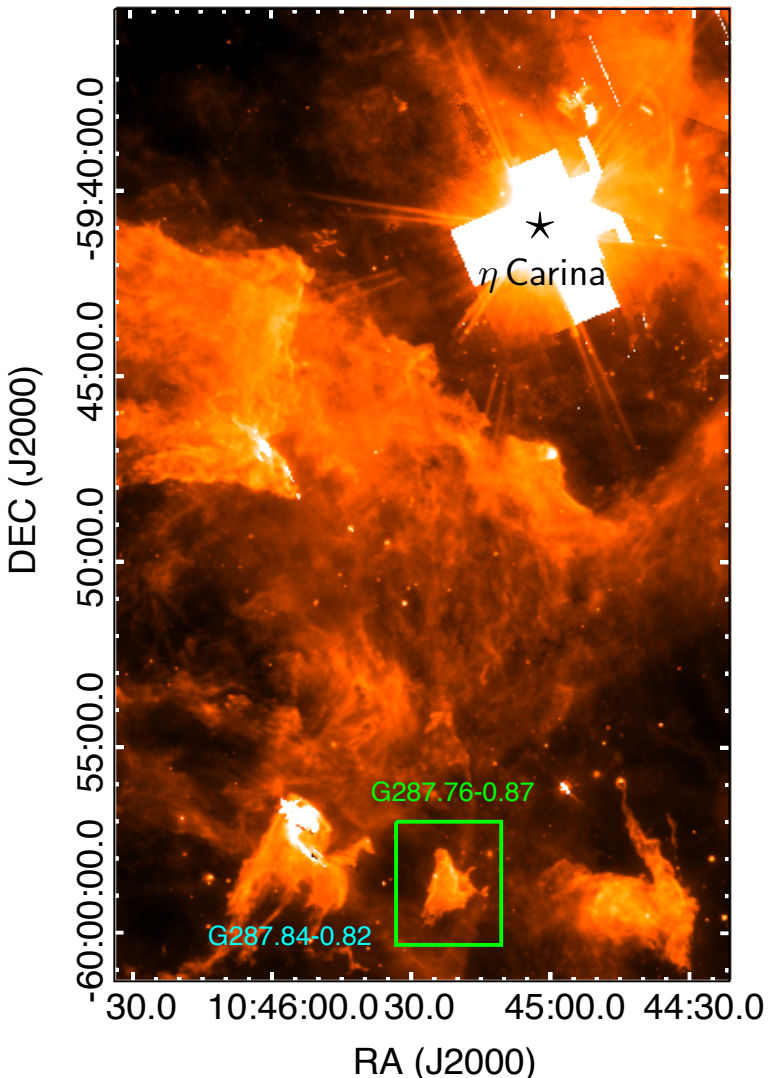
$$\boxed{f_j \left[\sum_i n_{\rm coll} C_{ji} + \sum_{i<j} A_{ji} \right] = \sum_i f_i n_{\rm coll} C_{ij} - \sum_{i>j} f_i A_{ij}}$$

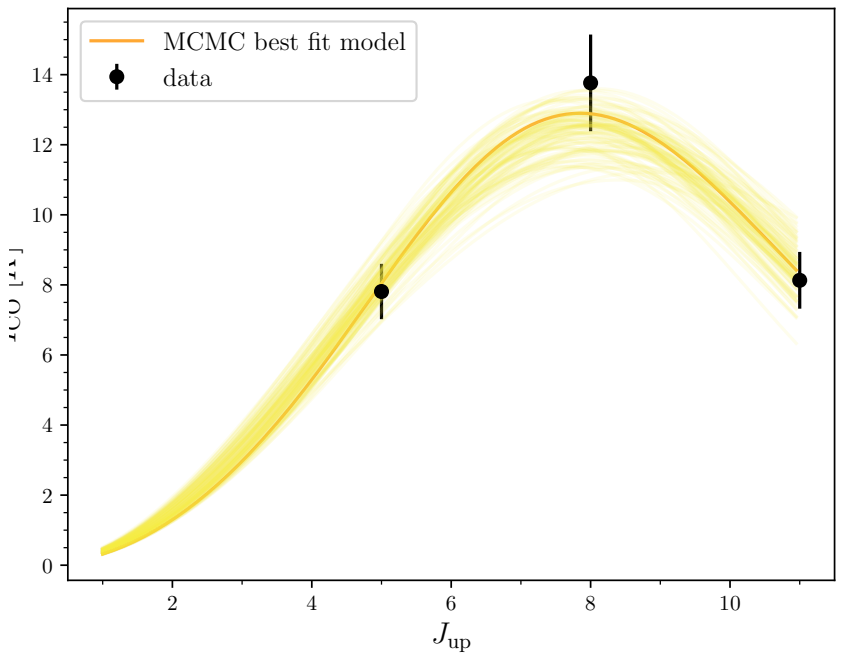
$$f_i = n_i / n_{\rm tot}$$
$$f_j = n_j / n_{\rm tot}$$

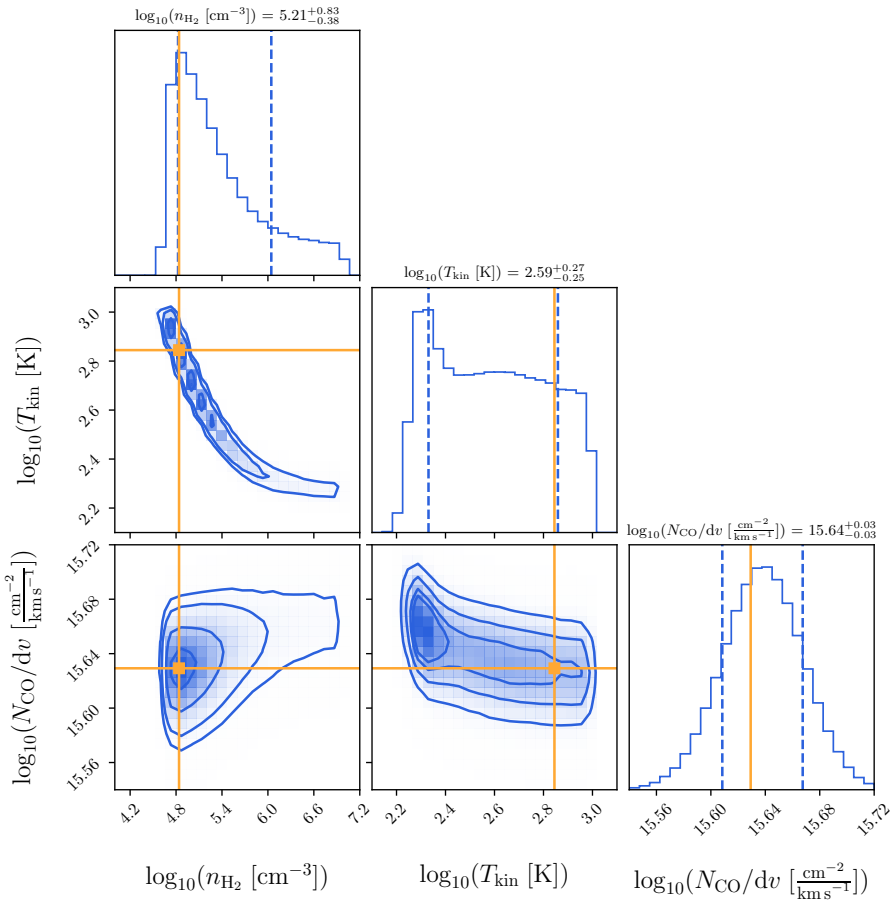
Non-Local Thermal Equilibrium (non-LTE): practical



Non-Local Thermal Equilibrium (non-LTE): practical

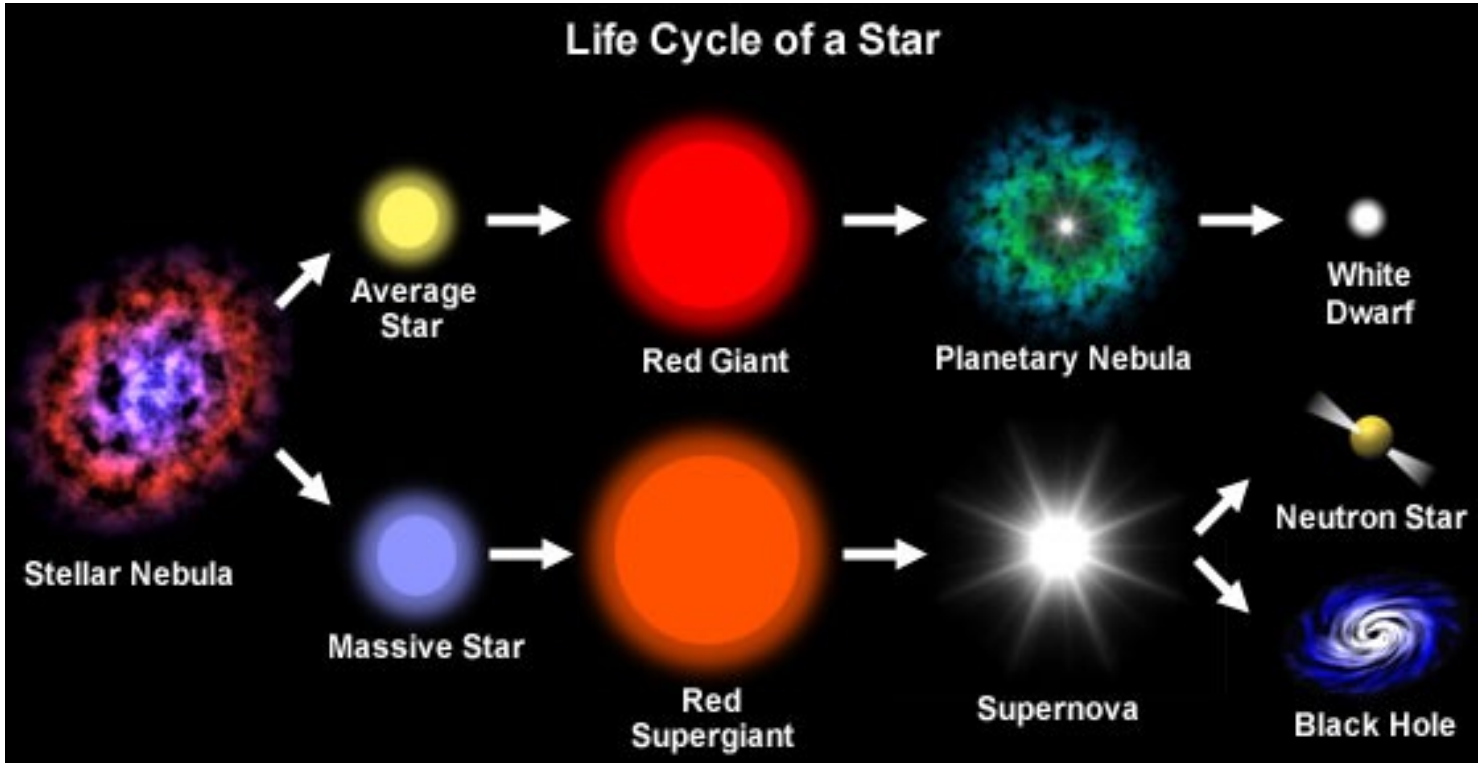






RADEX + MCMC (Tung et al. subm)

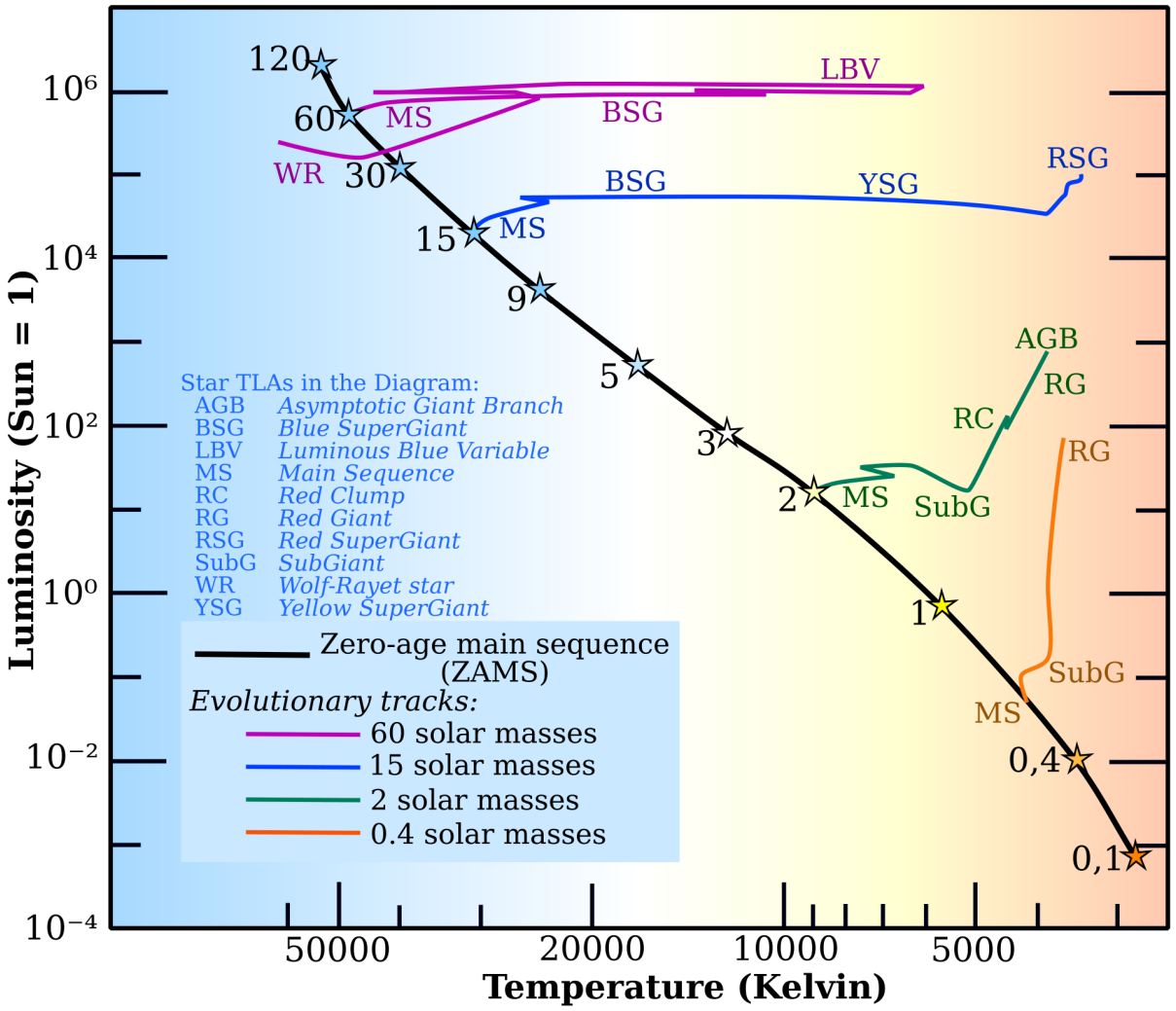
Photo-Dissociation Region: PDR



- Low- Intermediate mass star: $M_* < 8M_\odot$
- Massive star: $M_* > 8M_\odot$

Photo-Dissociation Region: PDR

HR diagram



Surface temperature of O/B associations
T< 50,000 K (depending on their mass)

$$\lambda_{max} > \frac{0.29\text{x}10^7(\text{nm K})}{5\text{x}10^4(\text{K})} = 58\text{nm}$$

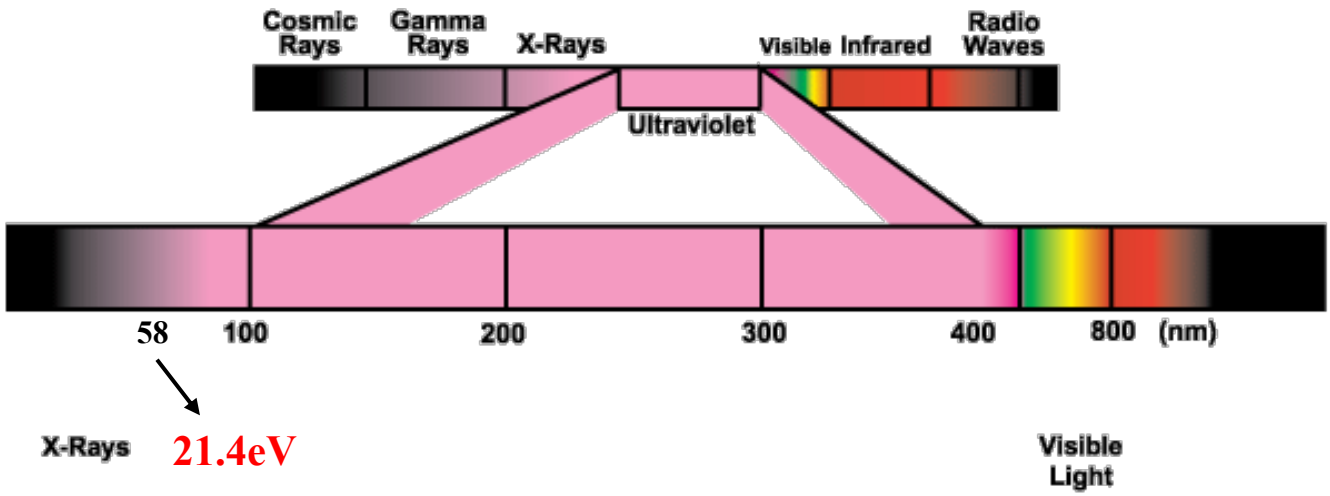
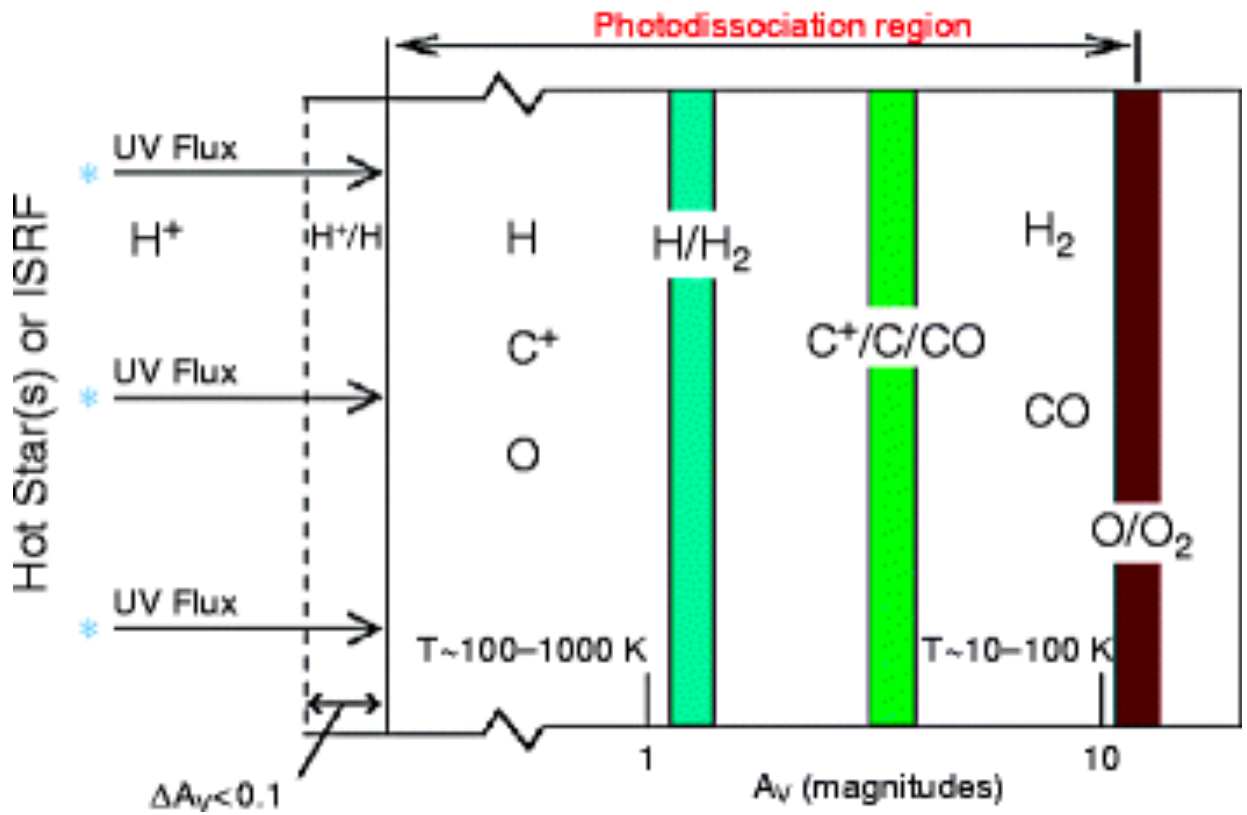


Photo-Dissociation Region: PDR



Ionization energy:

- $H + 13.6eV \rightarrow H^+$ (i.e., H II)
- C + 11.26eV → C^+ (i.e., C II) (remove outermost *e*)

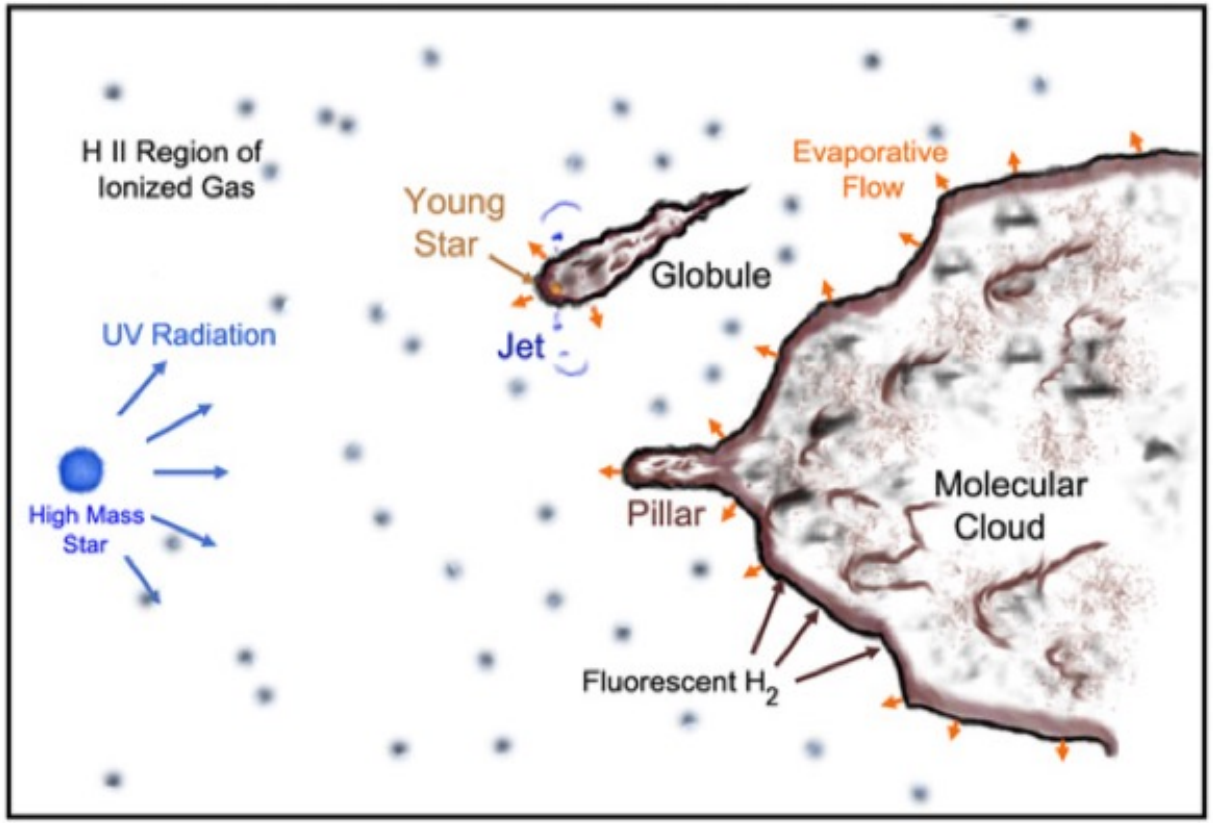
Dissociation energy:
(Energy to break the bonding)

- $H_2 + 4.5eV \rightarrow H$
- CO + 11.09eV → C + O (ground state)

General picture:

- Intense UV radiation ionizes an 'H II region' within which H is nearly fully-ionized
- At the boundaries of an H II region, H is in neutral state → define a photodissociation region or PDR
- Radiation (<13.6 eV) penetrates into the PDR; ionizing and dissociating molecules; heating dust grains
- Further in PDR region, gas could be in molecular form

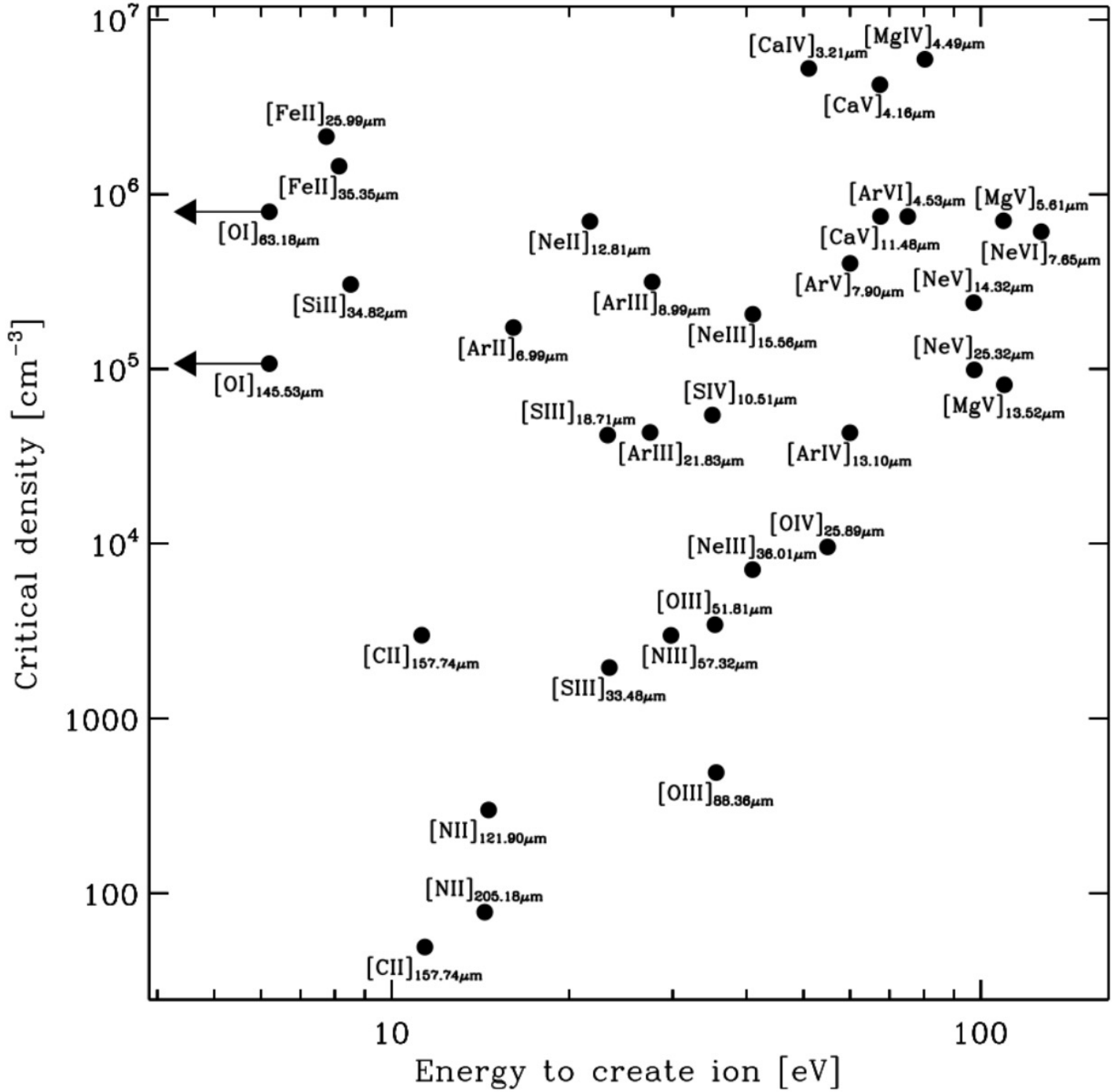
Photo-Dissociation Region: PDR



Sketch of a photodissociation region
(Hartigan et al. 2015)

Pillars: a column-like shape and a physical connection to the gas reservoir of the molecular cloud.

Globules: a head-tail structure pointing toward the illuminating source and isolated to the molecular cloud.


Critical density [cm^{-3}]
Energy to create ion [eV]
10^7
10^6
10^5
10^4
1000
100
10
100
[CaIV]$_{3.21\mu m}$
[MgIV]$_{4.49\mu m}$
[CaV]$_{4.16\mu m}$
[FeII]$_{25.99\mu m}$
[FeII]$_{35.35\mu m}$
[OI]$_{63.18\mu m}$
[ArVI]$_{4.53\mu m}$
[MgV]$_{5.61\mu m}$
[NeII]$_{12.81\mu m}$
[CaV]$_{11.48\mu m}$
[NeVI]$_{7.65\mu m}$
[ArV]$_{7.90\mu m}$
[NeV]$_{14.32\mu m}$
[SiII]$_{34.82\mu m}$
[ArIII]$_{8.99\mu m}$
[NeIII]$_{15.56\mu m}$
[ArII]$_{6.99\mu m}$
[NeV]$_{25.32\mu m}$
[OI]$_{145.53\mu m}$
[SIV]$_{10.51\mu m}$
[MgV]$_{13.52\mu m}$
[SIII]$_{18.71\mu m}$
[ArIII]$_{21.83\mu m}$
[ArIV]$_{13.10\mu m}$
[OIV]$_{25.89\mu m}$
[NeIII]$_{36.01\mu m}$
[OIII]$_{51.81\mu m}$
[CII]$_{157.74\mu m}$
[NIII]$_{57.32\mu m}$
[SIII]$_{33.48\mu m}$
[OIII]$_{88.36\mu m}$
[NII]$_{121.90\mu m}$
[NII]$_{205.18\mu m}$
[CII]$_{157.74\mu m}$

Carina Nebula

Check out data