

Interstellar Medium 2020

# Lecture 8: Molecular clouds



**Paul van der Werf**

# Course Contents

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2. Physical conditions and radiative processes
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# Today's Lecture

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Molecules and their excitation

1. The  $\text{H}_2$  problem
2. Molecules as probes
3. Molecular clouds

Corresponding textbook material: Draine Ch. 5 & 31

# Rotational transitions for linear molecules

Start with **heteronuclear molecules** (CO, CS, HD, SiO, HCN, HCO<sup>+</sup>,...)

The charge distribution is now asymmetric, and the asymmetry is measured by the **permanent electric dipole moment  $\mu$**  [Debye].

The Einstein A coefficient for **electric dipole transitions** (rotating dipole with electric dipole moment  $\mu$ ) can be calculated:

$$A_{J,J-1} = \frac{128\pi^3}{3\hbar} \left( \frac{B_v}{hc} \right)^3 \mu^2 \frac{J^4}{J + \frac{1}{2}}$$

with the selection rule  **$\Delta J = \pm 1$**

so approximately:  $A_{J,J-1} \propto J^3$  and the other A's are zero.

e.g., for CO:  $A_{J,J-1} = 1.07 \cdot 10^{-7} \frac{J^4}{J + \frac{1}{2}}$  s<sup>-1</sup>, so **slow** transitions (nuclear inertia)

# How about homonuclear molecules?

**Homonuclear molecules** (principally  $\text{H}_2$ ) have no permanent dipole moment and hence **no electric dipole transitions**.

Now the strongest transitions are the (much weaker) electric quadrupole transitions with the selection rule  $\Delta J = \pm 2$

This results in 2 separate rotational ladders:

- ortho- $\text{H}_2$  ( $J$  odd)
- para- $\text{H}_2$  ( $J$  even)

Quantum physics also requires (see Draine Sect 5.1.6):

- for para- $\text{H}_2$ : nuclear spins antiparallel ( $J_{\text{nuc}} = 0, g_{\text{nuc}} = 1$ )
- for ortho- $\text{H}_2$ : nuclear spins parallel ( $J_{\text{nuc}} = 1, g_{\text{nuc}} = 3$ ).

So abundance ratio ortho/para  $\text{H}_2$  is expected to be 3.

# The H<sub>2</sub> problem

The lowest H<sub>2</sub> transition is the  $J = 2-0$  transition at  $\lambda = 28 \mu\text{m}$  (from the  $J=2$  level which is 511 K above the ground state).

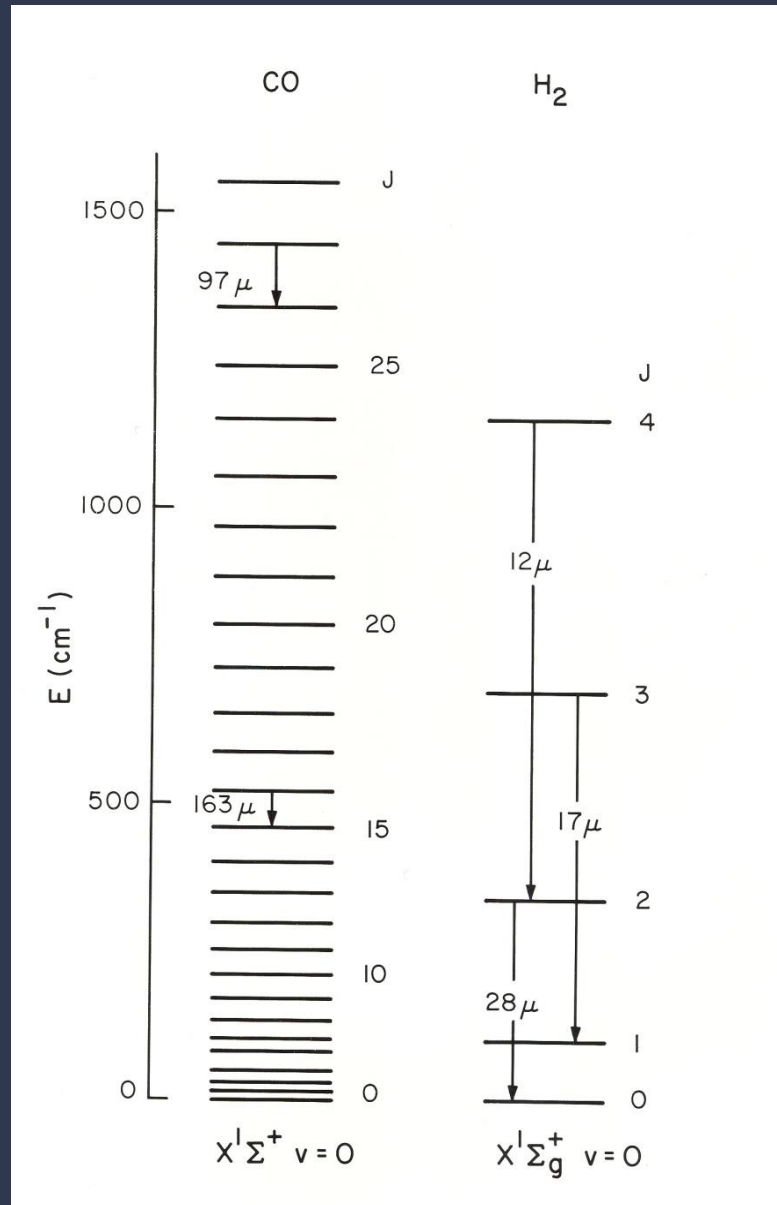
Hence:

- probes only warm H<sub>2</sub> (several 100K)
- can only be observed from space
- very weak line (quadrupole transition)

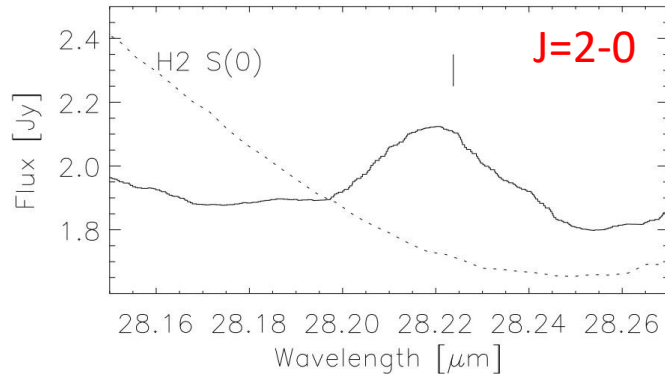
H<sub>2</sub> emission is very hard to observe directly and is not a tracer of bulk molecular gas.

In contrast: CO  $J = 1-0$ :  $\lambda = 2.6\text{mm}$  (accessible from the ground),  $J=1$  level is 5.5 K above ground state: promising probe of cold molecular gas.

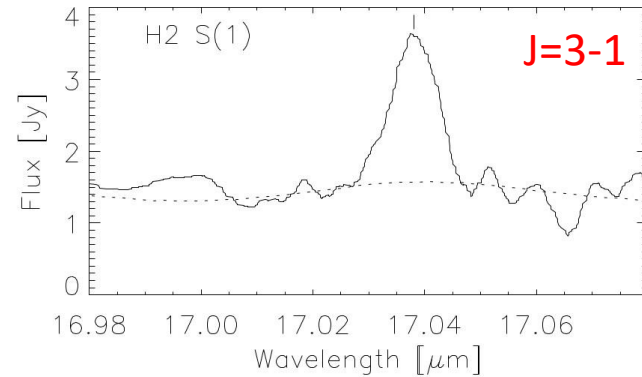
# Rotational line spectra: CO vs H<sub>2</sub>



# First detection of H<sub>2</sub> 28 $\mu$ m line in the ISM



**Fig. 3.** ISO-SWS spectrum of the H<sub>2</sub> S(0) line (28.21  $\mu\text{m}$ ) in the central regions of NGC 6946, with symbols as in Fig. 1.



**Fig. 1.** ISO-SWS spectrum of the H<sub>2</sub> S(1) line (17.03  $\mu\text{m}$ ) in the central regions of NGC 6946. The dotted line represents the RSRF of the instrument (see text). The vertical line is the expected wavelength for a heliocentric radial velocity of 48  $\text{km s}^{-1}$ .

(Valentijn, Van der Werf, De Graauw & De Jong 1996)



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# Critical densities for rotational lines

Recall  $n_{\text{crit}} = \frac{A_{J,J-1}}{k_{J,J-1}}$  and  $A_{J,J-1} = \frac{128\pi^3}{3\hbar} \left(\frac{B_v}{hc}\right)^3 \mu^2 \frac{J^4}{J + \frac{1}{2}}$

Since approximately  $A_{J,J-1} \propto J^3$ , and  $k_{J,J-1}$  is a slow function of  $J$ , we find that approximately  $n_{\text{crit}} \propto J^3$ .

We also had approximately  $E(J) \propto J^2$  for the level energy.

Implications:

- to excite high- $J$  lines efficiently, we need both high  $T$  and high  $n$ .
- since high- $J$  line fluxes depend on both  $T$  and  $n$ , they do not form a clean temperature or density probe.
- using multiple lines, the degeneracy can be broken (in principle)

# Tracing densities with molecular lines

Recall  $n_{\text{crit}} = \frac{A_{J,J-1}}{k_{J,J-1}}$  and  $A_{J,J-1} = \frac{128\pi^3}{3\hbar} \left(\frac{B_v}{hc}\right)^3 \mu^2 \frac{J^4}{J + \frac{1}{2}}$

So: molecules with large  $\mu$  will have large  $n_{\text{crit}}$   
molecules with low  $\mu$  will have low  $n_{\text{crit}}$ .

E.g., CO  $J=1-0$ :  $n_{\text{crit}} \sim \text{few } 100 \text{ cm}^{-3}$   
but HCN  $J=1-0$ :  $n_{\text{crit}} \sim \text{few } 10^5 \text{ cm}^{-3}$

Generally:

- low CO lines ( $J=1-0$ ,  $2-1$ ) are have low critical densities and good probes of bulk cold molecular gas
- lines of heavier molecules (HCN, CS,  $\text{HCO}^+$ ) probe denser molecular gas
- high lines of any molecule probe warm, dense gas

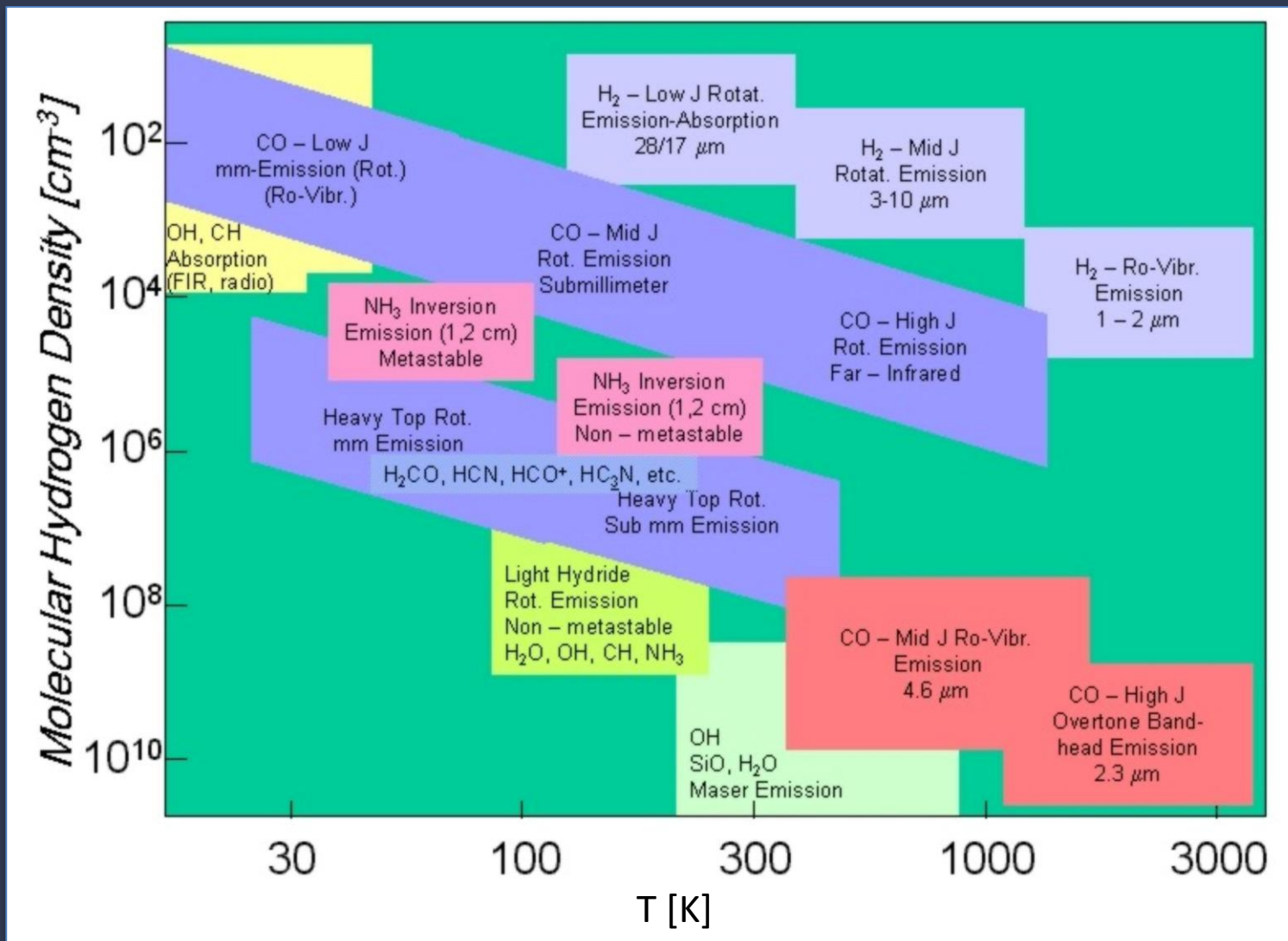
# Properties of some important molecules

MOLECULE	LOWEST ROTATIONAL LINE [ $\mu\text{m}$ ]	ROTATIONAL DIPOLE MOMENT [Debye]	VIBRATIONAL TRANSITIONS [ $\mu\text{m}$ ]
H <sub>2</sub>	28.1	0	2.3
HD	112.1	$5.8 \times 10^{-4}$	2.6
OH	119	1.7	2.7
NH	302		3.0
CH	149,562	1.46	3.5
HCl	479	1.11	3.3
CO	2600	0.112	4.8
CS	6110	2	7.8
HCN	3440	3	3.0, 4.9, 14
HCO <sup>+</sup>	3360	3.3	
NH <sub>3</sub>	524	1.5	2.9, 6.1, 10.5
H <sub>2</sub> O	538,269	1.85	2.7, 6.3
HDO	590	1.84	3.0, 3.7, 7.1
H <sub>2</sub> D <sup>+</sup>	806		
H <sub>3</sub> O <sup>+</sup>	760→830	≈1	
O <sub>2</sub>	5350	0	
SiO	6910	3.1	8.1

# Critical densities

Species	transition	$\nu_{ul}$ [GHz]	$E_u$ [K]	$A_{ul}$ [s <sup>-1</sup> ]	$n_{cr}$ [cm <sup>-3</sup> ]
CO	1 – 0	115.3	5.5	$7.2 \times 10^{-8}$	$1.1 \times 10^3$
	2 – 1	230.8	16.6	$6.9 \times 10^{-7}$	$6.7 \times 10^3$
	3 – 2	346.0	33.2	$2.5 \times 10^{-6}$	$2.1 \times 10^4$
	4 – 3	461.5	55.4	$6.1 \times 10^{-6}$	$4.4 \times 10^4$
	5 – 4	576.9	83.0	$1.2 \times 10^{-5}$	$7.8 \times 10^4$
	6 – 5	691.2	116.3	$2.1 \times 10^{-5}$	$1.3 \times 10^5$
	7 – 6	806.5	155.0	$3.4 \times 10^{-5}$	$2.0 \times 10^5$
CS	1 – 0	49.0	2.4	$1.8 \times 10^{-6}$	$4.6 \times 10^4$
	2 – 1	98.0	7.1	$1.7 \times 10^{-5}$	$3.0 \times 10^5$
	3 – 2	147.0	14	$6.6 \times 10^{-5}$	$1.3 \times 10^6$
	5 – 4	244.9	35	$3.1 \times 10^{-4}$	$8.8 \times 10^6$
	7 – 6	342.9	66	$1.0 \times 10^{-3}$	$2.8 \times 10^7$
	10 – 9	489.8	129	$2.6 \times 10^{-3}$	$1.2 \times 10^8$
HCO <sup>+</sup>	1 – 0	89.2	4.3	$3.0 \times 10^{-5}$	$1.7 \times 10^5$
	3 – 2	267.6	26	$1.0 \times 10^{-3}$	$4.2 \times 10^6$
	4 – 3	356.7	43	$2.5 \times 10^{-3}$	$9.7 \times 10^6$
HCN	1 – 0	88.6	4.3	$2.4 \times 10^{-5}$	$2.6 \times 10^6$
	3 – 2	265.9	26	$8.4 \times 10^{-4}$	$7.8 \times 10^7$
	4 – 3	354.5	43	$2.1 \times 10^{-3}$	$1.5 \times 10^8$
H <sub>2</sub> CO	2 <sub>12</sub> – 1 <sub>11</sub>	140.8	6.8	$5.4 \times 10^{-5}$	$1.1 \times 10^6$
	3 <sub>13</sub> – 2 <sub>12</sub>	211.2	17	$2.3 \times 10^{-4}$	$5.6 \times 10^6$
	4 <sub>14</sub> – 3 <sub>13</sub>	281.5	30	$6.0 \times 10^{-4}$	$9.7 \times 10^6$
	5 <sub>15</sub> – 4 <sub>14</sub>	351.8	47	$1.2 \times 10^{-3}$	$2.6 \times 10^7$
NH <sub>3</sub>	(1,1) inversion	23.7	1.1	$1.7 \times 10^{-7}$	$1.8 \times 10^3$
	(2,2) inversion	23.7	42	$2.3 \times 10^{-7}$	$2.1 \times 10^3$
H <sub>2</sub>	2-0	1.06E4 <sup>a</sup>	510	$2.9 \times 10^{-11}$	10
	3-1	1.76E4 <sup>b</sup>	1015	$4.8 \times 10^{-10}$	300

# Molecular lines as probes



(credit: Reinhard Genzel)

# Today's Lecture

Molecules and their excitation

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# Tracing molecular gas

We have already concluded:

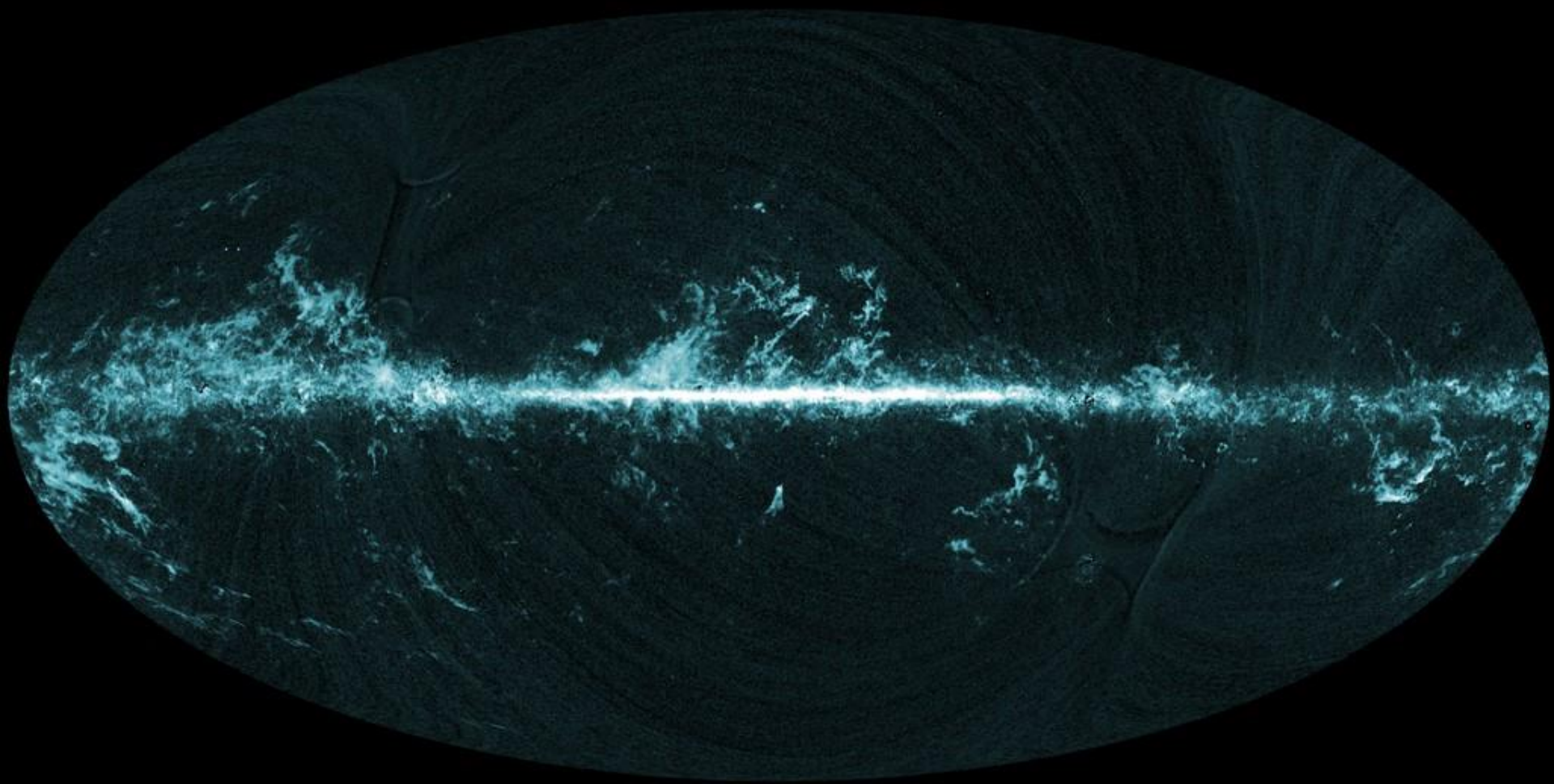
- By far the most important constituent (by mass) of molecular clouds is  $\text{H}_2$ , but we cannot determine  $\text{H}_2$  mass directly.
- But CO (the 2nd most abundant molecule) is a promising tracer of molecular gas, with an easily accessible line:  
 $\text{CO } J = 1 - 0 \text{ at } \lambda = 2.6 \text{ mm}$  ( $n_{\text{crit}} = 1.1 \cdot 10^{-3} \text{ cm}^{-3}$ ,  $E_u/k = 5.5 \text{ K}$ )

Remaining question: are CO and  $\text{H}_2$  co-spatial?

→ look at their formation and destruction mechanisms.

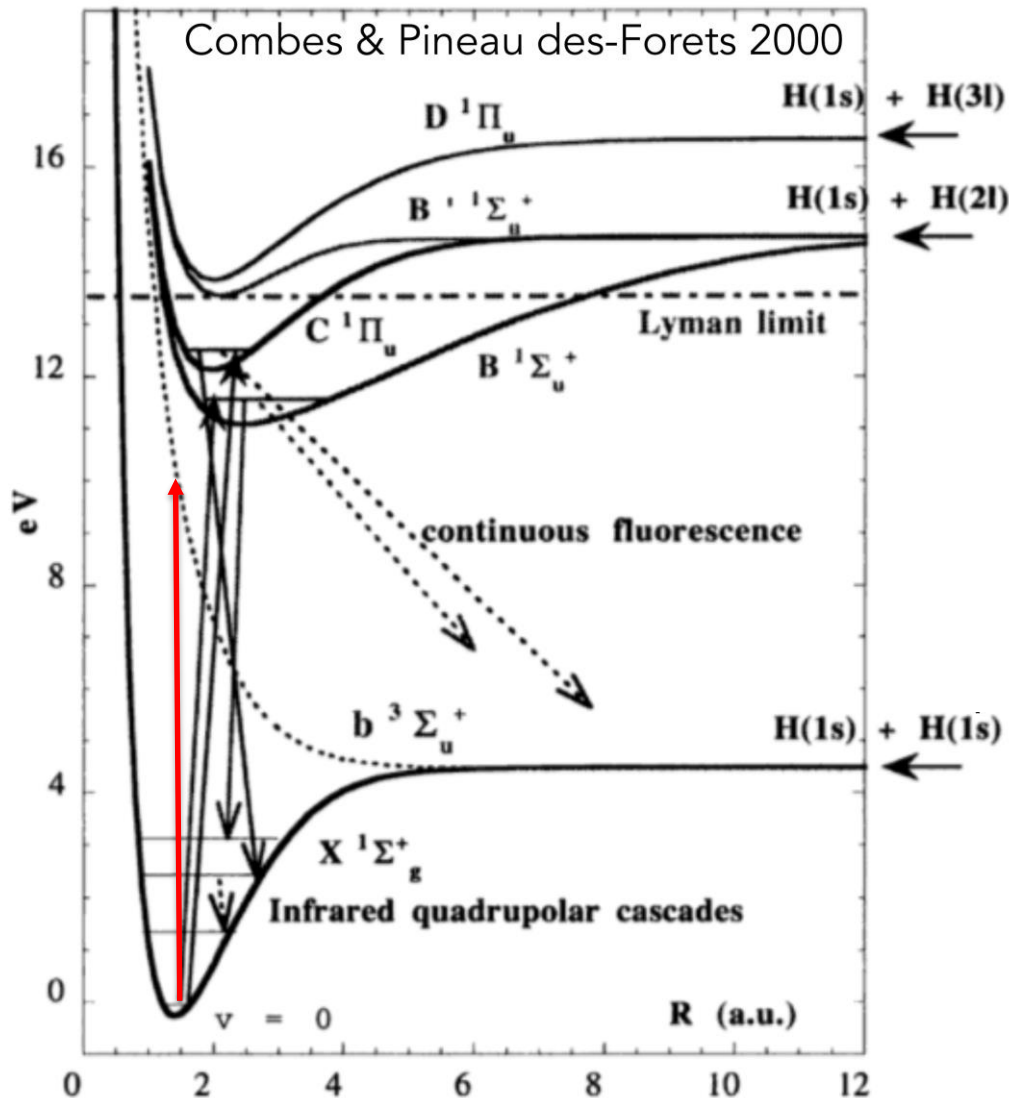


# All-sky CO emission

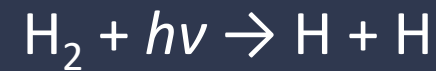


(Planck Satellite)

# H<sub>2</sub> photodissociation

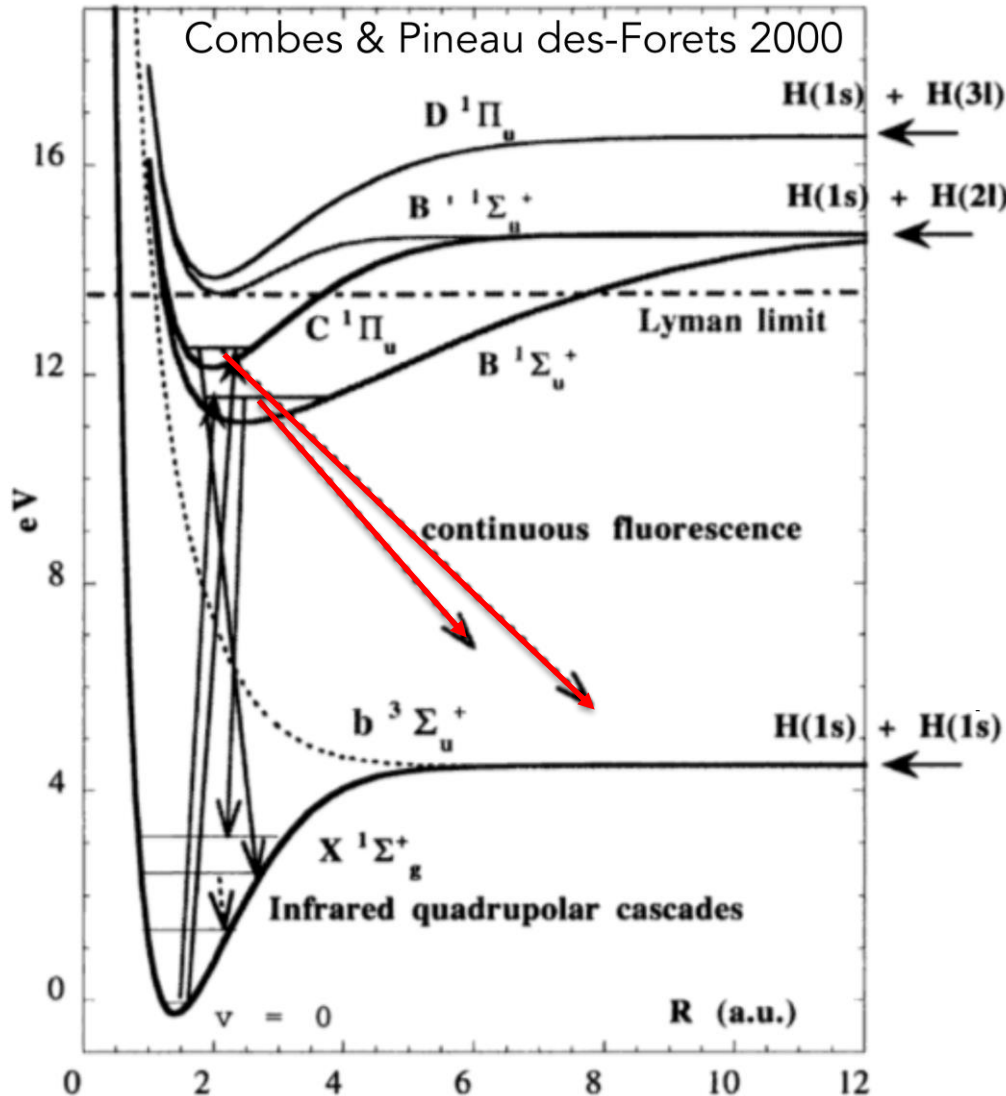


Direct photodissociation from the ground state:



This is a transition to the repulsive  $b^3\Sigma_u^+$  state (red arrow): **forbidden**

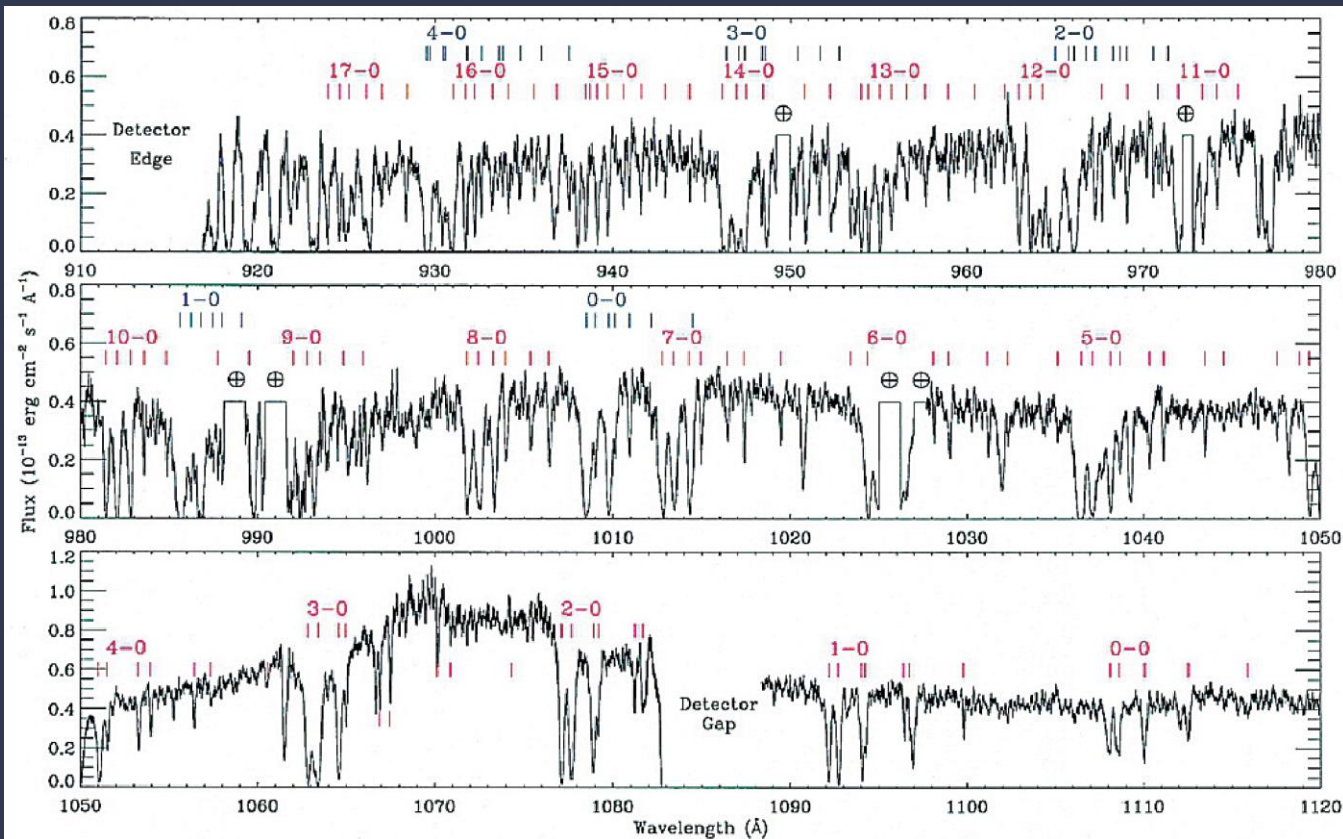
# H<sub>2</sub> photodissociation



H<sub>2</sub> photodissociation is a 2-step process:

1. Absorption in Lyman or Werner bands gives electronically excited molecule (black upwards arrows)
2. Cascading down, there is a 13% of ending up in the repulsive  $b^3\Sigma_u^+$  state → **dissociation (red arrows)**. Remaining 87% falls back to ground state emitting IR photons: vibrational fluorescence.

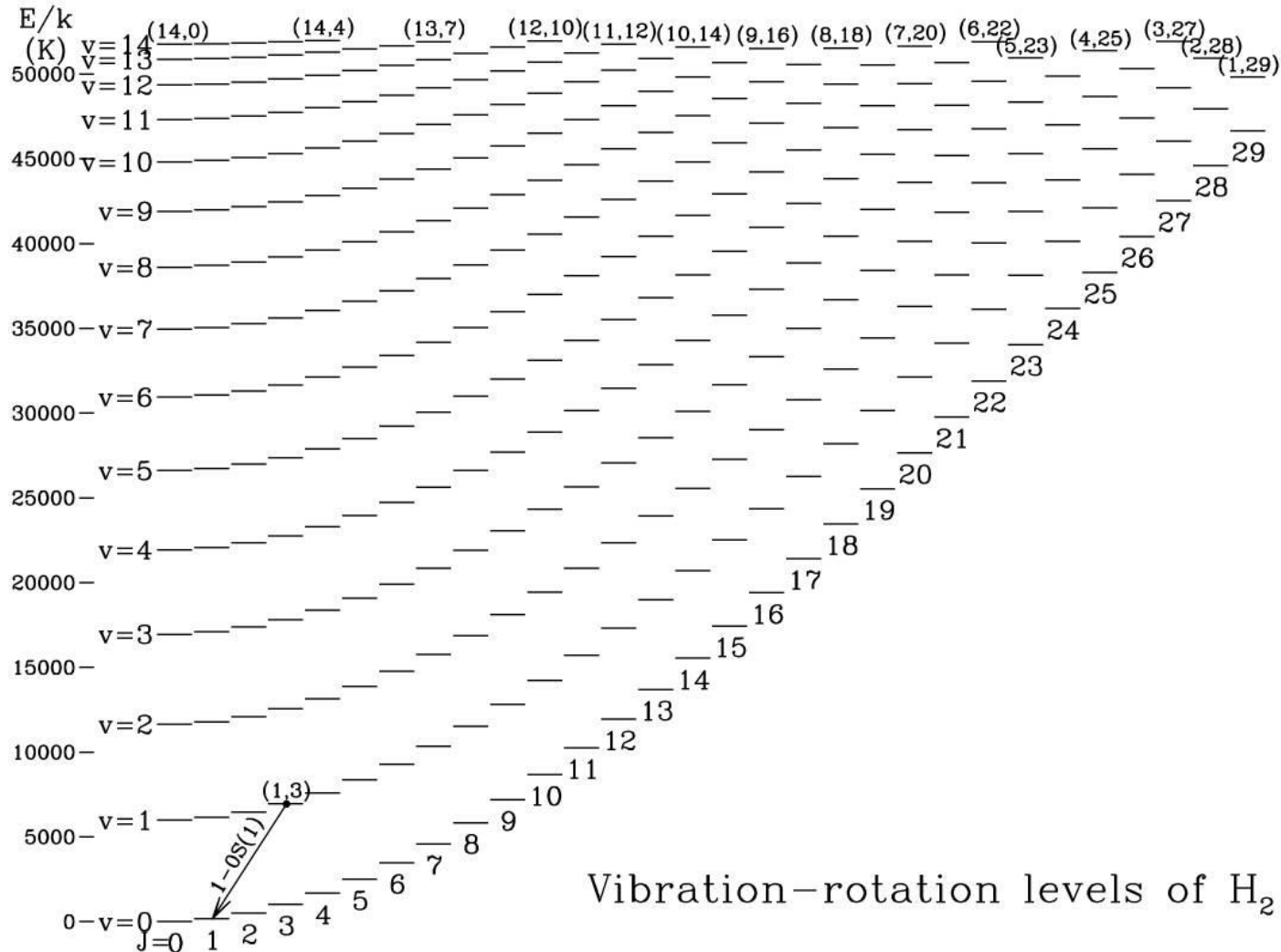
# H<sub>2</sub> UV absorption lines



FUSE spectrum  
towards a bright UV  
source, showing H<sub>2</sub>  
absorption lines  
(Shull *et al.*, 2000)

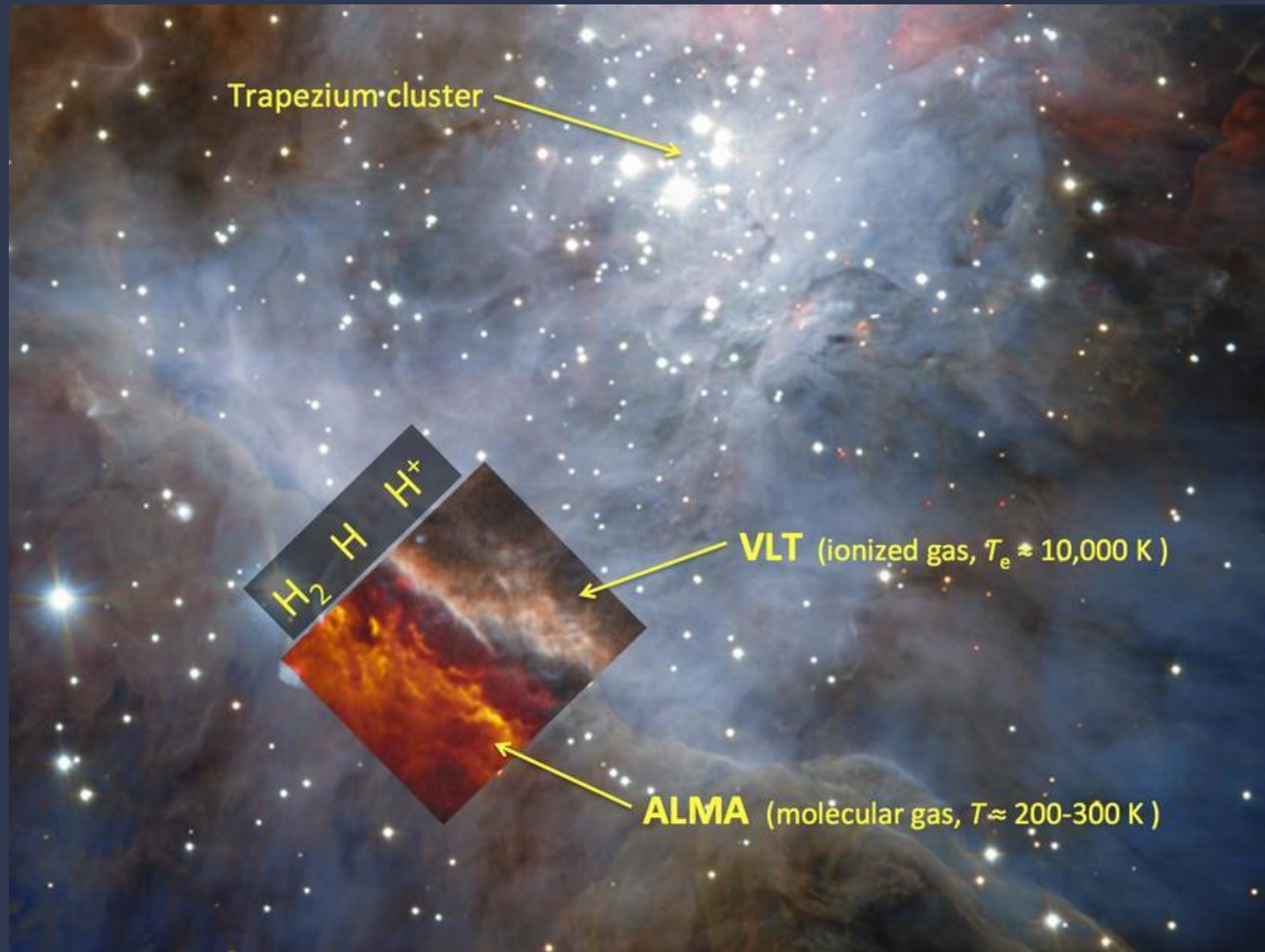
- blue tick marks: H<sub>2</sub> Werner band
- red tick marks: H<sub>2</sub> Lyman band

# H<sub>2</sub> rovibrational energy levels





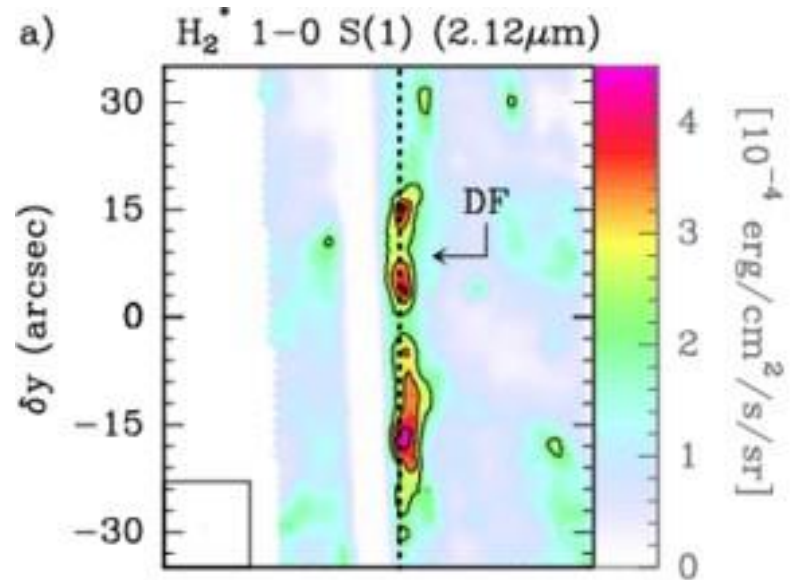
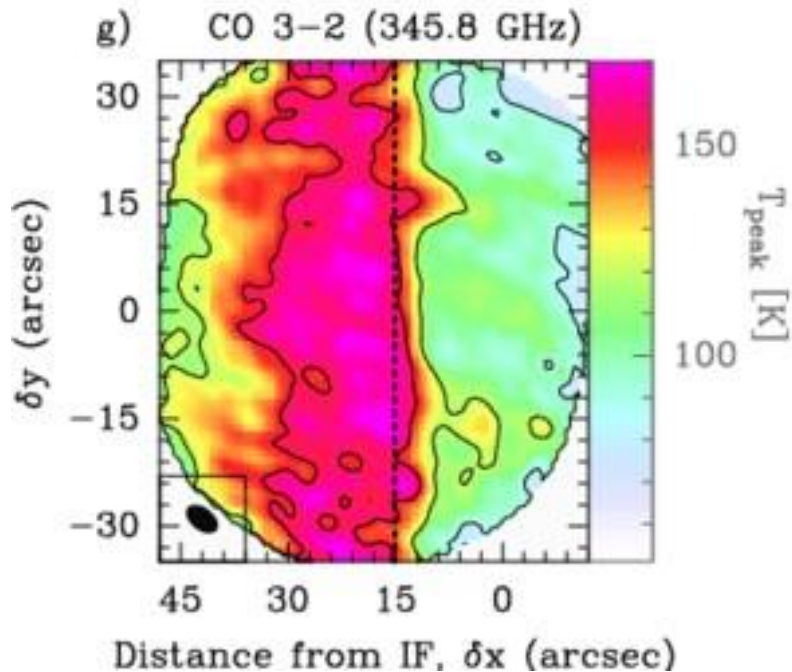
# Photodissociation regions (PDRs)



Orion Nebula

(Goicoechea *et al.*, 2016)

# The Orion Bar PDR



(Goicoechea *et al.*, 2016)

$\text{H}_2$  vibrational fluorescence delineates the dissociation front

# H<sub>2</sub> photodissociation rate

We can write the dissociation rate as  $\frac{dn_{\text{H}_2}}{dt} = -\zeta_{\text{diss}} n_{\text{H}_2}$

where  $\zeta_{\text{diss}}$  depends on the radiation field but nothing else (why not on  $n$  or  $T$ ?)

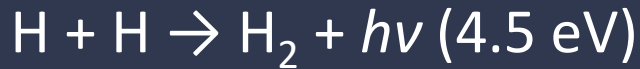
Given a radiation field,  $\zeta_{\text{diss}}$  can be calculated (summing over the UV absorption lines in the Lyman and Werner bands).

In the standard ISRF:  $\zeta_{\text{diss}} \approx 4 \cdot 10^{-11} \text{ s}^{-1}$

NB: the fact that photodissociation is a line process makes it very different from photoionization (which is a continuum process).



# H<sub>2</sub> formation in the gas phase



**extremely slow** reaction, since H<sub>2</sub> cannot radiate away the 4.5 eV

Alternative: use electrons as **catalyst**:



This is how the first H<sub>2</sub> molecule formed!

Reaction rates for these processes can be calculated and are **low**.

# Required H<sub>2</sub> formation rate

We can write the H<sub>2</sub> formation rate as

$$\frac{dn_{\text{H}_2}}{dt} = R n_{\text{H}}^2$$

where  $R$  is some constant (expected to depend on  $T$ ).

What value of  $R$  is required by the data?

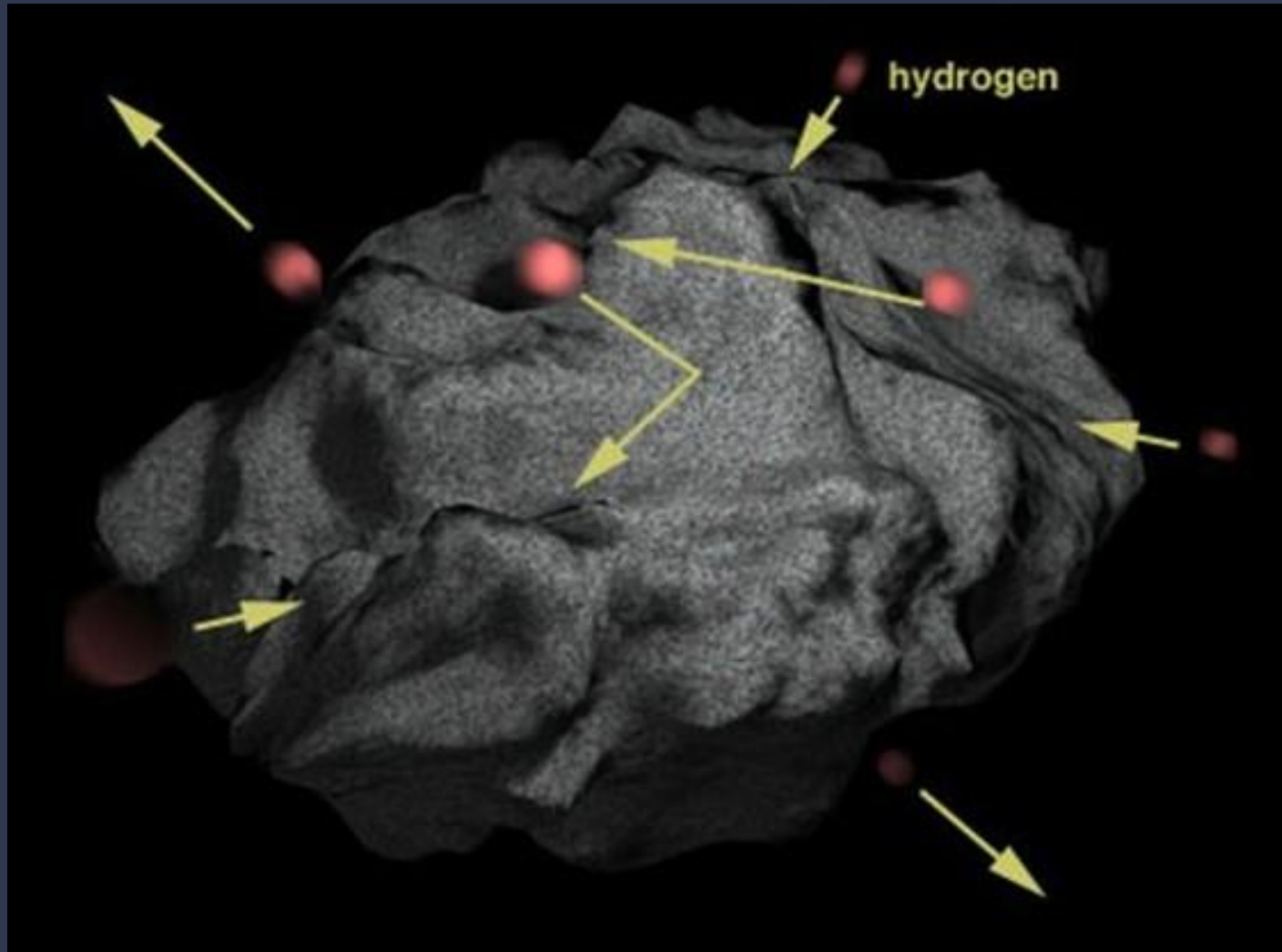
Equilibrium:  $\zeta_{\text{diss}} n_{\text{H}_2} = R n_{\text{H}}^2$

Since we know  $\zeta_{\text{diss}}$ , and we can measure  $n_{\text{H}}$  and  $n_{\text{H}_2}$  in some regions (from UV absorption line spectra), we can determine  $R$ .

Result:  $R \sim 3 \cdot 10^{-17} \text{ cm}^3 \text{ s}^{-1}$

This is about  $10^8 \times$  what can be produced gas-phase reactions!

# H<sub>2</sub> formation on dust grains



# H<sub>2</sub> formation on dust grains

The rate of H<sub>2</sub> formation on dust grains can be calculated, with

the result  $R_{\text{gr}} \approx 3 \cdot 10^{-17} \left( \frac{T}{70 \text{ K}} \right)^{\frac{1}{2}}$ , very close to what we need.

Now we can make a (failing) attempt to work out the equilibrium H<sub>2</sub> abundance:

$$\frac{n_{\text{H}_2}}{n_{\text{H}}} = \frac{R_{\text{gr}} n_{\text{H}}}{\zeta_{\text{diss}}} \approx 2.3 \cdot 10^{-5} \frac{n_{\text{H}}}{30 \text{ cm}^{-3}}$$

So we (incorrectly) conclude: mostly atomic, unless  $n_{\text{H}} > 10^6 \text{ cm}^{-3}$

But **this is not what is observed**: molecular gas can have densities down to  $100 \text{ cm}^{-3}$  → **what did we do wrong?**

# Self-shielding

H<sub>2</sub> photodissociation is a line absorption process and if the lines get optically thick, they will shield the deeper layers from dissociating photons: **self-shielding**

When does this happen?

We can calculate that  $\tau_{\text{H}_2 \text{ Lyman/Werner bands}} > 1$  if  $N(\text{H}_2) > 10^{17} \text{ cm}^{-2}$ , which is a very small value.

So only a very thin layer gets photodissociated. Molecular clouds are molecular because of self-shielding.

# CO formation and destruction

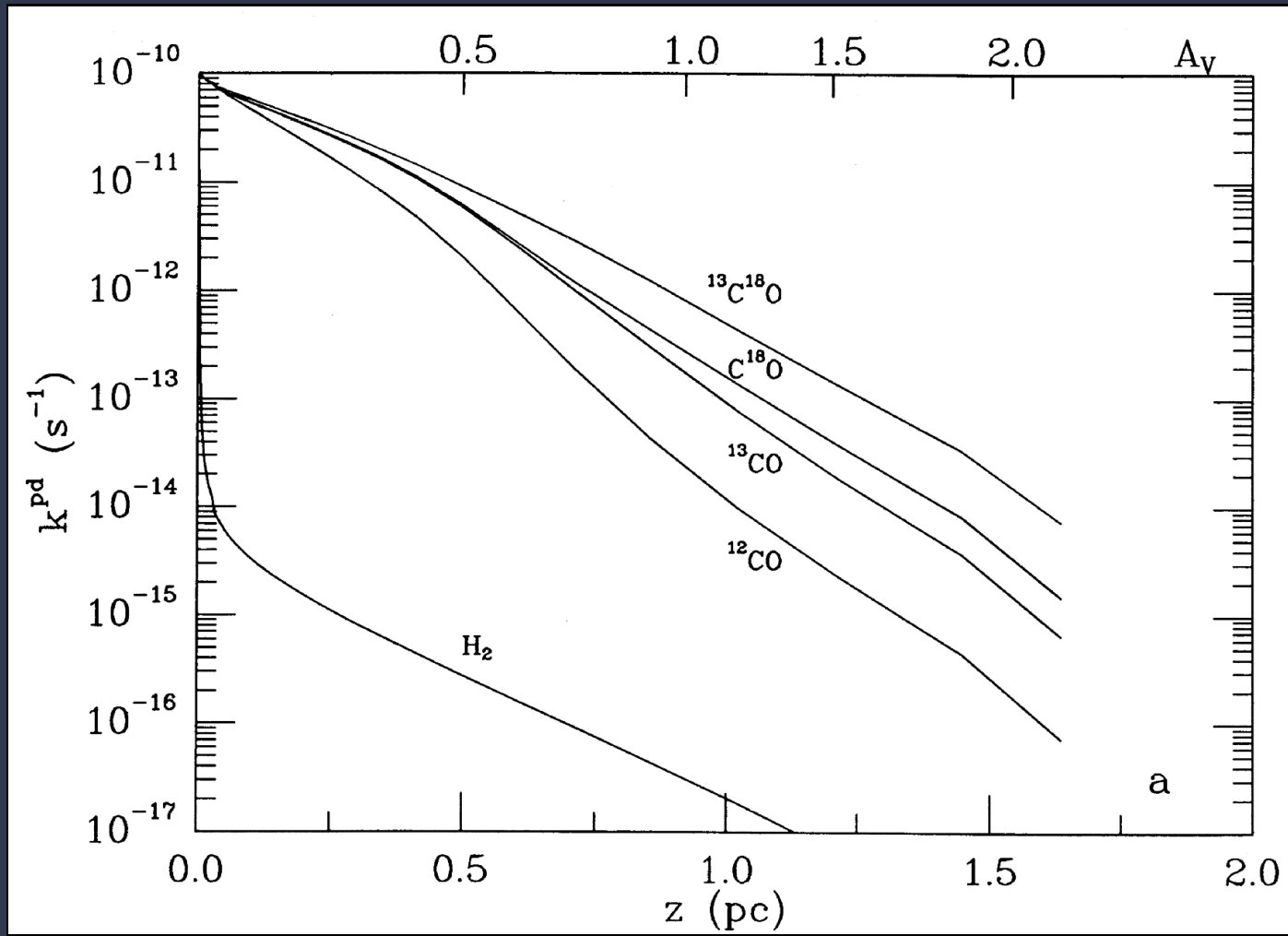
CO formation: gas-phase reactions

CO destruction: UV absorption line process with self-shielding, like  $H_2$

But: since in a given cloud layer  $N(CO) \ll N(H_2)$ ,  
 $\tau_{UV \text{ lines } CO} \ll \tau_{UV \text{ lines } H_2}$ , so the self-shielding layer needs to be thicker for CO.

Therefore a molecular cloud has an outer layer where CO is photodissociated (while  $H_2$  is molecular), resulting in free gas-phase O and  $C^+$ . The outer layer of a molecular cloud is essentially a PDR.

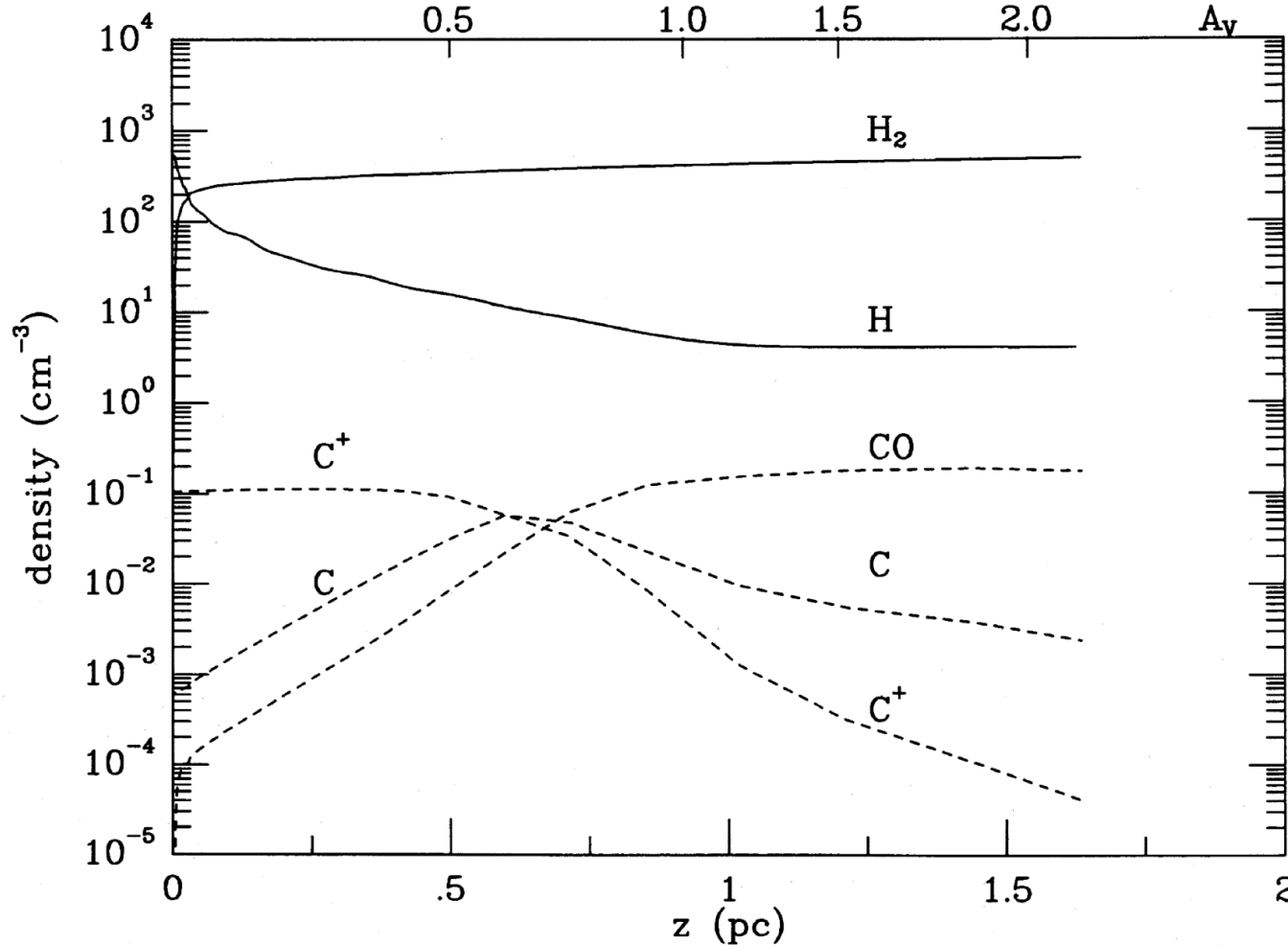
# Photodissociation rates in the ISRF



$T = 15 \text{ K}$   
 $n_{\text{H}} = 500 \text{ cm}^{-3}$

cloud  
edge

# Molecular cloud in the ISRF



$$T = 15 \text{ K}$$

$$n_{\text{H}} = 500 \text{ cm}^{-3}$$

cloud  
edge



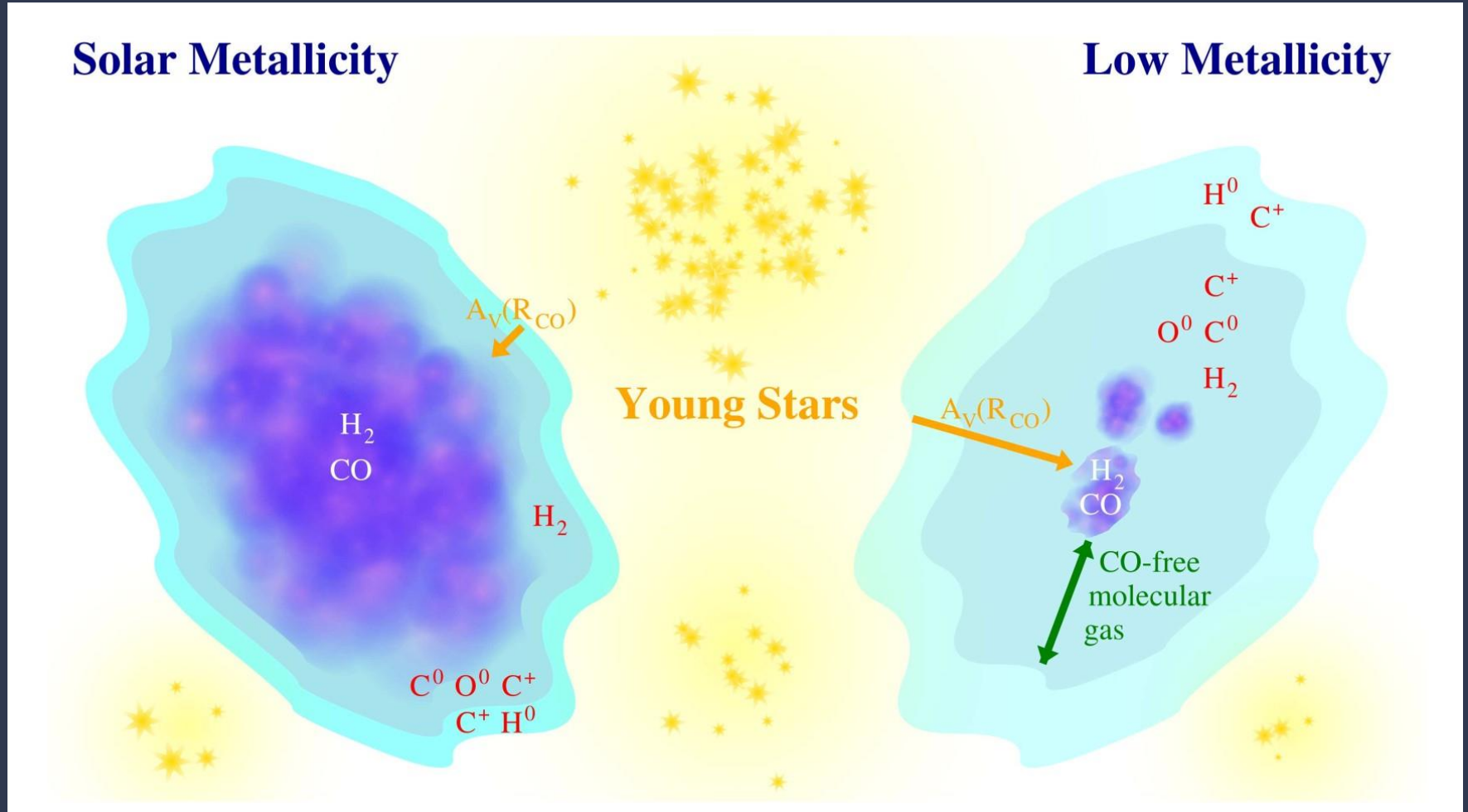
# Are CO and H<sub>2</sub> co-spatial?

In the Milky Way, the outer layers of molecular clouds where there is H<sub>2</sub> but no CO (“CO-dark gas”), contain only a small fraction of the H<sub>2</sub> mass (~10%, sometimes estimated up to 30%).

However, in low-metallicity galaxies a much higher column density is needed for CO self-shielding.

Conclusion: CO is a good tracer of H<sub>2</sub> in galaxies of ~ solar metallicity, but fails totally for low metallicity galaxies.

# Effect of metallicity on CO/H<sub>2</sub>



(Madden *et al.*, 2020)

# Next lecture

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## Thermal balance

1. What sets the temperature of the ISM?
2. Temperatures of HII regions
3. The origin of the 2-phase ISM
4. Temperatures of molecular clouds