

(AGN)<sup>2</sup>

## 8. Infrared Radiation and Molecules

Week 11

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updated on 05/13, 09:53

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## 8.1 Introduction

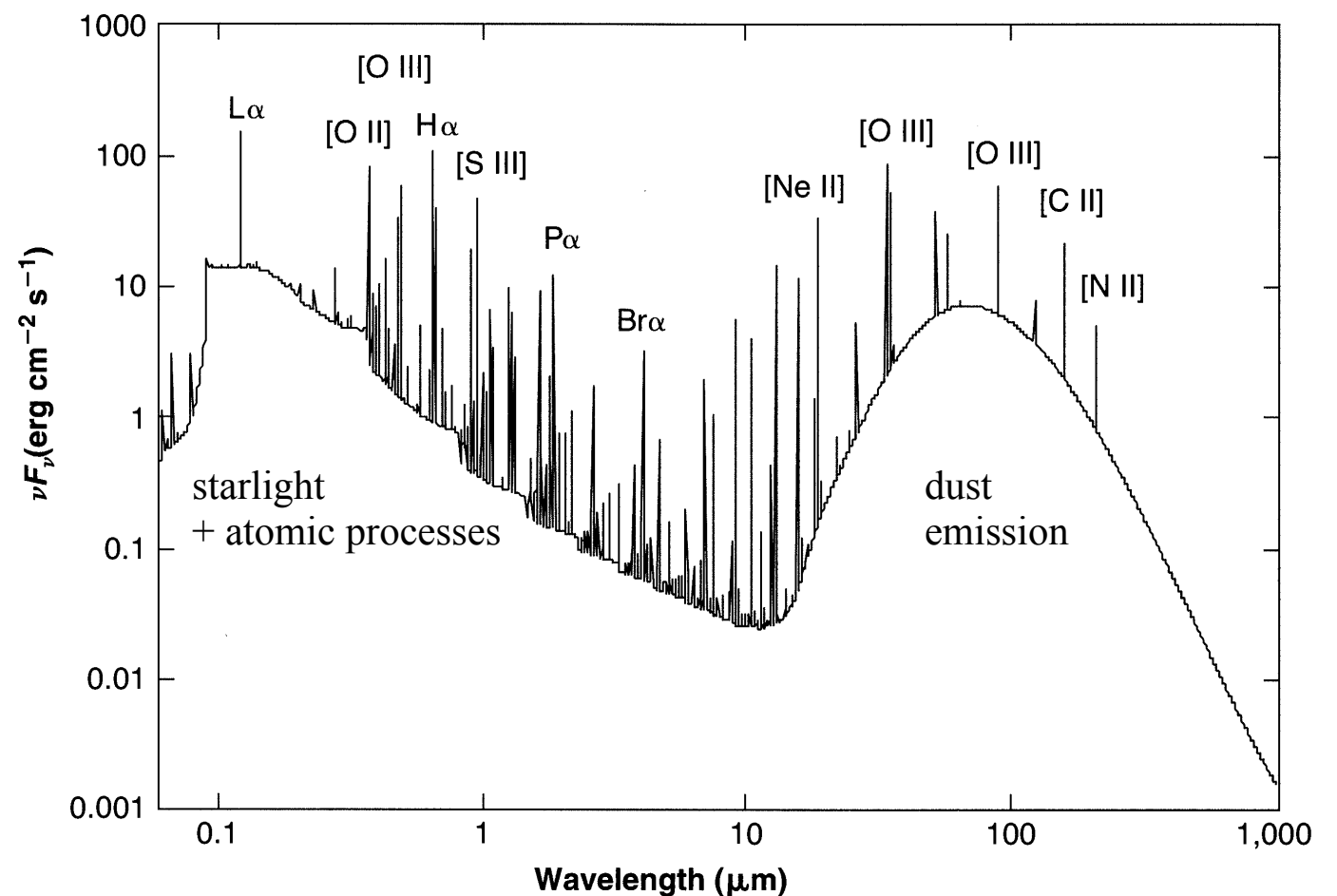
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- Photoionization
  - The light from nebulae comes from gas with temperature near  $10^4$  K.
  - The photoionization calculations are terminated where the hydrogen ionization front is reached.
  - Beyond it, the gas temperature would fall to a value too small to produce appreciable optical emission.
  - In visible light, the nebula appears to have an outer boundary at the ionization front.
- Gas beyond the visible edge (of a radiation-bounded nebula)
  - This gas is so cool that it emits mainly IR radiation.
  - In regions just outside the hydrogen ionization front, the gas is largely atomic and emits the FIR fine-structure lines, most notably [O I]  $\lambda 63 \mu\text{m}$  and [C II]  $\lambda 158 \mu\text{m}$ .
  - In regions even further from the ionization front, the gas is almost completely shielded and become quite cold, and molecular rather than atomic.
- Photodissociation region
  - The transition region between the fully ionized and fully molecular zones is known as the PDR (photodissociation region or photon dominated region).
  - This name indicates that molecules are dissociated by the radiation field, with energy less than  $h\nu_0$ .

## 8.2 The Structure of a PDR

- Radiation Field [Figure 8.1]

- The lines and continuum transmitted through the hydrogen ionization front of the simple model H II region.
- The continuum at shorter wavelengths is mainly due to the transmitted stellar continuum plus diffuse emission (free-bound, free-free, two-photon) from the H II region.
- The broad peak of emission near  $\sim 100 \mu\text{m}$  is produced by warm dust within the  $\text{H}^+$  zone.
- **The physical properties of gas within the PDR are determined by interactions between gas and this radiation field.**



# Habing's UV spectrum

- Radiation field striking the PDR

- Radiation field strength is specified by the intensity (into  $4\pi$  sr) integrated over the energy range 6.0 eV to 13.6 eV (which is capable of photoionizing grains), relative to the mean galactic radiation field in the solar neighborhood.

- Habing's UV spectrum gives

- ▶ an energy density  $u_{\text{Hab}}(6 - 13.6 \text{ eV}) = 5.29 \times 10^{-14} \text{ erg cm}^{-3}$

- ▶ mean intensity  $4\pi J_{\text{Hab}}(6 - 13.6 \text{ eV}) = 1.6 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1} \quad \Leftarrow J_{\nu} = \frac{c}{4\pi} u_{\nu}$

- The radiation field is given as the dimensionless ratio:

$$G_0 = \frac{\int_{6 \text{ eV}}^{13.6 \text{ eV}} 4\pi J_{\nu} d\nu}{1.6 \times 10^{-3} \text{ erg cm}^{-2} \text{ s}^{-1}}$$

- Observations indicates  $G_0 \approx 4 \times 10^5$  in the inner regions of the Orion Nebula.

- Calculation of the PDR structure

- The gas near the H ionization front is a complicated hydrodynamical environment. The evolution is rapid and the system changes toward the long-term constant-pressure case.
- For simplicity the calculation assumes constant pressure.

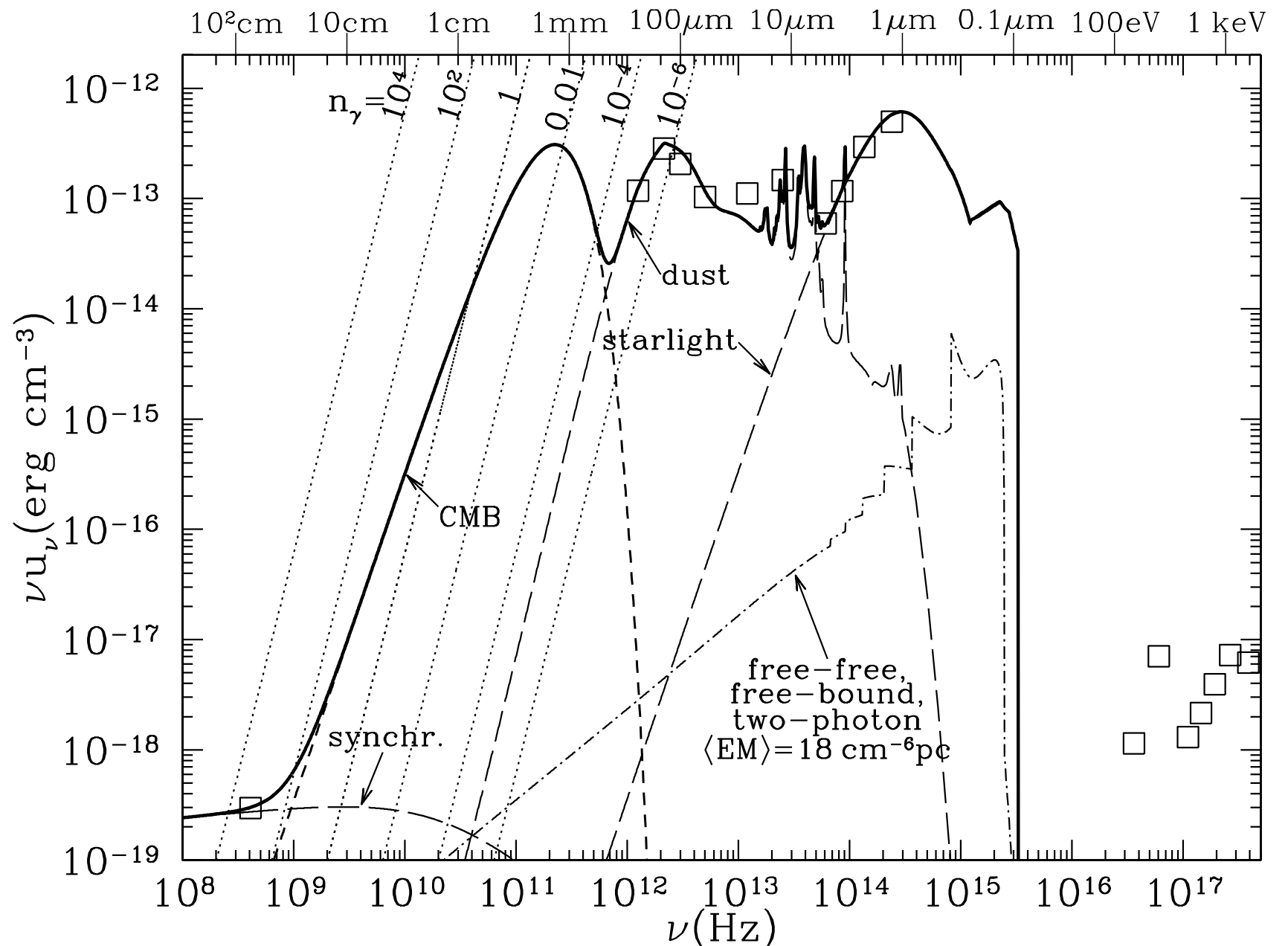
# Interstellar Radiation Fields (ISRF)

$$\nu u_\nu = \sum_{j=1}^3 \frac{8\pi h \nu^4}{c^3} \frac{W_j}{e^{h\nu/kT_j} - 1} \quad \text{for } \lambda > 2450 \text{ \AA},$$

Starlight:  $T_1 = 3000 \text{ K}, W_1 = 7 \times 10^{-13}$   
 $T_2 = 4000 \text{ K}, W_2 = 1.65 \times 10^{-13}$   
 $T_3 = 7500 \text{ K}, W_3 = 1 \times 10^{-14}$

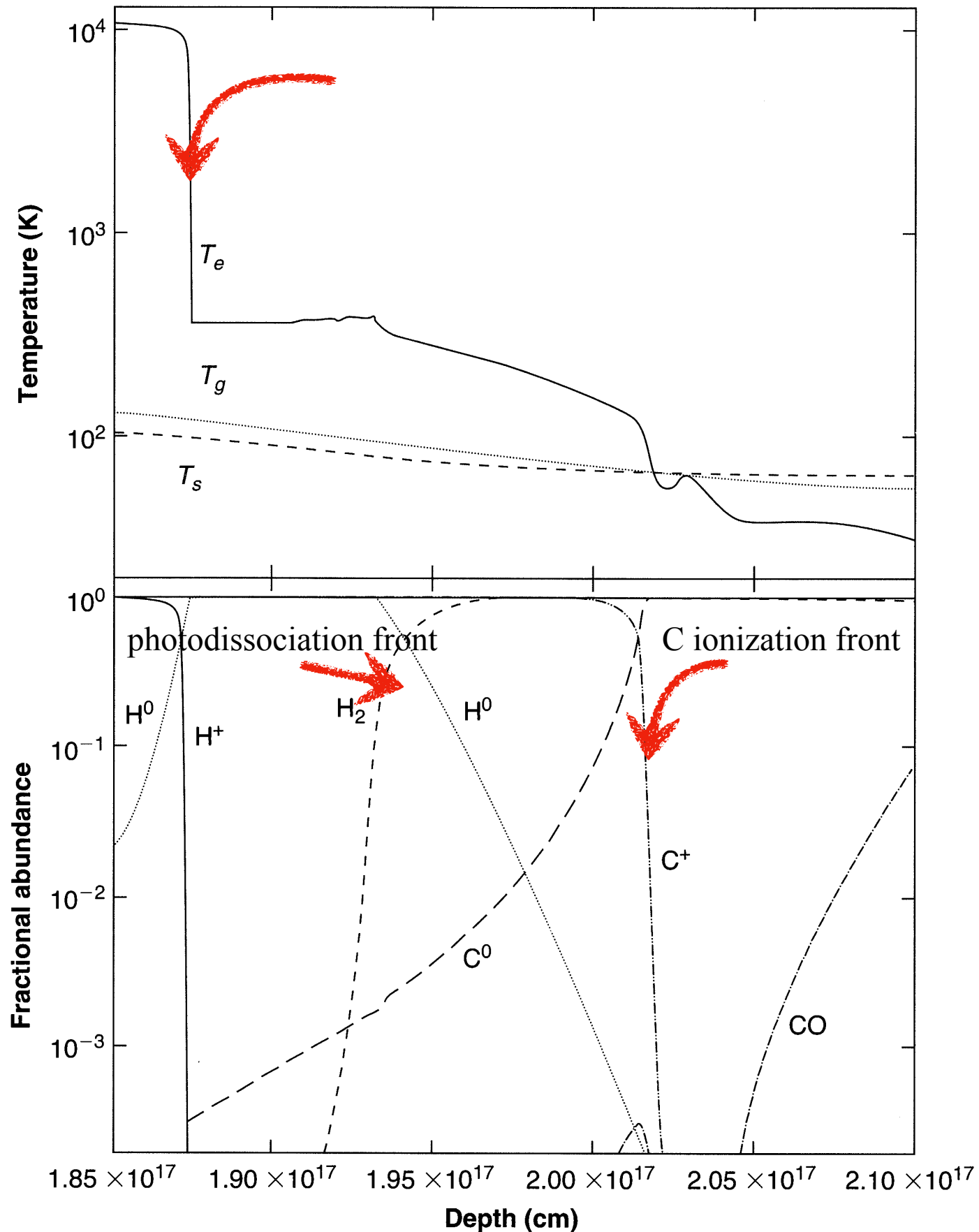
$$\nu u_\nu = \begin{cases} 2.373 \times 10^{-14} (\lambda / \mu\text{m})^{-0.6678} \text{ erg cm}^{-3} & 1340 - 2460 \text{ \AA} \\ 6.825 \times 10^{-13} (\lambda / \mu\text{m}) \text{ erg cm}^{-3} & 1100 - 1340 \text{ \AA} \\ 1.287 \times 10^{-9} (\lambda / \mu\text{m})^{4.4172} \text{ erg cm}^{-3} & 912 - 1100 \text{ \AA} \end{cases}$$

MMP83  
Mathis et al. (1983)



[Figure 12.1 in Draine]

[Figure 8.2]



- Opacity

- Grains are the dominant opacity source throughout the PDR. They absorb relatively low-energy photons from the H II regions.
- Grain photoionization is the dominant source at shallow depths within the PDR.
- At depths  $\gtrsim 2 \times 10^{17}$  cm, the higher-energy photons that photoionize grains are extinguished, and photoionization of  $C^0$  and  $Si^0$  becomes important.

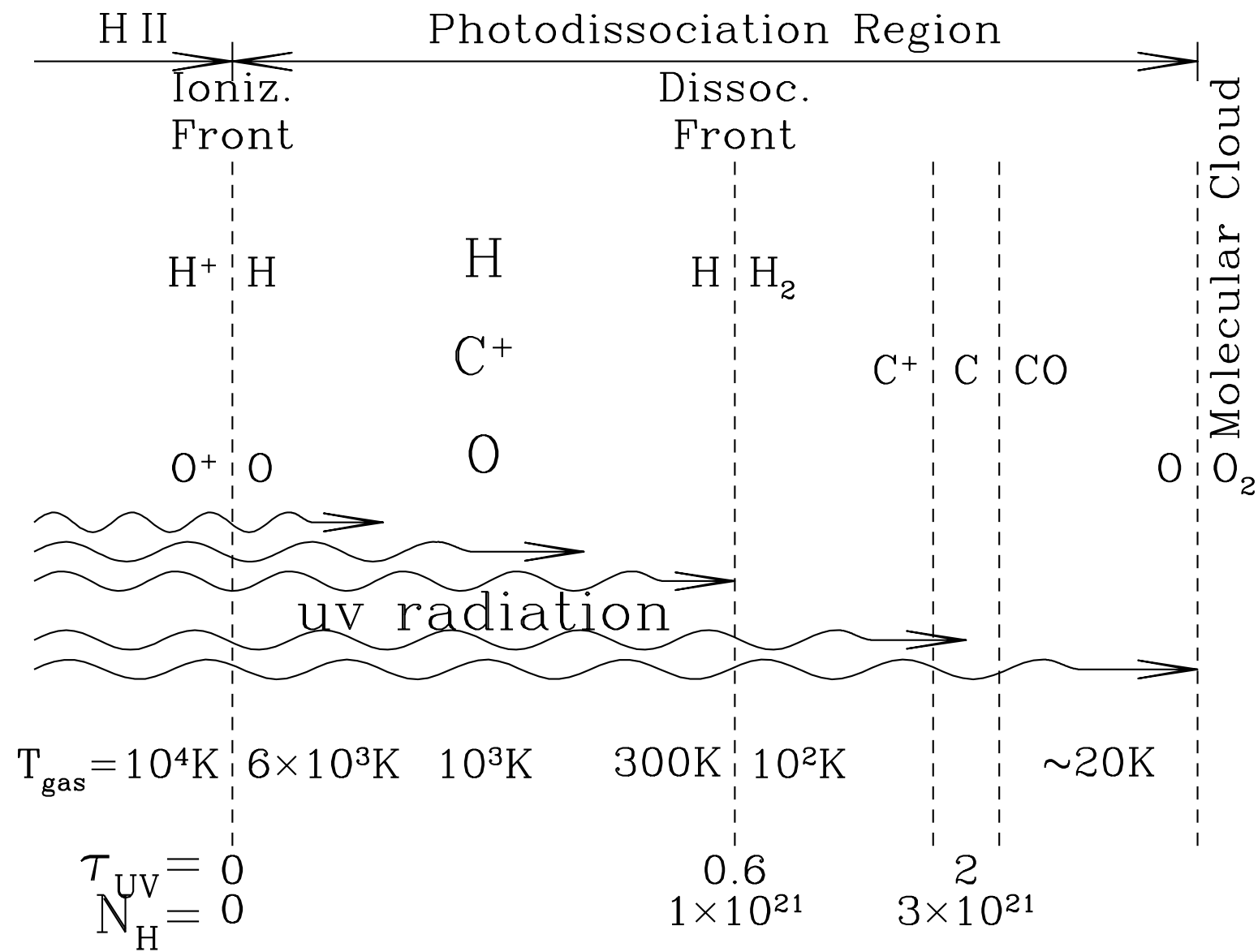
- Electrons

- Most of the free electrons come from abundant elements with atomic ionization potentials below 13.5 eV.
- For a solar composition, most electrons come from  $C^+$ . The electron density is nearly equal to the C density where C is mostly ionized.

- C ionization front (at  $d \approx 2 \times 10^{17}$  cm)

- $\tau(11.2 \text{ eV}) \approx 1$  and nearly all of the photons with  $h\nu > 11.2 \text{ eV}$  (ionization potential of C) have been absorbed.
- $A_V \approx 5 \text{ mag}$

- 
- Beyond C ionization front
    - C is neutral.
    - The higher-energy radiation that can photoionize grains have been completely absorbed.
    - Grains are heated by the radiation field.
    - $T_{\text{dust}} > T_{\text{gas}}$ : The gas temperature falls below the grain temperature, because there is no longer grain photoelectric heating.
    - **Collisions between the gas and dust grains heat the gas** by transferring energy from grains.
      - ▶ In other words, starlight heats the grains, followed by energy exchange between the gas and grains. Eventually, the gas is heated.
  - Heating source at the largest depths
    - Only the long-wavelength thermal emission from the grains is transmitted.
    - **Photoexcitation followed by collisional deexcitation**
      - ▶ Line photoexcitation of excited levels within the ground term of heavy elements (mainly [Si II]  $34.8 \mu\text{m}$ ), followed by collisional deexcitation, is the dominant heating process.
      - ▶ When the photoexcitation rate  $4\pi J_{\nu} B_{lu}$  is significant, the upper level can become overpopulated relative to the lower level.
      - ▶ In this case, the rate of downward collisions can exceed the upward collisional rate, and the line heats rather than cools the gas.
      - ▶ [O I]  $\lambda 63 \mu\text{m}$  is the dominant heating source in the deepest regions.



Structure of a PDR at the interface between an H II region and a dense molecular cloud.

[Fig 31.2, Draine]



## 8.3 The H<sub>2</sub> molecule

- H<sub>2</sub> is the most abundant molecular species in nebulae and interstellar matter.
- **Hyperfine splitting:** If one or more nuclei have nonzero nuclear spin and  $J_{ez} \neq 0$ , then there will be an interaction between the nuclear magnetic moment and the magnetic field generated by the electrons, resulting in “hyperfine splitting.” The energy will depend on the orientation of the nuclear angular momentum relative to the axis.
- **Ortho-H<sub>2</sub> and Para-H<sub>2</sub>**
  - In the case of H<sub>2</sub>, the electronic wave function is required to be antisymmetric under exchange of the two electrons.
  - The two protons, just like electrons, are identical fermions, and therefore, the Pauli exclusion principle antisymmetry requirement also applies to exchange of the two protons. The protons are spin 1/2 particles - the two protons together can have total spin 1 (parallel) or total spin 0 (antiparallel).
  - The consequence of the antisymmetry requirement is that

If the protons have spin 0, the rotational quantum number  $J$  must be even.  $\Rightarrow$  para-H<sub>2</sub> (even  $J$ )  
(an antisymmetric nuclear spin wave function ( $I = 0$ ) and a symmetric spatial wave function involving even values of the rotational quantum number  $J$ )

If the protons have spin 1, the rotational quantum number  $J$  must be odd.  $\Rightarrow$  ortho-H<sub>2</sub> (odd  $J$ )  
(a symmetric nuclear spin wave function ( $I = 1$ ) and an antisymmetric spatial wave function involving odd values of the rotational quantum number  $J$ )

- Because the nuclear spins are only weakly coupled to the electromagnetic field, ortho-H<sub>2</sub> and para-H<sub>2</sub> behave as almost distinct species.

# (Energy Levels)

- **Energy Levels**

- An electronic transition consists of vibrational bands, which in turn are made up of rotational transitions.

$$E_q(v, J) = V_q(r_0) + h\nu_0 \left( v + \frac{1}{2} \right) + B_v J(J + 1)$$

$$\nu_0 \equiv \frac{\omega_0}{2\pi} \quad B_v = \frac{\hbar^2}{2I} \quad I = \mu r_0^2 = \text{moment of inertia of the molecule.}$$

- Here,  $q$  denotes an electronic state.

- **Selection Rules**

- Electric-dipole selection rule for ro-vibrational transitions:

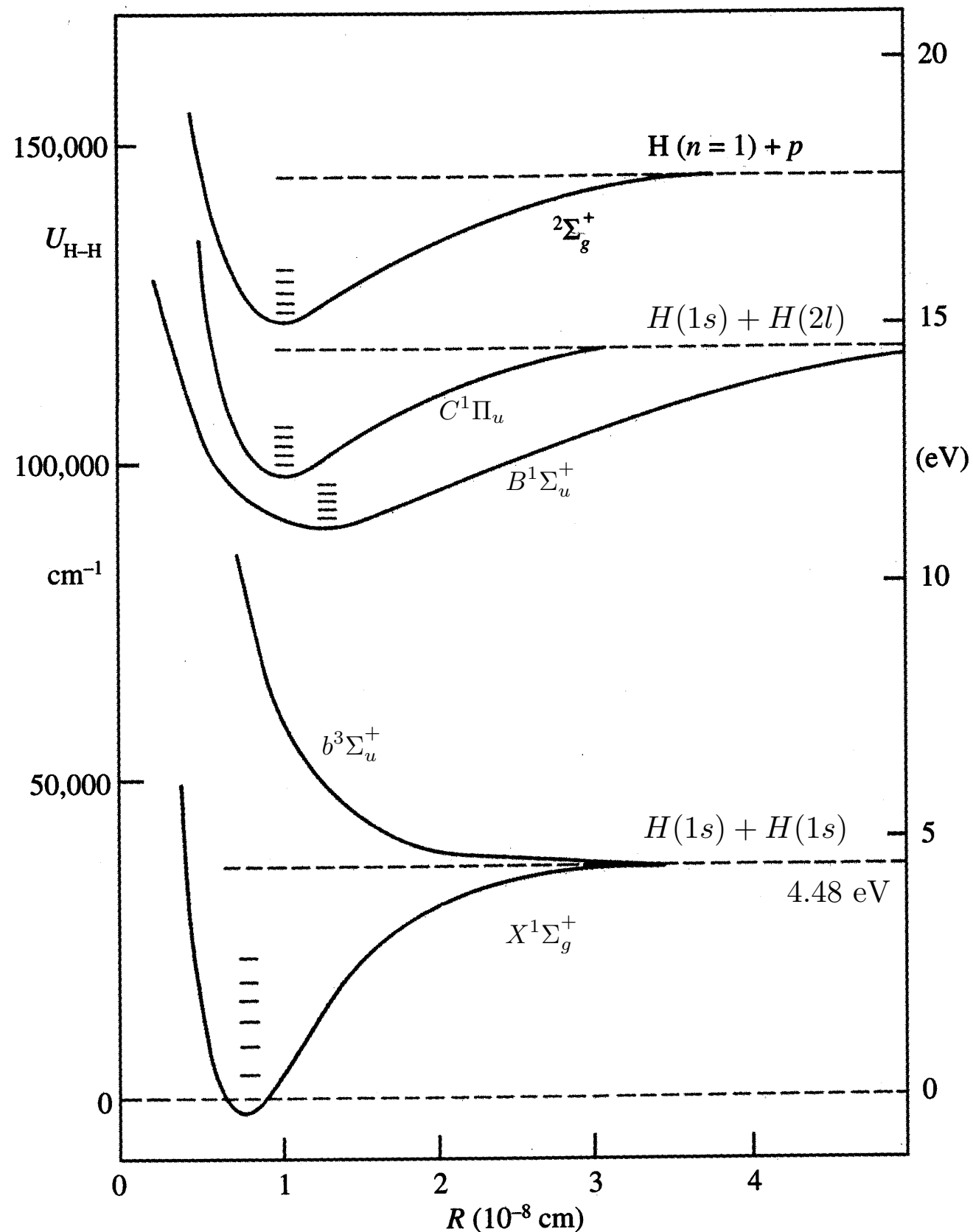
$$\Delta v = \text{any}$$

$$\Delta J = 0, \pm 1 \quad \text{not } J = 0 \leftrightarrow 0$$

- **Note that H<sub>2</sub> has no permanent electric-dipole moment.**

The electric-quadrupole are allowed for  $\Delta J = \pm 2$  within the ground electronic state.

# (Energy levels of Molecular Hydrogen)

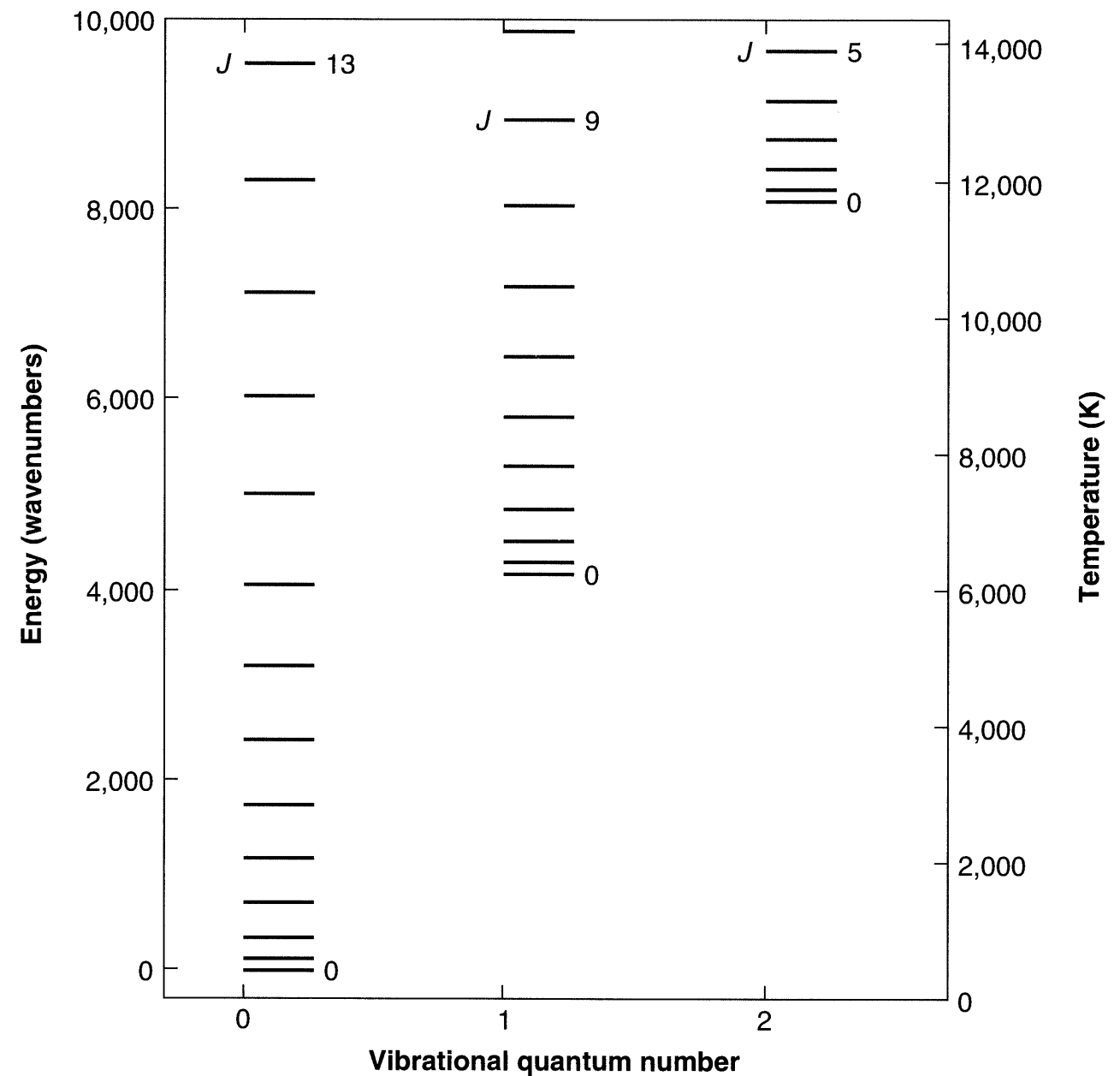


- The short horizontal lines in each of the bound states indicate the vibrational levels.
- The transition from the ground state  $X^1\Sigma_g^+$  to the excited states  $B^1\Sigma_u^+$  and  $C^1\Pi_u$  are called **Lyman and Werner bands**.

Werner band:  $C^1\Pi_u - X^1\Sigma_g^+$  at  $\lambda \approx 970 - 1650 \text{ \AA}$   
 Lyman band:  $B^1\Sigma_u^+ - X^1\Sigma_g^+$  at  $\lambda \approx 930 - 1240 \text{ \AA}$

- 
- For an isolated H<sub>2</sub> molecule in the ground electronic level, the odd  $J$  and even  $J$  rotational levels are effectively different species.
    - The radiative transition occurs by quadrupole radiation ( $\Delta J = 0, 2$ )
    - Spin-exchange collisions with H<sup>0</sup> and He<sup>+</sup>, and a process in which H<sub>2</sub> is captured on a grain surface can cause an ortho-para conversion.
    - Statistical weights are  $(2I + 1)(2J + 1)$ :  $3(2J + 1)$  for an ortho-H<sub>2</sub> and  $2J + 1$  for a para-H<sub>2</sub> level.
  - No permanent electric-dipole moment
    - no permitted pure rotational or rovibrational transitions.
    - But, electronic transitions are allowed.
  - Critical density
    - Typical transition probabilities for rovibrational transitions within  $X^1\Sigma$  (the ground electronic state) are  $A \approx 10^{-6}$  to  $10^{-7} \text{ s}^{-1}$ .
    - Typical collision rate coefficients for collisions with other H<sub>2</sub> molecules are  $\approx 10^{-12} - 10^{-11} \text{ cm}^3 \text{ s}^{-1}$ .
    - Then, the critical densities are in the range  $n_{\text{crit}} \approx 10^3 - 10^5 \text{ cm}^{-3}$ .
    - Below these densities nearly every H<sub>2</sub> collisional excitation will lead to emission of a photon (or photons).

- The very lowest energy quadrupole transition
  - ▶  $0-0 S(0)$  ( $v = 0 \rightarrow 0, J = 2 \rightarrow 0$ ) has a wavelength of  $28.2 \mu\text{m}$  and an excitation energy corresponding to 500 K.
- The temperature in a PDR is typically  $\lesssim 500 \text{ K}$ . Therefore, there are very few collisionally excited  $\text{H}_2$  lines from a PDR.
- However, collisional excitation is efficient in higher-temperature shocks.



[Figure 8.3]

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- Formation of H<sub>2</sub> molecules

- **[Direct Radiative Association]** H<sub>2</sub> cannot form in a collision between two free H atoms. This is because two colliding atoms have to lose enough energy to be captured into a bound state or it will break apart again. There is no electric dipole moment. Electric quadrupole transition rates are very low.
- **[Three-body reaction]** A third atom acts as a catalyst, carrying away the excess energy. In dense environments (atmosphere of a cool star, protostar, or protoplanetary disk), the three-body reaction is able to convert H to H<sub>2</sub>.
- **[Formation of negative hydrogen ion by radiative association followed by formation of H<sub>2</sub> by associative detachment]** (1)  $\text{H}^0 + e^- \rightarrow \text{H}^- + h\nu$  and (2)  $\text{H}^- + \text{H} \rightarrow \text{H}_2 + e^- + \text{KE}$ . This process occurs in the early universe.
- **[Catalysis on grain surfaces]** An H atom collides with a grain and, if it sticks to the surface, it may encounter another H<sup>0</sup> and form H<sub>2</sub>. The H<sub>2</sub> molecule may leave the grain surface in a variety of excited rovibrational states, and their decay produce emission.

- Ortho-para conversion

- Once H<sub>2</sub> in the gas phase may collide again with grains and be captured, it can undergo ortho-para conversion before escape.
- This is an important method by which ortho- and para-H<sub>2</sub> are converted into one another.

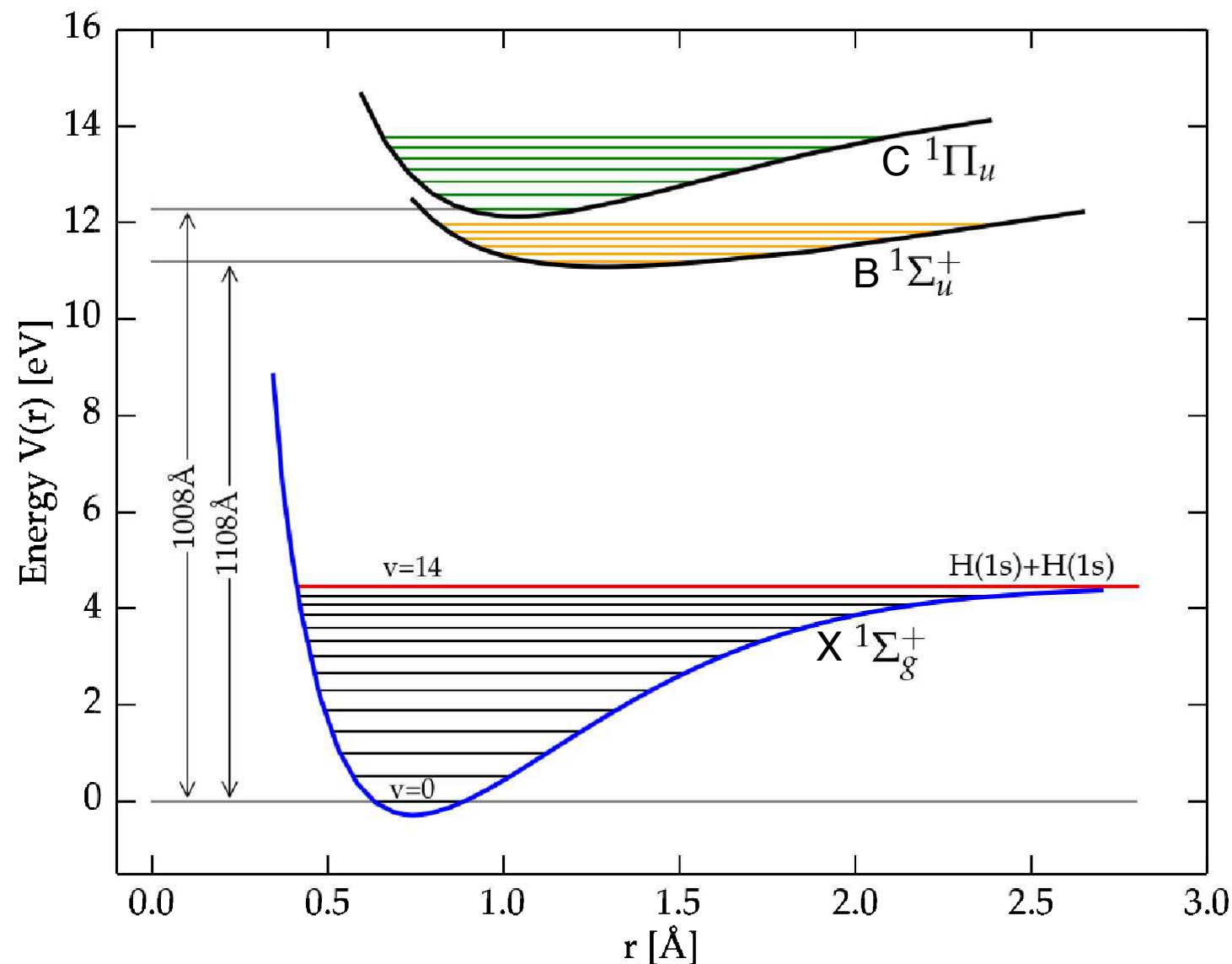
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- Dissociation of  $\text{H}_2$

- The binding energy of  $\text{H}_2$  is 4.5 eV (the energy needed to separate  $\text{H}_2$  into two  $\text{H}_0$  atoms).
- At the temperatures within a PDR, collisional dissociation is impossible.
- Direct photoionization is inefficient because there is little radiation with  $h\nu > h\nu_0$  within the PDR.
- **$\text{H}_2$  is predominantly destroyed by photoexcitation into excited electronic states, followed by decays into unbound levels of  $X^1\Sigma$ .**
  - ▶ Absorption of a stellar continuum photon in a line of one of the Lyman ( $B^1\Sigma - X^1\Sigma$ ) and Werner ( $C^1\Sigma - X^1\Sigma$ ) bands populates an excited electronic level.
  - ▶ About 90% of such photoexcitations decay into bound excited rovibrational levels within  $X^1\Sigma$ .
  - ▶ The remaining 10% decay into unbound levels in the  $X^1\Sigma$  and thus dissociate the molecule.
  - ▶ This mechanism is often referred to as the **Solomon process**.
  - ▶ The Solomon process can be efficient, and so the gas is largely atomic, until a column density of  $N(\text{H}_2) > 10^{14} \text{ cm}^{-2}$  is reached, when self-shielding becomes effective.
  - ▶ The gas predominantly molecular at larger column densities.

# (Photodissociation of H<sub>2</sub>)

- Photodissociation:  $\text{H}_2 + h\nu \rightarrow \text{H} + \text{H} + \text{KE}$ 
  - Photodissociation is the principal process destroying interstellar H<sub>2</sub>.



In the left potential energy curves, you might think that photodissociation of H<sub>2</sub> is a simple task; if H<sub>2</sub> absorb a photon of energy  $h\nu > 4.52 \text{ eV}$ , it will be excited to a vibrational state (*vibrational continuum*) with quantum number  $v > 14$ , which will be unbound.

However, absorbing a photon to lift the molecule to a  $v > 14$  vibrational state requires a quadrupole transition, which has a very small transition probability.

Schematic drawing of the potential energy curves of molecular hydrogen [Figure 7.4, Ryden]



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- H<sub>2</sub> decay process can be the dominant gas heating process in parts of a PDR.
    - 90% of the Lyman and Werner band photoexcitations results into H<sub>2</sub> decaying into excited rovibrational levels within  $X^1\Sigma$ .
    - These create a relatively large overpopulation of H<sub>2</sub> in excited levels. As a result, the collisional deexcitation rate per volume exceeds the collisional excitation rate per volume, and collisions involving these levels heat the gas (rather than cool it).
  - The H<sub>2</sub> emission spectrum of a PDR is highly non-thermal as a result of this process.

# The CO Molecule

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- Molecules other than H<sub>2</sub>
  - Once, the H<sub>2</sub> has been formed, other chemistry can follow.
  - Most of the gas will be neutral, but, *because of the presence of cosmic rays, there will always be some ions present in the gas.*
  - In the outer layers of molecular clouds, there may also be sufficient UV radiation to photoionize species with ionization potentials  $E_I < 13.6 \text{ eV}$ .
- Formation of CO
  - CO forms by a series of gas-phase chemical reactions.
  - Direct formation from atoms,  $\text{C} + \text{O} \rightarrow \text{CO}$ , is possible but unlikely due to the small cross sections of the atoms.
  - In the ISM, most molecules form by ion-molecule reactions, in which an ion approaches a molecule, inducing an electric dipole moment, and so increasing the capture cross section due to the electrostatic interactions.
  - CO forms at deeper regions in a PDR than H<sub>2</sub> because H<sub>2</sub> is an important first step in its formation.
  - CO is destroyed by photoexcitation processes similar to H<sub>2</sub>.

# (Formation of CO)

- In diffuse molecular clouds, most of the gas-phase carbon is in the form of  $C^+$ , and most of the H is in the form of  $H_2$ .

Carbon chemistry is initiated by the radiative association reaction of  $C^+$  with  $H_2$  forming  $CH_2^+$ .

CO is formed primarily by the sequence of the following reactions:

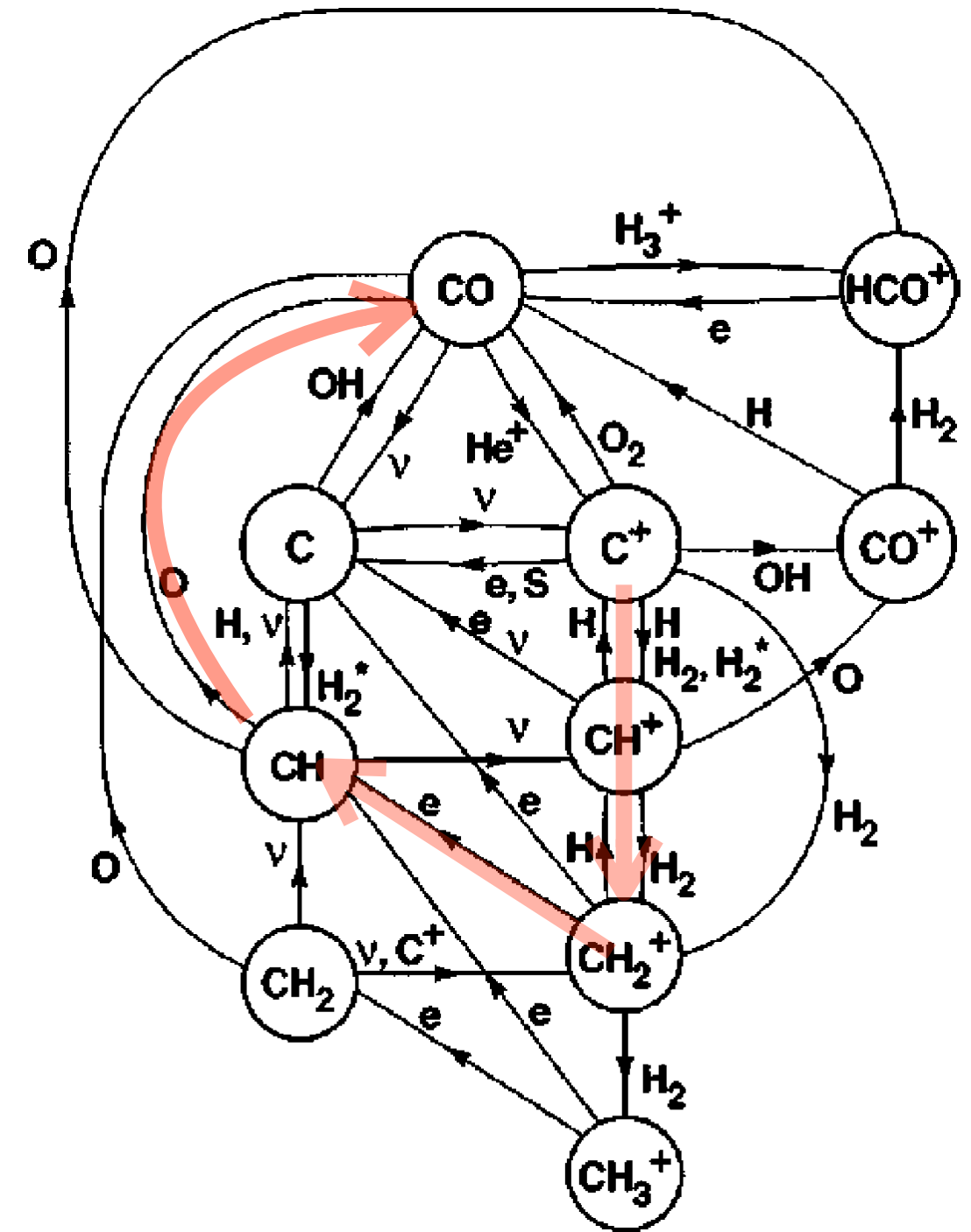
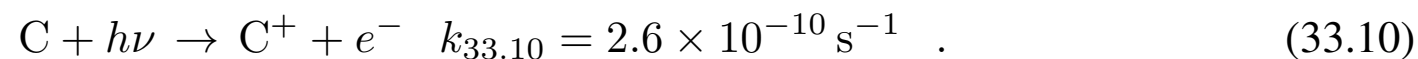
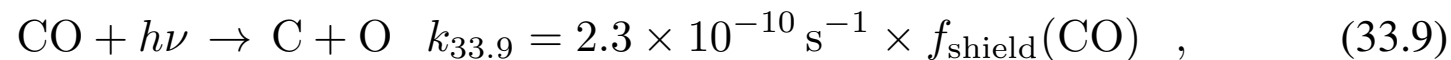
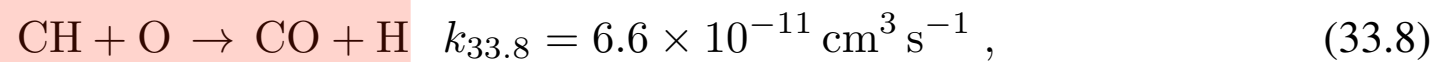
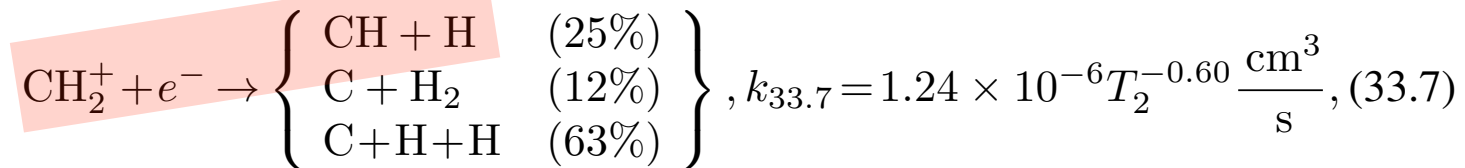
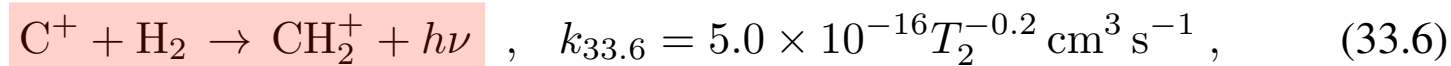
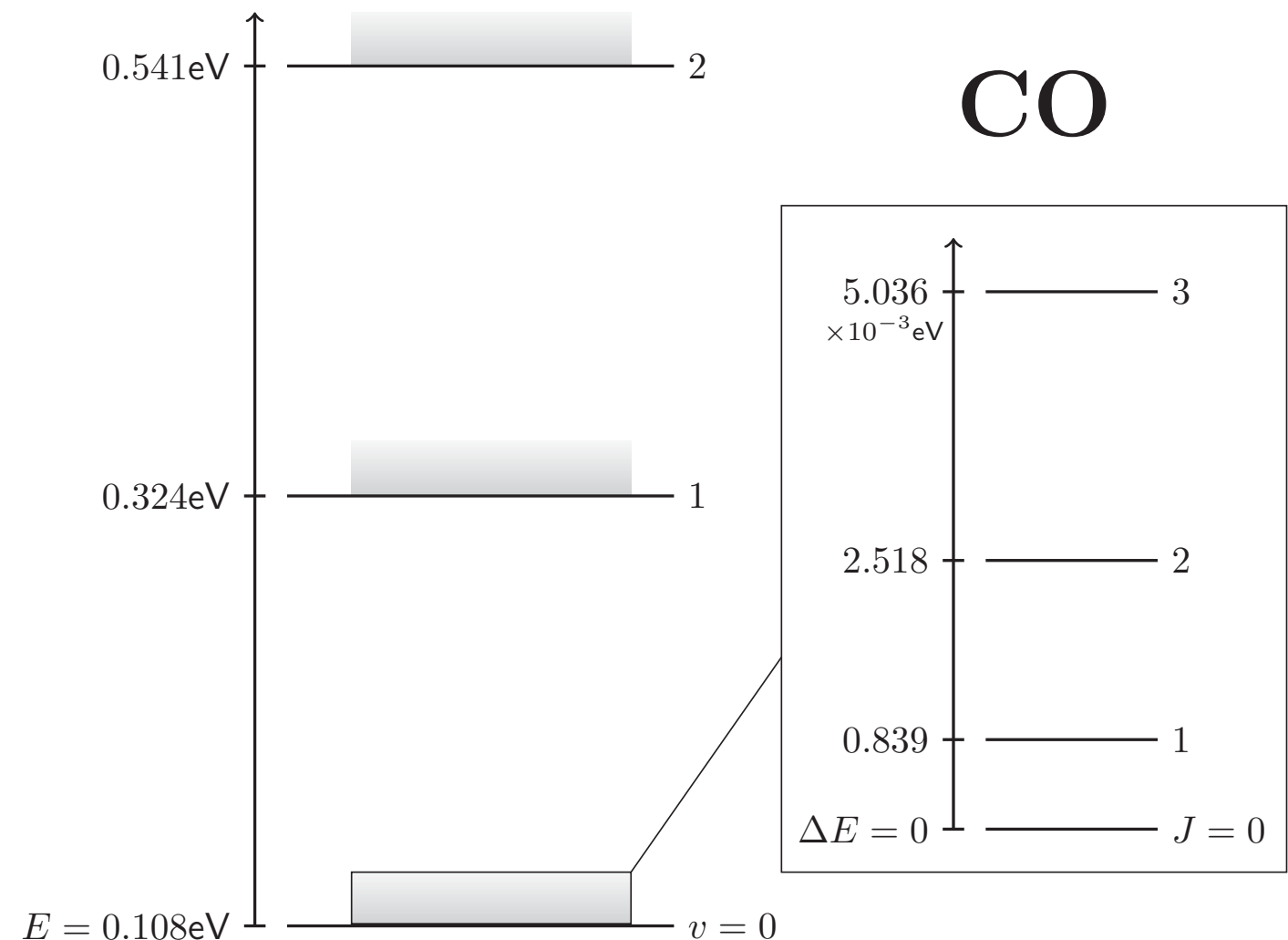


Fig 8.9, Tielens [The physics and chemistry of the interstellar medium]

From page 377 in [Draine]

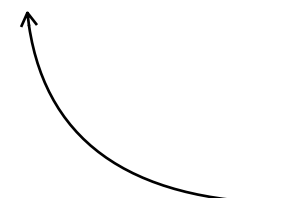
- Rovibrational structure of CO



The rotational and vibrational energy levels for CO. The left side show the vibrational energy for each level  $\nu$ . The rotational transitions are illustrated by the gray shading at each level. The rotational energies are about 100 times smaller than the vibrational and the inset on the right hand side shows a zoomed-in region of the J-ladder.

- The rotational energy levels depend inversely on the moment of inertia  $I$ .
  - The heavier nuclei and resulting larger rotational moment of CO means that its rotational levels have much smaller energies.
  - The lowest rotational transitions of CO has wavelength  $\lambda 2.59$  mm, corresponding to an excitation energy of 5.6 K.
  - Thus, CO is collisionally excited to much higher rotational levels in a PDR than is  $\text{H}_2$ .
  - The rotational (electric-dipole) transition probabilities increase with  $J$ , with  $A_{ul} \sim 10^{-7} - 10^{-5} \text{ s}^{-1}$  for  $J \leq 5$  levels.
  - The critical densities for collisions with  $\text{H}_2$  molecules are  $\sim 10^4 - 10^6 \text{ cm}^{-3}$ .
  
- **Optical Thickness of CO line ( $J = 1-0$ ):**
  - Because of the great abundance of CO and the long wavelengths of its lines, the lower  $J$  lines are optically thick under most circumstances.

$$\tau_0 = 297 \left( \frac{N_{\text{H}}}{10^{21} \text{ cm}^{-2}} \right) \left[ \frac{n(\text{CO})/n_{\text{H}}}{7 \times 10^{-5}} \right] \left[ \frac{n(J=0)}{n(\text{CO})} \right] \left( \frac{2 \text{ km s}^{-1}}{b} \right) \left( 1 - e^{-5.532 \text{ K}/T_{\text{exc}}} \right)$$



$$\kappa_{\nu} = n_0 \sigma_{01} \left( 1 - \frac{g_0}{g_1} \frac{n_1}{n_0} \right), \quad \sigma_{01} = \frac{g_1}{g_0} \frac{c^2}{8\pi\nu_{10}^2} A_{10} \phi_{\nu}, \quad \frac{n_1}{n_0} = \frac{g_1}{g_0} \exp \left( -\frac{h\nu_{10}}{kT_{\text{exc}}} \right)$$

# (Interstellar CO)

- Since the cold molecular hydrogen does not radiate (except the fluorescence UV line), the best tracer in galaxies is the most abundant molecule after H<sub>2</sub>, i.e. the carbon monoxide CO. *Much of what we know about molecular gas comes from observations of “tracer” molecules such as carbon monoxide (CO).*
- X-factor (<sup>12</sup>CO to H<sub>2</sub>) & Mass of molecular gas
  - Most of the interstellar molecular mass is in the form of H<sub>2</sub>, so it is only possible to estimate the total H<sub>2</sub> mass of a region roughly from CO line observations.
  - An empirical relationship has been found between the H<sub>2</sub> column density,  $N(\text{H}_2)$ , and the integrated intensity of the 1 - 0 CO line.

$$X_{\text{CO}} = \frac{N(\text{H}_2)}{\int T_{\text{A}} dv} = 1.56 \times 10^{20} \left( \frac{n_{\text{H}}}{10^3 \text{ cm}^{-3}} \right)^{1/2} \left[ \frac{\text{cm}^{-2}}{\text{K km s}^{-1}} \right]$$

Dame et al. (2001) observationally find  $X_{\text{CO}} = (1.8 \pm 0.3) \times 10^{20} \text{ cm}^{-2} / \text{K km s}^{-1}$ , where infrared emission from dust (Schlegel et al. 1998) was used as a mass tracer.

The most recent determination using gamma rays finds

$$X_{\text{CO}} = (1.76 \pm 0.04) \times 10^{20} \text{ cm}^{-2} / \text{K km s}^{-1} \quad \text{for the Orion A GMC (Okumura et al. 2009)}$$

- **Other galaxies:** Recent observations indicates that  $X_{\text{CO}}$  in Local Group galaxies is of order

$$X_{\text{CO}} \sim 4 \times 10^{20} \text{ cm}^{-2} / \text{K km s}^{-1} \quad (\text{Blitz et al. 2007})$$

with large variations from one galaxy to another.

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- The physical sources of scattering in the relationship include variations in (1) the C/H abundance ratio, (2) cloud temperature, (3) cloud mass, and (4) cloud size, of which all were taken as average values.
  - Isotopologue

CO is widely distributed in the interstellar medium and maps of the CO J = 1-0 transition are a standard tool for investigating the ISM.

If, as often happens, the CO 1-0 line is optically thick, one can use higher transitions such as the CO 2-1 line instead. **Another option to avoid the effects of optical thickness is to observe an isotopologue  $^{13}\text{CO}$** , which is present with much lower densities and whose transitions are therefore much less optically thick.

An isotopologue is a molecule that consists of at least one less abundant isotope of its constituent elements. They have the same transitions at nearby frequencies with similar decay and excitation rates. The main difference is in their abundance and observations of the rarer species help diagnose conditions in dense regions where lines from the primary species are optically thick.

Because of significant changes in the reduced mass of a diatomic molecule, the molecular lines occur as significantly different wavelengths. For instance

$^{12}\text{C}^{16}\text{O}$  1-0  $\lambda = 2.60$  mm vs.  $^{13}\text{C}^{16}\text{O}$  1-3  $\lambda 2.48$  mm

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- The abundance ratio between isotopes can be determined from their spectra.

However, there are complications.

- Optical depth effects

- ▶ The  $^{12}\text{CO}$  line with lowest  $J$  are usually optically thick, so the intensity near line center is often equal to that of a blackbody at the gas kinetic temperature, which is not directly related to the amount of CO.
- ▶ As a result, the ratio of the intensity of a line from the main isotope relative to a less common isotope is smaller than the isotopic abundance ratio itself.

- Chemical fractionation

- ▶ The dependence of chemical reaction-rate coefficients on nuclear mass causes the molecular and elemental isotope ratios to be different.
- ▶ For example, the  $^{12}\text{C}/^{13}\text{C}$  isotope ratio from CO is in the range of 57 - 96, while the terrestrial ratio is 89.