Interstellar Medium (ISM)

Lecture 14
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선광일 (Kwangil Seon)
KASI / UST

[Hyperfine Splitting & Ortho-H_2 and Para-H_2]

- **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_2 and Para-H_2 (spin isomers, 이상질체)**

In the case of H_2, 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 antisymmetric 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

<u>If the protons have spin 0, the rotational quantum number *J* must be even. ⇒ para-H_2 (even *J*)</u>

(an antisymmetric nuclear spin wave function ($I = 0$) and a symmetric spatial wave function having an even value of the rotational quantum number *J*)

<u>If the protons have spin 1, the rotational quantum number *J* must be odd. ⇒ ortho-H_2 (odd *J*)</u>

(a symmetric nuclear spin wave function ($I = 1$) and an antisymmetric spatial wave function having an odd value of the rotational quantum number *J*)

<u>Because the nuclear spins are only weakly coupled to the electromagnetic field, **ortho-H_2 and para-H_2 behave as almost distinct species.**</u>

H_2 has no permanent electric dipole moment.

- Thus, the vibrational states and the rotational states radiate very weakly, via the time-variation of the electric quadrupole moment and the molecule vibrates or rotates.

- Because the nuclear spin state does not change, the ro-vibrational radiative transitions of H_2 must have

$$\boxed{\begin{array}{l}\Delta J = 0 \text{ or } \Delta J = \pm 2, \text{ i.e., ortho} \rightarrow \text{ ortho or para} \rightarrow \text{ para} \\ (\text{not } J = 0 \leftrightarrow J = 0)\end{array}}$$

The vibration-rotation emission spectrum of H_2 therefore consists of electric quadrupole transitions. Therefore, the H_2 emission lines are faint and hard to detect. The downward transitions are identified by

$$\boxed{\begin{array}{rll} v_u - v_\ell & \mathrm{S}(J_\ell) & \text{if } J_\ell = J_u - 2 \quad , \\ v_u - v_\ell & \mathrm{Q}(J_\ell) & \text{if } J_\ell = J_u \quad , \\ v_u - v_\ell & \mathrm{O}(J_\ell) & \text{if } J_\ell = J_u + 2 \quad . \end{array}}$$

For example, 1-0 S(1) refers to the transition $(v = 1,\ J = 3) \rightarrow (v = 0,\ J = 1)$.

- $\boxed{\text{Spin-exchange collisions with } H^0 \text{ or } H^+\text{, and a process in which } H_2 \text{ is captured on a grain surface, can cause an ortho-para conversion.}}$

- The statistical weight of an ortho-H_2 rotational level J is $3(2J+1)$ [because $S_{\text{nucleus}} = 1$].

  For a para-H_2 it is $(2J+1)$ [because $S_{\text{nucleus}} = 0$].

Ortho/Para Ratios

- The ortho state of a molecule is defined as having the larger statistical spin weights and para as having the smaller weight.
- Since the typical energy separation between the ortho and para states of a molecule is comparable to the gas and dust temperature in the ISM and much smaller than the energy released in formation reactions, **it is expected that the abundance ratio between the two states will reflect the equilibrium values at high temperatures, that is, the ratio of their statistical weight.**

$$\frac{E_{J=1} - E_{J=0}}{k_{\rm B}} \approx 174.98\,{\rm K} \quad \text{for } H_2$$

  - Since g = 2I + 1, the usual ortho to para ratio is (2x1+1)/(2x0+1) = 3 for spin 1/2 systems such as H_2.

- If a molecule cannot be converted from ortho to para (or vice versa) by radiative or collisional processes, the two states can effectively be considered as two separate molecules. In this case, the ortho to para ratio at the time of molecule formation will be preserved.

Interstellar Molecules

- Interstellar Molecules
  - Interstellar molecules were first discovered in the late 1930s through the identification of optical lines seen in absorption against background starlight with electronic transitions of molecules.
  - The molecules first detected were CN ($B^2\Sigma^+ - X^2\Sigma^+$ at 3876.84Å), CH ($A^2\Delta - X^2\Pi$ at 4300.30Å) and CH^+ ($A^1\Pi - X^1\Pi^+$at 4232.54Å)
  - To date, over 200 interstellar molecules have been detected.

Interstellar molecules listed by number of atoms

Diatomic	Triatomic	Four atoms	Five atoms	Six atoms	Seven atoms	Eight atoms
H_2	C_3	c-C_3H	C_5	C_5H	C_6H	CH_3C_3N
AlF	C_2H	l-C_3H	C_4H	l-H_2C_4	CH_2CHCN	$HCOOCH_3$
AlCl	C_2O	C_3N	C_4Si	C_2H_4	CH_3C_2H	CH_3COOH(?)
C_2	C_2S	C_3O	l-C_3H_2	CH_3CN	HC_5N	C_7H
CH	CH_2	C_3S	c-C_3H_2	CH_3NC	$HCOCH_3$	H_2C_6
CH^+	HCN	C_2H_2	CH_2CN	CH_3OH	NH_2CH_3	CH_2OHCHO
CN	HCO	CH_2D^+(?)	CH_4	CH_3SH	c-C_2H_4O	CH_2CHCHO
CO	HCO^+	HCCN	HC_3N	HC_3NH^+	CH_2CHOH	
CO^+	HCS^+	$HCNH^+$	HC_2NC	HC_2CHO		
CP	HOC^+	HNCO	HCOOH	NH_2CHO		
CSi	H_2O	HNCS	H_2CHN	C_5N		
HCl	H_2S	$HOCO^+$	H_2C_2O	HC_4N		
KCl	HNC	H_2CO	H_2NCN			
NH	HNO	H_2CN	HNC_3			
NO	MgCN	H_2CS	SiH_4			
NS	MgNC	H_3O^+	H_2COH^+			
NaCl	N_2H^+	NH_3				
OH	N_2O	SiC_3				
PN	NaCN	C_4				
SO	OCS					
SO^+	SO_2					
SiN	c-SiC_2					
SiO	CO_2					
SiS	NH_2					
CS	H_3^+					
HF	SiCN					
SH	AlNC					
FeO(?)	SiNC					

Nine atoms	Ten atoms	Eleven atoms	Twelve atoms	Thirteen atoms
CH_3C_4H	CH_3C_5N(?)	HC_9N	$CH_3OC_2H_5$	$HC_{11}N$
CH_3CH_2CN	$(CH_3)_2CO$			
$(CH_3)_2O$	NH_2CH_2COOH			
CH_3CH_2OH	CH_3CH_2CHO			
HC_7N				
C_8H				

Table from A. Wootten (www.cv.nrao.edu/~awootten/allmols.html).

[Table 7.1, Kowk]

- Given the ubiquity of hydrogen in the ISM, and the inability of helium to form chemical bonds, we expect molecular gas in the ISM to consist primarily of H_2.
  - A hydrogen molecule, with the dissociation energy D_0 = 4.52 eV, is not very tightly bound. An UV photon can photodissociate it.
  - In a gas with temperature $T > D_0/k \sim 50{,}000$ K , collisions with other gas particles can collisionally dissociate it. Thus, we expect molecular hydrogen to survive for long periods of time **only in cold regions of the ISM that are shielded from UV radiation.**
  - Hydrogen has the lowest, reduced mass of any molecule, $\mu = m_{\rm H}/2$, hence, hydrogen molecules have a particularly high fundamental frequency of vibration compared to other diatomic molecules.

Properties of some diatomic molecules [Table 7.1, Ryden]

Molecule	D_0 [eV]	r_0 Å	B_0 [meV]	$\hbar\omega_0$ [eV]	μ_0 [debye]
H_2	4.52	0.74	7.36	0.516	0.000
CO	11.1	1.13	0.24	0.269	0.110
CH	3.51	1.12	1.76	0.339	1.406
OH	4.39	0.97	2.30	0.443	1.668
CN	7.57	1.17	0.23	0.253	0.557

$\mu_0 =$ permanent dipole moment

1 debye $= 10^{-18}$ statC cm

$D_0 =$ dissociation energy

$r_0 =$ speration

$$B_0 \equiv \frac{\hbar^2}{2I}$$

$\omega_0 = \sqrt{k/\mu}$ fundamental frequency of vibration

CO

- For any molecule to undergo a pure rotation transition, it must have a permanent dipole moment, μ. This means that **for any molecule to have a dipole-allowed rotational spectrum it must have an asymmetric charge distribution which gives rise to a permanent dipole moment.**

  Heteronuclear diatomics poses a permanent dipole moment but homonuclears, such as H_2, do not.

- CO

  Carbon monoxide, CO, is a particularly important species for astronomical observations.

  CO is the most stable diatomic molecule.

  It has a dissociation energy D_0 of 11.1 eV, which is more than double the D_0 value found for most other diatomic molecules. As a result, in astronomical environments where molecules form, C and O usually combine to form CO, which is very stable and long-lived.

  The wavelengths of the first few rotational transitions are 1-0 at λ = 2.60 mm, 2-1 at 1.30 mm, and 3-2 at 0.87mm.

  The J = 1-0 transition of CO is the second most important spectral line in radio astronomy after the hydrogen 21 cm line.

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.

One reason for this is that cold H_2 is very difficult to observe directly because its pure rotational transitions are not only very weak but lie in the near-infrared where ground-based observations are not possible. **The abundance of CO is therefore often used to estimate the total amount of molecular gas present in a given environment.** It is generally assumed that the number density of CO is approximately 10^{-4} of that of H_2.

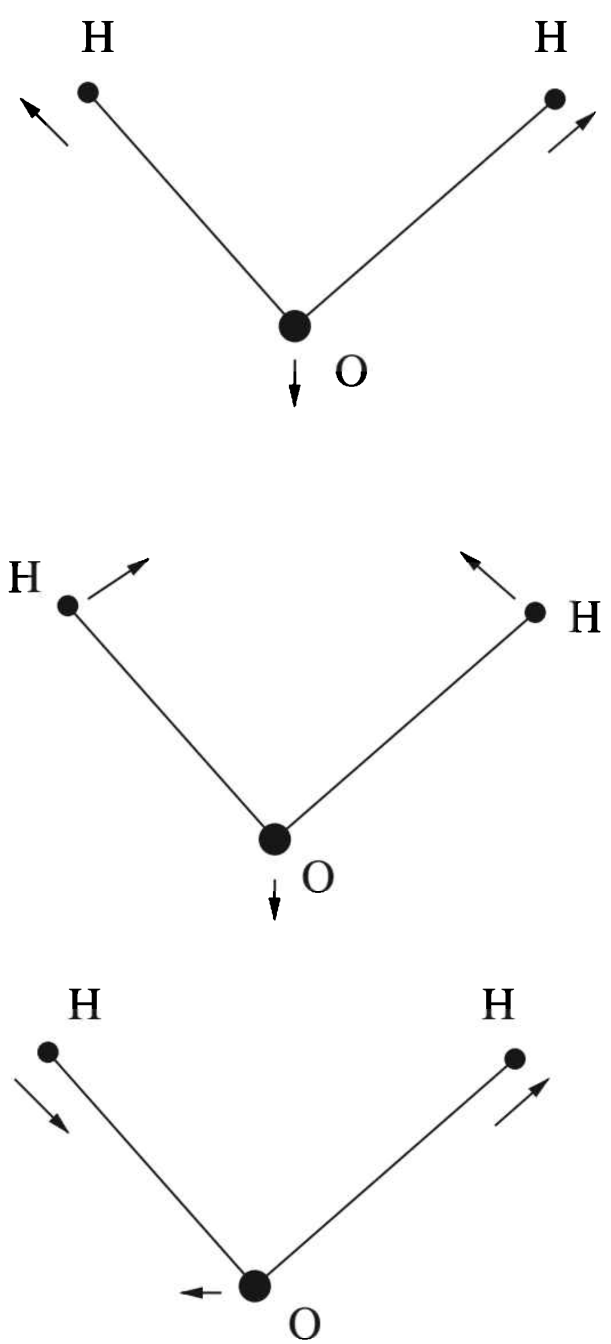
$$\boxed{n(\mathrm{CO}) \approx 10^{-4} n(\mathrm{H_2})}$$

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}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.

Vibrations in Polyatomic Molecules

H_2O



Symmetric stretch, ν_1

$\omega_1 = 3667\ \mathrm{cm}^{-1}$

Bend, ν_2

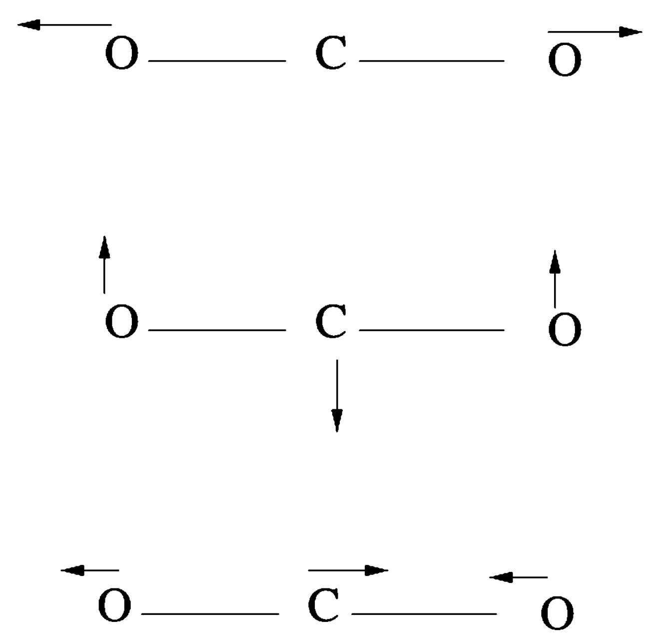
$\omega_2 = 1595\ \mathrm{cm}^{-1}$

Asymmetric stretch, ν_3

$\omega_3 = 3676\ \mathrm{cm}^{-1}$

The three vibrational modes of the **water molecule**

CO_2



Symmetric stretch, ν_1

$\omega_1 = 1388\ \mathrm{cm}^{-1}$

Bend (degenerate), ν_2

$\omega_2 = 667\ \mathrm{cm}^{-1}$

Asymmetric stretch, ν_3

$\omega_3 = 2349\ \mathrm{cm}^{-1}$

The vibrational modes of **carbon dioxide**; note that the bending mode is doubly degenerate as the motion can occur in the plane of the page, as drawn, or identically, perpendicular to the plane of the page.

[H_2 formation] (1) Gas-Phase Formation of H_2

- ***Direct Radiative Association***
  - When two free H atoms collide with each other, they create an excited hydrogen molecule that is unbound.

$$\mathrm{H} + \mathrm{H} \rightarrow \mathrm{H}_2^* \rightarrow \mathrm{H}_2 + h\nu$$

  - It must emit a photon carrying away enough energy to leave it a bound state, or it will break apart again. There is no electric dipole moment. As a result, there is no dipole radiation that could remove energy from the system and leave the two H atoms in a bound state. Electric quadrupole transitions are possible, but the rates are very low.

The lifetime of the excited hydrogen molecule until it breaks apart would be roughly one period of vibration:

$$\frac{2\pi}{\omega_0} = \frac{h}{E_{\mathrm{vib},0}} = \frac{6.626 \times 10^{-27}\,\mathrm{cm^2\,g\,s^{-1}}}{0.516\,\mathrm{eV}} \sim 8 \times 10^{-15}\,\mathrm{s}^{-1}$$

Rate for the electric quadrupole transition is $A_{u\ell} \sim 10^{-11}\,\mathrm{s}^{-1}$

Therefore, the probability of emitting a photon before it break apart is $\boxed{p \sim A_{u\ell}\,(2\pi/A_{u\ell}) \sim 10^{-25}}$

  - As a consequence, the rate coefficient for direct radiative association of H_2 is so small that this reaction can be ignored in astrochemistry.

- ***Three-body reaction***

$$3\mathrm{H} \rightarrow \mathrm{H}_2 + \mathrm{H} + \mathrm{KE}$$

  - The reaction can occur, when the third body carrying off the energy released when H_2 is formed, but the rate for this three-body reaction is negligible at interstellar or intergalactic densities.
  - At the high densities of a protostar or protoplanetary disk, the three-body reaction is able to convert H to H_2.

- ***Formation of negative hydrogen ion by radiative association followed by formation of H_2 by associative detachment***:
  - First step:

$$\mathrm{H}^0 + e^- \rightarrow \mathrm{H}^- + h\nu \qquad \text{rate coefficient:} \quad k \approx 1.9 \times 10^{-16}\,(T_{\mathrm{gas}}/100\,\mathrm{K})^{0.67}\ \mathrm{cm}^3\,\mathrm{s}^{-1}$$

  - Second step:

$$\mathrm{H}^- + \mathrm{H} \rightarrow \mathrm{H}_2 + e^- + \mathrm{KE} \qquad \text{rate coefficient:} \quad k \approx 1.3 \times 10^{-9}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

    This is an exothermic ion-molecule reaction.

  - The density of negative H ion is very low because the formation rate of H^- (first step) is slow while there are many, rapid processes that destroy H^-.

- $\mathrm{H^-}$ can be destroyed by reaction with protons:

$$\mathrm{H^- + H^+ \rightarrow H + H} \qquad k \approx 6.9 \times 10^{-7}\,(T/100\,\mathrm{K})^{-1/2}\,\mathrm{cm^3\,s^{-1}}$$

- $\mathrm{H^-}$ can be destroyed by reaction with other positive ions:

$$\mathrm{H^- + X^+ \rightarrow H + X} \qquad k \approx 4 \times 10^{-7}\,(T/100\,\mathrm{K})^{-1/2}\,\mathrm{cm^3\,s^{-1}}$$

- In the diffuse ISM, $n(\mathrm{H^+}) \approx 0.01\,\mathrm{cm^{-3}}$ or lower. Most of $\mathrm{H^-}$ is destroyed by ***photodetachment***, which is the inverse process to radiative association.

$$\mathrm{H^-} + h\nu \rightarrow \mathrm{H} + e^-$$

reaction rate: $\zeta \approx 2.4 \times 10^{-7} G_0\,\mathrm{s^{-1}}$

Here, G_0 is the strength of radiation in units of the interstellar radiation field (ISRF).

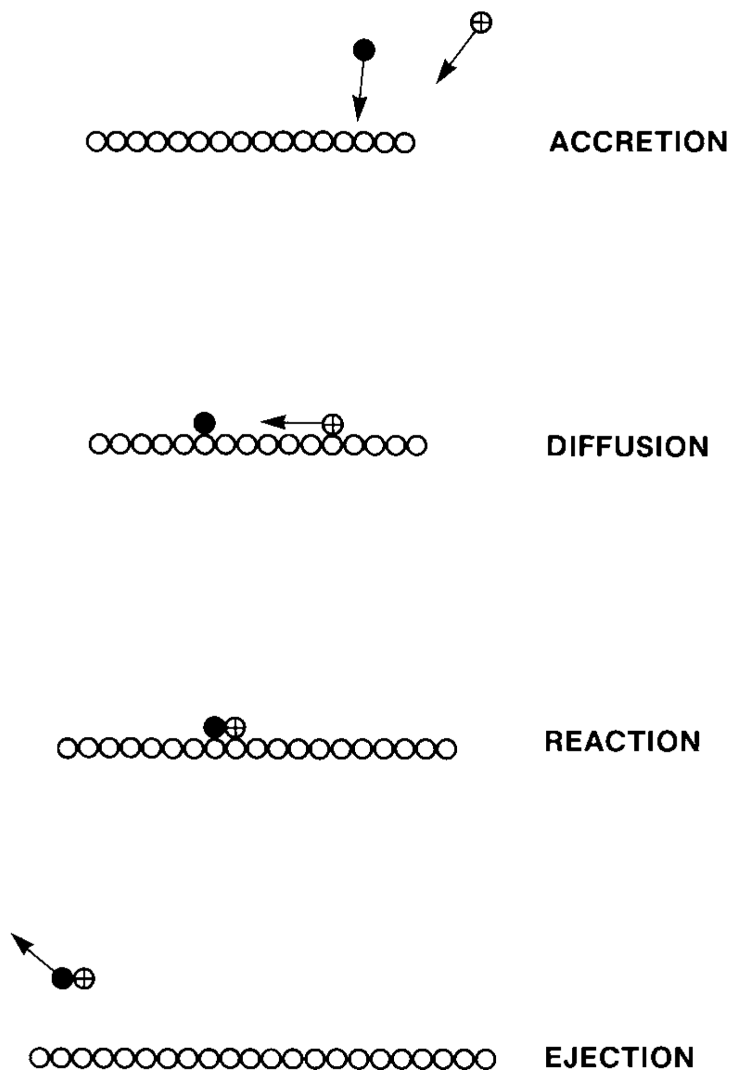
The photodetachment needs only $I = 0.77\,\mathrm{eV}$ to take away one of its electrons.

- ***In the absence of dust (e.g., in the early universe),*** $\mathrm{H^- + H \rightarrow H_2} + e^-$ ***is the dominant channel for forming H₂.***
  - Associative detachment and the resulting production of H_2 will only dominate over photodetachment when

$$n_{\mathrm{HI}} > \frac{\zeta_{\mathrm{pd}}}{k_{\mathrm{ad}}} \approx 120\,\mathrm{cm^{-3}}$$

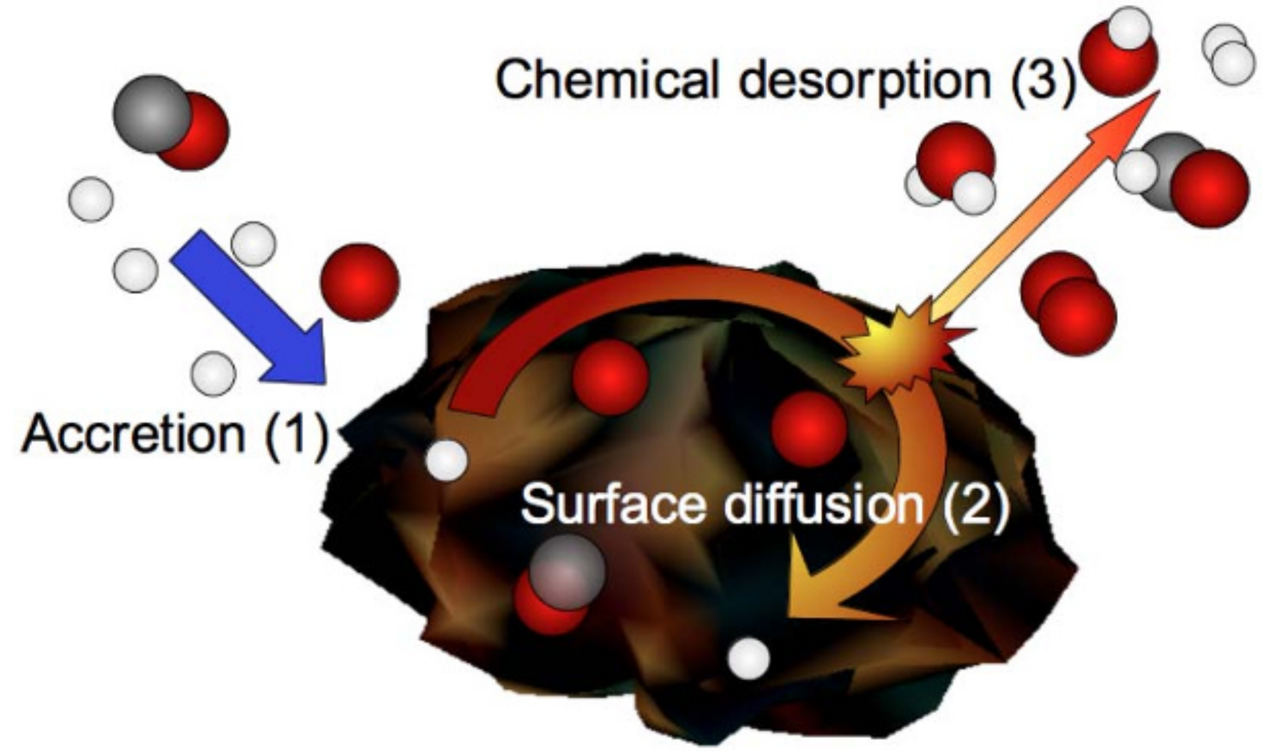
[H_2 formation] (2) Grain Catalysis of H_2

- The dominant process of H_2 formation in the Milky Way and other galaxies is via grain catalysis.
  - The surface of a dust grain acts as a lab of chemical activity.
  - ***Adsorption***:
    - A H atom colliding with a dust grain has some probability of sticking (bounding) to the grain.
    - The sticking probability depends (1) on the atom's speed (slower atoms are more likely to stick), (2) on the grain's temperature (hot grains are less sticky), (3) on the grain's size (smaller grains are less sticky), and (4) on the grain's composition.
    - Sticking probability: $\boxed{p_s \approx 0.3 \quad \text{for grains with } a \sim 0.1\mu\text{m}}$
  - ***Diffusion & Reaction***:
    - Initially, the binding may be weak enough that the H atom is able to diffuse (i.e., random-walk) some distance on the grain surface, until it happens to arrive at a site where it is bound strongly enough that it becomes "trapped."
    - Subsequent H atoms arrive at random locations on the grain surface and undergoes their own random walks until they also become trapped, but eventually one of the newly arrived H atoms encounters a previously bound H atom before itself becoming trapped.
    - When the two H atoms encounter one another, they react to form H_2.
  - ***Desorption***:
    - The energy released when two free H atoms react to form H_2 in the ground state is ΔE = 4.5 eV. This energy is large enough to overcome the forces that were binding the two H atoms to the grain, and the H_2 molecule is ejected from the grain surface.



A schematic of the formation of molecules on grain surfaces.

[Fig 4.1, Tielens]



Sketch that illustrates the chemical desorption process. Species coming from the gas accrete on the dust surface can meet each other to form other species. For some reactions, the formed product is ejected in the gas.

[Fig 1, Dulieu, 2003, Scietific Reports]

Formation rate of H_2

- Formation rate
  - The rate per unit volume at which H atoms collide with grains, averaged over the distribution of grain radii would be:

$$\Gamma_{\rm coll} = n_{\rm HI}\left(\frac{8kT_{\rm gas}}{\pi m_{\rm H}}\right)^{1/2}\int_{a_{\rm min}}^{a_{\rm max}}\frac{dn_{\rm gr}}{da}\pi a^2 da$$

Recall the mean speed of the Maxwell distribution

$$\langle v\rangle = \int_0^\infty v f(v) d^3 v = \sqrt{\frac{8kT}{\pi m}}$$

$$f(v) = \left(\frac{m}{2\pi kT}\right)^{3/2} e^{-mv^2/2kT}$$

  - It is customary to define *the total grain geometric cross section per H nucleon*.

$$\Sigma_{\rm gr} \equiv \frac{1}{n_{\rm H}}\int da\frac{dn_{\rm gr}}{da}\pi a^2 \longrightarrow \boxed{\Gamma_{\rm coll} = n_{\rm HI}n_{\rm H}\left(\frac{8kT_{\rm gas}}{\pi m_{\rm H}}\right)^{1/2}\Sigma_{\rm gr}}$$

  - Suppose that a fraction $\epsilon_{\rm gr}$ of the H atoms that collide with a grain depart from the grain as H_2. The rate for H_2 formation via grain catalysis would then be

$$\frac{dn({\rm H_2})}{dt} = \frac{1}{2}n_{\rm HI}n_{\rm H}\left(\frac{8kT_{\rm gas}}{\pi m_{\rm H}}\right)^{1/2}\int da\frac{dn_{\rm gr}}{da}\pi a^2\epsilon_{\rm gr}(a)$$

or

$$\frac{dn({\rm H_2})}{dt} = R_{\rm gr}n_{\rm H}n_{\rm HI}$$

The factor 1/2 is because two H atoms are required to form H_2, and the **"rate coefficient"** is given by

$$R_{\rm gr} = \frac{1}{2}\left(\frac{8kT_{\rm gas}}{\pi m_{\rm H}}\right)^{1/2}\langle\epsilon_{\rm gr}\rangle\,\Sigma_{\rm gr}$$

Here, the formation efficiency averaged over the grain surface area is:

$$\langle\epsilon_{\rm gr}\rangle \equiv \frac{1}{\Sigma_{\rm gr}}\int da\frac{dn_{\rm gr}}{da}\pi a^2\epsilon_{\rm gr}(a)$$

- Numerical values

  - Total grain geometric cross section per H nucleon: We note that

$$C(\lambda = 0.1\mu\mathrm{m}) \approx 2\times 10^{-21}\,\mathrm{cm}^2/\mathrm{H} \quad \text{suggests that} \quad \Sigma_{\mathrm{gr}} \gtrsim 10^{-21}\,\mathrm{cm}^2/\mathrm{H}$$

  The silicate-graphite-PAH grain model of Weingartner & Draine (2001) gives

$$\boxed{\Sigma_{\mathrm{gr}} \approx 6.0\times 10^{-21}\,\mathrm{cm}^2/\mathrm{H}}$$

  - The rate coefficient for H_2 formation is then

$$\boxed{R_{\mathrm{gr}} = 7.3\times 10^{-17}\,\mathrm{cm}^3\,\mathrm{s}^{-1}\left(\frac{T_{\mathrm{gas}}}{100\,\mathrm{K}}\right)^{1/2}\langle\epsilon_{\mathrm{gr}}\rangle\left(\frac{\Sigma_{\mathrm{gr}}}{10^{-21}\,\mathrm{cm}^2\,\mathrm{H}^{-1}}\right)}$$

  Jura (1975) used UV spectroscopy of diffuse clouds with $T_{\mathrm{gas}} \approx 70\,\mathrm{K}$ and determined that

$$R_{\mathrm{gr}} \approx 3\times 10^{-17}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$$

  The observed rate coefficient indicates

$$\boxed{\langle\epsilon_{\mathrm{gr}}\rangle \approx 0.08}$$

  This average is the result of a very low value of ϵ_{gr} for the PAHs, which dominate the surface area, and $\boxed{\epsilon_{\mathrm{gr}} \gtrsim 0.5}$ for the $a \gtrsim 0.01\mu\mathrm{m}$ "classical" silicate and carbonaceous grains.

- Time scale of H_2 formation: dust grains are converting atomic hydrogen into molecular hydrogen on a characteristic time scale:

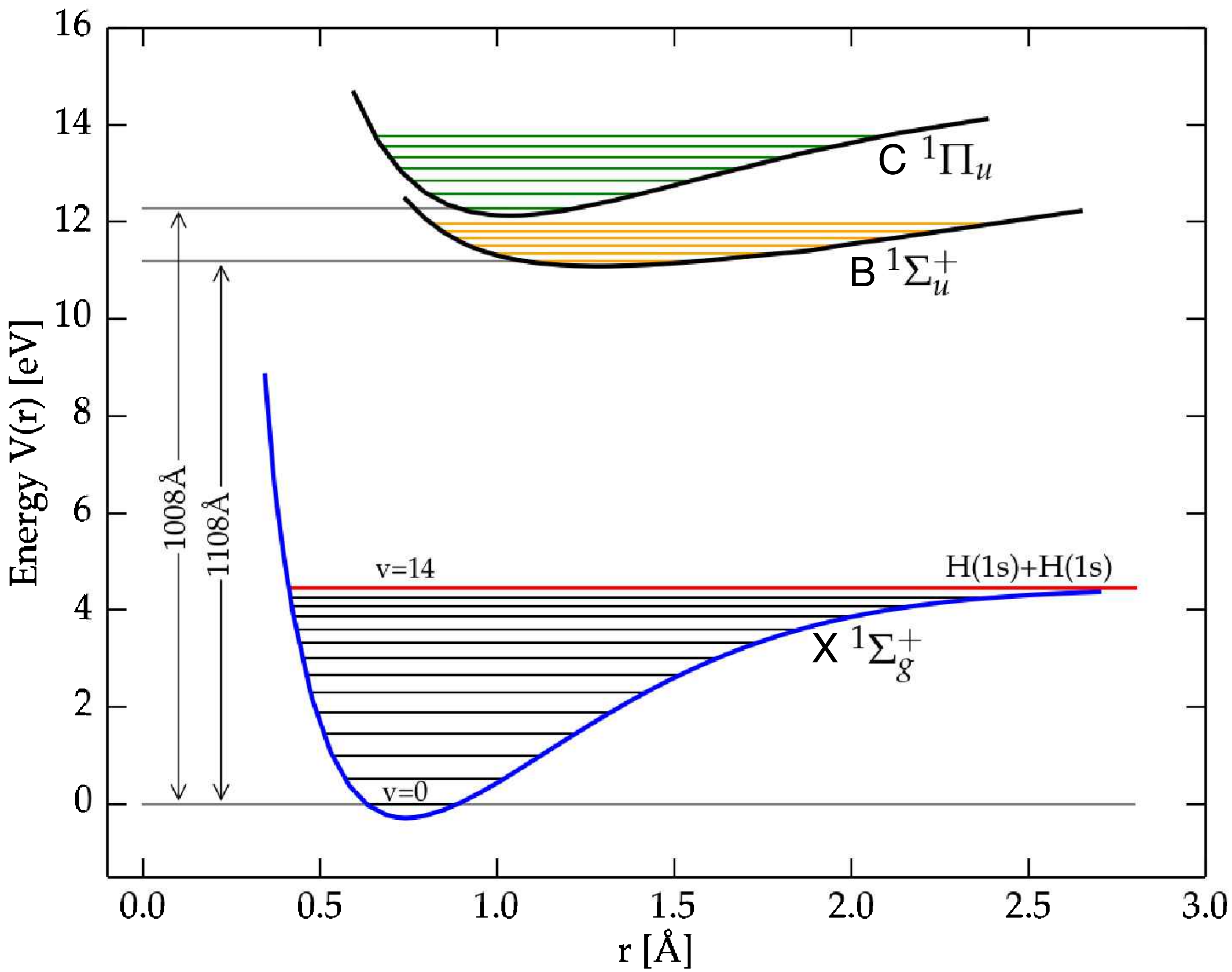
$$
\begin{aligned}
t_{\mathrm{H_2\,form}} &\approx \frac{\frac{1}{2}n_{\mathrm{HI}}}{R_{\mathrm{gr}} n_{\mathrm{H}} n_{\mathrm{HI}}} \\
&\approx 15\,\mathrm{Myr}\left(\frac{n_{\mathrm{H}}}{30\,\mathrm{cm^{-3}}}\right)^{-1}\left(\frac{T_{\mathrm{gas}}}{100\,\mathrm{K}}\right)^{-1/2}\left(\frac{\langle\epsilon_{\mathrm{gr}}\rangle}{0.08}\right)^{-1}\left(\frac{\Sigma_{\mathrm{gr}}}{6\times10^{-21}\,\mathrm{cm^2\,H^{-1}}}\right)^{-1}
\end{aligned}
$$

- Thus, **the CNM should be filled with molecular hydrogen** - unless there's a competing process that before the H_2 molecules as fast as grain surface make them.

- *The competing process is the photodissociation near bright stars.*

Photodissociation of H_2

- Photodissociation: $\mathrm{H_2} + h\nu \rightarrow \mathrm{H} + \mathrm{H} + \mathrm{KE}$
  - Photodissociation is the principal process destroying interstellar H_2.



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

In the left potential energy curves, you might think that photodissociation of H_2 is a simple task; if H_2 absorb a photon of energy $h\nu > 4.52\,\mathrm{eV}$, 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.

- Lyman-Werner band

- The energy difference between the $v = 0,\ J = 0$ level in the ground electronic state, and the $v = 0,\ J = 0$ level in the first excited electronic state is $E = 11.18\,\mathrm{eV}\ (\lambda = 1108\,\text{Å})$, which is a higher energy than the 10.2 eV energy of the Lyα line in atomic hydrogen.
- The transitions between the ro-vibrational levels in the ground electronic state and the ro-vibrational levels in the **first excited electronic states** produce a forest of lines that are referred to collectively as the ***Lyman band***.
- Emission and absorption between the ground electronic state and the **second excited electronic state** is called the ***Werner band***.
- The Lyman and Werner bands lie in the energy range 11.18 - 13.60 eV.

- The main mechanism by which H_2 is photodissociated is a two-step process.
  - The first step is absorption of a resonance line photon (λ = 912-1108Å), raising the H_2 from an initial level $X(v, J)$ to a level $B(v', J')$ or $C(v', J')$ of the first and second electronic states. This photoexcitation is via a permitted absorption line, and therefore the newly excited level is guaranteed to have electric dipole-allowed decay channels, with a large transition probability.
  - The excited level is most likely to decay to vibrationally excited bound levels $X(v'', J'')$ of the ground electronic state, and such decays occur ~85% of the time. However, a fraction of ~15% of the time, the downward spontaneous transition will be to the vibrational continuum ($v > 14$) of the ground electronic state: The two hydrogen atoms will then fly away from each other and the hydrogen molecule is dissociated.

- Photodissociation Rate:
  - The probability per unit time of photoexcitation of H_2 from lower level ℓ to upper level u is given by

$$\boxed{\zeta_{\ell\to u} = \frac{\pi e^2}{m_e c} f_{\ell u} \frac{u_\nu c}{h\nu_{\ell u}} \quad \to \quad \frac{\pi e^2}{m_e c^2 h} f_{\ell u} \lambda_{\ell u}^3 u_\lambda}$$

Eq (31.12) in Draine

  - There are many transitions out of a given lower vibration-rotation level. The total rate of photoexcitation out of ℓ is:

$$\zeta_{\mathrm{pe},\ell} = \sum_u \zeta_{\ell\to u}$$

  - The photodissociation rate is obtained by summing over all of the photoexcitation channels, each multiplied by the probability $p_{\mathrm{diss},u}$ that the upper level will decay to the vibrational continuum:

$$\boxed{\zeta_{\mathrm{diss},\ell} = \sum_u \zeta_{\ell\to u} p_{\mathrm{diss},u}}$$

  - The dissociation probability averaged over the photoexcitation channels is:

$$\boxed{\langle p_{\mathrm{diss}} \rangle_\ell \equiv \frac{\zeta_{\mathrm{diss},\ell}}{\zeta_{\mathrm{pe},\ell}}}$$

- Note that the photoexcitation and photodissociation rates are nearly independent of the level ℓ.

level ℓ (v, J)	$\zeta_{\mathrm{photoexc},\ell}/\chi$ [b] $(10^{-10}\,\mathrm{s}^{-1})$	$\zeta_{\mathrm{diss},\ell}/\chi$ $(10^{-11}\,\mathrm{s}^{-1})$	$\langle p_{\mathrm{diss}}\rangle_\ell$
(0,0)	3.08	4.13	0.134
(0,1)	3.09	4.20	0.136
(0,2)	3.13	4.23	0.135
(0,3)	3.15	4.57	0.145
(0,4)	3.21	4.94	0.154
(0,5)	3.26	5.05	0.155

Photoexcitation and Photodissociation Rates for Unshieled H_2

[Table 31.1, Draine; Draine & Bertoldi (1996)]

Here, the intensity of interstellar radiation field near 1000Å.

$$\chi \equiv \frac{(\nu u_\nu)_{1000\mathring{A}}}{4 \times 10^{-14}\,\mathrm{erg\,cm^{-3}}}$$

$$\begin{aligned}\chi &= 1 \text{ for the ISRF of Habing (1968)}\\ &= 1.71 \text{ for the ISRF of Draine (1978)}\\ &= 1.23 \text{ for the ISRF of Mathis et al. (1983)}\end{aligned}$$

- In the local diffuse neutral ISM, the H_2 photodissociation rate is:

$$\boxed{\zeta_{\mathrm{diss}} \equiv \langle p_{\mathrm{diss}}\rangle\,\zeta_{\mathrm{pe}} \approx 5 \times 10^{-11}\,\mathrm{s}^{-1}}$$

- The typical timescale for photodissociation of H_2 is the: $t_{\mathrm{diss}} \approx 1/\zeta_{\mathrm{diss}} \sim 640\,\mathrm{yr}$

  This is smaller by four orders of magnitude that the ~ 15 Myr timescale for creation of H_2 by grain surface catalysis in the CNM.

- Steady-state abundance of H_2
  - The steady-state abundance of molecular hydrogen is determined by a balance between formation on grains and photodissociation, resulting in a very low steady state abundance:

$$\zeta_{\rm diss} n({\rm H_2}) = R_{\rm gr} n_{\rm HI} n_{\rm H}$$

$$\begin{aligned} \frac{n({\rm H_2})}{n_{\rm HI}} &= \frac{R_{\rm gr} n_{\rm H}}{\zeta_{\rm diss}} \\ &\approx 1.8 \times 10^{-5} \left(\frac{n_{\rm H}}{30\,{\rm cm^{-3}}}\right) \left(\frac{R_{\rm gr}}{3 \times 10^{-17}\,{\rm cm^3\,s^{-1}}}\right) \left(\frac{5 \times 10^{-11}\,{\rm s^{-1}}}{\zeta_{\rm diss}}\right) \end{aligned}$$

  - ***In the absence of self-shielding***, diffuse H I clouds will contain only a tiny amounts of H_2. ***Molecular hydrogen shouldn't dominate over atomic hydrogen until the density reaches ~ 3x10^6 cm^{-3}***.
  - In reality, observations reveal that the molecular form dominates at densities as low as ~ 300 cm^{-3}. This is because the inner parts of molecular clouds are protected from UV light by ***self-shielding***.

Self-Shielding and Dust-Shielding

- ***Self-shielding*** refers to the phenomenon where the photoexcitation transitions become optically thick, so that the molecule in question is "shielded" from starlight by other molecules.
  - Self-shielding occurs on a line-by-line basis, with stronger self-shielding for the stronger lines (large oscillator strengths) from levels with large populations.
  - Recall that the equivalent width is the measure of absorbed light (EW = fraction of absorbed light). **The rate of photoexcitation** is given, in general, by

$$\Delta N_\ell \zeta_{\mathrm{pe},\ell\to\mathrm{u}} = \left(\frac{u_\nu c}{h\nu}\right)\Delta W$$

$$\zeta_{\mathrm{pe},\ell\to\mathrm{u}} = \left(\frac{u_\nu c}{h\nu}\right)_{\ell u}\frac{dW_\nu}{dN_\ell}$$

where

$$W_\nu = \int d\nu\left(1 - e^{-\tau_\nu}\right)$$

$$\tau_\nu = N_\ell \chi_0 \phi_\nu = N_\ell \frac{\pi e^2}{m_e c} f_{\ell u}\phi_\nu$$

$$\phi_\nu = \text{line profile}$$

u_ν = radiation energy density in the absence of H_2 line absorption

In the optical thin limt,

$$\frac{dW_\nu}{dN_\ell} = \frac{d}{dN_\ell}\int d\nu \tau_\nu = \chi_0 = \frac{\pi e^2}{m_e c} f_{\ell u}$$

Note that

$$\tau_\lambda = \tau_\nu = N_\ell \frac{\pi e^2}{m_e c} f_{\ell u}\phi_\lambda\left|\frac{d\lambda}{d\nu}\right|$$

  - Therefore, the self-shielding factor is defined to be:

$$f_{\mathrm{shield},\ell u} \equiv \frac{dW_\nu/dN_\ell}{(\pi e^2/m_e c) f_{\ell u}} < 1 \longrightarrow \zeta_{\mathrm{pe},\ell\to\mathrm{u}} = \left(\frac{u_\nu c}{h\nu}\right)_{\ell u}\left(\frac{\pi e^2}{m_e c} f_{\ell u}\right) f_{\mathrm{shield},\ell u}$$

- The photodissociation rate for H_2 in level ℓ is reduced by self-shielding:

$$\begin{aligned}\zeta_{\mathrm{diss},\ell} &= \sum_u \zeta_{\mathrm{pe},\ell\to u} p_{\mathrm{diss},u} \\ &= \frac{\pi e^2}{m_e c} \sum_u f_{\ell u} \left(\frac{u_\nu c}{h\nu}\right)_{\ell u} f_{\mathrm{shield},\ell u} p_{\mathrm{diss},u}\end{aligned}$$

Compare with Eq. (31.24) of [Draine]

$$u_\nu = u_\lambda \left|\frac{d\lambda}{d\nu}\right| = u_\lambda \frac{\lambda^2}{c}$$

$$\rightarrow \quad \frac{u_\nu c}{h\nu} = u_\lambda \frac{\lambda^3}{hc}$$

- The photodissociation rate per H_2 is obtained by averaging the above equation over the population levels. A reasonably accurate approximation is given by Draine & Bertoldi (1996).

$$\zeta_{\mathrm{diss}} \approx \zeta_{\mathrm{diss},0} f_{\mathrm{shield,\,diss}} e^{-\tau_{\mathrm{d},1000}}$$

$$f_{\mathrm{shield,diss}} \approx \frac{0.95}{(1+x/b_5)^2} + \frac{0.035}{(1+x)^{0.5}} \exp\left[-8.5\times10^{-4}(1+x)^{0.5}\right]$$

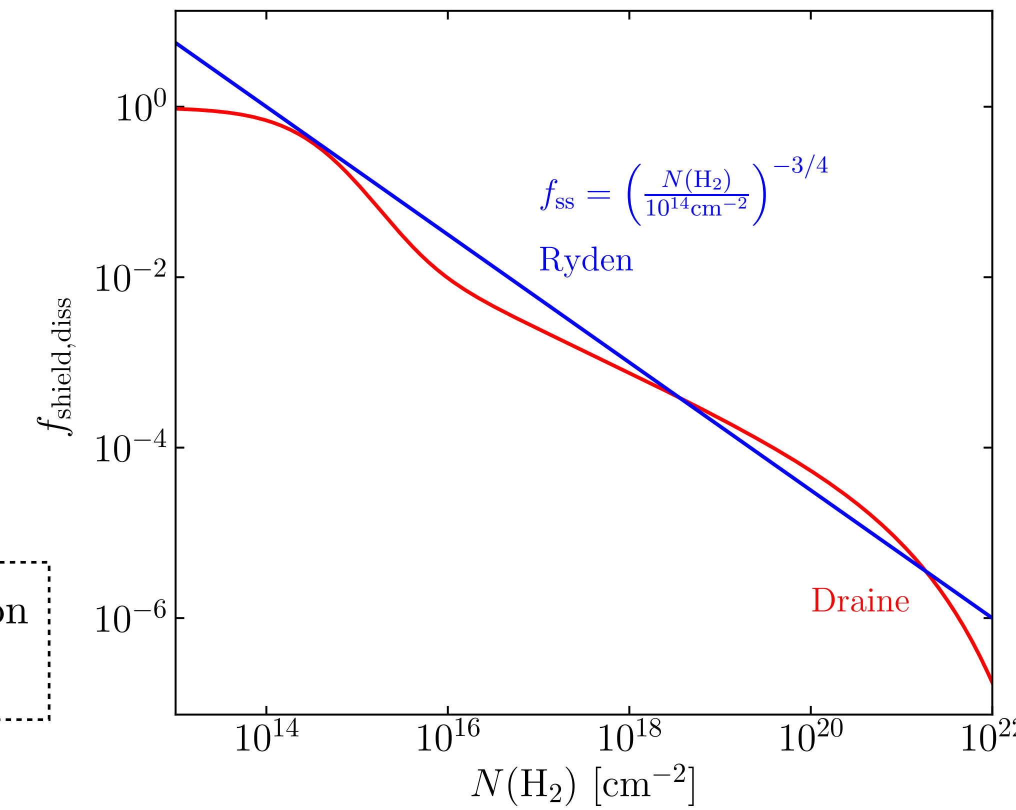
$$x \equiv \frac{N(\mathrm{H_2})}{5\times10^{14}\,\mathrm{cm^{-2}}}, \;\; b_5 \equiv \frac{b}{\mathrm{km\,s^{-1}}}$$

$\zeta_{\mathrm{diss},0}$ = the photodissociation rate in the absence of dust extinction or self-shielding

$\tau_{\mathrm{d},1000}$ = the dust optical depth by dust at 1000Å.

- Ryden provides a crude approximation for the self-shielding factor:

$$\boxed{f_{\text{shield,diss}} \approx \left(\frac{N(\text{H}_2)}{10^{14}\,\text{cm}^{-2}}\right)^{-3/4}}$$



- For a cloud with a density of 1000 cm^{-3},

$$\frac{n(\text{H}_2)}{n_{\text{HI}}} = \frac{R_{\text{gr}} n_{\text{H}}}{\zeta_{\text{diss}}}$$

n_{H} = number density of H nucleon
n_{HI} = number density of H atom

$$\approx 6 \times 10^{-4} \left(\frac{n_{\text{H}}}{1000\,\text{cm}^{-3}}\right)\left(\frac{1}{f_{\text{shield,diss}}}\right)$$

The ratio of H_2 molecules to H atoms becomes equal to one when the gas is self-shielded by a column density:

$$N_{\text{H}_2} \gtrsim 1.5 \times 10^{18}\,\text{cm}^{-2} \qquad \leftarrow \frac{n(\text{H}_2)}{n_{\text{HI}}} = 1$$

This corresponds to **an outer shelf-shielding skin to the cloud that is just 4x10^{-4} pc.**

$$d = \frac{N_{\text{H}_2}}{n_{\text{H}}} = 4 \times 10^{-4}\,\text{pc}\left(\frac{N_{\text{H}_2}/1.5\times10^{18}\,\text{cm}^{-2}}{n_{\text{H}}/1000\,\text{cm}^{-3}}\right)$$

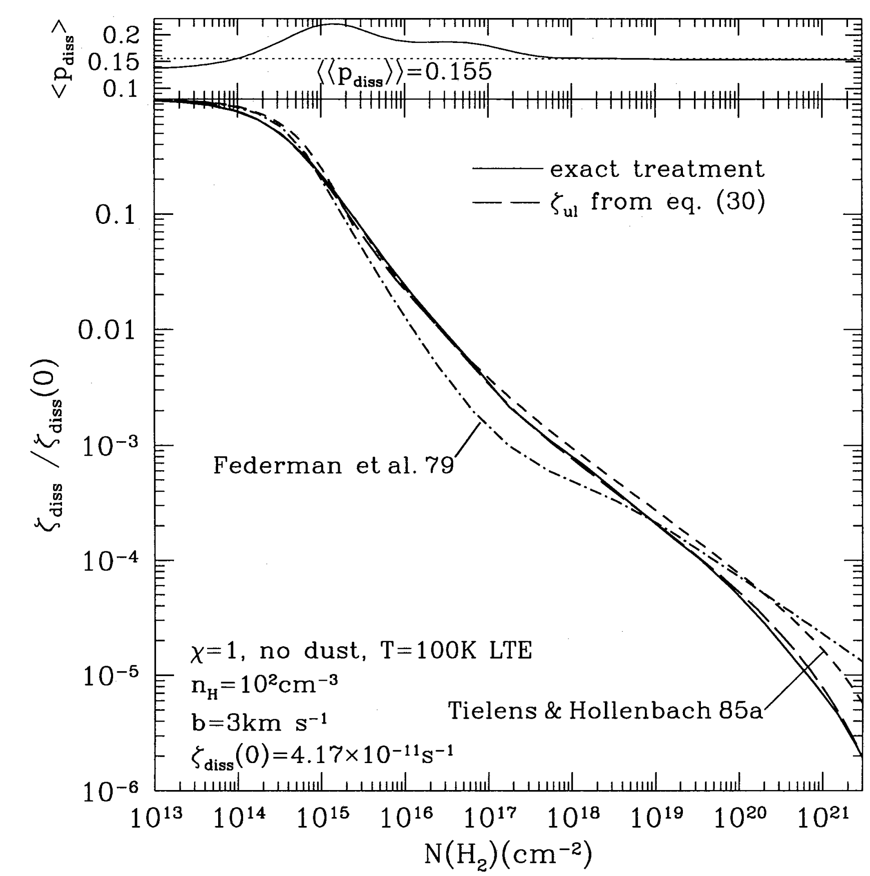


Fig 1, Draine & Bertoldi (1996)

- ***Dust*** can also shield molecular gas from UV light.
  - In our galaxy, the relation between dust extinction and column density of hydrogen nucleon and the ratio between extinctions 1100Å and V band are, respectively:

$$\frac{A_V}{N_{\rm H}} \approx 5.3 \times 10^{-22}\,{\rm cm}^2 \qquad \frac{A_{1100}}{A_V} \approx 4$$

  - When hydrogen is primarily molecular, $N({\rm H}_2) = N_{\rm H}/2$. This results in dust extinction in the Lyman and Werner bands of

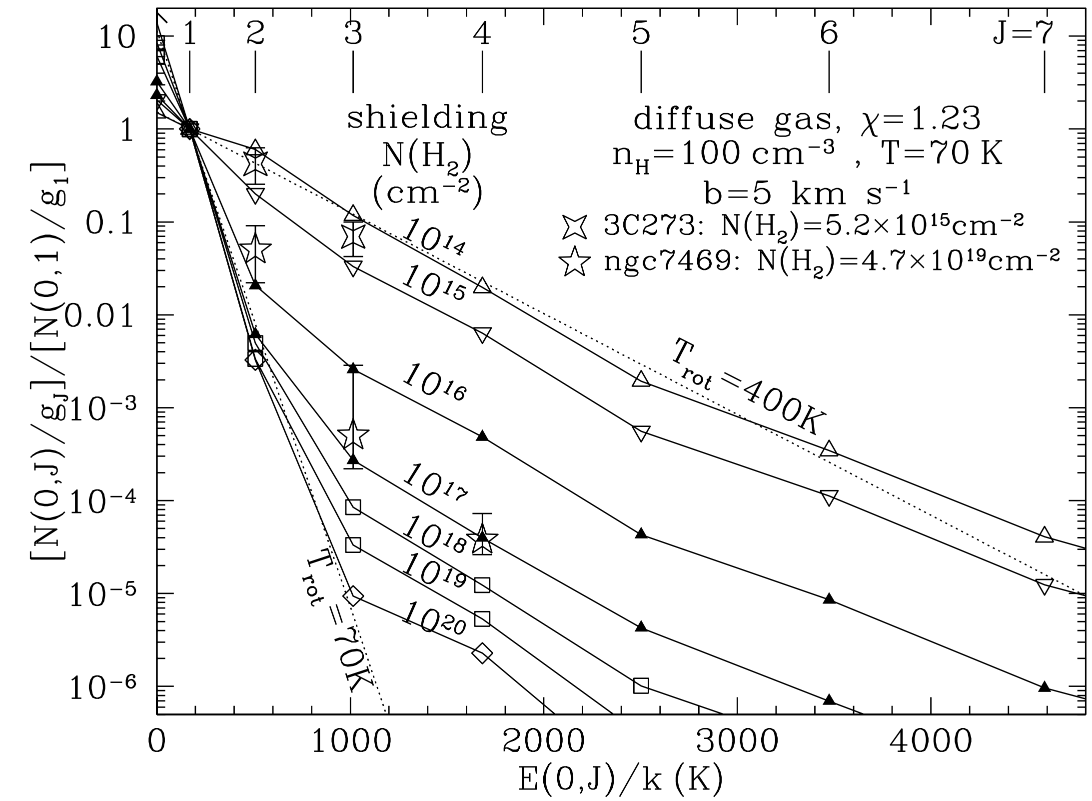
$$\boxed{\frac{A_{1100}}{N({\rm H}_2)} \approx \frac{4A_V}{N_{\rm H}/2} \approx 4.2 \times 10^{-21}\,{\rm cm}^2}$$

  - Thus, column densities $N({\rm H}_2) \gtrsim 2.4 \times 10^{20}\,{\rm cm}^{-2}$ have more than one magnitude of dust extinction in the Lyman and Werner bands. $\boxed{A_{1100} \gtrsim 1}$
  - This is 100 times higher than the H_2 column density that leads to self-shielding in typical molecular gas. Thus, **self-shielding by H_2 is much more effective than shielding by dust under ordinary circumstances.**

Vibrational and Rotational Level Population

- Vibrational Level Populations
  - Photoexcitation to some level $B(v', J')$ or $C(v', J')$ will be followed, within a few nanoseconds, by spontaneous decay to some level $X(v'', J'')$ of the ground electronic state. As a result, UV pumping of H_2 populates the vibrationally excited levels of the ground electronic state.
  - At low densities, these vibrationally excited levels will spontaneously decay to lower vibrational levels via electric quadrupole transitions. *This "radiative cascade" populates many lower levels, finally reaching the ground vibrational level.*
  - The vibrationally excited levels have radiative lifetimes of only ~ 10^6 sec, and collisional deexcitation by collisions with H, H_2, or He is unlikely at densities $n_{\rm H} \lesssim 10^4\,{\rm cm}^{-3}$.

- Rotational Level Populations
  - In the ground vibrational state, the lifetime of the lowest rotational levels are long enough that collisional effects can play a role in depopulating the lowest J levels. ***The populations of the lowest J levels are, therefore, sensitive to the density and temperature of the gas.***
  - For ***low levels of self-shielding*** ($N(\mathrm{H_2}) \lesssim 10^{15}\,\mathrm{cm^{-2}}$), the rotational distribution function for J > 2 is relatively insensitive to the gas temperature.
    - The rotational levels $J \geq 3$ have relative populations that can be approximately characterized by rotational temperature $T_{\mathrm{rot}} \approx 400\,\mathrm{K}$.
    - However, this has nothing to do with the actual temperature; ***it is entirely the result of the branching ratios in the vibration-rotation "cascade" that populates the high J levels***.
  - ***As the shielding column density increases***, the UV pumping rates decline, and the fraction of H_2 in levels J > 3 declines.
    - The relative populations of levels J = 0 and J = 2 can be used to estimate the gas temperature:



Rotational excitation of H_2 in diffuse clouds, for various $N(H_2)$.

Also shown is the rotational excitation of H_2 in diffuse clouds to the sightlines of the AGNs 3C273 and NGC 7469 (Gillmon et al. 2006).

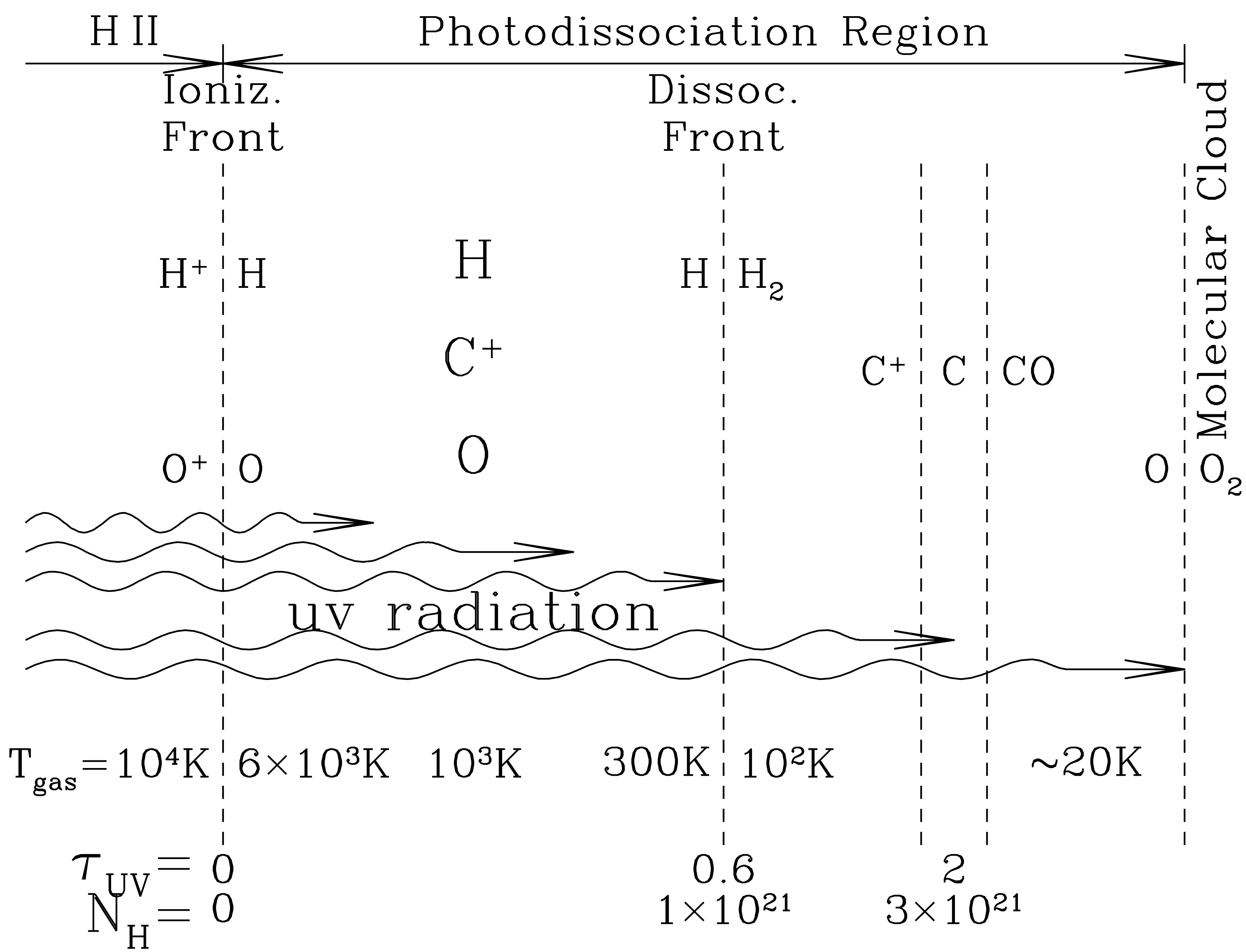
Fig 31.1, Draine

For $N(\mathrm{H_2}) \gtrsim 10^{18}\,\mathrm{cm^{-2}}$ high column density

$$T_{\mathrm{gas}} \approx \frac{510\,\mathrm{K}}{\ln\left[5N(0,0)/N(0,2)\right]}$$

Photodissociation Region (PDR)

- H II region + PDR
  - Stars are formed out of molecular gas, and when a massive star forms, it strongly irradiate the remaining molecular clouds with UV radiation, resulting in photoionization and photodissociation.
    - The photoionized gas, heated to ~ 10^4 K, will be overpressure, which will drive a compressive wave in the molecular cloud, and will also cause the ionized gas to try to flow toward lower-pressure regions nearby.
    - **The interface between the H II region and the dense molecular cloud is called a photodissociation region or PDR.**
    - PDR will be bounded by an ionization front - the surface where the hydrogen is 50% ionized - and will contain a photodissociation front - the surface where the hydrogen is 50% atomic and 50% molecular (by mass).
  - The overall physics and chemistry of PDRs is complex - see the review by Hollenbach & Tielens (1999).



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

[Fig 31.2, Draine]

[Molecular Clouds] Observations

- Cloud Structure
  - Local density estimates using line ratios often give larger densities than global mean densities found by averaging the observed molecular column densities along the line of sight.
  - The interpretation of this is that the ***clouds are very clumpy***, with the dense cores having typical sizes of < 1 pc or smaller, and densities > 10^6 cm^{-3}.
  - The overall cloud extends for 3—20 pc on average, with a mean density of $10^{3\text{-}4}$ cm^{-3}.
  - Most molecular clouds show **a number of discernible cores**. These are often detected as sources of molecular lines with high critical densities (e.g., CS), while the general cloud is mapped using lines of lower critical density (mainly CO).
  - Within the galaxies, molecular clouds are most often seen organized into complexes with **sizes from 20 pc to 100 pc, and overall H_2 masses of $10^{4\text{-}6}$ M_{sun}**. The distinction between “clouds” and “complexes” in terms of sizes and masses is somewhat artificial. A more precise statement would be that ***we see a wide range of structures***, from single small clouds to large complexes of clouds, with many complexes arrayed along the spiral arms of the Galaxy.

Molecular Clouds: Cloud Categories

- Cloud Categories (based on the total surface density)
  - Individual clouds are separated into categories based on their optical appearance: diffuse, translucent, or dark, depending on the visual extinction A_V through the cloud.

Category	A_V (mag)	Examples
Diffuse Molecular Cloud	$\lesssim 1$	ζ Oph cloud, $A_V = 0.84$ [a]
Translucent Cloud	1 to 5	HD 24534 cloud, $A_V = 1.56$ [b]
Dark Cloud	5 to 20	B68 [c], B335 [d]
Infrared Dark Cloud (IRDC)	20 to $\gtrsim 100$	IRDC G028.53-00.25 [e]

[a] van Dishoeck & Black (1986).
[b] Rachford et al. (2002).
[c] Lai et al. (2003).
[d] Doty et al. (2010).
[e] Rathborne et al. (2010).

[Table 32.1, Draine]

  - **Diffuse and translucent clouds** have sufficient UV radiation to keep gas-phase carbon mainly photoionized throughout the cloud.
    - Such clouds are usually pressure-confined, although self-gravity may be significant in some cases.
  - The typical **dark clouds have A_V ~ 10 mag, and is self-gravitating**. Some dark clouds contain dense regions that are extremely opaque, with $A_V > 20$ mag.
  - **Infrared Dark Clouds** are opaque even at 8 μm, and can be seen in silhouette against a background of diffuse 8 μm emission from PAHs in the ISM.

- Terminology for Cloud Complexes and Their Components

Categories	Size (pc)	$n_{\rm H}$ $(\rm cm^{-3})$	Mass $(M_\odot)$	Linewidth $(\rm km\,s^{-1})$	A_V (mag)	Examples
GMC Complex	$25-200$	$50-300$	$10^5-10^{6.8}$	$4-17$	$3-10$	M17, W3, W51
Dark Cloud Complex	$4-25$	10^2-10^3	$10^3-10^{4.5}$	$1.5-5$	$4-12$	Taurus, Sco-Oph
GMC	$2-20$	10^3-10^4	$10^3-10^{5.3}$	$2-9$	$9-25$	Orion A, Orion B
Dark Cloud	$0.3-6$	10^2-10^4	$5-500$	$0.4-2$	$3-15$	B5, B227
Star-forming Clump	$0.2-2$	10^4-10^5	$10-10^3$	$0.5-3$	$4-90$	OMC-1, 2, 3, 4
Core	$0.02-0.4$	10^4-10^6	$0.3-10^2$	$0.3-2$	$30-200$	B335, L1535

[Table 32.2, Draine]

- The **giant molecular cloud (GMC)** and **dark cloud** categories are distinguished mainly by total mass.
- Groups of distinct clouds are referred to as **cloud complexes**.
  - Molecular clouds are sometimes found in isolation, but in many cases molecular clouds are grouped together into complexes.
  - Since large clouds generally have substructure, the distinction between “cloud” and “cloud complex” is somewhat arbitrary.
  - Delineation of structure in cloud complexes is guided by the intensities and radial velocities of molecular lines (e.g., CO J = 1-0) as well as maps of thermal emission from dust at submm wavelengths.

Categories	Size (pc)	n_{H} (cm^{-3})	Mass ($M_\odot$)	Linewidth ($\mathrm{km\,s^{-1}}$)	A_V (mag)	Examples
GMC Complex	$25-200$	$50-300$	$10^5-10^{6.8}$	$4-17$	$3-10$	M17, W3, W51
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GMC	$2-20$	10^3-10^4	$10^3-10^{5.3}$	$2-9$	$9-25$	Orion A, Orion B
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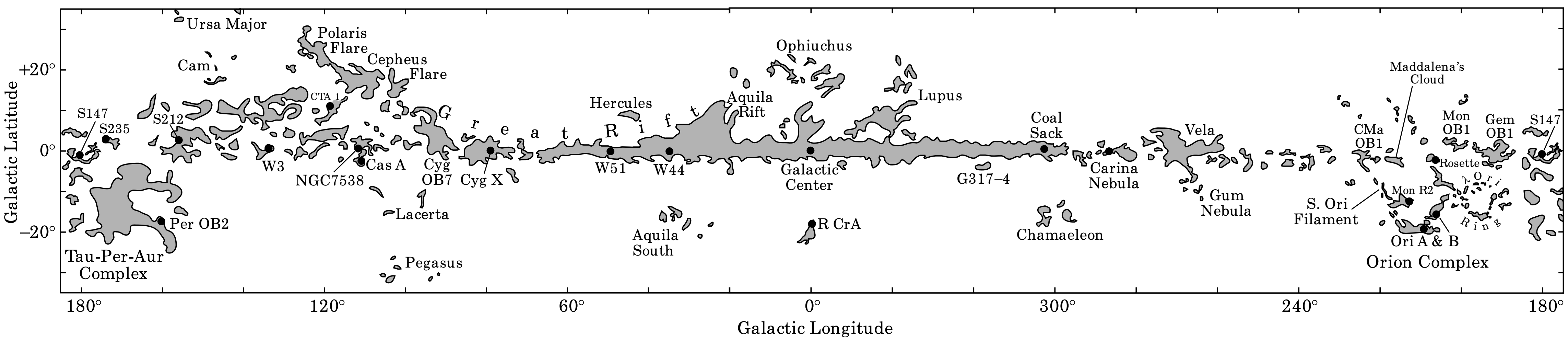
Star-forming Clump	$0.2-2$	10^4-10^5	$10-10^3$	$0.5-3$	$4-90$	OMC-1, 2, 3, 4
Core	$0.02-0.4$	10^4-10^6	$0.3-10^2$	$0.3-2$	$30-200$	B335, L1535

[Table 32.2, Draine]

- Structures within a cloud (self-gravitating entities) are described as **clumps**.
  - Clumps may or may not be forming stars; in the former case they are termed **star-forming clumps**. **Cores** are density peaks within star-forming clumps that will form a single star or a binary star.
- GMC and GMC complex
  - Much of the molecular mass is found in large clouds known as "giant molecular clouds", with masses ranging from $\sim 10^3\,M_\odot$ to $\sim 2.5\times10^5\,M_\odot$. Theses have reasonably well-defined boundaries.
  - A GMC complex is a gravitationally bound group of GMCs (and smaller clouds) with a total mass $\gtrsim 10^{5.3}\,M_\odot$.



Locations of prominent molecular clouds along the Milky Way

[Fig 32.2, Draine, Dame et al. (2001)]

Mass Distribution of GMCs

- Overall mass distribution of GMCs in the Milky Way
  - CO line surveys can detect GMCs at large distances, allowing the total number in the Galaxy to be estimated.

  - The overall mass distribution of GMCs in the Milky Way (excluding the molecular material within a few hundred pc of the Galactic center) can be approximated by a power-law:

$$\frac{dN_{\rm GMC}}{d\ln M_{\rm GMC}} \approx N_u \left(\frac{M_{\rm GMC}}{M_u}\right)^{-\alpha} \quad \text{for} \quad 10^3\,M_\odot \lesssim M_{\rm GMC} < M_u$$

$$M_u \approx 6\times 10^6 M_\odot$$
$$N_u \approx 63$$
$$\alpha \approx 0.6$$

  - Most of the mass is in the most massive GMCs:
    - ~ 80% of the molecular mass is in GMCs with $M > 10^5\,M_\odot$.

- Star Counts
    - Molecular clouds were originally discovered by star counts.
        - Herschel (1785) noticed that there were patches along the Milky Way where very few stars were seen. He incorrectly attributed this to a real absence of stars.
        - We now understand that the apparent deficiency of stars is the result of obscuration by dusty clouds.
        - Star counts using background stars is a good way to study the cloud structure.
        - Because the visual obscuration can be very large, studies of dark clouds using star counts are now usually done in the J, H, or K bands.

Gas Surface Density in the Milky Way

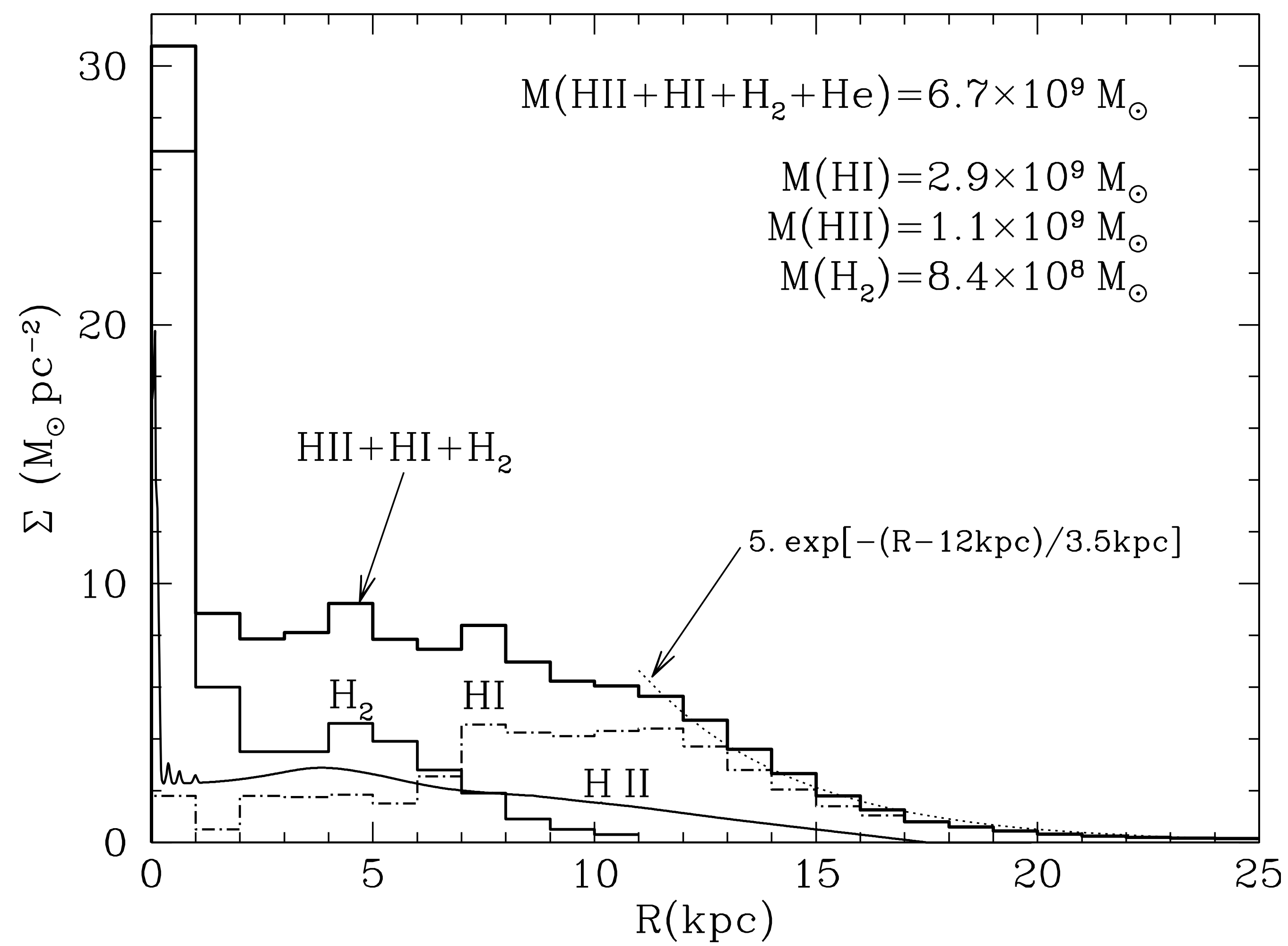
- The most common way to study molecular gas is through molecular line emission, and the primary line used is the J = 1-0 transition (2.6 mm) of CO.
  - This transition is often optically thick, but the CO 1-0 luminosity of a cloud is approximately proportional to the total mass.
  - ***Velocity-resolved mapping of CO 1-0 together with an assumed rotation curve and an adopted value of the "CO to H_2 conversion factor" X_{CO} have been used to infer the surface density of H_2 over the Milky Way disk.***

Gas surface densities as a function of galactocentric radius. The Sun is assumed to be at R = 8.5 kpc.

- Surface density of H_2 estimated from CO 1-0 observations (Nakanishi & Sofue 2006), assuming

$$X_{\rm CO} = 1.8 \times 10^{20}\,{\rm H_2\,cm^{-2}/K\,km\,s^{-1}}$$

- Surface density of H II derived from pulsar dispersion measures (Cordes & Lazio 2003).
- Surface density of H I from 21-cm studies (Nakanishi & Sofue 2003)



[Fig 32.4, Draine]

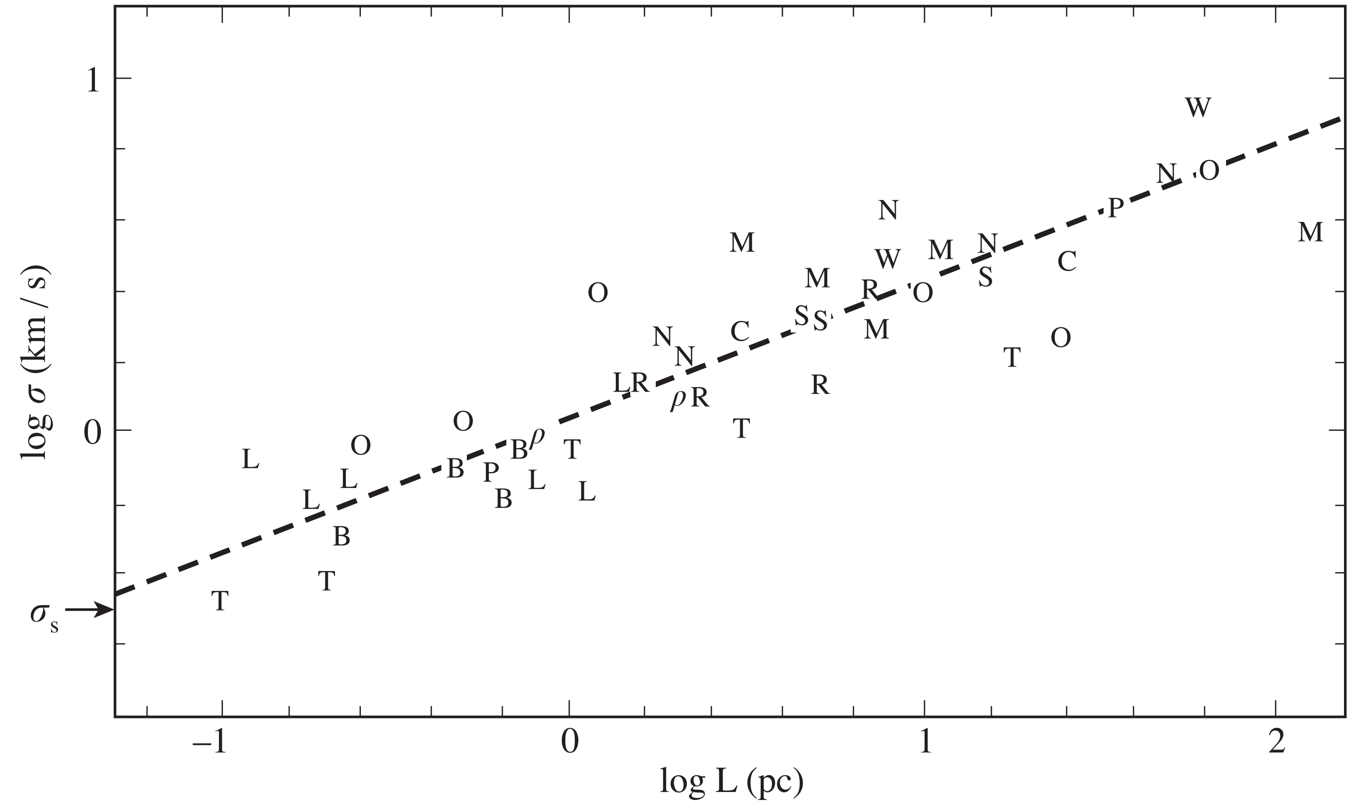
Size-Linewidth Relation in Molecular Clouds

- Larson (1981) noted that observations of molecular clouds in spectral lines of CO, H_2CO, NH_3, OH, and other species, were broadly consistent with a ***size-linewidth relation***, where a density peak of characteristic size *L* tends to have a 3D velocity dispersion given by

$$\sigma_v^* \approx 1.10\, L_{\rm pc}^{\gamma}\,{\rm km\,s^{-1}}, \quad \gamma \approx 0.38 \ \text{ for } 0.01 \lesssim L_{\rm pc} \lesssim 10^2 \quad (L_{\rm pc} = L/{\rm pc})$$

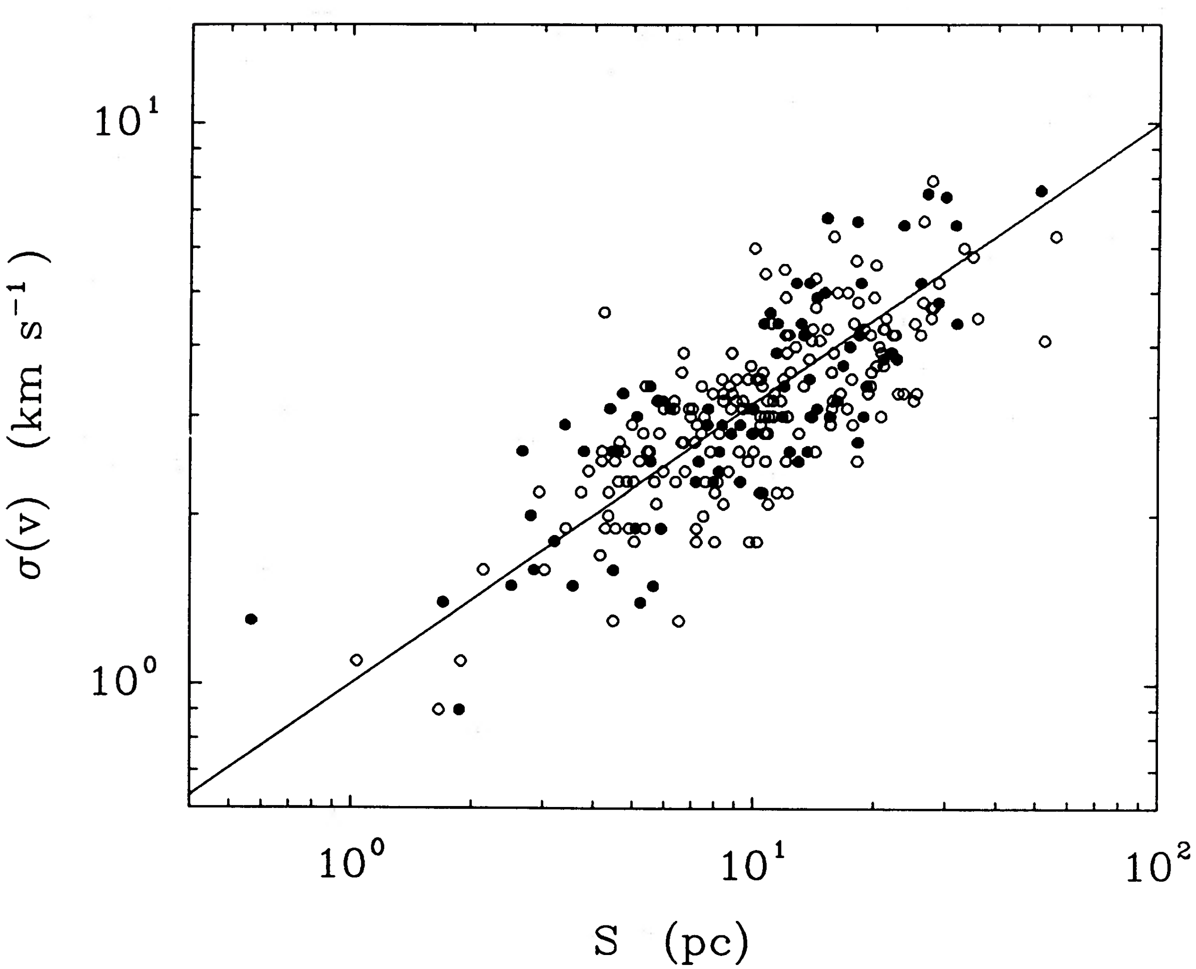
where *L* is the maximum projected dimension of the density peak.

- Larson noted that the power-law index $\gamma \approx 0.38$ is curiously close to the index 1/3 found by **Kolmogorov** for a turbulent cascade in an incompressible fluid.
- It therefore is tempting to refer to the observed fluid motion as “turbulence,” although in realty the motions are some combination of thermal motions, rotation, MHD waves, and turbulence.



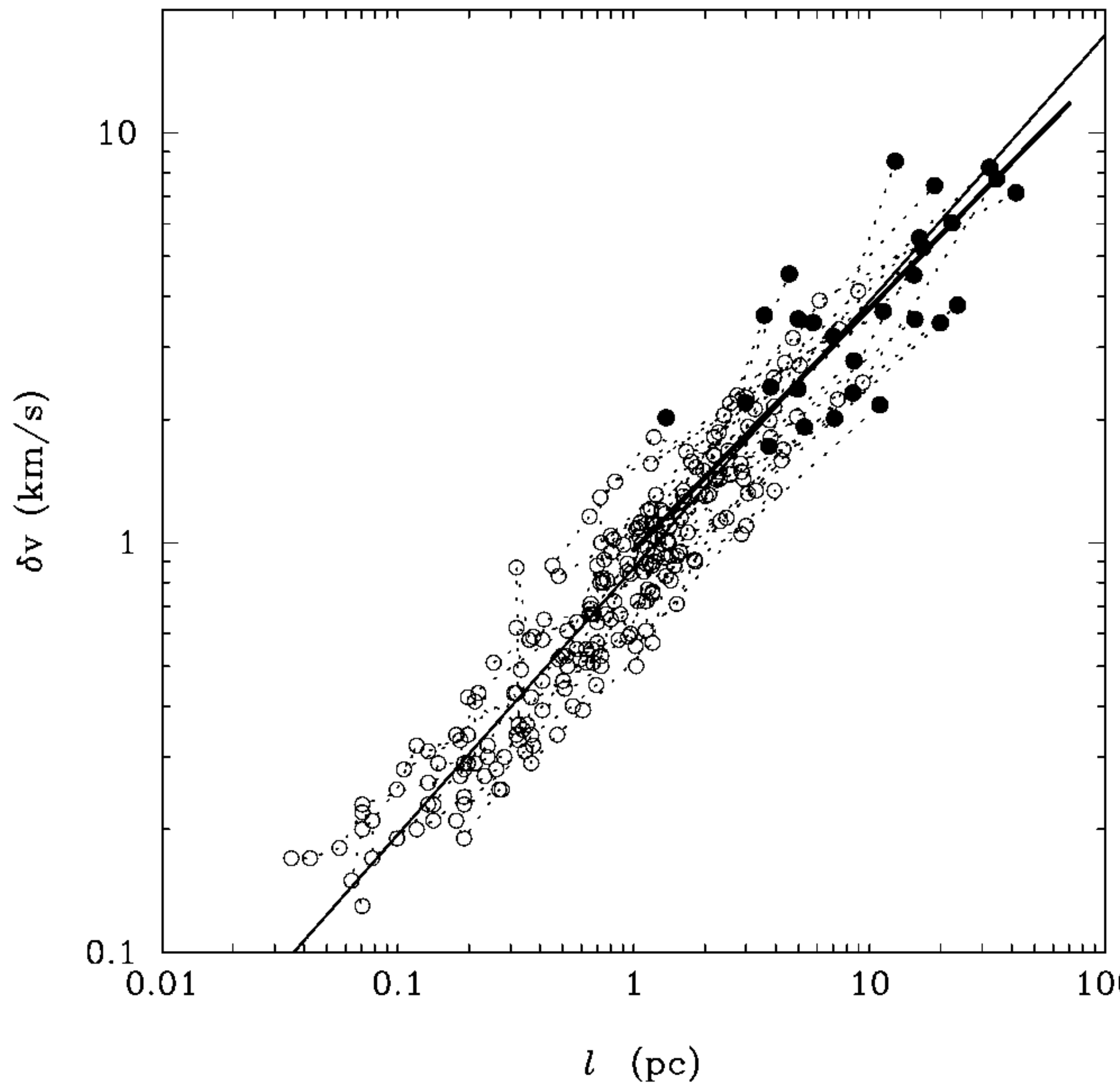
The 3D internal velocity dispersion versus maximum linear dimension *L* of the density peak.

Fig 32.5, Draine; Larson (1981)



Molecular cloud velocity dispersion as a function of size *S* for 273 clouds in the Galaxy

Fig 1, Solomon et al. (1987)



Velocity dispersion versus size ℓ from PCA decomposition of ^{12}CO J = 1-0 imaging observations of 27 individual molecular clouds

Fig 1, Heyer & Brunt (2004)

- However, the power-law index $\gamma \approx 0.38$ has been questioned.
  - Solomon et al. (1987) found $\sigma_v^* \approx 1.0\, L_{\rm pc}^{0.5}\,{\rm km\,s^{-1}}$ from a study of 273 molecular clouds.
  - Heyer & Brunt (2004) found $\sigma_v^* \approx 0.96\, L_{\rm pc}^{0.59}\,{\rm km\,s^{-1}}$.
- Note that
  - For $L \gtrsim 0.02\,{\rm pc}$, $\sigma_v^* \gtrsim (kT/\mu)^{1/2} \approx 0.23(T/15\,{\rm K})^{1/2}\,{\rm km\,s^{-1}}$ $\Rightarrow$ The linewidth is supersonic.
  - For $L \lesssim 0.02\,{\rm pc}$, the line width is nearly thermal, with only a small contribution from rotation, waves or turbulence.
- The density peaks are generally self-gravitating. If we assume them to be in approximate virial equilibrium, and consider only the kinetic energy associated with fluid motions, we can estimate the clump mass using the virial theorem.
  - For a uniform density sphere with a diameter *L*, we can obtain the follows:

$$\sigma_v^{*2} = 3\sigma_v^2 = 6GM/5L \quad (L = 2R)$$

However, this gives $\sigma_v^* \propto L$, which is not consistent with the size-linewidth relation

			for $\gamma \approx 0.38$
clump mass:	$M \approx \dfrac{5\sigma_v^{*2}L}{6G} \approx 230\, L_{\rm pc}^{2\gamma+1}\, M_\odot$	$\rightarrow$	$230\, L_{\rm pc}^{1.76}\, M_\odot$
density:	$n_{\rm H} \approx M/[(4\pi/3)(L/2)^3 1.4 m_{\rm H}] \approx 1.3\times10^4\, L_{\rm pc}^{2\gamma-2}\,{\rm cm^{-3}}$	$\rightarrow$	$1.3\times10^4\, L_{\rm pc}^{-1.24}\,{\rm cm^{-3}}$
column density:	$N_{\rm H} = n_{\rm H}L \approx 4.0\times10^{22}\, L_{\rm pc}^{2\gamma-1}\,{\rm cm^{-2}}$	$\rightarrow$	$4.0\times10^{22}\, L_{\rm pc}^{-0.24}\,{\rm cm^{-2}}$

- We recall that for the dust in diffuse clouds, $A_V / N_{\rm H} = 1.87 \times 10^{21}\,{\rm cm}^2$, and we would have

$$A_V \approx 21\, L_{\rm pc}^{2\gamma - 1}\,{\rm mag} \quad \rightarrow \quad 21\, L_{\rm pc}^{-0.24}\,{\rm mag}$$

The dust in dense clouds differs from that in the diffuse ISM, but this would give a reasonable estimate of the visual extinction through the cloud.

- If $\gamma \approx 0.38$, then **a GMC complex** with diameter $L \approx 50\,{\rm pc}$ would have

$$\boxed{\begin{aligned} M &\approx 2 \times 10^5\, M_\odot \\ n_{\rm H} &\approx 100\,{\rm cm}^{-3} \\ A_V &\approx 8\,{\rm mag} \end{aligned}}$$

whereas **a core** with diameter $L \approx 0.1\,{\rm pc}$ would have

$$\boxed{\begin{aligned} M &\approx 4\, M_\odot \\ n_{\rm H} &\approx 2 \times 10^5\,{\rm cm}^{-3} \\ A_V &\approx 40\,{\rm mag} \end{aligned}}$$

- Comments on the exponent: $N_{\rm H} \approx 4.0 \times 10^{22} L_{\rm pc}^{2\gamma-1}$
  - If $\gamma < 0.5$, smaller clouds tend to have a higher column density, meaning to be darker.
  - If $\gamma = 0.5$, small clouds and large clouds would all have the same column density and dust extinction (A_V).
  - However, **observationally, smaller structures tend to have higher A_V. This is consistent with exponent $\gamma < 0.5$.**
  - Therefore, ***the Larson's exponent would be better constrained with the observations***.

- Expressing the above relations with density as the independent variables, we obtain

$$L_{\rm pc} = (n_3/13)^{1/(2\gamma-2)} \rightarrow 7.94\, n_3^{-0.81} \quad ,$$

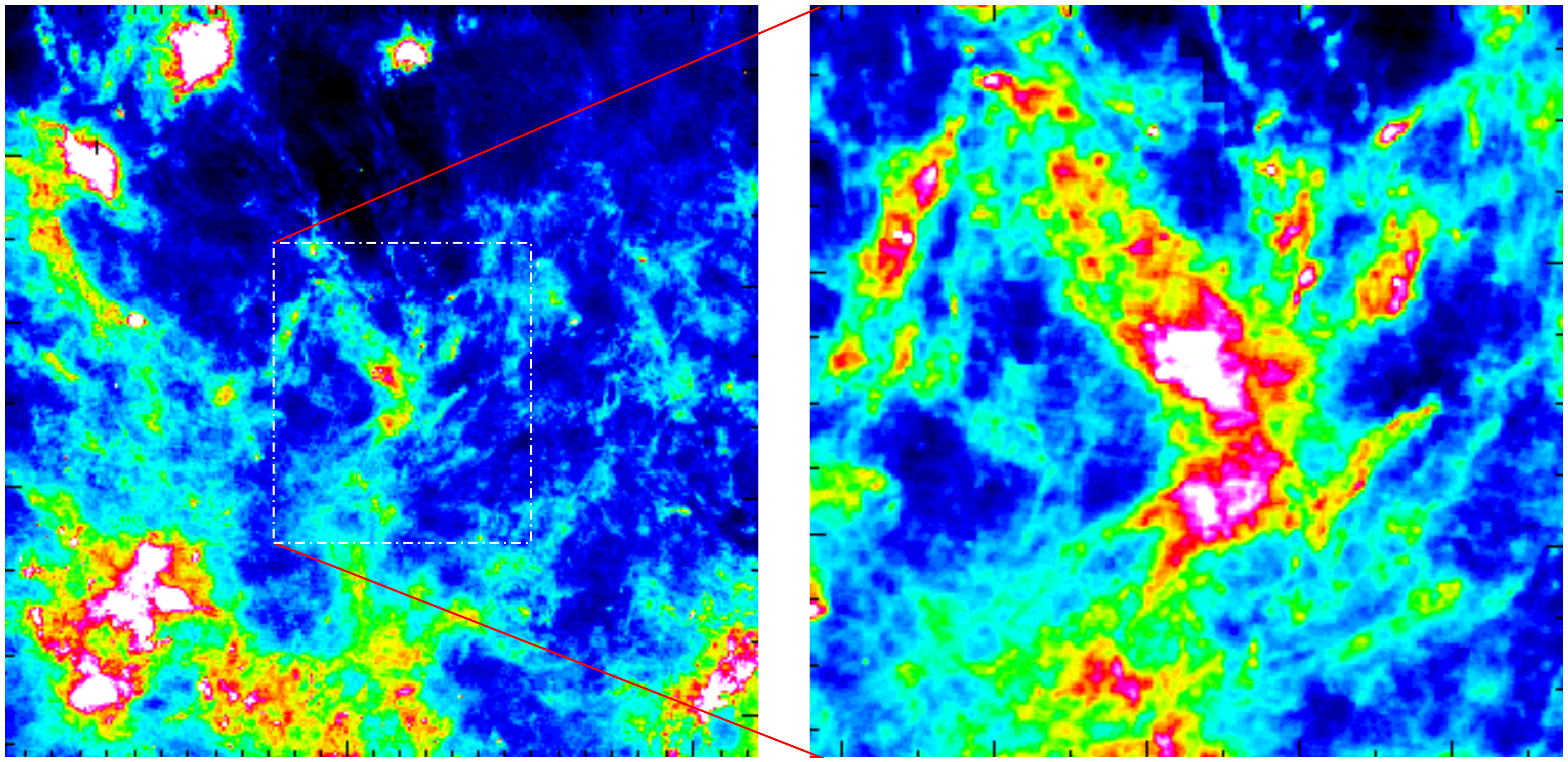
$$\sigma_v = 1.1(n_3/13)^{\gamma/(2\gamma-2)}\,{\rm km\,s^{-1}} \rightarrow 2.43\, n_3^{-0.31}\,{\rm km\,s^{-1}} \quad ,$$

$$M = 230(n_3/13)^{(2\gamma+1)/(2\gamma-2)}\,M_\odot \rightarrow 8940\, n_3^{-1.42}\,M_\odot \quad ,$$

$$A_V = 21(n_3/13)^{(2\gamma-1)/(2\gamma-2)}\,{\rm mag} \rightarrow 13\, n_3^{0.19}\,{\rm mag} \quad ,$$

The Fractal Structure of the Molecular Clouds

- Self-similarity of Clouds
  - The molecular interstellar medium is very clumpy and fragmented. Its hierarchical structure can well be described by a fractal, because of its self-similarity.
  - It has no characteristic scale. Fractals by definition are self-similar ensembles, that have a non-integer, i.e., fractional dimension.
  - ***The self-similar structures in the ISM extends over 6 orders of magnitude in scale, from about 10^{-4} to 100 pc.***
    - These are not observed for the same molecular cloud only because of technical problems, lack of spatial resolution on one side, and difficulty of mapping too large areas on the other.
    - The scaling relations all over the scales are however obtained by comparing various clouds observed with different resolutions.



IRAS 100 μm map of molecular clouds towards the Taurus complex, located at about 100 pc from the Sun.
The square is ~ 4000 pc^2.

Fig 14, Chap 2, Blain, Combes, Draine [The Cold Universe]

Excitation Temperature

- The excitation temperature for a given transition is defined as:

$$\frac{n_u}{n_\ell} = \frac{g_u}{g_\ell} e^{-h\nu_{ul}/kT_{\rm exc}}$$

  - For pure rotational transitions, the excitation temperature is often called the rotation temperature.
  - For vibrational transitions, it is called the vibrational temperature.
  - This nomenclature is analogous to the “spin temperature” defined for the H I 21-cm hyperfine transition.

[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_2, 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).***
- Fundamental frequencies
  - Vibrational frequency
    - The fundamental vibrational frequency corresponds to to a wavelength:

      $\lambda_0 = c/\nu_0 \approx 4.6\mu\mathrm{m}$ This energy is ~50% of the energy in the H_2 fundamental frequency.
  - Rotational frequency:
    - CO J=1-0, 2.60mm emission is the most important line used in studies of molecular gas.

      $$\lambda = 2.60\,\mathrm{mm} \rightarrow \nu = 115.3\,\mathrm{GHz} \rightarrow h\nu = 4.767\times10^{-4}\,\mathrm{eV} \rightarrow h\nu/k = 5.532\,\mathrm{K}$$
    - This energy level is therefore perfectly fitted to probe the cold molecular clouds.
    - The widely used CO lines (J = 1-0 at 2.6mm, J = 2-1 at 1.3 mm) are generally optically thick, for "standard" clouds of solar metallicity. This complicates the interpretation in terms of H_2 column densities and mass of the clouds.
- The line width b that we measure for molecular line emission is often much broader than the thermal value $b \sim 0.1(T_{\rm gas}/20\,\mathrm{K})^{1/2}\,\mathrm{km\,s^{-1}}$ that we expect. *The large broadening is similar for molecules of different molecular mass*, suggesting that ***the broadening is due to turbulent motions within the cloud.***

- ***Optical Depth & Velocity Structures***
  - Each individual molecular cloud is optically thick.
  - However, a giant molecular cloud is composed of many sub-structures, and there are many clouds along a line of sight. The "macroscopic" optical depth is in general not very large, due to velocity gradients: clouds do not hide each other at a given velocity, and therefore it is possible to "count" the clouds.
- ***Isotopic Species***
  - Since the CO lines are optically thick (on average $\tau_{\rm CO} \sim 10$), it might be interesting to observe the much less abundant isotope ^{13}CO.
  - At the solar neighborhood, the ^{12}CO/^{13}CO abundance ratio is ~90, and in individual molecular clouds, it is frequent that the ^{13}CO lines are optically thin.
    - However, when maps of the two isotopes are compared at millimeter wavelengths for well studied clouds, it appears that the ^{13}CO does not probe the entire extent of the clouds, but only the densest regions. This could be due to differences in excitation, self-shielding, or selective photo-dissociation.
  - The observed average ratio between integrated ^{12}CO and ^{13}CO intensities is of the order of 10.

Virial Theorem

- For a collection of N point particles, the total moment of inertia is given by

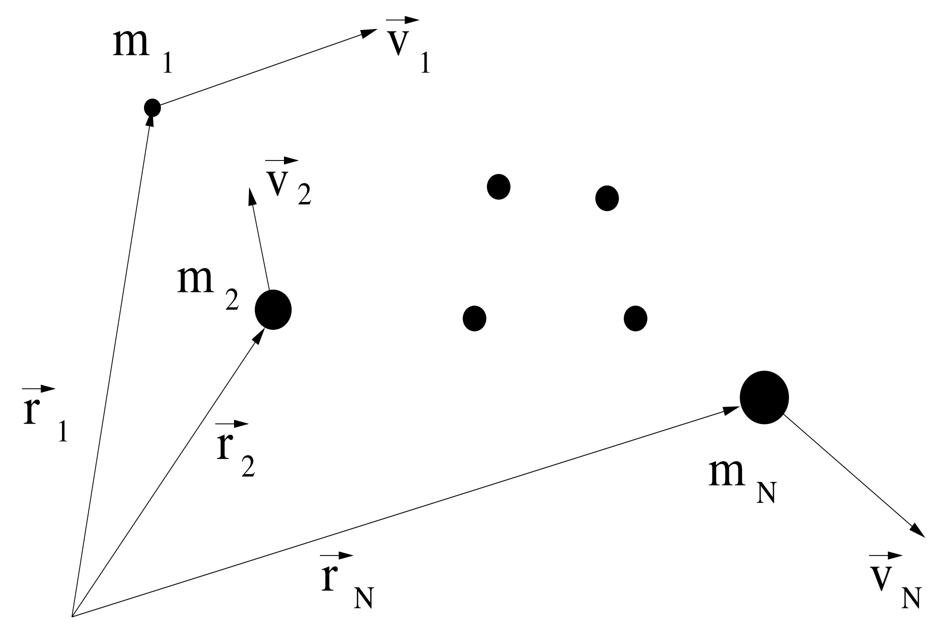
$$I = \sum_i m_i |\mathbf{r}_i|^2 = \sum_i m_i \mathbf{r}_i \cdot \mathbf{r}_i$$

- The time derivative of the moment of inertia is called the ***virial***:

$$Q = \frac{1}{2}\frac{dI}{dt} = \sum_i \mathbf{p}_i \cdot \mathbf{r}_i$$

Here, momentum vector:

$$\mathbf{p}_i = m_i \mathbf{v}_i \quad \left(= m_i \frac{d\mathbf{r}_i}{dt} \right)$$



Now take the time derivative of the viral

$$\frac{dQ}{dt} = \sum \mathbf{p}_i \cdot \mathbf{v}_i + \sum_i \frac{d\mathbf{p}_i}{dt} \cdot \mathbf{r}_i$$

$$= \sum_i m_i \mathbf{v}_i \cdot \mathbf{v}_i + \sum_i \mathbf{F}_i \cdot \mathbf{r}_i$$

Newton's second law:

$$\mathbf{F}_i = \frac{d\mathbf{p}_i}{dt} \quad \text{(the sum of all forces acting on particle } i\text{)}$$

The first term can be expressed in terms of the total kinetic energy of the system

$$\frac{dQ}{dt} = 2K + \sum_i \mathbf{F}_i \cdot \mathbf{r}_i \quad \left(\text{where } K = \sum_i \frac{1}{2} m_i |\mathbf{v}_i|^2 \right)$$

- The total force on particle i is the sum of all the forces from the other particles j in the system:

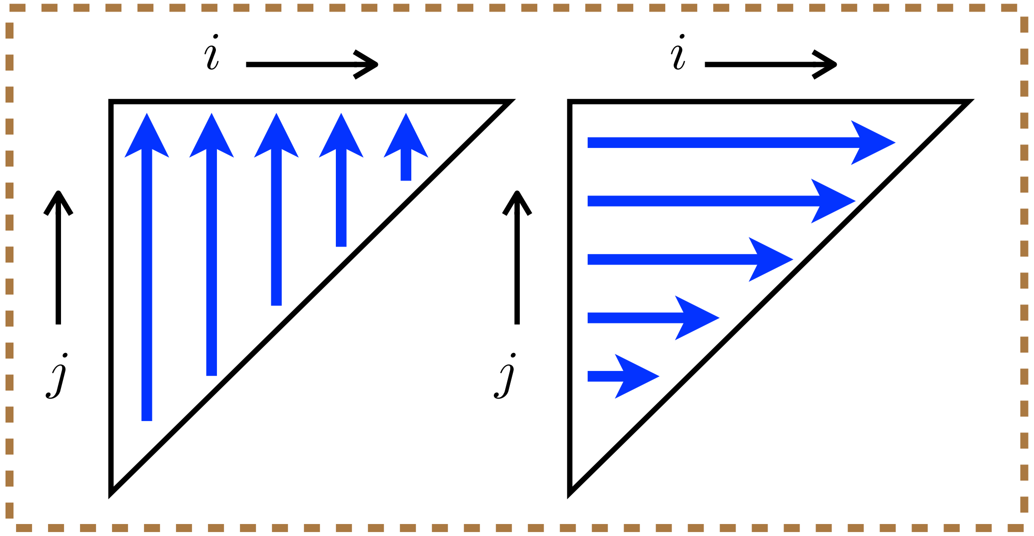
$$\mathbf{F}_i = \sum_{j \neq i} \mathbf{f}_{j \to i}$$

Here, $\mathbf{f}_{j \to i}$ is the force on particle i from particle j

Then,

$$\sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{r}_i = \sum_{i=1}^{N} \sum_{j \neq i} \mathbf{f}_{j \to i} \cdot \mathbf{r}_i$$

$$= \sum_{i=1}^{N} \sum_{j<i} \mathbf{f}_{j \to i} \cdot \mathbf{r}_i + \sum_{i=1}^{N} \sum_{j>i} \mathbf{f}_{j \to i} \cdot \mathbf{r}_i$$



The last term can be rewritten as follows:

$$\sum_{i=1}^{N} \sum_{j>i} \mathbf{f}_{j \to i} \cdot \mathbf{r}_i = \sum_{j=1}^{N} \sum_{i<j} \mathbf{f}_{j \to i} \cdot \mathbf{r}_i$$ interchange the ordering of the sums.

$$= \sum_{i=1}^{N} \sum_{j<i} \mathbf{f}_{i \to j} \cdot \mathbf{r}_j$$ interchange the name of the indices i and j.

$$= -\sum_{i=1}^{N} \sum_{j<i} \mathbf{f}_{j \to i} \cdot \mathbf{r}_j$$ Newton's third law: $\mathbf{f}_{i \to j} = -\mathbf{f}_{j \to i}$

Hence,

$$\sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{r}_i = \sum_{i=1}^{N} \sum_{j<i} \mathbf{f}_{j \to i} \cdot (\mathbf{r}_i - \mathbf{r}_j)$$

- Now, consider the gravitational force:

$$\mathbf{f}_{j\to i} = \frac{Gm_i m_j}{r_{ij}^3}(\mathbf{r}_j - \mathbf{r}_i) \longrightarrow \sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{r}_i = -\sum_{i=1}^{N}\sum_{j<i} \frac{Gm_i m_j}{r_{ij}}$$

where $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$

Note that the gravitational potential energy between particle i and j is given by $U_{ij} = -\frac{Gm_i m_j}{r_{ij}}$.

$$\sum_{i=1}^{N} \mathbf{F}_i \cdot \mathbf{r}_i = \sum_{i=1}^{N}\sum_{j<i} U_{ij} = U$$

=> total potential energy of the system

The total potential energy of the system is the sum of the potential energy between all possible pairs of particles (note that one pair of particle should be counted only once, this is why there is a $j < i$ in the second sum).

- We finally obtain the following. Now we take the mean value of the derivative of the virial over a long period of time:

$$\frac{dQ}{dt} = 2K + U \longrightarrow \left\langle \frac{dQ}{dt} \right\rangle = 2\langle K \rangle + \langle U \rangle$$

- If ***the system is bounded and the particles have finite momentum***, the average value will go to zero and we obtain the virial theorem:

$$\left\langle \frac{dQ}{dt} \right\rangle = \lim_{T\to\infty} \frac{Q(T) - Q(0)}{T} = 0 \longrightarrow \boxed{2\langle K \rangle + \langle U \rangle = 0}$$

$\langle\rangle$ denotes both the ensemble average and time average.

Ergodic hypothesis: Averaging system variables over a long time period is equal to averaging them over the ensemble.

$$\lim_{T\to\infty} \frac{1}{T}\int_0^T dt \to \lim_{N\to} \frac{1}{N}\sum_{i=1}^{N}$$

If a bound system has a huge number of particles, it is equivalent to seeing the system over a long period of time.

Virial Mass Estimate

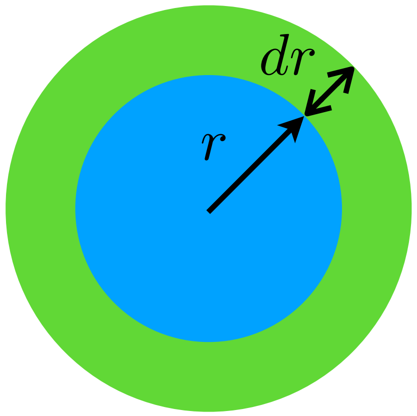
- A fundamental property is that GMCs are gravitationally bound and in viral equilibrium.
  - Their masses can then be estimated using line widths as a measure of the could velocities, following the arguments of Solomon et al.
  - The virial theorem provides a general equation that relates the average over time of the total kinetic energy of a stable, self-gravitating system of discrete particles, with the total potential energy of the system.

$$2\langle K\rangle + \langle U\rangle = 0$$

  - For a uniform density sphere with a mass M and radius R, the gravitational potential energy is

$$U = -\frac{3}{5}\frac{GM^2}{R}$$

$$\begin{aligned} U &= -\int_0^R \frac{GM_r dM_r}{r} \\ &= -\int_0^R \frac{G}{r}\left(\frac{4\pi}{3}r^3\rho\right)4\pi r^2 \rho dr \\ &= -\frac{(4\pi)^2}{3\times 5}G\rho^2 R^5 = -\frac{3}{5}\frac{GM^2}{R} \end{aligned}$$



Density $\rho = \frac{M}{(4\pi/3)R^3}$

Mass within a radius r

$$M_r = \int_0^r \rho(4\pi r'^2 dr') = \frac{4\pi}{3}r^3\rho$$

Mass between a shell $(r, r+dr)$

$$dM_r = \rho(4\pi r^2 dr)$$

- If the cloud is in equilibrium, with self-gravity being balanced by turbulent pressure, the virial theorem states that the turbulent velocity, in one dimension, to be

$$\langle K \rangle = \sum_i \frac{3}{2} m_i \langle v_i^2 \rangle = \frac{3}{2} \sum_i m_i \sigma_v^2 = \frac{3}{2} M \sigma_v^2$$

Here, σ_v is the rms velocity dispersion.

$$2\langle K \rangle + \langle U \rangle = 0 \quad \rightarrow \quad \sigma_v^2 = \frac{1}{5}\frac{GM}{R}$$

- Therefore, we obtain the total mass of the self-gravitation cloud in terms of the line width (broadening parameter):

virial mass:

$$M = \frac{5b^2 R}{2G} \approx 600\, M_\odot \left(\frac{b}{1\,\mathrm{km\,s^{-1}}} \right)^2 \left(\frac{R}{1\,\mathrm{pc}} \right)$$

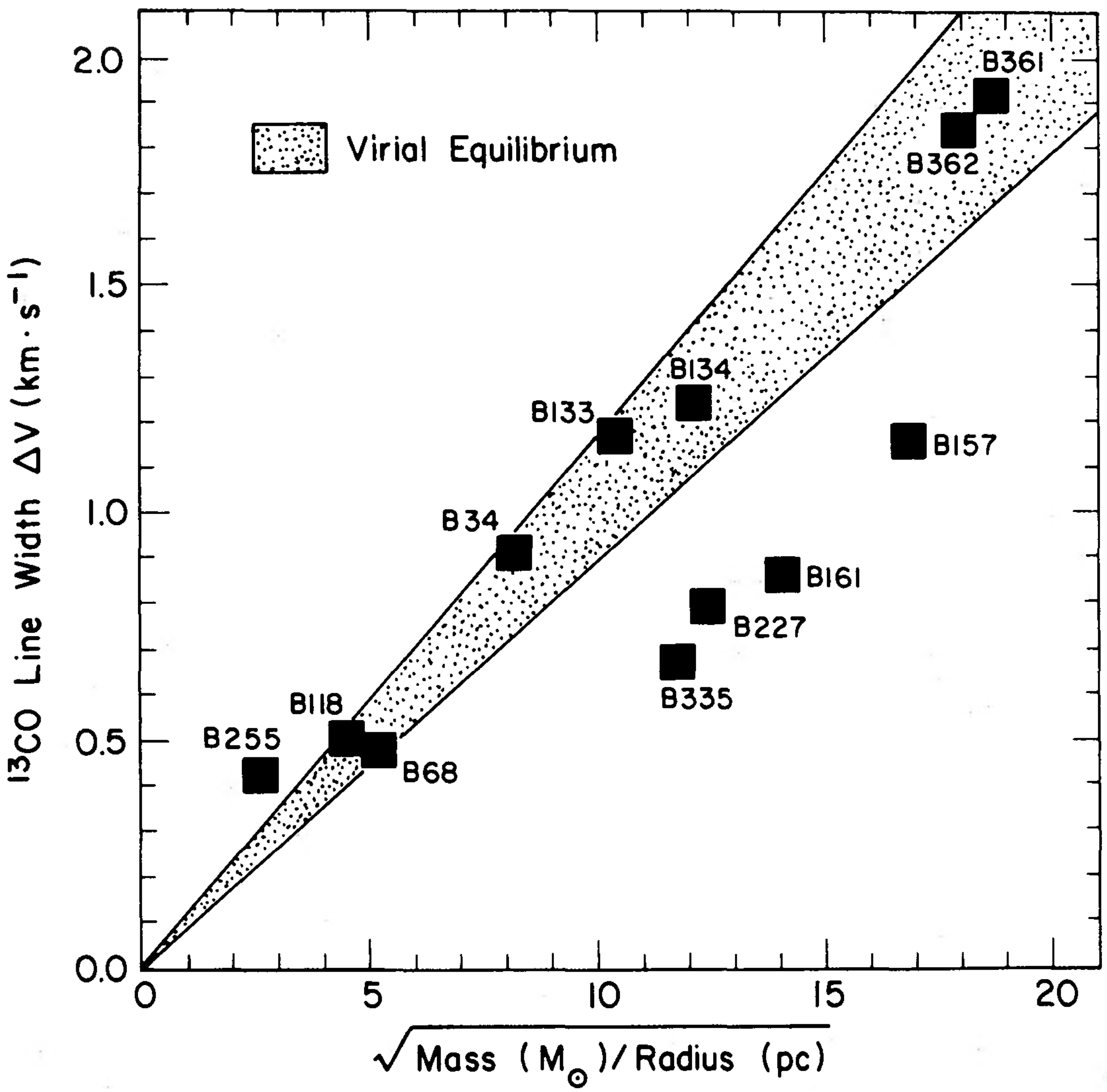
Here, $b = \sqrt{2}\sigma_v$

- Note that the virial theorem for a uniform density clouds indicates that the following size-linewidth correlation if the density is constant. But, it appears that the density is not a constant, but controlled by turbulence.

$$b^2 = \frac{2}{5}\frac{GM}{R} = \frac{8\pi}{15} G\rho R^2 \quad \rightarrow \quad b = \left(\frac{8\pi}{15} G\rho \right)^{1/2} R$$

- The ***line width - (mass/radius) correlation***:

$$b = \left(\frac{2G}{5}\right)^{1/2} \left(\frac{M}{R}\right)^{1/2}$$



The ^{13}CO line width versus (mass/radius)$^{1/2}$ for globules with $T < 10$K.

Fig 3, Leung et al. (1982, ApJ, 262, 583)

- The ***Mass - CO luminosity correlation***
  - Let $I_{\rm CO}$ the CO brightness temperature integrated over the line profile:

$$I_{\rm CO} \equiv \int T_{\rm CO} dv \approx T_{\rm CO} b \quad (b \approx \Delta v)$$

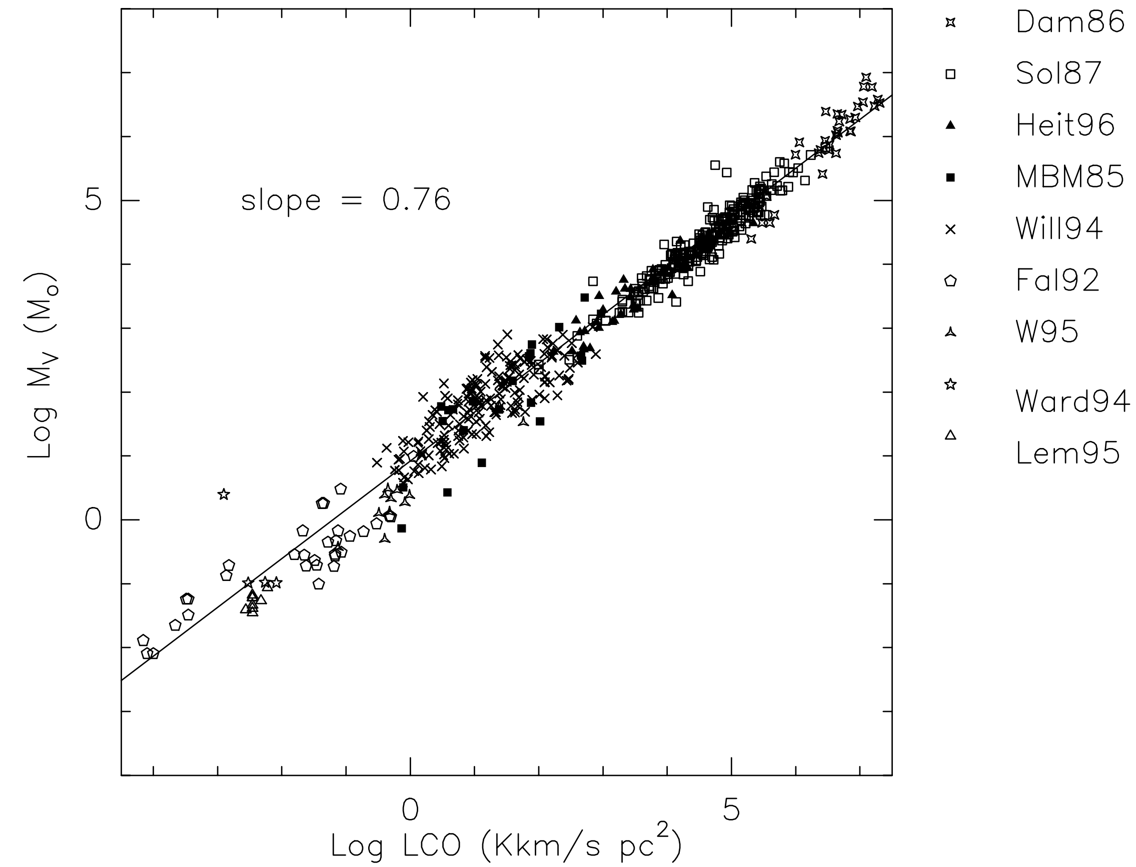
  - The CO luminosity of a cloud is:

$$L_{\rm CO} \equiv D^2 \int I_{\rm CO} d\Omega \approx \pi R^2 T_{\rm CO} b$$
$$= \sqrt{\frac{2\pi^2}{5} G M R^3} = \sqrt{\frac{6\pi}{20} G} \frac{T_{\rm CO}}{\sqrt{\rho}} M$$

Here, *D* = distance, and virial condition: $b \approx \sqrt{\frac{2}{5}\frac{GM}{R}}$

  - To the extend that the ratio $\sqrt{\rho}/T_{\rm CO}$ does not vary in the mean from cloud to cloud, this indicates that the total CO luminosity is directly proportional to the total mass of molecular clouds. However, in reality, the power-law slope is ~ 0.76.
  - ***This correlation supports the fundamental assumption that GMCs are in virial equilibrium.***

$$L_{\rm CO} \approx M \left(\frac{6\pi}{20} G\right)^{1/2} \frac{T_{\rm CO}}{\sqrt{\rho}}$$



Virial mass versus CO luminosity relation taken from various sources:

Fig 4, Chap 2, Blain, Combes, & Draine [The cold Universe]

Optical Thickness of CO (J = 1-0)

- The net absorption coefficient, taking into account both absorption and stimulated emission is:

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

- The optical depth of the thermally broadened CO line can be written as

$$\phi_\nu = \frac{1}{\sqrt{\pi}}\frac{\lambda}{b} e^{-\frac{v^2}{b^2}}$$

$$\tau_\nu = \int \kappa_\nu ds = \tau_0 e^{-v^2/b^2}$$

optical depth at line center =

$$\tau_0 = \frac{g_1}{g_0}\frac{c^2}{8\pi^{3/2}\nu_{10}^3} A_{10}\frac{c}{b}\left(1 - e^{-h\nu_{10}/kT_{\rm exc}}\right) N_0$$

$$A_{10} = 7.16 \times 10^{-8}\,{\rm s}^{-1}$$

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

Here, $N_{\rm H}$ is the column density of H nucleon in the J = 0 rotational level. Recall that the cosmic abundance of carbon is $n_{\rm C}/n_{\rm H} = 2.95\times 10^{-4}$ and a fraction $f_{\rm CO} \approx 0.25$ of the carbon is in CO molecules.

- The above equation seems to indicate that the CO J=1-0 line is optically thick. However, we need to estimate the fraction of the CO that is in the J = 0 level.

- The fraction of CO in a given rotational level J will be:

$$\frac{n(\mathrm{CO},J)}{n(\mathrm{CO})} = \frac{(2J+1)e^{-B_0 J(J+1)/kT_{\rm exc}}}{\sum_J (2J+1)e^{-B_0 J(J+1)/kT_{\rm exc}}}$$

$$E_J = B_0 J(J+1)$$

Here, B_0 is the "rotation constant."

- We can approximate the partition function in the denominator by

$$Z = \sum_{J=0}^{\infty}(2J+1)e^{-B_0 J(J+1)/kT_{\rm exc}} \approx \left[1+(kT_{\rm exc}/B_0)^2\right]^{1/2}$$

This approximation is exact in the limits $kT_{\rm exc}/B_0 \to 0$ and $kT_{\rm exc}/B_0 \gg 1$, and accurate to within 6% for all $T_{\rm exc}$.

$$\tau_0 = 297\left(\frac{N_{\rm H}}{10^{21}\,{\rm cm}^{-2}}\right)\left[\frac{n(\mathrm{CO})/n_{\rm H}}{7\times10^{-5}}\right]\frac{\left(1-e^{-5.532\,{\rm K}/T_{\rm exc}}\right)}{\left[1+(T_{\rm exc}/2.77\,{\rm K})^2\right]^{1/2}}\left(\frac{2\,{\rm km\,s^{-1}}}{b}\right)$$

Here, we used $B_0/k = 2.77\,\mathrm{K}$ for $^{12}C^{16}O$.

$$\tau_0 \approx 50\left(\frac{N_{\rm H}}{10^{21}\,{\rm cm}^{-2}}\right)\left[\frac{n(\mathrm{CO})/n_{\rm H}}{7\times10^{-5}}\right]\left(\frac{2\,{\rm km\,s^{-1}}}{b}\right)$$

for a typical CO rotation temperature $T_{\rm exc} \approx 8\,\mathrm{K}$.

- Thus, **the CO 1-0 transition is expected to be often quite optically thick.**

Radiative Trapping

- ***Radiative Trapping***:
  - In many situation of astrophysical interest, there is sufficient gas present so that, for some species X, a photon emitted in a transition $X_u \to X_\ell$ will have a high probability of being absorbed by another X_ℓ somewhere nearby, and, therefore, a low probability of escaping from the emitting region.
  - This phenomenon — referred to as radiative trapping — have two effects.

    (1) it reduces the emission in the $X_u \to X_\ell$ photons emerging from the region, and

    (2) it acts to increase the level of excitation of species X (relative to what it would be were the emitted photons to escape freely).
  - An exact treatment of the effects of radiative trapping is a complex problem of coupled radiative transfer and excitation — *it is nonlocal*, because photons emitted from one point in the cloud affect the level populations at other points.
  - The ***escape probability approximation*** is a simple way to take into account the effects of radiative trapping.

- ***Escape Probability Approximation***
  - Suppose that a some point $\mathbf{r}$ in the cloud, the optical depth $\tau_\nu(\hat{\mathbf{n}}, \mathbf{r})$ in direction $\hat{\mathbf{n}}$ and at frequency ν is know.
  - We define the direction-averaged "escape probability" for photons with frequency ν emitted from location $\mathbf{r}$:

$$\boxed{\bar{\beta}_\nu(\mathbf{r}) \equiv \int \frac{d\Omega}{4\pi} e^{-\tau_\nu(\hat{\mathbf{n}},\mathbf{r})}}$$

  Now define the direction-averaged and frequency-averaged escape probability:

$$\boxed{\langle\beta(\mathbf{r})\rangle = \int \phi_\nu \bar{\beta}_\nu(\mathbf{r}) d\nu} \qquad \text{Normalized line profile} = \int \phi_\nu d\nu = 1$$

  - Now we make two approximations:

  (1) we will approximate **the excitation in the cloud as uniform**.

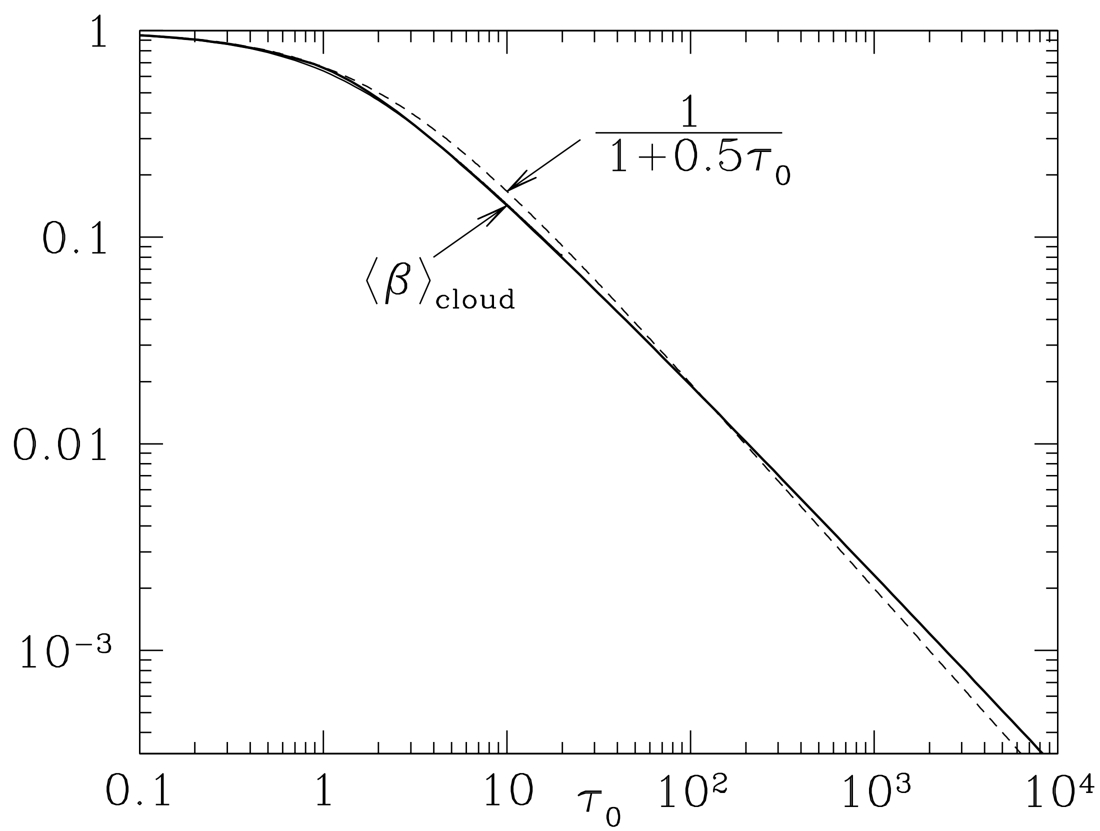
  (2) we make the **"on-the-spot"** approximation: we assume that if a radiated photon is going to be absorbed, it will be absorbed so close to the point of emission that we can approximate it as being absorbed at the point of emission.

    - These approximations replace a difficult nonlocal excitation problem with a much simpler local one! This is called the escape probability approximation.

- Homogeneous Static Spherical Cloud.
  - The angle-averaged escape probability $\bar{\beta}$ depends on the geometry and velocity structure of the region.

    For the case of a finite cloud, $\bar{\beta}$ will depend on position — it will be highest at the cloud boundary, and smallest at the cloud center.
  - We now define the escape probability averaged over the line profile and over the cloud volume. for a uniform density spherical cloud,

$$\boxed{\langle\beta\rangle_{\rm cloud} = \frac{1}{4\pi R^3/3}\int_0^R \langle\beta(\mathbf{r})\rangle\, 4\pi r^2 dr}$$



The left figure shows the mass-averaged escape probability calculated numerically for the case of a homogeneous spherical cloud, as a function of the optical depth τ_0 at line-center from the center of the cloud to the surface. The gas is assumed to have a Gaussian velocity distribution. [Fig 19.1, Draine]

A satisfactory approximation is provided by the simple fitting function.

$$\langle\beta\rangle_{\rm cloud} = \frac{1}{1+0.5\tau_0}$$

Critical Density of CO (J = 1-0)

- Conditions that are favorable for formation of CO are usually favorable for the formation of H_2.
  - Therefore, the main colliders that excite and de-excite the rotational states of CO are hydrogen molecules rather than hydrogen atoms of free electrons.
  - The collisional de-excitation rate coefficient of CO (J = 1) for collisions with H_2 collisions is

$$\boxed{k_{10} \approx 6 \times 10^{-11}\,(T/100\,\mathrm{K})^{0.2}\,\mathrm{cm^3\,s^{-1}}}$$

- The Einstein A coefficient for a rotational transition J → J-1 is given by

$$\boxed{A_{J\to J-1} = \frac{128\pi^3}{3\hbar}\left(\frac{B_0}{hc}\right)^3 \mu_0^2 \frac{J^4}{J+1/2} = 7.16 \times 10^{-8}\,\mathrm{s^{-1}} \ \text{ for } J = 1 \to 0}$$

- At the fundamental frequency, the dominant background radiation is the CMB.
  - The good news is that the 2.6 mm line of CO is radiatively excited by blackbody radiation, which is analytically tractable.
  - The bad news is that we can't use the Rayleigh-Jeans limit, as we did studying the 21 cm line.
  - The photon occupation number is: $$\bar{n}_\gamma = \frac{1}{e^{5.532\,\mathrm{K}/2.725\,\mathrm{K}} - 1} = 0.151 \qquad (T_{\mathrm{rad}} = T_{\mathrm{CMB}} = 2.725\,\mathrm{K})$$

- The critical density at which collisional de-excitation equals to radiative de-excitation is given by

$$\boxed{n_{\mathrm{crit,H_2}}(\mathrm{CO}, J=1) = \frac{(1+\bar{n}_\gamma)A_{10}}{k_{10}} \approx 1400(T/100\,\mathrm{K})^{-0.2}\,\mathrm{cm^{-3}}}$$

- Radiative trapping
  - The proceeding analysis has assumed that only photons from the external radiation field are used, ignoring contributions from emission line photons from the cloud material itself. This assumption is only strictly true in an optically thin cloud.
  - For lines in abundant molecular species, like the CO J = 1-0 line, the cloud will be optically thick, and we will have to include the effect of the radiative trapping.
  - Taking into account the radiative trapping, the actual Einstein A coefficient is replaced by an "effective" value $\langle\beta_{u\ell}\rangle_{\rm cloud} A_{u\ell}$ (see Chap 19.1 of Draine).
  - The critical density for the CO J = 1-0 line is:

$$\boxed{n_{\rm crit,H_2}({\rm CO}, J=1) = \frac{(1+\bar{n}_\gamma)\,\langle\beta_{10}\rangle_{\rm cloud}\,A_{10}}{k_{10}} \approx 54(T/100\,{\rm K})^{-0.2}\,{\rm cm}^{-3}}$$

$$\tau_0 \approx 50, \quad \langle\beta_{10}\rangle_{\rm cloud} \approx 1/(1+0.5\tau_0) \approx 0.04$$

for $N_{\rm H} = 10^{21}\,{\rm cm}^{-2}, b = 2\,{\rm km\,s}^{-1}, T_{\rm exc} = 8\,{\rm K}$

  - We, therefore, see that at least the J = 1 level of CO is expected to be thermalized in the central dense cores of molecular clouds with $n_{\rm H} \gtrsim 10^2\,{\rm cm}^{-3}$.

Excitation Temperature of CO (J = 1-0)

- No approximation is valid for CO.
  - We can't use the handy $kT_{\rm exc} \ll h\nu_{u\ell}$ approximation that was useful for Lyα line.
  - Neither can we use the $kT_{\rm exc} \gg h\nu_{u\ell}$ approximation that was used for 21-cm line.
- The radiative transfer equation is the usual

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

  - Emissivity and absorption coefficient are

$$j_\nu = n_1 \frac{A_{10}}{4\pi} h\nu_{10}\phi_\nu \qquad \kappa_\nu = n_0 \frac{g_1}{g_0} \frac{c^2}{8\pi\nu_{10}^2} A_{10}\phi_\nu \left(1 - \frac{g_0}{g_1}\frac{n_1}{n_0}\right), \quad \frac{n_1}{n_0} = \frac{g_1}{g_0} \exp\left(-\frac{k\nu_{10}}{kT_{\rm exc}}\right)$$

  - The source function can be written as

$$S_\nu \equiv \frac{j_\nu}{\kappa_\nu} = \frac{2h\nu_{10}^3}{c^2} \frac{1}{\exp\left(h\nu_{10}/kT_{\rm exc}\right) - 1} = B_\nu(T_{\rm exc})$$

  - If the excitation (rotation) temperature is constant over the entire region of emission, we have the solution:

$$I_\nu = I_\nu(0) e^{-\tau_\nu} + S_\nu\left(1 - e^{-\tau_\nu}\right)$$

  - The background radiation is the Cosmic Microwave Background: $I_\nu(0) = B_\nu(T_{\rm rad})$

- Now, we do perform the "on" observation toward a molecular cloud, and "off" observation over to a black sky.

$$I_\nu(\text{on}) = \frac{2h\nu^3}{c^2}\left[\frac{e^{-\tau_\nu}}{\exp\left(h\nu/kT_{\text{rad}}\right)-1} + \frac{1-e^{-\tau_\nu}}{\exp\left(h\nu/kT_{\text{exc}}\right)-1}\right]$$
$$I_\nu(\text{off}) = \frac{2h\nu^3}{c^2}\frac{1}{\exp\left(h\nu/kT_{\text{rad}}\right)-1}$$

The difference between the two observations is

$$\begin{aligned}\Delta I_\nu &= I_\nu(\text{on}) - I_\nu(\text{off}) \\ &= \frac{2h\nu^3}{c^2}\left[\frac{1}{\exp\left(h\nu/kT_{\text{exc}}\right)-1} - \frac{1}{\exp\left(h\nu/kT_{\text{rad}}\right)-1}\right]\left(1-e^{-\tau_\nu}\right)\end{aligned}$$

- It is customary to express the intensity in terms of an antenna temperature:

$$T_{\text{A}} \equiv \frac{c^2}{2k}\frac{\Delta I_\nu}{\nu^2} \approx \frac{h\nu}{k}\left[\frac{1}{\exp\left(h\nu/kT_{\text{exc}}\right)-1} - \frac{1}{\exp\left(h\nu/kT_{\text{rad}}\right)-1}\right]$$ for an optical thick cloud $\tau_\nu \gg 1$.

We can solve this for excitation temperature:

$$\frac{5.532\,\text{K}}{T_{\text{exc}}} \approx \ln\left(1+\frac{1}{T_{\text{A}}/5.532\,\text{K}+0.151}\right)$$

$$h\nu/k = 5.532\,\text{K}$$

- In our Galaxy, it is often found that $T_{\text{A}} \sim 5\,\text{K}$ at the line center, implying $T_{\text{exc}} \sim 8\,\text{K}$.

^{13}CO Column Density

- The ^{12}CO 2.6 mm line is optically thick. All the 2.6 mm emission that we see comes from a thin skin at the surface of the molecular cloud.
  - The column density of CO can be more easily derived from the optically thin ^{13}CO line. The rarer isotopes will refer to gas deeper in the molecular cloud.
  - The cosmic ratio of ^{13}CO to ^{12}CO is ~ 0.011. Hence, ^{13}CO is optically thin.
  - The frequency of ^{13}CO J = 1-0 transition is 110.20 GHz, 4.6% lower than that for ^{12}CO.

    ratio of the reduced masses:

$$\frac{\mu(^{13}\mathrm{C}^{16}\mathrm{O})}{\mu(^{12}\mathrm{C}^{16}\mathrm{O})} = \frac{13 \times 16/(13+16)}{12 \times 16/(12+16)} \approx 1.0460 \qquad \frac{B_0(^{13}\mathrm{C}^{16}\mathrm{O})}{B_0(^{12}\mathrm{C}^{16}\mathrm{O})} = \frac{\mu(^{12}\mathrm{C}^{16}\mathrm{O})}{\mu(^{13}\mathrm{C}^{16}\mathrm{O})} \approx 1/1.0460 = 0.9560$$

  - We assume that T_{ext} of ^{13}CO is the same as that of ^{12}CO. This is generally a safe assumption, since the two isotopes of carbon are intermingled in the ISM.

$$T_{\mathrm{A}}(^{13}\mathrm{CO}) \approx \frac{h\nu}{k}\left[\frac{1}{\exp\left(h\nu/kT_{\mathrm{exc}}\right)-1} - \frac{1}{\exp\left(h\nu/kT_{\mathrm{rad}}\right)-1}\right]\tau_\nu \qquad \leftarrow (1-e^{-\tau_\nu}) \approx \tau_\nu$$

$h\nu/k = 5.140\,\mathrm{K}$ for the ^{13}CO J = 1-0 transition.

  - The integrated line strength is then

$$\int T_{\mathrm{A}}(^{13}\mathrm{CO})dv \approx 5.140\,\mathrm{K}\left(\frac{1}{e^{5.140\,\mathrm{K}/T_{\mathrm{exc}}}-1} - 0.1787\right)\int \tau_\nu dv$$

- The optical depth, integrated over the thermally broadened line, is

$$\int \tau_\nu dv = \sqrt{\pi} b \tau_0 = \frac{1}{8\pi}\frac{g_1}{g_0}\frac{c^3}{\nu^3} A_{10}\left(1 - e^{-h\nu/kT_{\rm exc}}\right) N_0(^{13}{\rm CO})$$

$$\tau_0 = \frac{g_1}{g_0}\frac{c^2}{8\pi^{3/2}\nu_{10}^3} A_{10}\frac{c}{b}\left(1 - e^{-h\nu_{10}/kT_{\rm exc}}\right) N_0$$

Here, $N_0(^{13}{\rm CO})$ is the column density of ^{13}CO in its rotational ground state with J = 0.

Note: $$\begin{aligned} A_{10} &= 7.20 \times 10^{-8}\,{\rm s}^{-1} \quad \text{for } ^{12}{\rm CO} \\ &= 6.29 \times 10^{-8}\,{\rm s}^{-1} \quad \text{for } ^{13}{\rm CO} \end{aligned}$$

$$\int \tau_\nu dv \approx 1.52 \times 10^{-15}\left(1 - e^{-5.140\,{\rm K}/T_{\rm exc}}\right) N_0(^{13}{\rm CO}) \left[\frac{\rm km\,s^{-1}}{\rm cm^{-2}}\right]$$

- Therefore, we find:

$$\boxed{N_0(^{13}{\rm CO}) \approx 2.9 \times 10^{14} \frac{\int T_{\rm A}(^{13}{\rm CO}) dv}{1\,{\rm K\,km\,s^{-1}}} \left[{\rm cm^{-2}}\right] \quad \text{when} \quad T_{\rm exc} \approx 8\,{\rm K}}$$

X-factor (^{13}CO to H_2)

- X-factor (^{13}CO to H_2)
  - The fraction of ^{13}CO in its rotational ground state:

$$f_{J=0} = \frac{1}{\sum_J (2J+1) e^{-B_0 J(J+1)/kT_{\rm exc}}} \approx \left[\frac{1}{1 + \left(\frac{T_{\rm exc}}{2.766/1.0460\,{\rm K}} \right)^2} \right]^{1/2} \approx 0.314$$

  - Then, we obtain the CO to H_2 ratio:

$$\begin{aligned} N({\rm H_2}) =& 1.8 \times 10^6 \\ &\times \frac{1}{2} \frac{n_{\rm H}/n_{\rm C}}{(1/3.0 \times 10^{-4})} \frac{n({\rm C})/n(^{12}{\rm CO})}{4} \frac{n(^{12}{\rm CO})/n(^{13}{\rm CO})}{90} \frac{N(^{13}{\rm CO})/N_0(^{13}{\rm CO})}{3} N_0(^{13}{\rm CO}) \end{aligned}$$

$$N({\rm H_2}) \approx 5 \times 10^{20} \left[\frac{\int T_{\rm A}(^{13}{\rm CO}) dv}{1\,{\rm K\,km\,s^{-1}}} \right] \quad [{\rm cm^{-2}}]$$

$$X_{^{13}{\rm CO}} \equiv \frac{N({\rm H_2})}{W_{^{13}{\rm CO}}} \approx 5 \times 10^{20} \left[\frac{\rm cm^{-2}}{\rm K\,km\,s^{-1}} \right] \longleftarrow \quad W_{^{13}{\rm CO}} \equiv \int T_{\rm A}(^{1213}{\rm CO}) dv$$

X-factor (^{12}CO to H_2) - Correct Approach

(Chapter 19 of Draine's book)

- X-factor
  - It would be useful if we had a reliable way to convert from something easy to measure (the antenna temperature integrated over the line of ^{12}CO) to something difficult to measure (the column density $N(H_2)$ of molecular hydrogen).

$$W_{\rm CO} \equiv \int T_{\rm A}(^{12}{\rm CO})dv$$

$$\boxed{X_{\rm CO} \equiv \frac{N({\rm H_2})}{W_{\rm CO}}}$$

  - If the cloud is larger than our antenna beam, we can relate $W_{\rm CO}$ to $N({\rm H_2})$.
    - Recall that the optical depth at line-center from center to edge of the spherical cloud:

$$\tau_0 = \frac{g_1}{g_0}\frac{A_{10}c^2}{8\pi^{3/2}\nu_{10}^3}\frac{c}{b}\left(1-e^{-h\nu_{10}/kT_{\rm exc}}\right)n_0 R$$

Use virial theorem:

$$b = \left(\frac{2G}{5}\frac{M}{R}\right)^{1/2}$$

$$\tau_0 = \frac{g_1}{g_0}\frac{A_{10}\lambda_{10}^3}{8\pi}\left(\frac{5}{2\pi G}\right)^{1/2}\frac{n_0 R^{3/2}}{M^{1/2}}\left(1-e^{-h\nu_{10}/kT_{\rm exc}}\right)$$

    - The luminosity of the cloud in a spectral line (J = 1-0) is:

$$L_{10} = \int dr 4\pi r^2 n_1 A_{10} h\nu_{10}\left\langle\beta\right\rangle_{\rm cloud}$$
$$= \int dV 4\pi j_{10}\left\langle\beta\right\rangle_{\rm cloud}$$

Emissivity: $4\pi j_{10} = n_1 A_{10} h\nu_{10}$

Escape probability averaged over the line profile and over the cloud volume:

$$\left\langle\beta\right\rangle_{\rm cloud} = \frac{1}{4\pi R^3/3}\int_0^R \left\langle\beta({\bf r})\right\rangle 4\pi r^2 dr$$

- Using the escape probability $\langle\beta\rangle_{\rm cloud} \approx \dfrac{1}{1+0.5\tau_0}$

$$L_{10} \approx \frac{4\pi}{3} R^3 n_1 A_{10} h\nu_{10} \frac{2}{\tau_0}$$

Here, we assume $\tau_0 \gg 1$, thus $\langle\beta\rangle_{\rm cloud} \approx 2/\tau_0$.

$$L_{10} \approx \frac{64\pi^2}{3} \left(\frac{2\pi G}{5}\right)^{1/2} \frac{hc}{\lambda_{10}^4} M^{1/2} R^{3/2} \frac{n_1}{n_0} \frac{g_0}{g_1} \frac{1}{1-e^{-h\nu_{10}/kT_{\rm exc}}}$$
$$\approx \frac{64\pi^2}{3} \left(\frac{2\pi G}{5}\right)^{1/2} \frac{hc}{\lambda_{10}^4} M^{1/2} R^{3/2} \frac{1}{e^{h\nu_{10}/kT_{\rm exc}}-1}$$

- The line luminosity per unit mass is:

$$\boxed{\frac{L_{10}}{M} \approx 32\pi^2 \left(\frac{2G}{15}\right)^{1/2} \frac{hc}{\lambda_{10}^4} \frac{1}{\rho^{1/2}} \frac{1}{e^{h\nu_{10}/kT_{\rm exc}}-1}} \longleftarrow \quad M = \frac{4\pi R^3}{3}\rho$$

Note that for a give spectral line, **the luminosity per unit mass depends on the cloud density and on the excitation temperature.**

- Now, we relate (1) the mass to the average column density of hydrogen nucleon and (2) the luminosity to the average antenna (brightness) temperature.

$$\boxed{\text{Hydrogen column density: } N_{\rm H} = \frac{\Sigma}{1.4 m_{\rm H}} = \frac{\frac{M}{\pi R^2}}{1.4 m_{\rm H}}}$$

$$\Sigma = \text{ surface density}$$

Antenna temperature averaged over the projected surface area:

$$\int T_\mathrm{A} dv \equiv \frac{\int\int \frac{c^2}{2k\nu^2} I_\nu dv dA \left<\beta\right>_\mathrm{cloud}}{\int dA}$$

Here,

$dA =$ projected area

$ds =$ pathlength along a sightline

From the radiative transfer equation: $I_\nu = \int j_\nu ds$

$$\boxed{\begin{aligned}\int T_\mathrm{A} dv &= \frac{1}{\pi R^2}\int\left[\int \frac{c^2}{2k\nu^2} j_\nu \left<\beta\right>_\mathrm{cloud} dv\right] dV \\ &= \frac{1}{\pi R^2}\frac{1}{4\pi}\frac{c^3}{2k\nu_{10}^3} L_{10}\end{aligned}}$$

$$\frac{v}{c} \equiv \frac{\nu - \nu_{10}}{\nu_{10}}$$

$$j_\nu dv = j_\nu \left|\frac{dv}{d\nu}\right| d\nu = j_\nu \frac{c}{\nu_{10}} d\nu$$

- Then, we can relate the antenna temperature to the total H column density (averaged over the beam solid angle):

$$\begin{aligned}\frac{N_\mathrm{H}}{\int T_\mathrm{A} dv} &= \frac{8\pi k}{1.4 m_\mathrm{H}} \frac{M}{L_{10}} \\ &= \frac{1}{4\pi}\frac{k\lambda_{10}}{hc}\left(\frac{15}{2.8 G m_\mathrm{H}}\right)^{1/2} (n_\mathrm{H})^{1/2}\left(e^{h\nu_{10}/kT_\mathrm{exc}} - 1\right)\end{aligned}$$

Here, we used:

$\rho = 1.4 \times m_\mathrm{H} n_\mathrm{H}$

- If we assume $N(\mathrm{H_2}) = N_\mathrm{H}/2$, the above equation becomes:

$$X_\mathrm{CO} = \frac{N(\mathrm{H_2})}{\int T_\mathrm{A} dv} = \frac{1}{8\pi}\frac{k\lambda_{10}}{hc}\left(\frac{15}{2.8Gm_\mathrm{H}}\right)^{1/2}(n_\mathrm{H})^{1/2}\left(e^{h\nu_{10}/kT_\mathrm{exc}} - 1\right)$$
$$= 1.58 \times 10^{20}\left(\frac{n_\mathrm{H}}{10^3\,\mathrm{cm^{-3}}}\right)^{1/2}\left(e^{5.532\,\mathrm{K}/T_\mathrm{exc}} - 1\right)\left[\frac{\mathrm{cm^{-2}}}{\mathrm{K\,km\,s^{-1}}}\right]$$

- For $n_\mathrm{H} = 10^3\,\mathrm{cm^{-3}}$ and $T_\mathrm{exc} = 8\,\mathrm{K}$, this yields:

$$\boxed{X_\mathrm{CO} = \frac{N(\mathrm{H_2})}{\int T_\mathrm{A} dv} = 1.56 \times 10^{20}\left(\frac{n_\mathrm{H}}{10^3\,\mathrm{cm^{-3}}}\right)^{1/2}\left[\frac{\mathrm{cm^{-2}}}{\mathrm{K\,km\,s^{-1}}}\right]}$$

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

The most recent determination using gamma rays finds

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

<u>These results suggests that $n_\mathrm{H} = 10^3\,\mathrm{cm^{-3}}$ and $T_\mathrm{exc} = 8\,\mathrm{K}$ may be representative of self-gravitating molecular clouds in the local ISM.</u>

- Notes:
  - *Real molecular clouds have an outer layer where the hydrogen is molecular, but where the CO abundance is very low* because it is not sufficiently shielded from dissociating radiation.
  - *This does not show up in H I 21-cm or CO 1-0 surveys* — leading Wolfire et al. (2010) to refer to it as “the dark molecular gas” — but since it does contain dust, it does contribute to the Far-IR emission.
  - Wolfire et al. (2010) estimate that ~30% of the molecular mass in a typical Galactic molecular cloud may be in this envelope.
  - At constant $n_{\rm H}$ and $T_{\rm exc}$, this low-CO layer will result in an increase in $X_{\rm CO}$. This is in agreement with recent observations.
  - **Other galaxies:** Recent observations indicates that $X_{\rm CO}$ in Local Group galaxies is of order

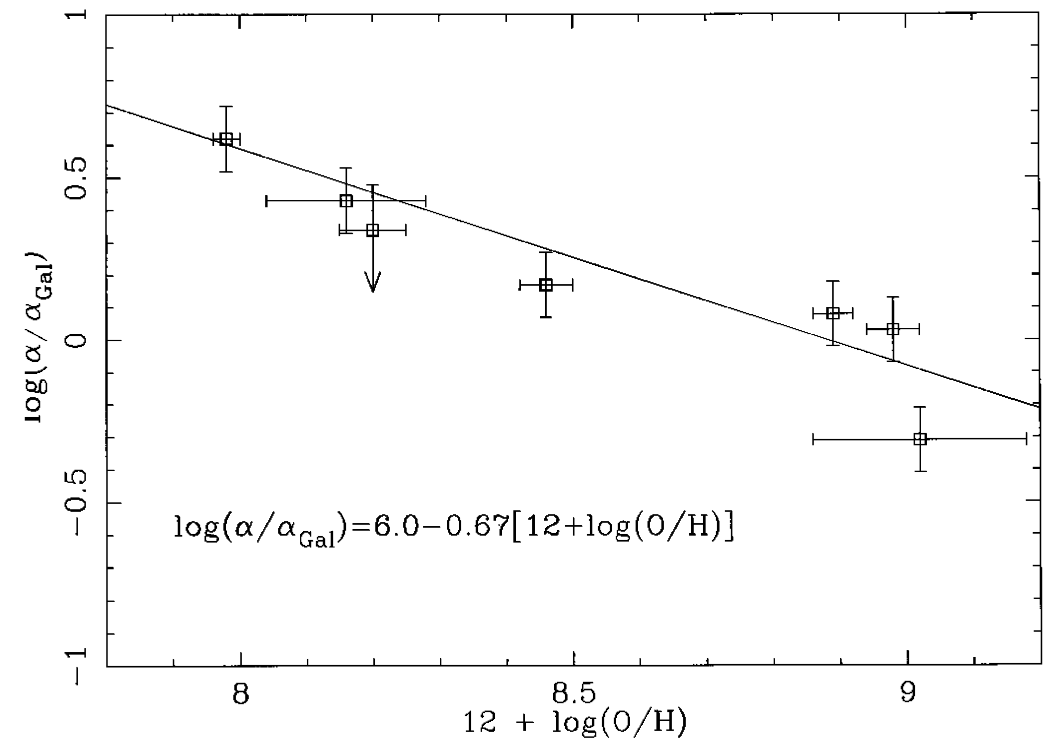
(Blitz et al. 2007)

$$X_{\rm CO} \sim 4 \times 10^{20}\,{\rm cm}^{-2}\,/{\rm K\,km\,s}^{-1}$$

with large variations from one galaxy to another.

An indirect estimate of the molecular gas mass based on modeling the IR emission from a sample of nearby galaxies also favored $X_{\rm CO} \approx 4 \times 10^{20}\,{\rm cm}^{-2}\,/{\rm K\,km\,s}^{-1}$ (Draine et al. 2007).

Metallicity dependence of the CO-to-H$_2$ conversion factor



The average CO-to-H$_2$ conversion factor in five Local Group galaxies (M31, M33, IC 10, NGC 6822, SMC) is plotted as a function of the oxygen abundance.

[Fig 2, Wilson, 1995, 448, L97]

X-factor (^{12}CO to H_2) - Approach of Ryden

- X-factor
  - Since a typical molecular cloud is optically thick at the J = 1-0 rotational transition of ^{12}CO, we use the radiative transfer solution for an opaque object:

$$I_\nu = \frac{2h\nu^3}{c^2}\left[\frac{e^{-\tau_\nu}}{\exp(h\nu/kT_{\rm rad})-1} + \frac{1-e^{-\tau_\nu}}{\exp(h\nu/kT_{\rm exc})-1}\right] \quad \rightarrow \quad \boxed{I_\nu \approx \frac{2h\nu^3}{c^2}\frac{1}{\exp(h\nu/kT_{\rm exc})-1}}$$

  - Expressed in terms of the antenna temperature, this is

$$T_{\rm A} \equiv \frac{c^2}{2k\nu^2} I_\nu \approx \frac{h\nu}{k}\frac{1}{\exp(h\nu/kT_{\rm exc})-1}$$

However, this is wrong by a geometrical factor because we are dealing with a sphere. Toward outer boundary of the sphere, the optical depth will be thin.

  - The observed emission lines is narrow, we can assume that $\nu = \nu_{10}$ over the entire line width.

$$\int T_{\rm A} dv \approx \sqrt{\pi} b T_{\rm A}(\nu_{10}) \approx \sqrt{\pi}\frac{h\nu_{10}}{k}\frac{b}{\exp(h\nu_{10}/kT_{\rm exc})-1}$$

Here, we assume a Gaussian line profile

$$T_{\rm A} = T_{\rm A}(0) e^{-v^2/b^2}$$

  - Then, the X-factor is

$$X_{\rm CO} = \frac{N({\rm H_2})}{b}\frac{1}{\sqrt{\pi}}\frac{k}{h\nu_{10}}\left(e^{h\nu_{10}/kT_{\rm exc}} - 1\right)$$

- Now let's use virial theorem for a uniform, spherical cloud:

$$\sigma_v^2 = \frac{GM_c}{5R_c},\ b = \sqrt{2}\sigma_v \quad \rightarrow \quad \boxed{M_c = \frac{5}{2}\frac{R_c b^2}{G}} \qquad M_c \equiv \frac{4\pi}{3}R_c^3\rho_c \quad \rightarrow \quad \boxed{\frac{b}{R_c} = \left(\frac{8\pi}{15}G\rho_c\right)^{1/2}}$$

- Surface density:

$$\Sigma = \frac{M_c}{\pi R_c^2} \xrightarrow{M_c = \frac{5}{2}\frac{R_c b^2}{G}} \Sigma = \frac{5}{2\pi G}\frac{b^2}{R_c}$$

- Column density of hydrogen nucleon in terms of velocity dispersion:

$$N(\mathrm{H}) \approx \frac{\Sigma}{1.4 \times m_\mathrm{H}} = \frac{5}{2.8\pi}\frac{1}{Gm_\mathrm{H}}\frac{b^2}{R_c} \qquad\qquad N(\mathrm{H}_2) = \frac{1}{2}N(\mathrm{H})$$

- The X-factor is:

$$\frac{N(\mathrm{H}_2)}{W_\mathrm{CO}} = \frac{5}{2 \times 2.8\pi\sqrt{\pi}}\frac{1}{Gm_\mathrm{H}}\frac{k}{h\nu_{10}}\frac{b}{R_c}\left(e^{h\nu_{10}/kT_\mathrm{exc}} - 1\right)$$

$$\frac{b}{R_c} = \left(\frac{8\pi}{15}G\rho_c\right)^{1/2} \approx \left(\frac{8\pi}{15}Gm_\mathrm{H}n_\mathrm{H} \times 1.4\right)^{1/2}$$

$$\frac{N(\mathrm{H}_2)}{W_\mathrm{CO}} = \frac{1}{2\pi}\frac{k}{h\nu_{10}}\left(\frac{20}{3}\frac{1}{2.8Gm_\mathrm{H}}\right)^{1/2} n_\mathrm{H}^{1/2}\left(e^{h\nu_{10}/kT_\mathrm{exc}} - 1\right)$$

This result gives a larger value than the correct one by a factor of 8/3 = 2.67.

Molecular Clouds: Chemistry and Ionization

- Molecular Hydrogen
  - In the Milky Way, **~ 22% of the interstellar gas is in molecular clouds**, where the bulk of the hydrogen is in H_2 molecules.
  - H_2 is formed primarily by due grain catalysis. Destruction of H_2 is primarily due to photodissociation, but self-shielding results in very low photodissociation rates in the central regions of molecular clouds.
- Other molecules
  - Once, the H_2 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 $E_I < 13.6\,\mathrm{eV}$.

- Five types of reactions
  - ***Photoionization***: $AB + h\nu \rightarrow AB^+ + e^-$
    - Many molecules (but not H_2) can be photo ionized by photons with $h\nu < 13.6\,\mathrm{eV}$ present in the ISRF in H I or diffuse H_2 clouds.
    - The ionization threshold for H_2 is 15.43 eV, hence H_2 will not be photo ionized even in H I regions.
  - ***Photodissociation***: $AB + h\nu \rightarrow (AB)^* \rightarrow A + B$
    - For some molecules (including H_2 and CO), photoexciation leading to ***dissociation occurs via lines rather than continuum***.
    - This allows such species either to self-shield (H_2), or to be partially shielded if there is accidental overlap between important absorption lines with strong lines of H_2, which will be self-shielded. This is the case with CO.
  - ***Neutral-neutral exchange reactions***: $AB + C \rightarrow AC + B$
    - Most species in molecular clouds are neutral, and neutral-neutral collisions are, therefore, frequent.
    - However, even when a neutral-neutral reaction is exothermic, there will often (but not always) be an energy barrier that must be overcome for the reaction to proceed.

- For instance,

  The following exothermic reaction has an energy barrier E/k = 1950 K, which causes the reaction to be negligibly slow at T < 100 K.

$$\mathrm{OH + H \rightarrow O + H_2} \qquad k = 1.5 \times 10^{-12}\, T_2^{2.8} e^{-19.50/T_2}\, [\mathrm{cm^3\, s^{-1}}]\ (300\,\mathrm{K} < T < 2500\,\mathrm{K})$$

  On the other hand, the reaction responsible for CO formation does not have any significant energy barrier, and can proceed at the low temperatures of molecular clouds.

$$\mathrm{C + OH \rightarrow CO + H} \qquad k = 1 \times 10^{-10}\, [\mathrm{cm^3\, s^{-1}}]\ (10\,\mathrm{K} < T < 300\,\mathrm{K})$$

- ***Ion-neutral exchange reactions***: $AB^+ + C \rightarrow AC^+ + B$
  - Ion-neutral reactions are very important in interstellar chemistry, for two reasons:

    (1) exothermic reactions generally lack energy barriers, allowing the reaction to proceed rapidly even at low temperature, and

    (2) the induced-dipole interaction results in ion-neutral rate coefficients that are relatively large, of order $\sim 2\mathrm{x}10^{-9}\ \mathrm{cm^3\ s^{-1}}$.

- ***Radiative association reactions***: $A + B \underset{k_d}{\overset{k_f}{\rightleftharpoons}} (AB)^* \xrightarrow{k_r} AB + h\nu$

  - The reaction first creates an excited complex. The complex will fly apart in one vibrational period (~ 10^{-14} s), unless a photon is emitted first; it can be thought of as having a probability per unit time $k_d \approx 10^{14}\,\mathrm{s}^{-1}$ of spontaneously dissociating.
  - If AB has an appreciable electric dipole moment (i.e., is not homonuclear), the probability per unit time that (AB)* will emit a photon is an electronic transition is $k_r \approx 10^6\,\mathrm{s}^{-1}$. Thus, a fraction $k_r/(k_r + k_d)$ of the (AB)* complexes formed will result in formation of stable AB.
  - Then, the effective rate coefficient for radiative association will be:

$$k_{\mathrm{ra}} = \frac{k_f k_r}{k_r + k_d}$$

For ion-neutral reactions, the "complex formation" (AB)* is $k_f \approx 10^{-9}\,[\mathrm{cm}^3\,\mathrm{s}^{-1}]$, and hence the rate coefficient for radiative association will be $k_{\mathrm{ra}} \approx 10^{-17}\,[\mathrm{cm}^3\,\mathrm{s}^{-1}]$.

  - For example, formation of CH^+ by radiative association:

$$\mathrm{C}^+ + \mathrm{H} \rightarrow \mathrm{CH}^+ + h\nu \qquad k = 4.45 \times 10^{-17}\, T_2^{-1/2} e^{-0.229 T_2^{-1/2}}\,[\mathrm{cm}^3\,\mathrm{s}^{-1}]$$

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:

$$\mathrm{C}^+ + \mathrm{H}_2 \rightarrow \mathrm{CH}_2^+ + h\nu \quad , \quad k_{33.6} = 5.0\times10^{-16}T_2^{-0.2}\,\mathrm{cm}^3\,\mathrm{s}^{-1} , \tag{33.6}$$

$$\mathrm{CH}_2^+ + e^- \rightarrow \left\{ \begin{array}{ll} \mathrm{CH}+\mathrm{H} & (25\%) \\ \mathrm{C}+\mathrm{H}_2 & (12\%) \\ \mathrm{C}+\mathrm{H}+\mathrm{H} & (63\%) \end{array} \right\} , k_{33.7} = 1.24\times10^{-6}T_2^{-0.60}\frac{\mathrm{cm}^3}{\mathrm{s}} , \tag{33.7}$$

$$\mathrm{CH}+\mathrm{O} \rightarrow \mathrm{CO}+\mathrm{H} \quad k_{33.8} = 6.6\times10^{-11}\,\mathrm{cm}^3\,\mathrm{s}^{-1} , \tag{33.8}$$

$$\mathrm{CO}+h\nu \rightarrow \mathrm{C}+\mathrm{O} \quad k_{33.9} = 2.3\times10^{-10}\,\mathrm{s}^{-1}\times f_{\mathrm{shield}}(\mathrm{CO}) \quad , \tag{33.9}$$

$$\mathrm{C}+h\nu \rightarrow \mathrm{C}^+ + e^- \quad k_{33.10} = 2.6\times10^{-10}\,\mathrm{s}^{-1} \quad . \tag{33.10}$$

From page 377 in [Draine]

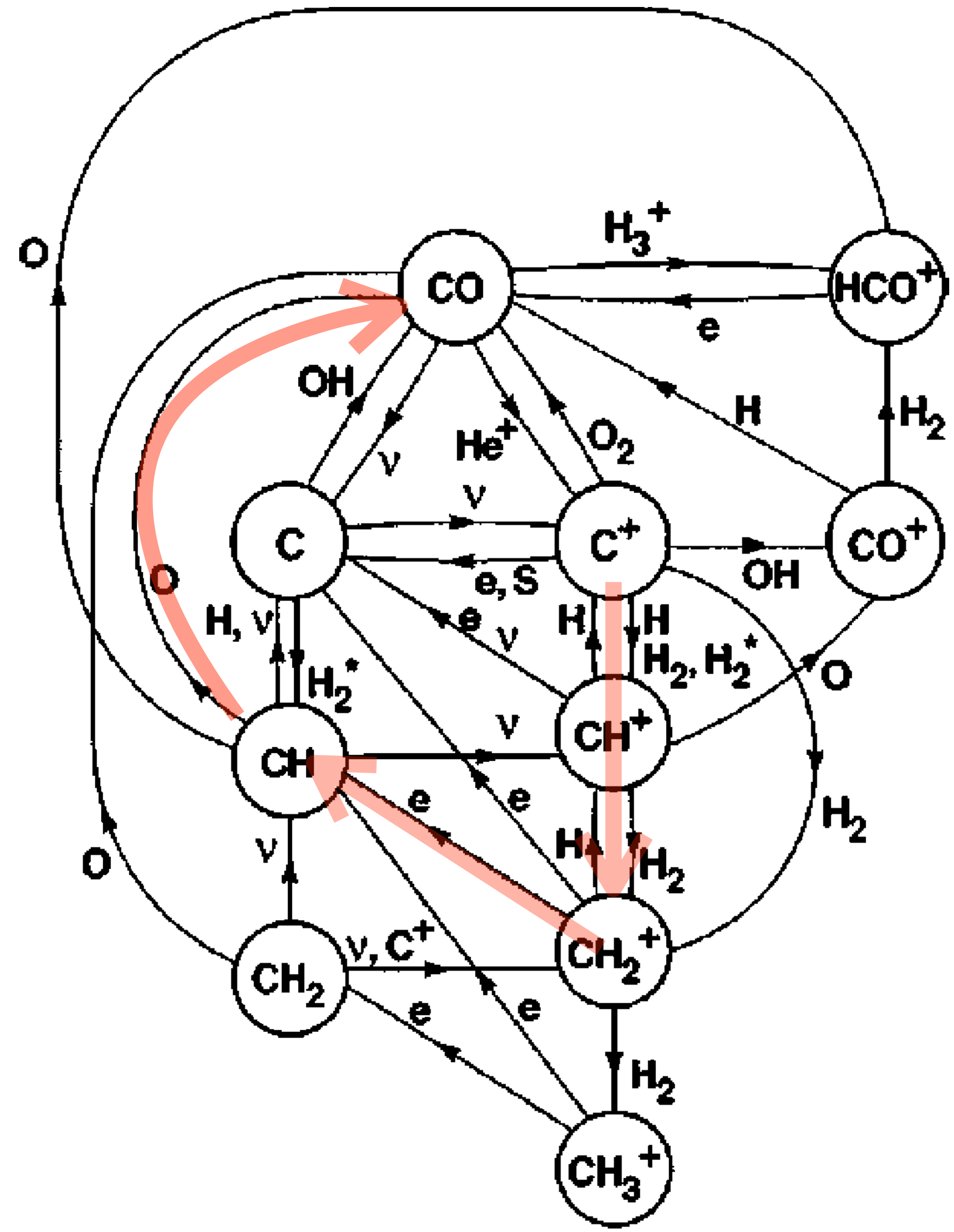


Fig 8.9, Tielens [The physics and chemistry of the interstellar medium]

Formation of OH and H_2O

- In diffuse H I clouds, cosmic-ray ionization produces H^+ — an important starting point of the O chemistry. Charge exchange of neutral O with H^+ yields O^+. Reaction of O^+ with H_2 then form OH^+.
- Deeper in the cloud, where H_2 is an important species, cosmic-ray ionization of H_2 leads to the formation of H_3^+, which readily reacts with O to form OH^+.
- This sequence of gas-phase reaction convert the gas-phase O to H_2O, yielding: $n(\mathrm{H_2O})/n_\mathrm{H} \approx 10^{-4}$
- However, observations indicate very low gas-phase abundance of H_2O:

$$n(\mathrm{H_2O})/n_\mathrm{H} \lesssim 3 \times 10^{-8}$$

  far below the predicted abundance of H_2O.
- The gas-phase H_2O is removed by freeze-out on grains, producing H_2O ice mantles which can contain a substantial fraction of the total oxygen.

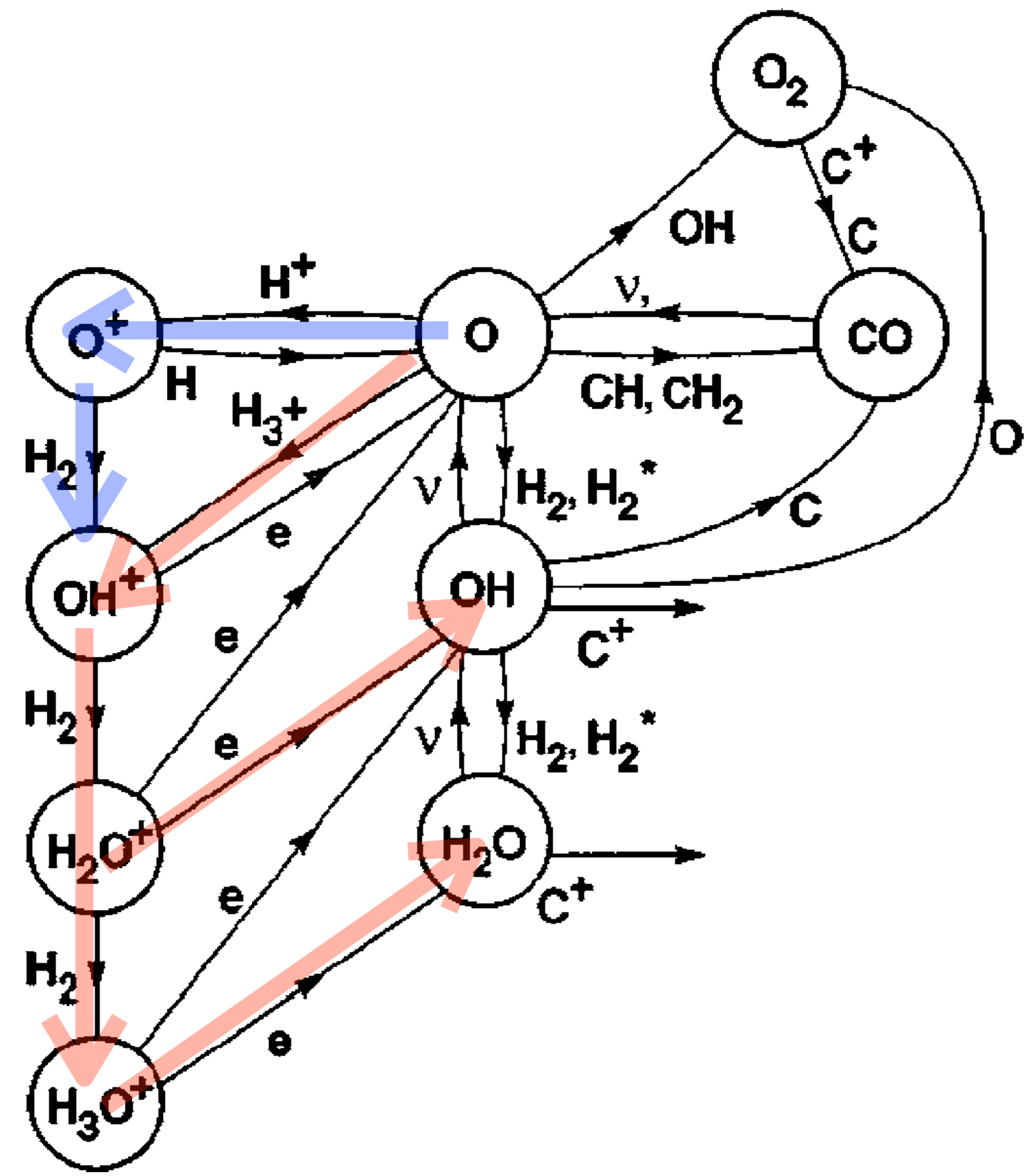


Fig 8.8, Tielens [The physics and chemistry of the interstellar medium]