

mm-submm emission

Basic Concepts of Molecular Structure

- Molecular structure is more complicated than atomic structure. The Schrodinger equation involves positions and moments of all constituents, both the nuclei and electrons.
- Transitions in a molecule can be put in 3 different categories according to energies W :
 1. electron transitions (a few eV) \rightarrow lines in visual UV regions
 2. vibrational transitions caused by oscillations of the relative positions of nuclei with respect to equilibrium positions (0.1-0.01 eV) \rightarrow lines in the IR region
 3. rotational transitions caused by the rotation of the nuclei (about 10^{-3} eV) \rightarrow lines in the cm, mm regions

The motion of nuclei is slow, the e make many cycles while the nuclei move to their new positions. The separation of the nuclear and electronic motions in molecular quantum mechanics is called Born-Oppenheimer approximation.

If we confine to the radio range, only transitions between different rotational levels and sometimes different vibrational levels will be involved.

Considering that the effective radius of a simple molecule is about 10^5 times the radius of the nucleus of an atom, the moment of inertia (Θ) of such a molecule is at least 10^{10} times that of an atom of the same mass. The kinetic energy of rotation is:

$$H_{rot} = (1/2)\Theta\omega^2 = J^2 / 2\Theta$$

J angular momentum (it is not the quantum number used in atomic physics). For a rigid molecule with two nuclei (A and B) the moment of inertia is:

J is perpendicular to the line connecting the two nuclei.

$$\Theta = m_A r_A^2 + m_B r_B^2 = m r_e^2$$

$$r_e = r_A - r_B$$

$$m = \frac{m_A m_B}{m_A + m_B}$$

$$\vec{J} = \Theta \vec{\omega}$$

More complicated expression for the moment of inertia can be obtained for molecules with two or more nuclei.

The solution of the Schrodinger equation:

J quantum number of angular momentum

$$E_{tot} = W(J) = \frac{\hbar^2}{2\Theta} J(J+1)$$
$$J = 0, 1, 2, \dots$$

This equation is correct for **rigid molecule**; for a slightly elastic molecule r_e will increase with the rotational energy due to centrifugal stretching. The actual frequencies are always lower than the frequencies predicted on the basis of a rigid rotor model; the deviations become rapidly larger with increasing J.

Allowed dipole radiative transitions will occur between different rotational states only if the molecule is polar. Homonuclear diatomic molecules (O_2 , H_2 , N_2) cannot undergo allowed transitions → difficult to detect.

For molecules with permanent dipole moments: in the plane of rotation the dipole moment can be viewed as an antenna, oscillating as the molecule rotates.

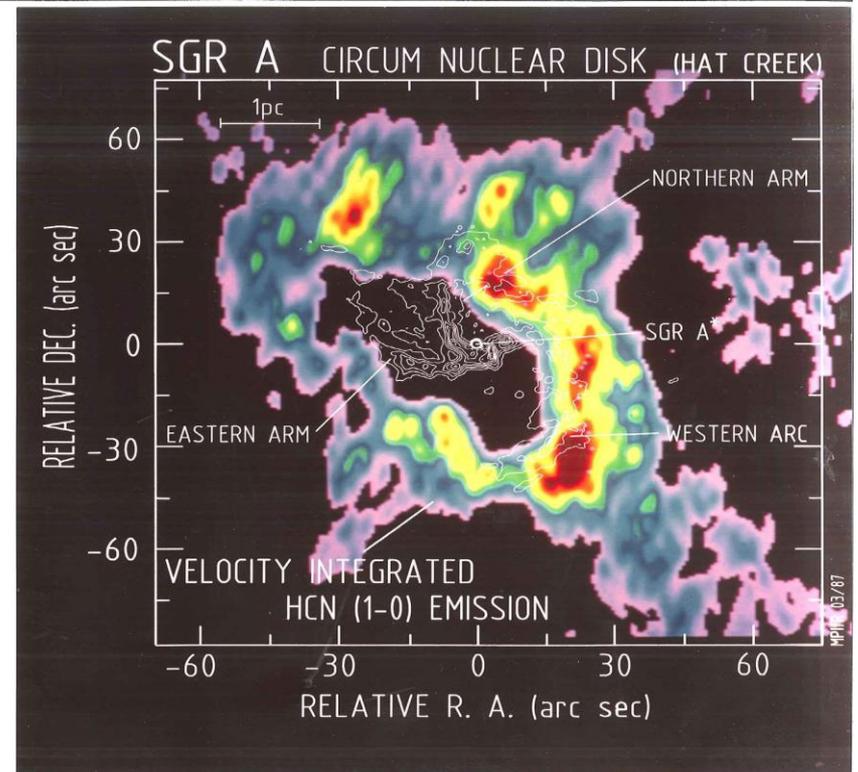
Classically, the acceleration of positive and negative charges gives rise to radiation whose frequency is that of rotation frequency.

In the quantum mechanical model, the angular momentum is quantized, so that the radiation is emitted in discrete frequencies.

Hyperfine Structure in Linear Molecules

The magnetic dipole or electric quadrupole of nuclei interacts with e and other nuclei. This gives rise to hyperfine structure in molecules such as HCN, HNC, HC₃N. The hyperfine splitting of energy levels depends on the position of the nucleus in the molecule; the effect is smaller for HNC than for HCN.

In general, the effect is of order of a few MHz, and decreases with increasing J.



Vibrational Transitions

If any of the nuclei of a molecule suffers a displacement from its equilibrium distance r_e it will on release perform an oscillation about r_e .

A molecule consisting of two atoms can vibrate only in one direction, the situation is more complex for molecules with two or three nuclei.

Relation between Line Intensity and Level Population

Relation between the observed line intensities and the column densities of the species emitting the transition

Considering rotational transitions

For an optically thin emission line

$$N_l = 2.07 \times 10^3 \frac{g_l \nu^2}{g_u A_{ul}} \int T_B dv$$

u=upper, l=lower level

A=Einstein coefficient, spontaneous transition probability from u to l

g=statistical weight of the state l and u

T_B=main beam brightness temperature

ν in GHz and linewidth in km/s

In a system that is in LTE the population of the energy levels is described by the Boltzmann distribution:

DeltaE=the energy difference of the two levels

$$\frac{N_2}{N_1} = \frac{g_2}{g_1} e^{-\Delta E/kT}$$

Molecules

(Tools of Radio astronomy, K. Rohlfs, T.L. Wilson)

First result from molecular line measurement is the conversion of line intensity, integrated over linewidth, into column density.

The aim is: to determine the complete chemical and isotopic content of a molecular cloud.

Then: to relate the molecular clouds to star formation, to interaction with very young stellar objects, to search prebiological molecules.

Ion-Molecule Chemistry

At typical densities neutral-neutral chemical reactions between atoms are too slow to form even triatomic molecules in a few 10^6 yr (for example H_2 forms on dust grain surfaces to conserve both energy and momentum)

The solution is ion-molecule chemistry.

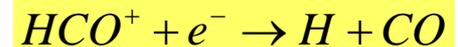
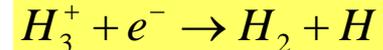
Simple example of gas phase production of molecules: HCO^+ .

Assume the interstellar radiation field plays no role.



Then reaction with many partners...e.g. $H_3^+ + CO \rightarrow HCO^+ + H_2$

The destruction of H_3^+, HCO^+ via reactions with e:



ζ total CR ionization rate per H_2 (in sec^{-1})

$\zeta/2$ ionization rate per H

Destruction of H_3^+ via reactions with e (either from those resulting from the formation of H_3^+ (rate k_e) or those resulting from other ions (rate k_i)).

When formation and destruction are in equilibrium we have a steady state relation for the abundance of H_3^+, HCO^+ in a cloud with local density $n(H_2)$.

Balancing formation and destruction:

$$k_e n_{H_3^+} + n_e + k_i n_{H_3^+} + n_{X_i} = \zeta n_{H_2}$$

Similarly

$$k_{HCO^+} n_{(HCO^+)} n_e + k'_i n_{(HCO^+)} n_{X_i} = k n_{(H_3^+)} n_{CO}$$

Dividing the previous two equations by the local density of H_2 and combining the two relations the abundance of HCO^+ (in [] concentrations):

$$[HCO^+] = \frac{k_{\zeta}[CO]/n(H_2)}{(k_{HCO^+}[e] + k_i[X_i])(k_e[e] + k_i[X_i])} \quad (1)$$

The abundance is obtained in terms of:

ζ cosmic ray rate

CO abundance

ionization fraction

where k ion-molecule rate which H_3^+ reacts with CO to form HCO^+

If

$$\sum X_i \ll 10^{-4}$$

$$R = \frac{n(H_2)n(HCO^+)}{n(CO)}$$

Then (1) is:

$$[e] \leq \sqrt{\frac{\zeta k}{Rk_{HCO^+} + k_e}}$$

Taking:

$$k_e = 4 \cdot 10^{-5} T^{-0.5} \text{cm}^{-3} \text{s}^{-1}$$
$$k_{\text{HCO}^+} = 6 \cdot 10^{-6} T^{-0.5} \text{cm}^{-3} \text{s}^{-1}$$
$$k = 10^{-9}$$

$$T_K = 10 \text{K}$$

$$R \approx 1$$

$$\zeta = 4 \cdot 10^{-17} \text{s}^{-1}$$

For molecular clouds typical values
are:



An upper limit to the
electron fraction is 10^{-8}

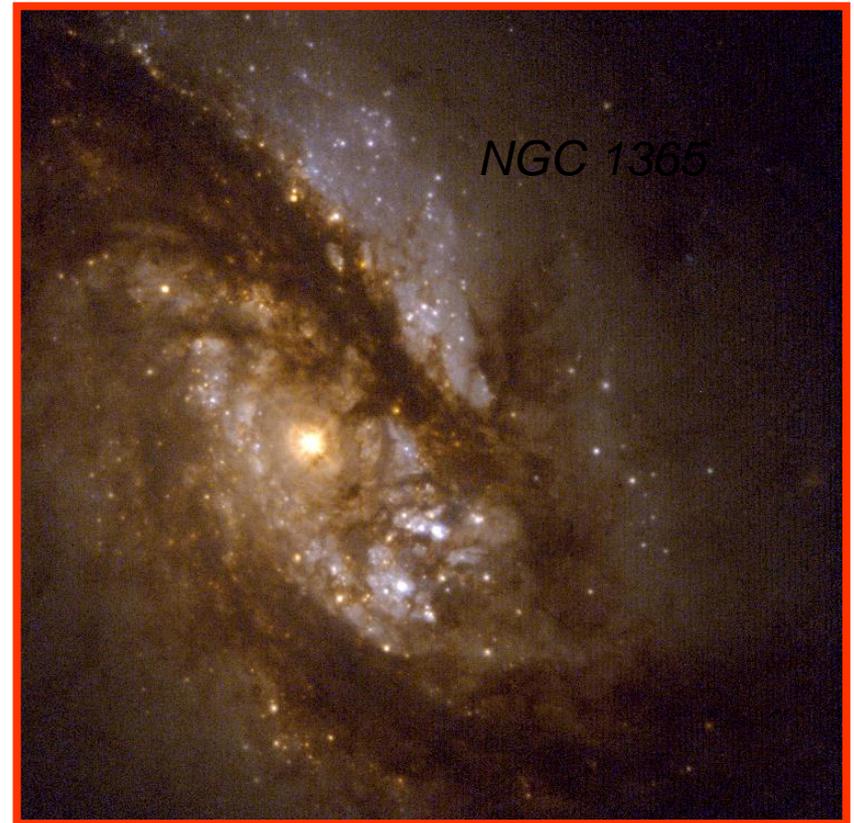
Effects on the computed value due to: inhomogeneous structure of clouds, possible non-LTE excitation and uncertain reaction rates for H_3^+

Productions of other species are more uncertain.

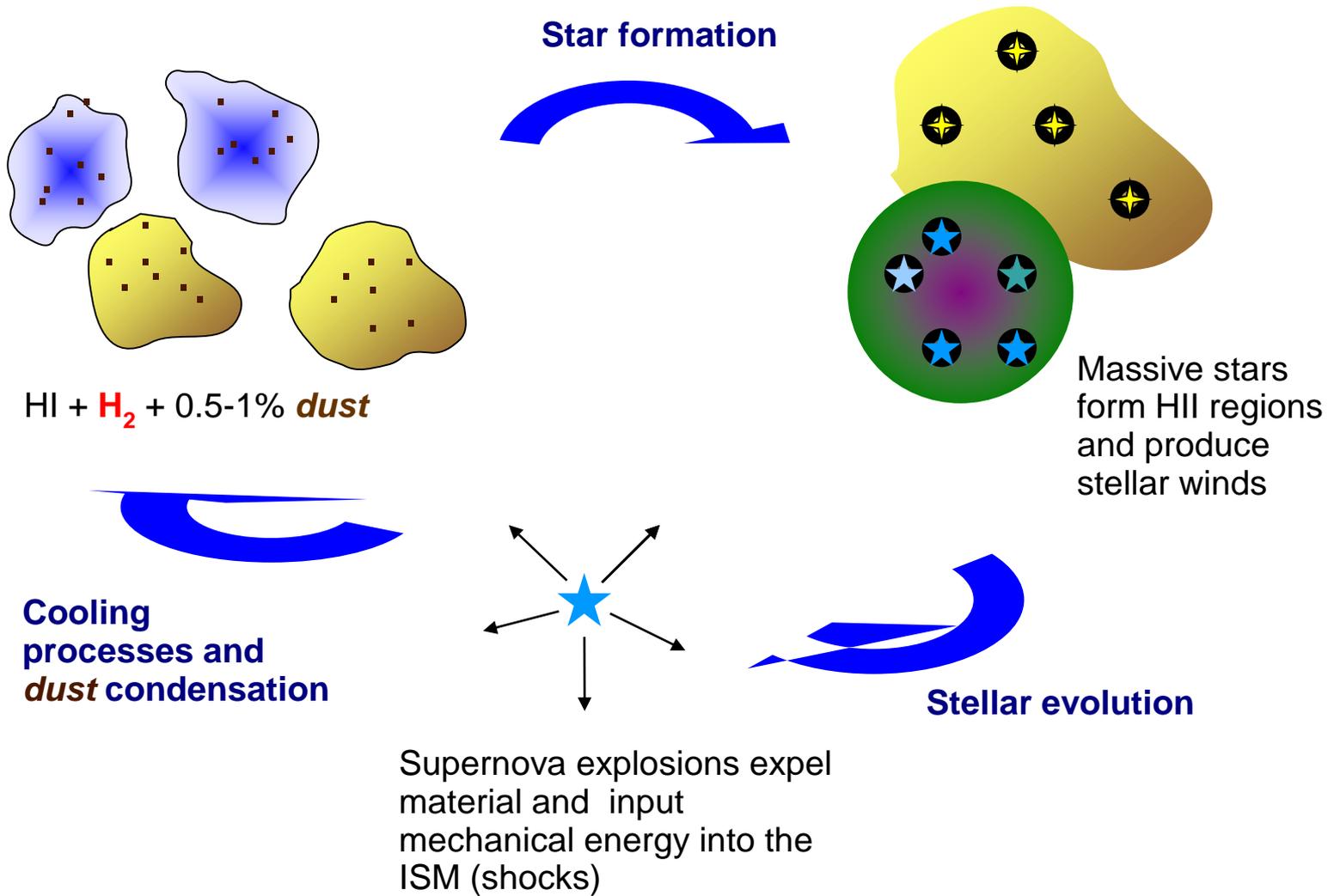
It is clear that the gas phase abundance of any species in a molecular cloud is a delicate balance between the production and destruction processes.

Molecular gas and ISM

- Stars form from dense , cool H_2
- The ISM plays an important role in the energy exchange and provide raw material
- Star formation occurs in dense dusty clouds so need some tracer that penetrates the dust ("extinction free" trace)
- Spectral observations also trace kinematics, so can be used to probe dynamical mass, gas motion, and gravitational torques
- Serves as fuel for both starburst and AGN activity
- Significant mass in galaxy nuclei
 - H_2 is a "silent" molecule –need tracer species (CO)



The interstellar medium energy cycle

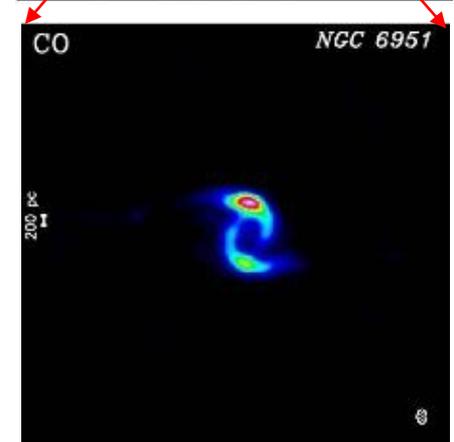
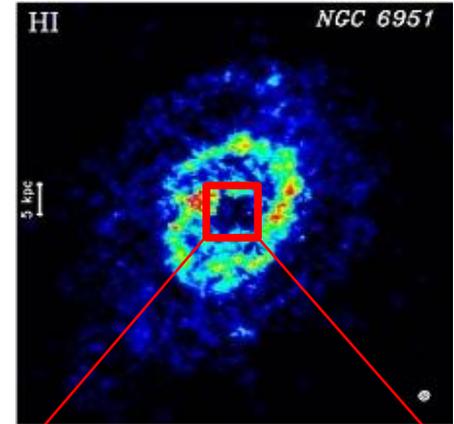
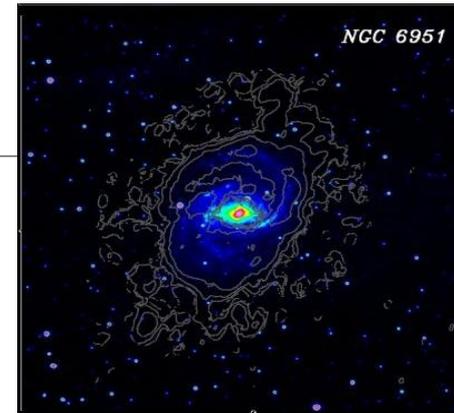
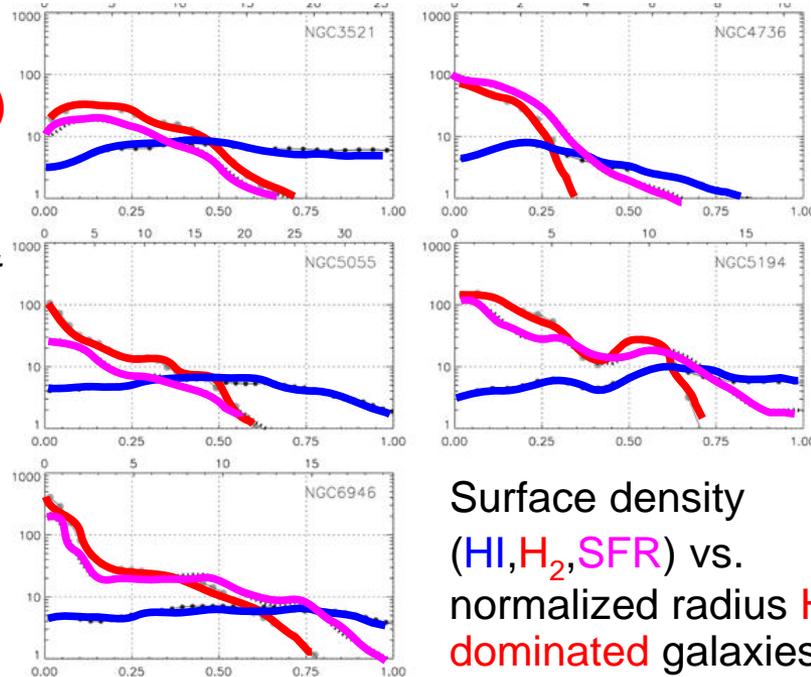


Where is the gas?

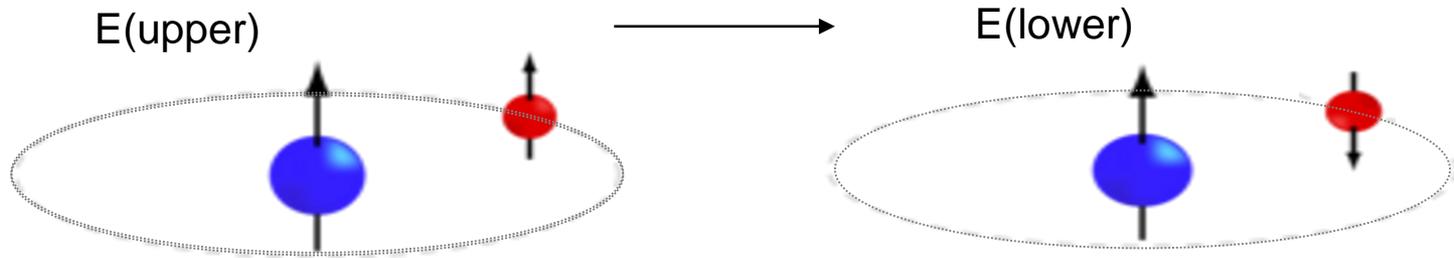
HI is usually much more extended than optical and H_2 (CO). The atomic gas (HI) distribution (middle panel) shows a much larger extent than the CO (bottom), or the optical (stellar) disk (top: optical in color, HI in contours) (see Haan+ 2008, 2009).

NOTE: CO traces H_2 which follows the star formation (see coming slides)...

HI and H_2 (CO) follow the exponential stellar disk, but usually with a central HI depression (hole) (see Kenney & Young 1989, Bigiel+ 2008)



Why don't stars form from atomic hydrogen?



HI emits at 1.42041 MHz (21.1 cm) by radiative transitions between the **two hyperfine levels of the ground electronic state**.

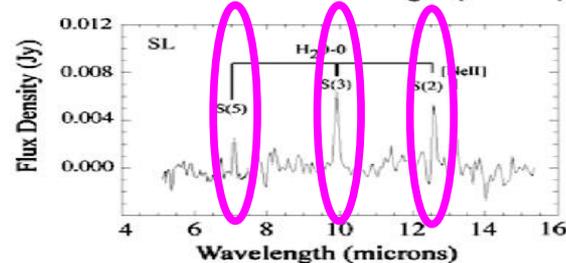
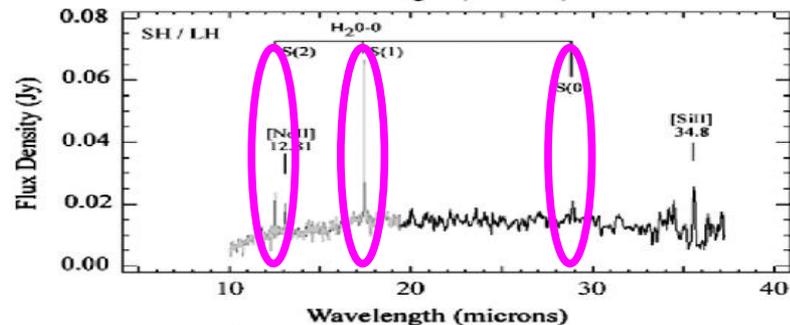
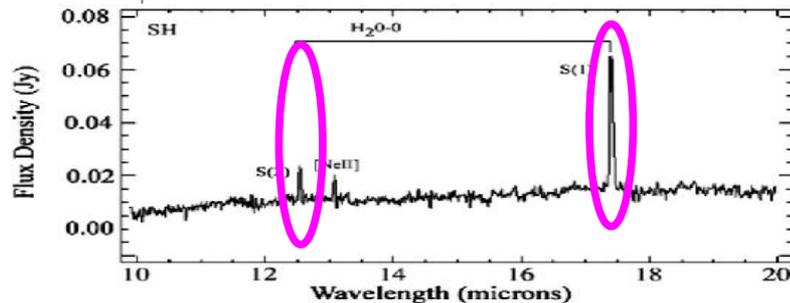
Transition is **highly forbidden**, with a probability of $2.9 \times 10^{-15} \text{ s}^{-1}$; time for a single (isolated) atom to emit a 21.1 cm photon is $\sim 1.1 \times 10^7$ yrs. (Collisions reduce this time drastically...)

Transition is thus inefficient for cooling, and the temperature T_{spin} of the HI clouds is ~ 60 -100K. HI clouds comprise $\sim 10\%$ of visible mass of a galaxy, but have typical densities $n_{\text{H}} \sim 1 \text{ cm}^{-3}$, so they

- ★ will never cool and collapse to form stars ($t_{\text{ff}} \sim 4 \times 10^7$ yrs)
- ★ need to be compressed to form molecular hydrogen

Cool H_2 not easy to observe directly (I)

H_2 homonuclear so no permanent dipole moment. *Only (symmetric) quadrupole transitions permitted*



MIR emission lines: Vibrational transitions in the **mid-infrared** (5-28 μm).

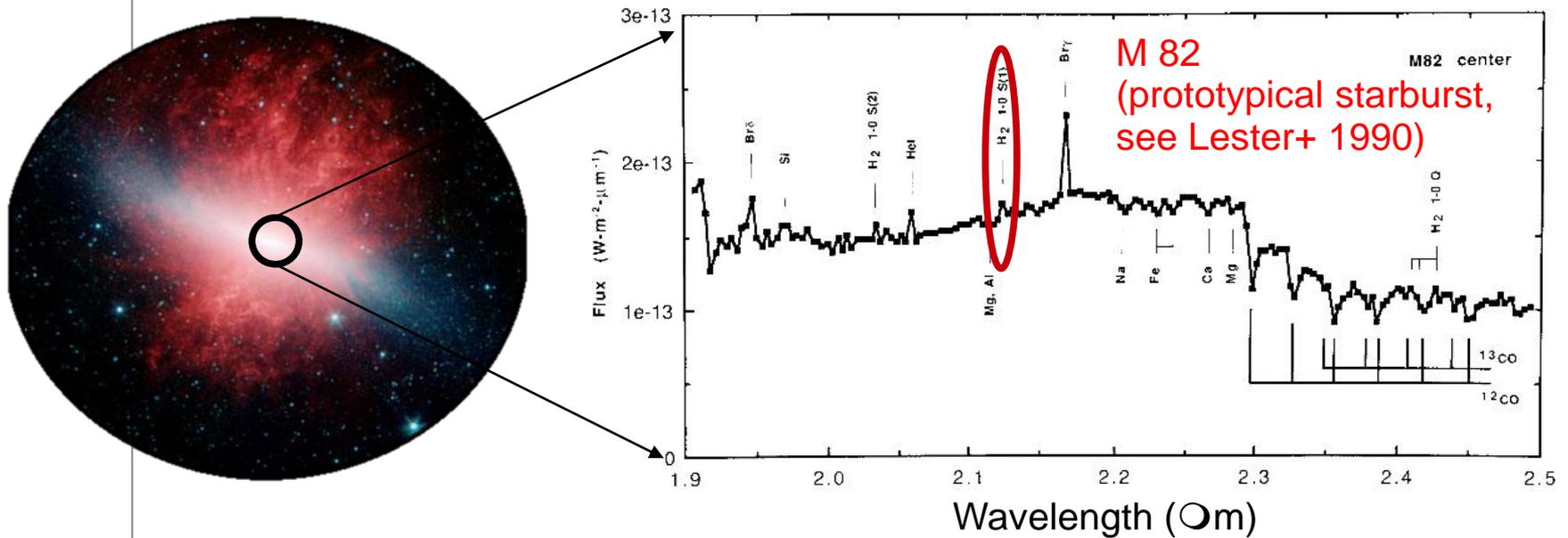
Relatively low critical densities ($>10^2 - 10^3 \text{ cm}^{-3}$) so usually thermally excited, although beware of fluorescence and shocks

However, the warm molecular gas at these temperatures (100-1000K) is **only a small fraction (~5%) of the cool molecular gas** (see Roussel et al. 2007).

Tip of the iceberg!

Spitzer IRS spectrum of brightest galaxy in Stephan's Quintet (Appleton+ 2006): shock excited!

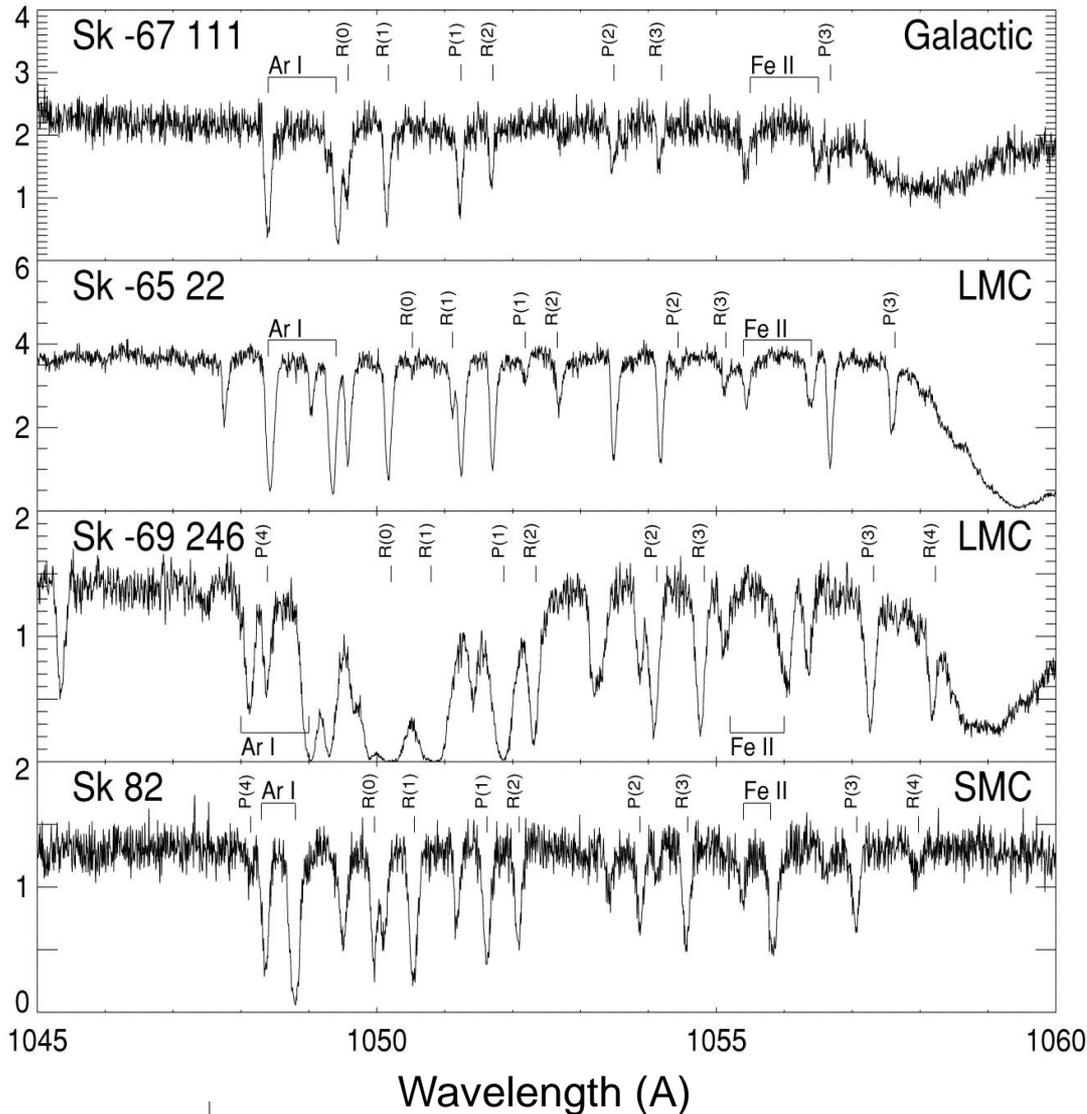
Cool H_2 not easy to observe directly (II)



NIR emission lines: Roto-vibrational transitions in the **near-infrared** ($1-2 \mu m$). Critical densities are sufficiently high ($> 10^4 \text{ cm}^{-3}$) that these transitions are usually **excited by fluorescence** (see Black & van Dishoeck 1987, Sternberg & Dalgarno 1989), rather than reflecting thermal equilibrium in the 1000-2000K regime.

AN EVEN SMALLER fraction ($< 10^{-5}$) of total cool molecular gas (see Dale et al. 2005)

Cool H_2 in *dusty* regions is virtually impossible



FUV (usually) absorption lines:

Electronic transitions in the **far-ultraviolet** (absorption of a Lyman-Werner photon with energies 11.2-13.6 eV, i.e. the origin of *fluorescence*, see Sternberg 1989).

~10-15% of these absorptions result in dissociation of the molecule.

But need a dust-free sightline ($A_V < 1$) in front of a bright star, so virtually **impossible to detect them in dusty regions** (see FUSE results, e.g., LMC/SMC: Tumlinson+ 2002).

CO to the rescue...

- ★ ^{12}CO is the most abundant molecule after H_2 :
 $N(\text{CO})/N(\text{H}_2) \sim \text{few } 10^{-5} \text{ to } 10^{-4}$
- ★ Permanent dipole moment with small value (0.112 Debye = 0.112×10^{-18} franklin cm)
★ Dipole transitions allowed
- ★ Rotational transitions visible at **sub-mm, mm wavelengths**
Collisions can populate lowest levels **even at low densities**
- ★ Excited by UV radiation field and collisions with H_2 , but too much radiation (from 11.1 to 13.6 eV) causes CO to dissociate, so **need self-shielding** (protection from the radiation field)
- ★ Must reside in **cold (10-40K) dense ($>10^3 \text{ cm}^{-3}$) clouds**

X factor: Relating CO luminosity to H₂ mass

CO emission is **optically thick** (e.g., Wilson+ 1974), hence traces surface area, not volume; need **proportionality constant X** to relate Intensity(CO) to mass or column density, N_{H₂}

Assumptions (e.g., Dickman+ 1986):

Extragalactic molecular emission distributed as an ensemble of independent discrete clouds (no overlap along LOS)

Individual clouds obeys the virial theorem

[line width (l.w.) \propto (dynamical mass/ diameter)^{1/2}]

$$I(\text{CO}) = \int T_b dv \sim \sum T_b (\Delta l.w.) \sim \sum T_b (M / r)^{1/2} \sim T_b \sum (n_{\text{H}_2})^{1/2} r$$

$$\sim [T_b (n_{\text{H}_2})^{-1/2}] N_{\text{H}_2} \quad \leftarrow \quad N_{\text{H}_2} = (n_{\text{H}_2}) r$$

X factor: Relating CO luminosity to H₂ mass ***(Bolatto et al. 2013)***

Hence, $N_{H_2} = X \cdot I(CO)$, where

$$X \sim (n_{H_2})^{1/2} / T_b$$

Empirically in the Milky Way disk, $X = 2 \times 10^{20} \text{ cm}^{-2} \text{ K}^{-1} \text{ km}^{-1} \text{ s}$ with +/- 30% uncertainty

Studies of other “normal galaxies” return similar values in Milky Way-like disks, but with greater scatter and systematic uncertainty.

Theoretical and observational arguments suggest that X increases with decreasing metallicity, turning up sharply below metallicity $\approx 1/3$ – $1/2$ solar.

A lower X is also present in the overwhelmingly molecular interstellar medium of starburst galaxies.

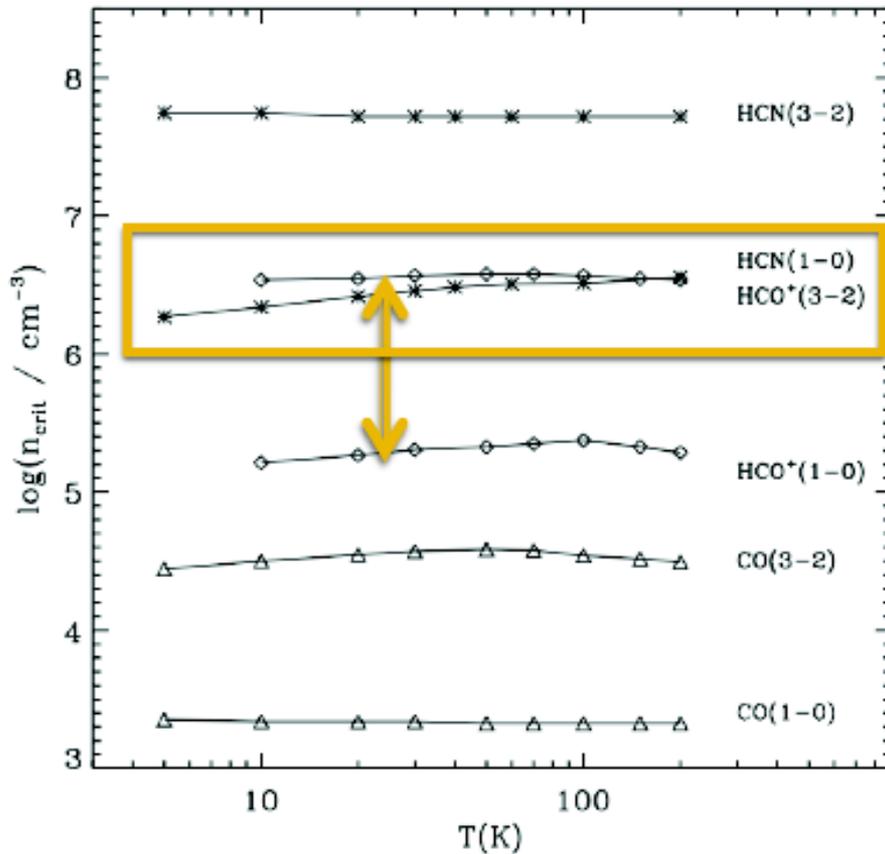
At high redshift, direct evidence regarding the conversion factor remains scarce.

Some other molecules

Molecular line ratios

- A. $^{12}\text{CO}/^{13}\text{CO}$ line ratio as a tracer of ISM-structure, temperature and dynamics.
 - B....and the dense gas:
 1. HCO^+/HCN
 2. HNC/HCN
 3. CN/HCN
 4. HC_3N
- Note: Even with existing telescope arrays, we are looking at **ensembles** of clouds ->
 - **Average** properties of the molecular gas within the beam – but ALMA is changing all of this.
 - Issues of radiative transfer and optical depth

High-density molecular tracers



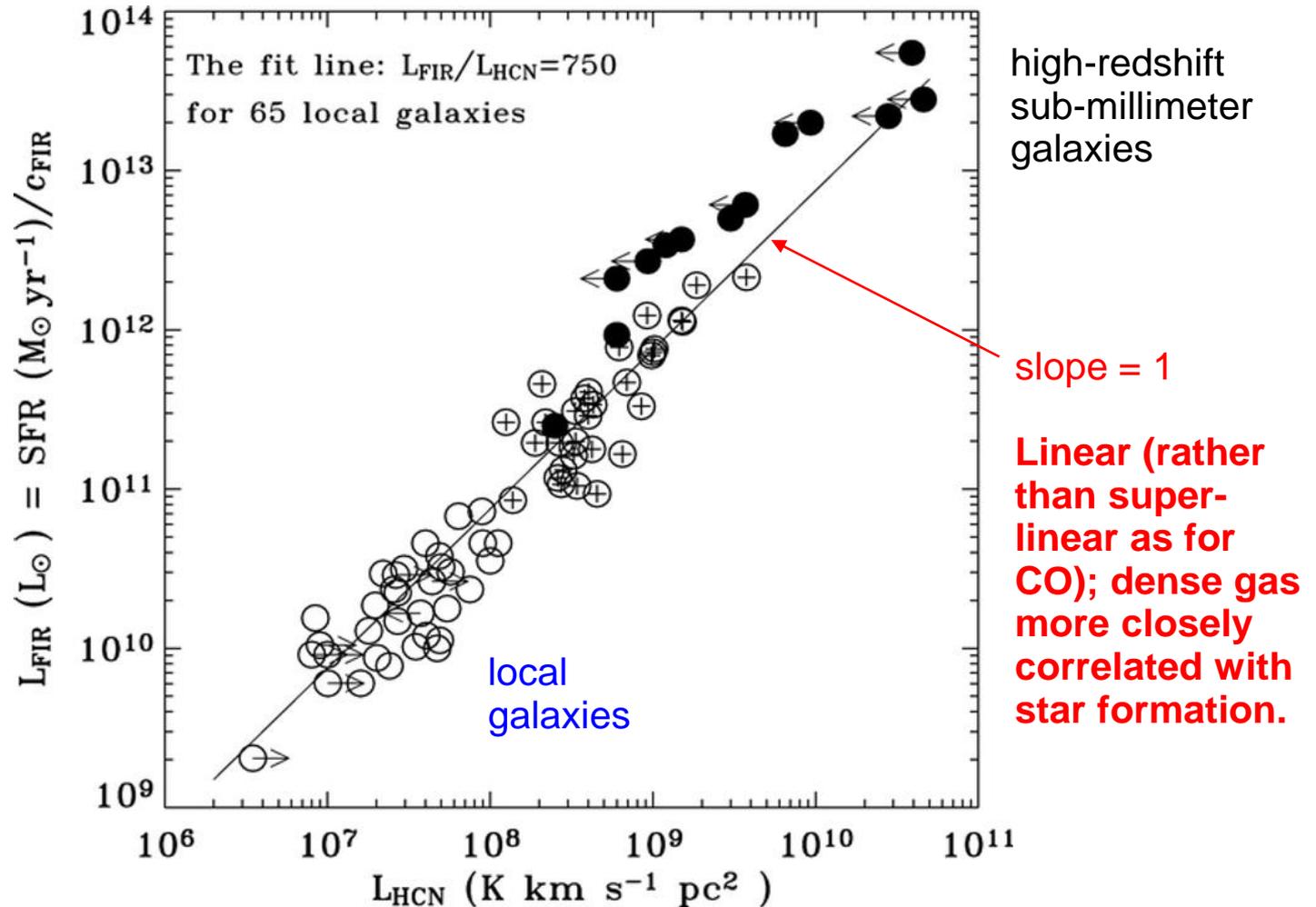
Competition between radiative and collisional de-excitation quantified by ratio C_{ul}/A_{ul}

Critical density n_{crit} for which $C_{ul}/A_{ul} = 1 \sim n(\text{H}_2)T^{1/2} / J^3 m_{el}^2$

where m_{el} = electric dipole moment,
 J = angular momentum quantum number

Because of their higher n_{crit} molecules with larger m_{el} (and higher-order transitions) trace hotter/denser molecular gas.

High-density molecular tracers: HCN(1-0)

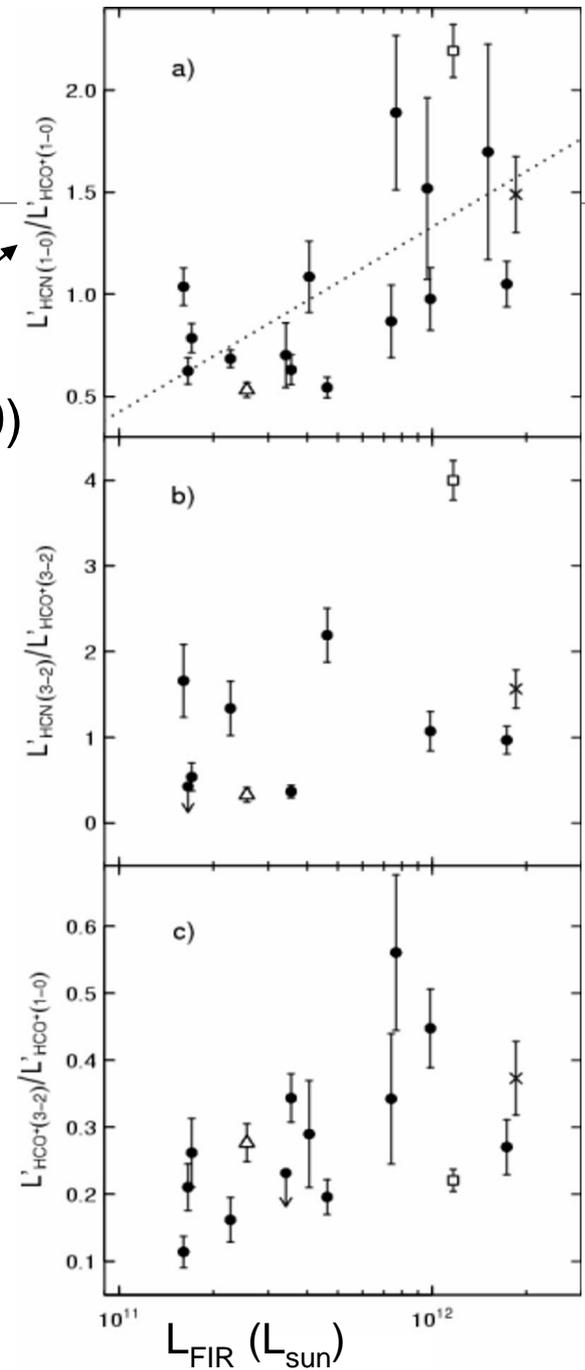


Correlation between IR (\sim SFR) and HCN J=1-0 luminosity (\sim mass of gas above critical density) (Gao & Solomon 2004, Gao+ 2007, see also Wu+ 2005)

High-density tracers: HCO^+

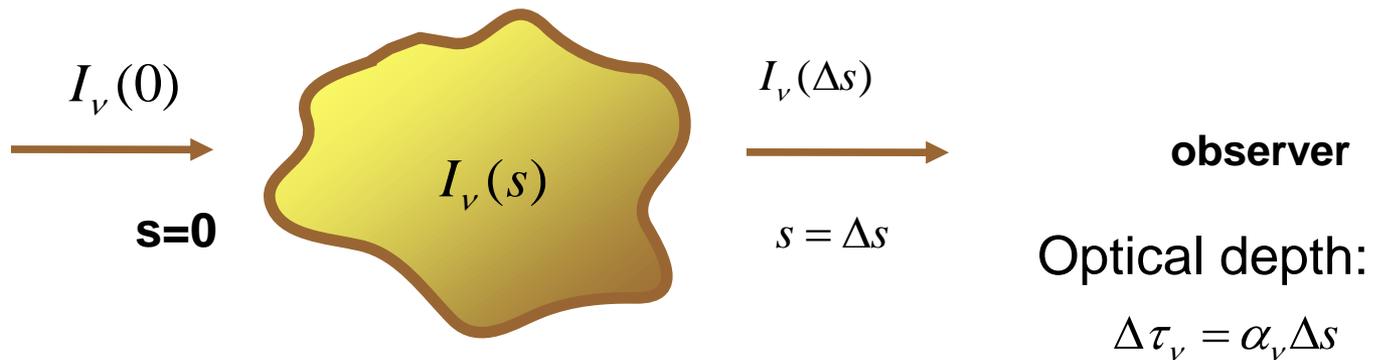
But at high densities (and high $L_{\text{IR}} > 10^{11} L_{\text{sun}}$), because of its higher n_{crit} $\text{HCN}(1-0)$ may be enhanced over other dense-gas tracers such as HCO^+ (Garcia-Carpio+ 2006, 2008).

$\text{HCN}(1-0)/\text{HCO}^+(1-0)$



Optically thin molecular tracers: ^{13}CO

$^{12}\text{C}/^{13}\text{C} \sim 50-70$, i.e. rare; ^{13}C likely optically thin. Thus, unlike ^{12}CO which is optically thick, ^{13}CO can be used to infer column densities $N(^{13}\text{CO})$ and $N(^{12}\text{CO})$, because of the relation between N and optical depth.



I_ν spectral intensity, j_ν spectral emission coefficient, α_ν spectral absorption coefficient.

Radiation transfer equation:
$$\frac{dI_\nu}{ds} = -\alpha_\nu I_\nu + j_\nu$$

Radiation transfer and thermal emission

After dividing by α_ν and substituting for τ_ν , the transfer equation can be written as:

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

where the “source function” is defined as: $S_\nu \equiv \frac{j_\nu}{\alpha_\nu}$

Thus, solution is:

$$I_\nu(\Delta s) = I_\nu(0)e^{-\tau_\nu} + \frac{j_\nu}{\alpha_\nu} [1 - e^{-\tau_\nu}]$$

For *thermal emission*: $j_\nu = \alpha_\nu B_\nu(T)$ (Kirchoff's Law)

and solution becomes:

$$I_\nu(\Delta s) = I_\nu(0)e^{-\tau_\nu} + \frac{2h\nu^3/c^2}{\exp(h\nu/k_B T) - 1} [1 - e^{-\tau_\nu}]$$

Radiative transfer and brightness temperature T_B

Rayleigh-Jeans approximation for low-energy transitions $h\nu \ll kT_B$ so that transfer equation becomes:

$$T_B(\Delta s) = T_B(0)e^{-\tau_\nu(\Delta s)} + T[1 - e^{-\tau_\nu(\Delta s)}]$$

Relate ***differences in intensity*** to ***the measurement unit of brightness temperature, T_B*** , and ***observed antenna temperature, T_A*** , via the Planck function:

$$T_B \equiv \frac{c^2}{2\nu^2 k_B} [I_\nu(\Delta\tau_\nu) - I_\nu(0)]$$

$$T_B = \frac{T_A}{\eta} \left(\frac{\theta_{source}^2 + \theta_A^2}{\theta_{source}^2} \right)$$

where η = main beam efficiency;
 $\mathcal{G}_A, \mathcal{G}_{source}$ = beam, source size

Conversion from T_A
to T_B depends on
source size!

Radiative transfer and “detection equation”

Assuming baseline subtracted (so omit term behind cloud), and remembering that cosmic background radiation is everywhere, we have the difference of two intensities as the “*detection equation*” (see Stahler & Palla 2004; Wilson, Rohlfs, & Hüttemeister 2009):

$$T_B(\nu) = T_0 \left(\frac{1}{e^{T_0/T_{ex}} - 1} - \frac{1}{e^{T_0/2.7} - 1} \right) (1 - e^{-\tau_\nu})$$

where $T_0 = h\nu/k$ [5.5K for $^{12}\text{CO}(1-0)$, 5.3K $^{13}\text{CO}(1-0)$].

One observable for each line: $T_B(\nu)$

Two unknowns for each line: T_{ex} and τ_ν

τ_ν *proportional to* α_ν , *hence to total volume density*; because of the Δs dependence, we can then infer *column density*!

Column density and optical depth of ^{13}CO

Hence need *two observables* (^{13}CO and ^{12}CO) and some *assumptions*:

- ✓ Uniform T_{ex} along the line of sight for $J=1 \rightarrow 0$ transition, and CO lines emitted from the same volume
- ✓ Same T_{ex} for ^{13}CO and ^{12}CO
- ✓ $T_{\text{kin}} = T_{\text{ex}}$ for ^{12}CO , and $\tau(^{12}\text{CO}) \gg 1$
- ✓ $\tau(^{13}\text{CO}) \ll 1$

Recipe



(1) Derive T_{ex} for $^{12}\text{CO}(1-0)$ by assuming $\tau(^{12}\text{CO}) \gg 1$ in det. eq.

(2) With T_{ex} , detection equation can be solved for $\tau(^{13}\text{CO})$

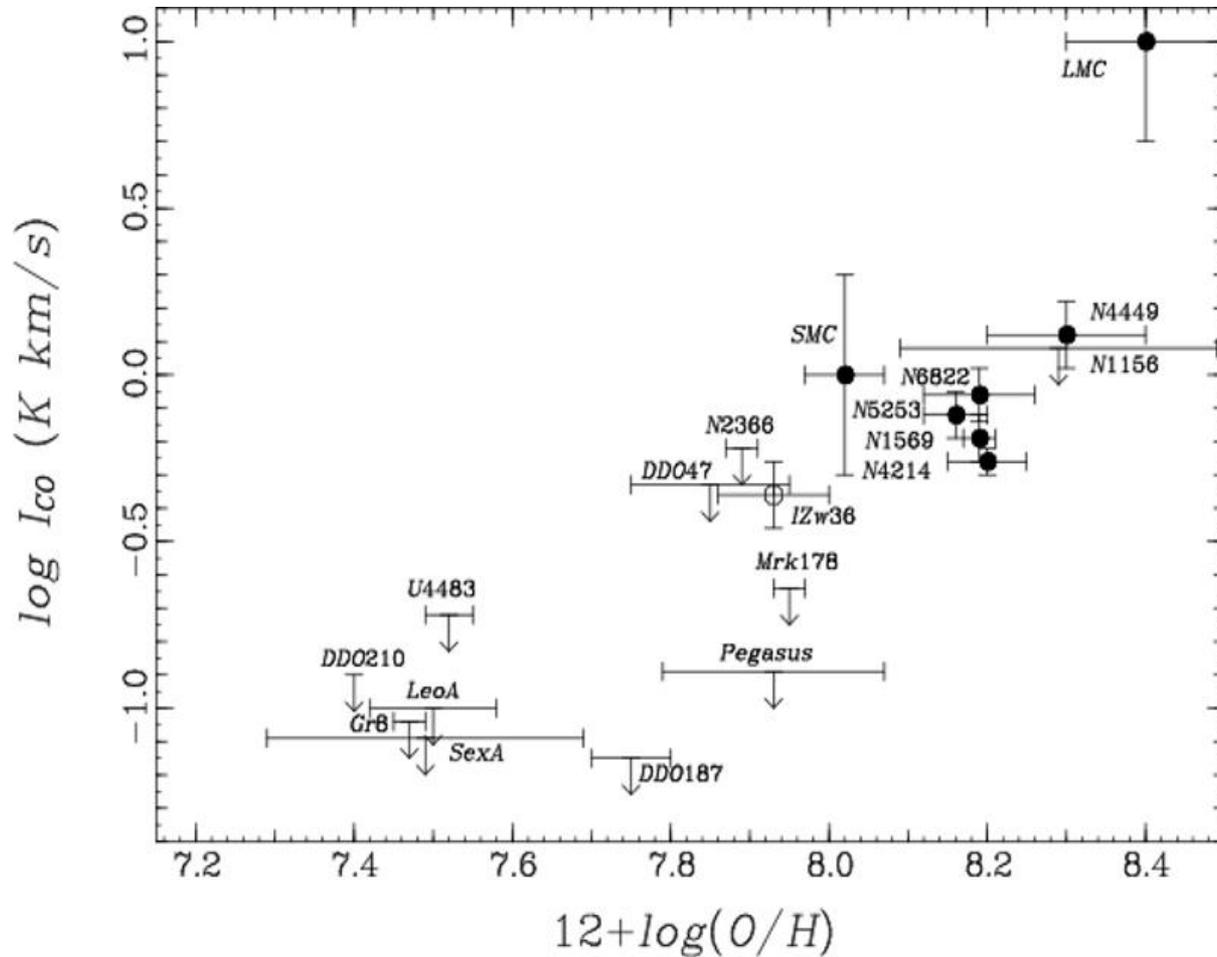
(3) $N(^{13}\text{CO}) \sim \tau(^{13}\text{CO}) f(T_{\text{B}}, T_{\text{ex}}, A_{\text{ul}}, \text{partition})$

(4) $N(^{12}\text{CO})/N(^{13}\text{CO}) = \tau(^{12}\text{CO})/\tau(^{13}\text{CO})$

$N(^{12}\text{CO}) = N(^{13}\text{CO}) \gamma [^{12}\text{C}/^{13}\text{C}]$, where $\gamma < 1$ (fractionation, shielding)

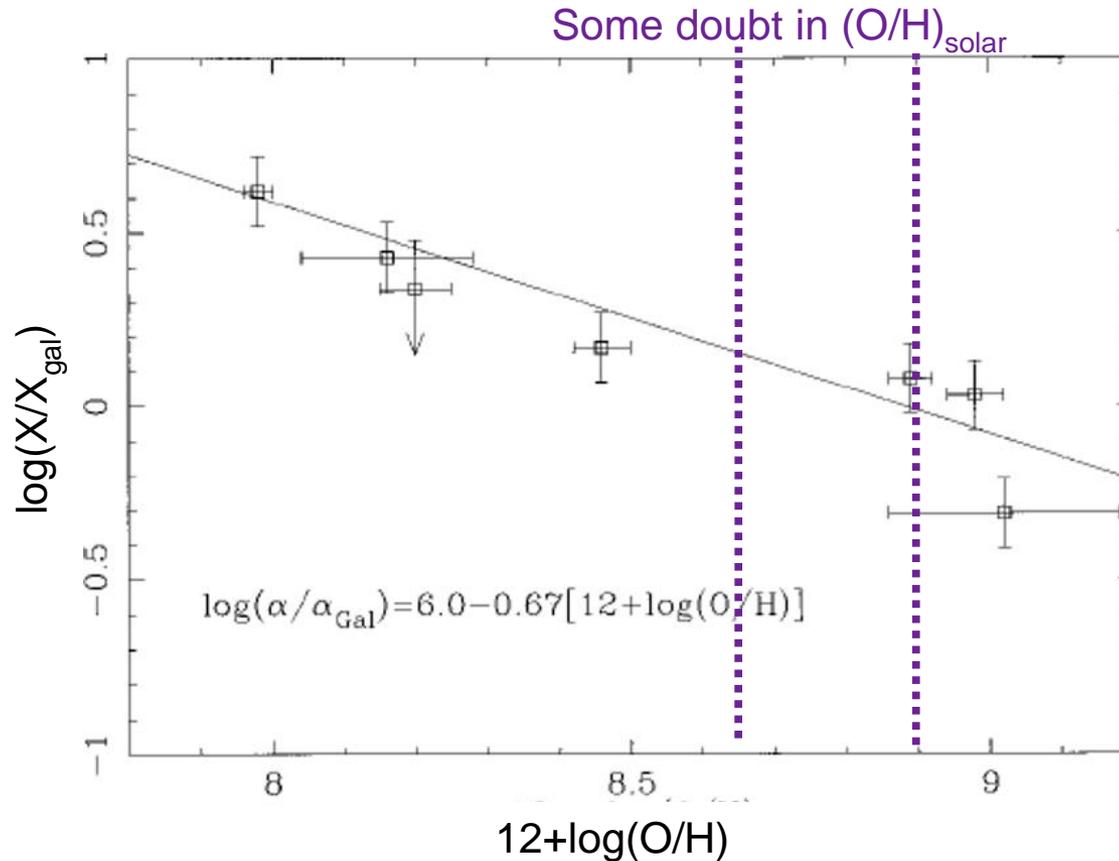
Molecule content at low metallicity

CO deficit in low-metallicity dwarf galaxies



CO intensity vs. oxygen abundance (Taylor+ 1998). Below $12 + \log O/H \sim 8$, virtually impossible to find CO!

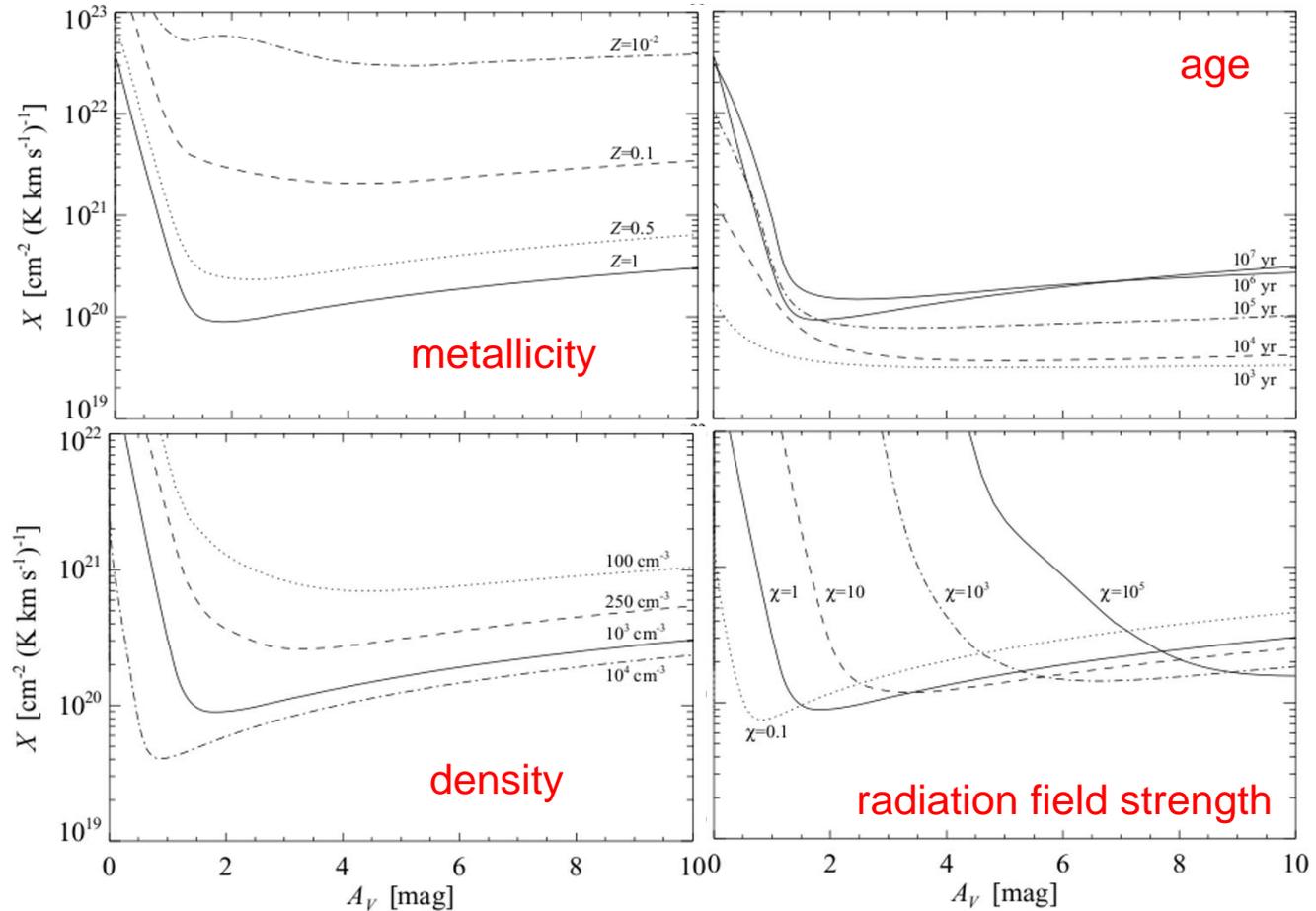
Variation with O/H of CO conversion factor X?



Observationally, resolved CO clouds in Local Group say **yes** (Wilson 1995).

Theoretical arguments (e.g., Maloney & Black 1988) also say **yes**.

Other factors also play a role...



In addition to the dependence of X on O/H and n_e , Bell+ (2006) find **variations with time and with radiation field strength!** Thus geometry of star-forming regions could be important.