9. Molecular Gas

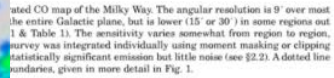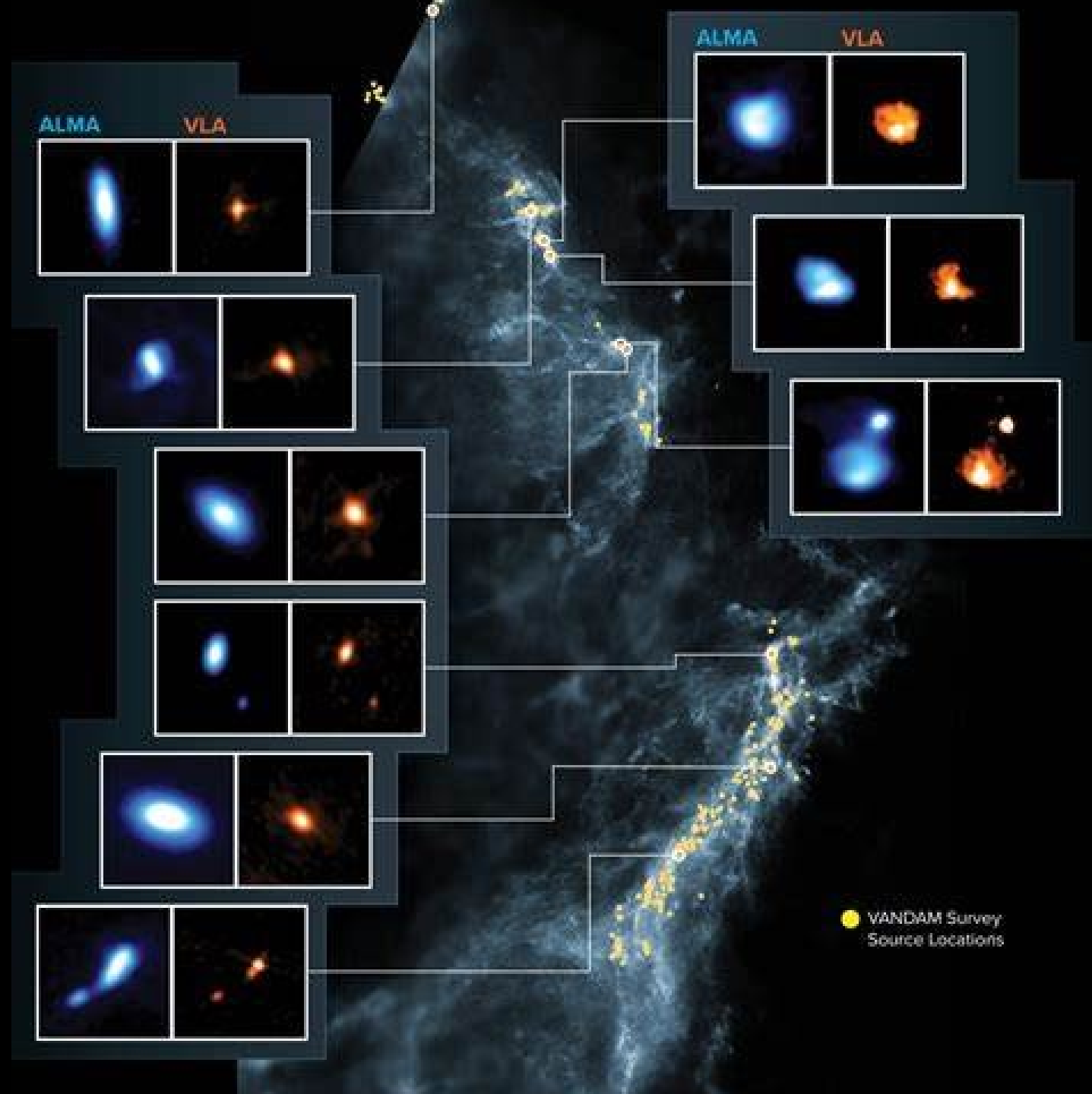Instructor: Hui Li   TA: Chengzhe Li

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Molecular phase is sooooooo fxxking complicated!!!!
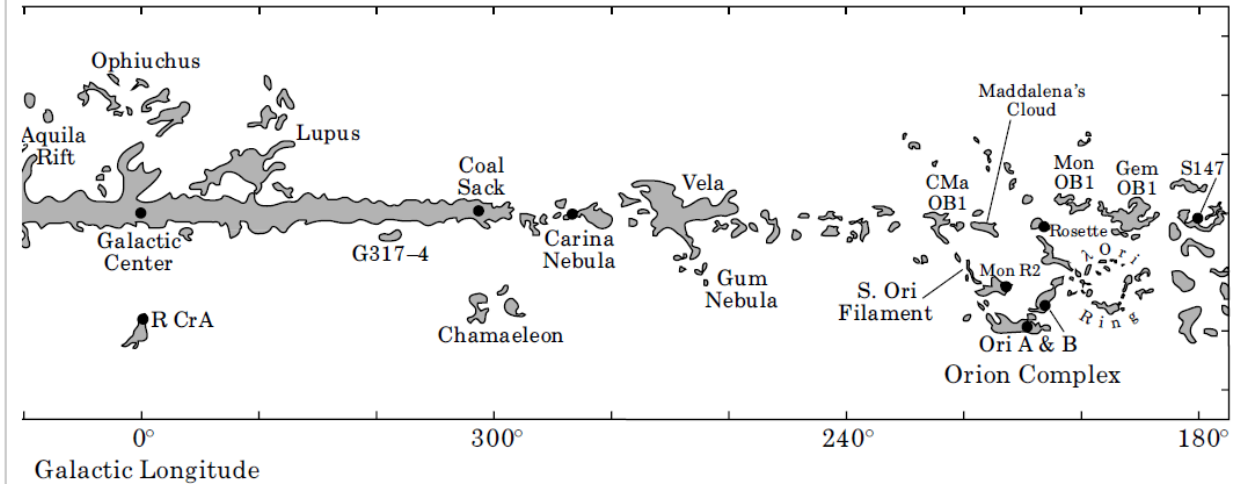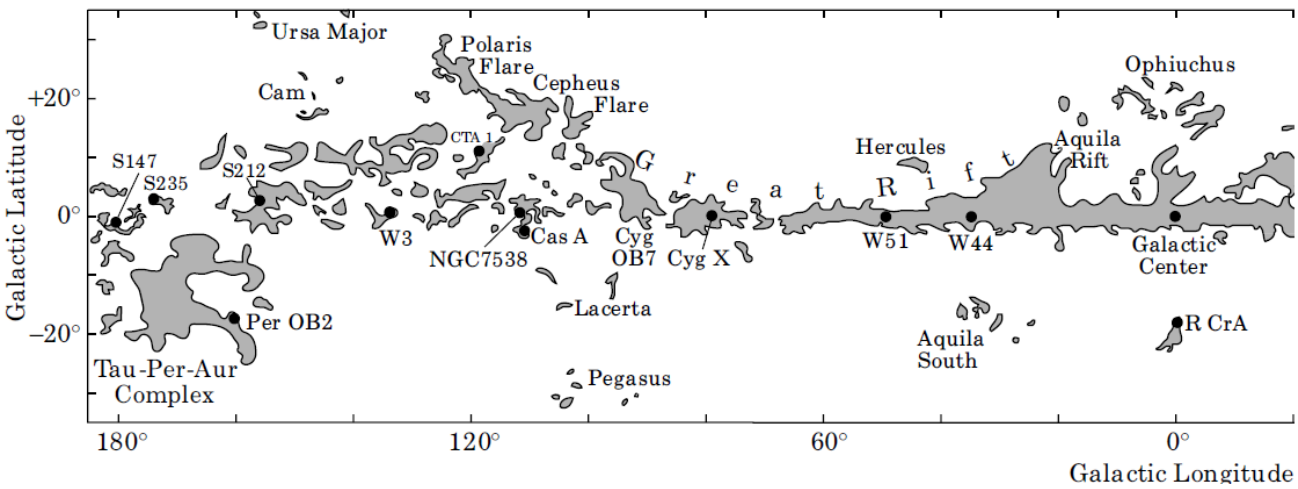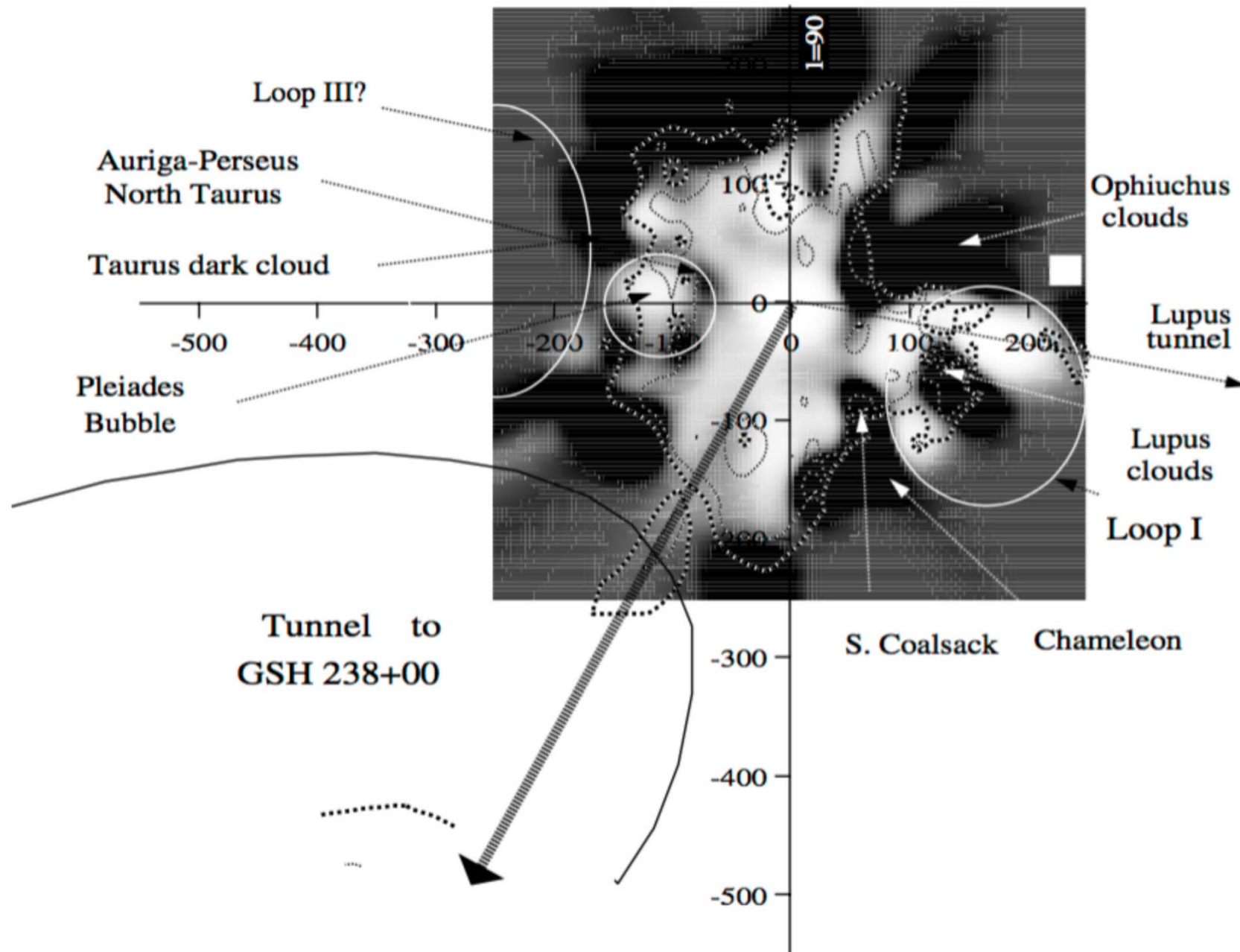
Observations of molecular gas in the ISM

Taurus

Perseus

Orion

Milky Way

ALMA VLA

ALMA VLA

VANDAND Survey
Source Locations

# Observations of molecular gas in the ISM

Cloud Categories and Terminology

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]

Categories	Size (pc)	n_H (cm^{-3})	Mass ($M_\odot$)	Linewidth ($km\,s^{-1}$)	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

Gas distribution in the Milky Way
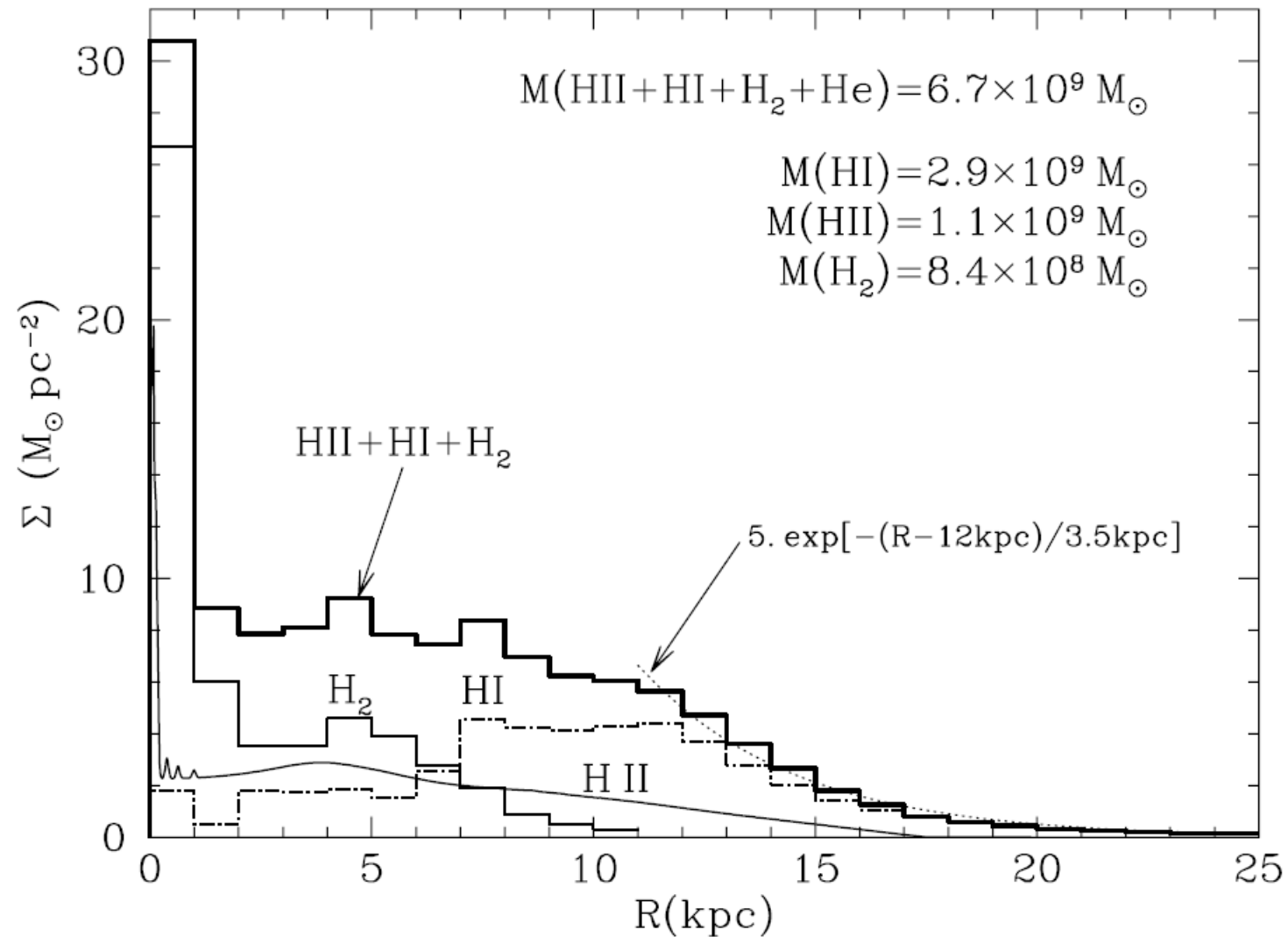
Kennicutt-Schmidt Relation

Larson's relation
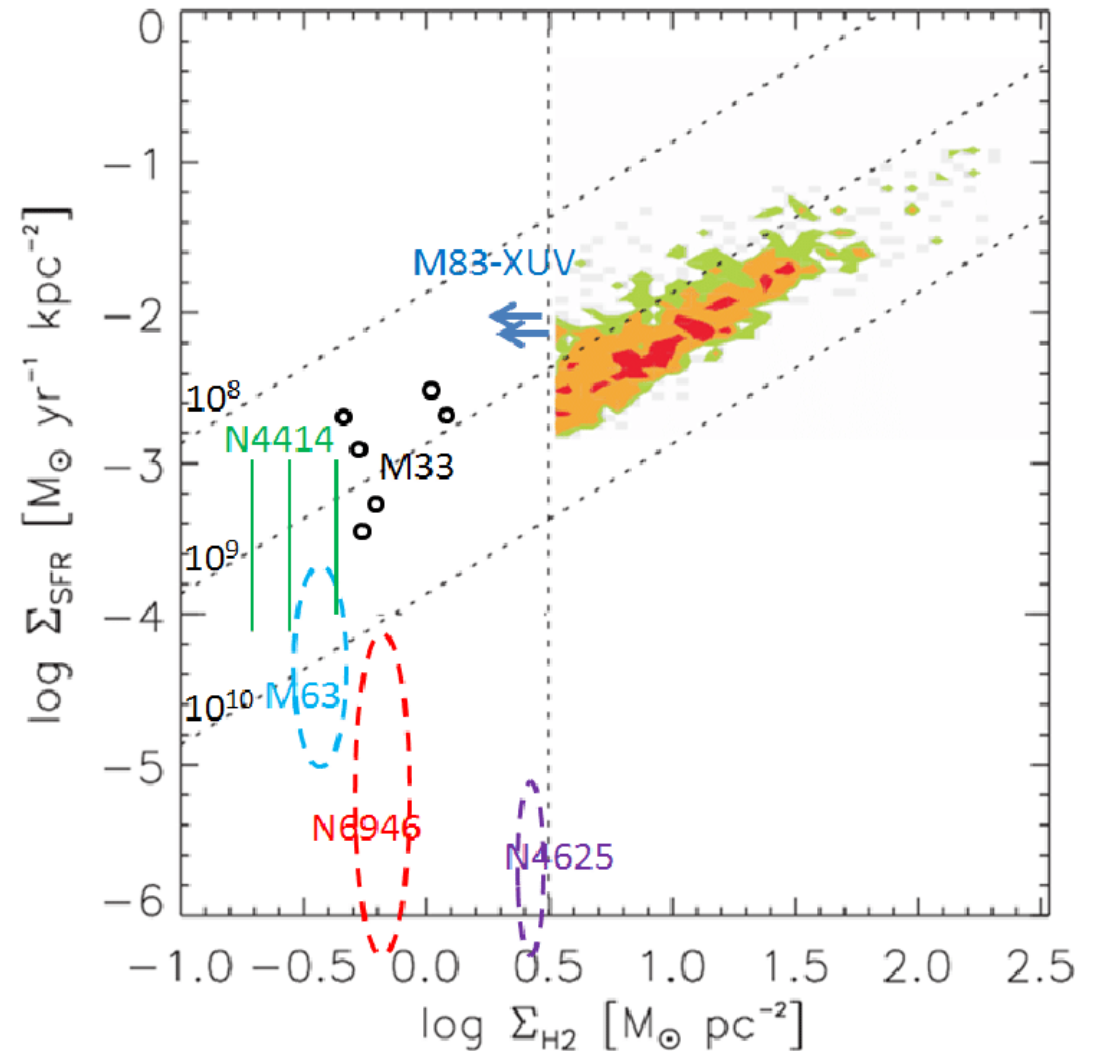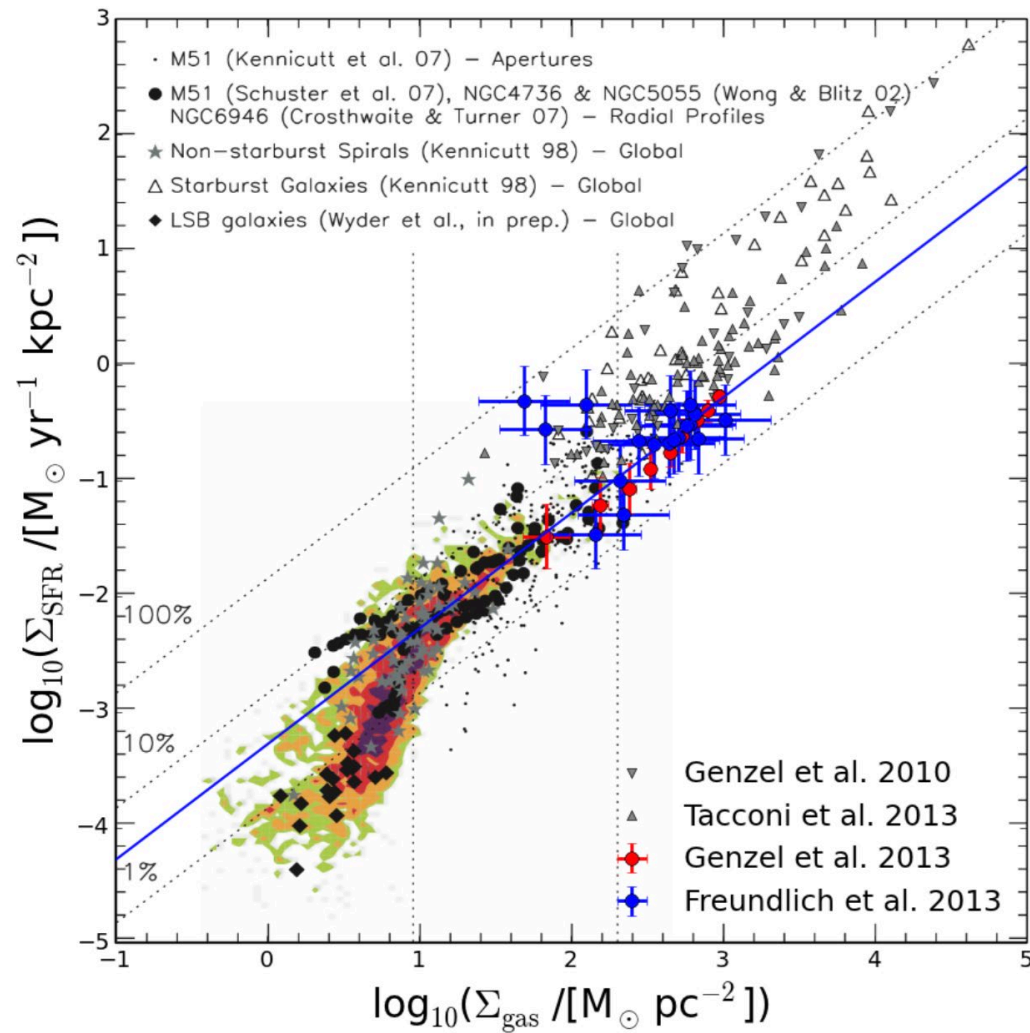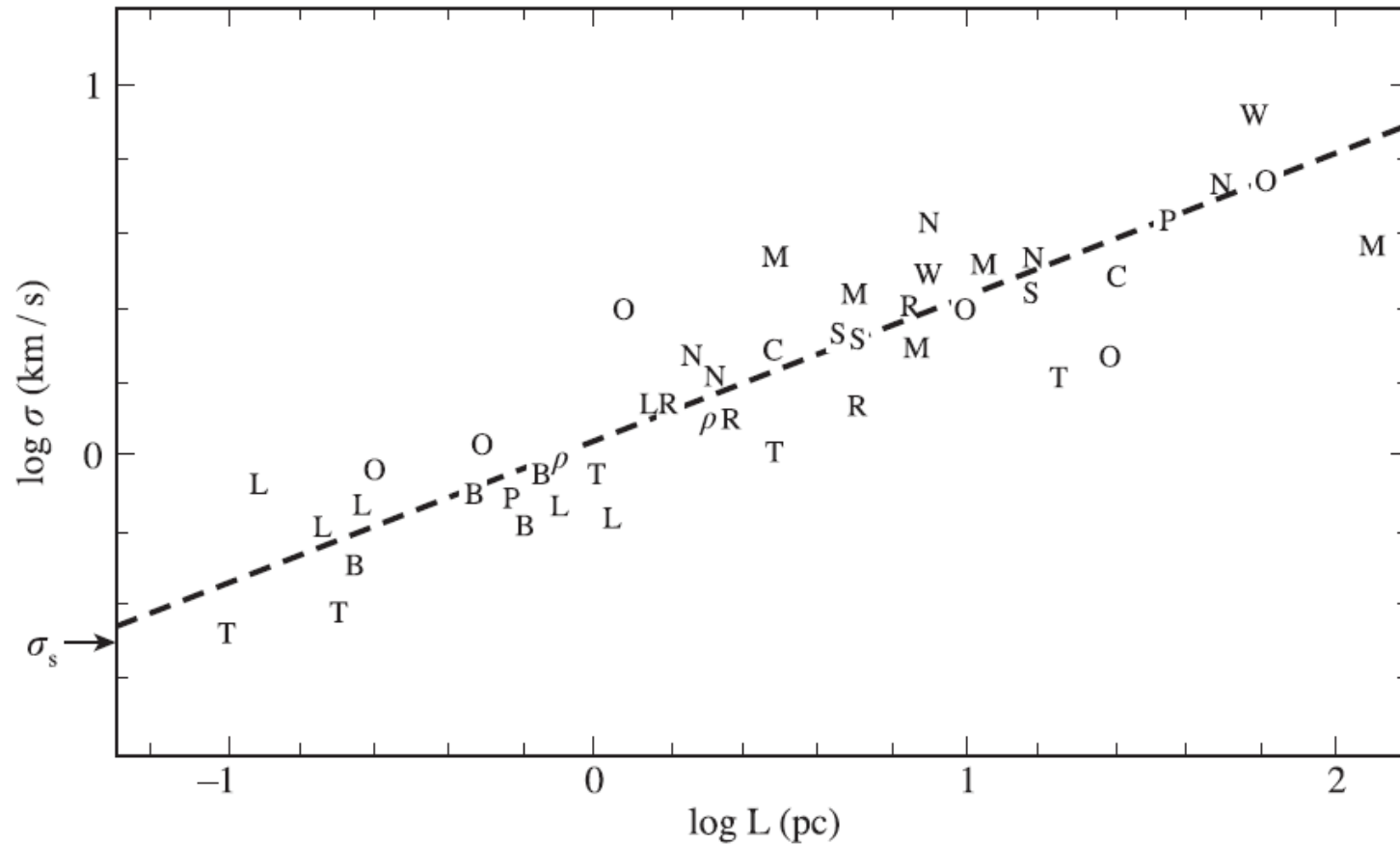
$$\sigma_v \approx 1.10 \, L_{\mathrm{pc}}^{\gamma} \, \mathrm{km \, s^{-1}}$$

$$M \approx \frac{5\sigma_v^2 L}{6G} \approx 230 L_{\mathrm{pc}}^{2\gamma+1} \, M_{\odot}$$

Crutcher's relation: magnetic fields in GMCs
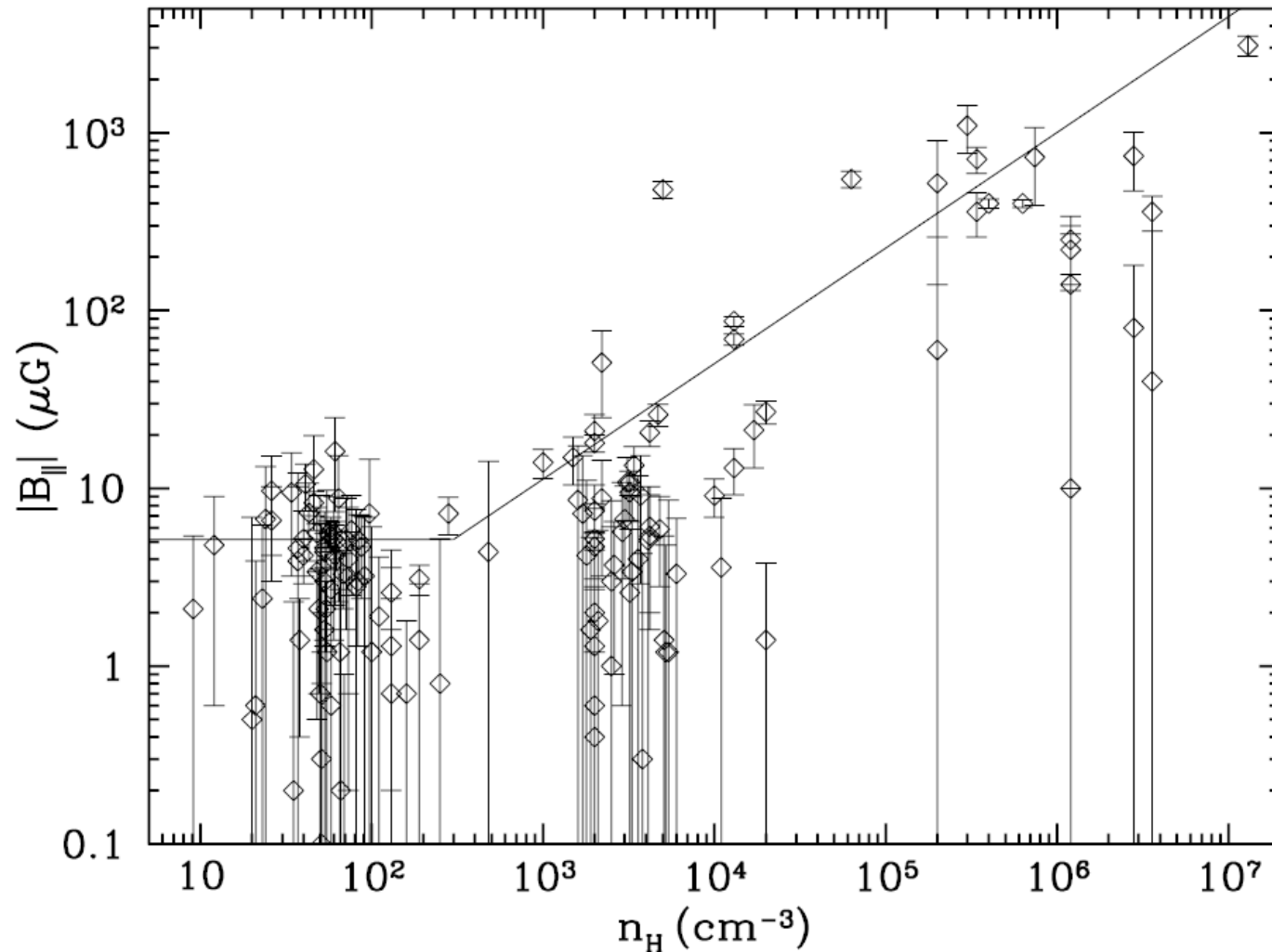
$$B_{0.5} \approx 5\,\mu\mathrm{G} \qquad \text{for } n_4 < 0.03$$
$$\approx 49 n_4^{0.65}\,\mu\mathrm{G} \qquad \text{for } 0.03 < n_4$$

$$\frac{(v_A)_{0.5}}{\sigma_v} \approx 0.85 \left(\frac{n_4}{1.3}\right)^{0.15+\gamma/(2-2\gamma)}$$

Different Probes of Molecular Gas

- Star counts / extinction or dust extinction/IR emission

- Molecular Radio Lines (e.g. 12CO 1-0, HCN, CS etc.)

- Gamma-rays

$$\mathrm{CR}p + p \;\rightarrow\; \mathrm{CR}p + p + \pi^0 \;,$$
$$\pi^0 \rightarrow 2\gamma \quad (\text{pion decay})$$
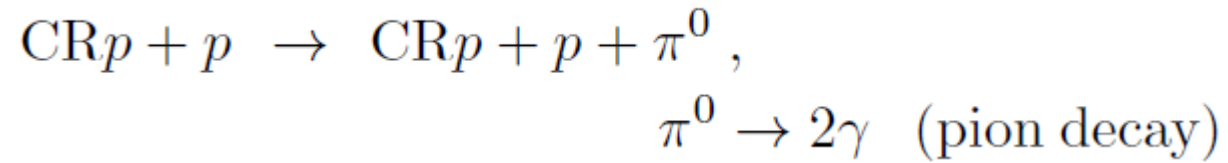
Composition of Molecular Gas

- The ubiquity of hydrogen in the ISM and the inert of helium to form chemical bonds, we expect the molecular gas consists primarily of H2.

- CO is usually the second most abundant molecule with one CO per ~20000 H2.

Molecule	Dissociation energy D_0 [eV]	Equilibrium separation r_0 [Å]	Rotational energy scale B_0 [meV]	Vibrational energy scale $\hbar\omega_0$ [eV]	Electric dipole μ_0 [debye]
H_2	4.48	0.741	7.554	0.546	0.000
CO	11.11	1.128	0.239	0.269	0.112
OH	4.41	0.970	2.345	0.463	1.66
CH	3.47	1.120	1.793	0.355	1.46
CN	7.72	1.172	0.236	0.256	1.45
CS	7.39	1.535	0.102	0.159	1.98

Electronic, Vibrational, and Rotational Levels

- Diatomic molecules can emit and absorb radiation due to electronic transitions.

- In addition, the vibrational quantum levels can be approximated as harmonic oscillators.

$$V(r) \approx V(r_0) + \frac{1}{2}k_s(r - r_0)^2 \qquad \omega_0 = (k_s/m_r)^{1/2}$$

- The vibrational energy level of a diatomic molecule must obey: $E_{vib} = \hbar\omega_0(v + 1/2)$

- The rotational energy levels must obey: $E_{\text{rot}} = \dfrac{\hbar^2}{2I}J(J + 1)$

Energy levels of H₂

The ground state is $X^1 \Sigma_g^+$.

The next state is $b^3\Sigma_u^+$. This state is unbound (electron spin repulsion), but the $\Delta S = 0$ dipole emission selection rule makes a transition between these two states forbidden.

Electronic transitions to the upper singlet levels are allowed; these are important in dissociating the molecule.
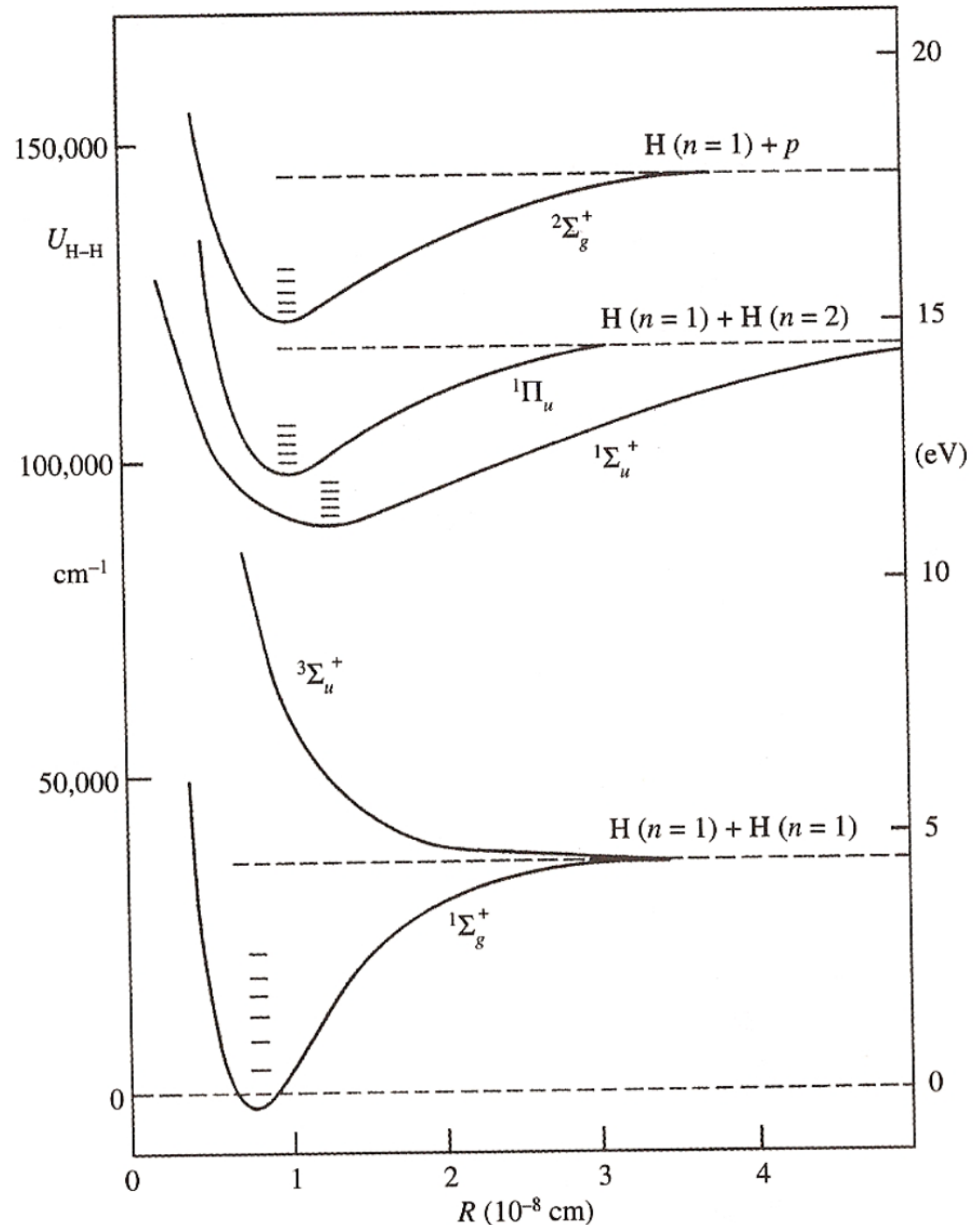
Problems with H$_2$ emission

- An H$_2$ molecule has no permanent electric dipole moment, and cannot produce the strong dipole radiation that is created, for example, by rotating OH and CO molecules.

- H$_2$ (J=1-0) is forbidden because its lack of electric dipole and the lowest permitted rotational transition is H$_2$ (J=2-0). E(J=2-0)=0.044eV (much much larger than typical rotational transition of other molecules) and wavelength 28.2 micro. The Einstein A coefficient is 3e-11/s!!!

- CO has a small but finite dipole moment and a relatively strong rotational and ro-vib transitions.

- CO (J=1-0) has an energy E(J=1-0)=4.8e-4eV, wavelength 2.6mm.

- It has many useful isotopes: 12CO, 13CO, C17O, C18O.

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

CO radiative transfer

- In the most general case with background source and CO emission and absorption, the solution of the radiative transfer equation is

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

$$\sigma_{01} = \frac{g_1}{g_0} \frac{c^2}{8\pi \nu_{10}^2} A_{10} \Phi_\nu$$

- The source function depends on the emissivity and absorption coefficient.

$$j_\nu = n_1 \frac{A_{10}}{4\pi} h\nu_{10} \Phi_\nu \qquad \kappa_\nu = n_0 \sigma_{01} \left[1 - \frac{g_0}{g_1}\frac{n_1}{n_0}\right] = n_0 \sigma_{01} \left[1 - \exp\left(-\frac{h\nu_{10}}{kT_{\text{exc}}}\right)\right]$$

- With the expression of the cross-section and assumed line profiles, the source function can be derived as

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

Excitation temperature of CO

- For CO (J=1-0) with energy $E_{10} = 0.4767\,\mathrm{meV}$ or temperature of 5.532 K, the dominant background radiation is the CMB.

$$I_\nu = B_\nu(T_{\mathrm{rad}}) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT_{\mathrm{rad}}} - 1}$$

- The critical density of CO (J=1-0) is

$$n_{\mathrm{crit}} = \frac{(1 + \bar{n}_\gamma)A_{10}}{k_{10}} \approx 2000\,\mathrm{cm}^{-3}\left(\frac{T_{\mathrm{gas}}}{15\,\mathrm{K}}\right)^{-0.2}$$

- For the central dense molecular cores with n>c_crit, collisional excitation dominates.

- For more diffuse regions with n<c_crit, radiative excitation dominates.

$$2.7K \sim T_{rad} < T_{exc} < T_{gas} \sim 15K$$

CO on-and-off strategy

- When we turn our radio antenna toward a molecular cloud, we detect an intensity

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

- When we "chop" our antenna over to a blank region of sky, we detect nothing but CMB

$$I_\nu(\text{off}) = \frac{2h\nu^3}{c^2}\frac{1}{\exp(h\nu/kT_{\text{rad}}) - 1}$$

- The difference between the two observations is

$$\Delta I_\nu = I_\nu(\text{on}) - I_\nu(\text{off})$$

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

Optically thin vs thick treatments

- If the emission is optically thin, the antenna temperature over the whole line profile depends linearly on the column density of the tracer and a weak excitation temperature dependence.

- On the other hand, if the emission is optically thick, we are only probing the surface of the molecular structure, and the antenna temperature is only a function of excitation temperature.

Optical depth of 12CO (J=1-0)

- Consider only thermal broadening of CO lines $\quad \tau_\nu = \int \kappa_\nu ds = \tau_0 e^{-v^2/b^2}$

- The line center optical depth is

$$\tau_0 = \frac{1}{(4\pi)^{3/2}} \frac{g_1}{g_0} \frac{c^2}{\nu_{10}^3} A_{10} \left[1 - e^{-h\nu_{10}/kT_{\text{exc}}} \right] \frac{c}{b} N_0$$

$$\approx 0.90 \left(\frac{T_{\text{gas}}}{15\,\text{K}} \right)^{-1/2} \left[1 - e^{-5.532\,\text{K}/T_{\text{exc}}} \right] \left(\frac{N_0}{10^{14}\,\text{cm}^{-2}} \right)$$

- From N_0 for CO to N_H for molecular hydrogen, we find that the transition column density from optically thin to thick is $N_H \sim 1e19/cm2$. (Lyman alpha: $1e12/cm2$; HI 21cm: $1e21/cm2$)

$$N_0 = 2.1 \times 10^{-5} N_H \left(\frac{n_C/n_H}{2.7 \times 10^{-4}} \right) \left(\frac{F_{CO}}{0.25} \right) \left(\frac{f_0}{0.31} \right)$$

How to proceed from CO observations to H2 component?

- From optically thick 12CO (J=1-0), we obtain the excitation temperature of the gas.

- From the optically think 13CO (J=1-0), by assuming the excitation temperature is the same for both lines, we obtain the column density of 13CO.

- From 13CO, column density, we obtain the H2 column density with a sequence of conversion factors!

$$N(\mathrm{H_2}) \approx \frac{1}{2} \times 3700 \times 4 \times 92 \times 3.2 \times N_0(^{13}\mathrm{CO}) \approx 2.2 \times 10^6 N_0(^{13}\mathrm{CO})$$

- The overall conversion factor from a specific molecular tracer to H2 is called X-factor!

$$X_{\mathrm{CO}} \equiv \frac{N(\mathrm{H_2})}{W_{\mathrm{CO}}} \qquad\qquad W_{\mathrm{CO}} \equiv \int T_A(^{12}\mathrm{CO})dv$$

Revisit the optical depth of 12CO

- Radiative trapping: for some species X, a photon emitted in a transition $Xu \rightarrow Xl$ will have a high probability of being absorbed by another Xl somewhere nearby, and a low probability of escaping from the emitting region. (the most extreme cases are called Case A and Case B.)

- It has two effects: (1) it reduces the emission in the $Xu \rightarrow Xl$ 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).

- Escape probability approximation: uniformly excitation & on-the-spot approximation.

- The effective rate equation can be simply expressed by replacing A with effective A!

$$\frac{dn_u}{dt} = n_c k_{\ell u} n_\ell - n_c k_{u\ell} n_u - \langle \bar{\beta} \rangle A_{u\ell} n_u + n_\ell \frac{g_u}{g_\ell} \langle \bar{\beta} \rangle A_{u\ell} n_\gamma^{(0)} \left(1 - \frac{n_u g_\ell}{n_\ell g_u} \right)$$

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

Spherical static clouds

- it is approximately the fraction of the cloud mass that is within optical depth ~2/3 of the cloud surface.

- Photons emitted near the surface have a high probability of escape.

- Photons emitted at the center have a negligible escape prob.

- The critical density for a level u is also reduced because of radiative trapping.

$$n_{\mathrm{crit},u}(c) \equiv \frac{\sum_{\ell<u} \langle \bar{\beta}_{u\ell} \rangle A_{u\ell}}{\sum_{\ell<u} k_{u\ell}(c)}$$

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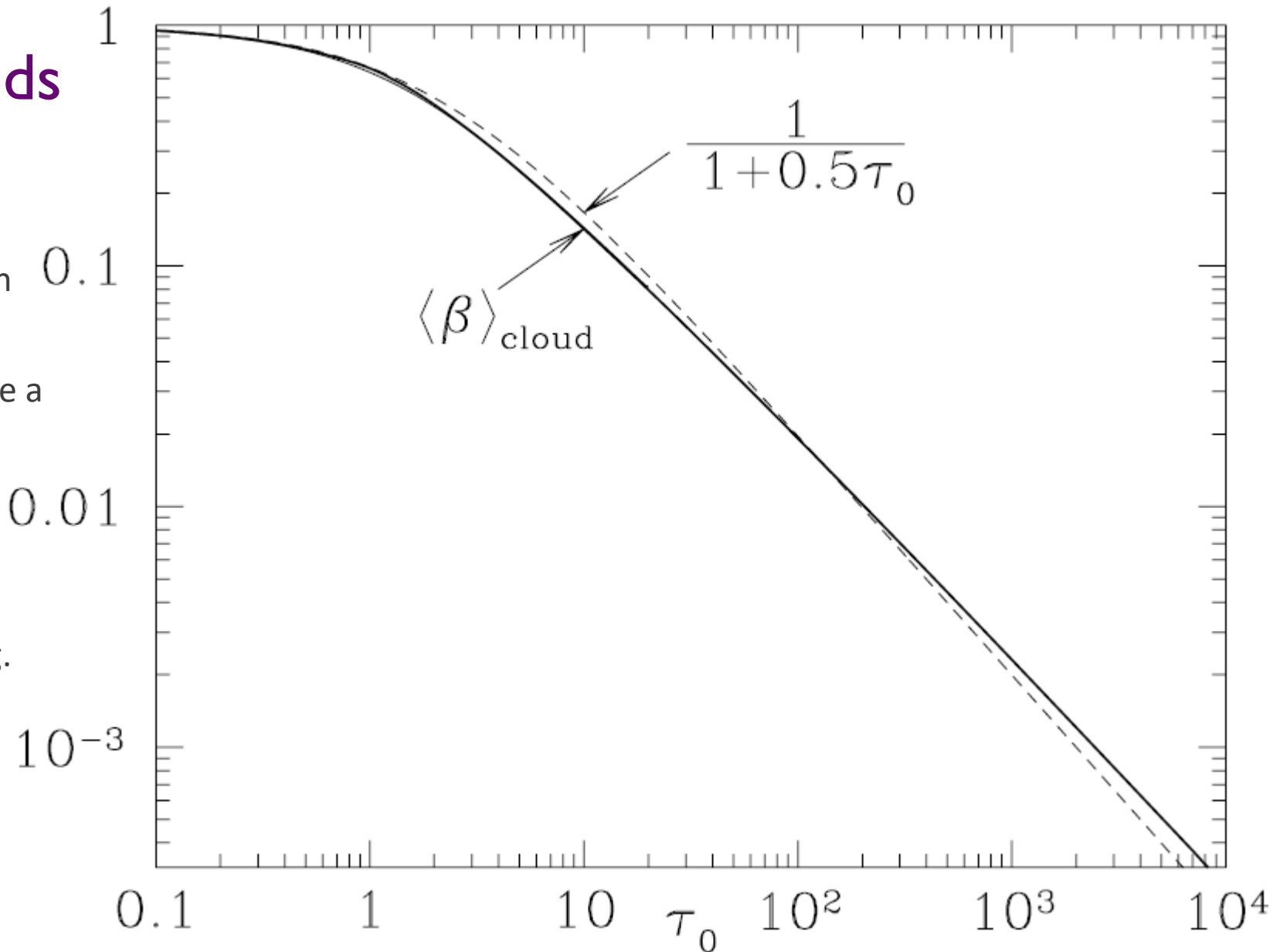
$$\langle \beta \rangle_{\mathrm{cloud}}$$

Sobolev (large velocity gradient; LVG) approximati

- Recall from the Larson's relation that molecular clouds are highly supersonic!

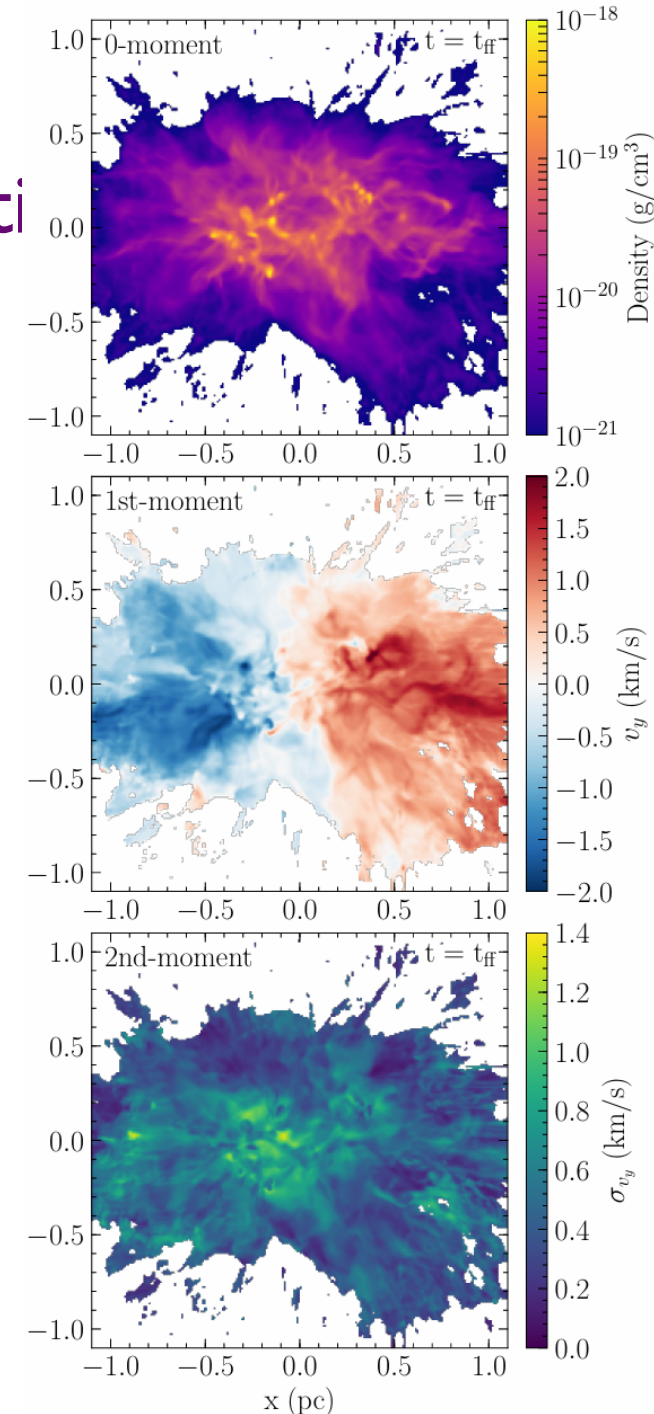- The previous estimated optical depth considered only static case.

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

- Optical depth is only relevant to nearby gas within Sobolev length:

$$S = \frac{v_t}{(dv_s/ds)} \sim \frac{v_t}{(v/R)} \sim v_t \tau_{tub}$$

- Only need to calculate the escape prob over S when evaluating tau.

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

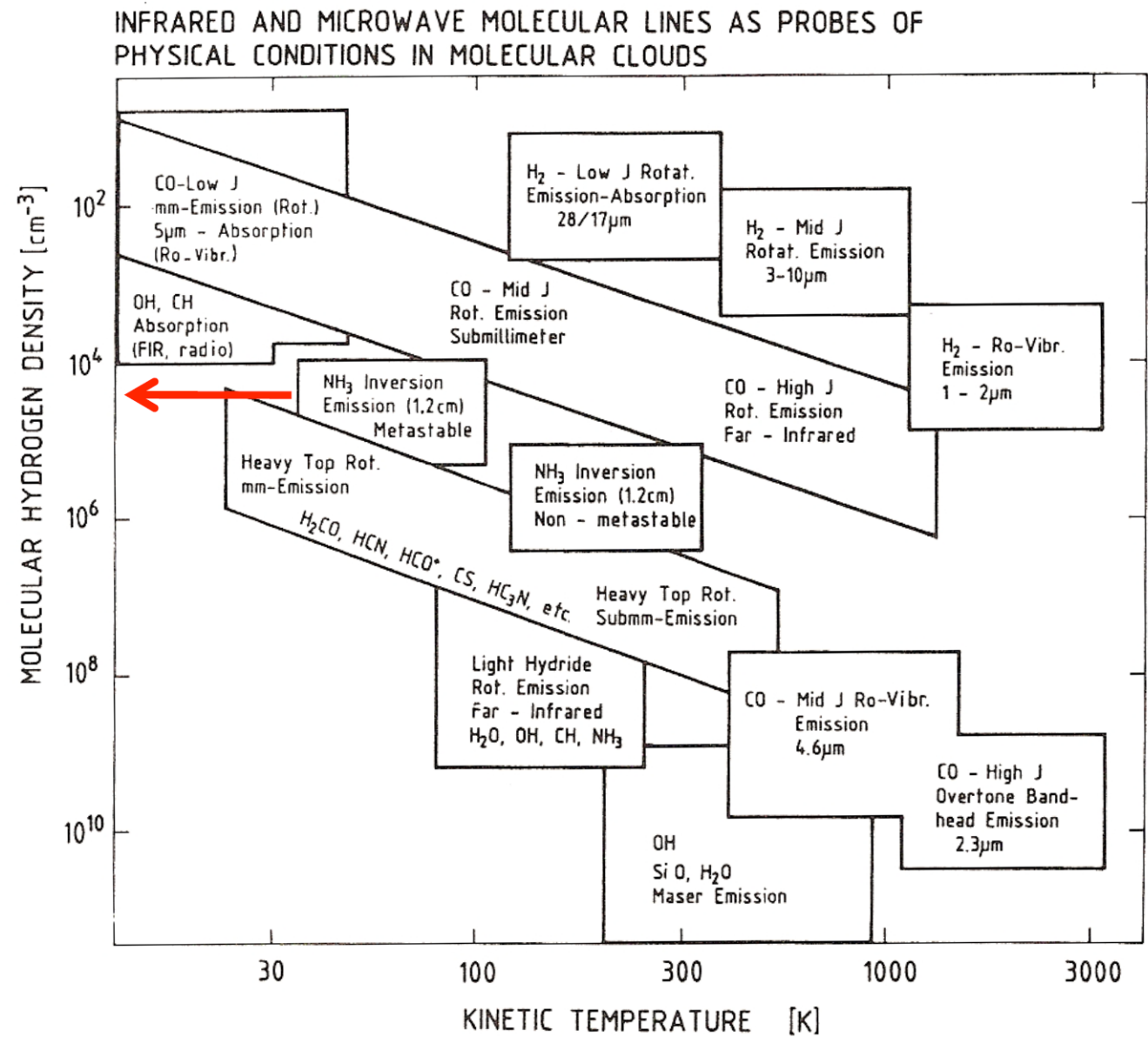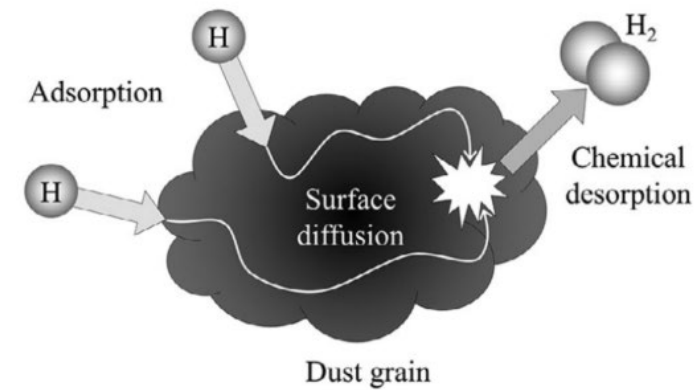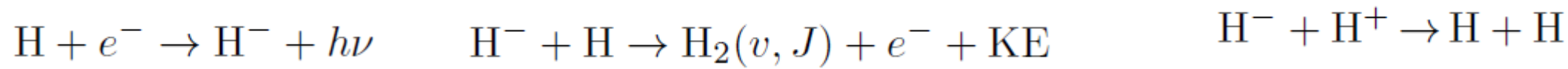# Molecular tracers for different rho and T

Genzel 1990, NATO ASI 342 (Lada & Kylafis, eds)

Molecular chemistry and ionization

H2 formation

- When two free H atoms approach one another, there is no electric dipole radiation that could remove energy from the system and leave the two H atoms in a bound state.

- The rate coefficient for $\mathrm{H+H} \rightarrow \mathrm{H_2}+h\nu$ is therefore so small and therefore can be ignored.

- The threr-body reaction $\mathrm{3H} \rightarrow \mathrm{H_2} + \mathrm{H} + \mathrm{KE}$ can occur, but it depends on nH^3.

- Gas-phase H2 formation depends on H-, which is really rare because of its rapid destruction!

$$\mathrm{H} + e^- \rightarrow \mathrm{H}^- + h\nu \qquad \mathrm{H}^- + \mathrm{H} \rightarrow \mathrm{H_2}(v, J) + e^- + \mathrm{KE} \qquad \mathrm{H}^- + \mathrm{H}^+ \rightarrow \mathrm{H} + \mathrm{H}$$

- Grain catalysis is the key to the formation of H2: 1) a first H atom arrives at a grain and becomes bound to the grain surface; 2) it happens to arrive at a site where it is bound strongly enough that it becomes "trapped"; 3) another H is also trapped at the same location and collides with the existing H atom; 4) They form H2 with exothermal reaction and release 4.5 eV energy that free them from dust surface.

Photodissociation of H2

Photodissociation ($H_2 + h\nu \rightarrow H + H + KE$) is the principal process destroying interstellar H_2 in galaxies. The first step in H_2 photodissociation is absorption of a resonance line photon, raising the H_2 from an initial level $X(v, J)$ of the ground electronic state $X\,{}^1\Sigma_g^+$ to a level $B(v, J)$ or $C(v, J)$ of the first and second electronic excited states, $B\,{}^1\Sigma_u^+$ and $C\,{}^1\Pi_u$. The original photoexcitation is via a permitted absorption line, and therefore the newly excited level $B(v', J')$ or $C(v', J')$ is guaranteed to have electric dipole-allowed decay channels. In general, the excited level $B(v', J')$ or $C(v', J')$ is most likely to decay to vibrationally excited bound levels $X(v'', J'')$ of the ground electronic state, and such decays occur $\sim 85\%$ of the time. Sometimes, however, spontaneous decay of the excited level $B(v', J')$ will be to the **vibrational continuum** of the ground electronic state: the H_2 molecule will fly apart in $\sim 10^{-14}$ s, separating into two free H atoms. Each electronically excited level u has some probability $p_{\mathrm{diss},u}$ of spontaneous decay to the vibrational continuum.
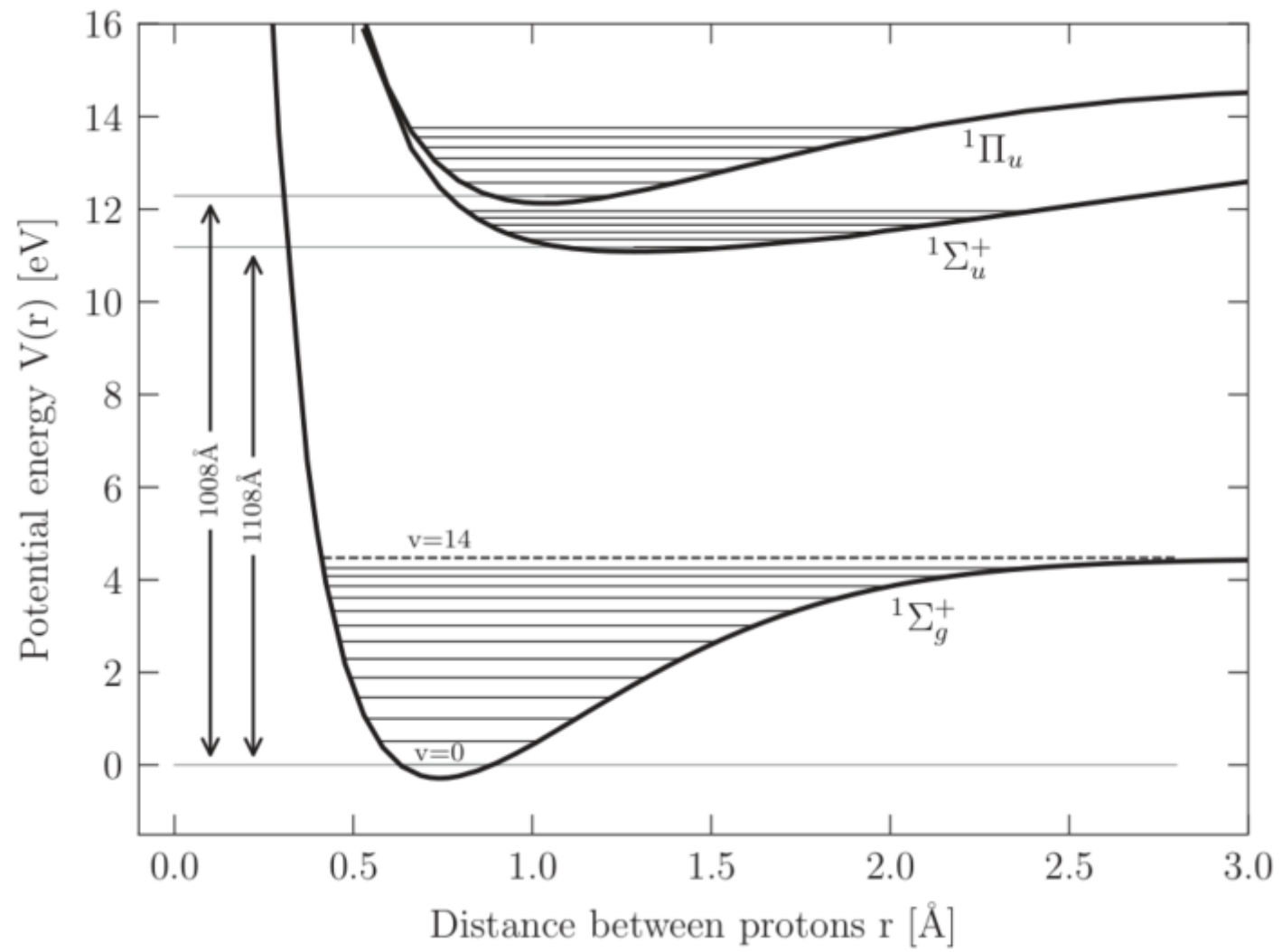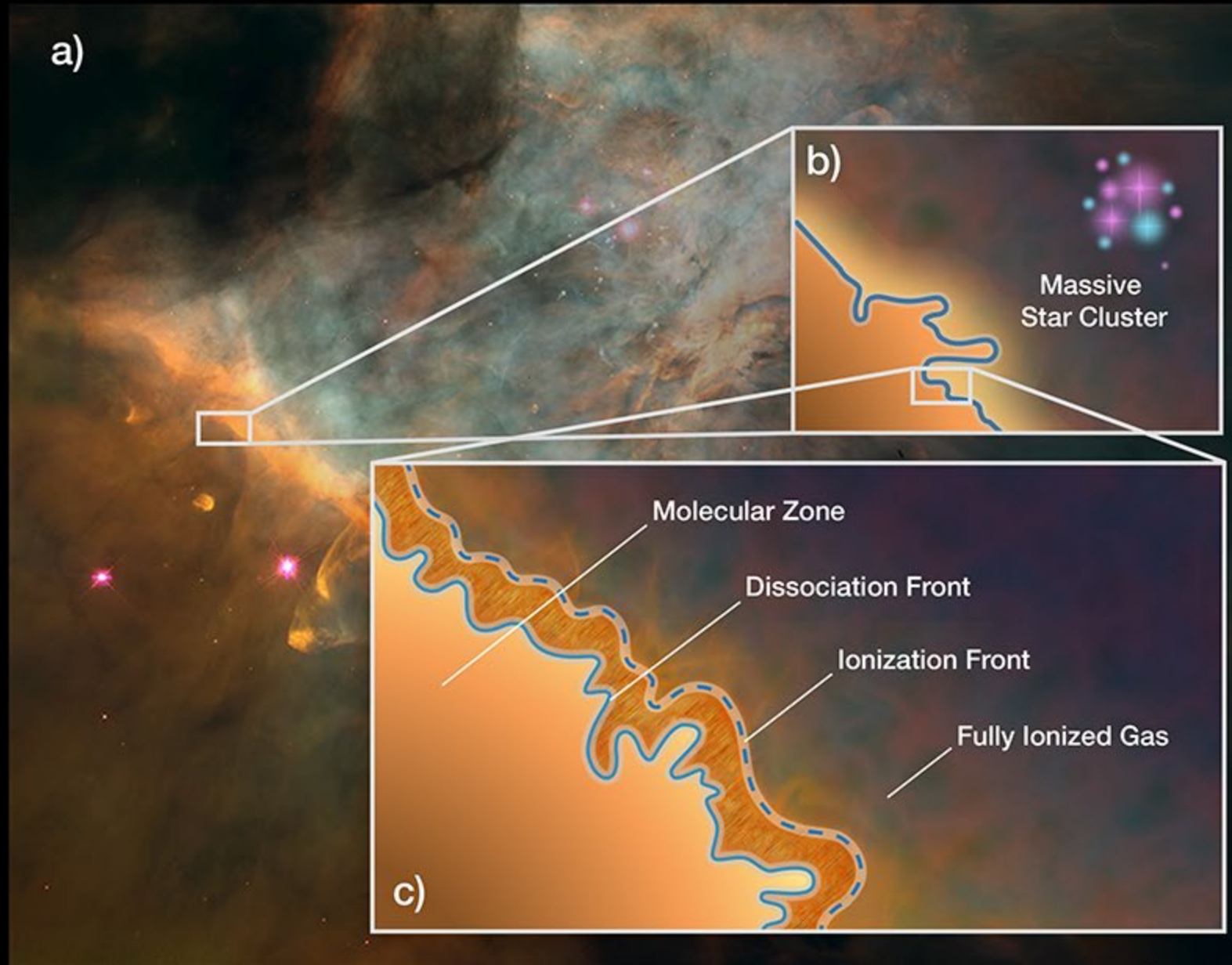
Self-Shielding of H₂
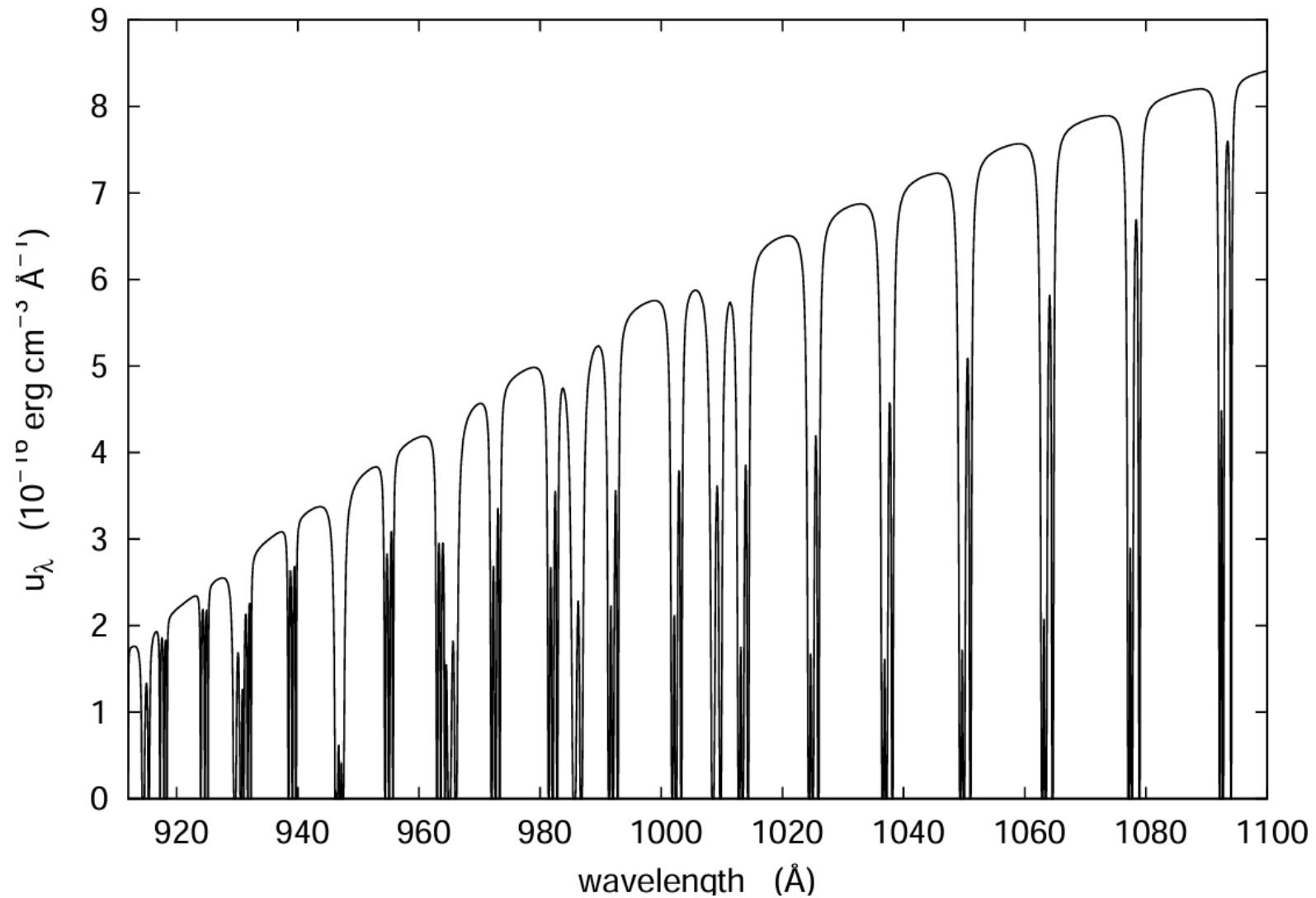
Structu

Anatomy of a Photodissociation Region

Formation of CO molecules

$$C^+ + H_2 \rightarrow CH_2^+ + h\nu \quad , \quad k_{33.6} = 5.0 \times 10^{-16} T_2^{-0.2} \, \mathrm{cm^3 \, s^{-1}} \, ,$$

$$CH_2^+ + e^- \rightarrow \begin{cases} CH + H & (25\%) \\ C + H_2 & (12\%) \\ C + H + H & (63\%) \end{cases} , \, k_{33.7} = 1.24 \times 10^{-6} T_2^{-0.60} \frac{\mathrm{cm^3}}{\mathrm{s}}$$

- Which is the key/bottleneck reaction?

$$CH + O \rightarrow CO + H \quad k_{33.8} = 6.6 \times 10^{-11} \, \mathrm{cm^3 \, s^{-1}} \, ,$$

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

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

$$CH_2^+ + h\nu \rightarrow \begin{cases} CH + H^+ & (1/3) \\ CH^+ + H & (1/3) \\ C^+ + H_2 & (1/3) \end{cases} , \, k_{33.11} = 1.38 \times 10^{-10} \, \mathrm{s^{-1}},$$

$$CH_2^+ + H_2 \rightarrow CH_3^+ + H \, , \quad k_{33.12} = 1.60 \times 10^{-9} \, \mathrm{cm^3 \, s^{-1}} \quad .$$