MOLECULAR COMPONENT

①

H_2 is the dominant species in MCs, but it does not emit (no permanent dipole) ⇒ we use other molecules as indirect tracers. Most important: CO and isotopes

^{12}CO, ^{13}CO, $C^{18}O$, $C^{17}O$, CS, HCN, HCO^+, NH_3, etc.

These probe different parts (densities) of MCs.

Overview of molec. spectroscopy

Born + Oppenheimer approx.: The dynamics and interaction w/ radiation of e and nuclei can be treated separately

$m_e \ll m_p$ ⇒ less inertia to react to $\vec{E}$ field

$$\omega_{pe}^2 = \frac{4\pi n_e e^2}{m_e}$$

$$\omega_{p_i}^2 = \frac{4\pi n_i e^2}{m_i}$$

→ plasma and ion freqs.

$\omega_{pi} \ll \omega_{pe}$

$$n_e \simeq n_i \sim \frac{1}{a_0^3} = \frac{1}{\left(\hbar^2/m_e e^2\right)^3}$$

$a_0 = \frac{\hbar^2}{m_e e^2}$ Bohr radius

$$E_{\text{vib, molec.}} \sim \hbar\omega_{pi} \sim \frac{\hbar}{a_0^{3/2}} \frac{e}{m_i^{1/2}}$$

$$E_{\text{vib},e} \sim \hbar\omega_{pe} \sim \frac{\hbar}{a_0^{3/2}} \frac{e}{m_e^{1/2}}$$

$$\Rightarrow E_{\text{vib, mol}} \sim \left(\frac{m_e}{m_i}\right)^{1/2} E_{\text{vib},e}$$

Rotation: $p \sim \frac{\hbar}{a_0}$ $\qquad E_{rot,mol} \sim \frac{p^2}{2m_i} \sim \frac{m_e}{m_i} E_{elec.}$

↑ quantiz. of angular mom.

$E_{elec} \sim$ a few eV, $\frac{m_e}{m_i} \sim 10^{-3}$,

$E_{rot,mol} \sim \frac{m_e}{m_i} E_{elect}$; $E_{vib,mol} \sim \left(\frac{m_e}{m_i}\right)^{1/2} E_{elect}$; $E_{elec} \sim E_{atom}$

$E_{rot,mol} \sim 0.001$ eV $\qquad E_{vib} \sim 0.01$ eV -0.1

Radio $\qquad$ IR

The wavefunction of the molecule can be separated in terms associated with these 3 energies

$$\psi = \varphi_{elec} \cdot \varphi_{vib} \cdot \varphi_{rot}$$

Because $E_{rot} \ll E_{vib} \ll E_{elec}$ we can separately think about their spectrum

$$E = E_{el} + E_{vib} + E_{rot}$$

$E_{vib} = \left(v + \frac{1}{2}\right)\hbar\omega_0$

↑ vib. quantum #

$v = 0, 1, 2, \ldots$

$E_{rot} = \frac{J(J+1)\hbar^2}{2\mu R_0^2}$

μ = reduced mass

R_0 = separation (diatomic)

$\sigma = J(J+1) \cdot B$

↑ rotational constant $\qquad J = 0, 1, 2, \ldots$

Note that $E = (J+1)\cdot J B \Rightarrow \Delta E(\Delta J = 1) = 2JB$

$$\Rightarrow E_{J_{1\to 0}} = 2B$$

$$E_{J_{2\to 1}} = 2E_{J_{1\to 0}}$$

$$\vdots$$

$$E_{J_{n\to n-1}} = n\, E_{J_{1\to 0}}$$

Usually because $E_{rot} \ll E_{vib}$ there is a pure rotational spectrum, but in general we have a mixed ro-vibrational spectral bands for high-lying transitions.

→ Mercifully, spectra of diatomic molecules is usually simple.

Transition rates?

$$H_{dipole} = -E_{rad}\cdot\vec{k}\cdot\vec{d}$$

$\vec{d} = \vec{d}_{elec} + \vec{d}_{nuclear}$ dipole moment

$$\Rightarrow \langle \psi_f | H_d | \psi_i \rangle = -\int_0^{2\pi} d\varphi \int_0^{\pi} d\theta \sin\theta \; Y^*_{Jm} Y_{J'm'}$$

$$\vec{E}_{rad} \underbrace{\langle \zeta_{vib} | \vec{d} | \zeta_{vib} \rangle}_{\text{for pure rot. transitions}}$$

$$= \int \vec{D}\, |\zeta_{vib}(R)|^2 dR$$

$$\vec{D}(R,\theta,\varphi) = \int (\vec{d}_{el} + \vec{d}_{nuc}) |\Psi_{el}|^2 d\vec{x}_{e}$$

$$\vec{d}_{nuc} = \frac{e}{M}(Z_A M_B - Z_B M_A)\vec{R}$$

lies along center line, zero for homonuclear molecules like H_2

Also, $\vec{d}_{el} = 0$ from parity considerations for homonuclear $\Rightarrow$

⇒ $\vec{D} = 0$ for homonuclear molecs.

⇒ no permitted pure rotational transitions

(but ∃ forbidden (quadrupole) + permitted vibrational)

Molecs. like CO have $\vec{D}$ nonzero

Rigid rotor approx. $\vec{D} \simeq \vec{D}_0$, and e-dipole selection rules are $\Delta J = \pm 1$, $\Delta m = 0, \pm 1$, $\hbar\omega = \Delta E = 2(J+1)B$ $\quad J+1 \to J$

$$A_{J+1,\,J} = \frac{4(J+1)\,\omega^3 D_0^2}{3(2J+3)\,\hbar c^3}$$

CO $1 \to 0$, $\lambda = 2.6$ mm $\quad A = 6\times10^{-8}\,s^{-1}$

Diagnostics

1) Vibrational transitions require $kT \sim 0.01-0.1$ eV ⟺ $T \sim 100-1000$ K

2) rotational trans. $kT \sim 0.001$ eV ⟺ $T \sim 10$ K
(if not homonuclear)

⇒ Cold molecular clouds have $T \sim 10-30$ K, too low to excite vibrational trans, but H_2 is homonuclear → look at other molecules.
CO, CS, etc.

CO : $\lambda(1\to0) = 2.6$ mm ⇒ $\lambda(J\to J-1) = \dfrac{2.6\text{ mm}}{J}$

Einstein As are ≫ than for HI
$6\times10^{-8}\,s^{-1}$ vs. $2.9\times10^{-15}\,s^{-1}$

and $h\nu/kT$ larger than @ 21cm ⇒ levels are not populated according to stat weights. $g_J = 2J+1$

$$S_\nu = \frac{2h\nu^3/c^2}{\frac{g_2}{g_1}\frac{n_1}{n_2} - 1} \qquad \left(S_\nu = \frac{n_2 A_{21}}{-n_2 B_{21} + n_1 B_{12}} \right)$$

$$\tau_\nu = \frac{h\nu}{4\pi} \frac{n_2 A_{21}}{S_\nu} \cdot s$$ (distance along los)

$$= \frac{h\nu}{4\pi} \frac{n_2 A_{21}}{2h\nu^3} \cdot c^2 \left(\frac{g_2}{g_1}\frac{n_1}{n_2} - 1 \right) \cdot s$$

$$\frac{n_2}{n_1} \triangleq \frac{g_2}{g_1} e^{-h\nu/kT_{ex}} \Rightarrow \tau_\nu = A_{21} \frac{h\nu}{4\pi} \cdot \frac{c^2}{2h\nu^3} \left(e^{h\nu/kT_{ex}} - 1 \right) \cdot n_2 s$$

$$= \frac{A_{21}}{8\pi} \lambda^2 \left(e^{h\nu/kT_{ex}} - 1 \right) n_2 s$$

$\uparrow$

CO is much more optically thick than HI ($A_{21}\lambda^2$ is much larger)

Besides, $\frac{h\nu}{kT_{ex}} = \frac{hc}{\lambda kT_{ex}} = \frac{1.44}{(\lambda/\text{mm})(T_{ex}/10\text{K})}$ $\Rightarrow$ not small, cannot simplify to R-J

for $\lambda = 2.6\,\text{mm}$, $\frac{h\nu}{kT_{ex}} = \frac{0.55}{T_{ex}/10\text{K}}$; $\lambda = 1.3\,\text{mm}$, $\frac{h\nu}{kT_{ex}} = \frac{1.1}{T_{ex}/10}$

$\Rightarrow$ generally more than 2 levels are excited (more complex than HI)

Rad. Transfer

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

$$I_\nu(0) = B_\nu(T_{CMB}) = \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT_{CMB}} - 1}$$

$\frac{h\nu}{kT_{CMB}} = 2$ for $J = 1-0$, 4 for $J = 2-1$, etc

$\Rightarrow \frac{1}{e^{h\nu/kT_{CMB}} - 1} = 0.16,\ 0.02,$ etc

$$S_\nu = \frac{2h\nu^3}{c^2}\frac{1}{e^{h\nu/kT_{ex}}-1}$$

$$\Rightarrow \Delta I_\nu = \frac{2h\nu^3}{c^2}\left[\frac{1}{e^{h\nu/kT_{ex}}-1} - \frac{1}{e^{h\nu/kT_{CMB}}-1}\right]\left(1-e^{-\tau_\nu}\right)$$

If equilibrium with CMB, $T_{CMB} = T_{ex} \Rightarrow \Delta I_\nu = 0$

For $T_{ex} \gtrsim 10K$, background correction is small

$J=1-0$ $\quad$ $J=2-1$

$$\frac{1}{e^{h\nu/kT_{ex}}-1} = 1.4\,,\ 0.5$$

Excitation is determined by detailed balance

$$n_2\left[A_{21} + \gamma_{21}\underbrace{n_{H_2}}_{} + B_{21}J_\nu\right] = n_1\left[B_{12}J_\nu + \gamma_{12}\,n_{H_2}\right] \rightarrow \text{collisional partner}$$

$$J_\nu = \frac{2h\nu^3/c^2}{e^{h\nu/kT_R}-1} \Rightarrow$$

down~~up~~ward: $n_2\left[A_{21}\frac{e^{h\nu/kT_R}}{e^{h\nu/kT_R}-1} + \gamma_{21}n_{H_2}\right]$ (after using Einstein's relations)

upward: $n_1\frac{g_2}{g_1}e^{-h\nu/kT}\left[\frac{A_{21}\,e^{h\nu/kT}}{e^{h\nu/kT_R}-1} + \gamma_{21}n_{H_2}\right]$ " + Boltzmann

Limiting cases: ① large n_{H_2} $\Rightarrow n_{H_2} \gg n_{crit} = \frac{A_{21}}{\gamma_{21}}$

Eg CO 1-0, $A_{10} = 6\times10^{-8}\,s^{-1}$, $\gamma_{10} = 1.8\times10^{-11}\,cm^3\,s^{-1}$ @ 10K

$\Rightarrow n_{crit,H_2} = 3,333\,cm^{-3}$

$\Rightarrow$ Unless T_R is very large, collisions dominate

$$\Rightarrow \frac{g_1}{g_2}\frac{n_2}{n_1} = e^{-h\nu/kT_K} \quad \text{and } T_{ex} = T_{kin}$$

②

Optically Thick line:

limiting value for T_R (except masers) is T_{kin}

			$J=1-0$	$J=2-1$
Eg: $T_R \to 10K$	$\dfrac{e^{h\nu/kT_R}}{e^{h\nu/kT_R}-1}$	$\to$	2.4	1.5
20K		$\to$	4.2	2.4
CMB		$\to$	1.15	1.02

$\Rightarrow$ If density is low $n_{H_2} \ll n_{crit}$ $\Rightarrow$ radiative terms dominate and $\dfrac{g_1 n_2}{g_2 n_1} \to e^{-h\nu/kT_R}$

Optically thick line has $I_\nu = S_\nu \Rightarrow T_{ex} = T_R \lesssim T_{kin}$

$\Rightarrow$ optically thick $\quad T_{ex} = T_R \sim T_K$

dense $\quad T_{ex} = T_K$

optically thin $\quad T_{ex} = T_R < T_K$

We can think in terms of photon escape probability

$$P_{esc} = \frac{1-e^{-\tau}}{\tau} \qquad \begin{array}{l} \tau \gg 1 \Rightarrow P_{esc} \to \frac{1}{\tau} \\ \tau \ll 1 \Rightarrow P_{esc} \to 1 \end{array}$$

If we think only of spontaneous + collis. de-exc

$\Rightarrow$ we reduce the spontaneous de-exc. by $P_{esc} \Rightarrow n_{cr} = \dfrac{A_{21}}{\gamma_{21}} \cdot P_{esc}$

$\Rightarrow$ The collision-dominated limit can hold at lower densities than otherwise possible $\Rightarrow T_{ex} \to T_{kin}$

Optical depth

$$\tau_\nu = \frac{A_{10}}{8\pi}\lambda^2\left(e^{h\nu/kT_{ex}}-1\right)N_1(\nu) \qquad N_1(\nu) = N_1\,\Phi(\nu)$$

line profile function

$$N_1(\nu) = N_1\Phi(v)\,\lambda \qquad N_1(\nu)d\nu = N_1(v)\,dv \qquad \frac{dv}{d\nu} = \frac{c}{\nu} = \lambda$$

$$\tau(v) = \frac{A_{10}}{8\pi}\lambda^3 \underset{N_{1,TOT}\,\Phi(v)}{\underset{\shortparallel}{N_1(v)}}\left(e^{h\nu/kT_{ex}}-1\right)$$

Write $N_1(v) = \frac{N_1}{N_{TOT}}\cdot\underset{\uparrow\text{ abundance}}{\frac{N_{TOT}}{N_{H_2}}}\,N_{H_2}(v)$

Eg: CO 1–0

$$\frac{N_1}{N_{TOT}} = \frac{g_1\,e^{-0.55/(T_{ex}/10K)}}{\underbrace{2kT_{ex}/h\nu_{10}}_{\text{partition function}}}$$

$$= \frac{3}{2}\cdot e^{-0.55/(T_{ex}/10K)}\cdot\frac{0.55}{(T_{ex}/10K)}$$

$$\frac{N_{CO}}{N_{H_2}} = 1.3\times10^{-4}$$

$$A_{10} = 6\times10^{-8}\,s^{-1}$$

$$\lambda = 0.26\,cm$$

$$\Rightarrow \tau_{10}(v) = 55\cdot\frac{0.82}{T_{ex}/10K}\cdot\left(1-e^{-0.55/(T_{ex}/10K)}\right)\frac{N_{H_2}(v)}{10^{21}\,cm^{-2}/km\,s^{-1}}$$

$$T_{ex} = 10K \Rightarrow \tau_{10}(v) = \frac{N_{H_2}(v)}{5\times10^{20}\,cm^{-2}/km\,s^{-1}}$$

$$20K \Rightarrow \tau_{10}(v) = \frac{N_{H_2}(v)}{2\times10^{20}\,cm^{-2}/km\,s^{-1}}$$

$$\tau_{21}(v) = \frac{N_{H_2}(v)}{3.8\times10^{19}\,cm^{-2}/km\,s^{-1}}$$

Typ. column densities are $N_{H_2} \sim$ [illegible], $10^{22}\ \text{cm}^{-2}/10\ \text{km s}^{-1}$

$\Rightarrow 10^{21}\ \text{cm}^{-2}/\text{km s}^{-1}$

more than enough for $\tau > 1$

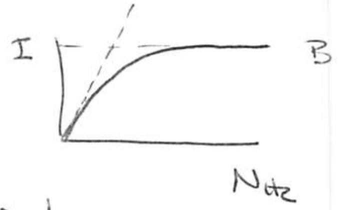
Isotopic forms, however, may be optically thin

Since $\dfrac{N_{\text{rare isotope}}}{N_{\text{common isotope}}} \ll 1$

E.g.: $\dfrac{N_{^{13}CO}}{N_{^{12}CO}} = \dfrac{1}{65}$, $\dfrac{N_{C^{18}O}}{N_{C^{16}O}} = \dfrac{1}{500}$

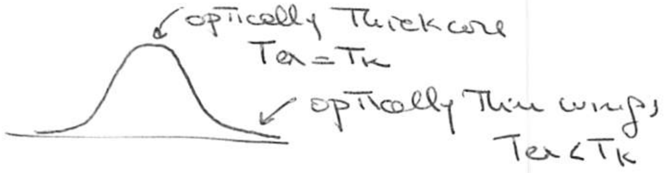
So, to the extent that ^{13}CO has $\tau \ll 1 \Rightarrow$

$$\Delta I_\nu = \underbrace{\tau_\nu}_{\propto N_{H_2}} \big(\underbrace{S_\nu}_{B_\nu(T_{ex})} - I_\nu(0)\big)$$



However, ^{13}CO is frequently thick.

Unequal line excitation:



<u>Estimating mass from optically thick lines:</u>

<u>If</u> a cloud is self-gravitating, we can use the linewidth to estimate mass:

$$I(v) = I_\nu d\nu/dv = I_\nu/\lambda \overset{\text{optically thick}}{=} B_\nu(T_{ex})/\lambda$$

$$\int I(v)dv = \int B_\nu(T_{ex}) \frac{dv}{\lambda} = \frac{B_\nu(T_{ex}) \cdot \Delta v}{\lambda}$$

Integrating over whole cloud area: $\pi R^2 \int I(v)dv = \underset{\text{distance}}{d^2} \cdot \int I(v)\,dv\,d\Omega$

$$L_{CO} \triangleq \pi R^2 \cdot \frac{B_\nu(T_{ex})\,\Delta v}{\lambda}$$

In virial equilibrium:

$$\Delta v \sim \left(\frac{GM}{R}\right)^{1/2} \qquad \left(M_{VIR} = \frac{9-3k}{G(5-2k)} R\sigma^2 , \quad \rho(r) \propto r^{-k} \right)$$

σ = 1D vel disp

$G = \frac{1}{232}\, p \left(\frac{km}{s}\right)^2 \frac{1}{M_\odot}$

$$\Rightarrow L_{CO} \propto R^2 \left(\frac{GM}{R}\right)^{1/2} \propto \left(GMR^3\right)^{1/2} \propto \left(GMR^3 \frac{\rho}{\rho}\right)^{1/2} \propto \left(\frac{G\,M^2}{\rho}\right)^{1/2}$$

$\Rightarrow L_{CO} \propto \frac{M}{\rho^{1/2}}$ $\Rightarrow$ if $\rho \sim$ constant from cloud to cloud,

$$L_{CO} \propto M \quad , \quad \int I(v)\,dv \propto \frac{M}{R^2} \propto N$$

Indeed, L_{CO} is observed to be prop. to M_{vir}, which yields the empirical relation

$$N(H_2) = 2.3\times10^{20}\ cm^{-2}\ \frac{I_{CO}}{K\ km\,s^{-1}}$$

$$I_{CO} = \int T_A\,dv$$

Other measures of mass agree: ^{13}CO and A_V, Total γ-ray, IR extinction, etc

$$\Rightarrow N_{H_2} = X_{CO} \cdot I_{CO} \qquad X_{CO} \sim 2.3-5\times10^{20}\ \frac{cm^{-2}}{K\,km\,s^{-1}}$$

$\uparrow$

most reliable calibrations are $\sim 2\times10^{20}$

Properties of molec. clouds

Temperatures: Estimated from multiline observations

$$I_\nu = B_\nu(T_{ex}) \propto \frac{1}{e^{h\nu/kT_{ex}}-1}$$

Typ. 10-30 K

Densities: ⓐ virial

$$\frac{GM}{R_{obs}} \sim (\Delta v)^2_{obs} \Rightarrow M \sim \frac{R(\Delta v)^2}{G}$$

$$\rho = \frac{M}{R^3}, \text{ or } \bar{\rho} = \frac{\langle N_{obs} \rangle}{\langle R \rangle}$$

Typ. value is $n_{H_2} \sim 100\ \mathrm{cm}^{-3}$

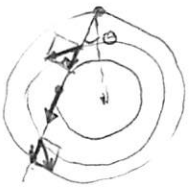
ⓑ excitation

Need $n_{H_2} \gtrsim n_{crit}$ to excite different transitions at least over a portion of the volume

⇒ filling factor of "moderate density gas" ($n_{H_2} \gtrsim 300\ \mathrm{cm}^{-3}$) is a few to 10%.

⇒ from turbulent simulations, this can be reproduced with $\frac{v_{turb}}{c_s} = 5-9$

Sizes & masses: Need to determine distances. Usually kinematic distances are used



$$\frac{dN}{dM} \propto M^{-\alpha} \qquad \alpha = 1.5 \text{ to } 1.7$$

Most of the mass is in the largest clouds $\sim 10^6 M_\odot$
Sizes ~ 50 pc

Velocity dispersion:

line widths well in excess of thermal ($v_{th} \sim 0.2\,\mathrm{km\,s^{-1}}$) by factors of $> \times 10$.

$\Rightarrow$ They are internally turbulent

Turbulent velocity dispersion is seen to increase as $\Delta v \propto R^{1/2}$

Virial equilibrium $\Delta v^2 \sim \frac{GM}{R}$

$\Rightarrow GM \sim R^2 \Rightarrow \frac{M}{R^2} \sim$ constant.

Surface density is indep. of cloud size,

$\Sigma \sim 170-200\ M_\odot\,pc^{-2}$

Note that this is ~10x larger than $\Sigma(ISM)$ in galaxies ($\Sigma \sim 12\,M_\odot\,pc^{-2}$)

Why this constancy? Clouds don't become molecular unless A_V is large (UV attenuation)

$$N_H = \frac{\Sigma}{1.4\,m_p} = 1.5\times10^{22}\ \mathrm{cm^{-2}} \text{ for } 170\ M_\odot\,pc^{-2}$$

↑ He correction by mass

We'll see that $\frac{A_V}{mag} = \frac{N_H}{1.9\times10^{21}\ \mathrm{cm^{-2}}} \Rightarrow A_V \simeq 8$ mag for average cloud

Heating and cooling:
- photoelectric heating from UV
- dissipation of turbulence
- CR heating, x rays

Cooling from ^{13}CO, CI, etc.

ASTR670
Spring 2009
Prof. Alberto Bolatto

Homework 3

1) Look at Figure 1 in page 223 of the Dickey & Lockman (1990) review. It represents the line profiles due to a combination of cold and warm HI along the line of sight.
   a. Using the cloud properties there listed, calculate the precise observed brightness temperature line profiles to reproduce both bottom panels of that figure. Consider both situations, with the warm gas in front and behind the cold gas. Assume that the intrinsic line profiles are Gaussian, with $\sigma=\Delta v/2.35$ (Δv is usually quoted as the full-width at half-maximum of a Gaussian in radioastronomy).
   b. What would be the sizes of these clouds, if they were spherical and virialized?
   c. What would be the column density of the warm cloud to obtain the same brightness temperature, if its kinetic temperature was 7,000 K?

2) What is wrong with this paper? Read Grimm et al. (2007), ApJS, 173, 70 and find the error that went past the authors and the referee. With your knowledge of the multiphase ISM, what would you do to improve Figure 6 of that paper? (Hint: it has something to do with a misused dataset)

3) The equation for the Einstein A coefficient for rotational dielectric dipole transitions is

$$A_{ul} = \frac{64\pi^4 \nu^3}{3hc^3} \mu^2 \frac{J_u}{g_u}$$

where J_u is the rotational quantum number of the upper level, g_u is the corresponding statistical weight, and μ is the electric dipole.
   a. Assuming that the excitation temperature T_{ex} is constant along the line of sight, show that the equation for the opacity τ_ν as a function of the column density of the upper level is

$$\tau_\nu = \frac{8\pi^3}{3h} \mu^2 \frac{J_u}{g_u} \left(e^{\frac{h\nu}{kT_{ex}}} - 1 \right) \frac{N_u}{\Delta V}$$

   where ΔV is the velocity line-width of the transition.
   b. Compute the ratio of brightness temperature for two consecutive transitions in the optically thin limit, and plot it as a function of excitation temperature.
   c. What is this ratio in the optically thick limit?

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