SPECTROSCOPY II

Rotational Transitions

- moment of inertia:

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

- angular momentum: $\bar{J} = \Theta_e \omega$
- kinetic energy of rotation:

$$H_{rot} = \frac{1}{2}\Theta_e \omega^2 = \bar{J}^2 / 2\Theta_e$$

- eigenvalues for the Schrödinger equation:

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

$$\nu(J) = \frac{1}{h}[W(J+1) - W(J)]$$

- centrifugal stretching, i.e. r_e increases with rotation:

$$E_{rot} = \frac{\hbar^2}{2\Theta_e} J(J+1) - hD[J(J+1)]^2$$

$$\nu(J) = 2B_e(J+1) - 4D(J+1)^3$$

where $B_e = \frac{\hbar}{4\pi\Theta_e}$ is rotational constant and D is the constant for centrifugal stretching.

- permanent electronic dipole moment is required (thus no rotational transitions for H_2,...)

Vibrational Transitions

- harmonic approximation of potential:

$$P(r) = \frac{k}{2}(r - r_e)^2 = a^2 D_e (r - r_e)^2$$

- classical oscillation: $\omega = \sqrt{\frac{k}{m}} = a\sqrt{\frac{2D_e}{m}}$
- energy levels: $W(v) = \hbar\omega(v + \frac{1}{2})$
- large perturbations require anharmonic factors:

$$W(v) = \hbar\omega(v+\frac{1}{2})+x_e\hbar\omega(v+\frac{1}{2})^2+y_e\hbar\omega(v+\frac{1}{2})^3+....$$

Line Intensity and Level Population

- spontaneous transition probability:

$$A_{ul} = \frac{64\pi^4}{3hc^3}\nu^3|\mu_{ul}|^2 = 1.165 \times 10^{-11}\nu^3|\mu_{ul}|^2$$

- dipole moment $|\mu|^2$:

$$|\mu_J|^2 = \mu^2\frac{J+1}{2J+1} \text{ for absorption}$$

$$|\mu_J|^2 = \mu^2\frac{J+1}{2J+3} \text{ for emission}$$

$$A_J = 1.165 \times 10^{-11}\mu^2\nu^3\frac{J+1}{2J+3}$$

- column density:

$$N_l = \frac{93.5 g_l\nu^3/g_u A_{ul}}{1 - exp(-0.048\nu/T_{ex})}\int \tau dv$$

$$N_l = 2070\frac{g_l\nu^2 T_{ex}}{g_u A_{ul}}\int \tau dv \text{ if } T_{ex}/\nu \gg 0.048$$

In optically thin case, $T_{mb} = \tau T_{ex}$ and

$$N_l = 2070\frac{g_l\nu^2}{g_u A_{ul}}\int T_B dv$$

CO under LTE Conditions

- dipole moment: $\mu = 0.112$ Debye
- low J transitions are usually close to LTE
- $T_B = \frac{h\nu}{k}[\frac{1}{exp(\frac{h\nu}{kT_{ex}})-1} - \frac{1}{exp(\frac{h\nu}{kT_{cmb}})-1}](1 - e^{-\tau_\nu})$
- $^{12}C^{16}O$ is almost always optically thick, and column density cannot computed this way. However, one can obtain directly

$$T_{ex} = 5.5[ln(1 + \frac{5.5}{T_B + 0.82})]^{-1}$$

  for $J = 1 \longrightarrow 0$ line at 115.271 GHz.

- for optically thin $^{13}C^{16}O$ (1–0) at 110.201 GHz,

$$\tau^{13} = -ln[1 - \frac{T_B^{13}}{5.3}([e^{5.3/T_{ex}} - 1]^{-1} - 0.16)^{-1}]$$

- In general we want total column density over all J. Rotational degeneracy is $2J + 1$

$$n(J)/n(total) = (2J+1)exp[-\frac{hB_e J(J+1)}{kT}]/Z$$

$$Z = \sum_J (2J+1)exp[-\frac{hB_e J(J+1)}{kT}]$$

- Under LTE, $Z \sim \frac{kT}{hB_e}$ for $hB_e \ll kT$. Boltzmann distribution applies, and $N_{total}(^{13}CO)$ can be derived from $J = 1 \rightarrow 0$ lines of CO.

$$N_{total}(^{13}CO) = 2.6 \times 10^{14} \frac{T \int \tau^{13}(v) dv}{1 - exp(-5.3/T)}$$

- optically thin limit:

$$T \int \tau^{13}(v) dv \sim \frac{\tau_0}{1 - e^{-\tau_0}} \int T_{mb}(v) dv$$

- limitations of the method:
  - uncertainty in T_{ex} – i.e., ^{12}CO easily thermalized but isotopes may be subthermal ($T_{ex} < T_K$).
  - spatial variations
  - large A coeff.. for high J states
  - selective photodissociation (self-shielding)

$\Rightarrow$ LTE over-estimates $N_{total}(^{13}CO)$ by 1-4

Radiative Transport of Optically Thick Lines

When $\tau > 1$, complex interactions among different levels important. Deviation from LTE should also taken into account.

LVG Treatment:

- populations n_i of level i at position r are given by

$$n_i(r) \sum_j P_{ij} = \sum_j n_j P_{ji}$$

$$P_{ij} = A_{ij} + B_{ij} < U_{ij} > + C_{ij} \text{ for } i > j$$

$$\text{and } P_{ij} = B_{ij} < U_{ij} > + C_{ij} \text{ for } i < j$$

- $< U_{ij} >$ is average radiation field and is related to the line source function S_{ij} via kernel $< K_{ij} >$

$$< U_{ij}(r) > = \int K_{ij}(|\vec{r} - \vec{r'}|) S_{ij}(r') dr'$$

- mean free path for a photon emitted $l \sim v_t R/V$ and absorption erases all previous memory

$$< U_{ij}(r) > = (1 - \beta_{ij}(r)) S_{ij} + \beta B_{ij}(\nu_{ij}, T_{cmb})$$

(see RW 14.10 for full discussion)

Spectral Line as Diagnostic Tools

1. T_K
   - CO peak intensity
   - LVG calculation
   - K ladders of symmetric tops (e.g. NH_3, CH_3CN)
2. **Linewidth**
   - $\Delta v_{1/2}$ and V_{LSR}
   - virial mass: $M_{vir} = 250(\frac{\Delta v_{1/2}}{km/s})^2(\frac{R}{pc})\ M_\odot$
   - free fall time:

$$t_{ff} \sim D/\Delta v_{1/2} \text{ or}$$

$$t_{ff} = \sqrt{\frac{3\pi}{32G\rho_0}} = 5 \times 10^7/\sqrt{n}\ yr$$

   - equipartition B field:

$$B = 15.2(\frac{\Delta v_{1/2}}{km/s})^2 R(pc)\ \mu G$$

3. **N(H$_2$) and mass**

- from LVG calculations,

  $N_{H_2} = 2.65 \times 10^{21} \int T_{mb}(C^{18}O(2-1))dv$

- from ^{12}CO intensity,

  $N_{H_2} = 2.3 \times 10^{20} \int T_{mb}(CO(1-0))dv$

  – γ-ray intensity
  – virialization
  – metallicity dependence
  – excitation conditions: $X \propto T/\sqrt{n}$
  – sub-thermal excitation

X-Factor: Virial Equilibrium Argument

(Dickman, Snell, Schloerb 1986; Scoville & Young 1991)

- For a uniform, spherical cloud

$$L_{CO} = \pi R^2 T_{CO} \Delta V$$

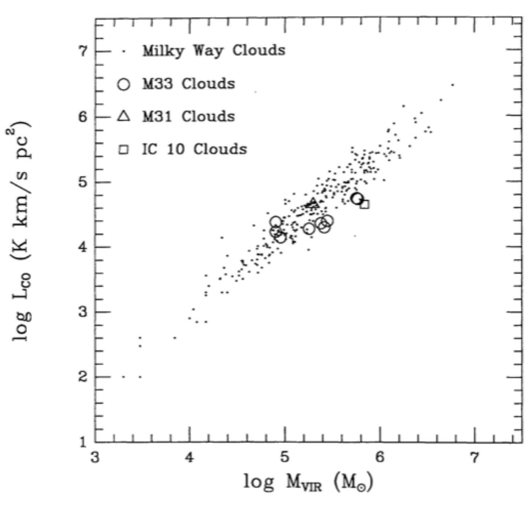
- For a self-gravitating GMC, $\Delta V = \sqrt{GM/R}$ and

$$M_{cl} = L_{CO} \sqrt{\frac{4\rho}{3\pi G}} \frac{1}{T_{CO}}$$

i.e., $M_{cl} \propto L_{CO}$ if $\sqrt{\rho}/T_{CO}$ does not vary much on average

- In external galaxies, $L_{CO} \propto N_{cl} \times M_{cl}$, and

$$N_{H_2} = 2.3 \times 10^{20} \int T_{mb}(CO(1-0))dv$$



X-Factor: Gamma-ray Method

(Bloemen et al. 1986; Hunter et al. 1997)

- γ-ray emission is mostly Galactic in origin
- MW transparent to γ-ray ($E \leq 10^{14}$ eV)
- Cosmic rays interact with ISM via
  - high energy electron bremsstrahlung
  - nucleon-nucleon interactions
  - plus inverse Compton, synchrotron,.....
- model the observed 3-D γ-ray distribution with the distribution of protons (HI, H II, H_2) via a cosmic ray coupling scale r_0 (=1.8 kpc)

$$N_{H_2} = (1.6 \pm 0.1) \times 10^{20} \int T_{mb}(CO(1-0))dv$$

- some discrepancy (60%) at >1 GeV (brighter than the model) and in the Outer disk

$$N_{H_2} = (2.7 \pm 0.1) \times 10^{20} \int T_{mb}(CO)dv$$

X-Factor: Metallicity Dependence

(Maloney & Black 1988; Elmegreen 1989; Arimoto et al. 1996)

- reduction in UV shielding may lead to smaller molecular cores in very low metallicity systems
- a threshold effect, however
- no radial dependence in MW, despite metallicity gradient

See Bolatto et al. (2008, ApJ, 686, 948) for the latest discussion.