Spectroscopy and Molecular Emission

Fundamental Probes of Cold Gas
Atomic Lines

- Few atoms have fine structure transitions at low enough energy levels to emit at radiofrequencies.

- Important exceptions:
  - HI (21cm)
  - CI (610 and 350 microns)
  - [N II] (205 microns)
  - [C II] (137 microns)
Molecules

- Molecules have many transitions at low energies, with lines at radioastronomical frequencies, hence are excellent probes of cold gas.
- Owing to the electron – nucleus mass difference, energetics decouple (Born-Oppenheimer approximation)

\[ E_{\text{TOT}} = E_{\text{el}} + E_{\text{vib}} + E_{\text{ROT}} \]

- \( E_{\text{el}} \sim 5-10 \text{ eV} \) at equilibrium nuclear distances
  - UV, optical transitions, not in cold regions
- \( E_{\text{vib}} \sim 0.1 \text{ eV} \)
  - 3-10 micron spectral region, too hot for most dark clouds
- \( E_{\text{rot}} \sim .0003 \text{ eV} \), smaller for heavier molecules
  - Perfect for radioastronomy, cold regions!
Molecular Energy Levels

- Upper levels depopulate by spontaneous radiative decay at a rate:
  \[ \Lambda_{ul} = \frac{64\pi^4\mu_{ul}^2}{3h\lambda_{ul}^3} = 0.3 \lambda_{100\,\mu m}^{-3} \mu_d^2 \, s^{-1}, \]
  \( \mu_d \sim 0.1 \text{ Debye CO} \)
  \( \mu_d \sim 1-4 \text{ Debye HCN, CS, HCO}^+ \) etc

- Radiative excitation in strong radiation fields...

- They populate and depopulate collisionally also at a rate
  \[ C_{ul} = n <\sigma_{ul}\nu> \text{ a function of T} \]
  \[ C_{lu} = C_{ul} (g_u/g_l) \exp(-h\nu_{ul}/kT) \]
  \[ <\sigma_{ul}\nu> \sim 10^{-11} \text{ for neutrals, } 10^{-10} \text{ for ions} \]

- Balance excitation, dexcitation, solve for density \( n \)
  - CO can be excited in less dense (>10^2 cm^{-3}) regions, a good gas tracer
    - \( \text{H}_2 \) being symmetric, has no suitable cold gas emission lines
  - HCN, CS, HCO^+, H_2CO, NH_3 require gas of \( \text{H}_2 \) density >10^4 cm^{-3}
Radiative Transfer

How does that photon find its way to us?

\[ I_{\text{obs}} = I_{\text{bgd}} e^{-\tau_\nu} + \varepsilon_\nu (1 - e^{-\tau_\nu}) \]

- \( I_{\text{bgd}} \) is the cosmic 3K background radiation
- \( \varepsilon_\nu \) is the source function; \( \tau_\nu \) is optical depth

For \( \tau_\nu \ll 1 \), for a collection of molecules

\[ I_\nu = \frac{h\nu ul}{4n} A_{ul} \text{ ergs cm}^{-3} \text{ s}^{-1} \text{ Hz}^{-1} \text{ sr}^{-1} \]

What does the telescope see???

- Now, for a blackbody,
  \[ I_\nu = \left( \frac{2h\nu^3}{c^2} \right) \left( e^{\frac{h\nu}{kT_B}} - 1 \right)^{-1} \text{ and for } h\nu \ll kT_B \text{ then} \]
  \[ I_\nu = 2kT_A \Delta \nu / \lambda^2 = 2kT_A \Delta V \nu^3/c^3 \]

Which we can substitute back into the equation for \( I \) above...
Physics from Molecular Emission

- $N_u = \frac{8\pi k \Delta V \nu^2 T_A}{hc^3 A_{ul}}$
- Which relates the antenna temperature and linewidth, measured quantities, to the total number of molecules in the beam in the upper excitation state.
- For $\tau << 1$, $T_A \sim T_x \tau$ from the transfer eqn

For everything in thermal equilibrium a molecule’s level populations are described by the kinetic temperature $T_{\text{kin}}$, so

$N_u/N_l = (g_u/g_l) \exp(-\Delta E_{ul}/kT_{\text{kin}})$ and $N_0 = h\nu/2kT_{\text{kin}}N_{\text{Total}}$

And
Eureka!

From the measurement of $T_A$ and assumption of $T_{\text{kin}}$, we have measured the total number of molecules. If we measure more than a single line, we can derive both the temperature and the number of molecules, the density of the emitting gas, and even test our assumption of thermal equilibrium!
Formaldehyde, an asymmetric rotor molecule, has many transitions. Some of these, at different energy levels, lie adjacent in frequency and may be observed simultaneously.

One useful grouping of lines includes lines at 211, 218.2, 218.5, 218.8 and 226 GHz. The cluster at 218 GHz is especially well suited to existing correlators. Note the line at 2 cm at similar energy.

Furthermore, these lines lie at 23 K (218.2 GHz line) and 64 K (the others) above ground, and are from the para form of formaldehyde.
Ammonia, an asymmetric top molecule, has a number of inversion lines lying close together in frequency near 1.3cm. The two lowest observable energy transitions lie at energies of 23 K and 64 K above ground.

Our hypothesis: With like energetics, the reasons for differences in the distribution of these two molecules must lie in their chemistry

Test: Image them in similar star forming regions
Cometary OH

- Comets, mostly made of water, sublime as they approach the Sun. Solar ultraviolet radiation dissociates the water, invisible owing to Earth’s watery atmosphere, into OH and H.

- Experiment—observe OH lines at 1665 and 1667 MHz with the GBT.
Assumptions…

- Assume:
  - OH lies in uniform density sphere of radius one dissociation scale length, \( \lambda \).
  - Uniform outflow velocity, \( V_{\text{out}} \), is given by the linewidth of the observation, \( \sim 1 \ \text{kms}^{-1} \).
  - Photodissociation timescale \( \tau_{\text{OH}} \) from OH physics, is \( 1.1 \times 10^5 \ \text{s} \) at 1 AU.
  - Therefore the OH sphere is 110,000 km in radius.
  - Compare beamsize of telescope to this sphere.
- Define \( Q_{\text{OH}} \) to be the production rate, per second, of OH molecules.
The Equation...

\[ Q_{\text{OH}} = 8(\pi \Delta \theta)^2 k V^2 \Delta V T_A / 4 \ln 2 h c^3 \tau_{\text{OH}} A_{\text{ul}} \]

- \( \Delta \) is the distance from Earth, \( \theta \) the beamsize, and the other parameters are as described before.

We can simplify this further:

\[ Q_{\text{OH}} = N \Delta V T_A \frac{\pi R^2}{\tau_{\text{OH}}} \]

Where \( N \) is the column density of OH which makes a line of 1 K km s\(^{-1} \) strength, and \( \beta \) is the fraction of cometary molecules lying within the beam (i.e. \( \beta = 1 \) for beamsize larger than the comet).

For Comet 1999H1Lee \( N = 1.37 \times 10^{14} \text{ cm}^{-2} (\text{K km s}^{-1})^{-1} \)
And the result!

- $Q_{\text{OH}} \approx 5.5 \times 10^{28}$ molecules s$^{-1}$
- Instant publication!
C/2002 Y1 (Juels-Holvorcem)

- Date TT R. A. (2000) Decl. Delta r Elong. Phase m1
- 2003 06 10 02 13.58 -15 58.6 1.514 1.306 58.3 41.4 8.6
- 2003 06 15 02 24.06 -20 04.1 1.500 1.378 63.0 41.1 8.8
- 2003 06 20 02 34.80 -24 16.8 1.491 1.450 67.6 40.4 9.0
- 2003 06 25 02 45.82 -28 35.3 1.487 1.521 72.1 39.5 9.2
- 2003 06 30 02 57.14 -32 57.9 1.490 1.593 76.3 38.3 9.4
- Rapidly heading south and not too close to Earth...
- How strong is its OH line????