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

Molecular Energy Levels

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

_____u

_____l
Simple
molecule
Energy levels

- Radiative excitation in strong radiation fields…
- They populate and depopulate collisionally also at a rate
  - $C_{ul} = n < \sigma_{ul} v>$ a function of T
  - $C_{lu} = C_{ul}\,(g_u/g_l)\,\exp(-h\nu_{ul}/kT)$
  - $< \sigma_{ul} v> \sim 10^{-11}$ for neutrals, 10^{-10} 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
    - H_2 b eing symmetric, has no suitable cold gas emission lines
  - HCN, CS, HCO^+, H_2CO, NH_3 require gas of H_2 density $>10^4\ cm^{-3}$

Radiative Transfer

- How does that photon find its way to us?

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

I_{bgd} is the cosmic 3K background radiation

ε_ν is the source function; τ_ν is optical depth

For $\tau_\nu << 1$, for a collection of molecules

$$I_\nu = \frac{h\nu_{ul}}{4\pi}\mathcal{N}u\, A_{ul} \text{ ergs cm}^{-3}\text{ s}^{-1}\text{ Hz}^{-1}\text{ sr}^{-1}$$

What does the telescope see???

- Now, for a blackbody,

$$I_\nu = (2h\nu^3/c^2)(e^{h\nu/kT_B}-1)^{-1} \text{ and for } h\nu << kT_B \text{ then}$$

$$I_\nu = 2kT_A\,\Delta\nu/\lambda^2 = 2kT_A\Delta V\,\nu^3/c^3$$

Which we can substitute back into the equation for I above...

Physics from Molecular Emission

- $\mathscr{N}_u = 8\pi k\, \Delta V\, \nu^2 T_A/hc^3 A_{ul}$

- 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_{kin}, so
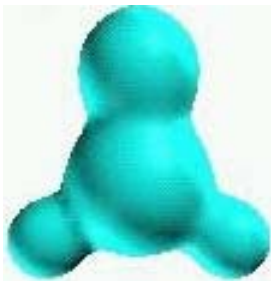
$\mathscr{N}_u/\mathscr{N}_l = (g_u/g_l)\exp(-\Delta E_{ul}/kT_{kin})$ and $\mathscr{N}_o = h\nu/2kT_{kin}\mathscr{N}_{Total}$
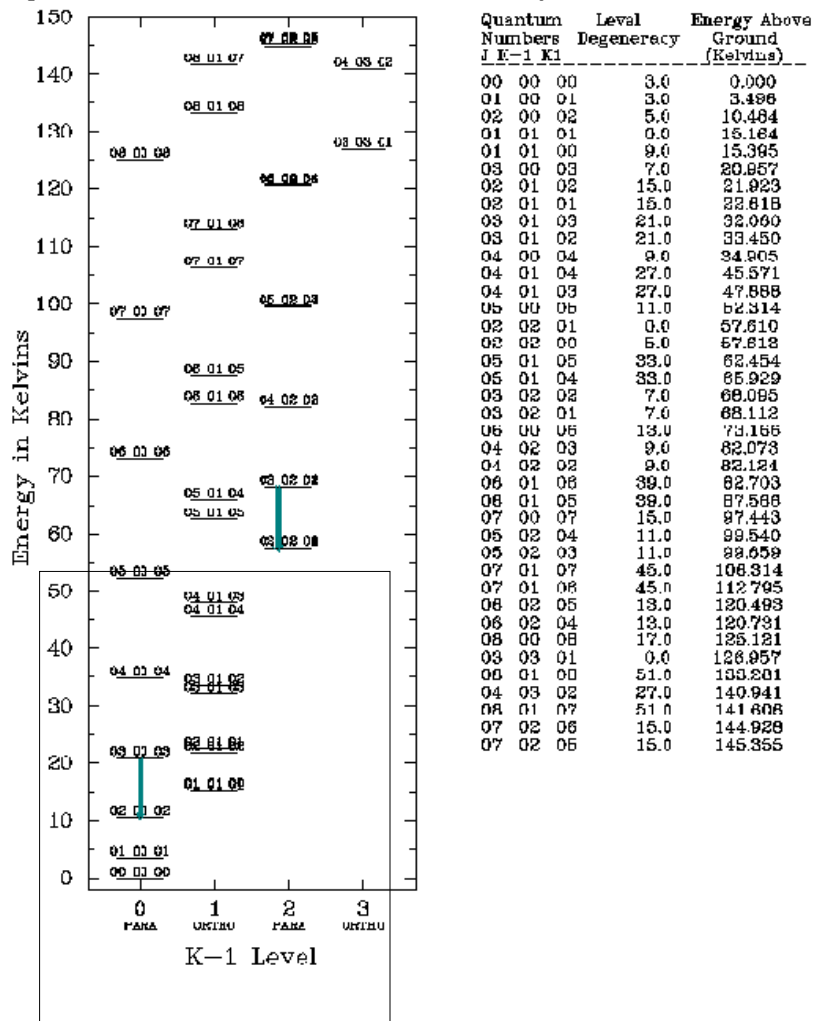
And

Eureka!

From the measurement of T_A and assumption of T_{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 2cm 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.

H2CO

AO: 281.9260 GHz   BO: 38.8368 GHz   CO: 38.8366 GHz
Dipole Moment: A=   2.331   B=   0.000   C=   0.000   Debye

Quantum Numbers J K−1 K1			Level Degeneracy	Energy Above Ground (Kelvins)
00	00	00	3.0	0.000
01	00	01	3.0	3.496
02	00	02	5.0	10.484
01	01	01	0.0	15.164
01	01	00	9.0	15.395
03	00	03	7.0	20.957
02	01	02	15.0	21.923
02	01	01	15.0	22.818
03	01	03	21.0	32.060
03	01	02	21.0	33.450
04	00	04	9.0	34.905
04	01	04	27.0	45.571
04	01	03	27.0	47.688
05	00	05	11.0	52.314
02	02	01	0.0	57.610
02	02	00	5.0	57.618
05	01	05	33.0	62.454
05	01	04	33.0	65.929
03	02	02	7.0	68.095
03	02	01	7.0	68.112
06	00	06	13.0	73.166
04	02	03	9.0	82.073
04	02	02	9.0	82.124
06	01	06	39.0	82.703
06	01	05	39.0	87.566
07	00	07	15.0	97.443
05	02	04	11.0	99.540
05	02	03	11.0	99.659
07	01	07	45.0	106.314
07	01	06	45.0	112.795
06	02	05	13.0	120.493
06	02	04	13.0	120.731
08	00	08	17.0	125.121
03	03	01	0.0	126.957
06	01	00	51.0	133.201
04	03	02	27.0	140.941
08	01	07	51.0	141.608
07	02	06	15.0	144.928
07	02	05	15.0	145.355

Energy in Kelvins (vertical axis, 0 to 150)

K−1 Level (horizontal axis): 0 PARA, 1 ORTHO, 2 PARA, 3 ORTHO

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.

ROTATIONAL ENERGY LEVELS OF NH$_3$

A = ORTHO
E = PARA

ENERGY IN cm^{-1}

EQUIVALENT TEMPERATURES (K)

J = 6
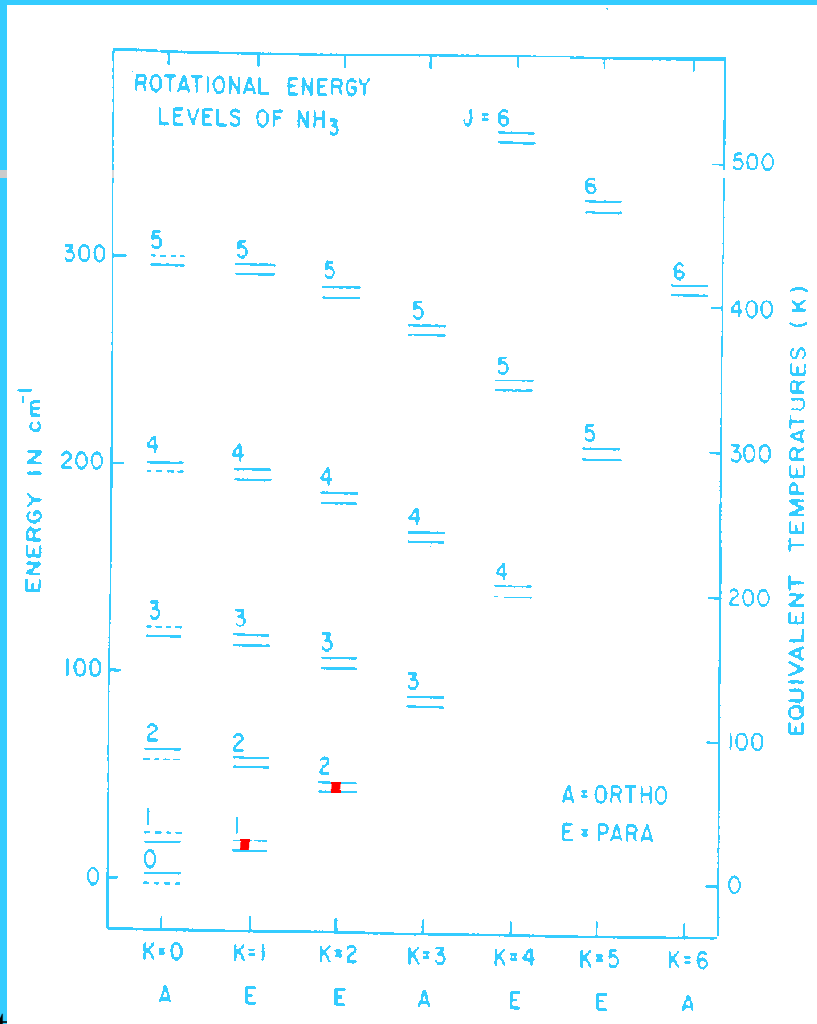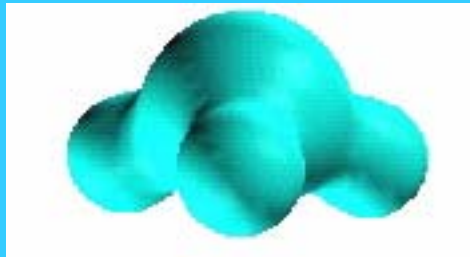
Our hypothesis: With like energetics, the reasons for differences in the distribution of these two molecules must lie in their chemistry

Test: Image them in similar star forming regions

Cometary OH

- Comets, mostly made of water, sublime as they approach the Sun. Solar ultraviolet radiation dissassociates 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, λ.
  - Uniform outflow velocity, V_{out}, is given by the linewidth of the observation, ~ 1 kms^{-1}
  - Photodissociation timescale τ_{OH} from OH physics, is 1.1×10^5 s at 1 AU
  - Therefore the OH sphere is 110,000 km in radius.
  - Compare beamsize of telescope to this sphere
- Define Q_{OH} to be the production rate, per second, of OH molecules.

The Equation...

- $Q_{OH} = 8(\pi\Delta\theta)^2 k \, \nu^2 \Delta V T_A / 4\ln 2 h c^3 \, \tau_{OH} A_{ul}$

  - Δ is the distance from Earth, θ the beamsize, and
  the other parameters are as described before

  We can simplify this further

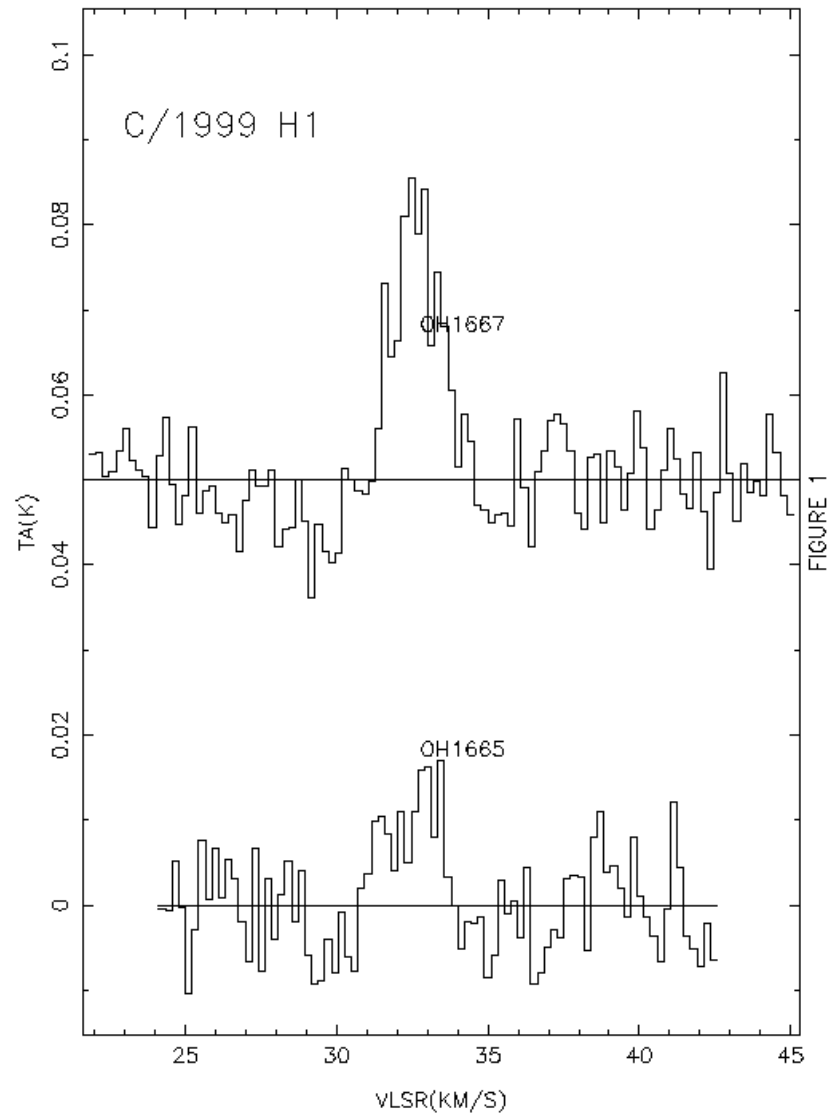 $Q_{OH} = N \, \Delta V T_A \, \pi R^2 / \tau_{OH} f$

  Where N is the column density of OH which makes a line of 1 K kms^{-1} strength, and f

  is the fraction of cometary molecules lying within the beam (i.e. $f=1$ for beamsize larger than the comet)

  For Comet 1999H1Lee $N = 1.37 \times 10^{14}$ cm^{-2} (K km s^{-1})$^{-1}$

And the result!

- $Q_{OH} \sim 5.5 \times 10^{28}$ molecules s^{-1}
- Instant publication!

C/1999 H1

OH1667

OH1665

TA(K)

VLSR(KM/S)

FIGURE 1

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????