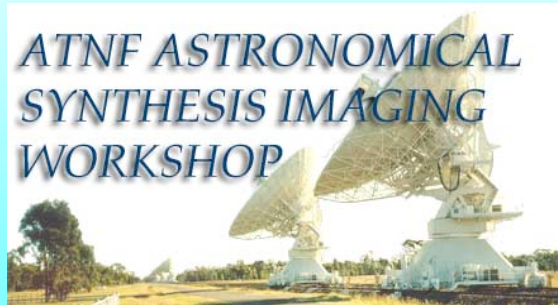


Narrabri, 12th–16th May 2003



Thermal Line mm Astronomy

16th May, 2003

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A word from our sponsor.....

Words ending in “-ic”:

mimic	□	mimicking, mimicked
panic	□	panicking, panicked
traffic	□	trafficking, trafficked
politic	□	politicking
magic	□	magicked
picnic	□	picnicking

mosaic? “c” followed by “i” or “e” makes the “c” soft (like an “s”)
□ mosaicking, mosaicked. Consistent with Greek root.

OED, MNRAS, ApJ all say: “k” is the way!

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Molecular Physics

1.1 Energies

At 100 GHz ($\lambda = 3\text{mm}$),

$$E = h\nu = 6.6 \times 10^{-23} \text{ J} = 4.1 \times 10^{-4} \text{ eV},$$

and

$$T = h\nu/k = 4.8 \text{ K}.$$

Thus, mm-spectroscopy is mostly about matter at low temperatures (or undergoing small ΔE changes). Although there are some exceptions, this is too cold for most electronic or vibrational transitions, and usually the only energy levels this low involve *rotational* transitions of *molecules*.

Molecular Physics 2

1.2 Quantum Mechanics and Simple Rotation Ladders

—————> See John Storey's lecture from 2001

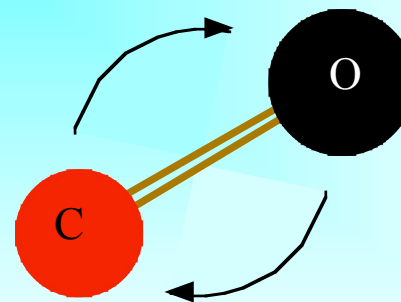
The simplest case is for linear (often just diatomic) molecules, of which CO is the prime example. Then we find there are quantised rotational energy levels, just like quantised electronic energy levels in (*e.g.*) the hydrogen atom.

The rotational quantum number is J . The angular momentum of a rotational level is

$$I\omega = Jh/2\pi,$$

while the energy above the ground state is

$$E = hBJ(J+1),$$



Molecular Physics 3

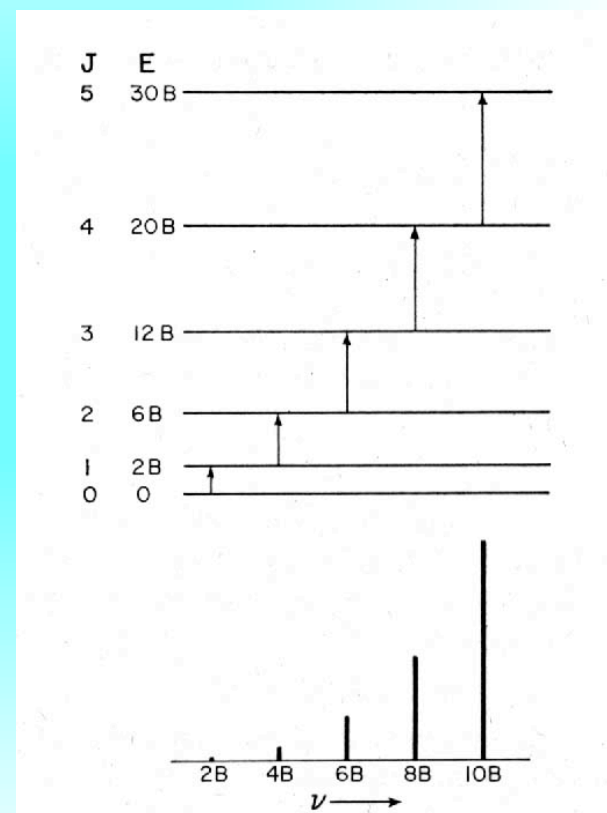
where

$$B = h/8\pi^2I$$

is the *rotational constant* for a given molecule. Quantum selection rules mean $\Delta J = \pm 1$ transitions are allowed. This leads to a “rotational ladder”, or just “*J*-ladder”, with transition frequencies

$$\nu = 2BJ_{\text{upper}}.$$

Note that molecules like H_2 , N_2 have no dipole moments, and so cannot have electric dipole *J*-lines.

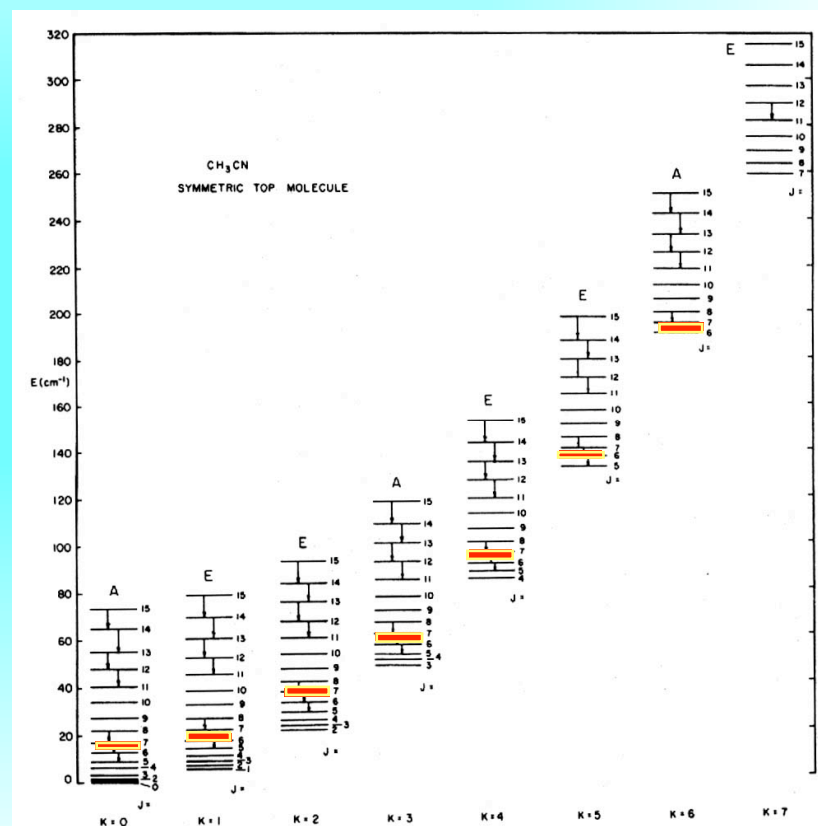


Molecular Physics 4

1.3 Complex Spectra

Linear molecules, or rigid rotors, have simple spectra. But more complex molecules are 3-D and have progressively more complex spectra: *symmetric tops*, both *prolate* (e.g. CH_3CN) and *oblate* (e.g. NH_3); and *asymmetric tops* (e.g. CH_3OH). The latter are a mess.

□ Look them up in the Lovas catalogue (on the web).



Molecular Physics 5

Other complications are possible as well, *e.g.* inversion transitions (NH_3), and hyperfine components (*e.g.* anything with a ^{14}N or ^{17}O). Hyperfines arise when the nuclear quadrupole I couples to the rotational J . A nice advantage: this splits the optical depth up into the components, so we can obtain \square from one J -line (see below). It also reduces “mismatched beam” problems.

1.4 Excitation

At a given T , the population of molecules will be distributed among the rotational energy levels, à la statistical mechanics (*e.g.* see below about the partition function). We can characterise this by an *excitation temperature* T_{ex} . Molecules make transitions between levels i and j either by collisions (probability $C_{ij} \text{ sec}^{-1}$ of going from level i to level j) or by radiation (probability $A_{ij} \text{ sec}^{-1}$).

Molecular Physics 6

Here,
and

$$C_{ij} = n \langle \sigma v \rangle$$
$$A_{ij} = 64\pi^4 \mu_{ij}^2 \nu_{ij}^3 S_{ij} / 3hc^3 g_i ,$$

where n is the number density of collision partners (usually H_2) for a given molecule, $\langle \sigma v \rangle$ is the mean cross-section for collisions at speed v (typically v is just the molecule's geometric size), μ_{ij} is the electric dipole moment of the molecule, ν_{ij} is the transition frequency, S_{ij} is the line strength, and g_i is the i -level degeneracy, usually $2i+1$. From this one can define a critical density for each molecule and transition,

$$n_{\text{cr}} \sim \mu^2 \nu^3 S / g \langle \sigma v \rangle (1 - e^{-h\nu/kT_r}),$$

at which the collisional and radiative probabilities will be equal (the bracketed term corrects for stimulated emission). So at higher densities (*e.g.* in planets'

Molecular Physics 7

atmospheres, or dense molecular cores), collisions dominate, and the level populations are *thermalised*, *i.e.*

$$T_{\text{kin}} = T_{\text{ex}}.$$

At densities below n_{cr} , radiative transitions are faster than collisions. Then higher-level populations rapidly collapse into the ground rotational state (or, collisions cannot significantly populate the higher- J levels):

$$T_{\text{kin}} > T_{\text{ex}} \sim T_{\text{bg}}.$$

Some examples:

	CO	CS	HCN	HC ₃ N	HCO ⁺
B	57.6	24.5	44.3	4.55	44.6
$\square_{J=1 \square 0}$	115	49.0	88.6	9.10	89.2
μ_{10}	0.11	1.96	2.98	3.6	4.07
$\log(n_{\text{cr}})$	3.6	5.0	6.2	4	5.3

So using the right J -transitions and molecules, we can (in principle) “peel away” the density structure of a given cloud with a suitable choice of n_{cr} .

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1.5 Radiative Transfer

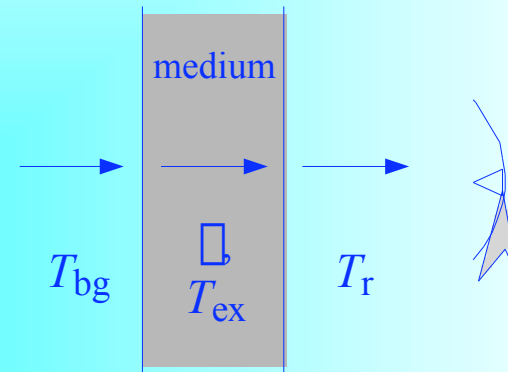
The holy equation is

$$T_r = (T_{\text{ex}} - T_{\text{bg}})(1 - e^{-\tau}),$$

where τ is the *optical depth* through the medium, T_{bg} is the background temperature (usually 2.7 K unless there's a nearby continuum source), and T_r is the observed *brightness temperature* or *radiation temperature*.

Optically thin ($\tau \ll 1$): then $T_r = (T_{\text{ex}} - T_{\text{bg}}) \tau = \tau T_{\text{ex}}$ if $T_{\text{ex}} \gg T_{\text{bg}}$.

Optically thick ($\tau \gg 1$): then $T_r = (T_{\text{ex}} - T_{\text{bg}}) = T_{\text{ex}}$ if $T_{\text{ex}} \gg T_{\text{bg}}$.



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So we have two main unknowns, τ and T_{ex} . We cannot get both from a single line (usually; hyperfines excepted), and need two pieces of data to solve for these, *e.g.* two different J -lines for the same molecule.

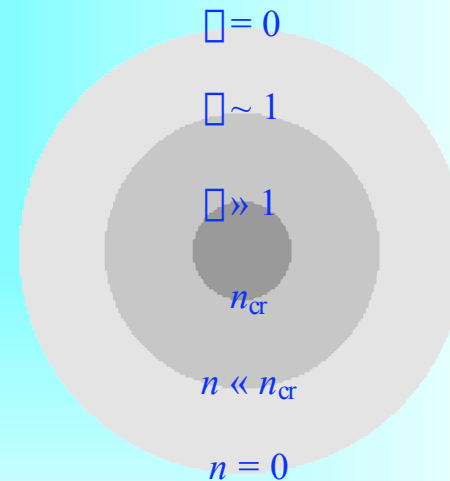
Remember, in general

$$T_r < T_{\text{ex}} < T_k.$$

1.6 Caveats

a) Radiative Trapping

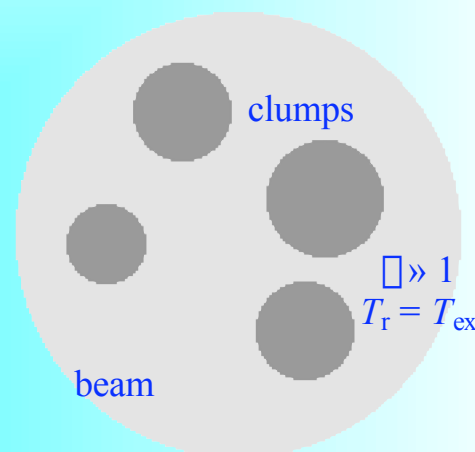
Particularly bad for CO. Note the low μ , n_{cr} : CO is very easily excited. It is also *very* abundant, so optical depths in molecular clouds are often $\gg 1$. In fact they are so high, that even looking from the outside, τ reaches ~ 1 before n reaches n_{cr} . So high τ makes the n_{cr} much lower than the statistical mechanics alone.



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b) *Filling Factor f*

This must depend on resolution. It's another way to get $T_r < T_{ex}$, even when $\Omega \gg 1$. It often makes estimates of T_{ex} and Ω indeterminate, and is worse when comparing “mismatched beams” (*i.e.* different resolutions for different J -lines) in T_{ex} calculations.



c) *Missing Flux at Short Spacings*

As described in previous talks, if short-spacing information is lacking, we don't have true intensities, and so can't get T_{ex} or Ω ; no abundances, chemistry, etc. Limited to kinematics (still useful!).

d) *Variations across the line for any/all the above!*

Observables

2.1 Velocity Field

————→ See Jürgen Ott's lecture

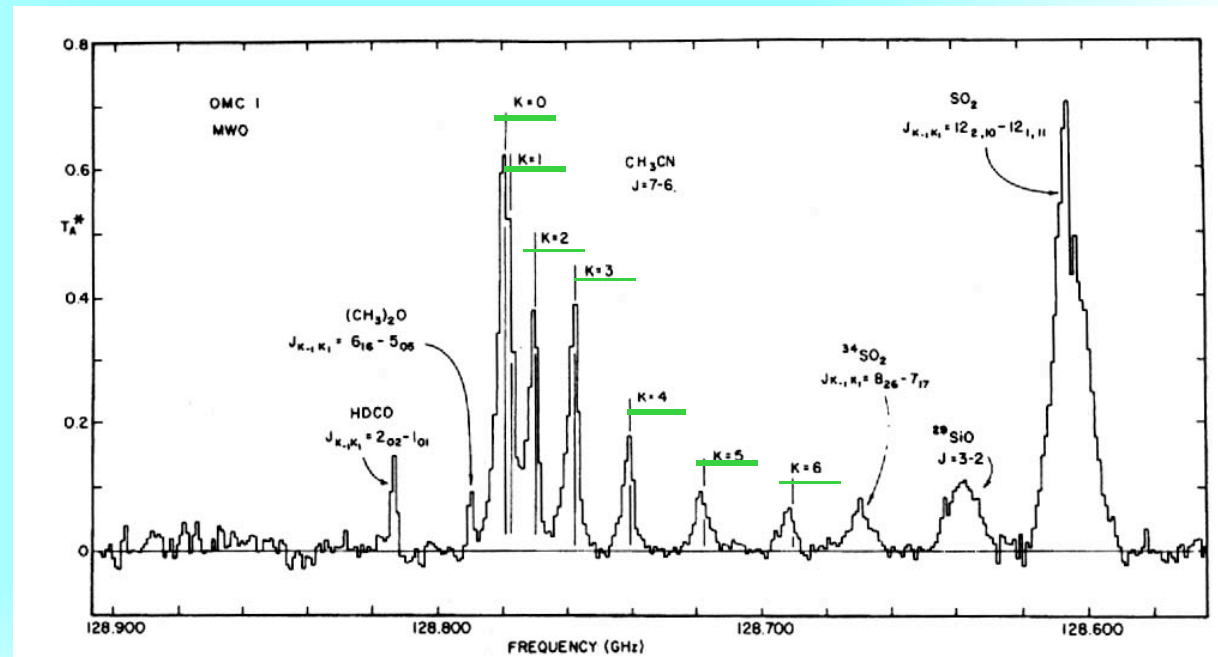
Doppler-shifted lines give velocities! We obtain channel maps, moment maps, kinematics. Can also get dynamics in some cases (rotation, Virial Theorem, oscillations, turbulence, outflows and infall). Thus carefully examining velocity data cubes is a very powerful astrophysical analysis technique.

2.2 Optical Depth, Excitation, and Filling Factor

With good data, avoiding pitfalls, we can obtain the total number of molecules emitting, and their thermodynamic state. *E.g.* with 3 beam-matched *J*-lines, or observing 2 lines at high enough resolution that $T_r \sim T_k$, we can be reasonably sure of our solution.

Observables 2

Alternatively, hyperfine components of 1 J -line, or symmetric-top molecules with many closely-spaced K -lines at one J , enable us to elegantly get around beam-matching problems.



Observables 3

Example: say we have 2 lines with matched beams, T_{ex} describes the line level populations, and let's assume $f = 1$ for both lines, for simplicity. Then we just solve the simultaneous equations

$$\begin{aligned} T_{r1} &= (T_{\text{ex}} - T_{\text{bg}}) \tau_1 \\ \text{and} \quad T_{r2} &= (T_{\text{ex}} - T_{\text{bg}}) \tau_2 = (T_{\text{ex}} - T_{\text{bg}}) \tau_1 (g_2/g_1) e^{-h\nu/kT_{\text{ex}}} . \end{aligned}$$

The same idea works whether we use different J -lines, a (J, K) set, or hyperfine components of one line. Note we must know the relationship between the optical depths: assuming LTE (or the T_{ex} description), this is given by the relative weights g ($= 2J+1$: level degeneracy factors).

We can also solve for a filling factor if we have a third line.

Observables 4

2.3 Column Density

Optical depths are fine, but physically we want column densities. These are related via Einstein A s:

$$N_{\text{tot}} = \frac{3kT_r Q(T_{\text{ex}}) e^{E_u/kT_{\text{ex}}} \int \tau d\nu}{8\pi^3 \nu \mu^2 S (1 - e^{-h\nu/kT_{\text{ex}}}} , \quad \text{note: cgs! (argh!)}$$

where $Q(T_{\text{ex}})$ is the partition function for the molecule. A more flexible way is to do this graphically, recasting the above as $y = mx + b$:

$$\ln \left[\frac{3kT_r \int \tau d\nu}{8\pi^3 \nu \mu^2 S} \right] = \ln \left[\frac{N_{\text{tot}}}{Q(T_{\text{ex}})} \right] - \left[\frac{E_u}{kT_{\text{ex}}} \right] .$$

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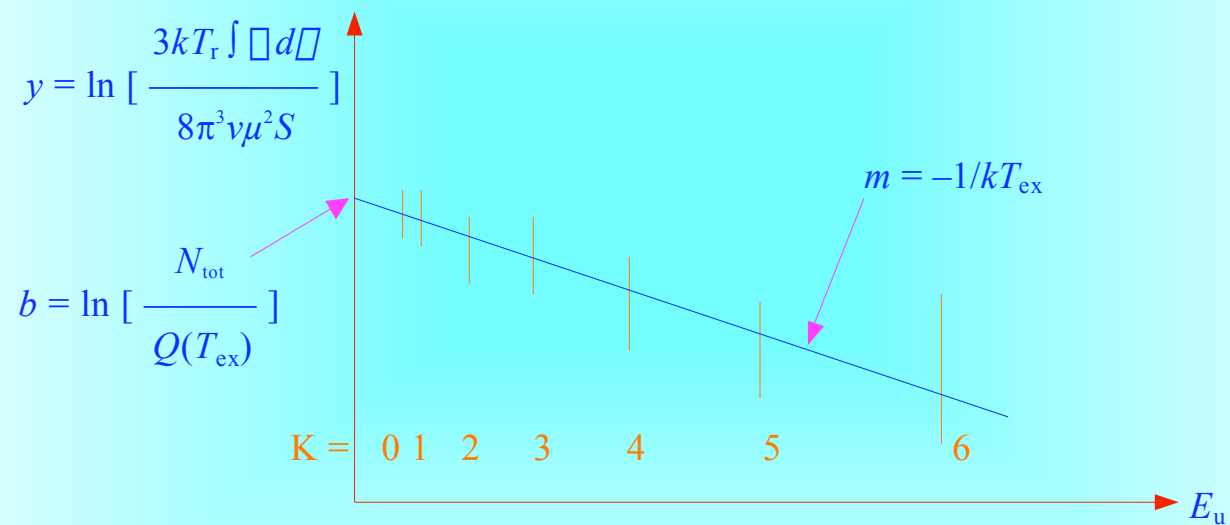
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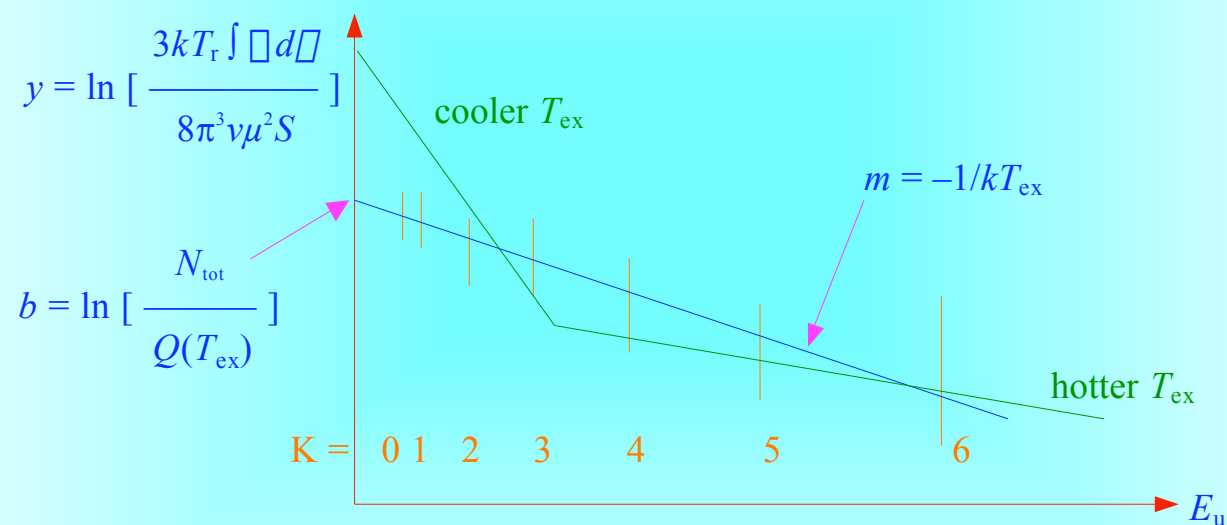
Observables 5

Example: recall the methyl cyanide (CH_3CN) spectrum.



Observables 5

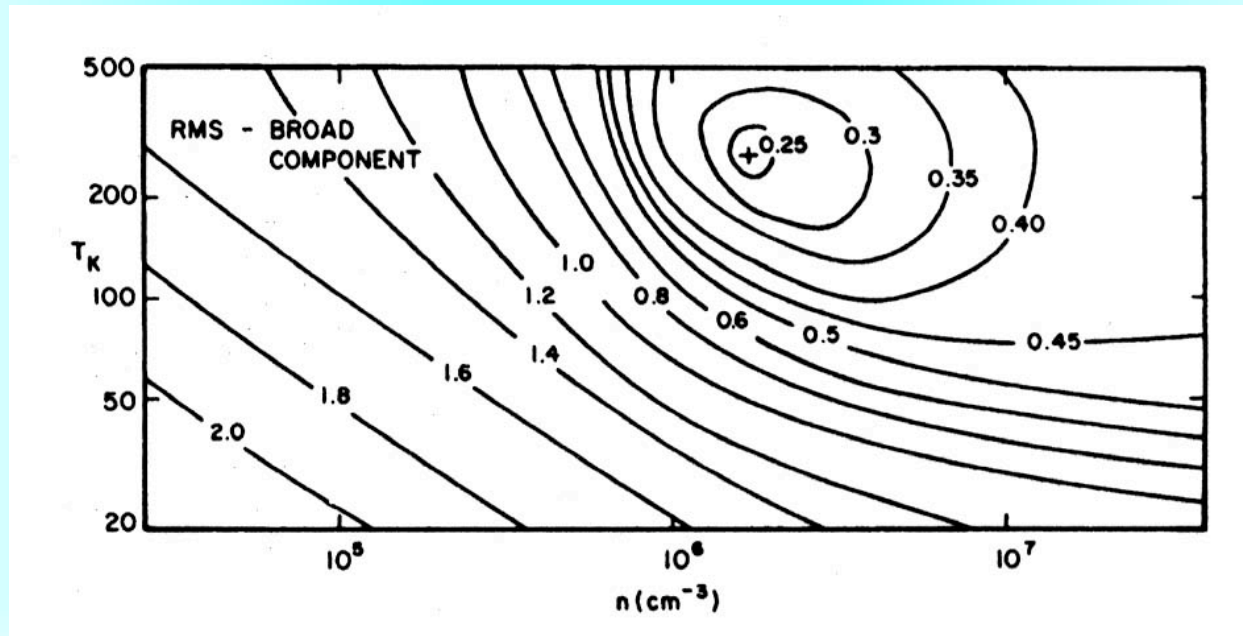
Example: recall the methyl cyanide (CH_3CN) spectrum.



A great advantage of this graph is eyeball physics: if there are 2 T_{ex} regimes (e.g. a hotter core and cooler envelope) it will show up as a **kink** in the fit (2 slopes).

Observables 6

We can play this game with densities too, *e.g.* formaldehyde (H_2CO) is very well-suited to density (n_{cr}) modelling, for a swag of lines from 5–50 GHz.



Observables 7

2.4 A Menagerie of Temperatures

A Cautionary Tale! The $N_{\text{tot}}-T_{\text{ex}}$ example shows that temperature is sometimes a slippery concept. There are even more diversions on this path. Ammonia (NH_3) has (J,K) inversion lines (which are actually hyperfine multiplets, each with its own T_{ex}) that together define a *rotation temperature* T_{rot} , which is $\neq T_{\text{kin}}$. (Here $T_{\text{ex}} < T_{\text{rot}} < T_{\text{kin}}$.) Formaldehyde (H_2CO) has a low-lying energy level that is often underpopulated relative to the radiative (J,K) ladder seen in emission. The transition from the ground state of the ladder to this “empty” level is thus seen *in absorption against the CMB!* Very widespread in galactic GMCs. And then of course, there are dust temperatures, which are also sometimes poorly defined. *E.g.* larger grains are “warmer” than small grains, and the smallest grains “spike”: they’re either “hot” or “cold” when they absorb or emit even low-energy photons.

Sample Results, Analysis, & Interpretation

3.1 Classes of Objects

—————▶ See Vincent Minier's lecture

Most often, mm telescopes spend time on PMS stars & molecular clouds. But Earth's atmosphere, comets, planets, AGB stars and PPNe, Sgr A*, spiral & irregular galaxies, AGNs & galaxy evolution, and cosmology & the CMB are studied too. What do we learn?

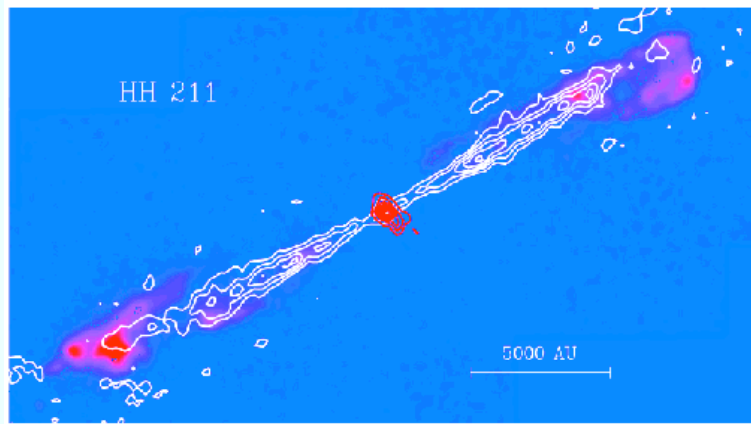
3.2 Motions

Doppler velocities reveal a rich variety of physical effects:

- orbital motions □ gravitating mass: disk? –properties
- expansion □ time since origin, evolution
- waves or shear motions □ MHD, equilibrium
- infall □ true protostars, accretion rate, heating
- outflows □ jets, angular momentum transfer, cloud dispersal

Sample Results 2

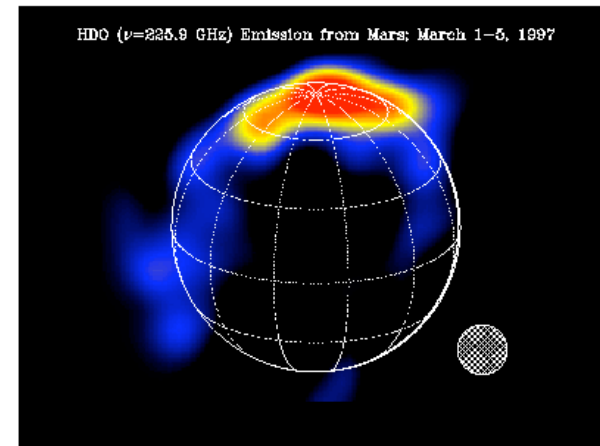
Molecular Clouds and Star Formation



CO J=2-1 map of the protostellar jet in HH211 from the IRAM PdBI overlaid on a near infrared image of excited H₂; red contours delineate a dust concentration around the protostar.

- probe the turbulence, fragmentation and gravitational collapse of star forming clouds
- determine the nature of protostellar outflows and measure mass-loss and accretion rates
- obtain abundances and study the chemistry of low temperatures and dissociative shocks

Planetary Sciences



OVRO Interferometer image of integrated HDO (3 1 2 - 2 2 1) line emission from Mars during northern summer solstice. Emission is concentrated over the Northern Polar Cap, indicating vigorous sublimation from water ice.

- study abundances of molecular species, probing atmospheric chemistry and transport
- resolve planetary disks to study variation of atmosphere with position and time
- study atmospheric dynamics through direct observation of doppler shifts in line cores

Sample Results 3

3.3 Abundances and Chemistry

Rare species in Earth's (or any other rocky planet's, or Titan's) atmosphere trace exotic chemistry, track down major, invisible counterparts.

Convert column density to abundance relative to H_2 , so we can compare to models of interstellar/circumstellar/planetary chemistry. There are >100 molecular species known, so the models have 1000s of chemical reactions in vast chemical networks. These are run as (usually) time-based simulations.

We often see different chemical domains operating in different physical conditions, *e.g.* “hot core”, “dark cloud”, and “diffuse cloud” chemistries can be distinguished. Recently, freeze-out (“depletion”) of some species onto dust grains has become better understood, based on maps of various species in cores: only a few species (*e.g.* NH_3 , N_2H^+) trace the total mass, best traced by

Sample Results 4

dust emission. CO freezes out in the densest, coldest parts!

The X-Factor: the conversion from $I_{\text{CO}} = \int T_{\text{r}} d\Omega$ to H_2 in the Milky Way is established (although still controversial). Incredibly, it has a different value in other galaxies! The cheek.

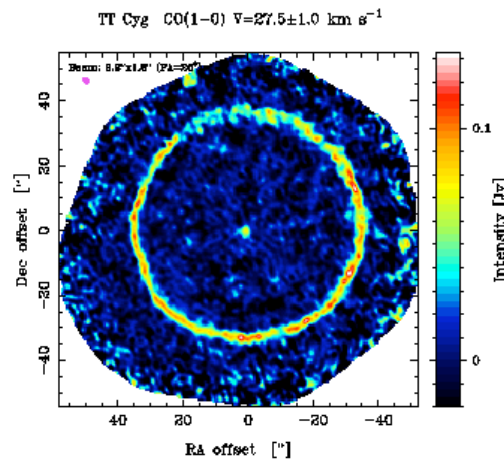
AGB stars/PPNe show a chemical “layering” in their ejecta, *i.e.* the gas chemically evolves as it flows away. Dramatic images show this directly, confirming chemical models.

3.4 Masses and Stability

Jeans masses or lengths in GMCs or cores are significant: ongoing star formation. Populations indicate time spent in each stage. Various dynamical considerations imply the importance of magnetic fields. Narrow line probes

Sample Results 5

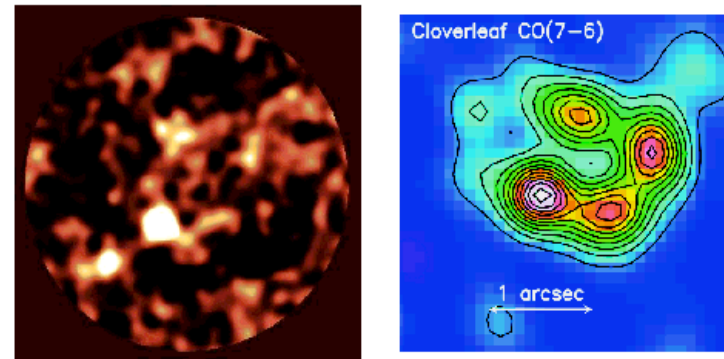
AGB Stars and Planetary Nebulae



CO J=1-0 image of the carbon star TT Cyg from the IRAM PdBI (Olofsson et al. 1999).

- Image (multi) thin shells to study episodic mass loss rate in the AGB phase (e.g. TT Cyg).
- Map disks and bipolar outflows associated with the transition from AGB to PN
- Detect polarization of molecular emission resulting from IR excitation.

Galaxy Evolution and Cosmology



Left: 850µm SCUBA image of the Hubble Deep Field showing a new population of dusty galaxies.

Right: Lensed CO J=7-6 emission from the Cloverleaf quasar imaged by the IRAM PdBI.

- probe the interstellar medium of evolving galaxies through CO, CI, and CII emission lines
- image dusty starbursts and gravitational lenses that cannot be penetrated at optical wavelengths
- obtain kiloparsec resolution maps of the nuclei of active galaxies in the early universe

Sample Results 6

are needed to measure *ambipolar diffusion* (the slip between ions and neutrals in dense cores). This governs quiescent cloud structure, and MHD waves in more massive or turbulent clouds. The Virial Theorem relates I_{CO} to cloud mass and size, but tends to be more relevant to GMCs than to cores. We still don't know how to make massive stars, or massive clusters.

3.5 The Larger Scale

GMCs in the Milky Way are the only way, besides HI, to get the rotation curve for the Galaxy. Critical for defining the kinematic distance scale, and size & mass of MW. Do the same in nearby galaxies, and get dark matter constraints: it doesn't dominate discs, but it does halos. Also inner CO defines *box orbits* which are characteristic of barred spirals: MW has a bar!

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