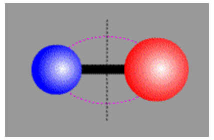
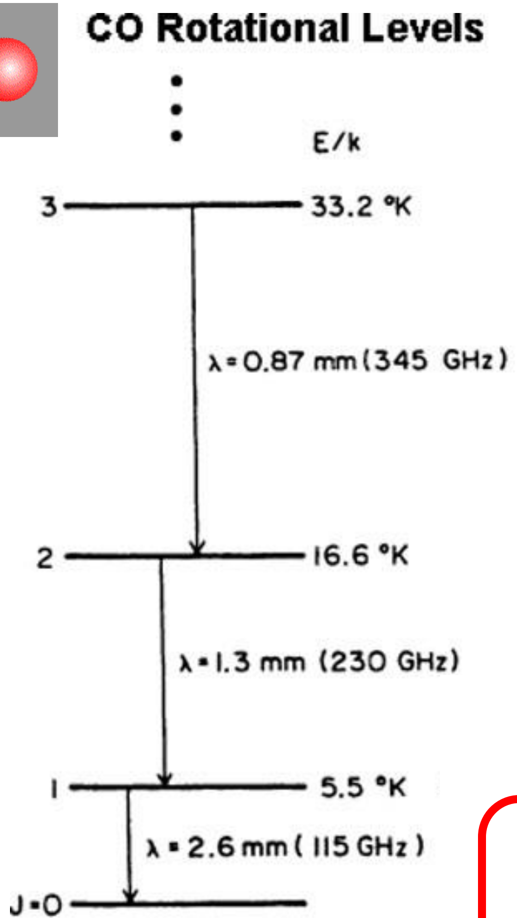

How cool was Green Bank?!?

Rotational Spectroscopy (from ERA):





Wilson et al., 1970

The rotational kinetic energy associated with the angular momentum is,

$$E_{\text{rot}} = \frac{I\omega^2}{2} = \frac{L^2}{2I}. \qquad (7.106)$$

Which of course also becomes quantized!

$$\boxed{E_{\text{rot}} = \left(\frac{\hbar^2}{2I}\right) J\,(J+1), \qquad J = 0, 1, 2, \ldots.} \qquad (7.107)$$

This quantization of rotational energy implies that changes in rotational energy are quantized, and the states permitted are restricted by quantum-mechanical **selection rules**, which in this simple case is,

$$\boxed{\Delta J = \pm 1.} \qquad (7.108)$$

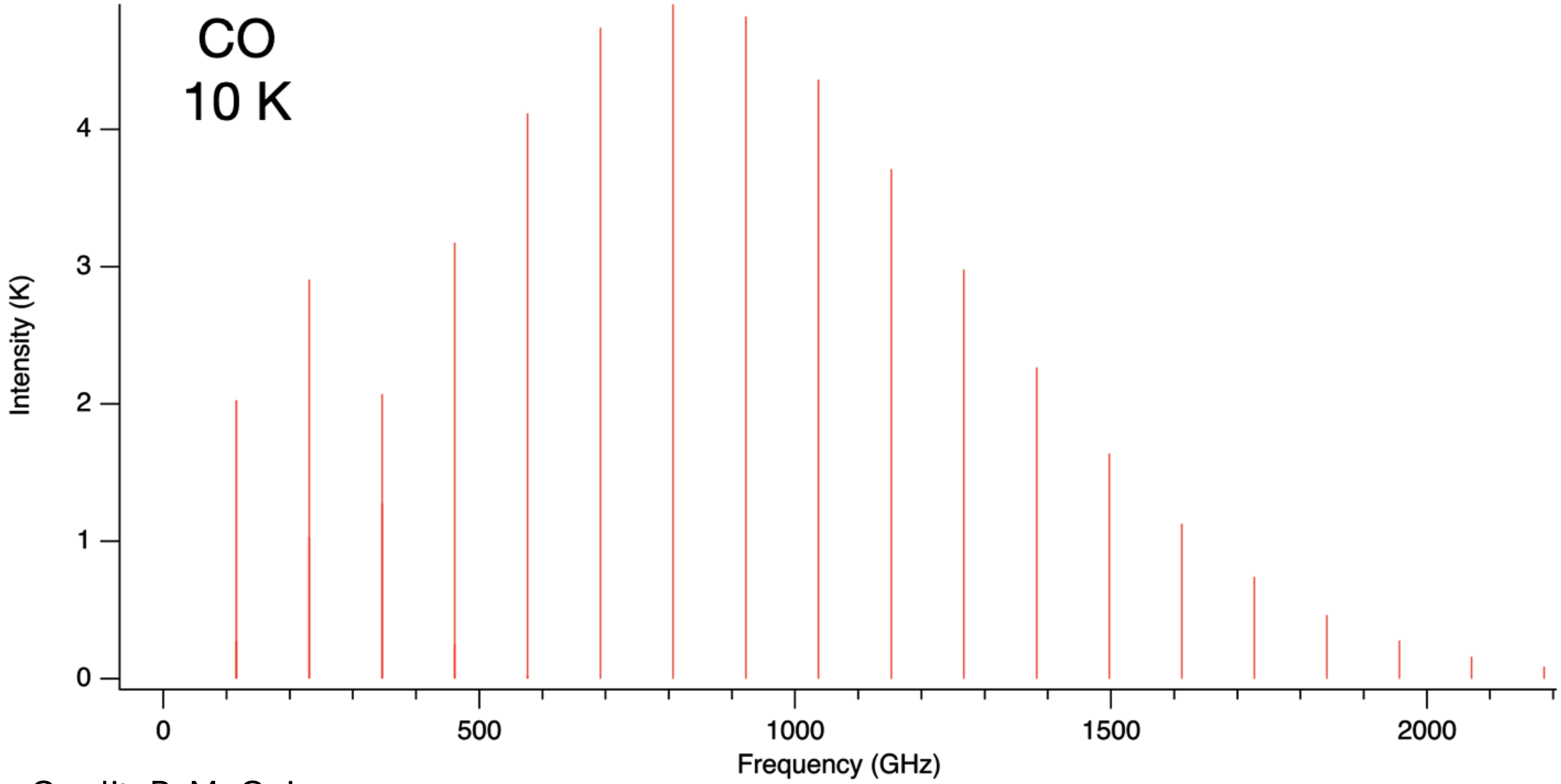
The frequency of the photon can be written,

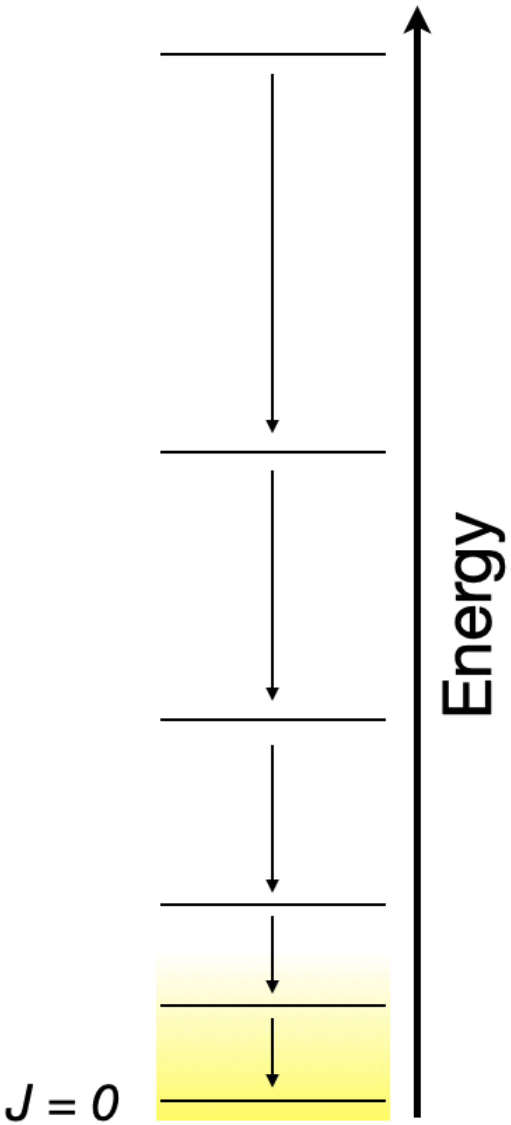
$$\nu = \frac{\Delta E_{\text{rot}}}{h} = \frac{\hbar J}{2\pi I}, \qquad J = 1, \; 2, \ldots, \qquad (7.109)$$

Use to calculate your rotational frequency → (structured like a ladder)

$$\boxed{\nu = \frac{hJ}{4\pi^2 m r_e^2}, \qquad J = 1, 2, \ldots.} \qquad (7.110)$$

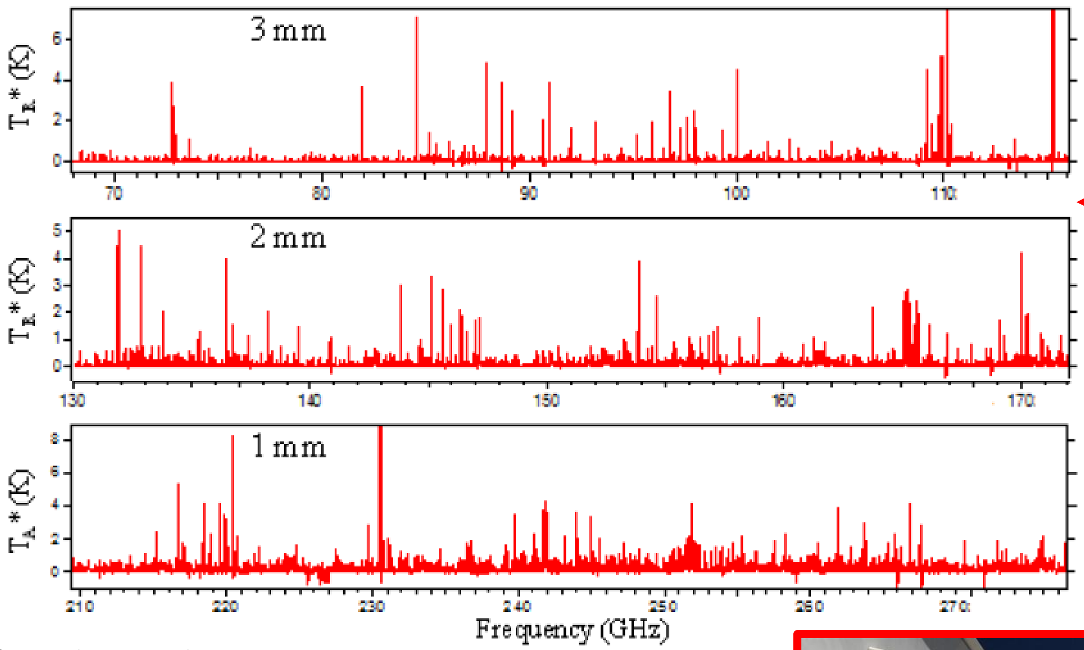
Rotational Spectroscopy:



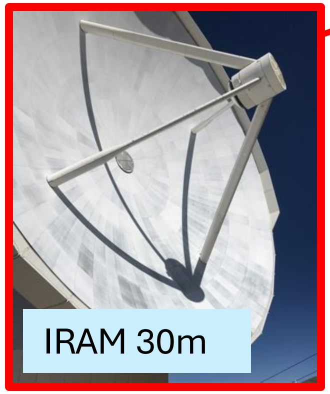


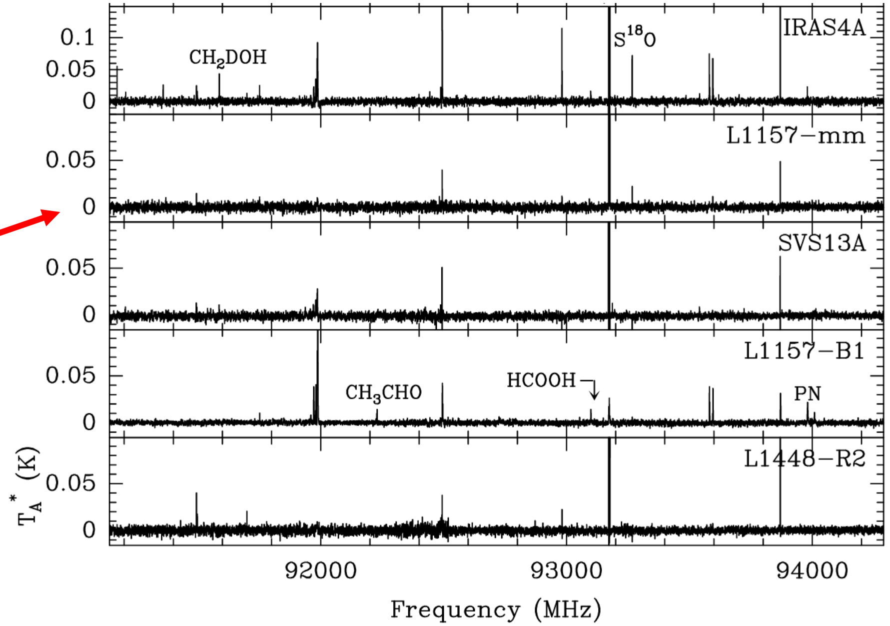
Credit: B. McGuire

Rotational Lines at Radio Wavelengths: The Best Probe of *Complex* Molecules



Credit: L. Ziurys





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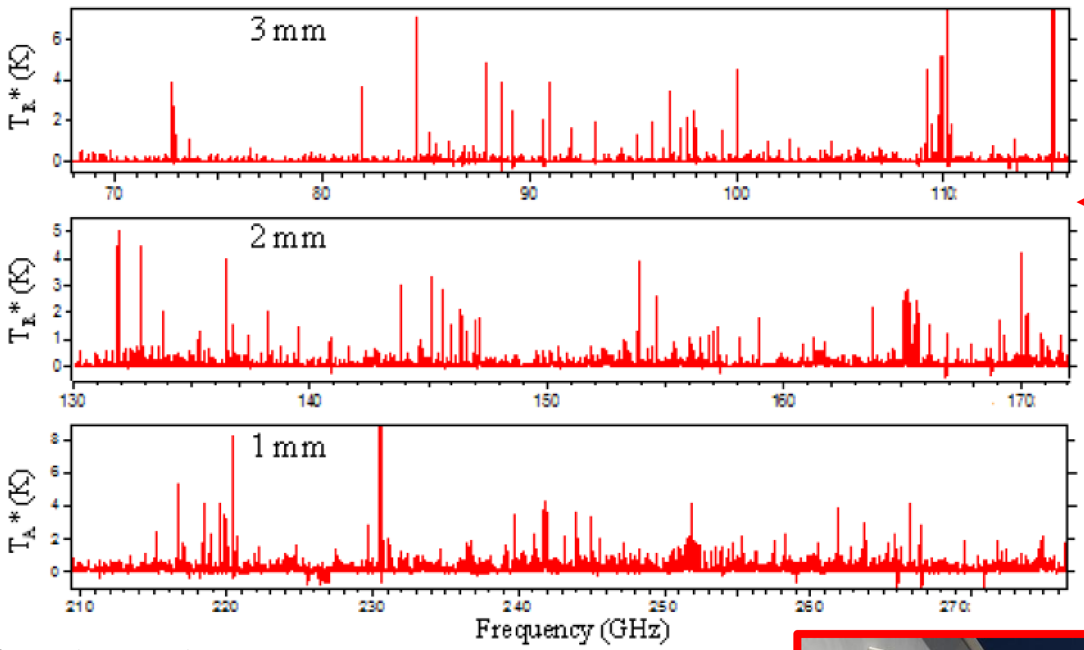

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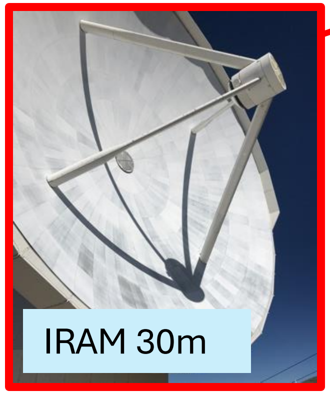

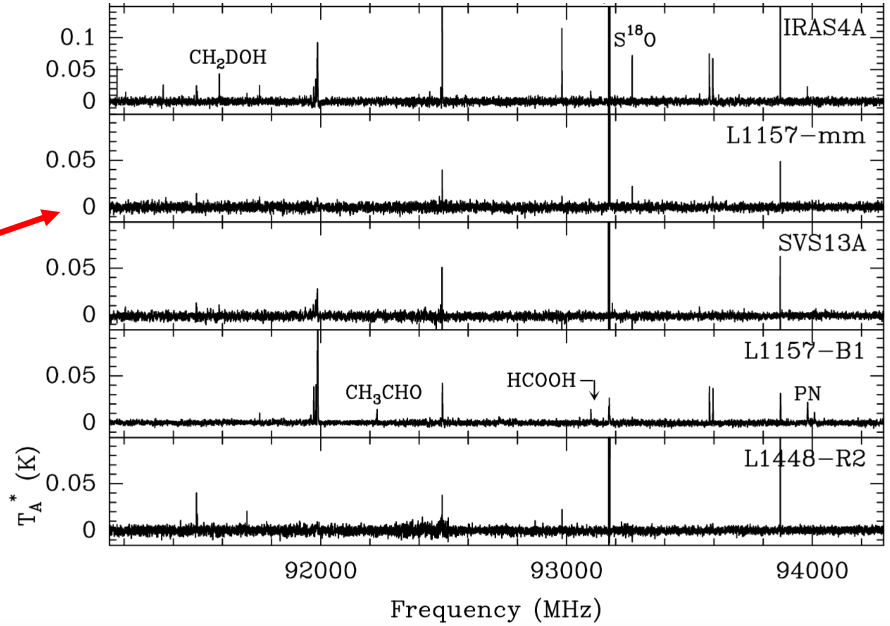

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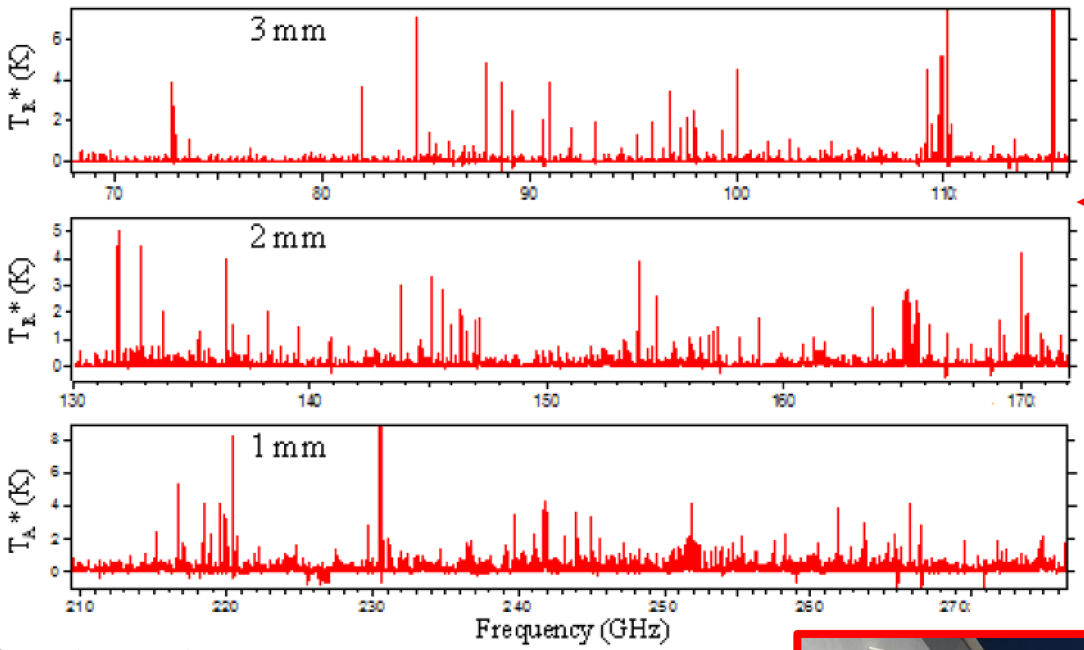
So, how do we know what molecules to look for, and in what ISM conditions? And how do we extract useful parameters out for our science? …

Rotational Lines at Radio Wavelengths: The Best Probe of *Complex* Molecules



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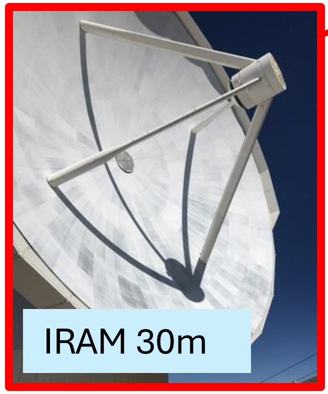

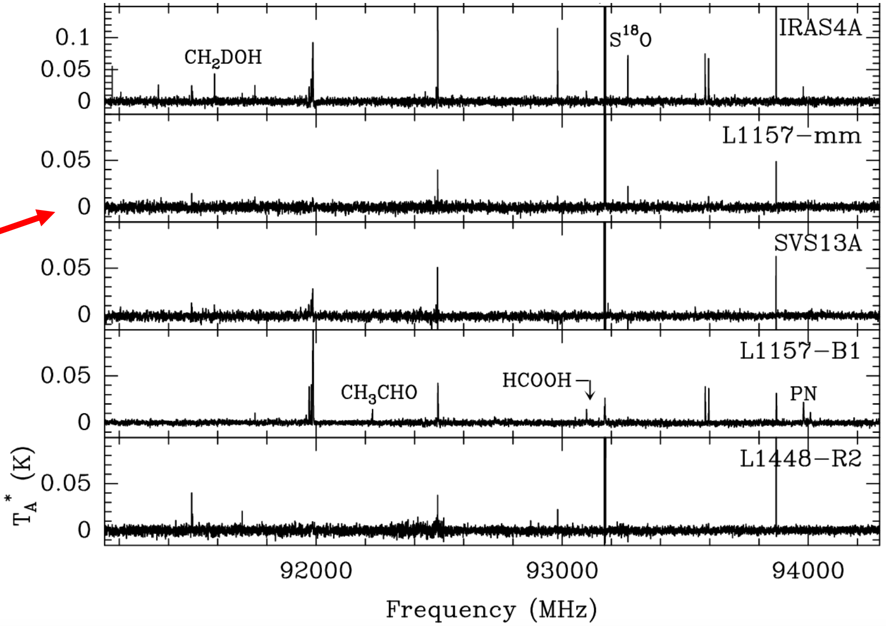

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Let's learn about **Line Radiative Transfer** and **Excitation**

GREEN BANK OBSERVATORY
AUI
NRAO National Radio Astronomy Observatory
NSF

Einstein Coefficients

To understand how emission, j_ν, and absorption, k_ν, coefficients are related to the atoms and molecules in a cloud, we must introduce the Einstein coefficients!

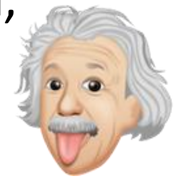
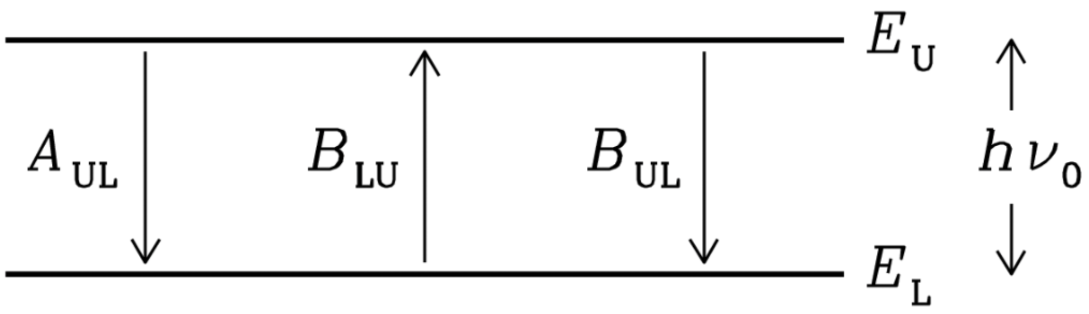


Fig. 7.5 (ERA)



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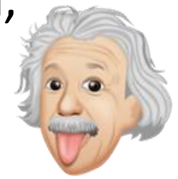

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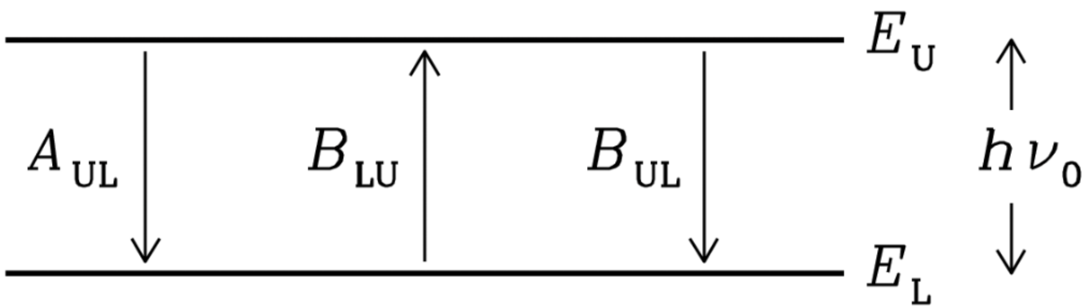

A_{UL} = spontaneous emission coefficient from level *u* to *l*, the probability per unit time that an atom or molecule in the upper state will emit a photon, and transition to the lower state (s^{-1}).

B_{UL} = induced (or stimulated) emission coefficient from level *u* to *l*, the probability per unit time per unit intensity at a given frequency that an atom or molecule in the upper state will emit a photon and transition to the lower state (s^{-1} or $s^{-1}\,erg^{-1}\,cm^2\,rad^2$).

B_{LU} = absorption coefficient from level *l* to *u*; induced emission from level *u* to *l*; the probability per unit time per unit intensity at a given frequency that an atom or molecule in the lower state will absorb a photon and transition to the upper state (s^{-1} or $s^{-1}\,erg^{-1}\,cm^2\,rad^2$).

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Einstein Coefficients

The photon emitted or absorbed during a transition between the upper and lower states will have energy and frequency related to,

$$E = E_U - E_L \qquad (7.38)$$

The rate (s^{-1}) for this process is proportional to the **profile-weighted mean radiation energy density** of the surrounding radiation field,

$$\bar{u} \equiv \int_0^\infty u_\nu(\nu) \;\; \phi(\nu) \;\; d\nu \qquad (7.39)$$

Where φ(ν) is your narrow line profile. Here a system in the lower energy stage may **absorb** a photon of frequency roughly equal to the rest frequency, $\nu \approx \nu_0$, and **transition to the upper state**.

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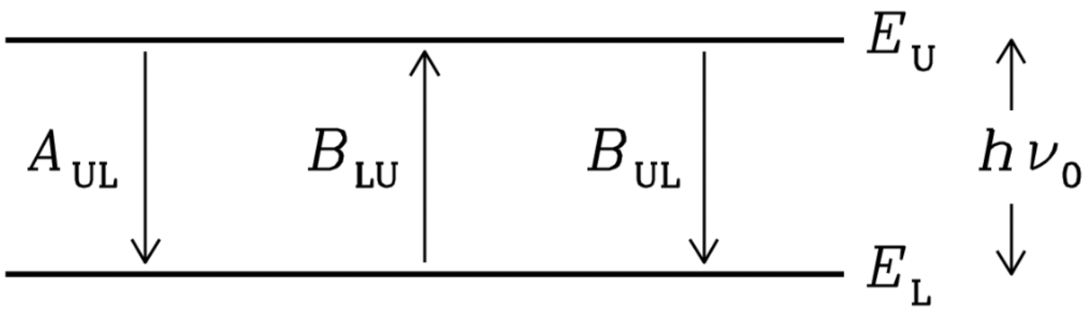

$$\rightarrow \boxed{B_{LU}\bar{u}} \qquad (7.40)$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

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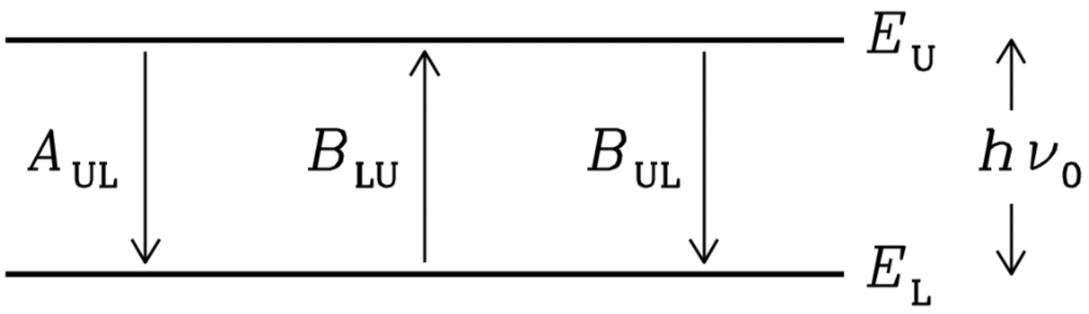

→ $$\boxed{B_{LU}\bar{u}} \qquad (7.40)$$

Analogous for 'stimulated emission' or **negative absorption:**

$$\boxed{B_{UL}\bar{u}} \qquad (7.41)$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

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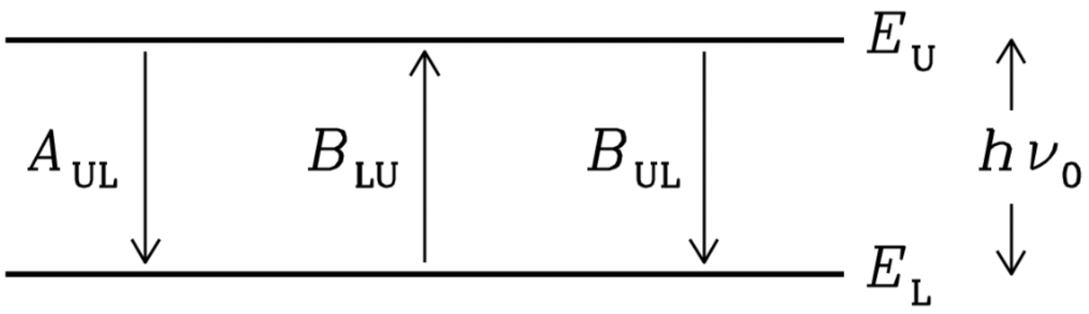

We can write this coefficients now in useful ways...

The first to **balance** the system, considering full thermodynamic equilibrium (TE) for 'n_U' or 'n_L' atoms or molecules per unit volume in 'upper' or 'lower' energy states:

$$\boxed{n_U A_{UL} + n_U B_{UL} \bar{u} = n_L B_{LU} \bar{u}.} \qquad (7.42)$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Einstein Coefficients

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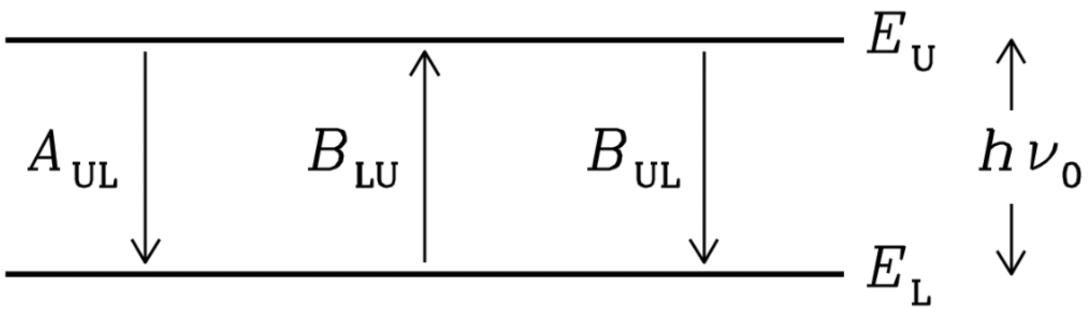

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And the ratio of n_U to n_L is fixed by the **Boltzmann equation**

$$\frac{n_U}{n_L} = \frac{g_U}{g_L} \exp\left[-\frac{(E_U - E_L)}{kT}\right] = \frac{g_U}{g_L} \exp\left(-\frac{h\nu_0}{kT}\right), \qquad (7.43)$$

where g_U and g_L are the numbers of distinct physical states or (**statistical weights**) having energies E_U and E_L

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Einstein Coefficients

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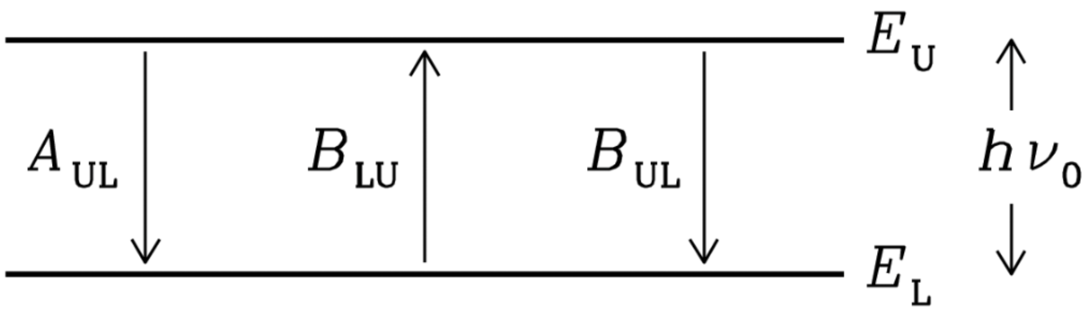

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→

Solving these two equations (see textbook) gets you the **equations of detailed balance**:

$$\boxed{\frac{g_L}{g_U} \frac{B_{LU}}{B_{UL}} = 1} \qquad (7.51)$$

$$\boxed{\frac{A_{UL}}{B_{UL}} = \frac{8\pi h \nu_0^3}{c^3}.} \qquad (7.52)$$

Einstein Coefficients

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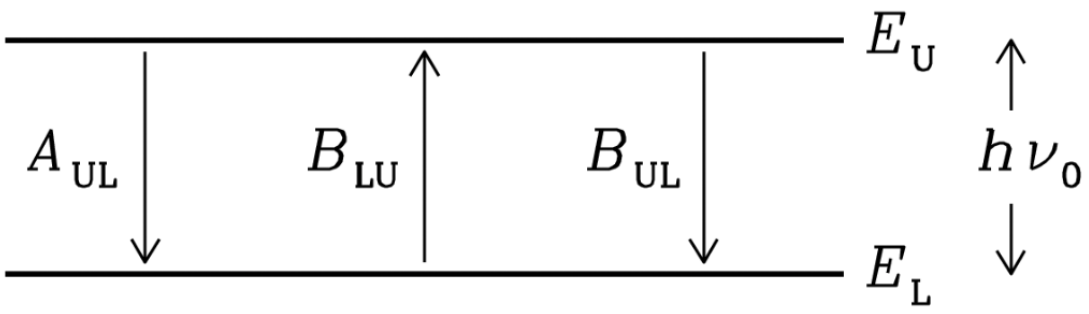

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→

Excitation Temperature is defined by the **Boltzmann equation** and gives the ratio of the populations in each level (T_{ex} or T_X)

$$T_{ex} = \frac{h\nu/k}{\ln \frac{n_l g_u}{n_u g_l}},$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Radiative Transfer with Einstein Coefficients

Remember our radiative transfer equation:

$$\frac{dI_\nu}{ds} = -\kappa I_\nu + j_\nu, \qquad \text{(2.27 and 7.52)}$$

We can construct **emission** and **absorption coefficients** from the Einstein coefficients,

$$\kappa = \left(\frac{h\nu_0}{c}\right)(n_L B_{LU} - n_U B_{UL})\,\phi(\nu)\,. \qquad (7.55)$$

$$\frac{dI_\nu}{ds} = j_\nu = \left(\frac{h\nu_0}{4\pi}\right) n_U A_{UL}\,\phi(\nu)\,. \qquad (7.56)$$

And write the line radiative transfer equation,

★ $$\boxed{\frac{dI_\nu}{ds} = -\left(\frac{h\nu_0}{c}\right)(n_L B_{LU} - n_U B_{UL})\,\phi(\nu)\,I_\nu + \left(\frac{h\nu_0}{4\pi}\right) n_U A_{UL}\,\phi(\nu)\,.} \qquad (7.47)$$

Radiative Transfer with Einstein Coefficients

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How does this determine what we observe with our radio telescope?

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Radiative Transfer with Einstein Coefficients

Remember our radiative transfer equation:

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We can simplify by defining a source function, S_ν, and writing in terms of the **optical depth, τ_ν**

$$\frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu \qquad \text{where} \qquad S_\nu = \frac{j_\nu}{k_\nu} \qquad \text{and} \qquad \tau_\nu = \int_0^L k_\nu \, dz$$

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by multiplying both sides by $e^{\tau\nu}$ a general solution to the equation of radiative transfer is found,

$$I_\nu = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau'} \exp[-(\tau_\nu - \tau')]\mathrm{S}_\nu \mathrm{d}\tau'$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

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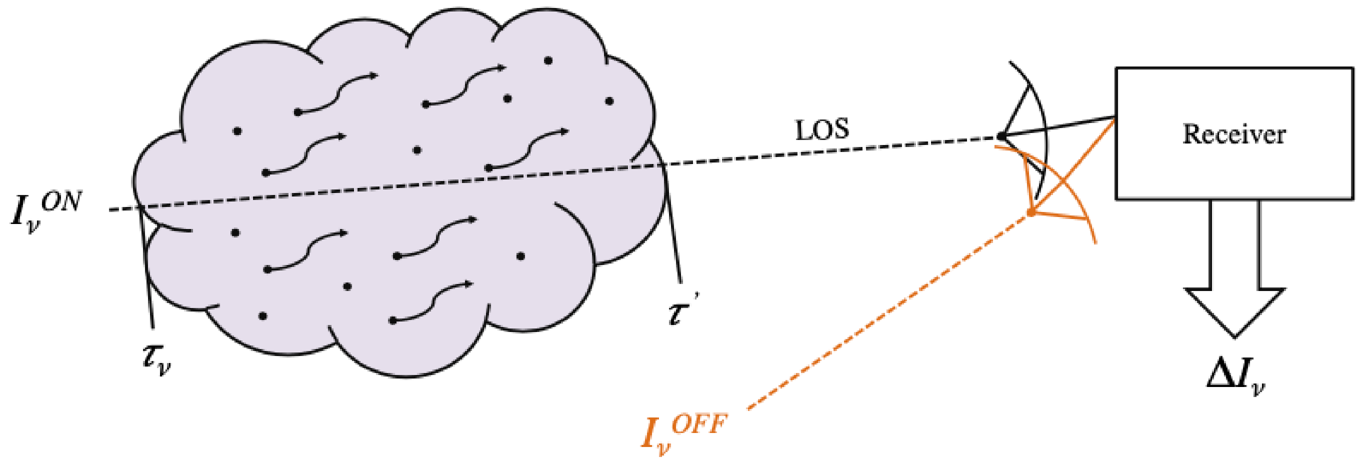
The sum of the background intensity attenuated by the interstellar medium plus the integrated emission attenuated by the effective absorption due to the ISM between the point of emission and the observer

Radiative Transfer with Einstein Coefficients

A standard observing mode in astronomy is to measure the intensity along a line-of-sight, LOS, to the object of interest (e.g., an interstellar cloud) and then along a LOS just off the object,

$$\Delta I_\nu = I_\nu^{ON} - I_\nu^{OFF} = [S_\nu - I_\nu](1 - e^{-\tau_\nu})$$



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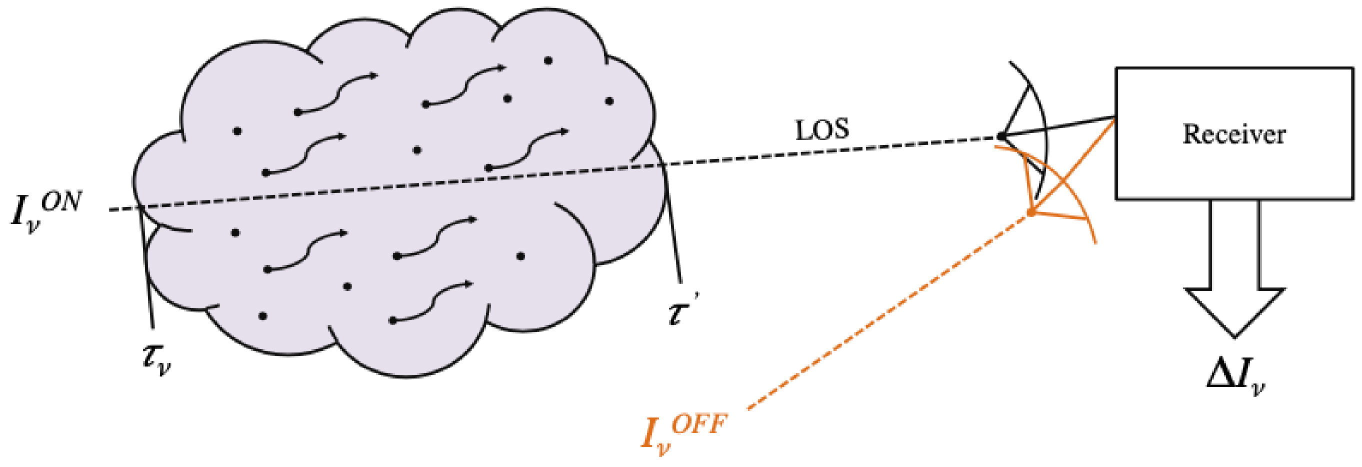

Now, in terms of Einstein coefficients,

$$S_\nu = \frac{j_\nu}{k_\nu} = \frac{n_u A_{ul}}{n_l B_{lu} - n_u B_{ul}} = \frac{A_{ul}/B_{ul}}{(n_l B_{lu}/n_u B_{ul}) - 1}$$

And, assuming the gas is in TE, the **Boltzmann equation and equations of detailed balance** can be substituted to yield,

$$S_\nu = \frac{(2h\nu^3/c^2)}{g_u n_l / g_l n_u - 1} \Leftrightarrow \frac{2h\nu^3}{c^2} \frac{1}{e^{h\nu/kT_{ex}} - 1}$$

Which is?!

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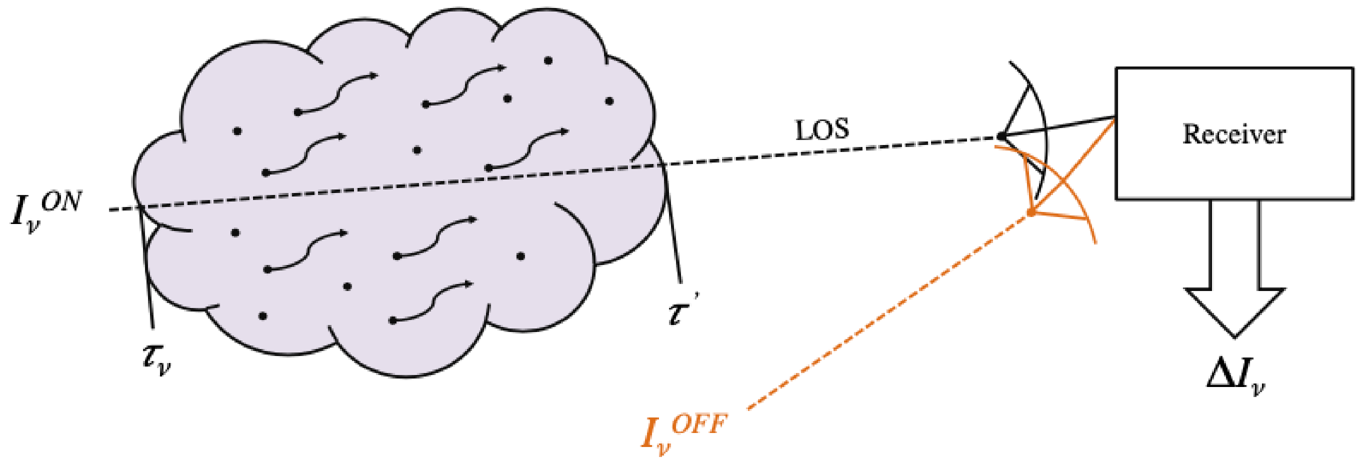

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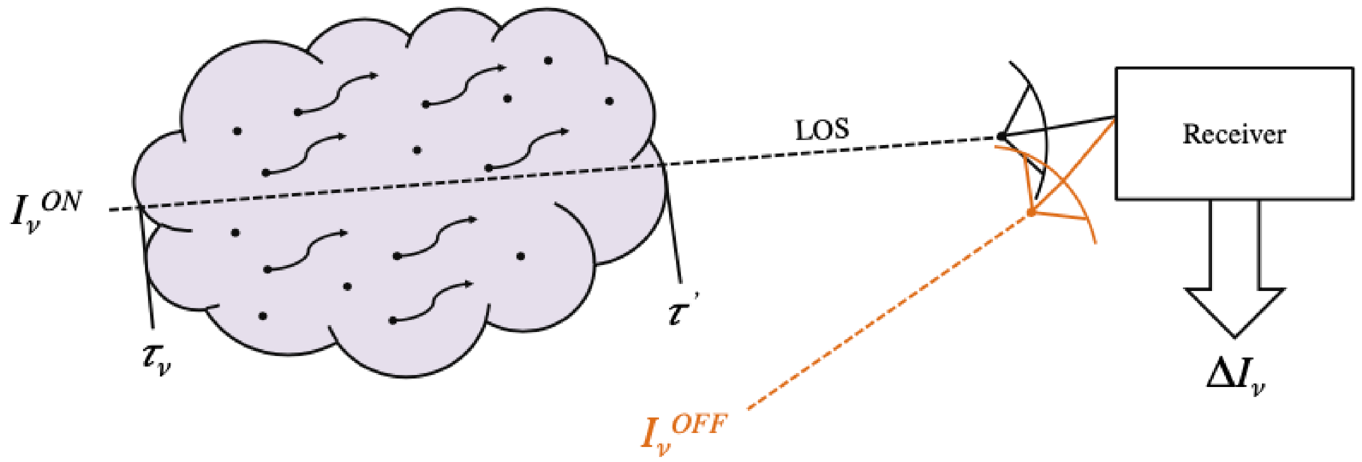
Your Planck Function! 

Radiative Transfer with Einstein Coefficients

In the case of **"local thermodynamic equilibrium" (LTE)** the radiative field is defined as a blackbody (Planck Function) with a constant excitation temperature, T_{ex} (where $T_k \sim T_{ex}$)

$$\Delta I_\nu = [B_\nu(T_{ex}) - B_\nu(T_{BG})](1 - e^{-\tau_\nu})$$



Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

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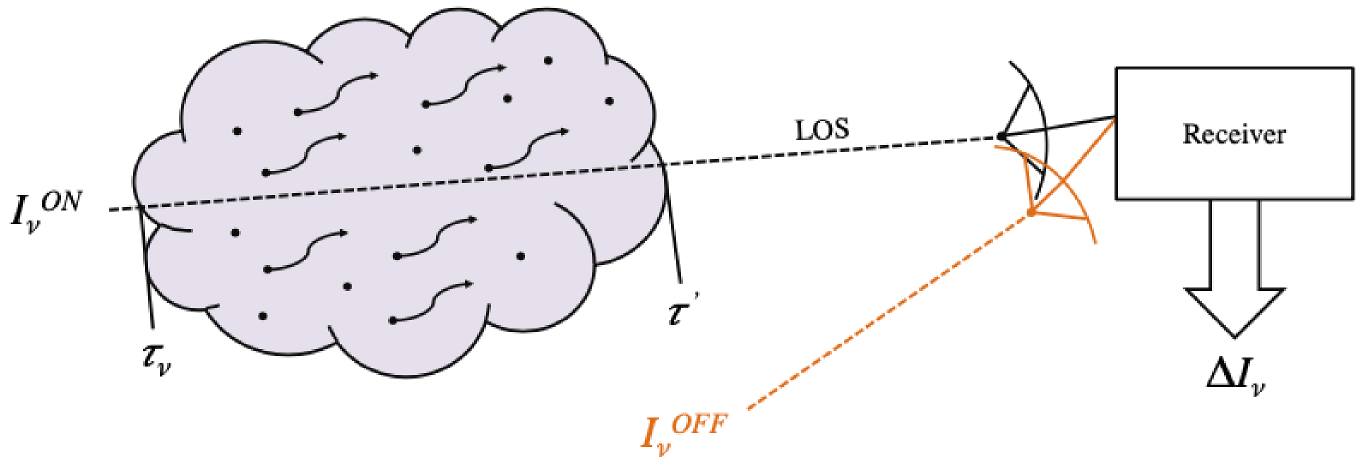
In the Rayleigh–Jeans limit:

$$B_\nu(T) = \frac{2\nu^2 kT}{c^2} \propto T$$

$$\Delta T = [T_{ex} - T_{BG}](1 - e^{-\tau_\nu})$$



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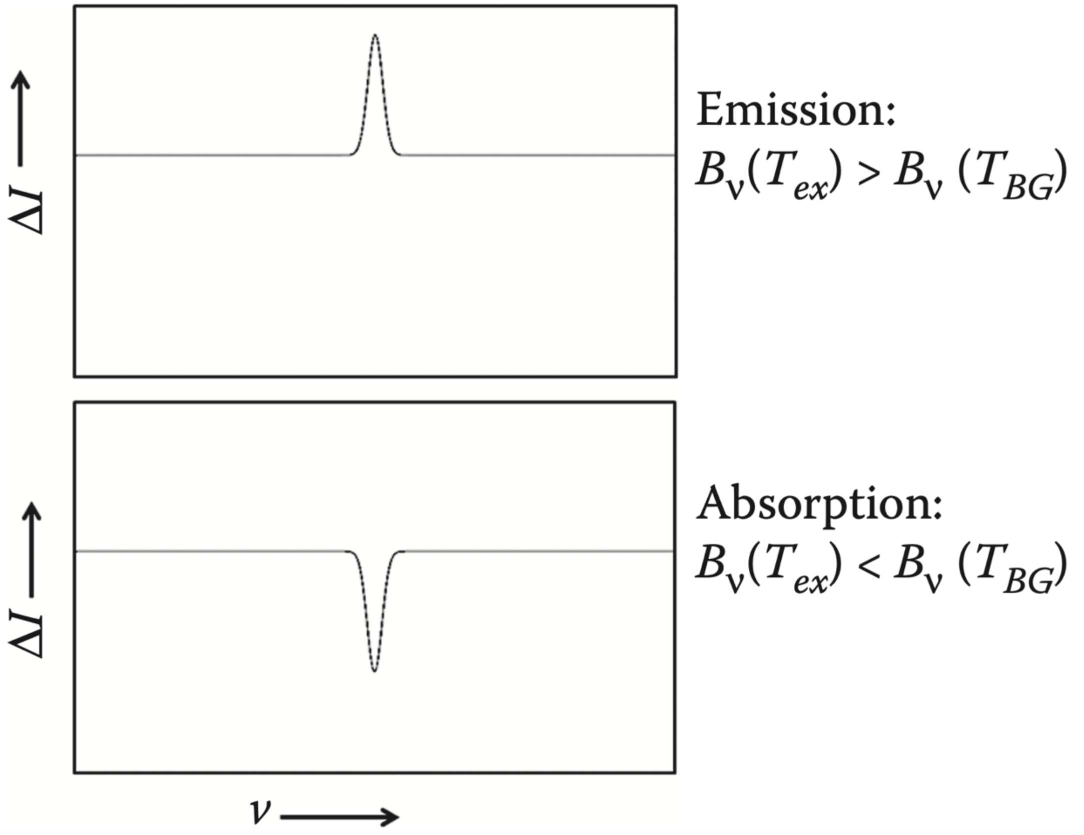

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In the limiting cases,

$$\Delta I_\nu = [B_\nu(T_{ex}) - B_\nu(T_{BG})] \quad \text{for } \tau_\nu \gg 1$$

$$\Delta I_\nu = [B_\nu(T_{ex}) - B_\nu(T_{BG})]\tau_\nu \quad \text{for } \tau_\nu \ll 1$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Radiative Transfer with Einstein Coefficients

In the case of **"local thermodynamic equilibrium" (LTE)** the radiative field is defined as a blackbody (Planck Function) with a constant excitation temperature, T_{ex} (where $T_k \sim T_{ex}$)

$$\Delta I_\nu = [B_\nu(T_{ex}) - B_\nu(T_{BG})](1 - e^{-\tau_\nu})$$

In the limiting cases,

$$\Delta I_\nu = [B_\nu(T_{ex}) - B_\nu(T_{BG})] \quad \text{for } \tau_\nu \gg 1$$

$$\Delta I_\nu = [B_\nu(T_{ex}) - B_\nu(T_{BG})]\tau_\nu \quad \text{for } \tau_\nu \ll 1$$

Optically thick lines (e.g., ^{12}CO) or dust emission can be used to determine the **temperature** of a cloud!

Optically thin lines (e.g., ^{13}CO or $C^{18}O$) or dust emission is directly proportional to the **cloud's optical depth** (and thus column density and cloud mass)!

Radiative Transfer with Einstein Coefficients

$$\Delta T_b \approx (T_x - T_c)\,\tau_0 = \left(\frac{T_x - T_c}{T_x}\right) N_L \frac{(\ln 2)^{1/2}}{4\pi^{3/2}} \frac{hc^3}{k\nu_0^2} \frac{g_U}{g_L} \frac{A_{UL}}{\Delta\nu} \qquad (7.139)$$

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To get column density, N_L, you need to know the <u>physical states</u> of your molecule and <u>calculate the spontaneous emission coefficient</u>

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Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Radiative Transfer with Einstein Coefficients

The spontaneous emission coefficient be calculated by writing in terms of the **mean electric dipole moment**,

$$\boxed{A_{\mathrm{UL}} = \frac{64\pi^4}{3hc^3}|\mu_{\mathrm{UL}}|^2\nu^3.} \quad (7.131)$$

For a linear rotating molecule,

$$\boxed{|\mu_{\mathrm{J}\to\mathrm{J}-1}|^2 = \frac{\mu^2 J}{2J+1}.} \quad (7.132)$$

$$\left(\frac{A_{J\to J-1}}{\mathrm{s}^{-1}}\right) \approx 1.165\times 10^{-11}\left|\frac{\mu}{\mathrm{D}}\right|^2\left(\frac{J}{2J+1}\right)\left(\frac{\nu}{\mathrm{GHz}}\right)^3. \quad (7.133)$$

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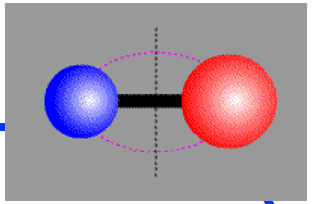


Example for CO (1-0):

$$A_{10} \approx 1.165\times 10^{-11}\cdot 0.11^2\cdot\left(\frac{1}{3}\right)\cdot 115^3$$
$$\approx 7.1\times 10^{-8}\ \mathrm{s}^{-1}$$

Solving for **critical density** assumes a typical collisional cross section and average velocity for H_2 molecules,

$$n^* \approx \frac{A_{\mathrm{UL}}}{\sigma v} \approx \frac{7\times 10^{-8}\ \mathrm{s}^{-1}}{10^{-15}\ \mathrm{cm}^2\cdot 5\times 10^4\ \mathrm{cm\ s}^{-1}}$$
$$\approx 1.4\times 10^3\ \mathrm{cm}^{-3}.$$

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Radiative Transfer with Einstein Coefficients

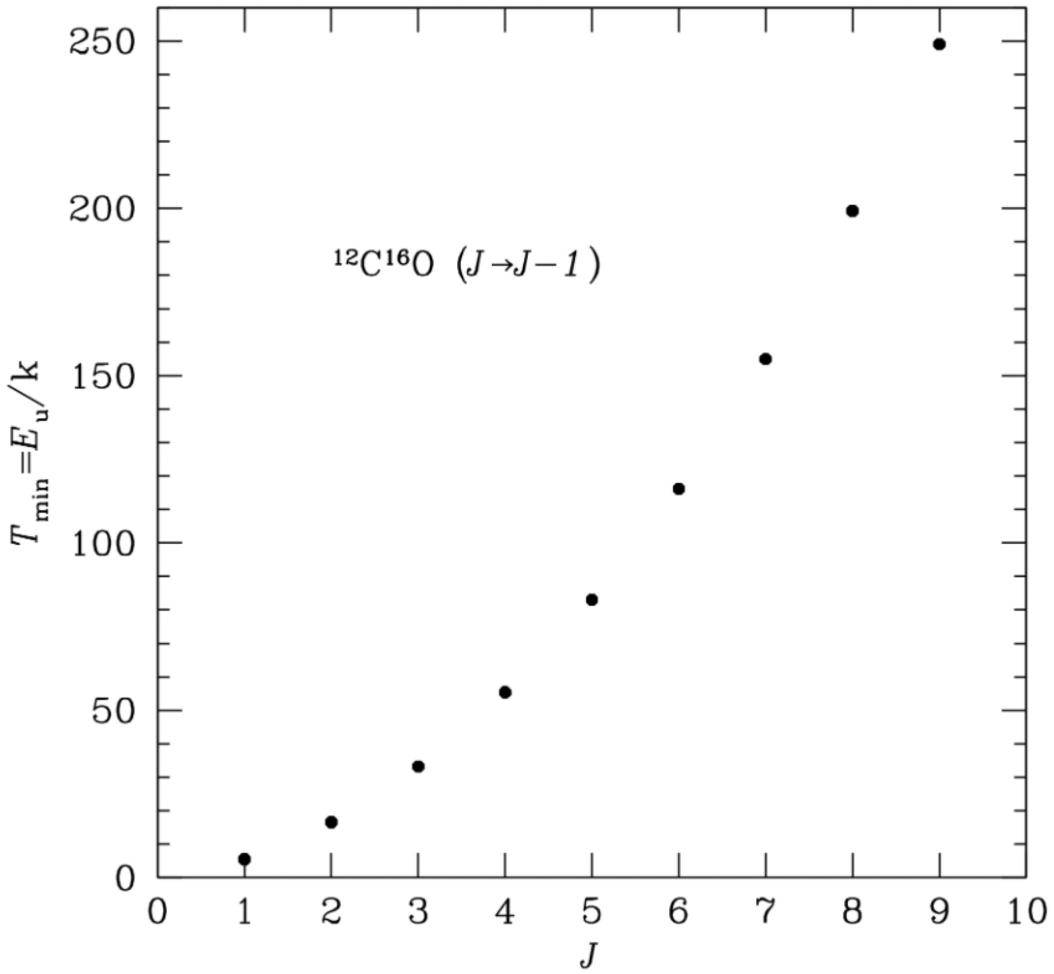
Related to A_{UL}, the **upper energies** give clues into what type of environments are molecular lines are likely to emit at and are directly connected to the minimum gas temperature needed for significant collisional excitation,

$$T_{\rm min} \sim \frac{E_{\rm rot}}{k}$$

$$\sim \frac{J\,(J+1)\,h^2}{2\cdot 4\pi^2 I k} = \frac{hJ}{4\pi^2 I}\,\frac{h\,(J+1)}{2k} = \frac{E_U}{k}$$

(7.116 & 7.118)

Fig. 7.15 (ERA)



Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

Radiative Transfer with Einstein Coefficients

$$\Delta T_{\mathrm{b}} \approx (T_{\mathrm{x}} - T_{\mathrm{c}})\,\tau_0 = \left(\frac{T_{\mathrm{x}} - T_{\mathrm{c}}}{T_{\mathrm{x}}}\right) N_{\mathrm{L}} \frac{(\ln\,2)^{1/2}}{4\pi^{3/2}} \frac{hc^3}{k\nu_0^2} \frac{g_{\mathrm{U}}}{g_{\mathrm{L}}} \frac{A_{\mathrm{UL}}}{\Delta v} \qquad (7.139)$$

To get column density, N_L, you need to know the <u>physical states</u> of your molecule and <u>calculate the spontaneous emission coefficient</u>

$$T_{\mathrm{min}} \sim \frac{E_{\mathrm{rot}}}{k}$$

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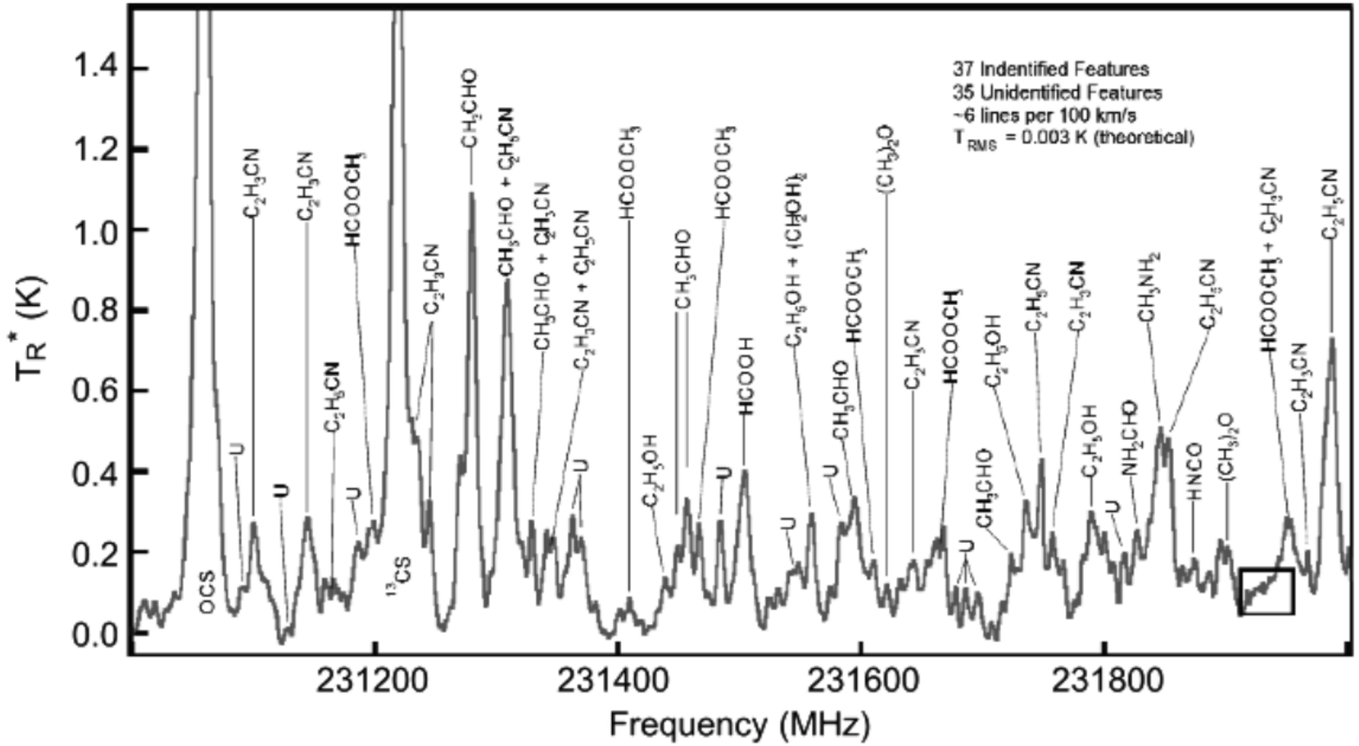
(7.116 & 7.118)

In practice… we look up these terms in Splatalogue!
https://splatalogue.online

Line Radiative Transfer (ERA 7.3, 7.4, +7.7, THz Astronomy Chap. 2)

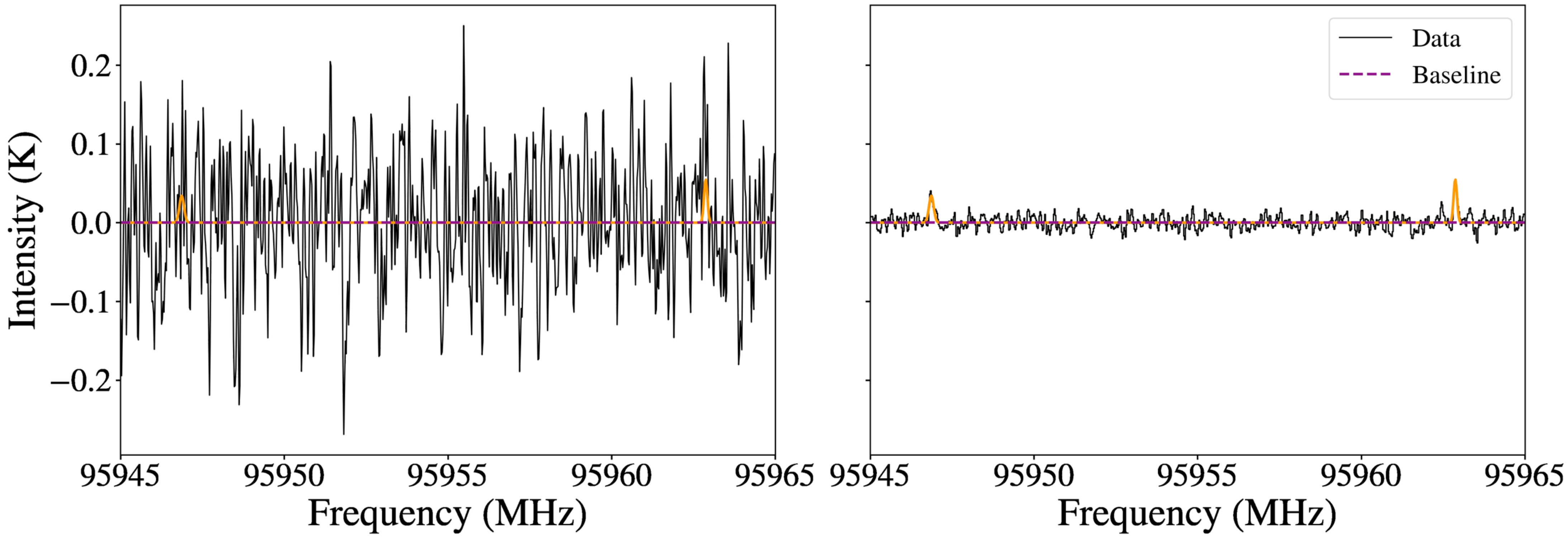
Radiative Transfer with Einstein Coefficients

Fig. 7.16 (ERA)



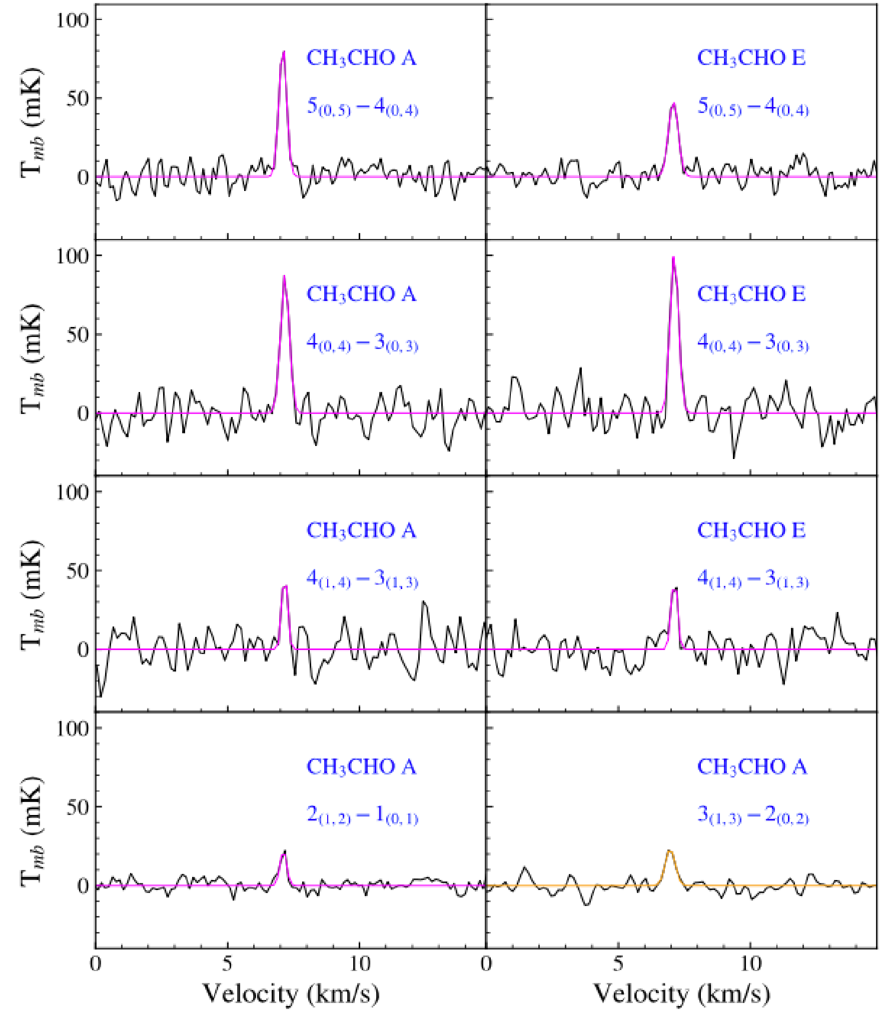
What spectral line are we looking at? Use Splatalogue!
https://splatalogue.online

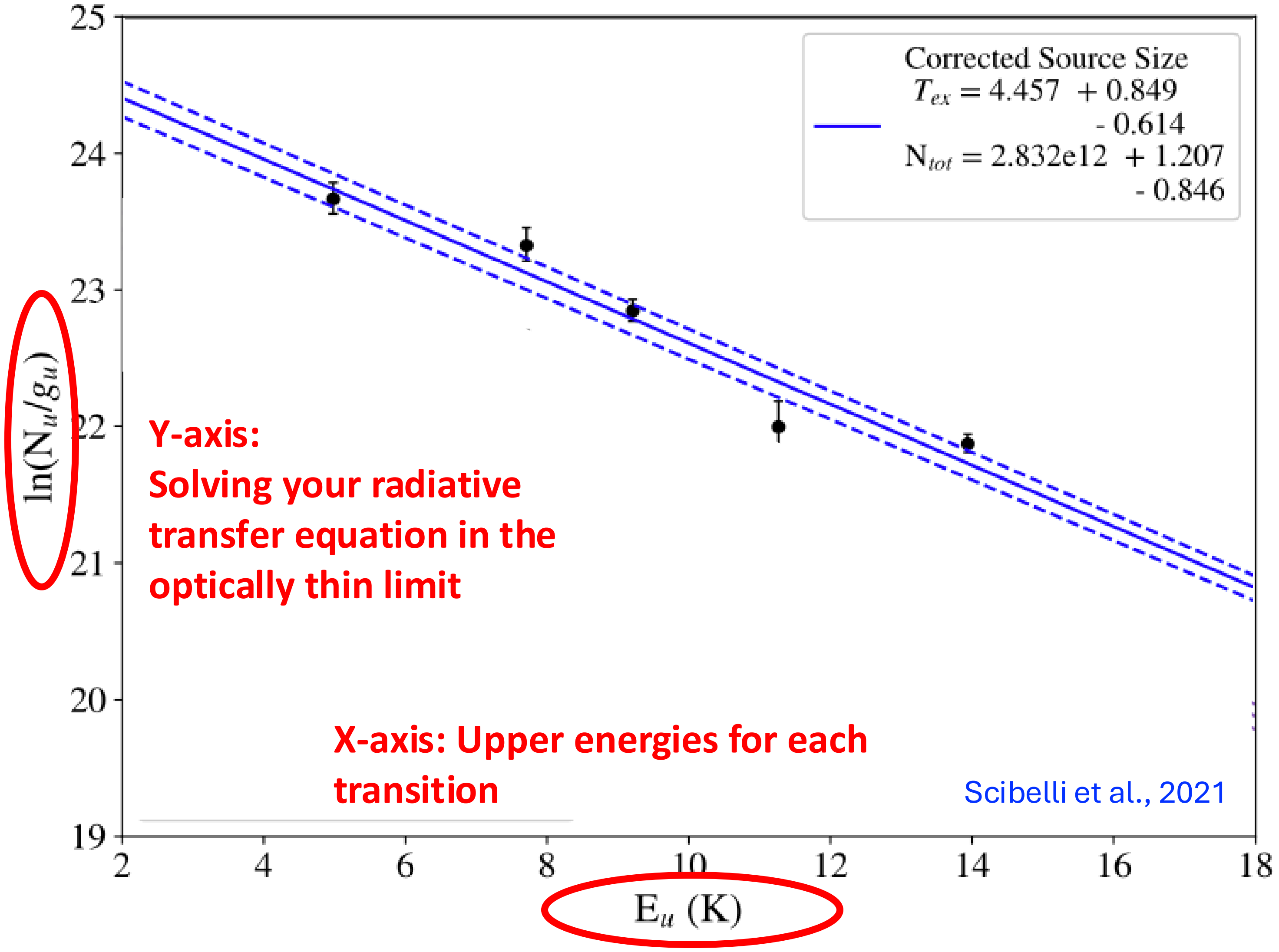
Example!



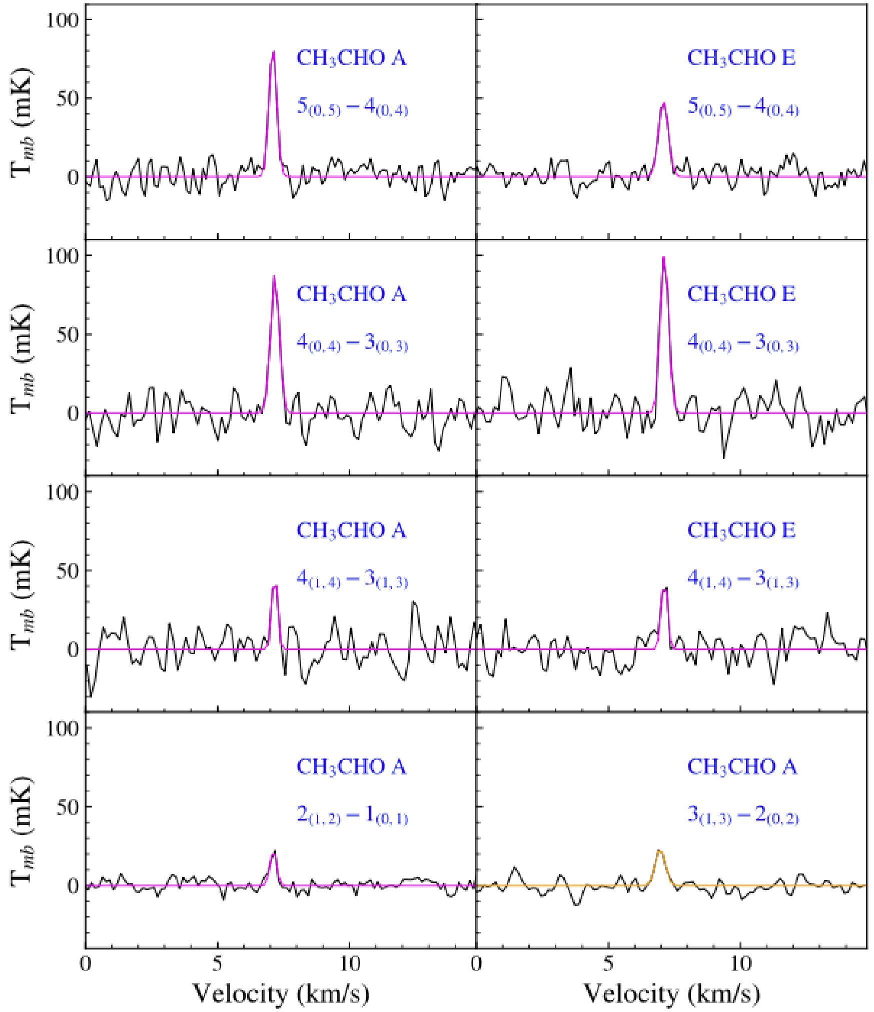
Intensity (K)
0.2
0.1
0.0
−0.1
−0.2
95945
95950
95955
95960
95965
Frequency (MHz)
Data
Baseline
95945
95950
95955
95960
95965
Frequency (MHz)

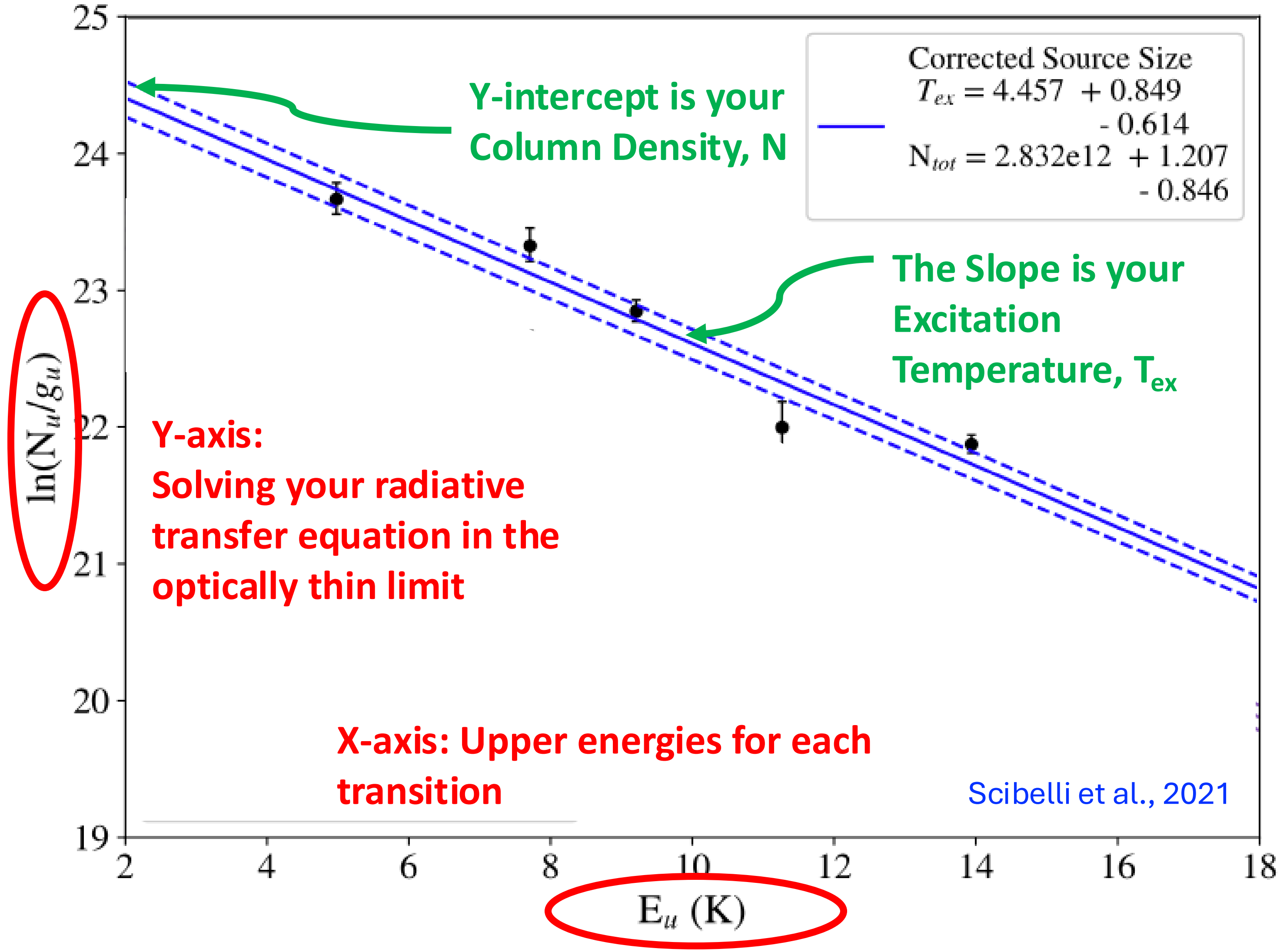
Practical use → Rotation Diagrams





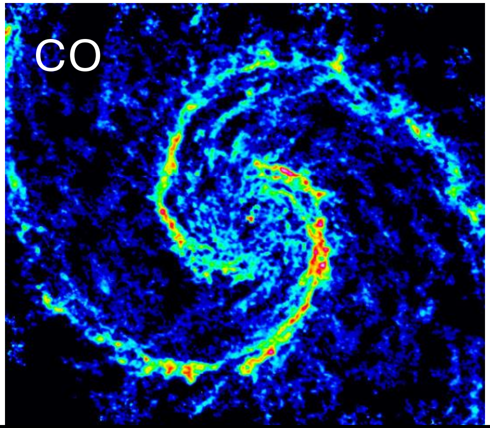
Practical use → Rotation Diagrams



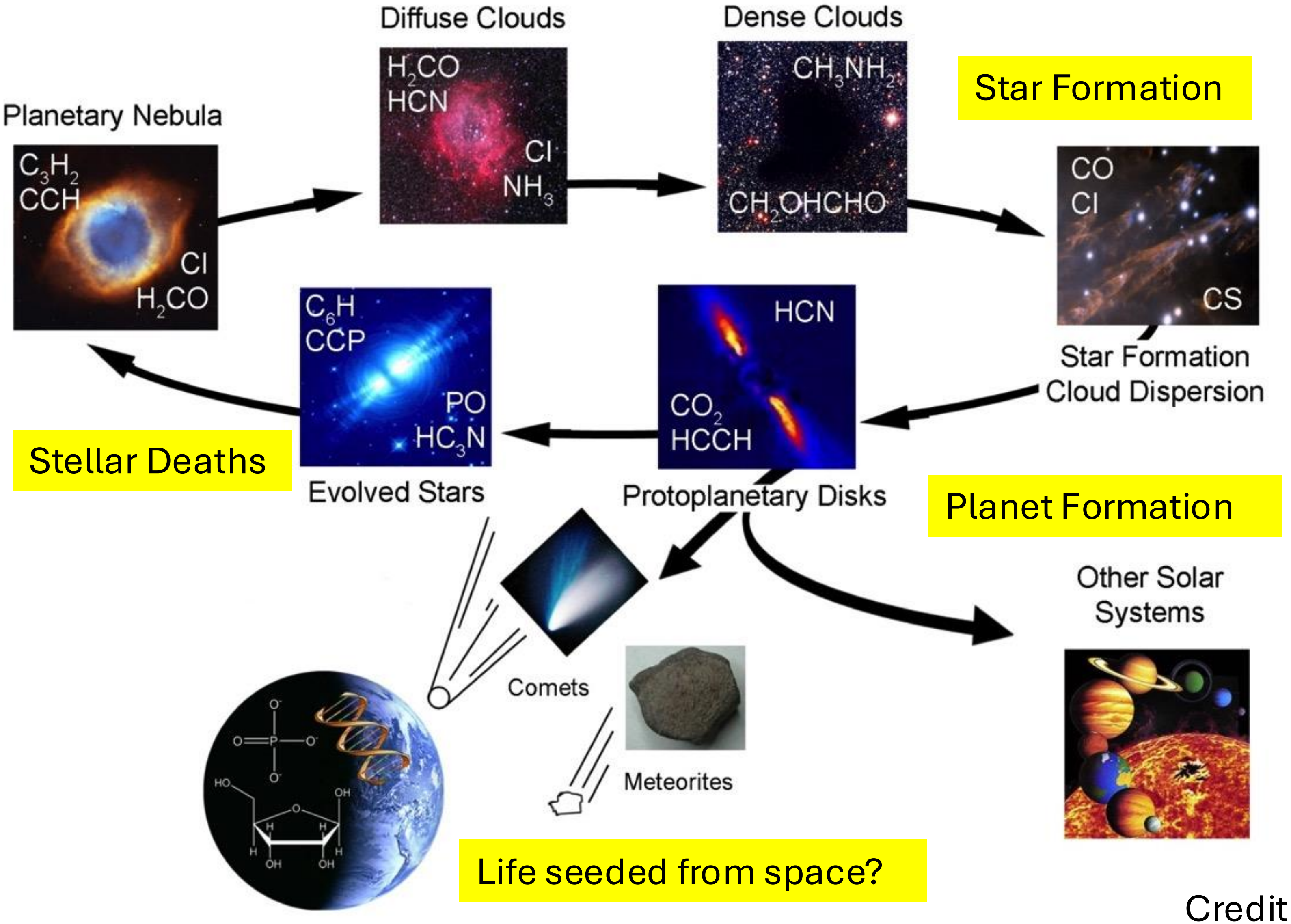


Molecular Life Cycle

Within Galaxies… →



M51 – Whirlpool Galaxy



Credit: L. Ziurys