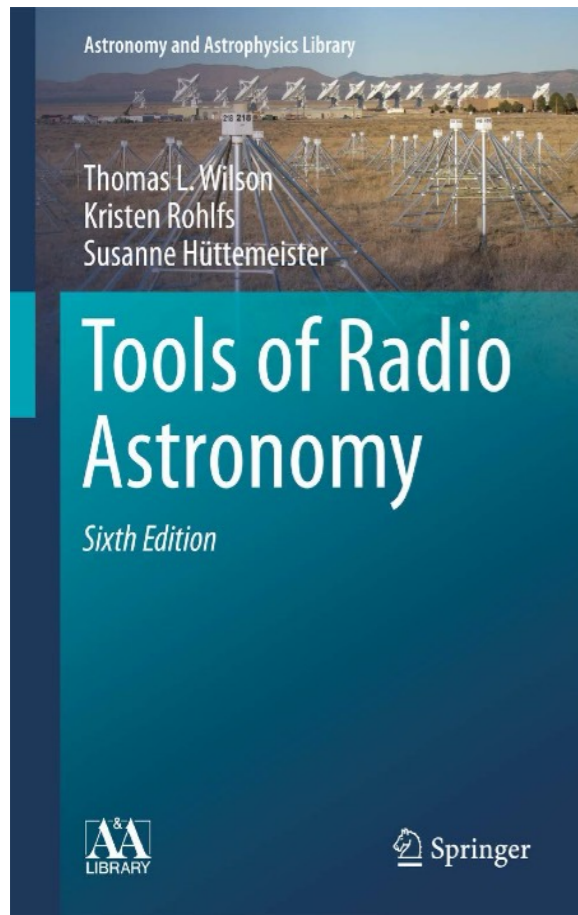




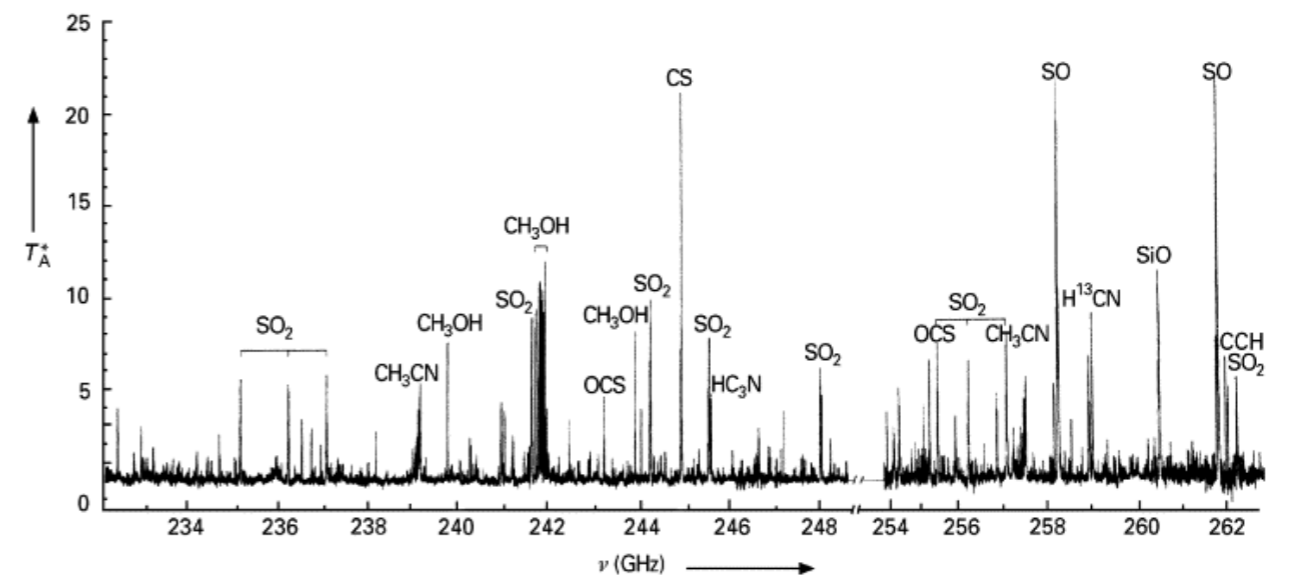
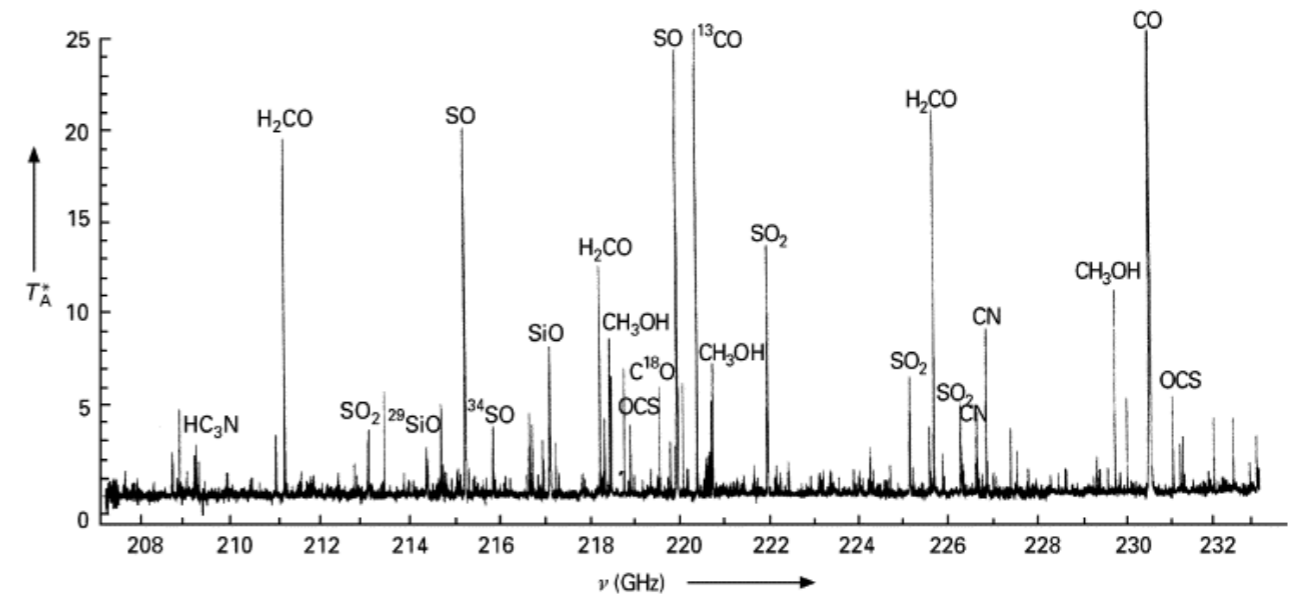
Radiative processes relevant to radioastronomy

A solid knowledge of the astrophysics behind radio observables is necessary to achieve a complete understanding of the various phenomena/astrophysical sources that will be investigated in this course.

Line emission/absorption processes



Chapters 12, 13, 14, 15, 16



Orion nebula, radio spectrum

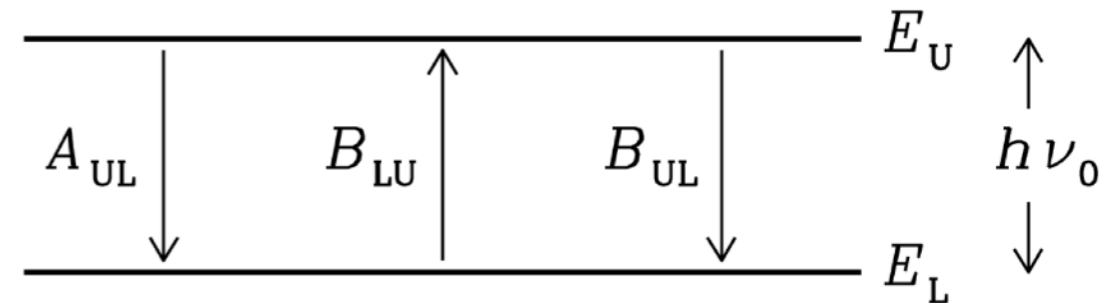


Statistical equilibrium equation

So far, we have considered the interaction between a single atom/molecule with radiation

$$N_U A_{UL} + N_U B_{UL} \bar{U} = N_L B_{LU} \bar{U}$$

But we have neglected that a system (atom or molecule) can be also excited/de-excited by collisions with other atom or molecules.



If collisions dominates the transitions between U and L:

$$N_U N_{\text{coll}} C_{UL} = N_L N_{\text{coll}} C_{LU} \quad \frac{C_{LU}}{C_{UL}} = \frac{N_U}{N_L} = \frac{g_U}{g_L} \exp\left(-\frac{h\nu_0}{kT_K}\right)$$

■■■ kinetic temperature

Where C_{LU} and C_{UL} are the excitation and de-excitation collisional coefficients ($\text{m}^3 \text{s}^{-1}$)

$$C_{ik} = \int_0^\infty \sigma_{ik}(v) f(v) dv$$

$f(v)$ velocity distribution function of the colliding particles
 σ_{ik} collision cross section

N_{coll} is the number density of the collisors



Statistical equilibrium equation and excitation temperature

In general both radiation and collisions regulate the transition rates

$$N_U A_{UL} + N_U B_{UL} \bar{U} + N_U N_{\text{coll}} C_{UL} = N_L B_{LU} \bar{U} + N_L N_{\text{coll}} C_{LU}$$

Statistical equilibrium equation

We can define an excitation temperature T_{ex} so that

$$\frac{N_U}{N_L} = \frac{g_U}{g_L} \exp\left(-\frac{h\nu_0}{kT_{ex}}\right)$$

■■■ excitation temperature

$$T_{ex} = T_K \frac{T_b A_{UL} + T_0 C_{UL}}{T_K A_{UL} + T_0 C_{UL}}$$

in the approximation that $T_{ex}, T_K, T_b \gg T_0$

$$T_0 = h\nu_0/k$$

$$T_{ex} \longrightarrow T_K \text{ when } C_{UL} \gg A_{UL}$$

$$T_{ex} \longrightarrow T_b \text{ when } A_{UL} \gg C_{UL}$$

We can define a **critical density** N^* as the density when $A_{UL} \sim C_{UL} \sim N^* \langle \sigma v \rangle$

If $N > N^*$ the upper level is de-excited by collisions rather than by photon emission

If $N < N^*$ the upper level is de-excited by emission of photons rather than collisions



Statistical equilibrium equation and excitation temperature

In general both radiation and collisions regulate the transition rates

$$N_U A_{UL} + N_U B_{UL} \bar{U} + N_U N_{\text{coll}} C_{UL} = N_L B_{LU} \bar{U} + N_L N_{\text{coll}} C_{LU}$$

Statistical equilibrium equation

The generalization of the statistical equilibrium equation to a multi-level system is obtained by adding all the excitation and de-excitation terms to and from a level. The results is a system of N_{lev} (= number of levels) equations:

$$N_U \sum_{L=U+1}^{N_{\text{lev}}} A_{UL} + B_{UL} \bar{U}_{UL} + N_{\text{coll}} C_{UL} = \sum_{L=1}^{U-1} N_L N_{\text{coll}} C_{LU} + N_L B_{LU} \bar{U}_{LU} \quad U = 1, \dots, N_{\text{lev}} - 1$$



Line formation (wrap up)

Consider a system (atom or molecule) with two energy levels only, U and L. The two levels are populated according to the statistical equilibrium equation.

Whatever is the mechanism governing the level population, there will always be N_U atoms/molecules in the upper level U, a fraction of which will decay in the lower level L by spontaneously emitting a photon at the frequency corresponding to the energy difference between the two levels, $h\nu_0 = E_U - E_L$. This occurs with a probability given by A_{UL} . If the gas is illuminated by a strong radiation field at the same frequency of the transition frequency, then there will also be stimulated emission.

The emitted photons will form an emission line at the frequency of the transition.

If the radiation field at the frequency ν_0 is strong enough, then the line will be in absorption. This happens when the atoms/molecules are excited to the upper level by the absorption of the radiation field photons rather than collisions. Quantitatively, absorption occurs when the excitation temperature (which is a measure of the processes regulating the level population) of the transition is lower than the radiation temperature.



✱ Use Boltzmann's relation to estimate T for a two-state system with equal statistical weight factors and level populations $N_1 = 1.01 N_2$ (upper state is 2).

✱ Suppose that the collision rate, C_{21} , is given by $n \langle \sigma v \rangle$, where the value of $\langle \sigma v \rangle$ is $\sim 10^{-10}$. For the 21 cm hydrogen line, $A_{21} = 2.85 \times 10^{-15} \text{ s}^{-1}$. Find the critical density N^* for this transition. Repeat this calculation for the $J = 1 - 0$ rotational transition of the molecule HCO^+ , modelling the molecule as a two-level system in which the Einstein A coefficient is $A_{21} = 3 \times 10^{-5} \text{ s}^{-1}$. What is the value of N^* ? Compare this to the value for the 21 cm line.

For HCO^+ ($\nu = 89.186 \text{ GHz}$), take $T_K = 100 \text{ K}$; find the value of the local density for which $T_{\text{ex}} = 3.5 \text{ K}$. $T_b = 2.7 \text{ K}$. For the same density, calculate N^* for the $J = 1 - 0$ transition of the carbon monoxide molecule CO ($\nu = 115.271 \text{ GHz}$), modelling this as a two-level system with $A_{21} = 7.4 \times 10^{-8} \text{ s}^{-1}$.



Line broadening mechanisms

Atomic/molecular levels are not infinitely sharp, nor are the lines connecting them.

Several physical effects determine the line shape, among which those we are mostly interested in are:
Natural broadening and Doppler broadening

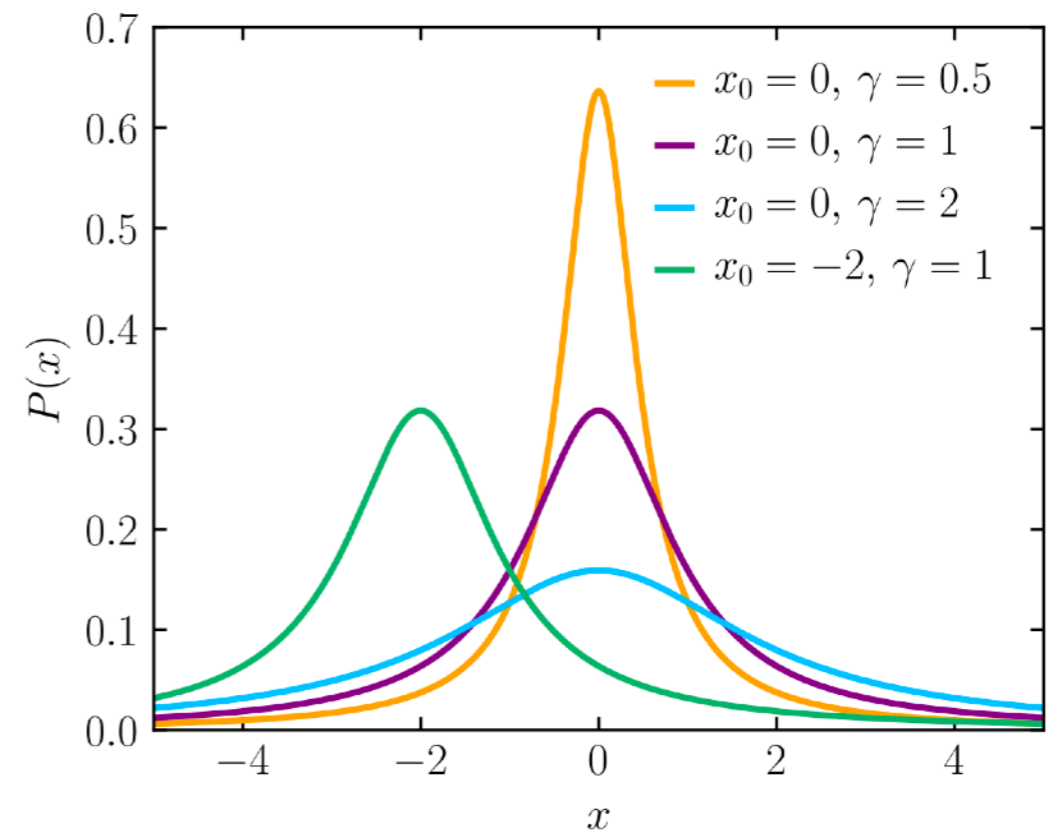
Natural broadening

$$\Delta E \Delta t \sim h/(2\pi)$$

The profile from this uncertainty is a Lorentz (or natural) profile

A given width to the atomic/molecular level is implied by the uncertainty principle. The spread energy ΔE and the duration Δt in the state have to satisfy

$$\phi_\nu = \frac{\gamma}{4\pi[(\nu - \nu_0)^2 + \left(\frac{\gamma}{4\pi}\right)^2]}$$





Doppler broadening

Any atom/molecule is in thermal motion, so that the frequency of emission or absorption in its own frame corresponds to a different frequency for an observer: Doppler shift with respect to the observer.

Atoms/molecules move according to the Maxwell distribution, the effect is a spread of the line over a frequency range.

The change in frequency is linked to the atom/molecule via the velocity along the line of sight:

$$\nu - \nu_0 = \frac{\nu_0 v_z}{c}$$

where ν_0 is the rest-frame frequency. The number of atoms/molecules with velocities in the range v_z to $v_z + dv_z$ is given by the Maxwellian distribution

$$N(v_z)dv_z = \sqrt{\frac{2kT}{\pi m}} \exp\left(-\frac{mv_z^2}{2kT}\right) \quad (\text{velocities})$$

From which the brightness profile is

$$I_\nu = \frac{1}{\sqrt{\pi}\Delta\nu_D} \exp\left[-\frac{(\nu - \nu_0)^2}{\Delta\nu_D^2}\right] \quad (\text{frequencies, Gaussian profile})$$

where $\Delta\nu_D$ is the Doppler width



Line broadening mechanisms

The Doppler width is defined as $\Delta\nu_D = \frac{\nu_0}{c} b$

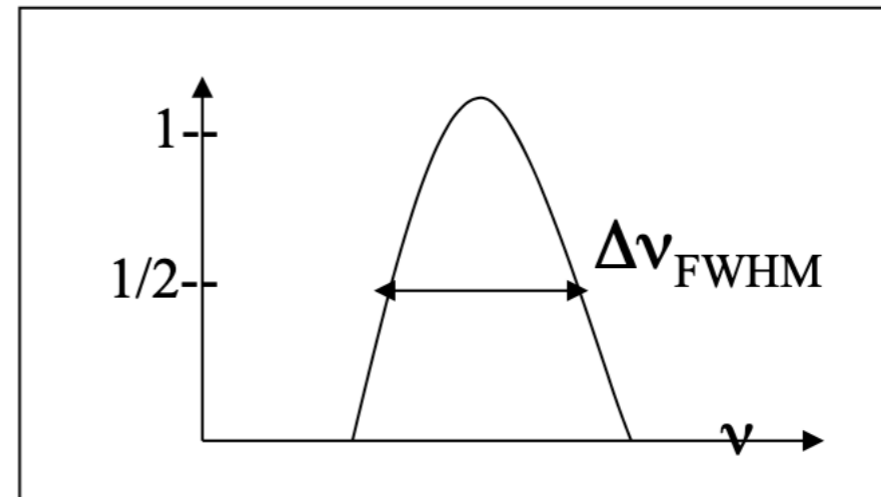
Where b is the Doppler parameter

$$b = \sqrt{\frac{2kT}{m_x}} = 0.129 \sqrt{\frac{T}{A_x}}$$

In which m_x is the mass of the species x and A_x is the atomic number

Then, if $\Delta\nu_{\text{FWHM}}$ is the full width at half maximum of the line profile, is related to b via the relation

$$\Delta\nu_{\text{FWHM}} = \frac{2\sqrt{\ln 2} b}{c} \nu_0$$



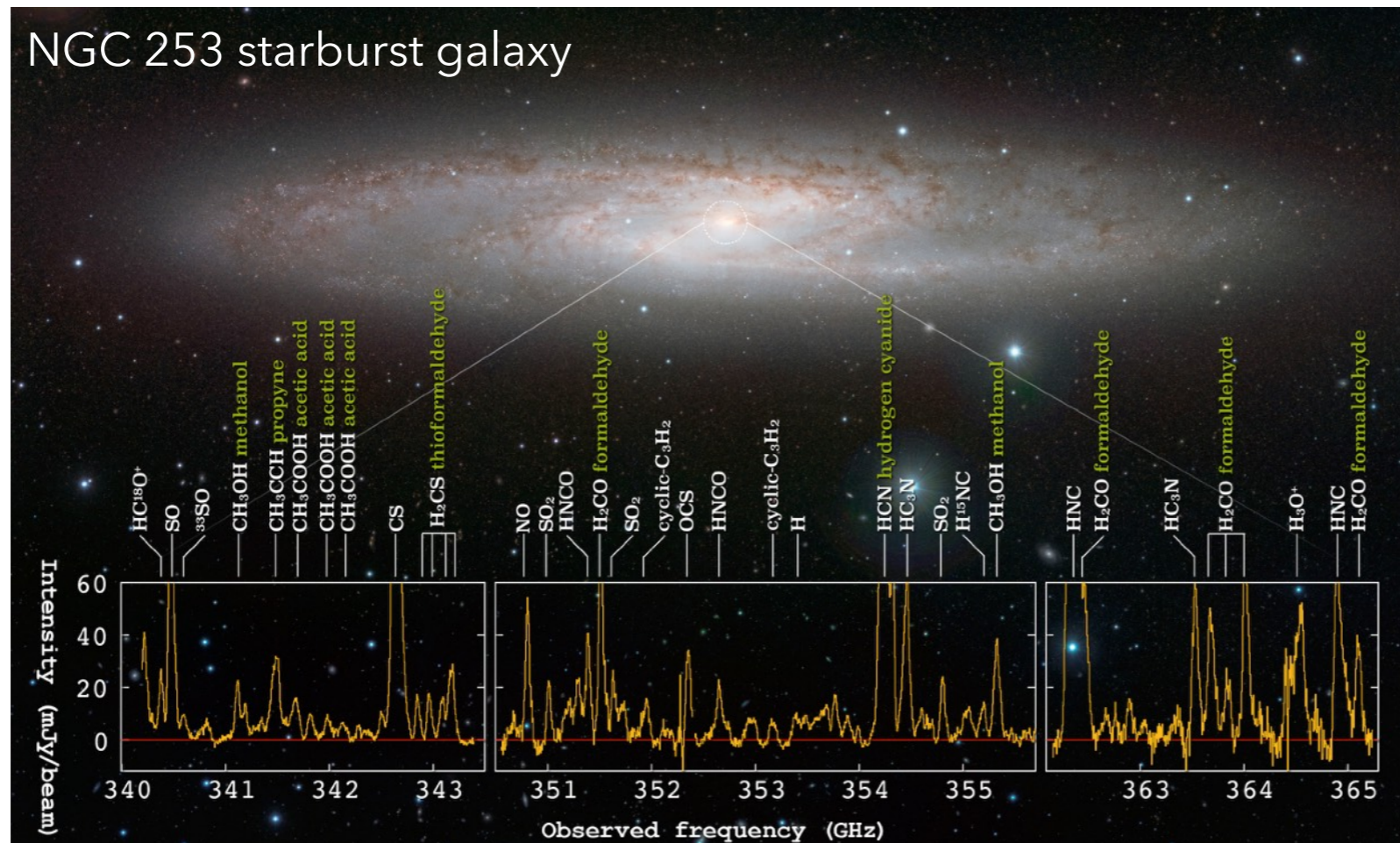
$\Delta\nu_{\text{FWHM}}$ is an observed parameter that provides a measurement of the gas temperature.

The larger the gas temperature, the larger the line width. Also, the larger the mass of the species, the smaller the line width caused by Doppler broadening.

Compared to atoms, molecules have a complicated structure and the Schrodinger equation of the system will be correspondingly complex, involving all nuclei and the electrons.

In principles, in a molecule we have three categories of transitions:

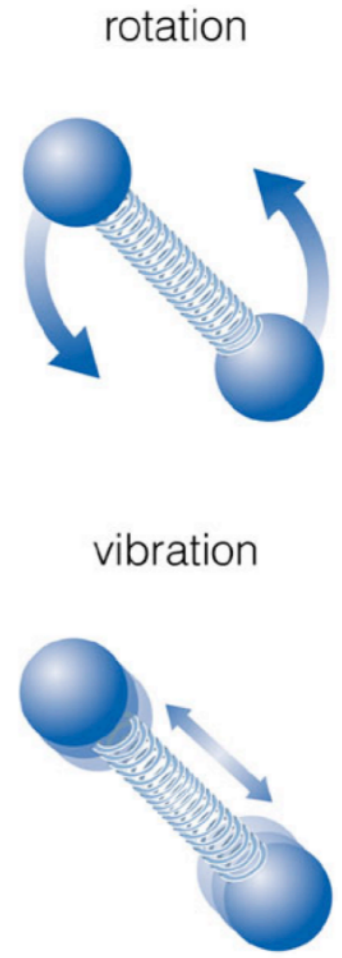
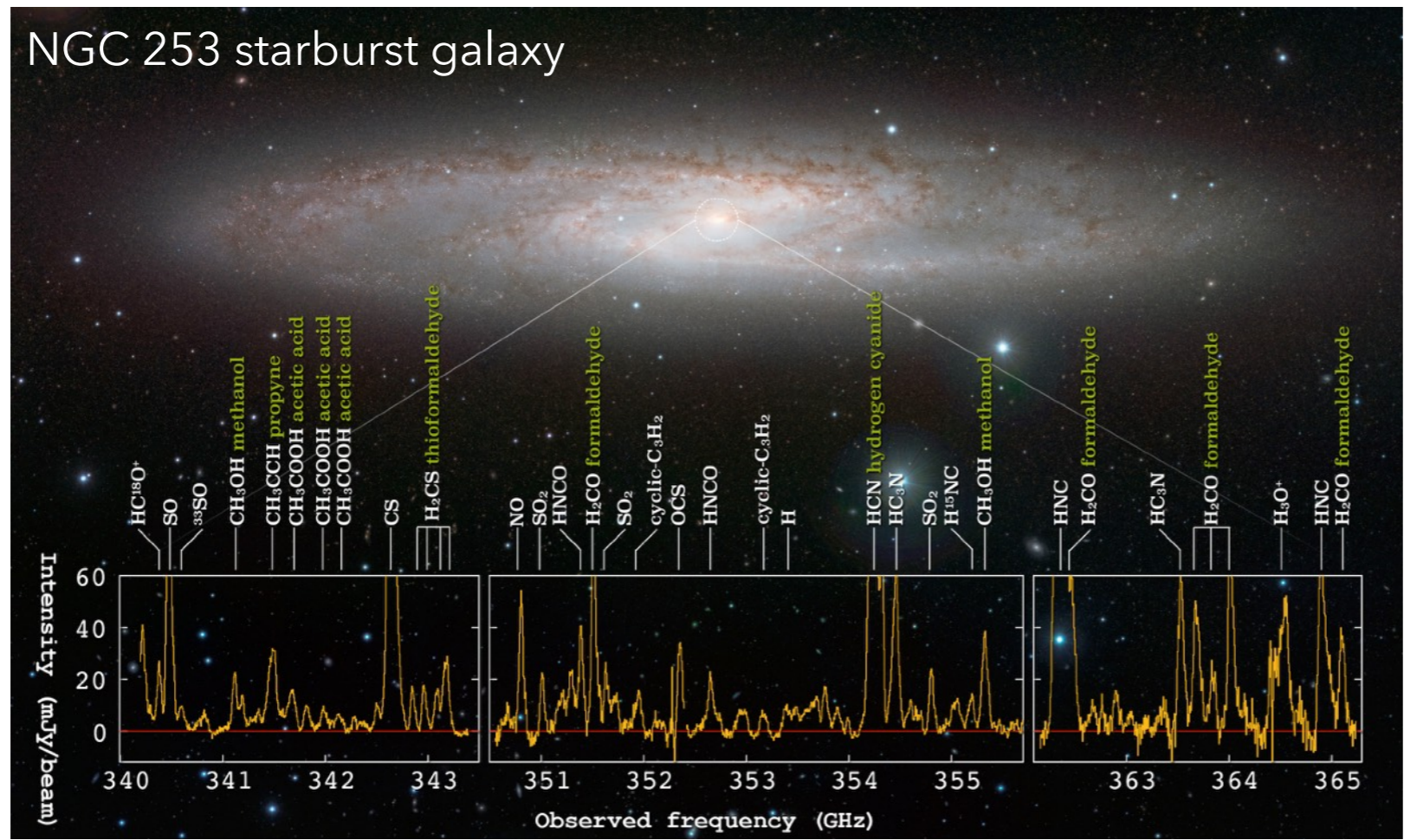
- electronic transitions (energies of a few eV, $T \sim 10^4$ K)
- vibrational transitions (energies of 0.01-0.1 eV, $T \sim 10^2 - 10^3$ K)
- rotational transitions (energies of 10^{-3} eV, $T \sim 10$ K)



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In principles, in a molecule we have three categories of transitions:

- electronic transitions (energies of a few eV, $T \sim 10^4$ K) ← **Optical-UV**
- vibrational transitions (energies of 0.01-0.1 eV, $T \sim 10^2 - 10^3$ K) ← **Infrared**
- **rotational transitions** (energies of 10^{-3} eV, $T \sim 10$ K) ← **mm and cm**



A molecule is **polar** if its permanent electric dipole moment is not zero.

$$\vec{p} = \int_V \vec{x} \rho(\vec{x}) d\vec{x}$$

$\rho(\vec{x})$ charge density

\vec{x} infinitesimal volume element

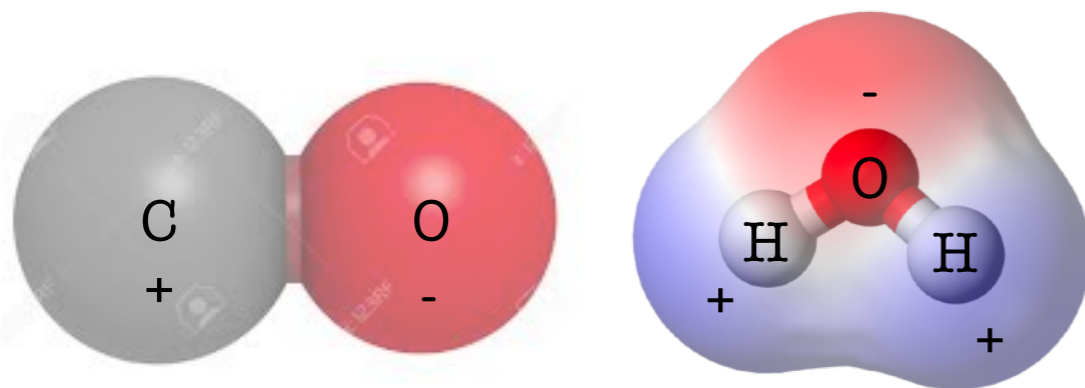
V volume containing the charges

Symmetric molecules (e.g. diatomic hydrogen H_2) have no permanent electric dipole moment, but most asymmetric molecules (e.g. carbon monoxide CO) have asymmetric charge distributions and are polar.

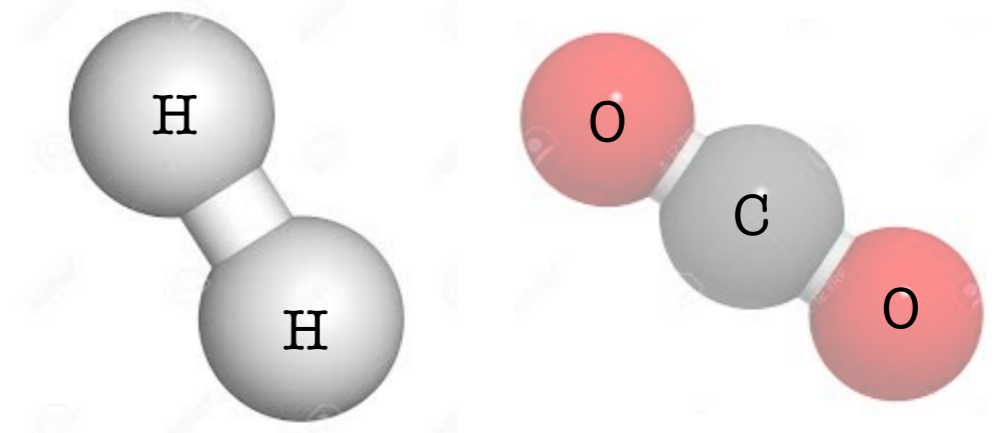
The electric dipole moment of polar molecules can be viewed as an antenna, oscillating as the molecule rotates. The acceleration of positive and negative charges gives rise to radiation whose frequency is that of the angular velocity ω of the rotation. **Polar molecules radiate at their rotation frequencies.**

(Longair 1992, *High-energy astrophysics*, chapter 2.7)

Polar



Non-polar





Diatomic molecules and angular momentum

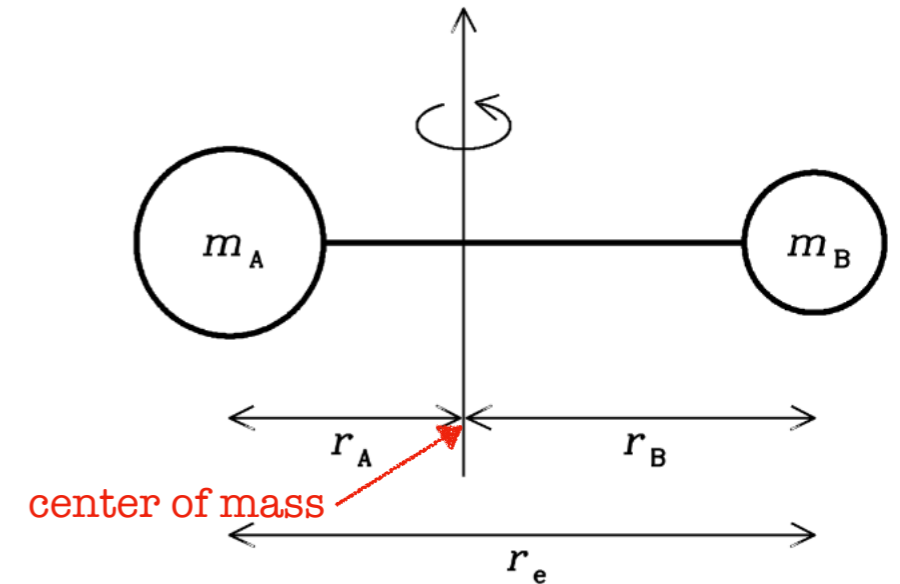
Consider a rigid diatomic molecule

two atoms

no internal motions (e.g. centrifugal forces)

$r_e = r_A + r_B$ equilibrium distance

r_A, r_B distances of the nuclei from center of mass: $r_A m_A = r_B m_B$



The angular momentum of a molecule rotating around its center of mass is simply

$$J = I\omega$$

where I is the moment of inertia and ω is the angular velocity of the rotation. As nearly all the mass is in the nuclei $I = m_A r_A^2 + m_B r_B^2$, from which

$$J = \frac{m_A m_B}{m_A + m_B} r_e^2 \omega = m r_e^2 \omega$$

.....

where m is the reduced mass of the molecule



Diatomic molecules and angular momentum

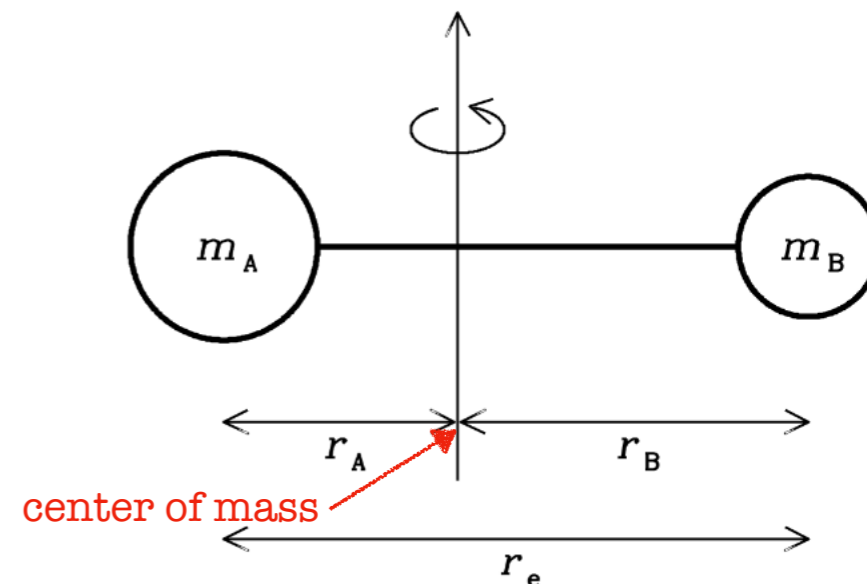
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$$J = \frac{m_A m_B}{m_A + m_B} r_e^2 \omega = m r_e^2 \omega$$

.....

where m is the reduced mass of the molecule

For our rigid diatomic molecule, J is simply the angular momentum perpendicular to the axis of the molecule. In the case of $N > 2$ molecules the angular momentum depends on the direction of the rotation:

$$\vec{J} = I\vec{\omega}$$

Similar (more complex) expressions can be calculated. In general I will be a three-axial ellipsoid and depend on the relative orientation of the nuclei.



Rotational energy

The effective radius of a (simple) molecule is about 10^5 times the radius of the nucleus of an atom ($R_{CO} \gtrsim \text{\AA}$). The moment of inertia I of such a molecule is $\gtrsim 10^{10}$ times that of an atom of the same mass. J is a quantity that cannot be neglected compared with the other internal energy states of the molecule, (e.g. translational, vibrational).

The **rotational kinetic energy** associated with the molecule angular momentum is:

$$H_{\text{rot}} = \frac{1}{2} I \omega^2 = \frac{J^2}{2I}$$

As the angular momentum of an atom/molecule is quantized (multiples of \hbar), the rotational energy is also quantized. The corresponding **energy eigenvalues** of the Schrödinger equation are:

$$H_{\text{rot}} = \left(\frac{\hbar^2}{2I} \right) J(J+1)^* \quad J = 0, 1, 2, \dots$$

The **energy change of permitted transitions** is restricted by the quantum-mechanical selection rule

$$\Delta J = \pm 1$$



Rotational ladder

For a transition from J to $J-1$ the energy released is:

$$\Delta H_{\text{rot}} = \frac{\hbar^2}{2I} [J(J+1) - (J-1)J] = \frac{\hbar^2 J}{I}$$

And the frequency of the emitted photons is therefore:

$$\nu = \frac{\Delta H_{\text{rot}}}{h} = \frac{\hbar J}{2\pi I} = \frac{hJ}{4\pi^2 m r_e^2} \quad J = 0, 1, 2, \dots \quad (\text{angular momentum of the upper level})$$

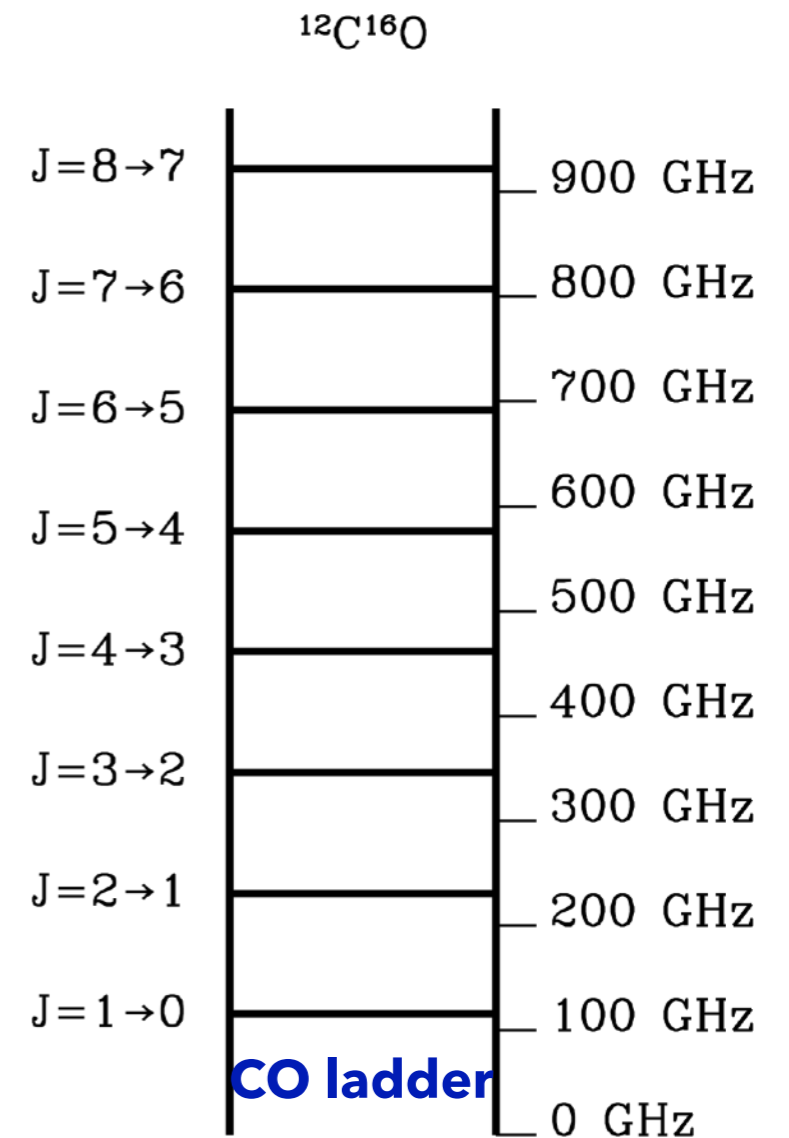
The radio spectrum of a particular molecular species will look like a ladder whose steps are all harmonics of the fundamental frequency.

The fundamental frequency ($J=1$) depends only on the moment of inertia, i.e. it depends only on the reduced mass and equilibrium distance of the molecule.

$$\nu \propto m^{-1} r_e^{-2}$$

small molecules --> mm

large molecules --> cm





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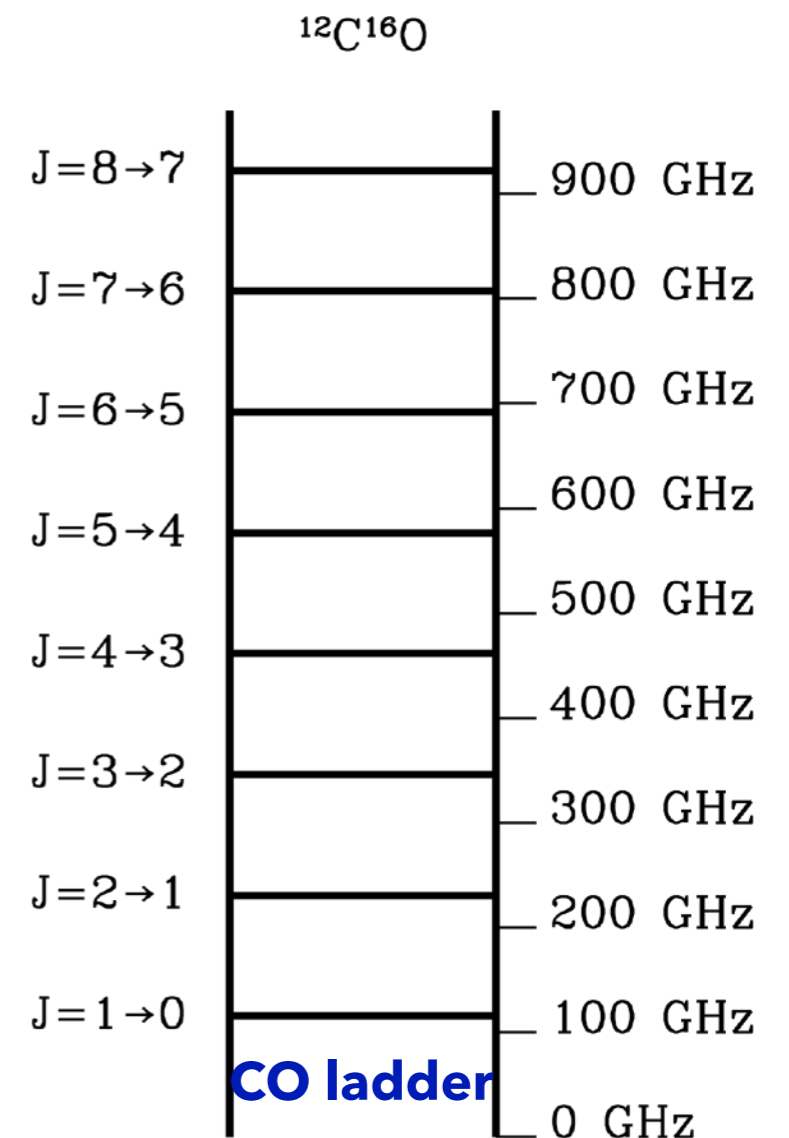
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$^{12}\text{C}^{16}\text{O}$ has a relatively small moment of inertia, so its fundamental frequency is at $\nu \approx 115.271 \text{ GHz}$ ($\lambda \approx 2.6 \text{ mm}$)



Rotational ladder

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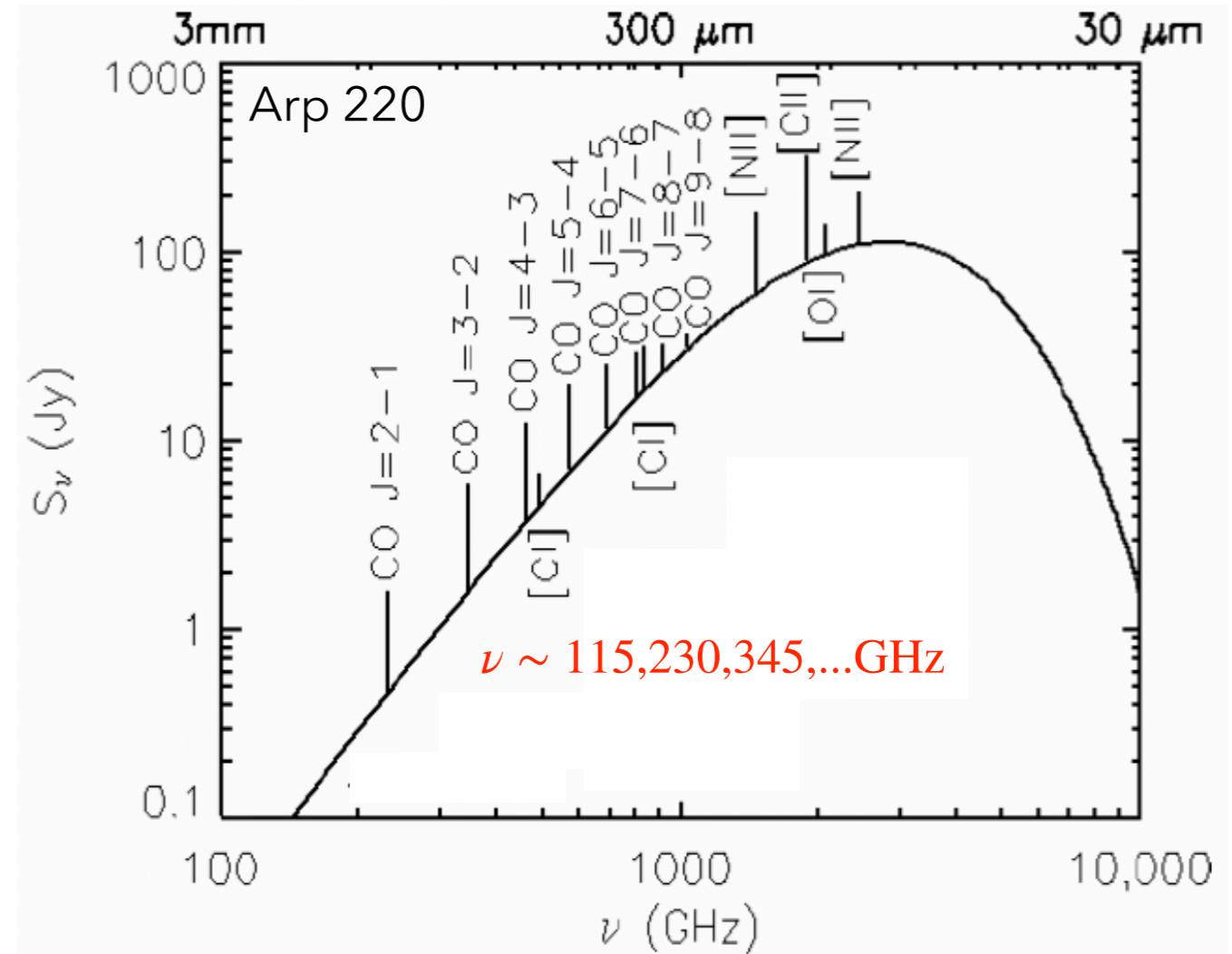
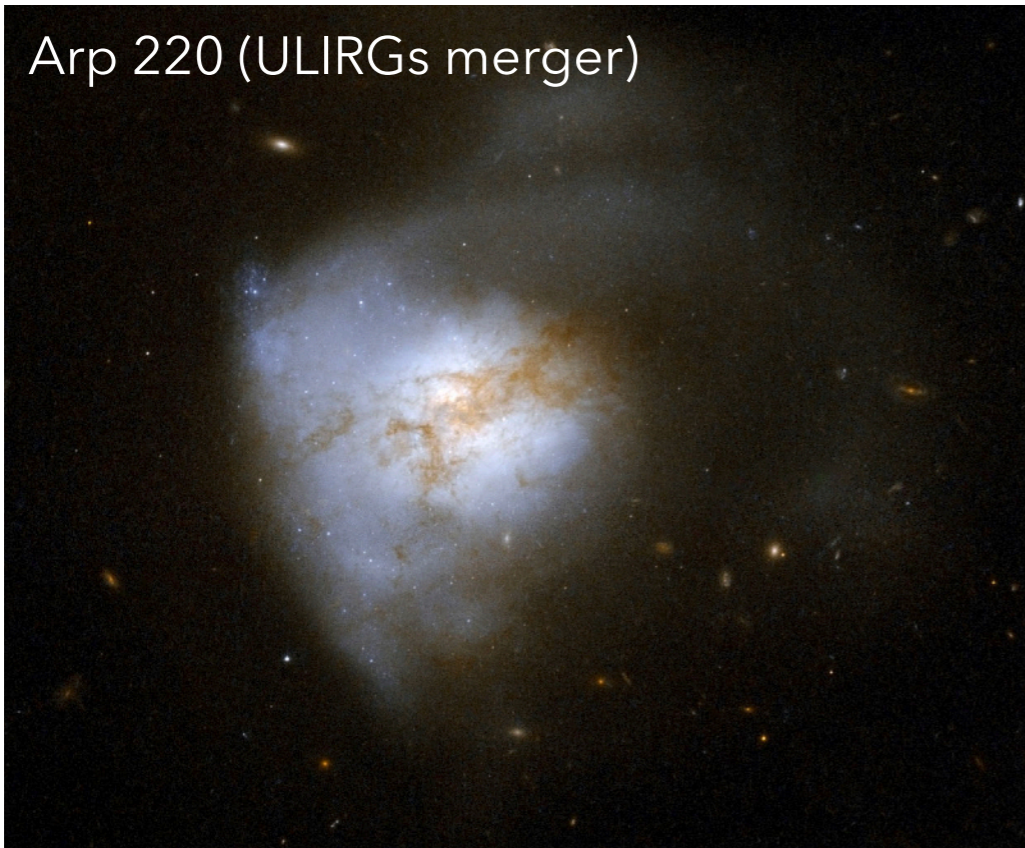
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$J = 0, 1, 2, \dots$ (angular momentum of the upper level)

Arp 220 (ULIRGs merger)





Radio spectra of complex molecules

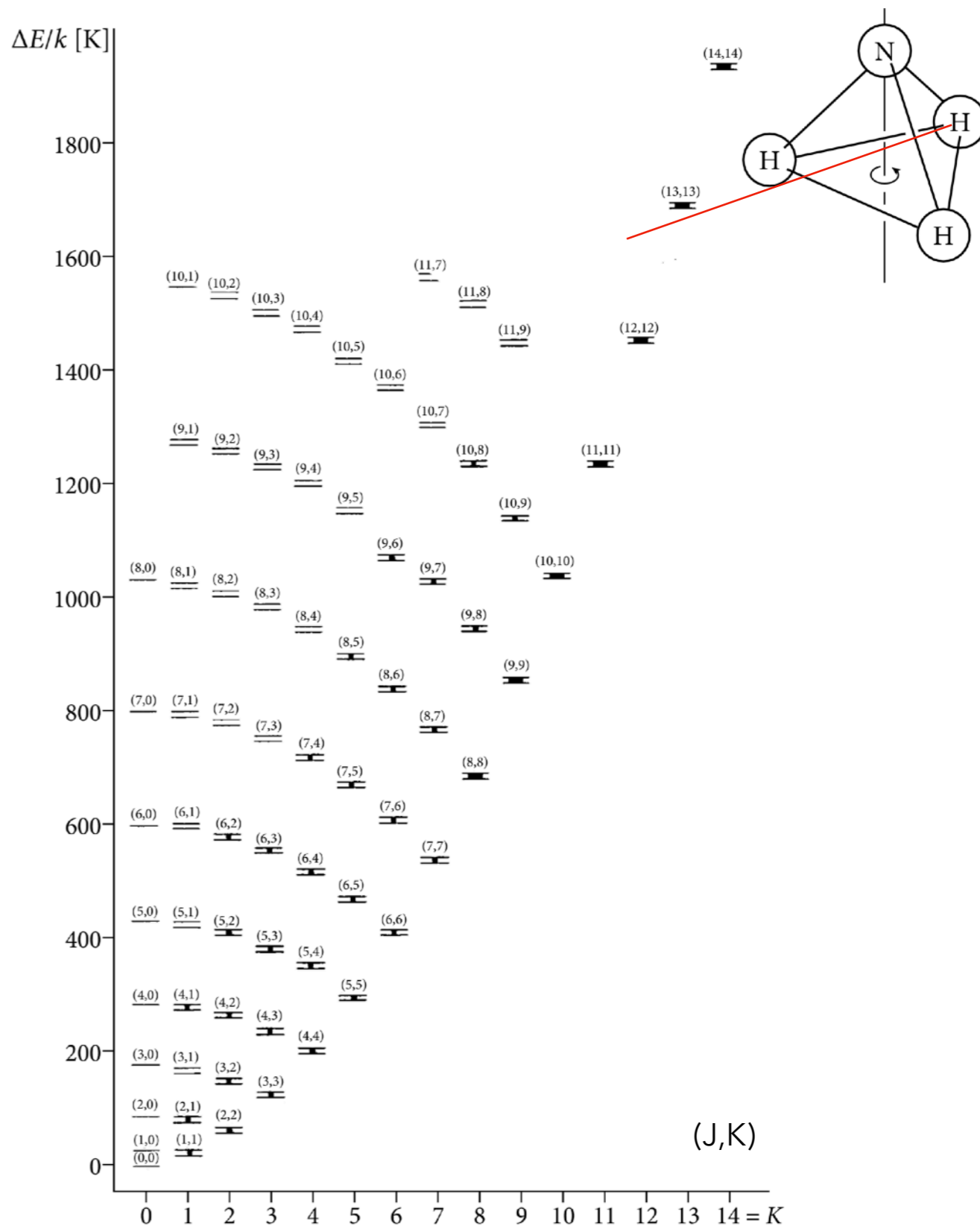
Spectra of non-linear molecules can be very complex!

e.g. NH_3 ammonia is a triaxial molecule with two rotation axes. Its spectrum is a combination of several ladders, one for each K .

J angular momentum

K angular momentum along the z-axis

Core of Orion nebula.
Spectrum between 0.9 and 1.3 cm





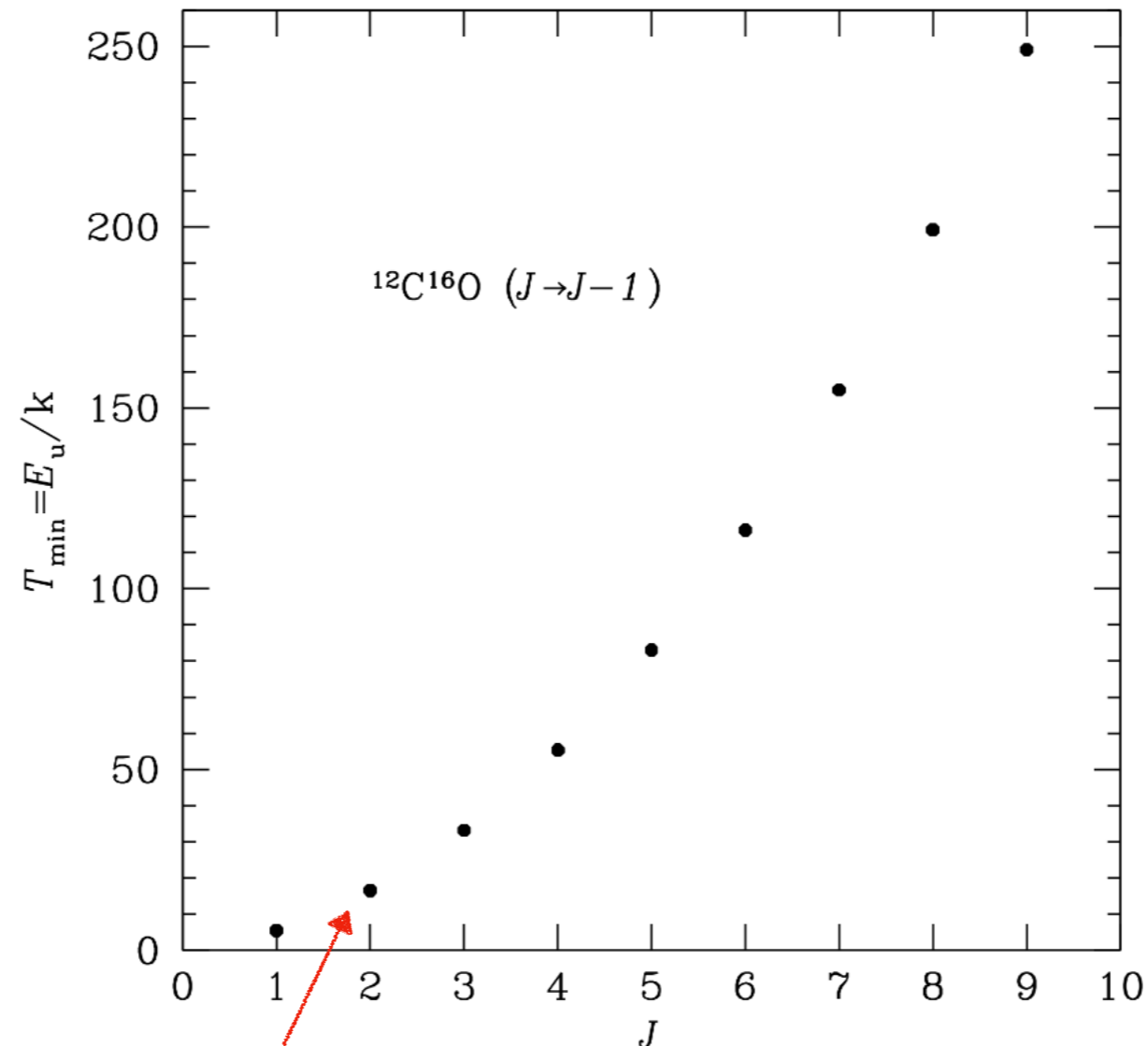
Collisional excitation and minimum temperature

We have seen that molecules can be excited into by ambient radiation and by collisions in a dense gas. The minimum gas temperature needed for significant collisional excitation

$$T_{\min} \sim \frac{H_{\text{rot}}}{k} \sim \frac{\nu h(J+1)}{2k}$$

Using * and **

that is the minimum temperature to excite the $J \rightarrow J-1$ transition at frequency ν



$$T_{\min}[\text{CO}(2 \rightarrow 1)] \sim \frac{230 \times 10^9 \text{ Hz} \cdot 6.6 \times 10^{-27} \text{ erg s} (2+1)}{2 \cdot 1.4 \times 10^{-16} \text{ erg K}^{-1}} \sim 17\text{K}$$



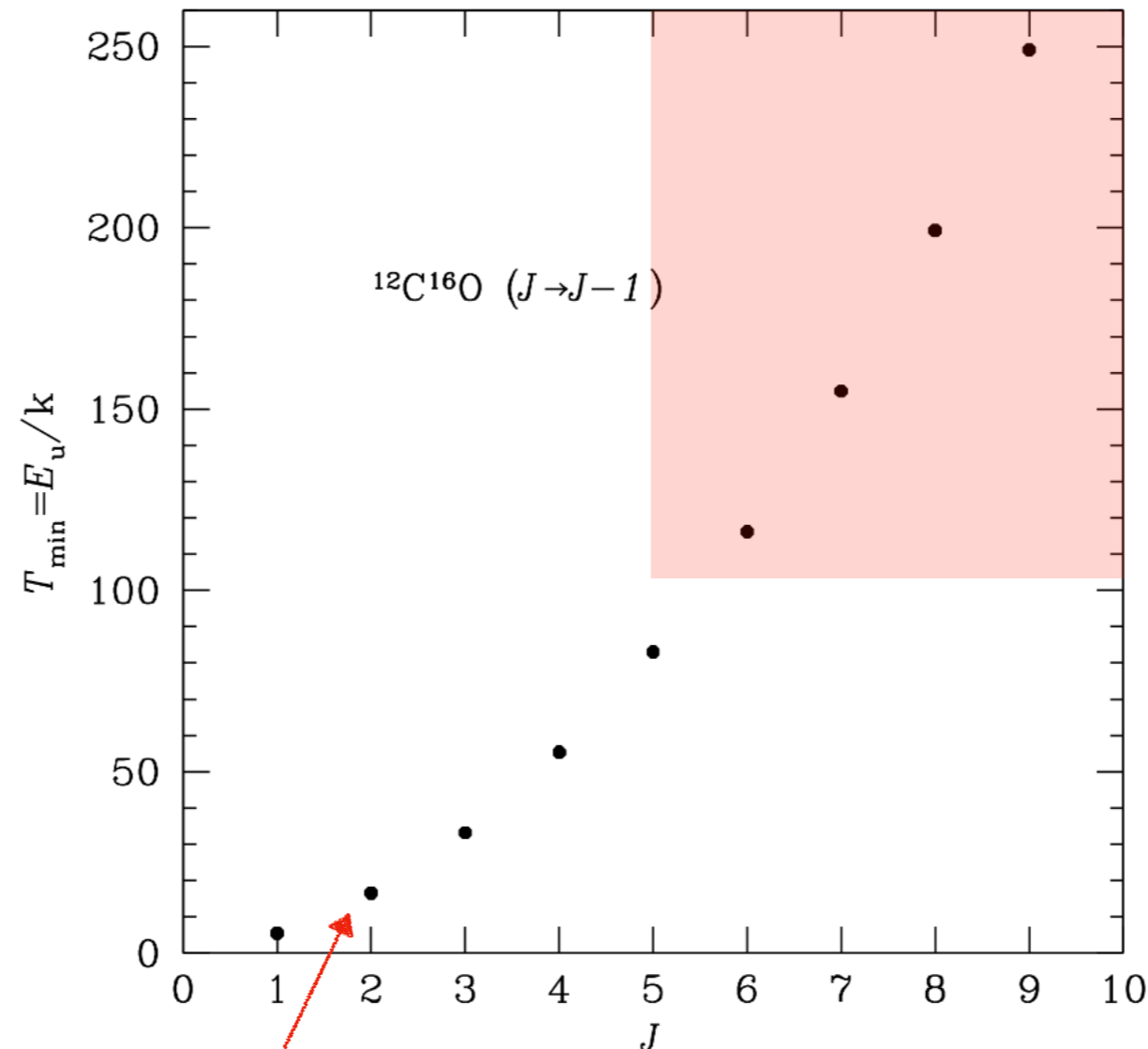
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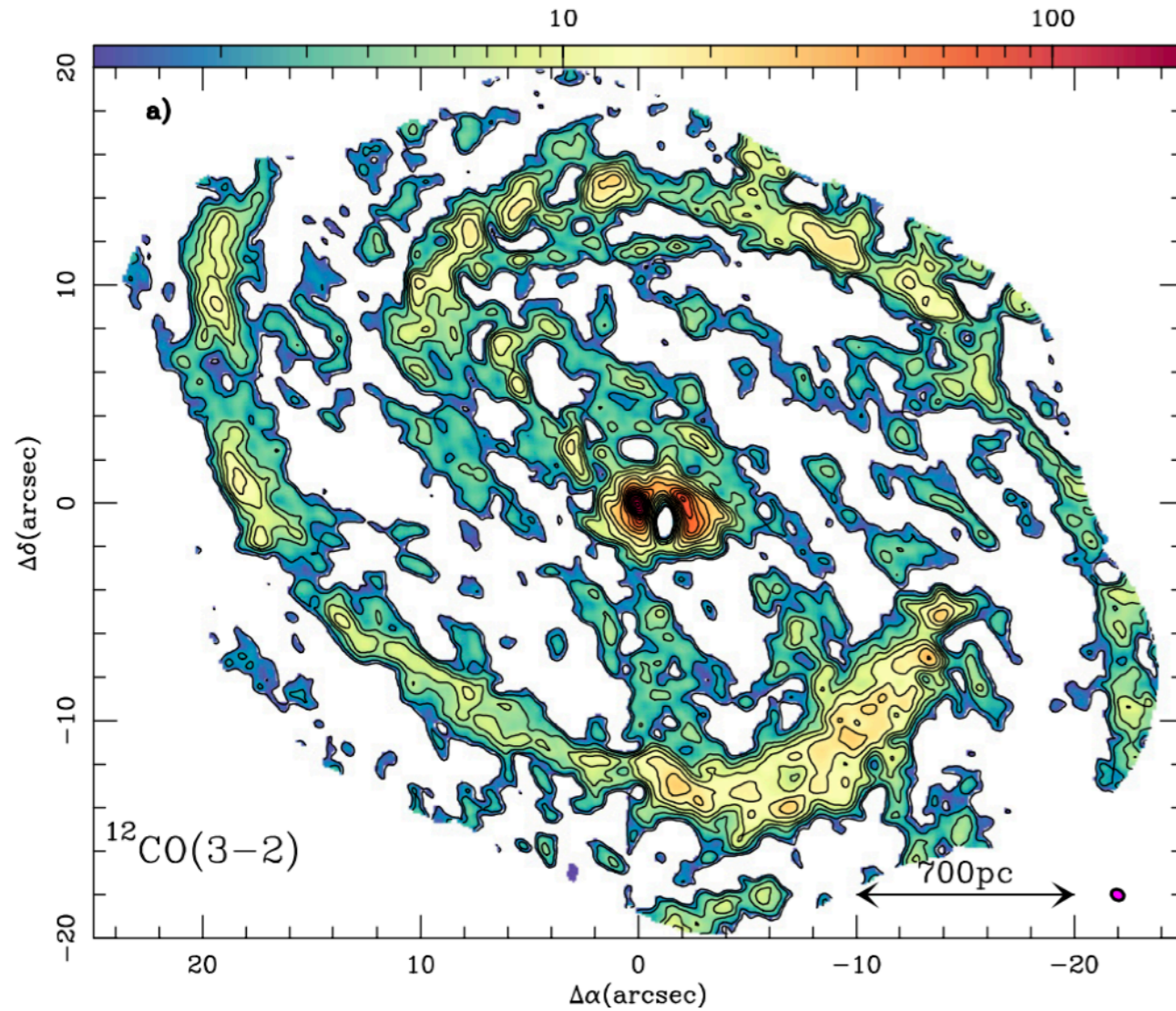
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Emission from high- J rotational transitions will be very weak in cold gas.

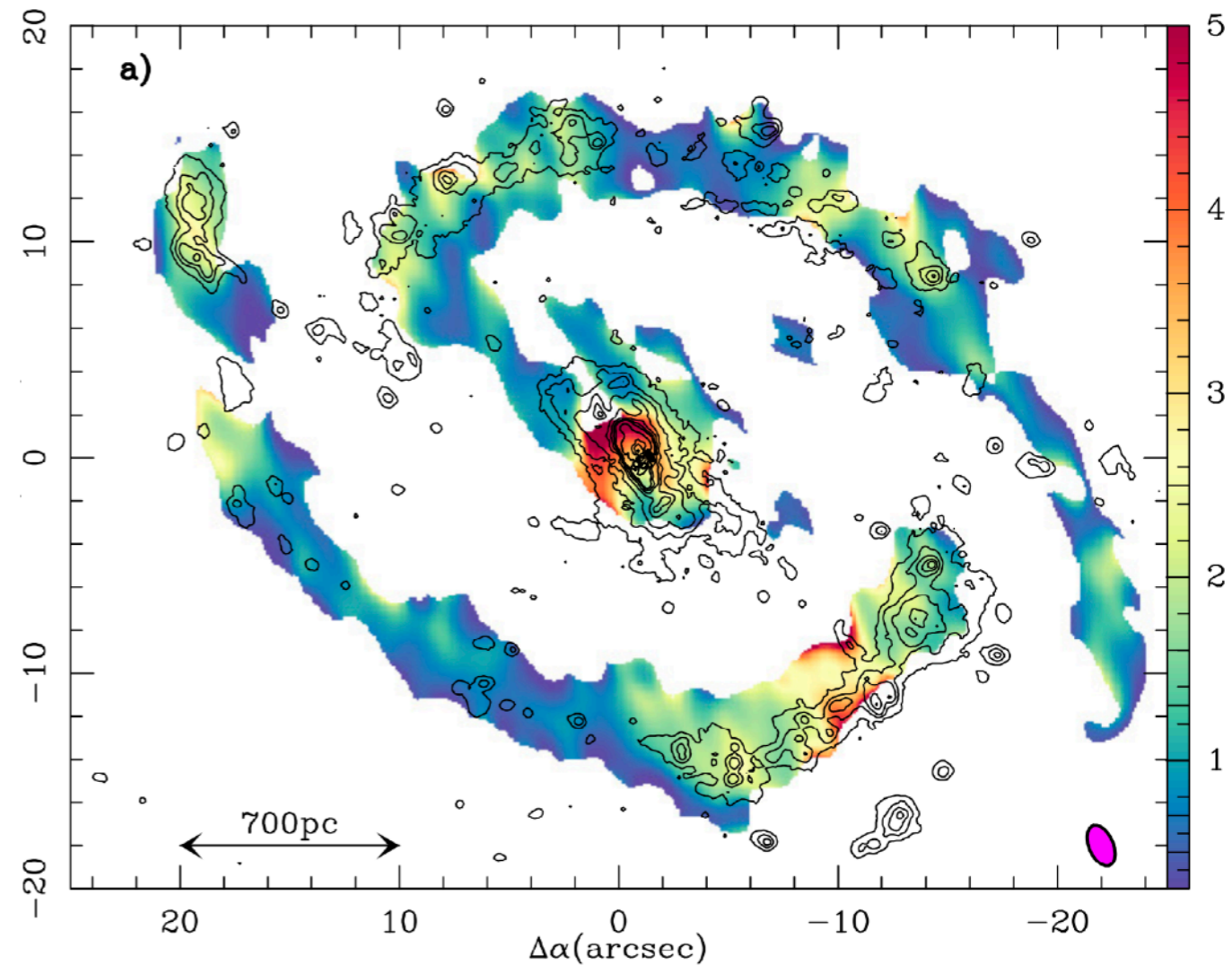
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Example: spiral galaxy NGC1068 (Garcia Burillo et al. 2014)



CO(3-2) $T_{\min} \sim 60 \text{ K}$ $n_{\text{crit}} \sim 10^4 \text{ cm}^{-3}$

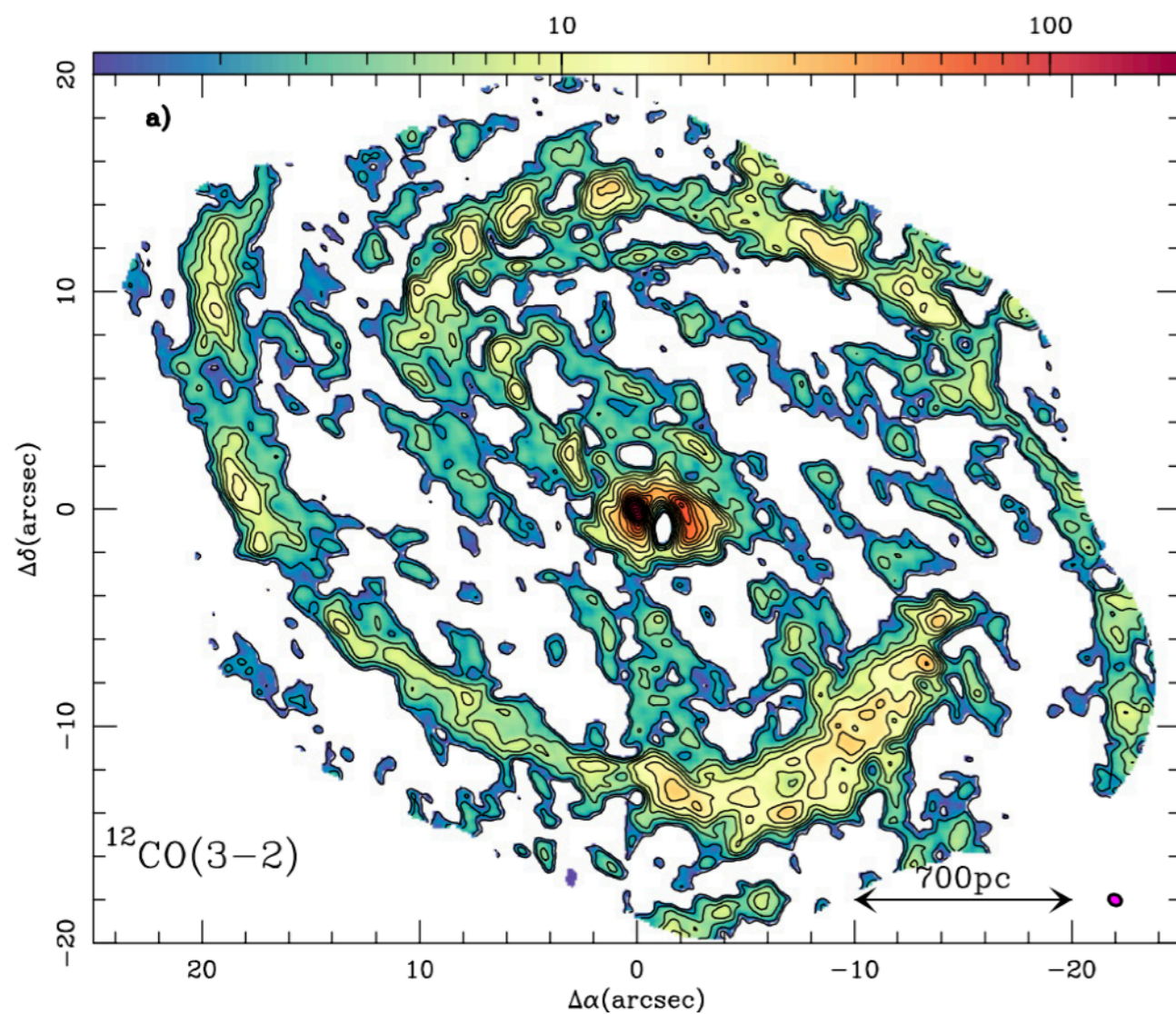
CO(1-0) $T_{\min} \sim 17 \text{ K}$ $n_{\text{crit}} \sim 10^3 \text{ cm}^{-3}$



CO(3-2)/CO(1-0) line ratio

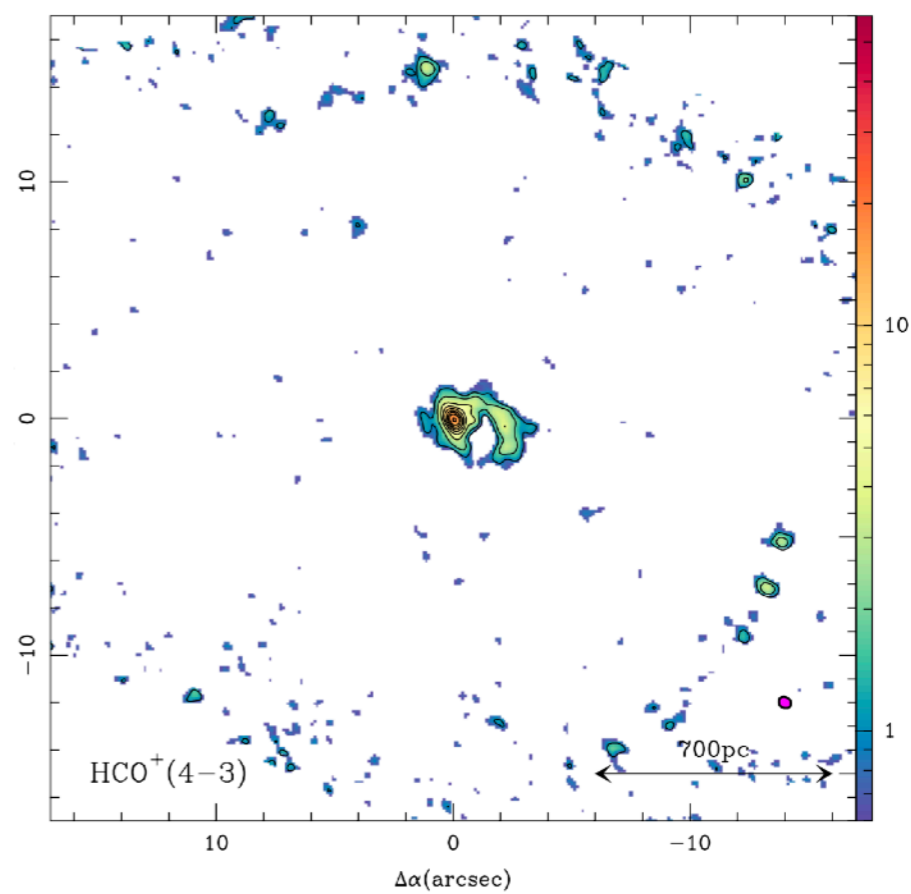
contours = PAH (recent star formation)

Example: spiral galaxy NGC1068 (Garcia Burillo et al. 2014)



CO(3-2) $T_{\min} \sim 60$ K $n_{\text{crit}} \sim 10^4$ cm⁻³

CO(1-0) $T_{\min} \sim 17$ K $n_{\text{crit}} \sim 10^3$ cm⁻³



HCO⁺(4-3) $T_{\min} \sim 43$ K $n_{\text{crit}} \sim 10^7$ cm⁻³



Fine-structure transitions

In atomic physics, the “gross structure” of line spectra describes the energy levels expected by the quantum mechanics of non-relativistic electrons with no spin. For a hydrogen atom, the gross structure energy levels only depend on n , the principal quantum number.

The “**fine structure**” takes into account relativistic and spin effects. The corresponding corrections to the non-relativistic Schrödinger equation break the degeneracy of the energy levels and split the corresponding spectral lines. The scale of the fine structure splitting relative to the gross structure energies is on the order of $(Z\alpha)^2 \sim 10^{-5} \text{ eV}$, where Z is the atomic number and $\alpha \sim 1/137$ is the fine-structure constant.

The most important relativistic correction to the kinetic energy is the correction due to the **spin-orbit coupling**, that is a relativistic interaction of a particle's spin with its motion inside a potential.

Bransden & Joachain, *Physics of atoms and molecules*, Addison-Wesley ed.



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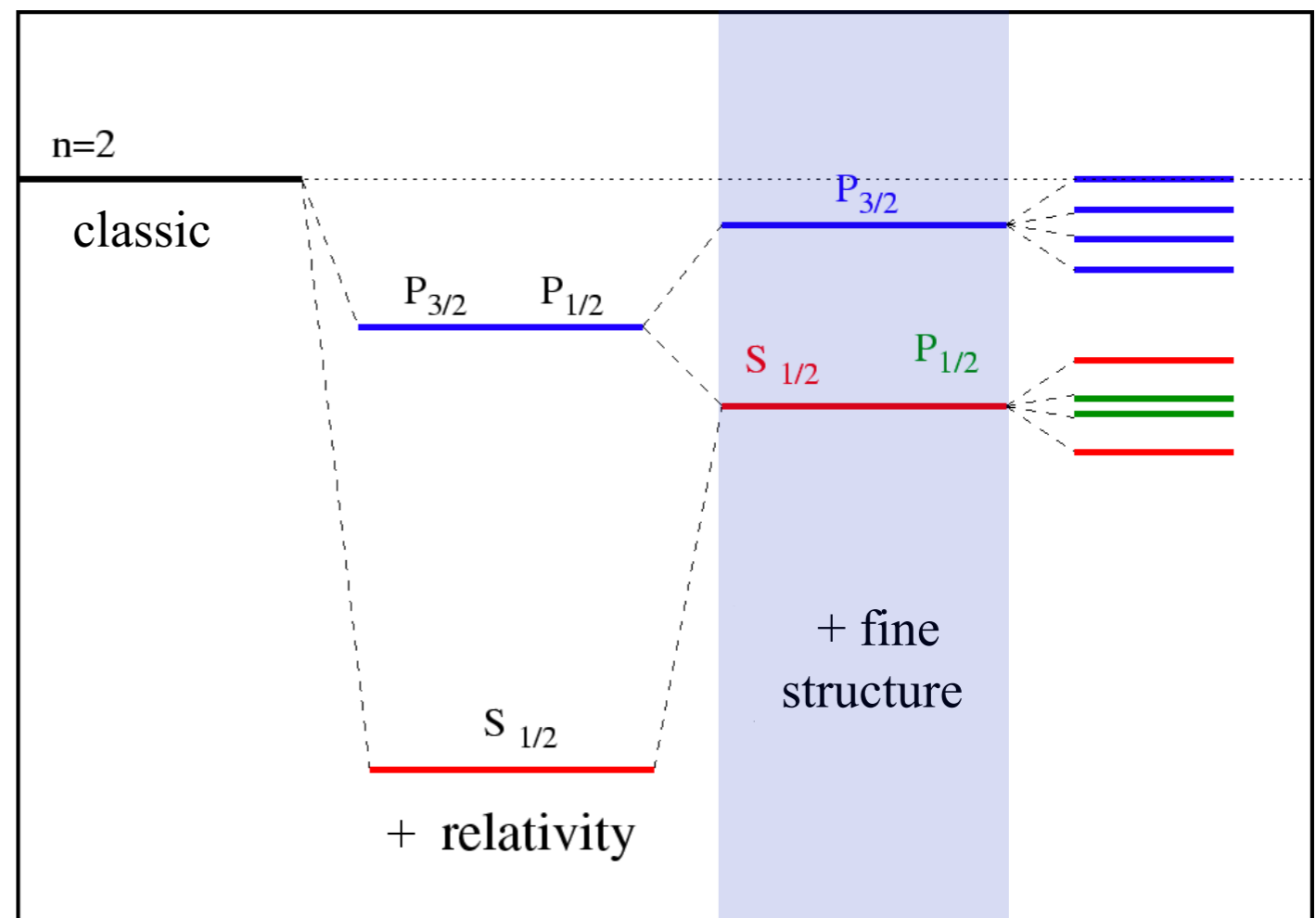
$$\mathbf{J} = \mathbf{L} + \mathbf{S} \text{ total angular momentum}$$

↑ orbital angular momentum ↑ spin magnetic momentum

P orbital corresponding to $L=1$

$$J = 3/2, 1/2$$

$$S = 1/2$$

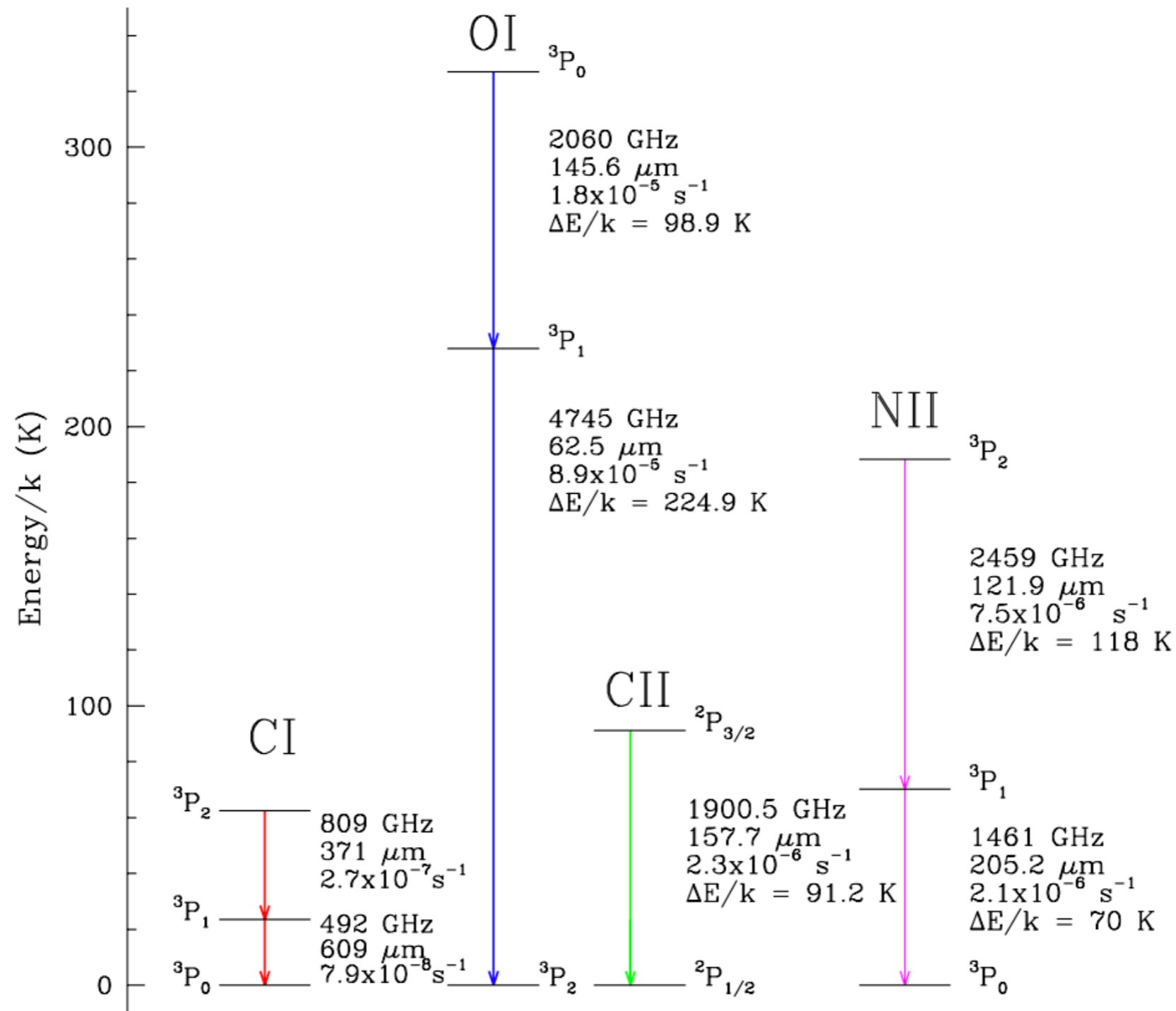


Hydrogen atom



Fine-structure transitions

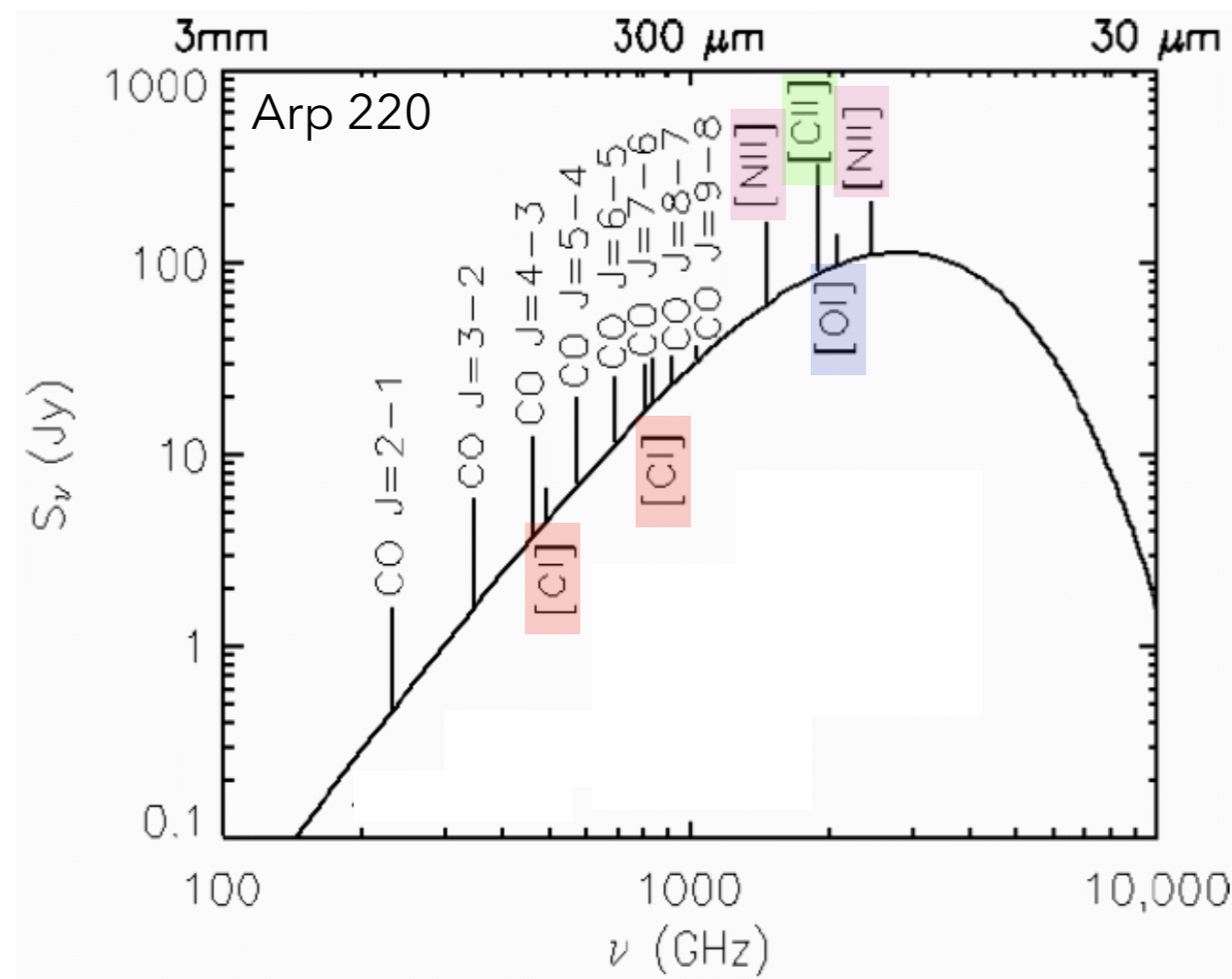
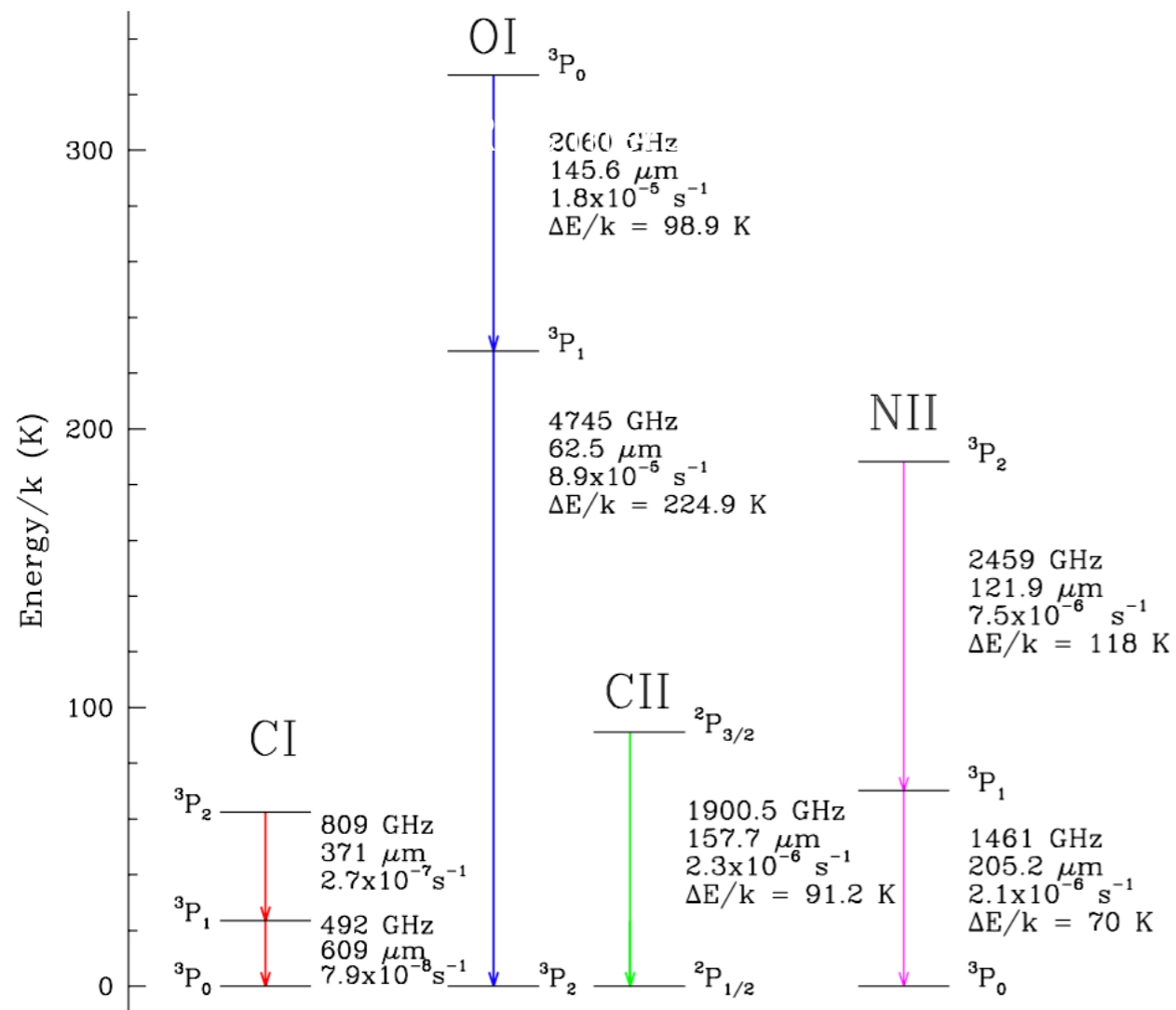
Examples of fine-structure transitions in the interstellar medium of galaxies





Fine-structure transitions

Examples of fine-structure transitions in the interstellar medium of galaxies

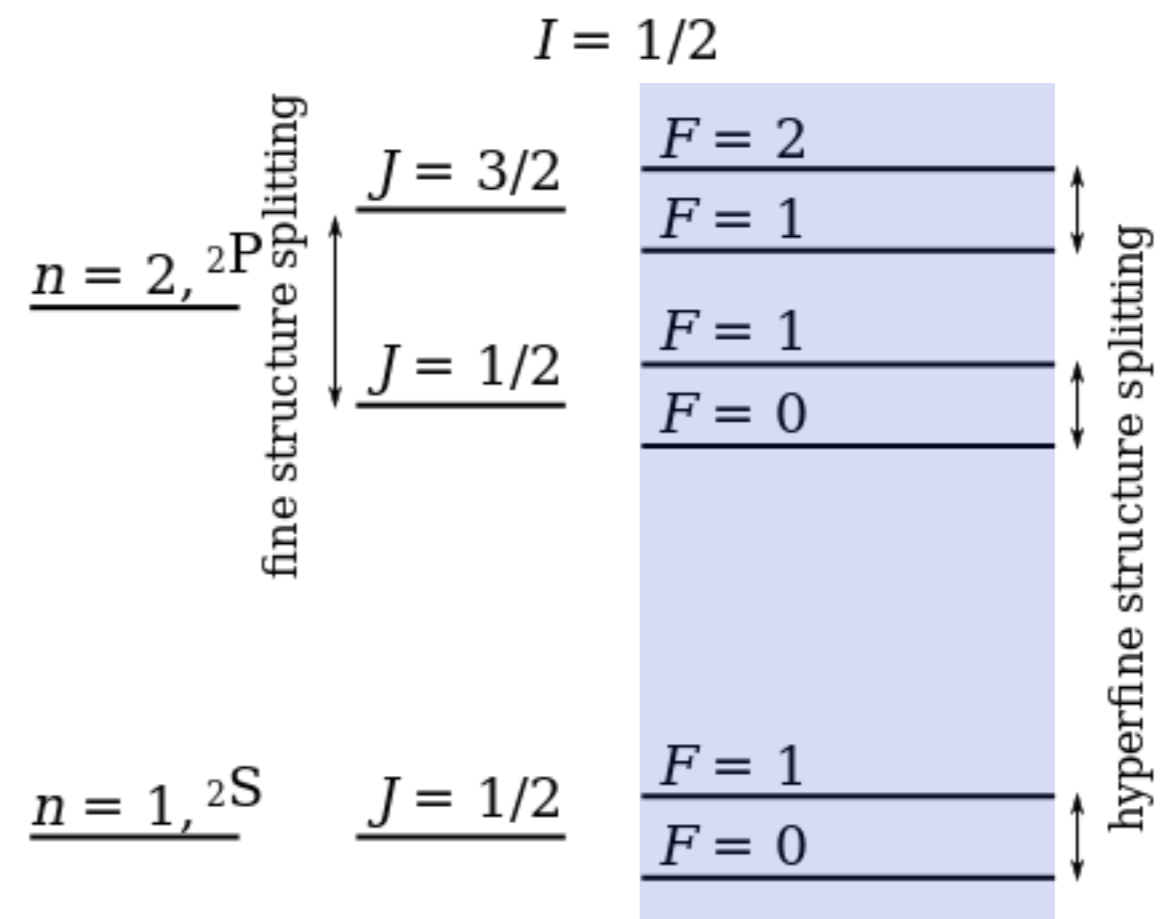




Hyperfine structure transitions

In atomic physics, hyperfine structure is defined by small shifts in otherwise degenerate energy levels. It arises from the energy of the nuclear magnetic dipole moment interacting with the magnetic field generated by the electrons.

Hyperfine structure \neq fine structure. Fine structure which results from the spin-orbit interaction the magnetic moments associated with electron spin and the electrons' orbital angular momentum. Hyperfine structure, with energy shifts typically $\lesssim 10^{-6}$ eV, results from the interactions of the nucleus (or nuclei, in molecules) with internally generated electric and magnetic fields.



The energy levels are split according to the total spin

$$F = |I + S|$$

$I = \pm 1/2$ nuclear spin

$S = \pm 1/2$ electronic spin

$F = 0, 1$ (for the ground level)



Hyperfine structure transitions: the 21 cm hydrogen line

In atomic physics, hyperfine structure is defined by small shifts in otherwise degenerate energy levels. It arises from the energy of the nuclear magnetic dipole moment interacting with the magnetic field generated by the electrons.

Hyperfine structure \neq fine structure. Fine structure which results from the spin-orbit interaction the magnetic moments associated with electron spin and the electrons' orbital angular momentum. Hyperfine structure, with energy shifts typically $\lesssim 10^{-6}$ eV, results from the interactions of the nucleus (or nuclei, in molecules) with internally generated electric and magnetic fields.

Radio emission of the hydrogen line come from the transition of an electron between the two hyperfine levels of the hydrogen 1 s ground state. It is called the **spin-flip transition**.

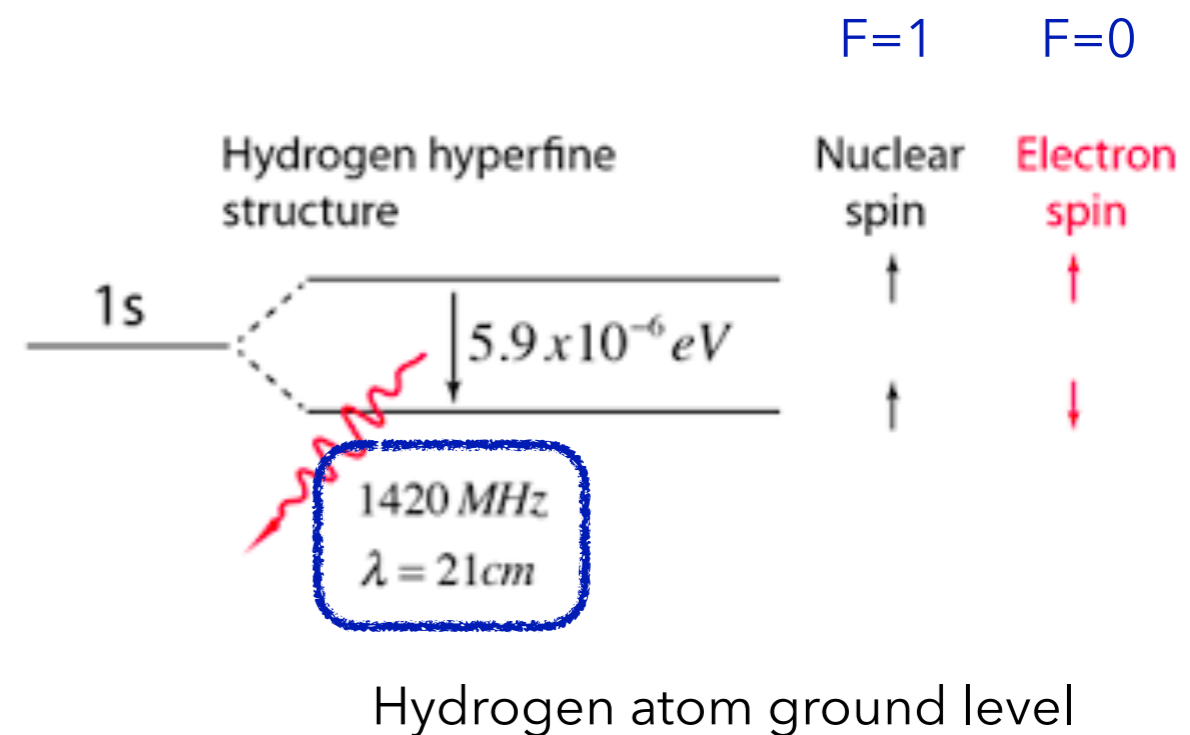
The energy levels are split according to the total spin

$$F = |I + S|$$

$I = \pm 1/2$ nuclear spin

$S = \pm 1/2$ electronic spin

$F = 0, 1$ (for the ground level)





Atomic lines: examples

Table 13.1 Parameters of some atomic lines

| Element and ionization state | Transition | ν/GHz | A_{ij}/s^{-1} | Critical density n^* |
|------------------------------|----------------------------|------------------|------------------------|------------------------|
| DI | $^2S_{1/2}, F = 3/2 - 1/2$ | 0.327 | 4.65×10^{-17} | ~ 1 |
| HI | $^2S_{1/2}, F = 1 - 0$ | 1.420 | 2.87×10^{-15} | ~ 1 |
| $^3\text{He}^+$ | $^2S_{1/2}, F = 0 - 1$ | 8.665 | 1.95×10^{-12} | ~ 10 |
| CI | $^3P_1 - ^3P_0$ | 492.16 | 7.93×10^{-8} | 5×10^2 |
| CI | $^3P_2 - ^3P_1$ | 809.34 | 2.65×10^{-7} | 10^4 |
| CII | $^2P_{3/2} - ^2P_{1/2}$ | 1900.54 | 2.4×10^{-6} | 5×10^3 |
| OI | $^3P_0 - ^3P_1$ | 2060.07 | 1.7×10^{-5} | $\sim 4 \times 10^5$ |
| OI | $^3P_1 - ^3P_2$ | 4744.77 | 8.95×10^{-5} | $\sim 3 \times 10^6$ |
| OIII | $^3P_1 - ^3P_0$ | 3392.66 | 2.6×10^{-5} | $\sim 5 \times 10^2$ |
| OIII | $^3P_2 - ^3P_1$ | 5785.82 | 9.8×10^{-5} | $\sim 4 \times 10^3$ |
| NII | $^3P_1 - ^3P_0$ | 1473.2 | 2.1×10^{-6} | $\sim 5 \times 10^1$ |
| NII | $^3P_2 - ^3P_1$ | 2459.4 | 7.5×10^{-6} | $\sim 3 \times 10^2$ |
| NIII | $^2P_{3/2} - ^2P_{1/2}$ | 5230.43 | 4.8×10^{-5} | $\sim 3 \times 10^3$ |

