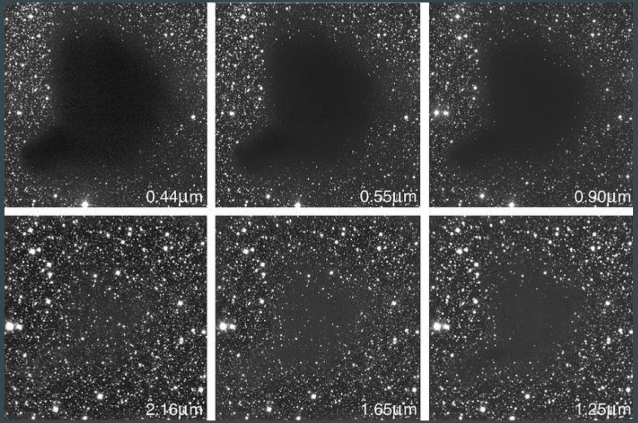
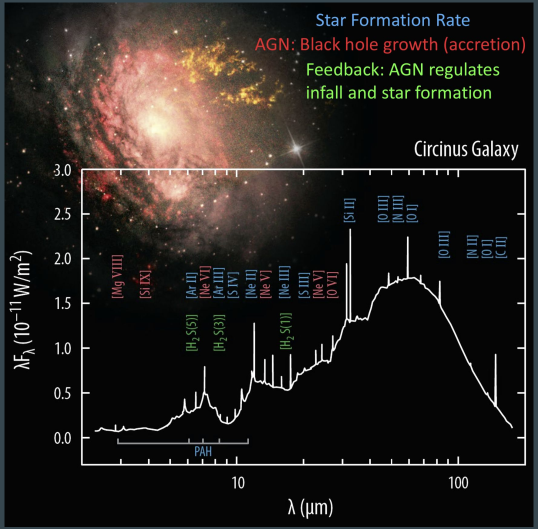
Infrared emission lines in the dusty interstellar medium



Elijah Kane
ARC Seminar 2/7/2025

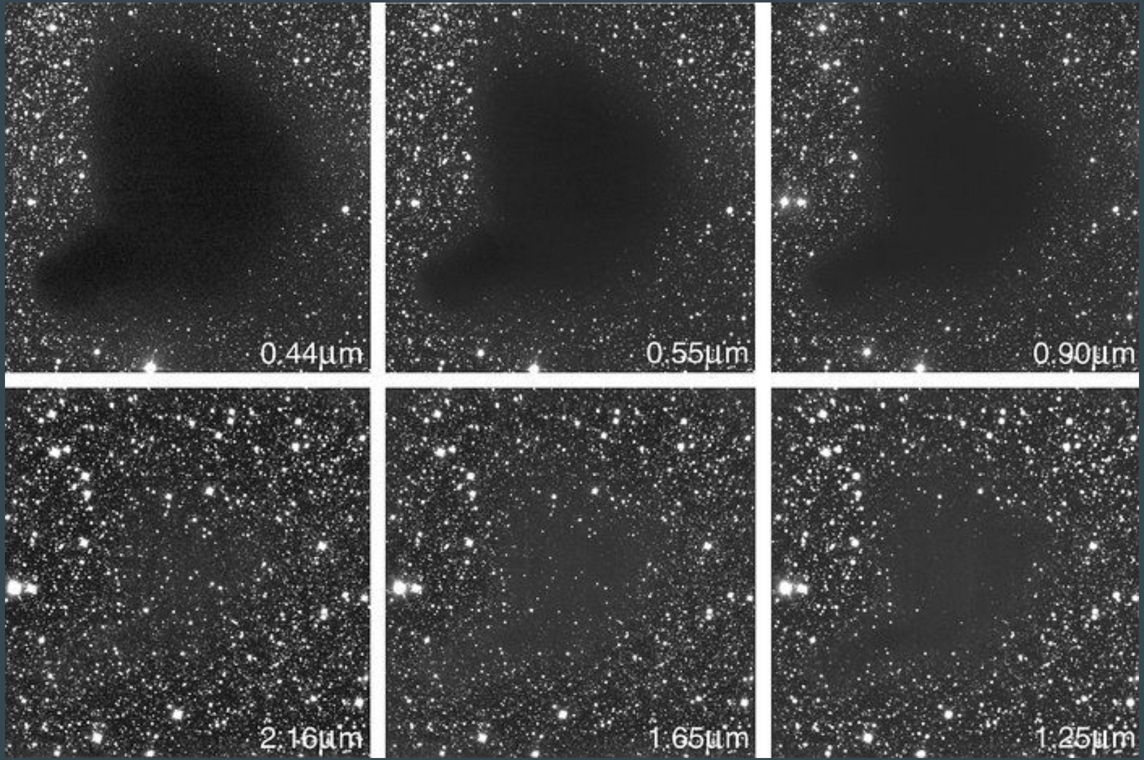


Outline

Mostly a review of some theory and observation papers from the 80s.

1. What is dust and why do we care?
2. Why do we see infrared emission lines from the dusty ISM?
   a. Derive collisional excitation rates – quantum scattering problem
   b. Relate the rates to observable quantities (i.e. luminosity)
3. What can we learn by observing emission lines?
   a. Starburst activity in an extragalactic source (M82 galaxy)
   b. Star formation in a nearby molecular cloud (M17)

What is dust?



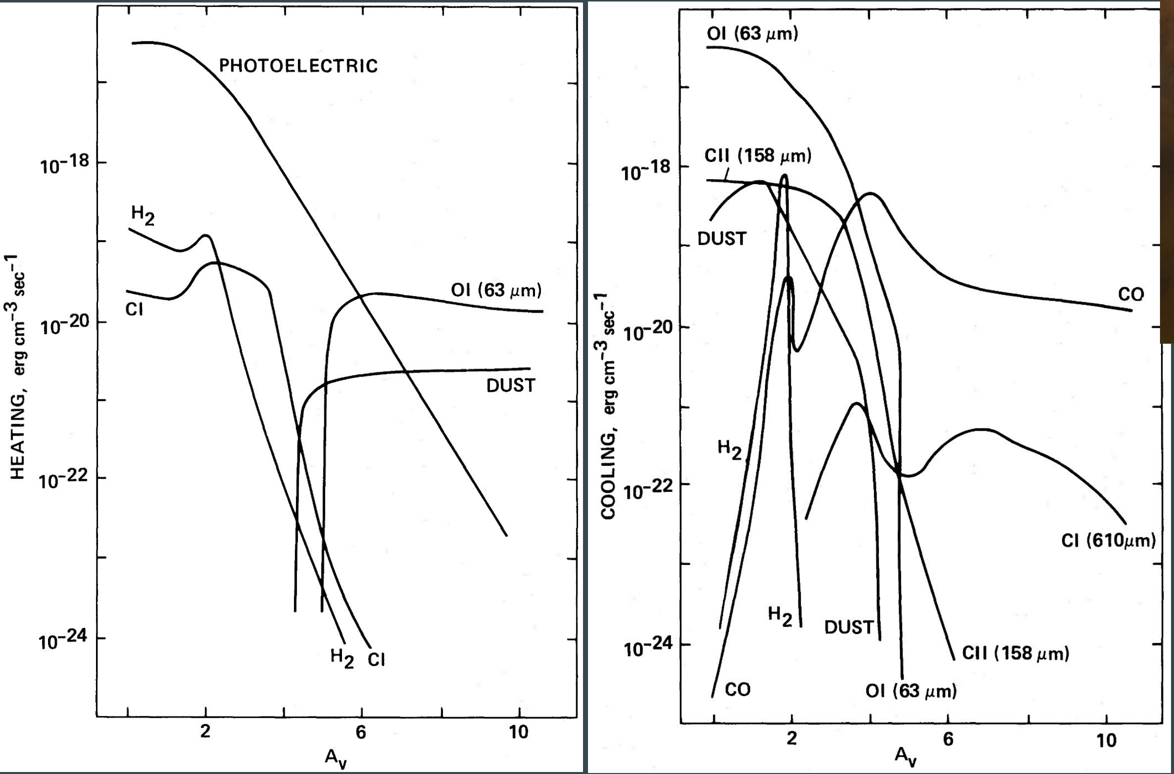
Barnard B68 molecular cloud from the visible through the near-IR.
Credit: ESO (https://www.eso.org/public/images/eso9934b/)

Dust = solid particles of heavy elements (O, C, Si, Mg, Fe) with sizes 0.3nm < r < 0.3um in the interstellar medium

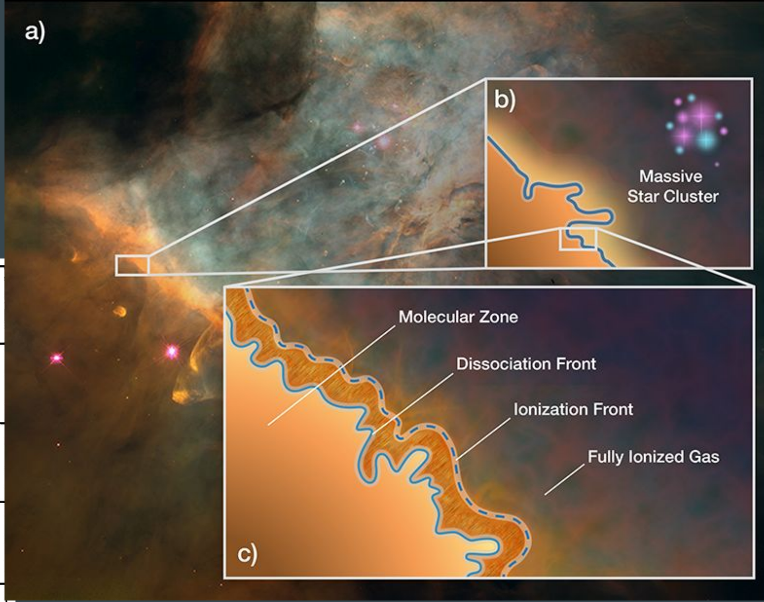
About 1% of the ISM mass

Dust is a highly efficient absorber of energetic UV and visible photons, but is largely transparent in the IR

Dust in star-forming regions



Tielens + Hollenbach 1985 (ApJ 291)



Photodissociation region in the Orion Nebula.
(JWST release 2021-024)

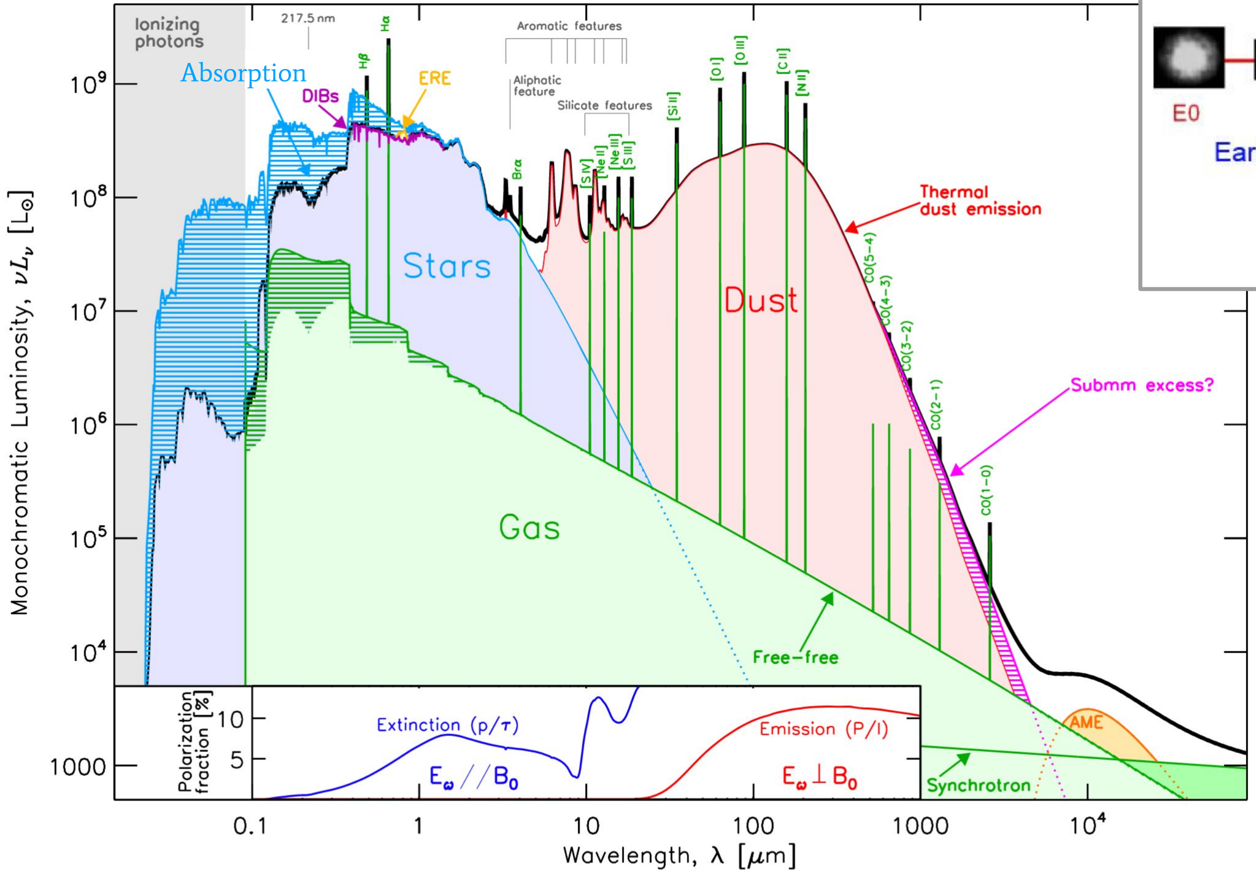
Dust absorbs UV from young stars and heats the ISM through photoelectric heating

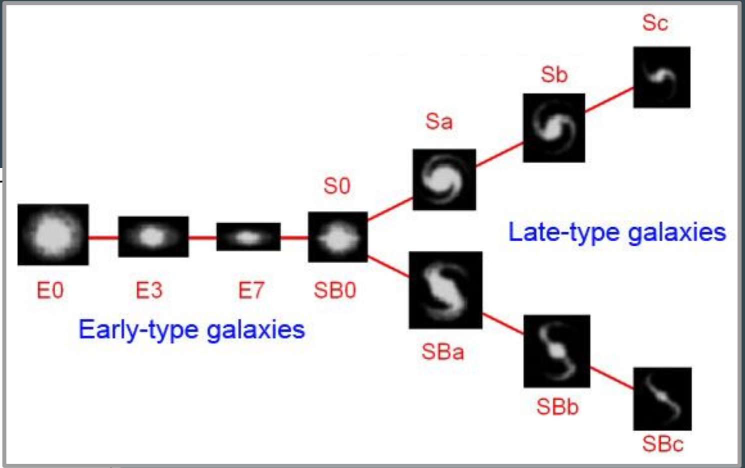
Carbon, Oxygen, Nitrogen, ... can also be photoionized

The dust cools itself with thermal greybody emission

The ISM gas cools itself through emission lines

Dust + gas emission from galaxies





https://astronomy.swin.edu.au/cosmos/L/late-type+galaxies

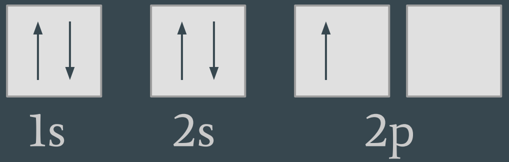
Example: typical late-type galaxy

Dust absorbs and scatters starlight

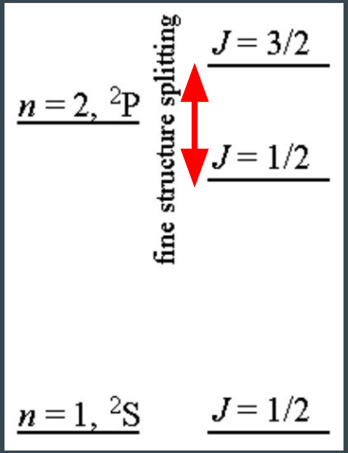
Absorbed UV/vis light is "re-processed" into the far-infrared

Example: The [CII] 158 micron line

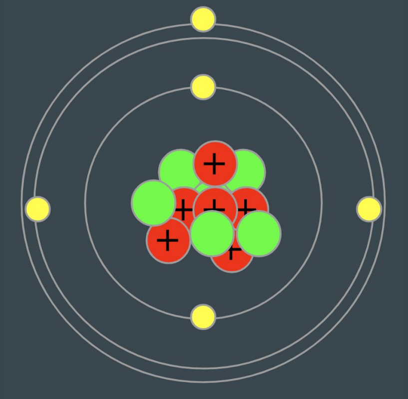
Electronic structure of C^+



Spin-orbit coupling + relativistic correction
→ Fine structure splitting of the ^{2}P level



7.9 meV
92 K
158 μm



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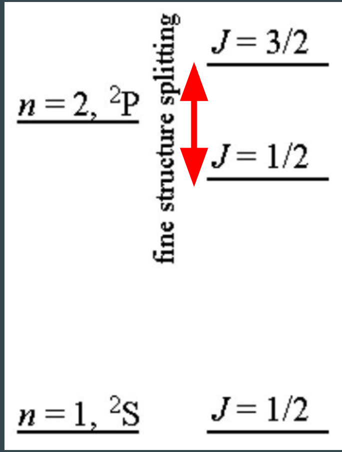

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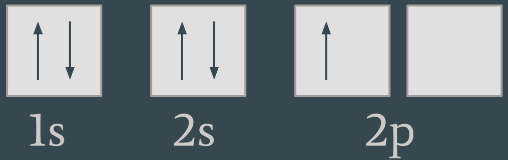

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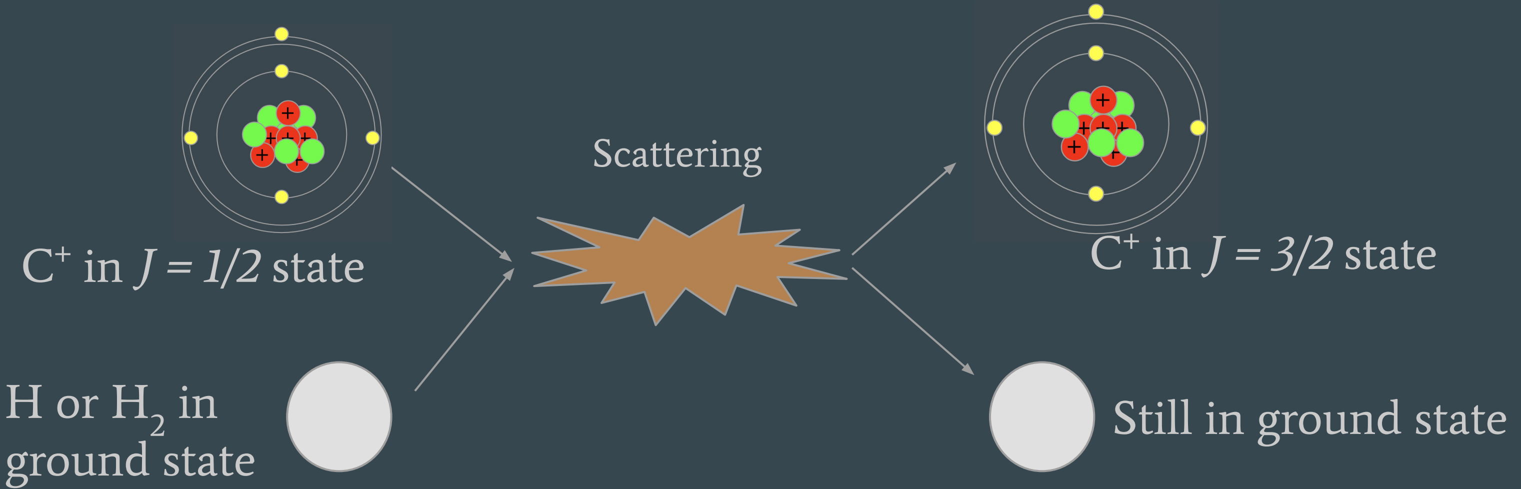
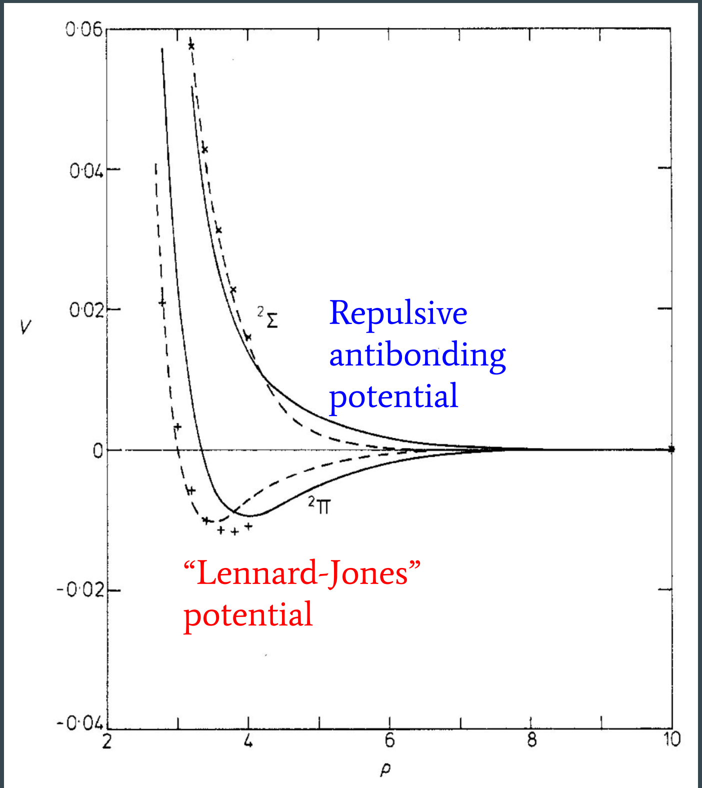
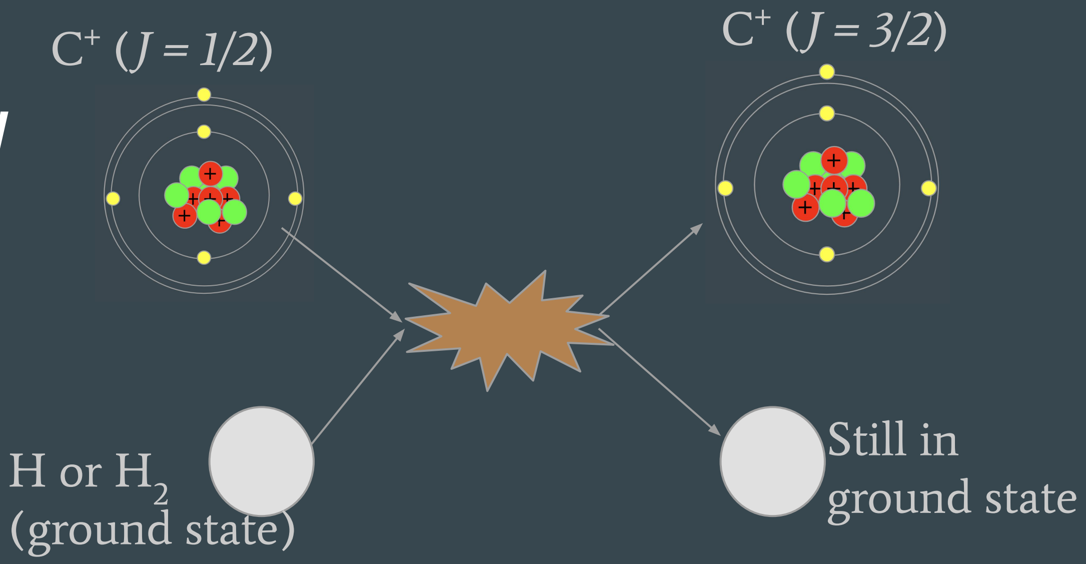
Collisional excitation by warm gas:

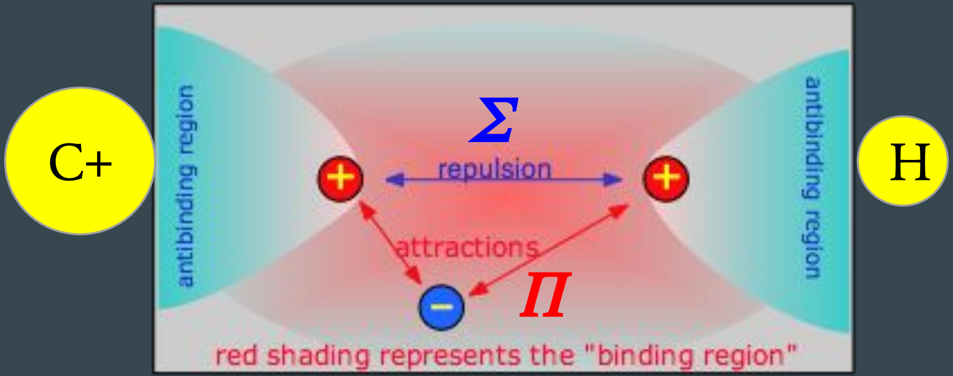


Interatomic potential energy



Flower + Launay 1977
(J.Phys.B:Atom.Mol.Phys. 10 3673)





https://chem.libretexts.org/Bookshelves/General_Chemistry/Chem1_(Lower)/09%3A_Chemical_Bonding_and_Molecular_Structure/9.08%3A_Molecular_Orbital_Theory

Schrödinger equation for colliding atoms

Relative kinetic energy of atoms A and B

Internal Hamiltonians of atoms A and B

Relative potential energy of atoms A and B

$$\left[-(1/2\mu)\nabla_R^2 + H_A + H_B + V\right]\Psi = E\Psi$$

The Hamiltonian is invariant with respect to spatial rotations, so it commutes with J and J_z

$$\Psi^{JM} = \sum_\gamma \left[(1/R) f_\gamma^J(R)\Gamma_\gamma^{JM}\right]$$

Relative angular momentum of the atoms

$$\gamma \equiv \{j_\alpha, j_\beta, \ell\}$$

Internal angular momenta of atoms $\{A, B\}$ in states $\{\alpha, \beta\}$

$\Gamma_\gamma^{JM} =$ Some mess of spherical harmonics and Clebsch-Gordan coefficients from adding the angular momenta.

$f_\gamma^J(R) =$ Radial parts of the wavefunction, we need to solve for these to get the inelastic scattering probabilities.

"Inelastic" because the internal angular momentum states can change:

$$\{j_{\alpha_1}, j_{\beta_1}\} \to \{j_{\alpha_2}, j_{\beta_2}\}$$

Schrödinger equation for colliding atoms

Apply the kinetic energy operator to each term in the sum:

Define:

$$u_\gamma^J \equiv (1/R) f_\gamma^J$$

$$\nabla_R^2(u_\gamma^J \Gamma_\gamma^{JM}) = \underbrace{\frac{1}{R^2}\frac{\partial}{\partial R}\left(R^2 \frac{\partial(u_\gamma^J \Gamma_\gamma^{JM})}{\partial R}\right)} + \underbrace{\frac{1}{R^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial(u_\gamma^J \Gamma_\gamma^{JM})}{\partial\theta}\right) + \frac{1}{R^2\sin^2\theta}\frac{\partial^2(u_\gamma^J \Gamma_\gamma^{JM})}{\partial\phi^2}}$$

$$= \Gamma_\gamma^{JM}\frac{1}{R}\frac{\partial^2 f_\gamma^J}{\partial R^2} + f_\gamma^J \frac{\hat{L}^2}{\hbar^2 R^3}\Gamma_\gamma^{JM}$$

$$= \Gamma_\gamma^{JM}\frac{1}{R}\frac{\partial^2 f_\gamma^J}{\partial R^2} + f_\gamma^J \frac{\ell(\ell+1)}{R^3}\Gamma_\gamma^{JM}$$

Also, the full wavefunction is an eigenstate of H_A and H_B:

$$H_A\Psi^{JM} = E_A(\alpha)\Psi^{JM} \qquad H_B\Psi^{JM} = E_B(\beta)\Psi^{JM}$$

$\alpha, \beta =$ Internal energy states of atoms A and B

Schrödinger equation for colliding atoms

Putting it all together (drop J and M superscripts for now):

$$\sum_\gamma \left[-(1/2\mu)\nabla_R^2 + H_A + H_B + V\right](u_\gamma \Gamma_\gamma) = \sum_\gamma \Bigg[-(1/2\mu)\frac{1}{R}\frac{\partial^2 f_\gamma}{\partial R^2}\Gamma_\gamma + \frac{1}{R} f_\gamma \Gamma_\gamma \left(\frac{-\ell(\ell+1)}{2\mu R^2} + E_A(\alpha) + E_B(\beta) + V\right)\Bigg]$$

Apply $\int d\Omega\, \Gamma^*_{\gamma'}$ to both sides:

$$\left[\frac{d^2}{dR^2} - \frac{\ell(\ell+1)}{R^2} + k_\gamma^2\right] f_\gamma^J(R) = 2\mu \sum_{\gamma'} V^J_{\gamma\gamma'}(R) f^J_{\gamma'}(R)$$

$$k_\gamma^2 = 2\mu\left[E - E_A(\alpha) - E_B(\beta)\right]$$

$$V^J_{\gamma\gamma'}(R) = \int d\Omega\ \left[\Gamma_\gamma^{*JM} V \Gamma_{\gamma'}^{JM}\right]$$

Coupled set of differential equations which we solve to get $f_\gamma^J(R)$

Calculating the scattering cross sections

When the particles are separated far enough, $V^J_{\gamma\gamma'} \simeq 0$

$$\left[\frac{d^2}{dR^2} - \frac{\ell(\ell+1)}{R^2} + k_\gamma^2\right] f_\gamma^J(\text{large } R) \simeq 0$$

(Bessel's equation)

Solutions are spherical Bessel functions:

$$f_\gamma^J(\text{large } R) = A_\gamma R\, j_\ell(k_\gamma R) + B_\gamma R\, n_\ell(k_\gamma R)$$

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$$f^J_\gamma(\text{large } R) = A_\gamma R\, j_\ell(k_\gamma R) + B_\gamma R\, n_\ell(k_\gamma R)$$

We get A_γ and B_γ as follows:

1) Solve $\left[\frac{d^2}{dR^2} - \frac{\ell(\ell+1)}{R^2} + k_\gamma^2\right] f^J_\gamma(R) = 2\mu \sum_{\gamma'} V^J_{\gamma\gamma'}(R) f^J_{\gamma'}(R)$ $\rightarrow$ Get $f^J_\gamma(R)$ for all R

2) Apply boundary condition: $\lim_{R\to\infty} f^J_\gamma(R) = A_\gamma R\, j_\ell(k_\gamma R) + B_\gamma R\, n_\ell(k_\gamma R)$

Scattering cross section can be calculated from A_γ and B_γ

$$\sigma = 4\pi \sum_{\ell=0}^{\infty} (2\ell+1)\, |a_\ell|^2$$

(With a more general form of this elastic scattering equation from Griffiths QM)

Collisional excitation rate in thermal equilibrium

Average the cross section over a Maxwellian kinetic energy distribution.

(For excitation of [CII] 158μm line, we use the cross section for going from $j_0 = 1/2 \rightarrow j = 3/2$)

$$\langle \sigma_{j_0 \rightarrow j} \rangle = (kT)^{-2} \int \sigma_{j_0 \rightarrow j}(E) E \exp(-E/kT) dE$$

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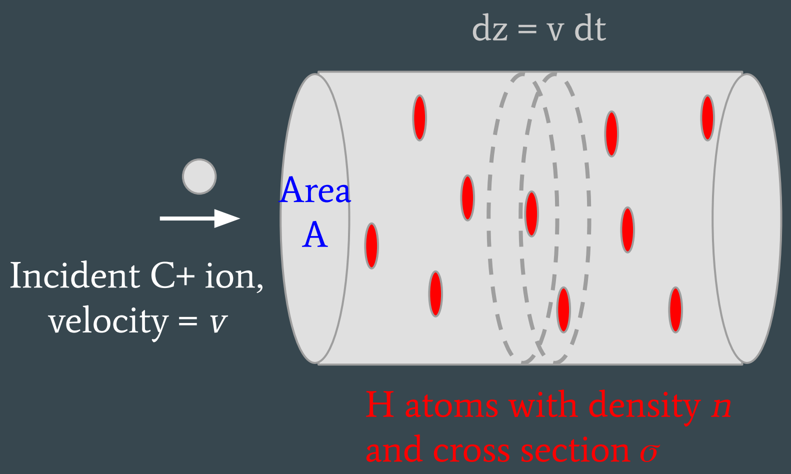

$$\frac{dP(\text{scatter})}{dt} = \frac{dP(\text{scatter})}{dz}\frac{dz}{dt} = n\langle \sigma_{j_0 \rightarrow j} \rangle \langle v \rangle$$

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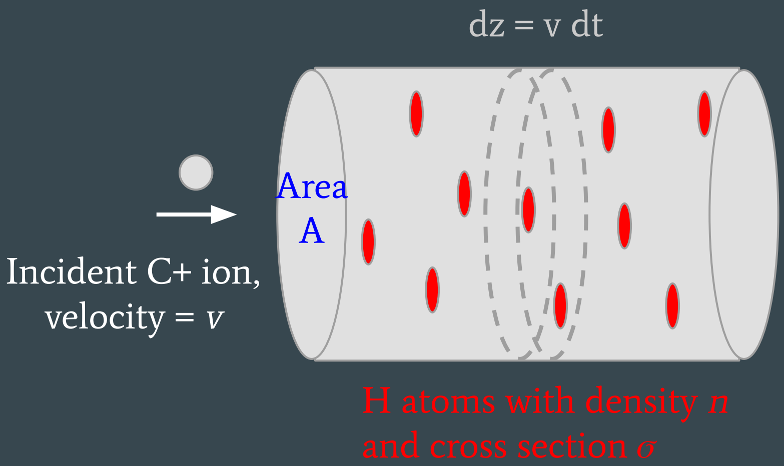

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$$\boxed{\gamma_{21} \equiv \langle v \rangle \langle \sigma_{j_0 \rightarrow j} \rangle}$$

Collisional excitation rate from ground state to excited state.

Collisional excitations / cm^3 / sec = $\gamma_{21} n_1 n$

Relating collisional excitation and de-excitation

Since Maxwell's equations obey time reversal symmetry, the collisional excitation/de-excitation rates must obey detailed balance.

$$\gamma_{21} n_2 n = \gamma_{12} n_1 n$$

The level population ratio in thermal equilibrium is given by the Boltzmann factor.

$$\frac{n_2}{n_1} = \frac{g_2 \exp(-E_2/kT)}{g_1 \exp(-E_1/kT)}$$

→ Expression relating collisional excitation and de-excitation rates. Holds even when we add other types of excitation/de-excitation processes!

$$\gamma_{12} = \frac{g_2}{g_1} \exp(-E_{21}/kT) \gamma_{21}$$

Adding in spontaneous emission

Balance collisional de-excitation + spontaneous emission with collisional excitation

$$\gamma_{21} n_2 n + A_{21} n_2 = \gamma_{12} n_1 n$$

(This is assuming the gas is optically thin – no absorption or stimulated emission)

Using the relationship between collisional excitation and de-excitation:

$$\frac{n_2}{n_1} = \frac{(g_2/g_1)\exp(-E_{21}/kT)}{1 + A_{21}/\gamma_{21} n}$$

Note - the level populations no longer follow the Boltzmann factor, although they are in a steady state

Define a "critical density" of colliding partners:

$$n_{crit} \equiv A_{21}/\gamma_{21}$$

When $n = n_{crit}$, collisional excitation and spontaneous emission rates balance each other.

And when $n \ll n_{crit}$, $n_2 \ll n_1$.

Calculating the line intensity

Intensity = (Photon energy) x (Spontanous decay rate) x (# of excited state atoms per area) x (1/4π)

C+ column density

$$I_{[\mathrm{CII}]} = \frac{1}{4\pi} h\nu A_{21} N_{C+} \frac{n_2}{n_{tot}}$$

(ergs s^{-1} cm^{-2} sr^{-1})

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Conservation of total particle number:

$$n_1 + n_2 = n_{tot}$$

$$\frac{n_2}{n_1} = \frac{(g_2/g_1)\exp(-E_{21}/kT)}{1 + n_{crit}/n}$$

Fraction of particles in the excited state:

$$\frac{n_2}{n_{tot}} = \left[1 + \frac{g_1}{g_2}\exp(E_{21}/kT)\left(1 + \frac{n_{crit}}{n}\right)\right]^{-1}$$

Optical depth

The line emission will interact with ground-state atoms through absorption and excited-state atoms through stimulated emission.

$$\alpha_\nu = \frac{c^2}{8\pi\nu^2} g_2 A_{21} \left(\frac{n_1}{g_1} - \frac{n_2}{g_2} \right) \phi(\nu)$$

(Rybicki + Lightman)

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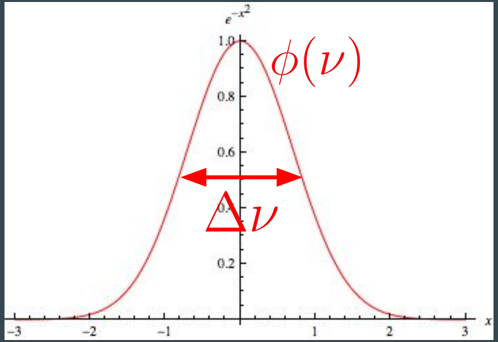

For spectral lines that are Doppler broadened:

$$\Delta\nu = \nu \frac{\Delta v}{c} \sim \frac{1}{\phi(\nu)}$$

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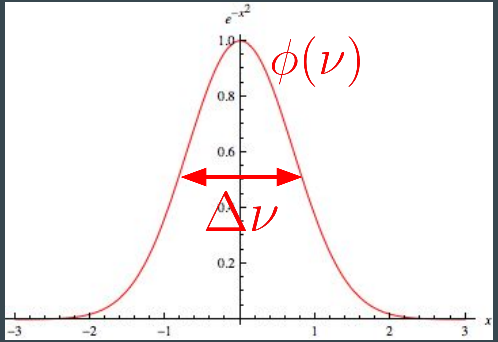

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$$\tau = \int \alpha_\nu ds = \frac{A_{21} c^3}{8\pi\nu^3 \Delta v} \left[\left(1 + \frac{n_{crit}}{n} \right) \exp(h\nu/kT) - 1 \right] N_{C^+} \frac{n_2}{n_{tot}}$$

Example: [CII] emission from an extragalactic source

Crawford+ 1985 (ApJ 291, 755-771)

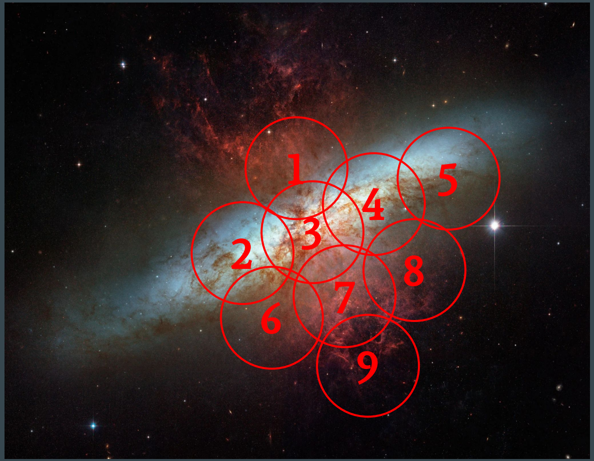
Messier 82: A gas-rich galaxy forming stars >10x as fast as our galaxy

Strong [CII] emission from around the nucleus

$$I_{[CII]} = \frac{1}{4\pi} h\nu A_{21} N_{C+} \frac{n_2}{n_{tot}}$$

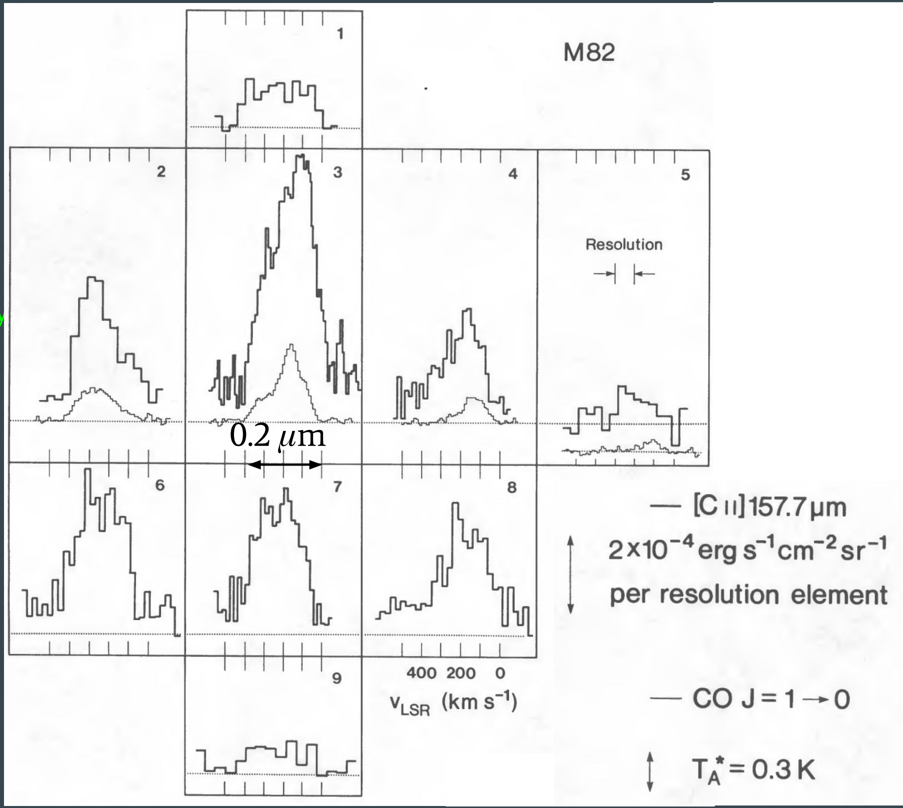
Implies warm, dense gas

Implies high C+ column density

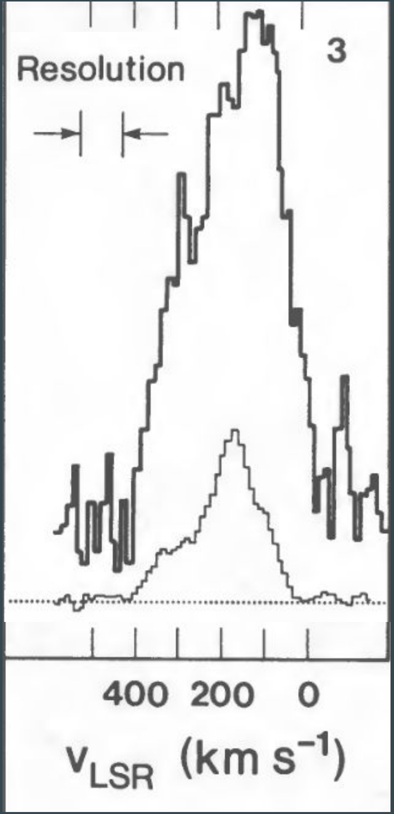


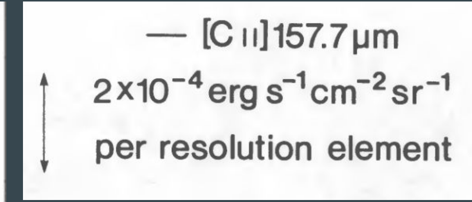
(Red = infrared, Blue/yellow = visible)

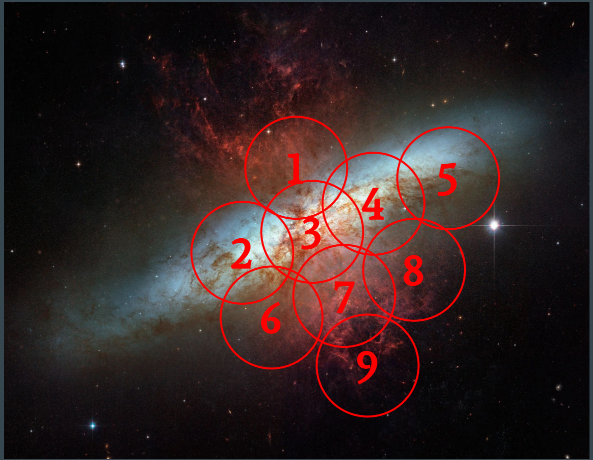
https://science.nasa.gov/mission/hubble/science/explore-the-night-sky/hubble-messier-catalog/messier-82/



Calculating [CII] luminosity







Measured [CII] line intensity:

$$I_{[\mathrm{CII}]} = 1.5 \times 10^{-3} \text{ ergs s}^{-1} \text{ cm}^{-2} \text{ sr}^{-1}$$

Beam size: $A_{beam} \sim 0.8 \text{ kpc}^2$

$$L_{[\mathrm{CII}]} = I_{[\mathrm{CII}]} \times 4\pi \times A_{beam}$$

$$= 4.6 \times 10^{7}\, L_{\odot}$$

(about 0.5% of the total infrared luminosity of this galaxy!)

Calculate optical depth

Can we assume the gas is optically thin? (this makes our lives easier)

We're assuming the emission comes from warm ($T >> 92$ K), dense ($n >> n_{crit}$) gas.

$$I_{[\mathrm{CII}]} = \frac{1}{4\pi} h\nu A_{21} N_{C+} \frac{n_2}{n_{tot}}$$

Implies warm, dense gas

Implies high C+ column density

$$\tau = \frac{A_{21} c^3}{8\pi\nu^3 \Delta v} \left[\left(1 + \frac{n_{crit}}{n}\right) \exp(92\ \mathrm{K}/T) - 1 \right] \frac{n_2}{n_{tot}} \chi N_H$$

$$\frac{n_2}{n_{tot}} = \left[1 + \frac{g_1}{g_2} \exp(92\ \mathrm{K}/T) \left(1 + \frac{n_{crit}}{n}\right) \right]^{-1}$$

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$$\tau \simeq \frac{A_{21} c^3}{8\pi\nu^3 \Delta v} \left(\frac{92\,\mathrm{K}}{T}\right) \chi N_H = 0.16 \left(\frac{N_H}{10^{21}\,\mathrm{cm}^{-2}}\right) \left(\frac{5\,\mathrm{km\ s}^{-1}}{\Delta v}\right) \left(\frac{92\ \mathrm{K}}{T}\right)$$

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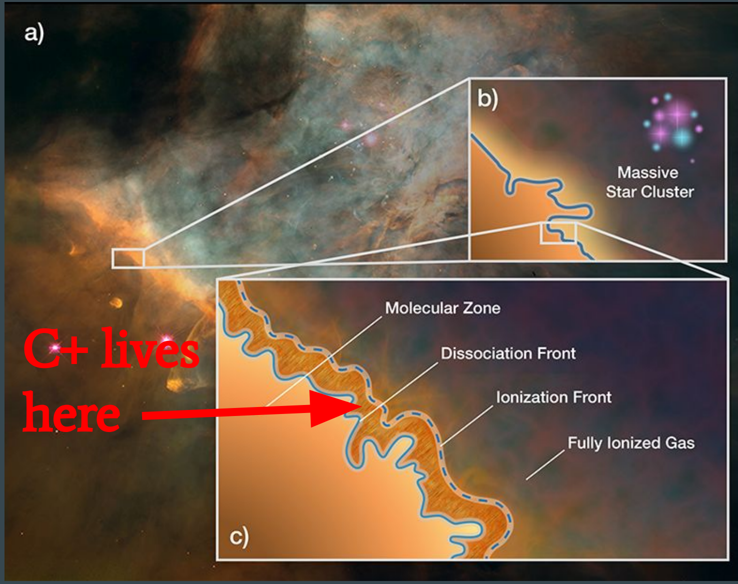
Models of photodissociation regions suggest the following:

$$N_H \lesssim 10^{22}\ \mathrm{cm}^{-2} \qquad \Delta v \sim 5\ \mathrm{km\ s}^{-1} \qquad T \gtrsim 300\ \mathrm{K}$$

Thus $\tau \lesssim 0.5.$ (optically thin)



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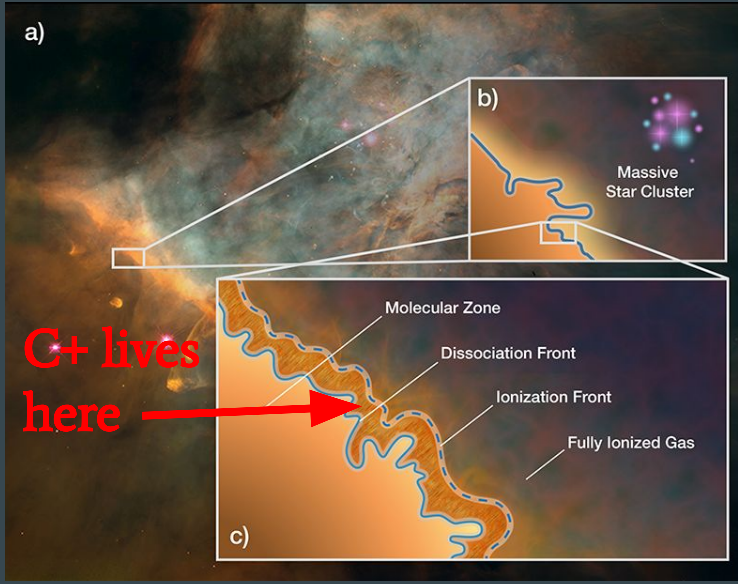
(I know this is handwavy please don't shoot the messenger)



Calculating C+ and H column densities

Assuming the emission comes from warm ($T >> 92$ K), dense ($n >> n_{crit}$) gas:

$$\frac{n_2}{n_{tot}} = \left[1 + \frac{g_1}{g_2} \exp(92 \text{ K}/T) \left(1 + \frac{n_{crit}}{n}\right)\right]^{-1} \simeq \left(1 + \frac{g_1}{g_2}\right)^{-1}$$

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Assuming the emission comes from warm ($T >> 92$ K), dense ($n >> n_{crit}$) gas:

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J = 1/2 state: g_1 = 2J+1 = 2

J = 3/2 state: g_2 = 4

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(These are lower bounds because the gas is not perfectly optically thin)

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Standard value for C+ abundance: $[\mathrm{C}^+]/[\mathrm{H}] \simeq 3 \times 10^{-4}$

$$N_{C+} \gtrsim 9 \times 10^{17}\ \mathrm{cm}^{-2}$$

$$N_H \gtrsim 3 \times 10^{21}\ \mathrm{cm}^{-2}$$

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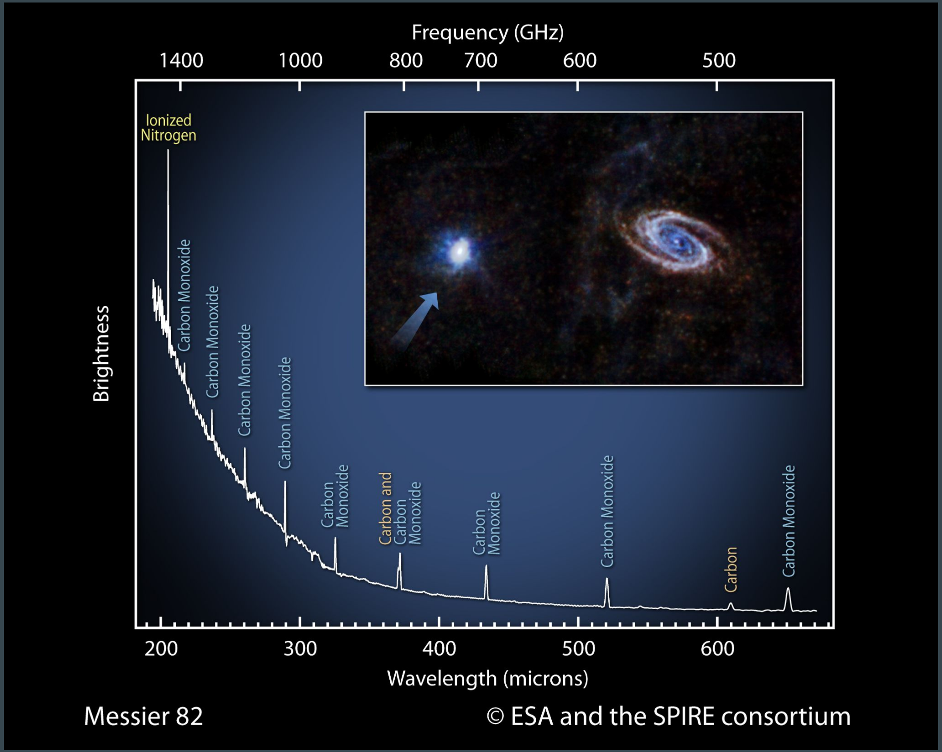
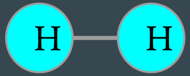
More complicated example: the CO rotational ladder

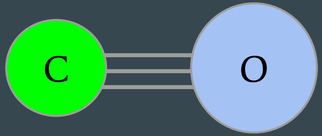


Molecular gas is mostly H_2, but it's hard to measure direct emission from it

$$L = h\nu A_{21} (\chi N_H) \frac{n_2}{n_{tot}}$$



No electric dipole moment
→ no dipole transitions
→ small A coefficient



Larger A coefficient,
Most common molecule after H_2

$$H_{rot} = \frac{\hat{L}^2}{2I} \qquad E_\ell = \frac{\hbar^2 \ell(\ell+1)}{2I}$$

$$\boxed{E_\ell - E_{\ell-1} = \frac{\hbar^2 \ell}{I}}$$

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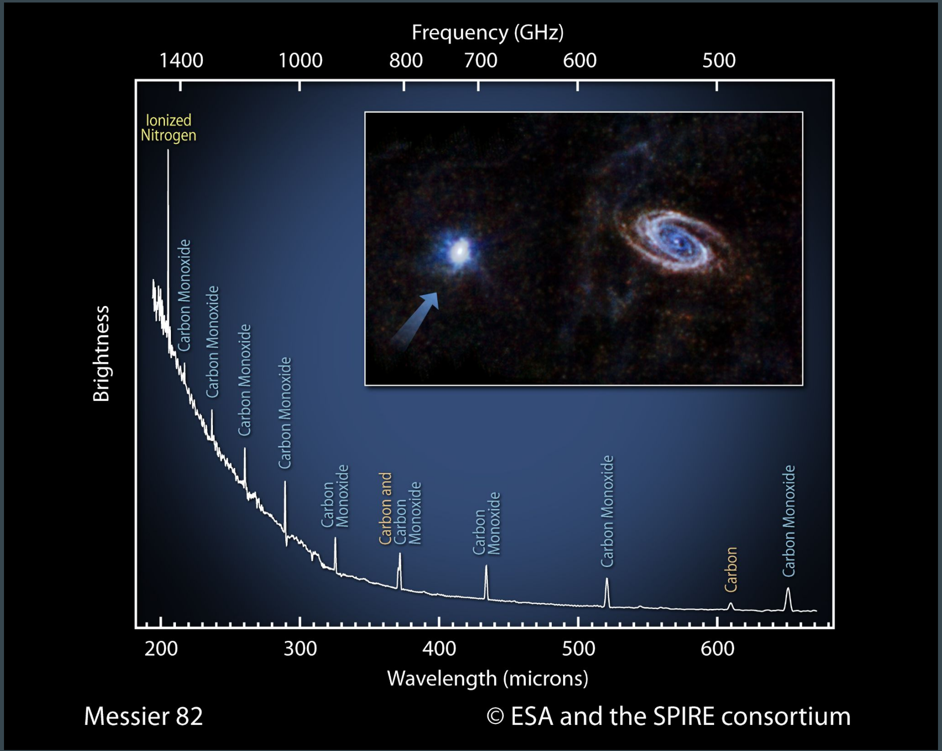
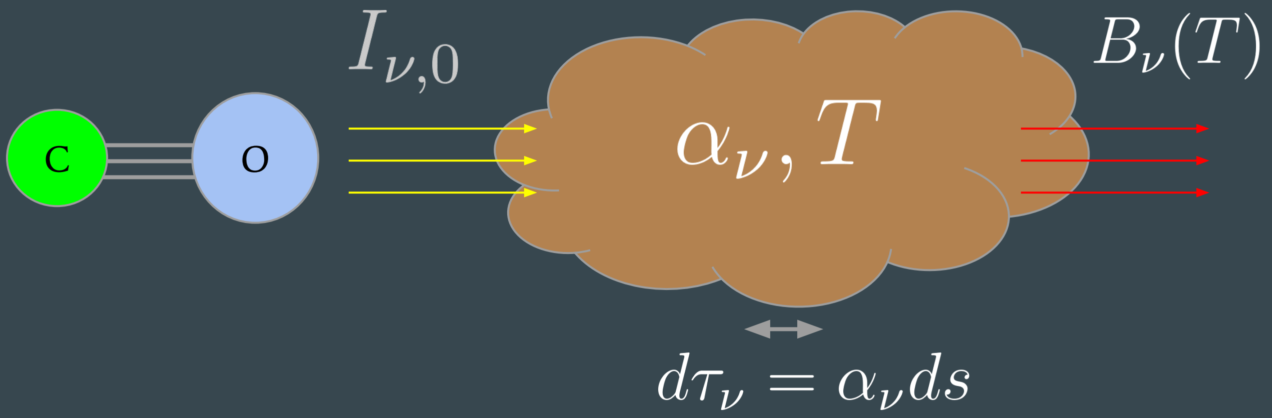


Because there is a lot of CO, it usually ends up being optically thick (the J = 1 → 0 transition in particular)

This factor is large

$$\alpha_\nu = \frac{c^2}{8\pi\nu^2} g_2 A_{21} \overbrace{\left(\frac{n_1}{g_1} - \frac{n_2}{g_2}\right)} \phi(\nu)$$

Optically thick emission



$$\frac{dI_\nu}{d\tau_\nu} = -I_\nu + B_\nu(T)$$

High optical depth “thermalizes” the line emission to the blackbody value

Example: CO in a molecular cloud

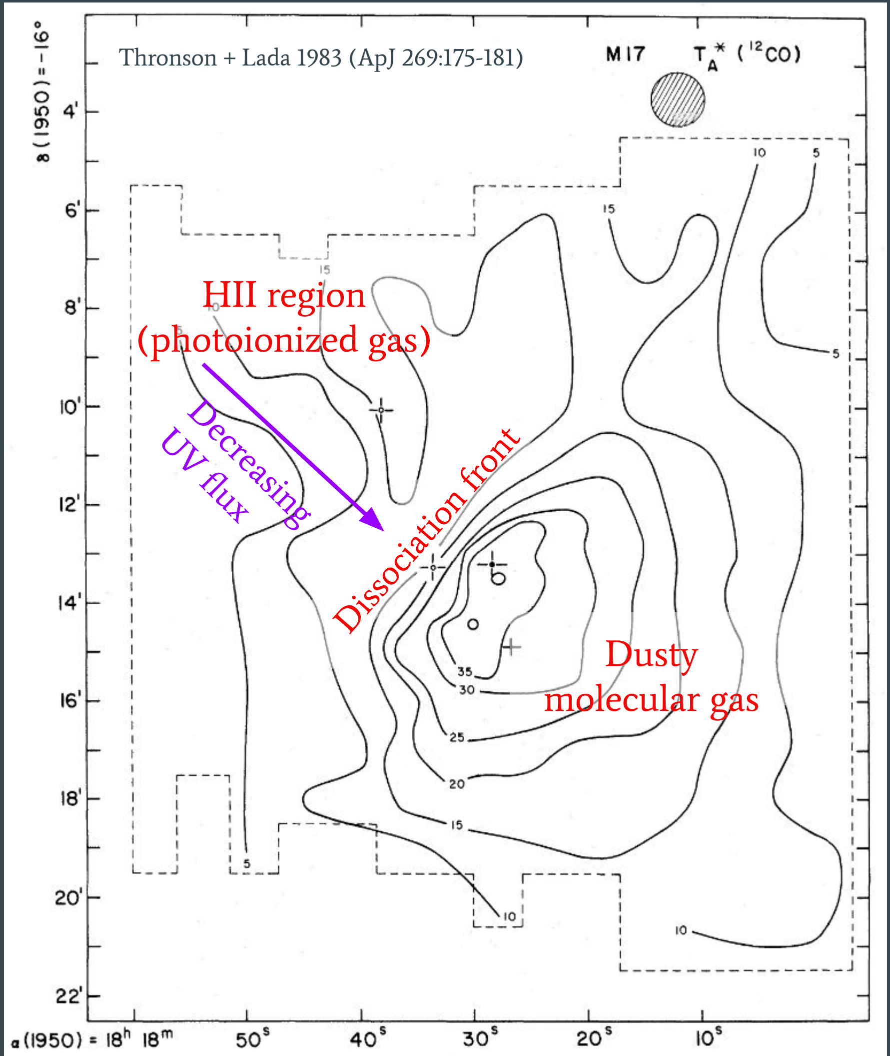
M17 SW molecular cloud imaged in ^{12}CO J 1→0

One of the most active sites of star formation known in our galaxy – viewed edge-on

As you move further from the stars, the UV flux decreases because of dust absorption

→ there is more CO farther into the cloud

The brightest emission comes from near the dissociation front because the hottest CO is located here



Sources

- Weisheit + Lane, Phys Rev A Vol 4, Issue 1 (1971) → Deriving the Schrodinger equation for two-atom inelastic scattering
- Griffiths QM chapter 10 → Calculating the scattering cross sections
- Launay + Roueff 1977, Fine structure excitation of ground-state C+ ions by hydrogen atoms → Thermal scattering cross section