Radiative Transfer,
Spectroscopy & Collisions - I

Jacques Le Bourlot
Observatoire de Paris & Université Paris-Cité

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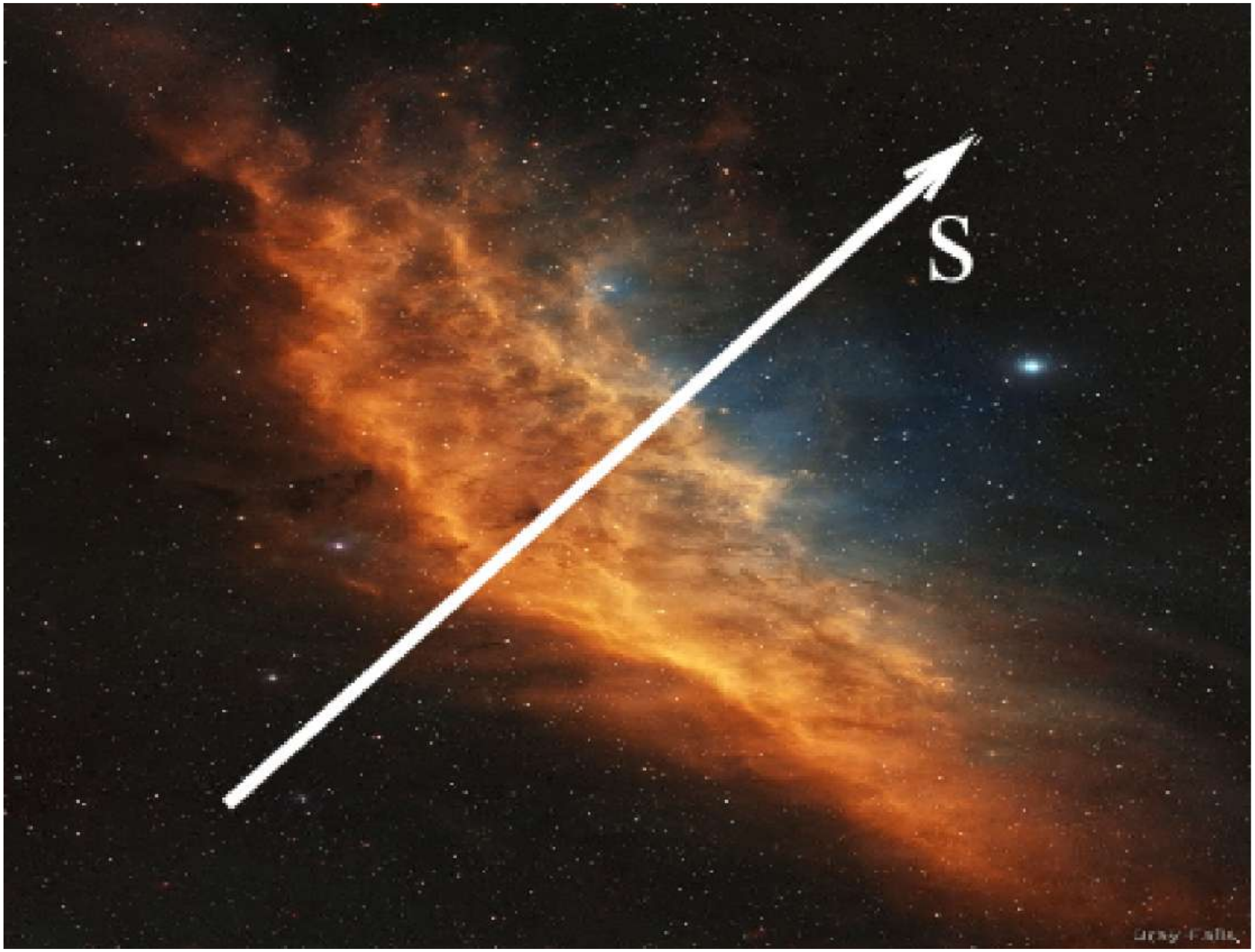
Funded by the European Union

What?



California Nebulae © (Astrofalls)

Plan

- Radiative transfer I:
  - Definitions & Problems
  - Matter properties

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- Spectroscopy:
  - Atomic structure and transitions.
  - Molecular structure.
  - Example: C lines in Orion proplyds.

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- Radiative transfer II:
  - Interstellar extinction
  - Non LTE situation
  - Some codes

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- Radiative transfer II:
  - Interstellar extinction
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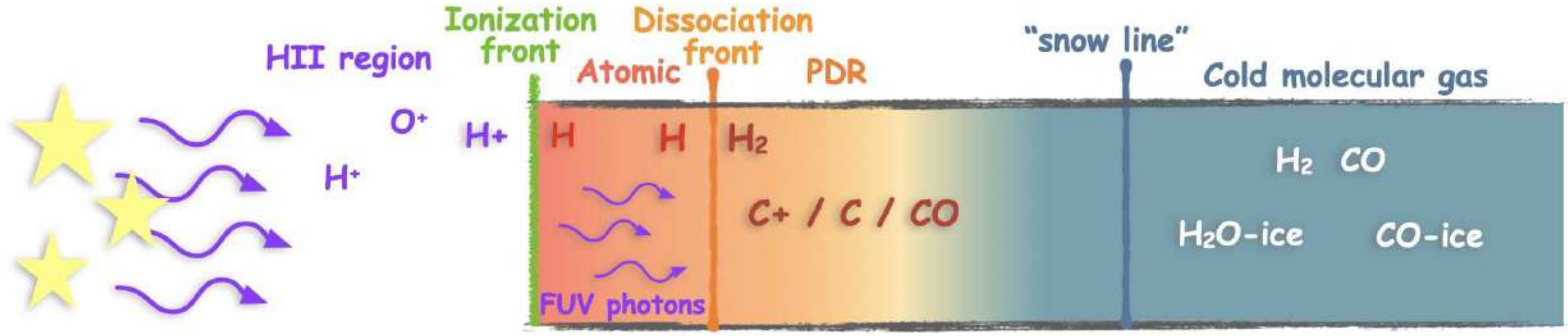
  - Some codes
- Collisions:
  - PES.
  - Collision computations.
  - Example: H_3^+ excitation in diffuse clouds.

PDR

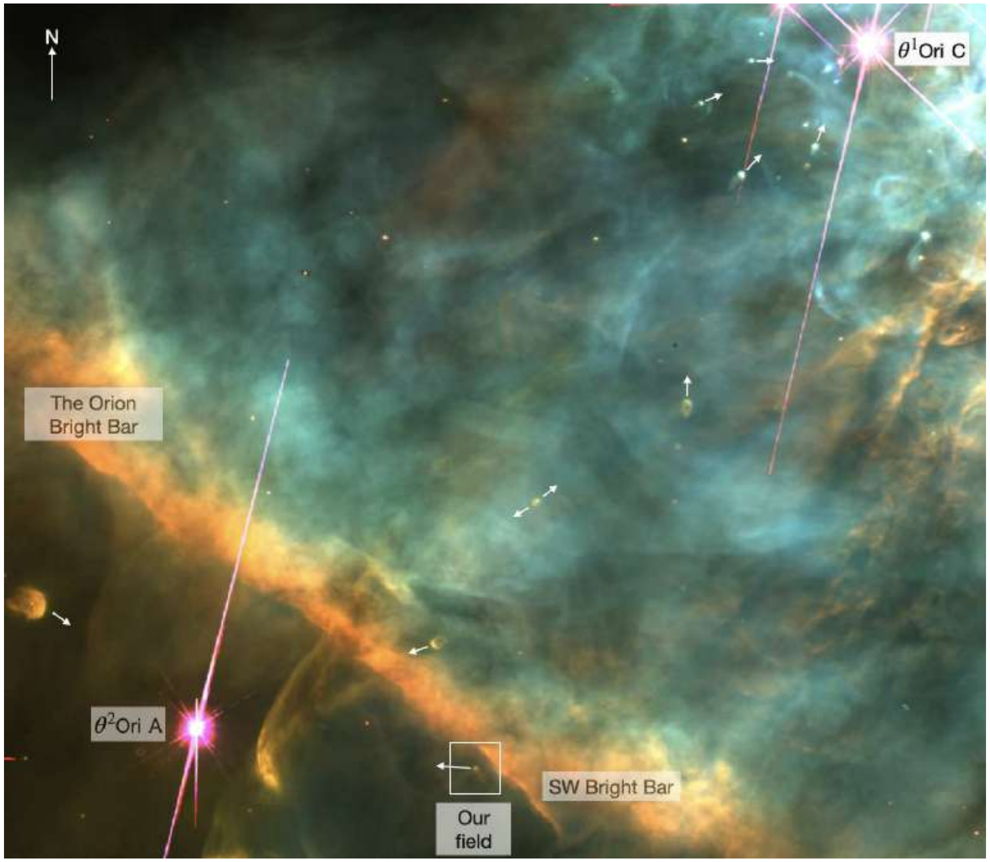


- **Meudon PDR code.**
  - 1D plane parallel steady-state.
  - Sophisticated micro-physics

New version 1.7 available (soon).

PDR

- Observations: Orion (Bar and d203-506). HST + JWST + ALMA + ...



Haworth et al. (2023) $0.1\,\mathrm{pc} \simeq 1\,\mathrm{arc\,mn}$

PDR

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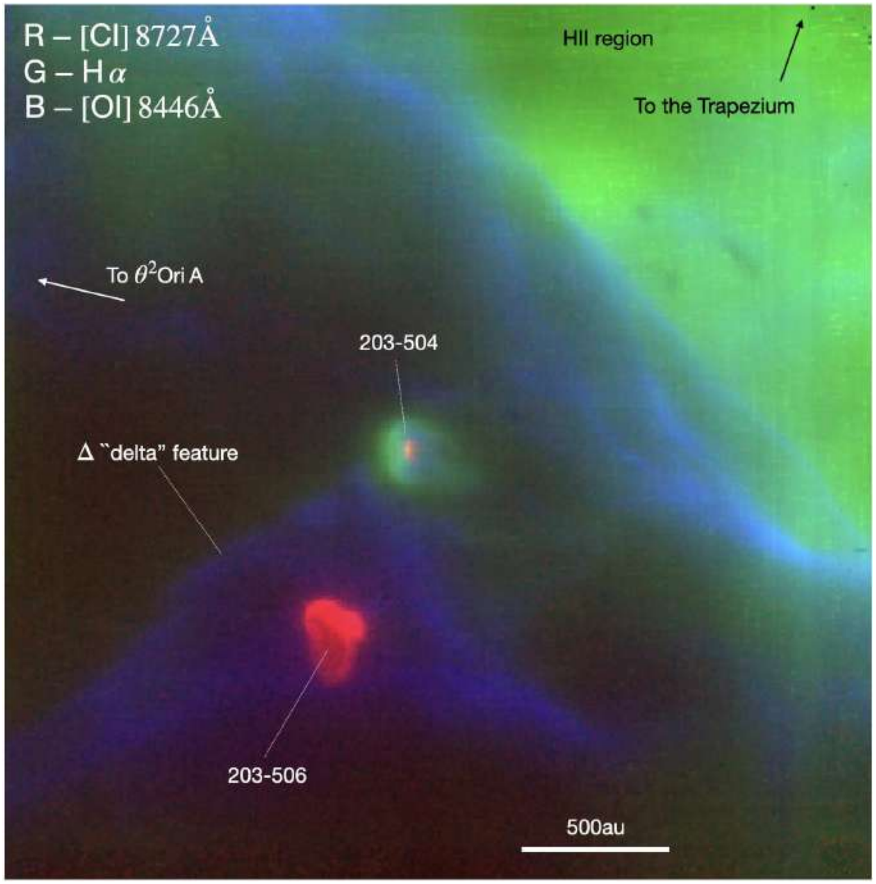
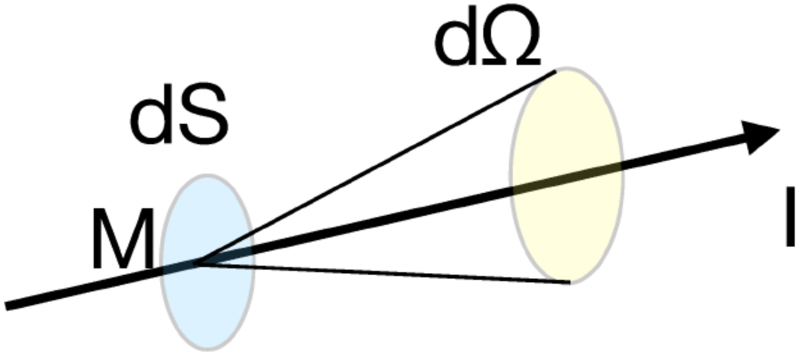


Haworth et al. (2023) $500\text{au} \simeq 1.2\,\text{arc sec}$

Specific Intensity (aka Spectral Radiance)



I: Energy transported by the radiation along a “ray”.

$$I_\nu : \mathrm{J\,s^{-1}\,m^{-2}\,ster^{-1}\,Hz^{-1}}$$

$$I_\lambda : \mathrm{J\,s^{-1}\,m^{-2}\,ster^{-1}\,m^{-1}}$$

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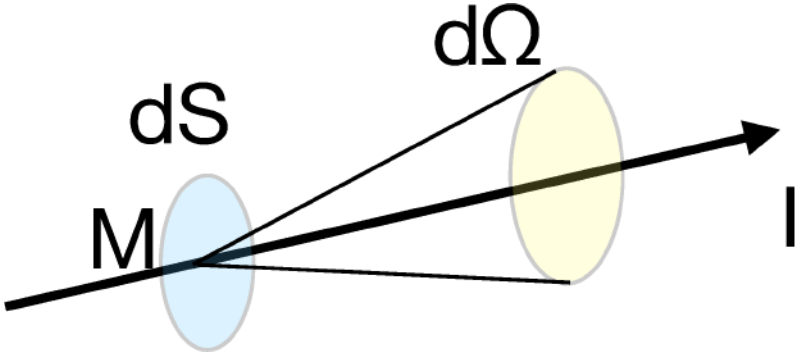

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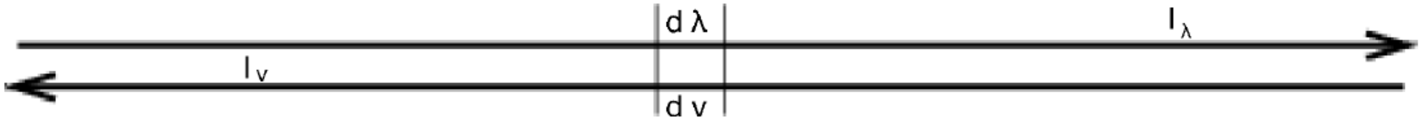
Conversion: $I_\lambda \, d\lambda = I_\nu \, d\nu \;\Rightarrow\; I_\lambda = \dfrac{c}{\lambda^2} I_\nu = \dfrac{\nu^2}{c} I_\nu$



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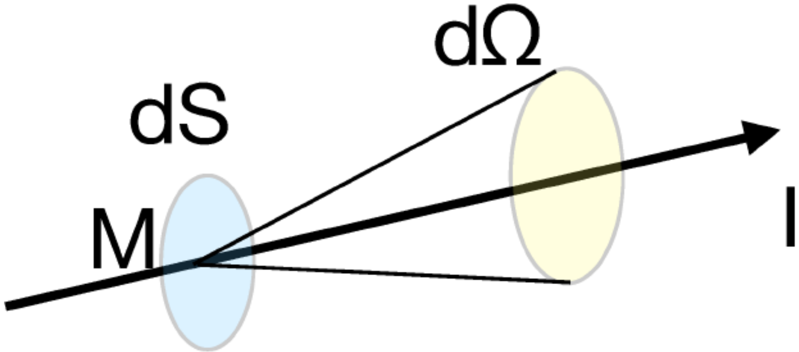

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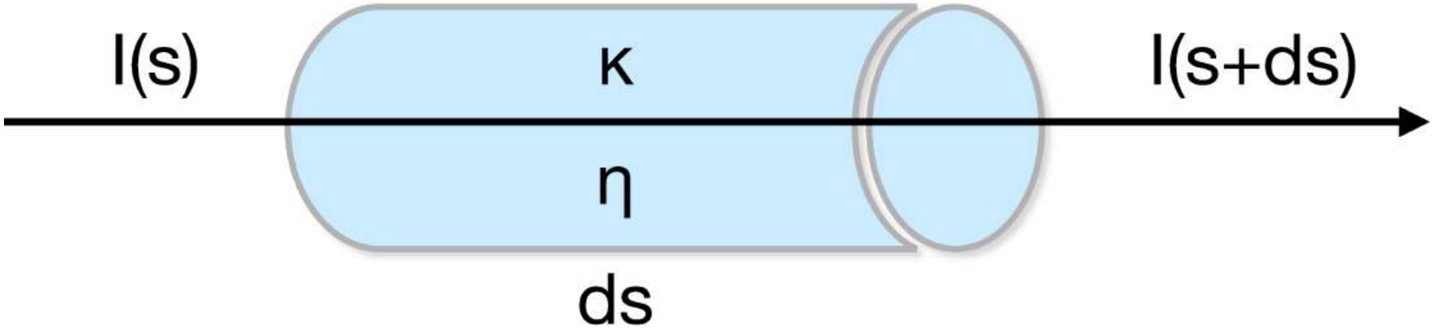
$$I_\lambda : \mathrm{J\,s^{-1}\,m^{-2}\,ster^{-1}\,m^{-1}}$$

$$J_\nu = \frac{1}{4\pi}\int_{4\pi} I_\nu\left(\Omega\right)\,d\Omega\,; \quad u_\nu = \frac{4\pi}{c}\,J_\nu\,\left(\mathrm{J\,m^{-3}\,Hz^{-1}}\right)$$

$$F_\nu = \int_{2\pi} I_\nu\left(\Omega\right)\,\cos\theta\,d\Omega\,; \quad F_\nu = \pi\,I_\nu\,\left(I_\nu = Cte\right)$$

Transfer



"OUT" = "IN" + "injected" − "removed":

$$\frac{dI}{ds} = -\kappa\, I + \eta$$

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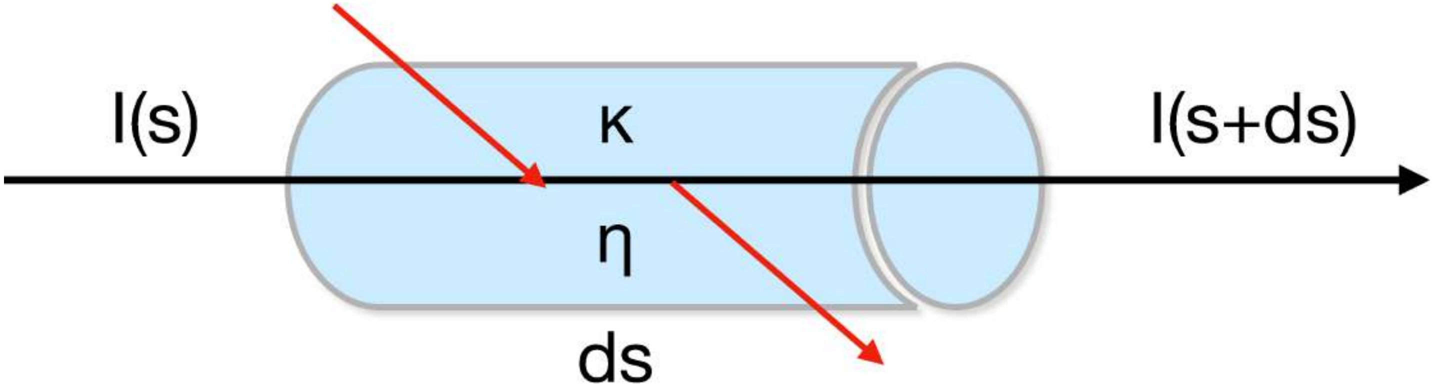

"OUT" = "IN" + "injected" − "removed":

$$\frac{dI}{ds} = -\kappa\, I + \eta$$

With scattering:

$$\frac{dI_\Omega}{ds} = -\left(\kappa + \sigma\right)\, I_\Omega + \eta + \sigma \int_{4\pi} p\left(\Omega, \Omega'\right)\, I_{\Omega'}\, d\Omega'$$

Space (reality vs. models)

Cygnus © APOD - J.-P. Metsavainio

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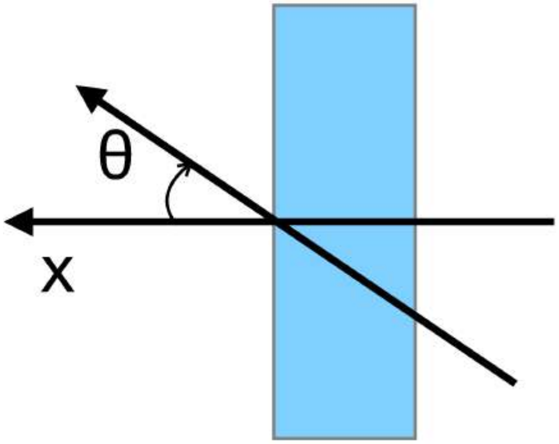

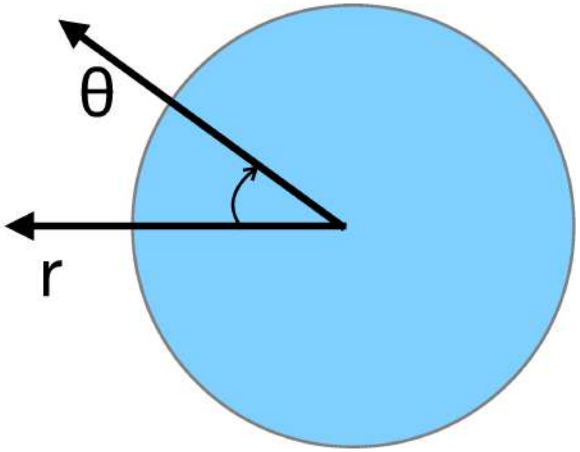

Models

- Building a model:

World

Models

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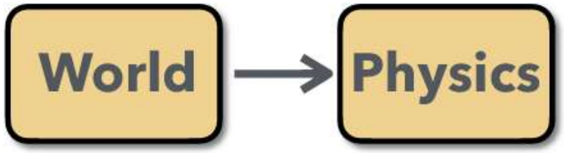

Models

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World → **Physics** → **Maths**

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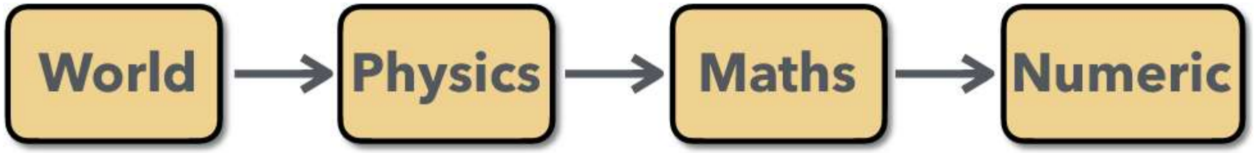

World → Physics → Maths → Numeric

Models

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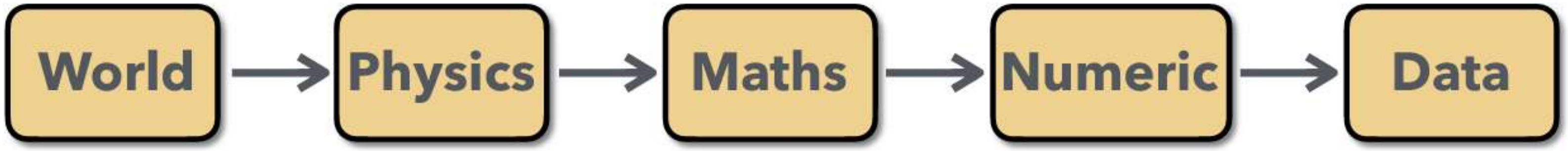

World → Physics → Maths → Numeric → Data

Models

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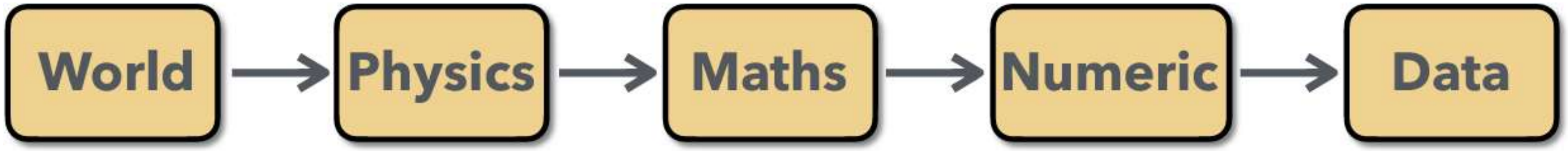

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- Start from the real problem.

Models

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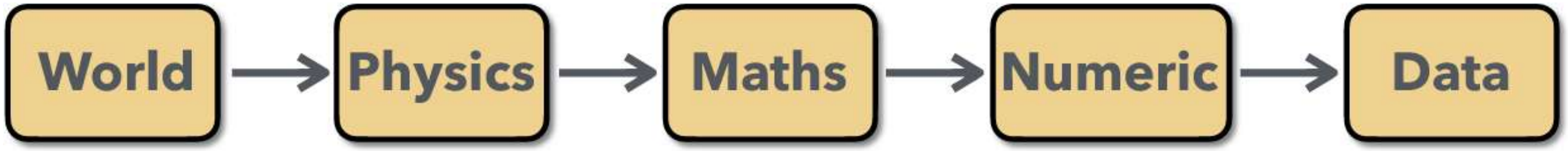

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- Start from the real problem.
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Models

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World → **Physics** → **Maths** → **Numeric** → **Data**

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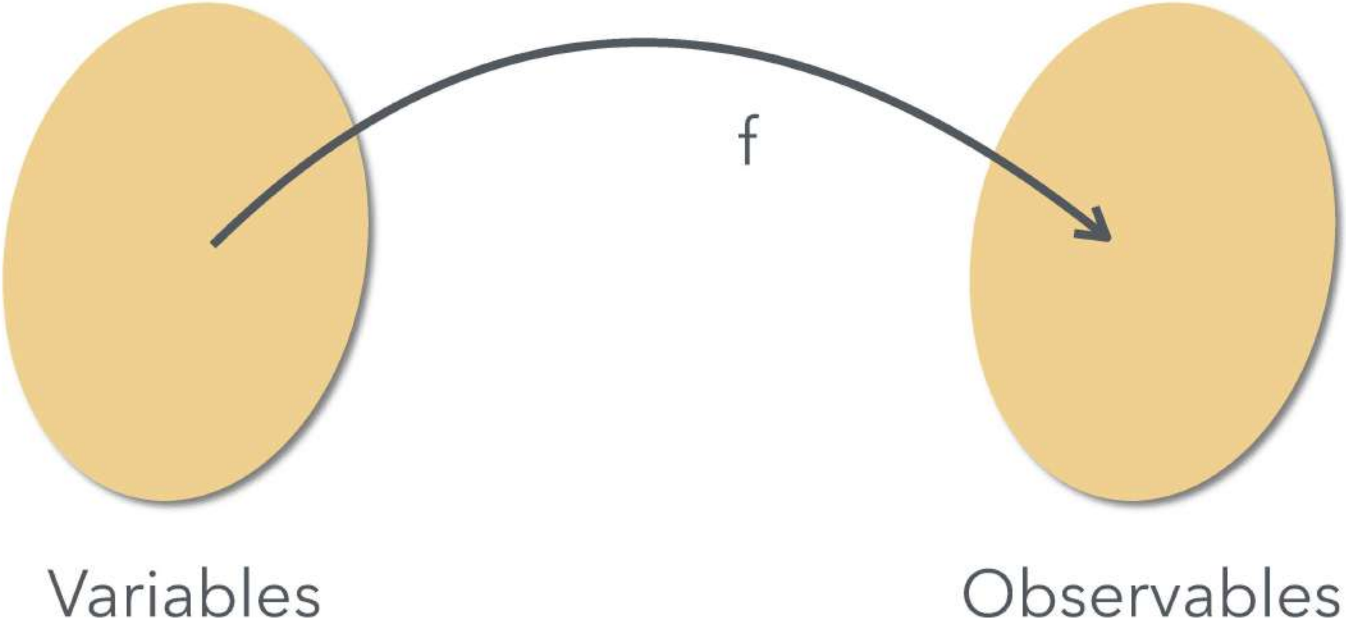
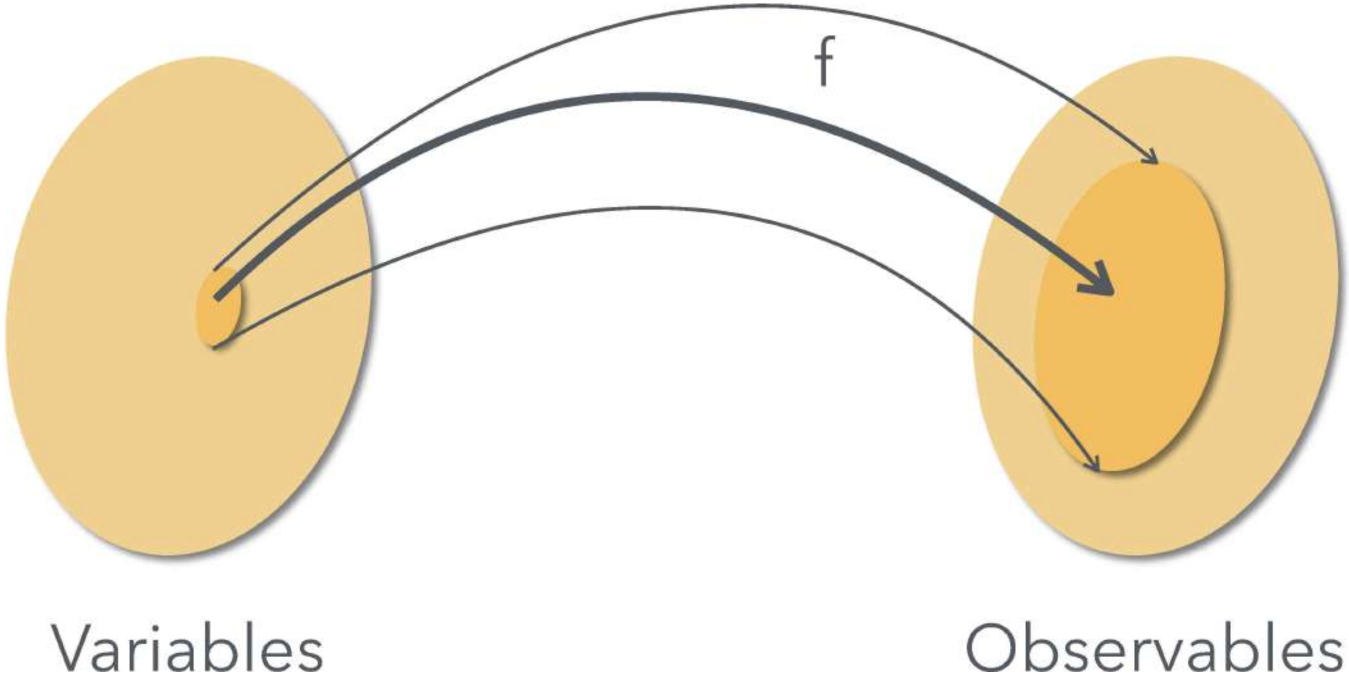
- Consequence: There are many radiative transfer theories.

Inverse problem



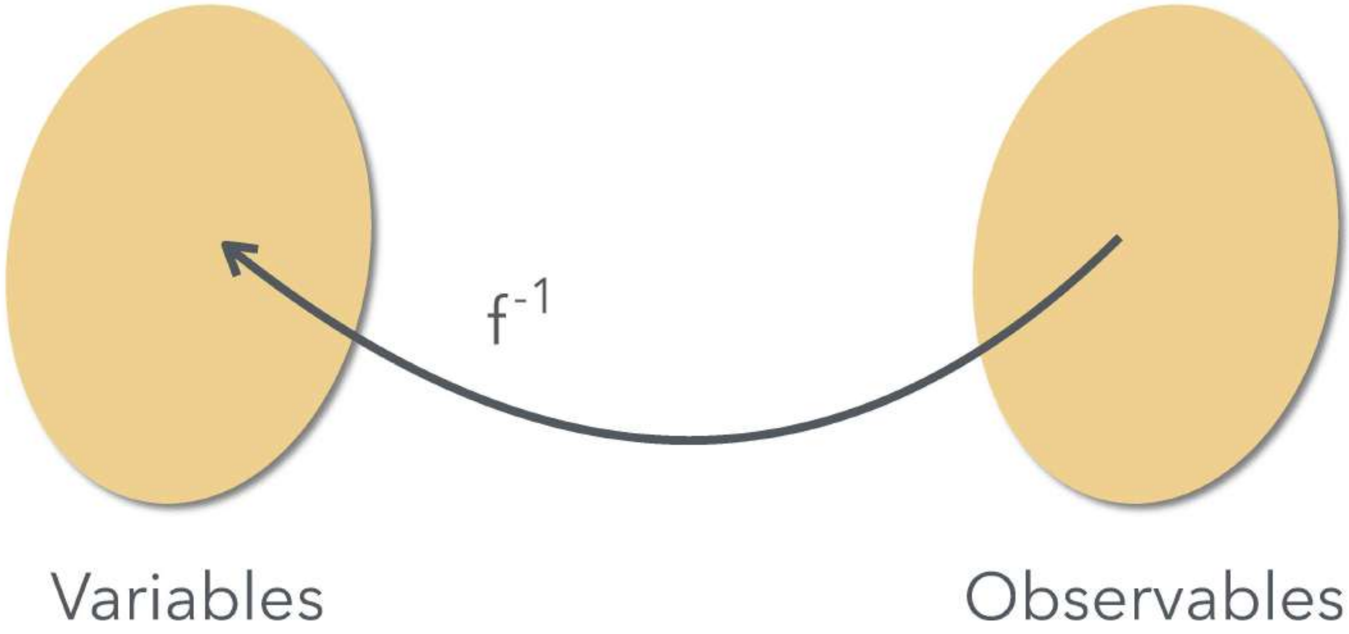
Model: 1 to 1 application (most of the time).

Inverse problem



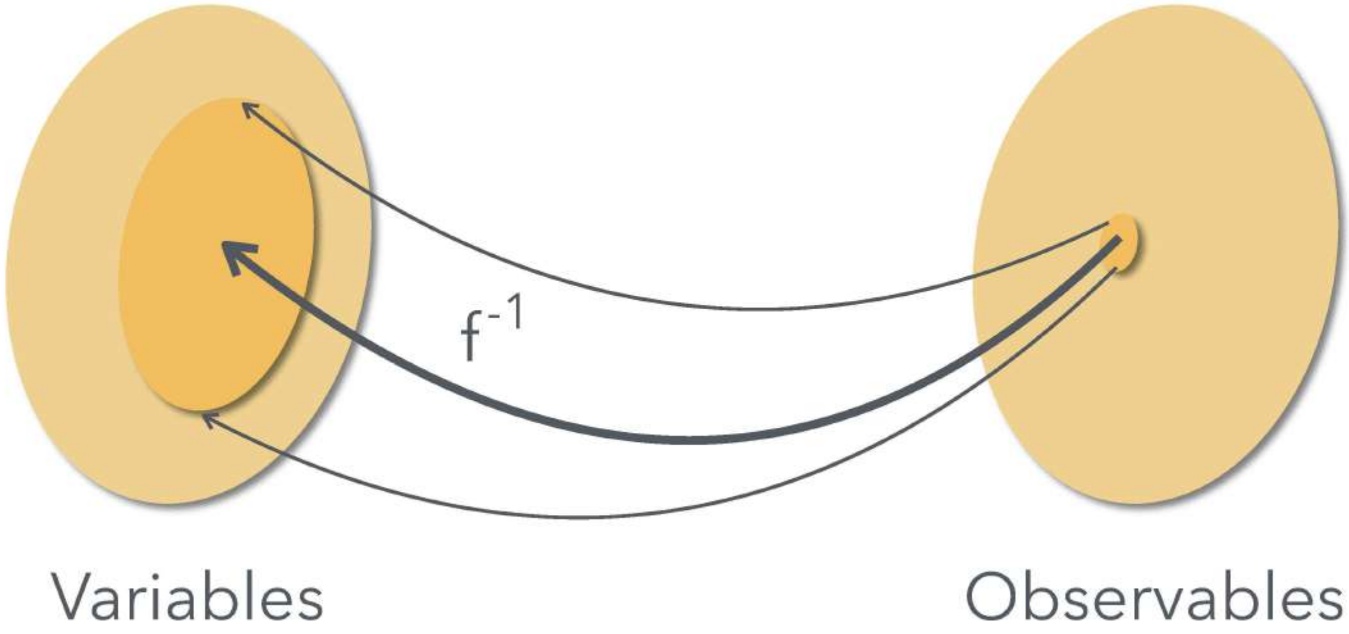
Explore sensitivity analysis!

Inverse problem



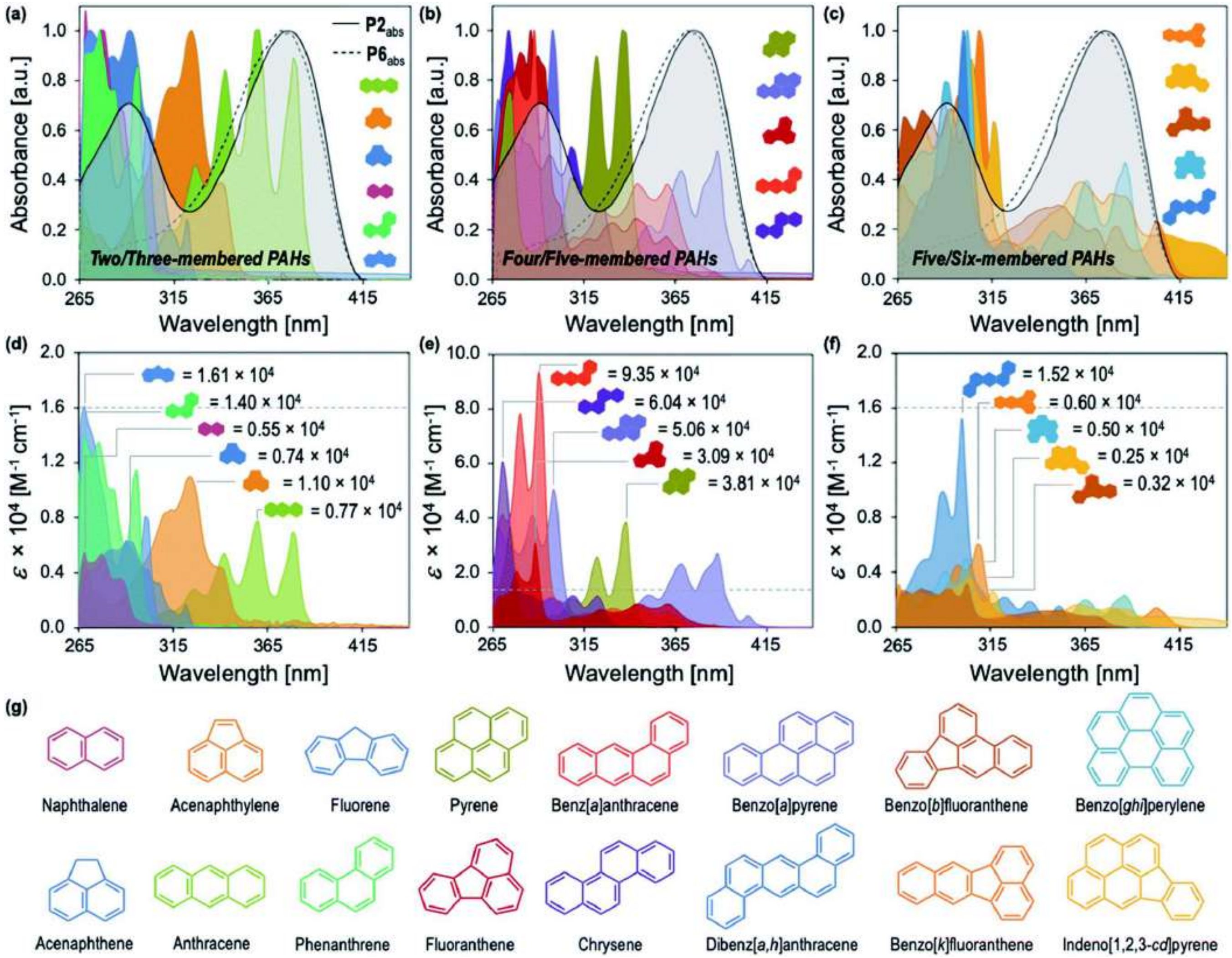
What you really need.

Inverse problem



What you get.

Different problems



© Tropp et al. (2019)

Divide & conquer

- Choose a geometry
  - 3D $\Rightarrow I\left(x, y, z, \theta, \phi\right)$: Use Monte-Carlo (see e.g. LIME (Brinch & Hogerheijde))
  - 1D (maybe 2+1D) $\Rightarrow$ Check the physics

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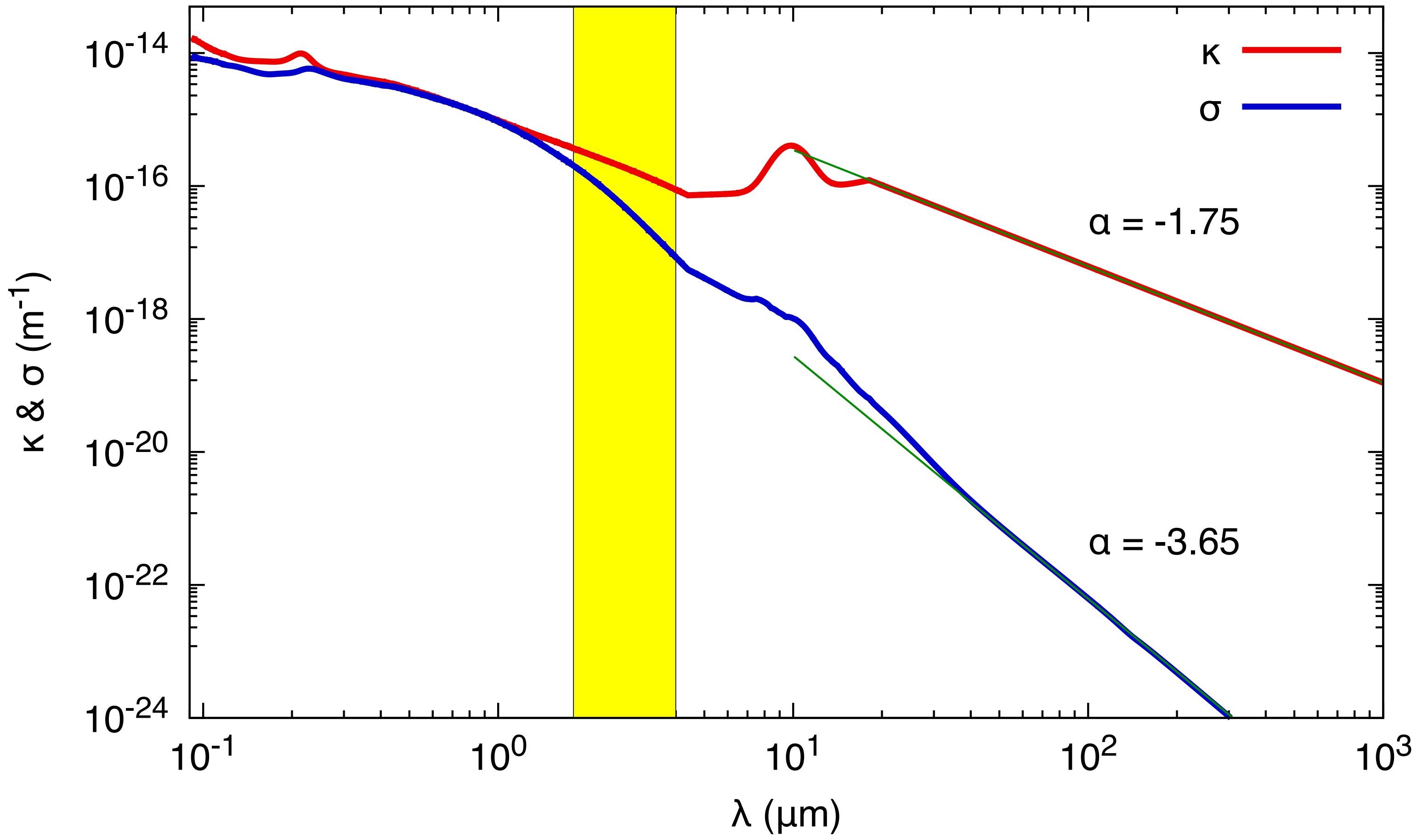
- Is scattering significant?
  - Yes: all directions coupled. No: "follow that ray".

Dust Absorption and Scattering



"Somewhere" around $2\,\mu m$

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- Is line transfer significant?
  - Yes: detailed balance is required.

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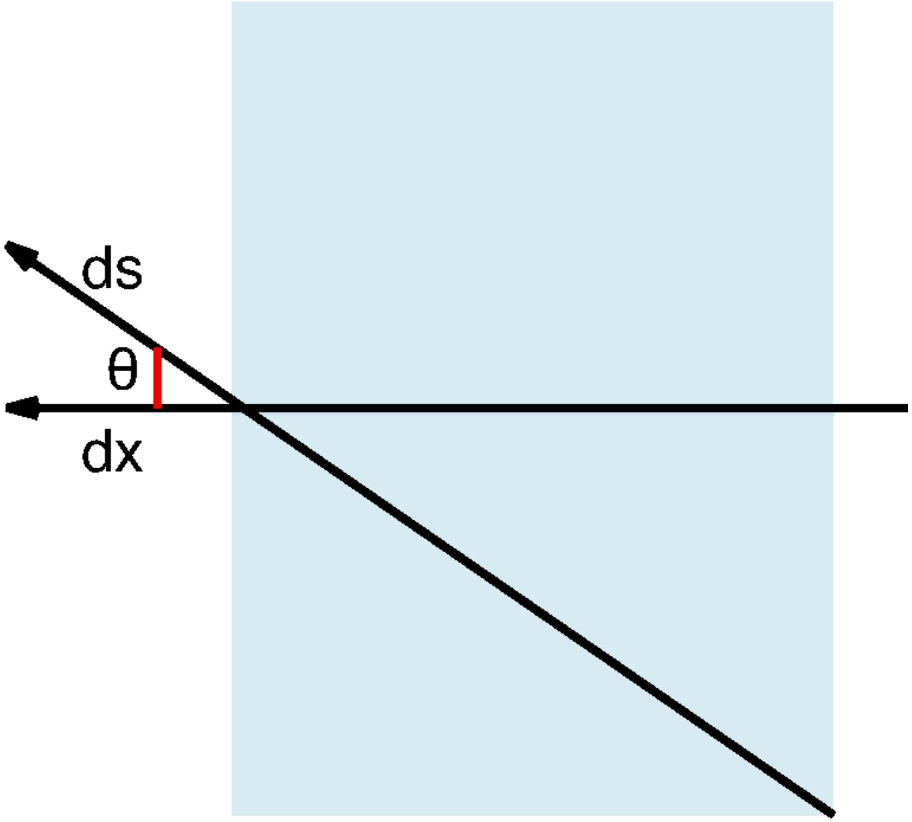
	No scattering	Scattering
No lines	**Easy**	**Doable**
Lines	**Hard**	**Really tough**

No scattering - No lines

1D transfer equation:

$$\frac{dI\left(s,\theta\right)}{ds} = -\kappa\left(x\right)\, I\left(s,\theta\right) + \eta\left(x\right)$$



$$\mu = \cos\theta$$

$$ds = \frac{dx}{\mu}$$

$$d\tau = \kappa\, dx$$

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1D transfer equation:

$$\frac{dI\left(s,\theta\right)}{ds} = -\kappa\left(x\right)\, I\left(s,\theta\right) + \eta\left(x\right)$$

Change of variables:

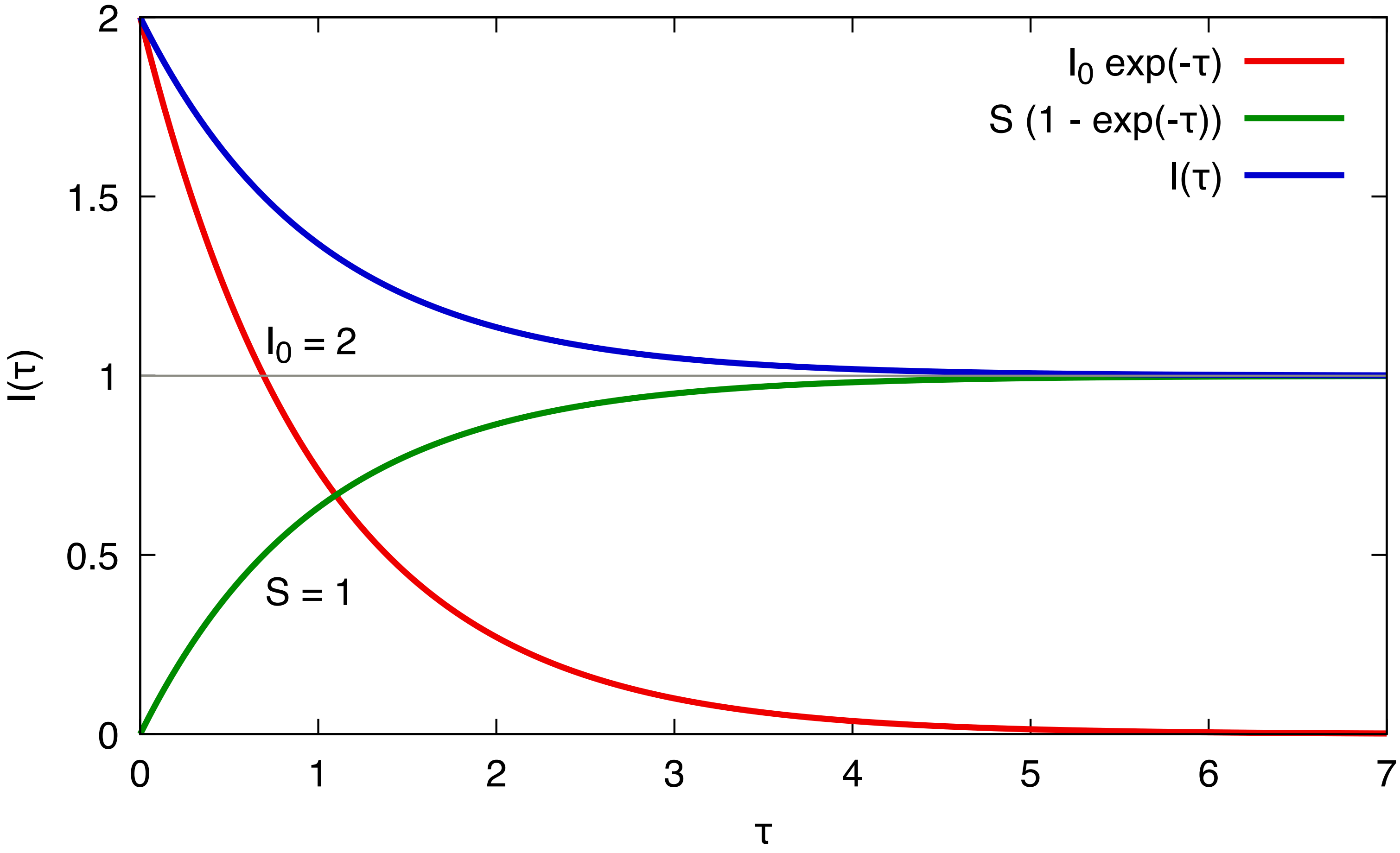
$$\mu = \cos\theta\,; \quad ds = \frac{dx}{\mu}\,; \quad d\tau = \kappa\, dx$$

$$\mu\,\frac{dI}{d\tau} = -I + \frac{\eta}{\kappa} = -I + S$$

Constant properties ($S = Cte$):

$$I\left(\tau,\mu\right) = I_0\left(\mu\right)\,\exp\left(-\frac{\tau}{\mu}\right) + S\,\left(1 - \exp\left(-\frac{\tau}{\mu}\right)\right)$$

No scattering - No lines



$$I_0 = 2\,; \quad S = 1$$

Formal solution to the transfer equation

If κ and η depend on position:

$$\tau\left(s\right) = \int_0^s \kappa\left(t\right)\, dt$$

$$I\left(\tau\right) = I_0 \exp\left(-\tau\right) + \int_0^\tau S\left(t\right) \exp\left(-\left(\tau - t\right)\right)\, dt$$

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Check:

$$\begin{aligned}\frac{I\left(\tau\right)}{d\tau}&=-I_{0}\,\exp\left(-\tau\right)+S\left(\tau\right)\,\exp\left(-\left(\tau-\tau\right)\right)\\&\quad-\int_{0}^{\tau}S\left(t\right)\,\exp\left(-\left(\tau-t\right)\right)\,dt\end{aligned}$$

$$\frac{I\left(\tau\right)}{d\tau}=-I\left(\tau\right)+S\left(\tau\right)$$

Formal solution if κ and η are known (or given...).

Scattering

What if ($\mu = \cos\theta$, $d\tau = (\kappa + \sigma)\ ds$):

$$\mu \frac{dI(\tau,\mu)}{d\tau} = -I(\tau,\mu) + \frac{\omega}{2}\int_{-1}^{+1} p\left(\mu,\mu'\right)\ I\left(\tau,\mu'\right)\ d\mu' + S(\tau)$$

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In 1D: use Legendre expansion
(see Roberge (1983) for an introduction).

$$I(\tau,\mu) = \sum_{l=0}^{\infty} (2l+1)\ f_l(\tau)\ P_l(\mu)$$

$$p(\mu,\mu') = \sum_{l=0}^{\infty} (2l+1)\,\sigma_l\,P_l(\mu)\ P_l(\mu')$$

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A bit of math magic leads to ($\forall l$):

$$l\ f'_{l-1} + (l+1)\ f'_{l+1} = (2l+1)\ (1-\omega\,\sigma_l)\ f_l + s\,\delta_{l0}$$

Scattering

Truncate at L finite $\Rightarrow$ set of linear equation with non-constant coefficients and boundary conditions at both edges:

$$\mathbf{A}\,\mathbf{f}'\left(\tau\right) = \mathbf{B}\,\mathbf{f}\left(\tau\right) + \mathbf{g}\left(\tau\right)$$

$\mathbf{A}$ and $\mathbf{B}$ diagonally dominant matrices.

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- Solved by diagonalization.
- Formal solution used for each f_l.
- Requires iterations.
- Very sensitive to numerical errors (precision).

$\Rightarrow$ Quite tricky, but doable.

May be extended to include lines.

General case strategy

Possible strategy:

1. Assume values of $\kappa(x)$ and $\eta(x)$ from educated guesses.
2. Compute $I(x)$ by the formal solution.
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4. Iterate...

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$\Rightarrow$ needs special methods (ALI: “Accelerated Lambda Iteration”).

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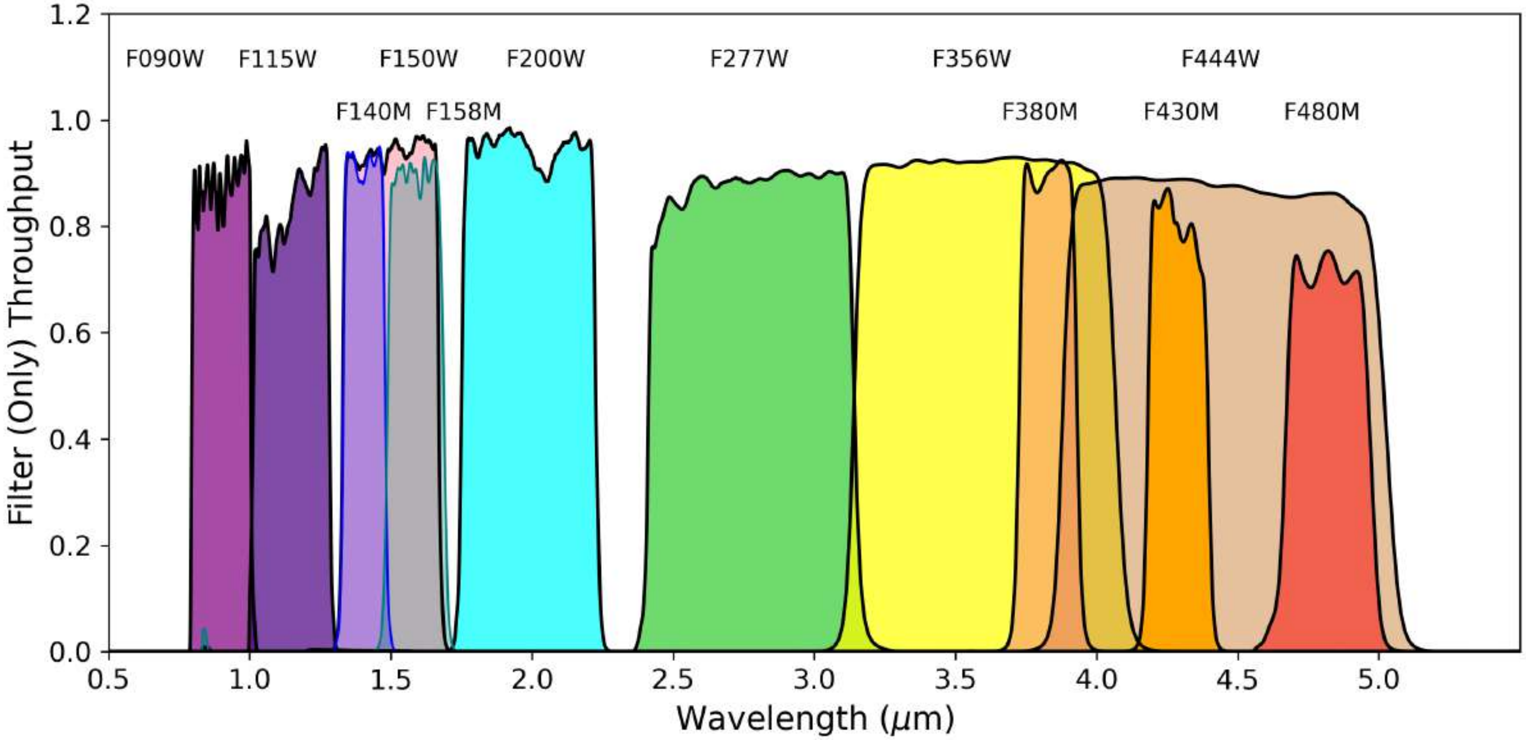
Requirement:

Finding κ and η.

Matter properties



Transmission curves for the NIRISS filters aboard the JWST.

Continuous processes

- Many possibilities:
  - Dust properties: absorption is constant, emission depends on temperature (radiative balance)
  - Free-free emission and absorption, electron scattering, bremsstrahlung, ...
  - Bound-free continuous absorption by species (Photo-destruction cross-sections.)
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    - ...
- Transfer usually converges rapidly.
- Requires access to many data bases for micro-physics processes. E.g.:
    - Dust: Bruce Draine's web site.
    - Photo-destruction: Ewine van Dishoeck web site.
    - Stellar models. E.g. CESAM2k20.
- Check detailed balance!

Lines

Absorption and emission coefficients depend on species level populations (n_u and n_l):

$$\kappa_{lu} = \frac{h\,c}{4\pi\,\lambda}\,\left(B_{lu}\,n_l - B_{ul}\,n_u\right)\,\phi_\lambda$$

$$\eta_{ul} = \frac{h\,c}{4\pi\,\lambda}\,A_{ul}\,n_u\,\phi_\lambda$$

- A_{ul}, B_{ul} and B_{lu}: Einstein coefficients.
- ϕ_λ: Line profile - Gaussian or Voigt (see later).
- n_u (resp. n_l): Population of “upper” (resp. “lower”) level of the transition.

Einstein coefficients

- A_{ul}: Probability of spontaneous transition, in s^{-1}.
  $\Rightarrow$ Find in relevant data bases (e.g. NIST)
- B_{ul} and B_{lu}: Induced transitions. Depend on the radiative field representation. For I_λ and specific intensity:

$$A_{ul} = \frac{2\,h\,c^2}{\lambda^5}\,B_{ul}\,; \quad g_u\,B_{ul} = g_l\,B_{lu}$$

- Conversion $\lambda \leftrightarrow \nu$ and/or $I_\lambda \leftrightarrow u_\lambda$ is a nightmare...

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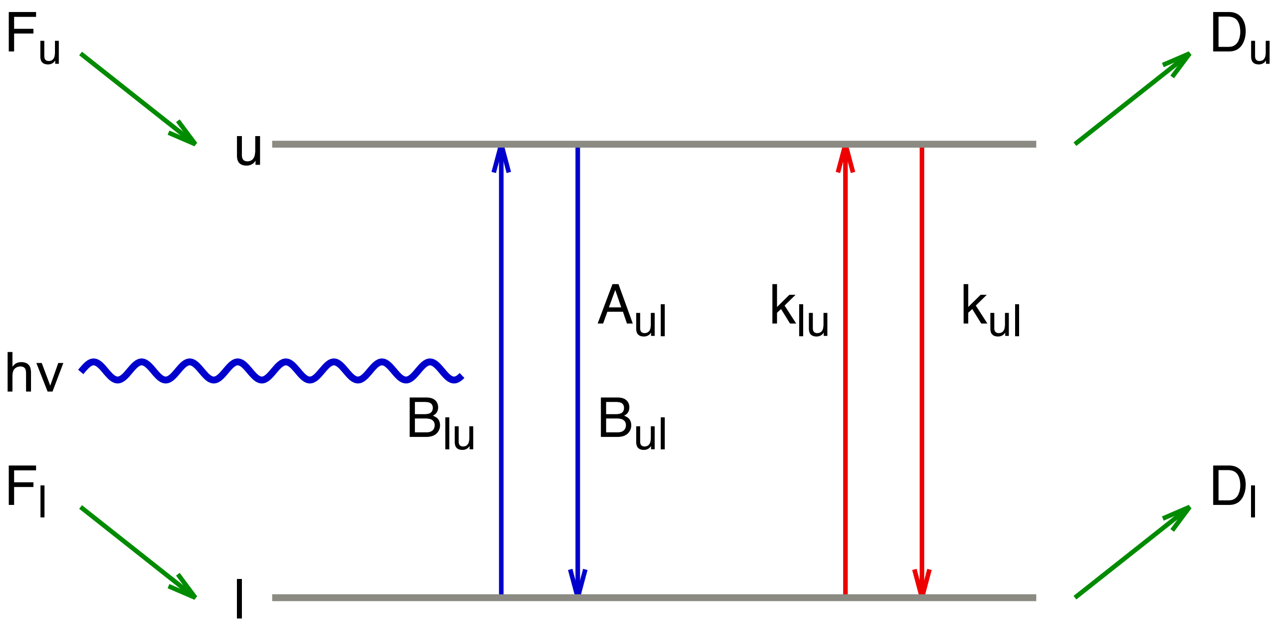
Compute populations

Detailed balance (2 levels)



- Detailed balance:

$$n_l \left(B_{lu}\,\bar{J}_{lu} + k_{lu}^{X}\,n_X + D_l\right) = n_u \left(A_{ul} + B_{ul}\,\bar{J}_{ul} + k_{ul}^{X}\,n_X\right) + F_l$$

$$n_u \left(A_{ul} + B_{ul}\,\bar{J}_{ul} + k_{ul}^{X}\,n_X + D_u\right) = n_l \left(B_{lu}\,\bar{J}_{lu} + k_{lu}^{X}\,n_X\right) + F_u$$

Comments

- Collisional rates linked by detailed balance:

$$g_l \, k_{lu} = g_u \, k_{ul} \, \exp\left(-\frac{E_{ul}}{k \, T}\right)$$

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  But $D_l \neq D_u$ and $F_l \neq F_u$ in general!
  - System is well behaved. $n_l + n_u = n_{tot}$ not needed.
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$$n_l \, k_{lu} \, n_X = n_u \, \left(A_{ul} + k_{ul} \, n_X\right)$$

$$\frac{n_u}{n_l} = \frac{1}{1 + \frac{A_{ul}}{k_{ul}^X \, n_X}} \, \frac{g_u}{g_l} \, \exp\left(-\frac{E_{ul}}{k \, T}\right)$$

Critical density

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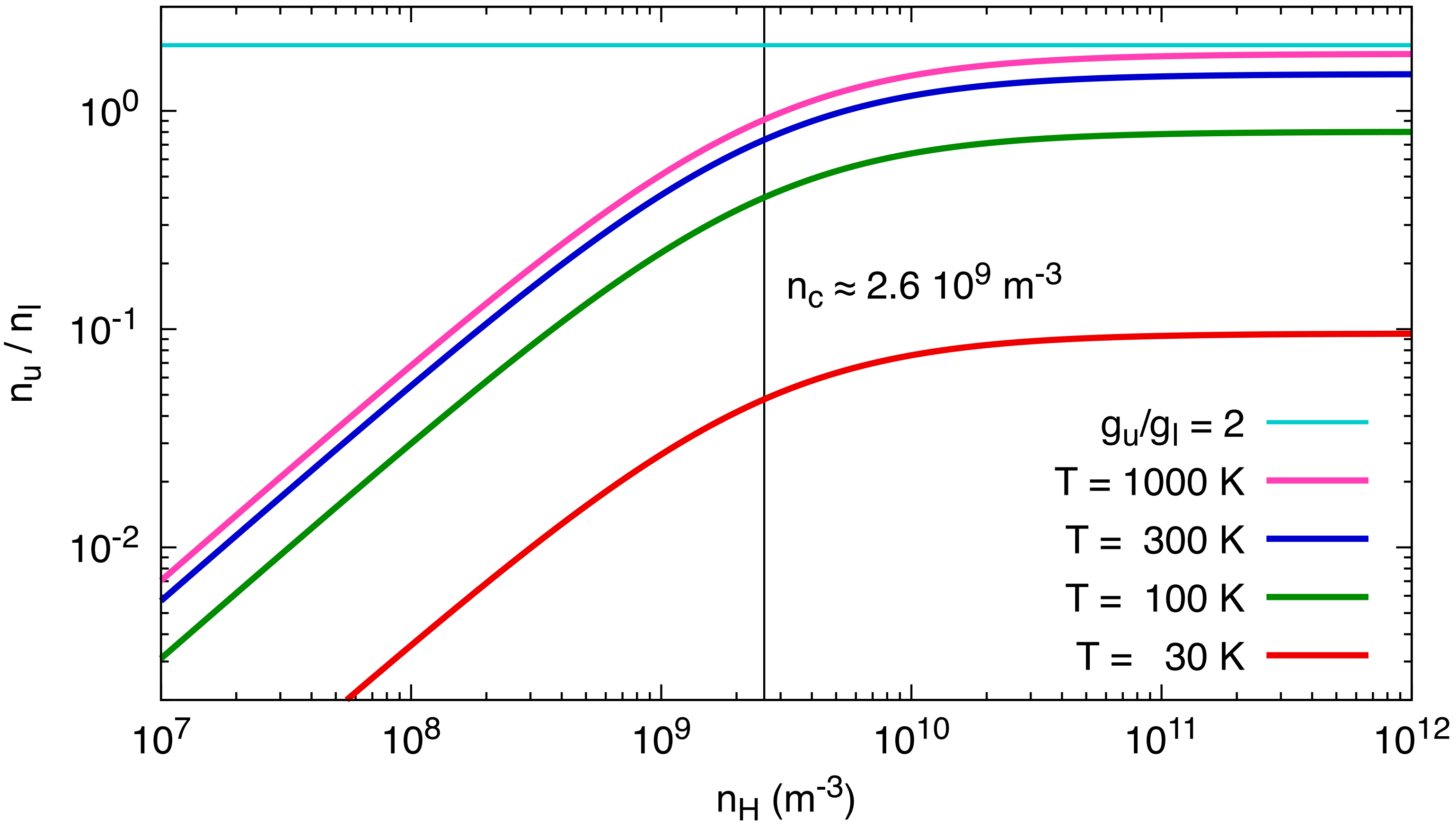
- Low density: Upper level is radiatively depopulated, with correction factor $1/\left(1 + \frac{A_{ul}}{k_{ul}\, n_X}\right)$.
- Critical density: n_c such that:

$$\frac{A_{ul}}{k_{ul}\, n_c} = 1\,; \quad n_c = \frac{A_{ul}}{k_{ul}}$$

- n_c depends on the line considered!

Critical density - C^+



Example: C^+ - $A_{ul} = 2.29\,10^{-6}\,\mathrm{s}^{-1}$, $\dfrac{E_{ul}}{k} = 91.25\,\mathrm{K}$,
$k_{ul} \simeq 8.9\,10^{-16}\,\mathrm{m}^3\,\mathrm{s}^{-1}$ with H (dominates e^-).

Excitation diagram

- Pure Boltzmann distribution:

$$n_j \propto g_j \exp\left(-\frac{E_j}{k\,T}\right) \; ; \quad \ln\left(\frac{n_j}{g_j}\right) = -\frac{1}{T}\,\frac{E_j}{k} + Cte$$

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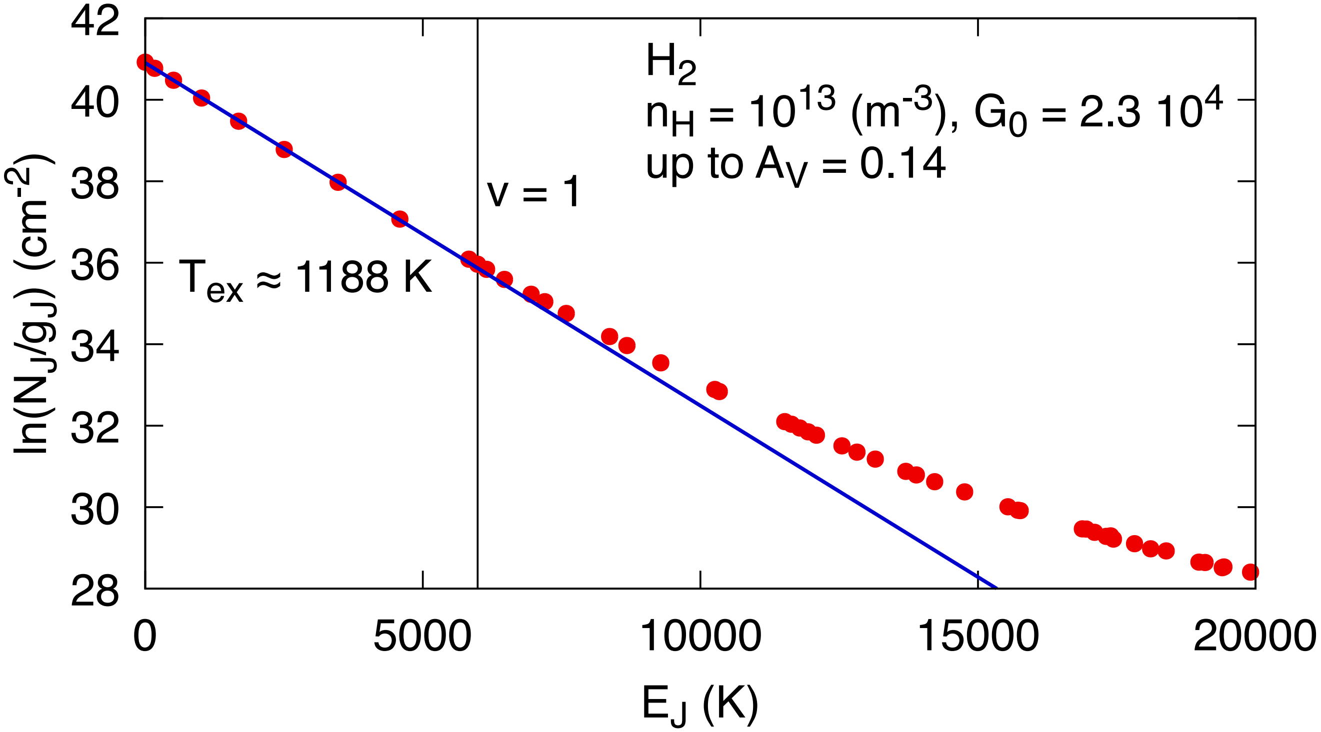
- Example: H_2 in a strong PDR:



Mean radiation field ($B_{ul}\,\bar{J}_{ul}$)

- $\bar{J}_{ul}$ is the local mean radiation field. That is:

$$\bar{J}_{ul} = \int_{-\infty}^{+\infty} \left(\frac{1}{4\pi} \int_{4\pi} I_\nu \left(\Omega\right) \, d\Omega \right) \phi_\nu \, d\nu$$

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- Broadening:
  - Thermal ⇒ Gaussian profile.
  - Turbulent ⇒ Gaussian profile.
  - Collisional ⇒ Lorentz profile.
  - Natural ⇒ Lorentz profile.
  - Combined ⇒ Convolution of Gaussian and Lorentz ⇒ Voigt profile.

Lorentz profile

- Natural profile:

$$\phi_L\left(\nu\right) = \frac{1}{\pi}\frac{\Gamma/4\pi}{\left(\nu-\nu_{ul}\right)^2+\left(\Gamma/4\pi\right)^2}$$

- Γ: “damping constant”: sum of all spontaneous transition probabilities (inverse radiative lifetime).
- Full width at half maximum (FWHM):

$$\gamma_L = \frac{\Gamma}{2\pi}$$

Gaussian profile

- Combine thermal and micro-turbulent velocity v_t
- Doppler width:

$$\Delta\nu_D\left(s\right) = \frac{\nu_{ul}}{c}\sqrt{\frac{2k\,T\left(s\right)}{\mu} + v_t^2\left(s\right)} = \frac{\nu_{ul}}{c}\,v_T\left(s\right)$$

- Profile:

$$\phi_D\left(\nu\right) = \frac{1}{\sqrt{\pi}\,\Delta\nu_D}\exp\left(-\left(\frac{\nu-\nu_{ul}}{\Delta\nu_D}\right)^2\right)$$

$$= \frac{1}{\sqrt{\pi}\,\nu_{ul}}\,\frac{c}{v_T\left(s\right)}\exp\left(-\left(\frac{\nu-\nu_{ul}}{\nu_{ul}}\,\frac{c}{v_T\left(s\right)}\right)^2\right)$$

- Full width at half maximum (FWHM):

$$\gamma_D = 2\sqrt{\log 2}\,\Delta\nu_D$$

Voigt profile

- Convolution of Gaussian and Lorentz:

$$\phi_V\left(\nu\right)=\int_{-\infty}^{+\infty}\phi_L\left(\nu_{ul}+\nu-\nu'\right)\,\phi_D\left(\nu'\right)\,d\nu'$$

Voigt profile

- Convolution of Gaussian and Lorentz:

$$\phi_V\left(\nu\right) = \int_{-\infty}^{+\infty} \phi_L\left(\nu_{ul} + \nu - \nu'\right)\, \phi_D\left(\nu'\right)\, d\nu'$$

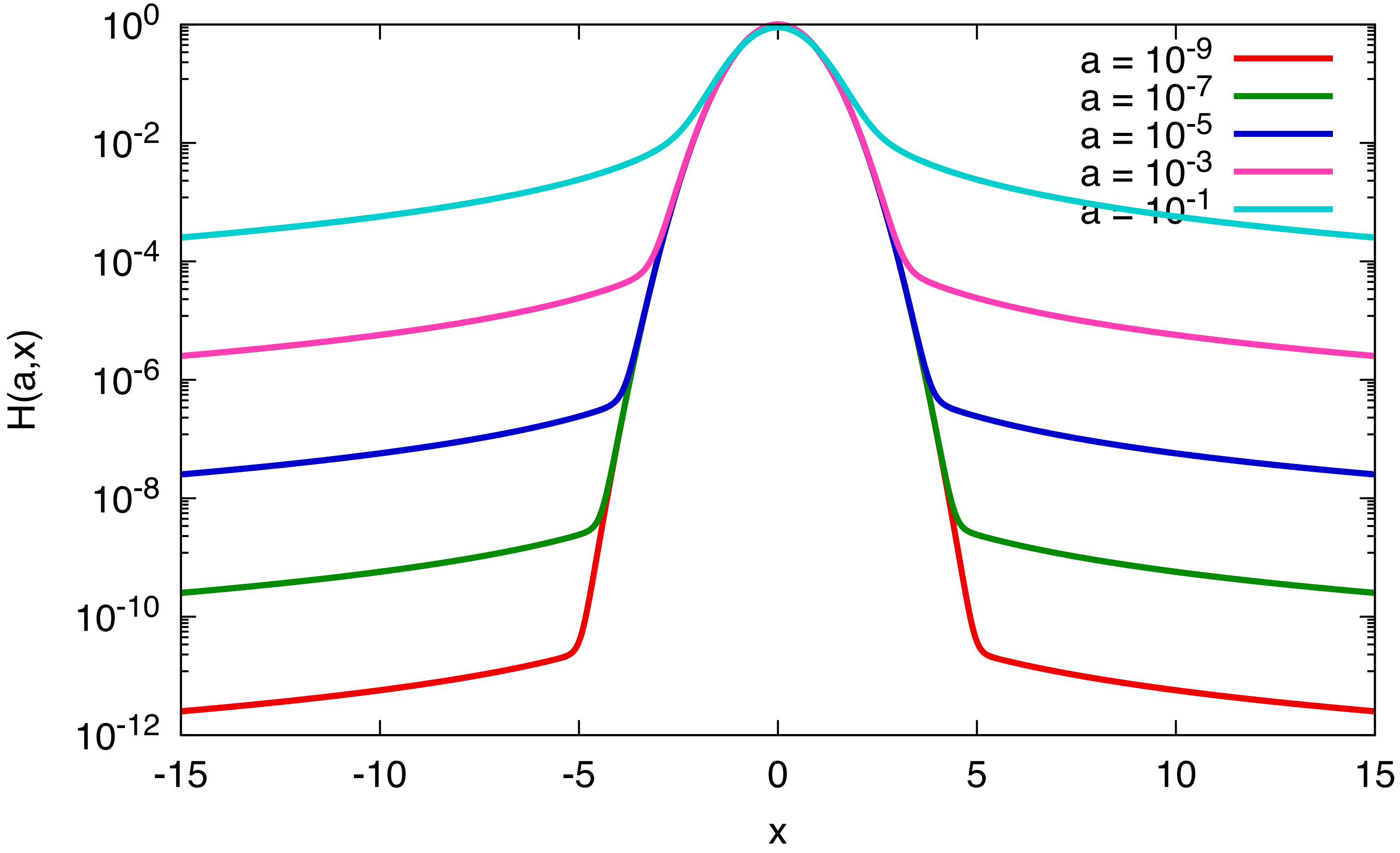
- Let $a = \frac{1}{\Delta\nu_D}\frac{\Gamma}{4\pi}$, $x = \frac{\nu-\nu_{ul}}{\nu_{ul}}$, then:

$$\phi_V\left(\nu\right) = \frac{1}{\Delta\nu_D}\frac{1}{\sqrt{\pi}} H\left(a, x\right)$$

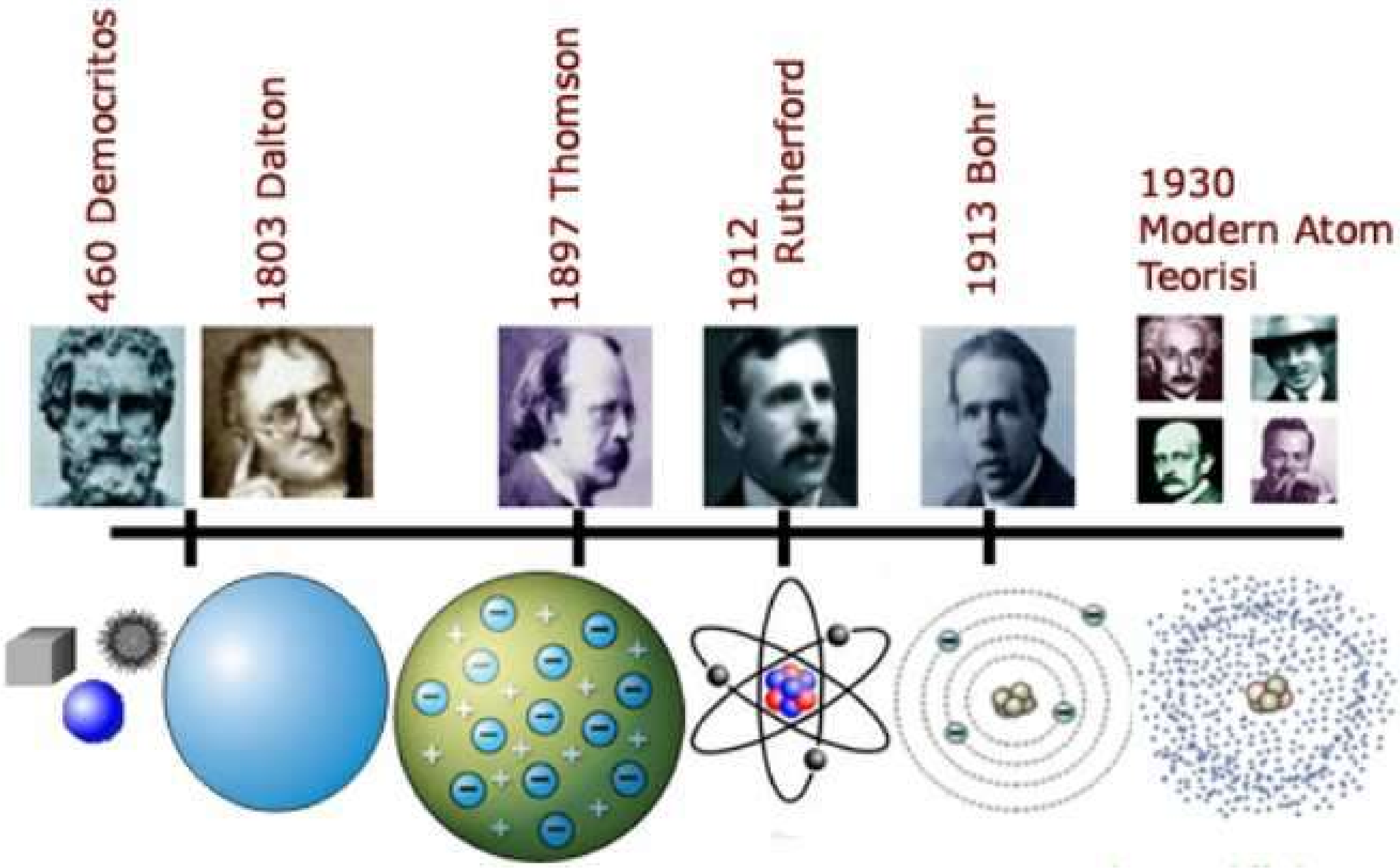
with:

$$H\left(a, x\right) = \frac{a}{\pi}\int_{-\infty}^{+\infty} \frac{\exp\left(-y^2\right)}{\left(x-y\right)^2 + a^2}\, dy$$

Voigt profile



Atomic structure and transitions



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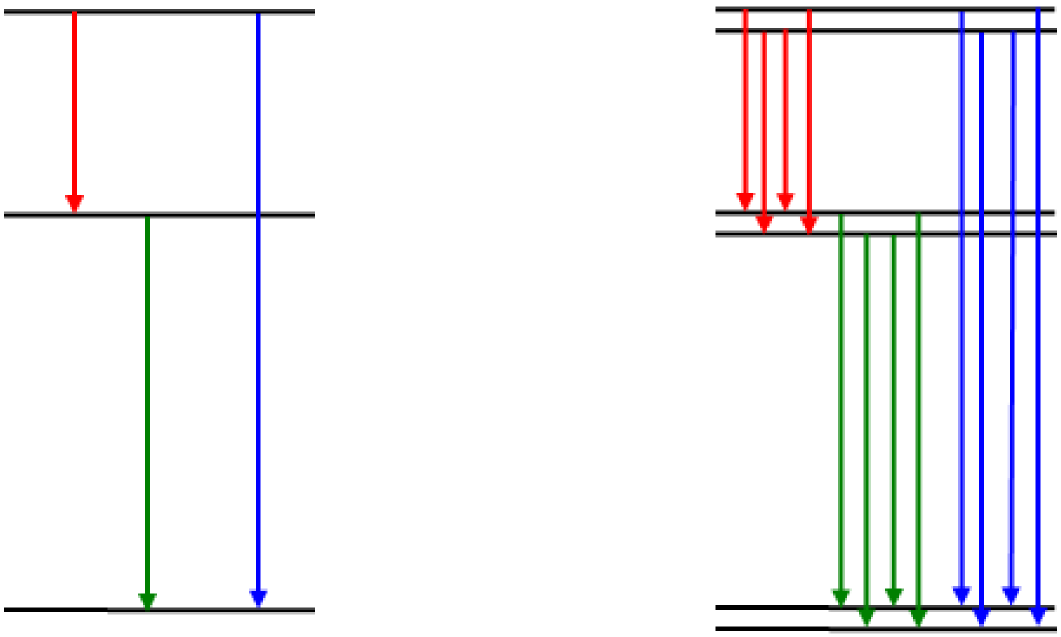
Radiative transitions

- Governed by selection rules.
- Based on quantum mechanics constraints.
  - Transition probability: $\langle \Psi_i \,|\mu|\, \Psi_f \rangle$: an integral…
  - Is 0 if some symmetry properties are not met.
  - Depend mostly on total angular momentum of initial (Ψ_i) and final (Ψ_f) state.



Electrons arrangement

- Electrons are characterized by quantum numbers:
  - n: number of nodes in the wave function. $n > 0$
  - l: quantum of angular momentum. $l < n$
  - m_z: projection of angular momentum on $\overrightarrow{Oz}$. $-l \leqslant m_z \leqslant +l$
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- Standard notation for l: s, p, d, f...
- Example: 6 e^- (C, N^+, O^{++},...):

$$1s^2\,2s^2\,2p^2$$

Total Angular momentum

- $1s$ and $2s$ shells are full: contribute 0.
- $2p$ shell: 6 possibilities for each e^- and only 2 e^-.
- Same n and same l, so they must have different m_z (3 possibilities) and s (2 possibilities).
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- Terms (with $L = S$, P, D, ...):

$$^{2S+1}L_J$$

Terms for C

Scan possibilities for m_z and s, for fixed $n = 2$ and $l = 1$:

- Case 1: Both e^- have $m_z = 1$.
    - Then, $L = 2$, which implies $S = 0$ and $J = 2$.
    - Only one possibility: ${}^1D_2$, $g = 2J + 1 = (2S + 1)\,(2L + 1) = 5$.

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  - But $L = 2$ is not possible, so $L = 1$.
  - Hence it is ${}^3P$, $g = 9$. 3 possibilities for J: 0, 1 or 2.
  - ${}^3P_0$, $g = 1$, ${}^3P_1$, $g = 3$, ${}^3P_2$, $g = 5$ and $1 + 3 + 5 = 9$.

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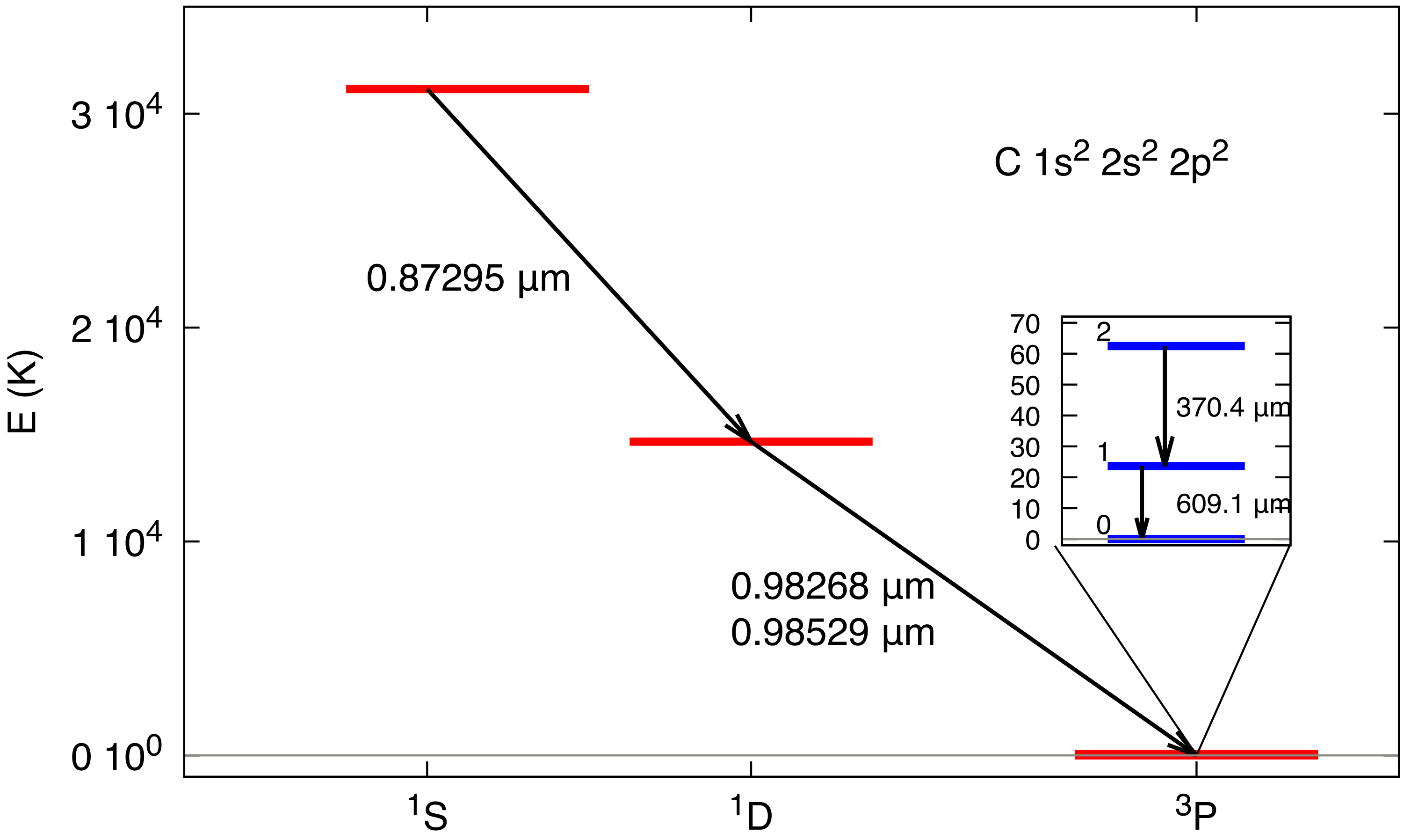
  - So the last one is ${}^1S_0$.
- Energies: Solve Schrödinger.

C $(1s^2\,2s^2\,2p^2)$


E (K)
3 10^4
2 10^4
1 10^4
0 10^0
C 1s^2 2s^2 2p^2
0.87295 µm
0.98268 µm
0.98529 µm
370.4 µm
609.1 µm
70
60
50
40
30
20
10
0
2
1
0
^1S
^1D
^3P

Selection rules

- In $\langle \Psi_i \left| \mu \right| \Psi_f \rangle$, μ is expended on spherical harmonics $Y_l^m\left(\theta, \phi\right)$.
- Expansion gives electric and magnetic multipoles contribution E_1, E_2, ... M_1, M_2...
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- Each term in the expansion has its symmetry and gives selection rules.
- Main ones:
  - If dipole transition $(E_1,\, M_1)$ are possible $(P,\, Q$ and R branches):

$$\Delta J = 0, \pm 1\,; \quad 0 \nleftrightarrow 0$$

$$P:\; J \rightarrow J+1,\, Q:\; J \rightarrow J,\, R:\; J \rightarrow J-1$$

  - For $J' \rightarrow J”$ transition: $P\,(J”)$, $Q\,(J”)$, $R\,(J”)$.

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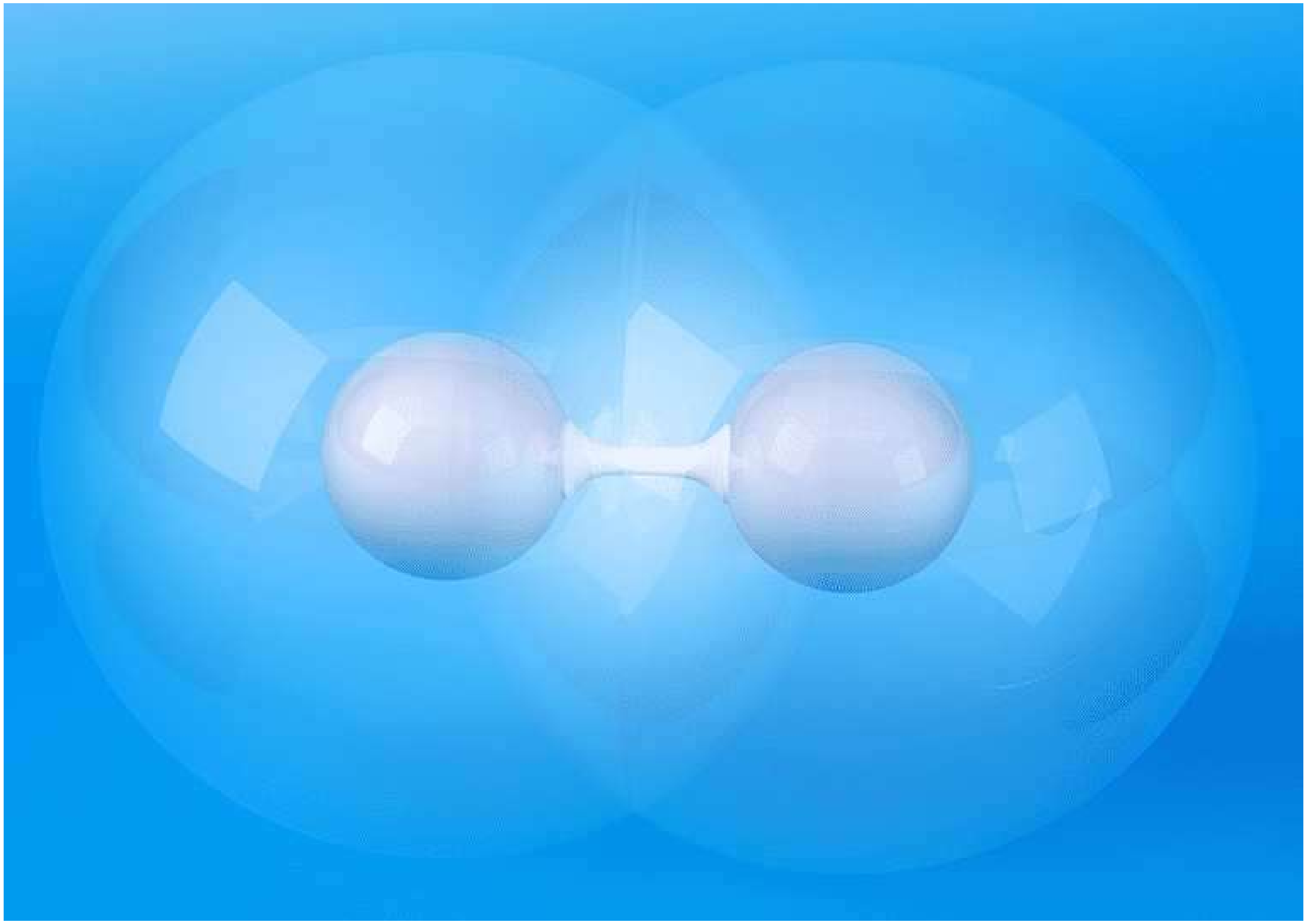
- Each term in the expansion has its symmetry and gives selection rules.
- Main ones:
  - If not: E_2, M_2 (O and S branches):

$$\Delta J = 0,\, \pm 1,\, \pm 2\,; \quad 0 \not\leftrightarrow 0,\, 1\,; \quad \frac{1}{2} \not\leftrightarrow \frac{1}{2}$$

  - Strongest: E_1, then $E_2 \sim M_1$, then $E_3 \sim M_2$...

Molecular structure



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Born-Oppenheimer approximation

- Separate electrons from nucleons.
- Electrons adapt adiabatically to nucleons positions.
- Nucleon motions:
  - Vibration ⇒ No selection rules.
  - Rotation ⇒ Angular momentum selection rules.
  - Branches: $v' - v''\,P\,(J'')$, $v' - v''\,Q\,(J'')$, $v' - v''\,R\,(J'')$.
- Database: HITRAN.

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Diagnostics possible from far UV to Radio

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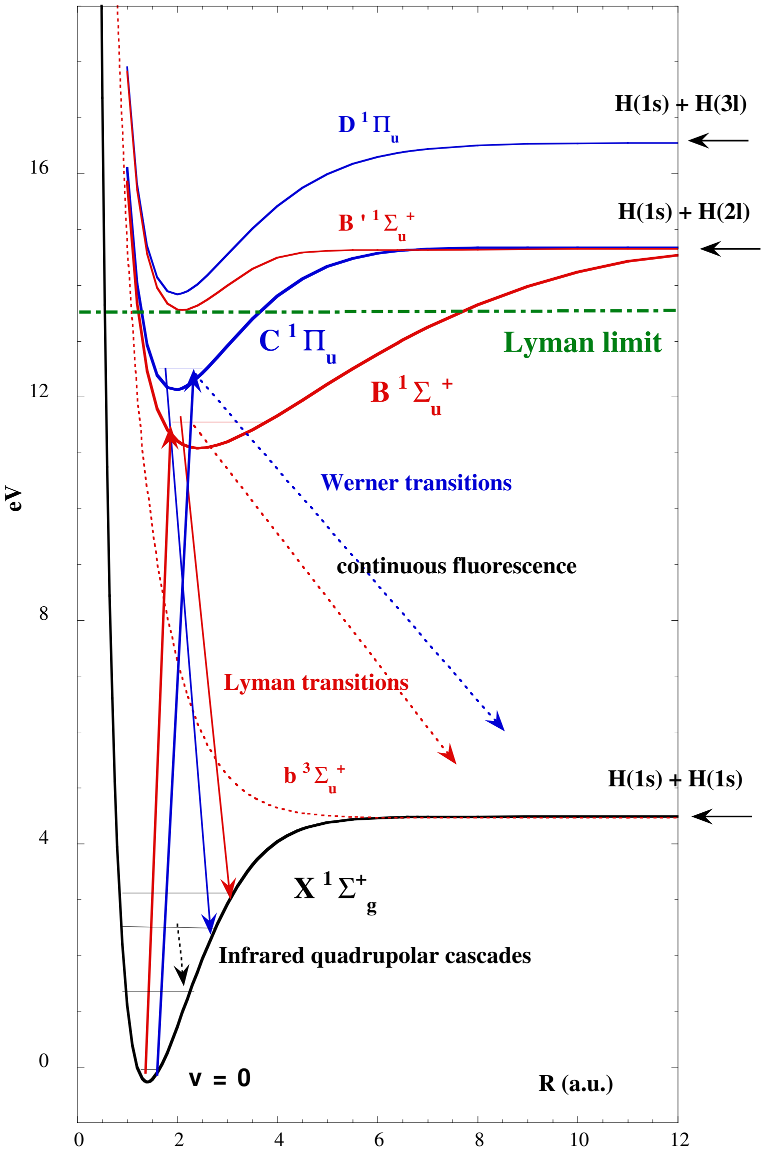
Molecular hydrogen



- Main electronic states: $X\,^1\Sigma_g^+$, $B\,^1\Sigma_u^+$ (Lyman transitions), $C\,^1\Pi_u$ (Werner transitions)

- Infrared spectrum: Ro-vibrational quadrupolar transitions within $X\,^1\Sigma_g^+$.
- Ultraviolet spectrum: Electronic transitions $\Rightarrow$ lead to dissociation ($\sim 10\%$).

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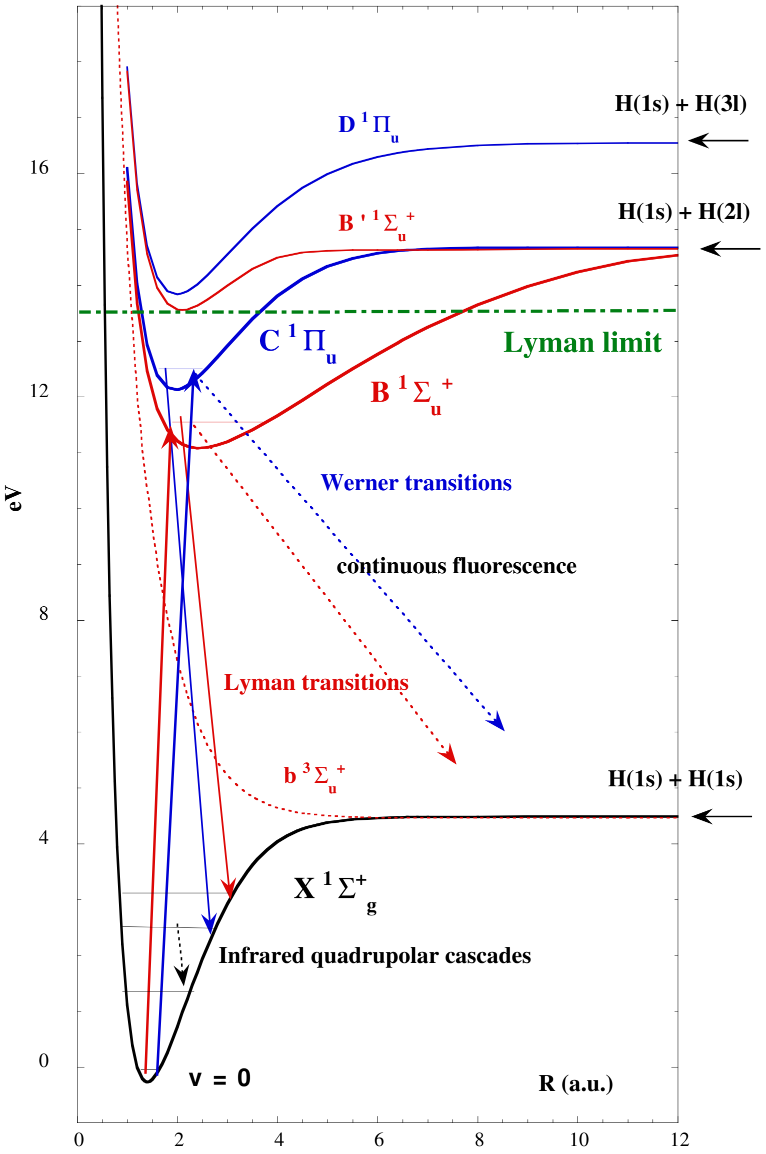

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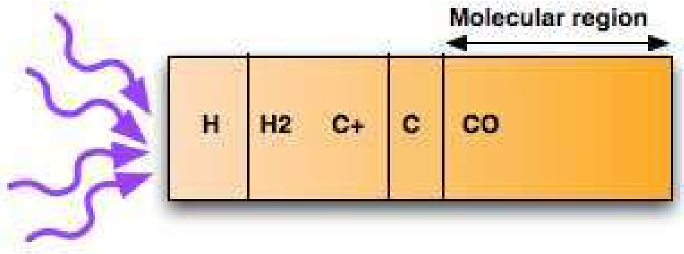
- Infrared spectrum: Ro-vibrational quadrupolar transitions within $X\,^1\Sigma_g^+$.
- Ultraviolet spectrum: Electronic transitions ⇒ lead to dissociation ($\sim 10\%$).
- Dominates edge of PDR.



Absorption from H_2

- UV pumping followed by radiative decay:
  - 10% dissociation.
  - 90% populates high v (up to $v = 14$), but low J.
  - $\lambda_{emis} > \lambda_{abs}$

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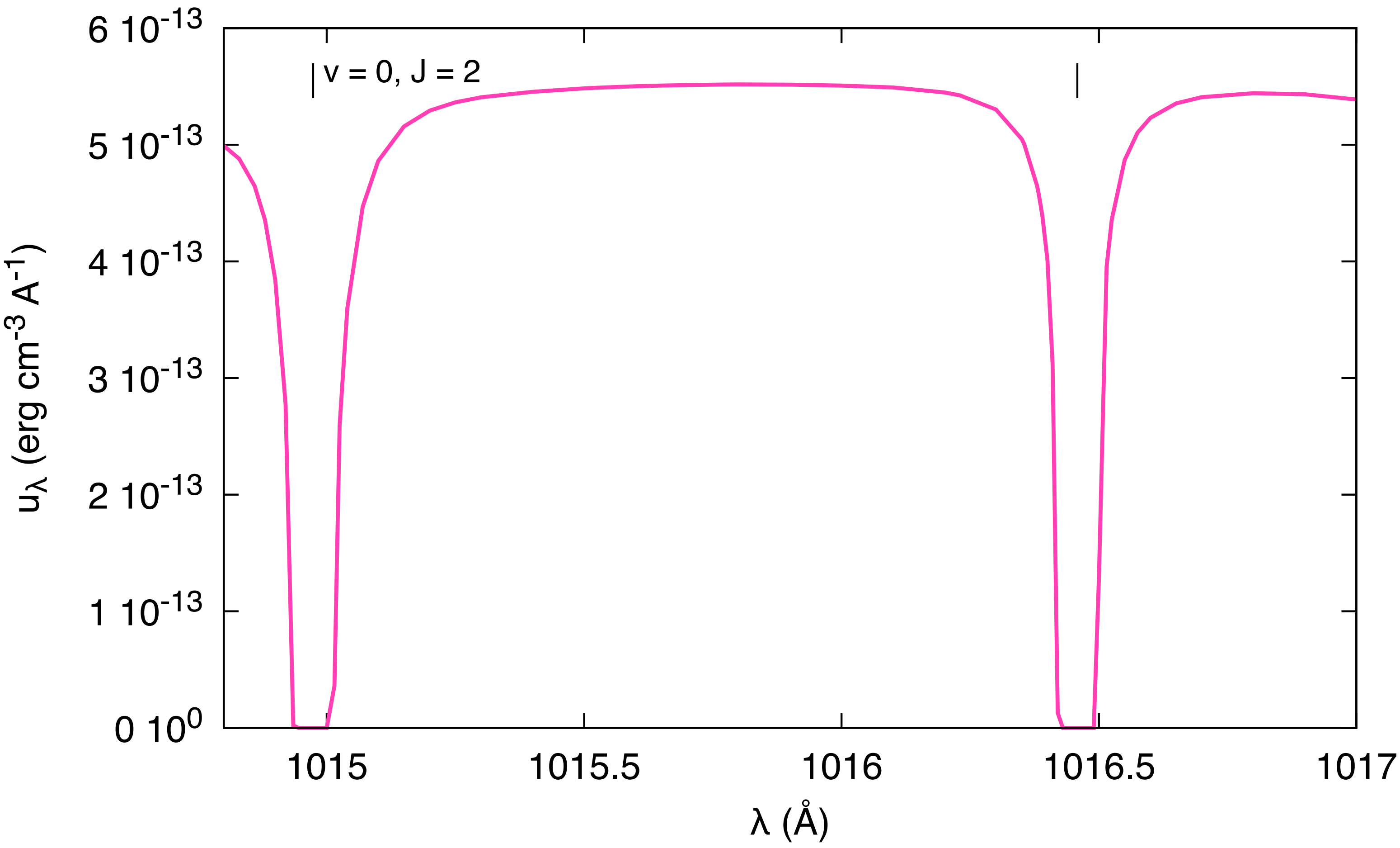
  - 10% dissociation.
  - 90% populates high v (up to $v = 14$), but low J.
  - $\lambda_{emis} > \lambda_{abs}$
- Dissociating photons disappear close to the cloud surface.
  - $\Rightarrow$ "Self-Shielding": H_2 protects H_2.
  - Less UV photons for heating, ionization, dissociation...
- Example: d203-506 (constant density model):

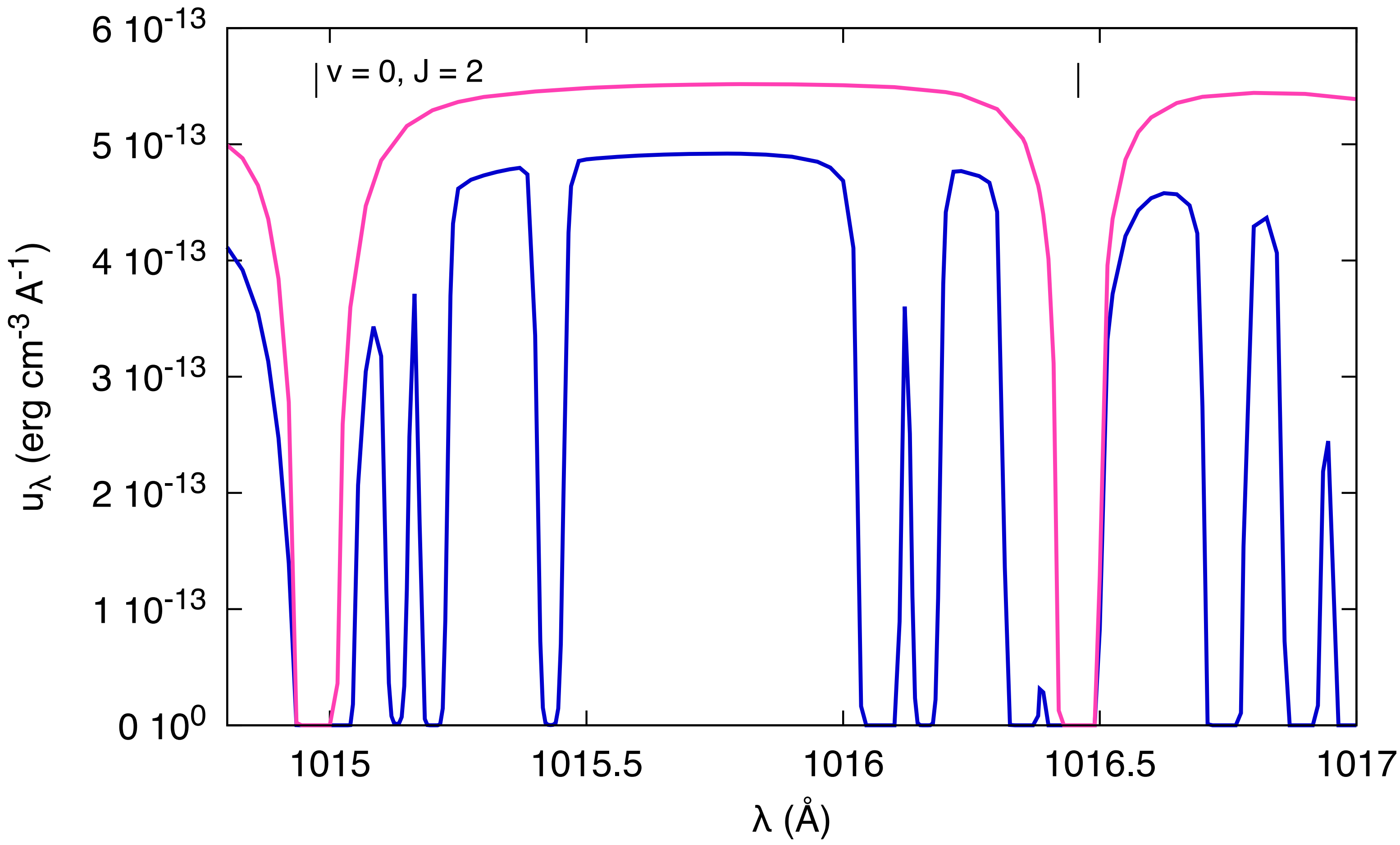
$n_{\rm H}$ $(\rm m^{-3})$	G_0	ζ $(\rm s^{-1})$
10^{13}	$2.3\,10^4$	10^{-16}

Transfer effects in d203-506



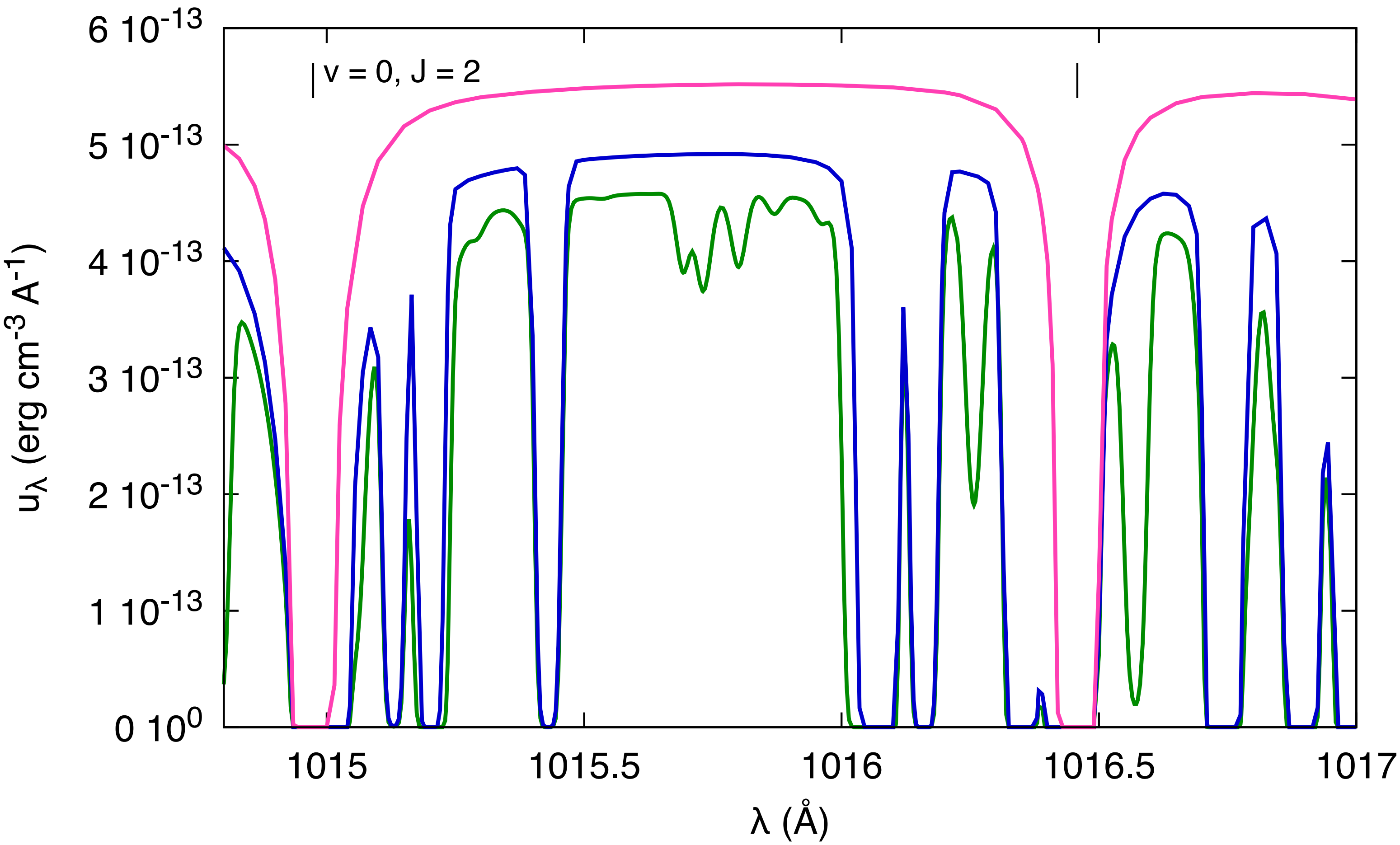
$A_{\rm V} = 0.1$, Absorption from 4 lowest levels.

Transfer effects in d203-506



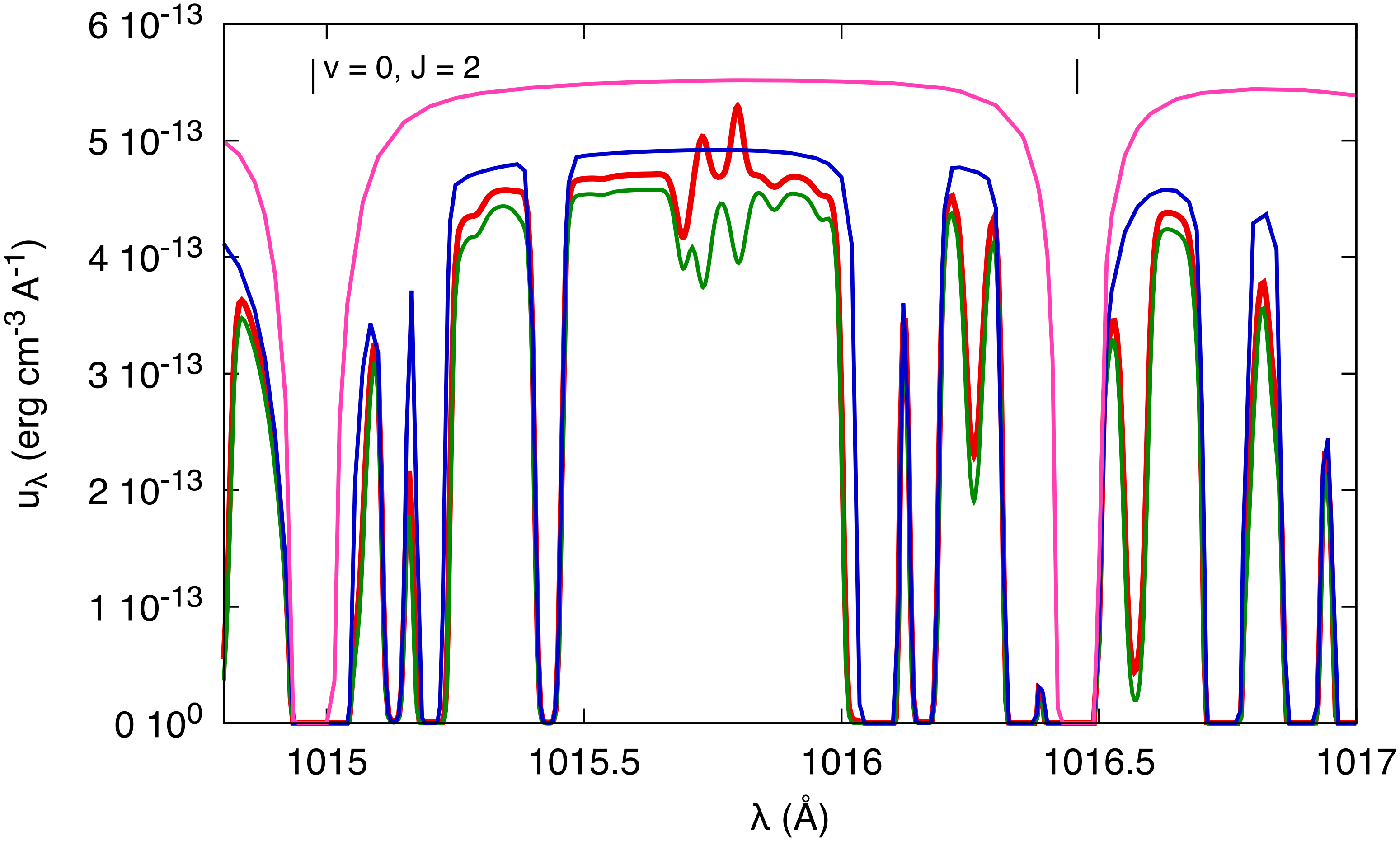
$A_{\rm V} = 0.1$, Absorption from 20 levels.

Transfer effects in d203-506



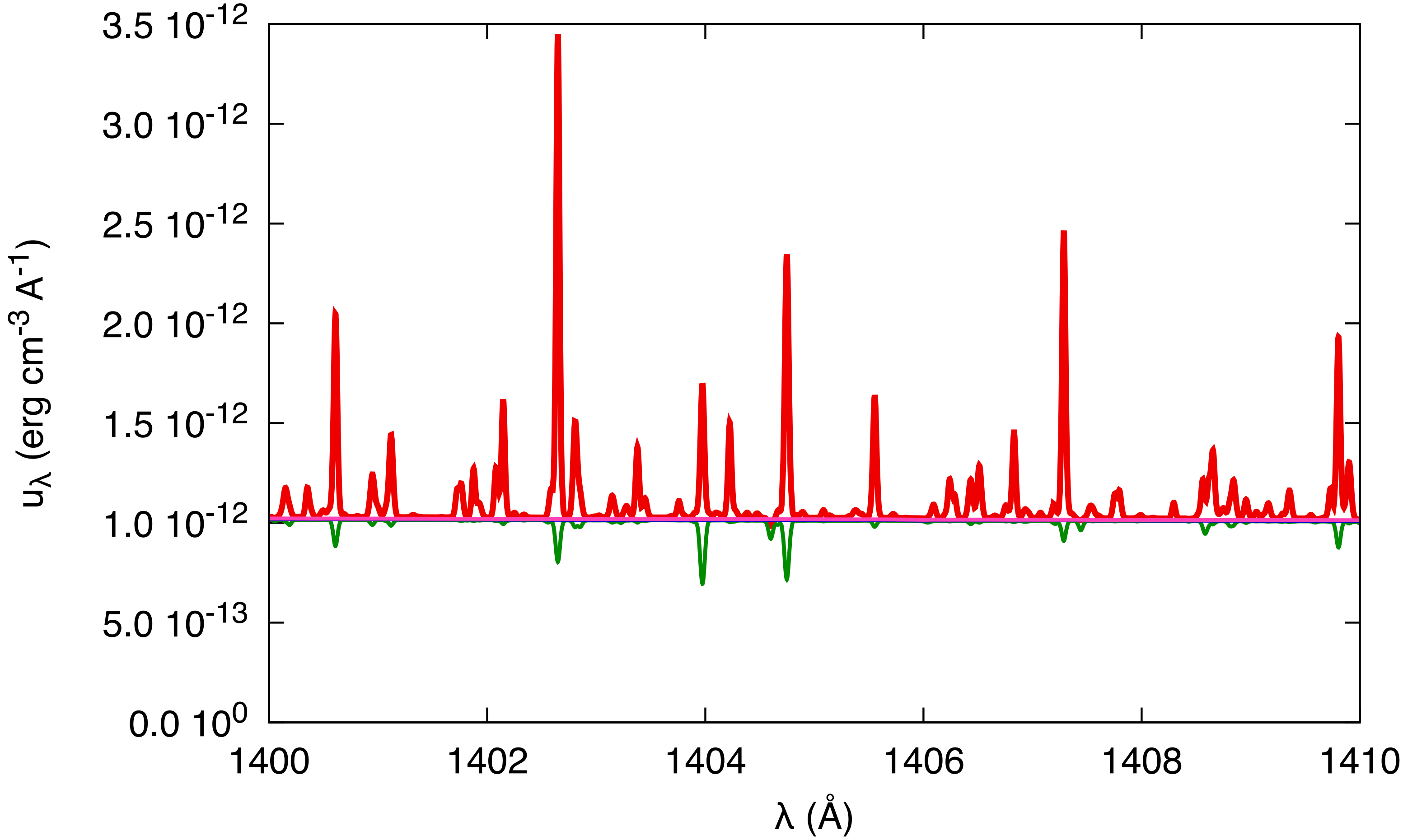
$A_V = 0.1$, Absorption from all 302 levels.

Transfer effects in d203-506



$A_V = 0.1$, Absorption from 302 levels + fluorescence.

Transfer effects in d203-506



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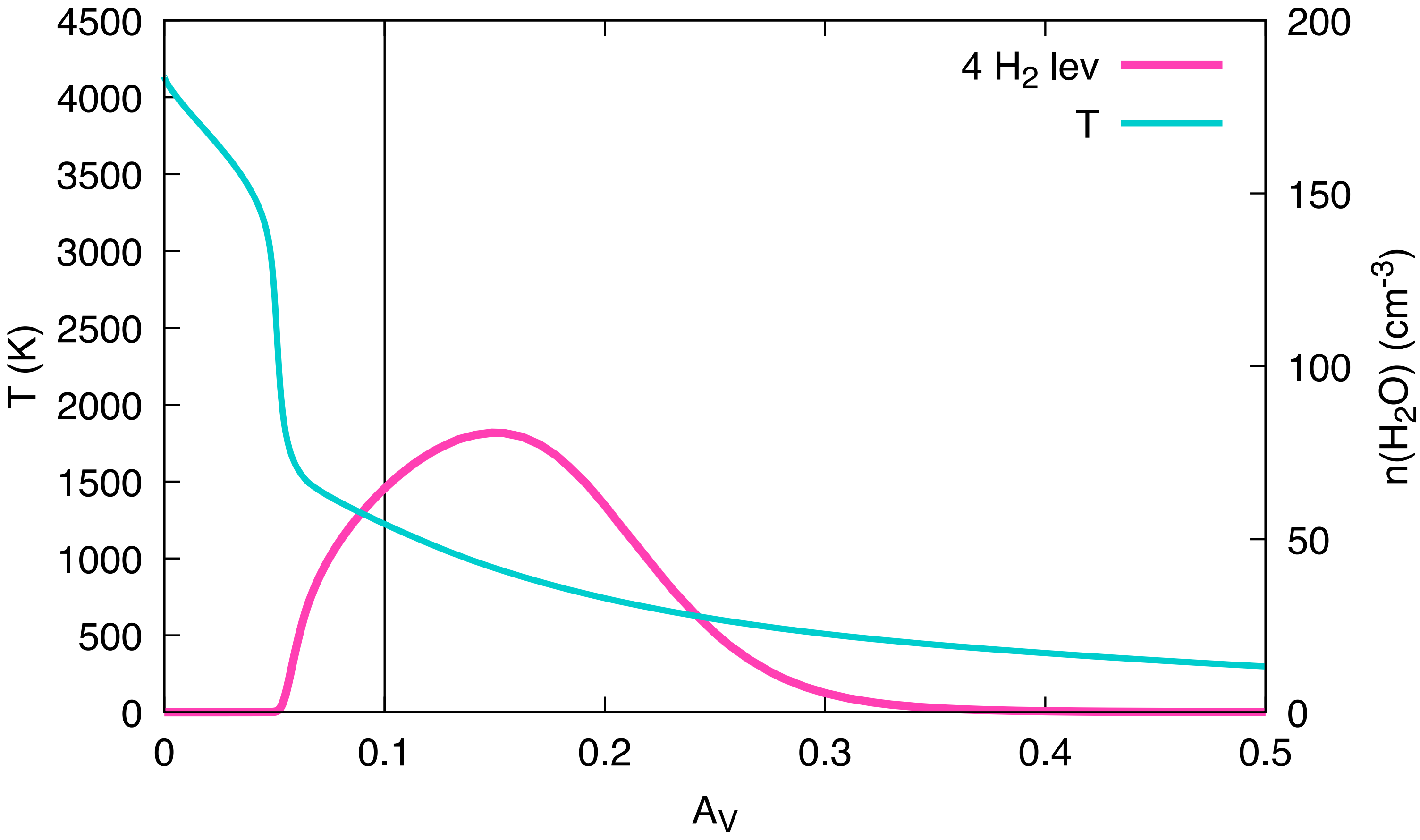
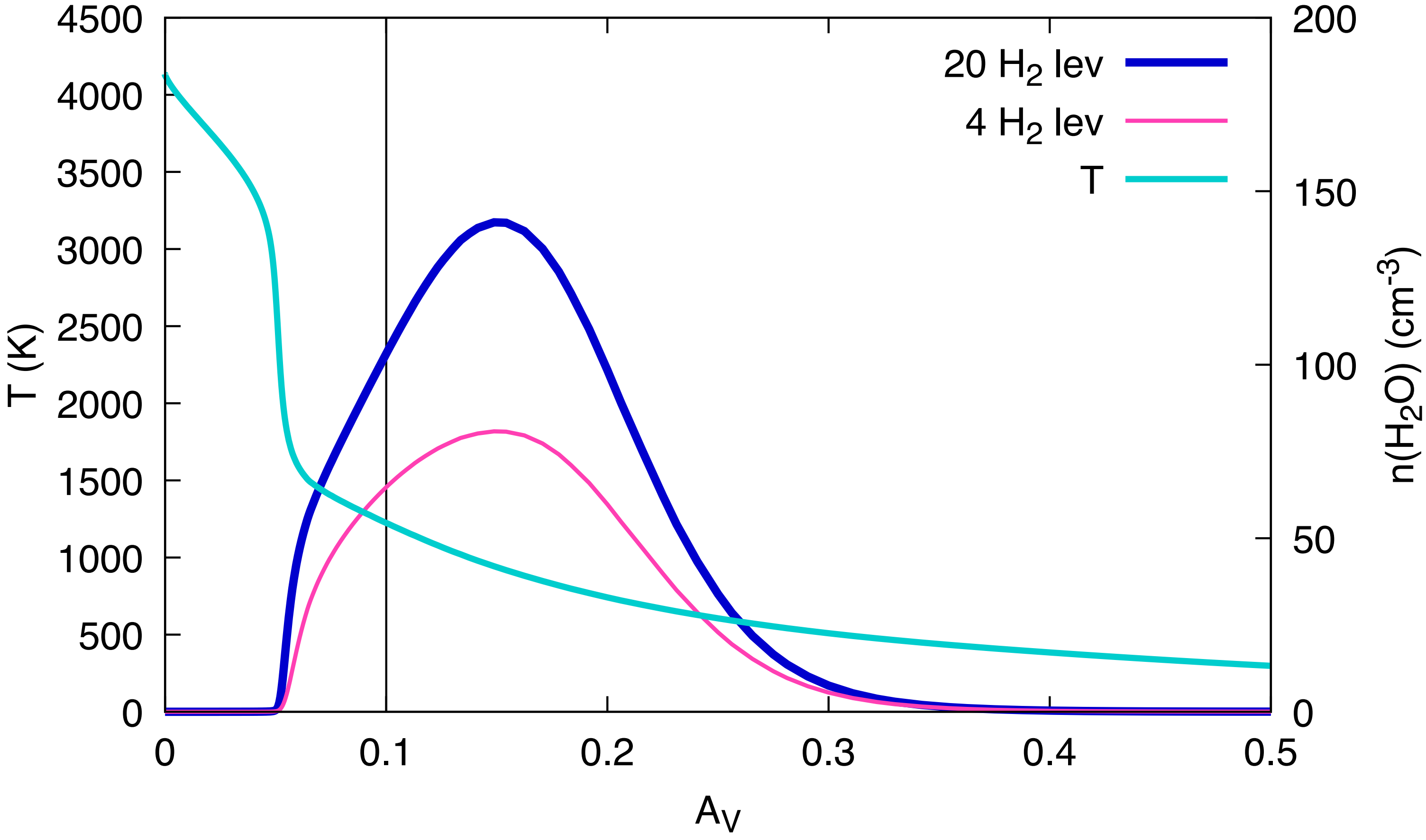
Water abundance in d203-506



Effect of number of H_2 levels included in transfer.

Water abundance in d203-506



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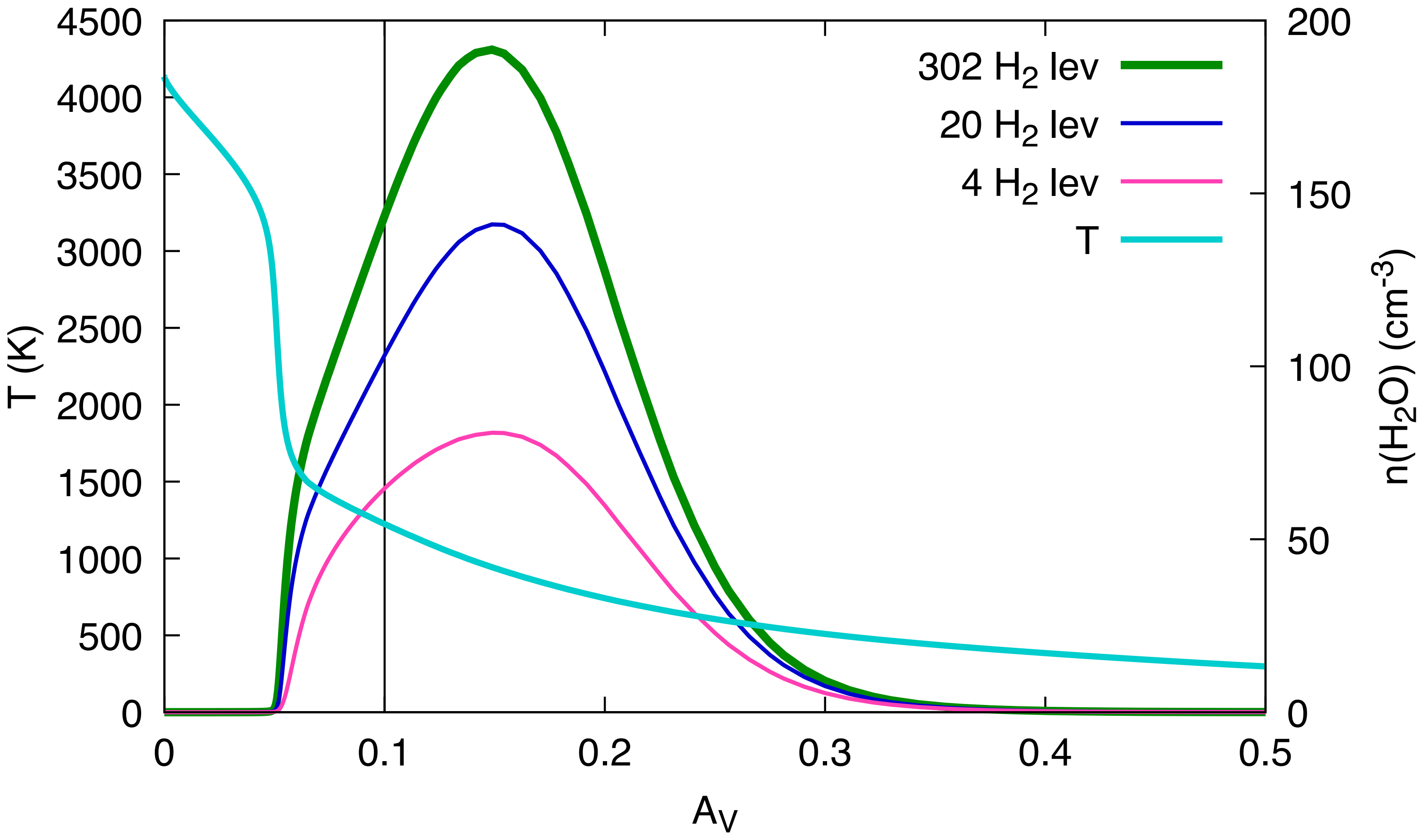

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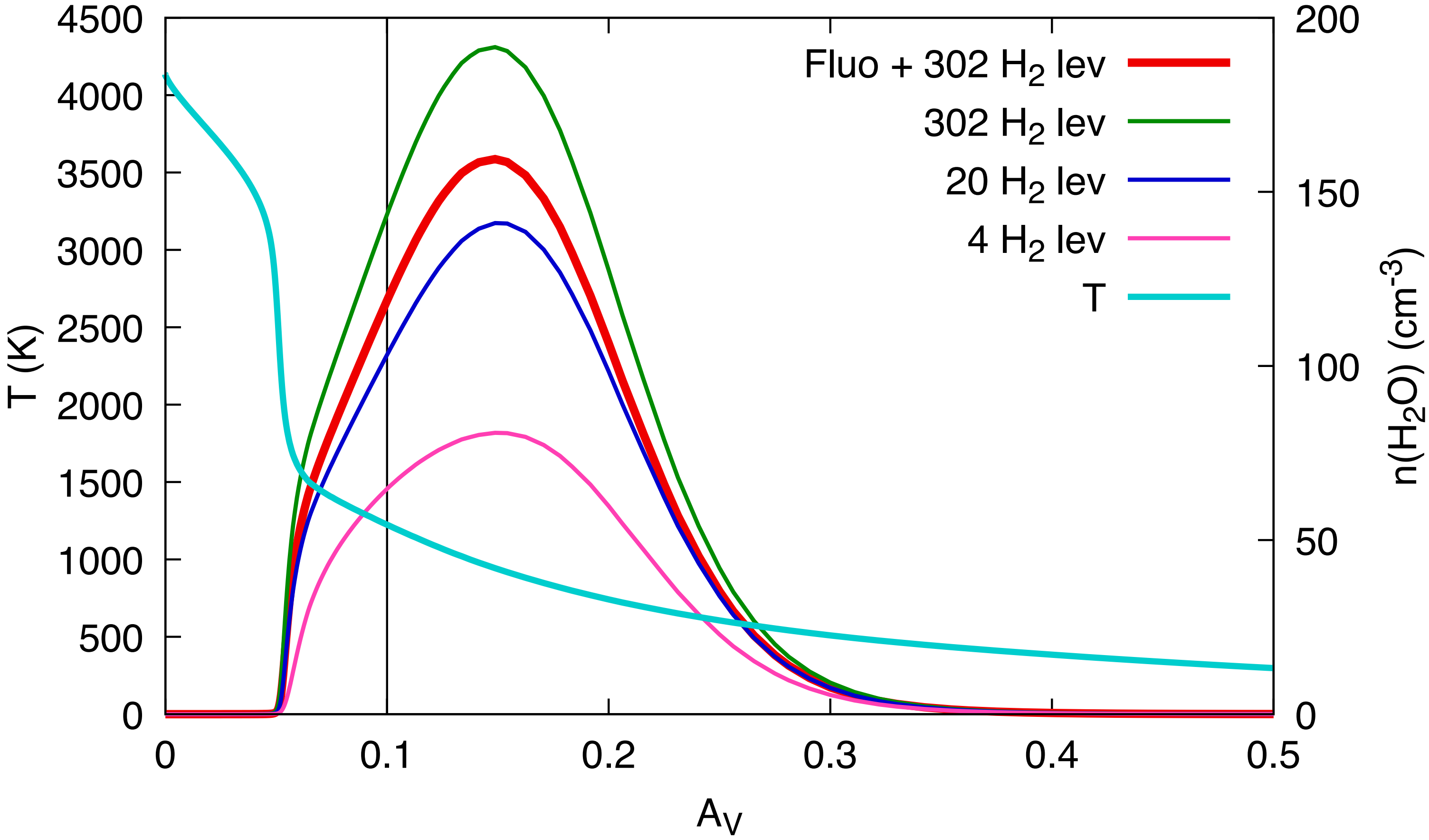
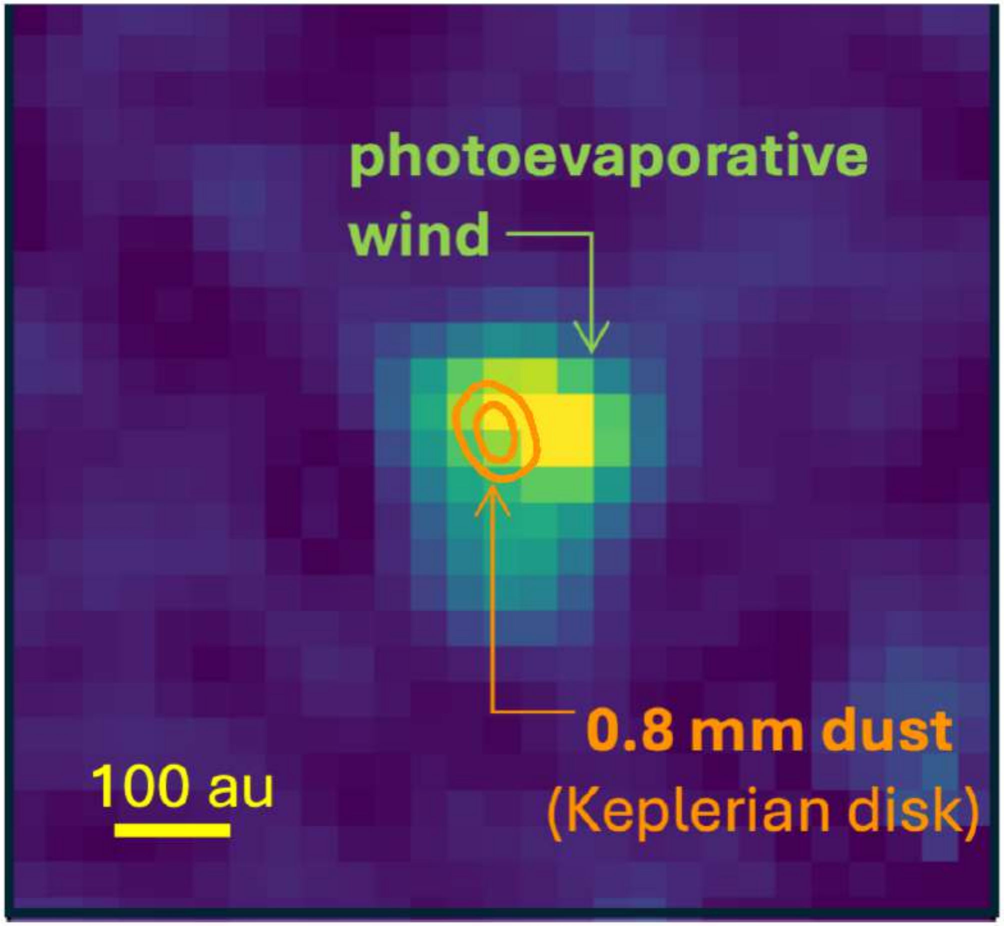


Effect of number of $\mathrm{H_2}$ levels included in transfer.

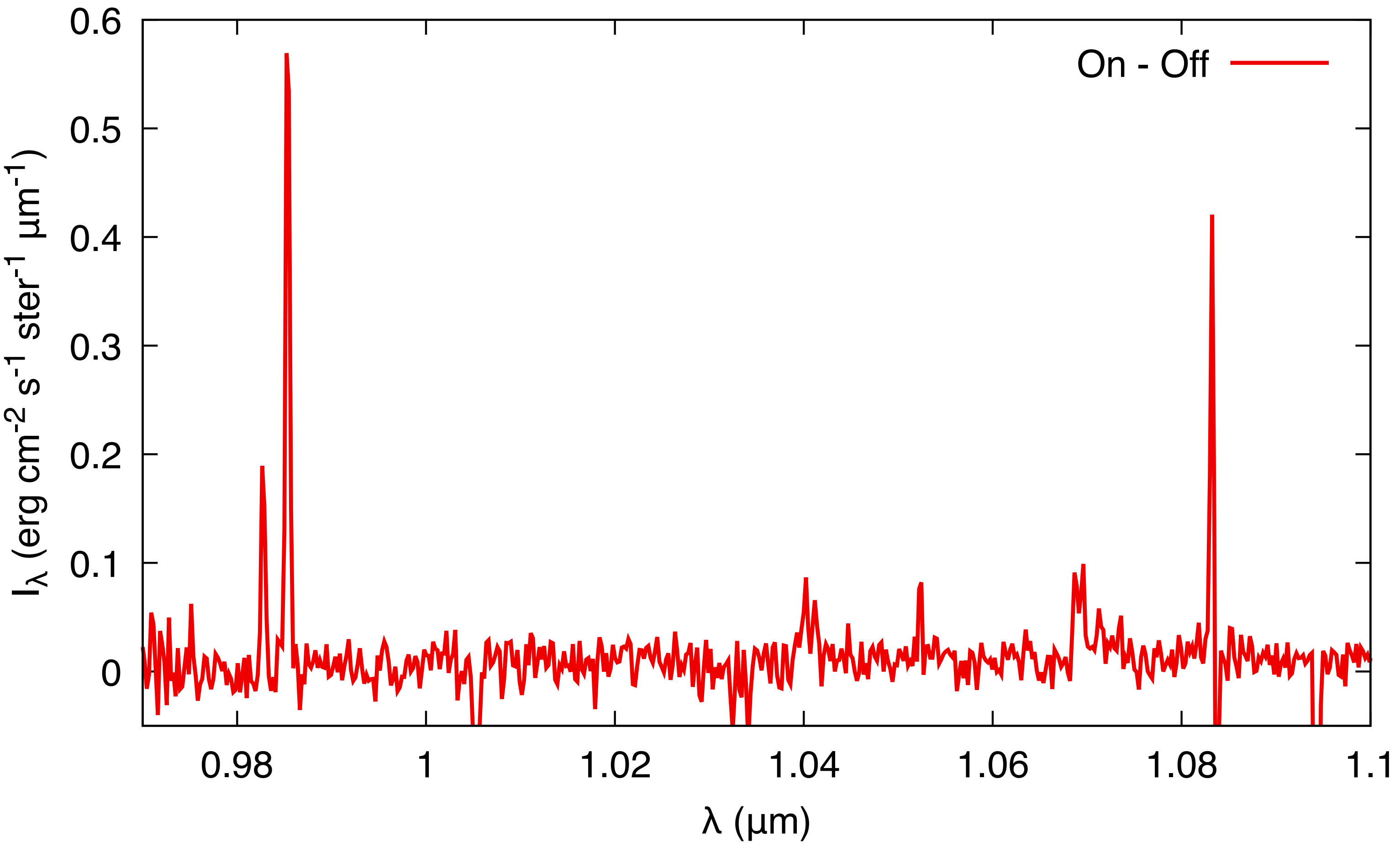
Carbon Excitation in d203-506

[CI] $^1D_2$-$^3P_2$ 0.9853μm



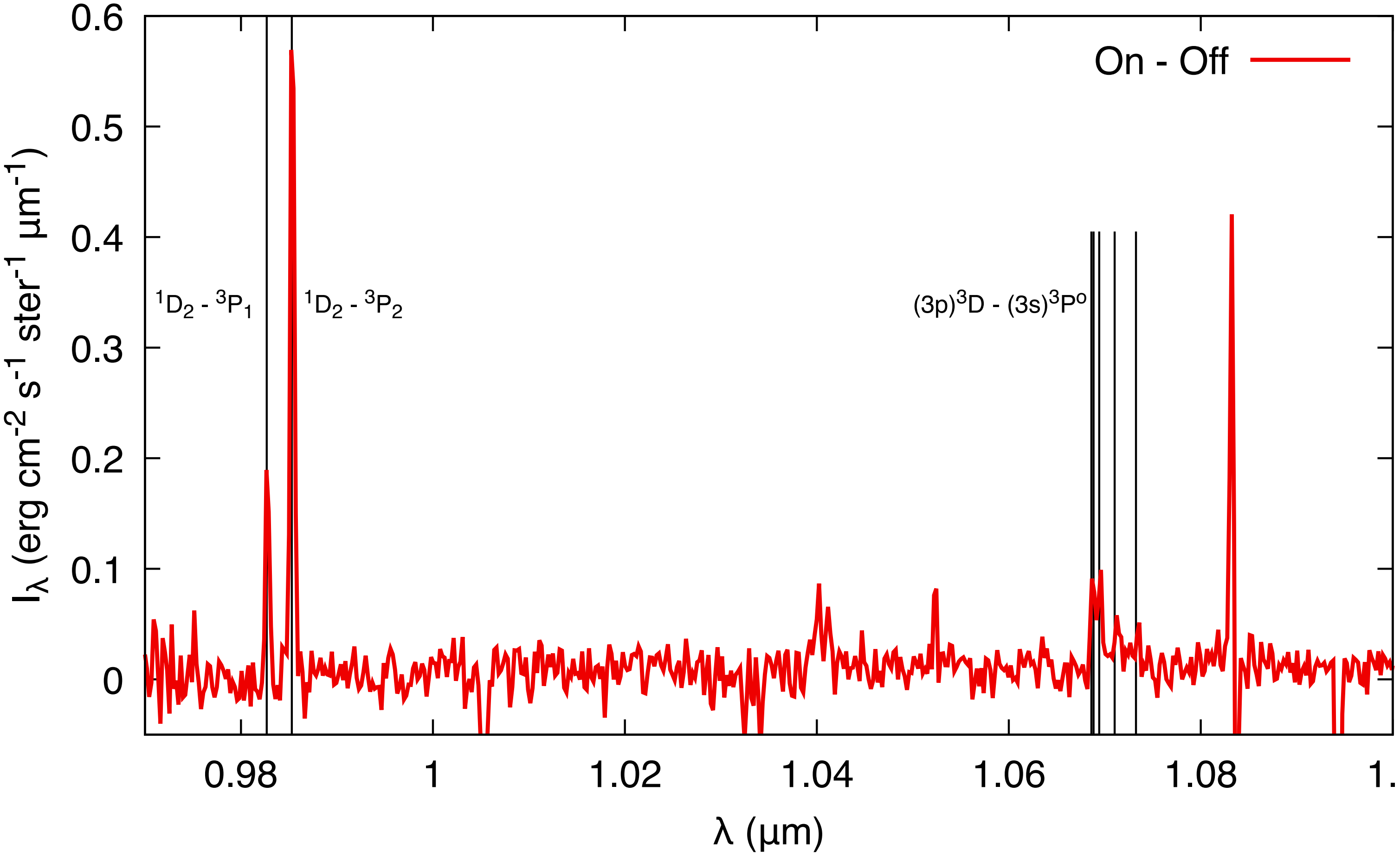
d203-506 in Orion bar - JWST - Goicoechea et al. (2024)

Spectrum d203-506



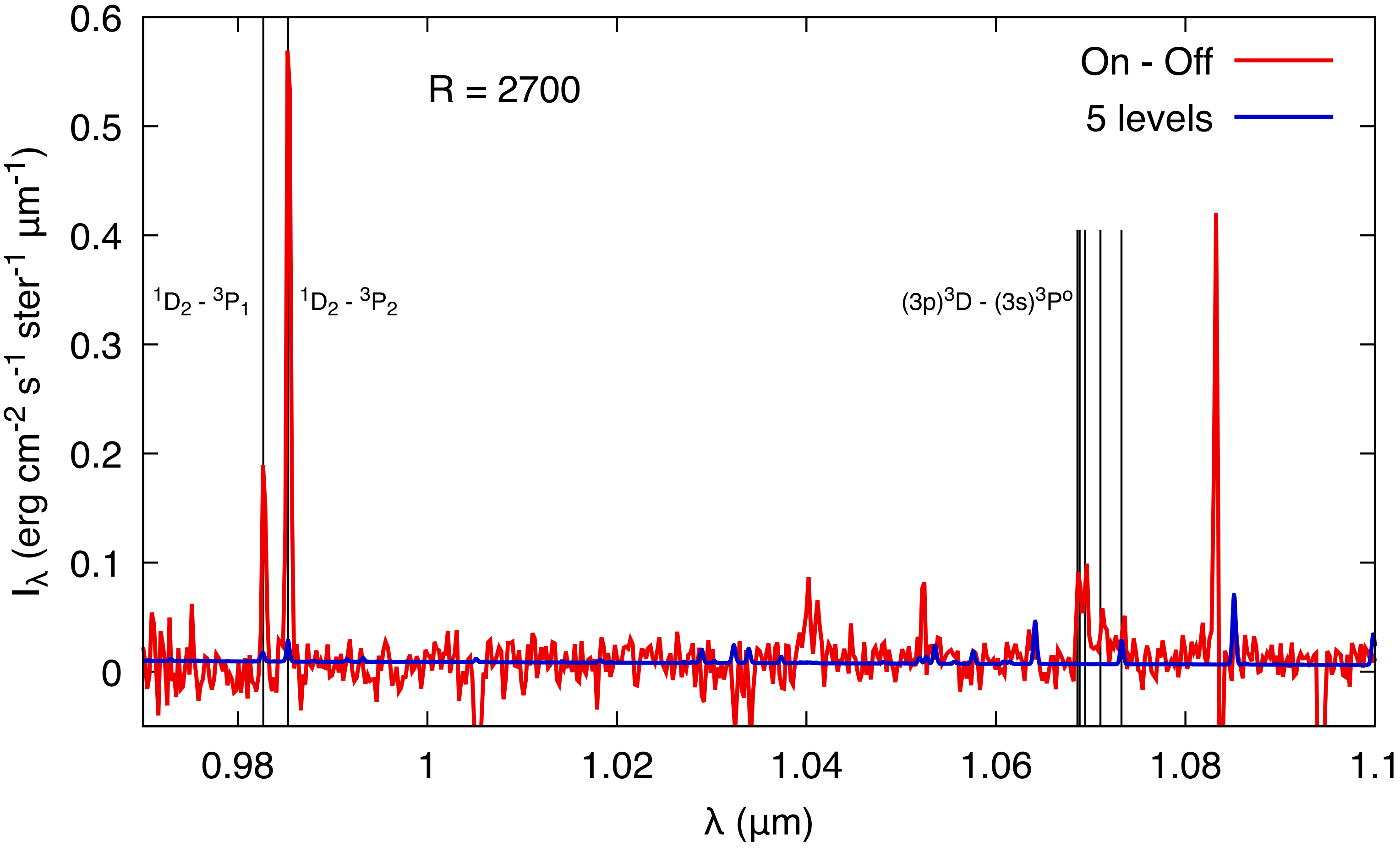
JWST - NIRSpec

Spectrum d203-506



JWST - NIRSpec

Simple model

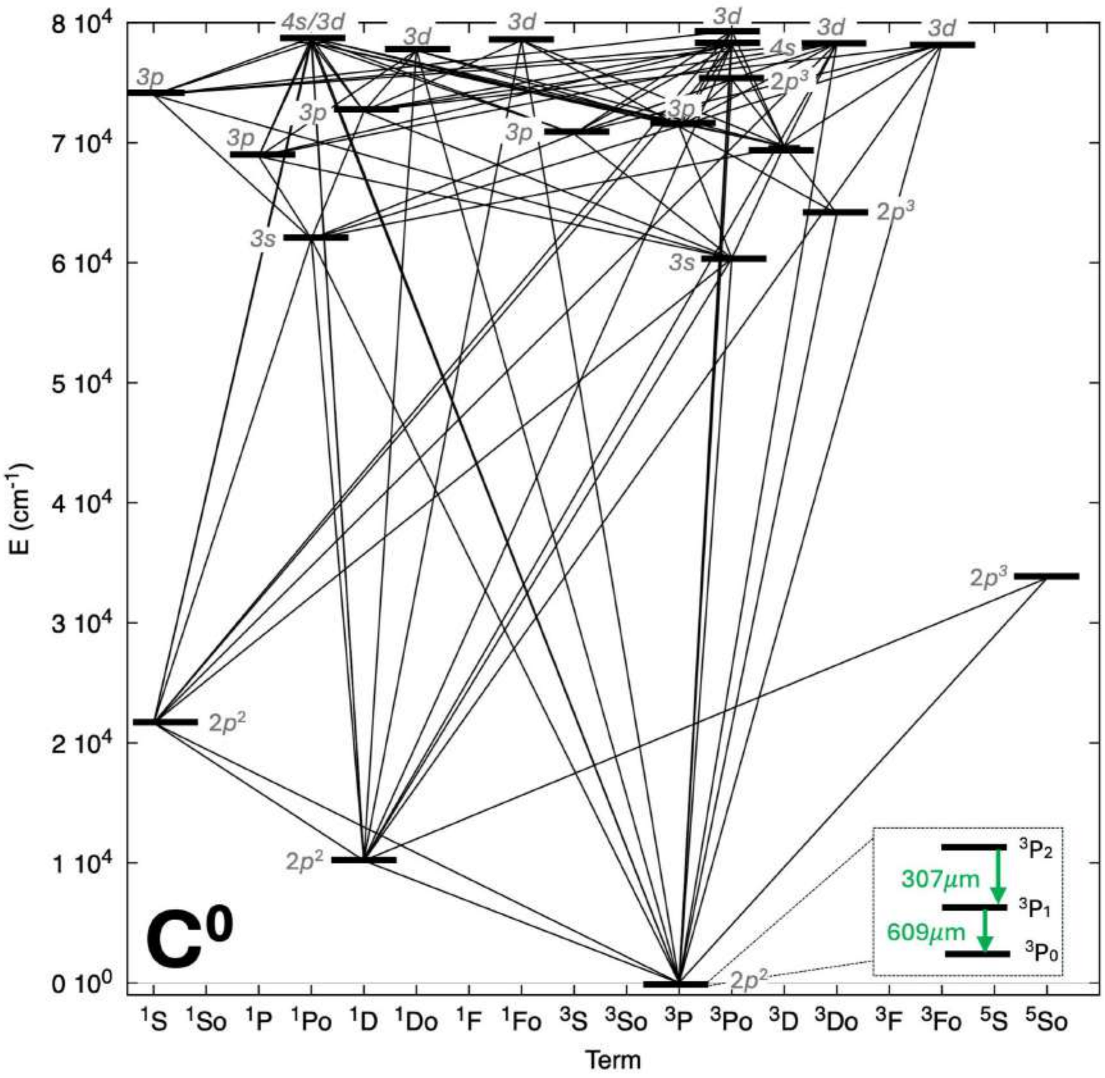


Meudon PDR code - Standard parameters

NIST Database

- Many reliable info at NIST:
  - Ions and atoms Levels.
  - Ions and atoms Lines.
- Good for ions and atoms
- No molecule...

Carbon structure



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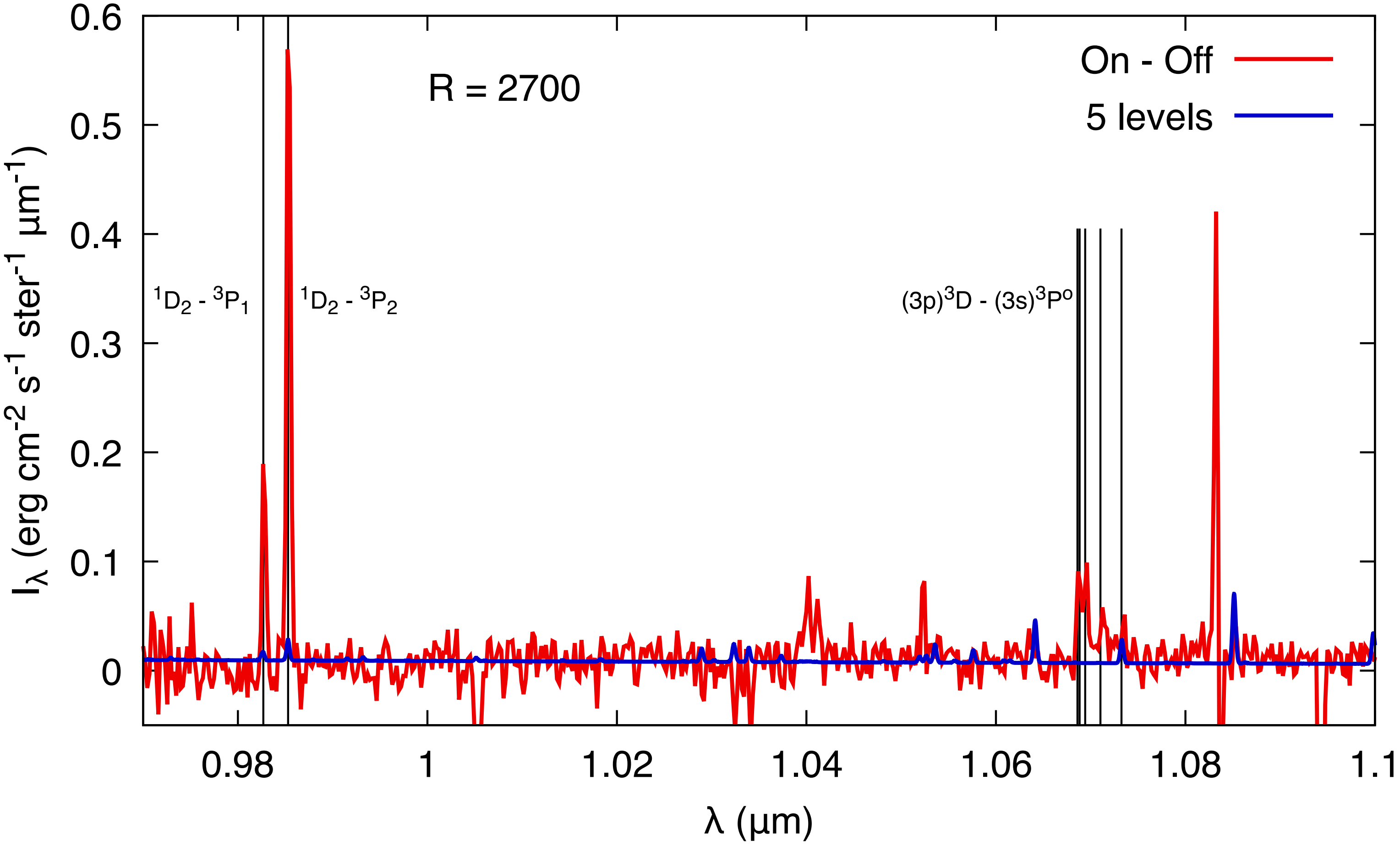
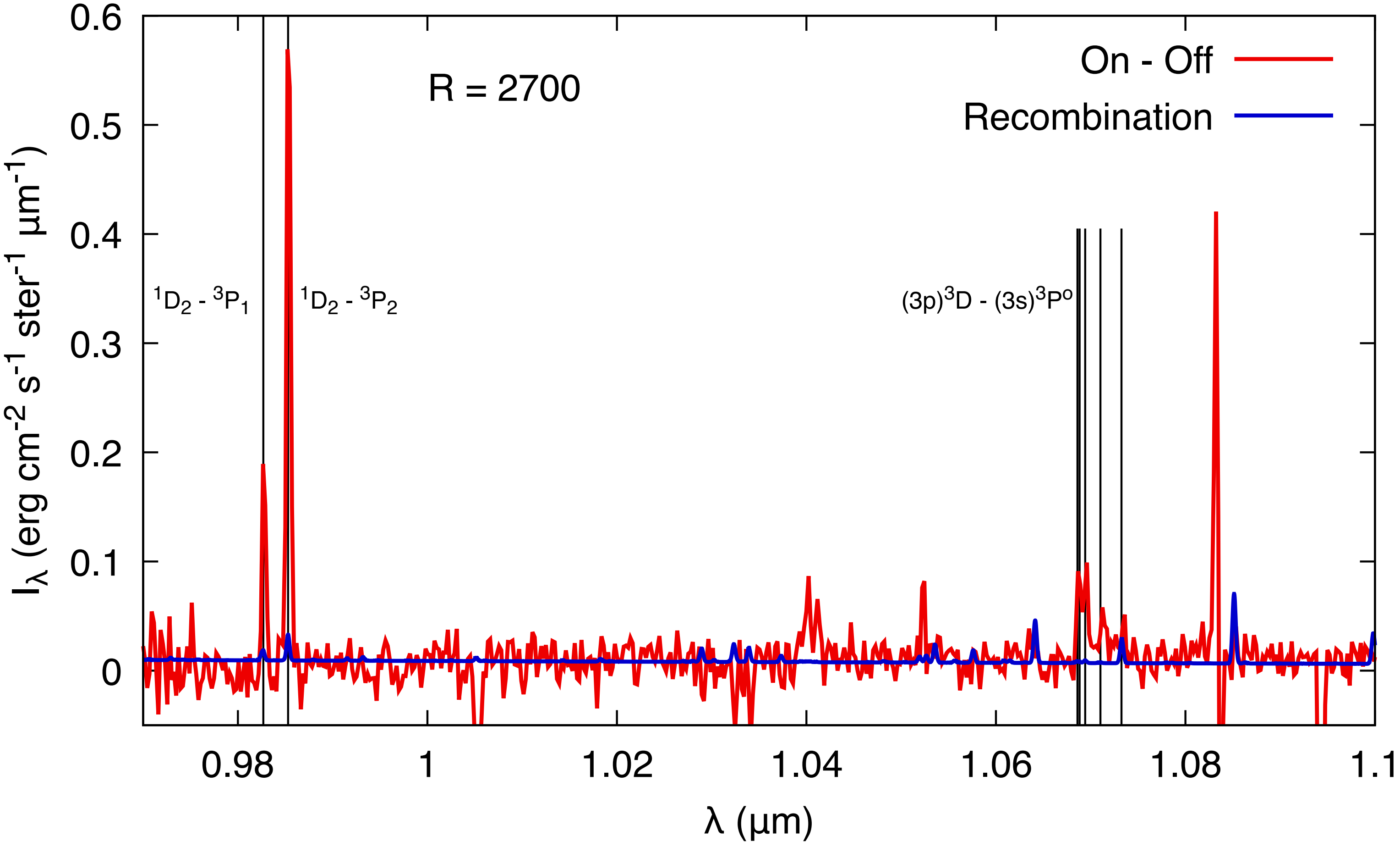


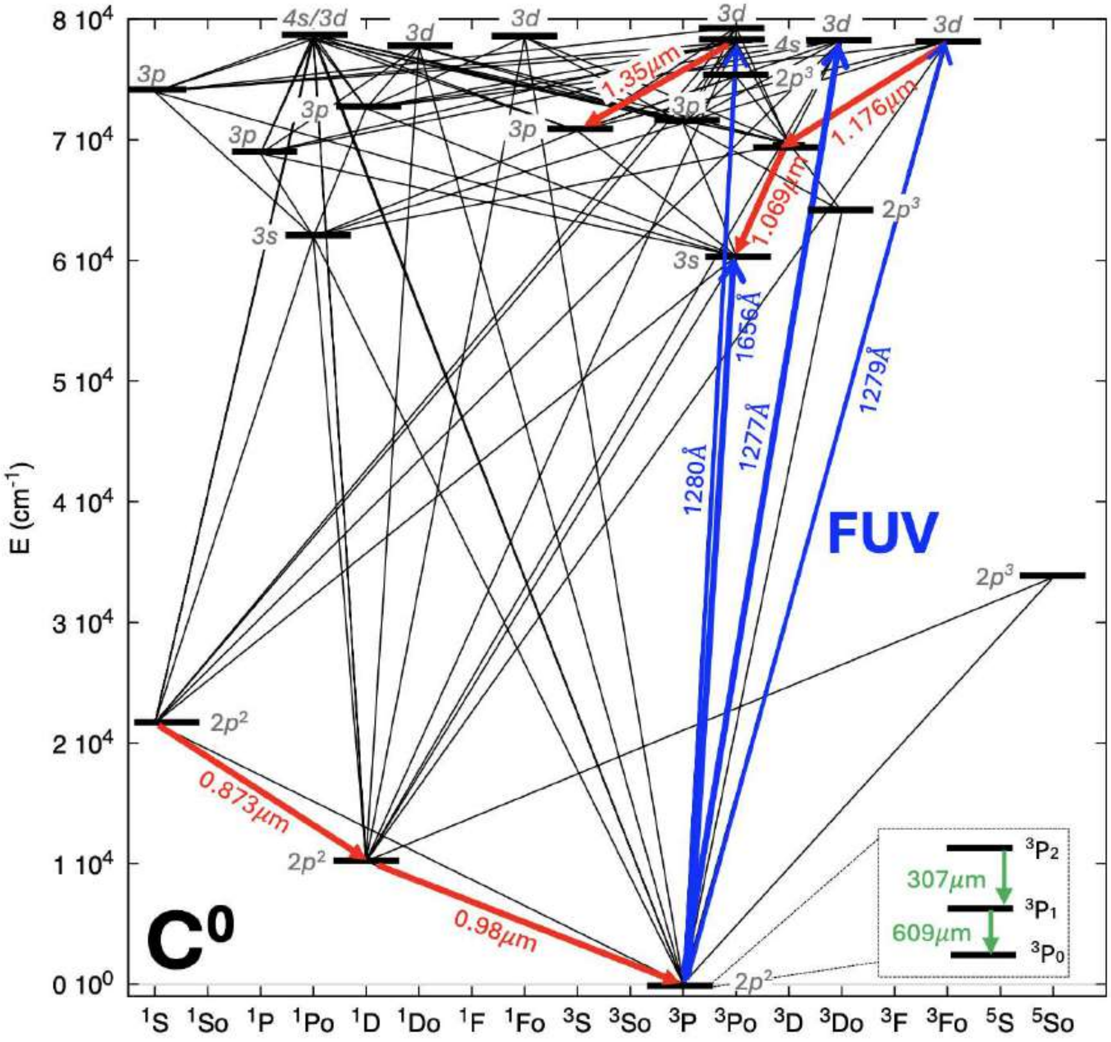
Meudon PDR code - Standard parameters

Simple model + Recombination



Meudon PDR code - Standard parameters
$+ \mathrm{C}^+ + e^-$ recombination

Carbon structure (bis)



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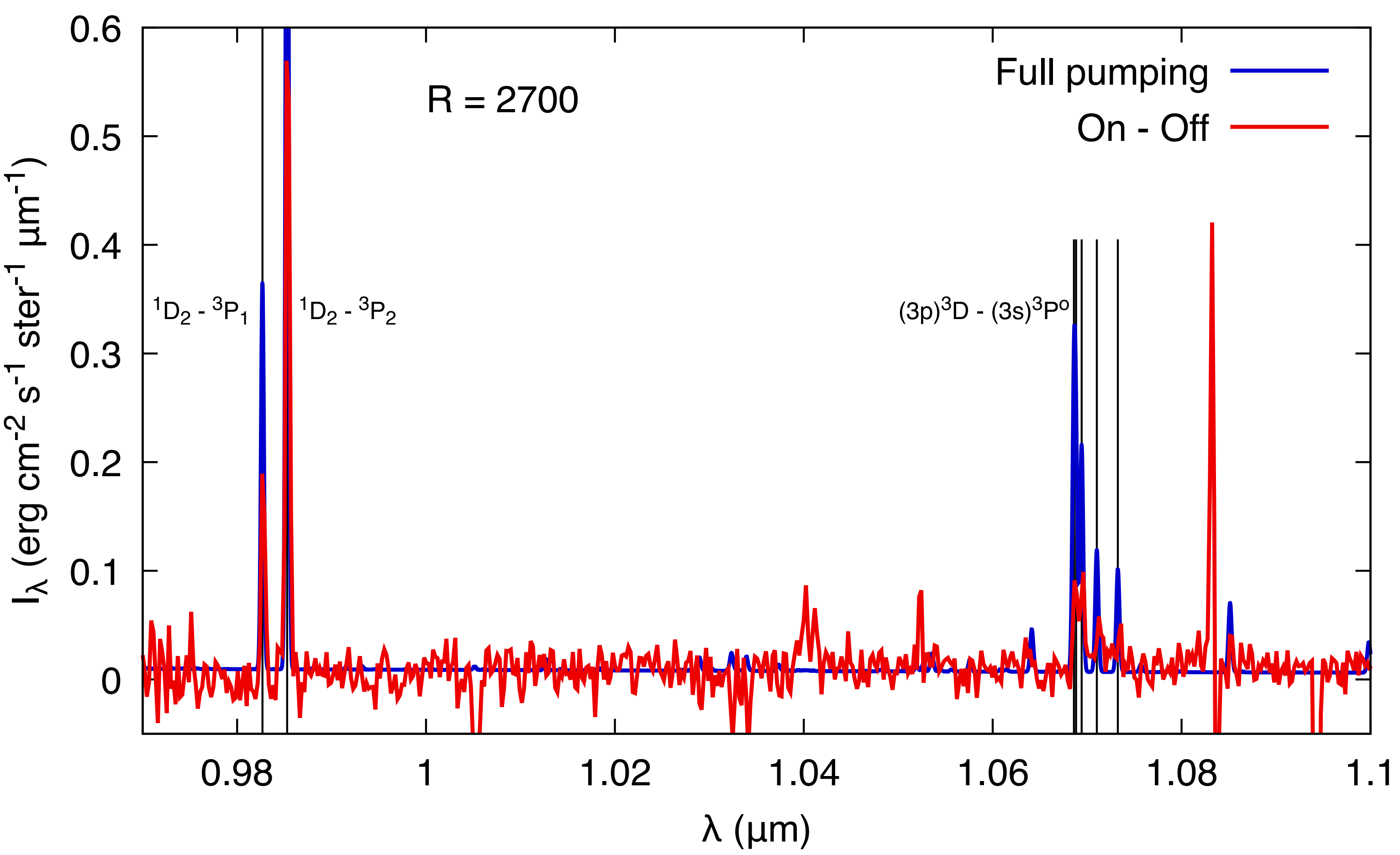
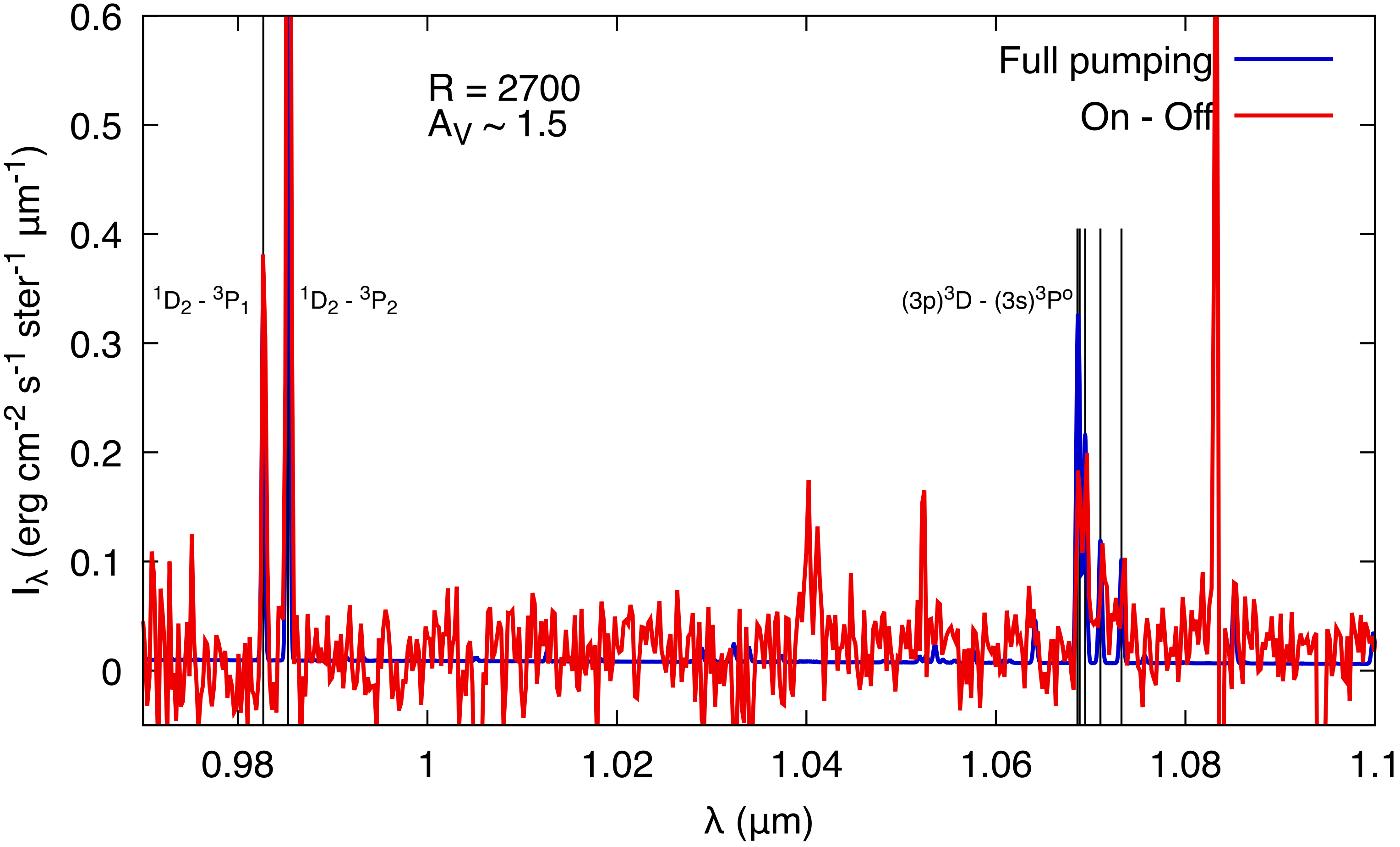
Spectrum d203-506



Meudon PDR code - Standard parameters
$+ \mathrm{C}^+ + e^-$ recombination + Radiative pumping

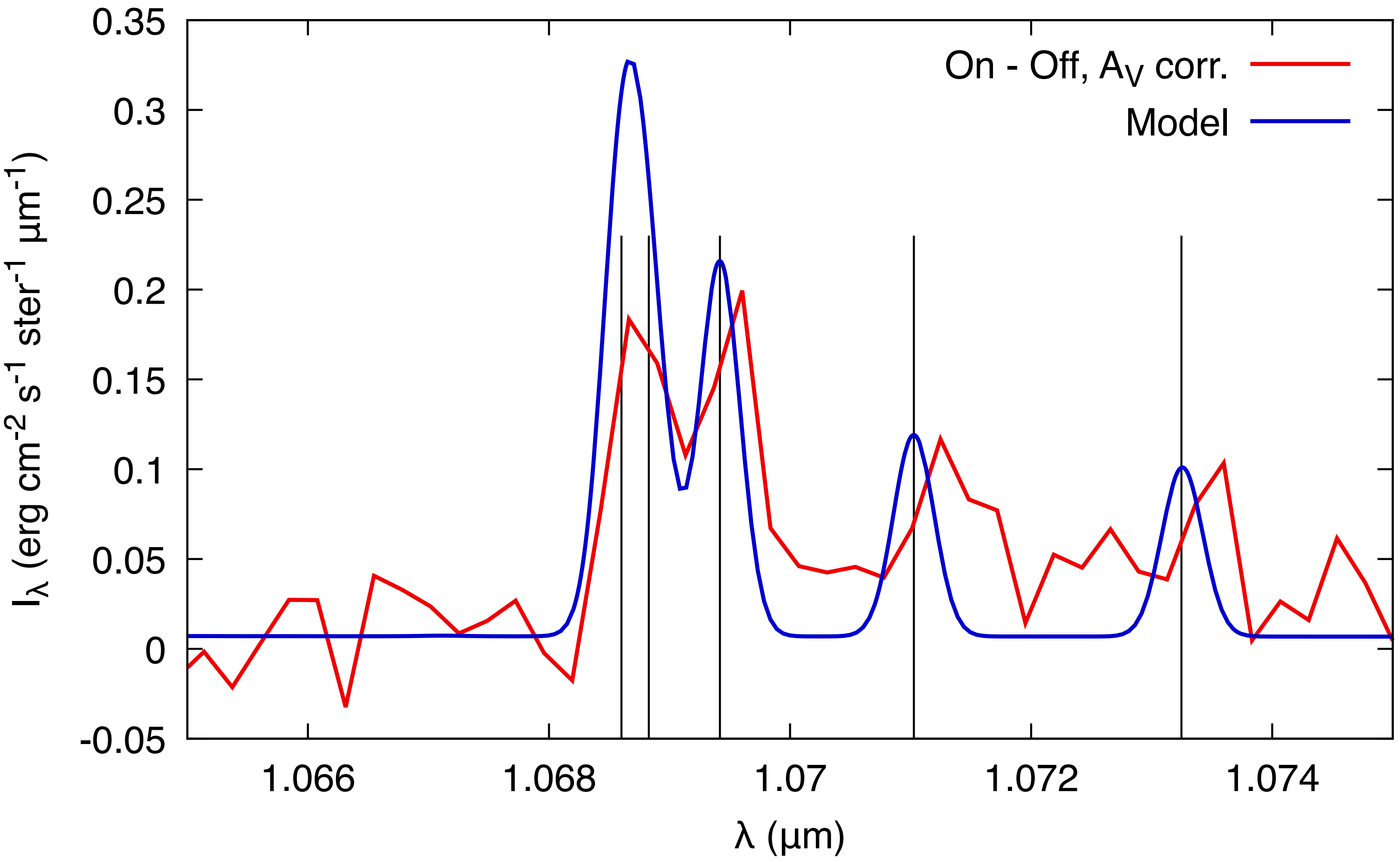
Spectrum d203-506



Meudon PDR code - Standard parameters

$+ \mathrm{C}^+ + e^-$ recombination + Radiative pumping

Spectrum d203-506



Meudon PDR code - Standard parameters

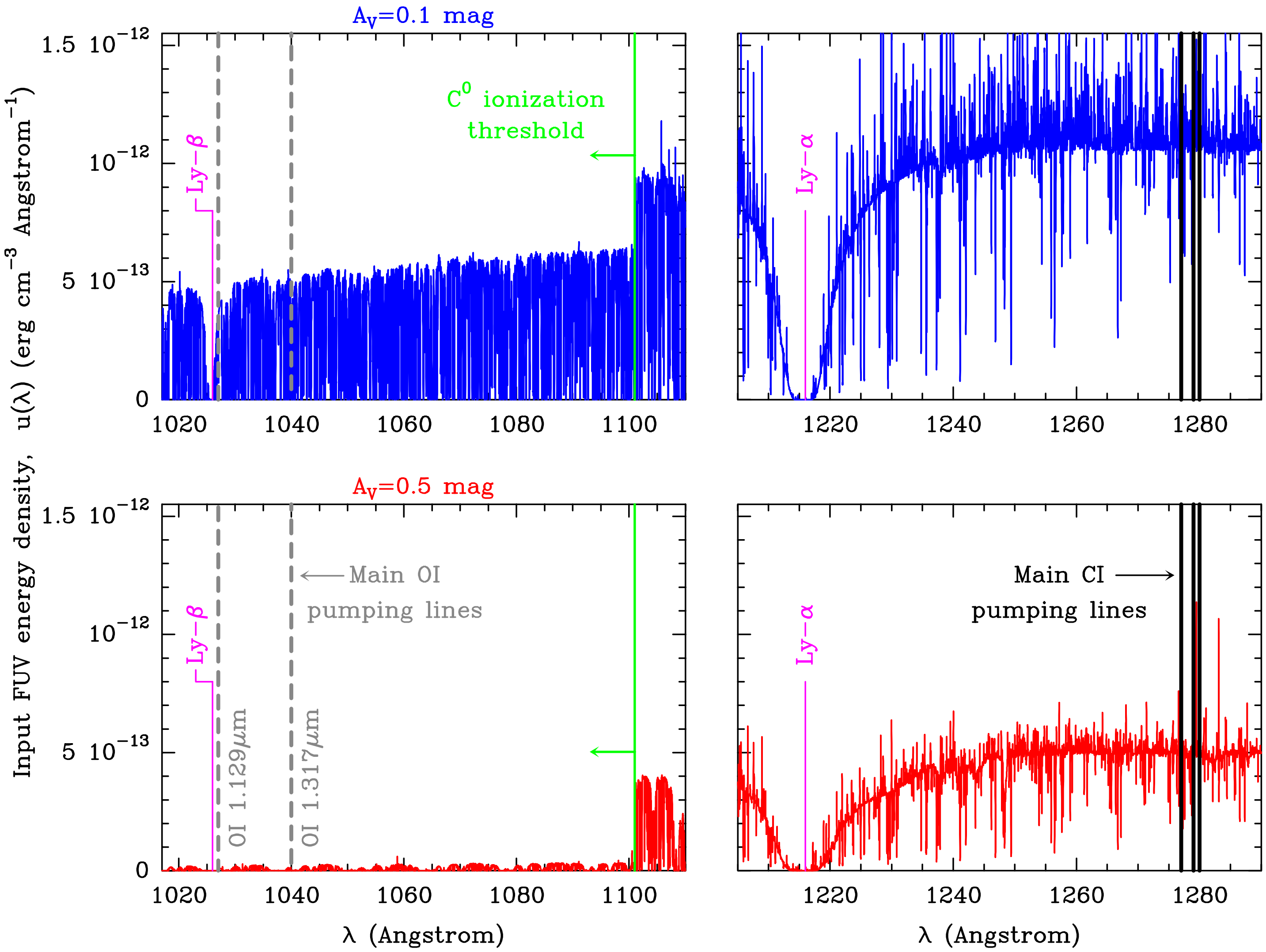
$+ \mathrm{C}^+ + e^-$ recombination + Radiative pumping

C in d203-506

Transition	λ	I_{Obs}^{On-Off} corrected	I_{PDR} (pump)	I_{PDR} (recomb)
	(μm)	$(\mathrm{erg\,cm^{-2}\,s^{-1}\,ster^{-1}})$		
$^3P_1 - {}^3P_0$	609.14	$1.62\,10^{-6}$	$1.60\,10^{-6}$	$1.60\,10^{-6}$
$^1D_2 - {}^3P_1$	0.9827	$1.94\,10^{-4}$	$1.13\,10^{-4}$	$2.02\,10^{-6}$
$^1D_2 - {}^3P_2$	0.9853	$6.57\,10^{-4}$	$3.38\,10^{-4}$	$9.17\,10^{-6}$
$(3p)\,{}^3D - {}^3P^o$	1.069	$3.23\,10^{-4}$	$2.34\,10^{-4}$	$1.40\,10^{-6}$
$(3d)\,{}^3F^o - {}^3D$	1.176	$3.08\,10^{-5}$	$4.78\,10^{-5}$	$6.40\,10^{-7}$
$(4s)\,{}^3P^o - (3p)\,{}^3S$	1.355	$4.55\,10^{-5}$	$3.30\,10^{-5}$	$8.34\,10^{-8}$

C lines come from UV pumping, not recombination.

No O lines?


A_V=0.1 mag
A_V=0.5 mag
Input FUV energy density, u(λ) (erg cm^{-3} Angstrom^{-1})
1.5 10^{-12}
10^{-12}
5 10^{-13}
0
1020
1040
1060
1080
1100
1220
1240
1260
1280
C^0 ionization threshold
Ly−β
Ly−α
Main OI pumping lines
OI 1.129μm
OI 1.317μm
Main CI pumping lines
λ (Angstrom)