The Meudon PDR code

Astrosim School

July 2017

Lecture description

Outline

- physics & algorithms
- applications
- recent updates
- conclusions

1. Introduction on PDRs
2. Assumptions
3. User Guide - first steps
4. Examples
5. Physics & algorithms
6. Applications
7. Recent updates
8. Conclusions

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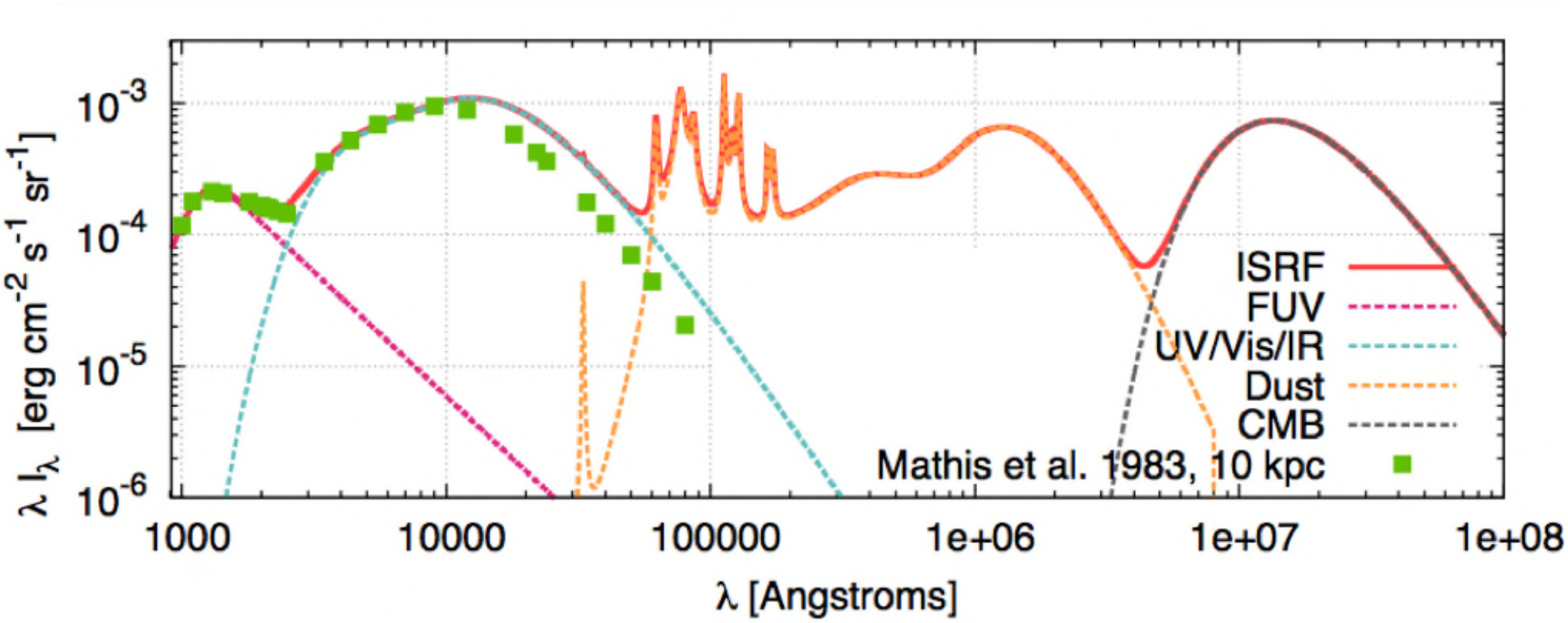
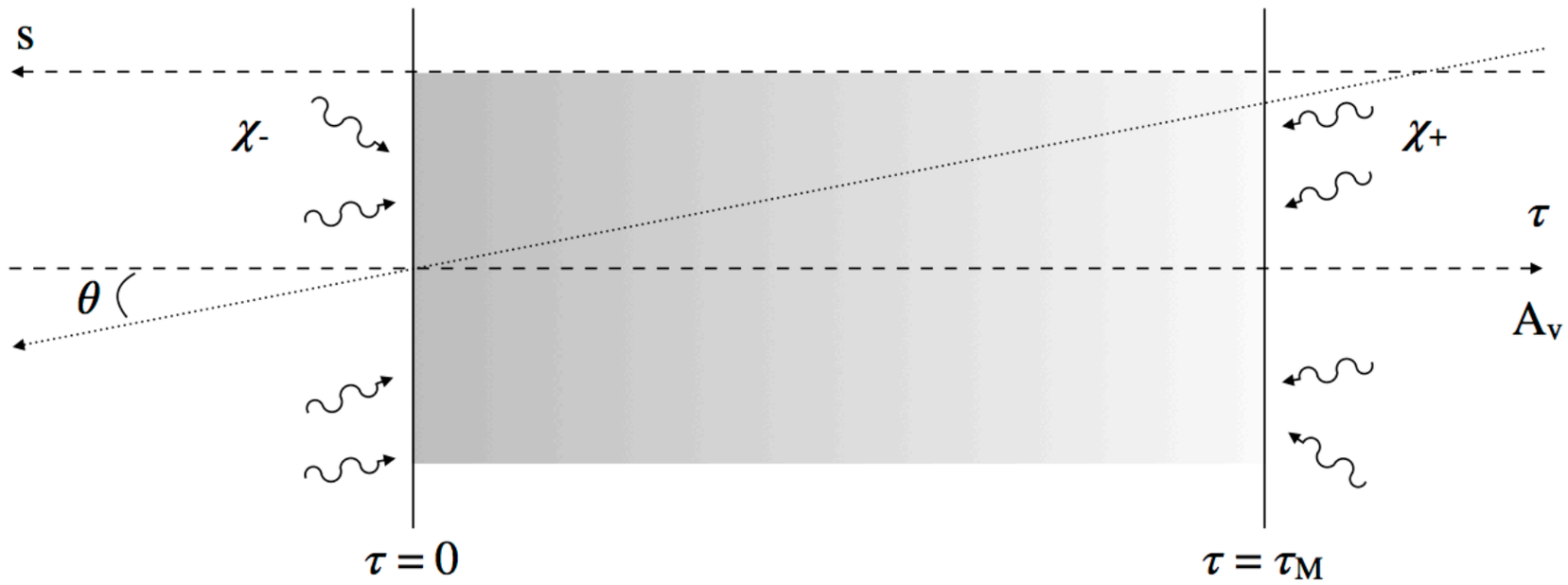
Standard interstellar radiation field



Radiative transfer



$$\mu \frac{\partial I_\lambda(s,\mu,\lambda)}{\partial s} = -\left[\kappa(s,\lambda)+\sigma(s,\lambda)\right] \times I_\lambda(s,\mu,\lambda) + \frac{\sigma}{2}\int_{-1}^{+1} p(\mu,\mu') I_\lambda(s,\mu',\lambda) d\mu' + \eta(s,\lambda)$$

Natural variables

- optical depth $\tau = -\int (\kappa+\sigma) ds$
- visible extinction $A_V = 2.5 \log_{10}(e)\ \tau(0.551\mu\mathrm{m})$

Radiative transfer

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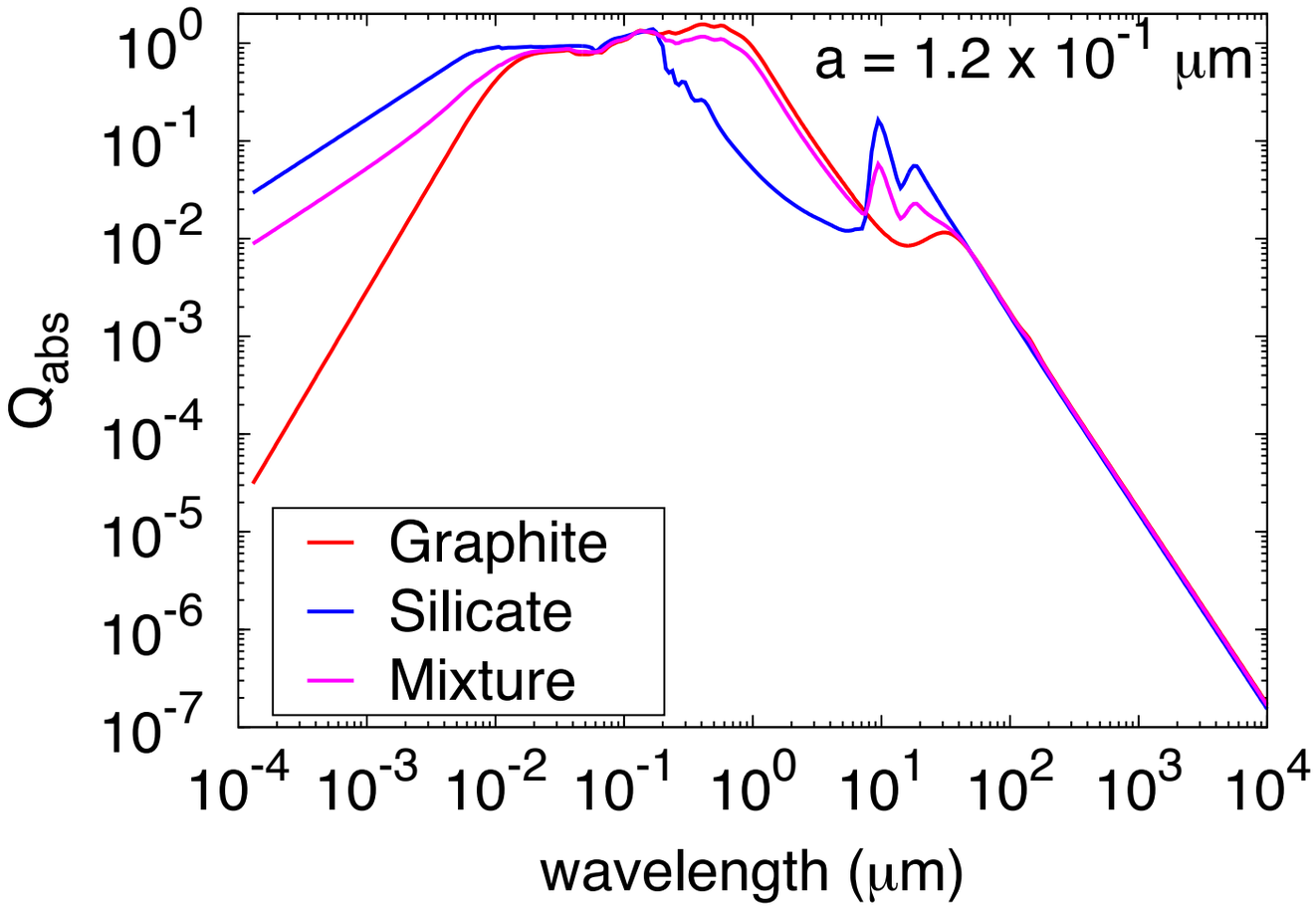
1 - absorption / emission by dust



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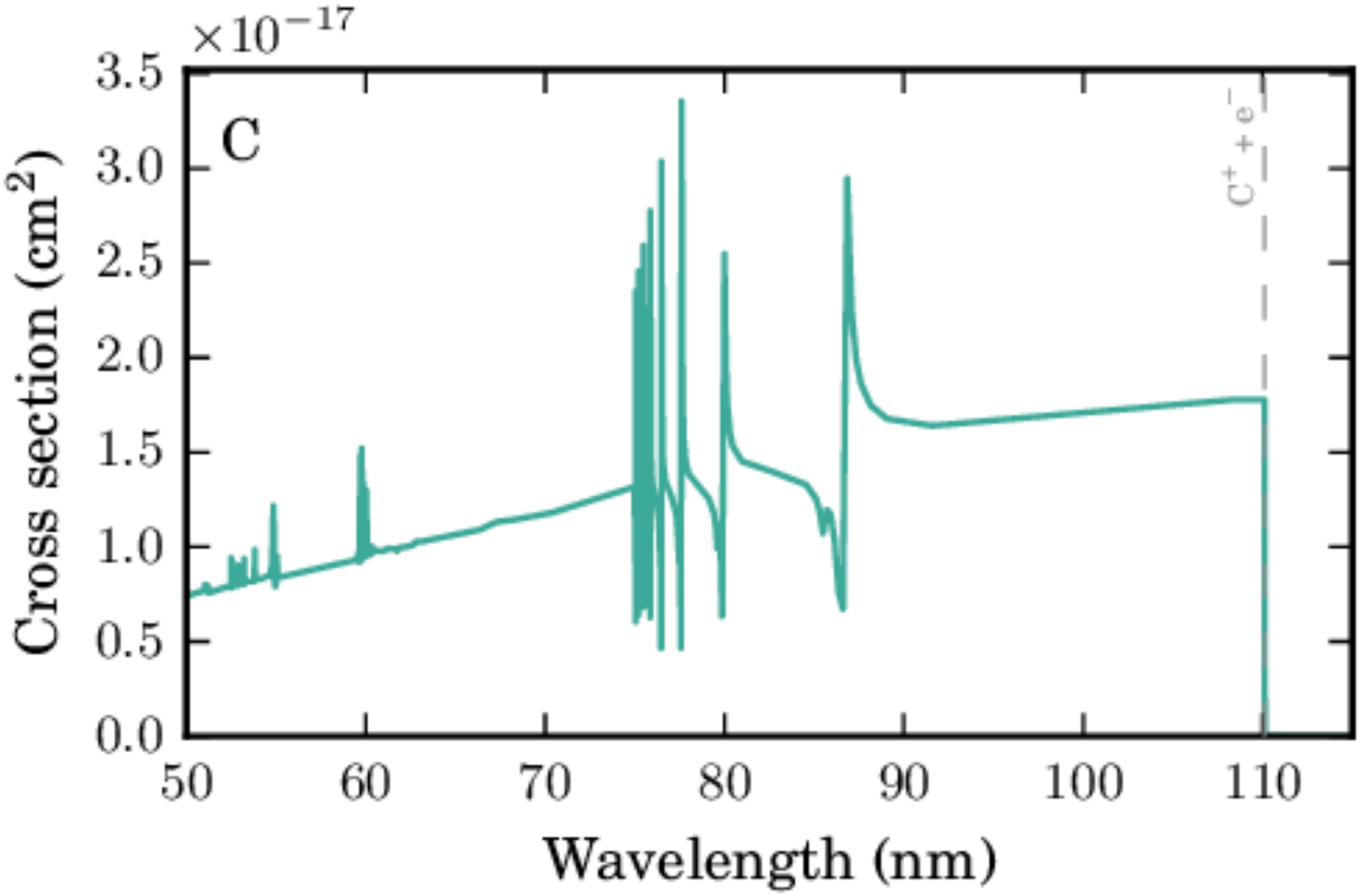
2 - absorption / emission by gas - continuum



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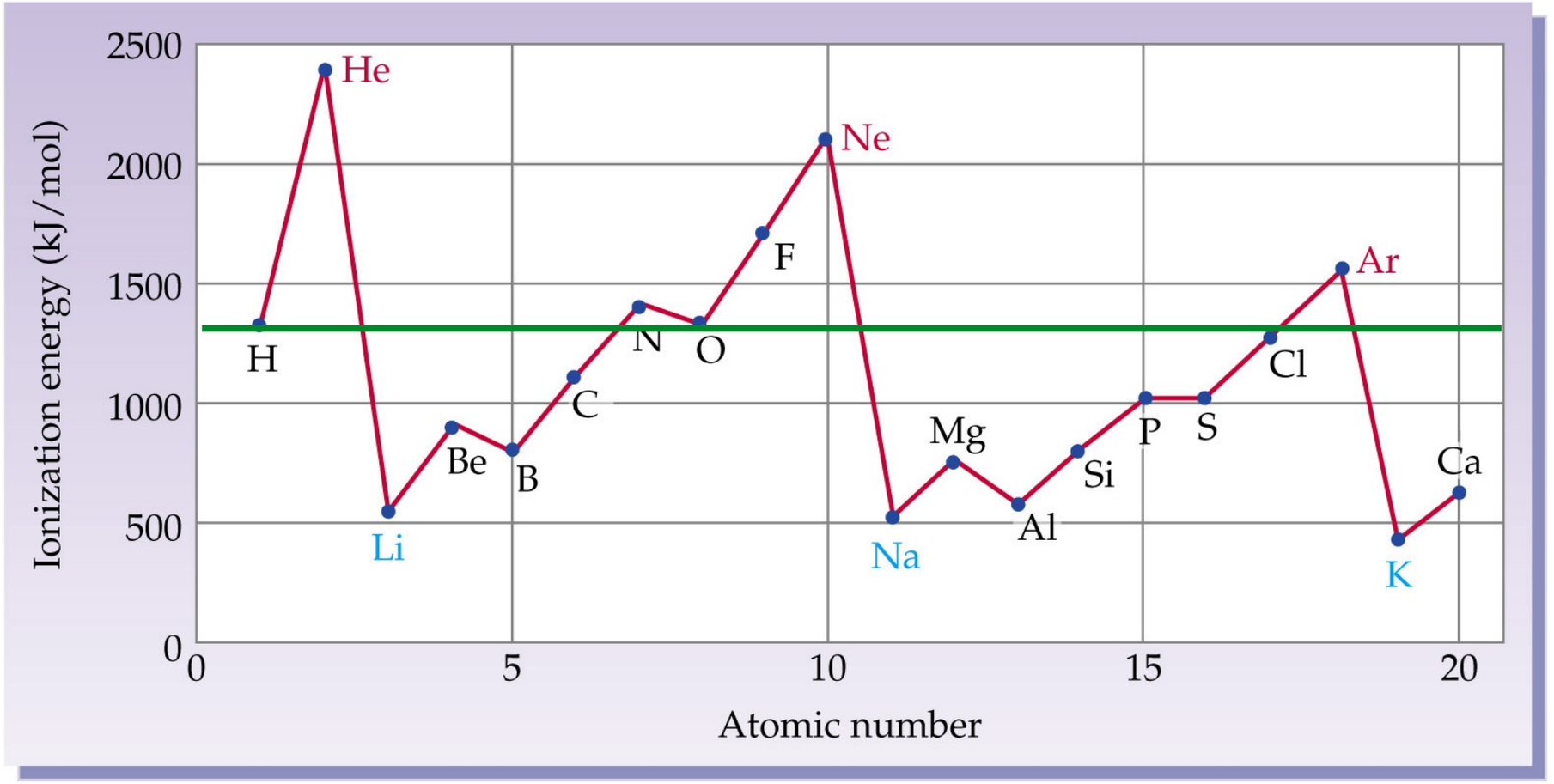

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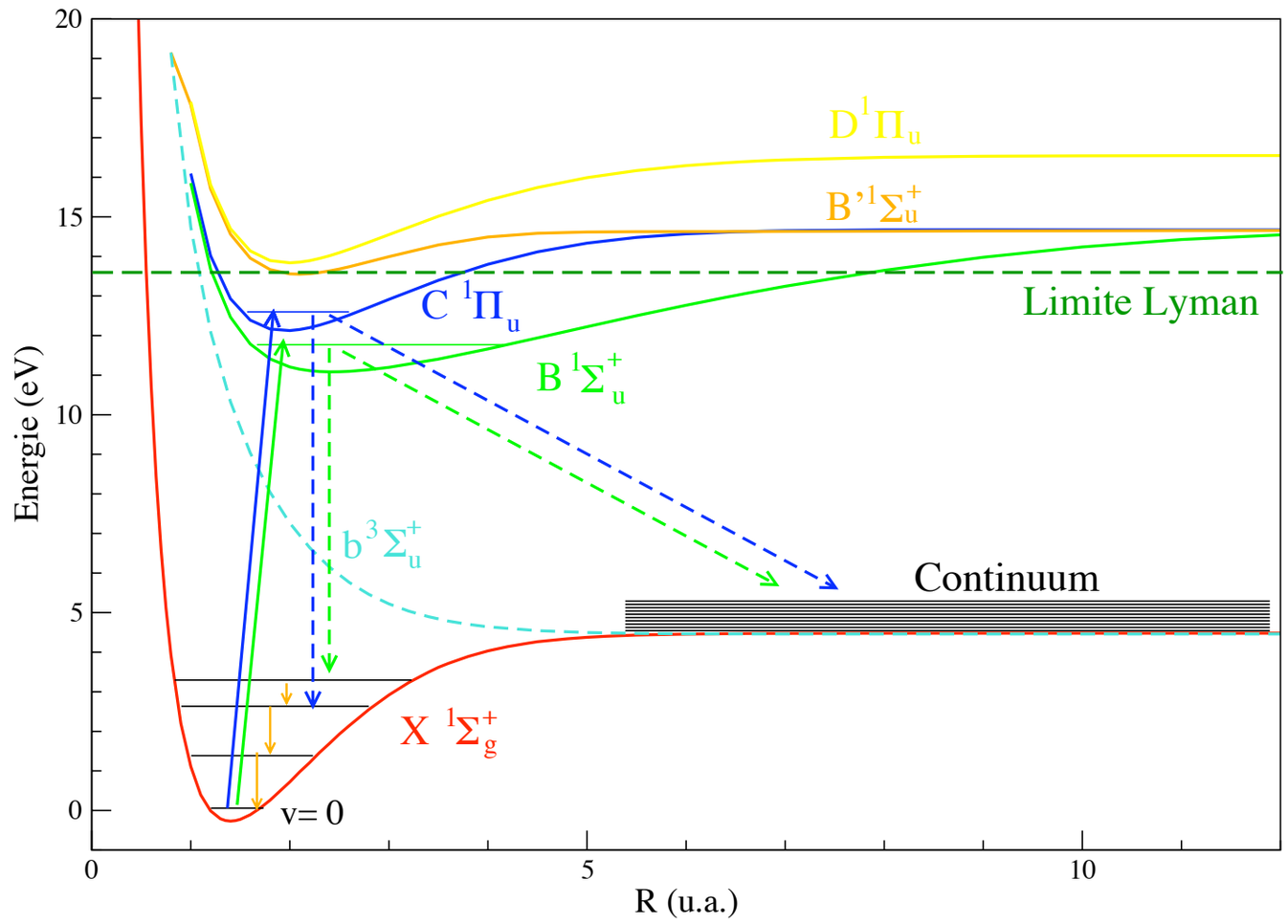
3 - absorption / emission by gas - line



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- expansion in Legendre polynomials
- linear set of partial differential equations
- boundary value problem with non constant coefficients

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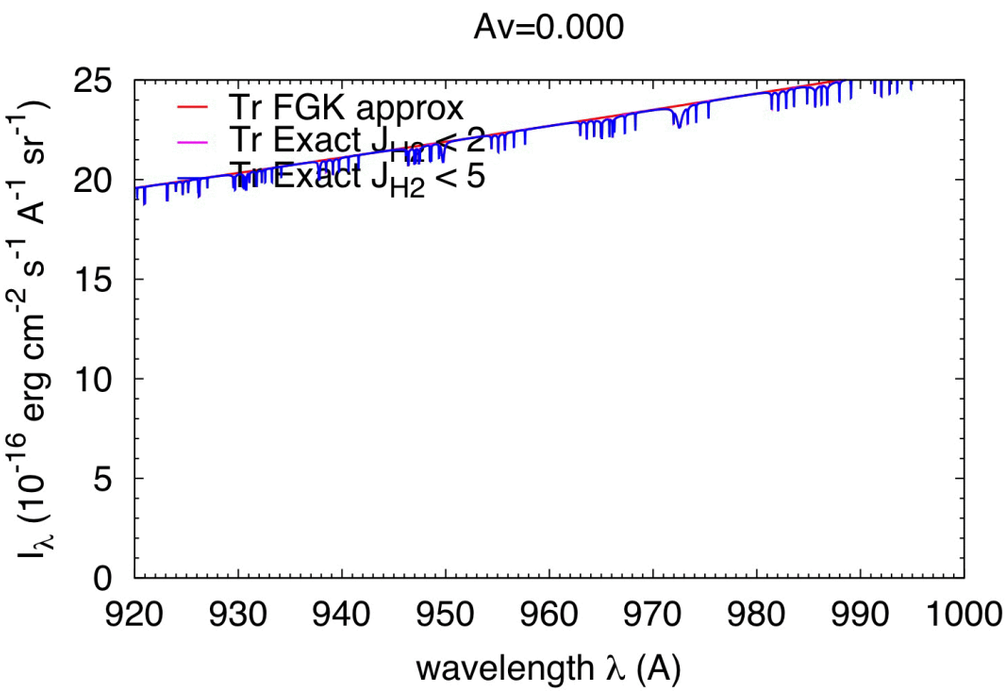

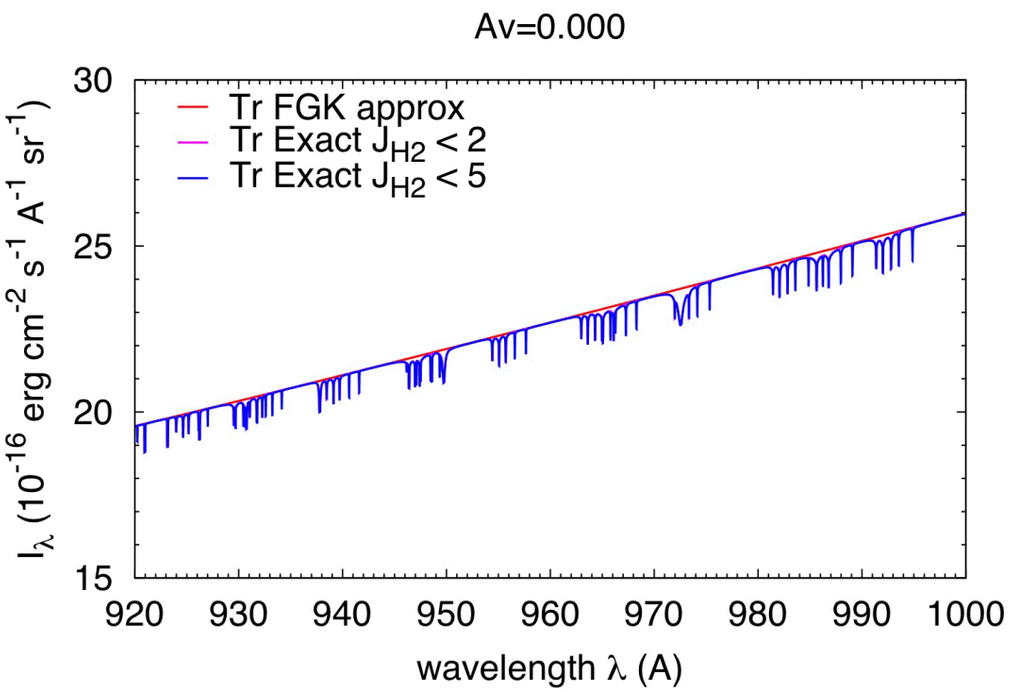

Dust treatments

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Size distribution

- big grains:

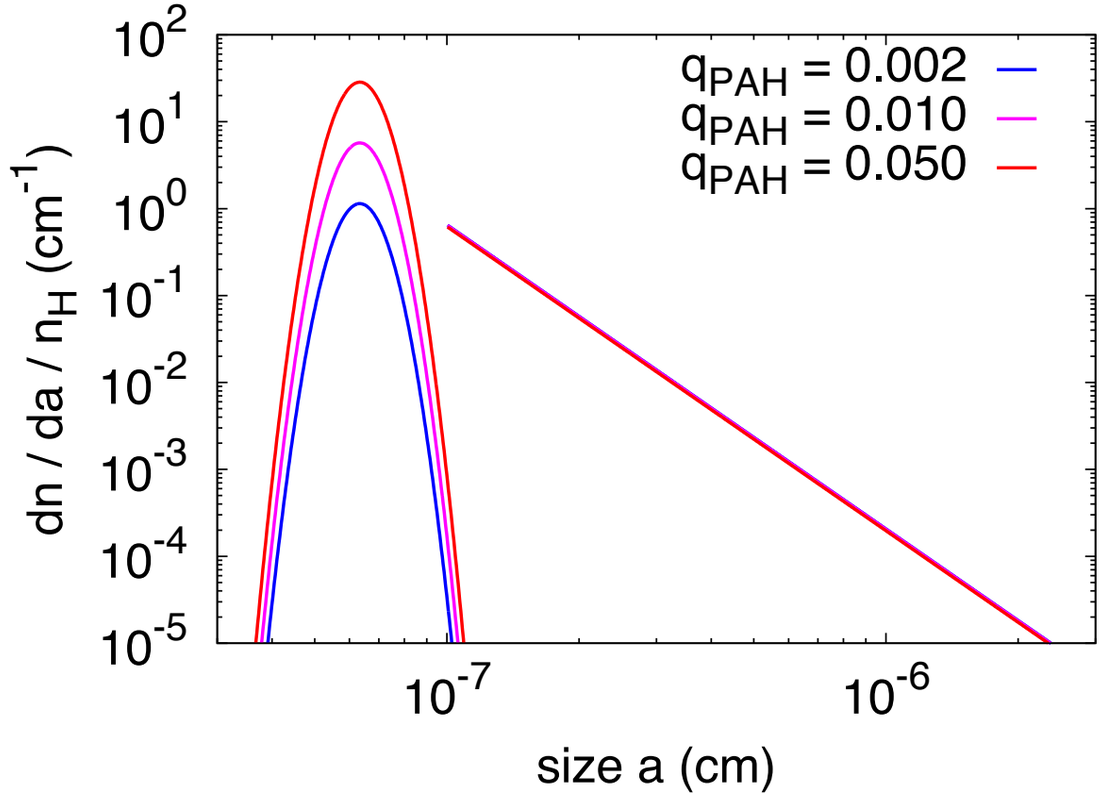
  MRN : a_{min} - a_{max}

  fixed dust / gas ratio

- PAHs

  log-normal : a_0

  fixed PAH fraction



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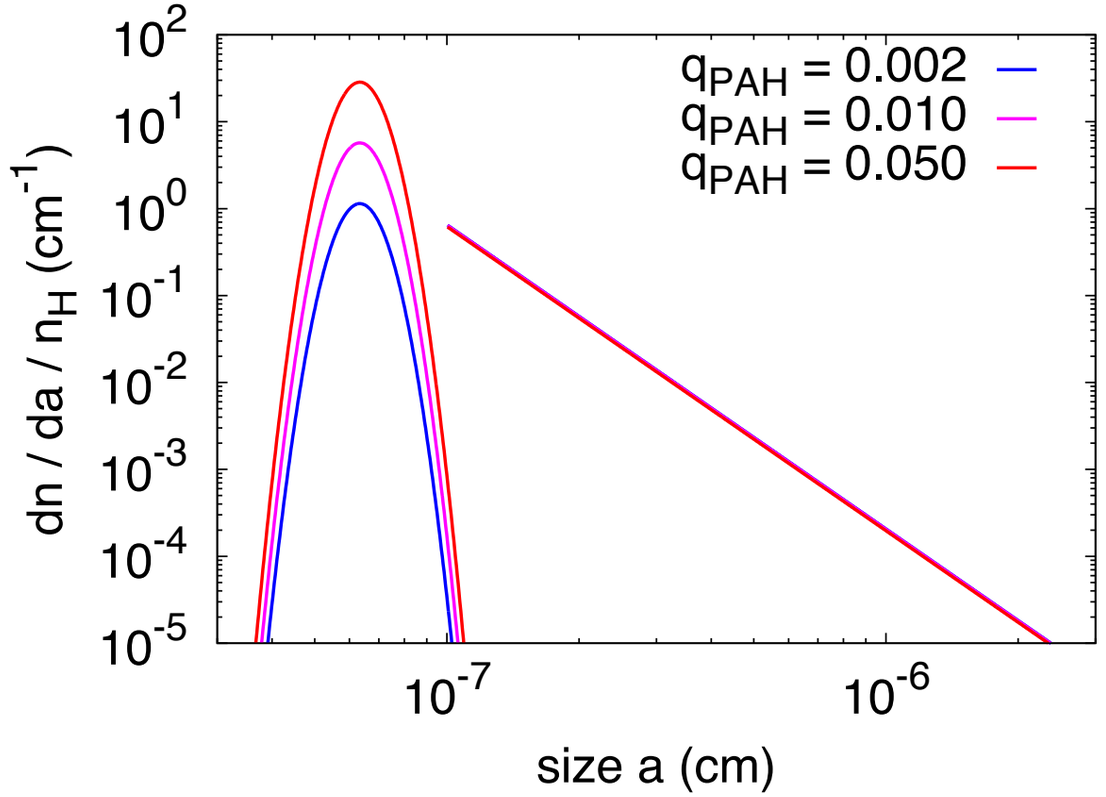

Thermal balance T_d

⇒ radiative equilibrium between absorption and emission

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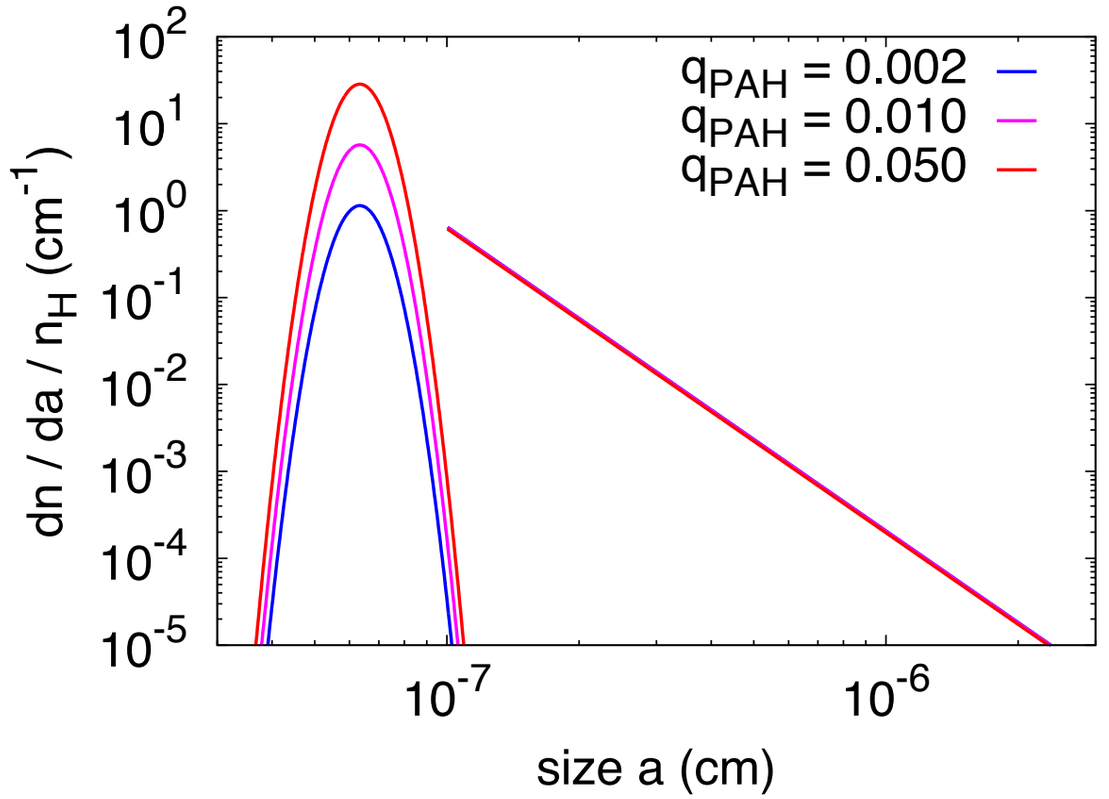

Charge distribution

GRAIN + γ → GRAIN$^+$ + e$^-$

GRAIN + C$^+$ → GRAIN$^+$ + C

GRAIN + e$^-$ → GRAIN$^-$

…

$$f_Z(Z)\left[J_{\rm pe}(Z)+\sum J_{\rm ion}(Z)\right] = f_Z(Z+1)J_e(Z+1)$$

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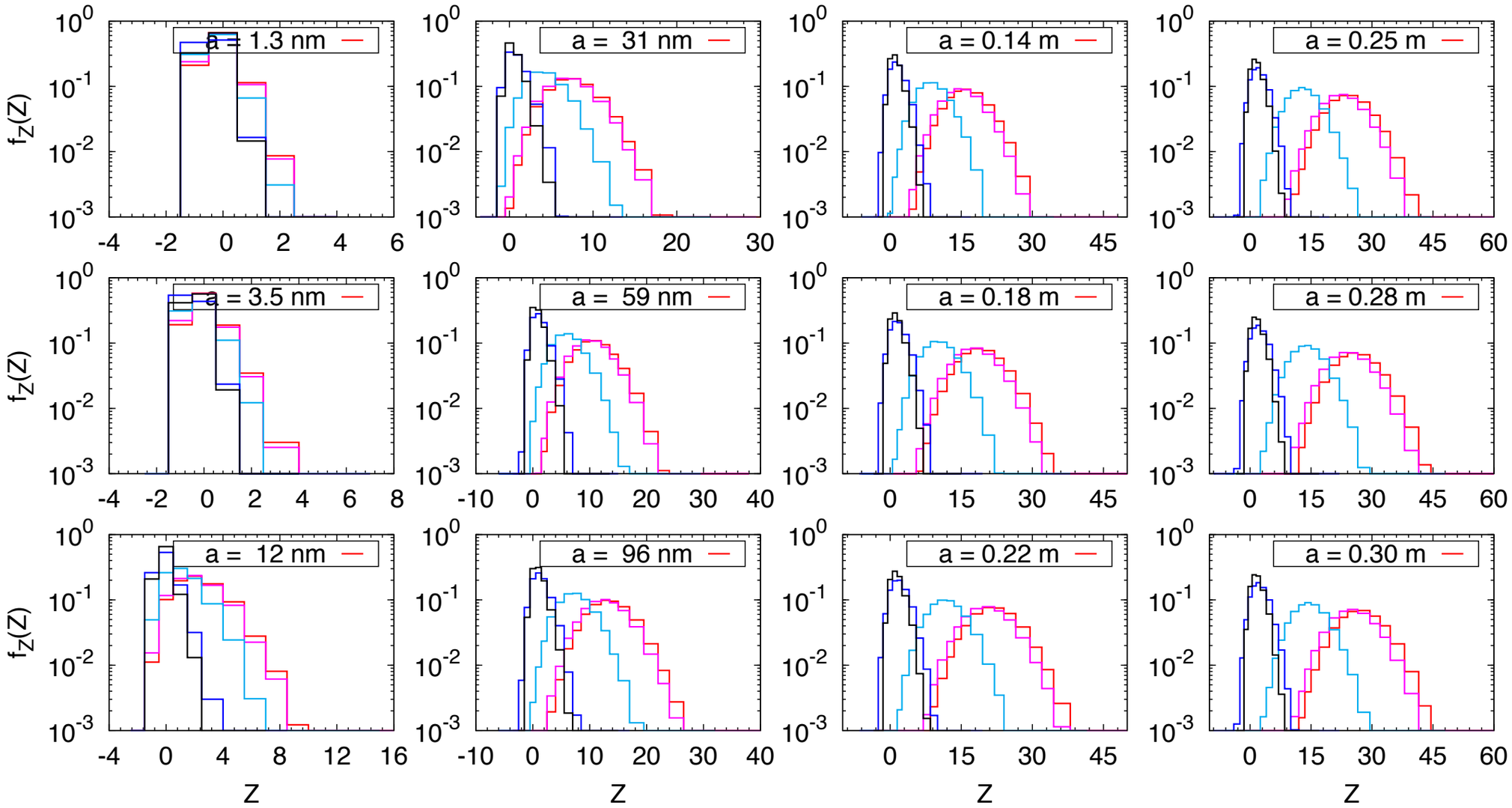

Chemistry

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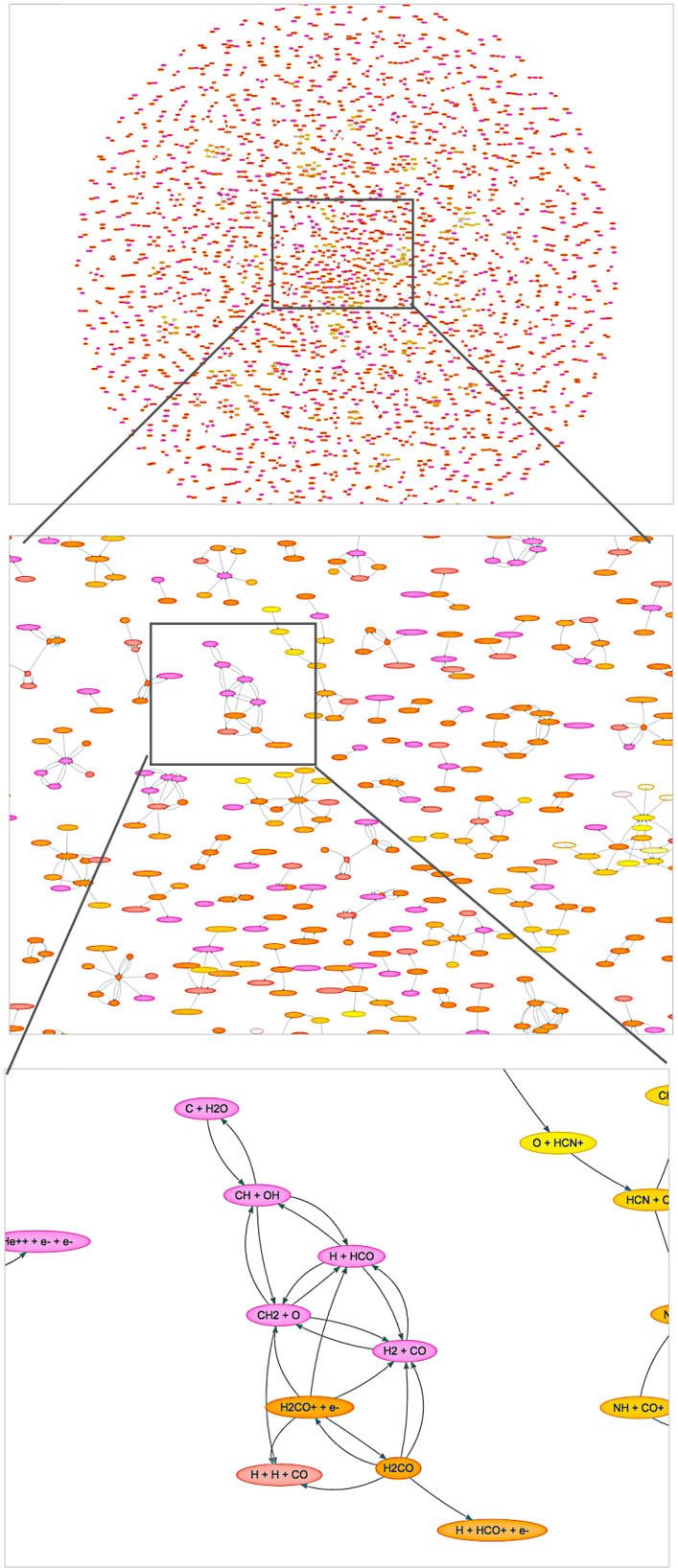
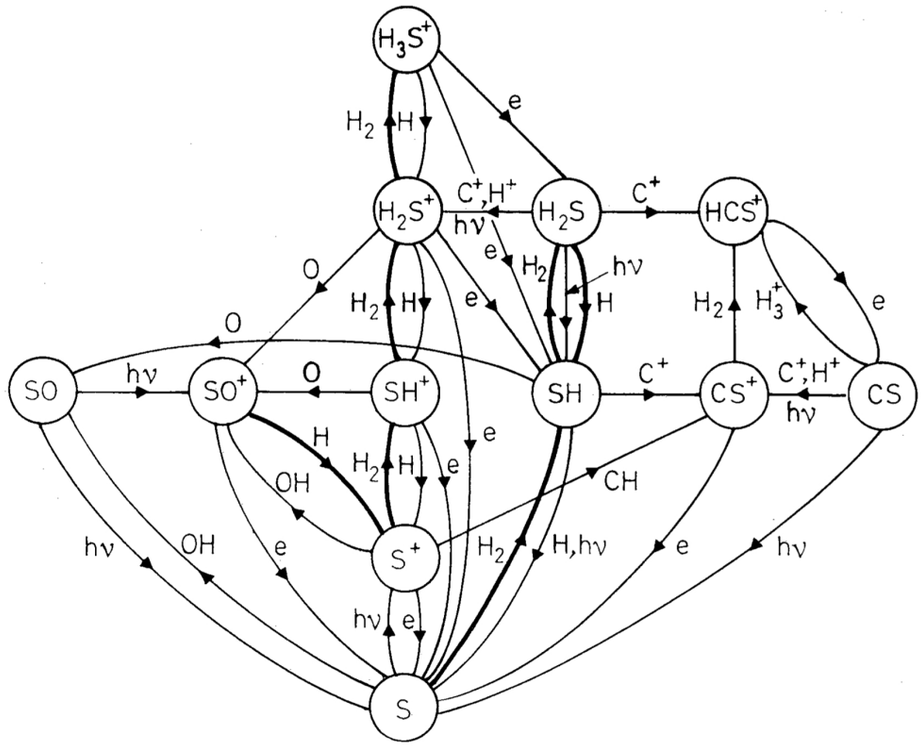
Gas phase chemistry

- hundreds species
- thousands reactions
  - ✓ photoionization
  - ✓ photodissociation
  - ✓ cosmic ray ionization
  - ✓ 2-bodies reactions





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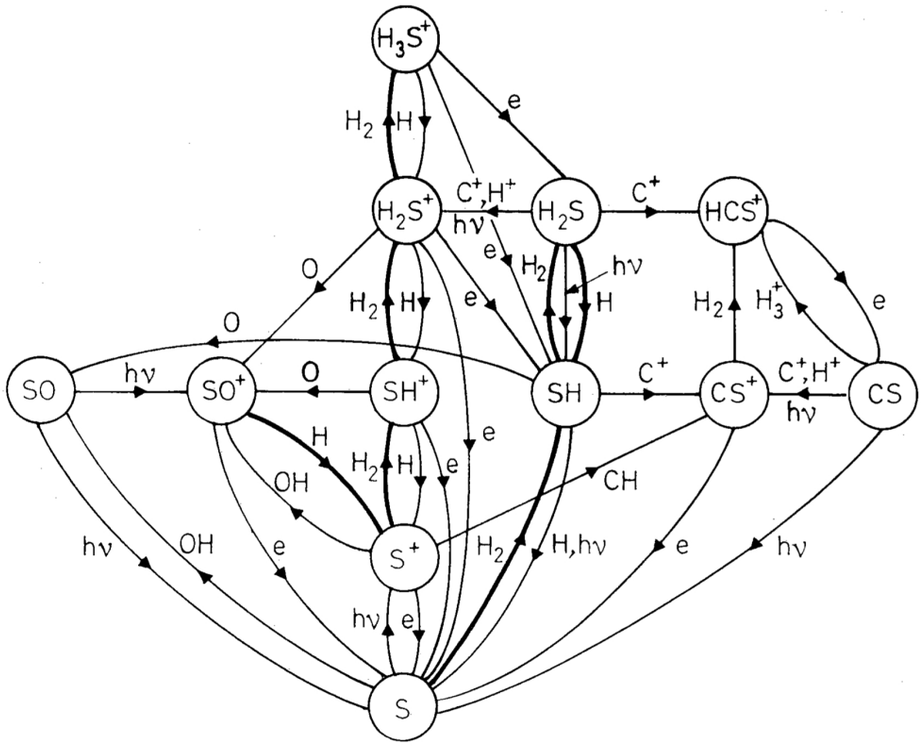
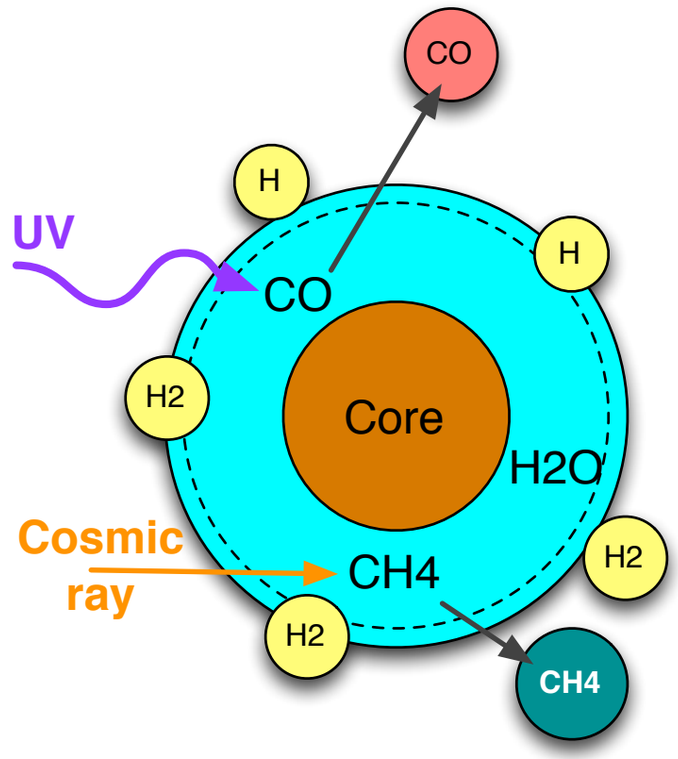


Surface chemistry

- adsorption, desorption
- migration
- mantle formation
- reactions on dust



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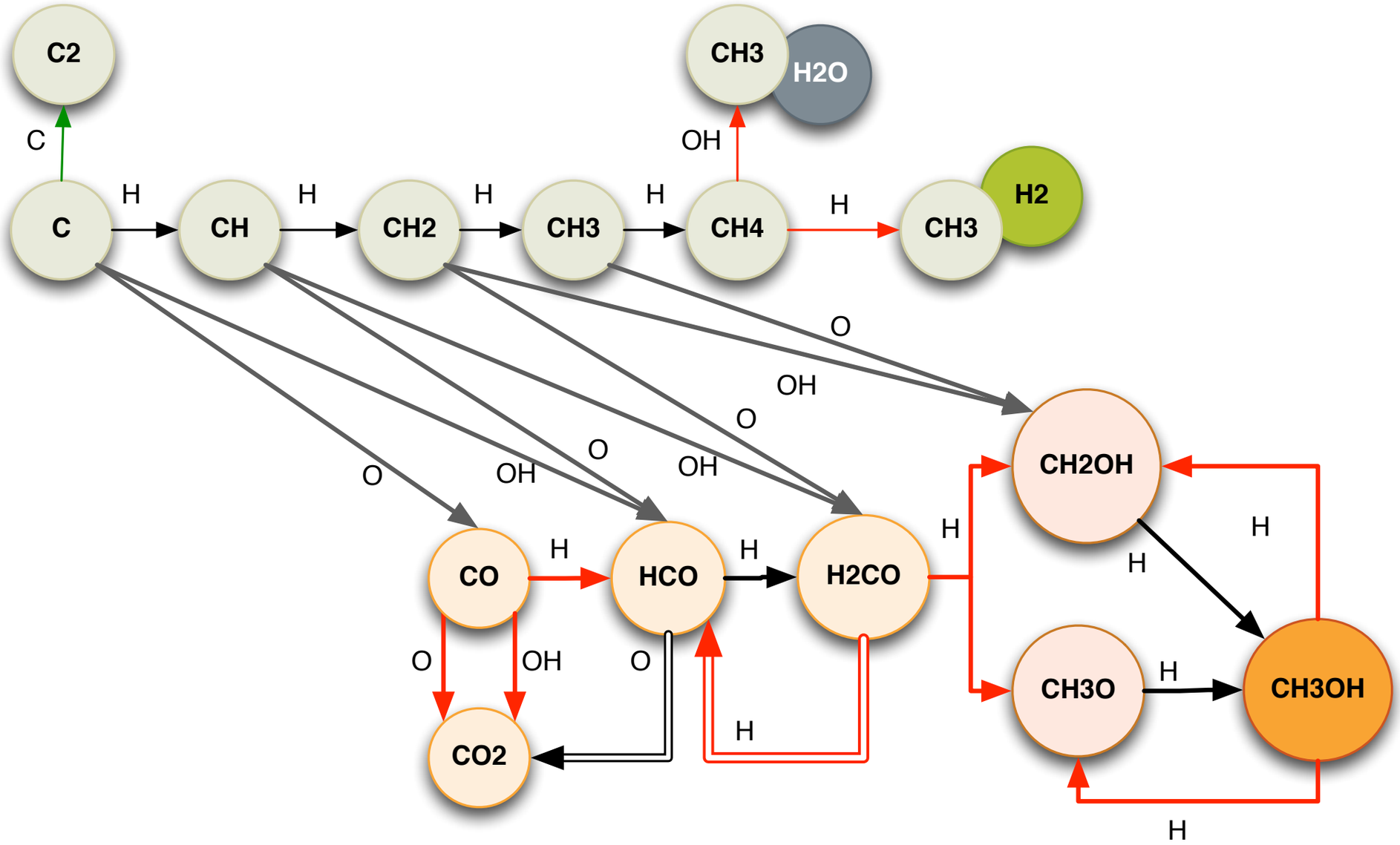

methanol network on dust surfaces

Le Petit et al. (in prep)

Chemistry

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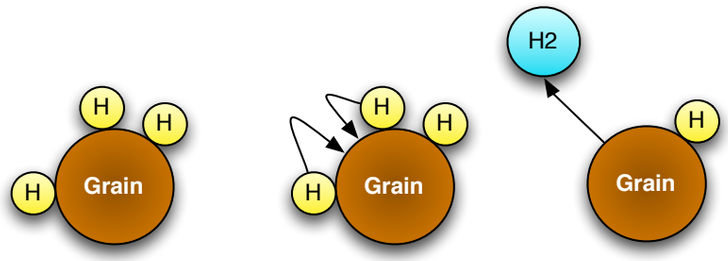
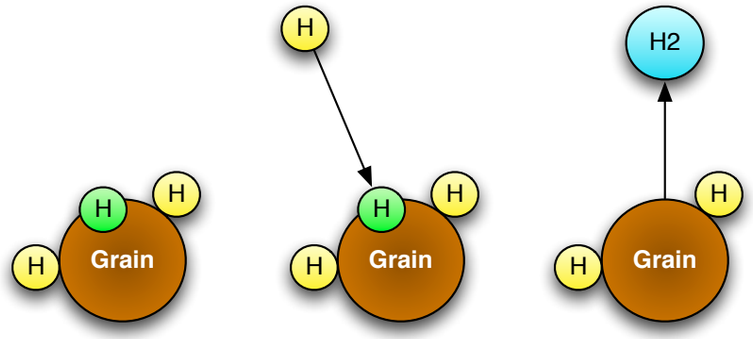
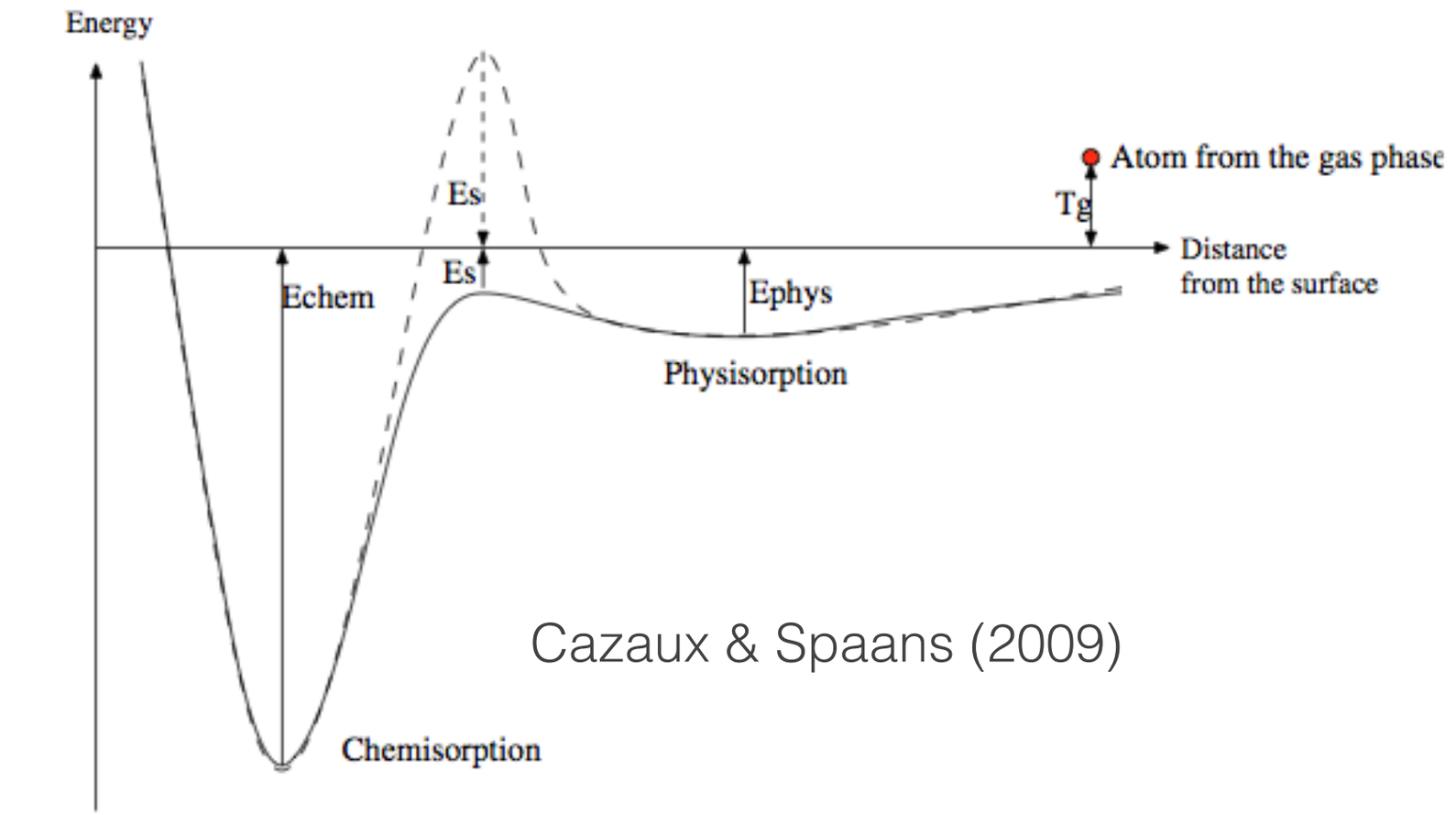
- Langmuir-Hinshelwood
  - ✓ physisorption (hundreds K)
  - ✓ efficiency depends on T_d



- Eley-Rideal
  - ✓ chemisorption (thousands K)
  - ✓ efficiency depends on T_g





Cazaux & Spaans (2009)

Initial conditions

element	X	[X] / [H]	gas phase	grains
helium	He	1.00×10^{-1}	1.00×10^{-1}	
carbon	C	3.55×10^{-4}	1.38×10^{-4}	2.17×10^{-4}
oxygen	O	4.42×10^{-4}	3.02×10^{-4}	1.40×10^{-4}
nitrogen	N	7.94×10^{-5}	7.94×10^{-5}	
sulfur	S	1.86×10^{-5}	1.86×10^{-5}	
magnesium	Mg	3.70×10^{-5}		3.70×10^{-5}
silicon	Si	3.37×10^{-5}		3.37×10^{-5}
iron	fe	3.23×10^{-5}	1.50×10^{-8}	3.23×10^{-5}

$$\frac{dn(\mathrm{X})}{dt} = \sum_{j}^{N_F(\mathrm{X})} n_j(V_j) n_j(W_j) k_{F,j} - n(\mathrm{X}) \sum_{j}^{N_D(\mathrm{X})} n_j(Y_j) k_{D,j} = 0$$

- chemical kinetics data required (e.g. KIDA)
- steady-state: ordinary algebraic equations
- closure: conservation of elemental abundances
- Newton-Raphson integrator

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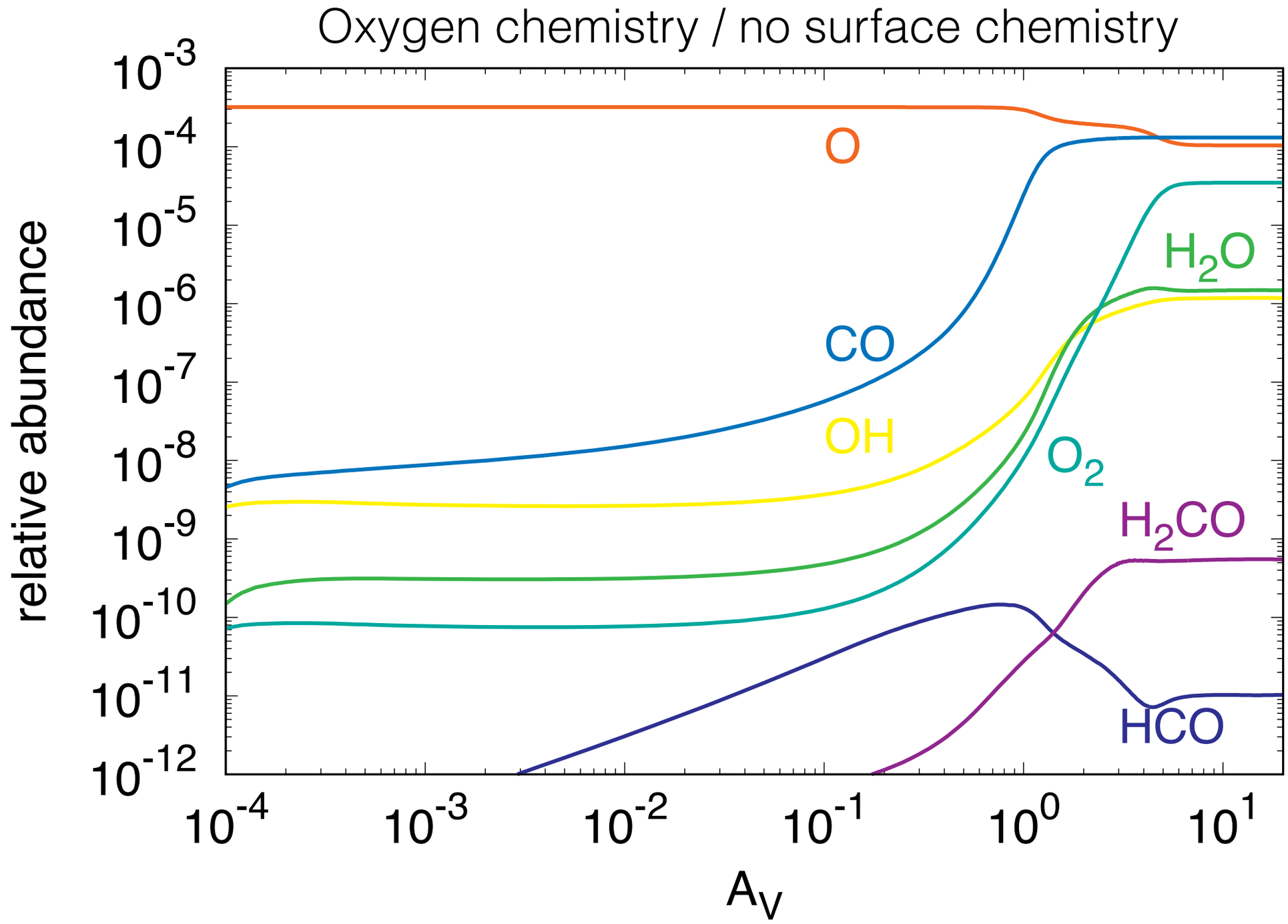

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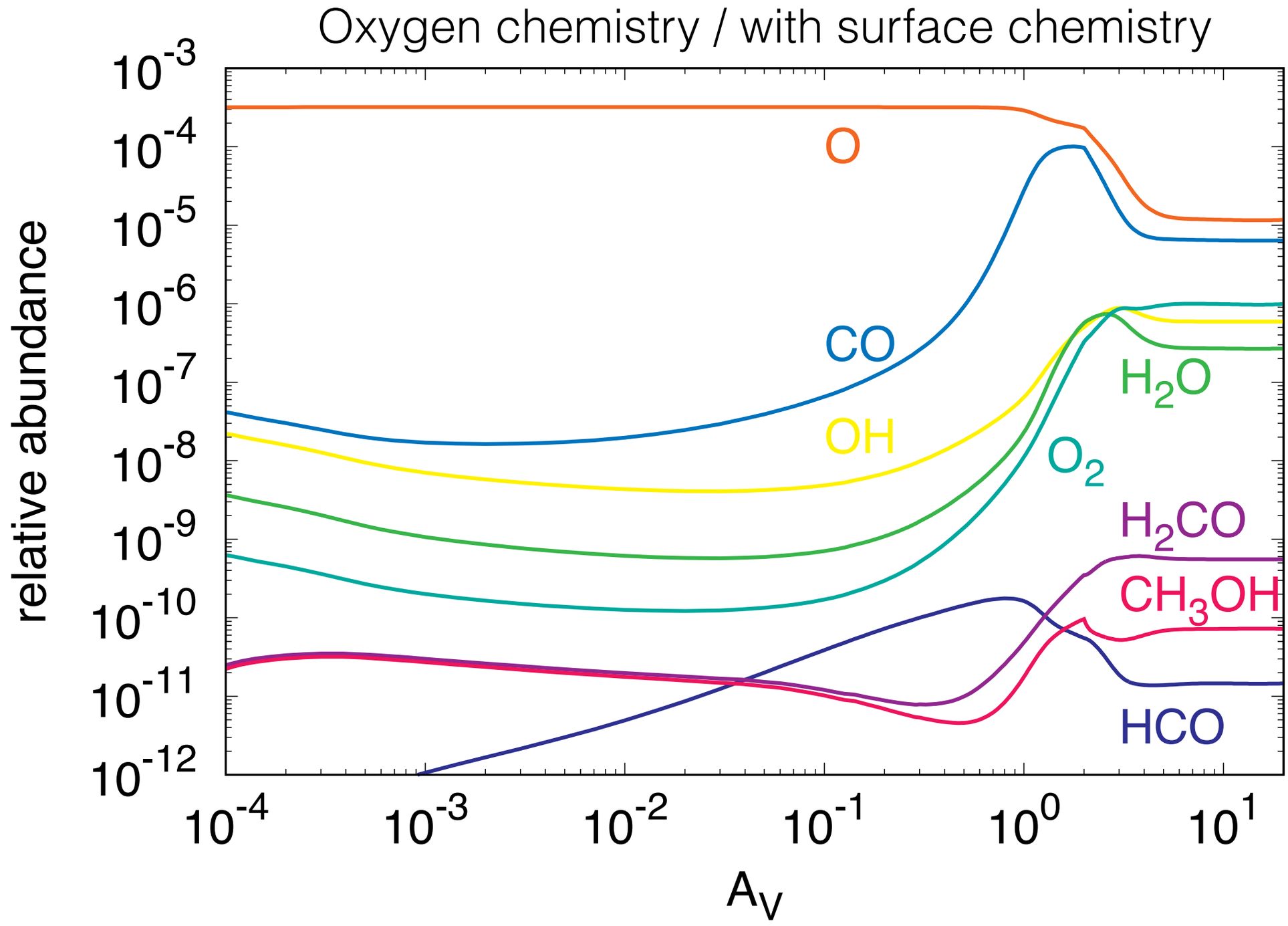

Excitation

$$\frac{dn_i}{dt} = \sum_F \langle n_{\gamma,\nu} \rangle n_{F_a} n_{F_b} k_i^F + \sum_c \sum_j n_c n_j k_{ji}^c +$$
$$\sum_j n_j (A_{ji} + \langle n_{\gamma,\nu} \rangle A_{ji} + \frac{g_i}{g_j} \langle n_{\gamma,\nu} \rangle A_{ij}) -$$
$$n_i \Bigg[\sum_D n_D k_i^D + \sum_C \sum_j n_C k_{ij}^C +$$
$$\sum_j (A_{ij} + \langle n_{\gamma,\nu} \rangle A_{ij} + \frac{g_j}{g_i} \langle n_{\gamma,\nu} \rangle A_{ji}) +$$
$$\int \frac{4\pi}{h\nu} \sigma_i^\gamma(\nu) I_\nu d\nu \Bigg] = 0$$

- tens species, thousands levels
- radiative pumping,fluorescence
- collisions (H, H_2, He, e^-)
- (de)excitation formation / destruction
- set of linear equations

Excitation

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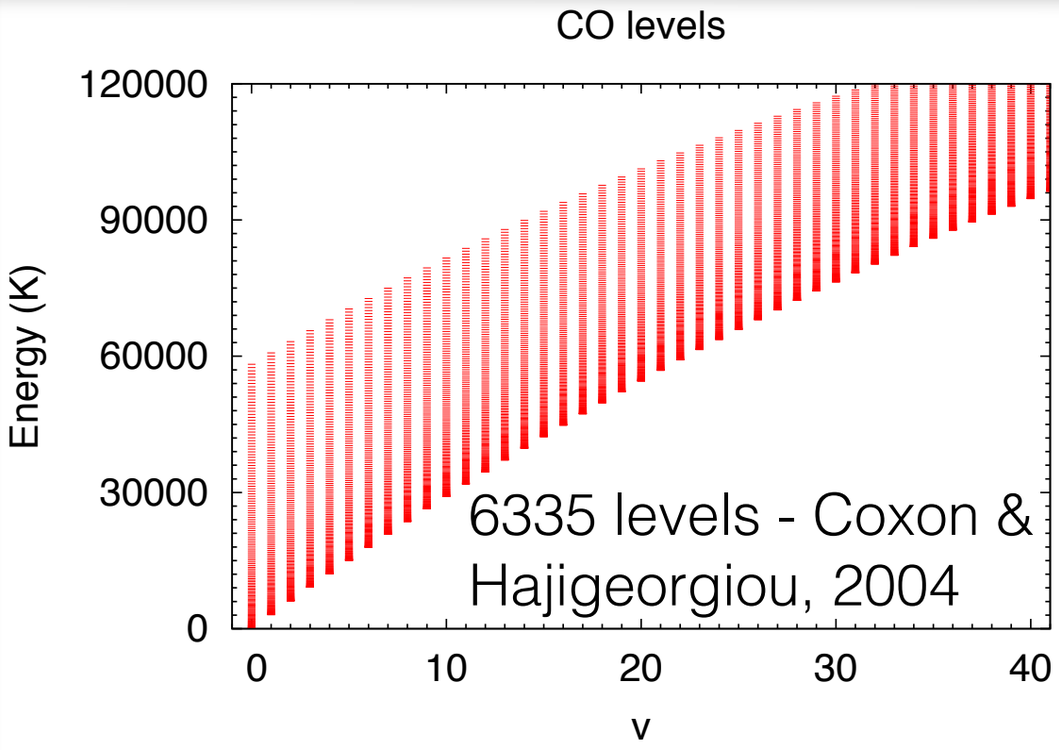

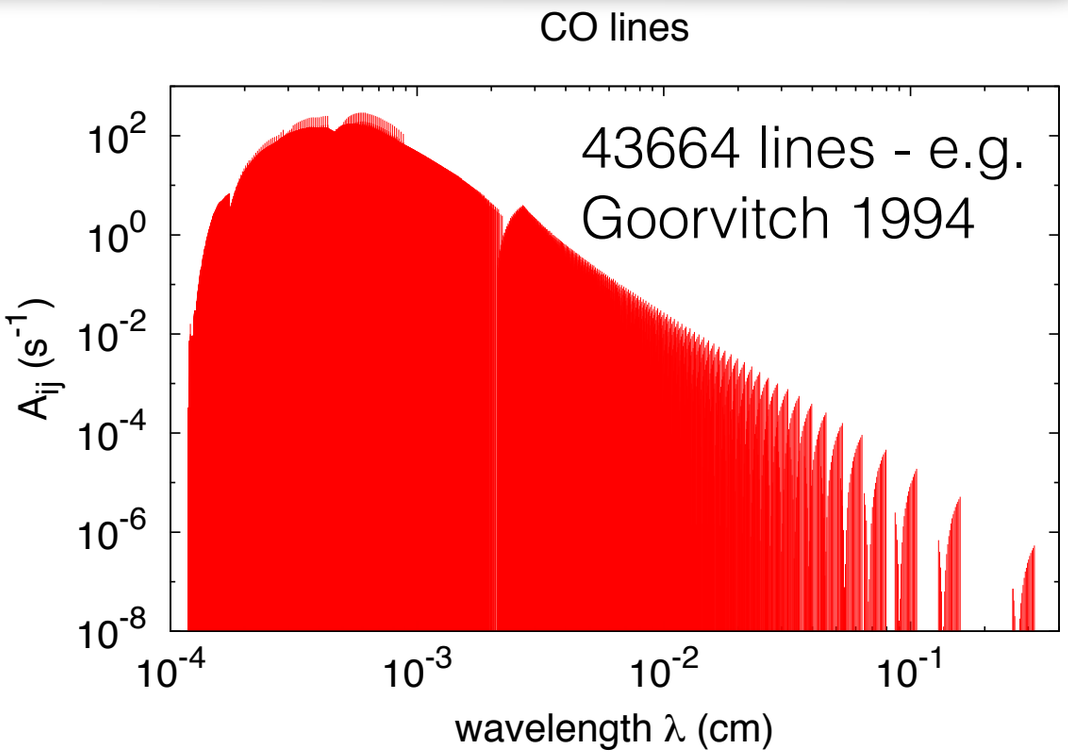

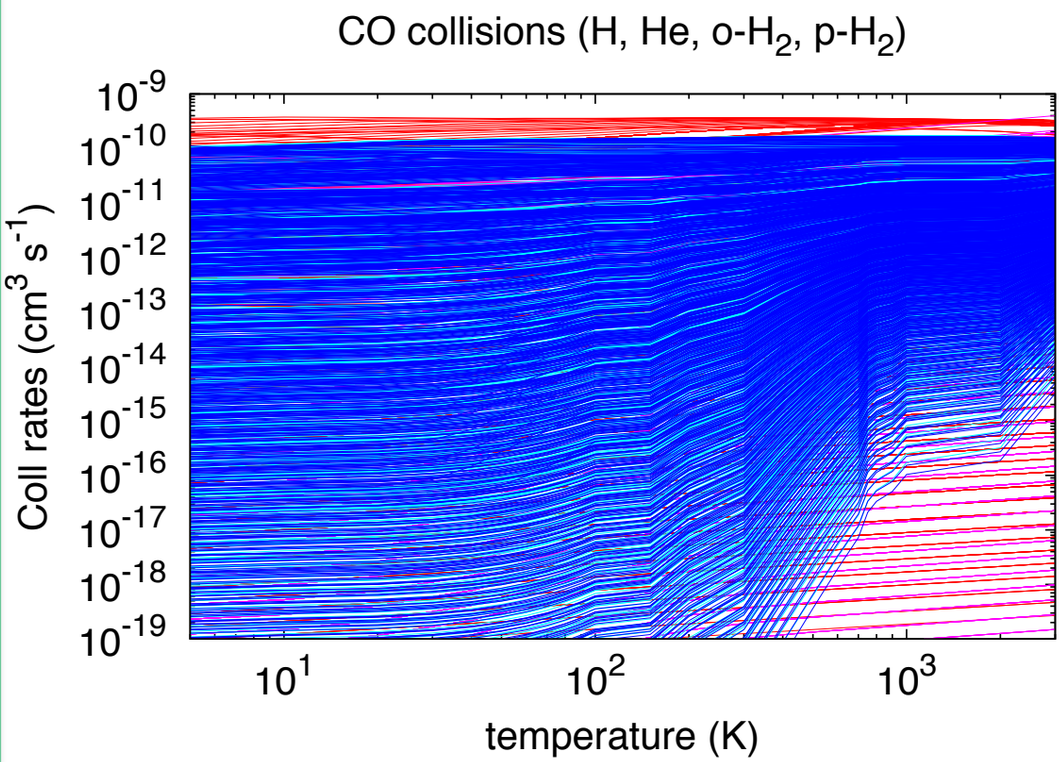

State-to-state chemistry ?

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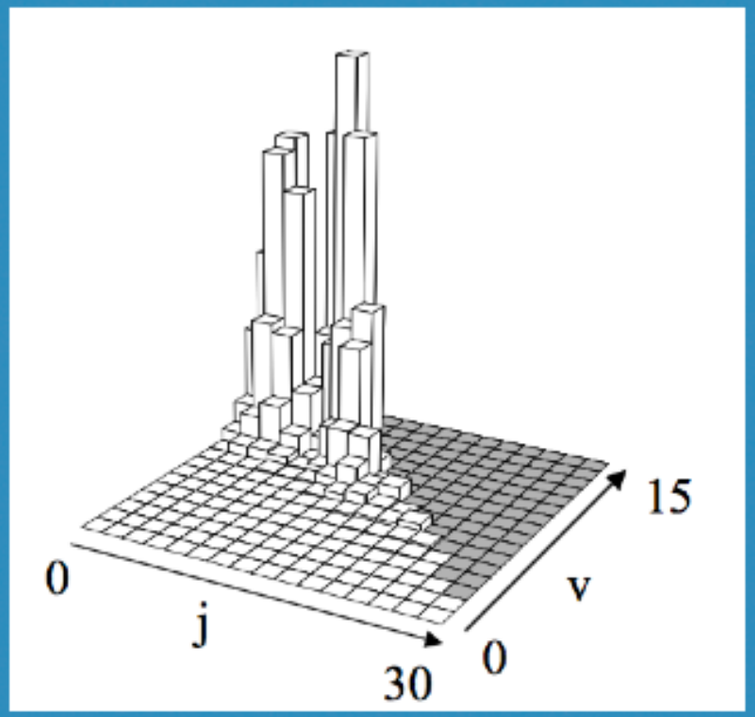
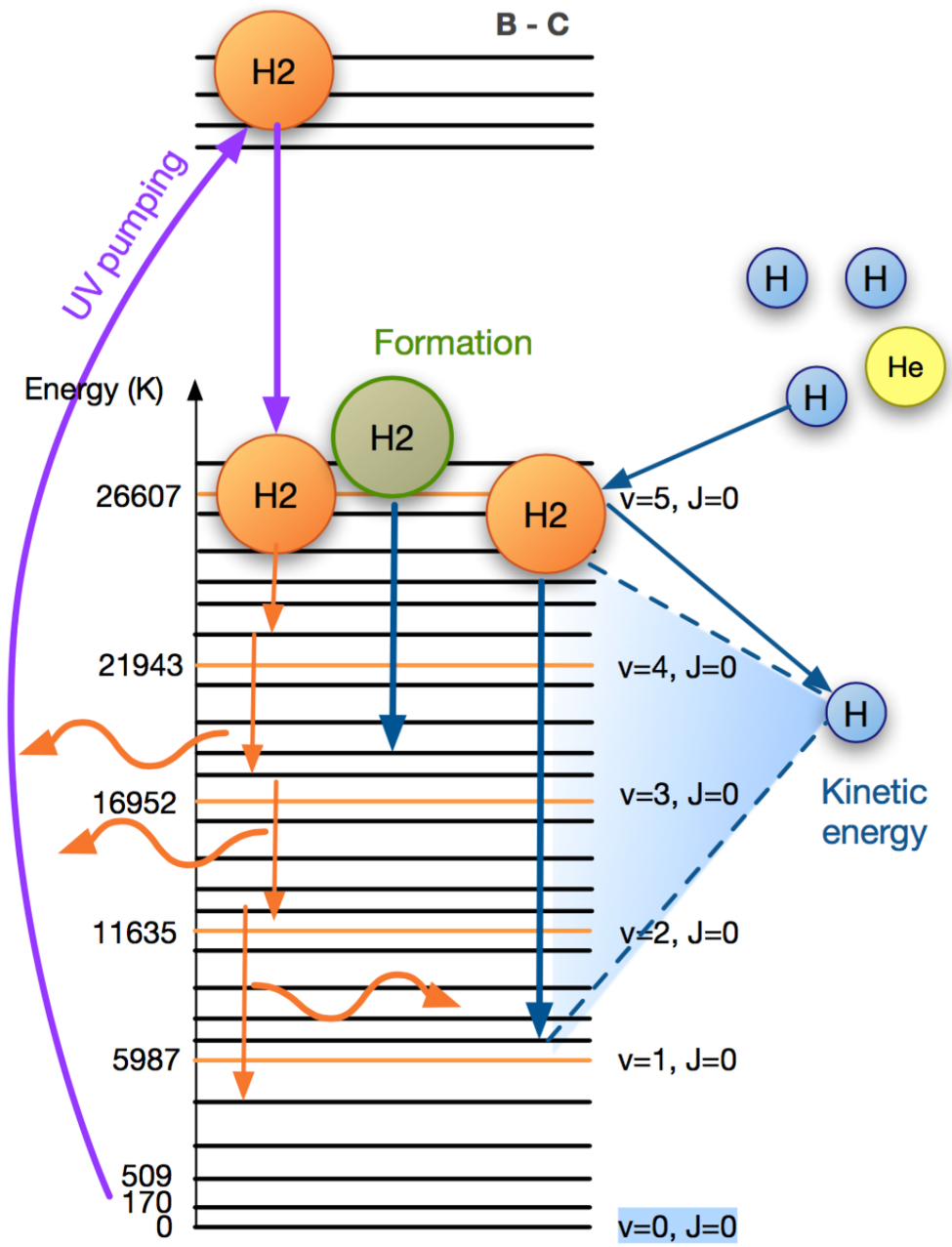
H_2 excitation at formation

Langmuir-Hinshelwood



Moriset S. (PhD thesis)
Sizun et al. (2010)



Thermal balance

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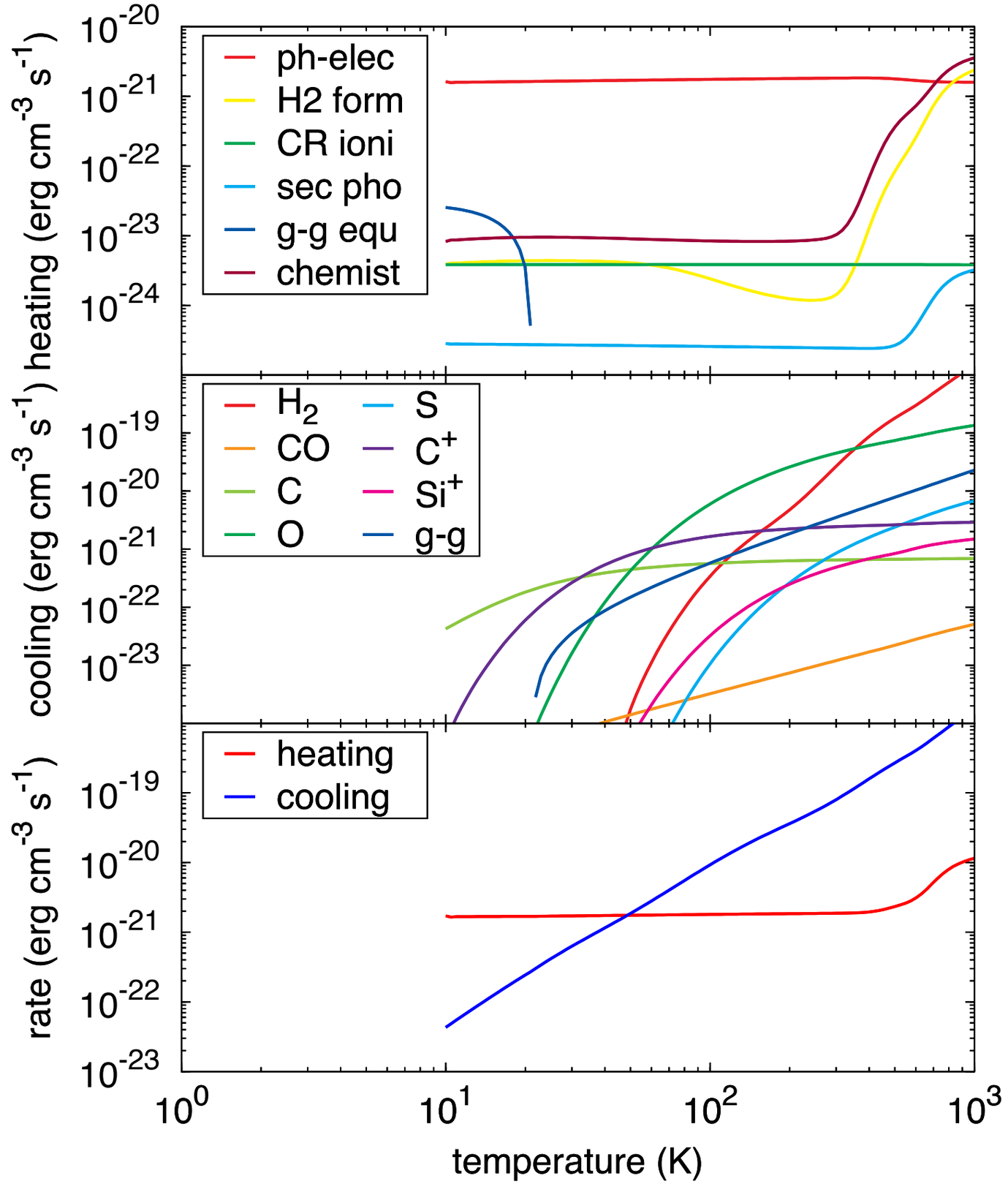

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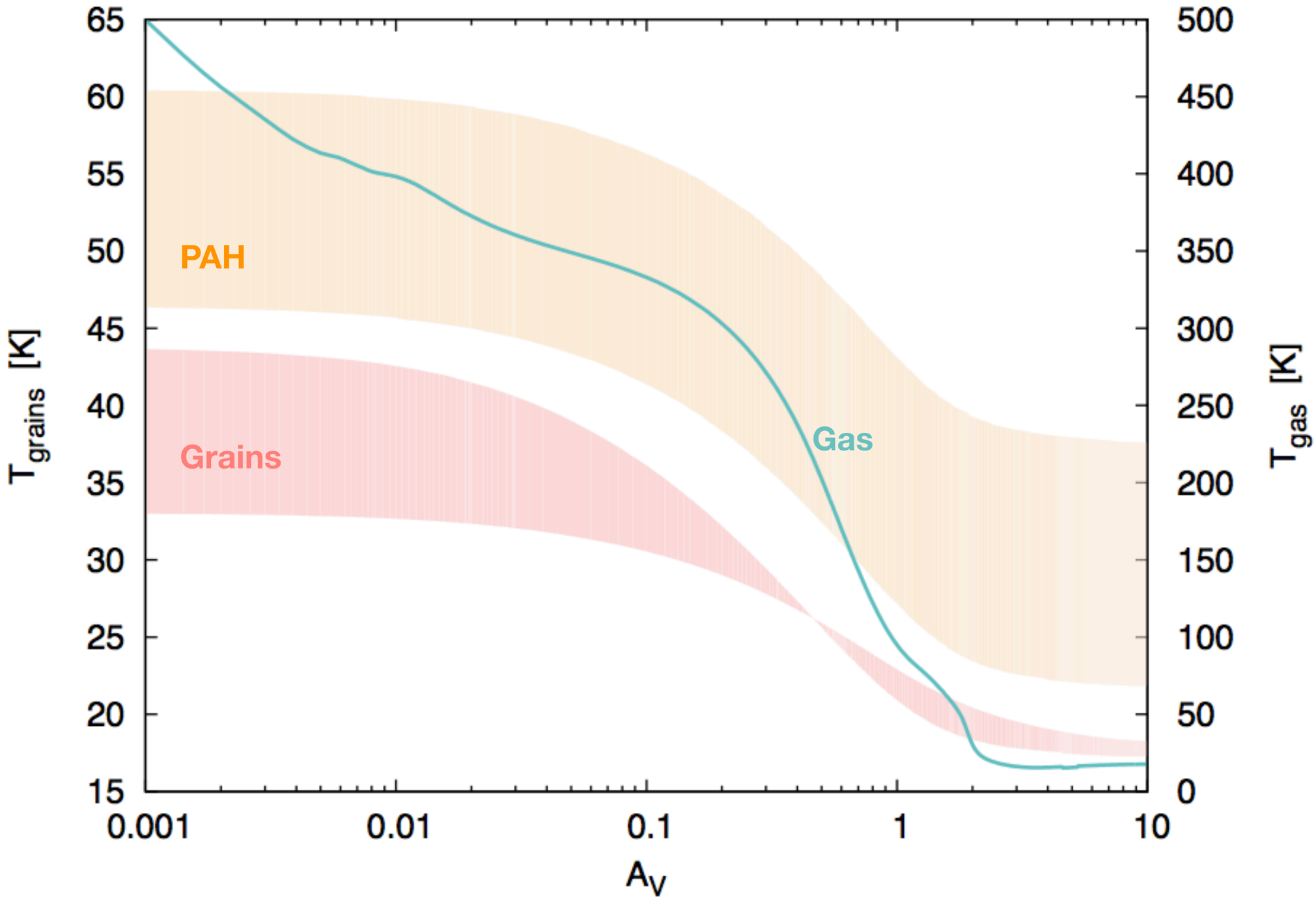

Exemple

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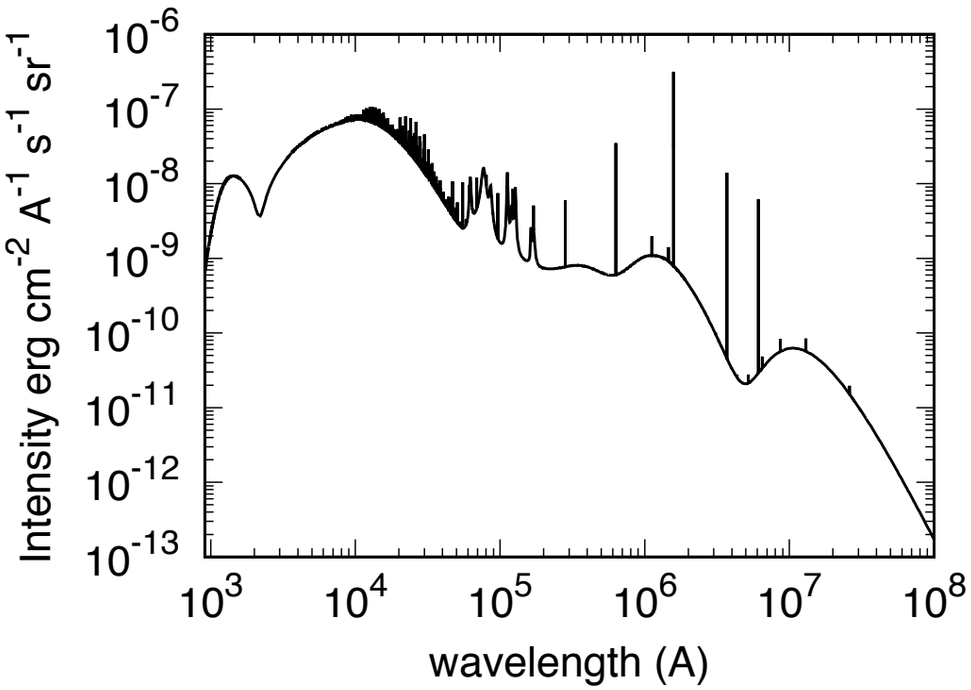

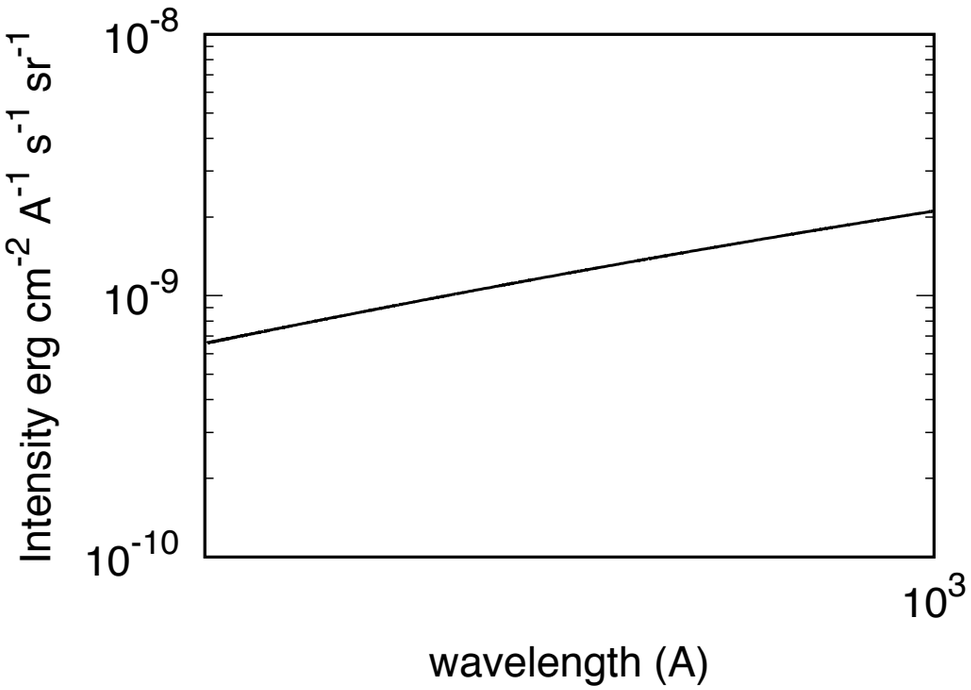

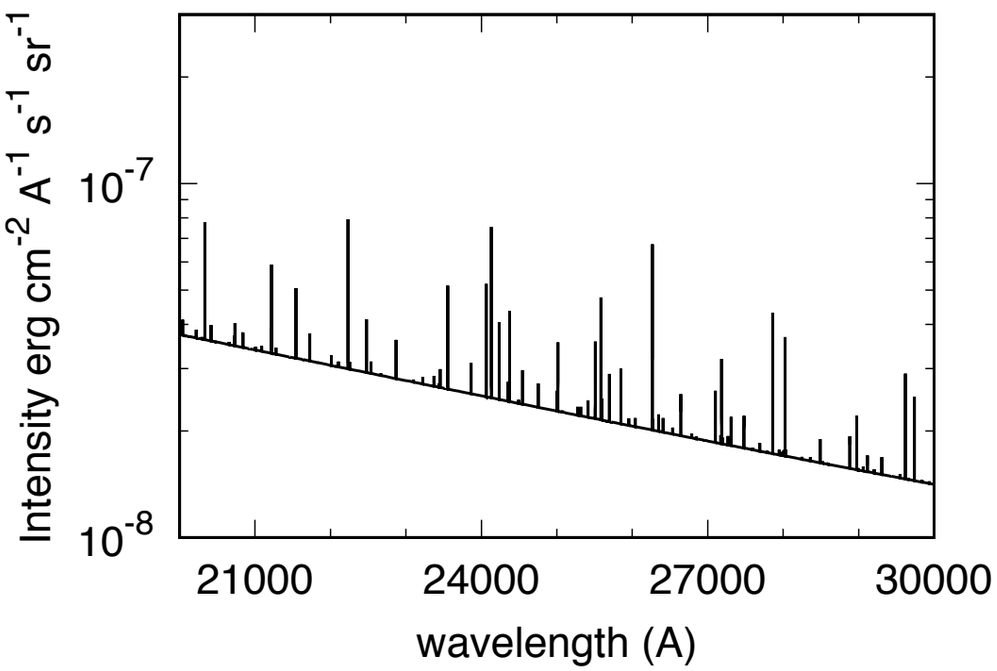

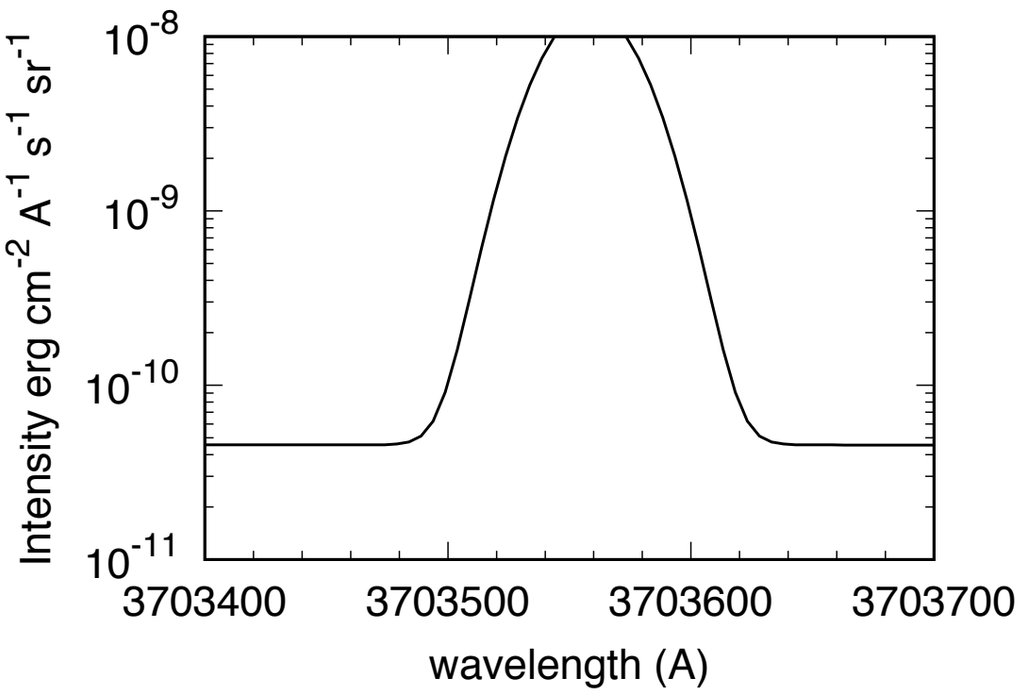

Dense PDRs

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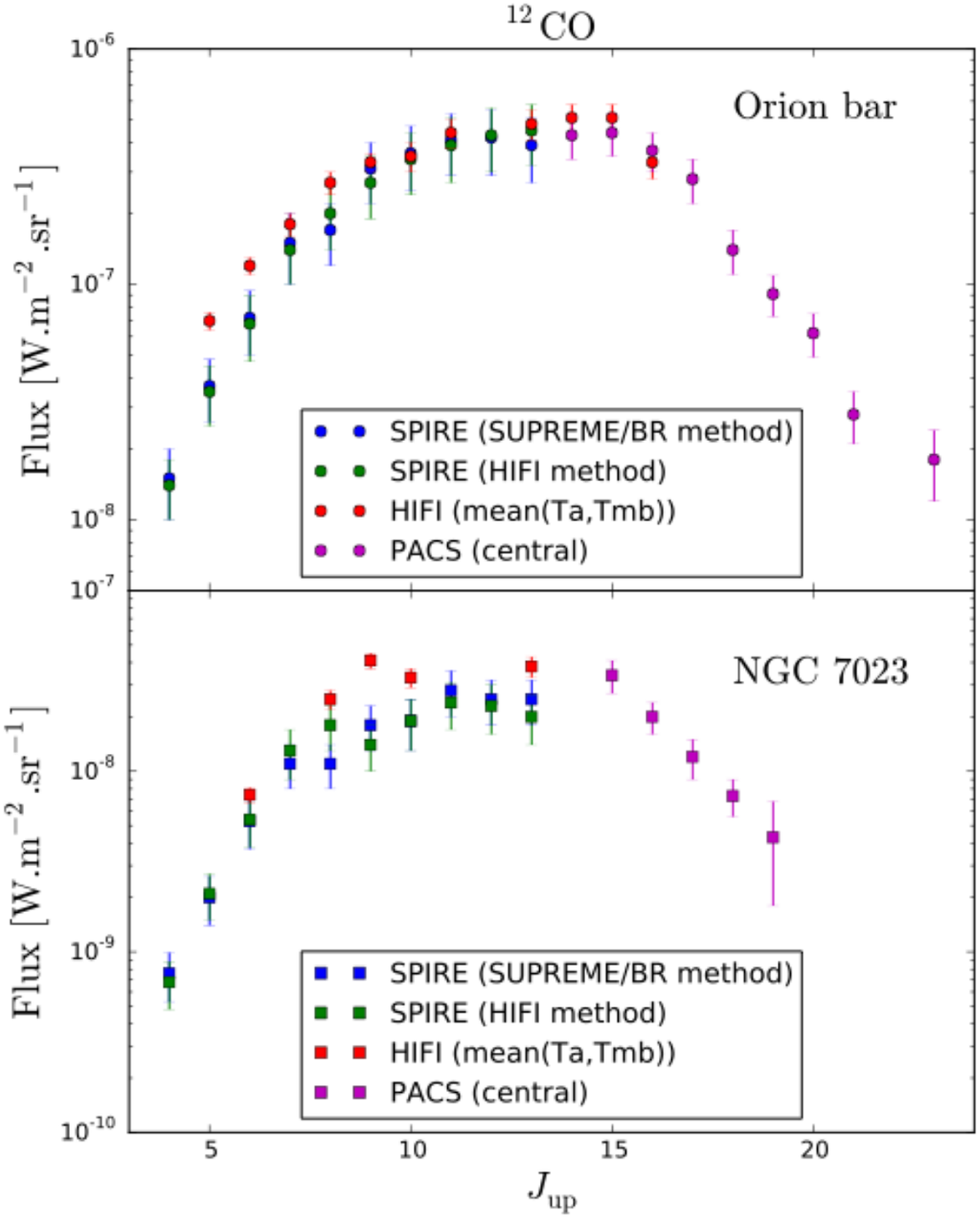
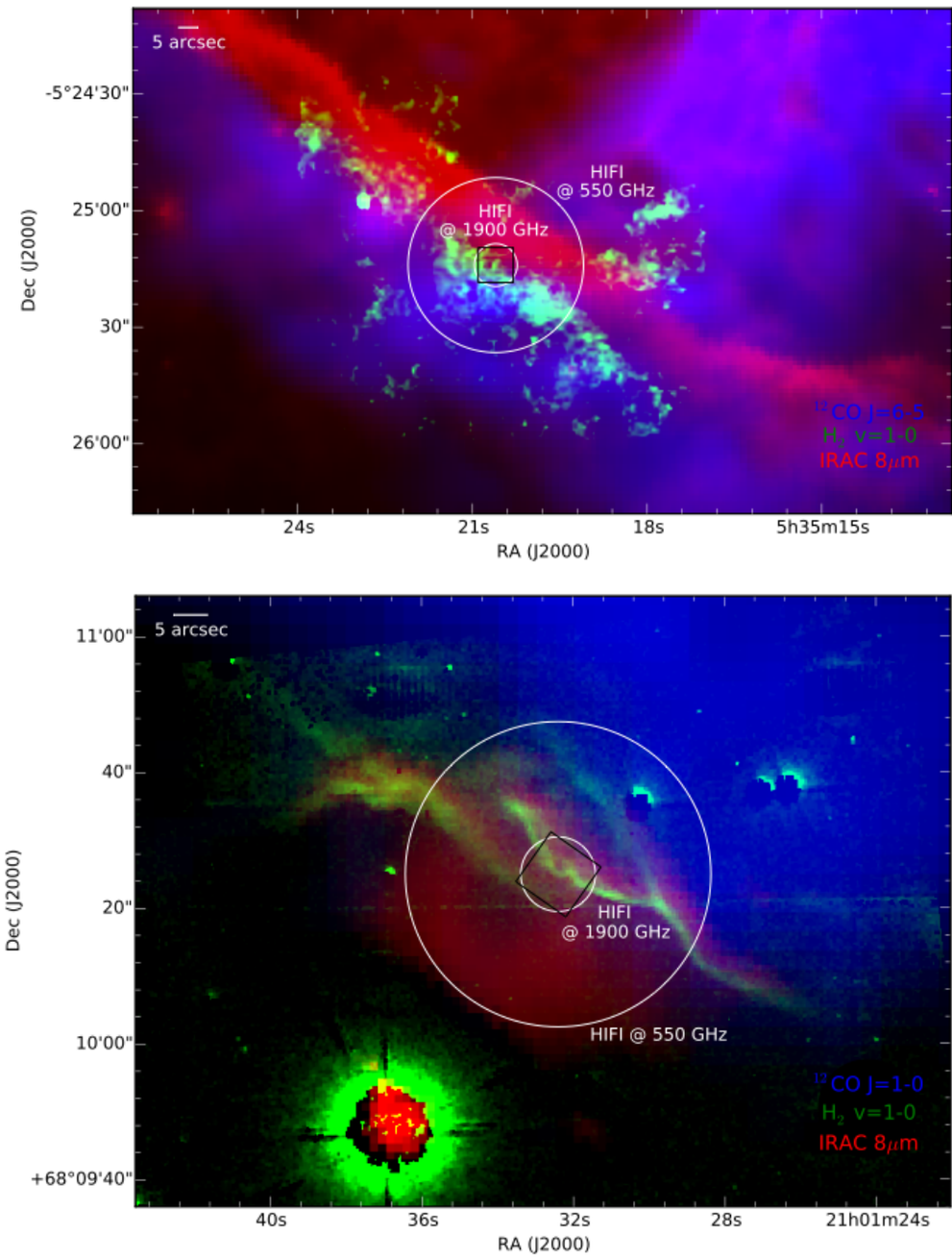
Observations





Jobin et al. (in prep)

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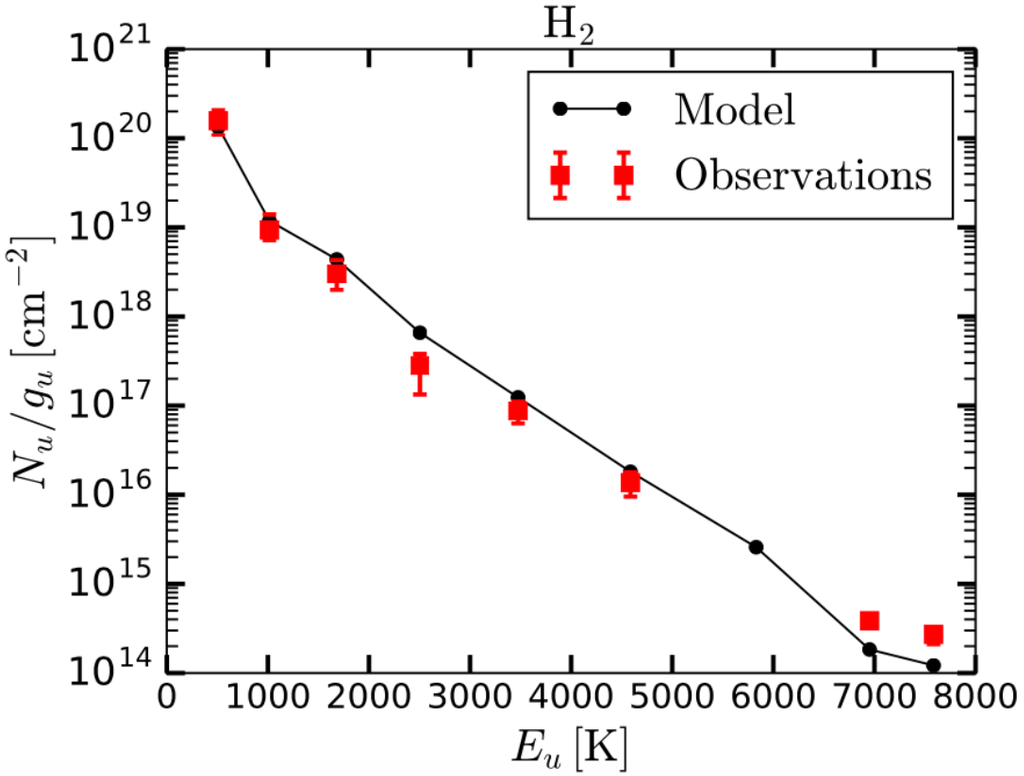
Model of NGC 7023 (joblin et al. in prep)



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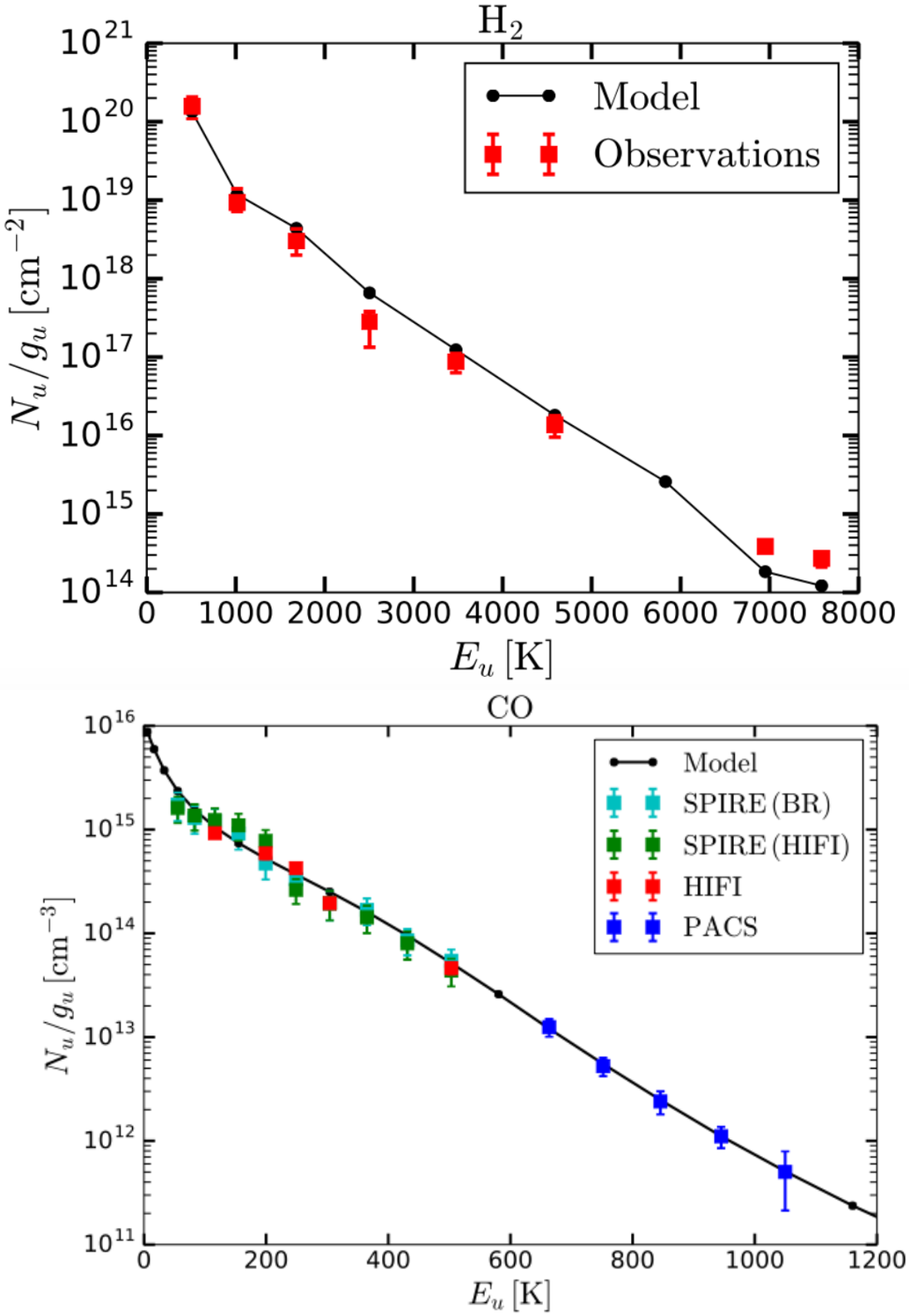

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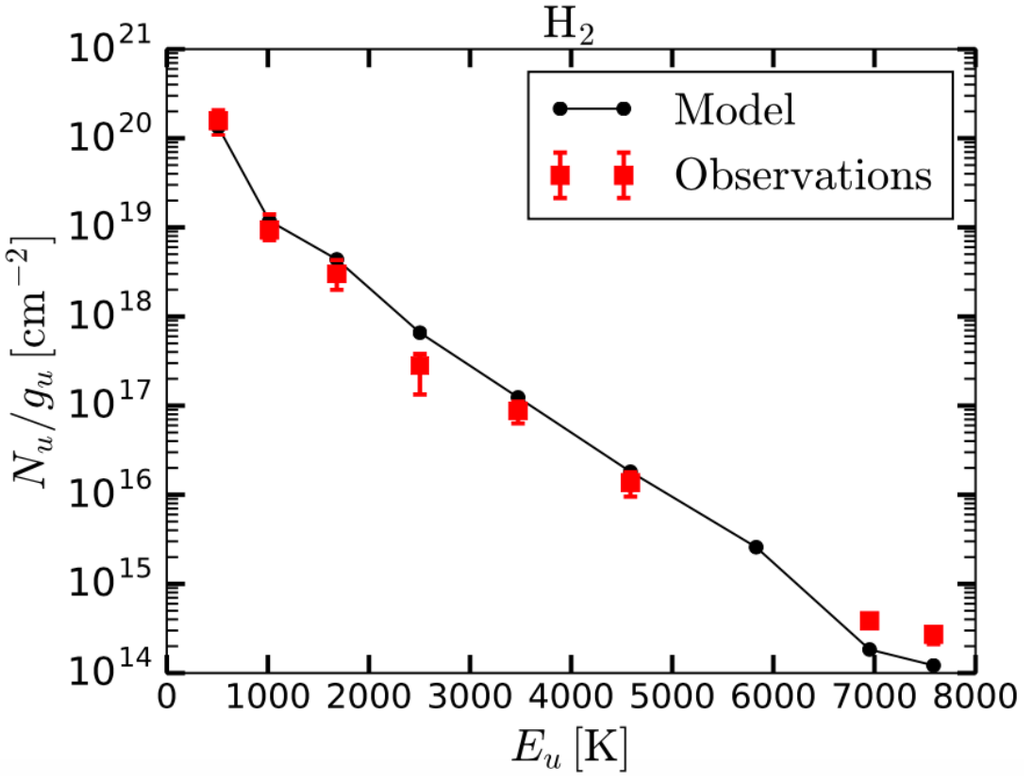

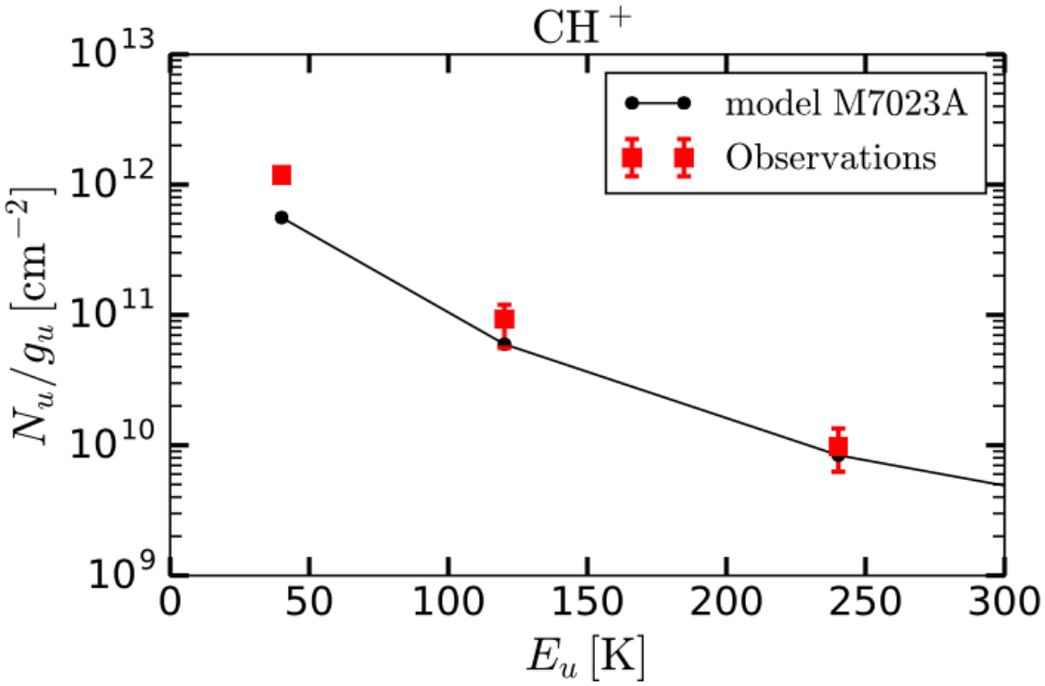

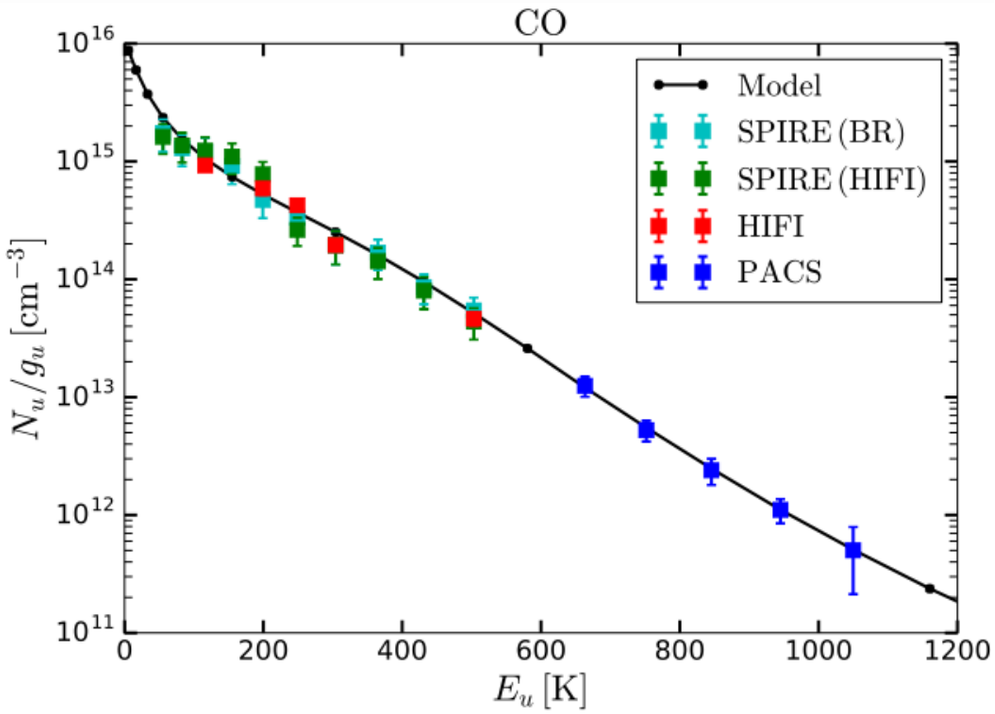

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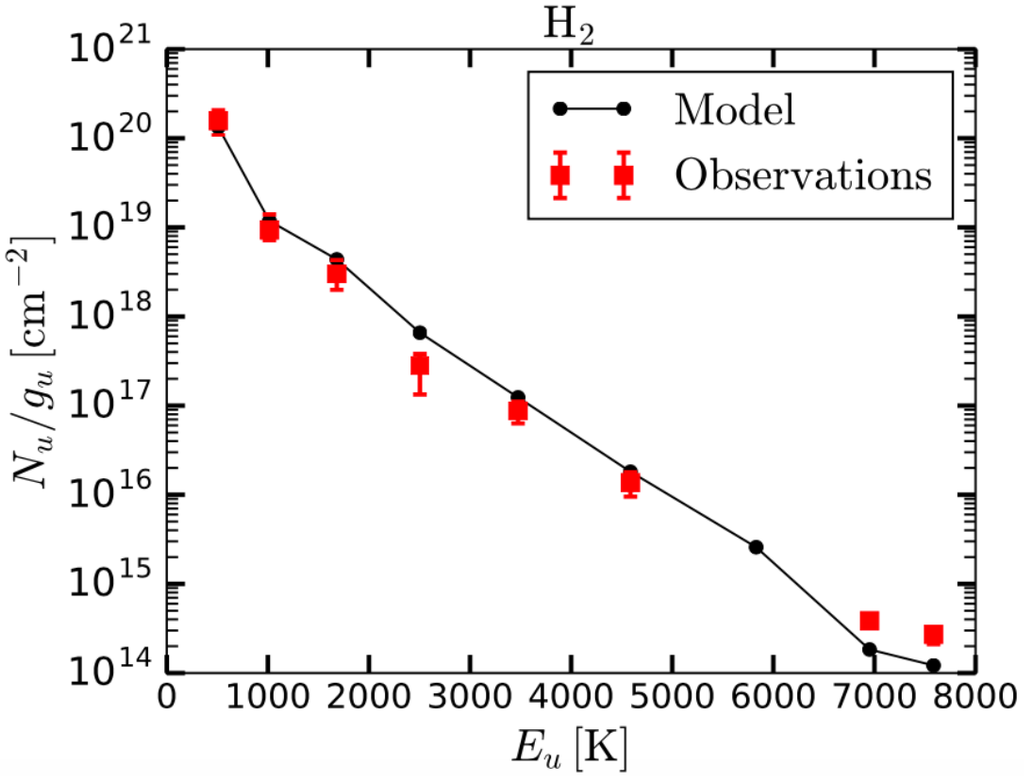

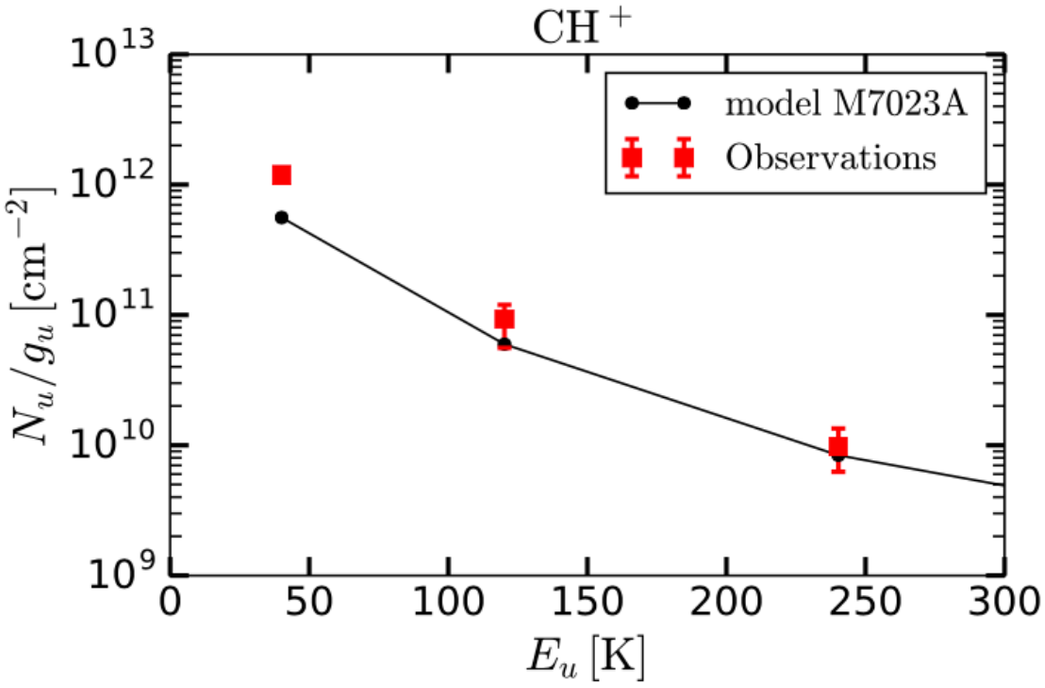

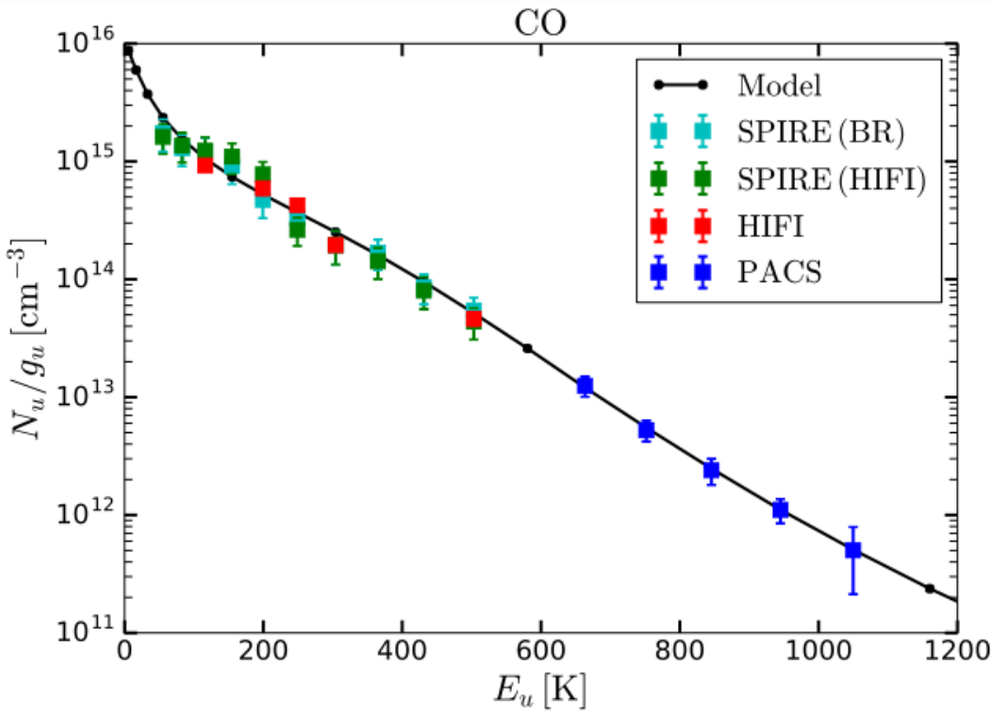

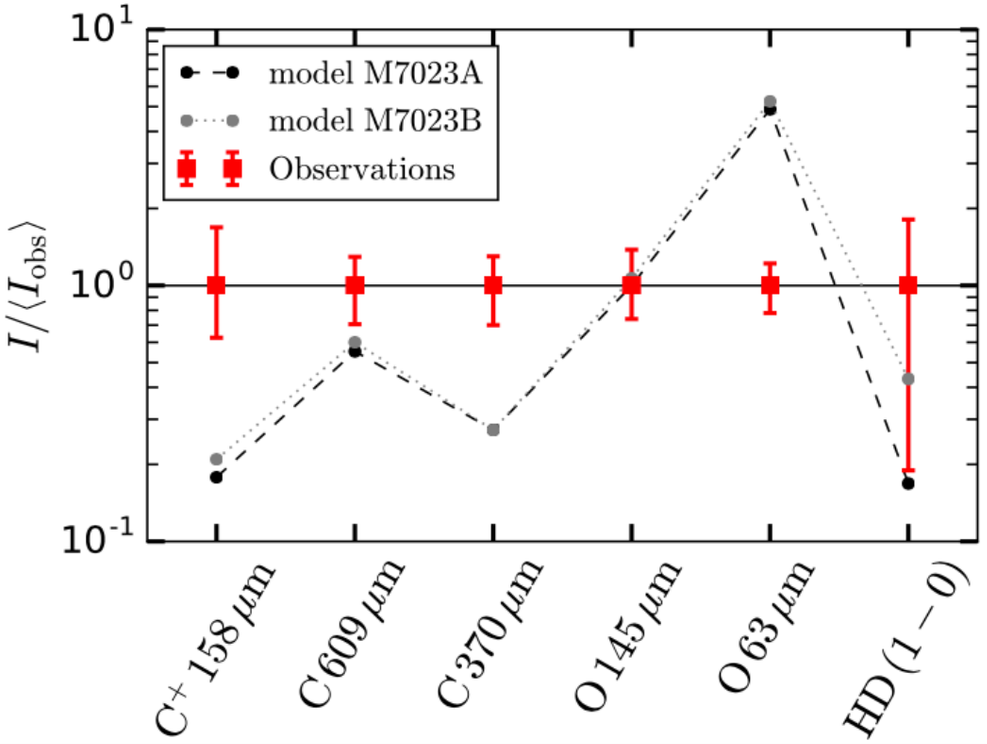

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- physics & algorithms
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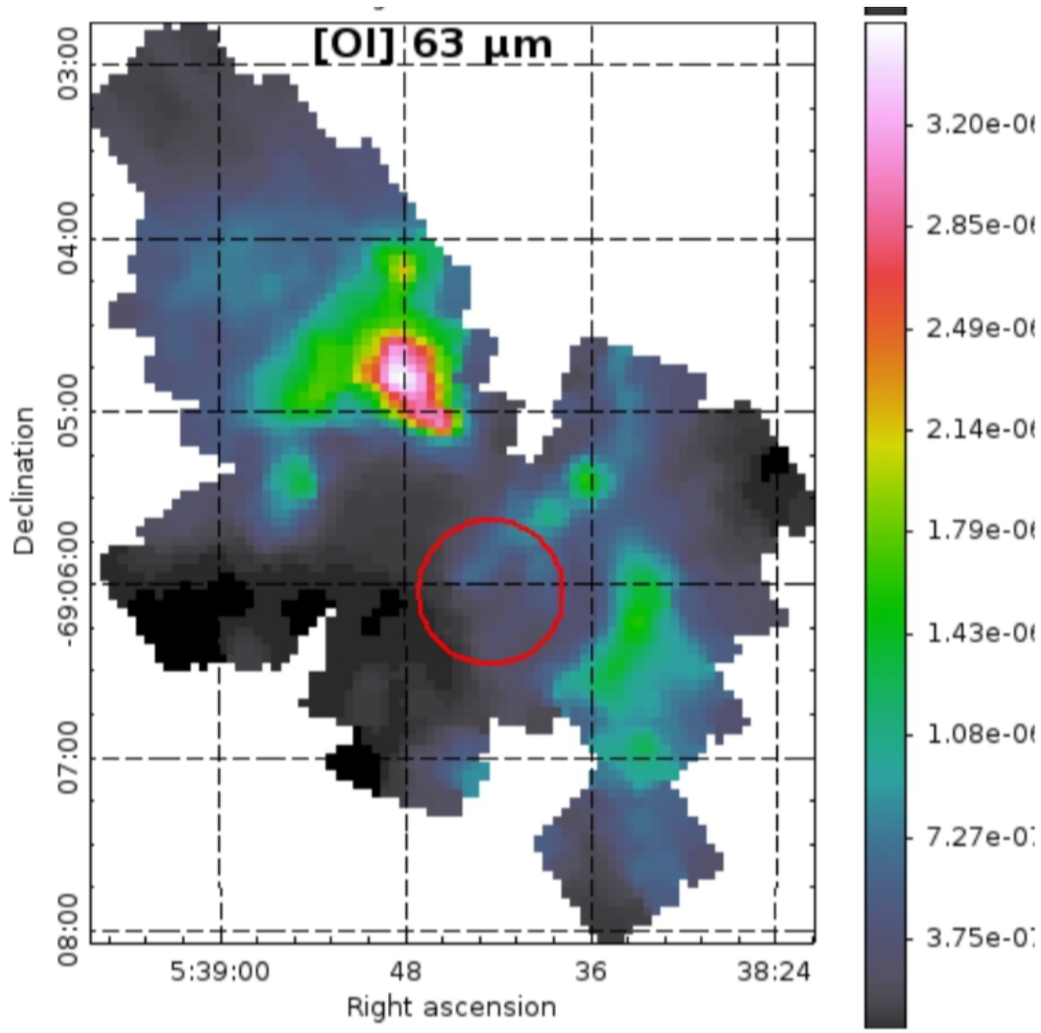
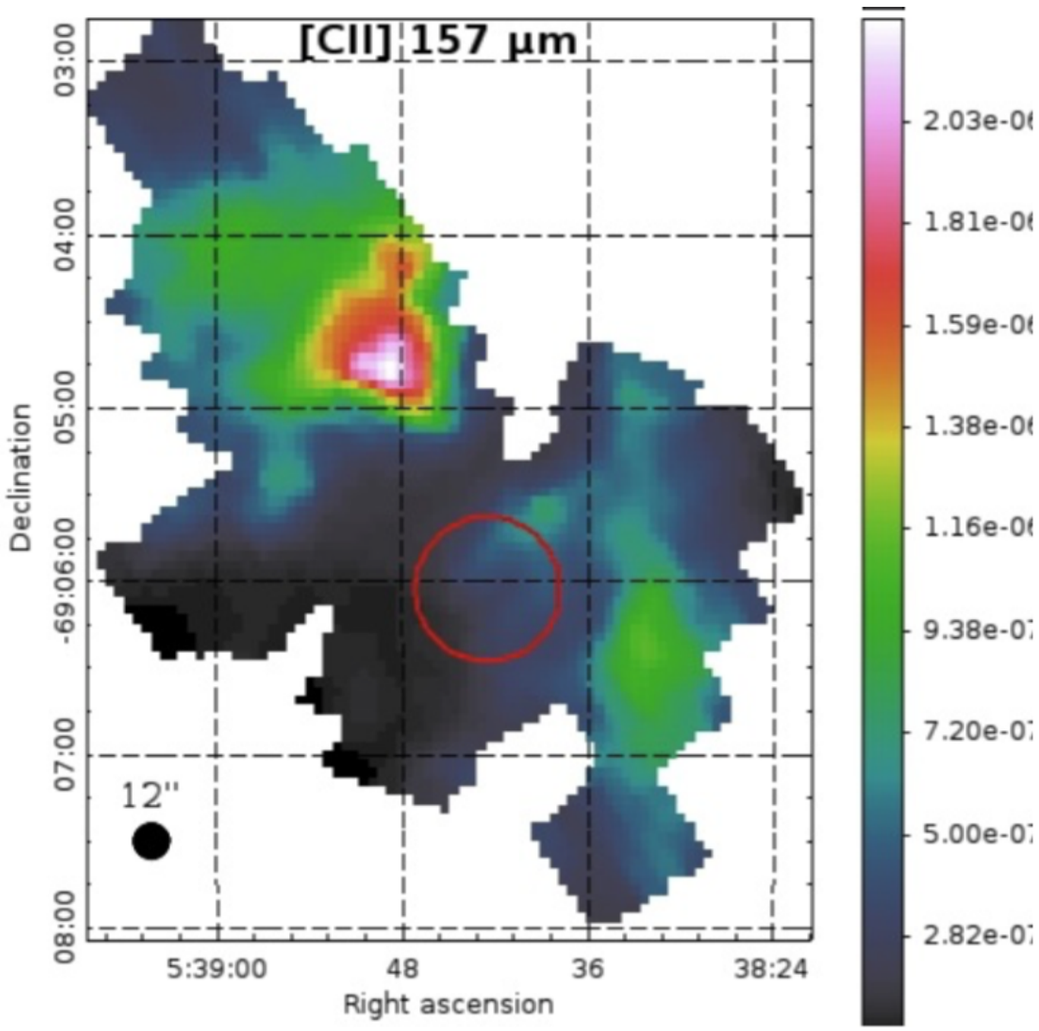
Model of 30 Doradus (Chevance et al. 2015)





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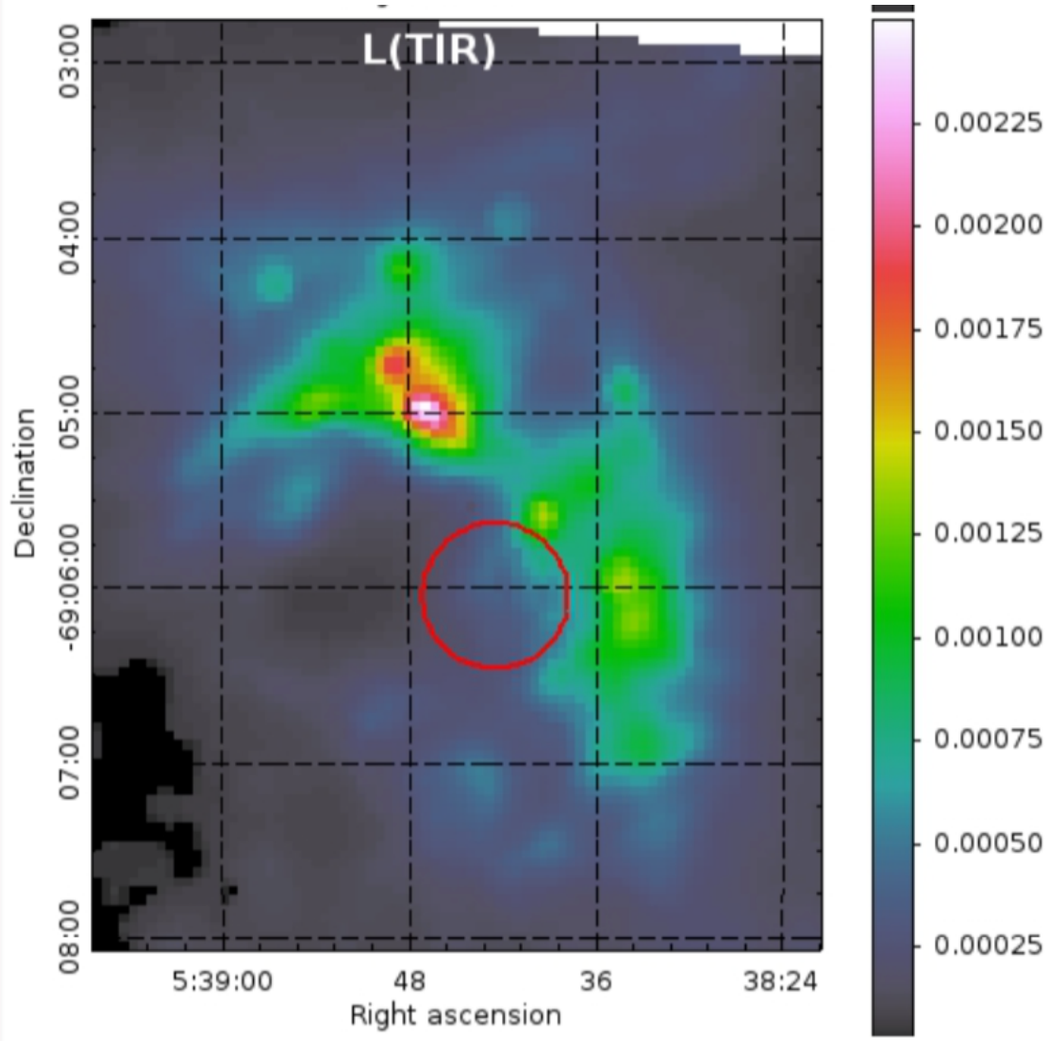

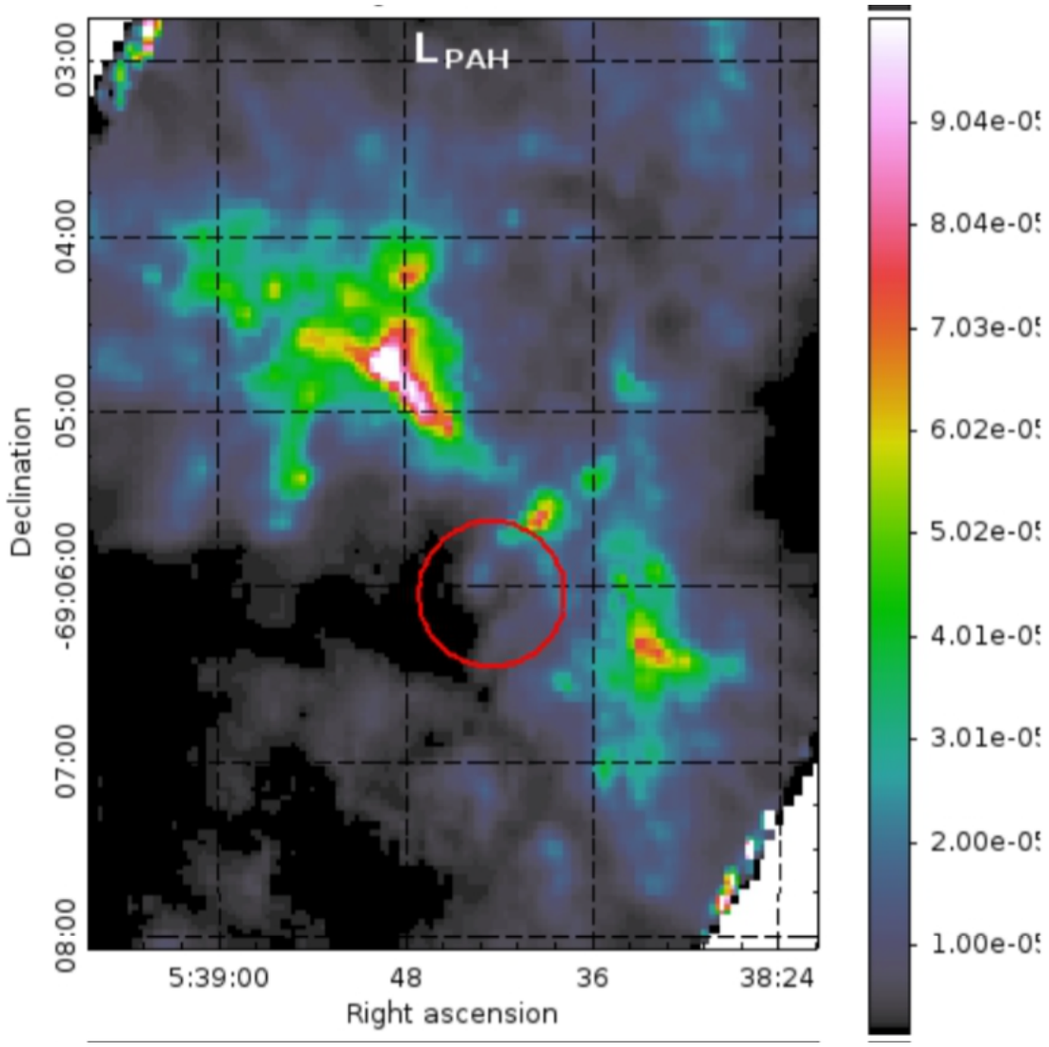

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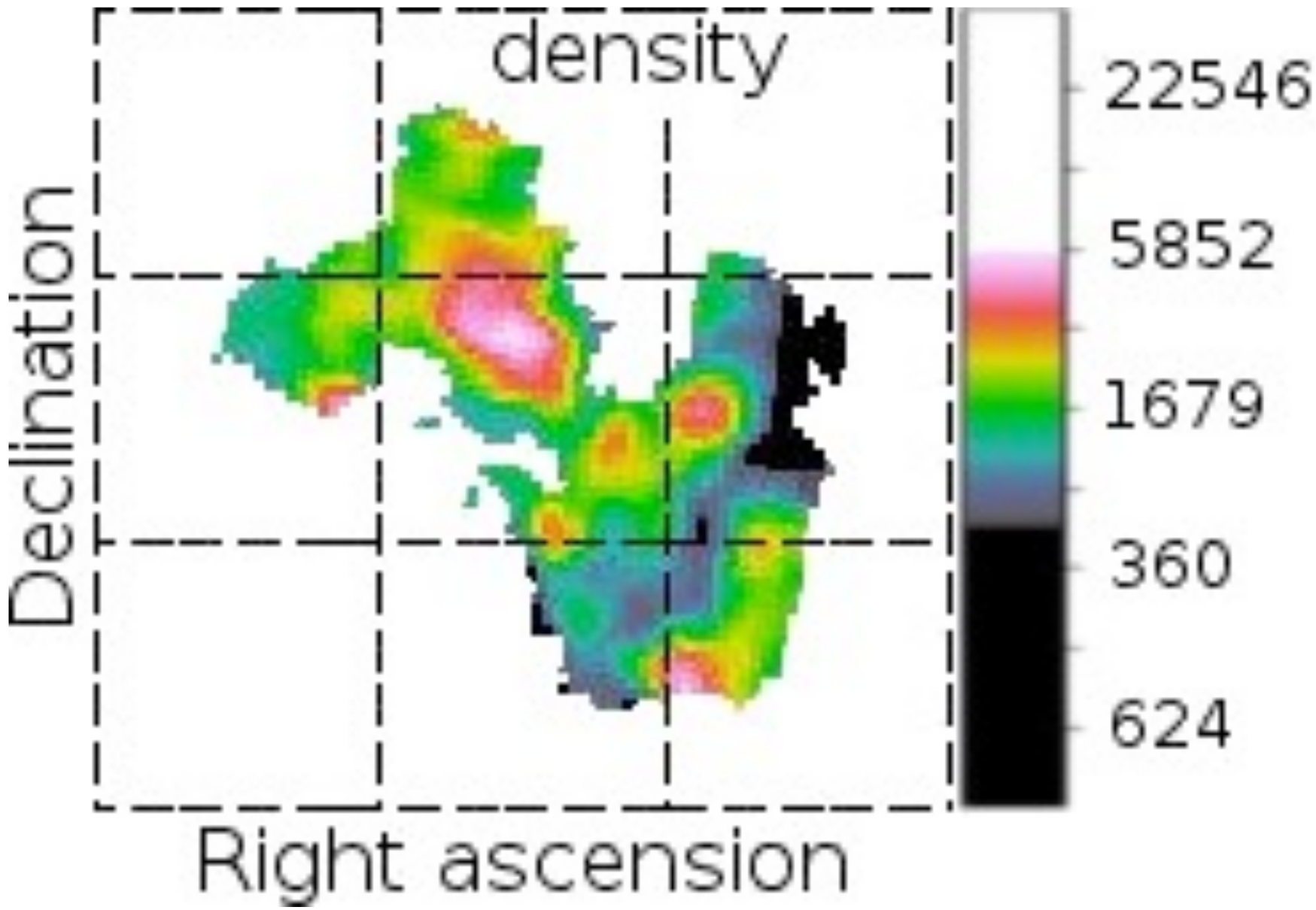

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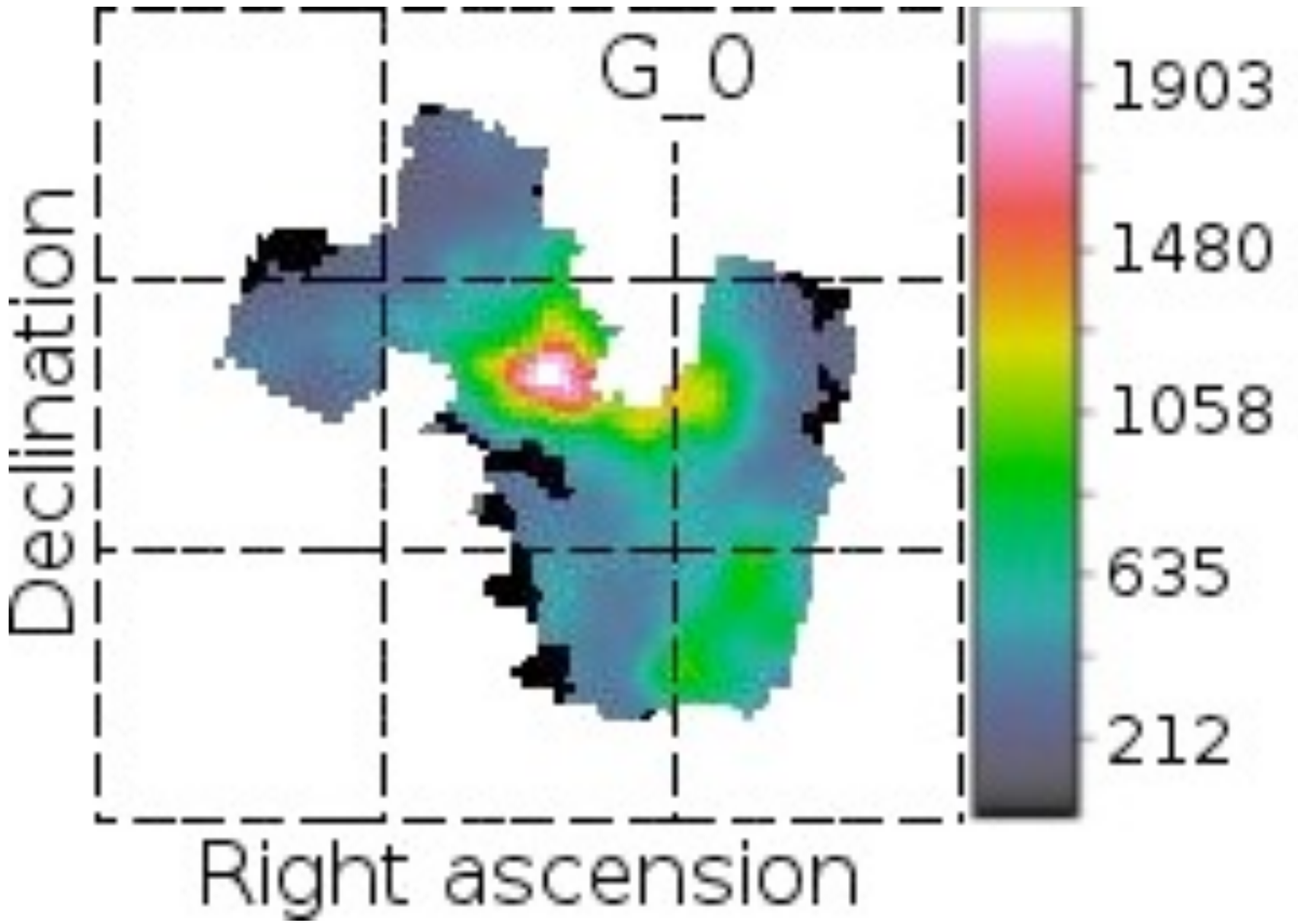

Post-treatment of simulations

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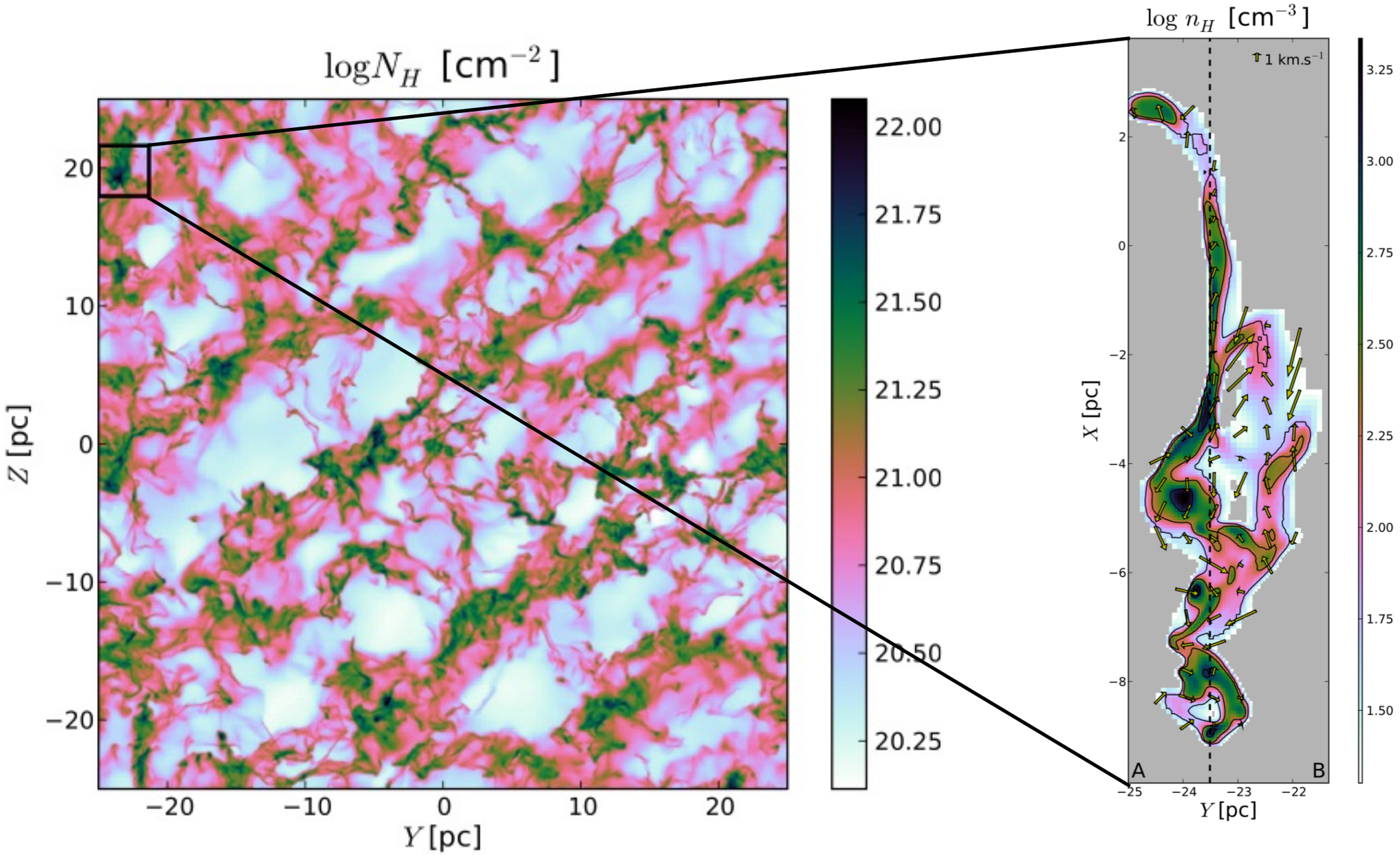
Simulated 3D diffuse cloud (Levrier et al. 2012)



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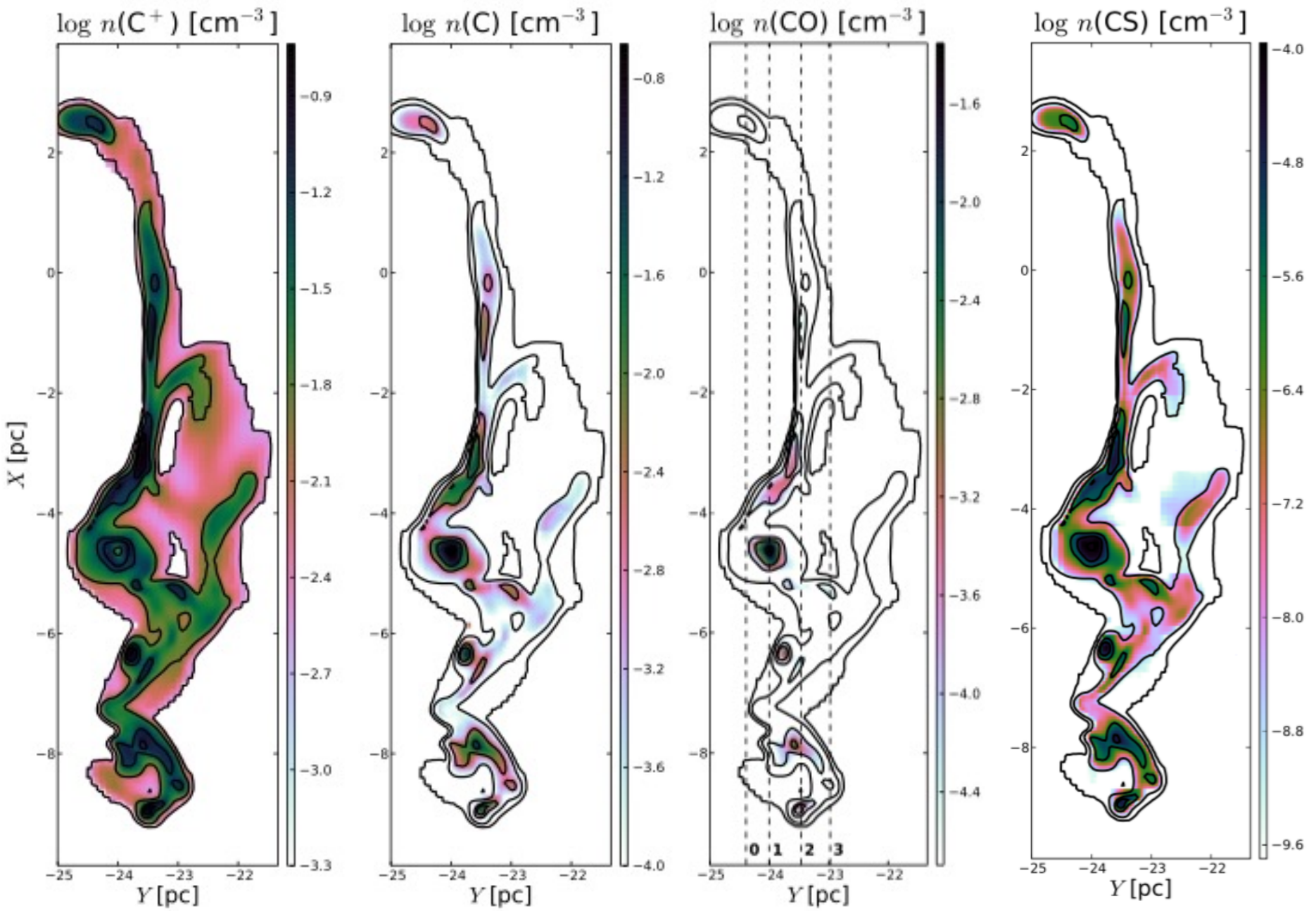
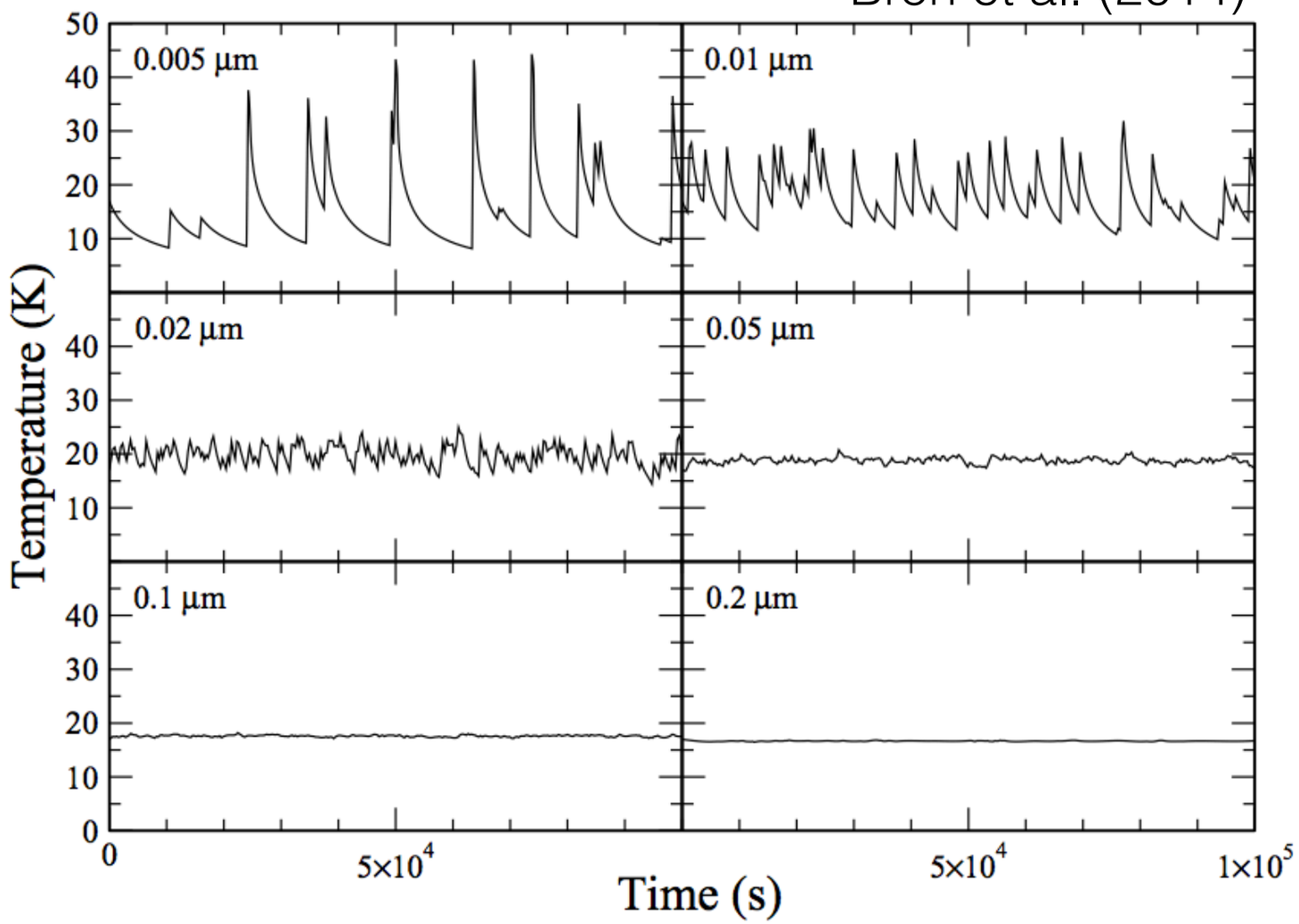


Dust temperature fluctuations

- Master equation $\int dY\, p_{Y\to X} f(Y) = f(X) \int dY\, p_{X\to Y}$
- Improve efficiency of processes
- Reduce importance of barriers

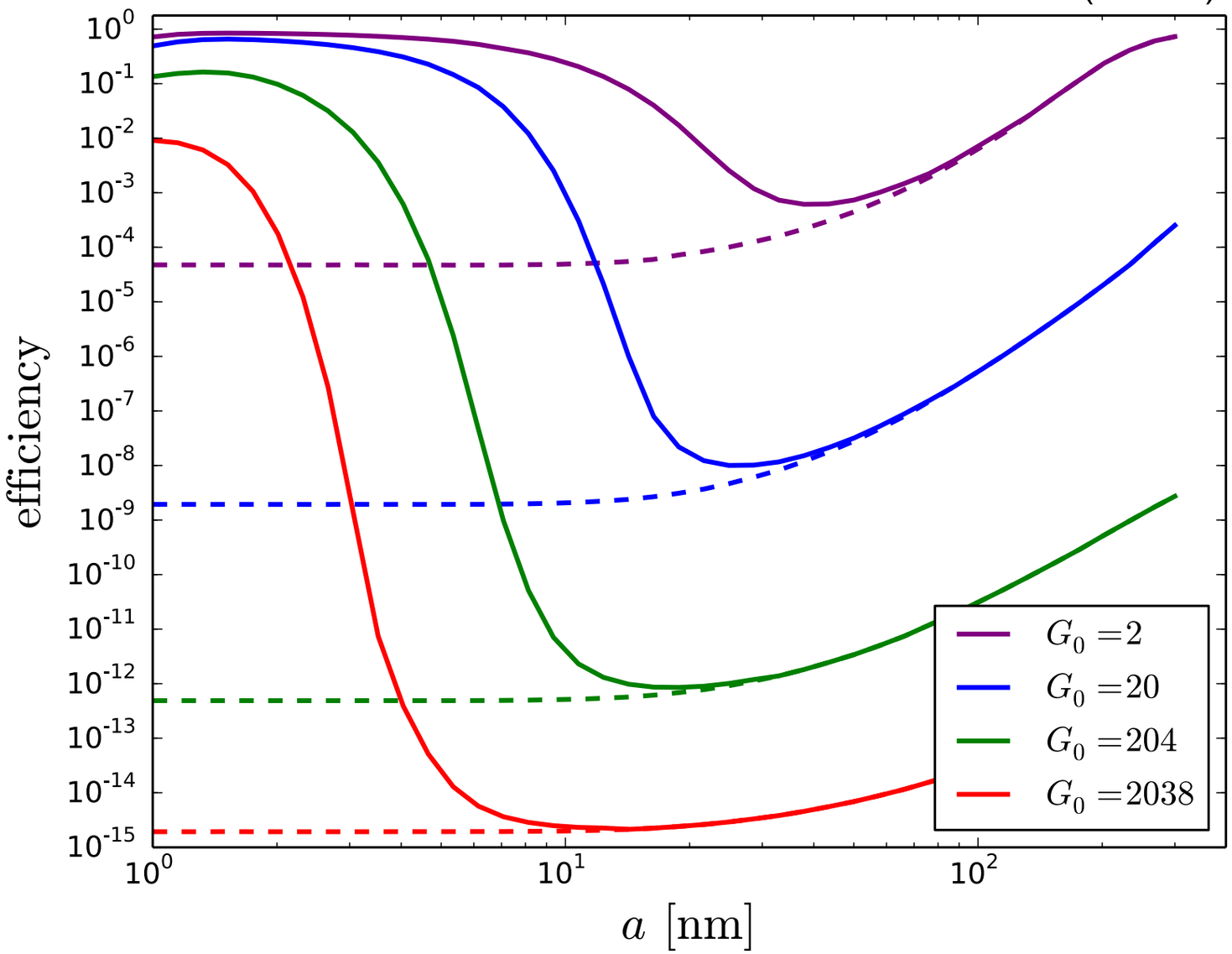
Bron et al. (2014)



Impacts of dust temperature fluctuations

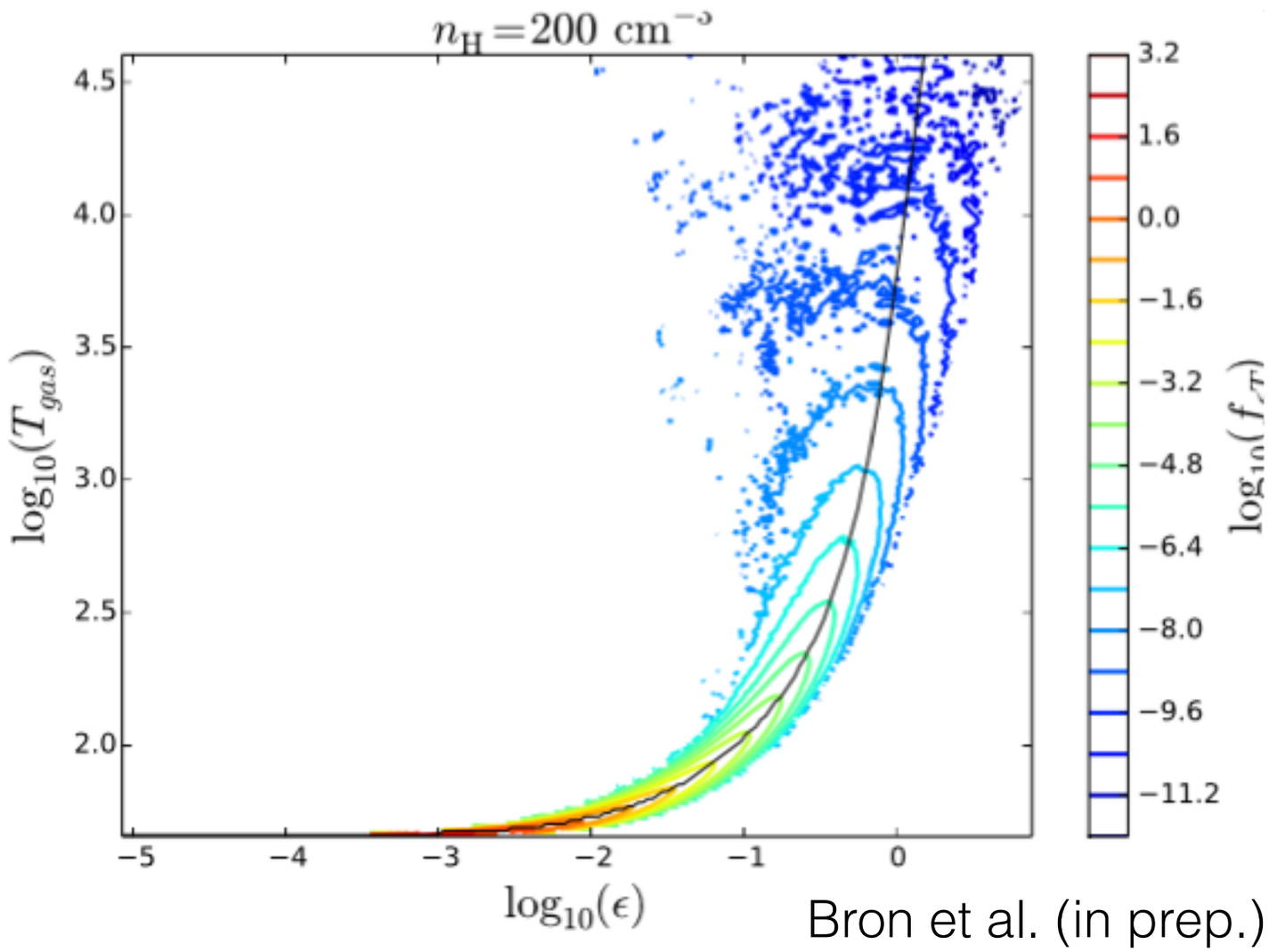
- Formation of H_2 on grains
- Conversion ortho / para

Bron et al. (2014)



Dissipation of turbulence

- Fluctuations of gas temperature
- Same formalism / only requires dissipation
- Help overcoming reaction endothermicities



Bron et al. (in prep.)

Interactions with X-rays

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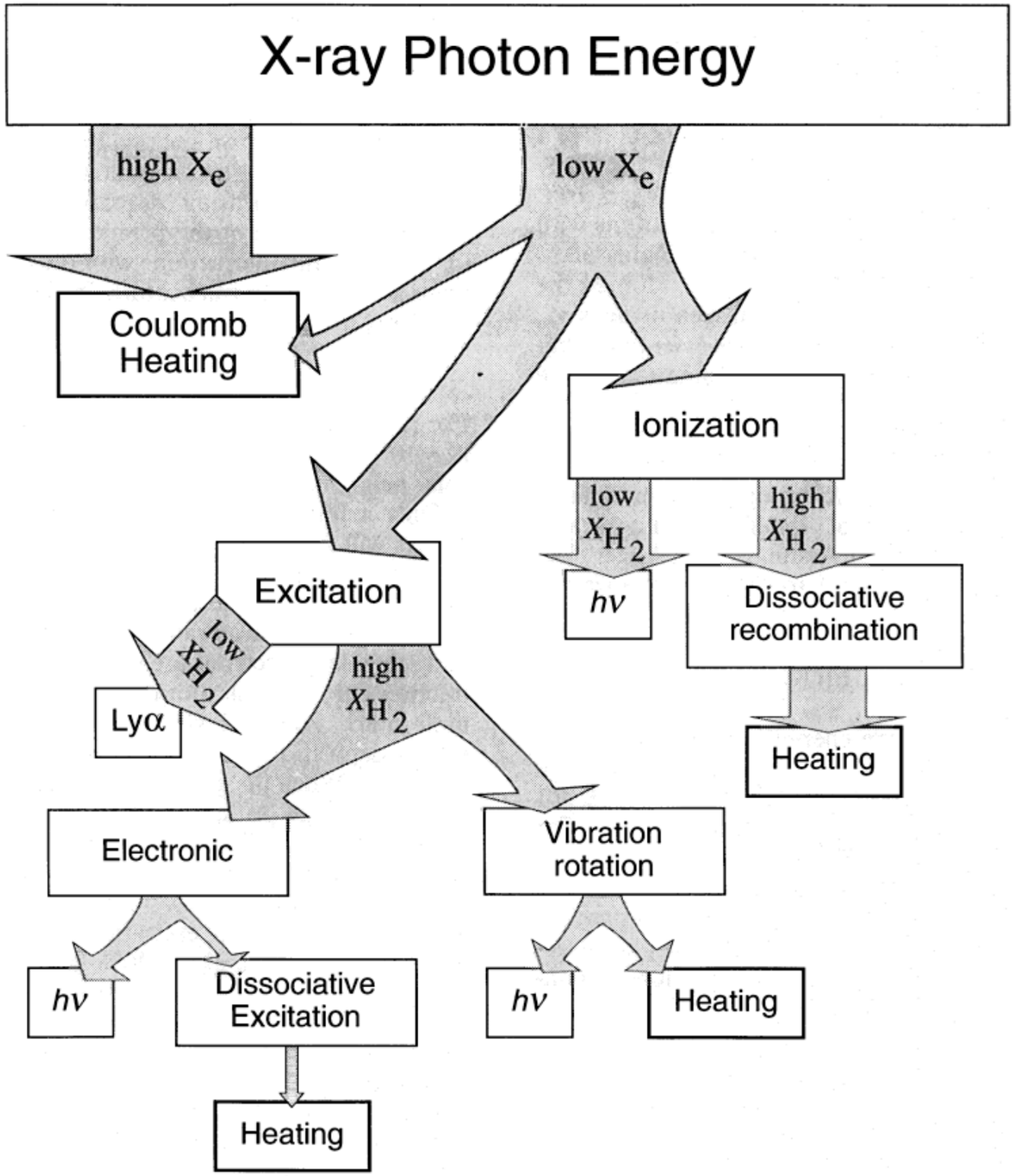

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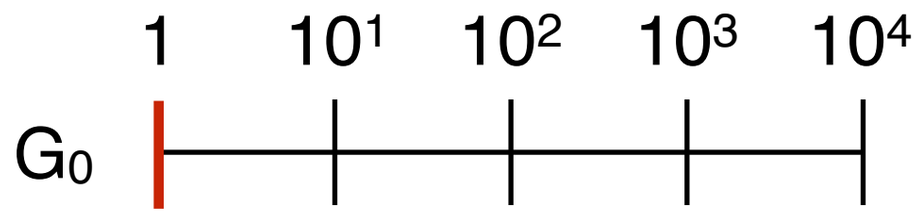

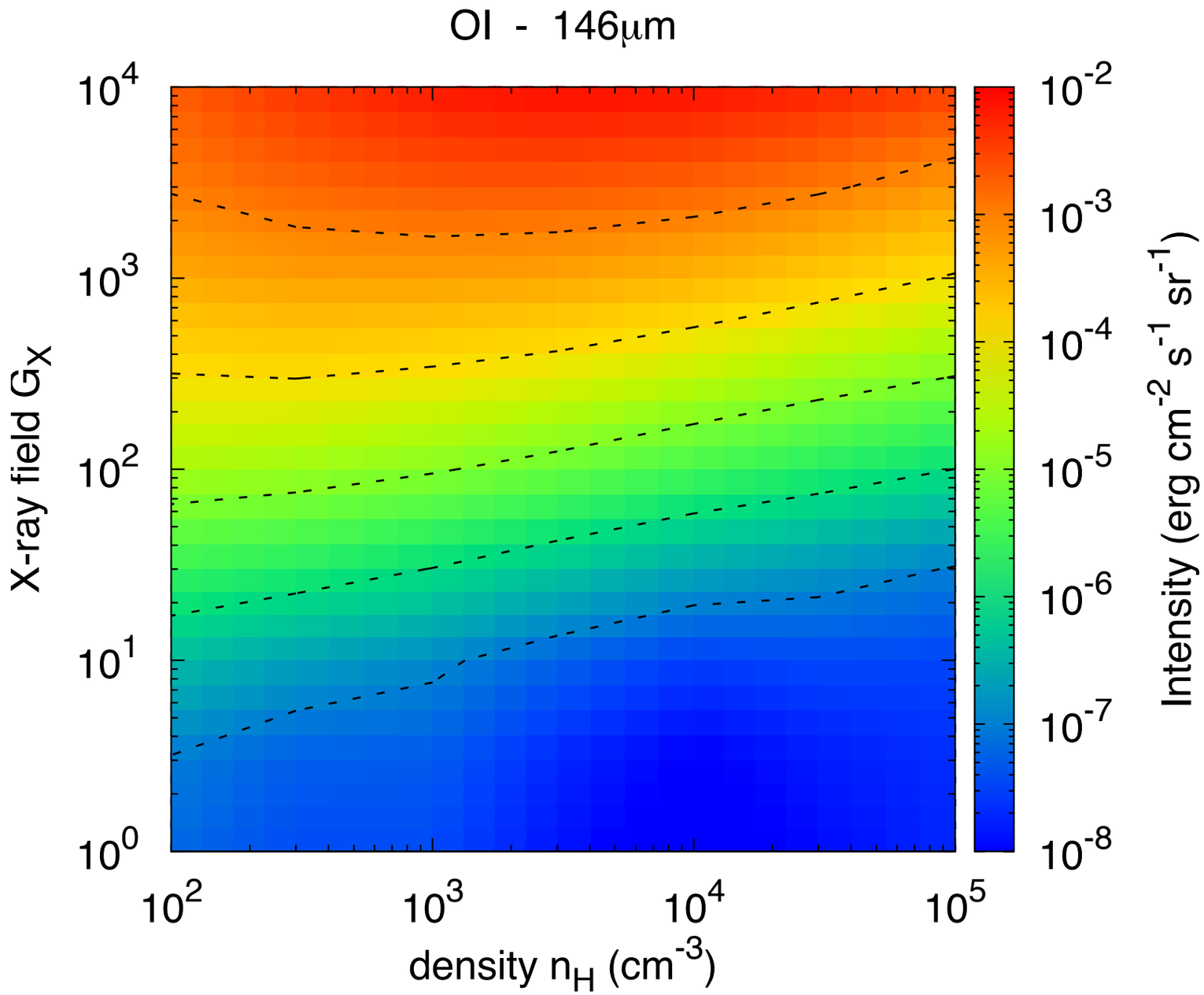

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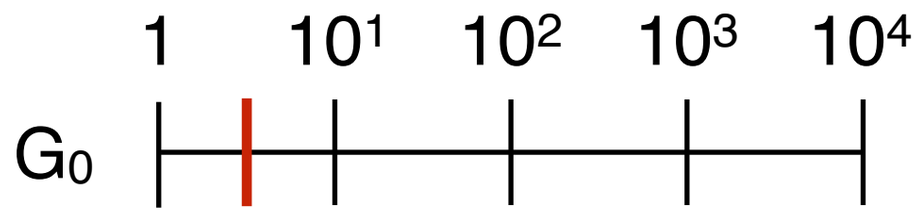

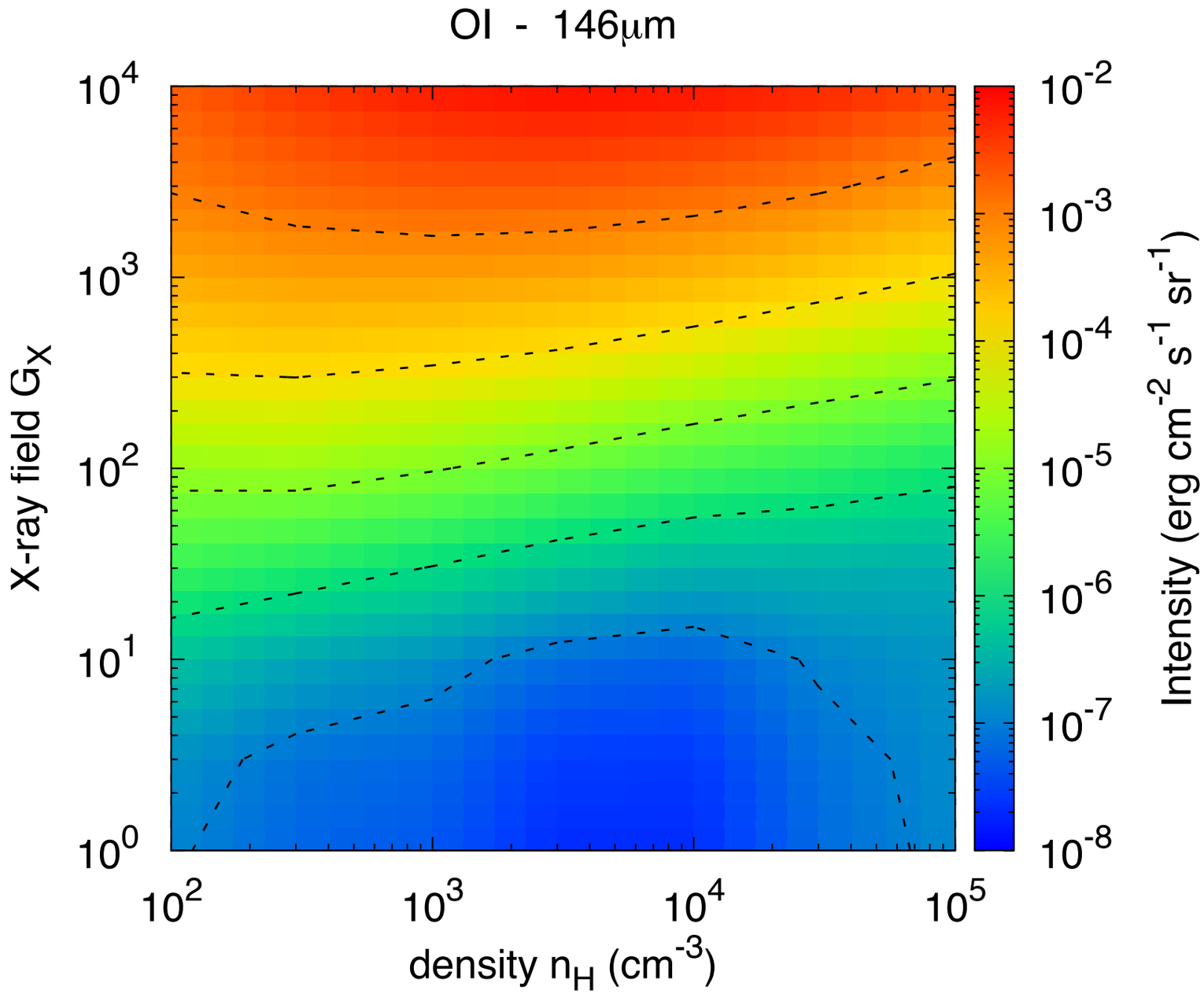

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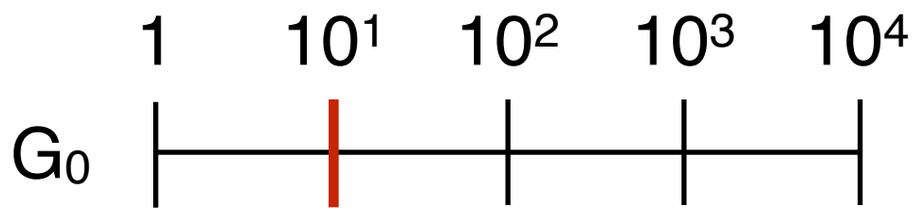

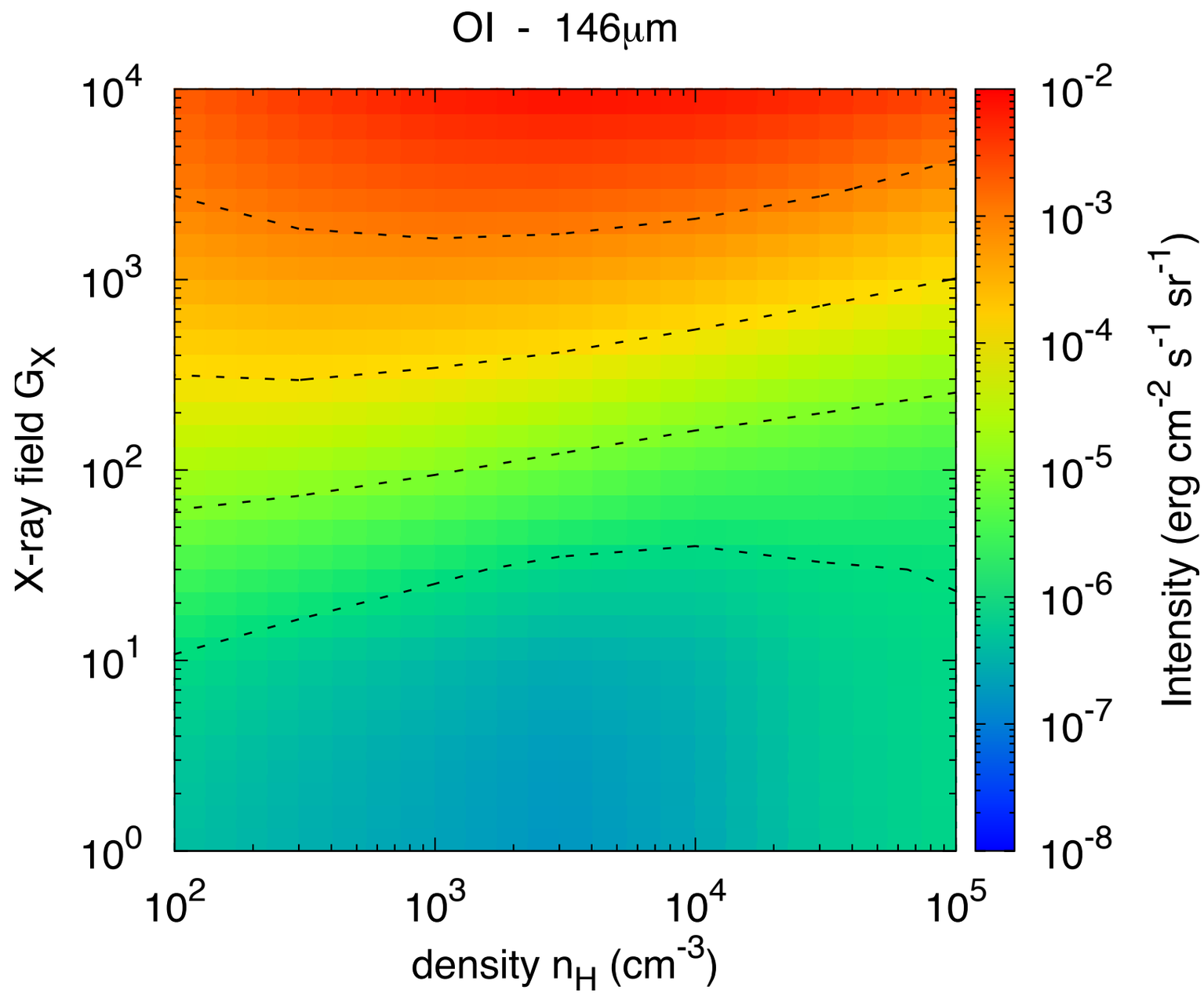

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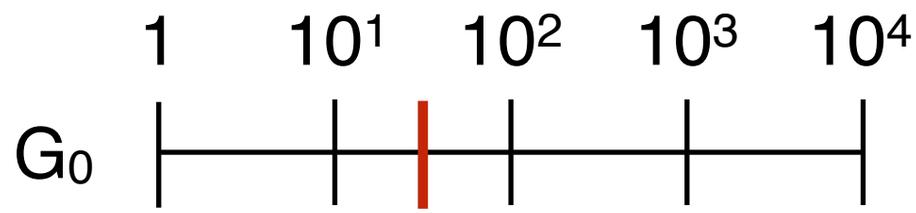

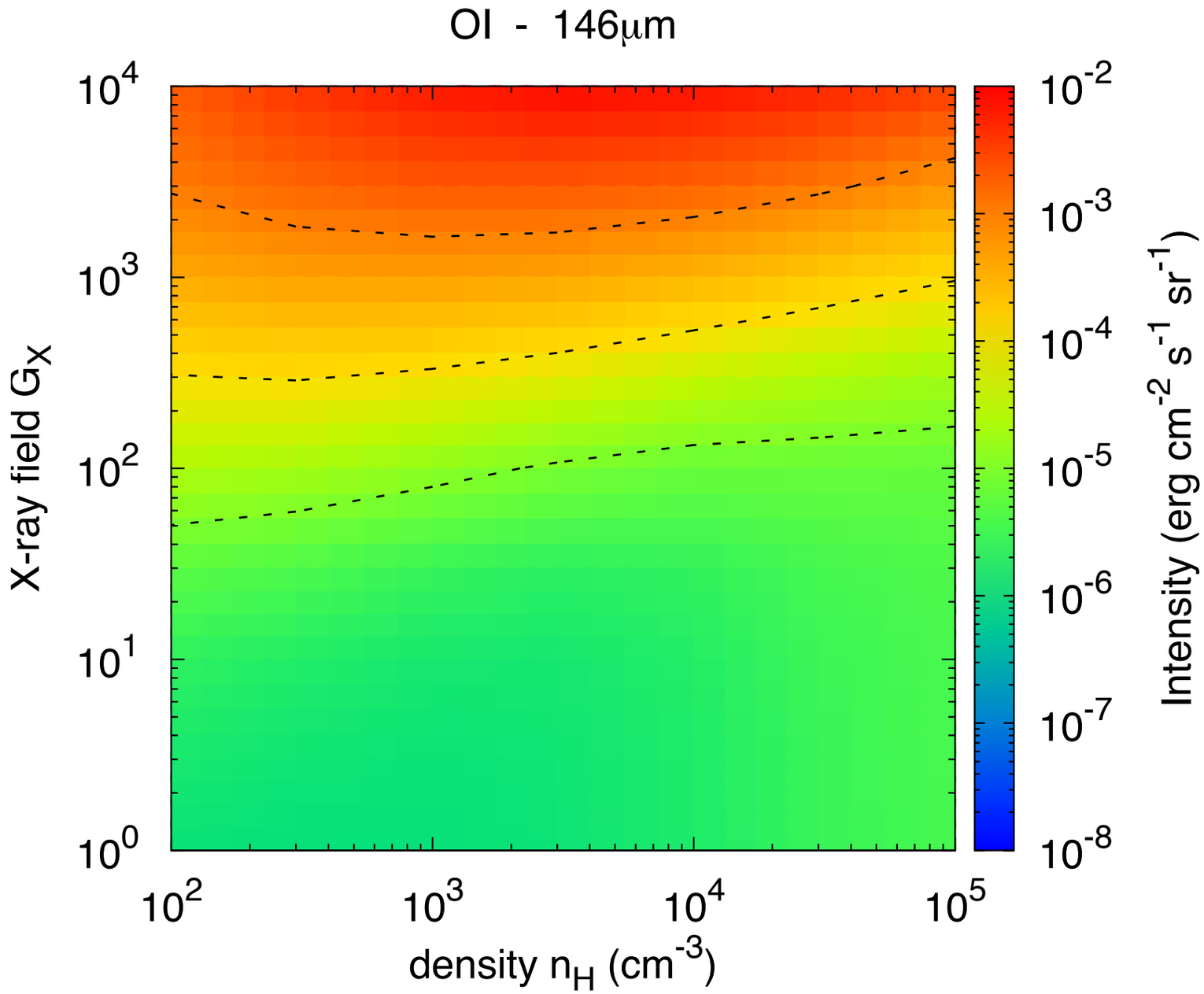

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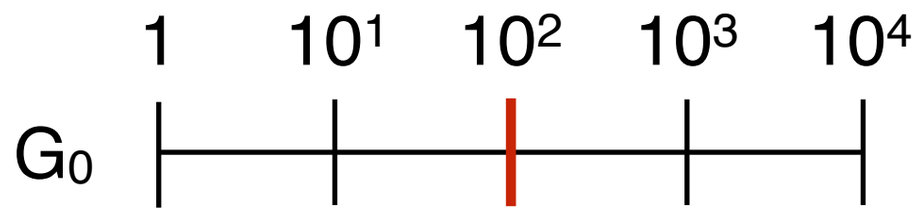

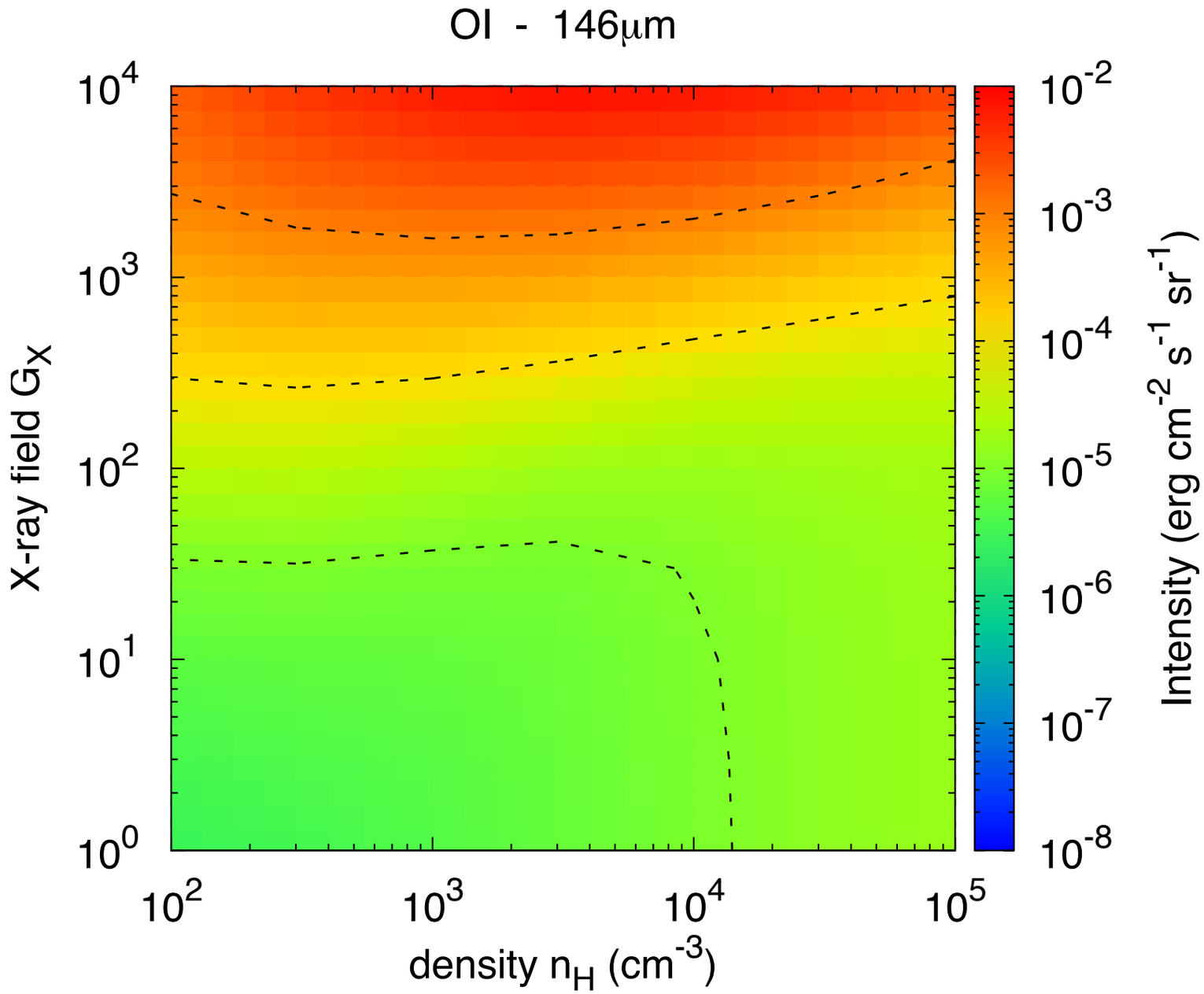

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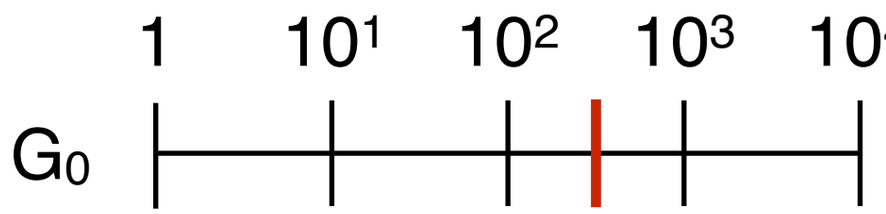

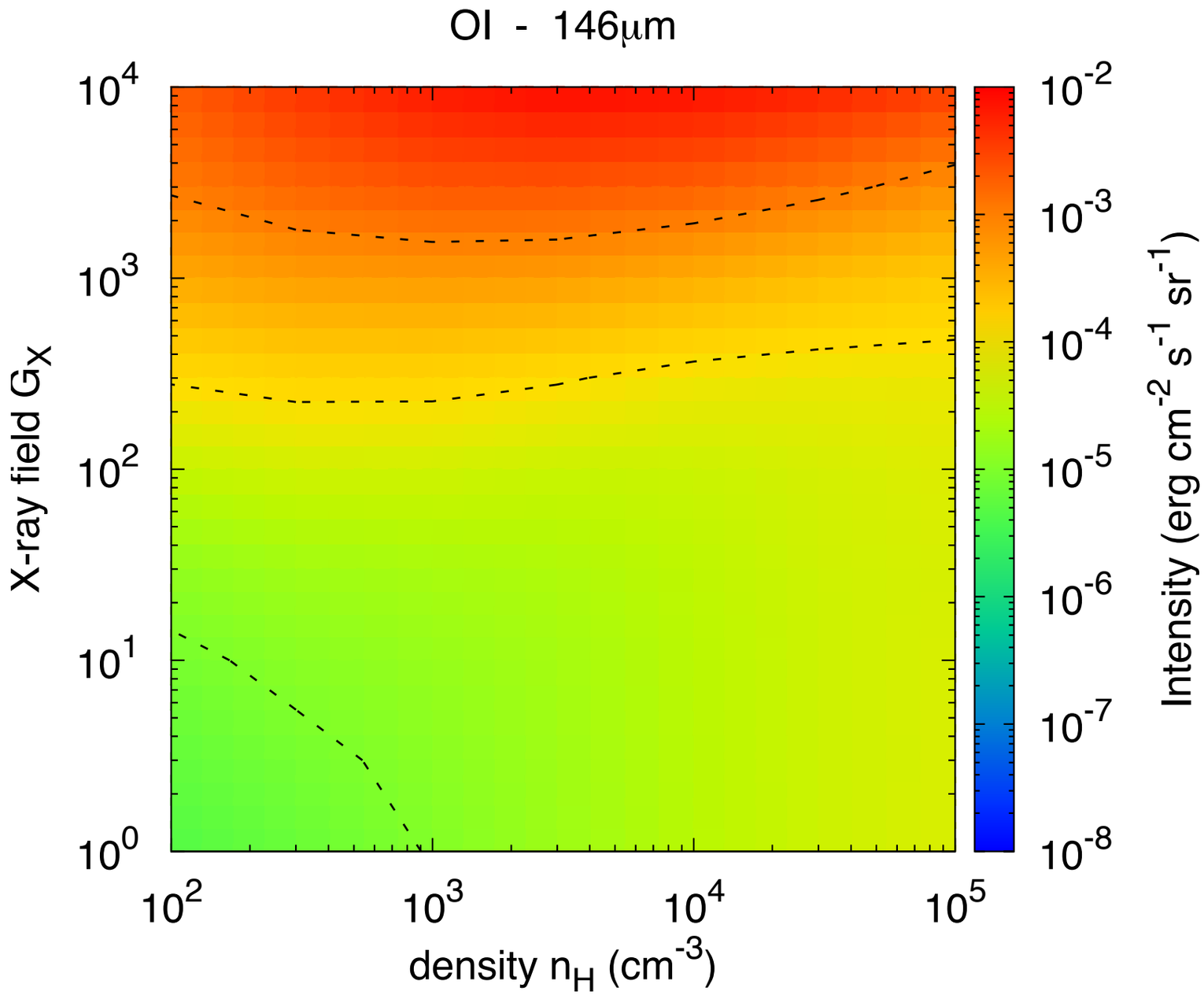

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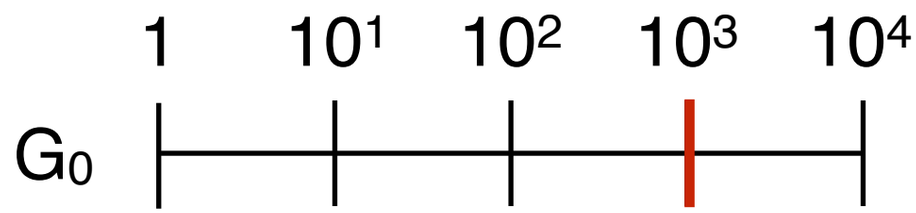

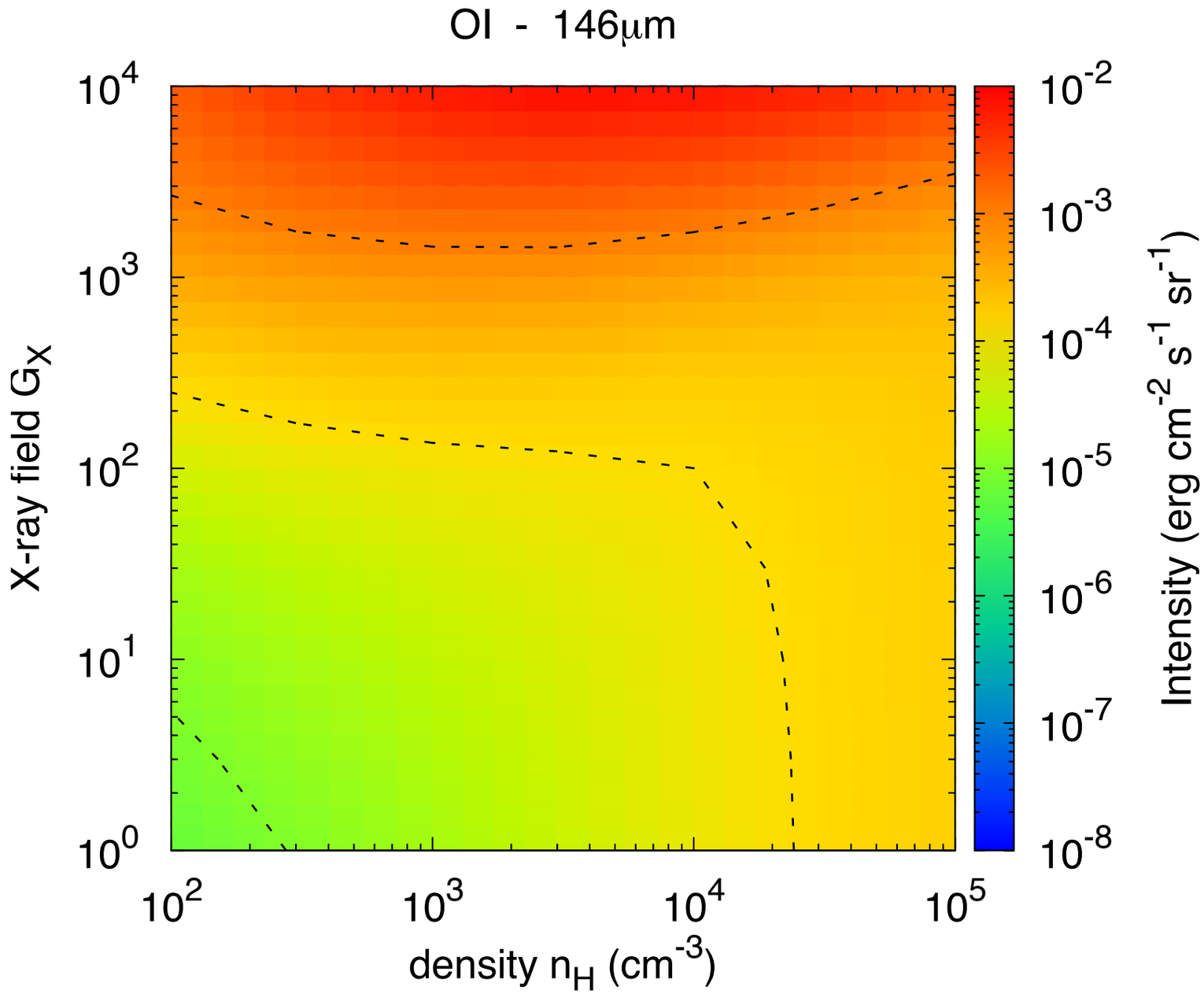

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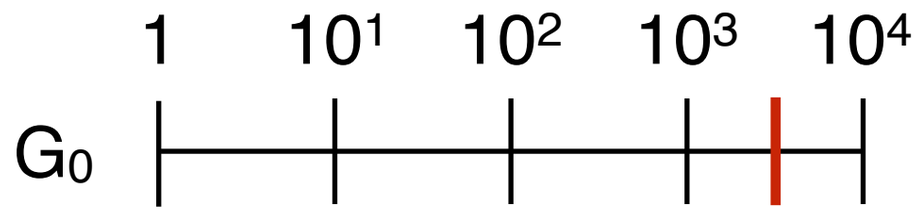

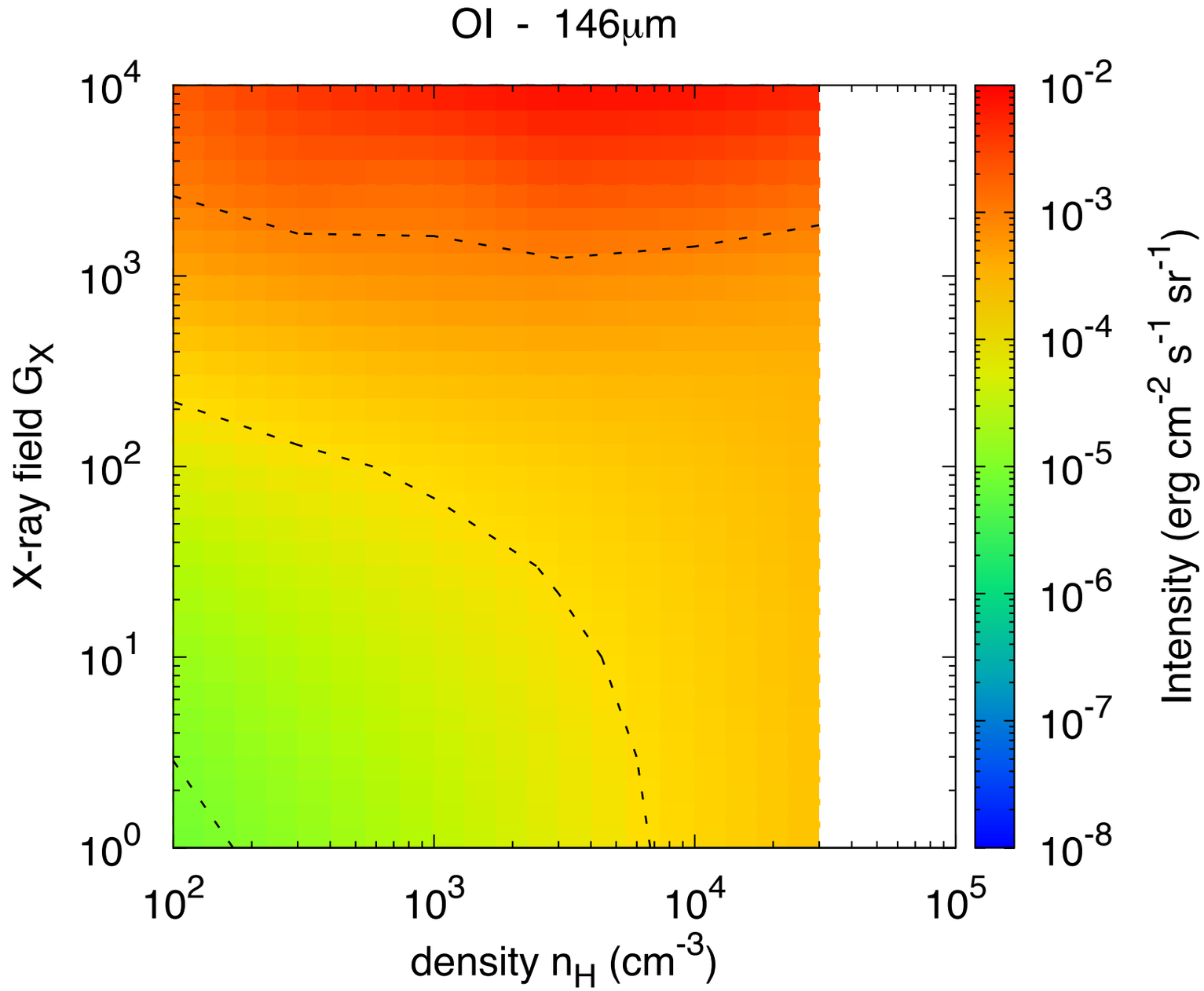

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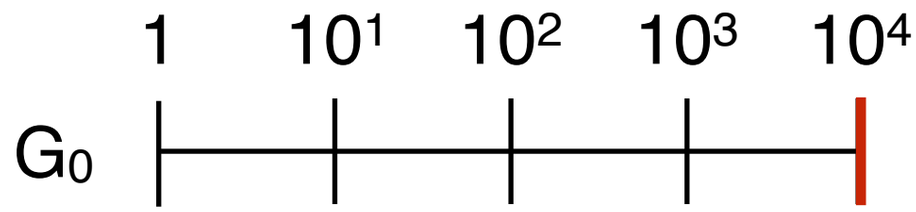

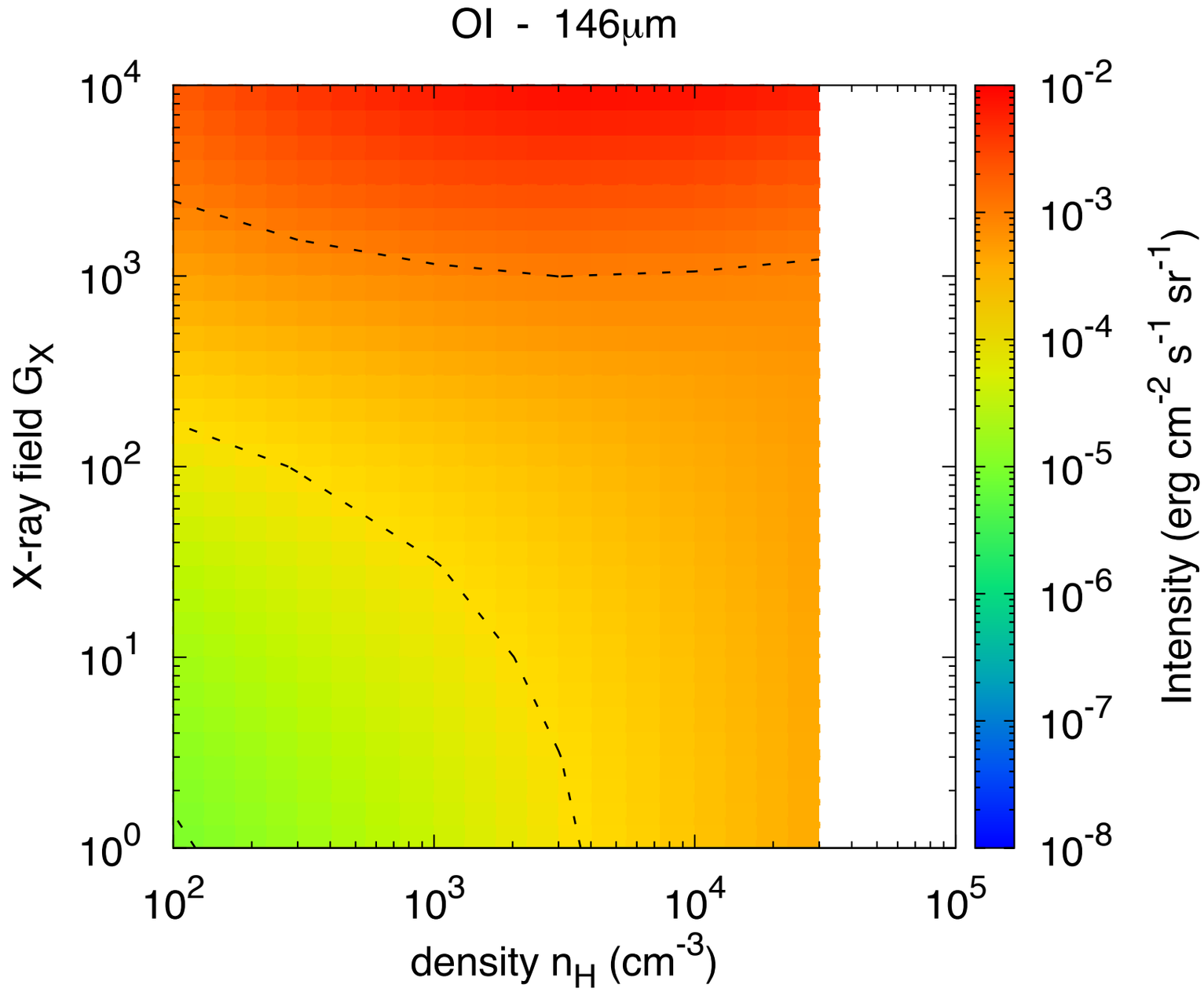

Conclusions

PDR code

- state-of-the-art numerical model
- 1D, static, steady-state BUT
- treats hundreds of microphysical processes

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Physical building blocks

- radiative transfer
  - ✓ continuum
  - ✓ line
- dust
  - ✓ thermal balance
  - ✓ emission
  - ✓ charge
- chemistry
  - ✓ gas phase
  - ✓ surface
- excitation
- gas thermal balance
  - ✓ heating
  - ✓ cooling

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Input data building blocks

- Atom & molec structures
- Collisional Rates
- Chemical properties
- Chemical rates
- Cross Sections
- Grains properties
- Yields

Numerical building blocks

- Ordinary Algebraic Eqs.
- Ordinary Differential Eqs.
- Partial Differential Eqs.
- Initial Value Problems
- Boundary Value Problems
- Linear Algebra
- Numerical Integration & Differentiation