Physics of Photon Dominated Regions

PDR Models

SS 2007

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The standard view from plane-parallel models

- So far: all necessary components of a PDR model introduced:
  - energy balance: important heating and cooling processes
    - PE heating
    - H_2 vibrational deexctiation
    - H_2 formation heating
    - H_2 photodissociation heating
    - CR heating
    - fine-structure emission ([CII], [CI], [OI])
    - line emission (CO, H_2O, OH, Ly α, ...)
    - gas-grain collision (heating and cooling)

The standard view from plane-parallel models

- chemical network:
  - N species (e.g. 99)
  - L reactions (e.g. 1548)
  - M elements (e.g. 7)
  - system of chemical **rate equations**
    - N+M+1 equations for N unknowns
    - numerical complexity scales $\propto N^2 ... N^3$

The standard view from plane-parallel models

- radiative transfer
  - incoming radiation (radiation hitting the PDR surface from outside)
  - outgoing radiation (radiation leaving the PDR)

or

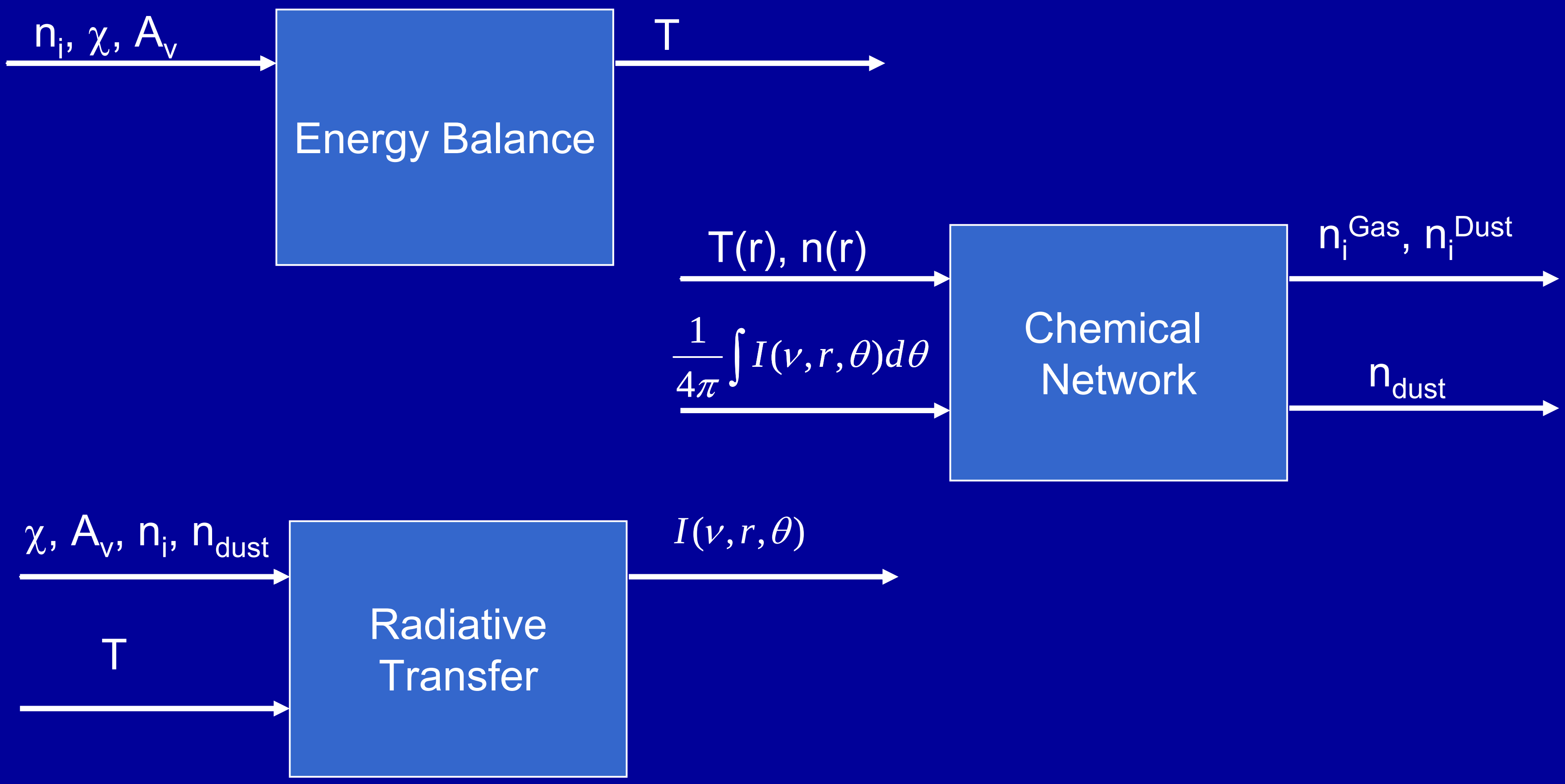
  - emission of radiation
  - absorption of radiation

these two descriptions are not fully exchangeable, since outgoing radiation means emitted radiation, which has partly been re-absorbed in the cloud.

or

  - FUV radiation
  - IR and FIR radiation

The standard view from plane-parallel models



Energy Balance

- PE heating $\Gamma_{PE} = 10^{24} \varepsilon G_0 n$ [erg s^{-1} cm^{-3}]
  Γ denotes heating rates
  ε: PE efficiency, e.g.:

$$= 3\times10^{-2} < f(O) >= \frac{3\times10^{-2}}{1+4.2\times10^{-4} G_0 T^{1/2} / n_e}$$

<f(O)>: neutral fraction $\propto \frac{\text{ionization rate}}{\text{recombination rate}} \propto \frac{G_0 T^{1/2}}{n_e}$
(Bakes&Tielens, 1994)

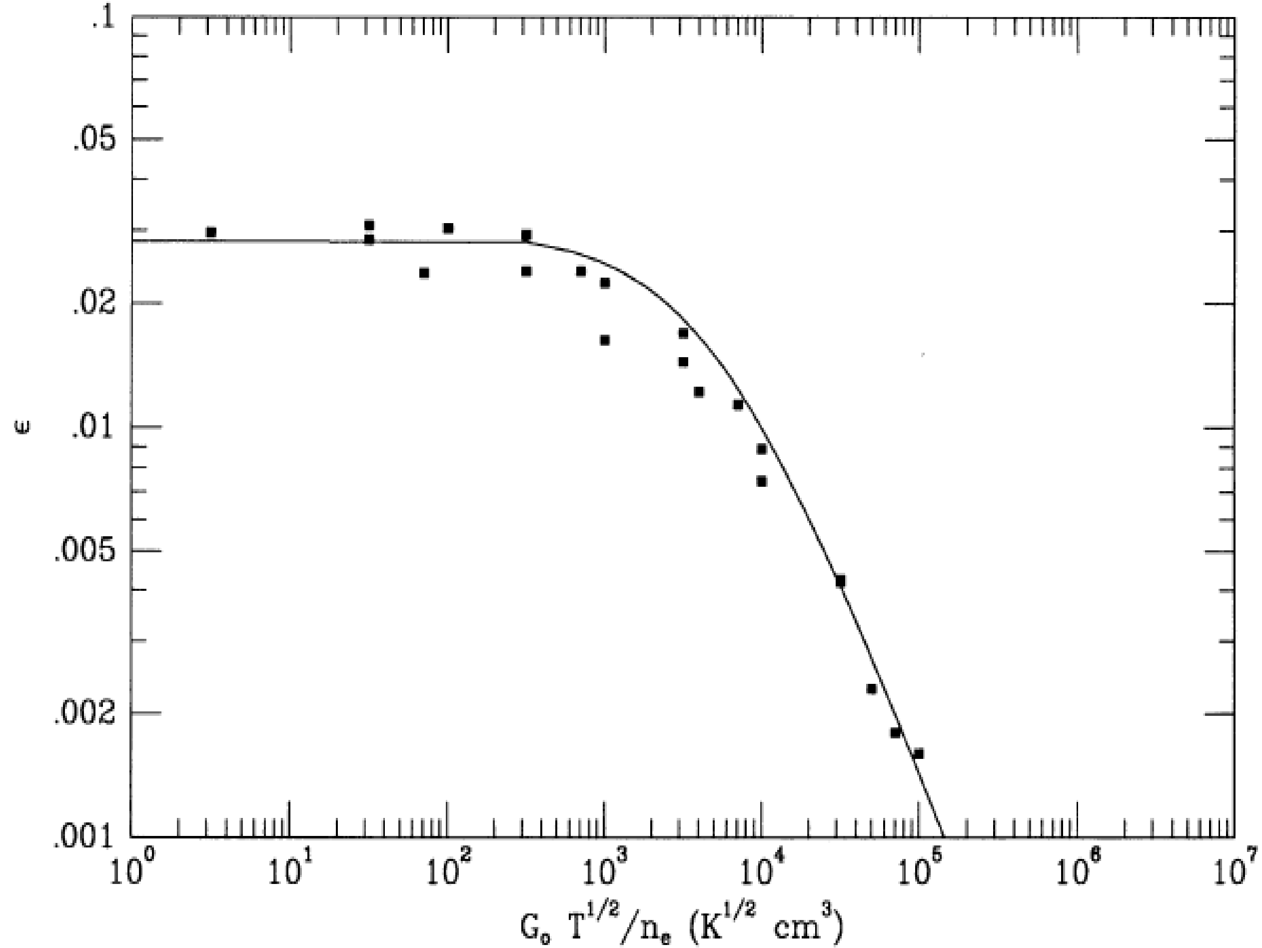


FIG. 11.—The numerically calculated efficiency (*squares*) of the net photoelectric heating rate per hydrogen atom for a range of different interstellar environments defined by the intensity of the incident UV field, G_0, gas temperature, T, and electron density, n_e. The analytic fit (*solid line*) compares well with the numerical results for all gas temperatures less than 10^4 K.

(Bakes&Tielens, 1994)

G_0 vs. χ

- G_0 : FUV flux normalized to the Habing field for the solar neighborhood (Habing 1968) integrated over 6-13.6 eV

  $G_0 = 1.6 \times 10^{-3}$ erg cm^{-2} s^{-1}

  $$\lambda u_\lambda = \left(-\frac{25}{6}\lambda_3^3 + \frac{25}{2}\lambda_3^2 - \frac{13}{3}\lambda_3 \right) \times 10^{-14} \text{ ergs cm}^{-3}$$

- χ: FUV flux normalized to the Draine field (Draine 1978)

  G_0=1.71 χ (isotropic radiation from 4π)

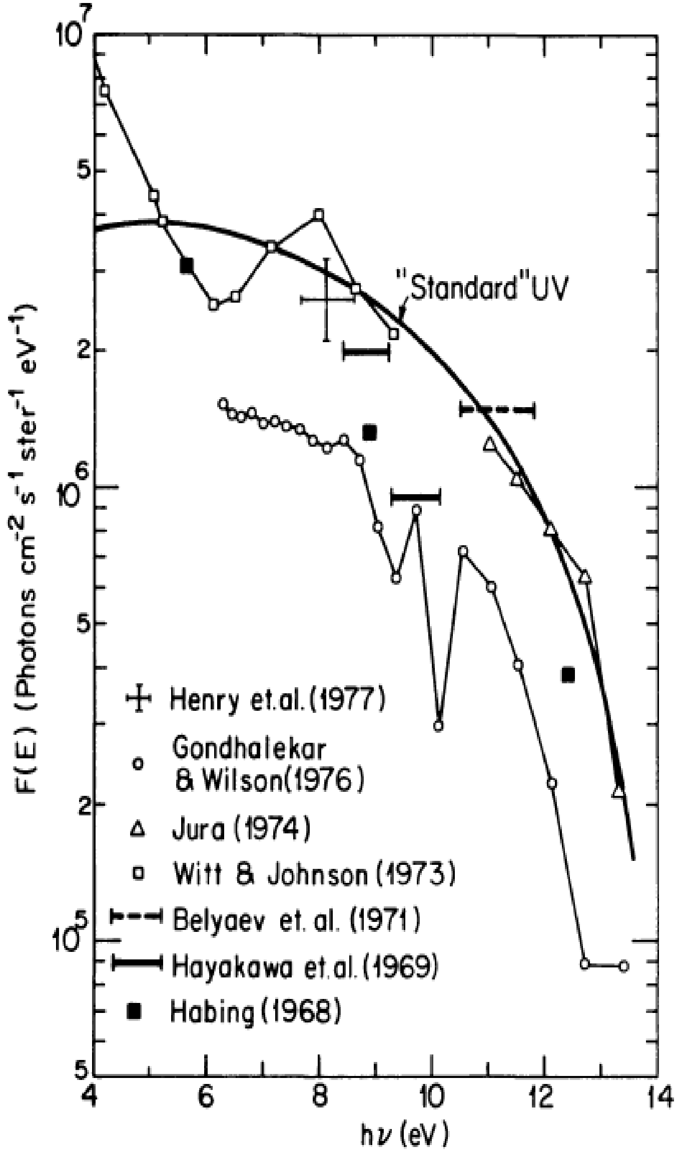


FIG. 3.—The ultraviolet background $F_E = \lambda^3 u_\lambda (4\pi h^2 c)^{-1}$ below 13.6 eV: theoretical estimates of Habing (1968), Witt and Johnson (1973), Jura (1974) and Gondhalekar and Wilson (1975); observations of Hayakawa *et al*. (1969), Belyaev *et al*. (1971), and Henry *et al*. (1977). The smooth curve labeled "standard UV" is the spectrum adopted in the present work.

(Draine, 1978)

G_0 vs. χ

- Draine intensity:

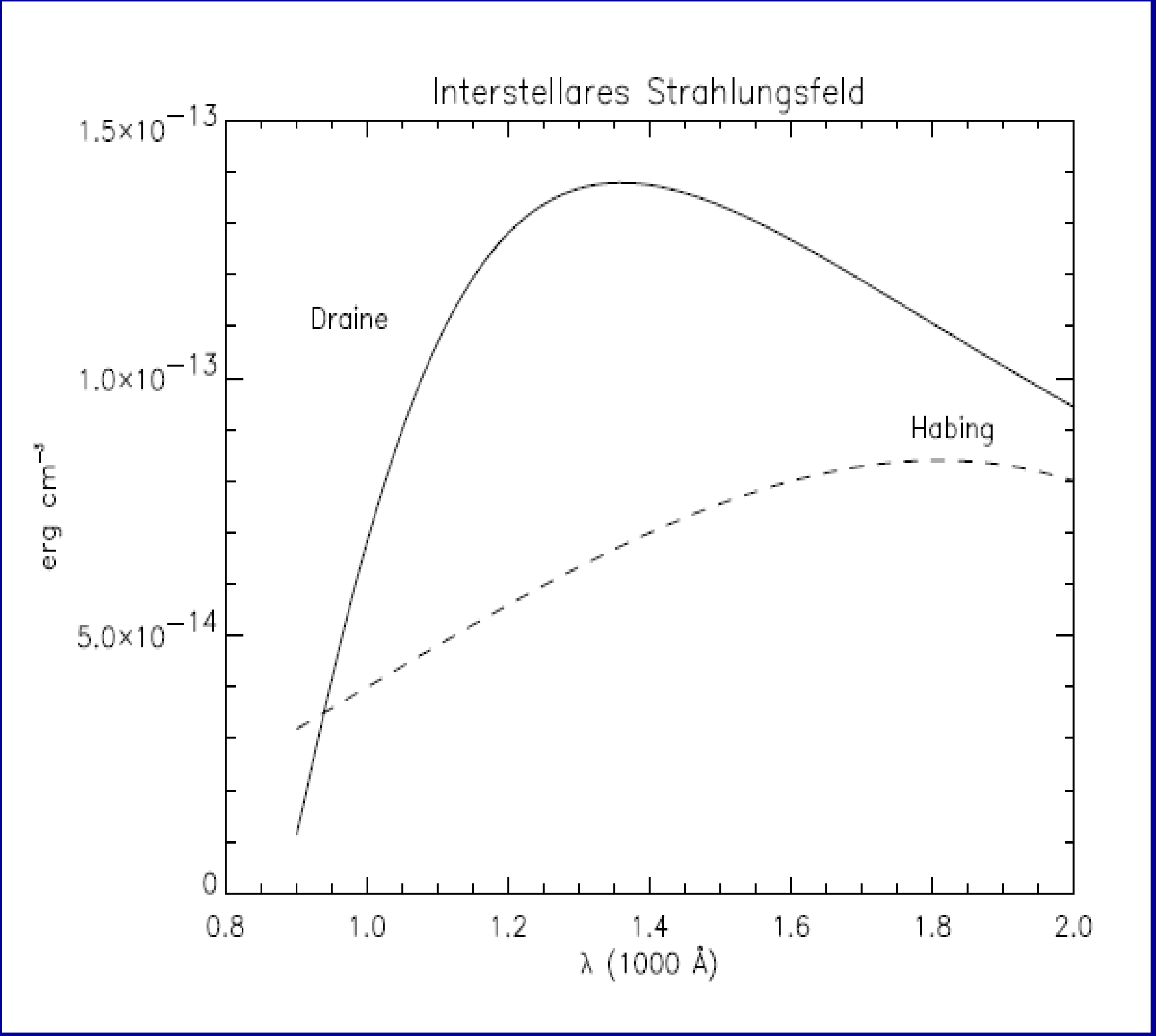
$$I(\lambda) = \frac{1}{4\pi}\left(\frac{6.3000\times10^{7}}{\lambda^{4}} - \frac{1.0237\times10^{11}}{\lambda^{5}} + \frac{4.0812\times10^{13}}{\lambda^{6}}\right)$$

λ in [Å], I(λ) in erg s^{-1} cm^{-2} ster^{-1} Å^{-1}

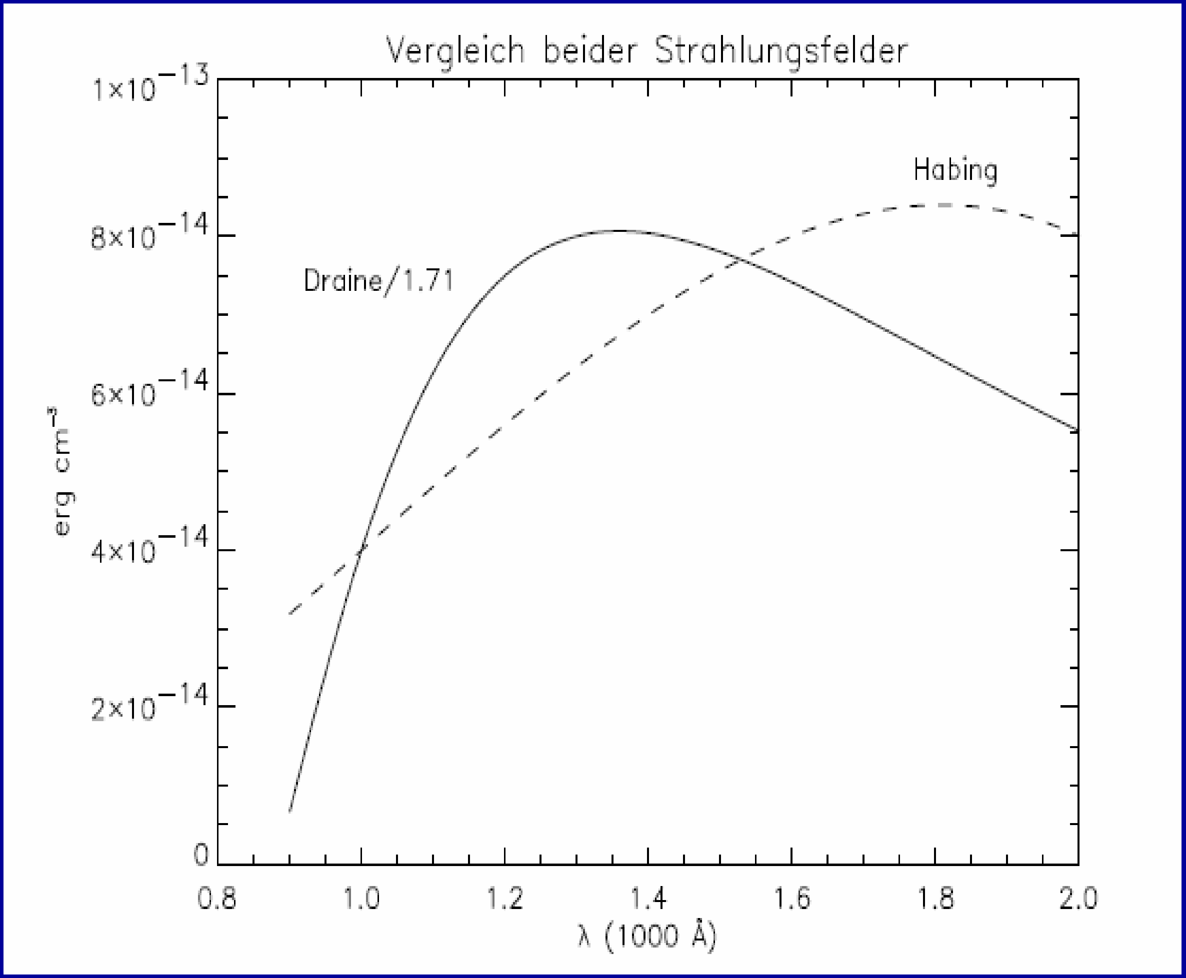
$$u(\lambda) = \frac{1}{c}\int I(\lambda)\,d\Omega$$

$$G = \frac{1}{5.6\times10^{-14}}\int_{912\text{Å}}^{2400\text{Å}} u(\lambda)\,d\lambda$$

Draine vs. Habing

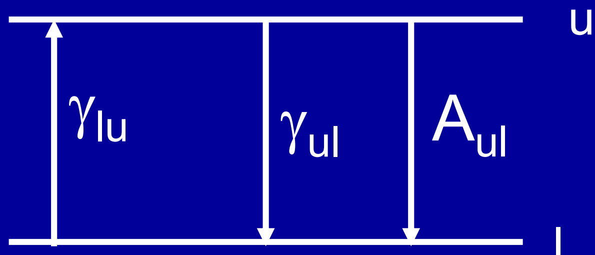


Draine vs. Habing



Cooling

- [CII] 158μm fine structure emission $^2P_{3/2} \rightarrow {}^2P_{1/2}$
- 2-level system (collision + spont. emission)



$$n_l n \gamma_{lu} = n_u n \gamma_{ul} + n_u A_{ul}$$

$$\gamma_{lu} = \frac{g_u}{g_l} \gamma_{ul} e^{-\frac{E_{ul}}{kT}}$$

detailed balance

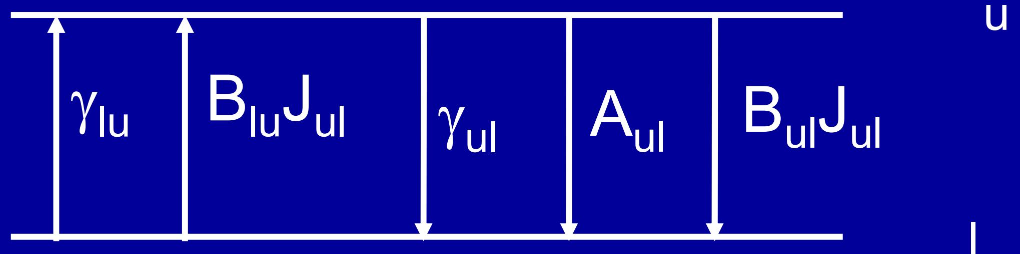
$$n_{cr} = \frac{A_{ul}}{\gamma_{ul}}$$

critical density:
$n > n_{cr}$: collisions dominate

$$\frac{n_u}{n_l} = \frac{\left(\frac{g_u}{g_l}\right) e^{-\frac{E_{ul}}{kT}}}{1 + \frac{n_{cr}}{n}}$$

Escape Probability

- now including absorption



J_{ul}: mean intensity
B: Einstein coefficients for absorption and stimulated emission

$$n_l n \gamma_{lu} + n_l B_{lu} J_{ul} = n_u n \gamma_{ul} + n_u A_{ul} + n_u B_{ul} J_{ul}$$

Attention:
- local population depends on J
- J depends on population everywhere

new concept: escape probability $\beta(\tau_{ul})$

Escape Probability

Assumptions:

- photons produced locally can only be absorbed locally
- in calculating τ_{ul} we assume that the local population holds globally

STRONG ASSUMPTIONS!

now: photon balance

net absorption = emitted photons that do not escape

$$\left(n_l B_{lu} - n_u B_{ul}\right) J_{ul} = n_u \left(1 - \beta\left(\tau_{ul}\right)\right) A_{ul}$$

net # of photons used up for absorptions

net # of photons made available for local absorptions

Escape Probability

- $\beta(\tau_{ul})$: probability that a photon formed at opt. depth τ escapes through the surface

$$n_l n\gamma_{lu} + n_l B_{lu} J_{ul} = n_u n\gamma_{ul} + n_u A_{ul} + n_u B_{ul} J_{ul}$$

$$n_l n\gamma_{lu} + \left(n_l B_{lu} - n_u B_{ul}\right) J_{ul} = n_u n\gamma_{ul} + n_u A_{ul}$$

$$n_l n\gamma_{lu} + n_u \left(1 - \beta(\tau_{ul})\right) A_{ul} = n_u n\gamma_{ul} + n_u A_{ul}$$

$$n_l n\gamma_{lu} = n_u n\gamma_{ul} + n_u \beta(\tau_{ul}) A_{ul}$$

simple 2-lev corrected with β factor

$$n_l n\gamma_{lu} = n_u n\gamma_{ul} + n_u A_{ul}$$

Cooling

- Line cooling rate $n^2\Lambda = n_u A_{ul} E_{ul} \beta(\tau_{ul})$ (erg s^{-1} cm^{-3})
- n_u: number of atoms in upper level

$$\left.\begin{aligned} \frac{n_u}{n_l} &= \frac{\left(\frac{g_u}{g_l}\right) e^{-\frac{E_{ul}}{kT}}}{1+\frac{n_{cr}\beta}{n}} \\ n_u + n_l &= n_{tot} \end{aligned}\right\} \quad n_u = \frac{n_{tot}}{1+\left(\frac{g_l}{g_u}\right) e^{\frac{E_{ul}}{kT}}\left(1+\frac{n_{cr}\beta}{n}\right)}$$

Escape Probability

- β=??
- depends e.g. on geometry
- turbulent, homogeneous, semi-infinite slab
- line-averaged opt. depth:

$$\tau_{ul} = \frac{A_{ul} c^3}{8\pi \nu_{ul}^3} \frac{n_u}{b/\Delta z} \left[\frac{n_l g_u}{n_u g_l} - 1 \right]$$

  b: Doppler broadening parameter
  Δz: distance from the surface
- instead of thermal motion:
  velocity gradient b/Δz$\rightarrow$dv/dz
- once a photon has traveled a distance $\Delta v_D/(dv/dz)$, with Δv_D its Doppler width of the line, it will be shifted to the line-wings, where the opt. depth is small, and the photon will escape

Escape Probability

- For various geometries, β can be given analytically.
- For a semi-infinite, plane-parallel slab:

$$\beta(\tau) = \frac{1-\exp(-2.34\tau)}{4.68\tau} \qquad \tau<7$$

$$\beta(\tau) = \left[4\tau \left(\ln\left(\frac{\tau}{\sqrt{\pi}} \right) \right)^{1/2} \right]^{-1} \qquad \tau>7$$

small τ: β→1/2 (photons escape through half the hemisphere)
large τ: $\beta \propto \tau^{-1}$

Emergent Intensities

2π: photons only escape through the front surface

$$I = \frac{1}{2\pi}\int_0^z n^2 \Lambda(\tilde{z})d\tilde{z}$$

In thermodynamic equilibrium ($n \gg n_{cr}\beta$)

$$I = B(T)\frac{\nu b}{c}f(\tau)$$

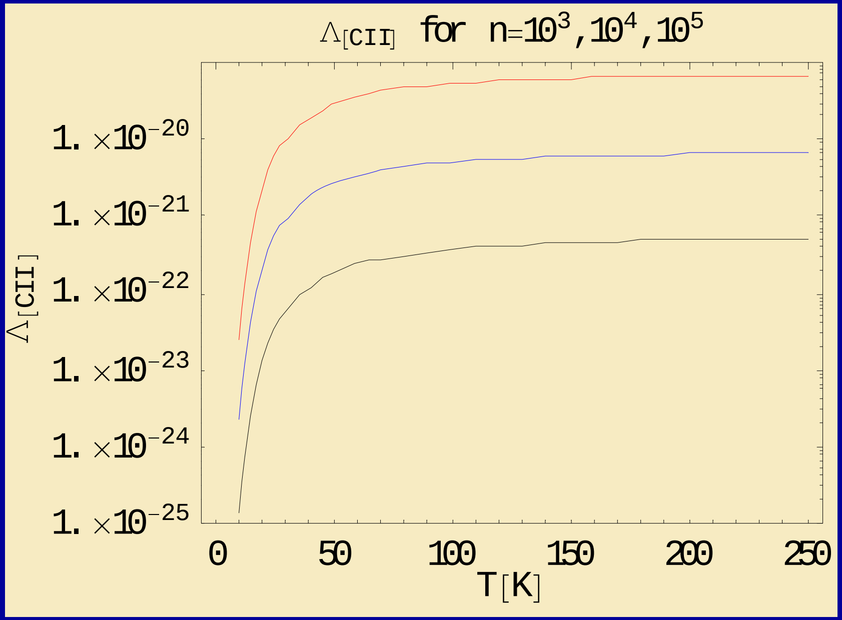
$$f(\tau) = 2\int_0^\tau \beta(\tau)d\tau = 0.428\left[E_1(2.34\tau) + \ln(2.34\tau) + 0.57721\right]$$

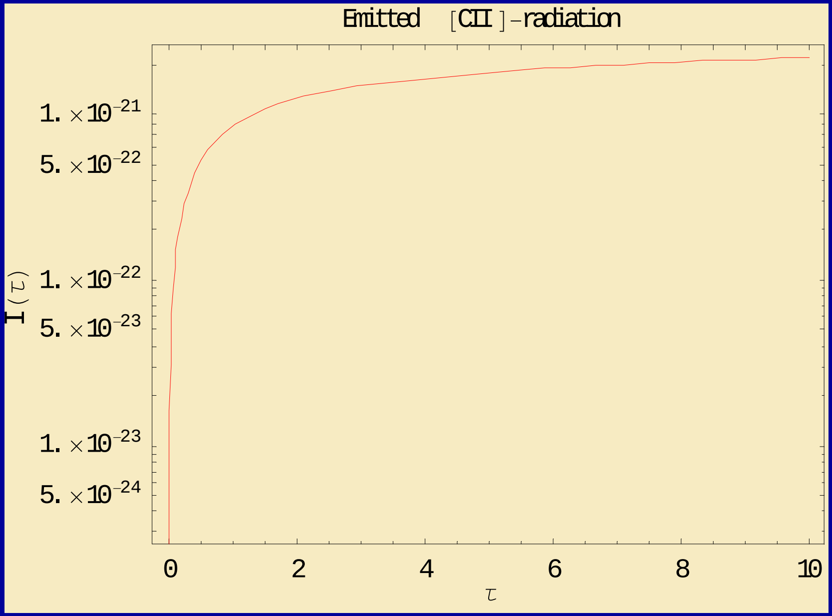
for $\tau \ll 1$: $f(\tau)=\tau$ $\quad I = \frac{A_{ul}N_u h\nu_{ul}}{4\pi}$

Cooling

- [CII] 158μm

$$n^2\Lambda = \frac{1.4\times10^{-4}\cdot 2.29\times10^{-6}\cdot 1.26\times10^{-14}\, n\beta}{1+\frac{1}{2}e^{\frac{92\mathrm{K}}{T}}\left(1+\frac{2600\beta}{n}\right)} \quad \mathrm{erg\ cm^{-3}\ s^{-1}}$$





3-Level System [OI]

$$\Lambda_{12} = A_{12} E_{12} \beta Z \left(\frac{n_{\rm OI} \exp(E_{01}/T)\, g_1\, n\, (n + \beta\, n_{cr,01})}{g_0\, n^2 \;\; \exp(E_{01}/T)\, (n + \beta\, n_{cr,01})\, (g_1\, n \; + \exp(E_{12}/T)\, g_2\, (n + \beta\, n_{cr,12}))} \right) \quad \mathrm{erg\, cm^{-3}\, s^{-1}}$$

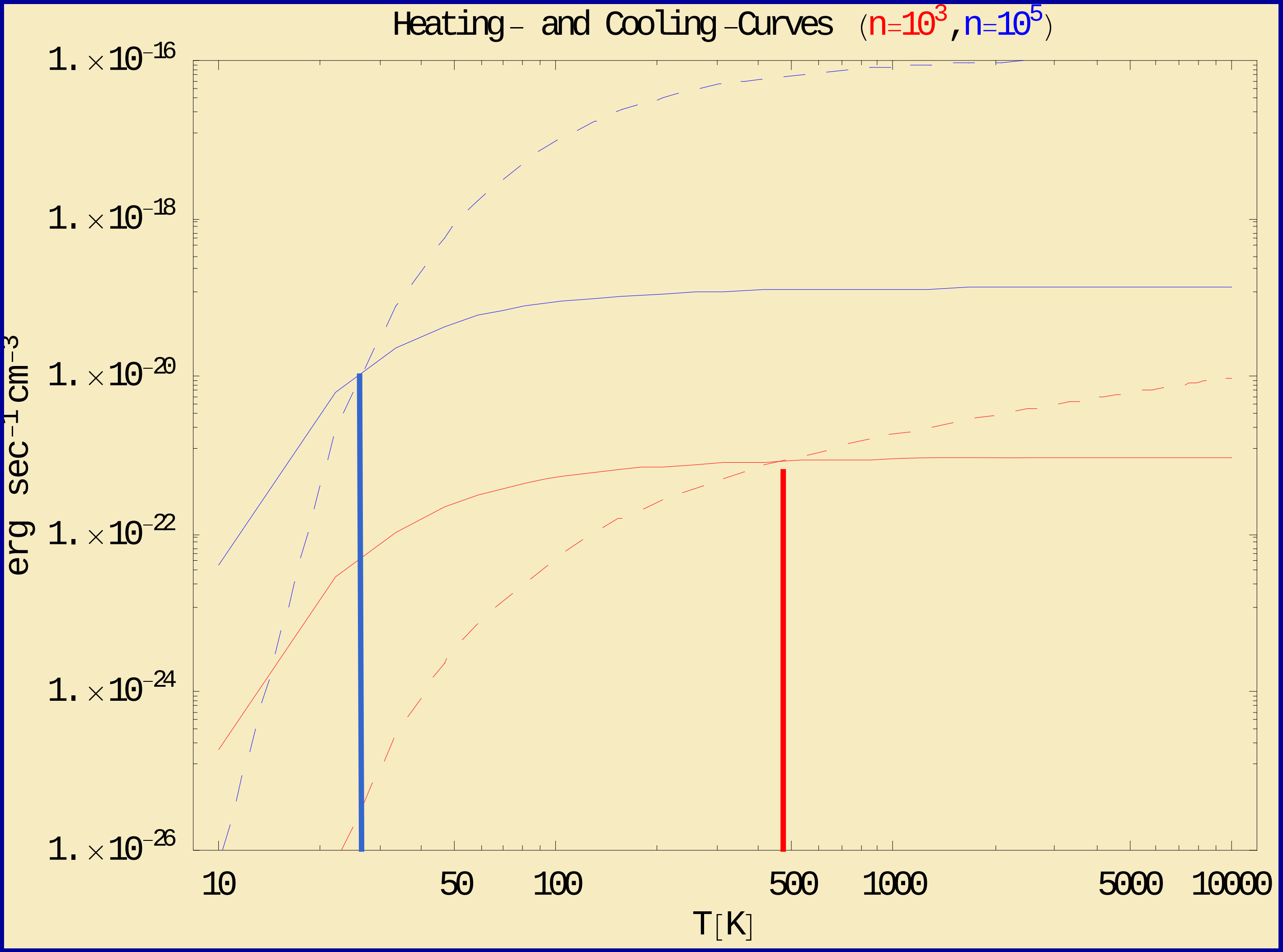
$$\Lambda_{01} = A_{01} E_{01} \beta Z \left(\frac{n_{\rm OI}\, g_0\, n^2}{g_0\, n^2 \;\; \exp(E_{01}/T)\, (n + \beta\, n_{cr,01})\, (g_1\, n \; + \exp(E_{12}/T)\, g_2\, (n + \beta\, n_{cr,12}))} \right) \quad \mathrm{erg\, cm^{-3}\, s^{-1}}.$$

$$\Lambda_{63\,\mu\mathrm{m}} = 3.15 \times 10^{-14}\, 8.46 \times 10^{-5}\, \frac{1}{2} Z$$
$$\times \frac{3 \times 10^{-4}\, n\, \exp(98\,\mathrm{K}/T)\, 3\, n \left(n + \frac{1}{2} \frac{1.66 \times 10^{-5}}{1.35 \times 10^{-11}\, T^{0.45}} \right)}{n^2 \; + \exp(98\,\mathrm{K}/T) \left(n \; + \; \frac{1}{2} \frac{1.66 \times 10^{-5}}{1.35 \times 10^{-11}\, T^{0.45}} \right) \left(3\, n \; + \; \exp(228\,\mathrm{K}/T)\, 5 \left(n \; + \; \frac{1}{2} \frac{8.46 \times 10^{-5}}{4.37 \times 10^{-12}\, T^{0.66}} \right) \right)} \quad \mathrm{erg\, cm^{-3}\, s^{-1}}$$

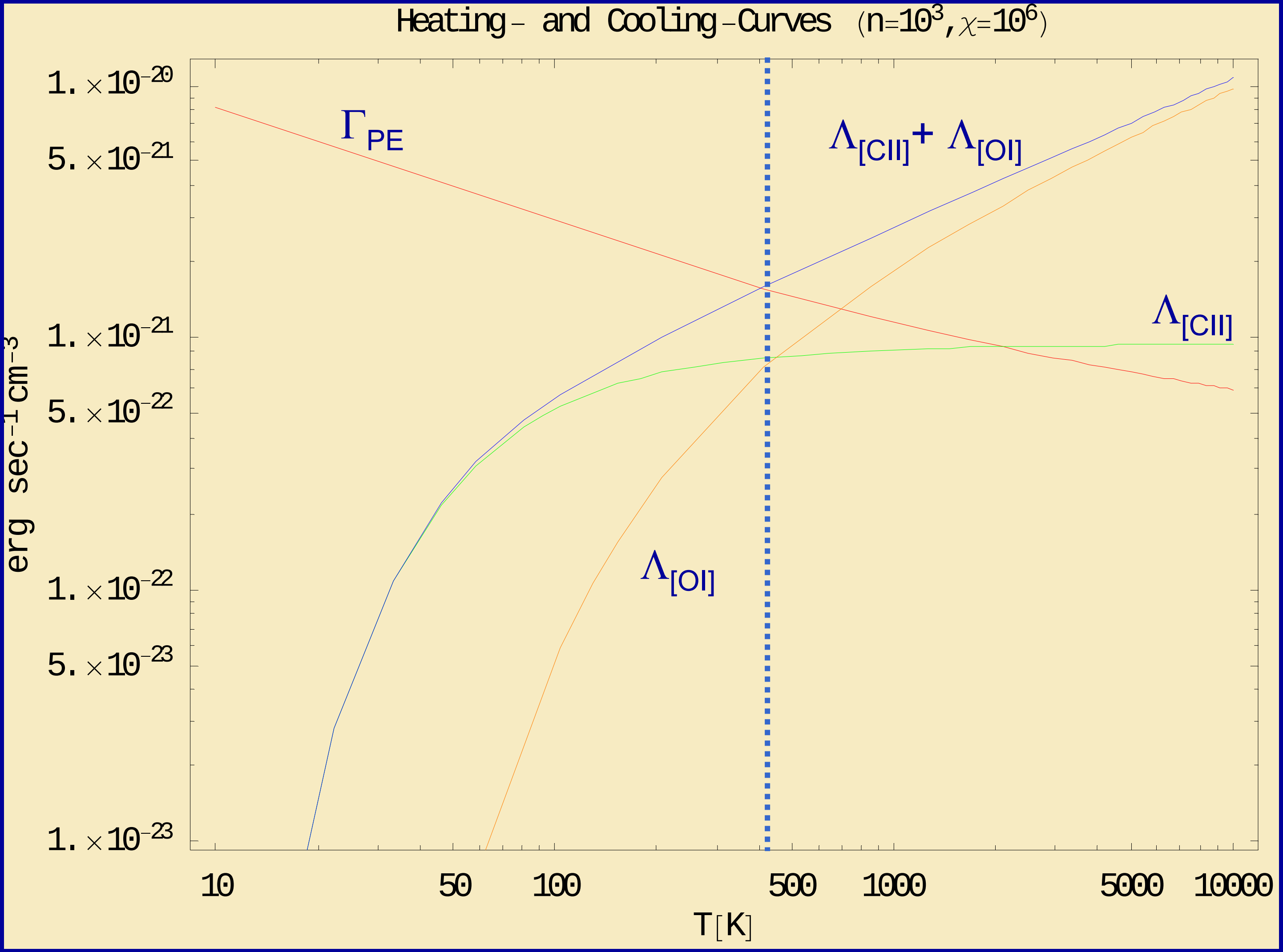
$$\Lambda_{146\,\mu\mathrm{m}} = 1.35 \times 10^{-14}\, 1.66 \times 10^{-5}\, \frac{1}{2} Z$$
$$\times \frac{3 \times 10^{-4}\, n\, n^2}{n^2 \; + \exp(98\,\mathrm{K}/T) \left(n \; + \; \frac{1}{2} \frac{1.66 \times 10^{-5}}{1.35 \times 10^{-11}\, T^{0.45}} \right) \left(3\, n \; + \; \exp(228\,\mathrm{K}/T)\, 5 \left(n \; + \; \frac{1}{2} \frac{8.46 \times 10^{-5}}{4.37 \times 10^{-12}\, T^{0.66}} \right) \right)} \quad \mathrm{erg\, cm^{-3}\, s^{-1}}.$$

!! β=0.5, Z: metallicity

Cooling – [CII] vs. [OI]



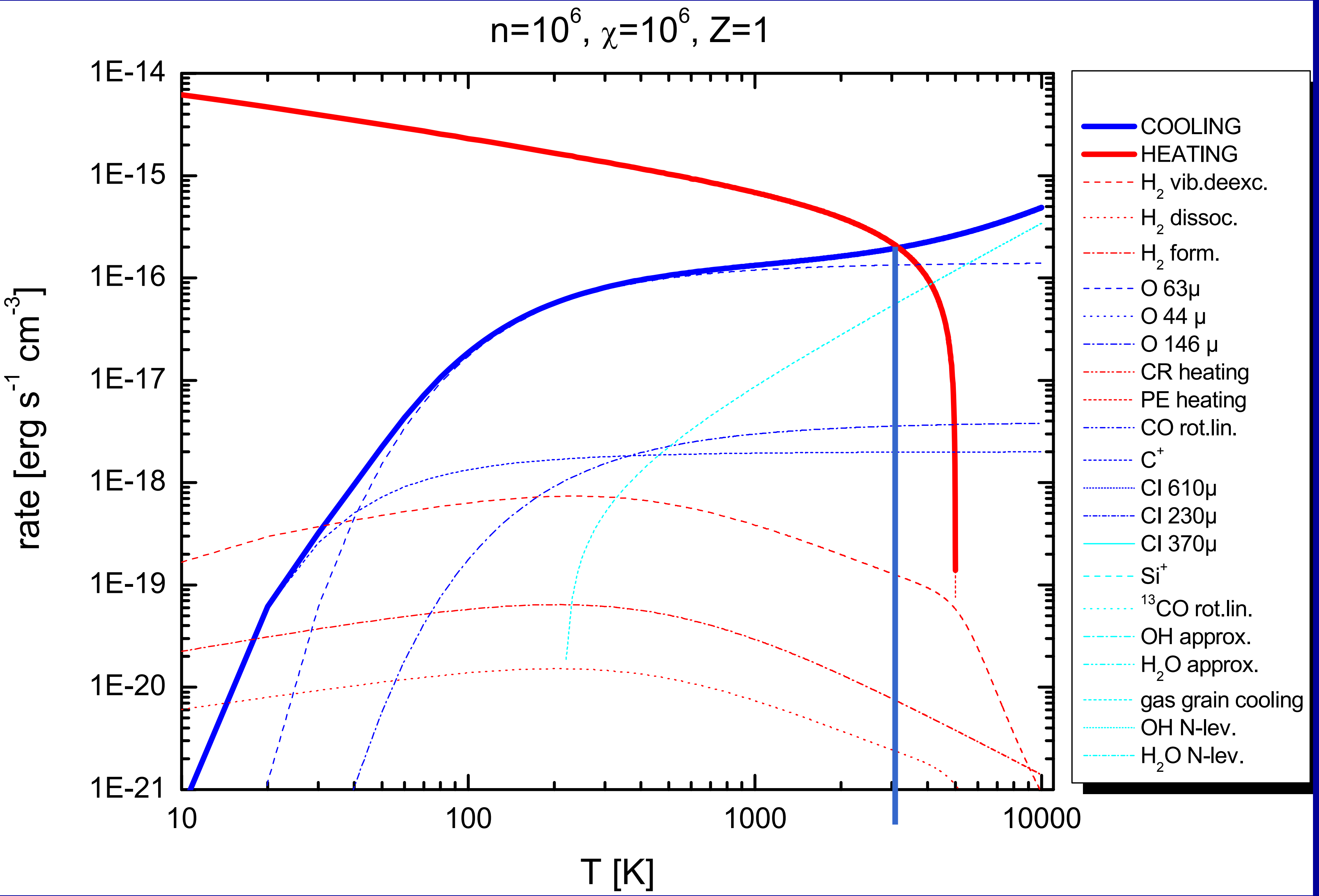
Energy Balance



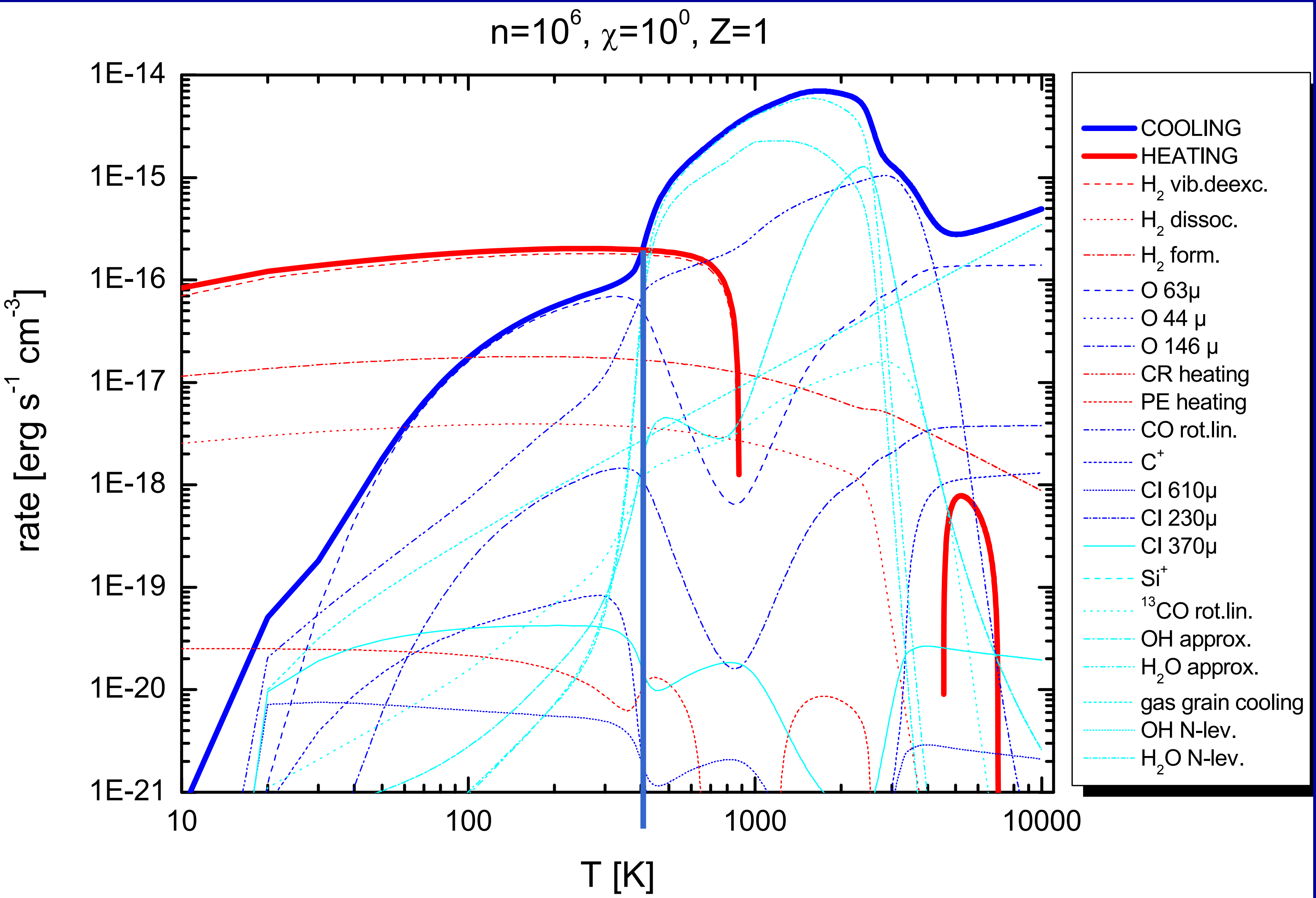
Heating and Cooling

- H_2 vib. deexcitation
- H_2 dissociation
- H_2 formation
- CR heating
- PE heating
- gas-grain collisions

- [OI] 63, 146, 44μm
- CO rot. lines
- [CII]158μm
- [CI] 610, 370, 230μm
- Si^+
- ^{13}CO rot. lines
- OH
- H_2O
- gas-grain collisions



n=10^6, χ=10^6, Z=1
rate [erg s^-1 cm^-3]
T [K]
1E-14
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
1E-21
10
100
1000
10000
COOLING
HEATING
H2 vib.deexc.
H2 dissoc.
H2 form.
O 63μ
O 44 μ
O 146 μ
CR heating
PE heating
CO rot.lin.
C+
CI 610μ
CI 230μ
CI 370μ
Si+
13CO rot.lin.
OH approx.
H2O approx.
gas grain cooling
OH N-lev.
H2O N-lev.



n=10^6, χ=10^0, Z=1
rate [erg s^-1 cm^-3]
1E-14
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
1E-21
10
100
1000
10000
T [K]
COOLING
HEATING
H2 vib.deexc.
H2 dissoc.
H2 form.
O 63μ
O 44 μ
O 146 μ
CR heating
PE heating
CO rot.lin.
C+
CI 610μ
CI 230μ
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OH approx.
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OH N-lev.
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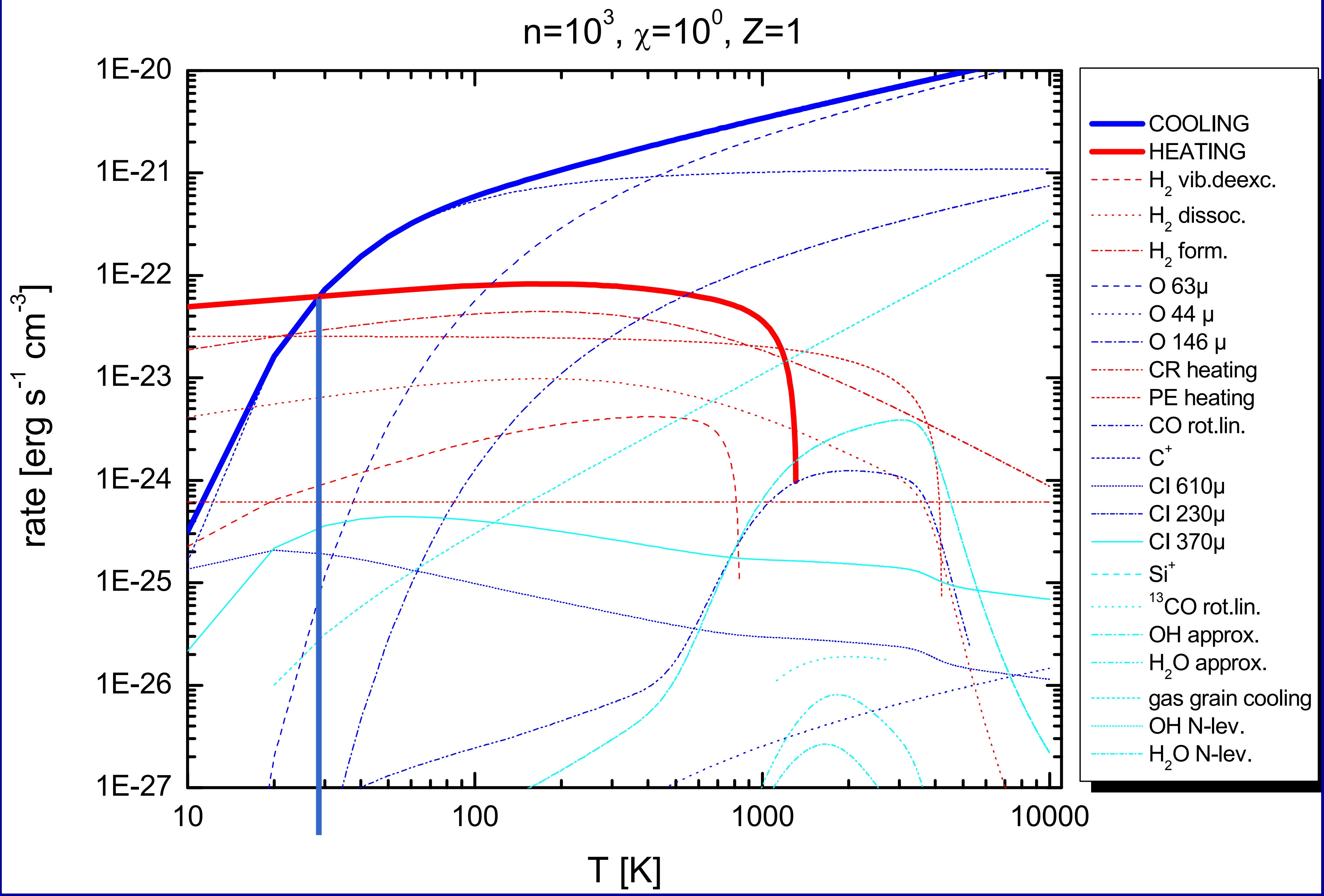

n=10^3, χ=10^0, Z=1
rate [erg s^-1 cm^-3]
T [K]
1E-20
1E-21
1E-22
1E-23
1E-24
1E-25
1E-26
1E-27
10
100
1000
10000
COOLING
HEATING
H2 vib.deexc.
H2 dissoc.
H2 form.
O 63μ
O 44 μ
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CR heating
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OH approx.
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OH N-lev.
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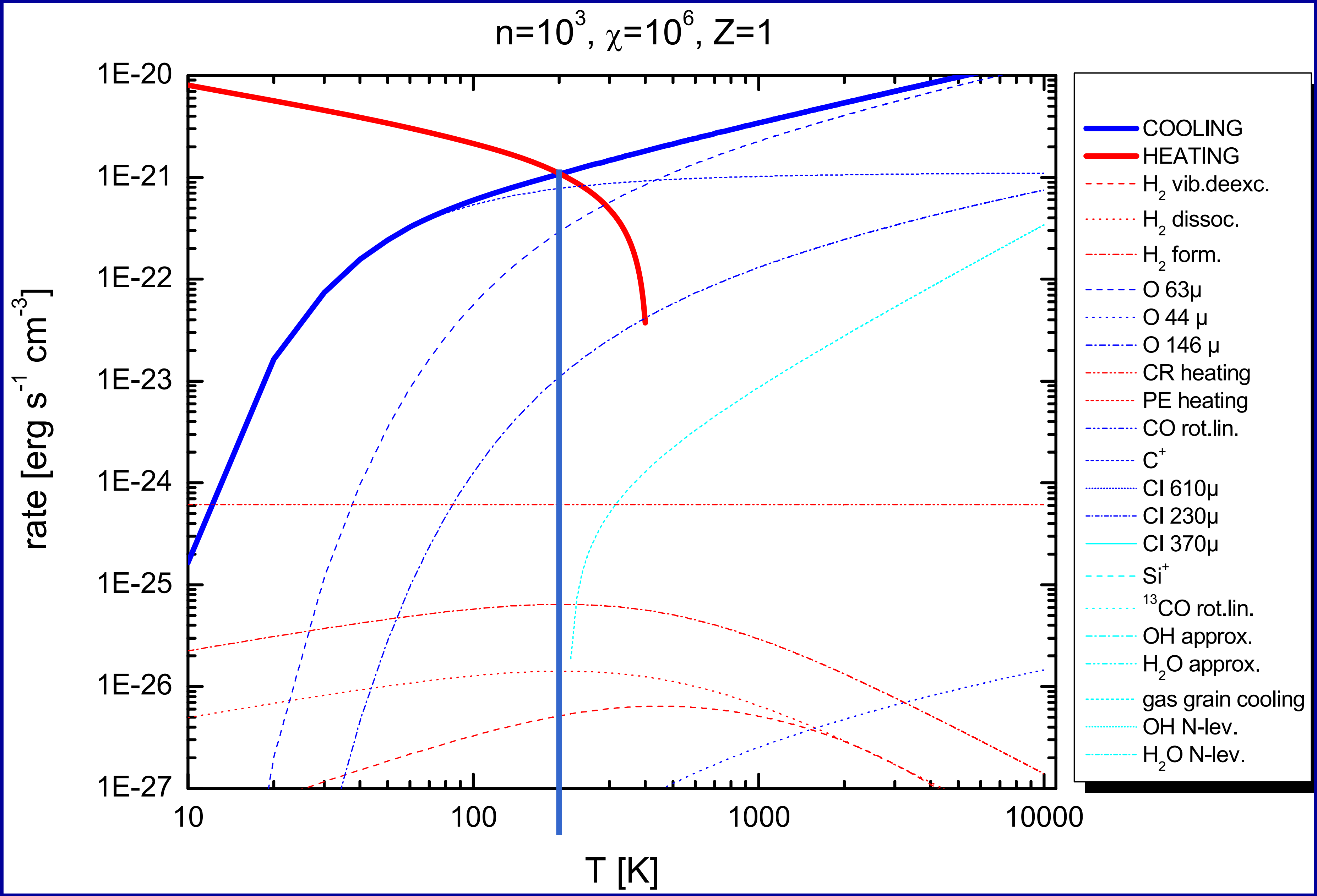


n=10^3, χ=10^6, Z=1
1E-20
1E-21
1E-22
1E-23
1E-24
1E-25
1E-26
1E-27
rate [erg s^-1 cm^-3]
10
100
1000
10000
T [K]
COOLING
HEATING
H2 vib.deexc.
H2 dissoc.
H2 form.
O 63μ
O 44 μ
O 146 μ
CR heating
PE heating
CO rot.lin.
C+
CI 610μ
CI 230μ
CI 370μ
Si+
13CO rot.lin.
OH approx.
H2O approx.
gas grain cooling
OH N-lev.
H2O N-lev.

Chemistry

- N species, M elements
- one rate equation per species

$$\frac{\partial n_i}{\partial t} = -n_i \left\{ \tilde{\zeta}_i + \sum_q n_q k_{qi} \right\} + \sum_r \sum_s k_{rs} n_r n_s + \sum_t n_t \tilde{\zeta}_{ti} \qquad \text{, i=1,...,N}$$

destruction reactions formation reactions

$\tilde{\zeta}_i = \zeta_i^{diss} + \zeta_i^{ion}$ rate coefficient for photo-destruction of i

k_{qi} rate coefficient for $X_i + X_q \rightarrow ...$

k_{rs} rate coefficient for $X_r + X_s \rightarrow X_i + ...$

$\tilde{\zeta}_{ti} = \zeta_{ti}^{diss} + \zeta_{ti}^{ion}$ rate coefficient for $X_t + h\nu \rightarrow X_i + ...$

Chemistry

particle conservation

$$n_M = \sum_i n_i c_i^M \qquad \mathrm{c_i^M : number\ of\ atoms\ of\ element\ M\ in\ species\ i}$$

e.g.: $\mathrm{n = n_H + 2n_{H_2}}$

charge conservation

$$n_e = \sum_i n_i c_i^{charge} \qquad \mathrm{c_i^{charge} : number\ of\ charges\ in\ species\ i}$$

e.g.: $\mathrm{n_e = n_{C^+}}$

<u>N+M+1 quations for N unknown quantities</u>

Chemistry

- e.g.: H/H_2 balance

advection

$$\frac{\partial n(H_2)}{\partial t} = R_f - f_{shield} e^{-\tau} I_{diss}(\tau = 0) \chi n_{H_2} - \frac{\partial (n_{H_2} v)}{\partial z}$$

$$R_f \sim 3\times 10^{-17} n n_H \quad \text{cm}^3\text{s}^{-1} \quad \text{(observation)}$$

$$R_f = \frac{1}{2} S(T, T_D)\eta(T_D) n_D n_H \sigma_D v_H \quad \text{(theory)}$$

$$I_{diss}(\tau = 0) \approx 5.2\times 10^{-11} \quad \text{s}^{-1}$$

Chemistry

Assumptions:

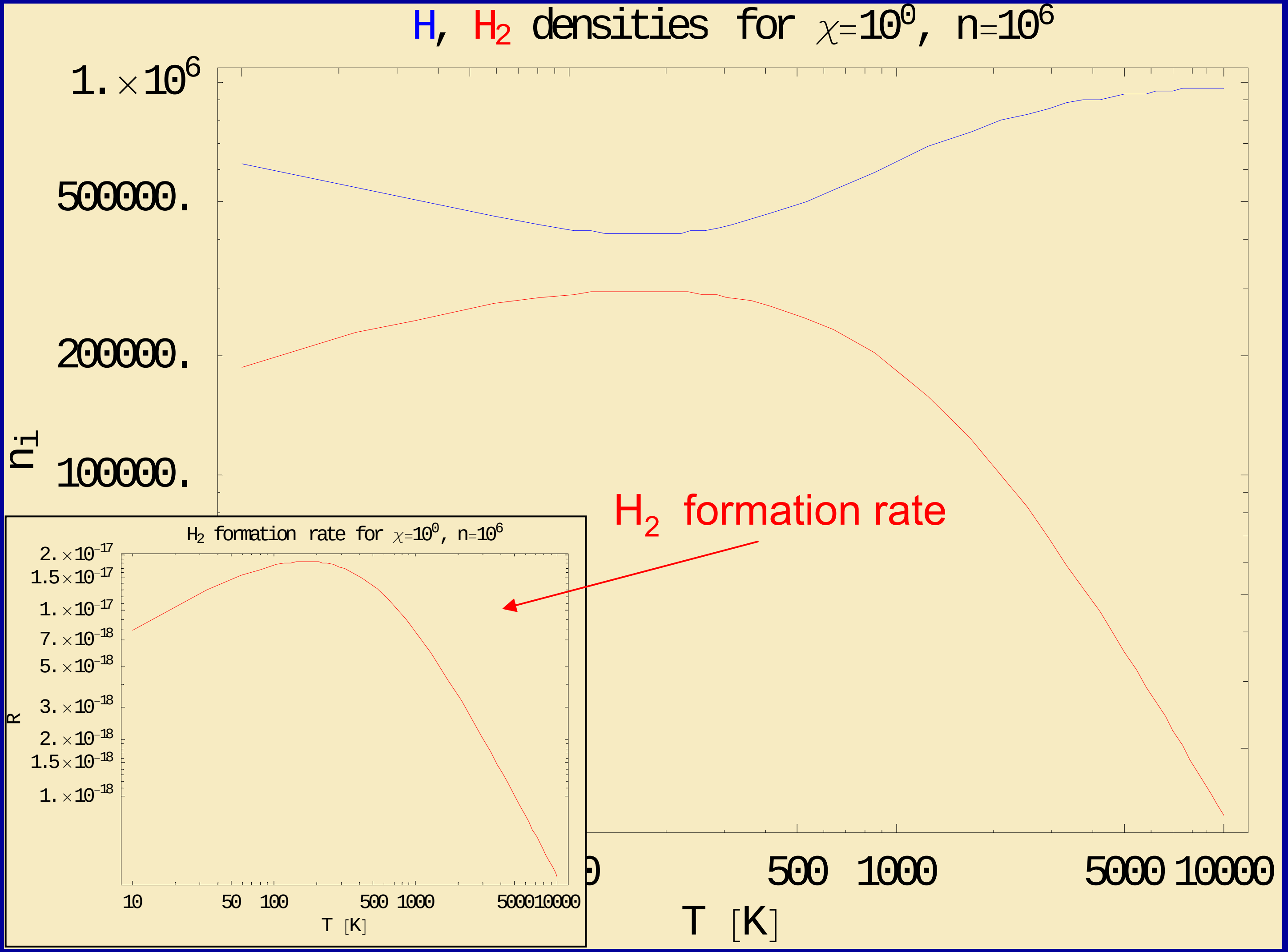
- steady-state chemistry $\Rightarrow$ $\frac{\partial n}{\partial t} = 0$
- τ=0 : cloud surface

$$Rnn_H = I_{diss}(0)\chi n_{H_2}$$

$$n = n_H + 2n_{H_2}$$

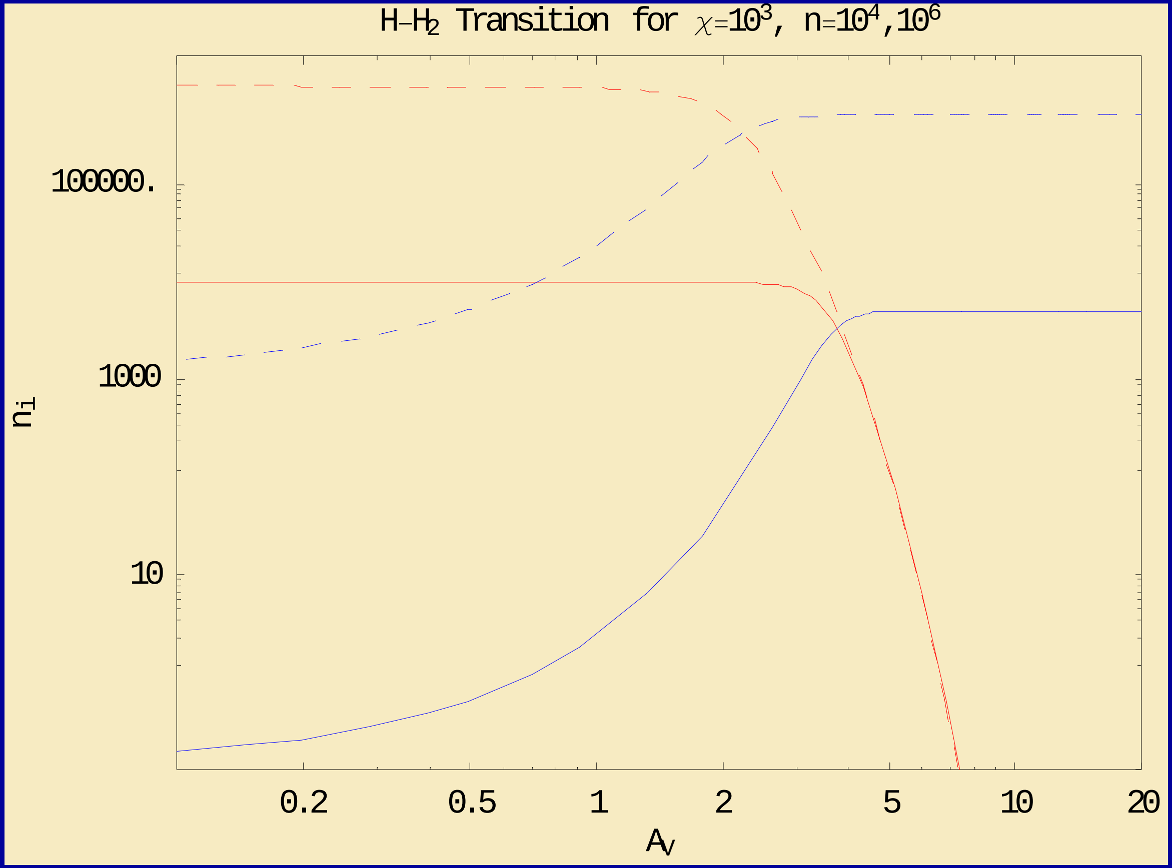
$$n_H = n\frac{1}{1+2\alpha}, n_{H_2} = n\frac{\alpha}{1+2\alpha}, \alpha = \frac{nR}{\chi I(0)}$$

Chemistry



H, H2 densities for χ=10^0, n=10^6
1.×10^6
500000.
200000.
100000.
n_i
500
1000
5000
10000
T [K]
H2 formation rate
H2 formation rate for χ=10^0, n=10^6
2.×10^-17
1.5×10^-17
1.×10^-17
7.×10^-18
5.×10^-18
3.×10^-18
2.×10^-18
1.5×10^-18
1.×10^-18
R
10
50
100
500
1000
5000
10000
T [K]

Chemistry



$$\tau \neq 0 : I \rightarrow I(0)e^{-\tau_{UV}}$$

$$\Rightarrow \alpha = \frac{nR}{\chi I(0)e^{-\tau_{UV}}}$$

$\tau \longrightarrow$ connection to RT

τ_{UV}=k A_v (e.g. k=3.02)
$A_V = 6.289 \times 10^{-22} N_{Htot}$
$\Rightarrow$
A_V=1 entspricht
$N_H = 1.59 \times 10^{21}$ cm^{-2}

Chemistry

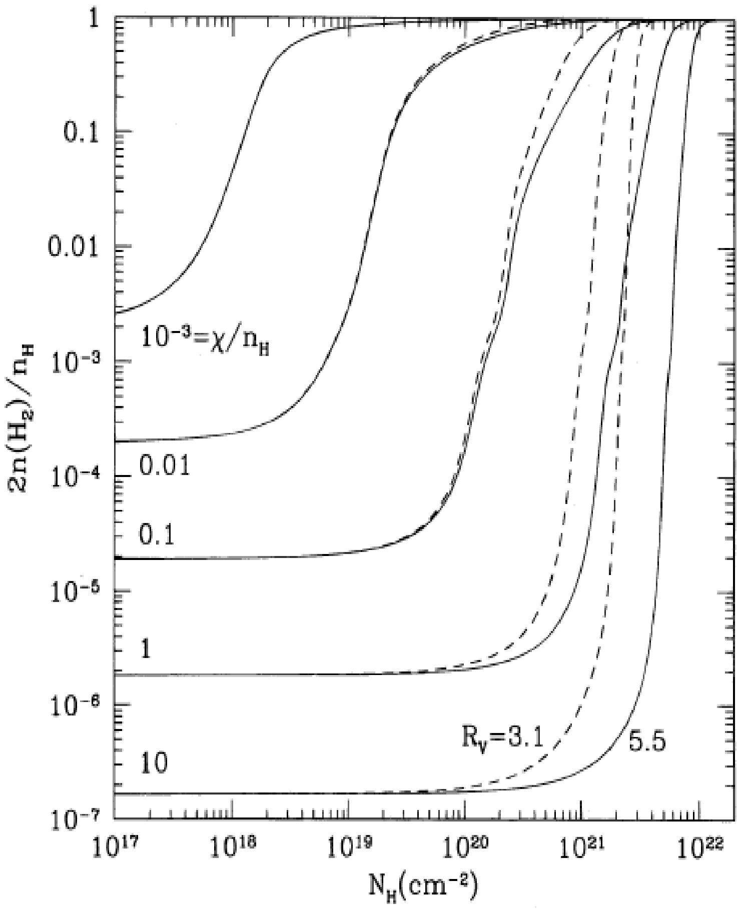


FIG. 8.—H_2 fractions in stationary, plane-parallel photodissociation fronts for $n_H = 10^2$ cm^{-3} and $T_0 = 200$ K, for selected values of χ/n_H (cm^3) and dust with $R_V = 3.1$ ($\sigma_{d,1000} = 2 \times 10^{-21}$ cm^2) and $R_V = 5.5$ ($\sigma_{d,1000} = 6 \times 10^{-22}$ cm^2). $\lambda > 912$ Å radiation with $u_\nu \propto \nu^{-2}$ is propagating in the $+x$ direction at $N_H = 0$. N_H is the total column density of H nucleons. Self-shielding of the H_2 is computed for 27,983 lines using eq. (30) with $W_{max} = 0.2$.

dust shielding important $G_0/n \geq 4\times10^{-2}$ cm^3

self shielding important $G_0/n \leq 4\times10^{-2}$ cm^3

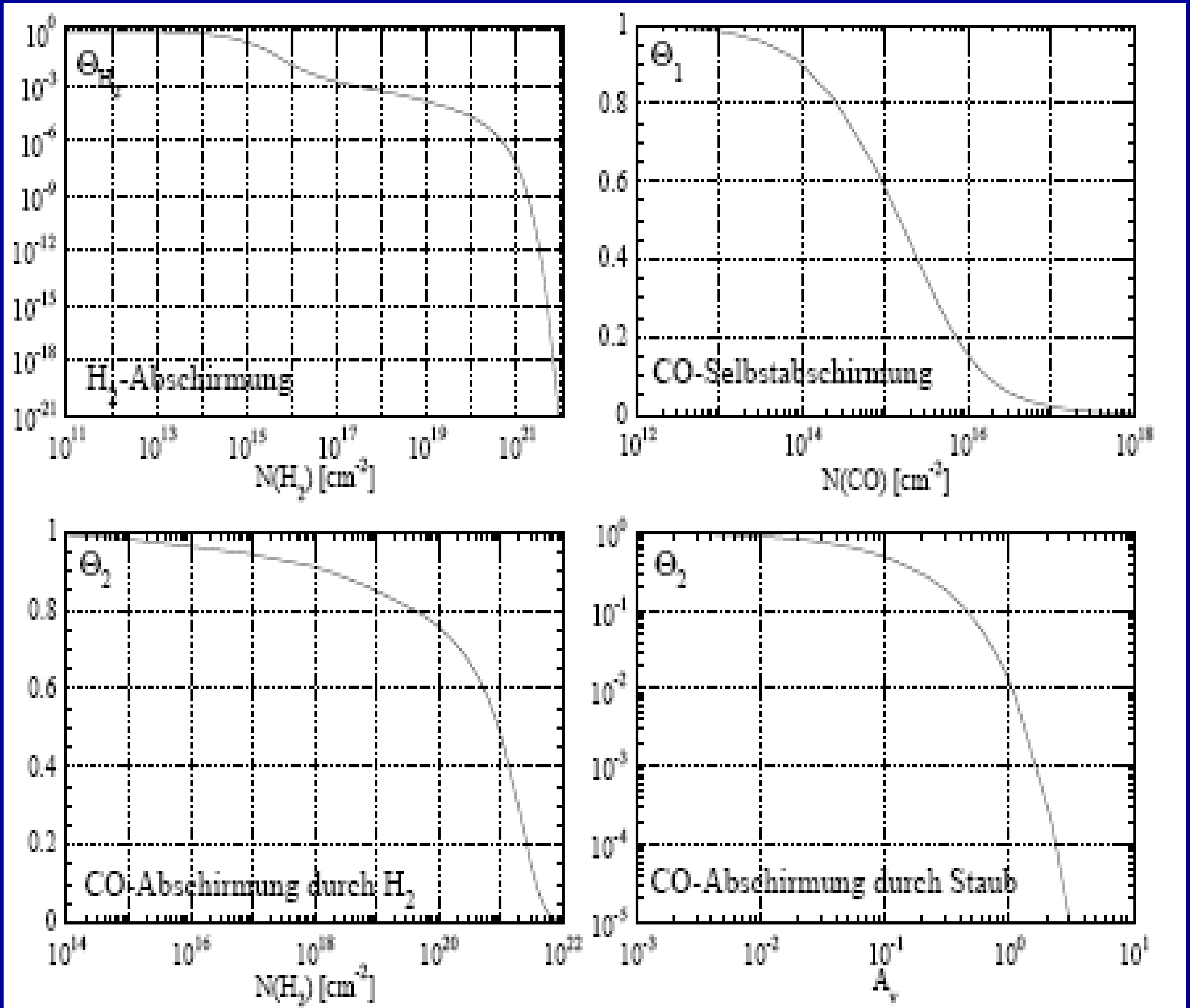
self shielding factor approximation

$$\beta_{SS} = \left(\frac{N(H_2)}{N_0}\right)^{-0.75}$$

$$N_0 = 10^{14} \leq N(H_2) \leq 10^{21}\ \text{cm}^{-2}$$

Draine & Bertoldi, 1996, Ap.J., 468

Chemistry



H2 and CO are photodissociated via line absorption, hence they are both subject to line shielding effects

(see. e.g. van Dishoeck & Black, 1988)

Lee et al. 1996

Chemistry

- τ, A_V, N are exchangeable measures of the amount of matter passed by radiation.
- Pay attention when you exchange them!

Radiative Transfer

- pure absorption $$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu$$

- absorption +emission $$\frac{dI_\nu}{ds} = -\kappa_\nu I_\nu + \varepsilon_\nu$$

$$\text{with } d\tau_\nu = \kappa_\nu ds, \qquad \frac{dI_\nu}{d\tau_\nu} = -I_\nu + \frac{\varepsilon_\nu}{\kappa_\nu} = -I_\nu + S_\nu$$

- extinction $$k_\nu = \kappa_\nu + \sigma_\nu \quad \Rightarrow \quad d\tau_\nu = k_\nu ds$$

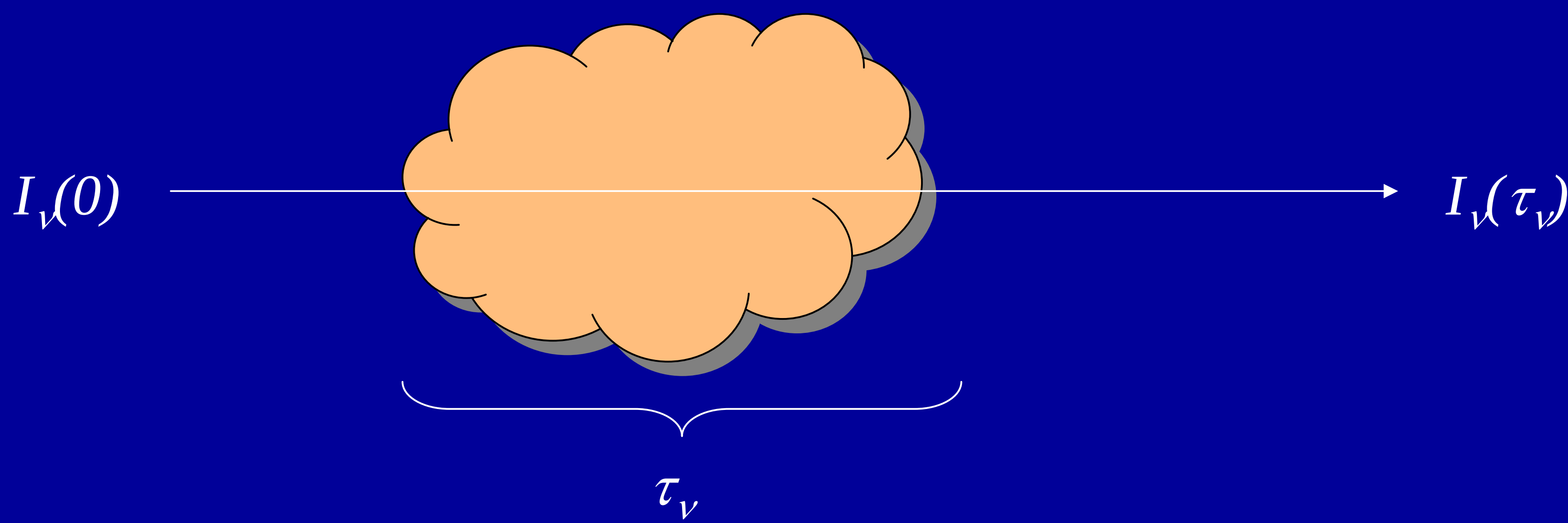
$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-\tau'_\nu} S_\nu(\tau'_\nu) d\tau'_\nu$$

Radiative Transfer

$$I_\nu(\tau_\nu) = I_\nu(0)e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-\tau'_\nu} S_\nu(\tau'_\nu)\,d\tau'_\nu$$

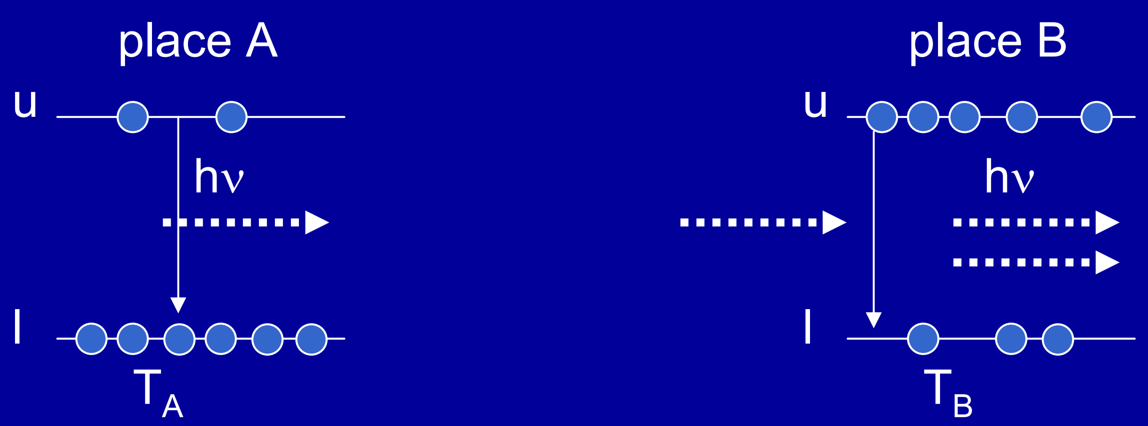
background radiation

radiation emitted inside the cloud and partly re-absorbed within the cloud



Radiative Transfer

- in case of LTE (local thermodynamic equilibrium) und e.g. constant temperature $S_\nu \rightarrow B_\nu(T)$ (black body)
- Problem:



emission depends on n_u/n_l and T_A

emission depends on n_u/n_l and T at A and n_u/n_l and T at B

Radiative Transfer

- radiative properties at plave B depends on conditions at place A! → non-local problem
- To solve the RT problem at B it is necessary to have it already solved at all other places. Same argument holds for all positions.
- Analytical solution only for special cases possible.
  - numerical, iterative solution
  - special simplifications to de-couple the RT
    - escape probability
    - LVG (large velocity gradient) (Sobolov approx.)

Radiative Transfer

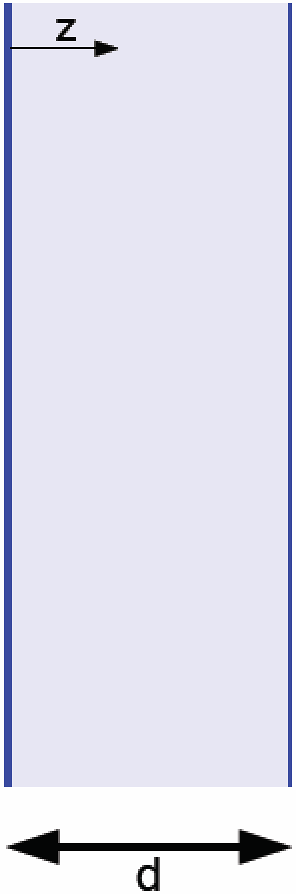
- Through RT geometry enters the stage
- Since RT couples distant mass elements to each other it becomes necessary to define the model geometry

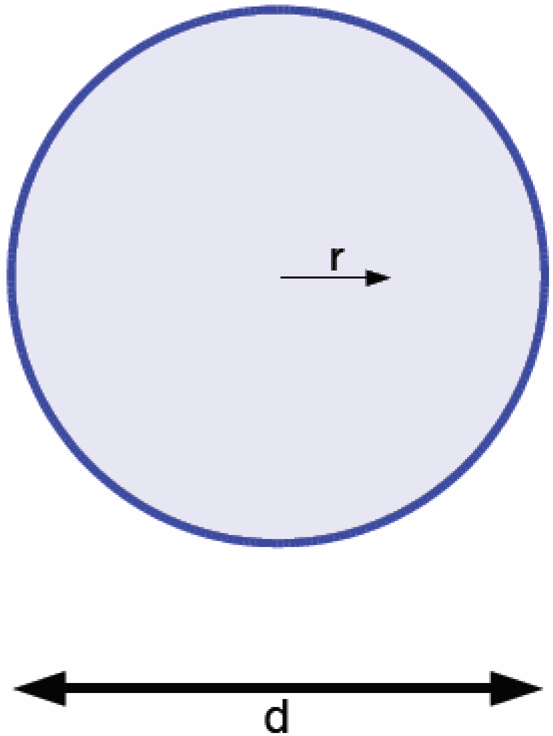
Geometry

- Cloud
  - plane-paralle (semi-infinite or finite), spherical, disk
  - spatial size
  - structure (density/velocity gradient or fluctucations)
- Environment
  - FUV field (isotropic?, strength)
  - other radiation background (IR?)
  - density, presure, temperature of the ambient medium

Some configurations more advantageous due to their symmetry.

  - pp-models with directed or isotropic FUV
  - spherical clouds with isotropic FUV





<u>plane parallel</u>

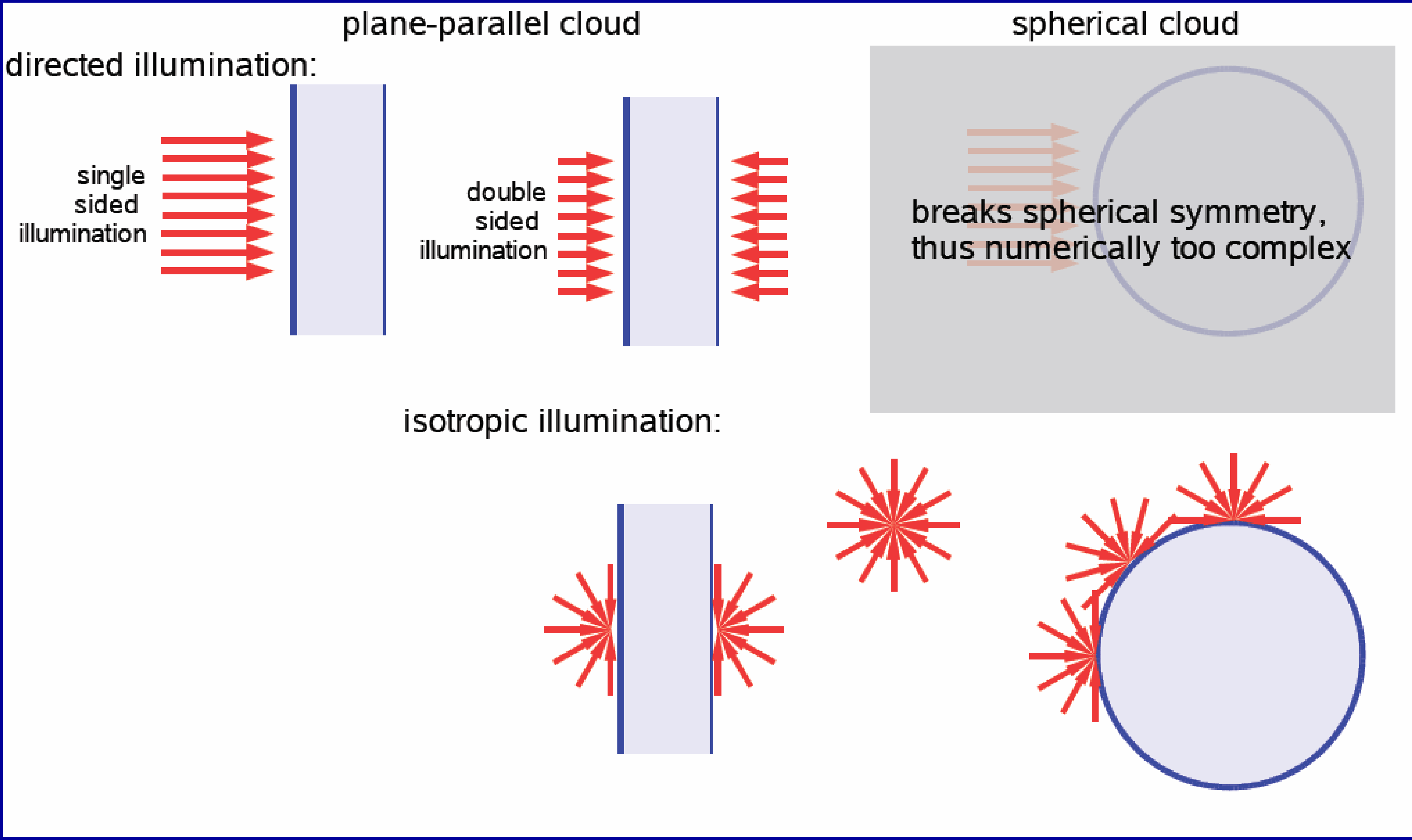
$d \rightarrow \infty$: semi-infinite

τ or $A_v \propto z$ (homogenous)

<u>spherical</u>

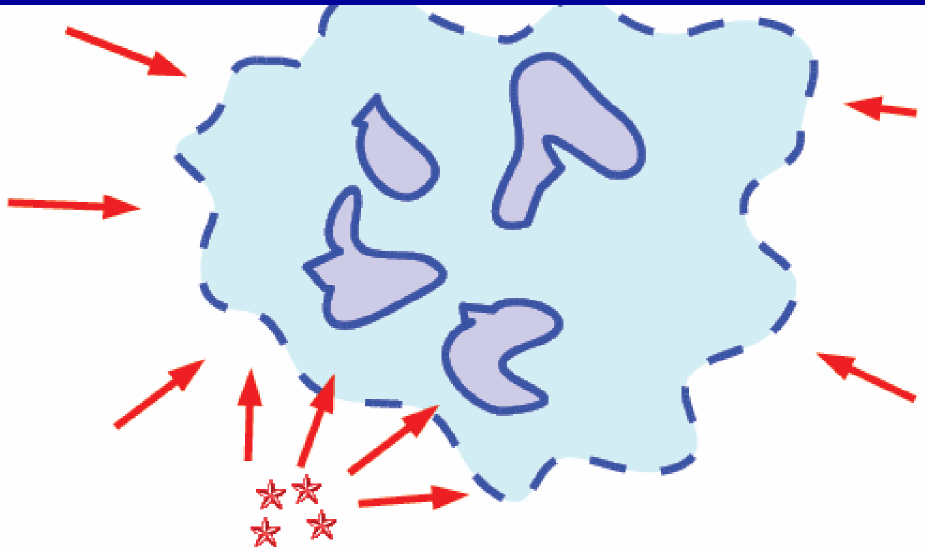
$d \rightarrow \infty$: semi-infinite

τ or $A_v \propto (d/2-r)$ (homogenous)


plane-parallel cloud
spherical cloud
directed illumination:
single sided illumination
double sided illumination
breaks spherical symmetry, thus numerically too complex
isotropic illumination:

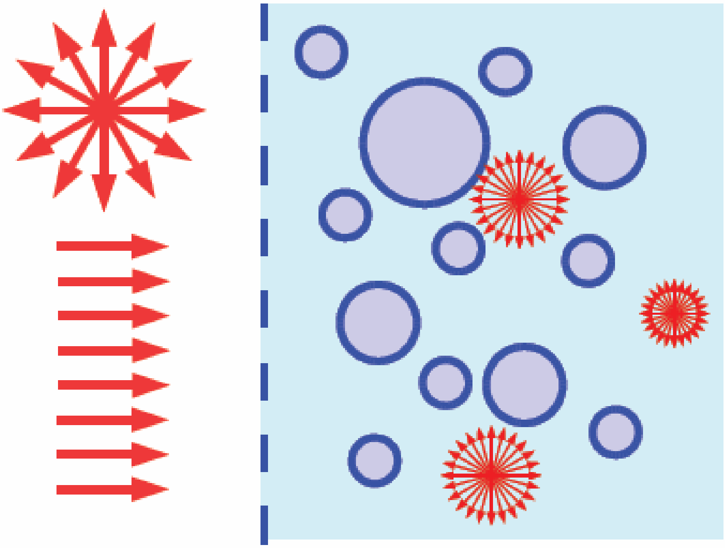
real clouds:

- fractal or clump ensemble
- diffuse interstellar radiation field
  plus
  local young stellar clusters

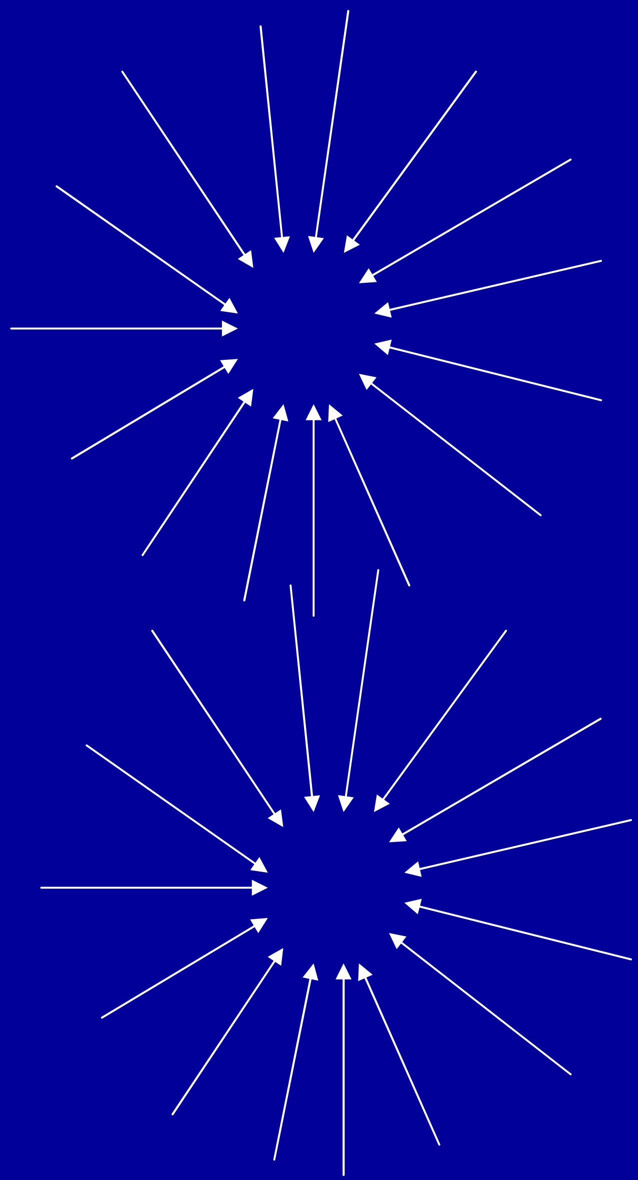


modelling:

- 3D density/velocity structure and Monte-Carlo rad. transfer plus PDR physics
- sperical clump ensemble
  - directed and/or isotropic illumina-tion
  - interclump p.p. PDR
  - pre-shielding of clumps by inter-clump medium

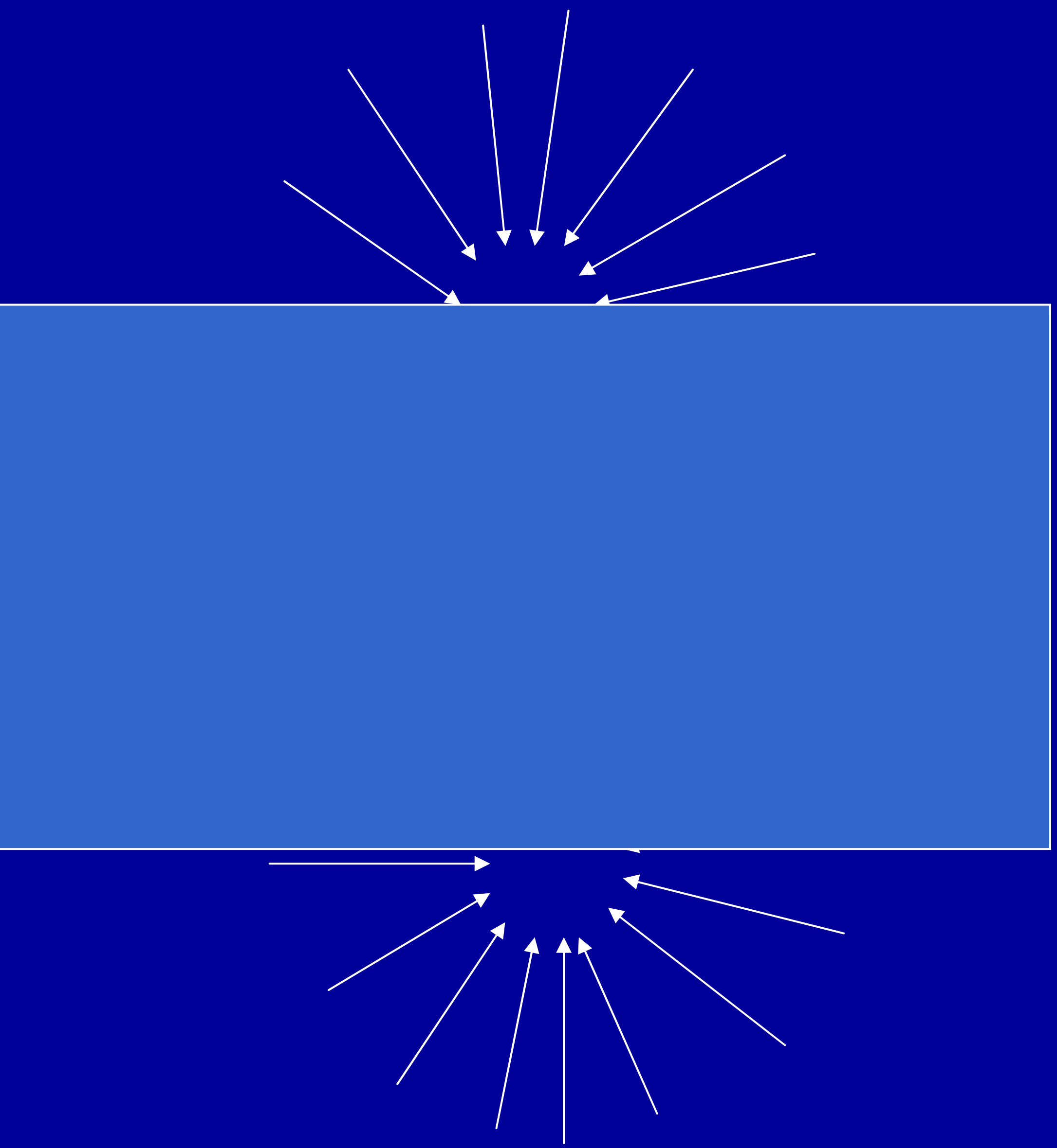


Geometry



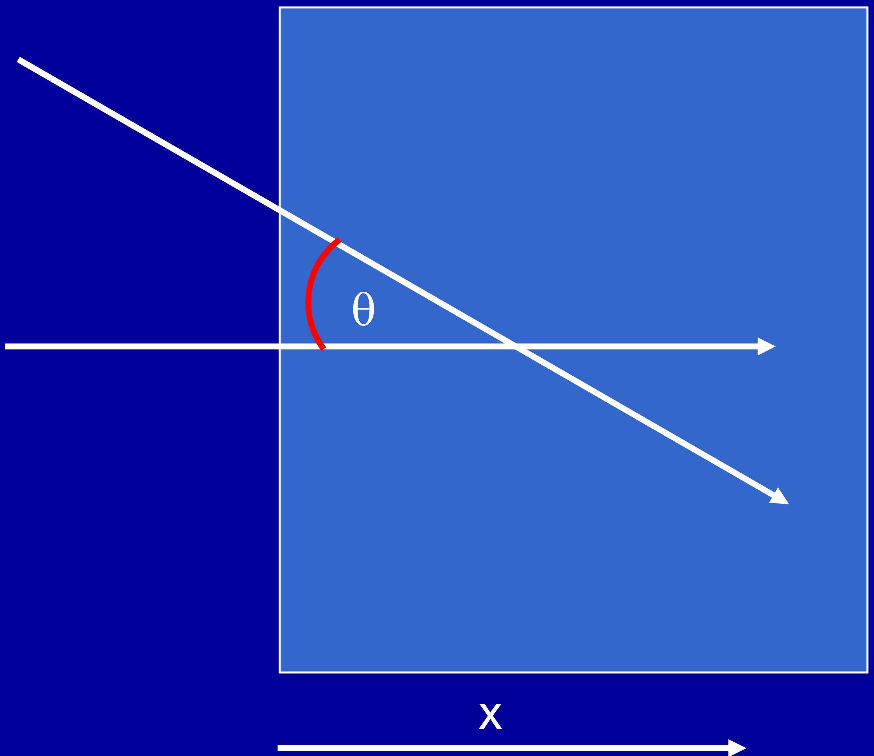
If we put a model cloud in an isotropic FUV field with G_0=1, the flux at the cloud's edge is 0.8×10^{-3} erg s^{-1} cm^{-2} (1/2 G_0)

Geometry



If we put a model cloud in an isotropic FUV field with G_0=1, the flux at the cloud's edge is 0.8×10^{-3} erg s^{-1} cm^{-2} (1/2 G_0)

Geometry



irradiation with inclination angle

$$\mu = \cos\theta$$

$$\mu \frac{dI_\nu(\mu, x)}{dx} = -\kappa_\nu(x) I_\nu(\mu, x) + \varepsilon_\nu(x)$$

for pure absorption:

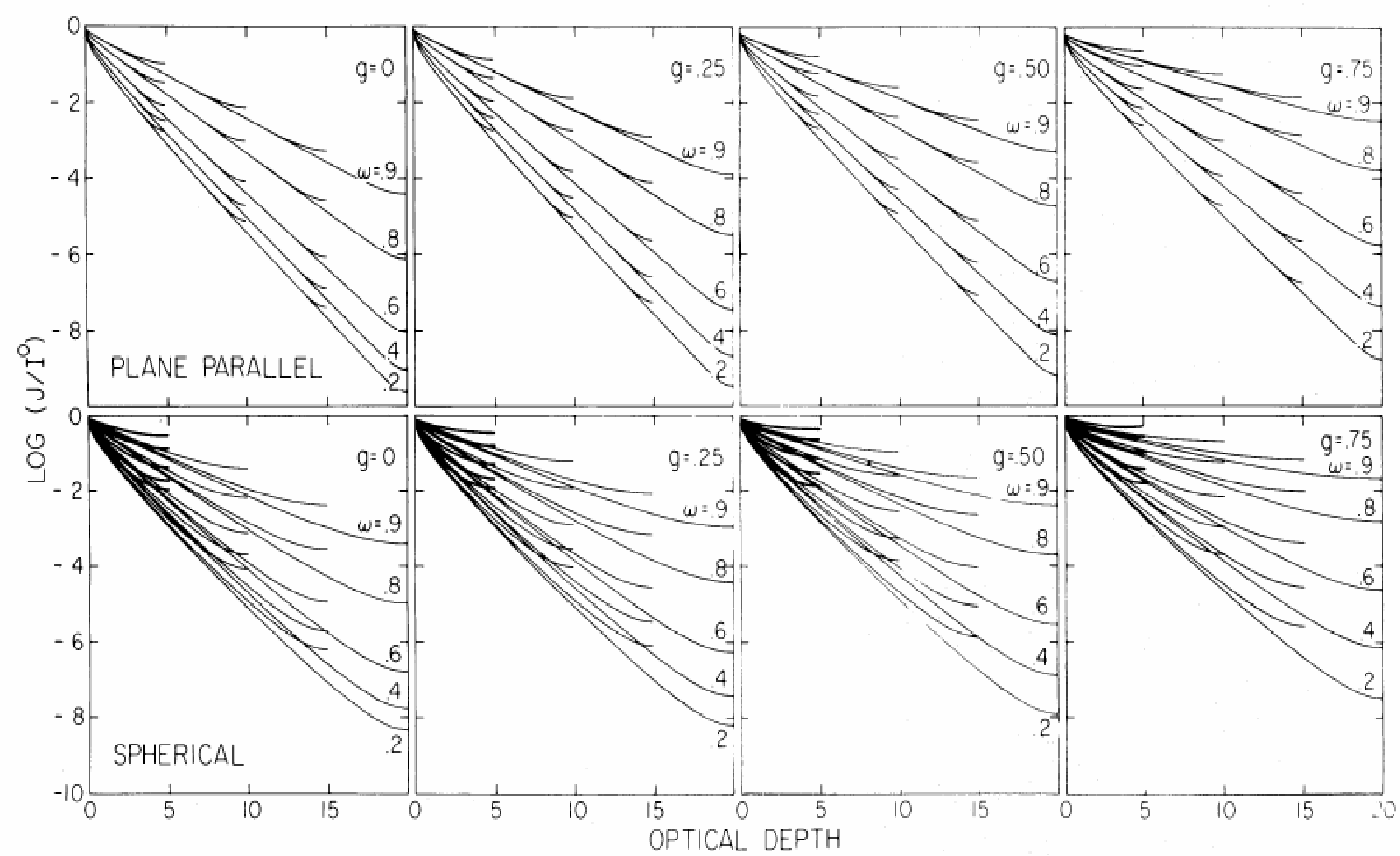
$$J/J_0 = E_2(\tau) = \int_0^1 \frac{\exp(-\tau\mu)}{\mu^2} d\mu$$

E2: second order elliptical integral
J: mean intensity, integral over 4π

Geometry

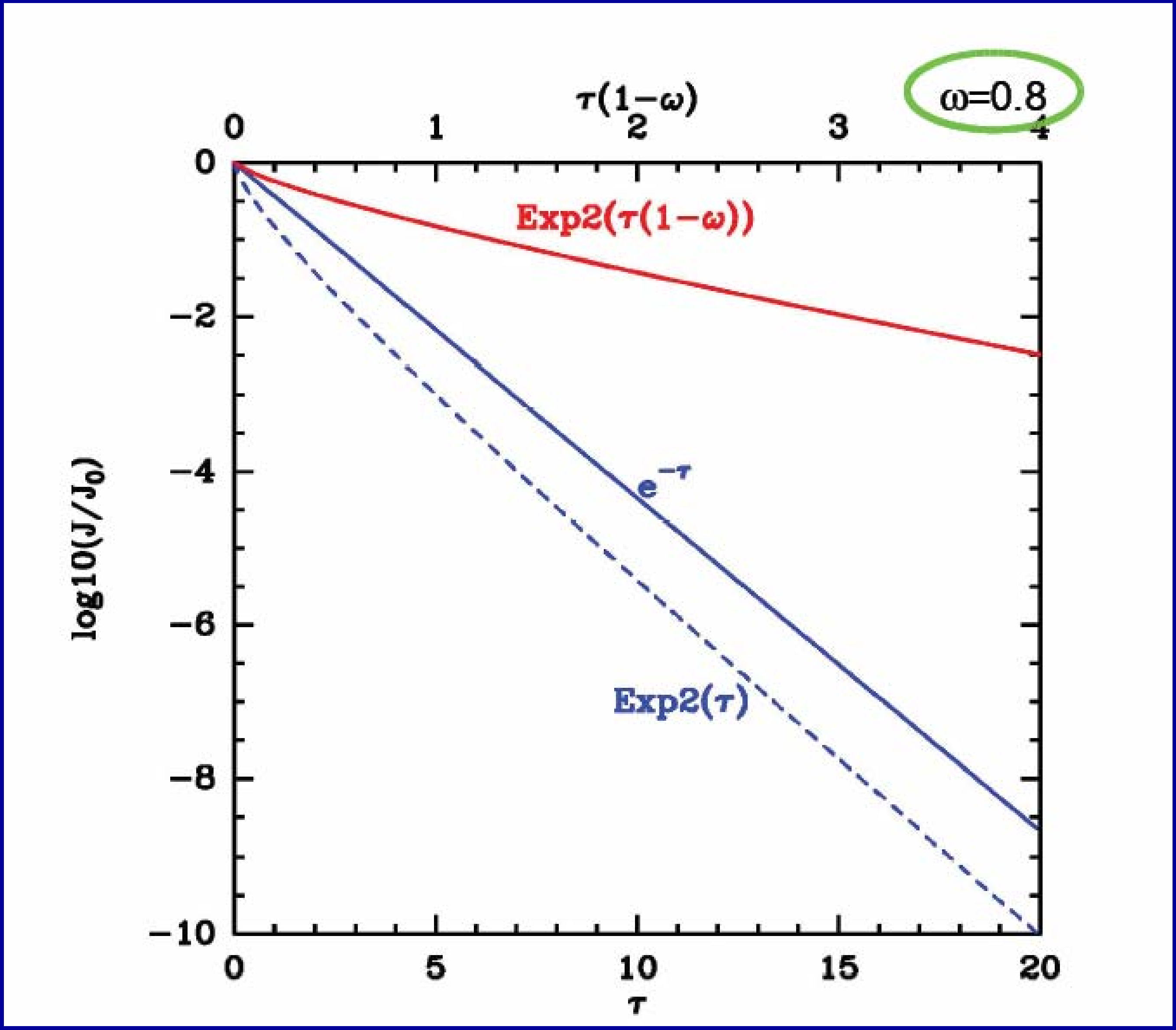
directed vs. isotropic attenuation
1.0
0.8
0.6
0.4
0.2
0.0
0
2
4
6
J/J0
τ
e-τ
Exp2(t)

Geometry



Flannery et al. 1980
(Legendre polynomial expansion)

g: mean cosine of scattering angle (1=forward)
ω: scattering albedo



ω: single scattering albedo
$0 \le \omega \le 1$
the fraction of light that is actually absorbed is 1- ω

Flannery et al. 1980

Geometry

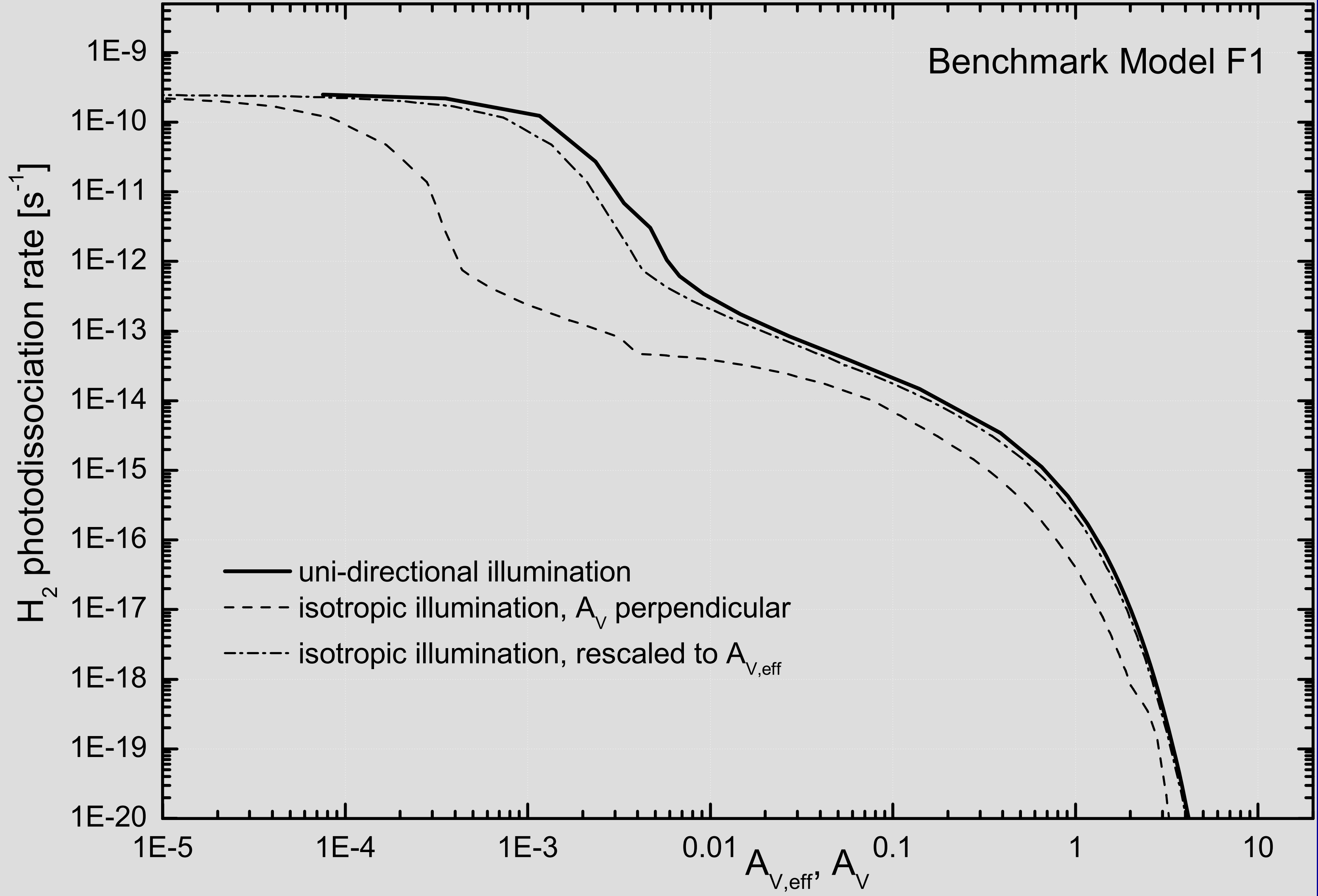
- uni-directional: A_V is a function of depth
- isotropic: A_V depends on the depth and the angle

- it is difficult to directly compare the output of isotropic models with uni-directional models.
- Solution: definition of an effective A_V

$$e^{-A_{V,eff}} = E_2(A_V)$$

$$A_{V,eff} = -\ln\left(E_2(A_V)\right)$$

Geometry



Benchmark Model F1
H2 photodissociation rate [s-1]
1E-9
1E-10
1E-11
1E-12
1E-13
1E-14
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
1E-5
1E-4
1E-3
0.01
0.1
1
10
AV,eff, AV
uni-directional illumination
isotropic illumination, AV perpendicular
isotropic illumination, rescaled to AV,eff

Solution scheme

Solve chemical network

$$\frac{\partial n^i}{\partial t} = -n_i \left\{ \tilde{\varsigma}_i + \sum_q n_q \cdot k_{qi}(T) \right\} + \sum_r \sum_s k_{rs}(T) \cdot n_r \cdot n_s + \sum_t n_t \cdot \tilde{\varsigma}_{ti}$$

destruction formation

$I_\nu(\tau(r))$

$n_i(r) \Rightarrow \tau$

$n_i(r) \Rightarrow \tau$

$T(r)$

Solve radiative transfer

$$I_\nu(\tau_\nu) = I_\nu(0) e^{-\tau_\nu} + \int_0^{\tau_\nu} e^{-\tau'_\nu} S_\nu(\tau'_\nu) d\tau'_\nu$$

$T(r)$

$S(r)$

$I_\nu(\tau(r))$

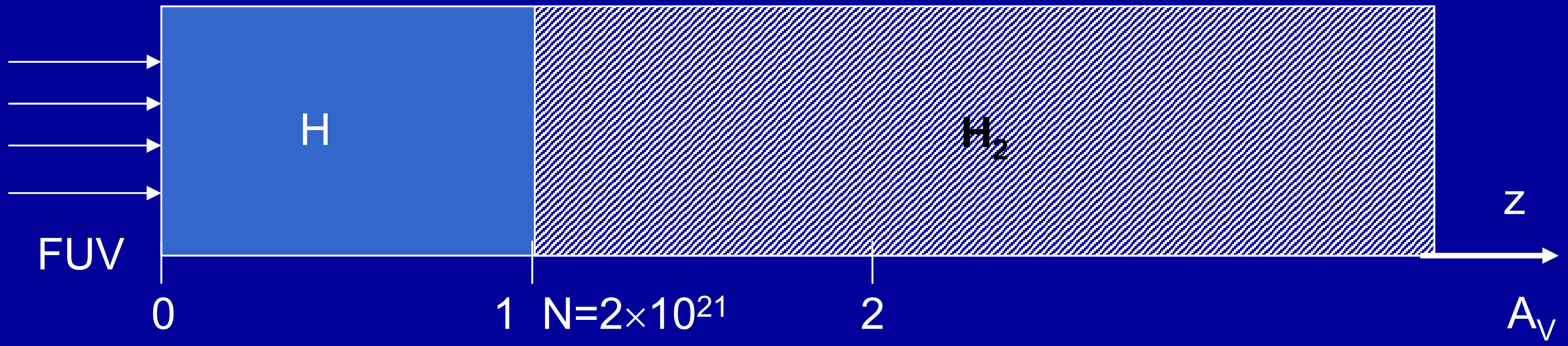
Solve energy balance

$$\sum_i \Gamma_i(\vec{r}, \vec{n}, \chi, T) = \sum_i \Lambda_i(\vec{r}, \vec{n}, \chi, T)$$

heating cooling

Standard Setup

- plane-parallel slab, semi-infinite
- FUV radiation hits surface perpendicular
  extinction $\propto \exp(-A_V)$
- total gas density $n=n(H)+2n(H_2)=\mathrm{const.}$
  $\Rightarrow A_V \propto N_H \propto z$
- steady-state chemistry $\Rightarrow \partial n/\partial t=0$



Standard Setup

- Example: C^+/C

$$C + h\nu \rightarrow C^+ + e^-$$
$$C^+ + e \rightarrow C + h\nu$$

} small A_V

$$C^+ + H_2 \rightarrow CH_2^+ + h\nu$$

larger A_V

$$\chi I \exp(-A_V k) n_C = a_C n_C + n_e + k_C n_{C^+} n_{H_2}$$

$$n_C + n_{C^+} = X_C n$$

$$n_C = \left(X_C n - n_{C^+} \right)$$

$$n_{C^+} = n_e$$

$$\alpha = 2.5\times10^{-11}, I = 3\times10^{-11}, k_C = 7\times10^{-16}, k = 1.8$$

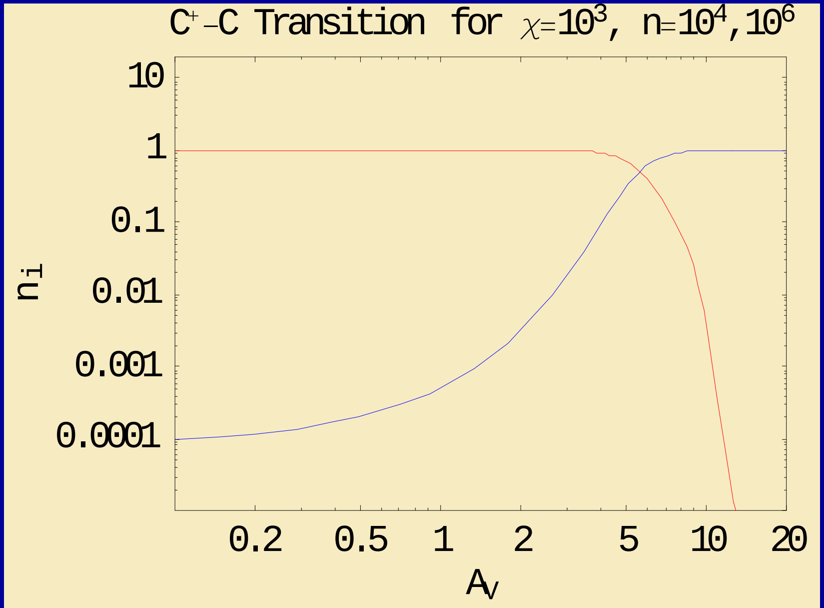
Standard Setup

$$\chi I \exp(-A_V k)\left(X_C n - n_{C^+}\right) = a_C n_{C^+}^{\ 2} \qquad ,\mathrm{n}=10^4, \mathrm{X_C}=10^{-4}$$

$$n_{C^+}^{\ 2} + \frac{\chi I \exp(-A_V k)}{a_C} n_{C^+} - \frac{\chi I \exp(-A_V k)}{a_C} X_C n = 0$$

$$n_{C^+} = -6000 \exp(-1.8 A_V) +$$

$$+2\times10^{10}\sqrt{9\times10^{-14}\exp(-3.6A_V)+3\times10^{-17}\exp(-1.8A_V)}$$



layers: C^+ outsinde, C inside

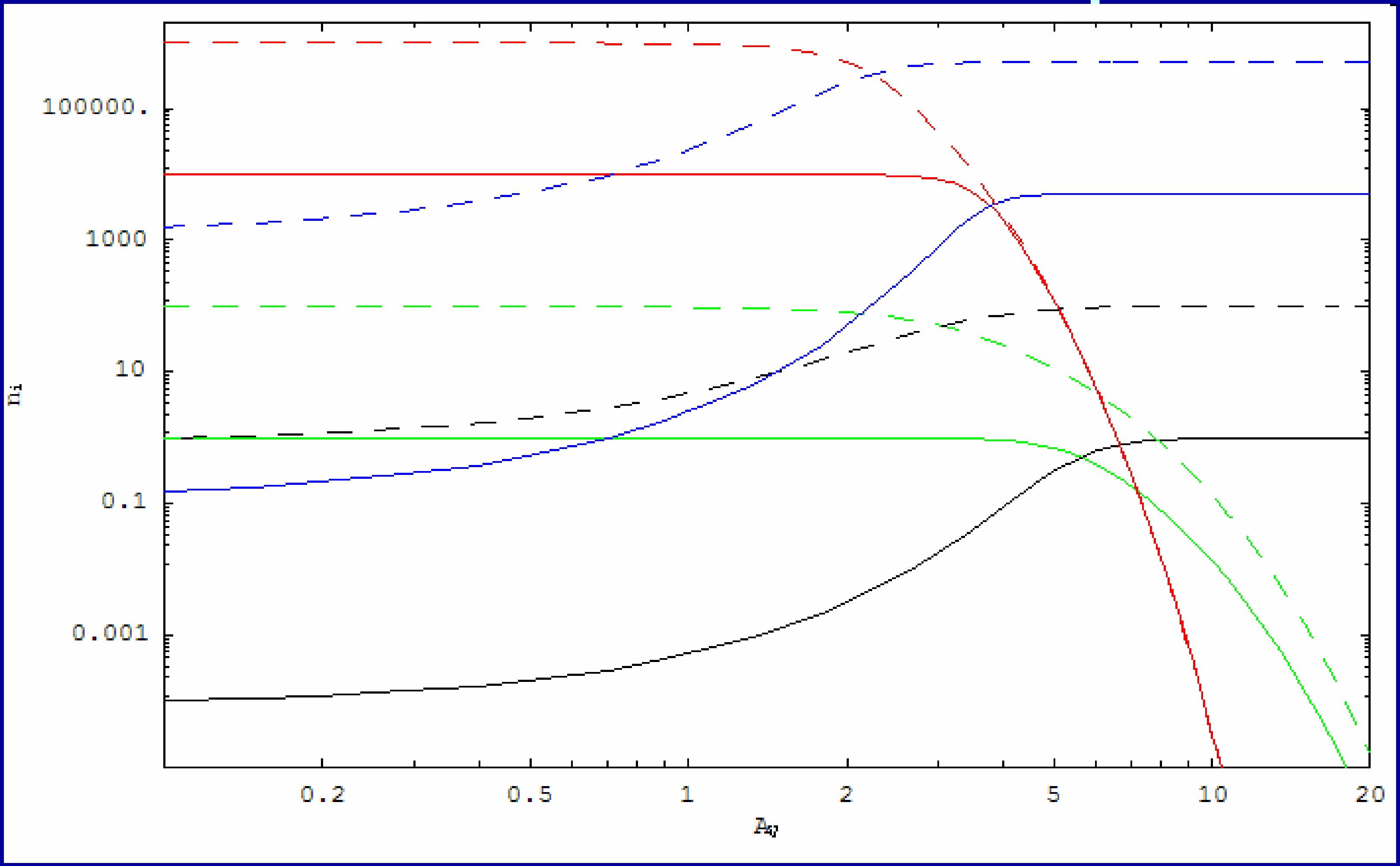
next step C → CO

C + OH → CO + H

C + O_2 → CO + O

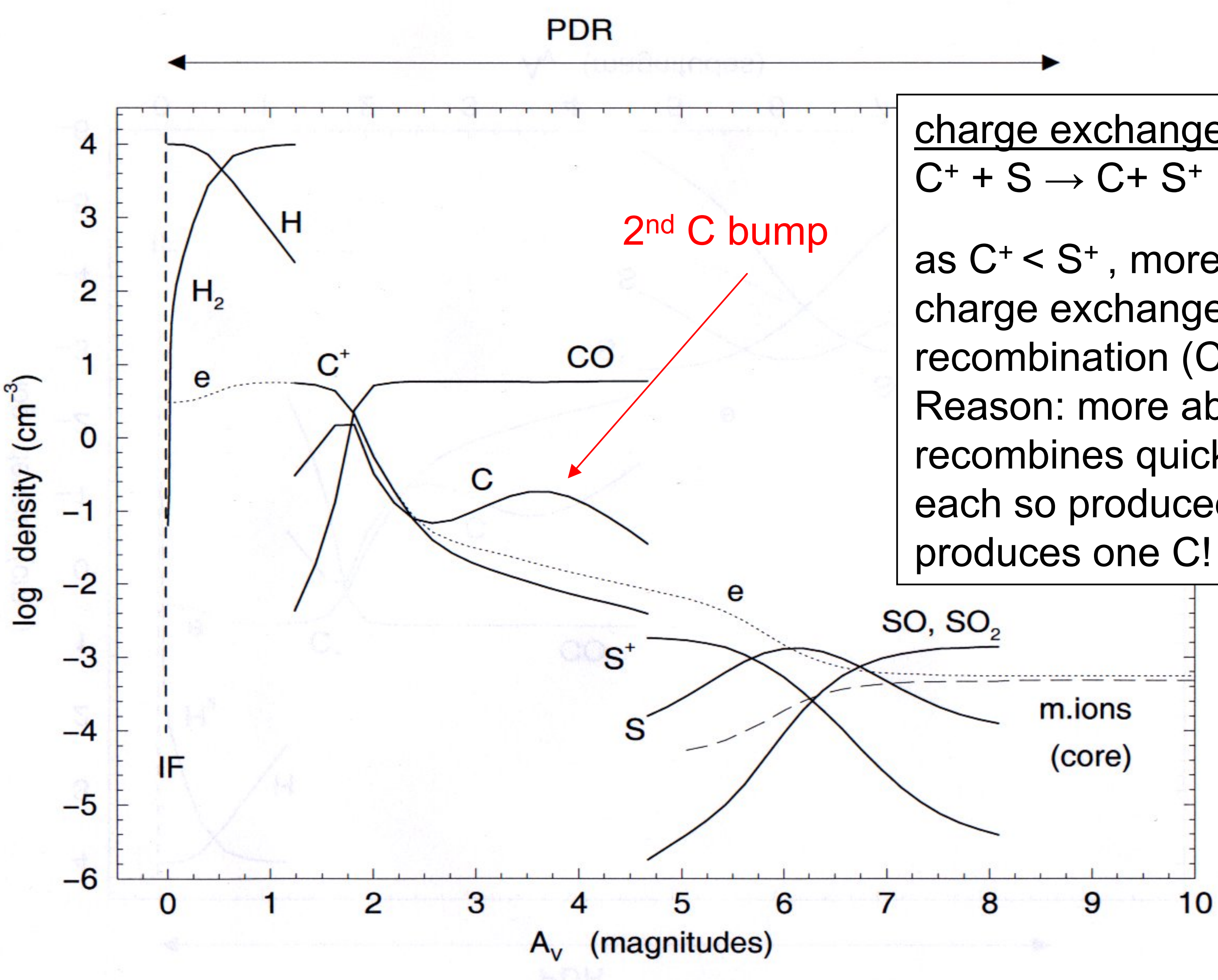
⇒classical C^+-C-CO stratification

Standard Setup



$\chi=10^3$, C/H=10^{-4}, n=10^4 cm^{-3} (solid), n=10^6 cm^{-3} (dashed)
H (red), H_2 (blue), C^+ (green), C (black)

Standard Setup

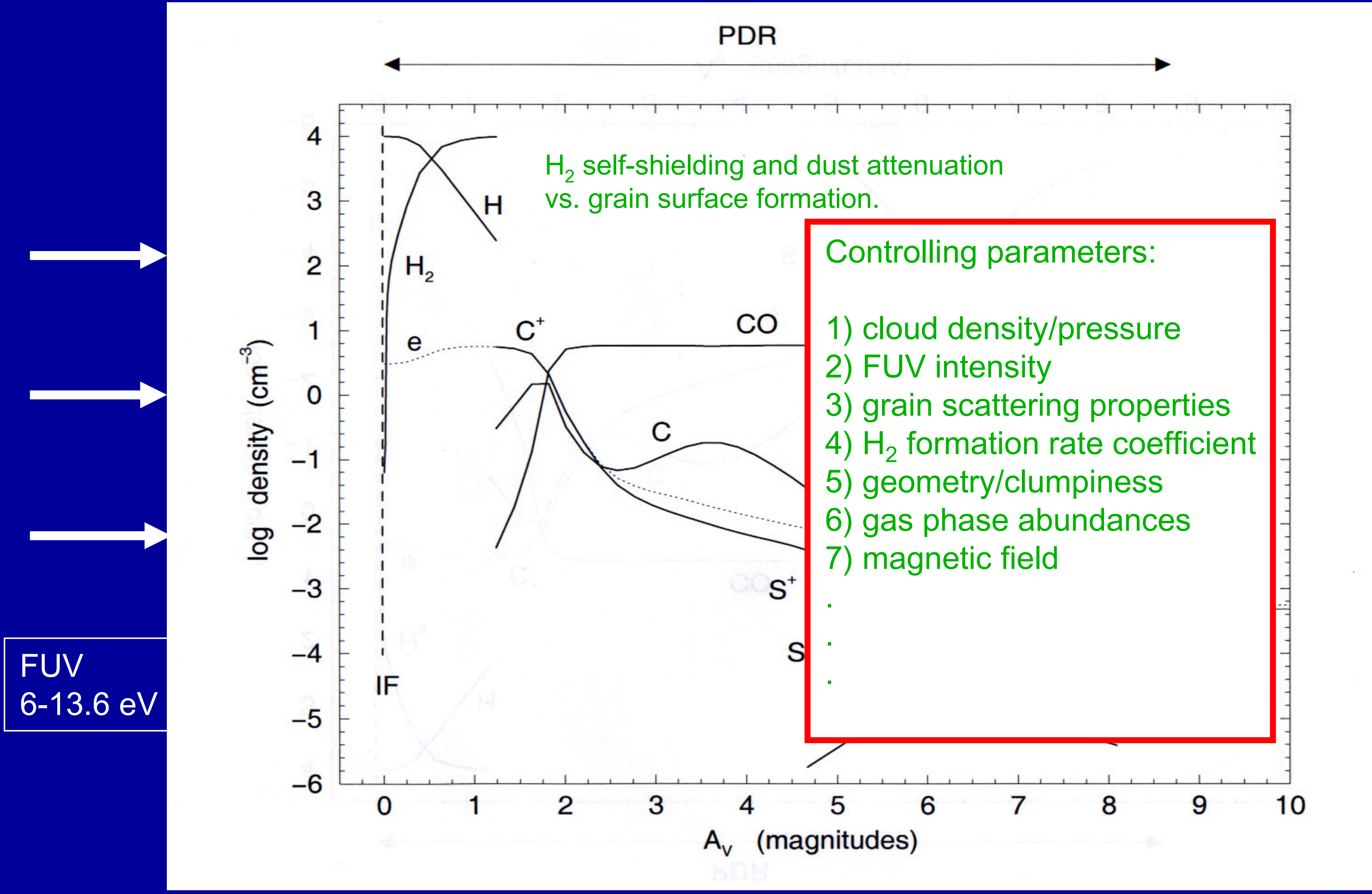


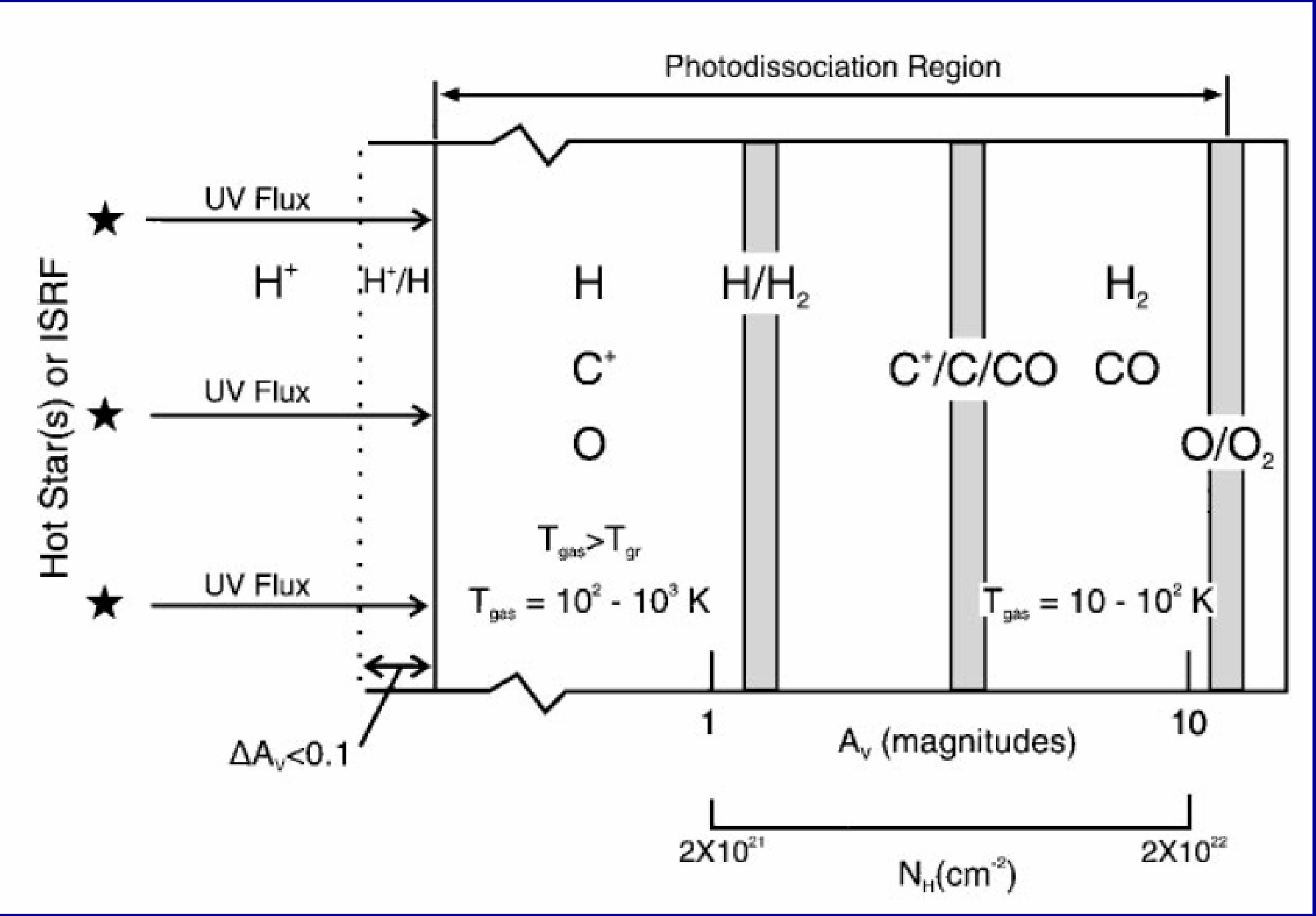
<u>charge exchange</u>

$C^+ + S \rightarrow C + S^+$

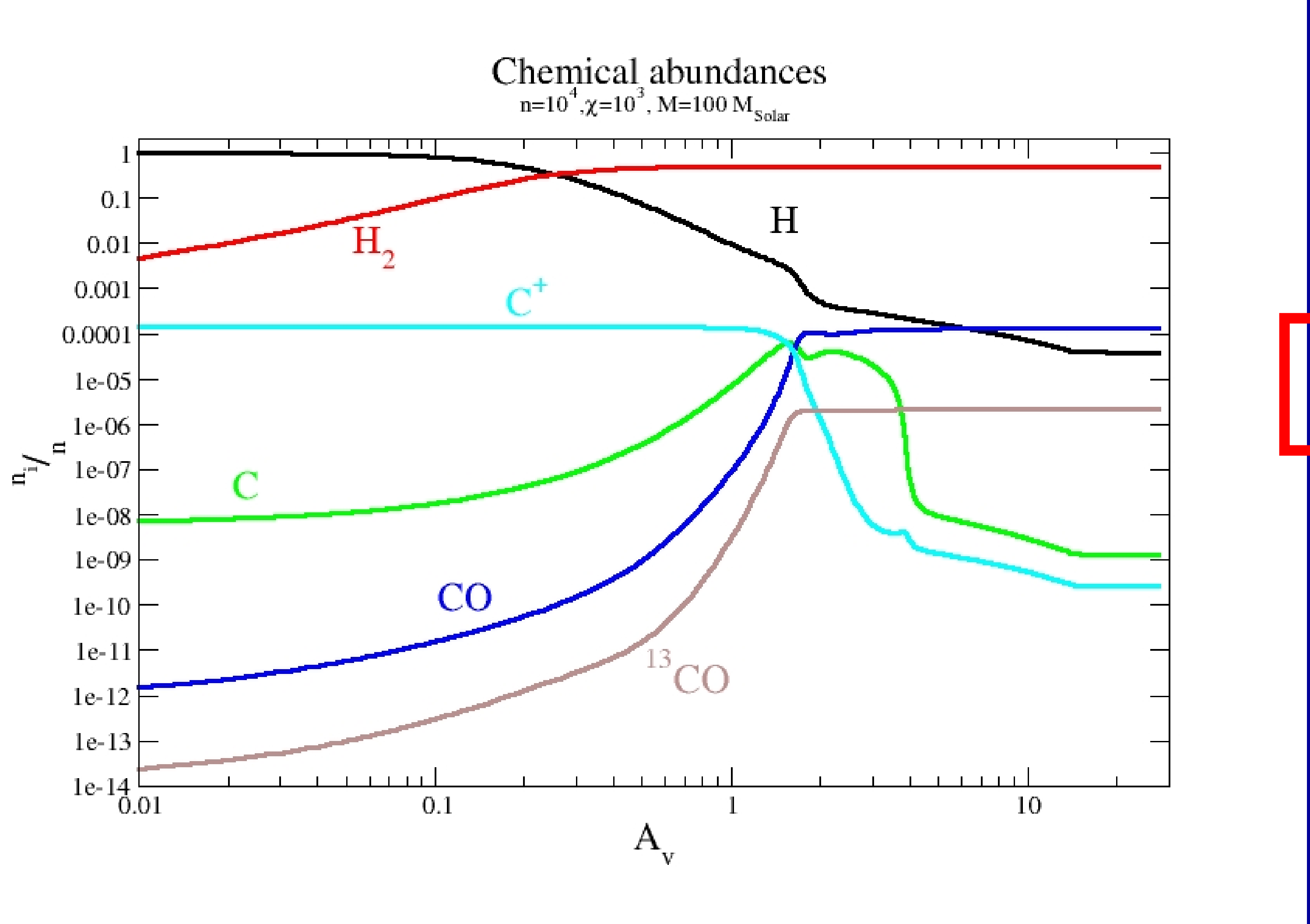
as $C^+ < S^+$, more C produced via charge exchange with S than via recombination ($C^+ + e^-$). Reason: more abundant S^+ recombines quicker than C^+, and each so produced S then produces one C!

Basic structure: 1-D steady-state model, escape probability method.



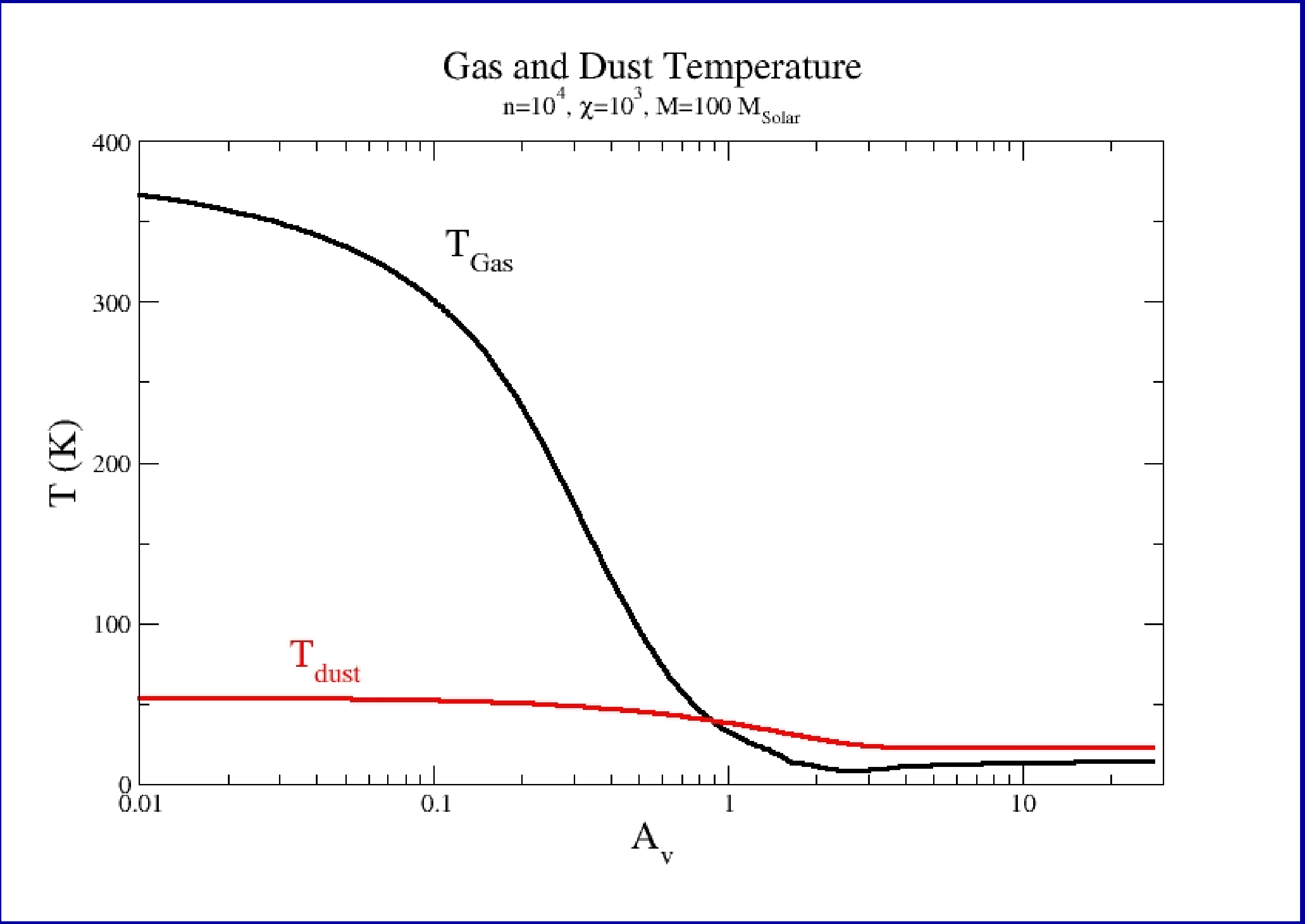


Hollenbach&Tielens, 1999



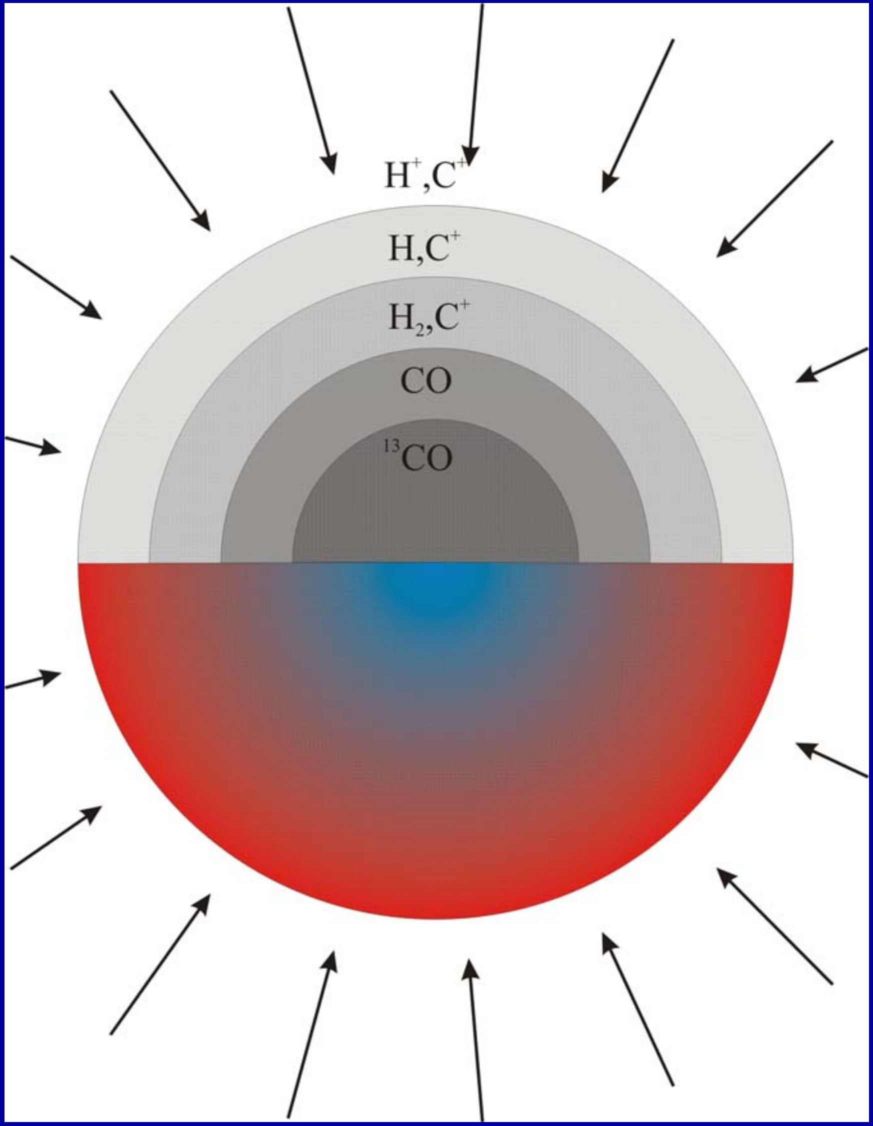
Chemical abundances
n=10^4, χ=10^3, M=100 M_Solar
H
H2
C+
C
CO
13CO
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1e-07
1e-08
1e-09
1e-10
1e-11
1e-12
1e-13
1e-14
0.01
0.1
1
10
A_V
n_i/n

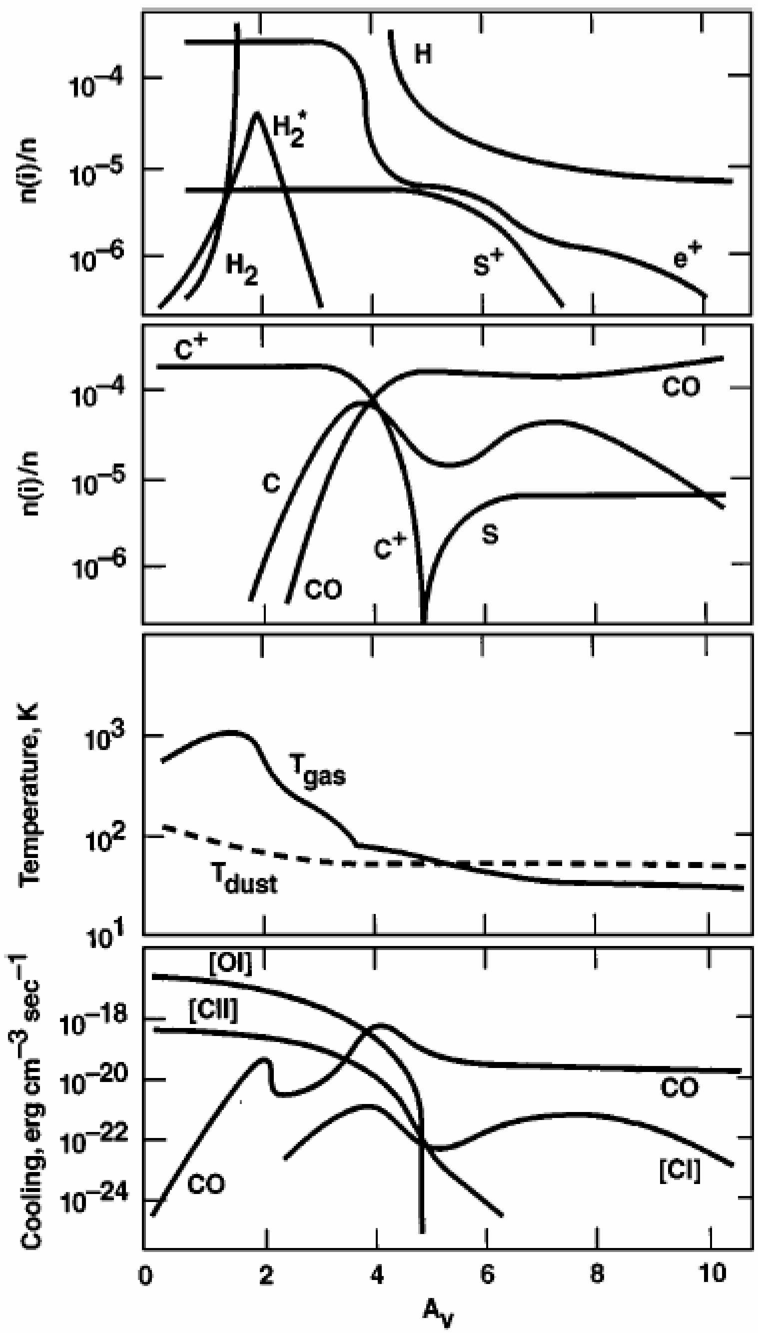
$\vec{n}(\vec{r})$



$$T_{dust,gas}(\vec{r})$$

Resulting Model Cloud



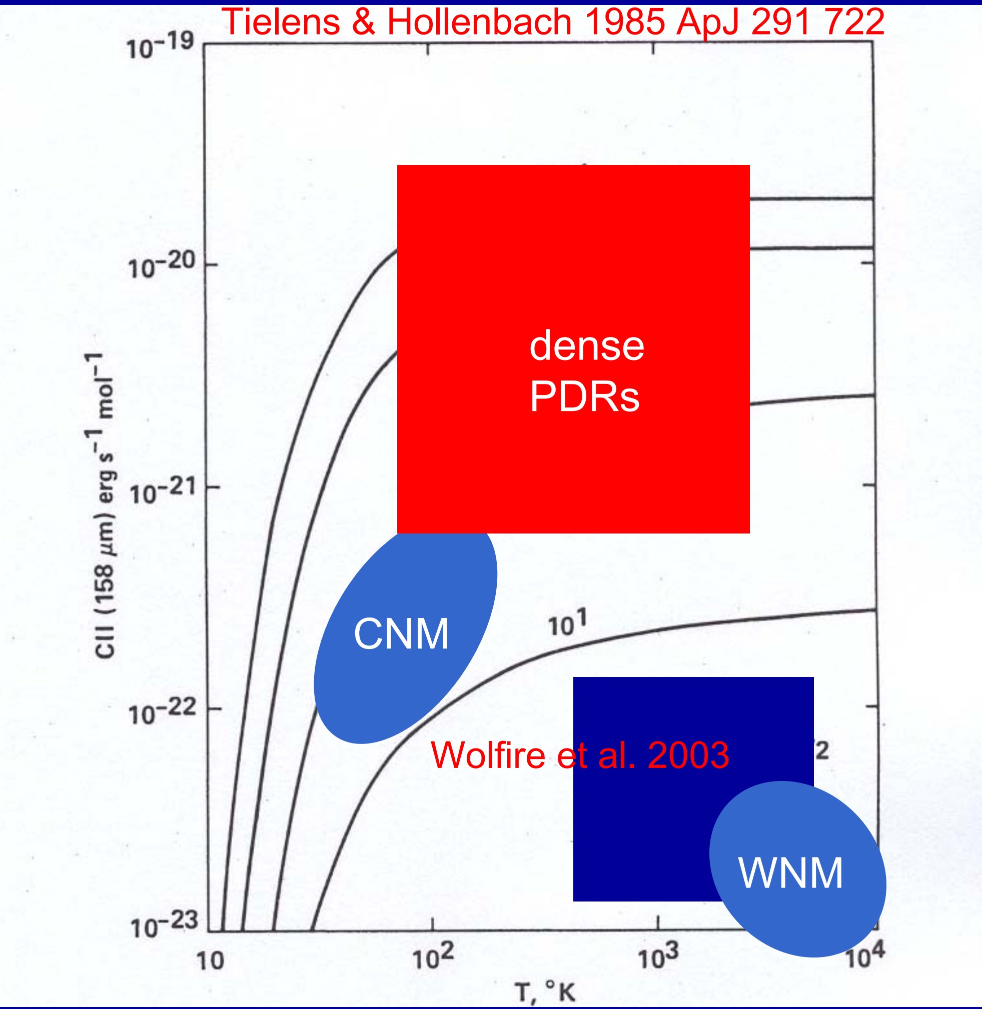


PDR model for Orion

$n=2.3*10^5\ cm^{-3}$
$G_0=10^5$

Tielens & Hollenbach 1985

CII 158 μm fine-structure line cooling:

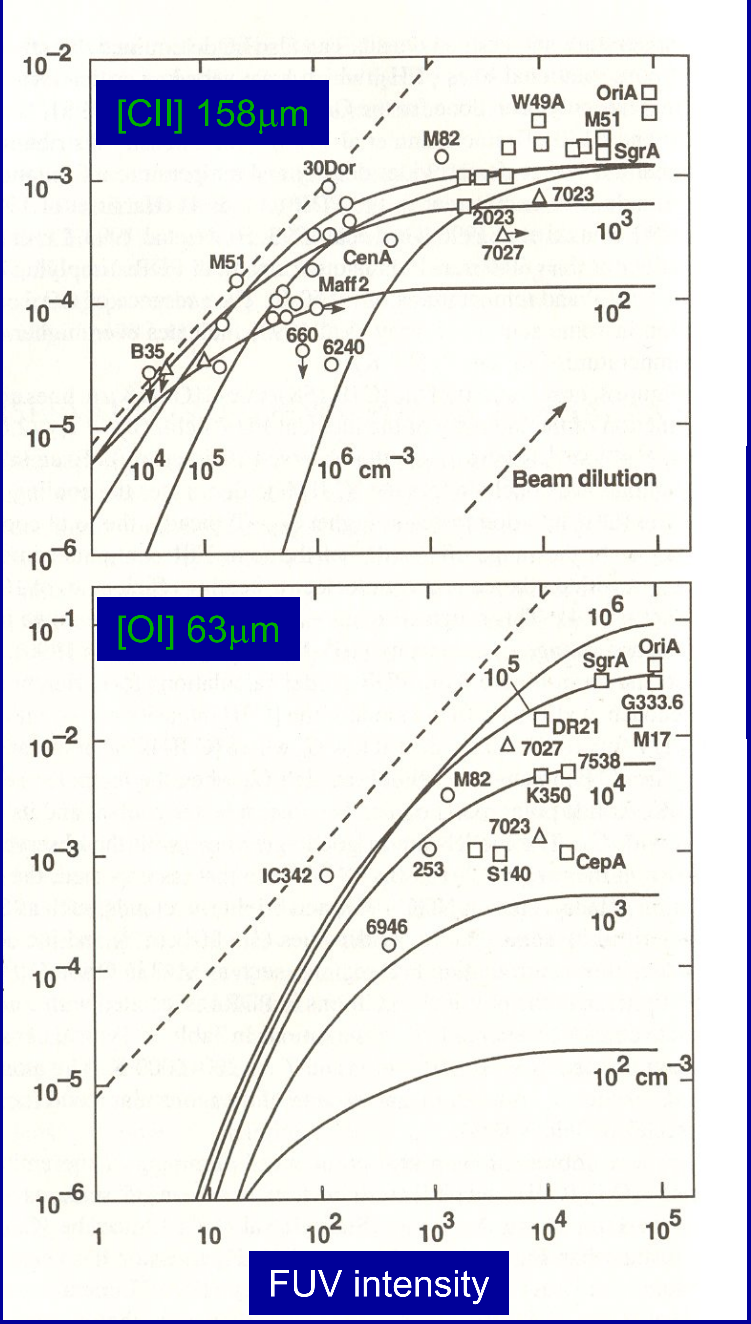


Expected theoretically -
e.g. Dalgarno & McCray 1972.

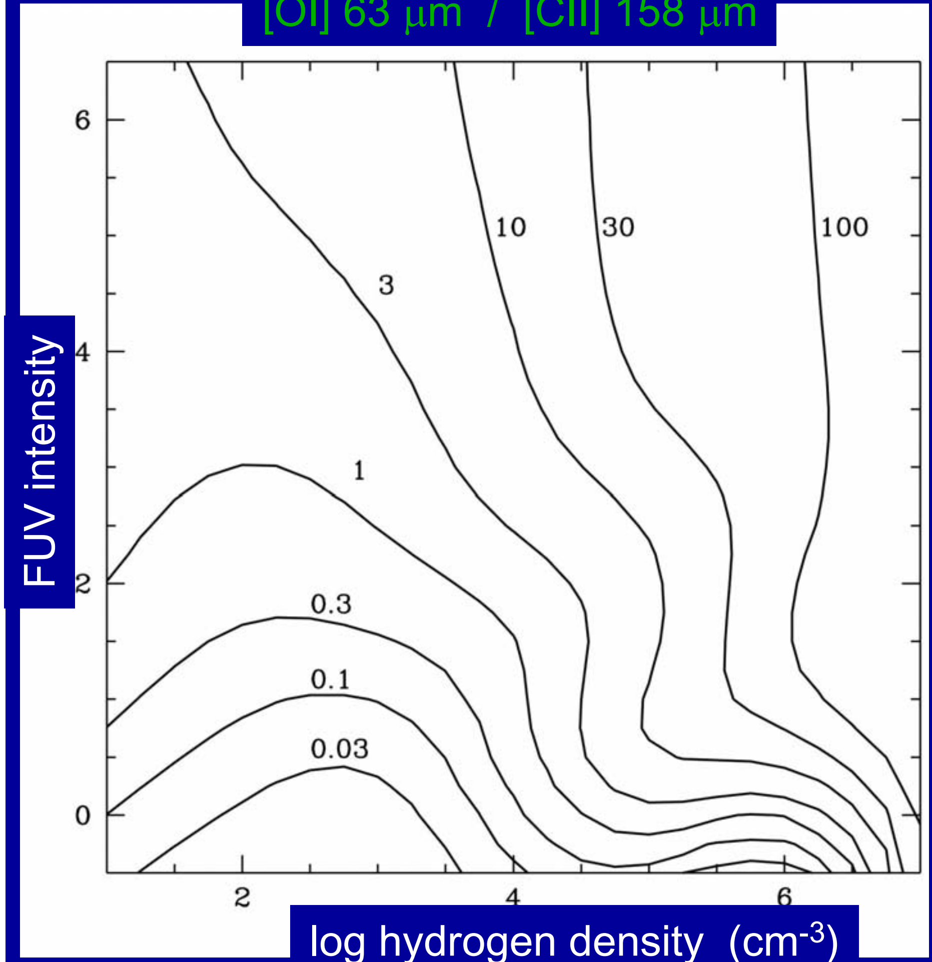
First far-IR (Lear jet) detections by
Russell et al. 1980
in NGC 2024 and Orion.

Widely detected since with
KAO, ISO...

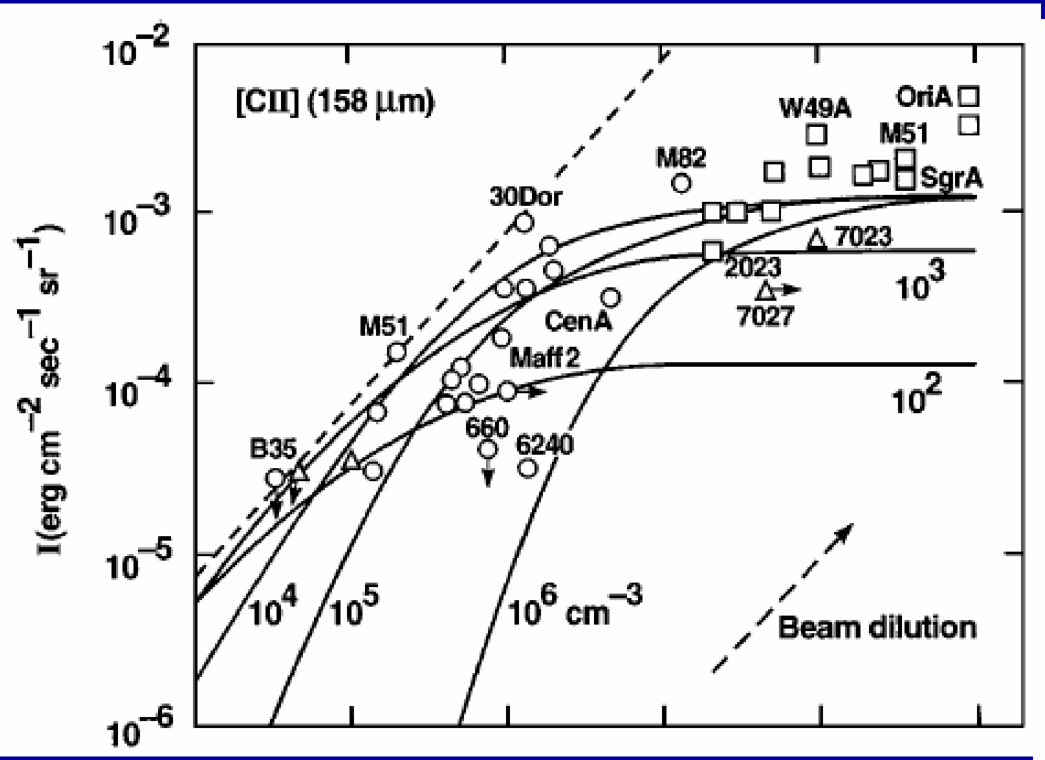
Fine-Structure Line Emission:

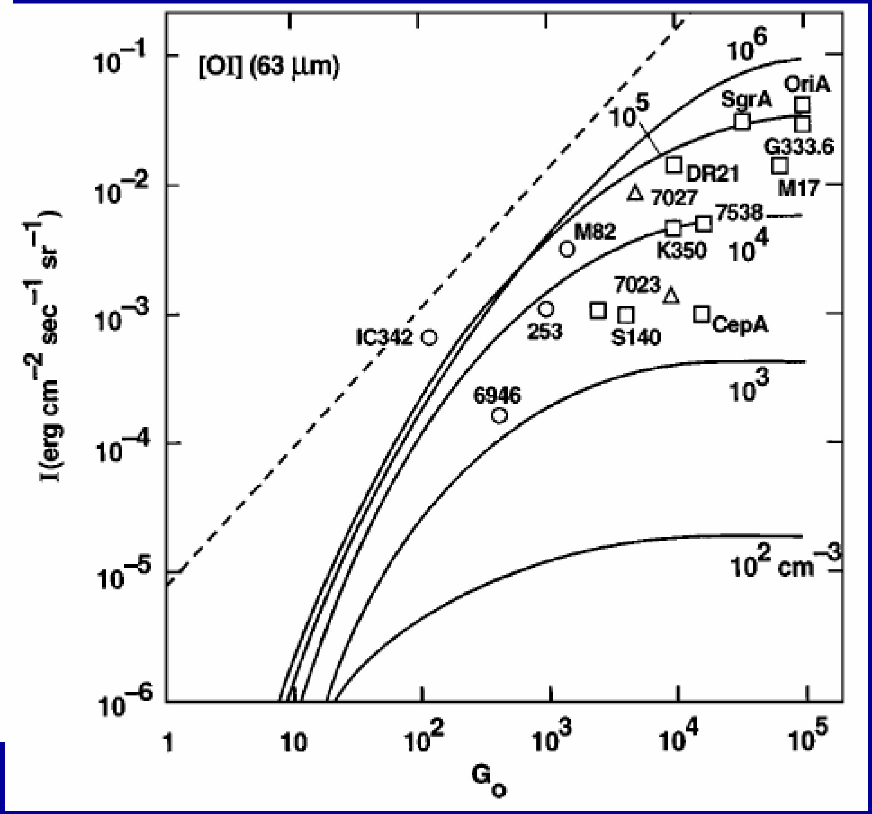


Kaufman et al. 1999 ApJ, 527, 795

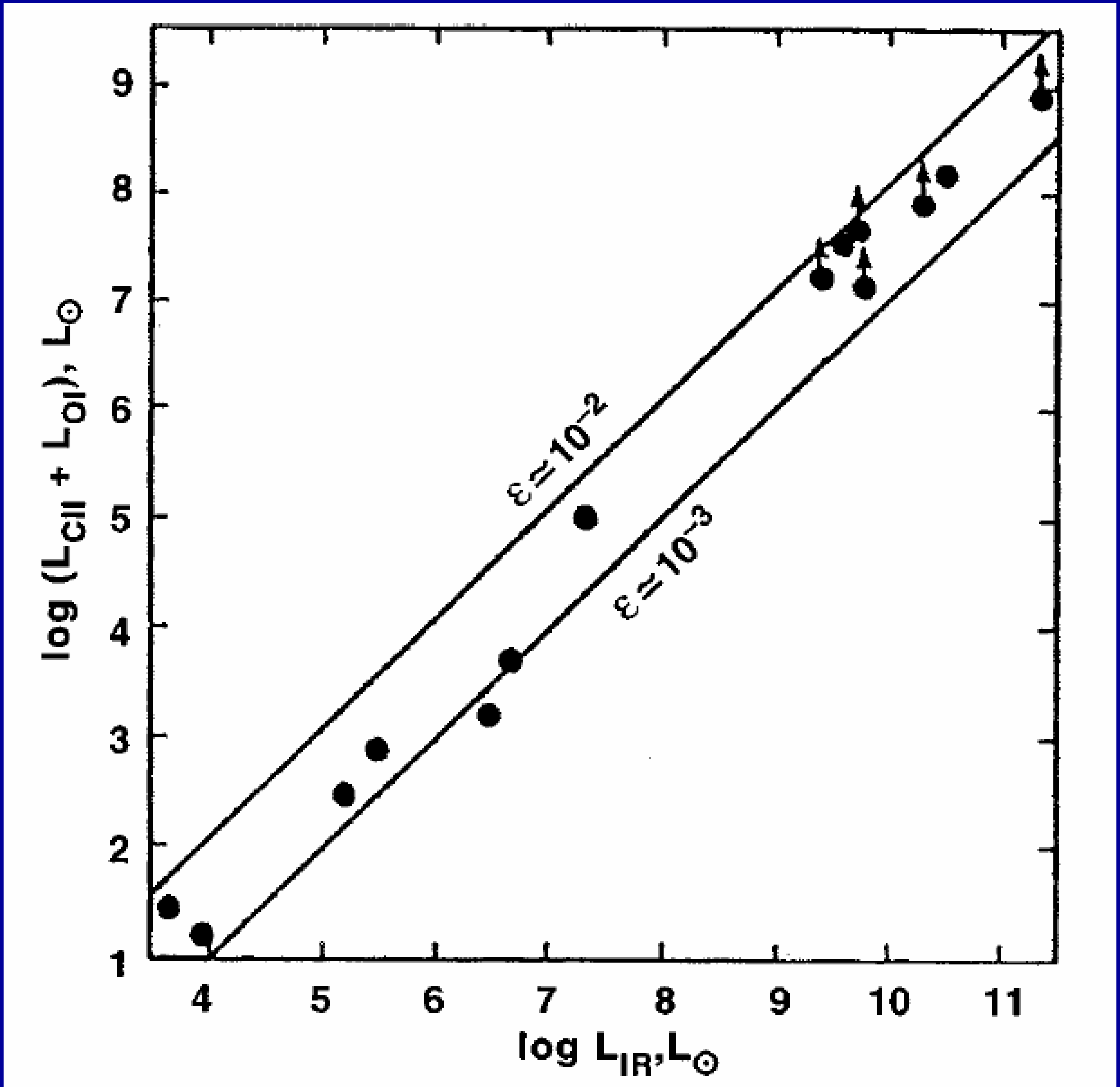


[OI] 63μm can become optically thick.

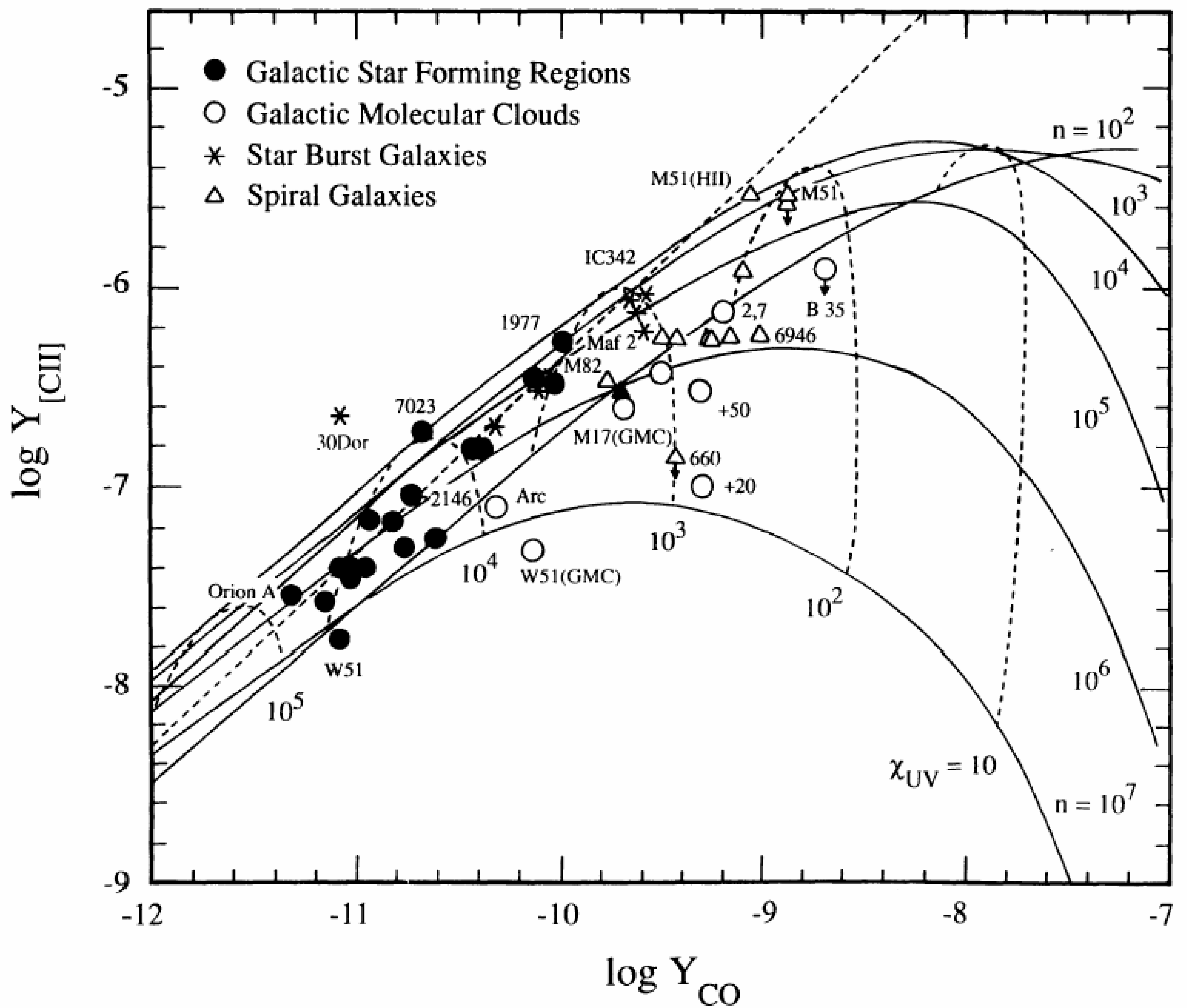




Hollenbach et al. 1991



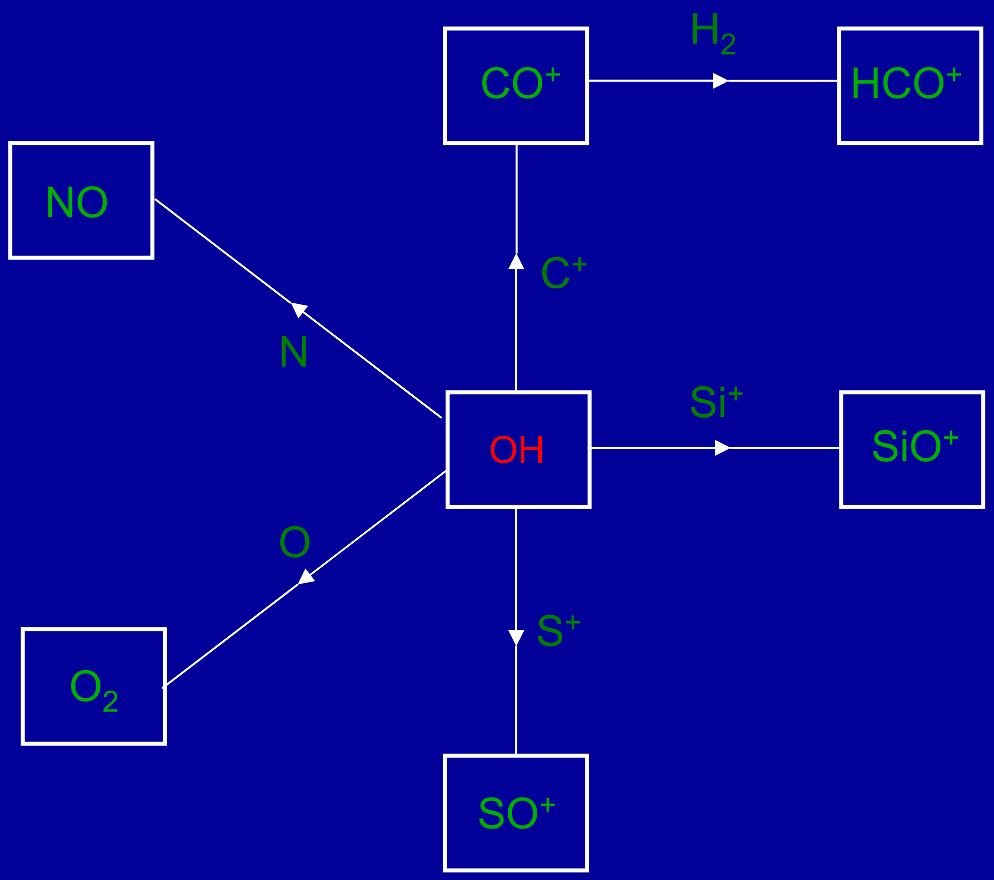
Hollenbach et al. 1990



Stacey et al. 1991

OH driven chemistry in warm H/H_2 transition zone:

T = 300 – 1000 K

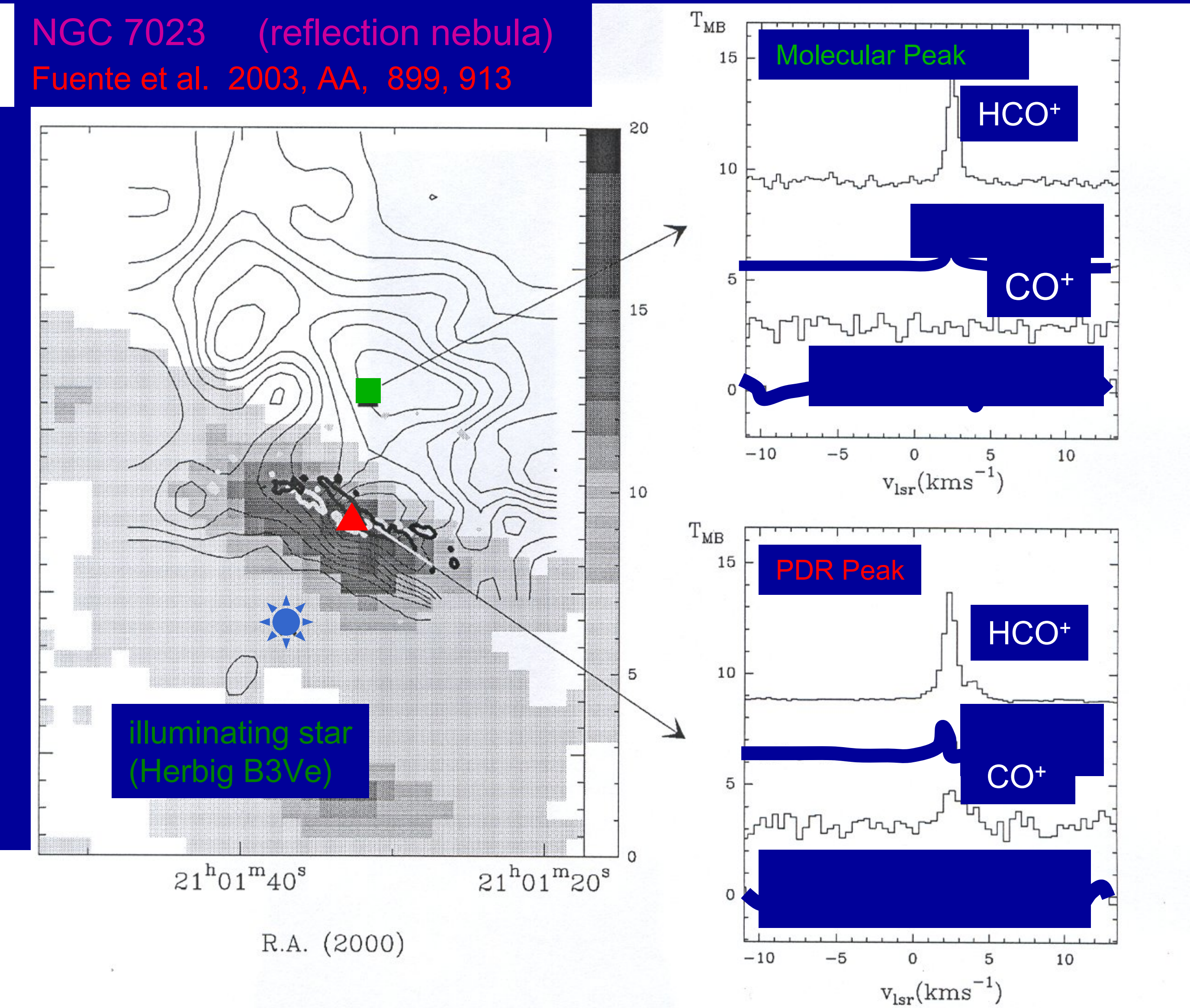


Prediction:

CO^+/HCO^+ large in PDR

CO^+/HCO^+ small in dark core

For example, CO^+ / HCO^+



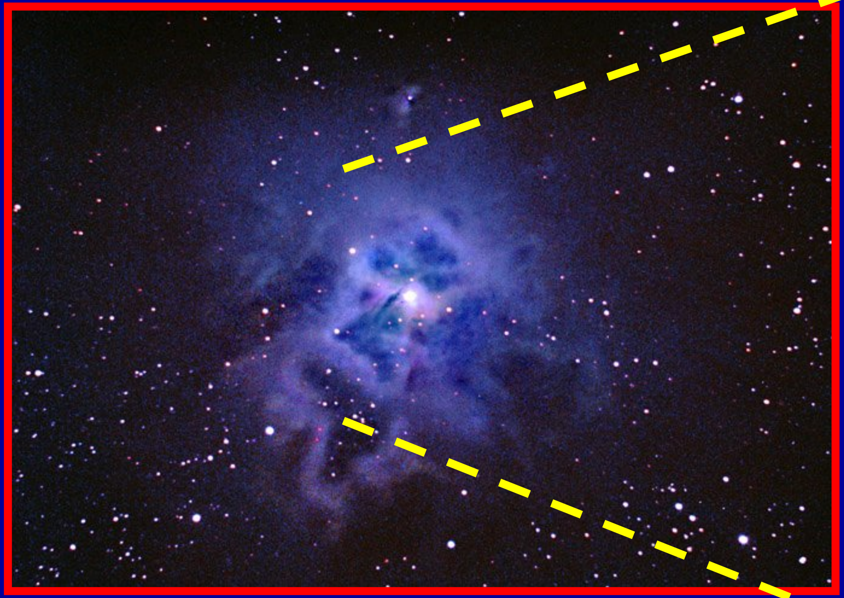
	CO^+/HCO^+
Molecular Peak	< 0.001
PDR Peak	~ 0.1

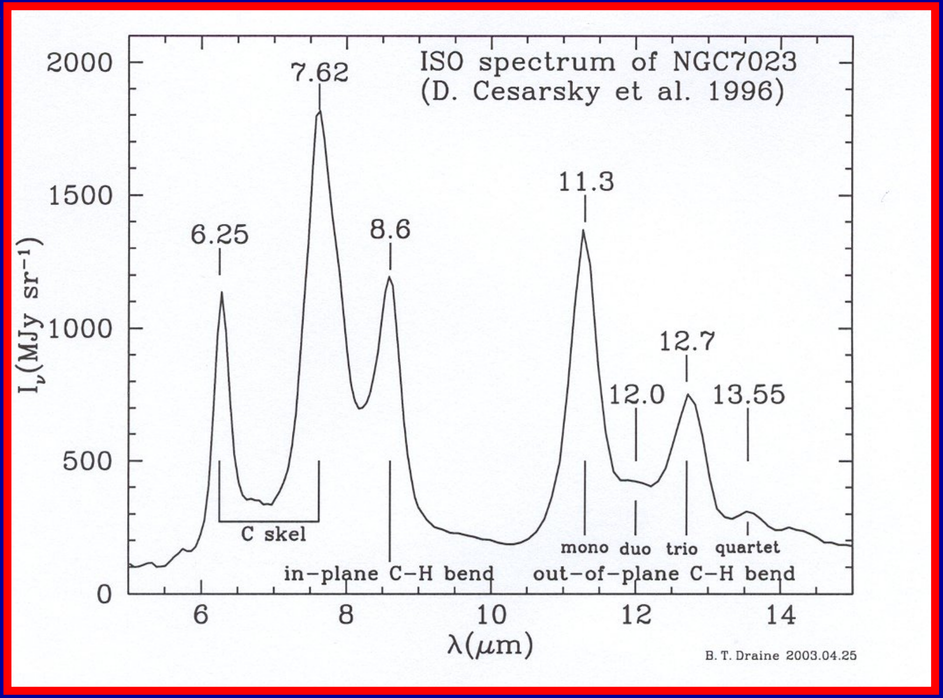
At interface:
G_0 = 2.4 x 10^3
n = 10^4 cm^{-3}

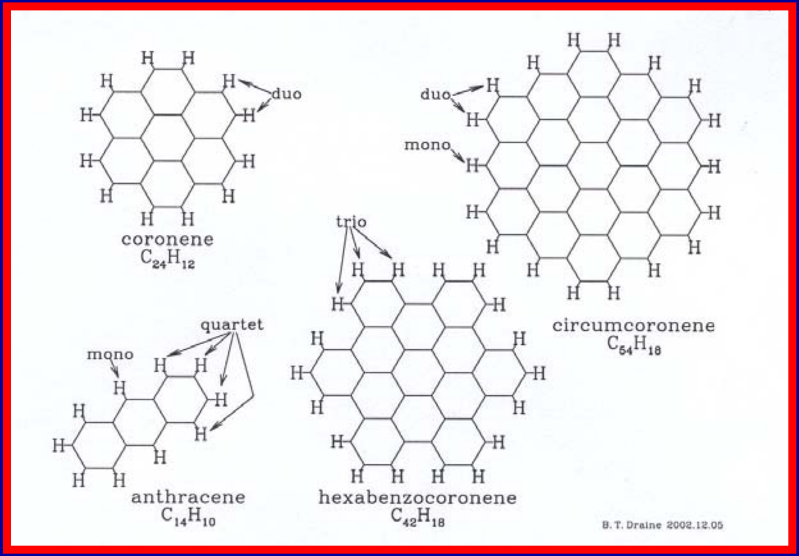
Polycyclic Aromatic Hydrocarbons (PAHs):

Optical → "internal conversion" → IR

NGC 7023 (reflection nebula)





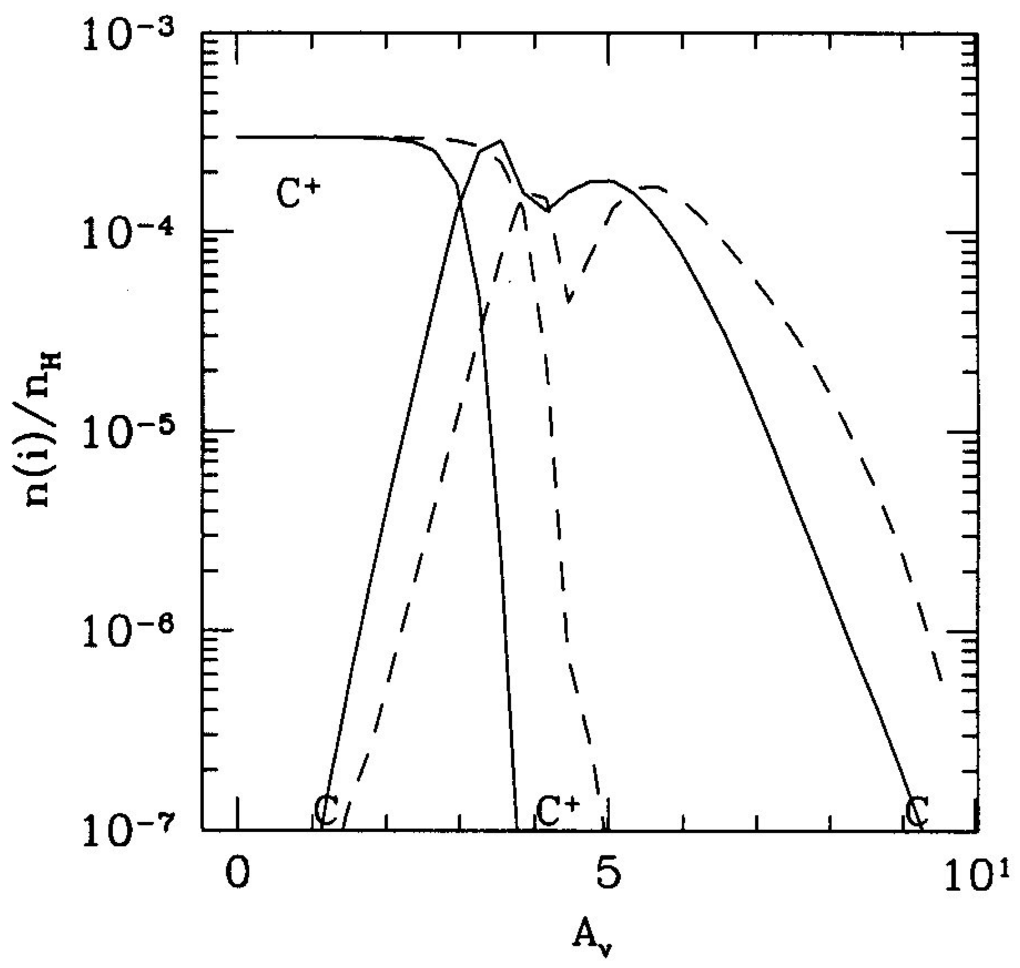


PAHs in PDRs:

Bakes & Tielens 1998 ApJ 499, 258

PAH+ ⟷ PAH ⟷ PAH-

dashed – without PAHs



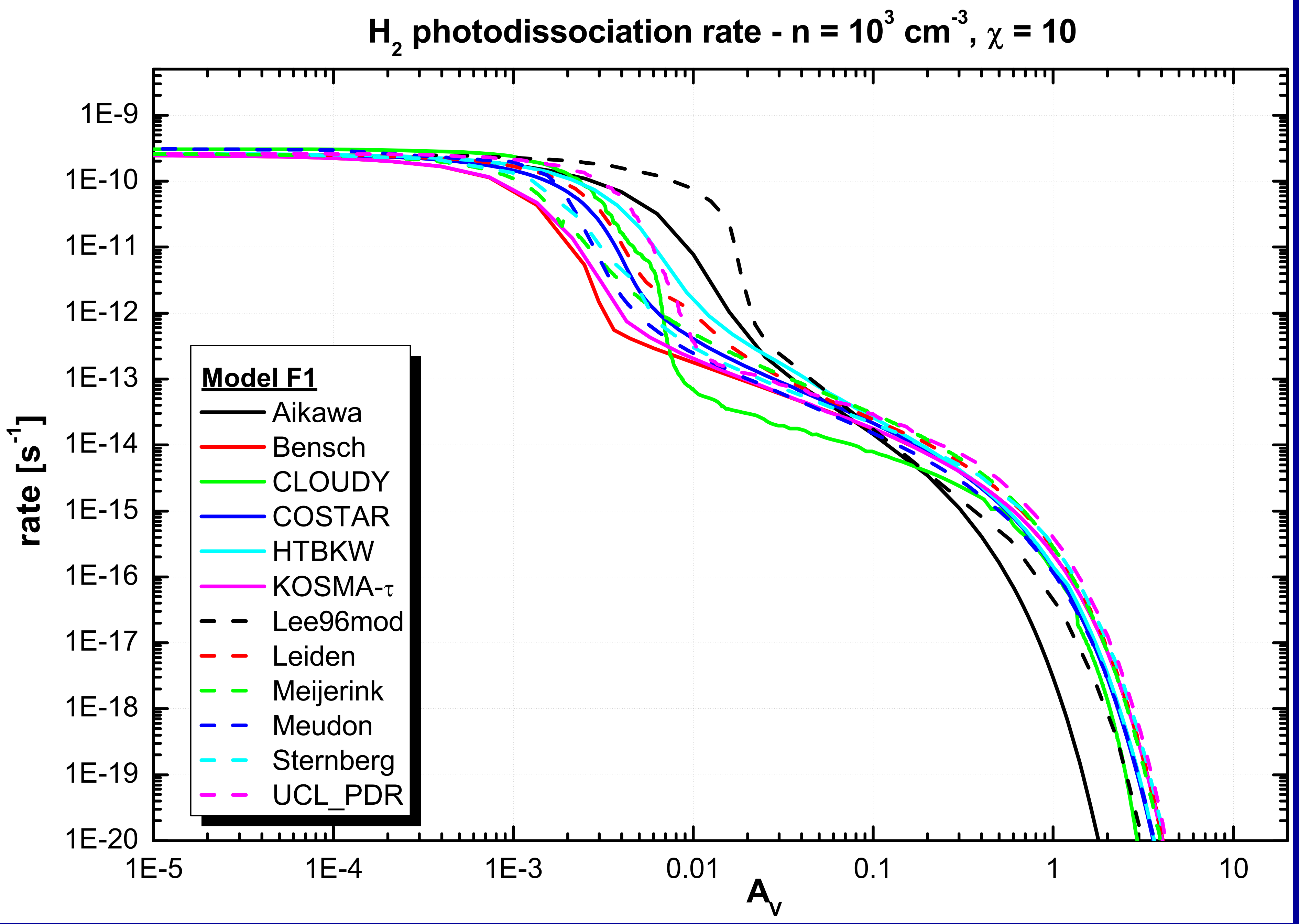
mutual neutralization

X^+ + PAH- → X + PAH

competes with or dominates radiative recombination

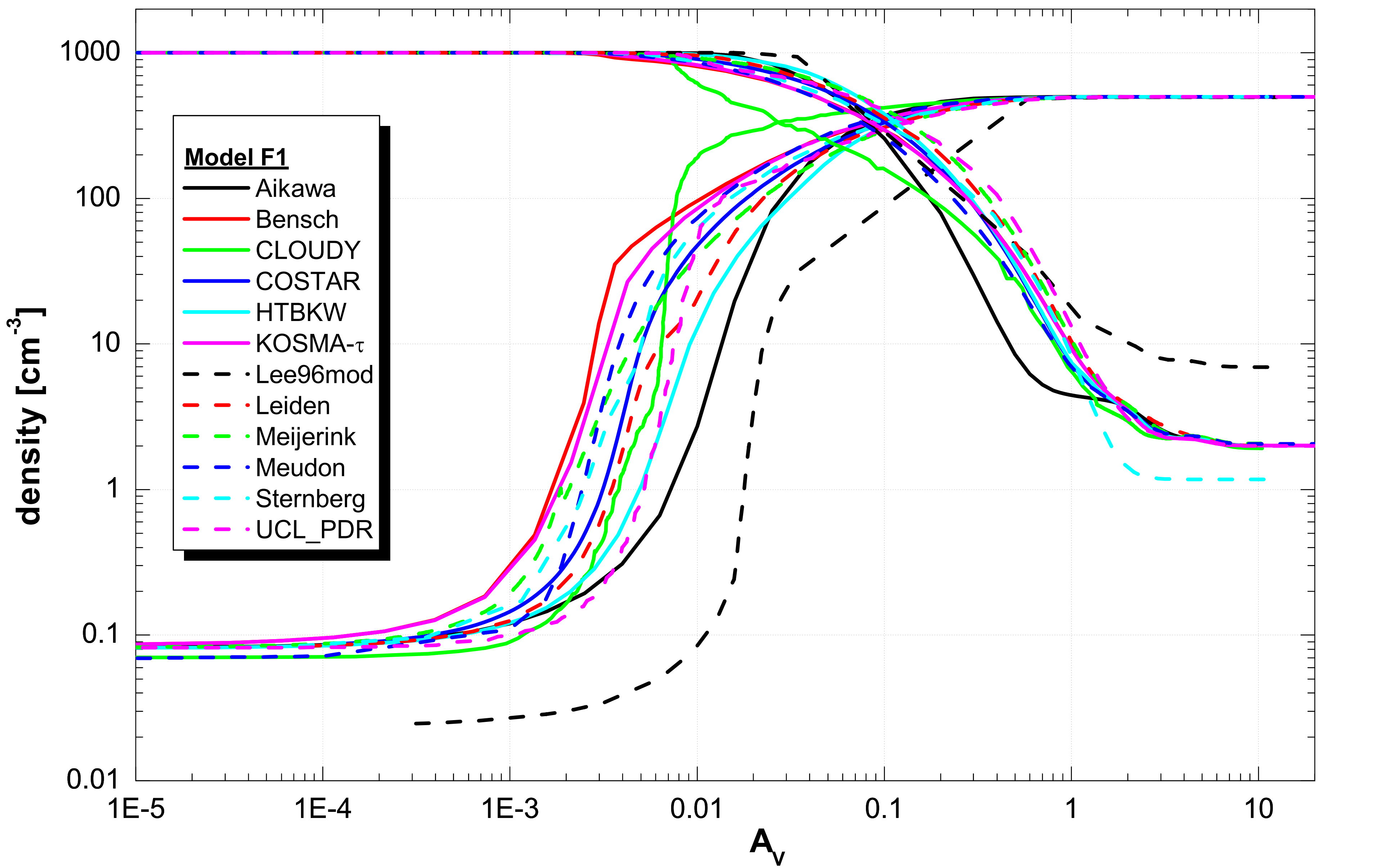
X^+ + e → X + hν

Lepp & Dalgarno 1988, ApJ, 335, 769

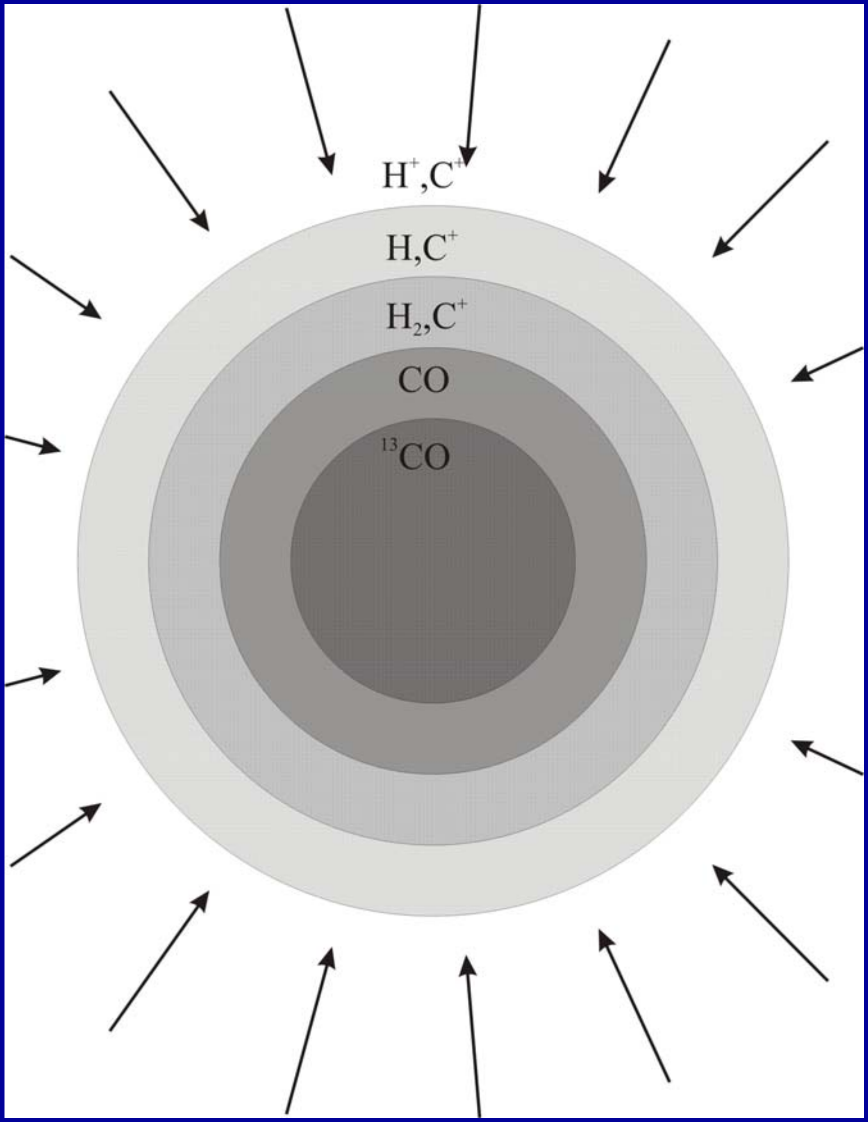


H2 photodissociation rate - n = 10^3 cm^-3, χ = 10
rate [s^-1]
1E-9
1E-10
1E-11
1E-12
1E-13
1E-14
1E-15
1E-16
1E-17
1E-18
1E-19
1E-20
1E-5
1E-4
1E-3
0.01
0.1
1
10
A_V
Model F1
Aikawa
Bensch
CLOUDY
COSTAR
HTBKW
KOSMA-τ
Lee96mod
Leiden
Meijerink
Meudon
Sternberg
UCL_PDR

H density - $n=10^3$ cm^{-3}, $\chi=10$



Resulting Model Cloud



Resulting Model Cloud