The Meudon PDR code

J. Le Bourlot
F. Le Petit
E. Roueff

- ✧ Introduction
- ✧ Benchmark exercise
- ✧ Photoprocesses and UV radiative transfer
    - exact / approximate
    - diagnostic tool?
- ✧ Chemical processes
    - H_2 formation
- ✧ Conclusions

l'Observatoire de Paris LUTH
Laboratoire de l'Univers et de ses Théories

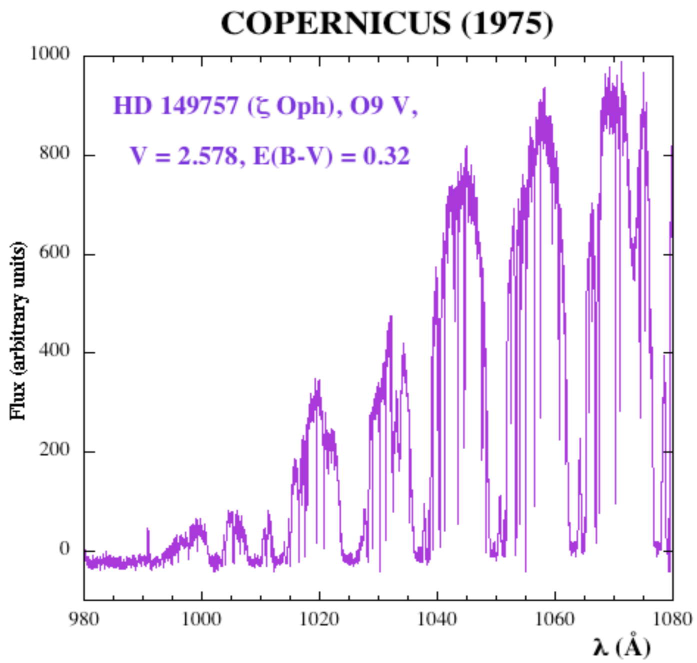
PDR models

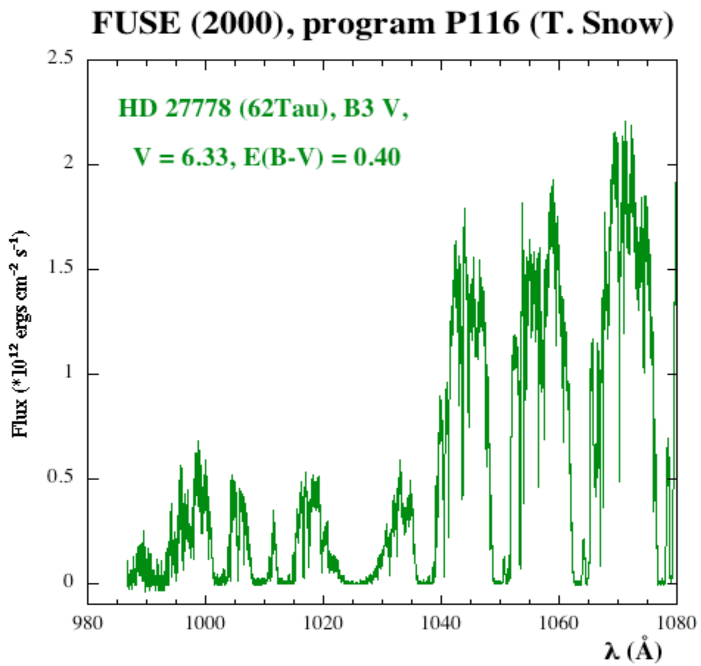
Photon Dominated Regions :

- Diffuse and translucent clouds
- Edge of molecular clouds
- Damped Lyman α systems
- Circumstellar disks
- ...
- Dark clouds

Some historical facts

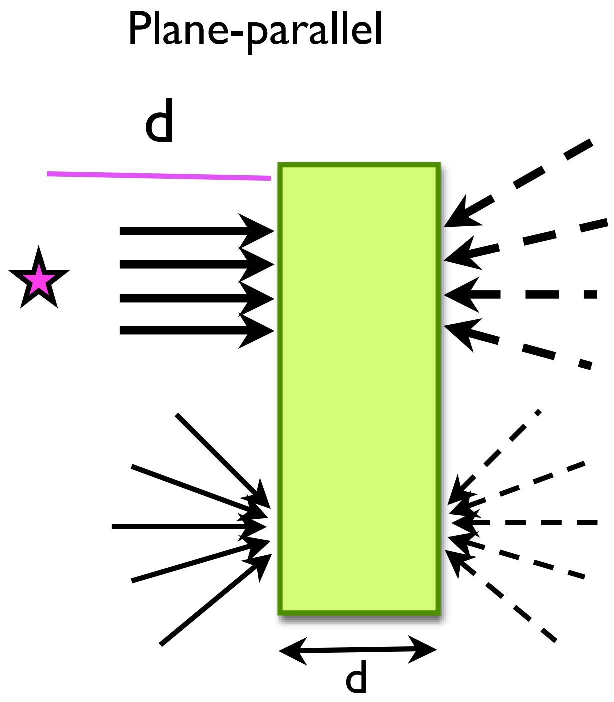
- 70's : first detection of H_2 with Copernicus toward bright stars : Black, Dalgarno, Glassgold, Hollenbach, Jura, …. Stationary models - H/H_2 transition-
- 80's : GHRS of HST UV spectra longwards 120 nm C^+/ C / CO transition : van Dishoeck, Black, Sternberg, Viala, Flower, Pineau des Forêts, Le Bourlot, Roueff …
- 90's : ISO H_2 and atomic fine structure line seen in emission !
- 2000's : FUSE : fainter sources
- present and future : Spitzer, Herschel, ALMA, JWST, … ?



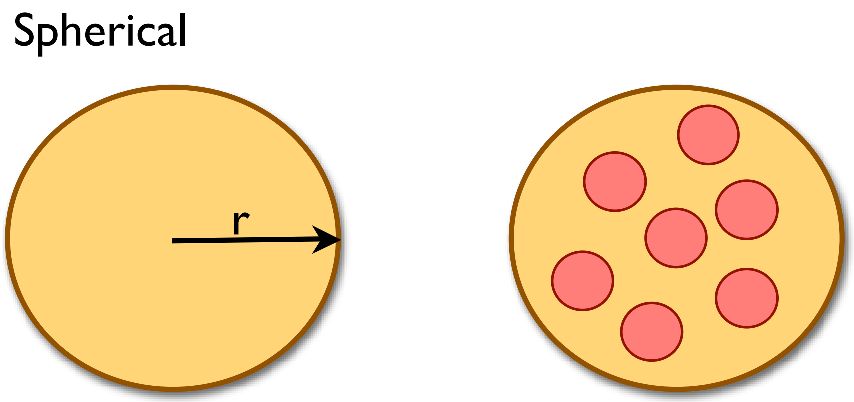


PDR models

Geometry

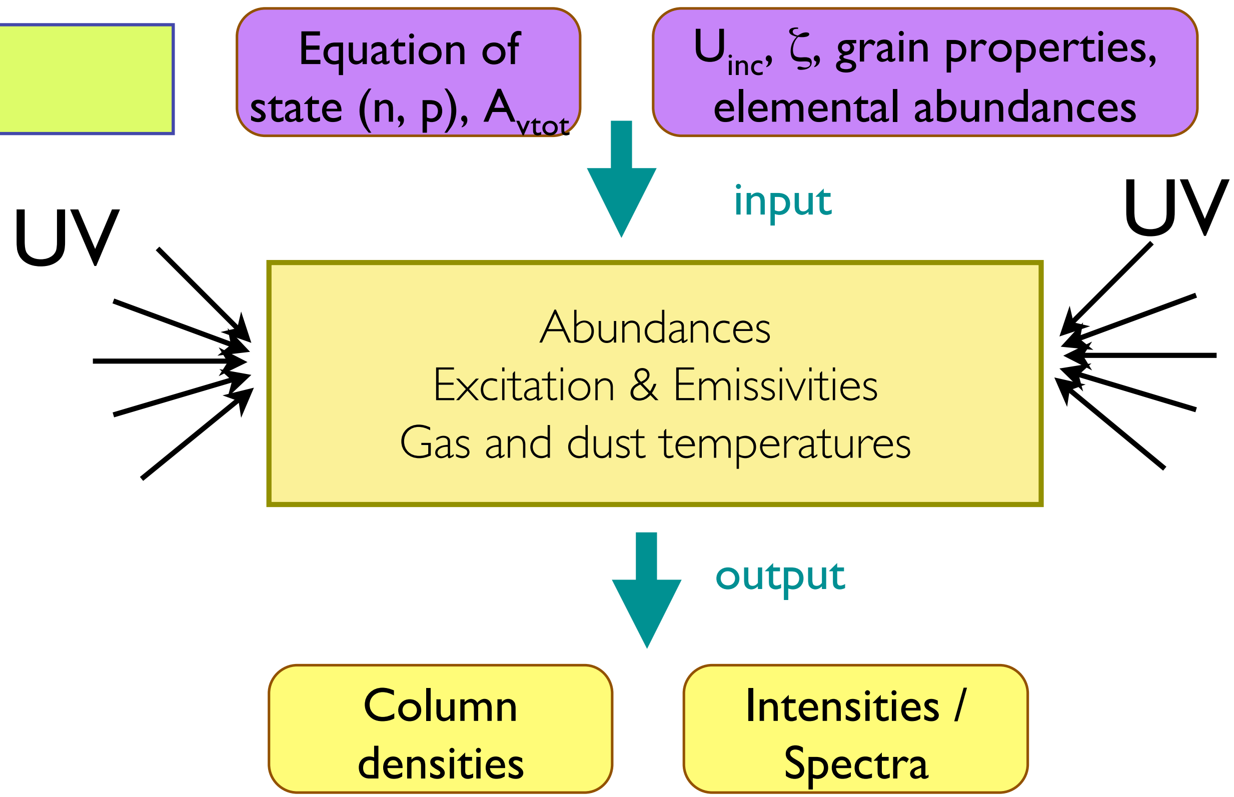


- 1 or 2 side illumination
- Isotropic or perpendicular



- Isotropic illumination
- r $\longrightarrow$ ∞ to mimic a plane parallel case

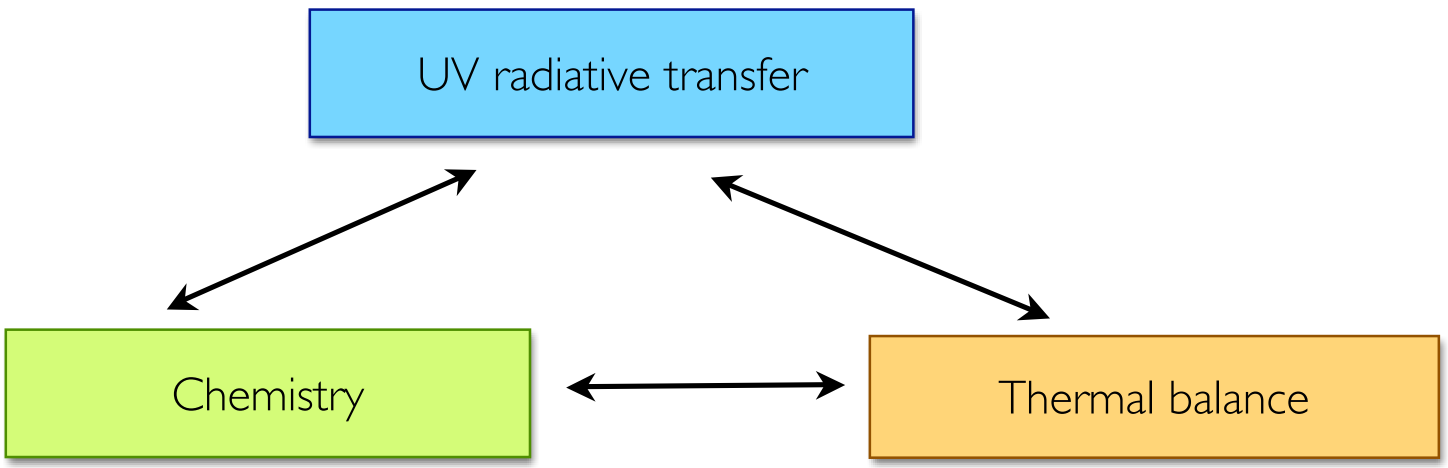
PDR models



Problem to be solved :

Compute all local quantities :

- abundances
- populations
- local emissivities
- Heating/cooling processes
- temperatures : gas and dust particles



Benchmark of PDR codes (Leiden)

(Röllig et al. - A&A 467, 187, 2007)

Aikawa	Lee, Herbst, Pineau des Forêts, Le Bourlot, Aikawa	**Analytical formulae for H_2 and CO photodissociation**
Lee96mod	Lee, Herbst, Pineau des Forêts, Roueff, Le Bourlot	**Analytical formulae for H_2 and CO photodissociation**
Kosma	Störzer, Köster, Zilinsky, Jeyakumar, Röllig	**spherical geometry**
Bensch	Störzer, Köster, Zilinsky, Jeyakumar, Bensh	**spherical geometry**
HTBKW	Hollenbach, Tielens, Burton, Kaufman, Wolfire	**Simplified H_2**
Leiden	Black, van Dishoeck, Jansen, Jonkheid	**Detailed physics**
Cloudy	Ferland, van Hoof, Abel, Shaw	**Detailed physics**
Meudon	Le Bourlot, Roueff, Le Petit	**Detailed physics**
Sternberg	Sternberg, Dalgarno	**Detailed physics**
Meijerink	Meijerink, Spaans	**XDR**
Costar	Kamp, Bertoldi, van Zadelhoff	**Circumstellar disks**
UCL	Viti, Thi, Bell	**Time dependence**

Benchmark exercise

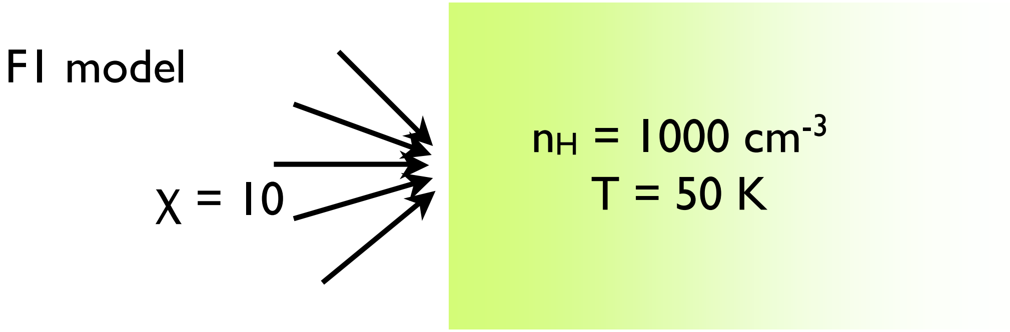
Simplification

Chemistry based on : H, He, C, O
31 species
Chemistry : UMIST99
H_2 formation rate fixed : $R = 3\times10^{-18}\ T^{1/2}\ cm^3\ s^{-1}$ (2×10^{-17} at 50 K)

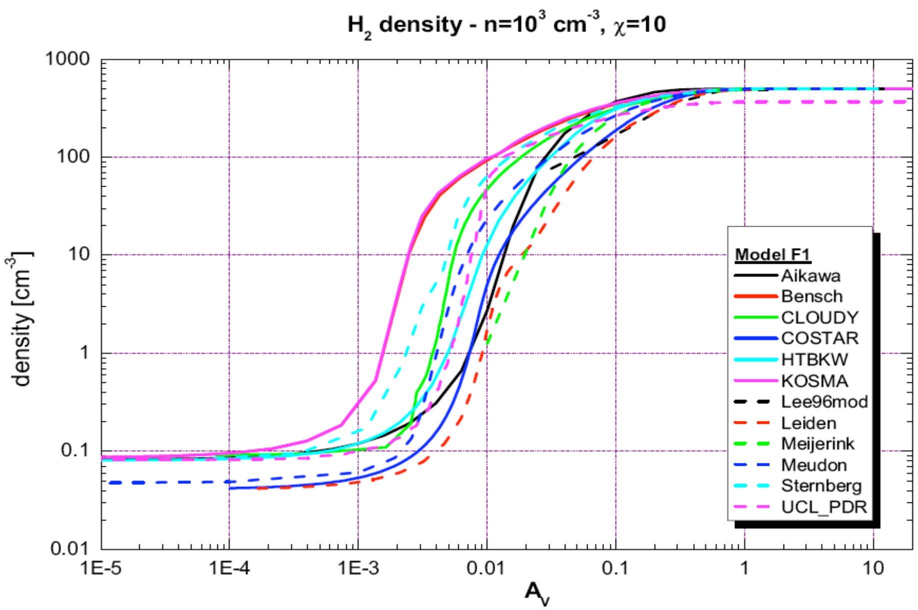
2 types of models

F1 $n = 10^3\ cm^{-3}$, $\chi = 10$	F2 $n = 10^3\ cm^{-3}$, $\chi = 10^5$	T fixed 50 K	Test of photo-processes
F3 $n = 10^{5.5}\ cm^{-3}$, $\chi = 10$	F4 $n = 10^{5.5}\ cm^{-3}$, $\chi = 10^5$		
V1 $n = 10^3\ cm^{-3}$, $\chi = 10$	V2 $n = 10^3\ cm^{-3}$, $\chi = 10^5$	T variable	Test of thermal balance
V3 $n = 10^{5.5}\ cm^{-3}$, $\chi = 10$	V4 $n = 10^3\ cm^{-3}$, $\chi = 10^5$		

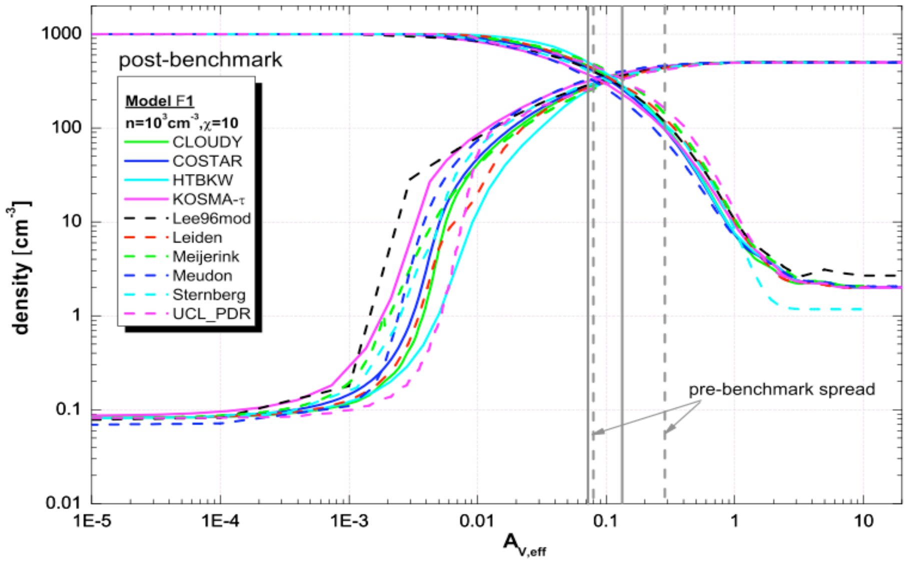
Benchmark exercise



Before comparaison



After comparaison



Meudon PDR code

Characteristics

- Plane parallel & steady state
- Detailed UV radiative transfer for photo-processes
  - with discrete gas absorption in H, H_2, HD, CO, ... (~35000 transitions)
  - continuous absorption from dust particles
- Chemistry
- Thermal balance
- Detailed balance of molecular populations in H_2, CO, CS, H_2O, HCO^+, H_3^+, …

http://aristote.obspm.fr/MIS

Various improvements since benchmark exercise

- exact radiative transfer (Goicoechea & Le Bourlot, AA 467, 1, 2007)
- infrared pumping of H_2O by dust radiation (Gonzalez-Garcia et al. submitted)
- H_2 formation with moment equations (work in progress with O. Biham)

….

Meudon PDR code

Inversion tool

- analyse lines
- derive physical conditions (T, n_H, …)
- Hint at evolution paths
- Caveat : Reality is too sophisticated

Experiment *in silico*

- Test physical hypothese
- Assert importance of physical parameters
- Suggest new paradigms
- Caveat : Reality is too sophisticated

We must adapt our limited tols and computing power to our goals

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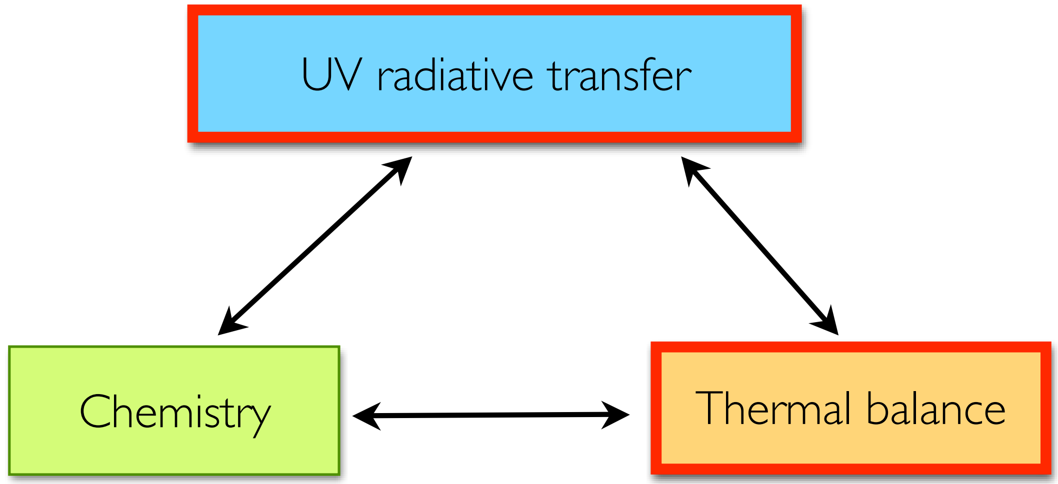
Radiative transfer

Decoupling between UV and IR / radio



UV radiative transfer

- dependence on the excitation status (H_2, HD, CO)
- dependence on the grain properties
- absorption
- angular redistribution
- different levels of approximations
    - ✧" FGK" (Federman et al. 1979, ApJ 227, 466) self shielding approximation
    - ✧ "exact"

•IR / radio radiative transfer :

Statistical equilibrium equations (collisional + radiative excitation and de-excitation)

- [C II] 158 μm and [Si II] 35 μm (Barinovs & van Hemert, 2005, ApJ 620, 537)
- [O I] 63, 145 μm (Abrahamson et al. 2007, ApJ 654, 1171)
- [C I] 370, 610 μm (Abrahamson 2007)
- CO [H_2 : Flower 2001, H revisited by Shepler et al, 2007)
- H_2O [H_2 : Green, Phillips, revisited by Dubernet, Grosjean et al.)
- H_2 : collisions with H, revisited by Wrathmall and Flower, 2006; non-reactive only

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One can not avoid the transfer equation

$$\mu \frac{\partial I_\lambda(\tau_\lambda,\mu)}{\partial \tau_\lambda} = I_\lambda(\tau_\lambda,\mu) - S_\lambda(\tau_\lambda) - \frac{\omega_\lambda(\tau_\lambda)}{2}\int_{-1}^{+1} p_\lambda(\mu,\mu') I_\lambda(\tau_\lambda,\mu') d\mu'$$

with $$\omega_\lambda(\tau_\lambda) = \frac{\sigma_\lambda^D(\tau_\lambda)}{\kappa_\lambda^G(\tau_\lambda) + \kappa_\lambda^D(\tau_\lambda) + \sigma_\lambda^D(\tau_\lambda)}$$

I_λ : specific intensity
S_λ : Source function
ω_λ : effective albedo
p_λ : angular redistribution function

Solution through spherical harmonics

- First proposed by Flannery et al., ApJ 236, 598, 1980
- Extended by Roberge, ApJ 275, 292, 1983 to include embedded sources
- Extended by Goicoechea & Le Bourlot (2007) with variable coefficients including discrete transitions

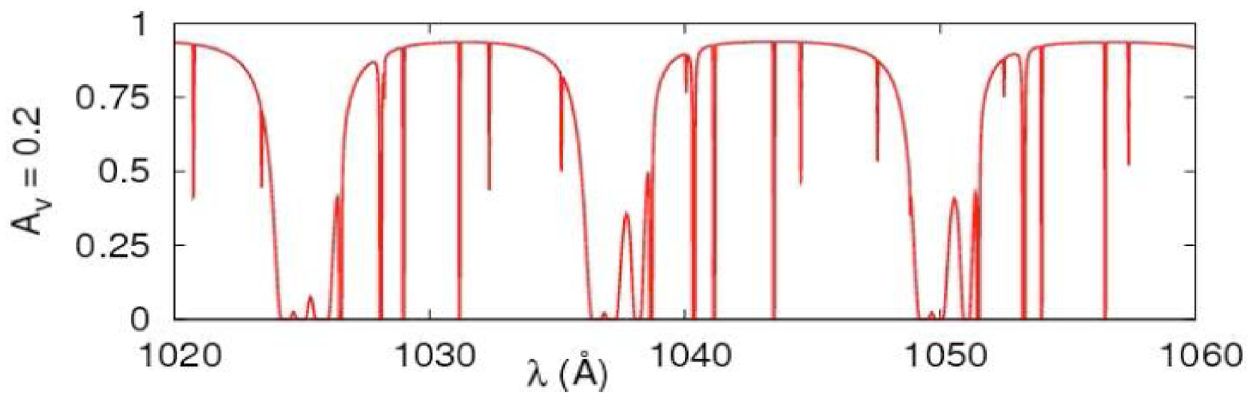

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Photo-reactions probability calculations

$$k = \int \sigma(\lambda) I(\lambda) d\lambda$$

$\sigma(\lambda)$: photodissociation cross section cm^2

$I(\lambda)$: mean intensity of the radiation in photons $cm^{-2}\ s^{-1}\ Å^{-1}$

In presence of resonances : $$k = \frac{\pi e^2}{mc^2} \lambda_u^2 f_u \eta_u I_u$$

8.85×10^{-21}

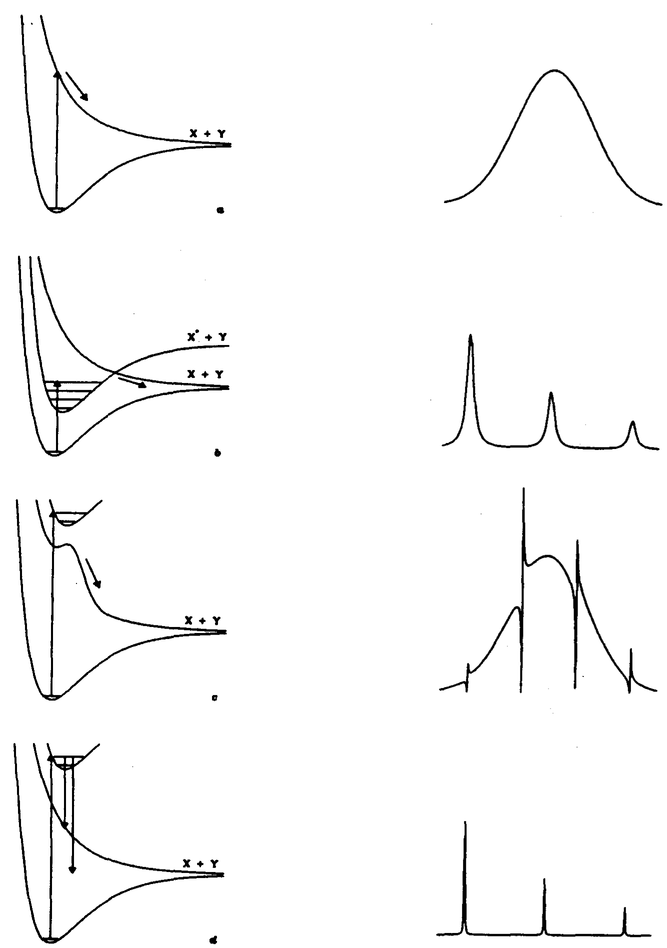
Frequent approach : $k = k_0 \cdot \chi \cdot \exp(-\beta A_V)$

Example : $S + h\nu \rightarrow S^+ + e^-$ $\quad k = 5.9 \times 10^{-10}\, e^{-2.58\, Av}$

- All possible channels should be considered
- dependence on the grain properties and intensity of the radiation field (values different for “Mathis” and “Draine” radiation fields)

cf Ewine’s talk

Photodissociation mechanism **Cross section**



From van Dishoeck (1988)

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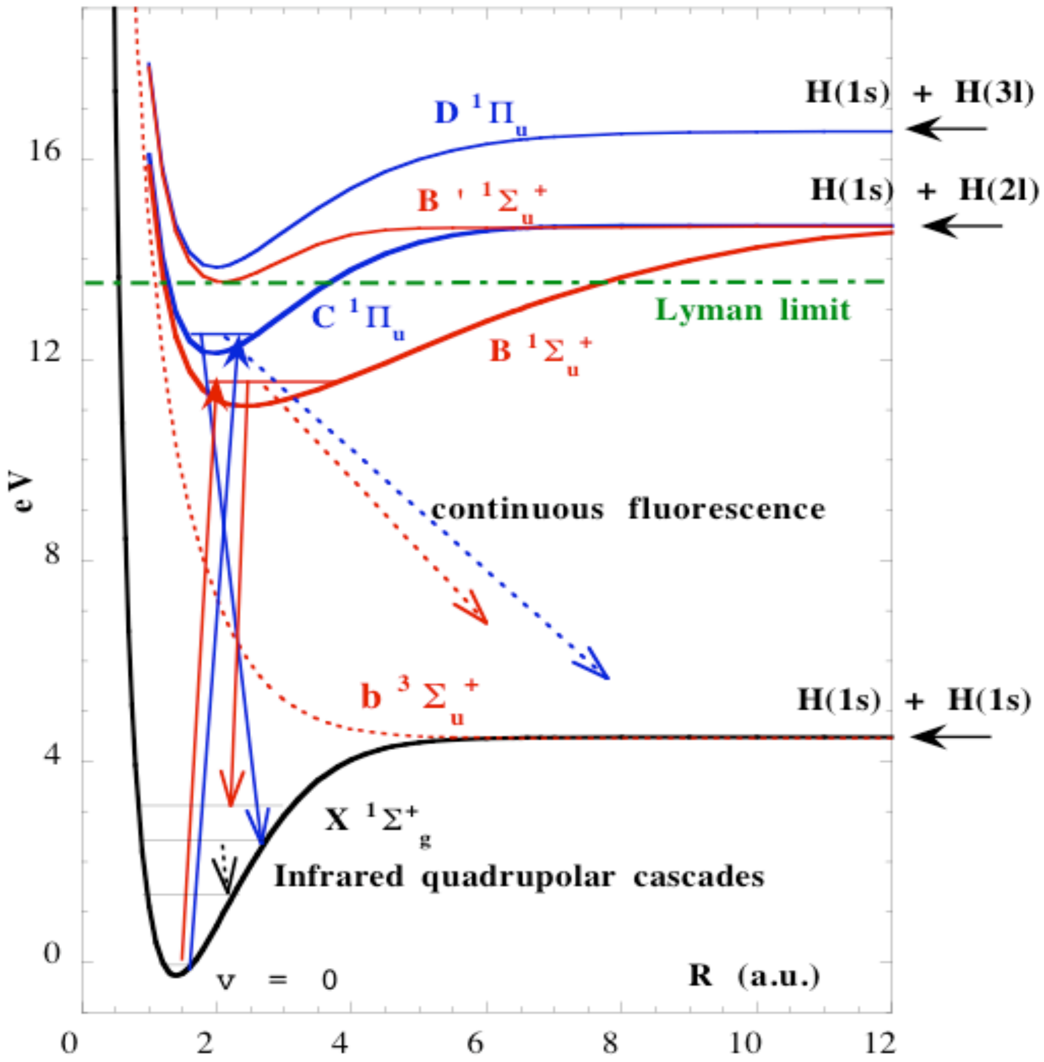
H_2 photodissociation probability

Dependence on

- incident radiation
- H_2 excitation
- molecular physics data
  - J dependent oscillator strengths and photodissociation probabilities (Abgrall & Roueff) data available at http://molat.obspm.fr
  - (de)excitation collision rates by H, He, H_2, electrons, H^+, … (new calculations by Wrathmall & Flower in J. Phys B 39, L249 (2006) for H_2 + H data available at http://massey.dur.ac.uk/saw/website_data



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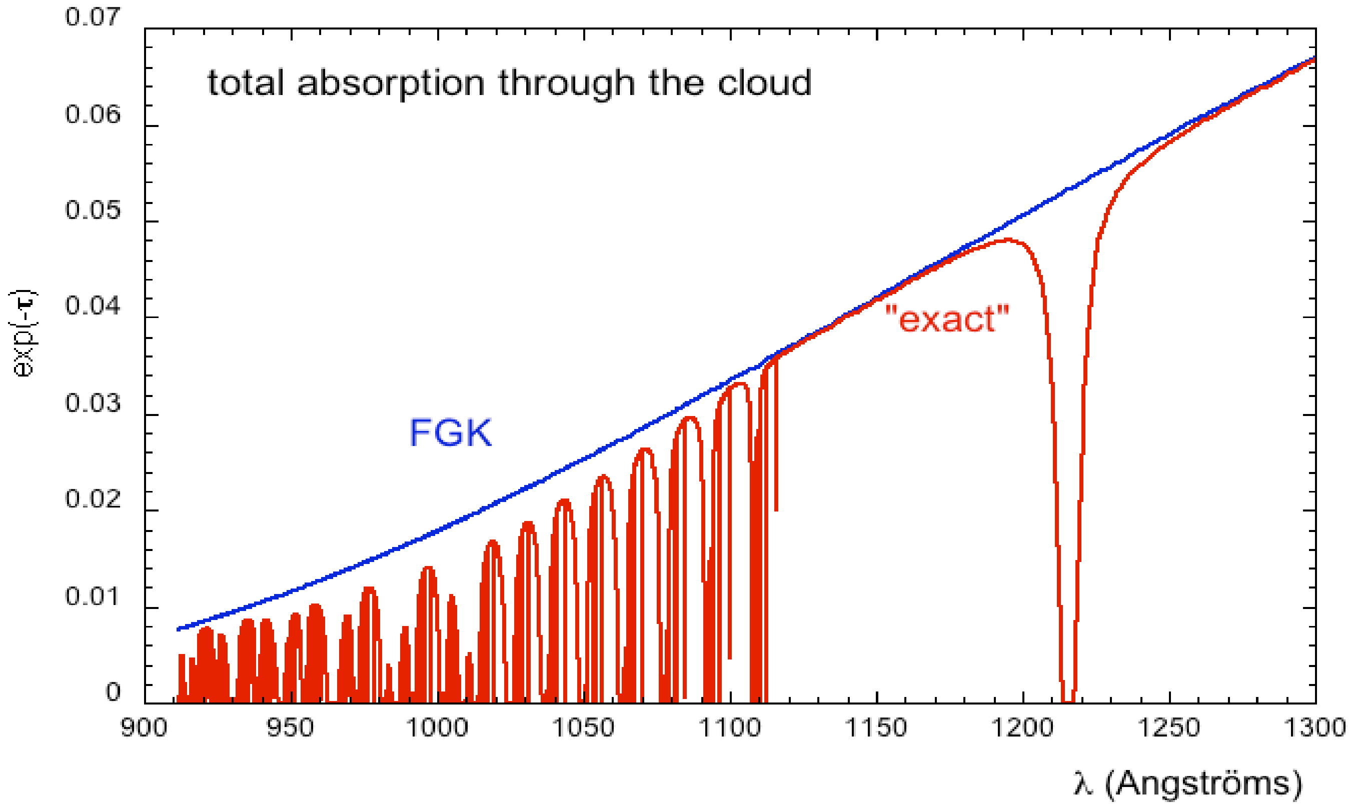
FGK versus "exact" UV transfer

✧ 2-side illumination model with $\chi = 1$, $n_H = 100\ cm^{-3}$
✧ exact radiative transfer for H and H_2 absorption up to J = 4



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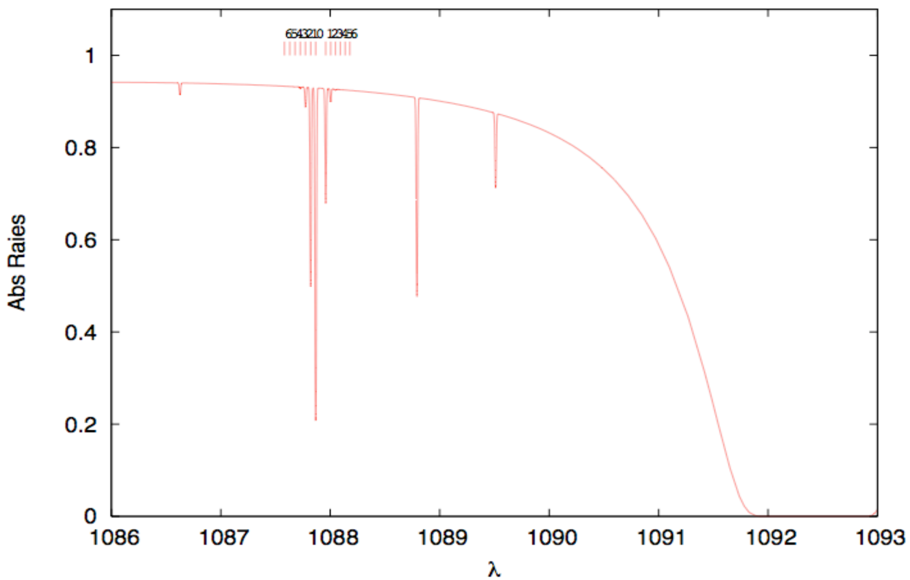
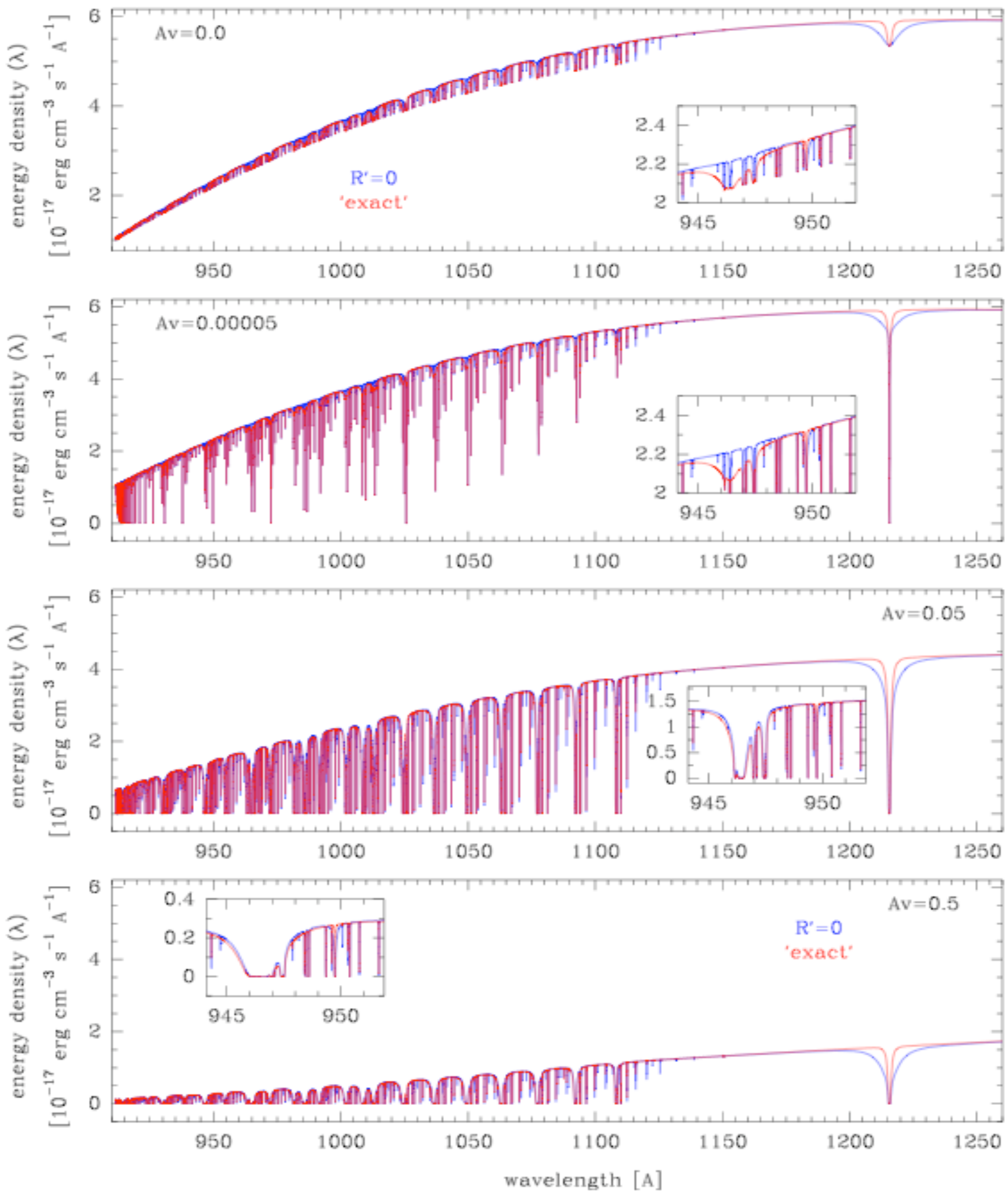
Exact Transfer :

Goiecoechea & Le Bourlot (AA 467, 1, 2007)

CO transitions:





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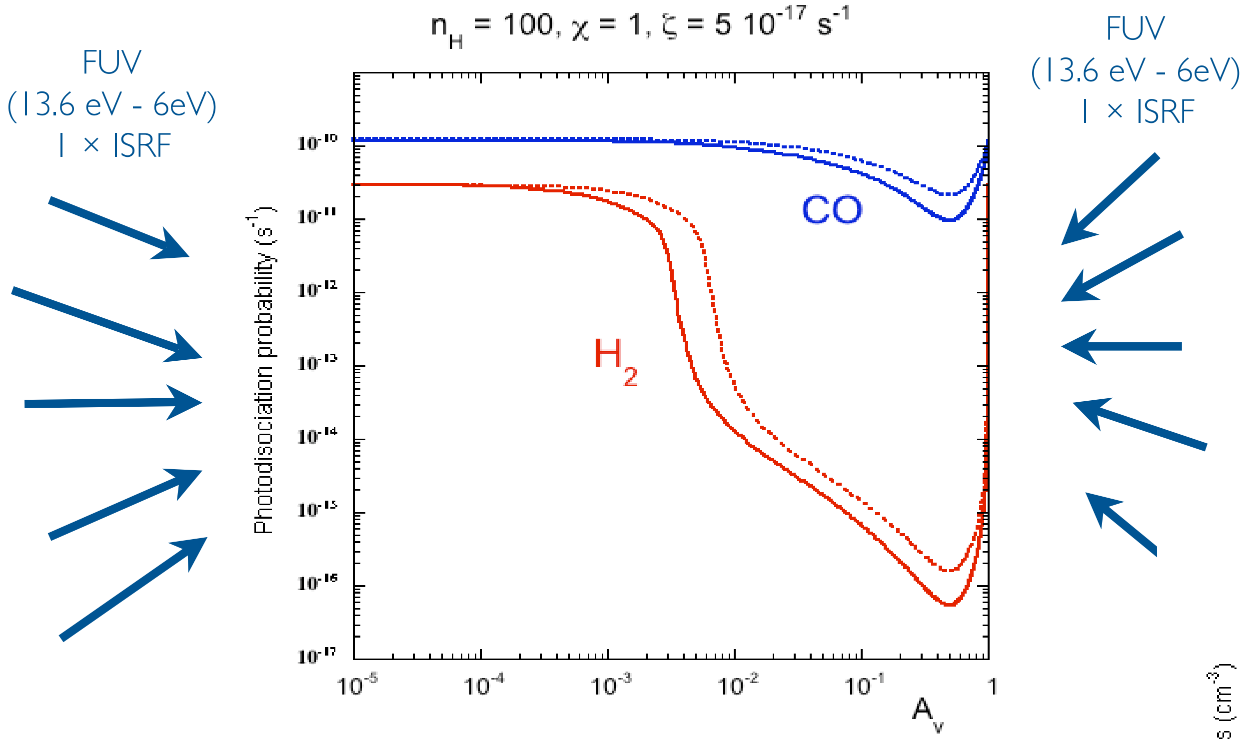
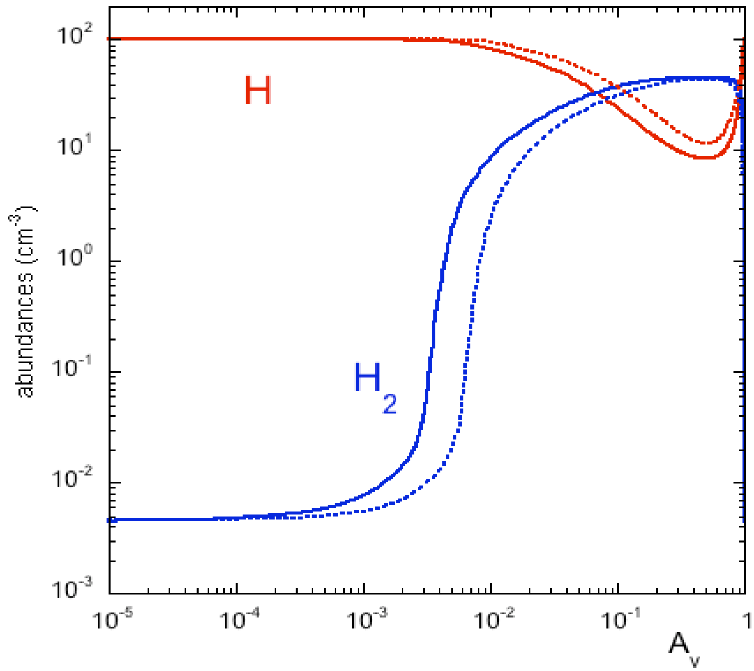
Included cross-sections :

H_2 : PD
CO : PD
C : PI
S : PI
CH : PD + PI
C_2 : PD + PI
C_3 : PD + PI
CN : PD
OH : PD + PI
H_2O: PD + PI
NH : PD
HF : PD

FGK (dotted lines) versus “exact” (full lines) UV transfer





✧ Decrease of photodissociation probabilities when exact transfer is included (role of overlap with H_2 transitions)
✧ H/H_2 transition towards smaller A_v
✧ same trend for all photodissociation rates

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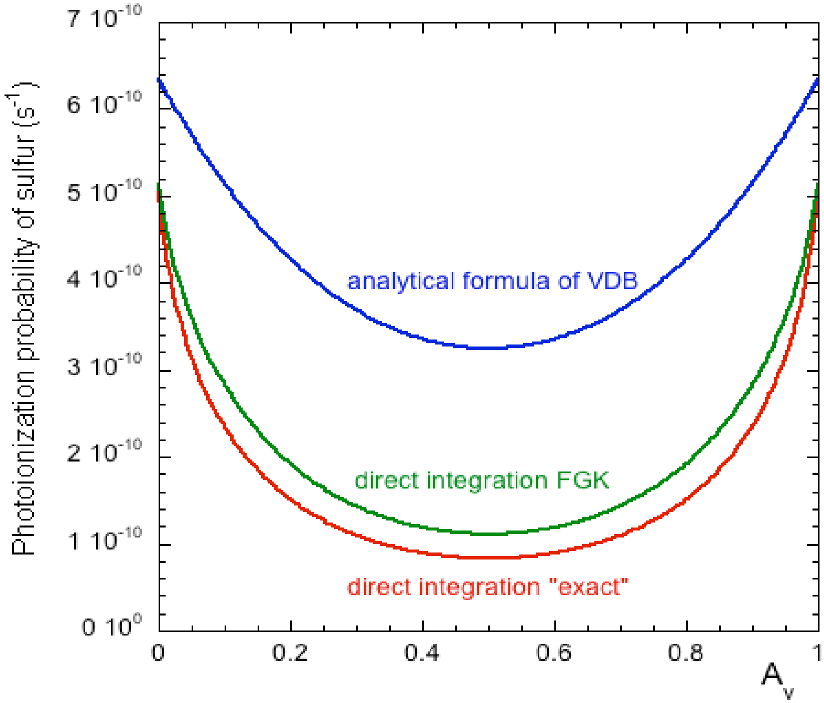
Exact transfer allows to know the radiation field at each point;

Photodissociation probability

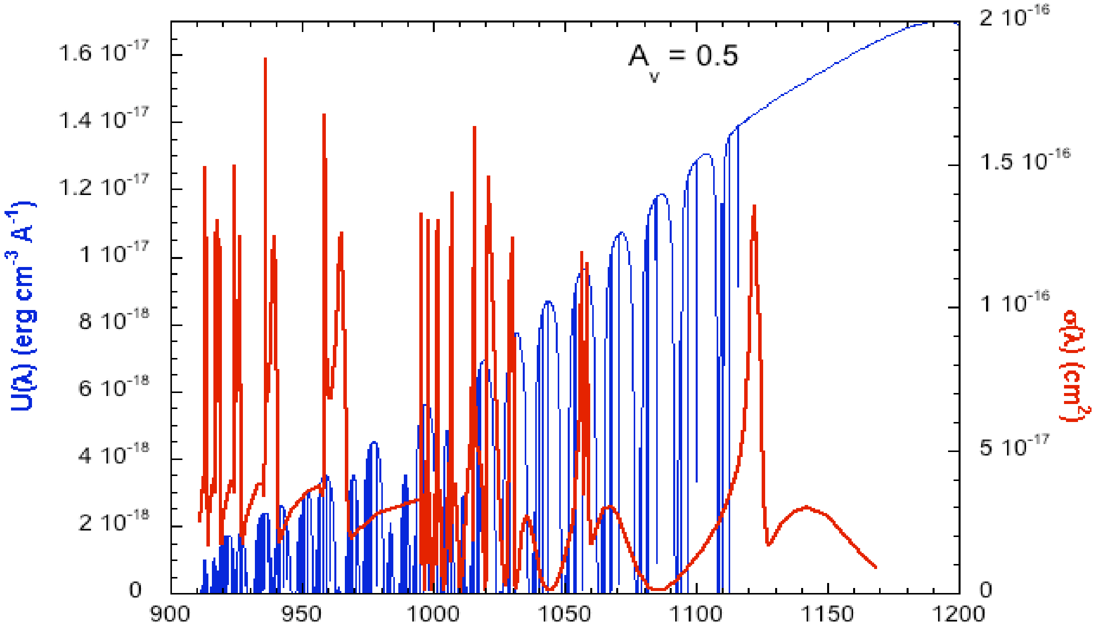
$$k = \int \sigma(\lambda) I(\lambda) d\lambda$$

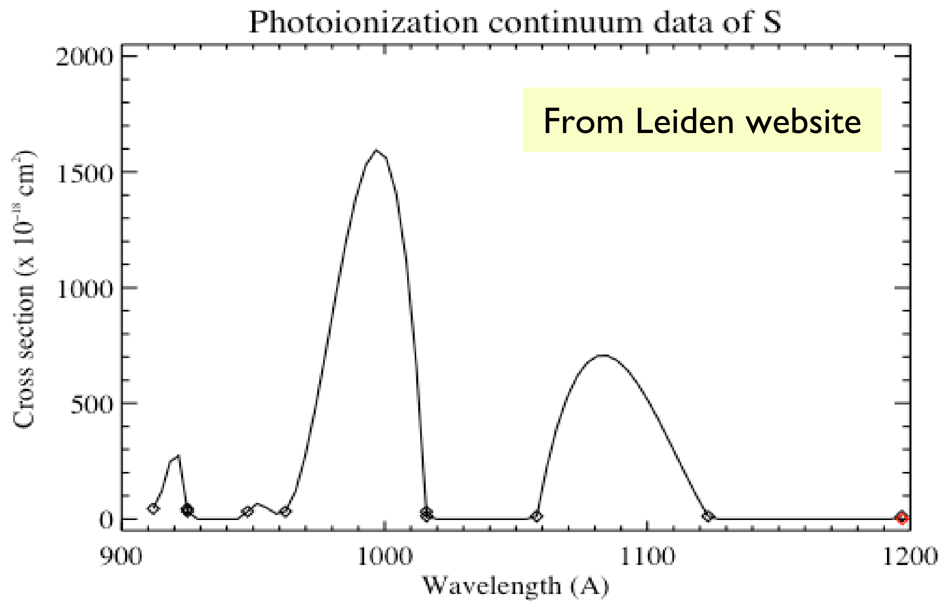
Sulfur example :

n_H = 100 cm^{-3}, ζ = 5 10^{-17} s^{-1},
χ = 1, 2-side illumination



σ from Topbase





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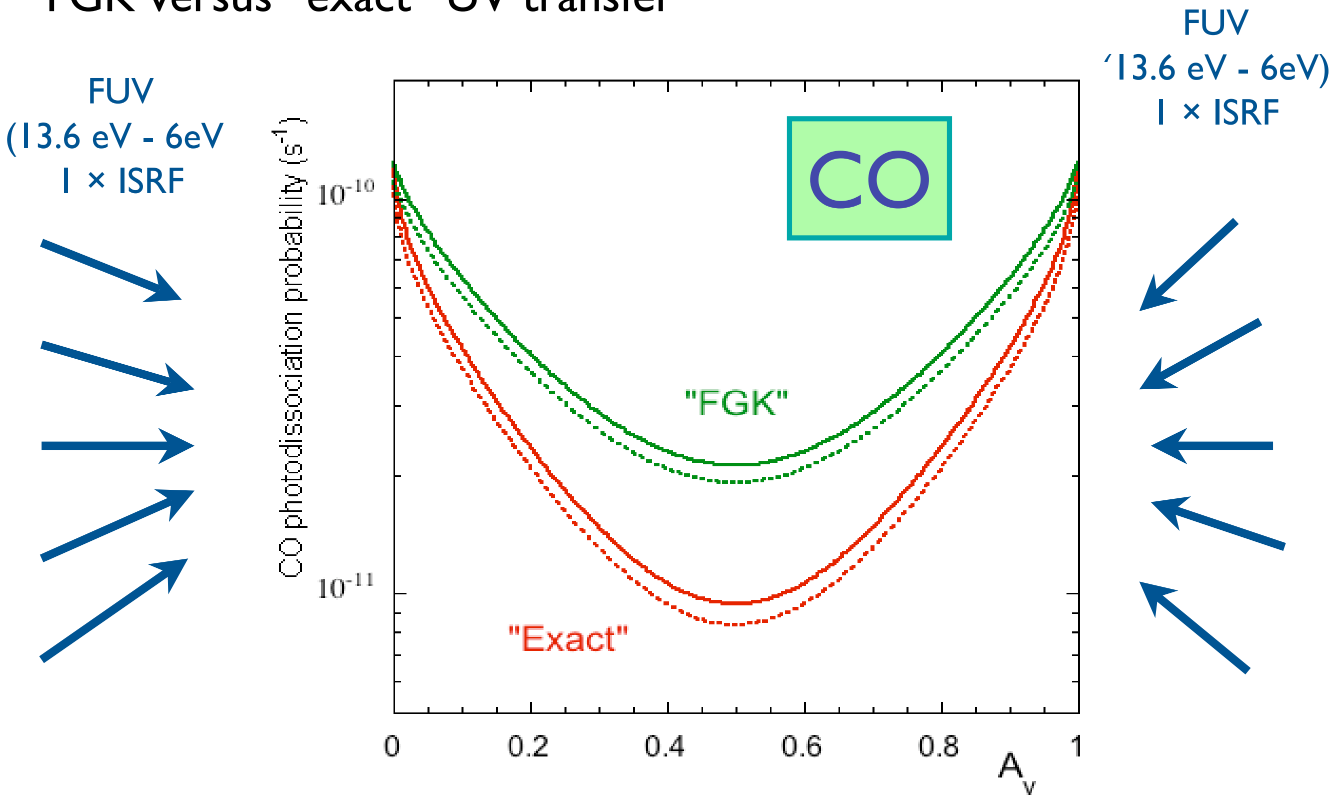
FGK versus "exact" UV transfer



Modelled column densities

species	exact	FGK
H	3.6(20)	5.0(20)
H_2	7.6(20)	6.9(20)
C^+	1.5(17)	1.5(17)
C	1.3(15)	8.1(14)
S	3.2(13)	2.7(13)
CO	1.2(13)	6.5(12)
CH	1.5(13)	1.2(13)
CN	9.1(10)	4.0(10)
OH	4.3(12)	3.8(12)
H_3^+	1.4(13)	1.2(13)

☛ full lines: with revised oscillator strengths of Eidelsberg et al. 2006, ApJ 647, 1543, for E-X, B-X and W-X transitions

E. Bayet et al., in preparation

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Example of diffuse clouds

2-side model : $\chi = 1$

''exact '' transfer required for diffuse regions

2 cases : - FGK
- ''exact'' transfer up to J = 3

n_H (cm^{-3})		N(H)	N(H_2)	f	T_{moy}	T_{01}
10	FGK	1.3E20	7.3E15	1.1(-4)	695	-2080
	exact	1.3E20	6.2E16	9.5(-4)	655	321
30	FGK	1.2E20	4.2E18	6.5(-2)	221	151
	exact	1.1E20	9.8E18	0.15	192	142

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Thermal balance

Several uncertainties

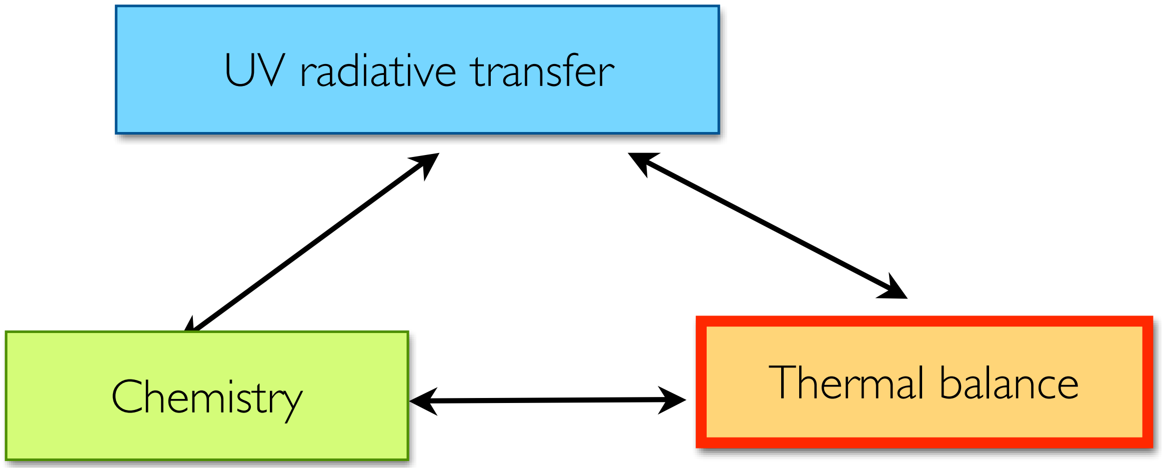
Heating :

- Photo-electric effect on grains
- H_2 : vibrational de-excitation, dissociation, formation
- Cosmic ray ionization; secondary UV photons
- Gas/grain interaction (if $T_{grain} > T_{gas}$)
- chemical heating

Cooling :

- [C II] 158 µm
- [O I] 63, 145 µm
- [C I] 370, 610 µm
- H_2, CO, H_2O, HCO^+, CS, OH, …
- Gas/grain interaction (if $T_{grain} < T_{gas}$)

Escape probabilities



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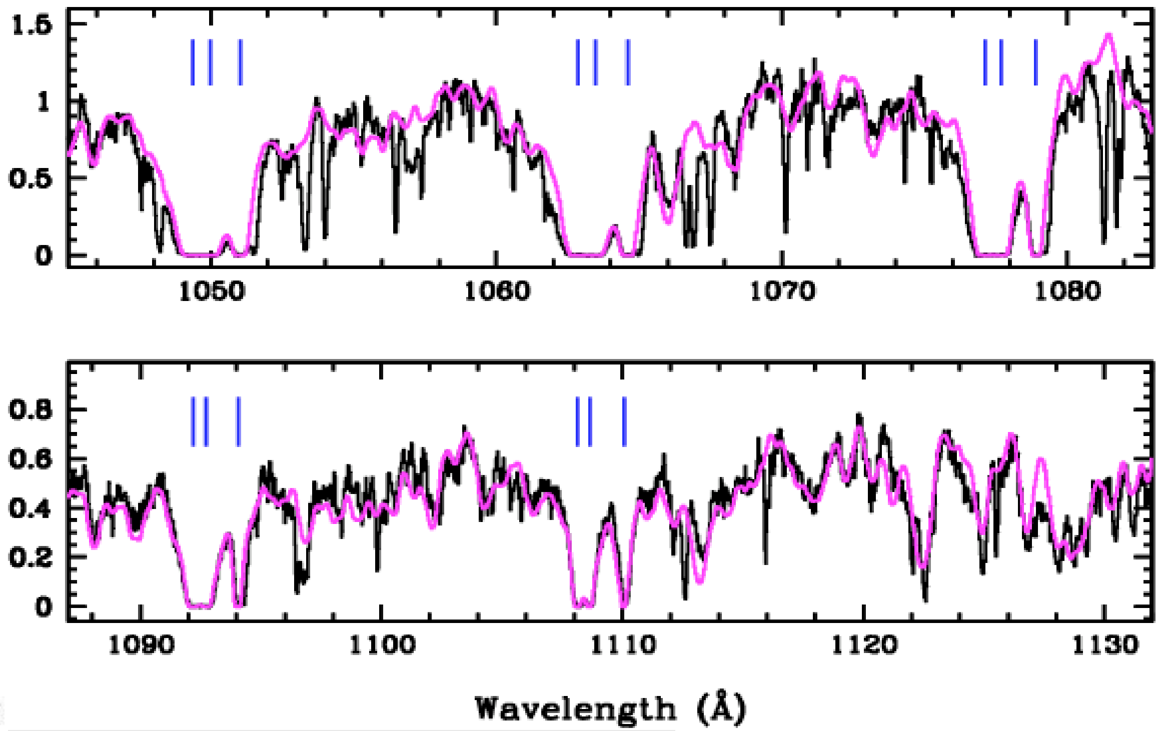
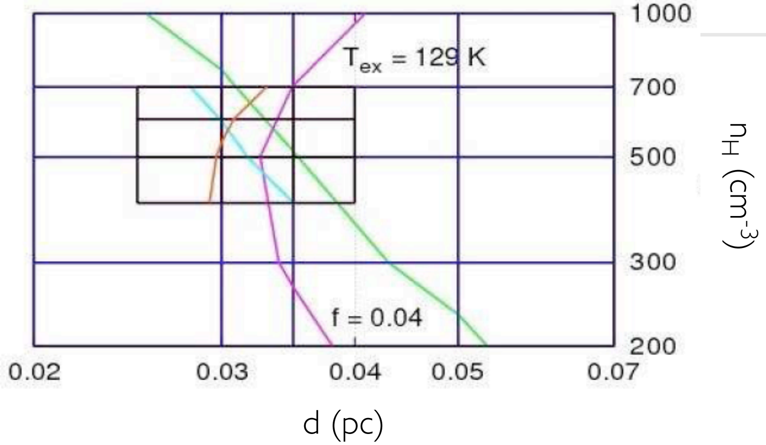
Observation of circumstellar H_2 towards HD 76534

Martin-Zaïdi et al.
submitted



Observational information

- ✧ f molecular fraction
- ✧ excitation temperature of lowest H_2 levels



Space parameters

- ✧ n_H
- ✧ Distance of the star to the enveloppe

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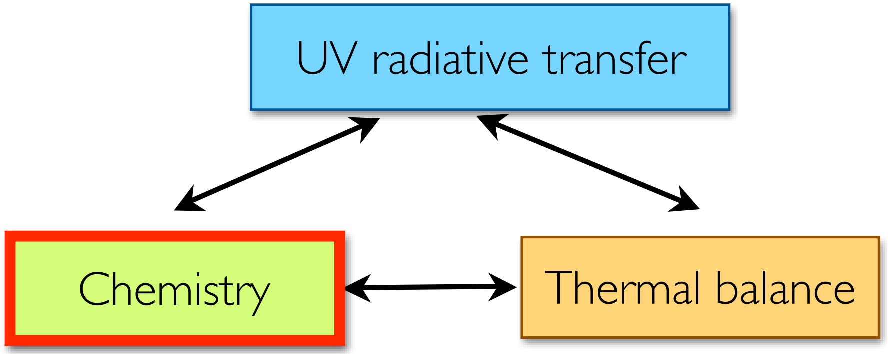
Chemistry

Typically 10 more reactions than involved species



All binary reactions relevant to dark cloud chemistry (cf Eric's and Tom's talk) + :

- Photo-reactions
- Formation reaction of H_2 on grains
- Reactions with atoms (H, N, O, C, S, …) and ions (charge transfer included)
- Small endothermicities may be overcome at the edge of the PDRs ; role of reactions with vibrationally excited H_2

Free chemical reaction rates data bases

UMIST : http://www.udfa.net/
E. Herbst : http://www.physics.ohio-state.edu/~eric/research.html
M. Larsson : Dissociative recombination reactions : http://mol.physto.se/moldata
Photoprocesses : Leiden : http://www.strw.leidenuniv.nl/~ewine/photo
SWRI : http://amop.space.swri.edu/
Meudon : http://aristote.obspm.fr/MIS
KIDA : future

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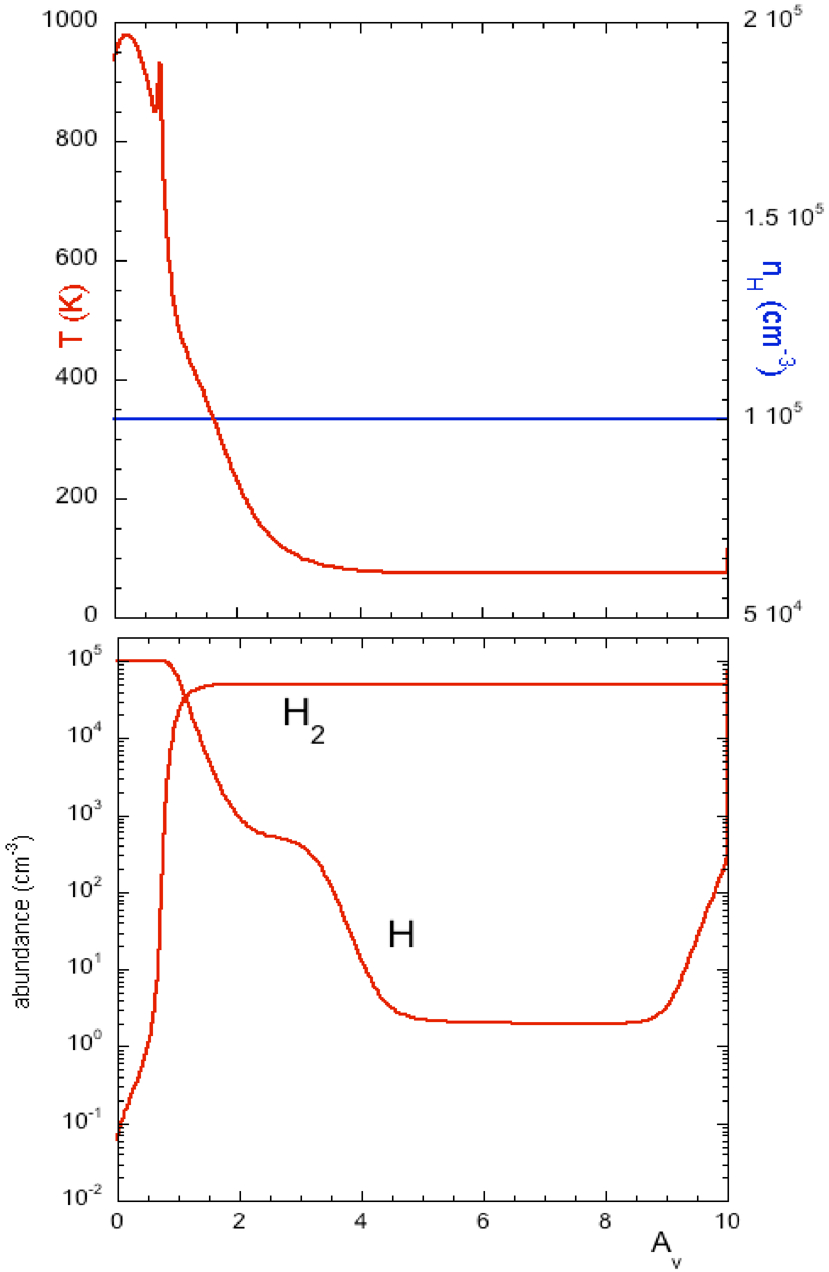

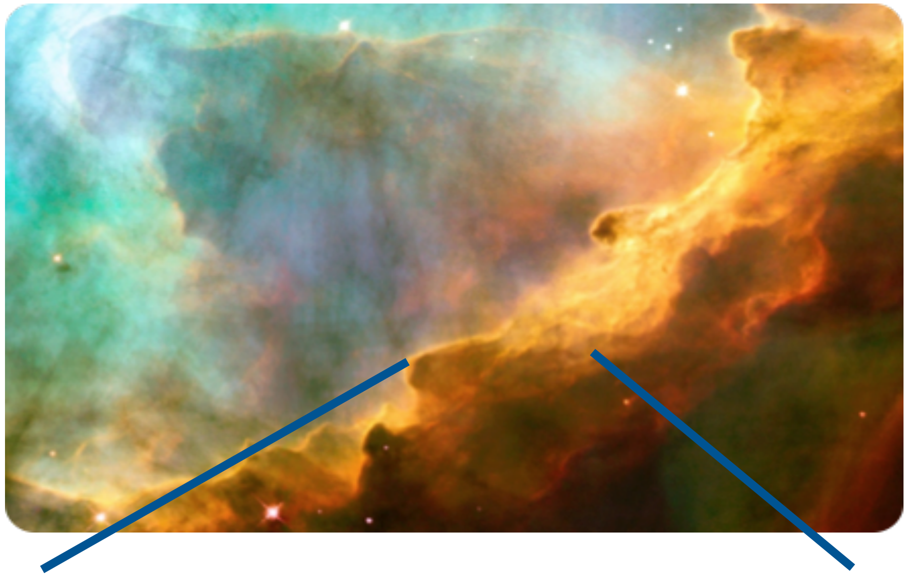

Physical structure

$n_H = 10^5$ cm^{-3}

$Av_{tot} = 10 \approx d = 0.061$ pc

$\chi_{left} = 10^5$

$\chi_{right} = 1$

$\zeta = 5\ 10^{-17}$ s^{-1}

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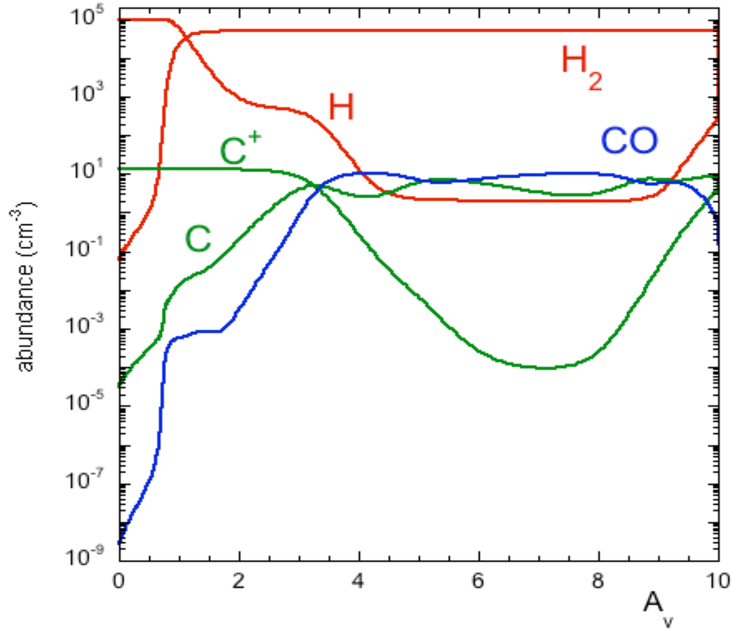

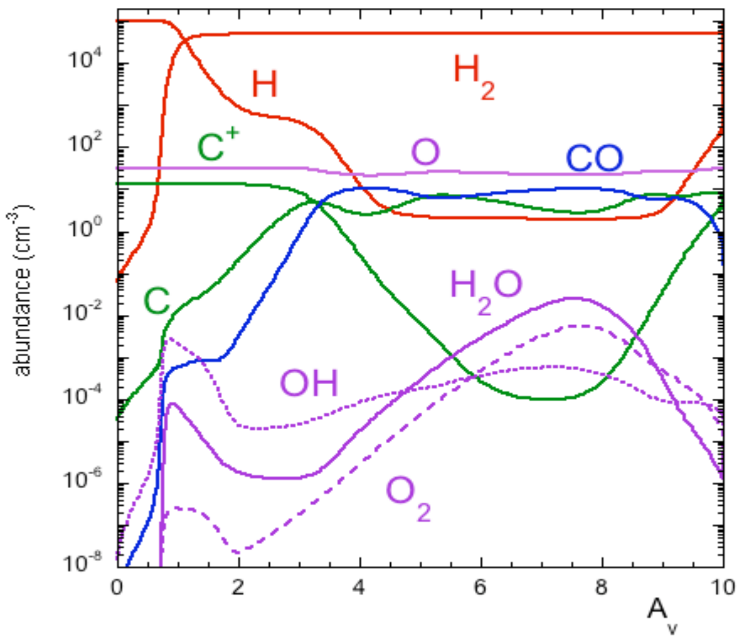

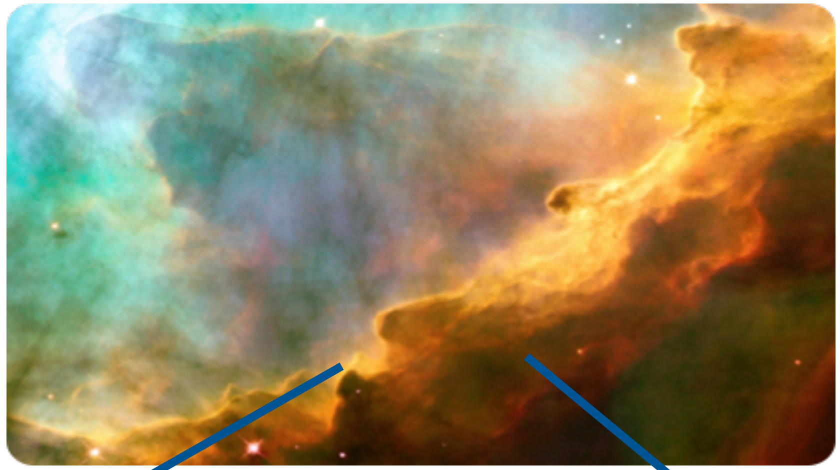

$n_H = 10^5$ cm^{-3}
$Av_{tot} = 10 \approx d = 0.061$ pc
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Carbon and oxygen chemistry

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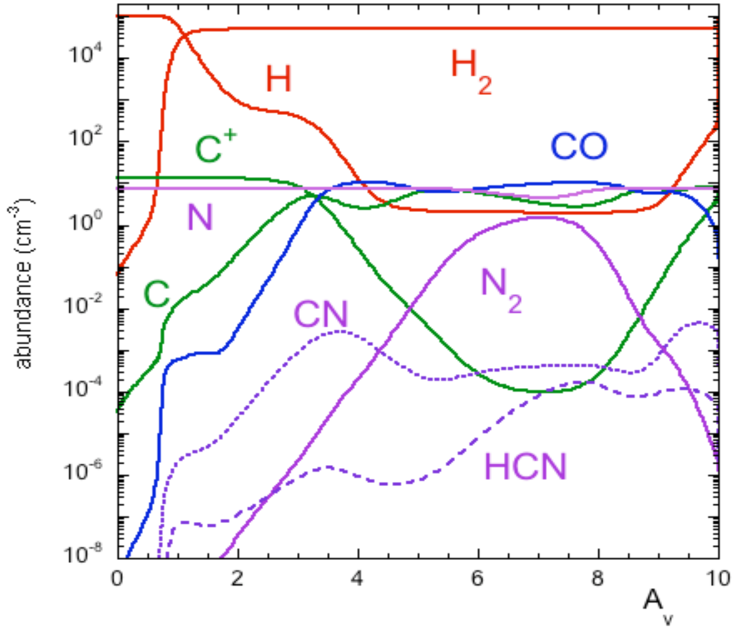
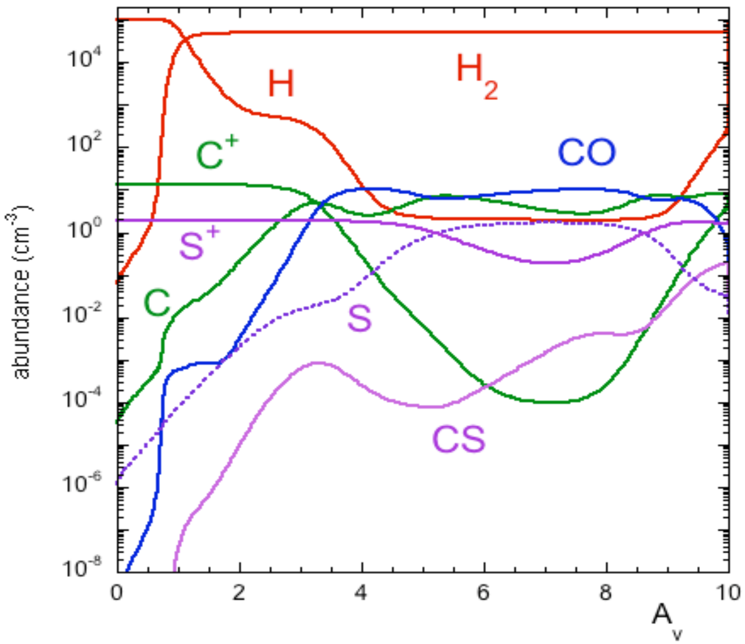
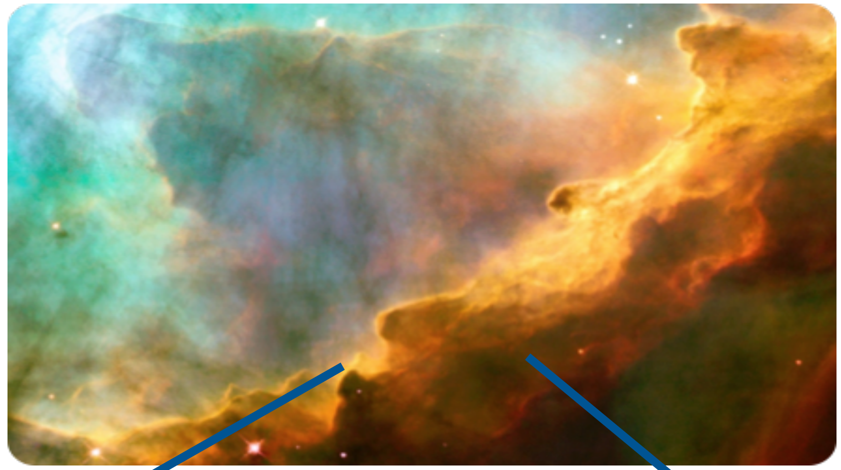






$n_H = 10^5\ cm^{-3}$

$Av_{tot} = 10 \approx d = 0.061$ pc

$\chi_{left} = 10^5$

$\chi_{right} = 1$

$\zeta = 5\ 10^{-17}\ s^{-1}$

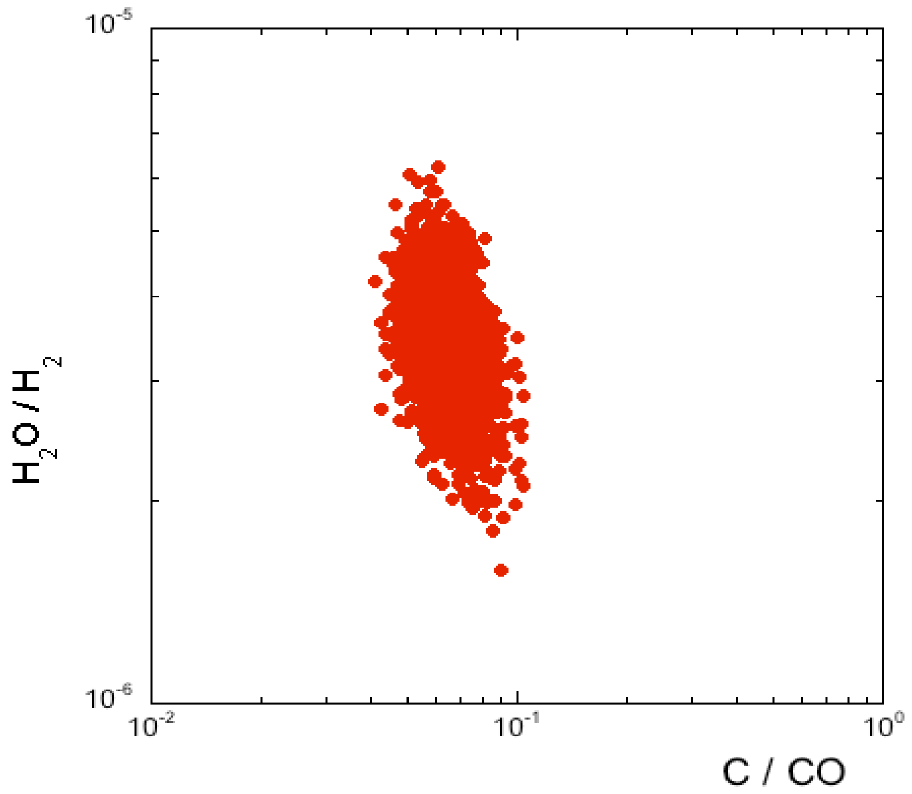
Nitrogen and sulfur chemistry

Chemical uncertainties

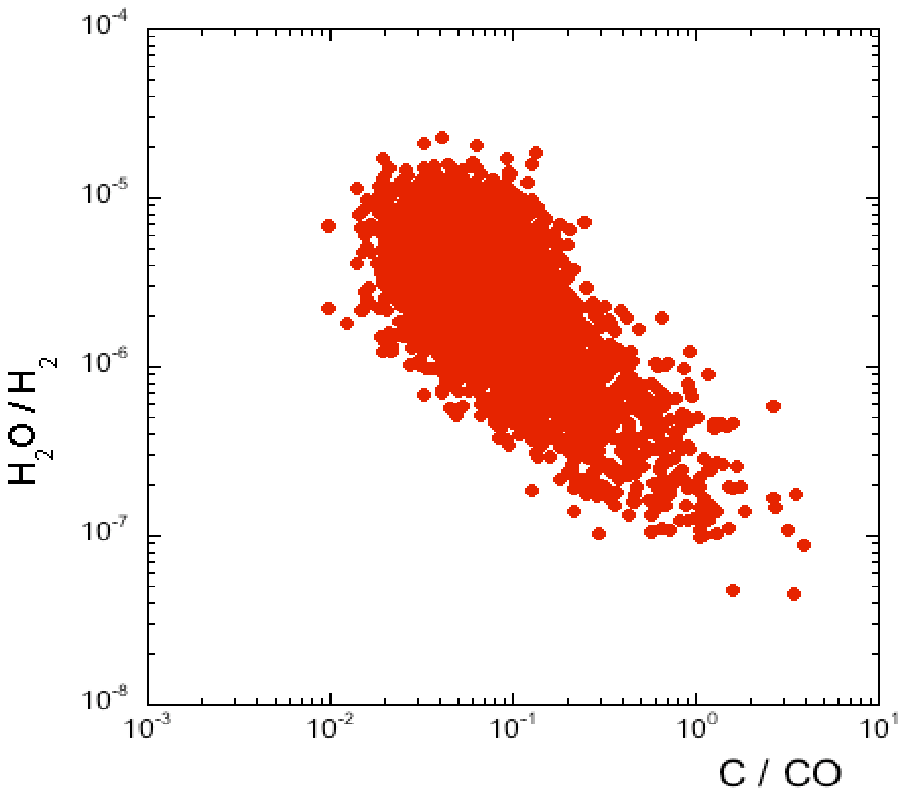
Basic question for models of any region

- Example : $n_H = 2\ 10^3\ cm^{-3}$, $T = 10\ K$ et $\zeta = 5 \times 10^{-17}\ s^{-1}$
- chemical network : 200 species - ≈ 2000 reactions

Random variation of reaction rate coefficients by a factor of 2



Random variation of reaction rate coefficients by a factor of 10

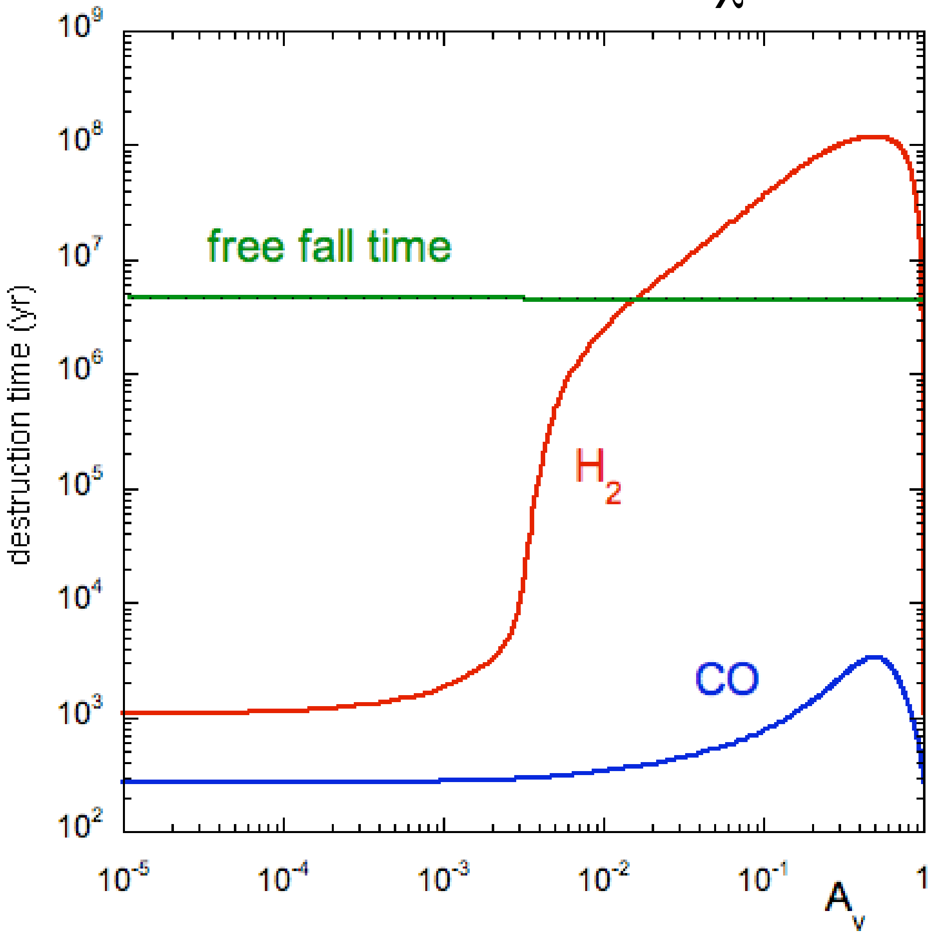


PDR models

Stationarity & time dependence

$$t_{dest}(X) = \frac{n(X)}{\text{destruction rate in cm}^{-3}\ \text{s}^{-1}}$$

$n_H = 100$ cm^{-3}, $\zeta = 5\ 10^{-17}$ s^{-1},
2 side illumination : $\chi = 1$



Compare chemical times to dynamical times

$$t_{\text{free fall}} = \sqrt{\frac{3\pi}{32G\rho(0)}} = \frac{4.3 \times 10^7}{\sqrt{n_H(0)}}\ \text{yrs}$$

- at the edge, destruction by photons
- At higher Av, destruction by chemical processes, cosmic rays

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H_2 Formation

"Observational" determination of H_2 formation rate in diffuse clouds

- Jura (1975) Copernicus $R = 3\times10^{-17}$ cm^3 s^{-1}
- Gry et al. (2002) FUSE $R = 3.1 - 4.5 \times 10^{-17}$ cm^3 s^{-1}

H_2 formation rate in the Meudon PDR code

- fixed formation rate
- calculated from grain properties
- calculated from rate equations, moment equations (in progress)

Grain size distribution : $dn(a) \propto a^{\alpha} da$ with α = -3.5 Mathis et al. (1983)

$$\frac{dn(H_2)}{dt} = \frac{1}{2} s\, v_H\, n(H) \left\langle \sigma_g \cdot n_g \right\rangle$$

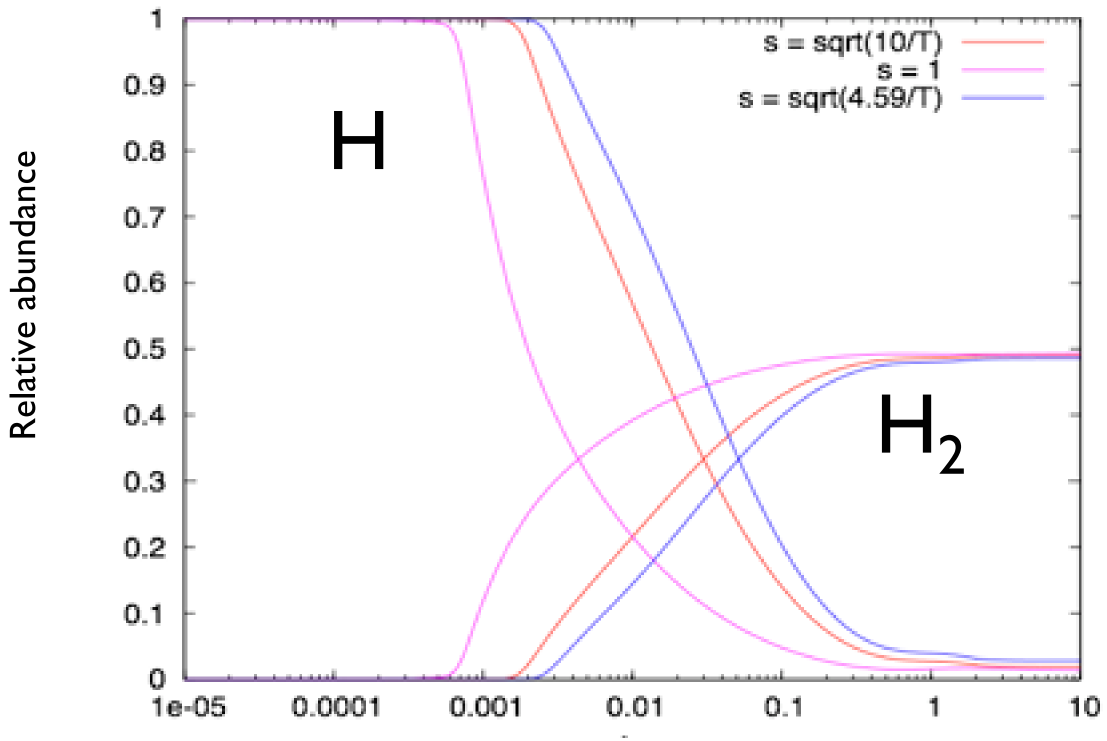
$$< \sigma_g \cdot n_g >= \frac{3}{4} \frac{1.4\, m_H\, G}{\rho_g} \frac{1}{\sqrt{a_{min} \cdot a_{max}}} n_H$$

$$\left.\frac{dn(H_2)}{dt}\right|_{form.gr.} = s \cdot 1.4 \times 10^{-17} \sqrt{T_K}\, n_H\, n(H)$$

H_2 Formation

Different choices for s :

- s = √(10/T)   : R independent de T
- s = 1
- s = √(4.59/T) gives R = 3×10^{-17} cm^3 s^{-1}
- ...



H_2 Formation

case of small grains
I the mean number of H atoms is about 1, the rate equations formalism does not apply anymore.

Master equation approach: Biham et al. 2001, ApJ 553, 595

$$\frac{dP_H(N_H)}{dt} = F_H\left[P_H(N_H-1) - P_H(N_H)\right]$$
$$+W_H\left[(N_H+1)P_H(N_H+1) - N_H P_H(N_H)\right]$$
$$+A_H\left[(N_H+2)(N_H+1)P_H(N_H+2) - N_H(N_H-1)P_H(N_H)\right]$$

with :
F_H : flux of H atoms impinging on the surface
W_H : desorption rate of H atoms : $W_H = \nu \exp(-E_1/kT_g)$
A_H : scanning of the surface by H atoms: $A_H = a/S$, where S is the number of adsorption sites on the grain ($S=4\pi r^2 s$) and $a = \nu \exp(-E_0/kT_g)$

$\nu(s^{-1})$	10^{12}
s (cm^{-2})	5 10^{13}
E_0 (K)	510.6
E_1 (K)	658

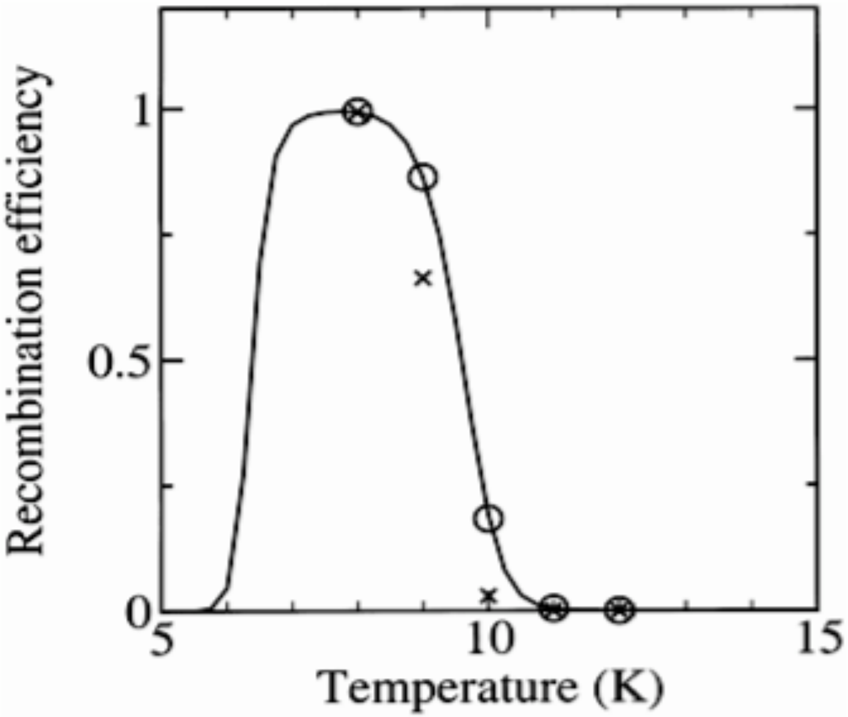
Katz et al. 1999, ApJ 522, 305

H_2 formation rate:

$$R_{H_2}^{grain} = A_H\left(\langle N_H^2\rangle - \langle N_H\rangle\right)$$

H_2 Formation

Biham et al. 2001



× master equation, d = 0.01 μm

○ master equation, d = 0.1 μm

- rate equation

H_2 formation efficient only in a narrow window of grain temperatures

$T_0 < T_g < T_1$

$$T_0 = \frac{E_0}{k_B \; ln(\nu S/F)}$$

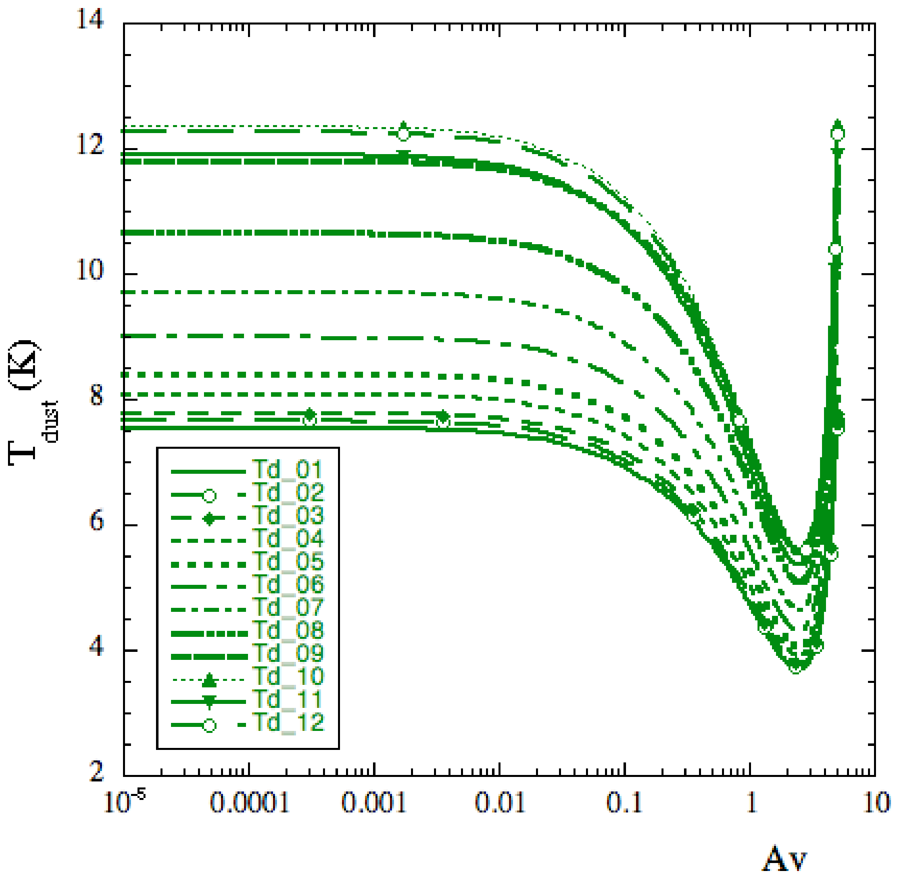
$$T_1 = \frac{2E_1 - E_0}{k_B \; ln(\nu S/F)}$$

Determination of Tg essential

Determination of grain temperatures

- Observational information ?
- Thermal balance : approximate formula of Tielens & Hollenbach with simple assumptions on the grain absorption and emission coefficients (used in the Meudon PDR code)
- detailed calculations (cf Cuppen, Herbst, …)

$n_H = 100\ cm^{-3}$, $\xi = 1$, $A_v^{tot} = 5$, $\zeta = 5\ 10^{-17}\ s^{-1}$



Case of the MRN size distribution

$dn_g \approx a^{-3.5}$

$a_{min} = 3\ 10^{-7}$ cm

$a_{max} = 3\ 10^{-5}$ cm

The temperatures at the edge have the right order of magnitude for H_2 formation.

Meudon PDR code

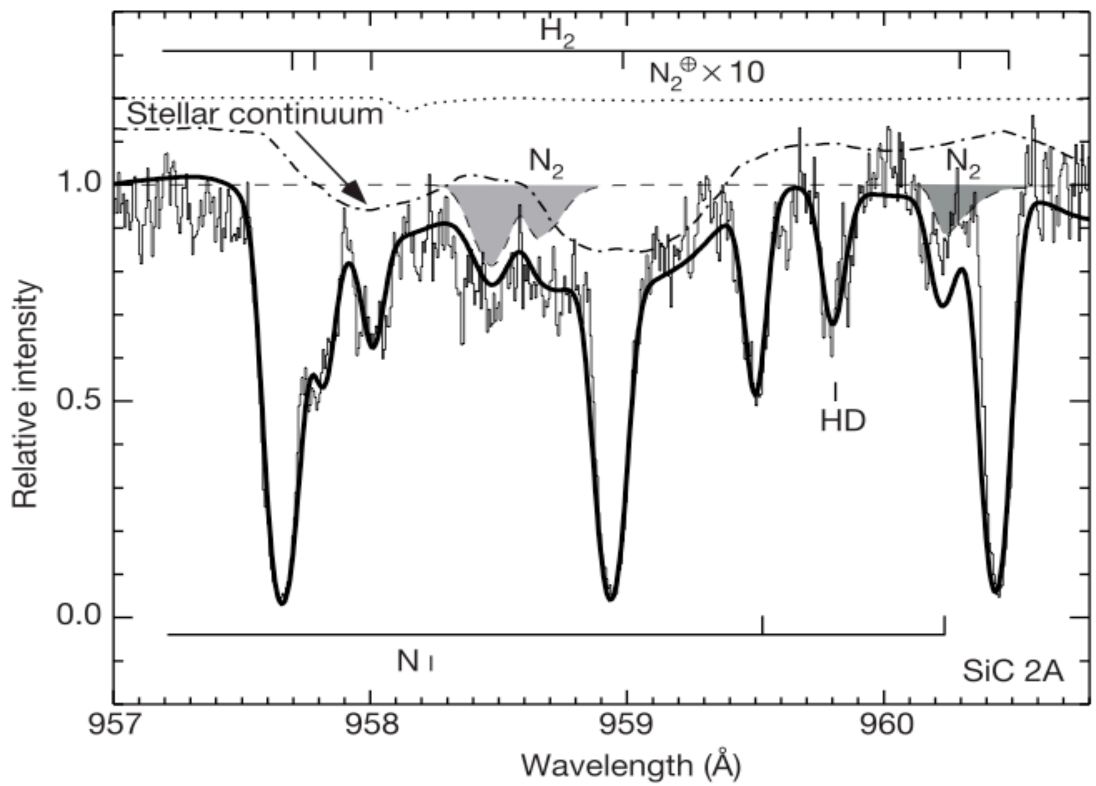
Conclusions

Detailed UV radiative transfer
Introduction of the impinging radiation field (from 912 Å to IR)
Detailed microscopic physics
Versatile chemistry; possibility of state to state chemistry
Source and input data downloadable from http://aristote.obspm.fr/MIS
Inclusion in the Virtual Observatory

Plane parallel geometry
Steady state
Extension to X radiation
Grain physics and chemistry should be improved (in particular H_2 formation)
Computing time becomes excessive when "exact" transfer is performed (but essentially needed for diffuse environments)

Meudon PDR code

Knauth et al., Nature, 429, 2004



Exemple : Detection of N_2

- HD 124314 (Knauth et al. 2004)
- 20 Aquilae (Knauth et al.)