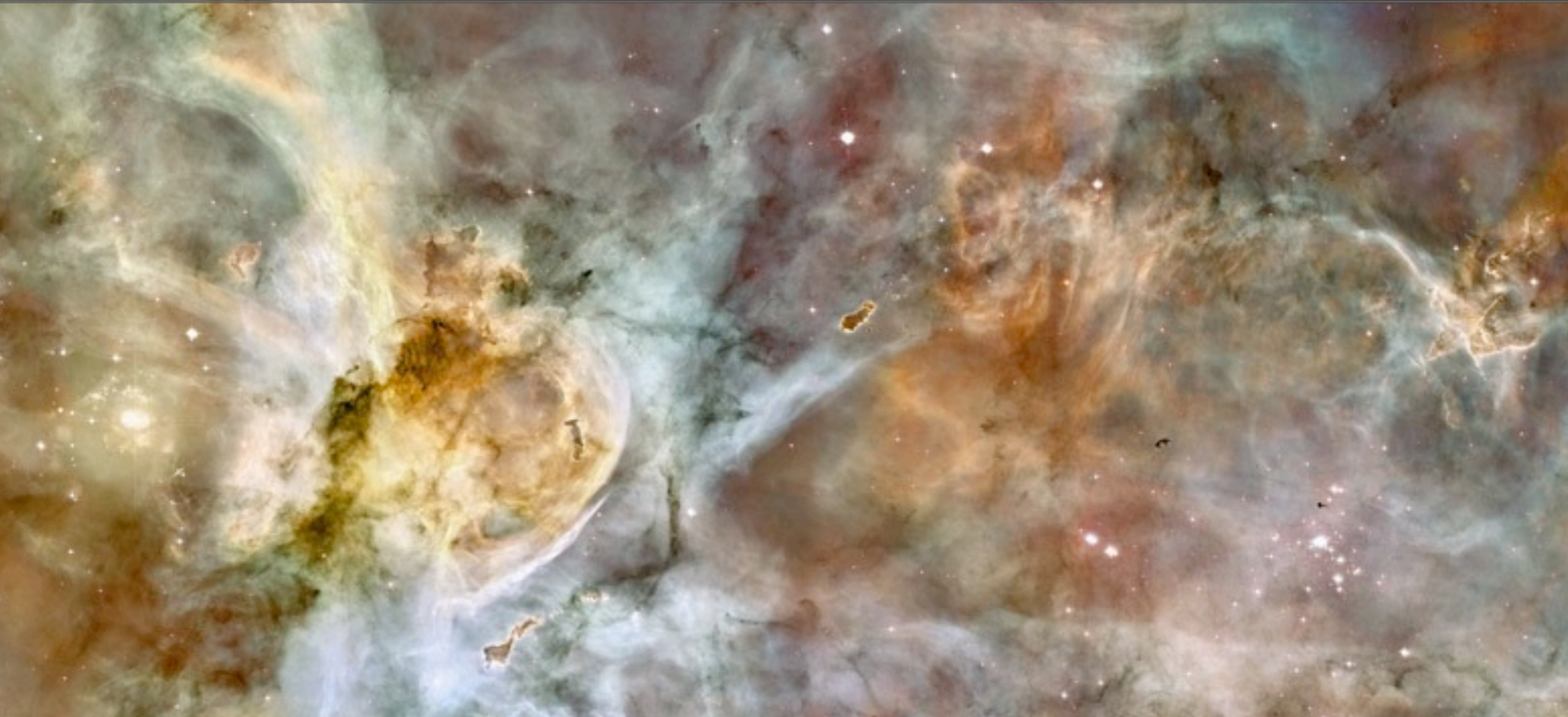
**Colloque PCMI**
Paris - 19-21 novembre 2012



# New processes in the PDR code

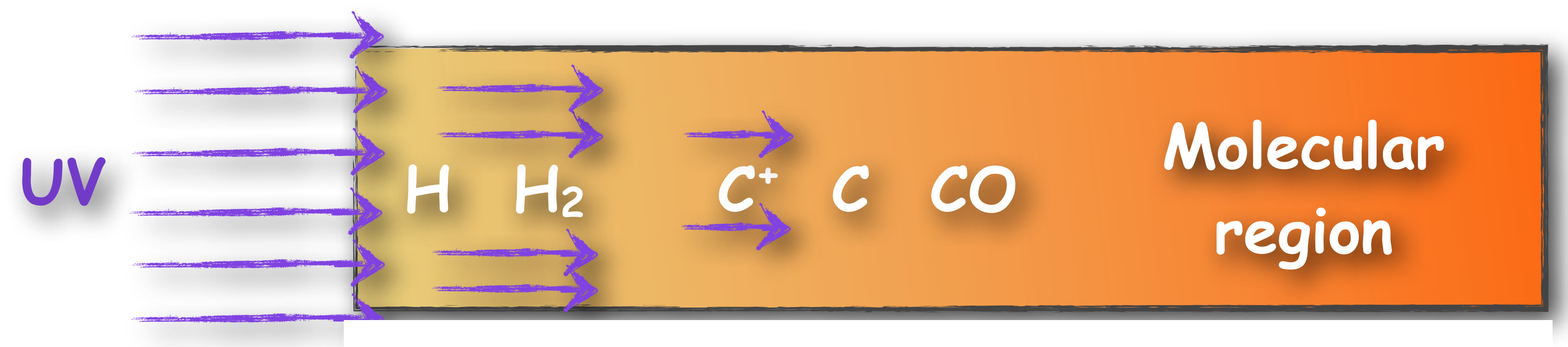
**Franck Le Petit, E. Roueff, J. Le Bourlot, C. Pinto, E. Bron**
LUTH - Observatoire de Paris, CNRS, Université Paris Diderot

# The Meudon PDR code

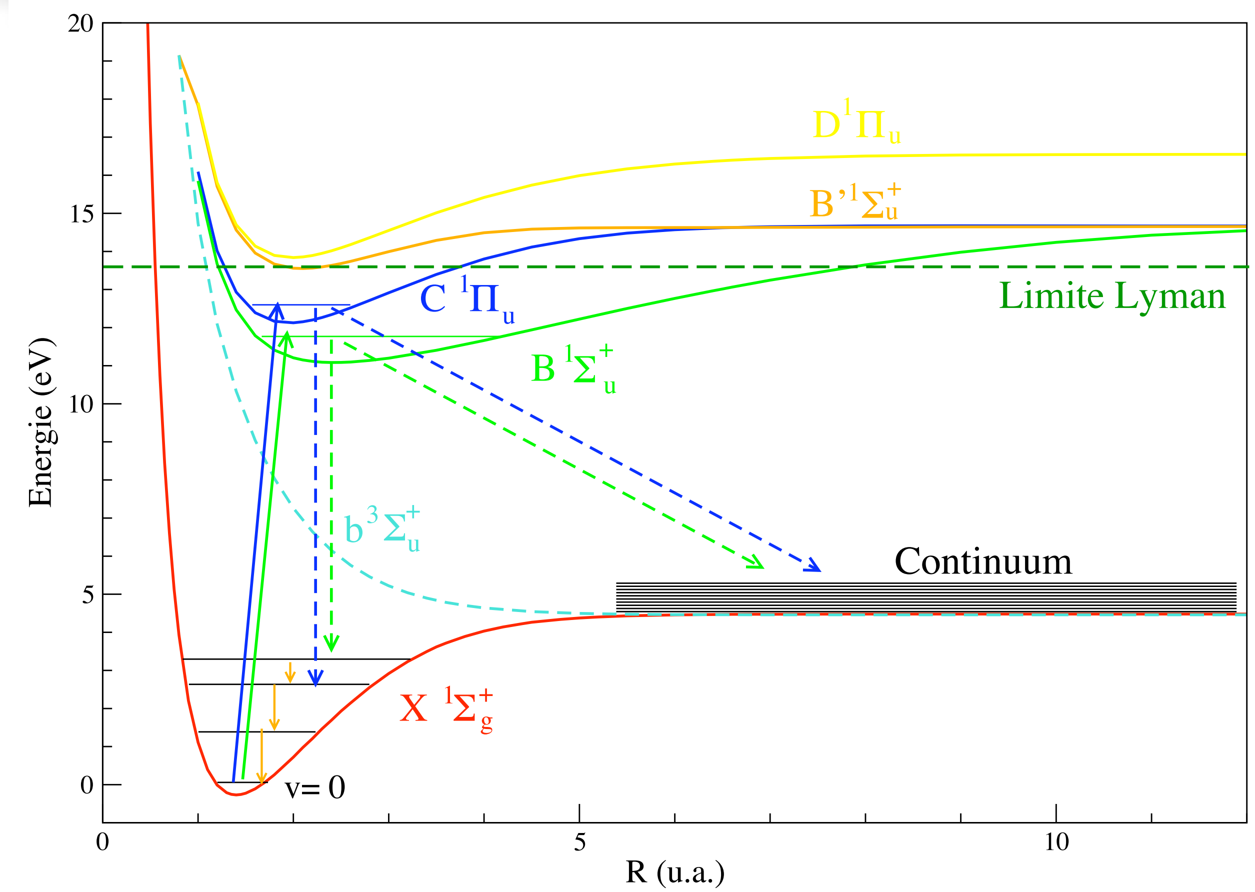
**PDR code :**

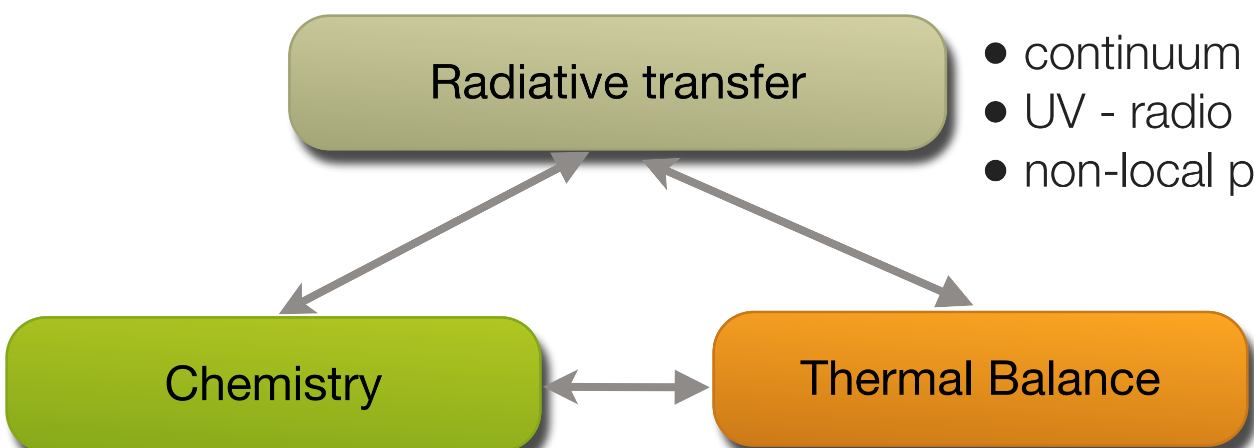
- computes atomic and molecular structure of interstellar clouds
- interpret observations & understand physical and chemical processes
- 1D & stationnary

- densities of chemical species
- level excitations
- gas and grains temperature
- ...




- line intensities ($H_2$, CO, $H_2O$, ...)
- column densities
- spectra




- continuum & lines
- UV - radio
- non-local pumping

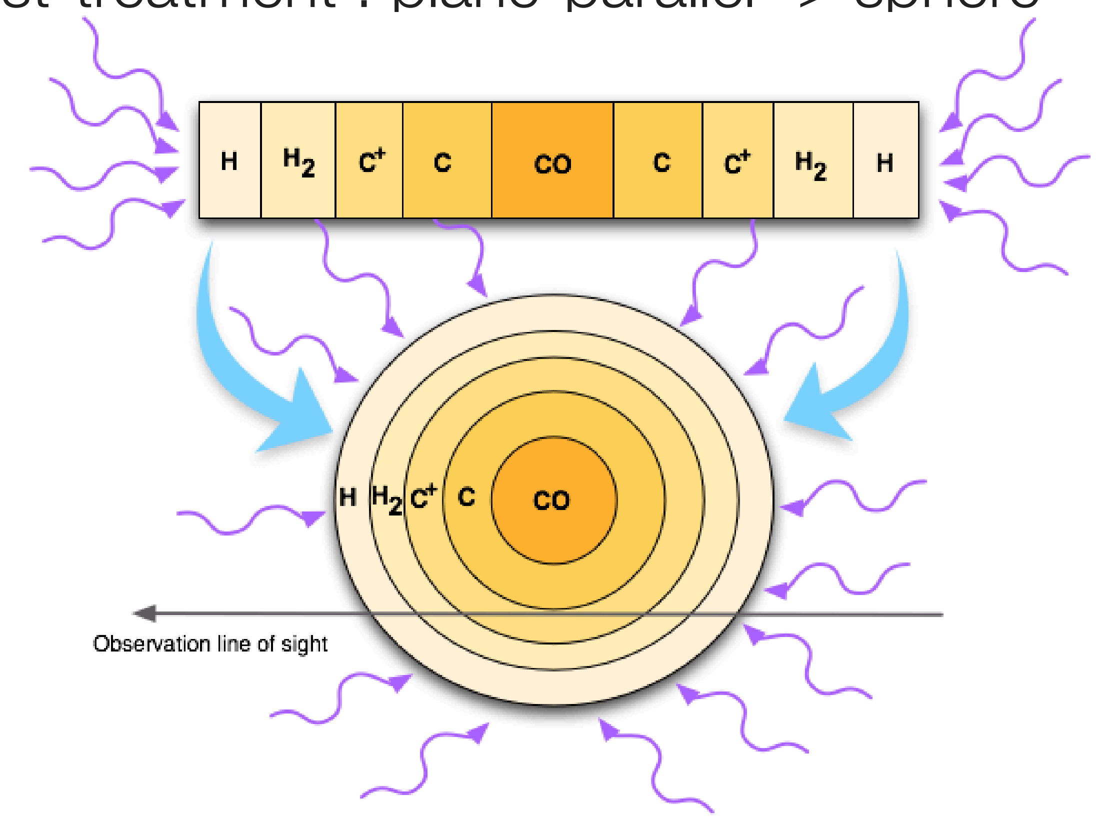
- hundreds species
- thousands reactions

- non LTE
- Statistical equilibrium in levels populations
- Detailed heating mechanisms
- Cooling - non local radiative transfer

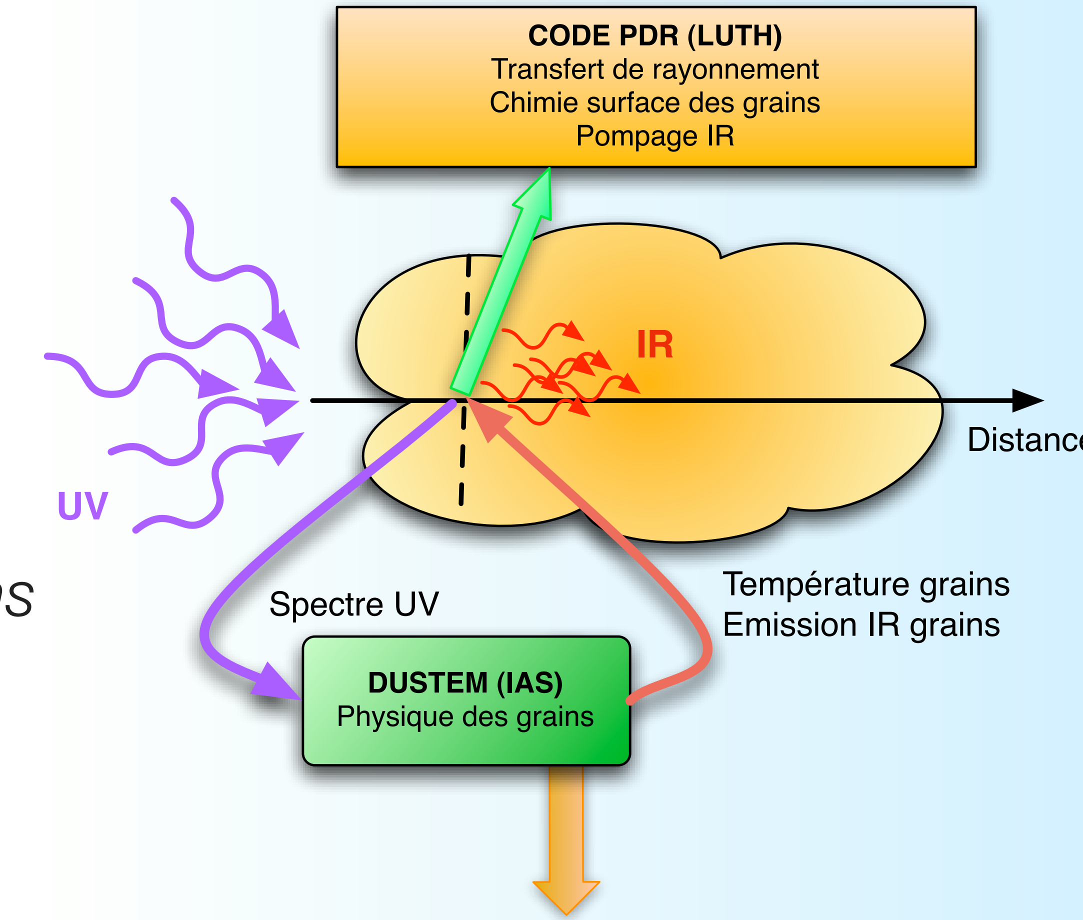
# The Meudon PDR code

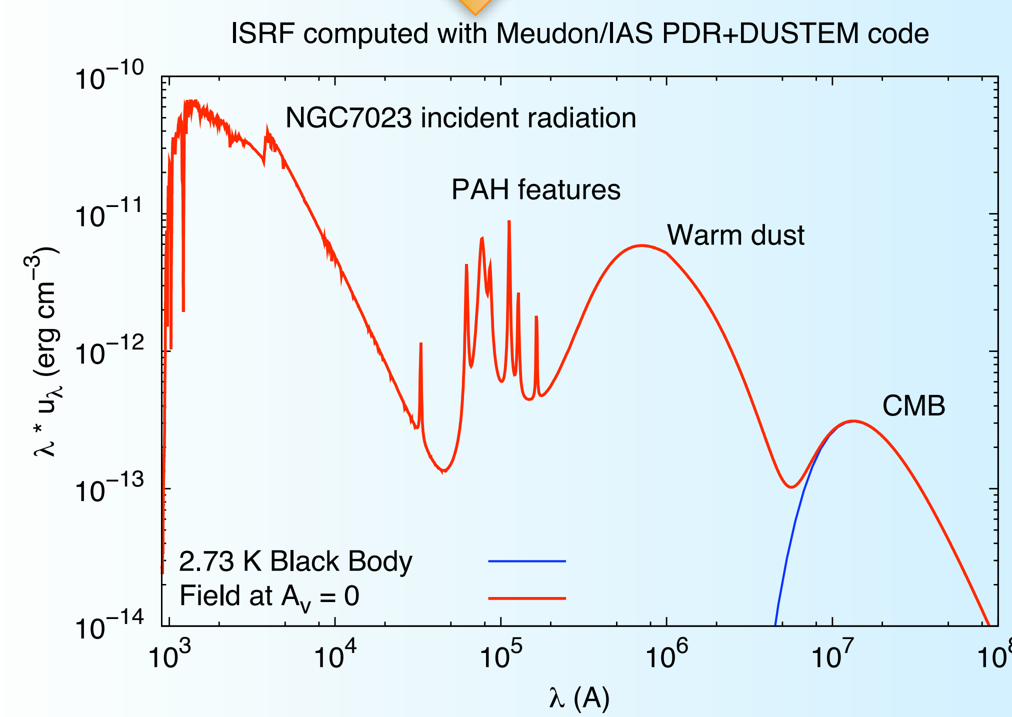
New developments :

- **Grains**
  - modified Hollenbach et al. prescription
    - MRN grains size distribution
    - Simple prescriptions for $T_{gr}(r,A_V)$
  - PDR + DustEM
    - computes I.R. emission by dust
    - *Ex : non-local pumping of $H_2O$ by warm grains*
- **Spherical geometry**
  - Post-treatment : plane-parallel -> sphere




**PDR (LUTH) + DUSTEM (IAS)**



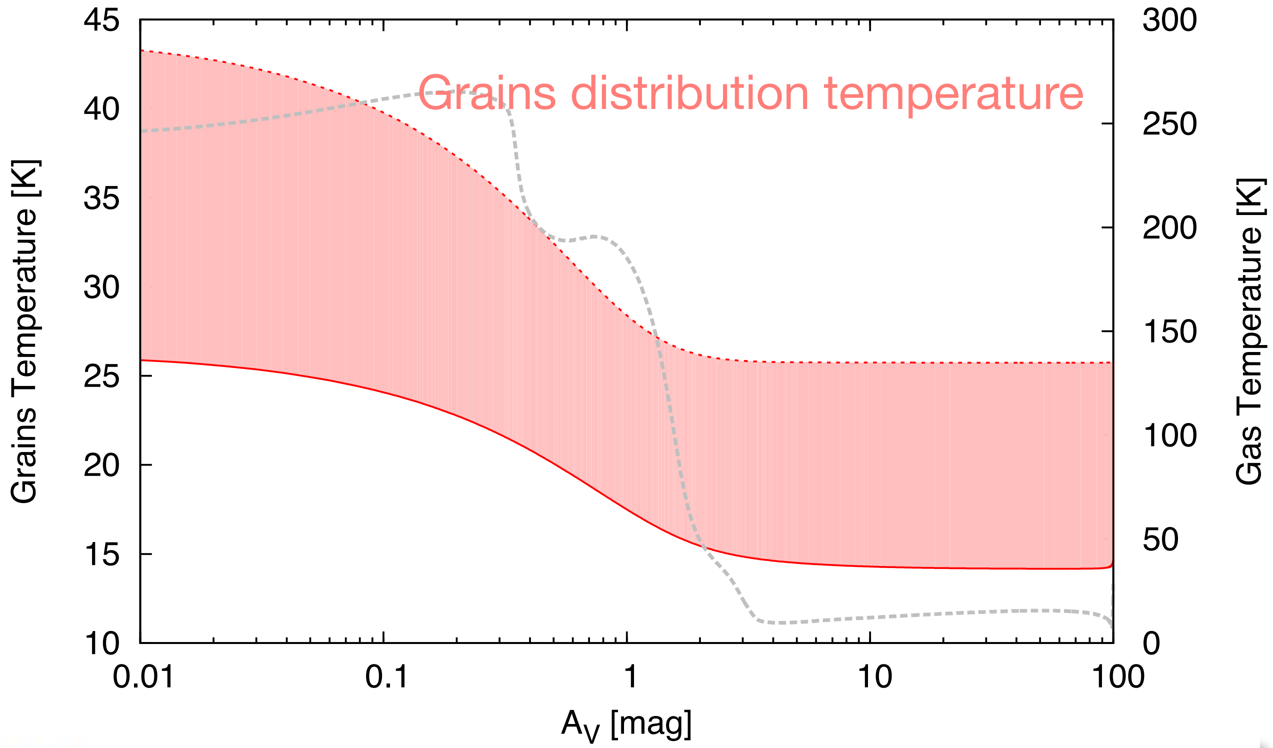



# Surface chemistry : $H_2$ formation

**Observations :**

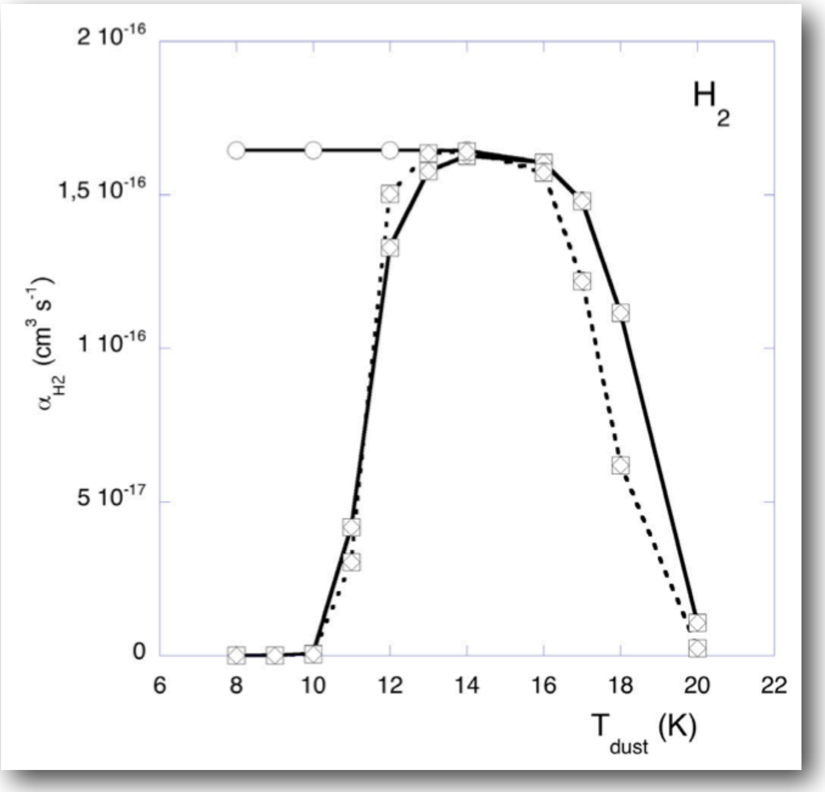
ISO - Spitzer : **Models underestimate $H_2$ line intensities in PDRs** (Habart et al.)

- $H_2$ formation rate on grains in models is too low
- Impacts the transition atoms / molecules
- Impacts interpretations of all species




**Laboratory experiments :**

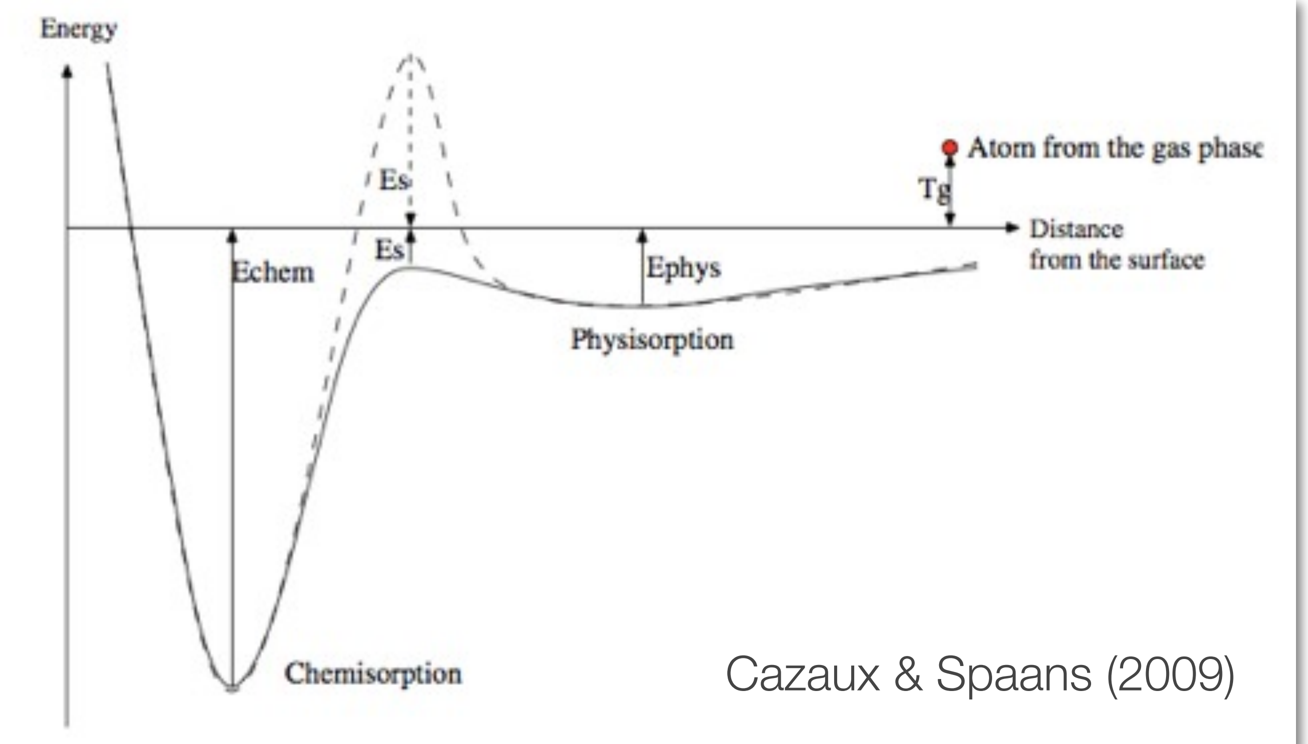
- $H_2$ forms in a narrow window of $T_{dust}$
- ~ 11 - 20 K




Edge of clouds :

Physisorption :

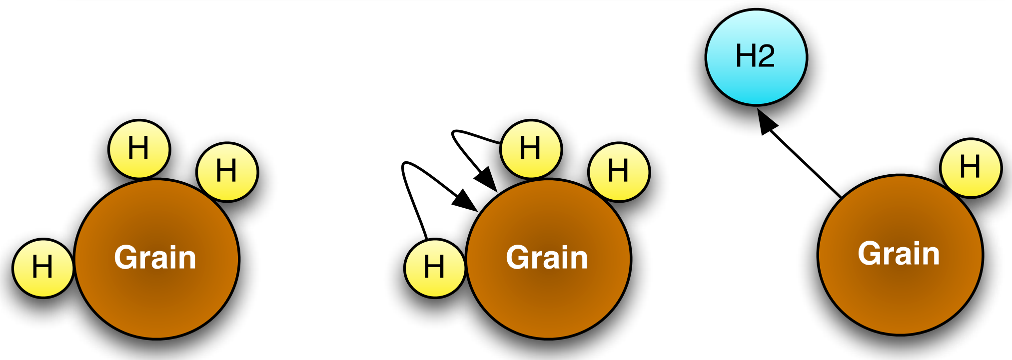
- $T_{dust}$ > 20 K => Thermal desorption
- not in agreement with observations



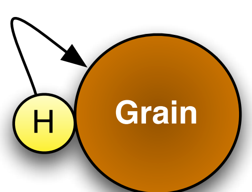

Cazaux & Spaans (2009)

# Surface chemistry : $H_2$ formation (Le Bourlot et al. 2012)

## Langmuir-Hinshelwood (LH)

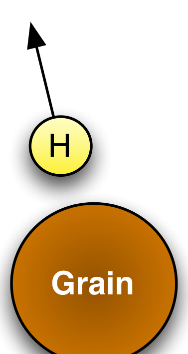



- **Diffusion**




$$A = \frac{\nu}{S} \cdot exp\left(\frac{-E_0}{kT_d}\right)$$

- **Desorption**

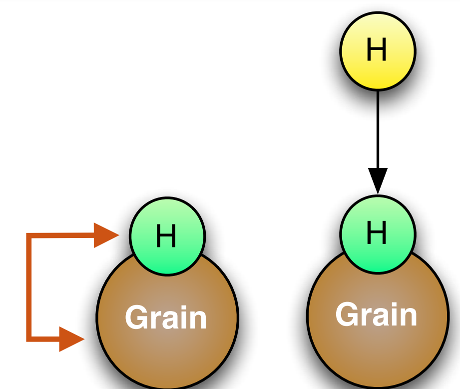



$$W = \nu \cdot exp\left(\frac{-E_1}{kT_d}\right)$$

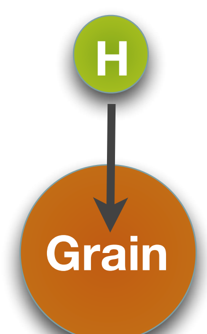
The formation rate by LH mechanism depends on **grains temperature**

## Eley-Rideal (ER) on chemisorption sites

Binding energy ~ 5000 K

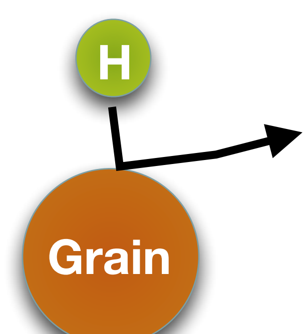



- **Chemisorption efficiency**




T1 : chemisorption barrier
~ [100 - 1000]
our choice : 300 K

- **Reaction efficiency**



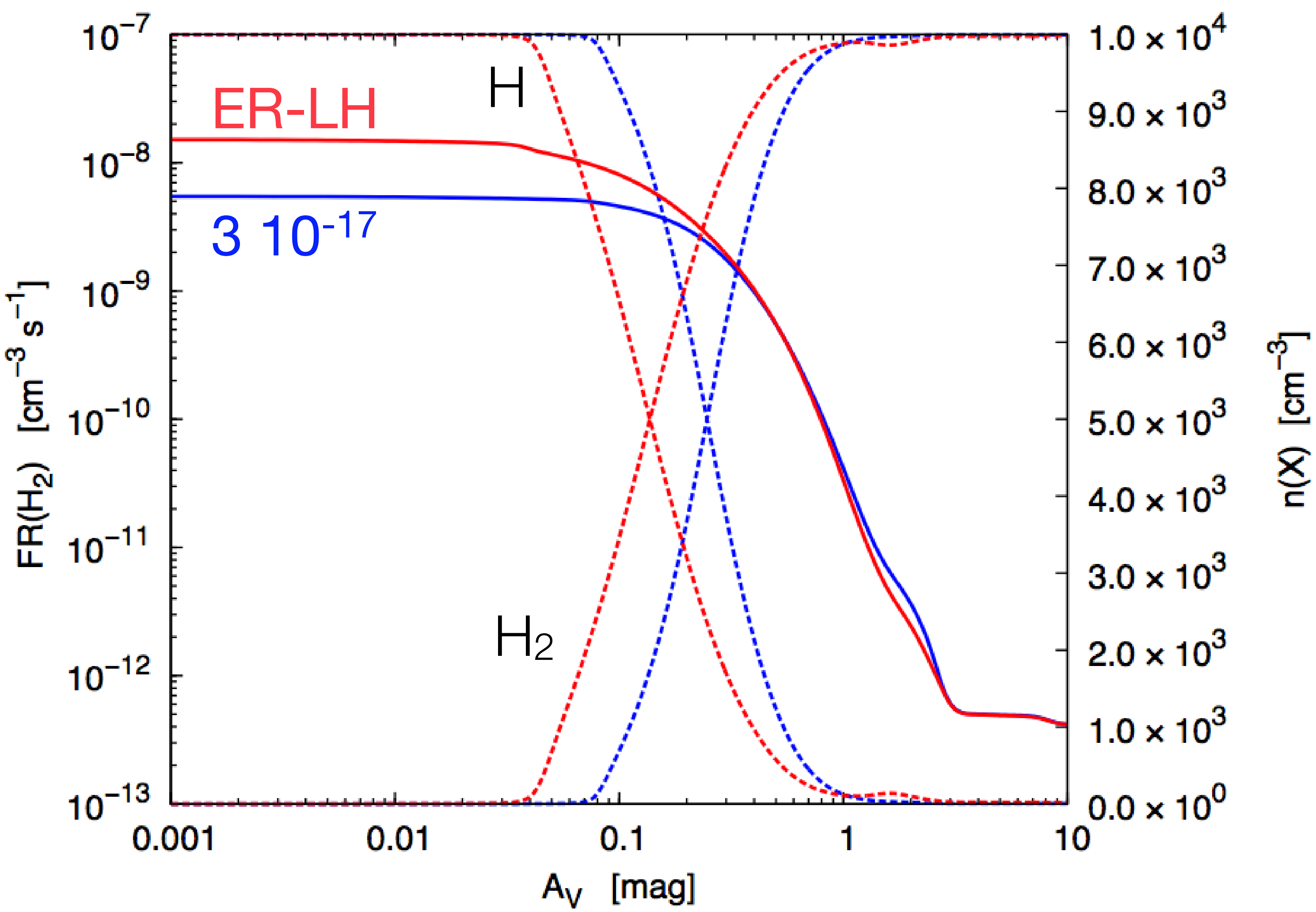

T2 : bounce back efficiency
T2 ~ 400 K

The formation rate by ER mechanism depends on **gas temperature**

# Surface chemistry : $H_2$ formation

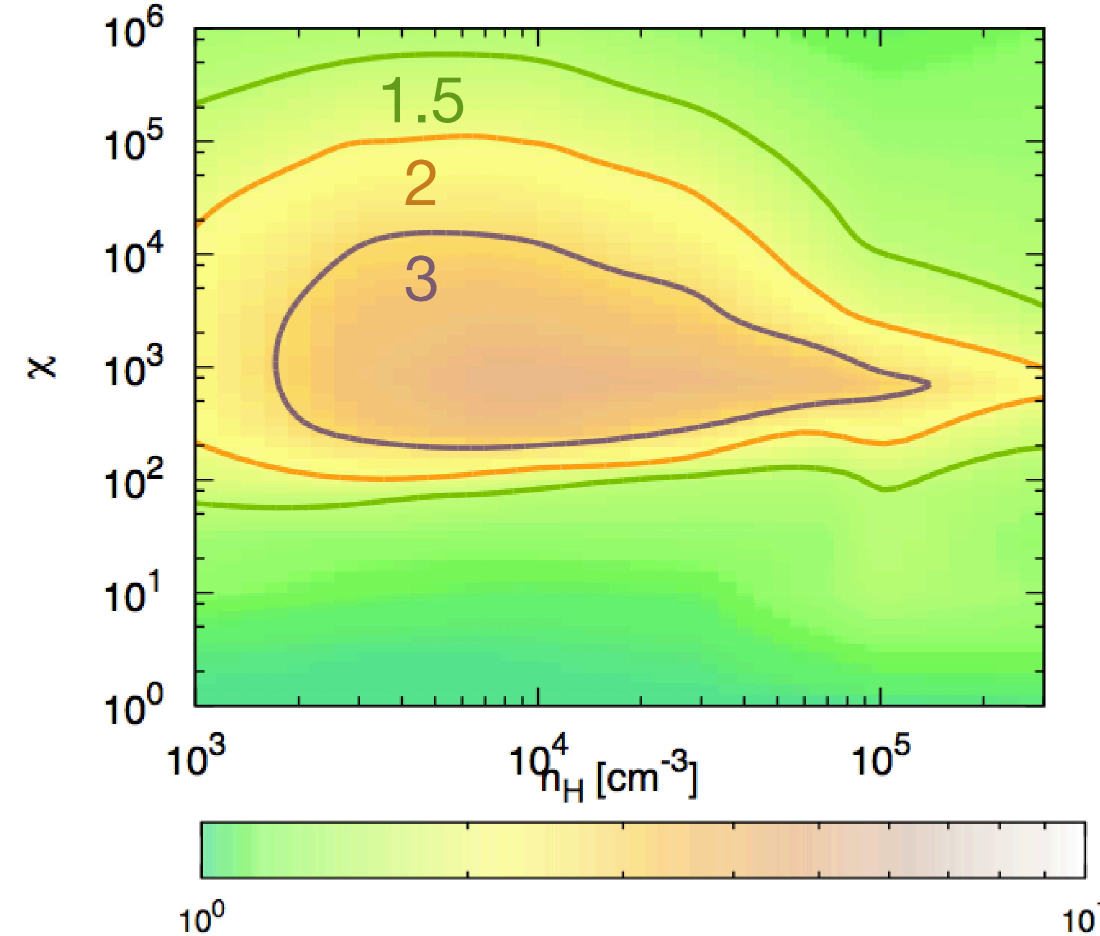
## Impact on $H_2$ line intensities

PDR : $n_H = 10^4$ cm$^{-3}$, G = $10^3$ ISRF




H$_2$, 0-0 S(2)

I(ER-LH) / I(R = 3x10$^{-17}$)




Eley-Rideal mechanism :

- shifts $H_2$ formation towards the edge of PDRs
  Efficient formation on warm grains
- $H_2$ line intensities can be increased up to a factor 3

# $H_2$ formation by Eley-Rideal : Heating mechanism

Theoretical results of Eley-Rideal (Sizun et al. 2010)

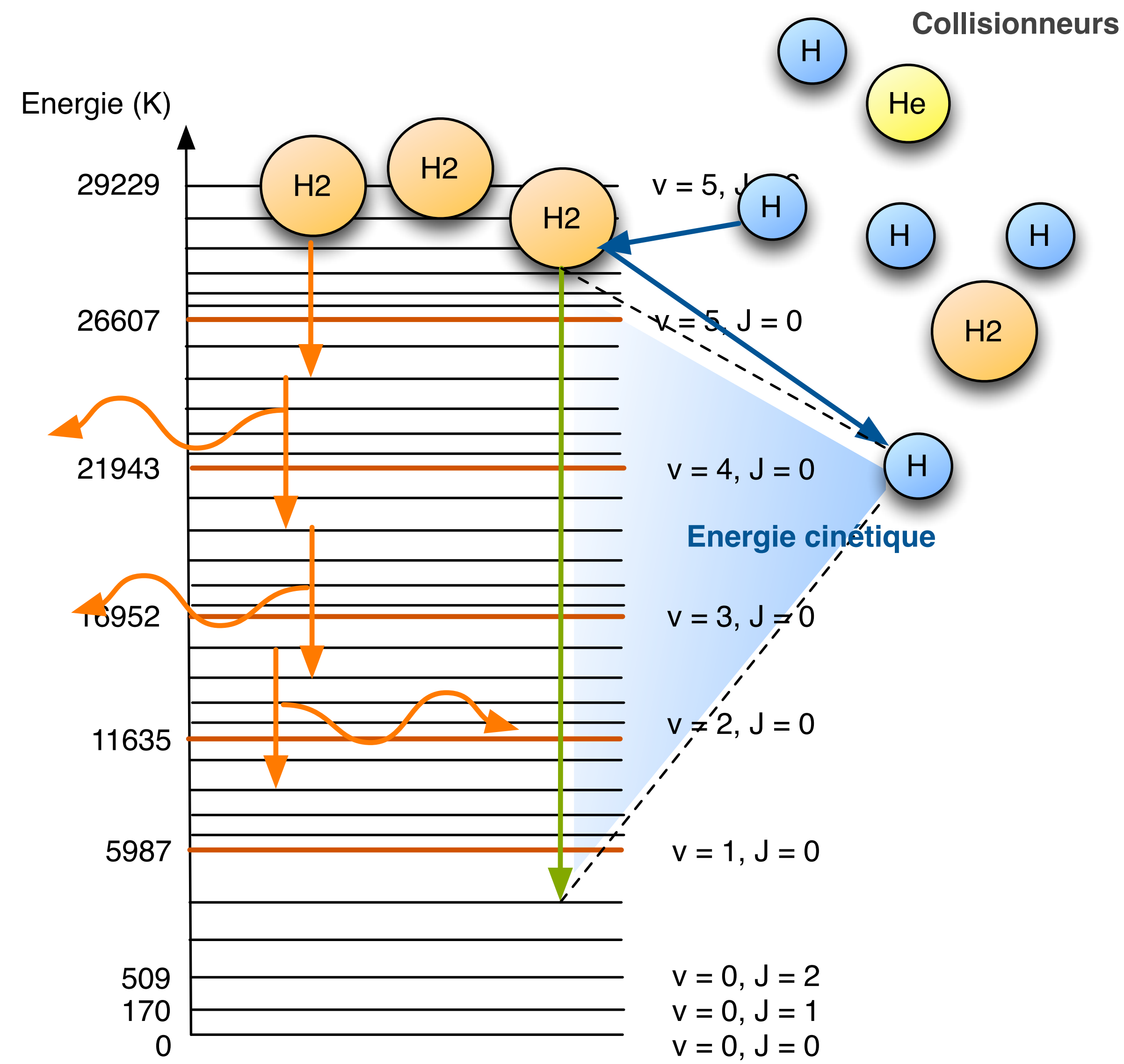
$H_2$ formation produces 4.5 eV

7 % Extraction

**60 % $H_2$ intenal energy**

13 % $H_2$ kinetic energy

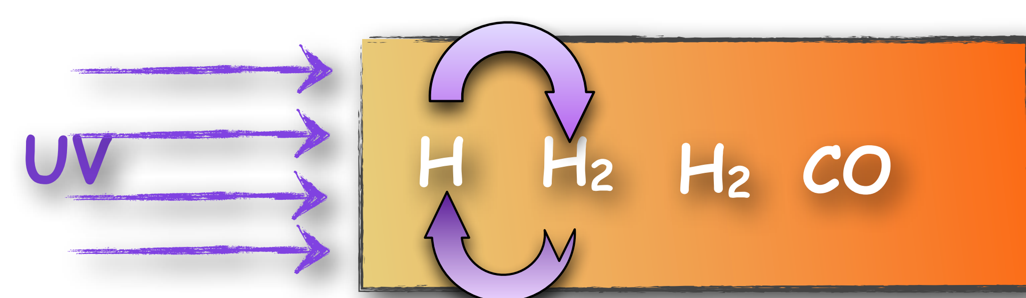
20 % Grain internal energy




In star forming regions (Ex : Orion)

- High density
  - collisinal de-excitations are efficient
  - $E_{internal}$ -> $E_{kinétic}$ (gaz)

- High UV radiation field
  - Fast cycle : formation - destruction
  - Fast conversion of the UV energy in kinetic energy of the gas



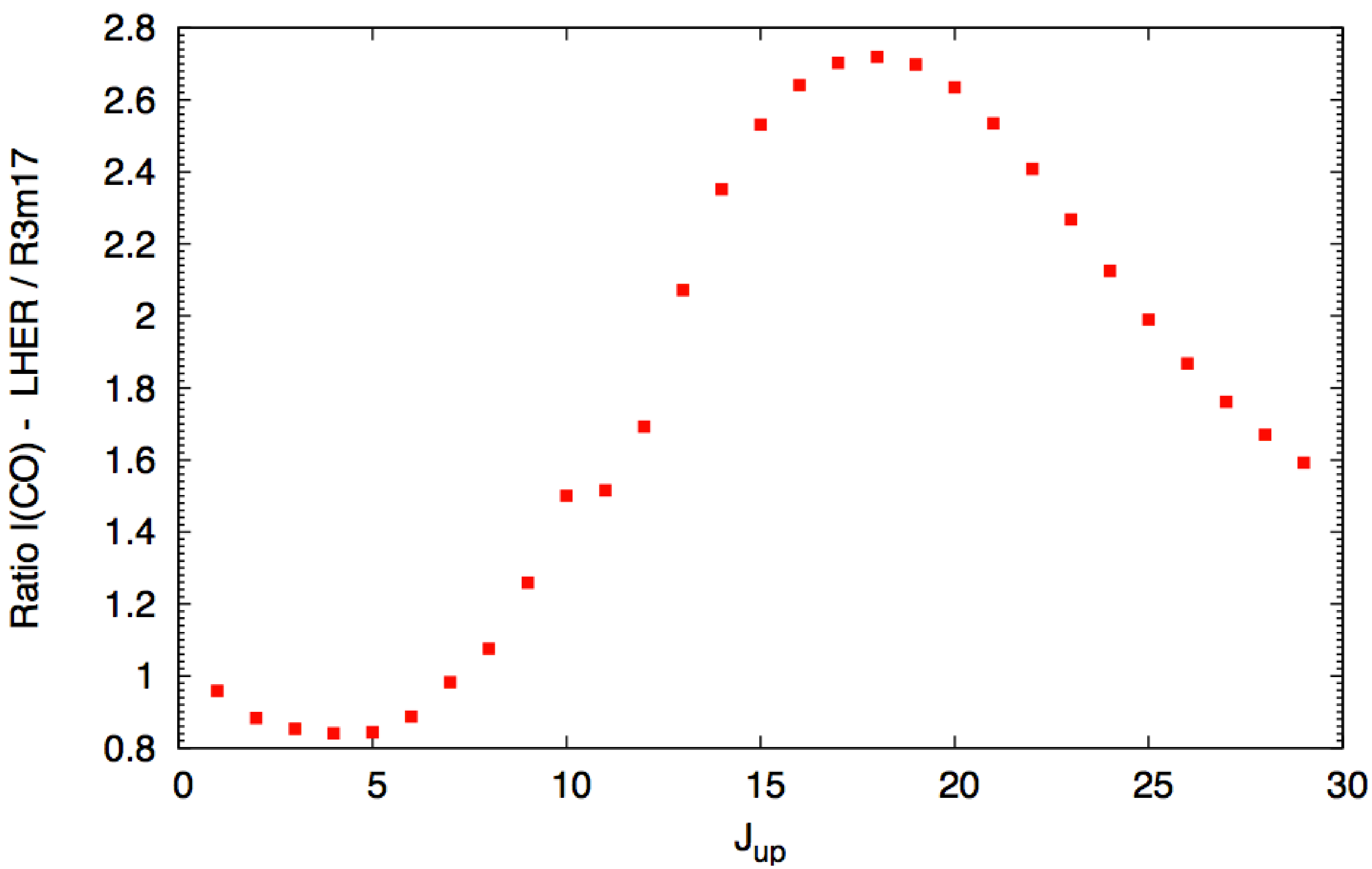

Eley-Rideal mechanism can be **an efficient heating process** in dense and strongly illuminated regions

# **Surface chemistry** : $H_2$ formation

PDR code : everything is coupled !

=> Impact of $H_2$ formation by E.R. on CO excitation

- Comparison of CO line intensities between models with ER and R = 3 $10^{-17}$




Parameters

- $n_H = 10^5$ $cm^{-3}$
- rad = $10^4$ ISRF

**Some CO lines intensities can be increased up to a factor ~ 3**

(dependent on gas density and intensity of radiation field)

# **Surface chemistry** : $H_2$ formation

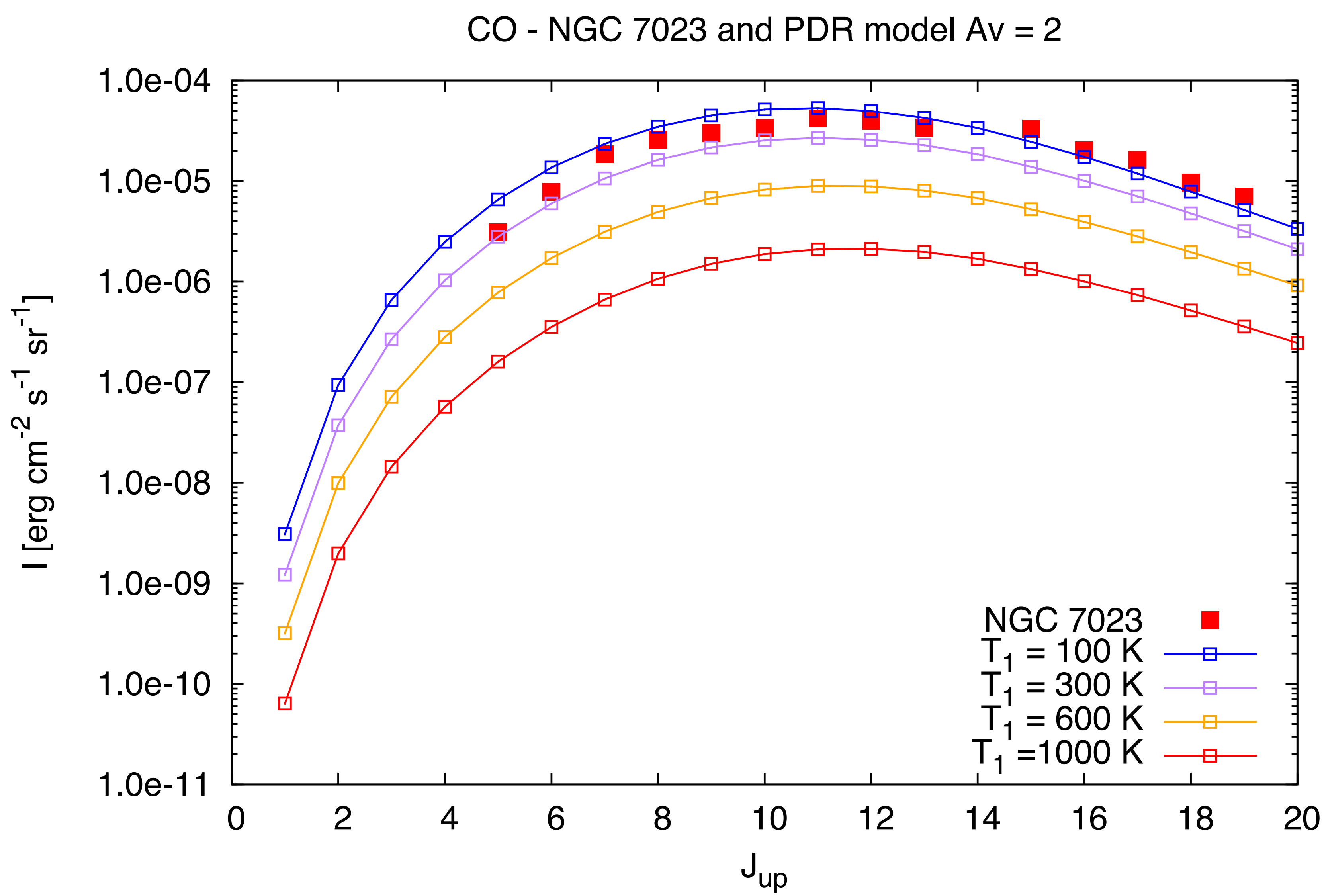
## Application to NGC 7023 & Orion Bar

- Herchel observations of CO up to J ~ 19

(Joblin et al. in prep)

**Model parameters :**

- Specific radiation field
- isobaric model (P ~ $10^7$ $cm^{-3}$ K)




Limits to have better agreement :

- geometry
- grain size distribution / composition profile

- **Poster 32 :** Impact of PAH evolution on the energetic of photon-dominated regions (C. Joblin)

# Complex surface chemistry

**Implementation of surface chemistry in the PDR code**
Rate equation formalism

**Two kind of species**

- Mantle / Ice : $C$, $CH$, $CH_2$, $CH_3$, $CH_4$,
  $O$, $OH$, $H_2O$,
  $CO$, $HCO$, $H_2CO$, $H_3CO$, $O_2$, $CO_2$, $CH_3OH$
  F, HF, Cl, HCl...
- Surface species : H

**Reactions**

- Adsorption / Bouncing
- diffusion reactions
- Desorption due to :
  - UV photons (primary & secondary)
  - cosmic rays

**Important chemical parameters**

- adsorption efficiencies
- surface reaction rates
- photo & cosmic rays desorption rates

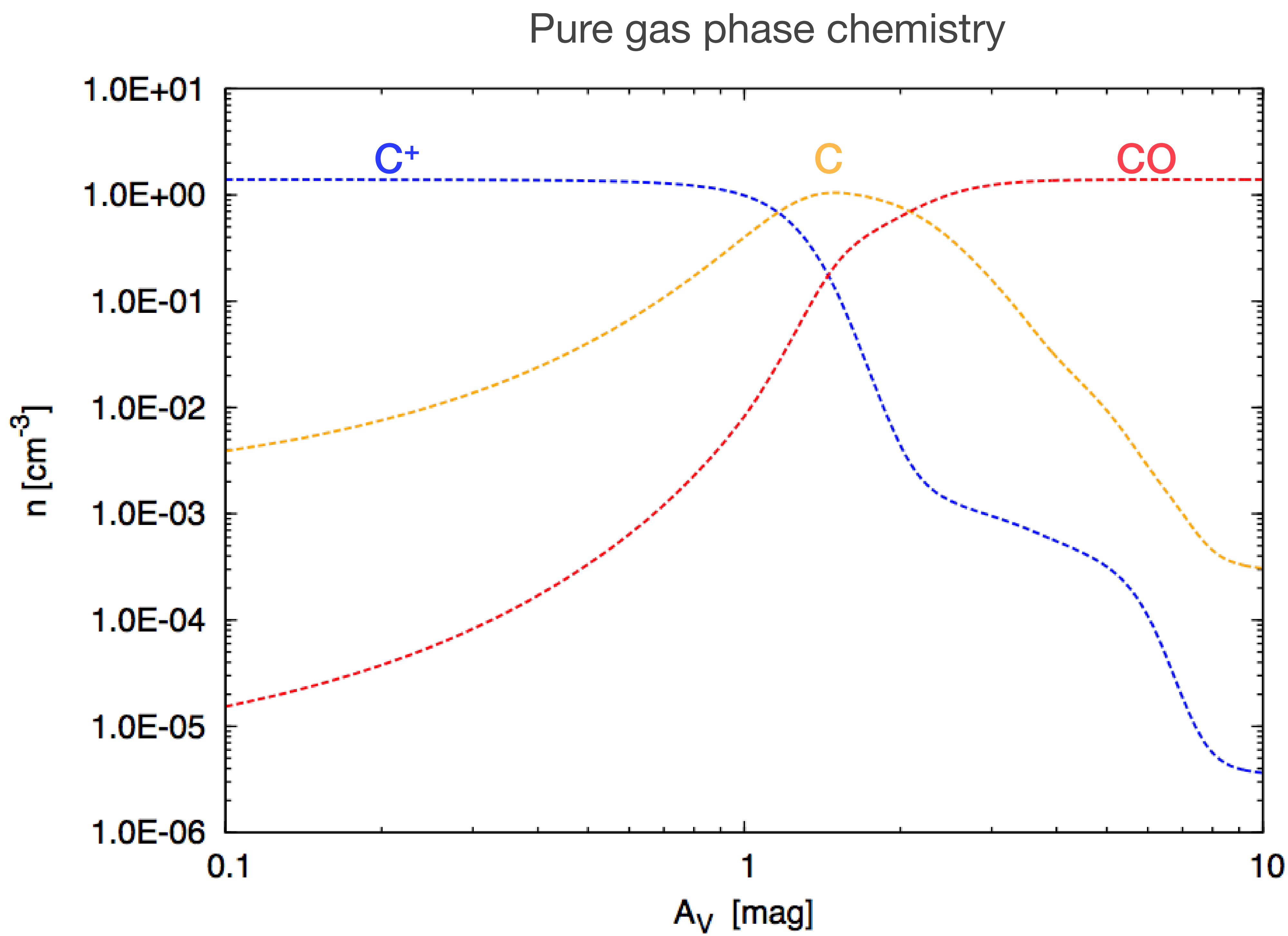
Only a few of these chemical parameters are known

| | Barrier [K] | |
|---|---|---|
| | Diffusion | Desorption |
| H | 100 | 350 |
| O | 240 | 800 |
| OH | 378 | 1260 |
| $H_2$ | 135 | 450 |
| $O_2$ | 363 | 1210 |
| $H_2O$ | 558 | 1860 |
| CO | 363 | 1210 |
| HCO | 453 | 1510 |
| $H_2CO$ | 528 | 1760 |
| $CH_3O$ | 651 | 2170 |
| $CH_3OH$ | 618 | 2060 |
| $CO_2$ | 750 | 2500 |

Stantcheva et al. (2002)

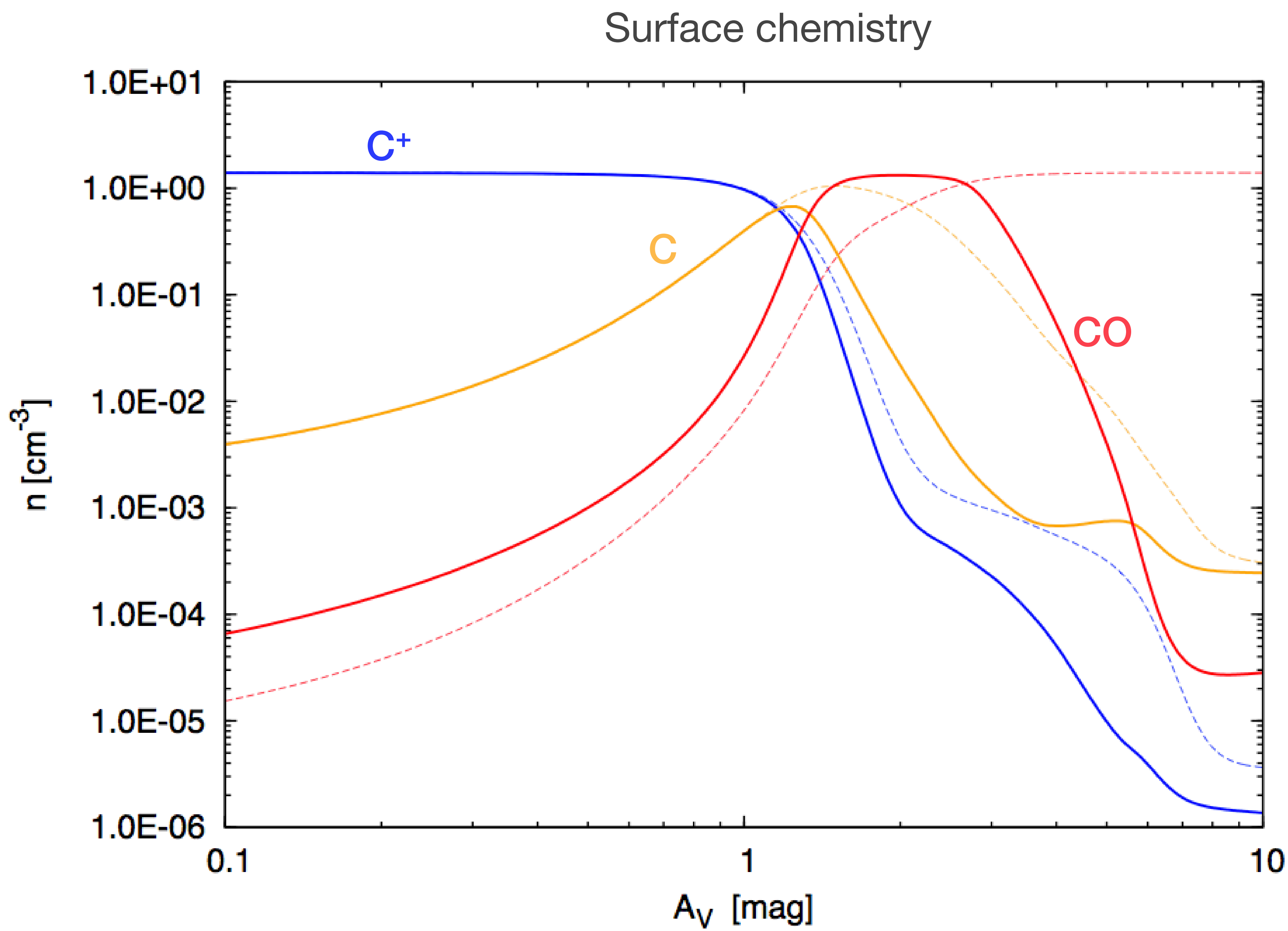
# Complex surface chemistry

Impact of surface chemistry on a typical PDR
$n_H = 10^4$ cm$^{-3}$, G = $10^3$ Mathis

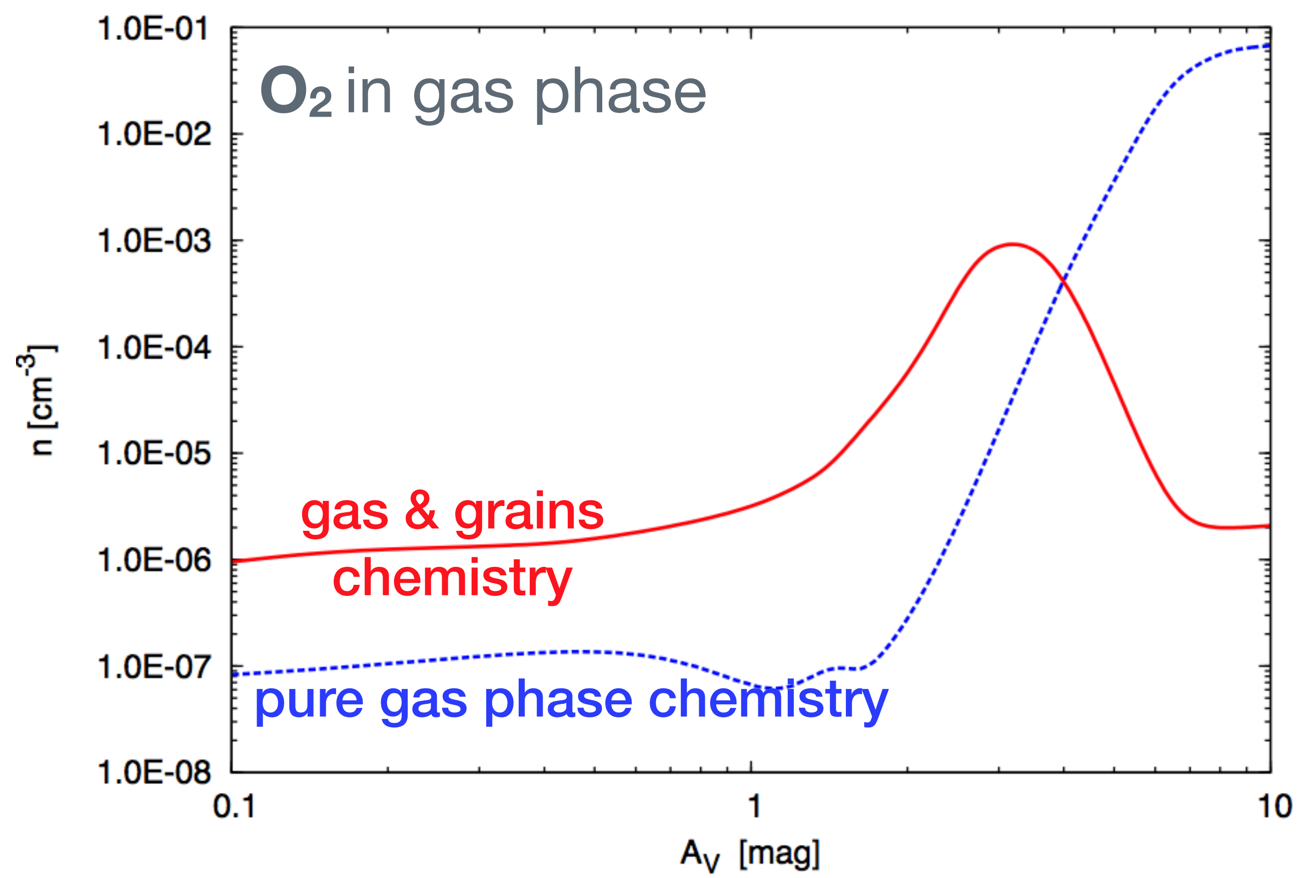


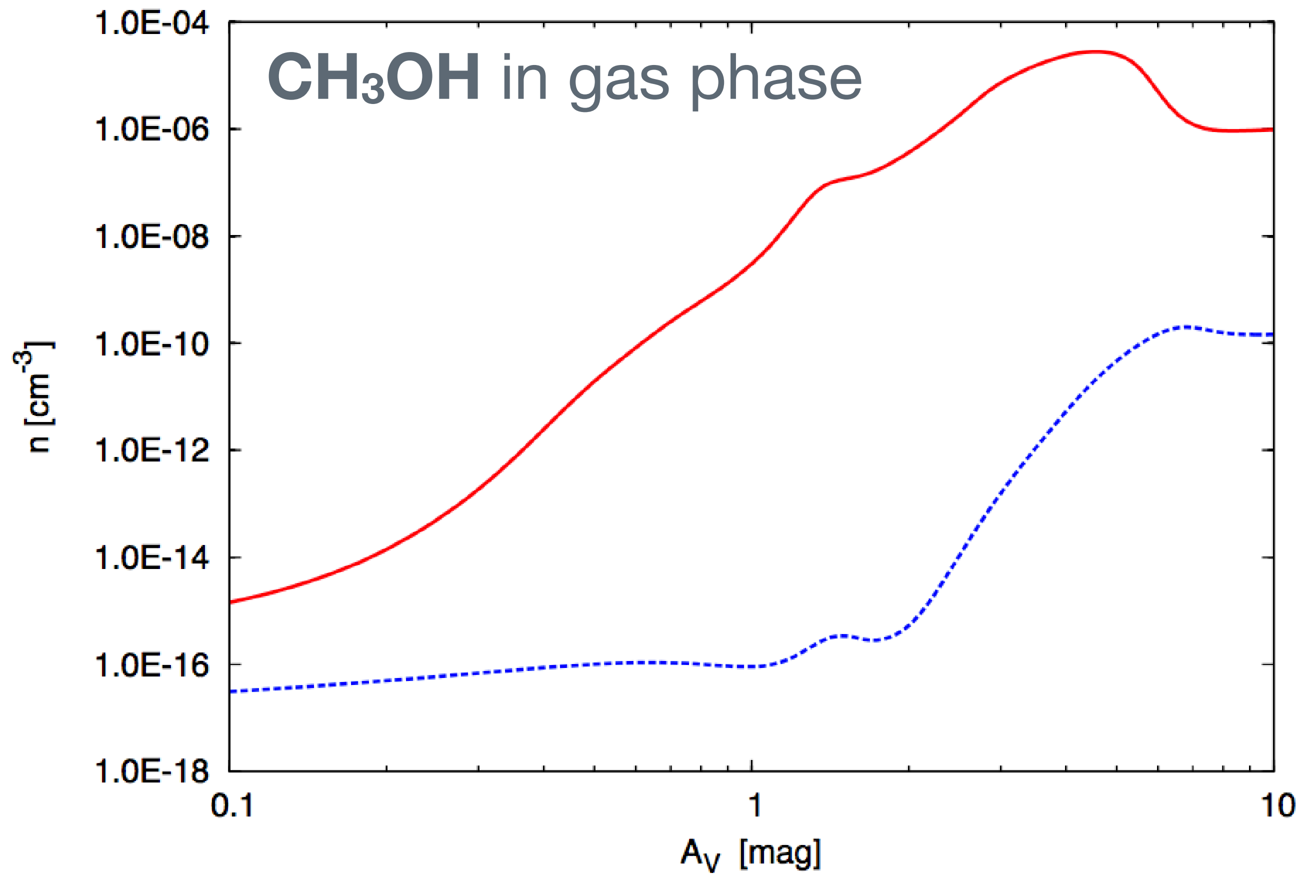
# Complex surface chemistry

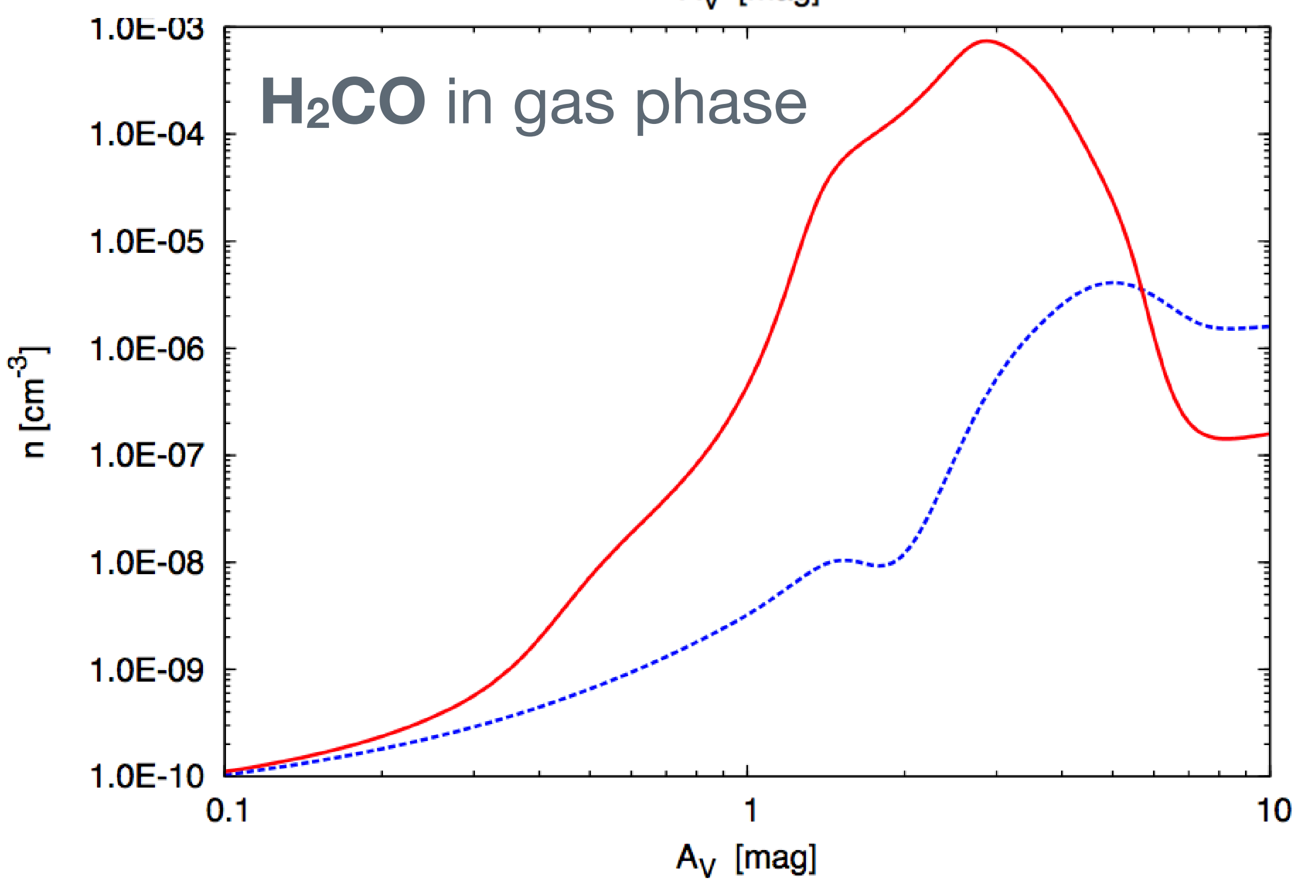
Impact of surface chemistry on a typical PDR
$n_H = 10^4$ cm$^{-3}$, $G = 10^3$ Mathis



# Complex surface chemistry

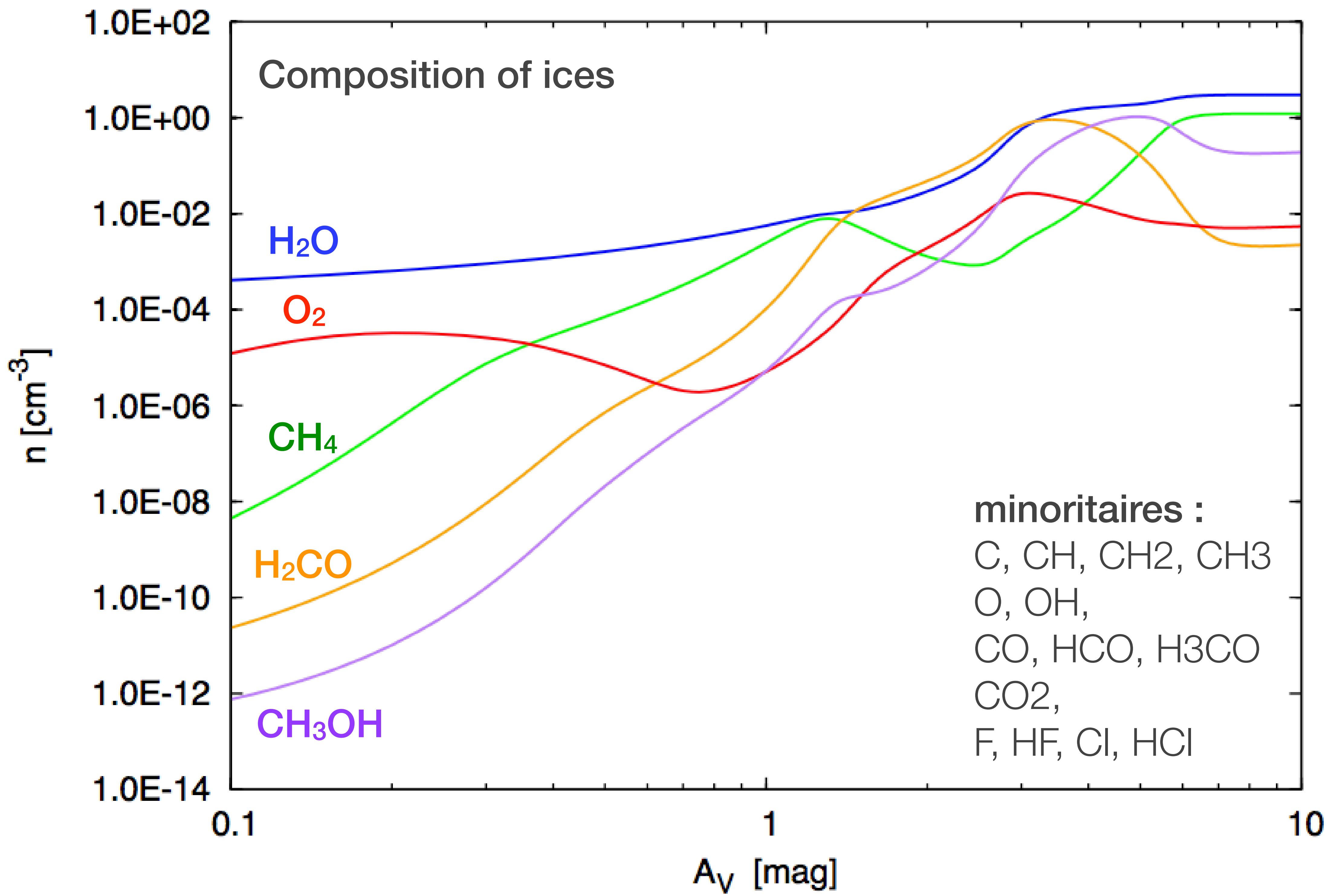



| N(X) [cm$^{-2}$] | Gas chemistry | Gas & Surface chemistry |
|---|---|---|
| CO | 2.0E+18 | 4.2E+17 |
| $O_2$ | 4.0E+16 | 2.6E+14 |
| $CH_3OH$ | 1.4E+08 | 1.2E+13 |
| $H_2CO$ | 3.0E+12 | 2.0E+14 |

# Complex surface chemistry

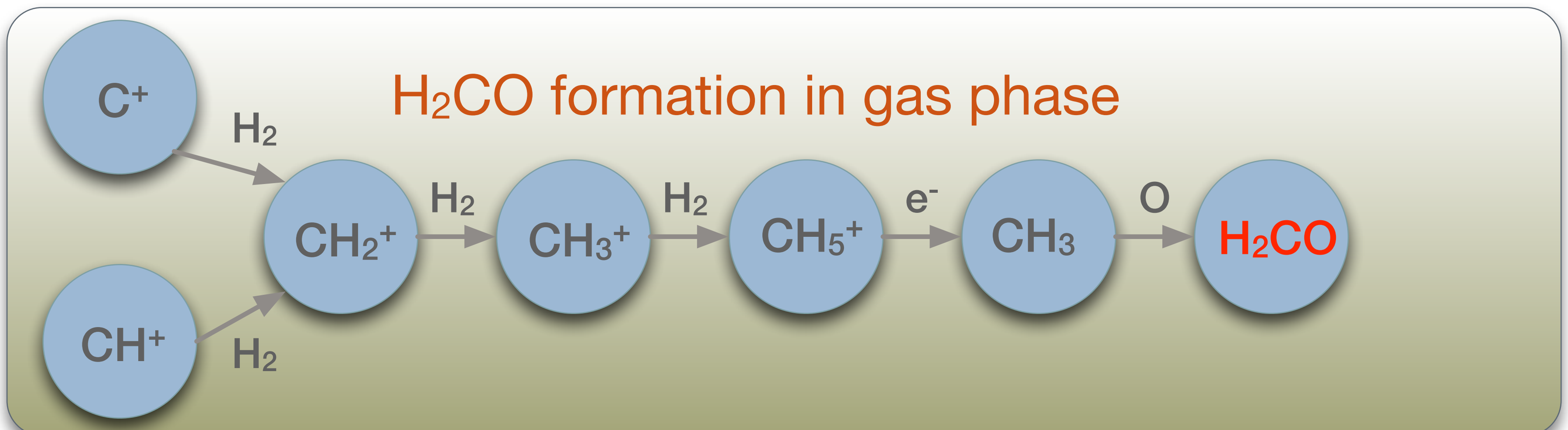


# Complex surface chemistry

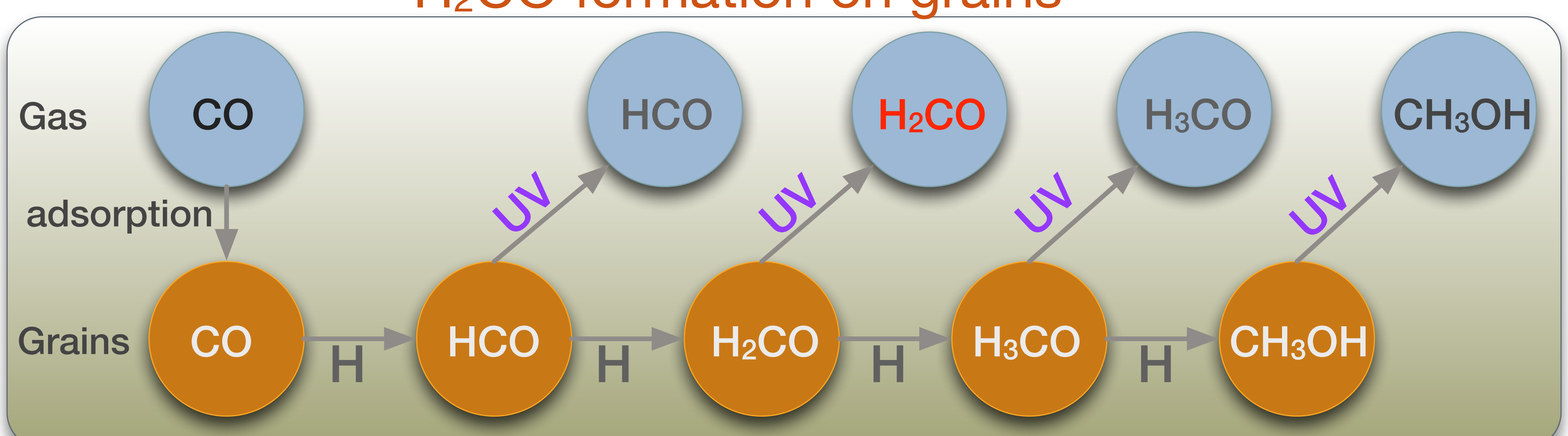
## Application to $H_2CO$ towards the Horsehead

(V. Guzman et al. - A&A, 2012)

Chemistry of $H_2CO$ :




H2CO formation on grains



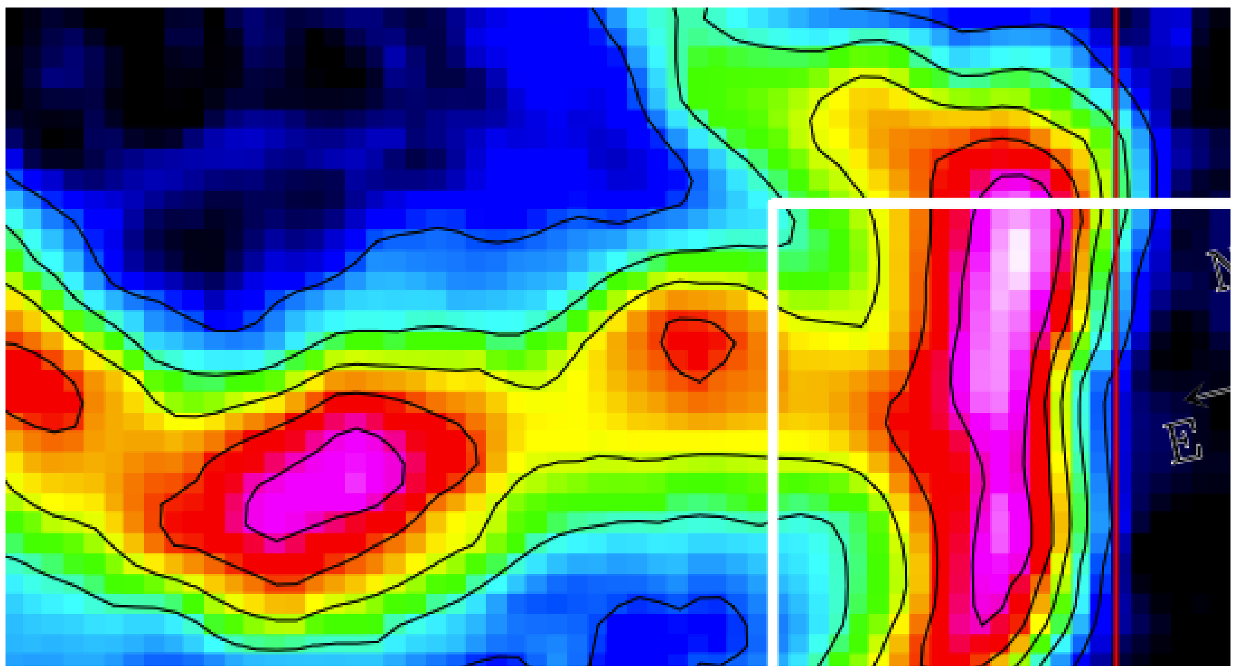
# Complex surface chemistry

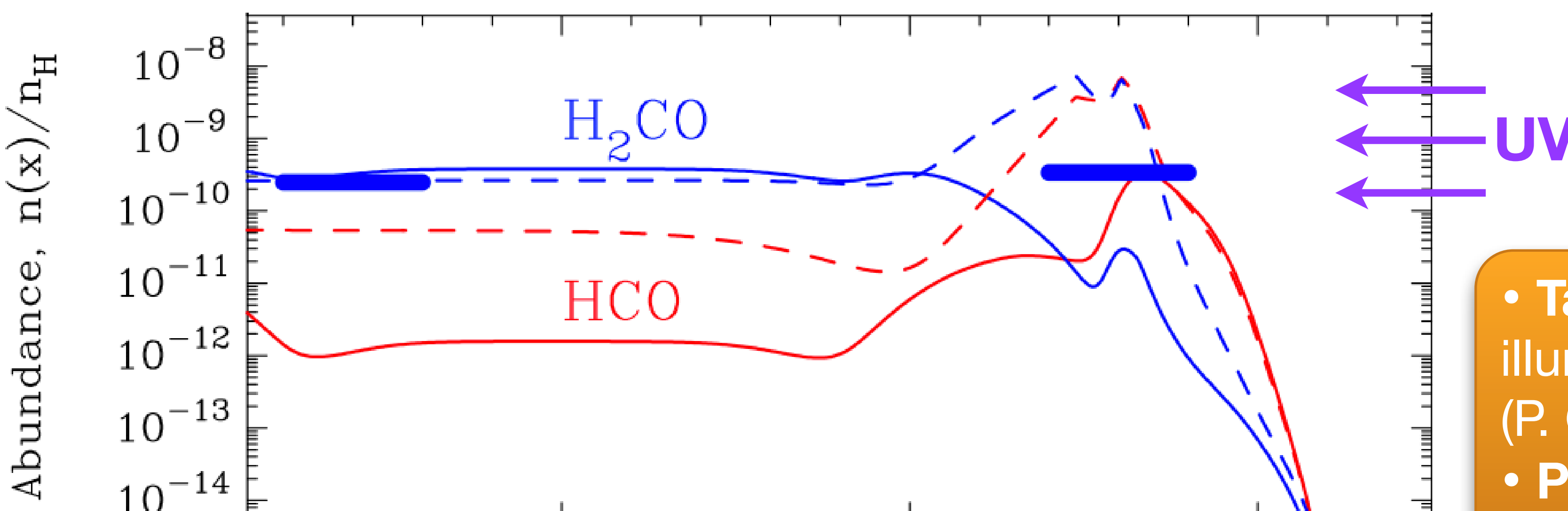
## Application to $H_2CO$ towards the Horsehead

(V. Guzman et al. - A&A, 2012)

IRAM obs. of $H_2CO$ at 2 positions

- PDR
- dense core






Model :

- Specific density profile
- G ~ 100 ISRF

Formation of $H_2CO$

In dense core

- Formation in gas

In the PDR

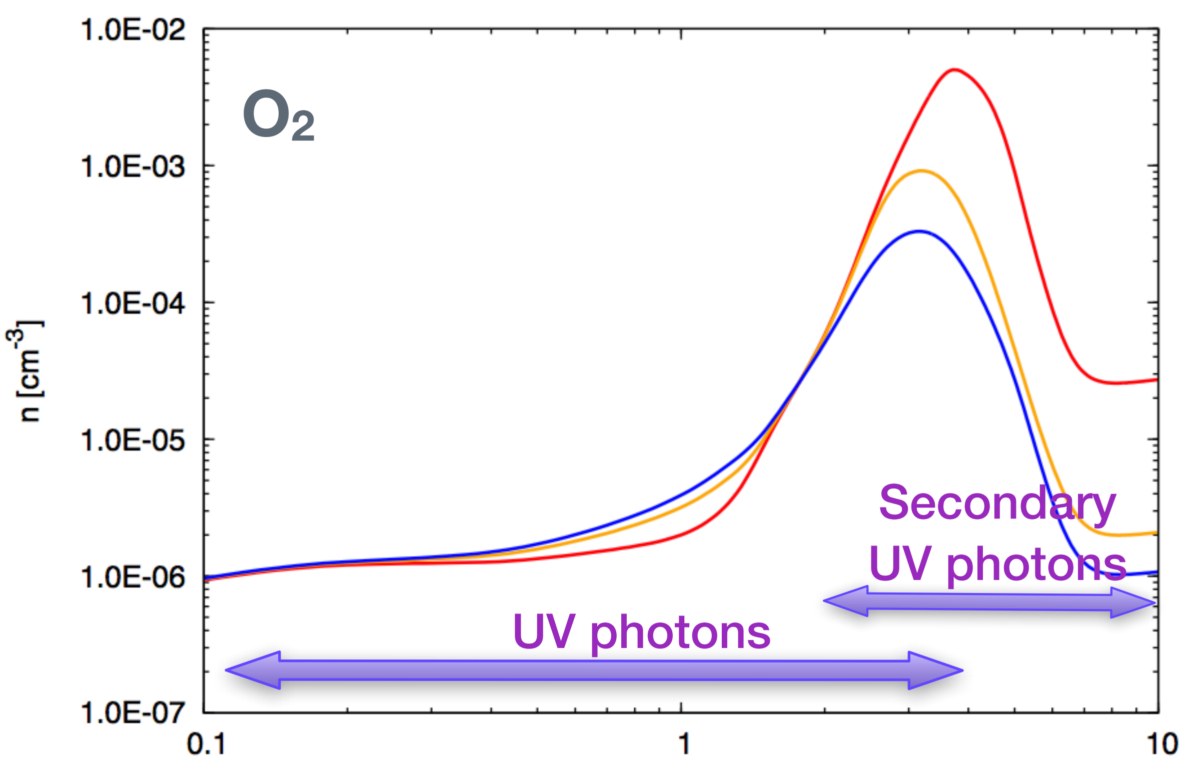
- Formation on grains
- **Photo-desorption**

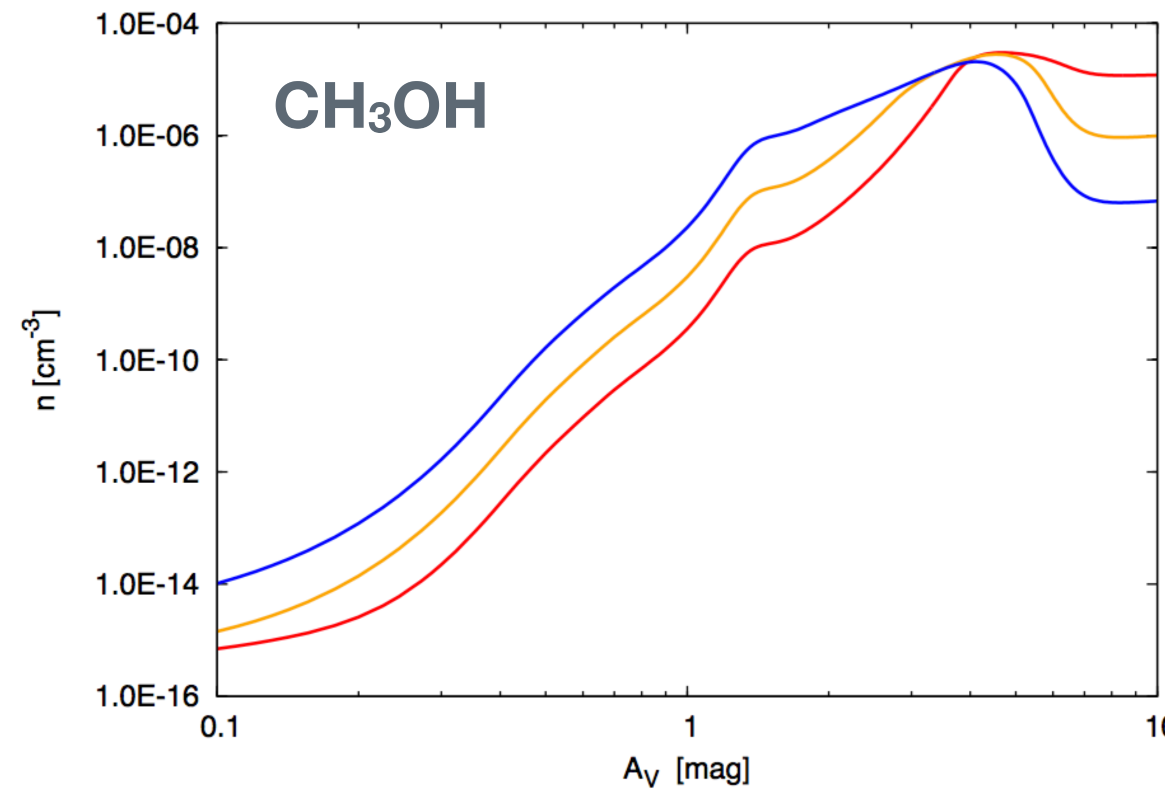
- **Talk :** Physics and chemistry of UV illuminated neutral gas: The Horsehead case (P. Gratier)
- **Poster 30 :** The Horsehead WHISPER line survey (V. Guzman et al.)

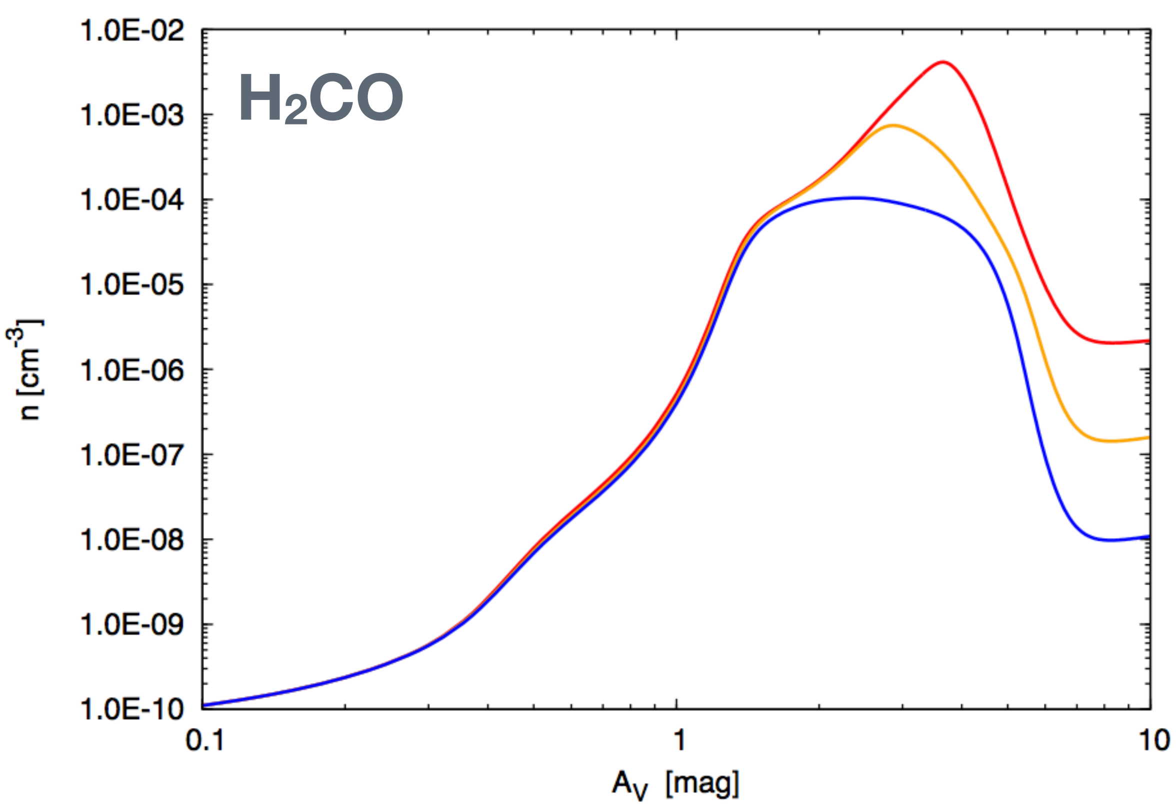
# Complex surface chemistry

**Impact of desorption by UV photons** (and cosmic rays)

**rate = k** x **f**$_{UV}$




| N(X) [cm$^{-2}$] | k = $10^{-4}$ | k = $10^{-3}$ | k = $10^{-2}$ |
|---|---|---|---|
| CO | 1.9E+17 | 4.2E+17 | 6.5E+17 |
| $O_2$ | 1.1E+14 | 2.6E+14 | 1.4E+15 |
| $CH_3OH$ | 7.6E+12 | 1.2E+13 | 2.2E+13 |
| $H_2CO$ | 4.4E+13 | 2.0E+14 | 9.4E+14 |

# Conclusions

Implementation of detailed physics :

- ER, LH mechanisms for $H_2$ formation
- complex surface chemistry

- **Better agreement observations - models**
  - $H_2$ line intensities
  - CO excitation properly reproduced up to J ~ 20 in PDRs by models
  - Proper order of magnitudes for species linked to surface chemistry : $H_2CO$, $O_2$, hydrids, ...

▸ **thanks to many years of laboratory experiments & theoretical studies of grains physics PDR models begin to give proper results !**

Still some ad-hoc parameters

**Laboratory experiments & theoretical studies more and more mandatory**

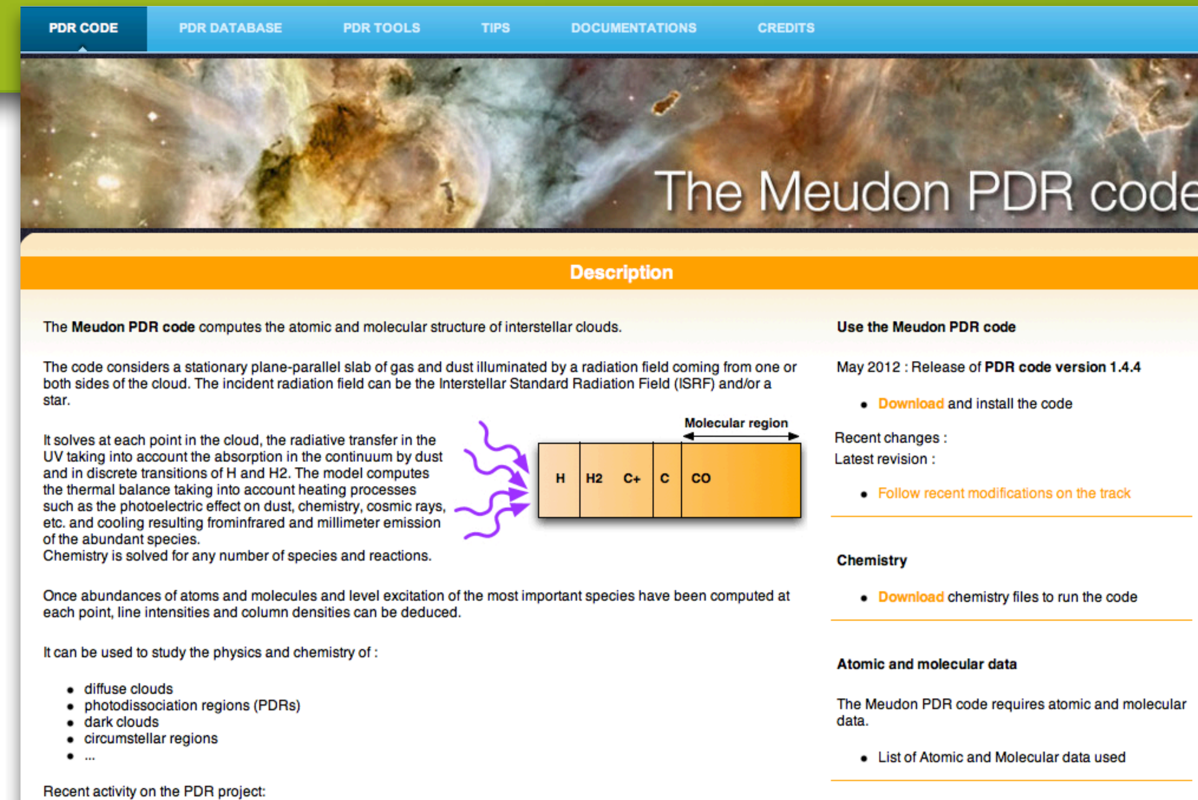
- adsorption barriers on non-perfect surfaces
- surface reaction rates
- photo-desorption rates
- cosmic rays effects on grains

# Future of the PDR code

Present public version : PDR 1.4.4

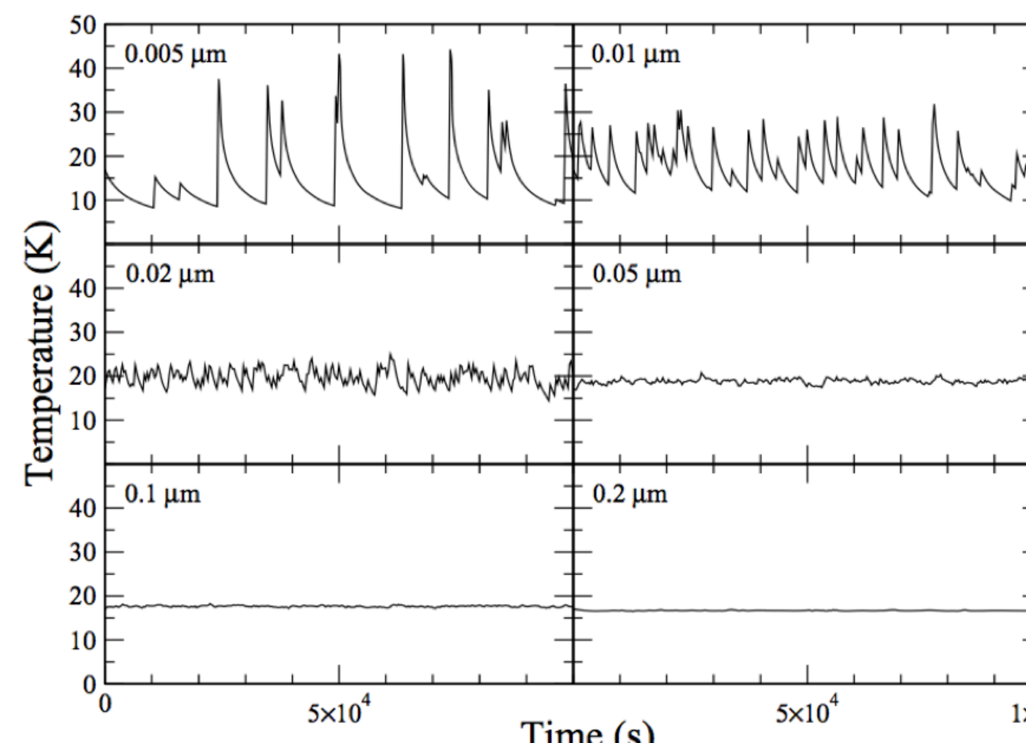
- $H_2$ formation by ER and LH
- DustEM 4.0 coupling
- non local I.R. pumping effects
- Several updated at. mol. data

Download at : http://pdr.obspm.fr




Next version : beginning 2013

- Complex surface chemistry
- UV pumping for more molecules as CO




Cuppen et al. (2006)

What's next

- Stochastic effects on grains (T, n(H))
- Turbulence and diffusion
- Better implementation of X-rays and cosmic rays
  - Environments : Extragalactic medium, young stars, Galactic center, ...

**Poster 8 :** Formation de H2 : Influence des fluctuations de la température des grains (E. Bron)