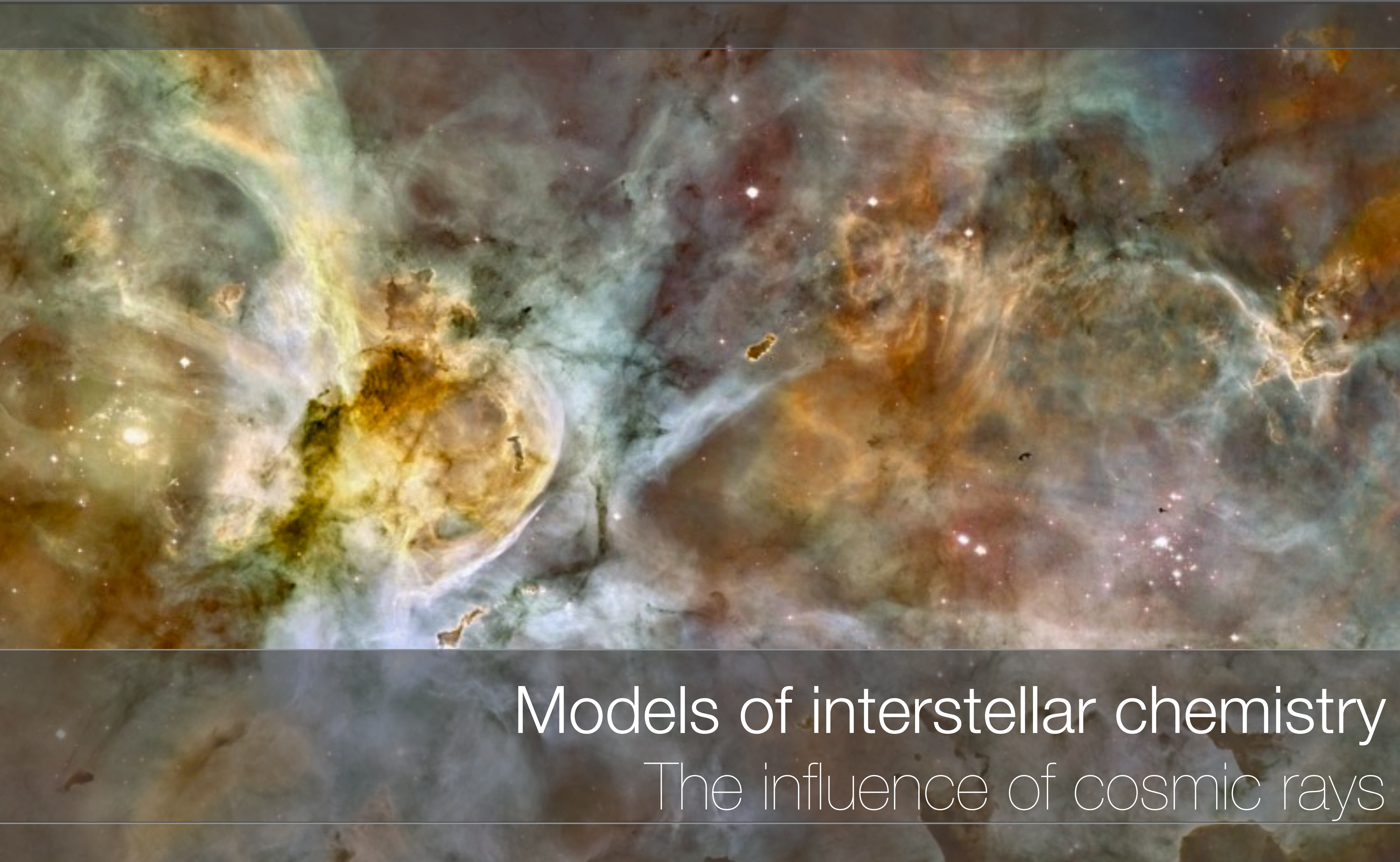


Models of interstellar chemistry

The influence of cosmic rays

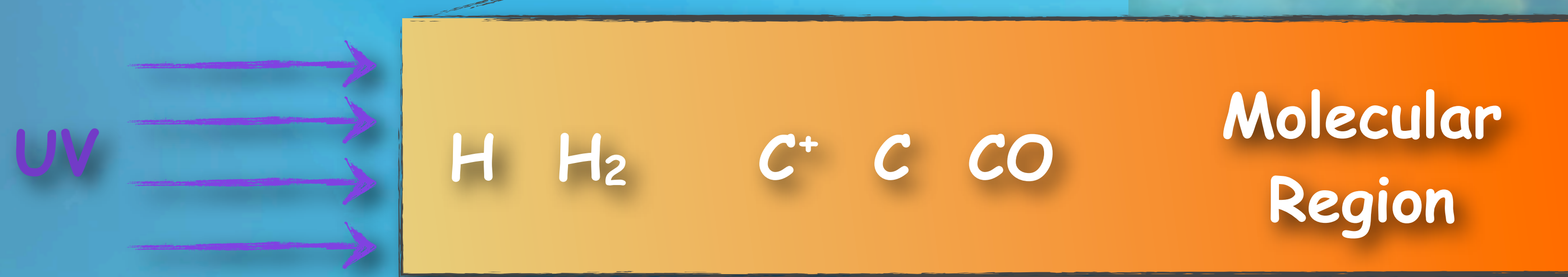
CRISM
1 july 2011

Franck Le Petit
LUTH - Observatoire de Paris

The Meudon PDR code

PDR code models the astrochemistry of interstellar gas

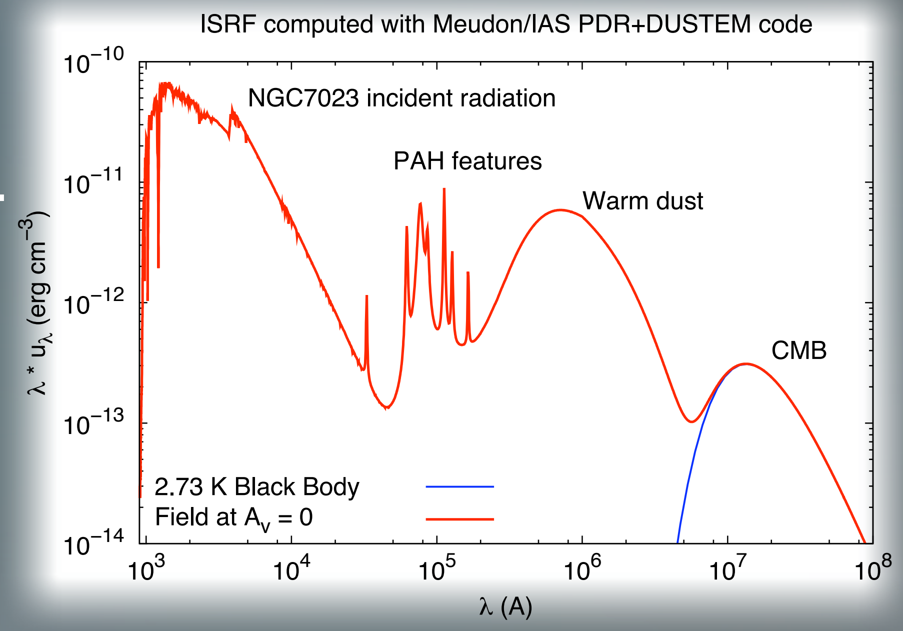
Development of a PDR code at Paris Observatory from more than 10 years.
Jacques Le Bourlot, Evelyne Roueff, Franck Le Petit, ...



Hypothesis & geometry :
- Plan-parallel
- Stationnary

The Meudon PDR code

Stationnary model solving:

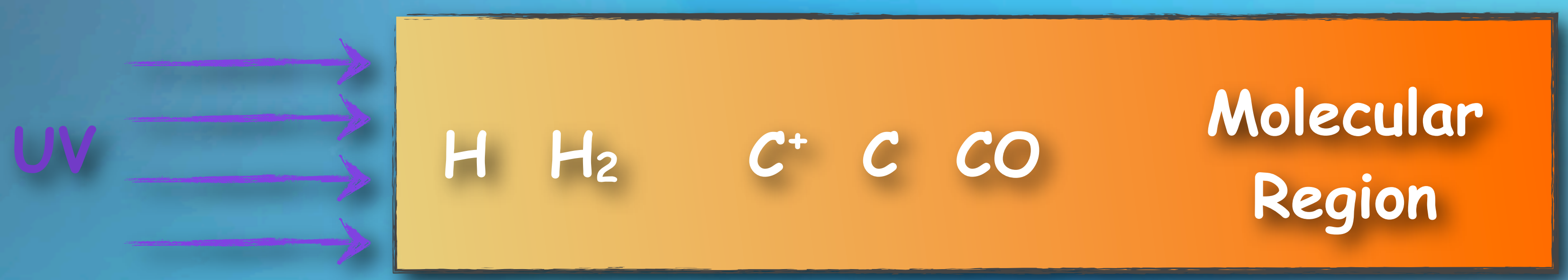


- **Radiative transfer**: absorption in the lines of H, H_2, CO, HD, …
  absorption in the continuum
  UV to sub-mm
- **Chemistry**: more than 100 chemical species
  network of more than 1000 chemical reactions
  grain surface chemistry (formation of mantles)
- **Statistical equilibrium of the populations** in the levels of H_2, HD, CO, HCO^+, H_2O, CS, H_3^+, …
  takes into account: radiative and collisional excitation / de-excitations, photodissociation
- **Thermal balance**: heating by photoelectric effect, chemistry, cosmic rays …
  cooling in the lines of atoms and molecules

The Meudon PDR code

Input parameters
- density of the medium
- intensity of the radiation field
- metallicities
- grains properties
- flux of cosmic rays
- ...

Atomic and molecular data :
- Radiative transitions : Einstein coefficients / wavelengths
- Collision rates
- Photo-reaction cross sections
- Chemical reaction rates



Solves :
- Radiative transfer
- Chemistry
- Thermal balance

Provides :
- Abundance profiles
- Gas temperature
- Excitation of atoms and molecules
- Local emissivities
- Temperature and charge of grains
- ...

Post-processing :
- Column densities
- Line intensities
- Spectra

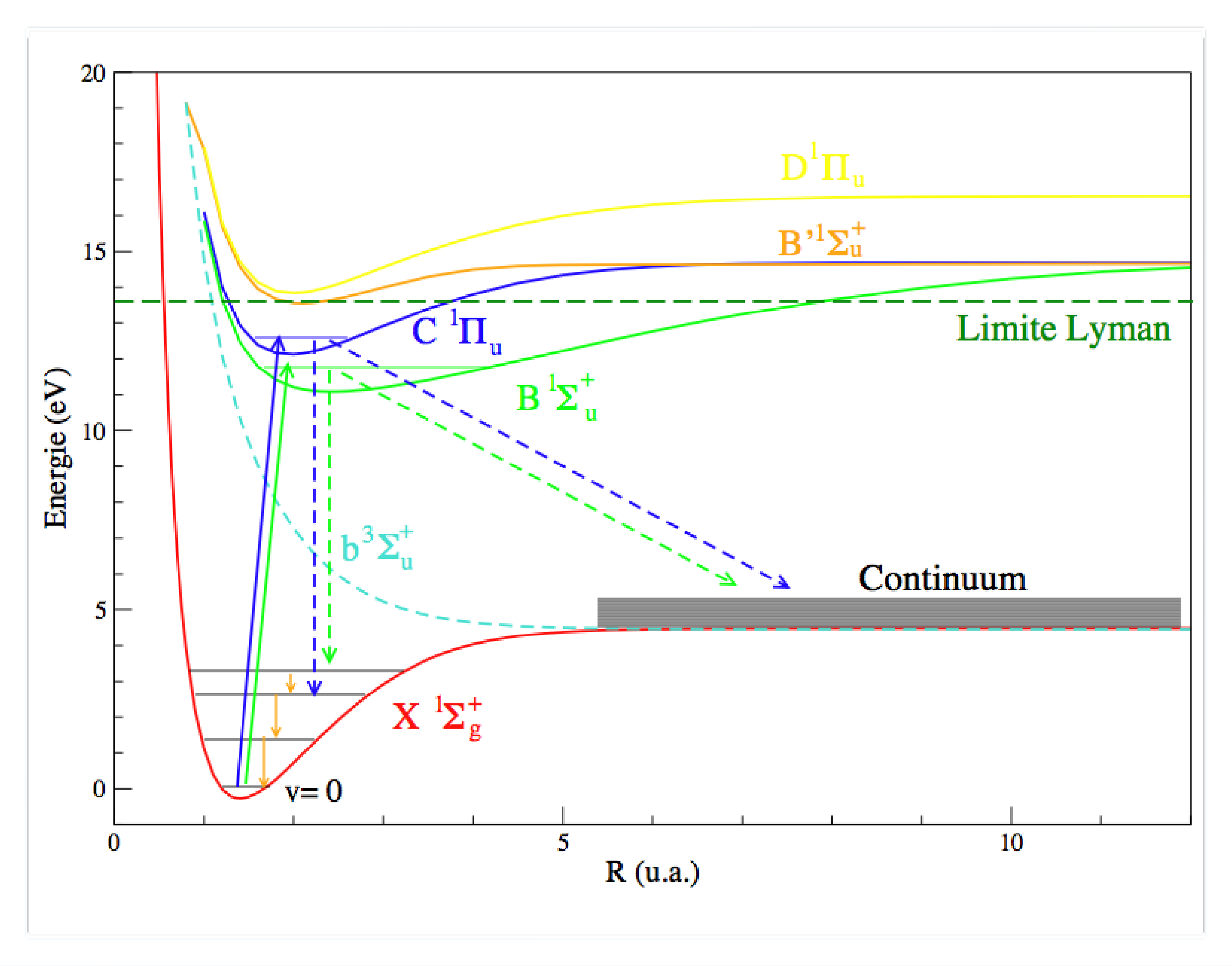
- Spherical approximation

Public code :
http://pdr.obspm.fr

Interstellar chemistry & cosmic rays

Cosmic rays have a strong influence on interstellar chemistry

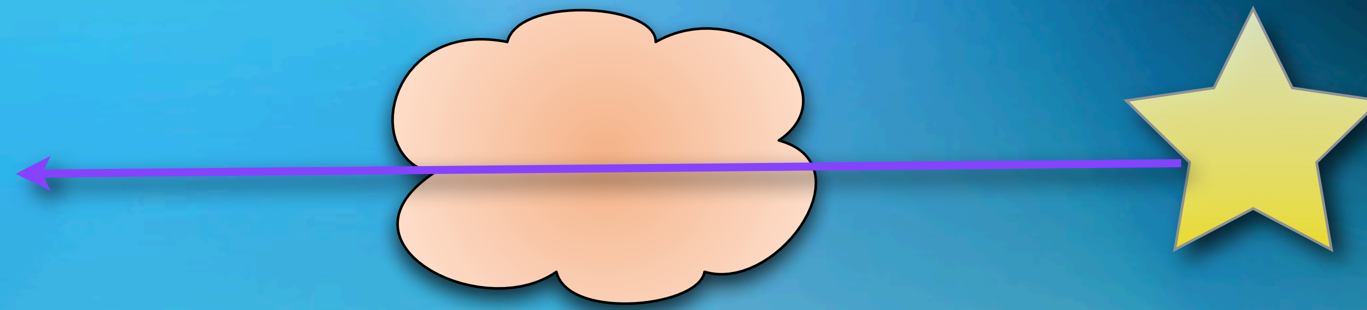
- Induce desorption of molecules from grains
- stochastic heating of grains
- Production of secondary photons
- Ionize partially the gas
  => can take control of the chemistry
  - (fast) ion-neutral reactions
  - no energy thresholds



Molecules directly linked to cosmic rays : OH, HD, H_3^+, OH^+, H_2O^+, ...

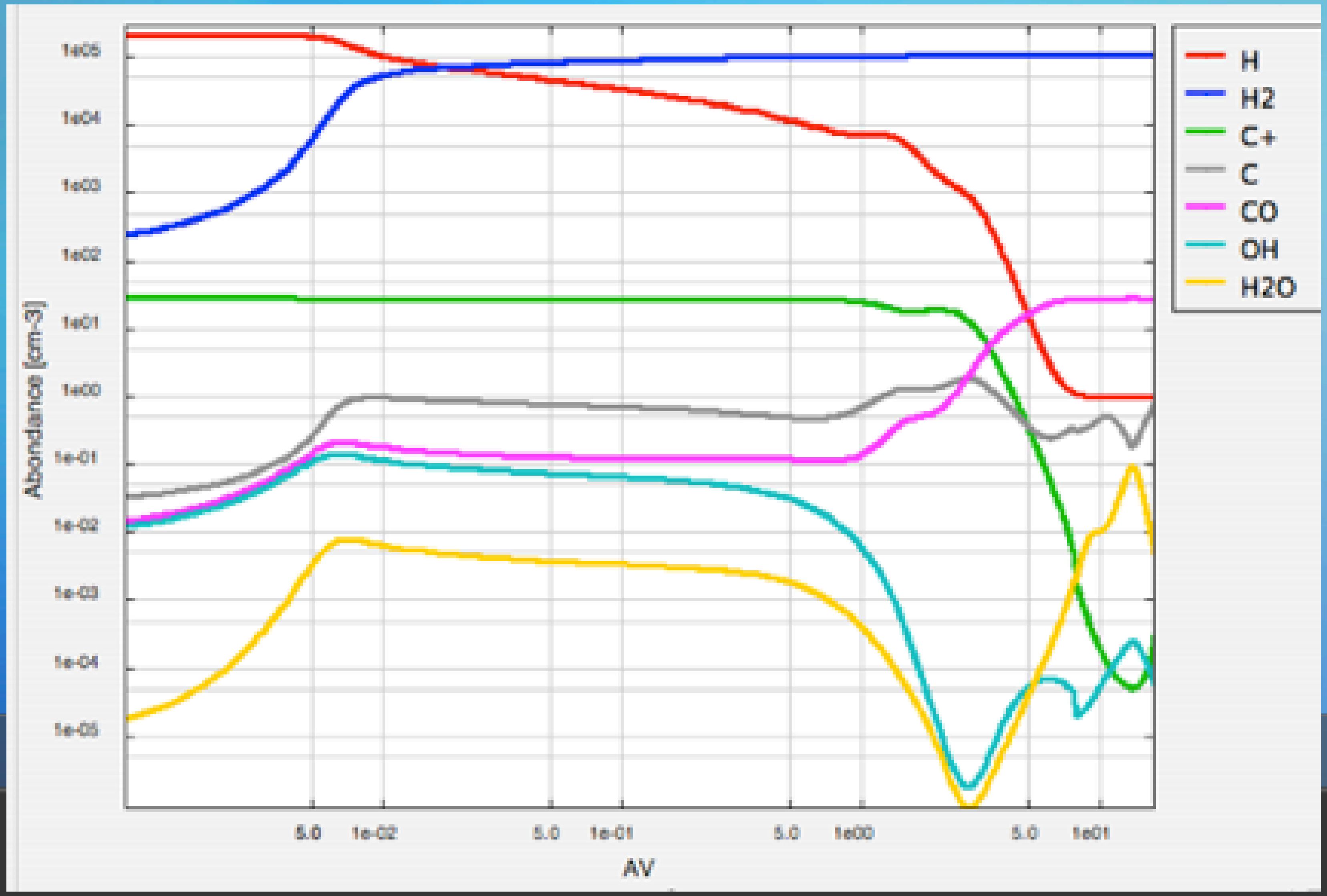
Diffuse clouds

- Density : n_H ~ 100 cm^{-3}
- illuminated by to the ISRF



Very interesting objects :

- observations in absorption => direct access to abundances
- small molecules => simplified chemistry => study in detail physical processes



Diffuse clouds : OH and HD

Determination of the flux of cosmic rays

(Black & Dalgarno 1973, Black et al. 1978, Federman et al. 1996, Le Petit et al. 2001)

① Observe OH

$$H \xrightarrow{cosmic} H^+ \xrightarrow{O} O^+ \xrightarrow{H_2} OH^+ \xrightarrow{H_2} H_2O^+ \xrightarrow{H_2} H_3O^+ \xrightarrow{e^-} OH$$

n(OH) is proportional to ζ and to O/H → O/H has been determined by observations

② Observe HD

$$H \xrightarrow{cosmic} H^+ \xrightarrow{D} D^+ \xrightarrow{H_2} HD$$

n(HD) is proportional to ζ and to D/H

Get ζ

Get D/H

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

Diffuse clouds : H_3^+

The abundance of H3+ is also directly linked to the flux of cosmic rays

Formation :

$$H_2 + \text{cosmic} \rightarrow H_2 + e^-$$
$$H_2^+ + H_2 \rightarrow H_3^+ + H$$

Destruction : recombination with electrons

$$H_3^+ + e^- \rightarrow \ldots$$

Observations : $N(H_3^+) / E(B\text{-}V) \sim 10^{14}$
=> 10 times higher than dense clouds

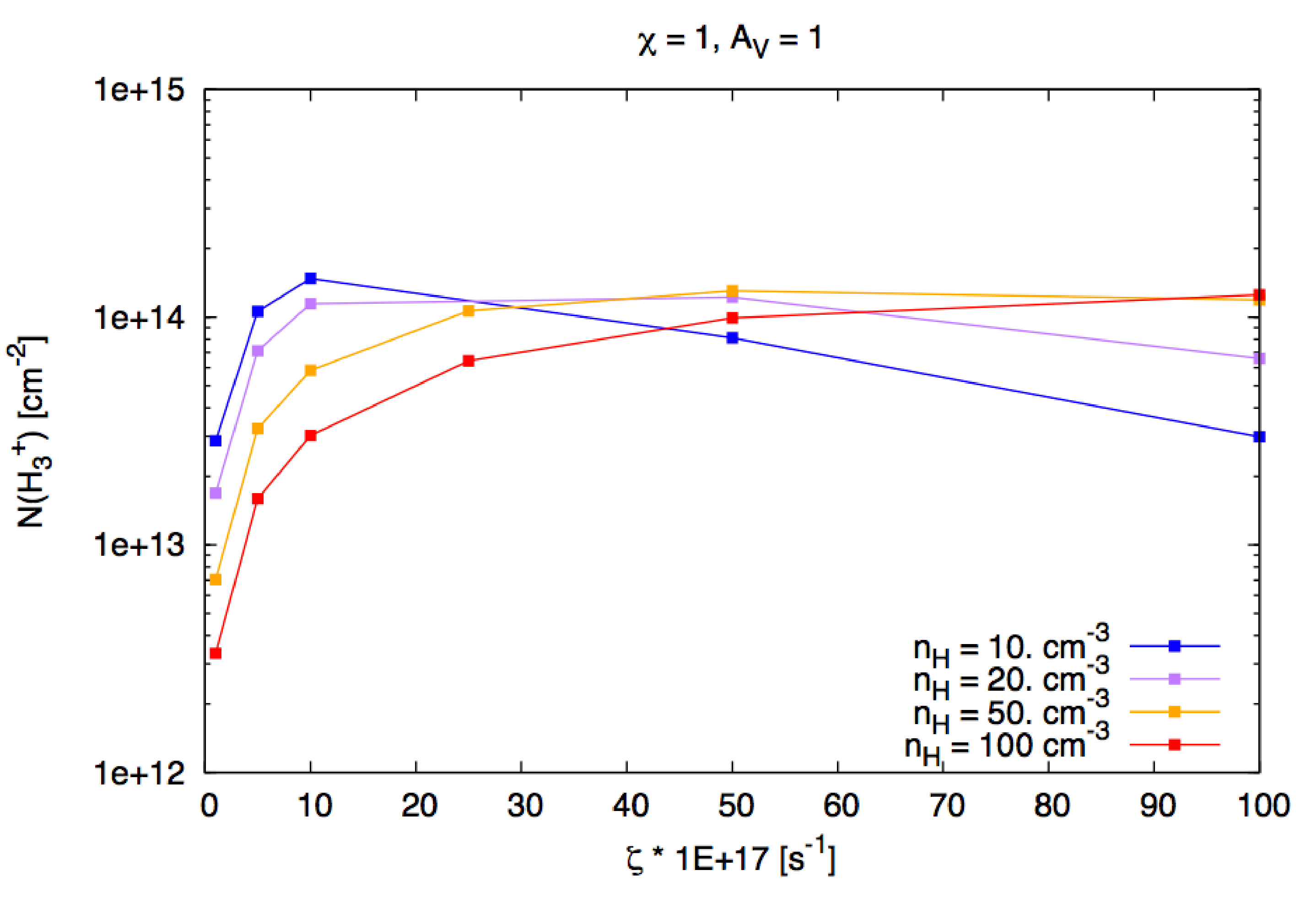
Typical model: $n_H = 100\ cm^{-3}$
$\chi = 1$
$T = 60\ K$
$\zeta = 5 \times 10^{17}\ s^{-1}$
$N_H = 10^{21}\ cm^{-2}$

→ $N(H_3^+) = 8 \times 10^{12}\ cm^{-2}$

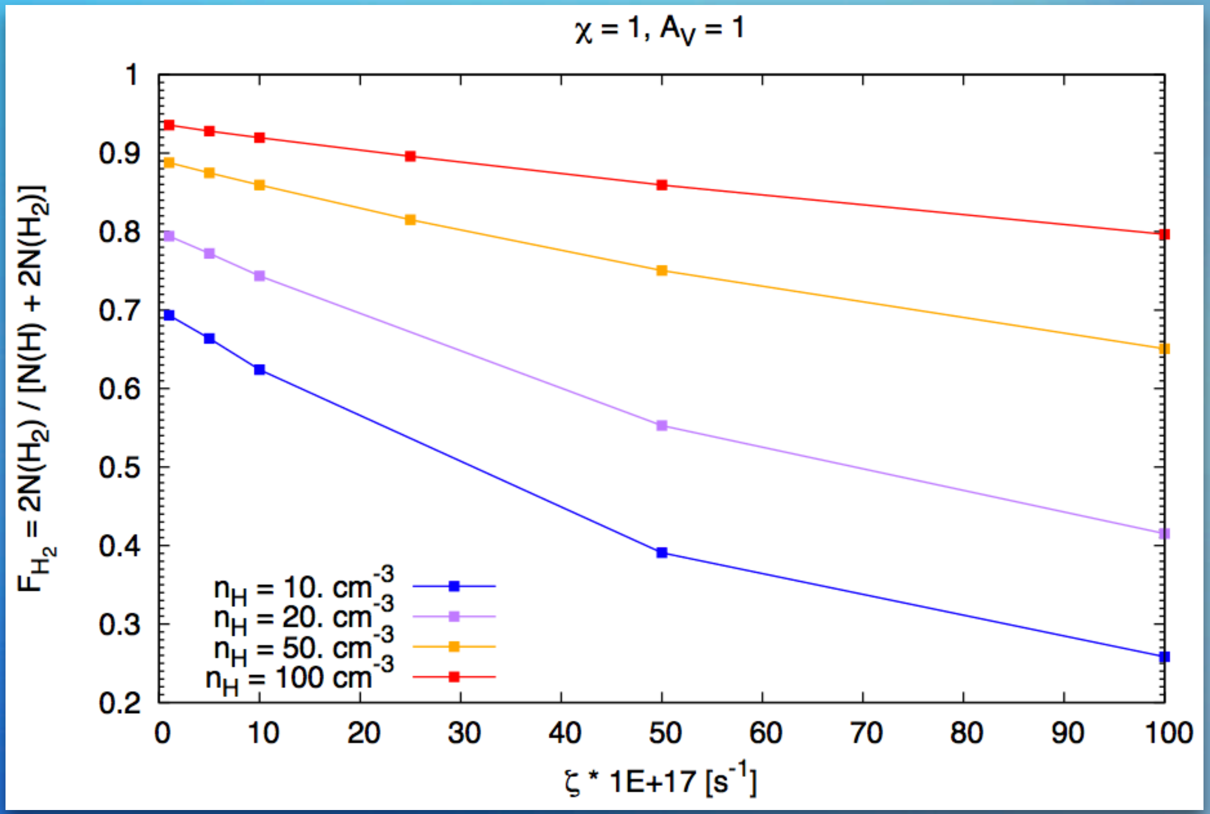
	E(B-V)	$N(H_3^+)$
HD 183143	1.28	~ 2 (14)
HD 20041	0.70	1.74 (14)
WR 104	2.10	~ 2 (14)
WR 118	4.13	~ 4 (14)
WR 121	1.68	1.12 (14)
ζ Per	0.32	8.0 (13)
...		

Diffuse clouds : H_3^+

$$n(H_3^+) = 7.76 \cdot 10^{-4} \cdot \zeta \cdot \frac{f_{H_2}^2 n_H^2}{n(e^-)} \cdot \frac{1}{1.04 \cdot 10^{-9} f_{H_2} n_H + 2.53 \cdot 10^{-7} \frac{T}{300}^{-0.5} n(e^-)}$$



- N(H_3^+) as a function of ζ has maximum
- Effect of the molecular fraction and n(e^-)



Application : the Zeta Perseus line of sight

Zeta Perseus is one of the line of sight used to get

$\zeta \sim 1\ 10^{-17}\ s^{-1}$

McCall et al. (2004) : detection of H_3^+ towards Zeta Perseus

From a simple relation between N(H3+) and ζ they find :

$$\zeta = 100\ 10^{-17}\ s^{-1}$$

Zeta Perseus is a very well studied line of sight

Temperature of the gas : 45 - 75 K

	Observations min	Observations max
H	5.7 (20)	7.1 (20)
H_2	3.2 (20)	7.1 (20)
H_2 (J=0)	0.53	0.66
H_2 (J=1)	45	75
H_2 (J=2)	2.0 (15)	1.1 (16)
H_2 (J=3)	8.0 (13)	
H_2 (J=4)	1.8 (17)	
H_2 (J=5)	2.9 (15)	3.6 (15)

	Observations min	Observations max
H	5.7 (20)	7.1 (20)
H_2	3.2 (20)	7.1 (20)
f	0.53	0.66
T_{01}	45	75
HD	2.0 (15)	1.1 (16)
H_3^+	8.0 (13)	
C^+	1.8 (17)	
C	2.9 (15)	3.6 (15)
CO	5.4 (14)	
CH	1.9 (13)	2.0 (13)
CH^+	3.5 (12)	
C_2	1.6 (13)	2.2 (13)
C_3	1.0 (12)	
CN	2.7 (12)	3.3 (12)
NH	9.0 (11)	
O	0.2 (18)	1.0 (18)
OH	4.0 (13)	
S^+	1.7 (16)	2.3 (16)
S	1.5 (13)	2.2 (13)
Si^+	2.8 (16)	2.8 (14)

Application : the Zeta Perseus line of sight

Determination of the flux of cosmic rays

- **Black, Hartquist and Dalgarno (1978)**
  2 components models
  - cold zone : $T = 45$ K, $n_H = 267$ cm^{-3}
  - warm zone: $T = 120$ K, $n_H = 100$ cm^{3}

  $\zeta = 2.2\ 10^{-17}\ s^{-1}$

- **van Dishoeck & Black (1986)**
  - take into account all constraints at this time
  - model with T and n_H profile

  $\zeta = 2 - 4\ 10^{-17}\ s^{-1}$

- **Federman & al. (1996)**
  - from OH only

  $\zeta = 1.7\ 10^{-17}\ s^{-1}$

- **McCall & al. (2004)**
  - **$N(H_3^+) = 8\ 10^{13}$ cm^{-2}**

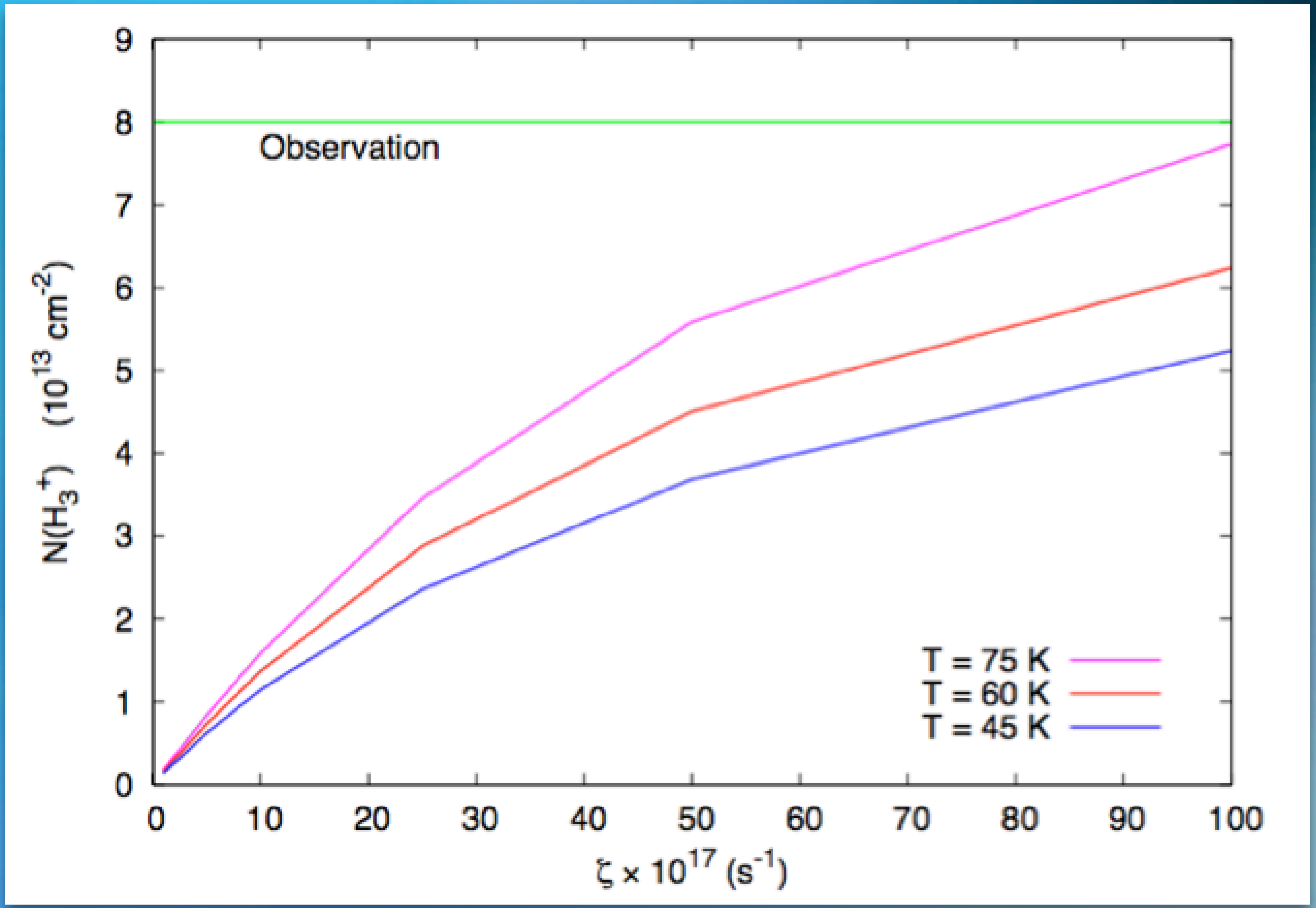
  $\zeta = 120\ 10^{-17}\ s^{-1}$

Application : the Zeta Perseus line of sight

Parameters
$n_H = 100\ cm^{-3}$
UV Flux : 2 * ISRF

Column density of H_3^+

- small dependance on T
- Observations require $\zeta = 100\ 10^{-17}\ s^{-1}$



Application : the Zeta Perseus line of sight

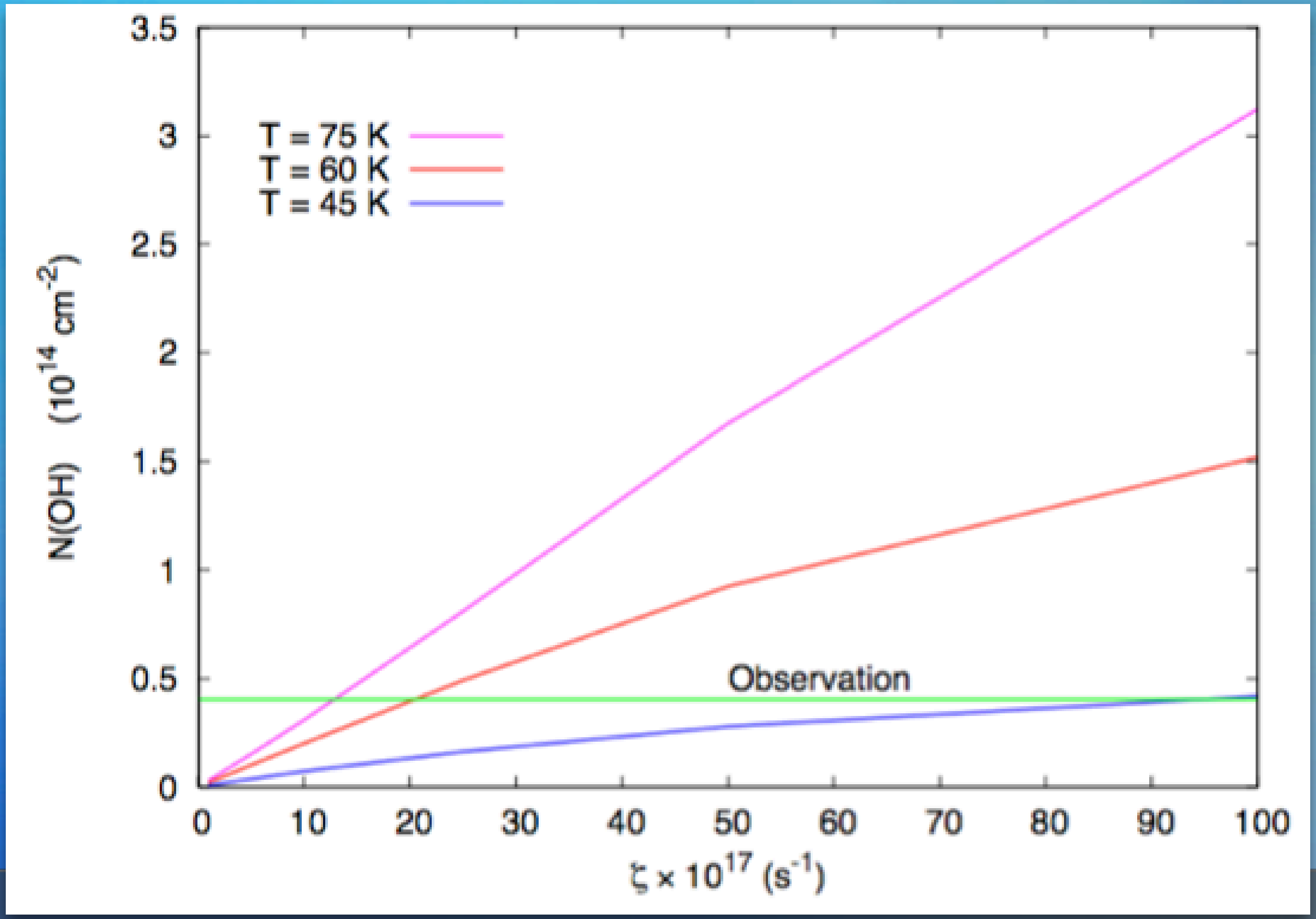
Column density of OH

- n(OH) depends strongly on T

$H^+ + O \rightarrow O^+ + H$ $k = 6\ 10^{-10}\ e^{-227/T}\ cm^3\ s^{-1}$

45 K $k = 3.9\ 10\text{-}12\ cm^{+3}\ s^{-1}$

75 K $k = 2.9\ 10\text{-}11\ cm^{+3}\ s^{-1}$



Application : the Zeta Perseus line of sight

Column density of HD

- n(HD) does not depend on T

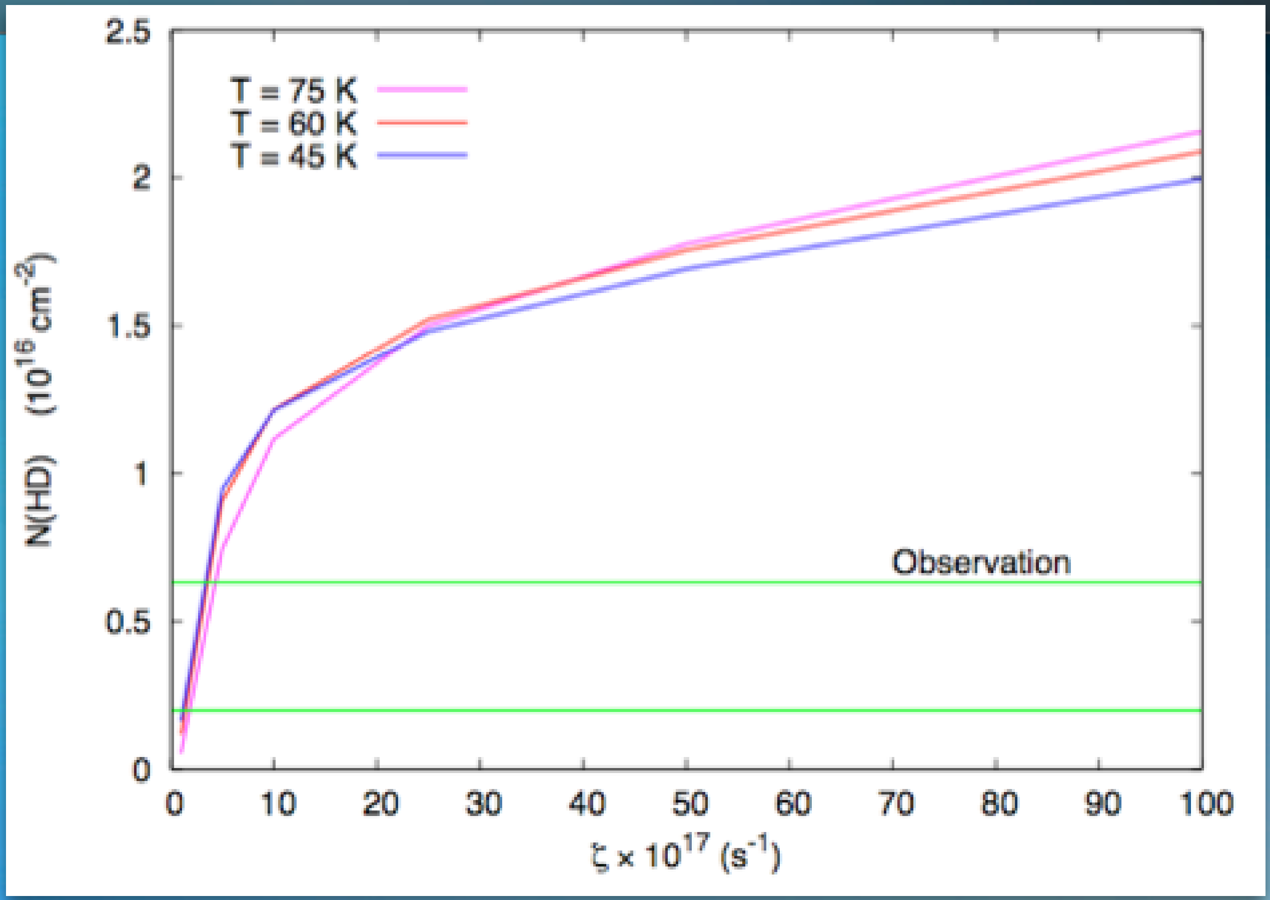
$H^+ + D \rightarrow D^+ + H$ $k = 10^{-9} e^{-41/T} cm^{+3} s^{-1}$
$D^+ + H \rightarrow HD + H^+$ $k = 1.2\ 10^{-9}$

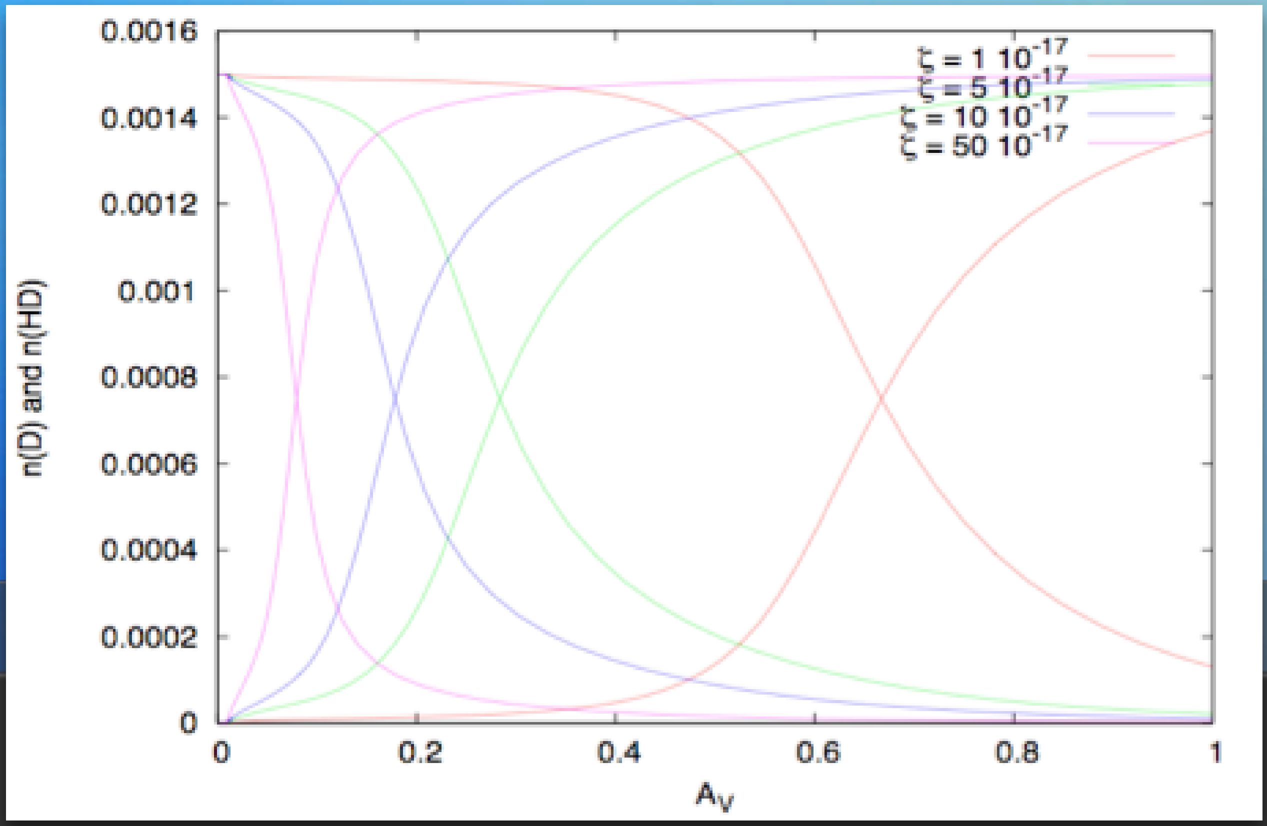
N(HD) is a good constraint for $\zeta < 10\text{-}16\ s^{-1}$

n(HD) is proportionnal to ζ if :
1) it is formed in gas phase by $D^+ + H_2$
2) it is destroyed by photodissociation

after the D/HD transition
$HD + H_3^+ \rightarrow H_2D^+ + H$

n(HD) is no more proportionnal to ζ





Application : the Zeta Perseus line of sight

Sulfur ionization

High value of ζ increases the ionization degree

Efficient recombination with electrons :

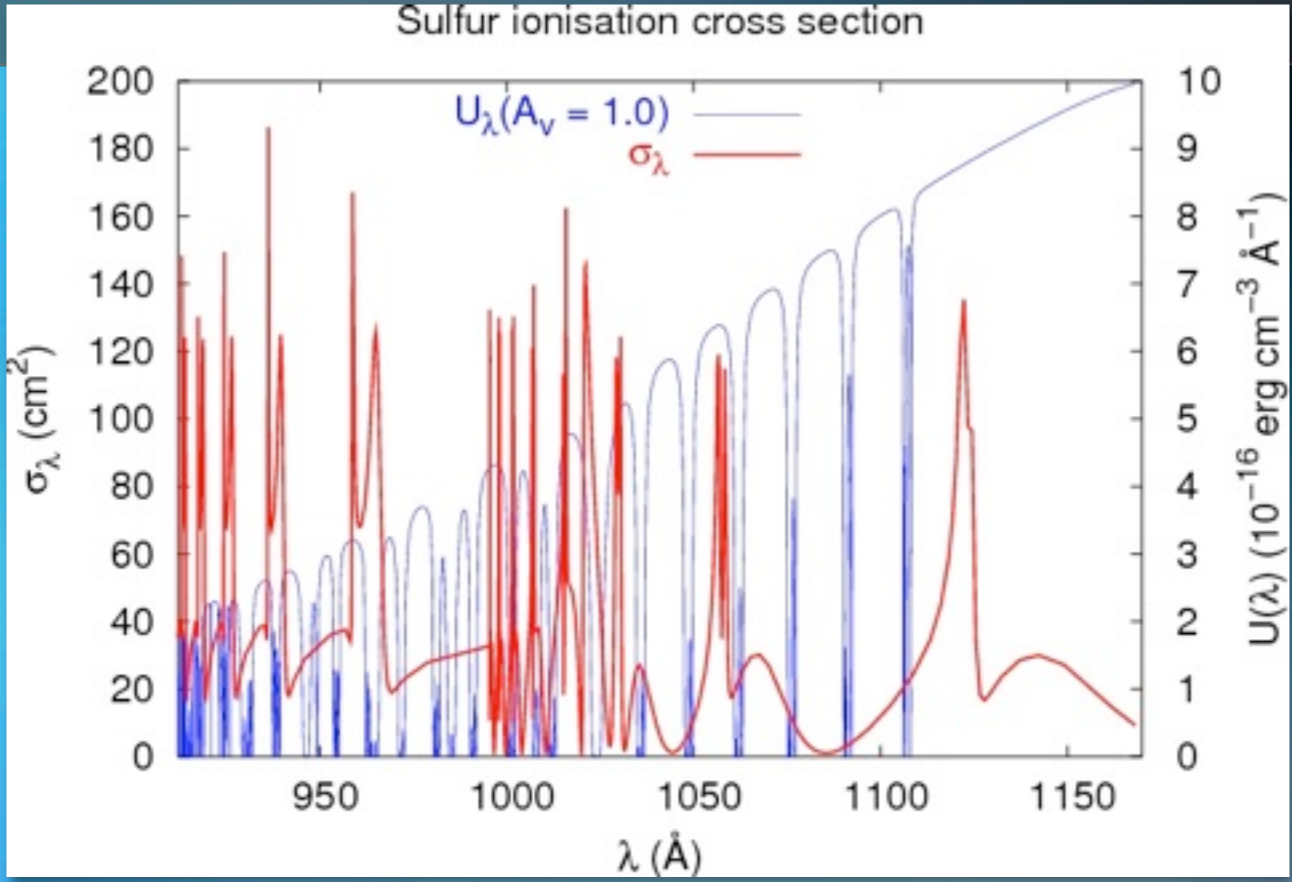
S + photon -> S+ + e-

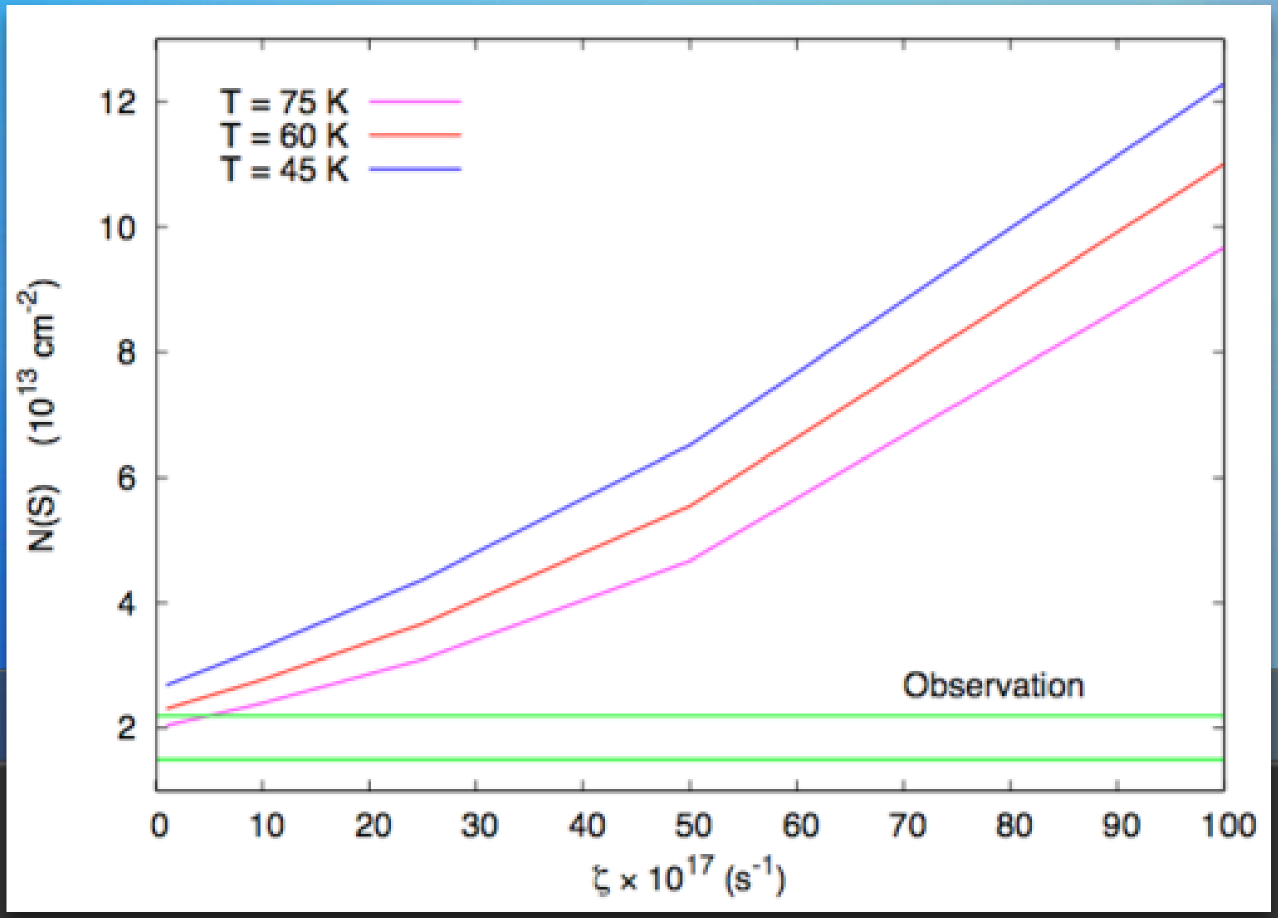
S+ + e- -> S + photon

ζ = 100 10-17 s-1

↓

overproduction of neutral sulfur





Application : the Zeta Perseus line of sight

Conclusion about the ζ Perseus line of sight

- **Standard value of ζ :**
  Underestimate N(H_3^+) by a factor 50

- **ζ = 100 times the standard value and T = 60 K**
  Reproduce N(H3+) but overproduce :
  OH by a factor 4
  S by a factor 6

ζ [10^{-17} s^{-1}]	H_3^+ [cm^{-2}]	OH [cm^{-2}]	HD [cm^{-2}]	S [cm^{-2}]
1	1.5 (12)	1.6 (12)	1.7 (15)	1.7 (13)
25	3.0 (13)	4.1 (13)	1.5 (16)	2.6 (13)
100	6.3 (13)	1.4 (14)	2.0 (16)	8.2 (13)
Obs.	8.0 (14)	4.0 (13)	2.0 (15) 1.1 (16)	1.5 (13) 2.2 (13)

good compromise : ζ = 25 10-17 s-1
(considering the uncertainties on the observatons and the simplifications of the model.)

Interpretation of observations : use as much observations as possible

H_3^+ in the Galactic center

Observations towards the Galactic Center
Works done by : Geballe, Oka, McCall, Indriolo, ...

From 2005, they observed **level excitation of H_3^+** on different lines of sight in the central molecular zone

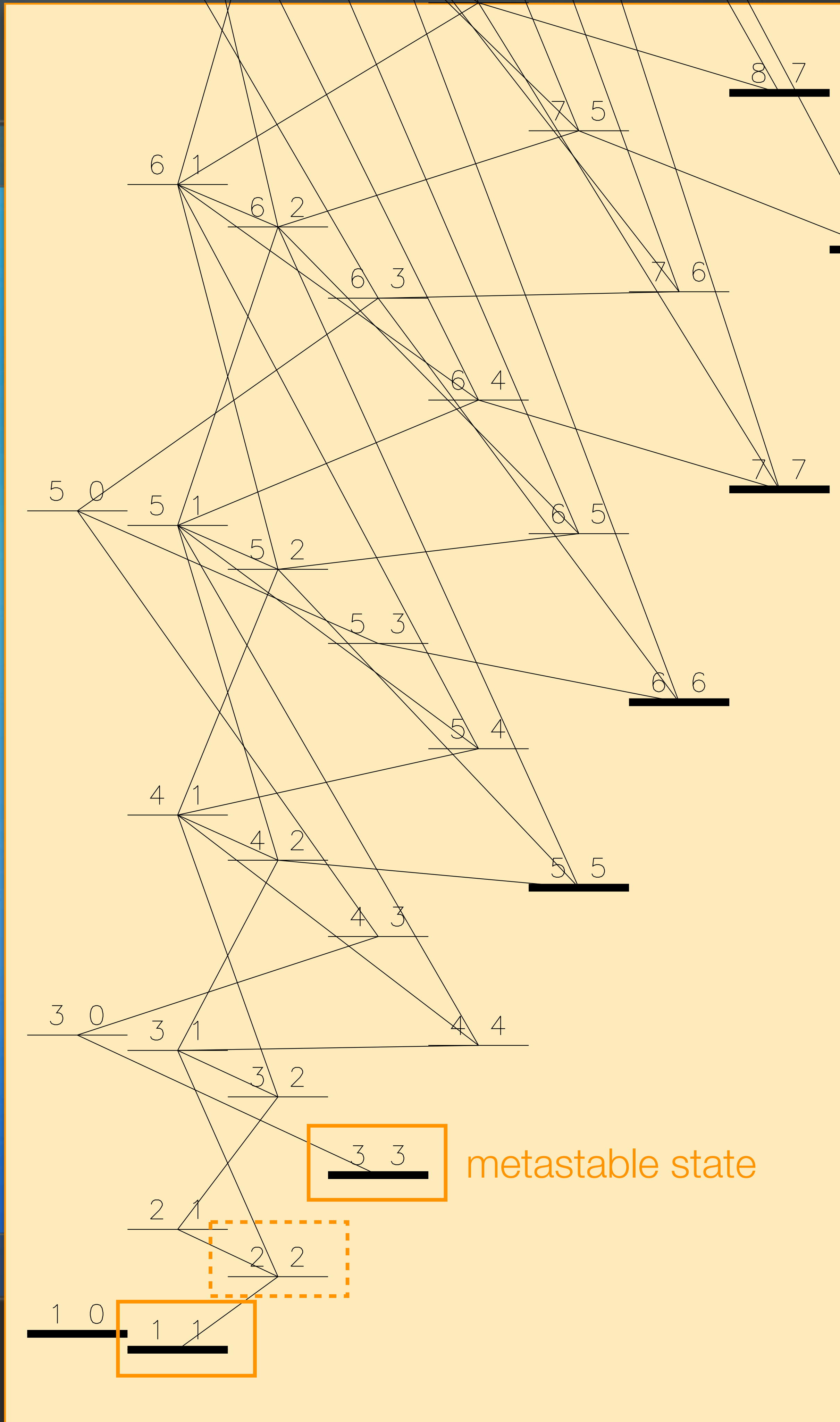
They conclude to a high ionization rate by cosmic rays

Is it cosmic rays or X-rays which are responsible ?
(see T. Montmerle remarks at IAU Symposium 280)

Observation of (3,3), (2,2) (upper limit) and (1,1) show that H_3^+ is present in :

- diffuse medium n_H = 50 - 200 cm^{-3}
- warm gas T = 200 - 300 K

The observation of H3+ not only gives access to the **cosmic rays flux** but also to the **density** and **temperature** of the medium.



H_3^+ in the Galactic center

Atomic and molecular data concerning H_3^+

- Levels energies and radiative transitions
  - B. McCall PhD theses
  - Neal et al. (1996)
  - Miller & Tennyson, ApJ (1988)
  - Lindsay & McCall, JMoSp (2001)

- Collisionnal data : no precise data
  - Expression by Oka & Epp (2004)
  - Our prescription
  - Hugo et al. (2010) : collision rates at low temperature (T < 50 K)
    - show existence of selection rules

$$k_{JK}^{J'K'} = C_{JK}^{J'K'} \sqrt{\frac{g_{JK}}{g_{J'K'}}} \exp\left(-\frac{E_{JK}-E_{J'K'}}{2kT}\right)$$

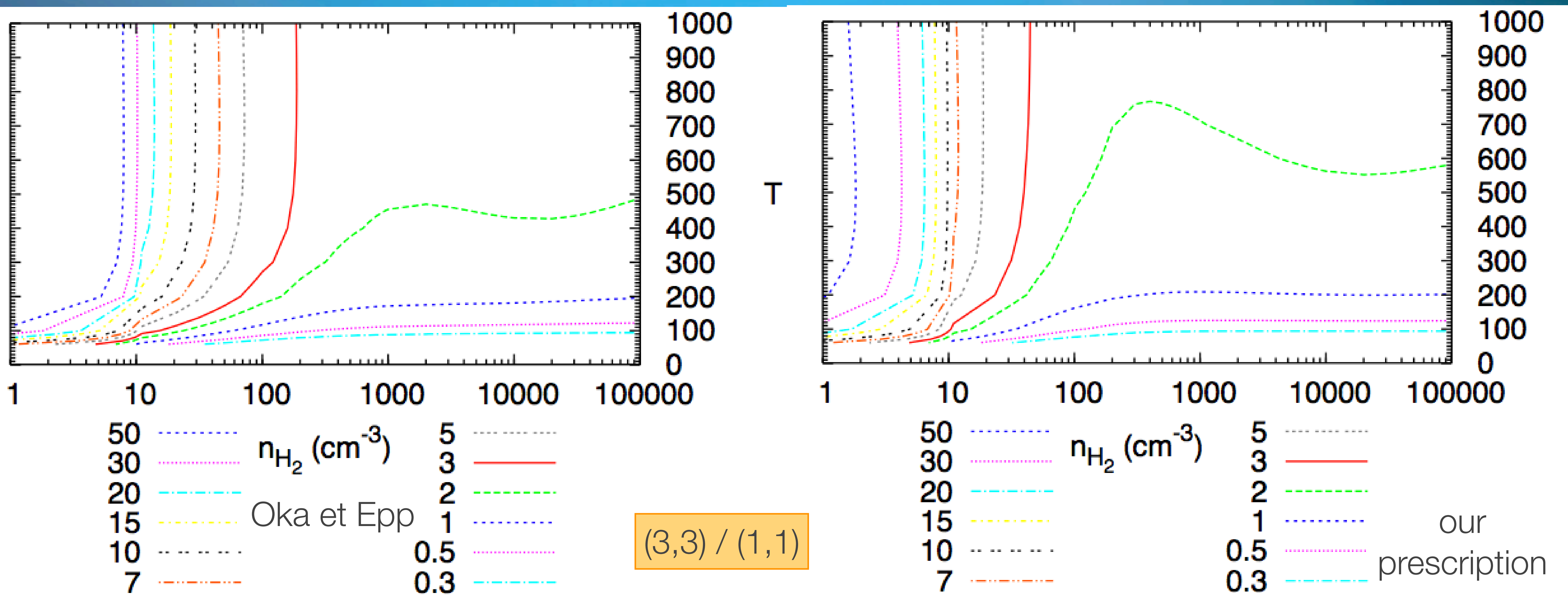
$$C_{JK}^{J'K'} = C_{J'K'}^{JK} = C\left\{1+\sum_{J''K''}\left(\frac{g_{J''K''}}{\sqrt{g_{JK}g_{J'K'}}}\right)^{1/2}\exp\left[-\frac{E_{J''K''}-(1/2)(E_{JK}+E_{J'K'})}{2kT}\right]\right\}^{-1}$$

C = 2×10^{-9} cm^3 s^{-1} : Langevin rate constant for H_3^+ + H_2

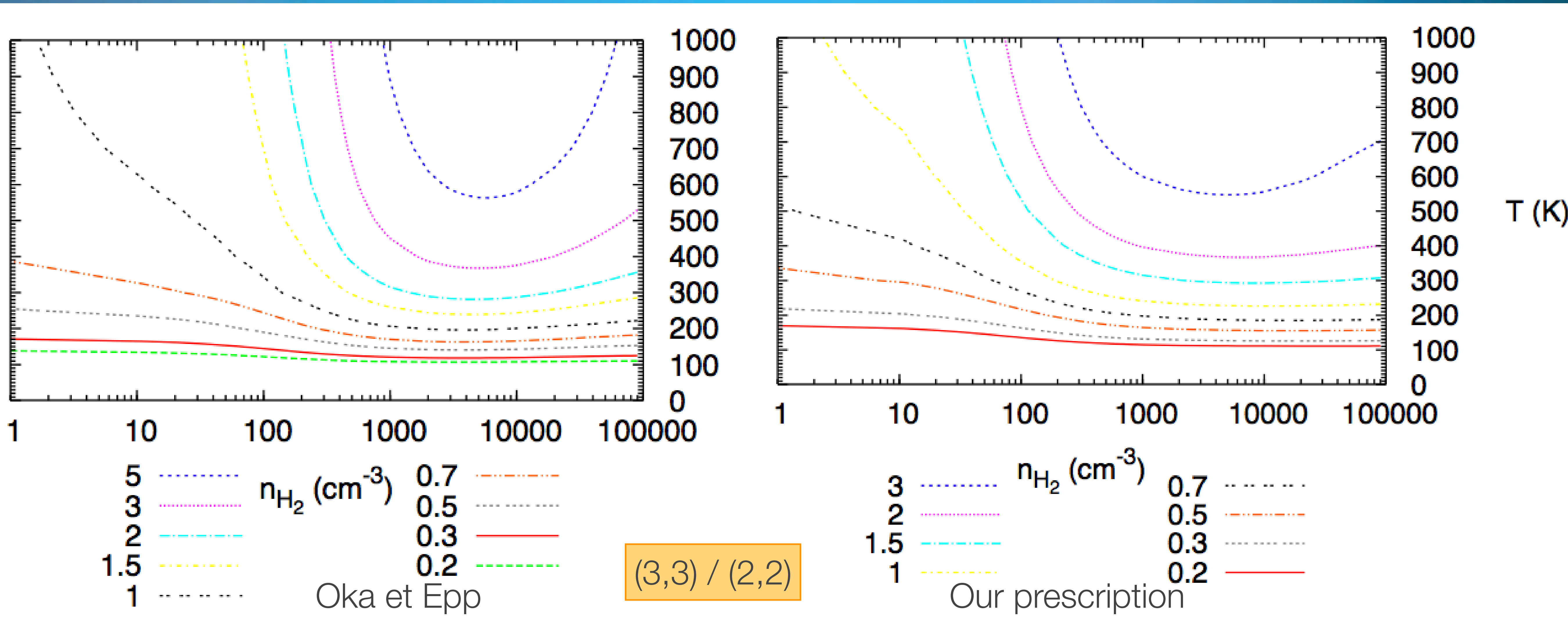
Poor knowledge of H_3^+ + H_2 collision rates

		p-H_3^+ p-H_2	p-H_3^+ o-H_2	o-H_3^+ p-H_2	o-H_3^+ o-H_2
p-H_3^+	p-H_2	1.89(−9) 0.00	8.16(−10) 164.9	F	5.88(−10) 198.2
p-H_3^+	o-H_2	2.98(−10) −0.69	1.13(−9) −0.19	3.46(−10) −0.69	8.03(−10) 32.6
o-H_3^+	p-H_2	F	1.50(−9) 136.2	1.84(−9) −0.26	8.84(−9) 170.0
o-H_3^+	o-H_2	1.04(−10) 0.00	4.00(−10) −0.19	9.67(−11) −0.14	1.29(−9) 0.07

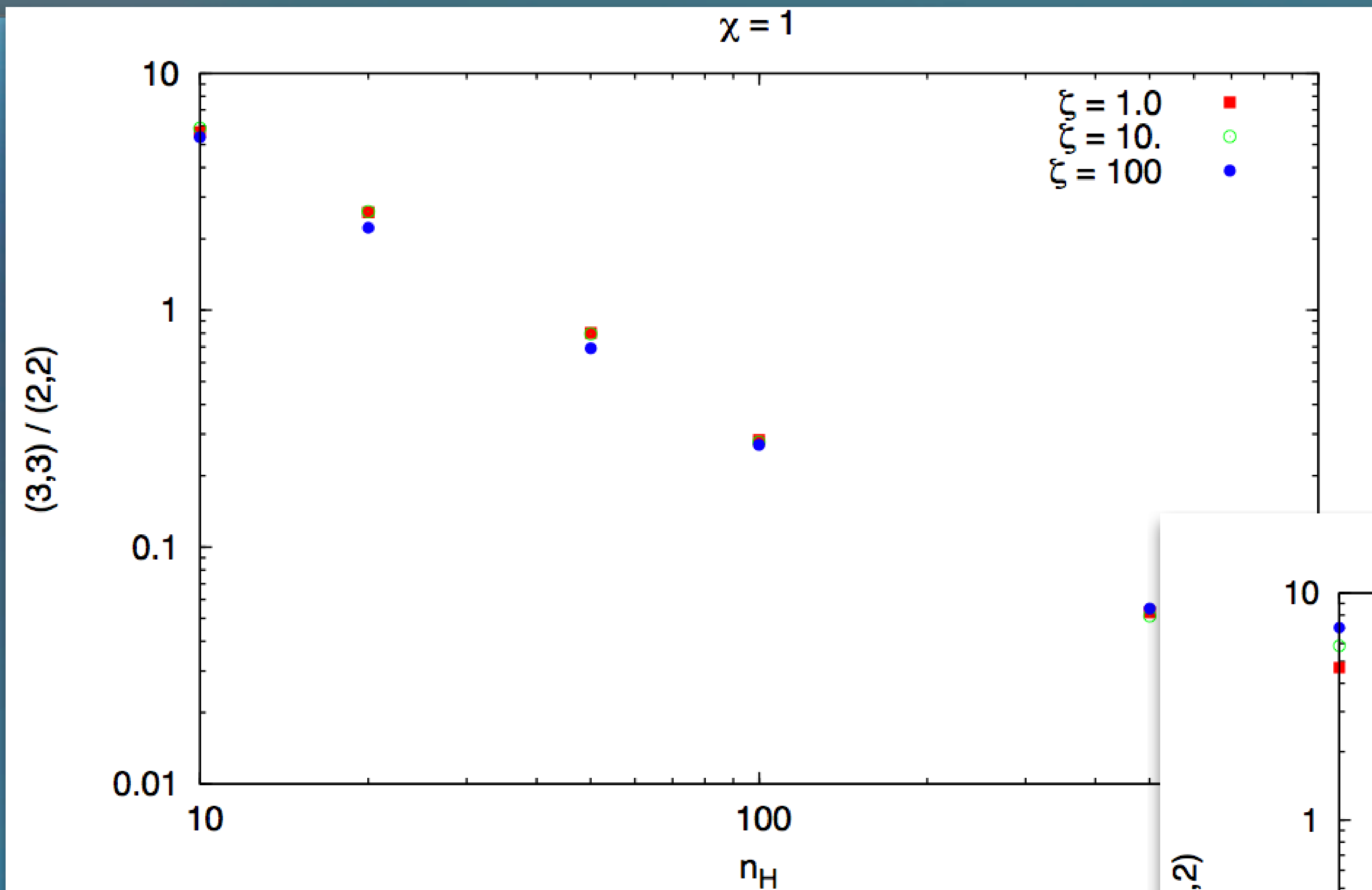
H_3^+ in the Galactic center



H_3^+ in the Galactic center

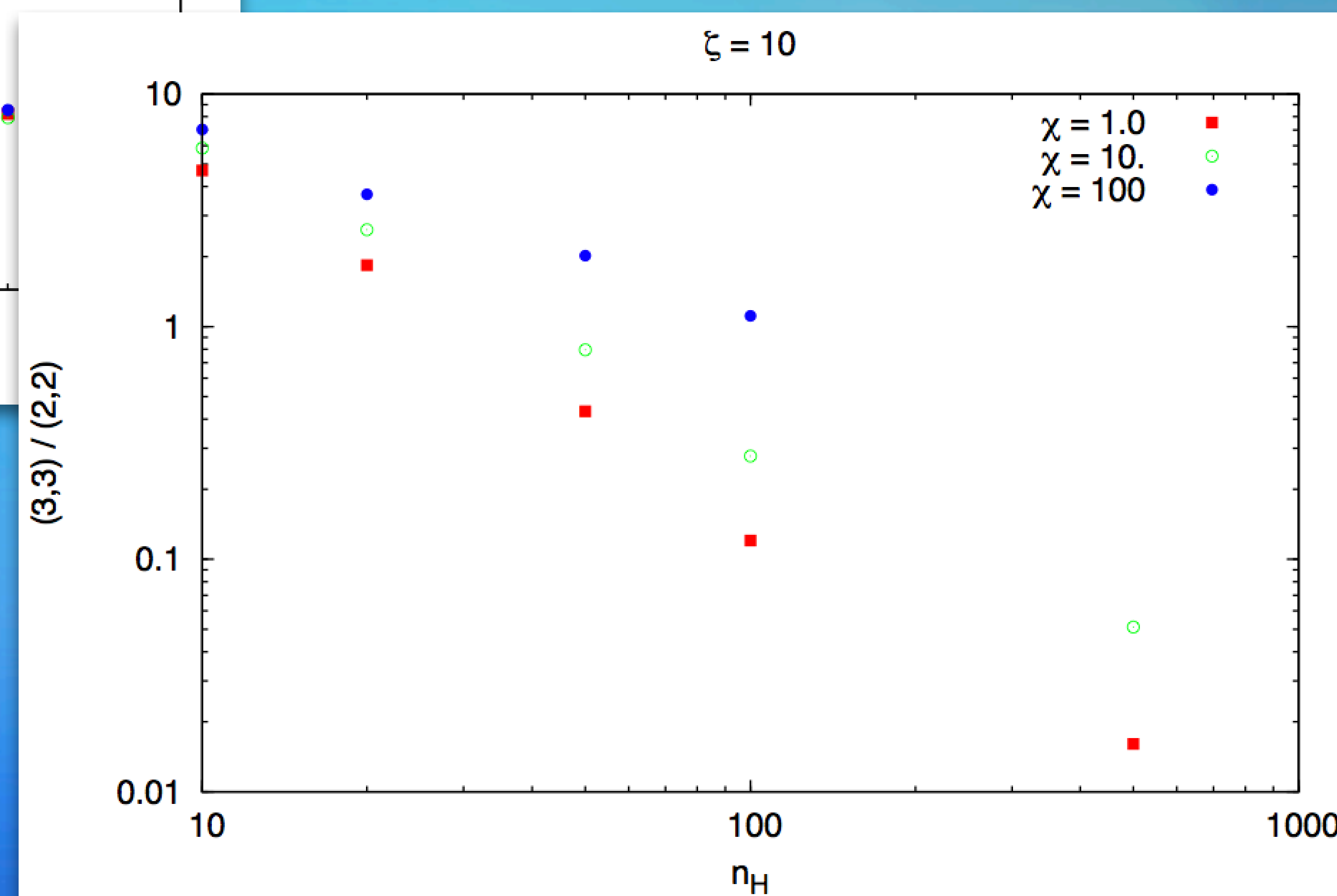


H_3^+ in the Galactic center



PDR model

- ζ has no impact on (3,3) / (2,2)
- PDR models confirm a low density



- The intensity of the UV flux has not a significant role for low density medium

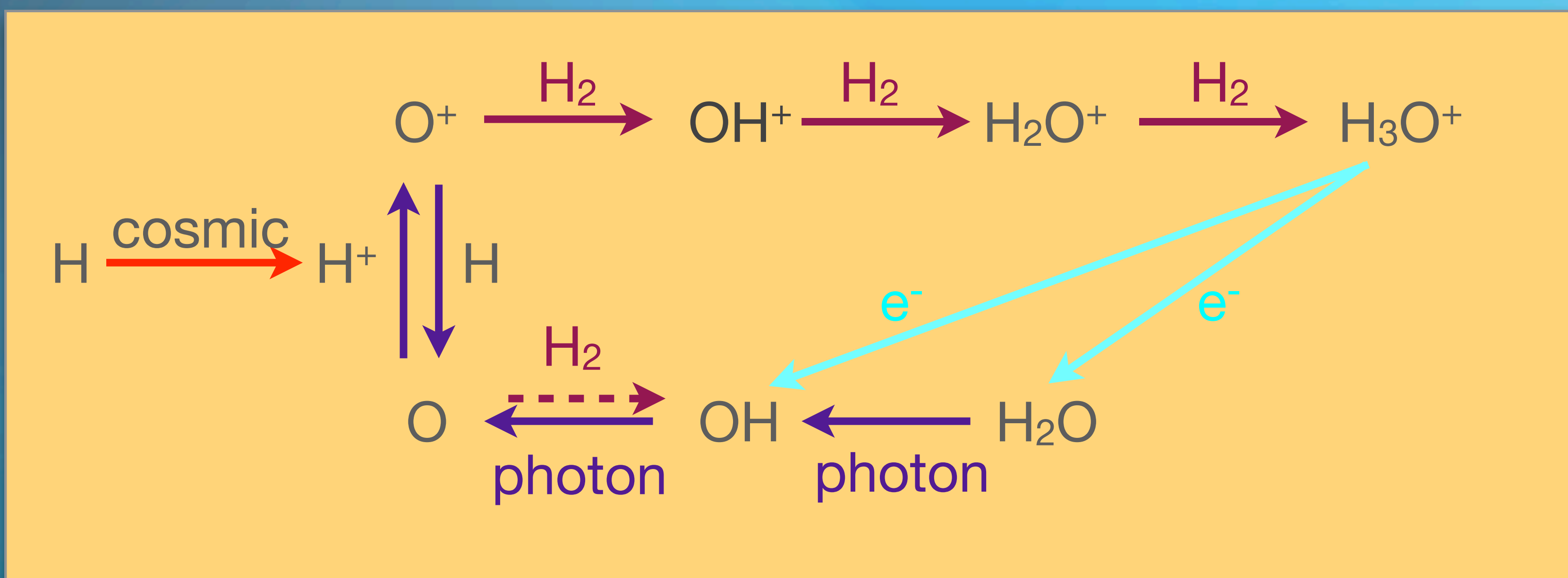
These models confirm the results obtained by Geballe, Oka et al.

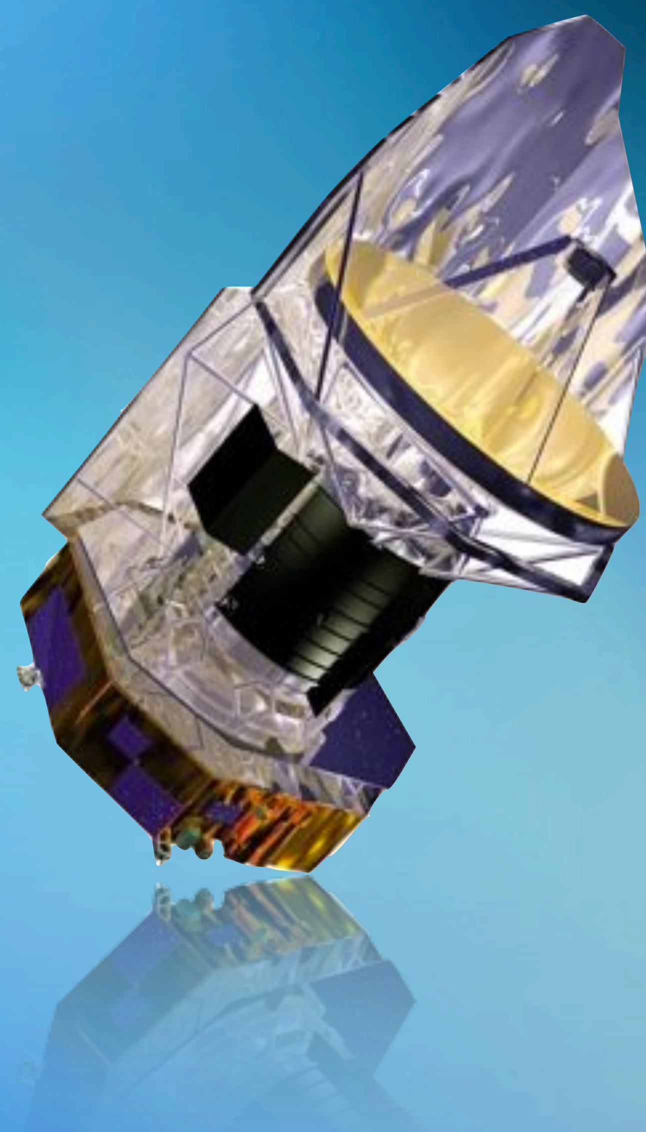
Herschel results : OH^+ and H_2O^+

Key program PRISMAS (M. Gerin et al.)

Search for hydrids in diffuse medium

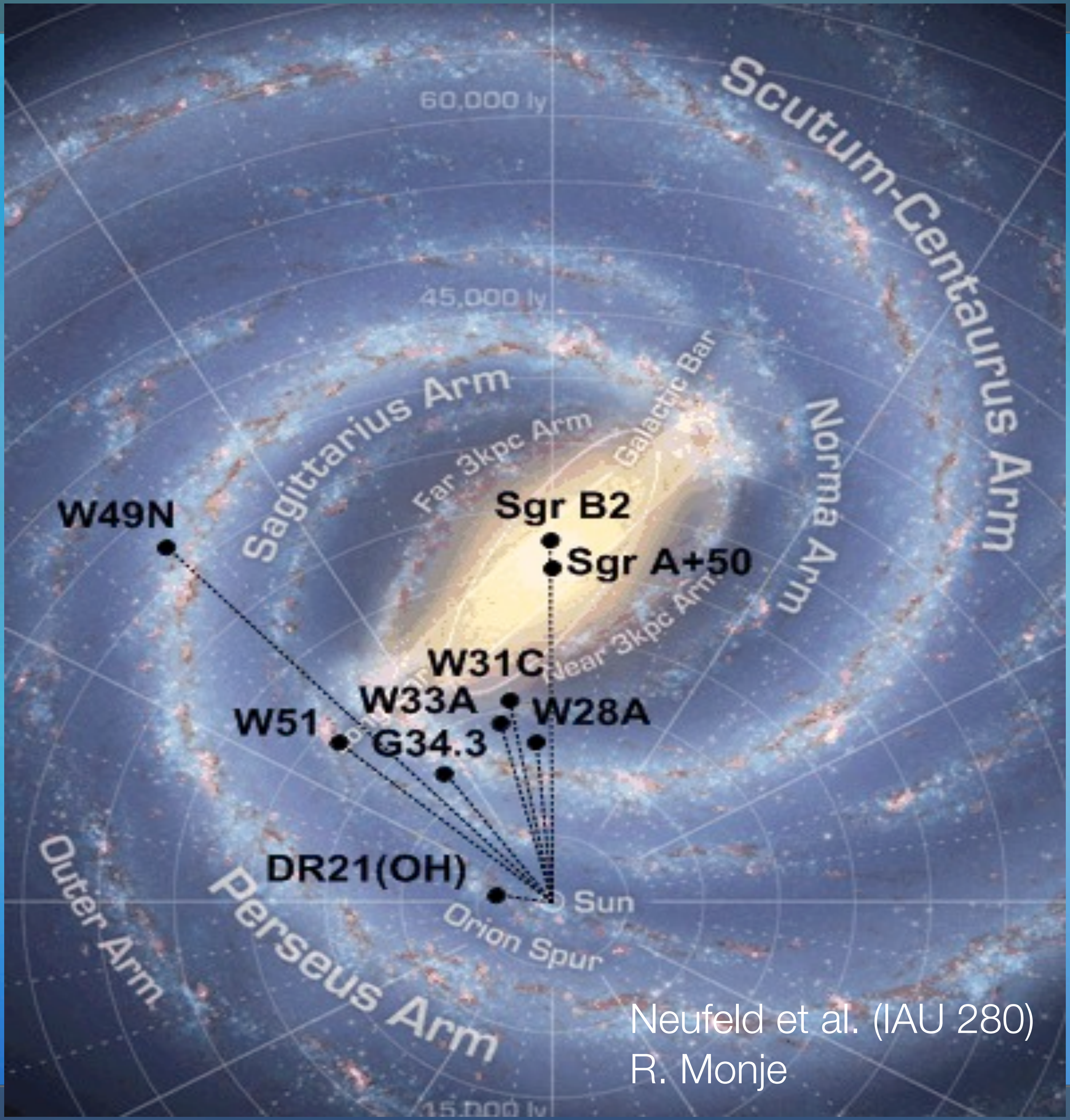
Among them : OH^+, H_2O^+
Chemistry initiated by cosmic rays





O cannot react with H_2 for $T < 300$ K

Herschel results : OH^+ and H_2O^+

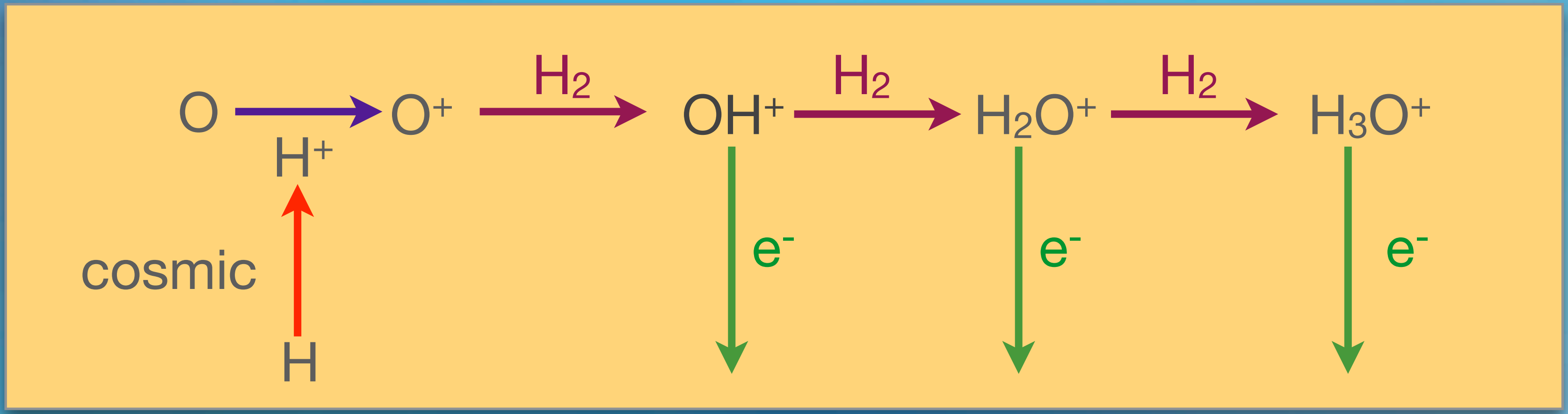


Neufeld et al. (IAU 280)
R. Monje

Herschel results : OH^+ and H_2O^+

Detection of OH^+ and H_2O^+
Neufeld et al. (2010), Gerin et al. (2010)

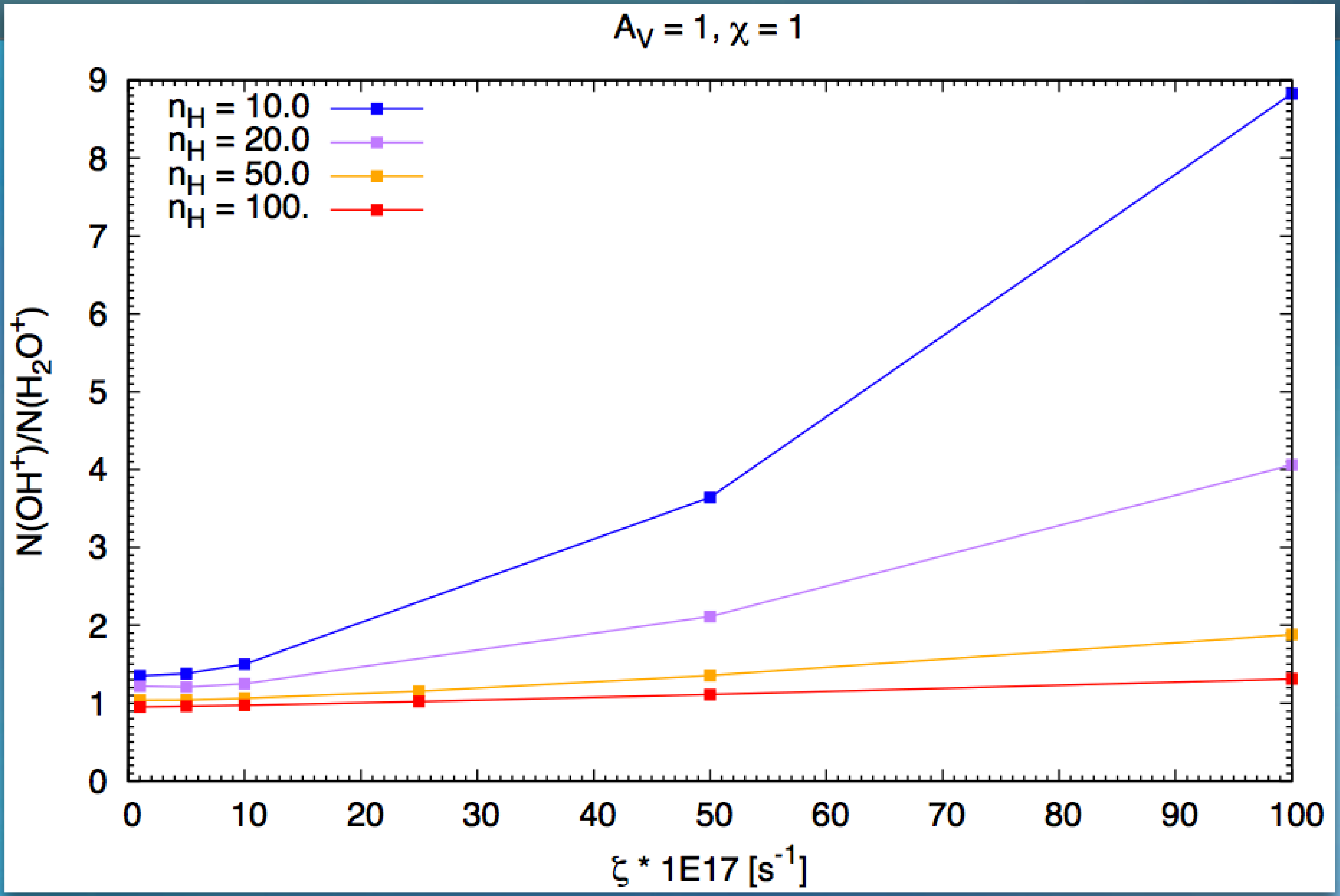
Unexpected result : OH^+ / H_2O^+ = 3 - 15
This means that dissociation with electrons compete with H_2 reactions



$$\frac{n(OH^+)}{n(H_2O^+)} = 0.63 + \frac{0.11}{f_{H_2}} \left(\frac{T}{300}\right)^{-0.5}$$

The ratio does not depend directly on ζ but on f_{H2} and T

Herschel results : OH^+ and H_2O^+



The lower the density, the higher $N(OH^+) / N(H_2O^+)$ depends on the flux of cosmic rays

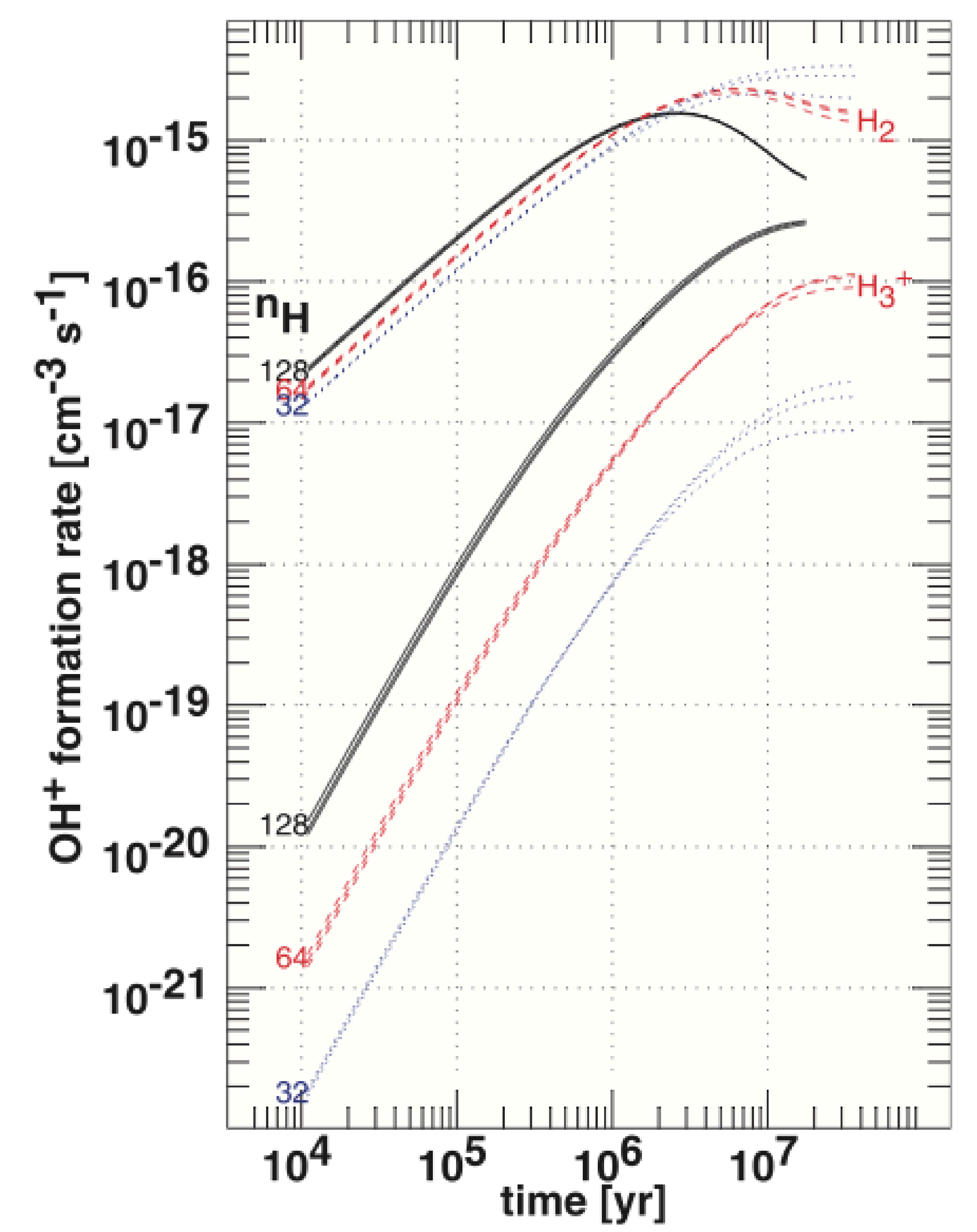
High flux of cosmic rays helps to maintain a high OH^+ / $H2O^+$ ratio

Herschel results : OH^+ and H_2O^+

Other explanation : time dependent effect

Liszt (A&A - 2007) predicted the abundance of OH^+

He showed that OH^+ could be quite abundant before the gas reaches a steady state.



Conclusions

Diffuse interstellar clouds are wonderful places to study cosmic rays chemistry

To interpret observations :

simple formula are nice, but it is even better to :

- try to gather as much constraints as possible
- try to build a consistent model with more constraints as parameters

We have now several observations that shows that :

- zeta is a few 1E-16 up to 1E-15 in some diffuse interstellar clouds
- the density of diffuse clouds can be quite low
- OH^+ and H_2O^+ seems to be present in low density, low molecular fraction clouds

- H_3^+ is a wonderful molecule
  - flux of cosmic rays
  - density of the gas
  - temperature of the gas

but we need its collision rates.

Future developments of the PDR code
http://pdr.obspm.fr

- Implementation of X-rays physics
- Better implementation of cosmic rays
  - Energy deposit of supra-thermal electrons
  - stochastic heating of grains
  - effect on grain surface chemistry

ANR Sympatico