H_3^+ in the Diffuse Interstellar Medium
The Problem of the Ionization

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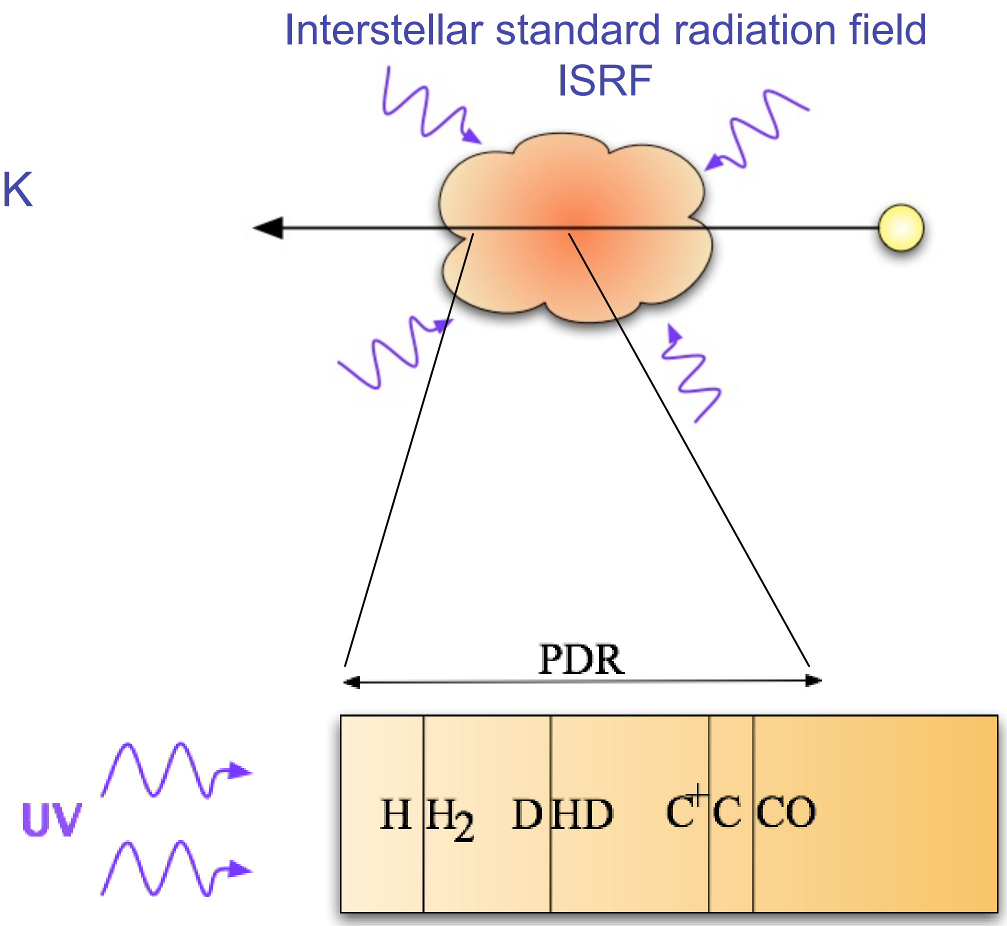
Diffuse clouds

Properties:

- Density: $n_H \approx 100\ cm^{-3}$
- embedded in the ISRF
- Kinetic temperature $T_{kin} \approx T_{01} \approx 70$ K
- Transition between atomic and molecular hydrogen



Observation in absorption possible

- Far UV : H, H_2, HD, CO, …
- Visible: OH, CH, CH^+, CN, C_2, C_3, …
- IR: H_3^+
- Radio : HCO^+, HOC^+, NH_3, HCN, HNC, H_2S, …

Interest to study diffuse clouds

Simple chemistry ➔ good place to understand the physics of ISM

Two fundamental questions:

- **dissipation of energy**
  - formation process of CH^+
  - rotationnal excitation of H_2

- **ionization**
  - the formation of many molecules is initiated by cosmic rays ionization
    H_3^+, HD, OH, …

Formation:	H_2 + cosm. ray $\longrightarrow$	$H_2^+ + e^-$	$k = 0.96 \times \zeta$
	$H_2^+ + H_2$ $\longrightarrow$	$H_3^+ + H$	$k = 2.1\ 10^{-9}$
Destruction:	$H_3^+ + e^-$ $\longrightarrow$	…	$k = 6.80{\times}10^{-8}\ (T/300)^{-0.5}$

$$n(HD),\ n(OH),\ n(H_3^+) \propto \zeta$$

Determination of the ionization rate by cosmic rays

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

$$H + \text{cosmic ray} \rightarrow H^+ + e^-$$
$$H^+ + O \rightarrow O^+ + H$$
$$O^+ + H_2 \rightarrow OH^+ + H$$
$$OH^+ + H_2 \rightarrow H_2O^+ + H$$
$$H_2O^+ + H_2 \rightarrow H_3O^+ + H$$
$$H_3O^+ + e^- \rightarrow \mathbf{OH} + \ldots$$

n(OH) $\propto$ cosmic rays flux

determination of ζ

$$H + \text{cosmic ray} \rightarrow H^+ + e^-$$
$$H^+ + D \rightarrow D^+ + H$$
$$D^+ + H_2 \rightarrow \mathbf{HD} + H^+$$

n(HD) $\propto$ D/H $\times$ cosmic rays flux

D/H

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

H_3^+ in diffuse clouds

Observation:

- detected on 8 diffuse lines of sight
  $N(H_3^+) / E(B\text{-}V) \sim$ some 10^{14}
  => 10 × higher than dense clouds

- in diffuse medium near the Galactic center
  (Oka et al. 2005)

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)	$N(H_3^+)$
Cyg. OB2 12	3.35	2.02 (14)
Cyg. OB2 5	1.99	~ 3 (14)
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)
Gal. center		3.1 (15)

Ref: McCall et al. (2002)
McCall et al. (2003)
Oka et al. (2005)

The Zeta Per line of sight

A very well studied line of sight

Spectral type : B1
R_V = 2.8 (Cardelli et al. 1989)
E(B-V) = 0.32 (van Dishoeck & Black 1989)

A very good test for models

	Observation
H_2	3.2 - 7.1 (20)
H_2 (J=0)	2.2 - 4.8 (20)
H_2 (J=1)	1.0 - 2.3 (20)
H_2 (J=2)	1.1 - 2.4 (18)
H_2 (J=3)	2.0 - 9.6 (16)
H_2 (J=4)	1.1 - 2.0 (15)
H_2 (J=5)	2.3 - 2.8 (14)

	Observations	
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)

Determination of the flux of cosmic rays

- Black, Hartquist & Dalgarno (1978)
  2 components model
  - cold zone: T = 45 K, n_H = 267 cm^{-3}
  - hot zone: T = 120 K , n_H = 100 cm^{-3}

  $\zeta = 2.2\times10^{-17}\ s^{-1}$

- van Dishoeck & Black (1986)
  all constraints taken into account (at this time …)
  models with T and n_H profile

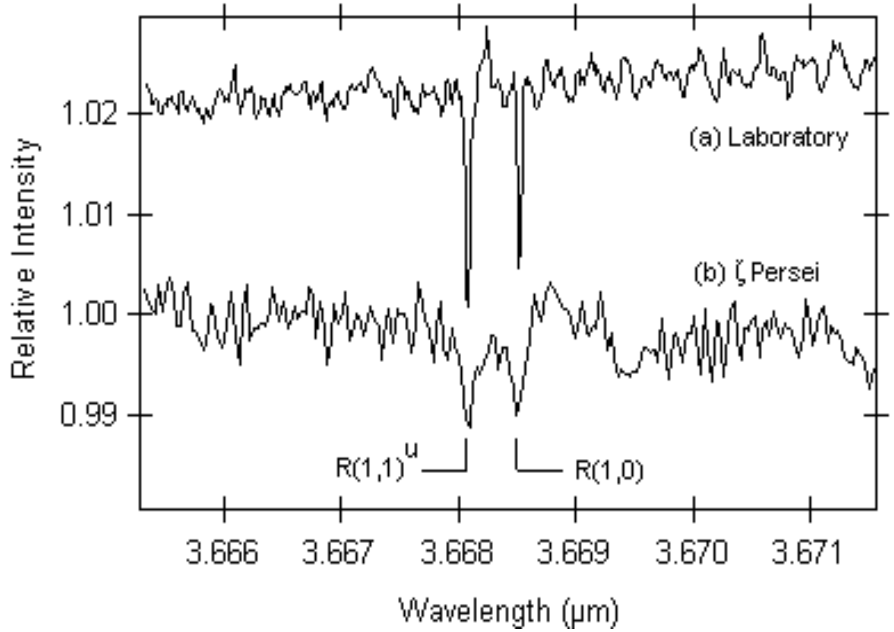
  $\zeta = 4\text{-}7\times10^{-17}\ s^{-1}$

- Federman et al. (1996)
  From OH only : $\zeta = 1.7\times10^{-17}\ s^{-1}$

Observation of H_3^+ towards ζ Per:

- McCall et al. (2003) :
  - -Determination of the recombination rate of H_3^+
  - $-N(H_3^+) = 8.0 \times 10^{13}$ cm^{-2}

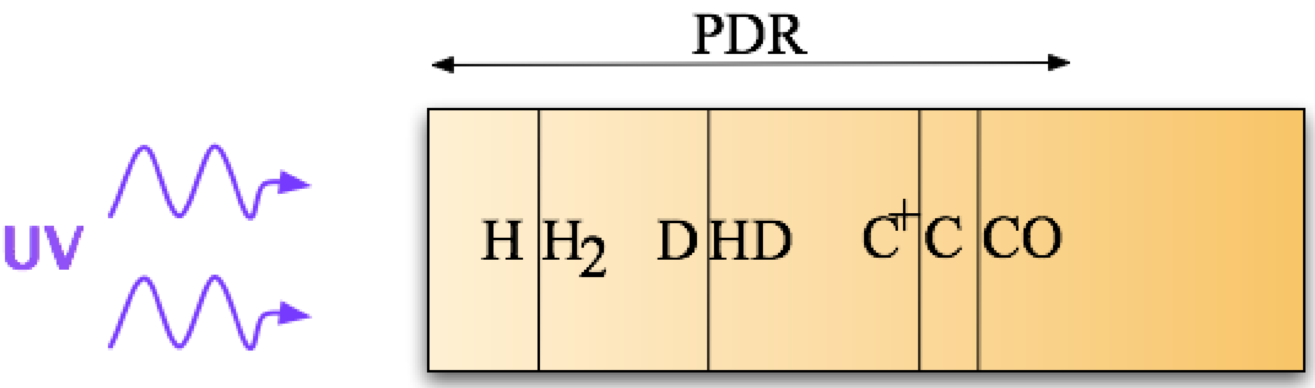
$\zeta = 1.2 \times 10^{-15}$ s^{-1}



Comparison of ζ between different authors not always simple:

H + cosm. ray	→ H^+ + e^-	$k = 0.46 \times \zeta$ (s^{-1})	- Prassad & Huntress (1980)
H_2 + cosm. ray	→ H_2^+ + e^-	$k = 0.96 \times \zeta$ (s^{-1})	- A. Dalgarno (priv. com.)
	H + H	$k = 1.50 \times \zeta$ (s^{-1})	- A. Dalgarno (priv. com.)
	H^+ + H + e^-	$k = 0.04 \times \zeta$ (s^{-1})	- A. Dalgarno (priv. com.)

The Meudon PDR code *(http://aristote.obspm.fr/MIS)*



Stationnary model solving:

- Radiative transfer: absorption in the lines of H, H_2, CO, HD, …
  absorption in the continuum

- Chemistry: more than 100 chemical species
  network of more than 1000 chemical reactions
  photoionization

- Statistical equilibrium of the populations in the levels of H_2, HD, CO, HCO^+, CS, …
  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

Modelisation of the ζ Per line of sight
(Franck Le Petit, Evelyne Roueff & Eric Herbst, A&A, 2004)

Parameters and hypothesis :

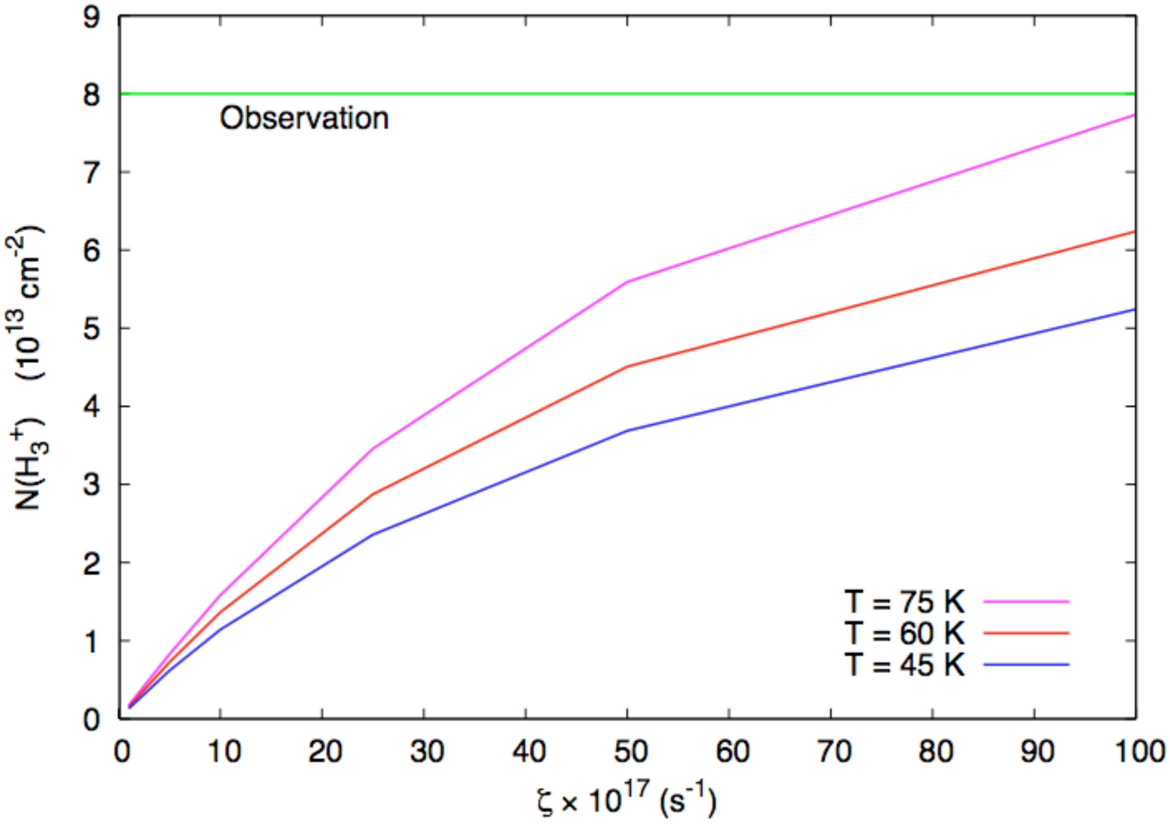
$R_V = 2.8$
Isothermal model : $T_{01} = 60$ K (45-75 K)
$N(H_2) = 4.5 \times 10^{20}$ cm^{-2}

$n_H = 100$ cm^{-3}
$\chi = 2$

	Relative abundance
D/H	1.5 (-5)
O/H	3.2 (-4)
N/H	7.5 (-5)
C/H	1.32 (-4)
S/H	1.86 (-5)
Si/H	2.9 (-5)

Variation of ζ between 1×10^{-17} and 100×10^{-17} s^{-1}
⇘ effect on species sensible to ζ

Determination of ζ from H_3^+



Depends on T

Observations require : $\zeta \sim 100 \times 10^{-17}\ cm^{-3}$

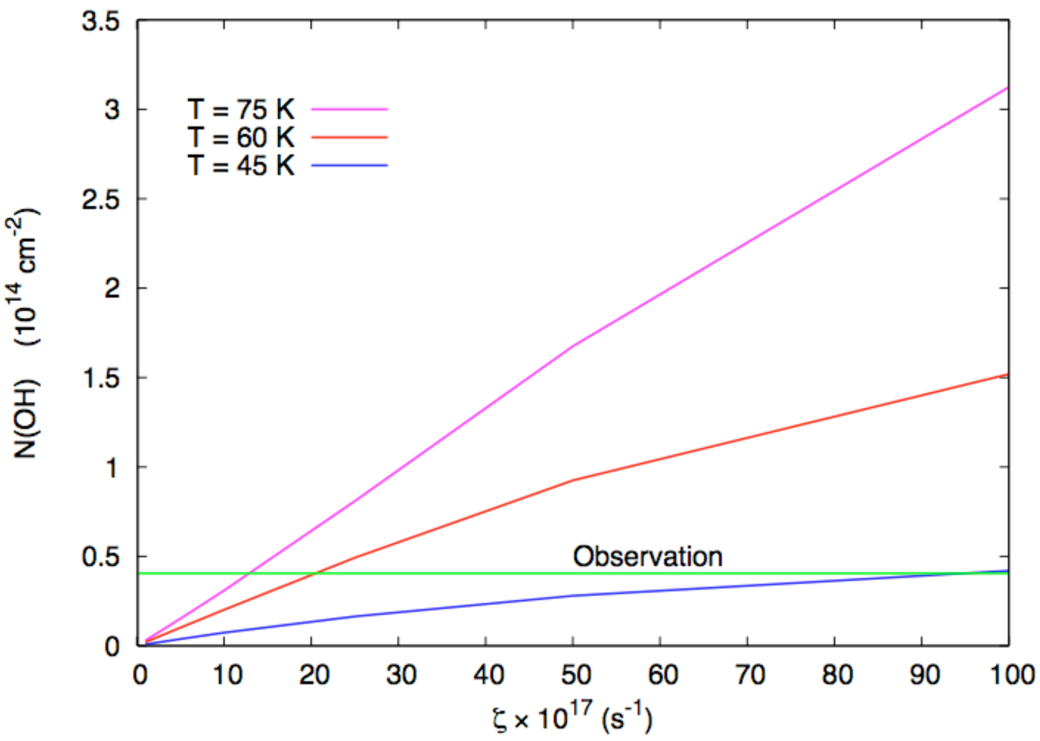
Determination of ζ from OH

n(OH) is highly dependent on T

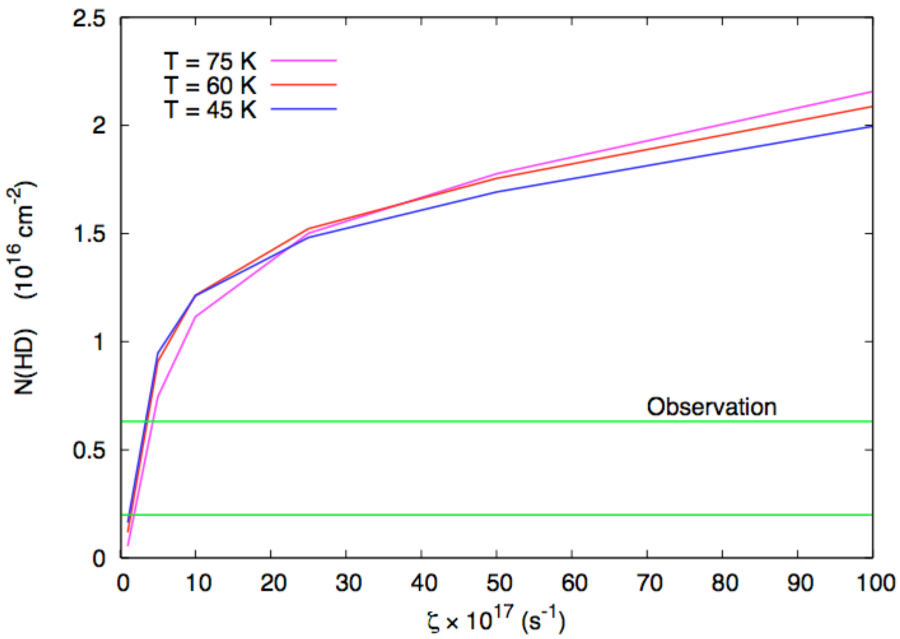
$$H^+ + O \longrightarrow O^+ + H \qquad k = 6\times10^{-10}\, e^{-227/T}\ cm^3\, s^{-1}$$

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

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



HD as a constraint on ζ



- **not much dependent on T**

$H^+ + D \longrightarrow D^+ + H \quad k = 10^{-9}\, e^{-41/T}$

$D^+ + H_2 \longrightarrow HD + H^+ \quad k = 1.2\ 10^{-9}$

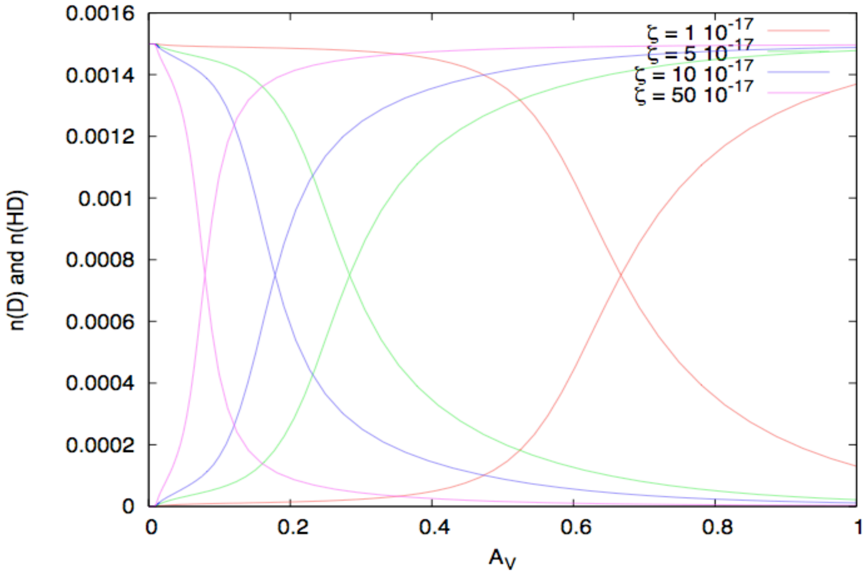
- **good constraint for $\zeta < 10^{-16}\ s^{-1}$**

n(HD) $\propto \zeta$ **if** : 1) It is formed in gas phase by $D^+ + H_2$
2) It is destroyed by photodissociation

after the D/HD transition :

$HD + H_3^+ \longrightarrow H_2D^+ + H$

n(HD) no more proportionnal to ζ



- still some debates on D/H
- difficult to get a precise value of N(HD)

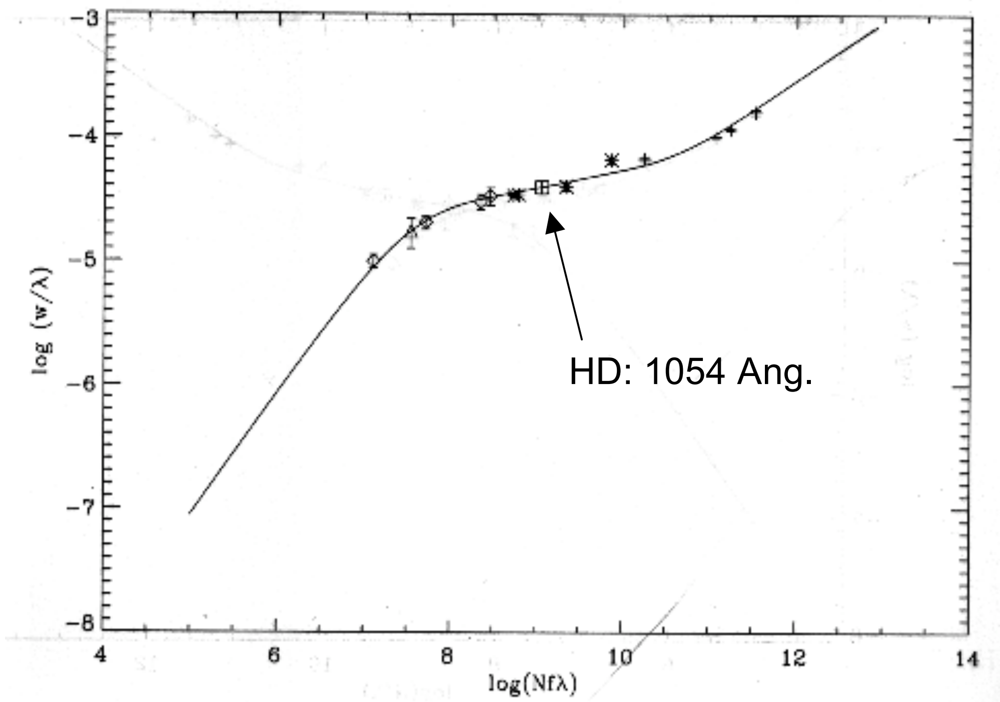
  Determination of N(HD) requires to know precisely the b Doppler parameter

<u>Towards ζ Per :</u>

- Only HD at 1054 Ang. detected
- flat part of the curve of growth

- Re-analysis with updated H_2, f values (Abgrall et al. 1993)
  - max value: 1.1×10^{16} cm^{-2}
  - instead of 5.1×10^{15} cm^{-2} (Snow 1977)

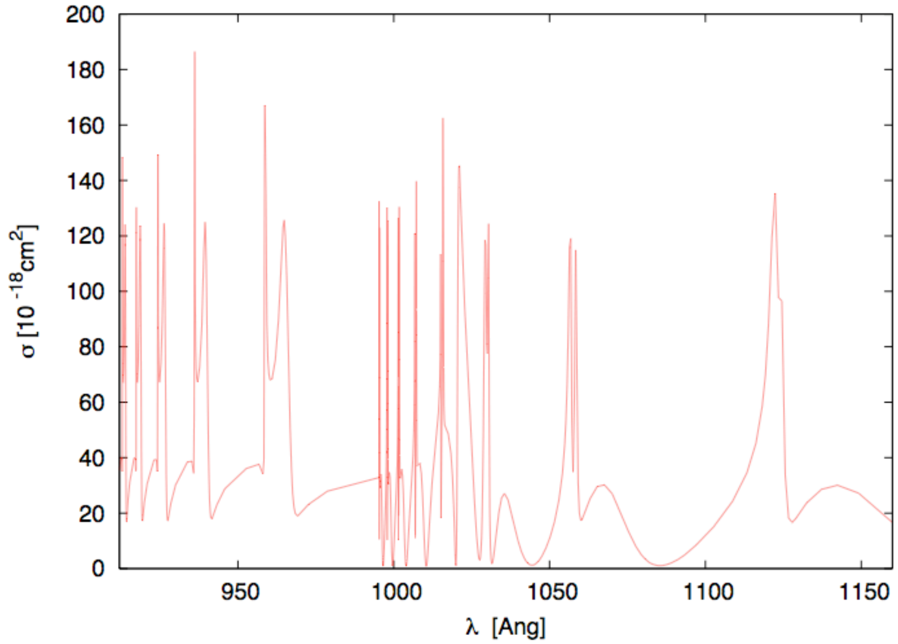
<u>Other lines of sight:</u> same problem



Conclusion from N(HD) : ζ> 5 10^{-17} s^{-1} overestimates slightly N(HD)

(with D/H = 1.5 10^{-5})

The neutral and ionized atoms



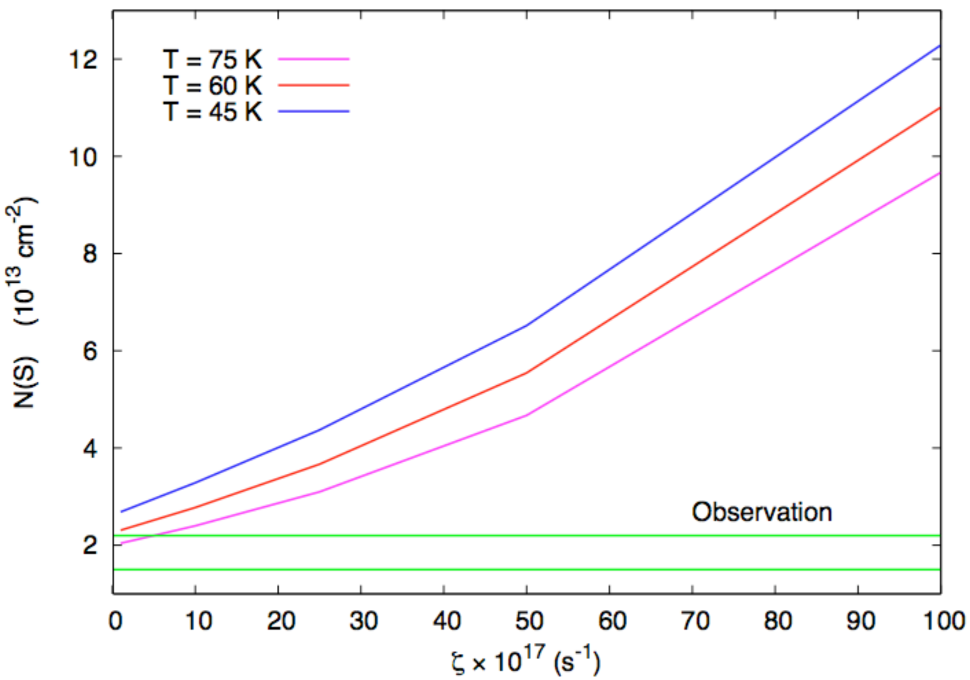
High ζ increases the ionization degree

Efficient recombination with electrons :

S^+ does not react with H or H_2

↳ reactive recombination dominates

$$S^+ + e^- \longrightarrow S + h\nu$$
$$S + h\nu \longrightarrow S^+ + e^-$$



$\zeta = 100\times10^{-17}\ s^{-1}$

⇩

overproduction of neutral sulfur

Conclusion about the ζ Per line of sight

n_H = 100 cm^{-3}, χ = 2
T = 60 K,
N(H_2) = 4.5 10^{20} cm^{-2}

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)

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

- **ζ = 100 times the standard value and T = 60 K**
  Reproduce N(H_3^+) but overproduce
  OH by a factor 4
  S by a factor 6

  T can be decreased to 45 K to match better OH
  negative impact on C, S, H_3^+

  χ can be increased to match better S
  molecules too much photodissociated

- **ζ = 25 × 10^{-17} s^{-1} good compromise to fit all abundances**

H_3^+ towards the Galactic center

Observations *(Oka et al. 2005)*

Clouds	N(H_3^+) [10^{14} cm^{-2}]						T [K]	n [cm^{-3}]
	(1,1)	(3,3)	(2,2)	(1,0)	HM	Total		
-100 km s^{-1}	**7.0±0.8**	**4.4 ± 0.9**	**≤ 0.7**	**2.9 ± 1.0**	***1.4 ± 0.7***	**15.7 ± 1.7**	**270 ± 70**	**≤ 50**
-50 km s^{-1}	2.6 ± 0.5	1.6 ± 0.6	0.4 ± 0.4	1.6 ± 0.9	0.4 ± 0.2	6.6 ± 1.3	250 ± 100	≤ 100
0 km s^{-1}	4.9 ± 05	1.0 ± 07	≤ 0.7	2.4 ± 1.3	0.1 ± 0.1	8.4 ± 1.6	130 ± 100	≤ 200

Constraints :

Populations ⟷ n_H, T : Parameters

N(H_3^+) ⟷ ζ, L, (χ)

N(CO, J=0) < 3 10^{16}

f = 0.5 - 1

H_3^+ excitation

- Oka & Epp (2004) prescription for collision rates:

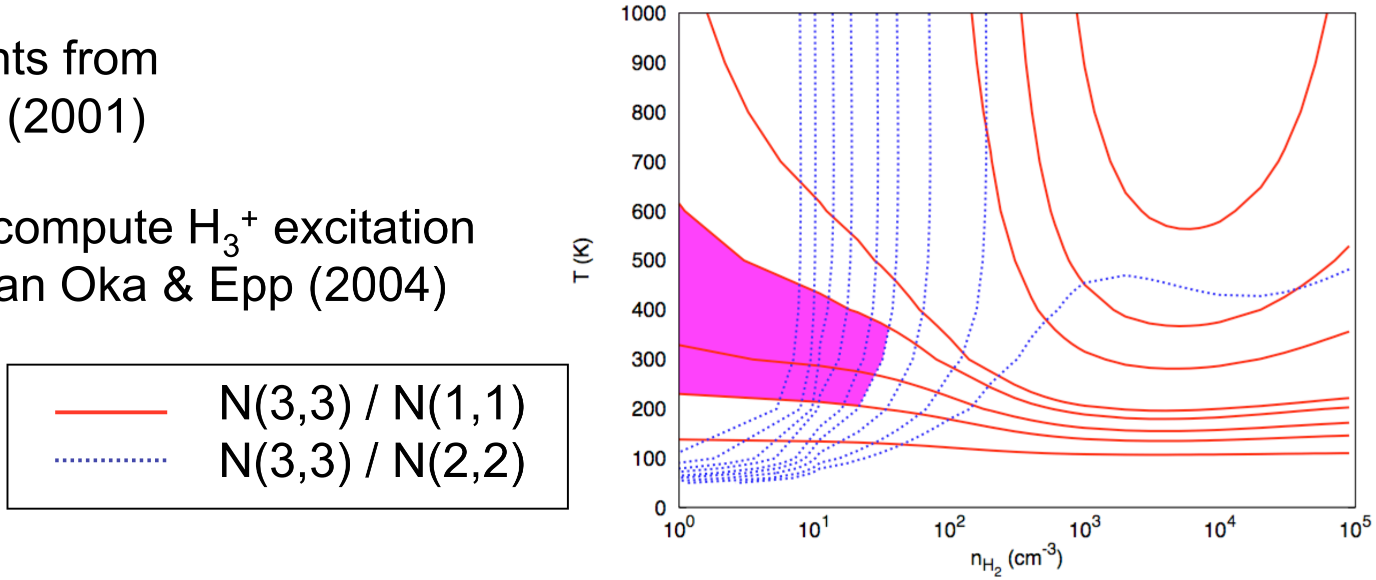
$$k_{JK}^{J'K'} = C_{JK}^{J'K'} \sqrt{\frac{g_{JK}}{g_{J'K'}}} \exp\left(-\frac{E_{JK} - E_{J'K'}}{2kT}\right)$$

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

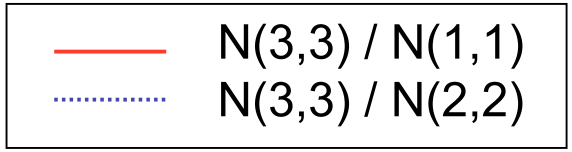
C = 2×10^{-9} cm^3 s^{-1} : Langevin rate constant for $H_3^+ + H_2$

- Einstein coefficients from Lindsay & McCall (2001)

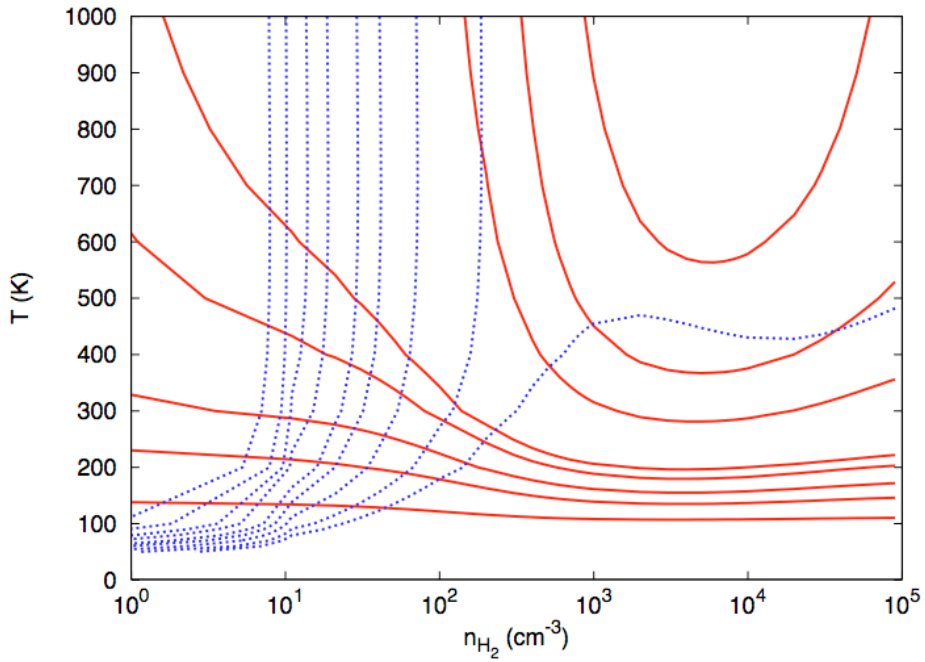
Small program to compute H_3^+ excitation
↳ same results than Oka & Epp (2004)



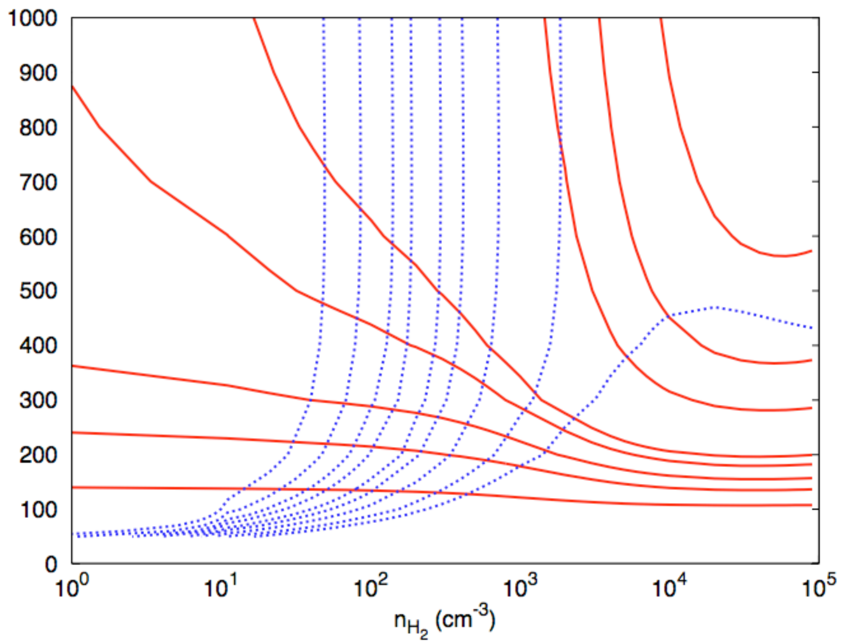
Variation of the collision rates



$C_{Langevin} = 2\ 10^{-9}$



$C_{Langevin} = 2\ 10^{-10}$



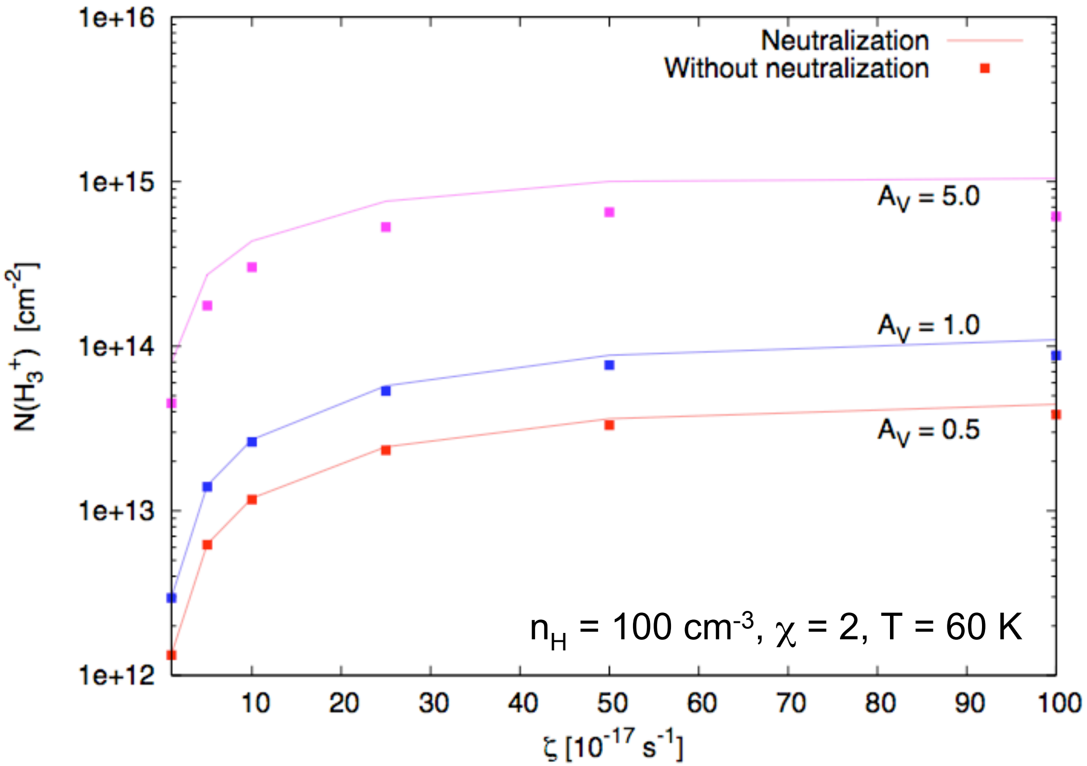
Reduction of $C_{langevin}$: n-T domain reproducing the observations increases higher densities & temperatures allowed

New implementations in the PDR code

1. **Statistical balance of H_3^+**
   - H_3^+ formed following a Boltzman distribution at T_{kin}
     - Tests: formation in specific levels
       - ↳ no significant differences
   - destruction independent of levels

2. **Neutralization of atomic ions on grains**
   (Previous study by H. Liszt 2003)

	$N(H_3^+)$	
$\zeta = 100 \times 10^{-17}$ s^{-1}	With neutr.	Without neutr.
Av = 0.5	4.4 (13)	3.8 (13)
Av = 1.0	1.1 (14)	8.8 (13)
Av = 5.0	1.0 (15)	6.1 (14)



Isothermal PDR models

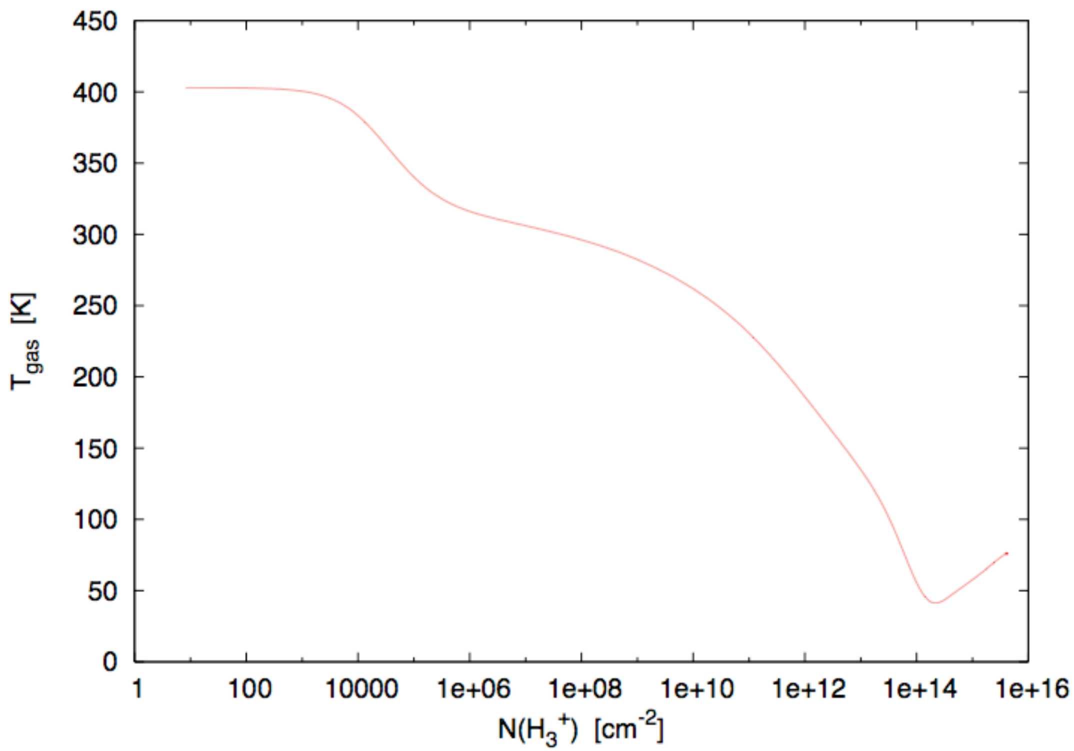
$\chi = 10, \quad R_X = 3$

n [cm^{-3}]	ζ [10^{-17} s^{-1}]	T [K]	L [pc]	f	N(CO) [cm^{-2}]	J = 1 [cm^{-2}]	N(H_3^+) [cm^{-2}]	1,1 [cm^{-2}]	2,2 [cm^{-2}]	3,3 [cm^{-2}]
10	25	270	100	0.61	1.3 (17)	6.6 (16)	1.2 (15)	5.2 (14)	1.2 (13)	3.0 (14)
	50	270	100	0.42	1.4 (17)	7.0 (16)	1.2 (15)	5.4 (14)	1.4 (13)	3.2 (14)
	100	270	100	0.23	4.4 (16)	1.7 (16)	5.7 (14)	2.5 (14)	7.4 (12)	1.5 (14)
50	50	270	20	0.82	1.5 (17)	6.6 (16)	8.7 (14)	3.5 (14)	3.3 (13)	2.3 (14)
		270	31	0.83	3.4 (17)	1.3 (17)	**1.8 (15)**	**7.3 (14)**	**6.9(13)**	**4.8(14)**
		200	31	0.83	3.9 (17)	1.5 (17)	1.6 (15)	7.0 (14)	6.0 (13)	**3.1 (14)**
		150	33	0.84	4.7 (17)	1.7 (17)	**1.5 (15)**	**7.0 (14)**	**5.4 (13)**	**1.9 (14)**
	100	270	22	0.70	2.4 (17)	1.0 (17)	**1.7 (15)**	**6.7 (14)**	**6.9 (13)**	**4.5 (14)**
	500	270	31	0.26	1.7 (17)	8.2 (16)	**1.5 (15)**	**5.5 (14)**	**7.5 (13)**	**3.8 (13)**
Observations		**min**	**15-20**	**0.5**		**< 3 (16)**	**1.4 (15)**	**6.2 (14)**	**< 7 (13)**	**3.5 (14)**
		max		**1**			**1.7 (15)**	**7.8 (14)**		**5.3 (14)**

Thermal Balance

How to have $N(H_3) = 10^{14}$ cm^{-2} in a diffuse medium ($n_H < 50$ cm^{-3}) at 270 K ?

Galactic center :
- Radiation field higher
- R_X = 3 - 10 => more coolants
- X-Rays and cosmic rays
- shocks & turbulence
- ⇘ 5-40 km s^{-1}
  (Rodiguez-Fernandez et al. 2004)



<u>Model with thermal balance :</u>

Medium : n_H = 50 cm^{-3}, R_X = 3,

Photoelectric effect : χ = 10

r_{min} = 1 nm

Cosmic ray heating : $\zeta = 100\times10^{-17}$ s^{-1}

Energy input by cosmic ray: γ = 4 - **6 eV**

Turbulence : Shocks & Vortex

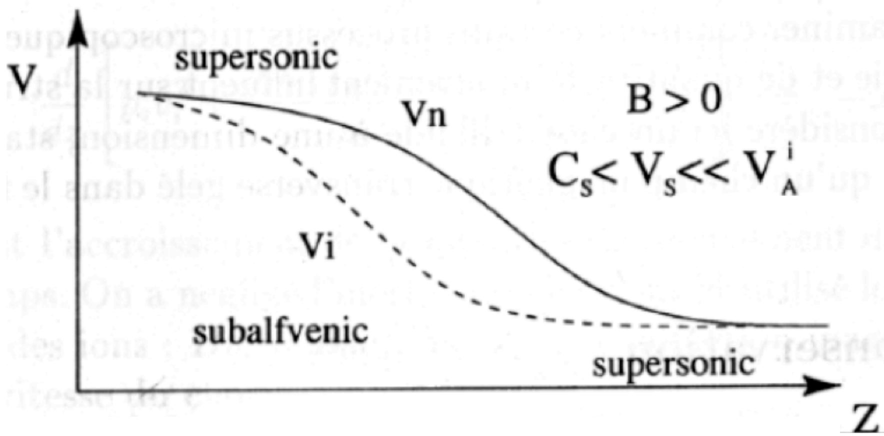
1 - C-shock model :

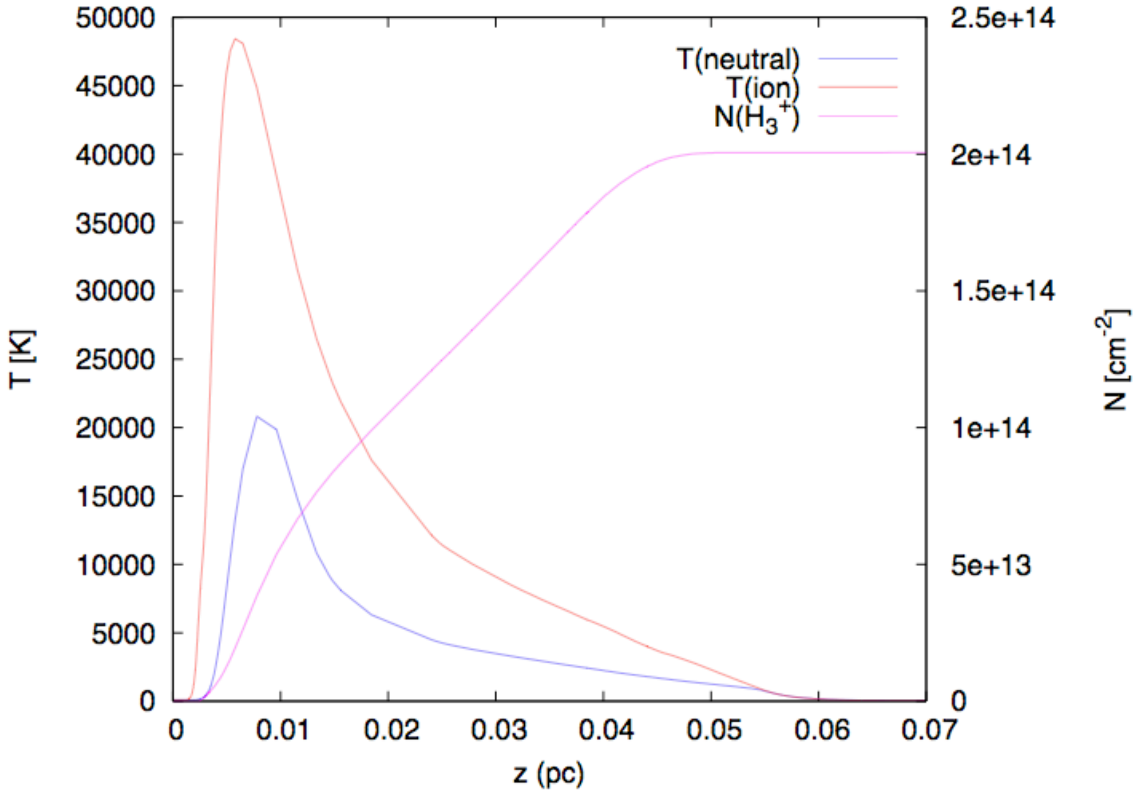
Pre-shock density : 20 cm^{-3}
v_{shock} = 50 km s^{-1}
B = 7 muG

$H^+ + H_2 \longrightarrow H_2^+ + H$
$k = 6.4 \times 10^{-10}\, e^{-21300/T}$

$N(H_3^+) = 2.0 \times 10^{14}$ cm^{-2} $N(CH^+) = 9.1 \times 10^{13}$ cm^{-2} $N(CO) = 5.0 \times 10^{13}$ cm^{-2}

Best PDR isothermal model
$N(H_3^+) = 1.7 \times 10^{15}$ cm^{-2}
$N(CH^+) = 1.1 \times 10^{12}$ cm^{-2}
$N(CO) = 2.4 \times 10^{17}$ cm^{-2}





2 - Vortex

Local and temporal heating of the gas allowing to overcome activation thresholds

- Introduced by K. Joulain & E. Falgarone (1998)
  ⇘ formation of CH^+

$$C^+ + H_2 \longrightarrow CH^+ + H \qquad k = 1.5\ 10^{-10}\ e^{-4640/T}\ cm^3\ s^{-1}$$

- Cecchi-Pestelini, Casu, Dalgarno (2005)
  Model of vortex to compute H_2 excitation

  ⇘ Reproduce rotationnal H_2 excitation (J > 2) in standard diffuse medium

=> test this on the H_3^+ excitation