H_3^+ and the cosmic-ray ionization rate in the Galactic Center: the dual role of (secondary) electrons

Alexandre Faure

Université de Grenoble-Alpes / CNRS, IPAG, Grenoble (France)

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Outline

1. H_3^+ as a probe of the ISM

2. A new excitation model of H_3^+

3. Concluding remarks

1. H_3^+ as a probe of the ISM

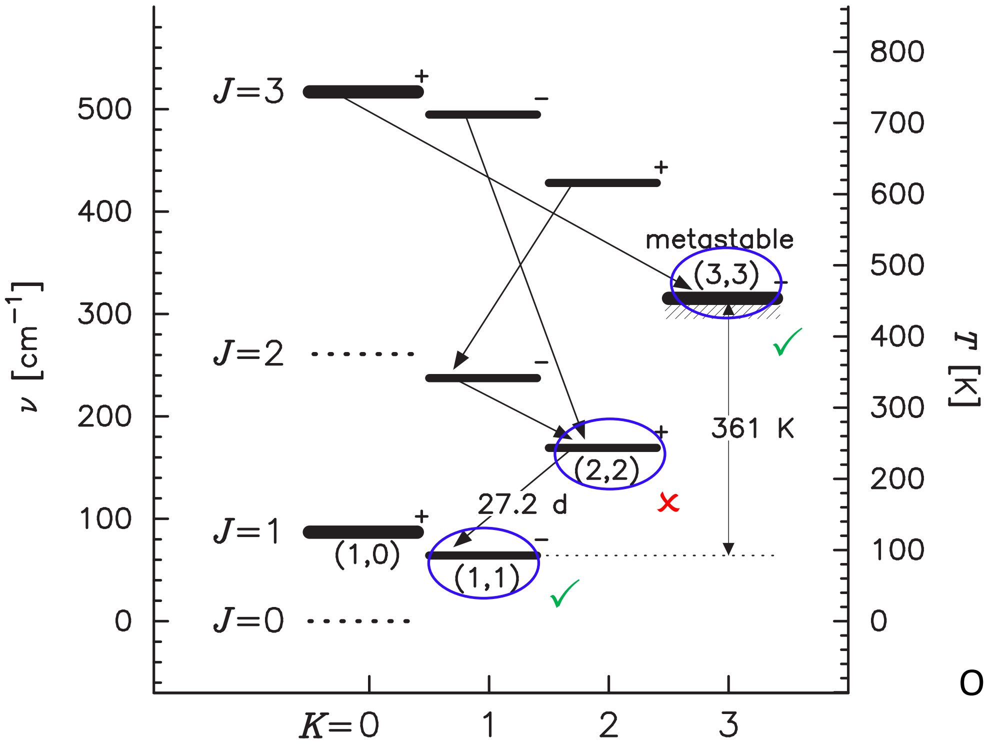
H_3^+ in the ISM

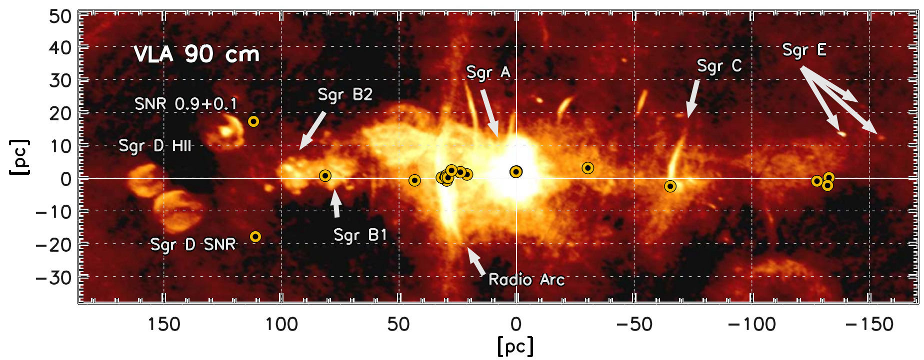
- H_3^+ is central in molecular astrophysics: initiator of chemistry and hence star formation

- Discovered in space by Geballe & Oka (1996) in dense clouds

- Powerful astrophysical probe of temperature, density and cosmic ray flux in the ISM (McCall et al. 2003)

H_3^+ in the Central Molecular Zone (CMZ): an extreme population inversion!





Oka et al. (2005), (2019)

Simple H_3^+ chemistry (Geballe & Oka)

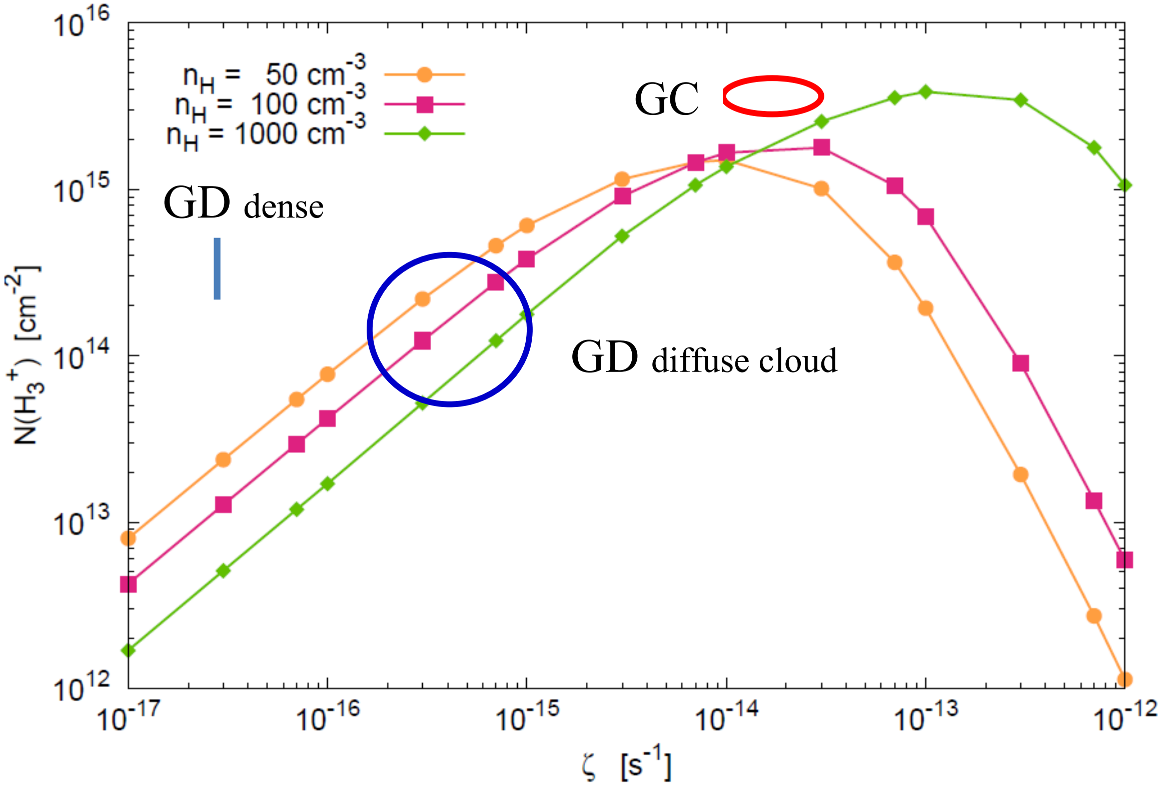
- Formation and destruction
  - $H_2 + \text{C.R.} \rightarrow H_2^+ + e^-$ $\zeta \sim 10^{-17}\ s^{-1}$ (3 x 10^9 years)
  - $H_2 + H_2^+ \rightarrow H_3^+ + H$ $k_L n(H_2) \sim 10^{-7}\ s^{-1}$ (4 months)
  - $H_3^+ + e^- \rightarrow H + H + H\ /\ H_2 + H$ $k_e n(e^-) \sim 10^{-9}\ s^{-1}$ (30 years)

- Production rate is $\zeta n(H_2)$ so that at steady-state $\zeta \propto \mathbf{N(H_3^+)}$:

$$\zeta L = k_e N(H_3^+)[n_e / n(H_2)]$$

- From measured $N(H_3^+)$ and estimated L (cloud depth) one can infer ζ !

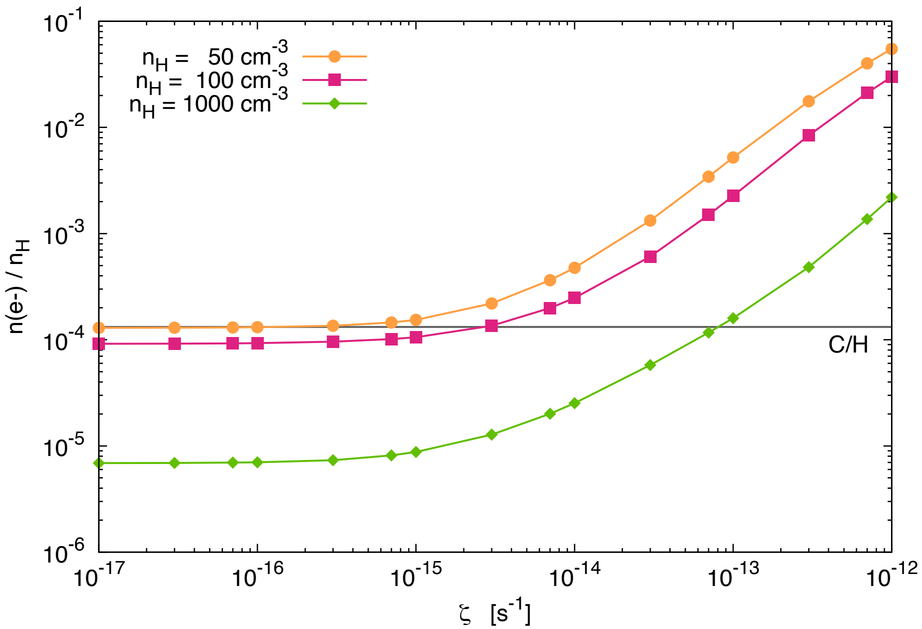
Departure from linearity



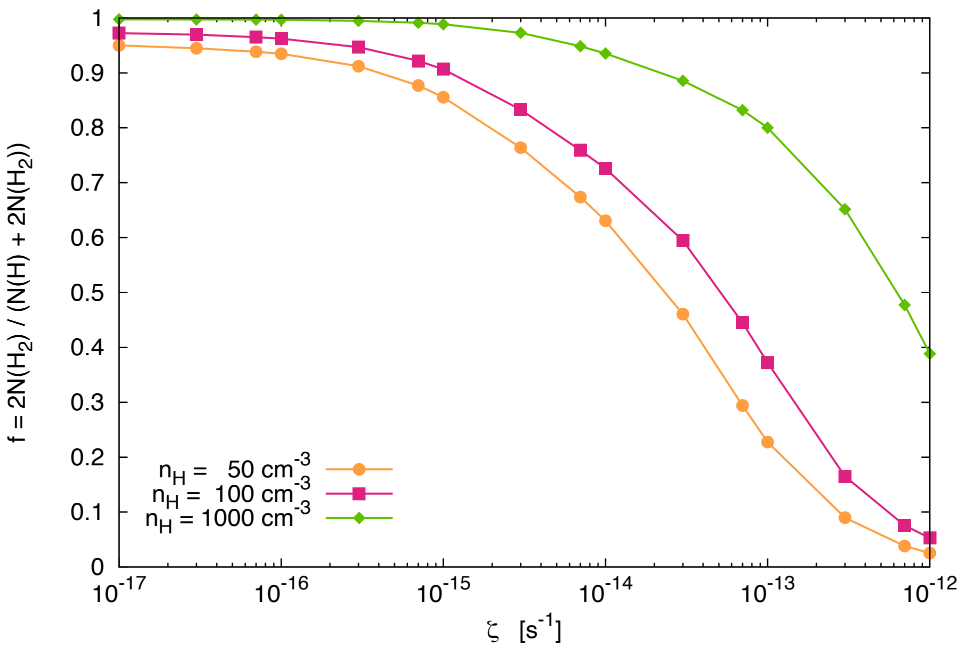
Le Petit et al. (2016); Oka (2019)

Origin of non-linearity ?

Electronic fraction



Molecular fraction: $f(H_2)=2n(H_2)/[n(H)+2n(H_2)]$



Le Petit et al. (2016)

The critical parameters

- Electron fraction due to H and H_2 ionization (in addition to C)
- Fraction of molecular hydrogen ($f(H_2) \sim 0.6 - 1$)
- Critical processes:
  - $H_3^+ + H_2 \rightarrow H_3^+ + H_2$
  - $H_3^+ + e^- \rightarrow H_2 + H$ / $H + H + H$; $H_2^+ + e^- \rightarrow H + H$
  - $H^+ + e^- \rightarrow H + h\nu$
  - $H_2^+ + H \rightarrow H_2 + H^+$

2. A new excitation model

- The role of electron collisions
- State-dependence of dissociative recombination in $H_3^+ + e^-$

Previous excitation models

- Oka & Epp (2004): assume that (1) lifetime of H_3^+ is much longer than the times of both spontaneous emission and collision and (2) electron-impact excitation is negligible

- Le Petit et al. (2016): take into account (1) chemical pumping (i.e. short lifetime of H_3^+) but (2) ignore electron-impact excitation and state-specific dissociative recombination

A fully **state-to-state** chemical pumping model

- Formation (chemical pumping) — $H_2^+(j) + H_2(j) \rightarrow H_3^+(j, k) + H$ (ΔH=-1.7 eV)
- Excitation — $H_3^+(j, k) + H_2(j) \rightarrow H_3^+(j', k') + H_2(j')$ (o/p conversion)
  $H_3^+(j, k) + e^- \rightarrow H_3^+(j', k') + e^-$ (no o/p conversion)
- Destruction — **$H_3^+(j, k) + e^- \rightarrow H_2 + H$ or $H + H + H$**

References for state-selected data:

Gomez-Carrasco et al. J Chem Phys (2012)	$H_3^+ + H_2$	statistical / QCT
Kokoouline et al. MNRAS (2010)	$H_3^+ + e^-$ coll	MQDT
Dos Santos et al. J Chem Phys (2007)	$H_3^+ + e^-$ DR	MQDT

Statistical equilibrium with **chemical pumping**

excitation

population

chemistry

$$\frac{dn_i}{dt} = \sum_{i \neq j}^{N} n_j P_{ji} - n_i \sum_{i \neq j}^{N} P_{ij} + F_i - n_i D_i$$

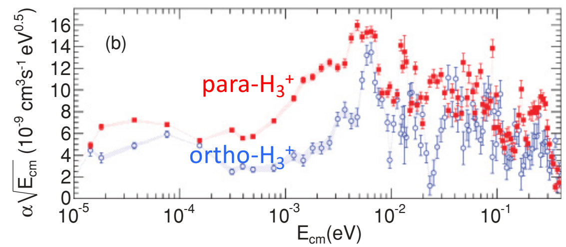
$$P_{ij} = \begin{cases} A_{ij} + B_{ij}\bar{J}_\nu + C_{ij} & (i > j) \\ B_{ij}\bar{J}_\nu + C_{ij} & (i < j) \end{cases}$$

Illustration: state-to-state DR of H_3^+

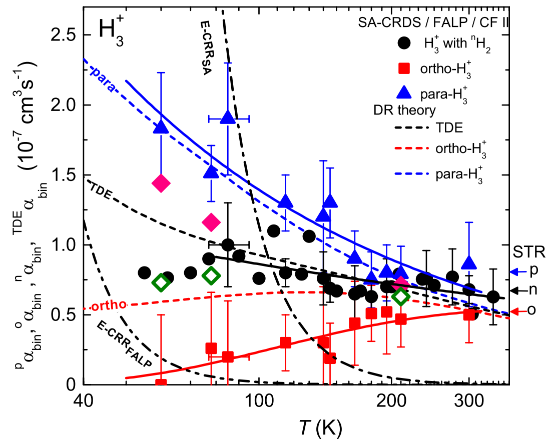
para-H_3^+

ortho-H_3^+

Dos Santos et al. (2007)
+ Kokoouline (2020) private communication

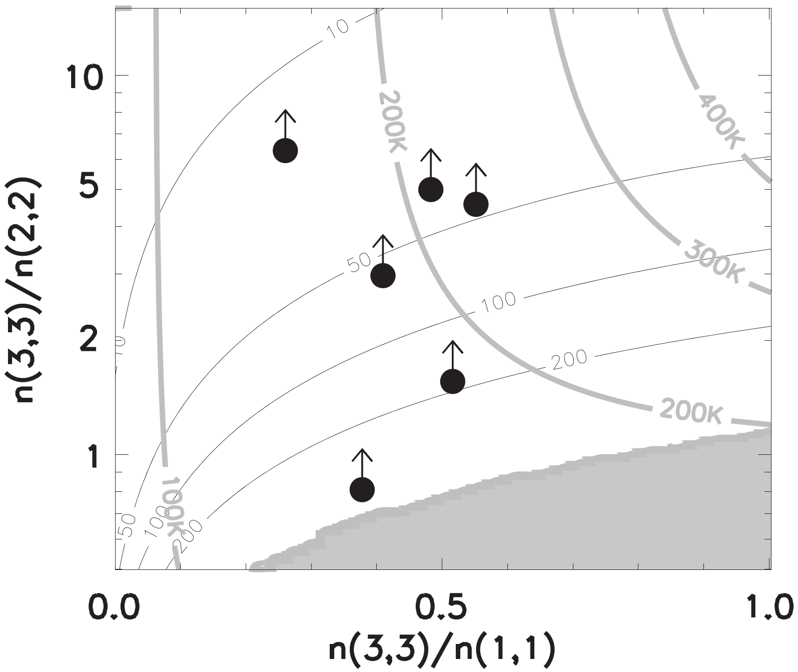


Kreckel et al. (2010)



Hejduk et al. (2015)

Physical conditions in the CMZ ?



Oka et al. (2019)

- 6 sources selected:
  α, α^+, γ, NHS 21, NHS 42, GCS 3-2
  (from Oka et al. 2019)

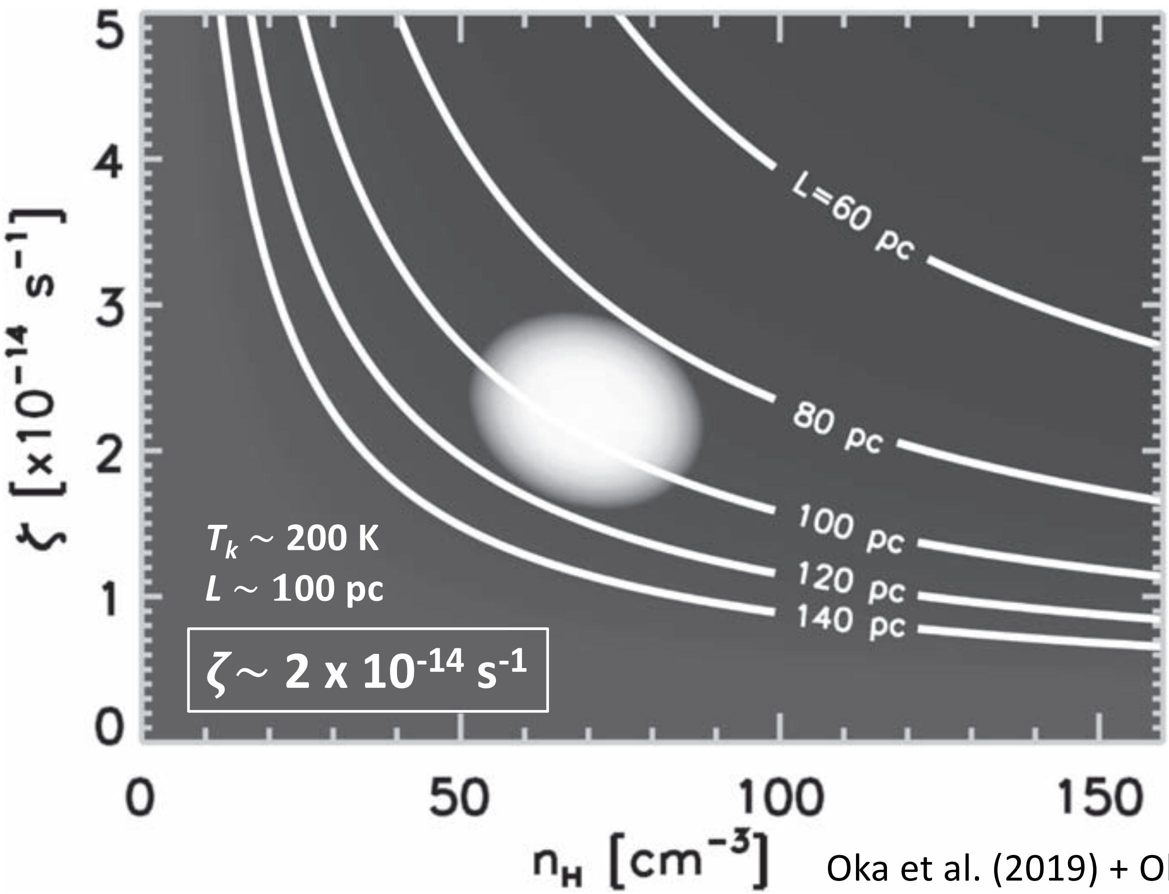
- Oka et al. (2019):

  $n <$ 20-650 cm^{-3}; $T_k \sim$ 140-230 K

- Present model:

  $n <$ 20-950 cm^{-3}; $T_k \sim$ 70-240 K

Most likely average values (Geballe & Oka)



Oka et al. (2019) + Oka & Epp (2004)

H_3^+ excitation as a probe of $n(e^-)$

- Best values from Oka et al. (2019):
  - T_k = 200K
  - n = 50 cm^{-3} with $f(H_2)$=0.6
  - $n(H_3^+)$ = 1 x 10^{-5} cm^{-3} ($L \sim$ 100 pc)
  - $n(e^-)$ = 0.33 cm^{-3}

- Chemical pumping model (with $f(H_2)$=1)
  - OFF $n(e^-) < 0.3$ cm^{-3}
  - ON $n(e^-) < 0.1$ cm^{-3}

Faure et al. in preparation

A new estimate of the CR ionization rate ?

- The electron fraction is a simple function of ζ (Oka et al. 2019):

$$n_{\rm e} = \left(\frac{n_{\rm C}}{n_{\rm H}}\right)_{\rm SV} R n_{\rm H} + \frac{k_{\rm e}}{2k_{\rm r}} n({\rm H}_3^+) \left[\sqrt{1 + \frac{2\zeta k_{\rm r} n_{\rm H}}{[k_{\rm e} n({\rm H}_3^+)]^2}} - 1\right]$$

- We obtain $\zeta \lesssim 2 \times 10^{-14}$ s^{-1}

- Problem: the degeneracy between density and temperature

Faure et al. in preparation

3. Concluding remarks

Conclusions

- Excitation of H_3^+ in the galactic centre is a challenging problem for molecular physics
- Because $x(e^-)$ is high, secondary electrons play a key role and it is crucial to couple inelastic AND reactive collisions between H_3^+ and H, H_2, and e^- (*H_3^+ + H collisions in progress in Grenoble*)
- Our model predicts an upper limit **$\zeta \lesssim 2 \times 10^{-14}$ s^{-1}** but more laboratory works are needed before a robust estimation of ζ can be made

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