Spin statistics of triatomic hydrides

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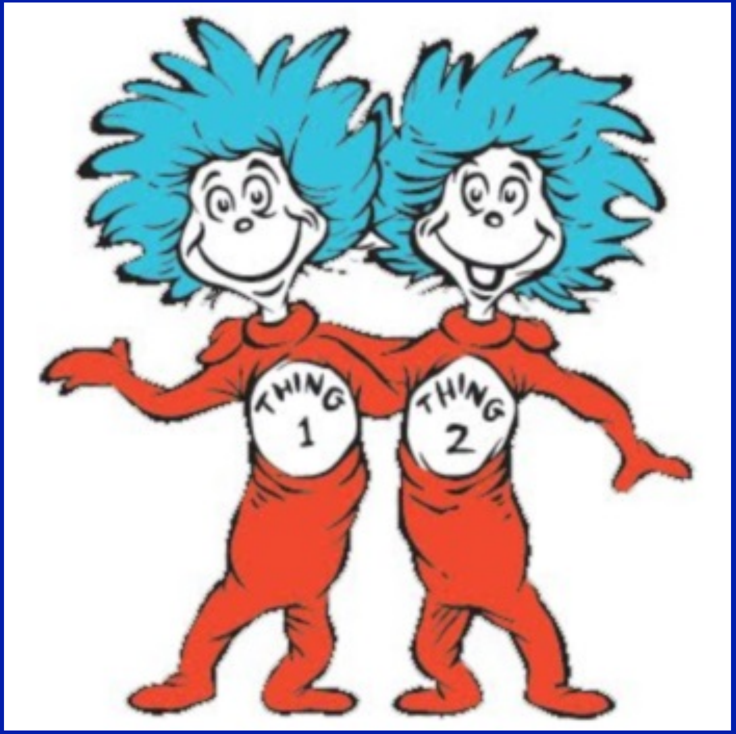
*pendant le mois de Mai….

Outline

I'll discuss 2 things:



1) Chloronium (H_2Cl^+)

Observed OPR ~ 3

(high-T equilibrium)

2) Trihydrogen cation (H_3^+)

Observed OPR ~ 0.4 – 1

(T_{spin} can be as low as ~ 20 K)

Outline

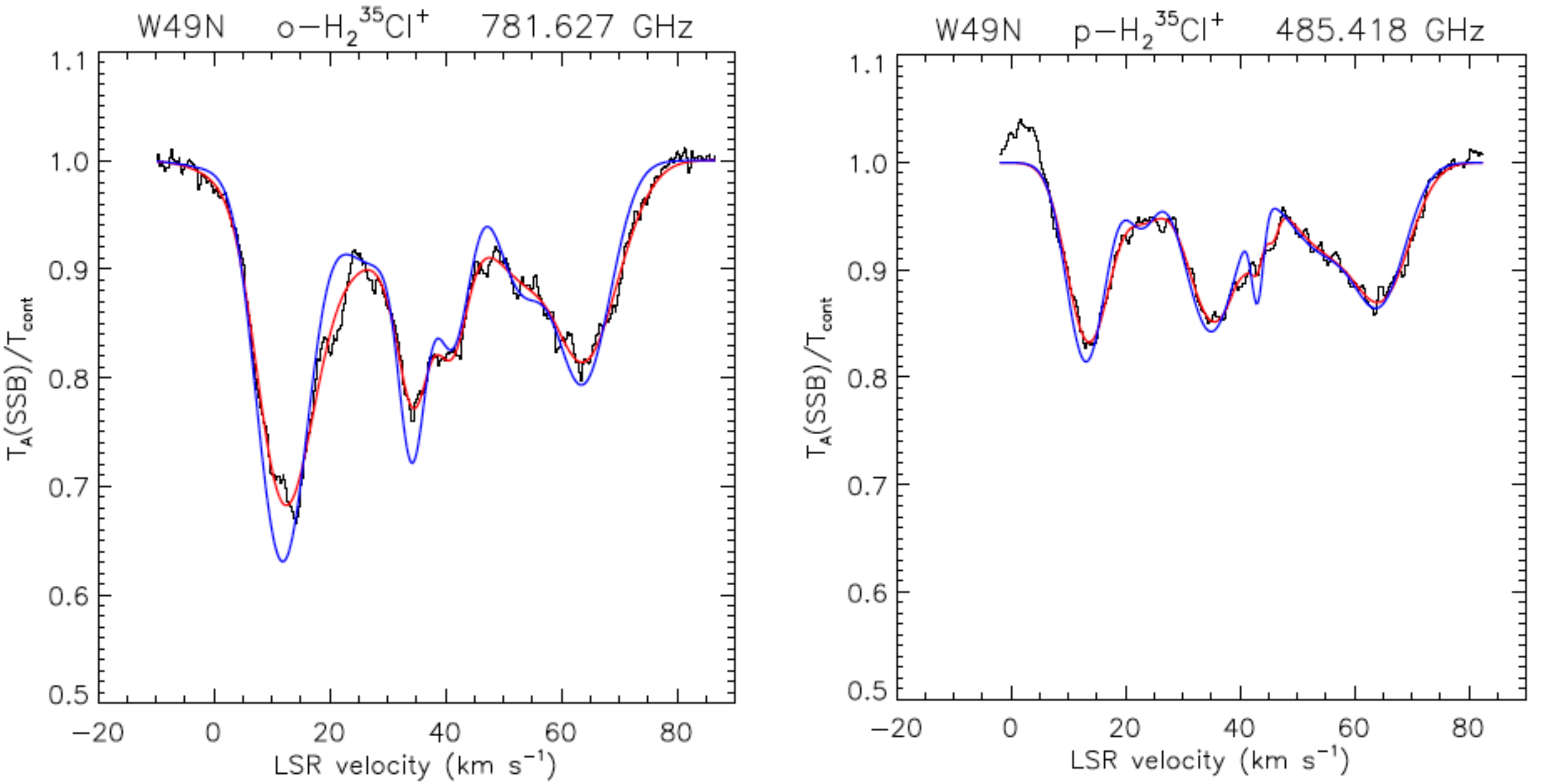
Chloronium (H_2Cl^+)

Observed OPR ~ 3
(high-T equilibrium)

Chloronium (H_2Cl^+)

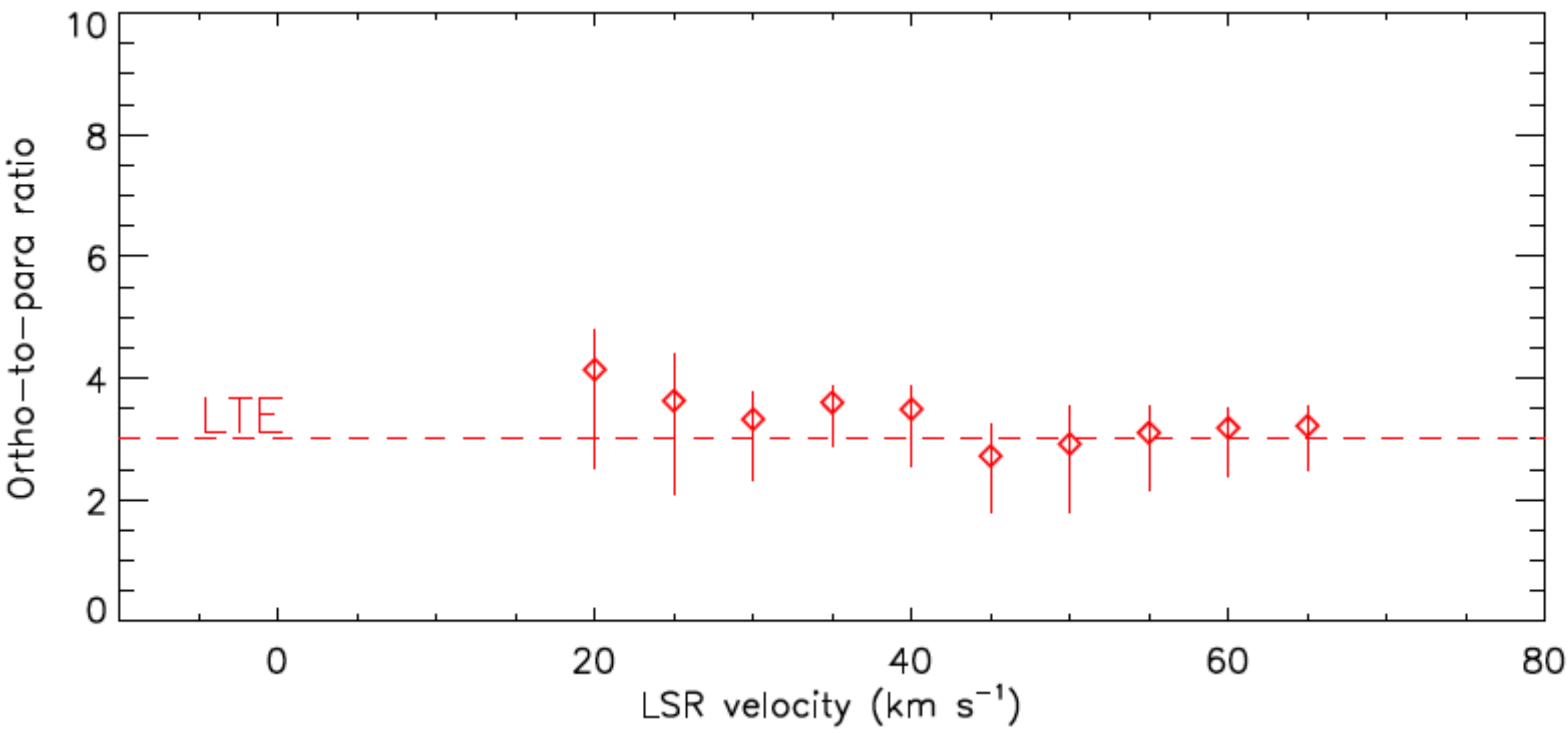
- Discovered with Herschel/HIFI (Lis et al. 2010)
- Asymmetric top (isoelectronic with H_2S)
- Ground state 0_{00} has nuclear spin 0
- Lowest ortho-state 1_{01} is 14.6 cm^{-1} above 0_{00}
- Equilibrium OPR ~ 3 above ~ 40 K
- In low temperature limit OPR ~ 9 $\exp(-20.2K / T)$

Chloronium observations with *Herschel* toward W49N



Neufeld et al. (2015, ApJ)

Chloronium observations with *Herschel* toward W49N



Neufeld et al. (2015, ApJ)

Expectations for the H_2Cl^+ OPR

Formation via the exothermic reactions:

$Cl^+ + H_2 \rightarrow HCl^+ + H$ *R1*

$HCl^+ + H_2 \rightarrow H_2Cl^+ + H$ *R2*

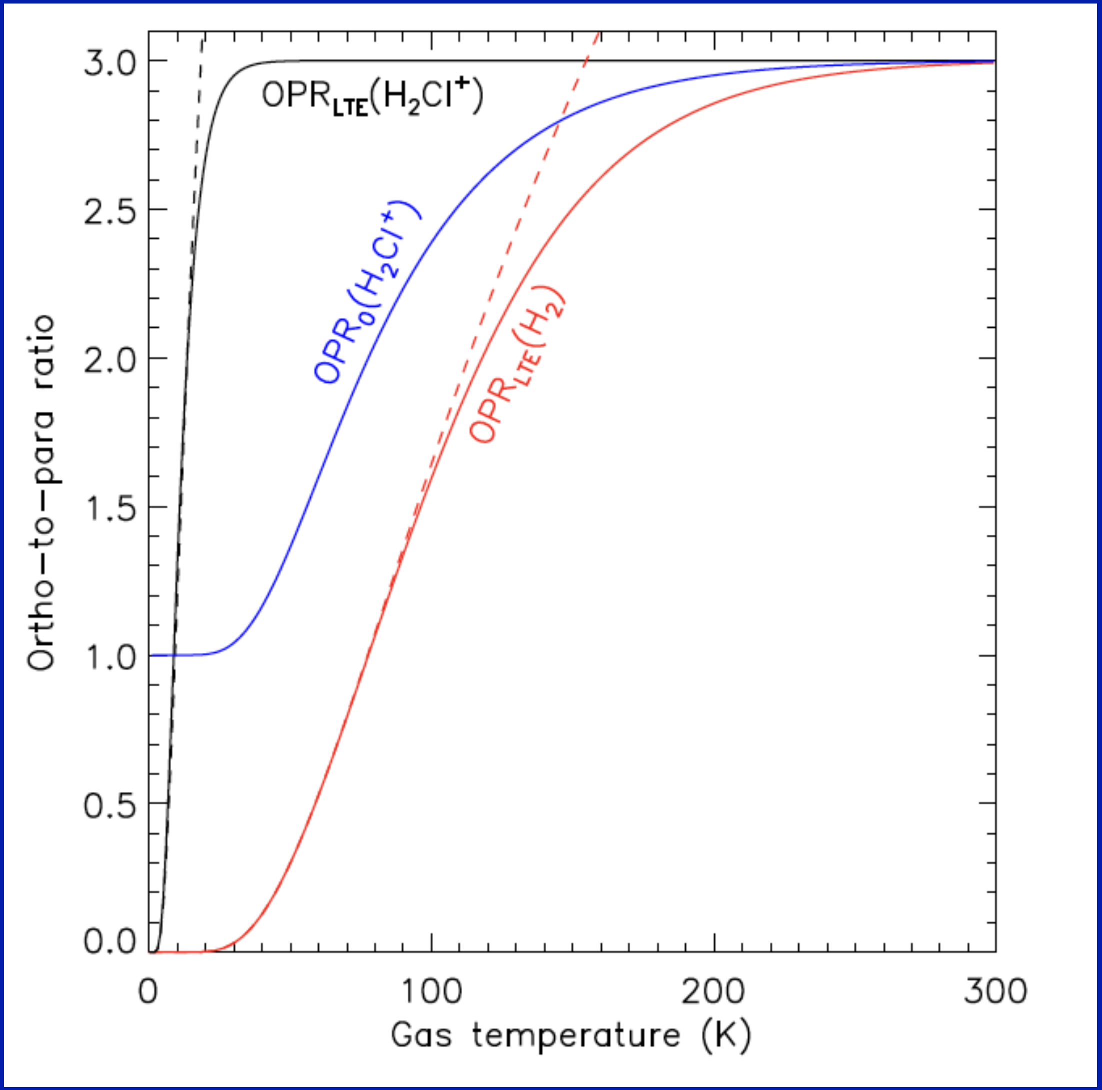
If the scrambling limit applies for *R2*, then the OPR for H_2Cl^+ reflects that of H_2

Expectations for the H_2Cl^+ OPR

$HCl^+ + o-H_2$	$\rightarrow o-H_2Cl^+ + H$	5/6
	$\rightarrow p-H_2Cl^+ + H$	1/6
$HCl^+ + p-H_2$	$\rightarrow o-H_2Cl^+ + H$	1/2
	$\rightarrow p-H_2Cl^+ + H$	1/2

$$\text{Formation OPR} = OPR_0 = \frac{5\,OPR\,(H_2) + 3}{OPR\,(H_2) + 3}$$

Expectations for the H_2Cl^+ OPR



Expectations for the H_2Cl^+ OPR

The actual H_2Cl^+ OPR depends on the relevant timescales for destruction (via dissociative recombination) and ortho-para conversion via

$$o - H_2Cl^+ + H \longleftrightarrow p - H_2Cl^+ + H$$

$$OPR(H_2Cl^+) = x\, OPR_{LTE}(H_2Cl^+) + (1 - x)\, OPR_0(H_2Cl^+)$$

$$\text{where } x = \frac{k_{op} n(H)}{k_{op} n(H) + k_{dr} n_e}$$

(assumes DR rate same for $o -$ and $p - H_2Cl^+$)

Observed H_2Cl^+

Assuming that H_2Cl^+ exists in a region with $T > 30$ K, the observed $H_2Cl^+ > 2.5$ implies

1) Scrambling mechanism does not apply

and/or

2) $T > 110$ K so that $OPR_{LTE}(H_2) > 1.8$

and/or

3) Ortho-para conversion is rapid with

$k_{op} > 1.5 \times 10^{-10}$ cm^3 s^{-1}

Outline

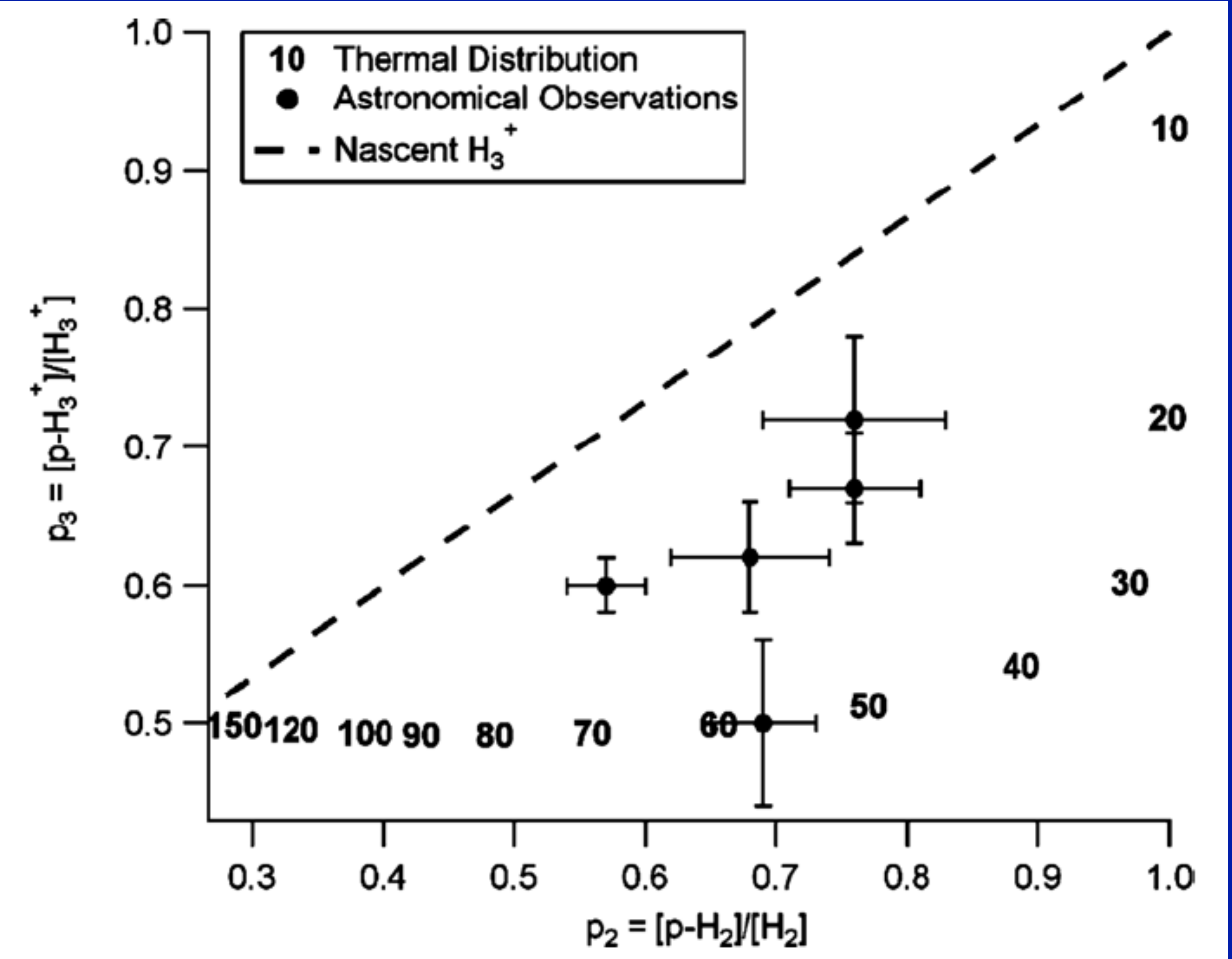
Trihydrogen (H_3^+)

Observed OPR ~ 0.4 – 1

(T_{spin} can be as low as ~ 20 K)

Observed H_3^+ and H_2 OPRs

Crabtree et al. (2011, ApJ)



Observed H_3^+ and H_2 OPRs

Observations indicate $T_{spin}(H_3^+) < T_{spin}(H_2)$

Various effects have been included in models

- State selective DR rates
- Time dependence
- Enhanced CR ionization rates

In general, models overpredict $T_{spin}(H_3^+)$
(recall Kyle Crabtree's talk)

Effect of T variations in diffuse clouds

Even if ortho-para conversion is very rapid, and the OPRs are everywhere in LTE,

$T_{spin}(H_2)$ does not have to equal $T_{spin}(H_3^+)$, because clouds are not isothermal

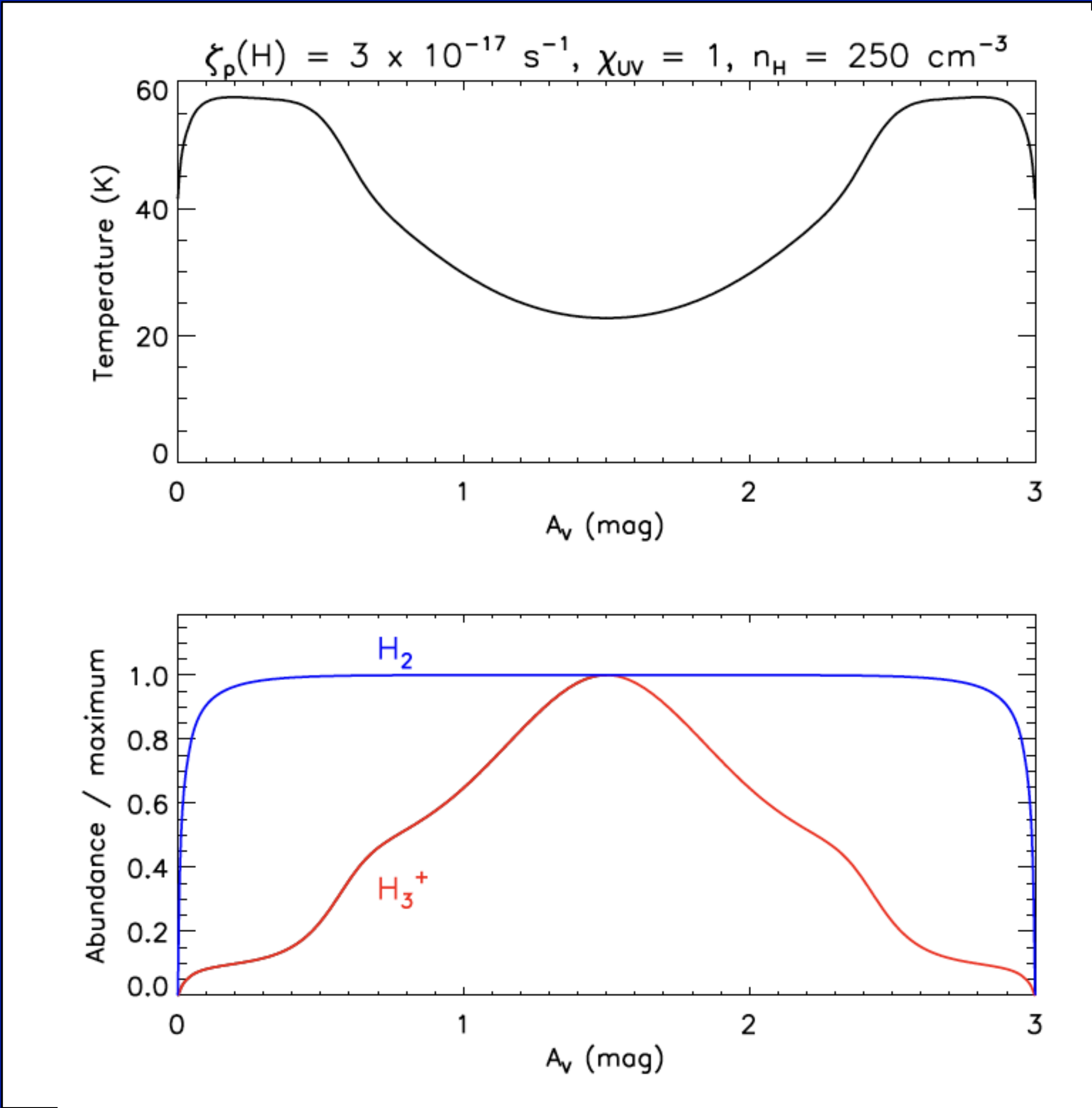
Effect of T variations in diffuse clouds

Averaging over this cloud, we find

T_{spin} (H_2) = 43 K

T_{spin} (H_3^+) = 29 K

This effect goes in the right direction



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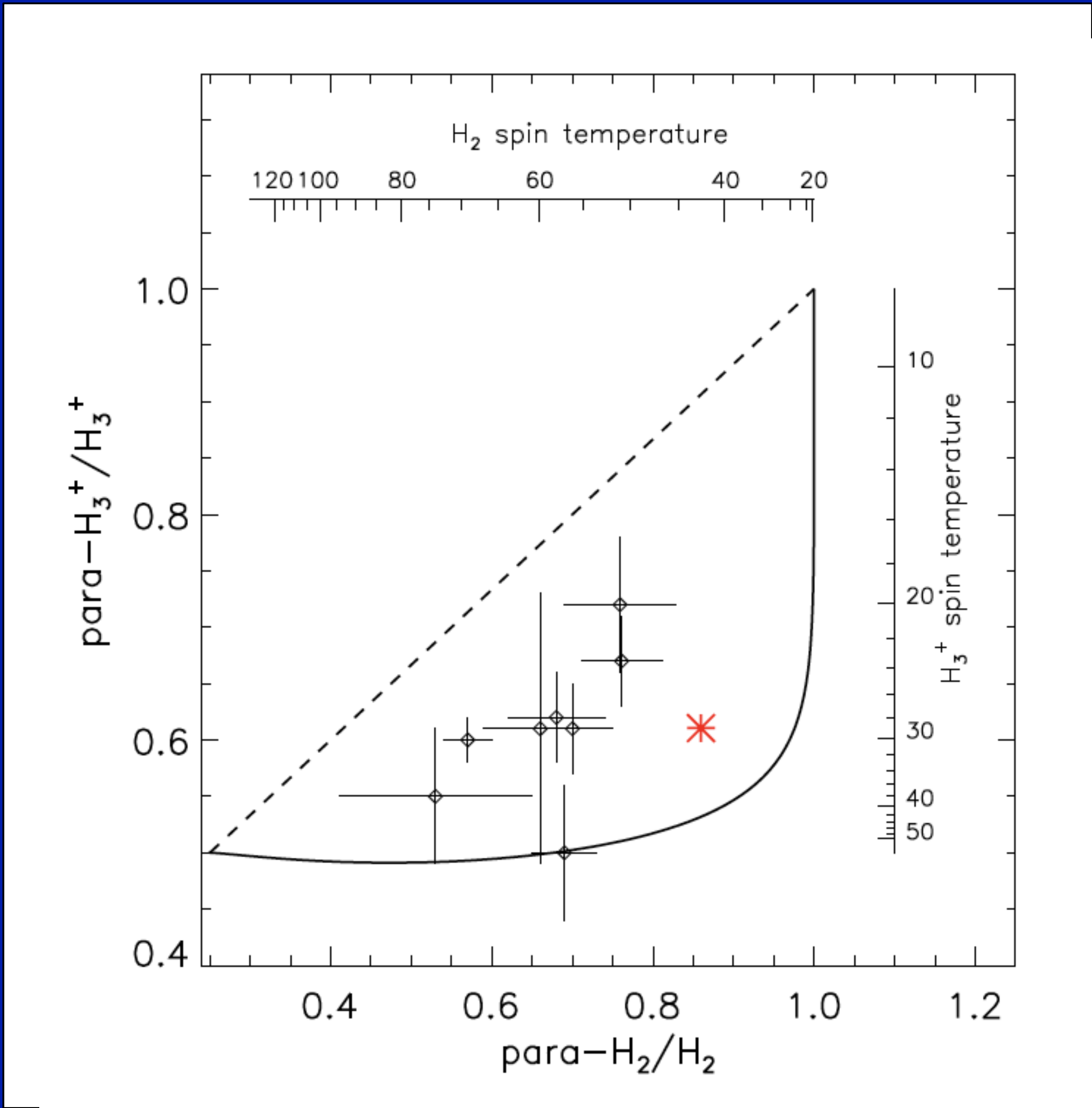


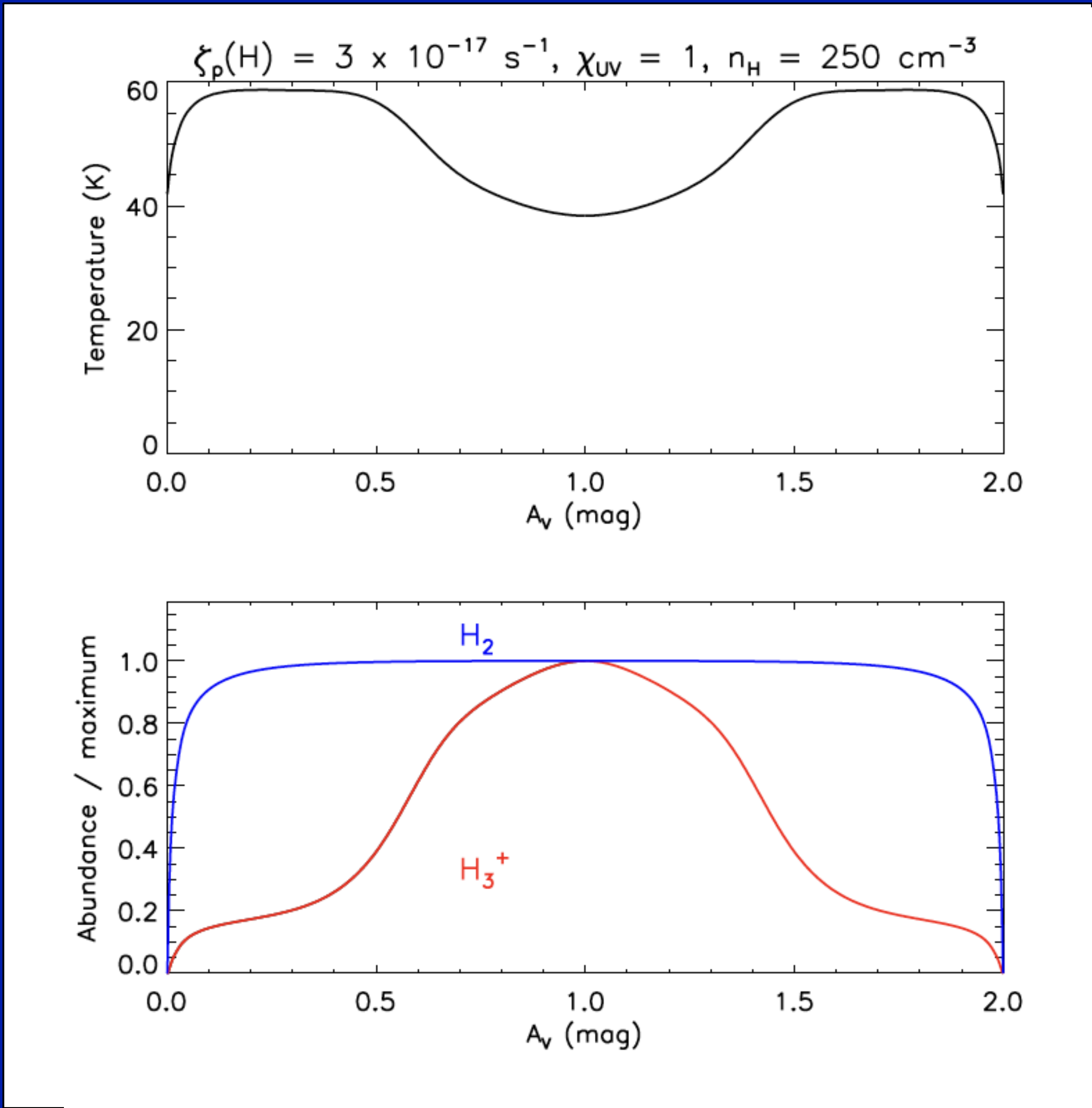
Effect of T variations in diffuse clouds

However, these cloud parameters overpredict $N(H_2)$ and underpredict $N(H_3^+)$

Decreasing A_V to 2, we find

T_{spin} (H_2) = 51 K

T_{spin} (H_3^+) = 45 K



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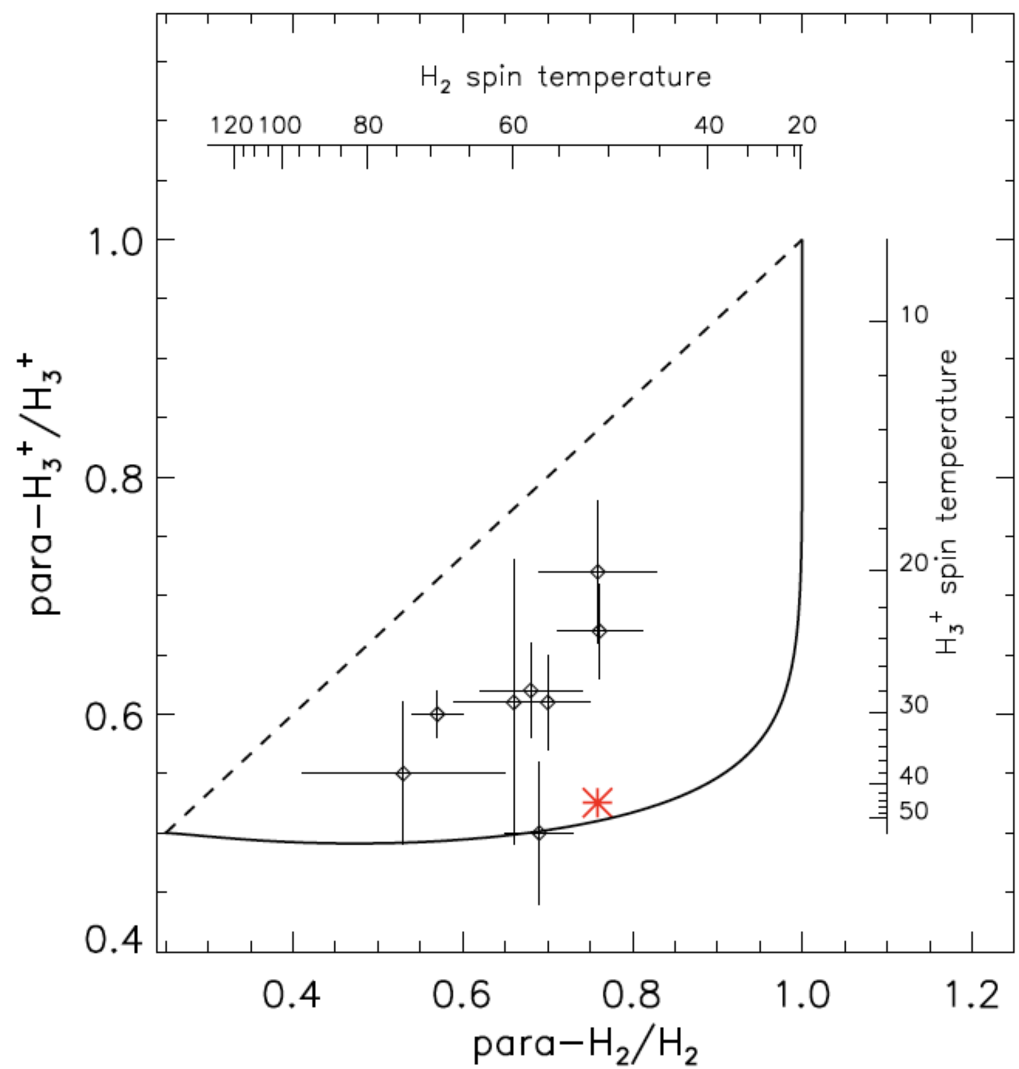
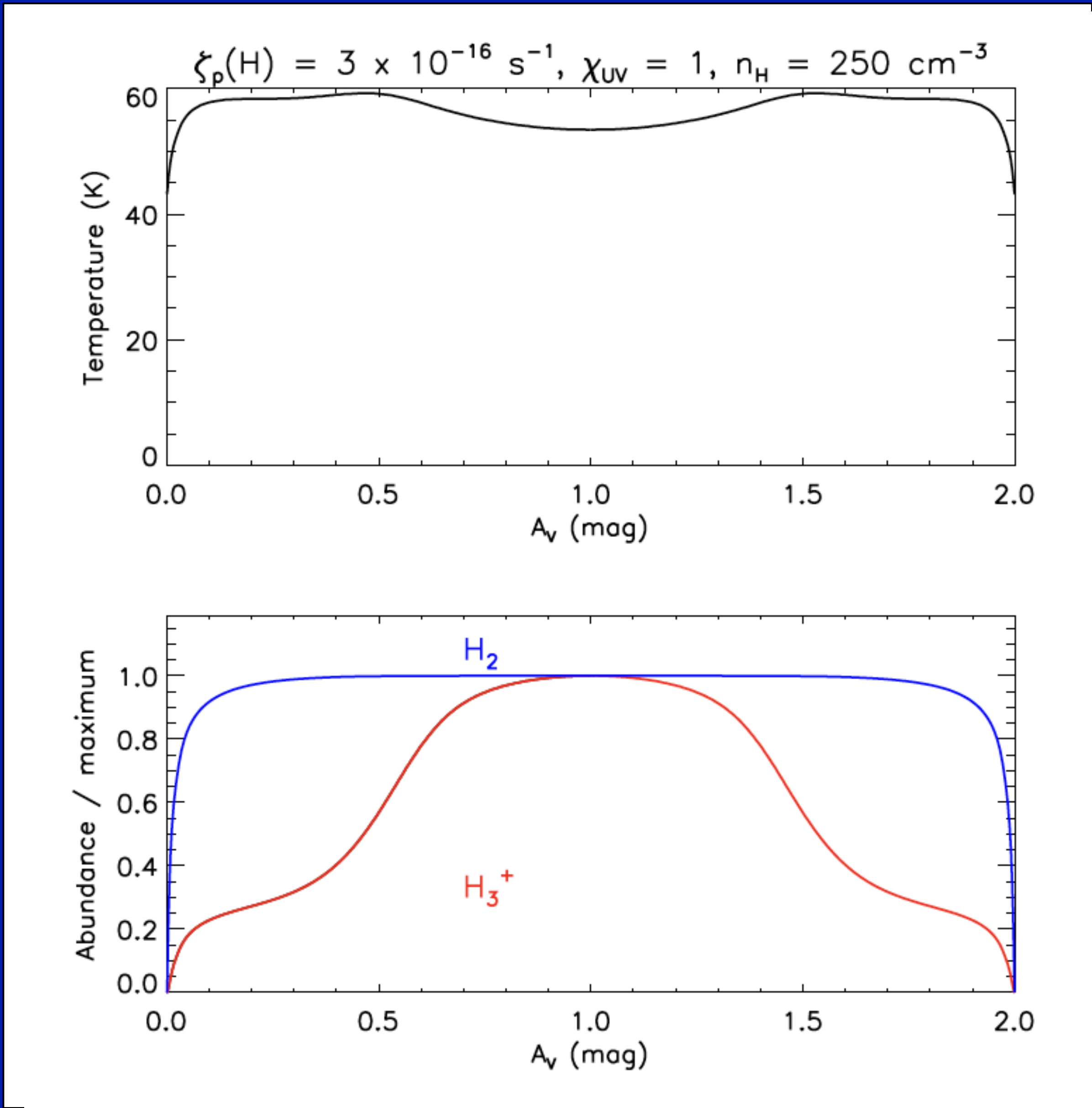


Effect of T variations in diffuse clouds

And now increasing the CRIR to 3×10^{-16} s $^{-1}$ as well

T_{spin} (H_2) = 57 K

T_{spin} (H_3^+) = 56 K



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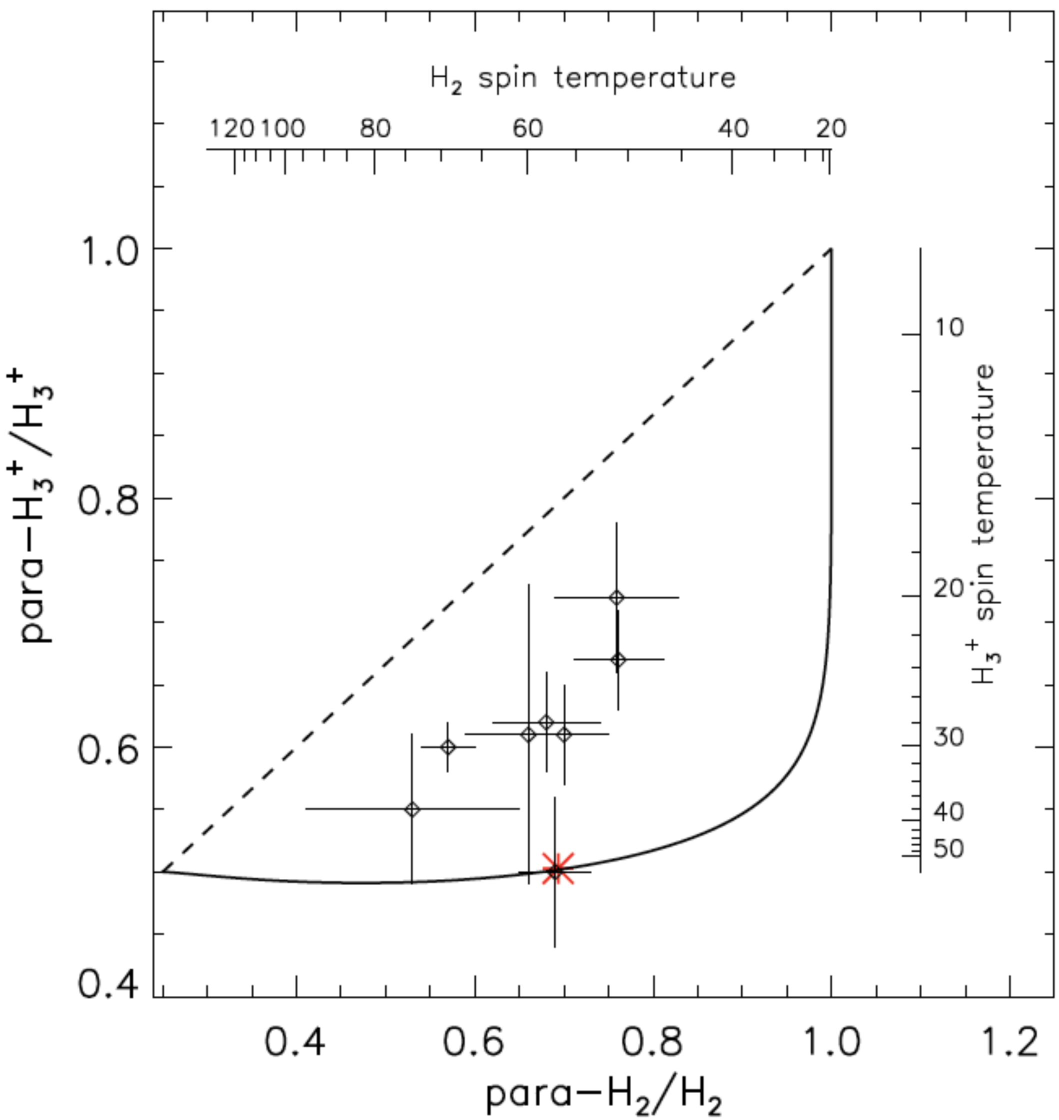

Effect of T variations in diffuse clouds

We still need to do a complete parameter study, but it's not clear that this effect can account for the observed H_3^+ spin temperature when all relevant observational constraints (e.g. $N(H_2)$, $N(H_3^+)$) are considered