Spin states of H_2D^+ and D_2H^+ as chemical age tracers

Olli Sipilä

Center for Astrochemical Studies (CAS)
Max Planck Institute for Extraterrestrial Physics

This presentation is based on the following two papers:

H_2D^+ observations give an age of at least one million years for a cloud core forming Sun–like stars

Sandra Brünken[1], Olli Sipilä[2,3], Edward T. Chambers[1], Jorma Harju[2], Paola Caselli[3,4], Oskar Asvany[1], Cornelia E. Honingh[1], Tomasz Kamiński[5], Karl M. Menten[5], Jürgen Stutzki[1] & Stephan Schlemmer[1]

Nature 515, 219

DETECTION OF INTERSTELLAR ORTHO-D_2H^+ WITH SOFIA

Jorma Harju[1,2,6], Olli Sipilä[1], Sandra Brünken[3], Stephan Schlemmer[3], Paola Caselli[1], Mika Juvela[2], Karl M. Menten[4], Jürgen Stutzki[3], Oskar Asvany[3], Tomasz Kamiński[4,5], Yoko Okada[3], and Ronan Higgins[3]

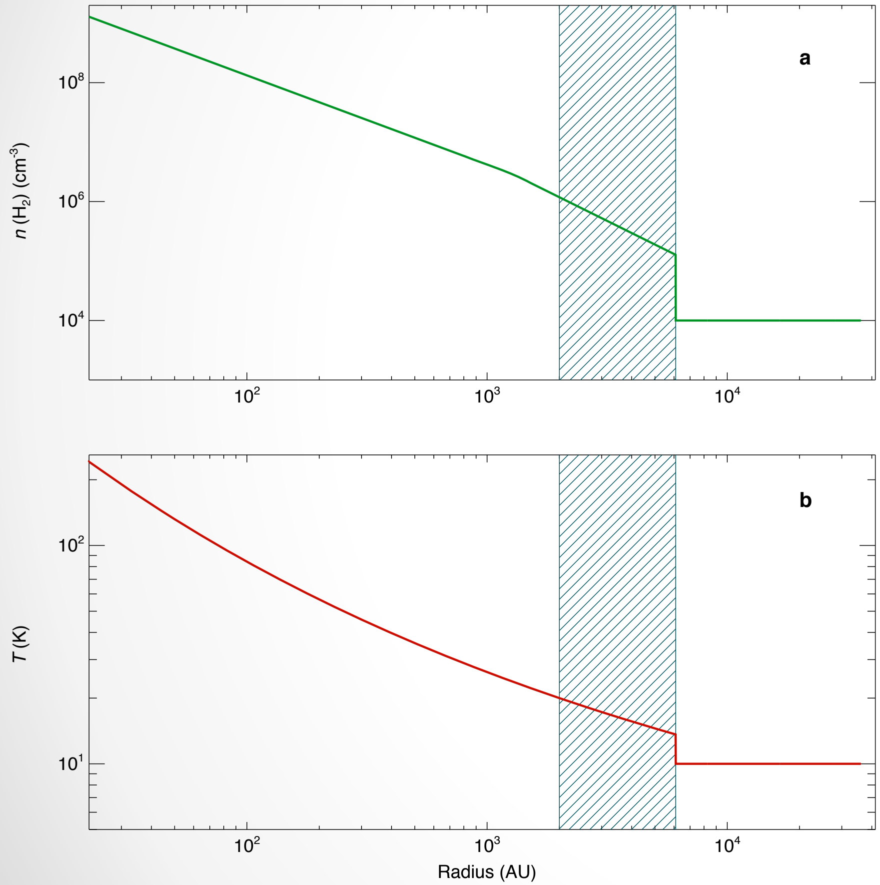
[1]Max-Planck-Institut für extraterrestrische Physik, Gießenbachstraße 1, 85748 Garching, Germany
[2]Department of Physics, P.O. BOX 64, 00014 University of Helsinki, Finland
[3]I. Physikalisches Institut, Universität zu Köln, Zülpicher Straße 77, 50937 Köln, Germany
[4]Max-Planck-Institut für Radioastronomie, Auf dem Hügel 69, 53121 Bonn, Germany
[5]Harvard-Smithsonian Center for Astrophysics, 60 Garden Street, Cambridge MA 02138, USA
[6]harju@mpe.mpg.de

ApJ accepted, arXiv:1704.02526

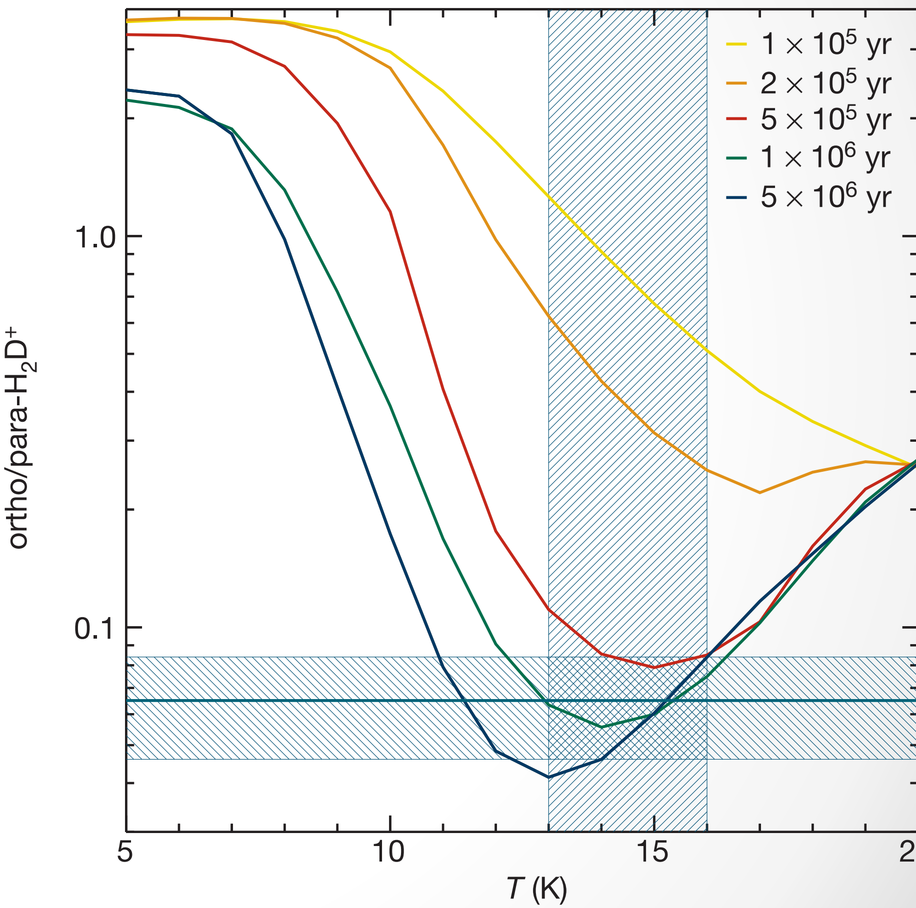
Spin states of H_2D^+ and D_2H^+ as chemical age tracers

- first confirmed detection of para-H_2D^+ in space, toward IRAS 16293-2422 A/B (*SOFIA* Cycle 2)
- we modeled the emission/absorption of ortho and para H_2D^+ using a pseudo-time-dependent chemical model + radiative transfer
- H_3^+ + H_2 chemistry from Hugo et al. (2009), rest of non-D chemistry from OSU
- deuterium and spin-state chemistry from Sipilä et al. (2013), where the spin-state chemistry was generated using the method of Oka (2004)
- physical model static, consists of two phases: 1) homogeneous dark cloud; 2) protostellar core (structure from Crimier et al. (2010))

density, temperature of the source model

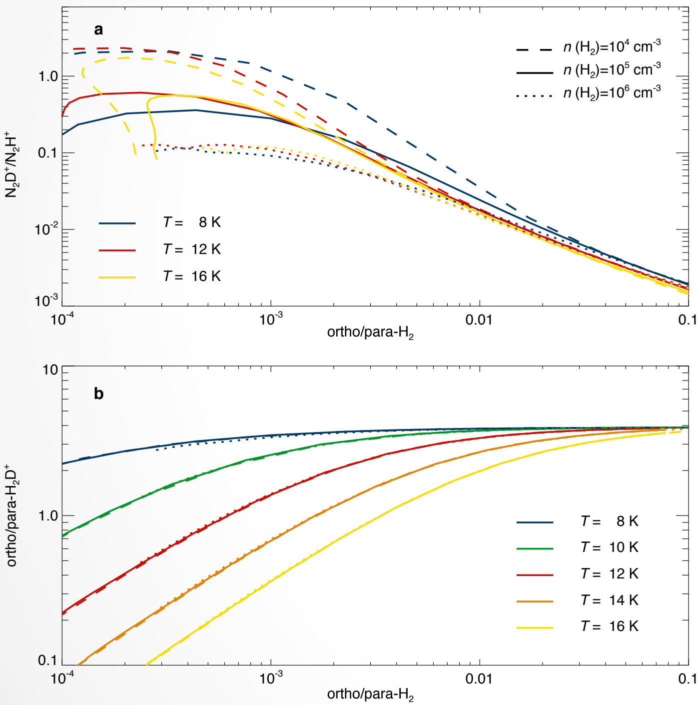


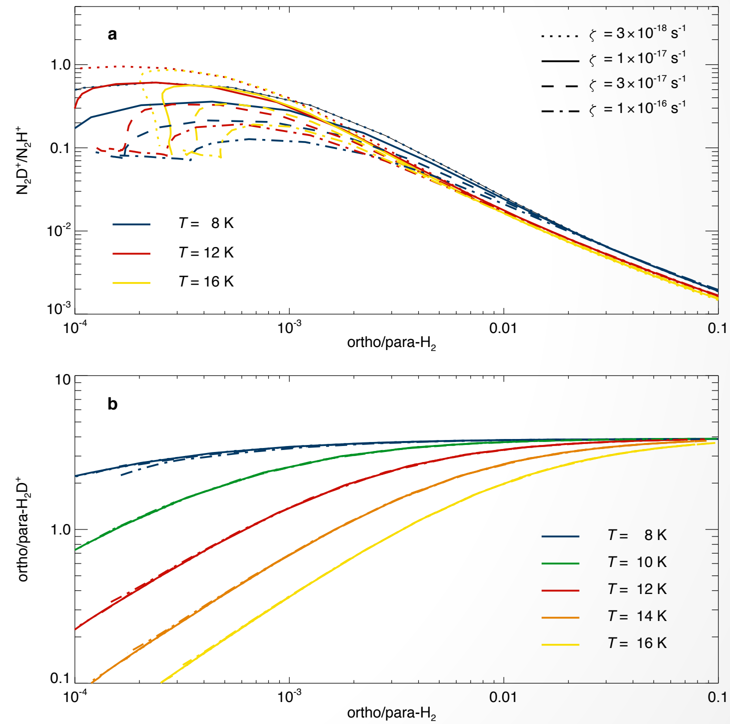
modeled H_2D^+ o/p ratio



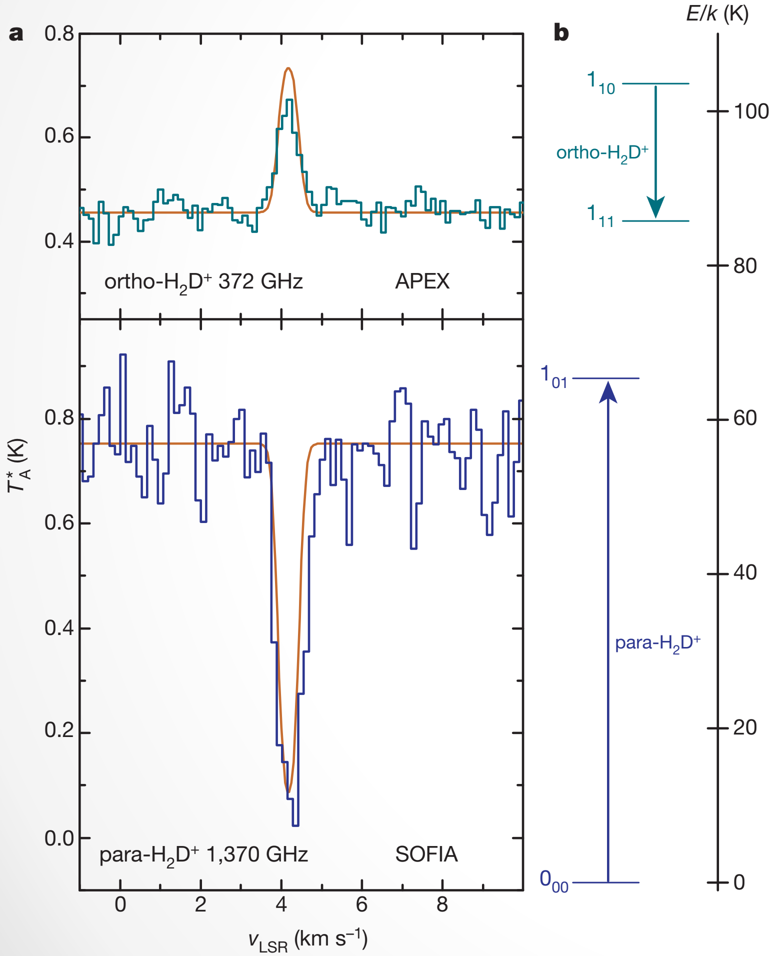
Spin states of H_2D^+ and D_2H^+ as chemical age tracers

H_2D^+ seems to be a more robust chemical age tracer than N_2D^+/N_2H^+





observed + modeled spectra



- observed H_2D^+ o/p ratio (0.065±0.019) implies a very low H_2 o/p ratio
- best-fit chemical age based on this analysis is 10^6+10^6 yr
- the model is rather simple, for example the continuum is added after the RT calculations
- we only had one pair of lines to fit

Spin states of H_2D^+ and D_2H^+ as chemical age tracers

- in *SOFIA* Cycle 3, we obtained the first detection of ortho-D_2H^+ in space
- coupled with an APEX observation of para-D_2H^+, we now have data on both spin states of H_2D^+ and D_2H^+ towards the same line of sight
- we proceeded to reanalyze the problem using an improved modeling approach
- the chemical model was updated based on Sipilä et al. (2015a,b); spin chemistry derived using a group-theoretical approach
- now using KIDA instead of OSU
- the RT calculations now consider the continuum as well; small velocity shift introduced between the core and the ambient cloud

- in Sipilä et al. (2015b; A&A 581, A122) we discussed the spin-state chemistry of deuterated ammonia in detail
- we constructed new gas-phase and grain-surface reaction sets where the spin chemistry of deuterated species was derived based on symmetry rules ($H_3^+ + H_2$ chemistry still taken from Hugo et al. 2009)
- the underlying assumption is complete scrambling

Table A.1. Statistical nuclear spin branching ratios for reactions $H_2 + H \rightleftharpoons H_3$ and $D_2 + D \rightleftharpoons D_3$.

H_3	$H_2 + H$ $A \otimes A$	$B \otimes A$	Σ
$4\,A_1$	4	0	4
$0\,A_2$	0	0	0
$2\,E$	2	2	4
Σ	6	2	8

D_3	$D_2 + D$ $A \otimes A$	$B \otimes A$	Σ
$10\,A_1$	10	0	10
$1\,A_2$	0	1	1
$8\,E$	8	8	16
Σ	18	9	27

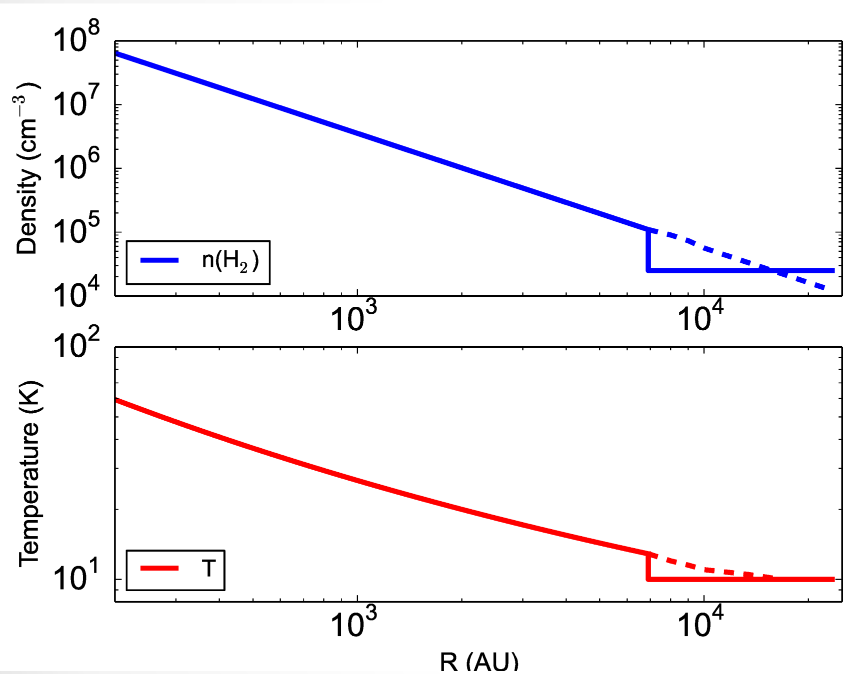
Table A.5. Statistical nuclear spin branching ratios of the reaction $D_6 \rightleftharpoons D_4 + D_2$.

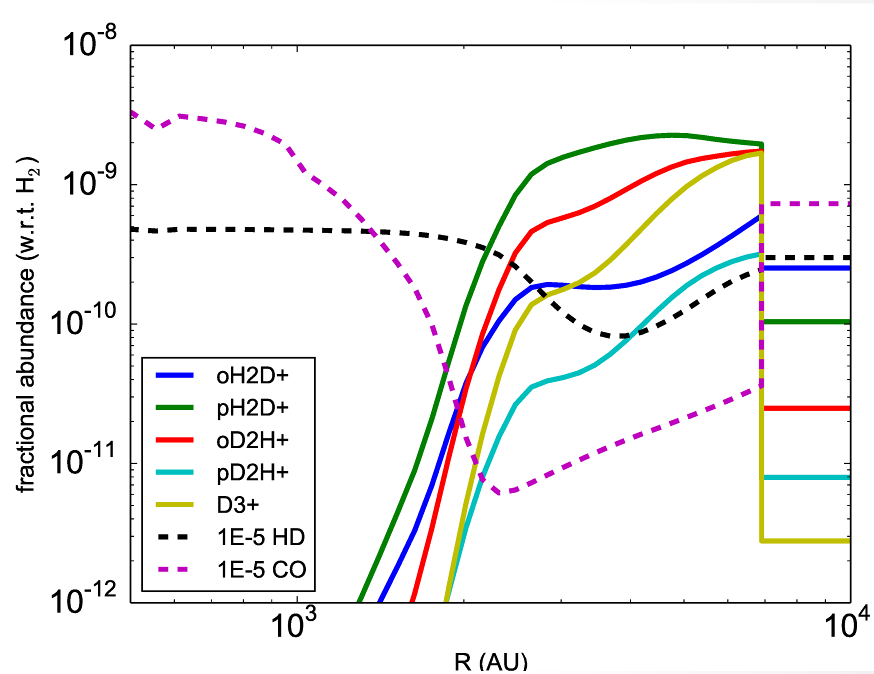
D_6	$D_4 + D_2$ A_1, A	A_1, B	E, A	E, B	F_1, A	F_1, B	F_2, A	F_2, B	Σ
$28\,A_1$	28	0	0	0	0	0	0	0	28
$35\,H_1$	35	35	0	0	105	0	0	0	175
$1\,H_3$	0	0	2	0	0	0	0	3	5
$10\,H_4$	0	0	0	20	30	0	0	0	50
$27\,L_1$	27	0	54	0	81	81	0	0	243
$10\,M_1$	0	10	0	0	30	30	30	0	100
$8\,S$	0	0	16	16	24	24	24	24	128
Σ	90	45	72	36	270	135	54	27	729

energy effects neglected so far, no vibrational excitation

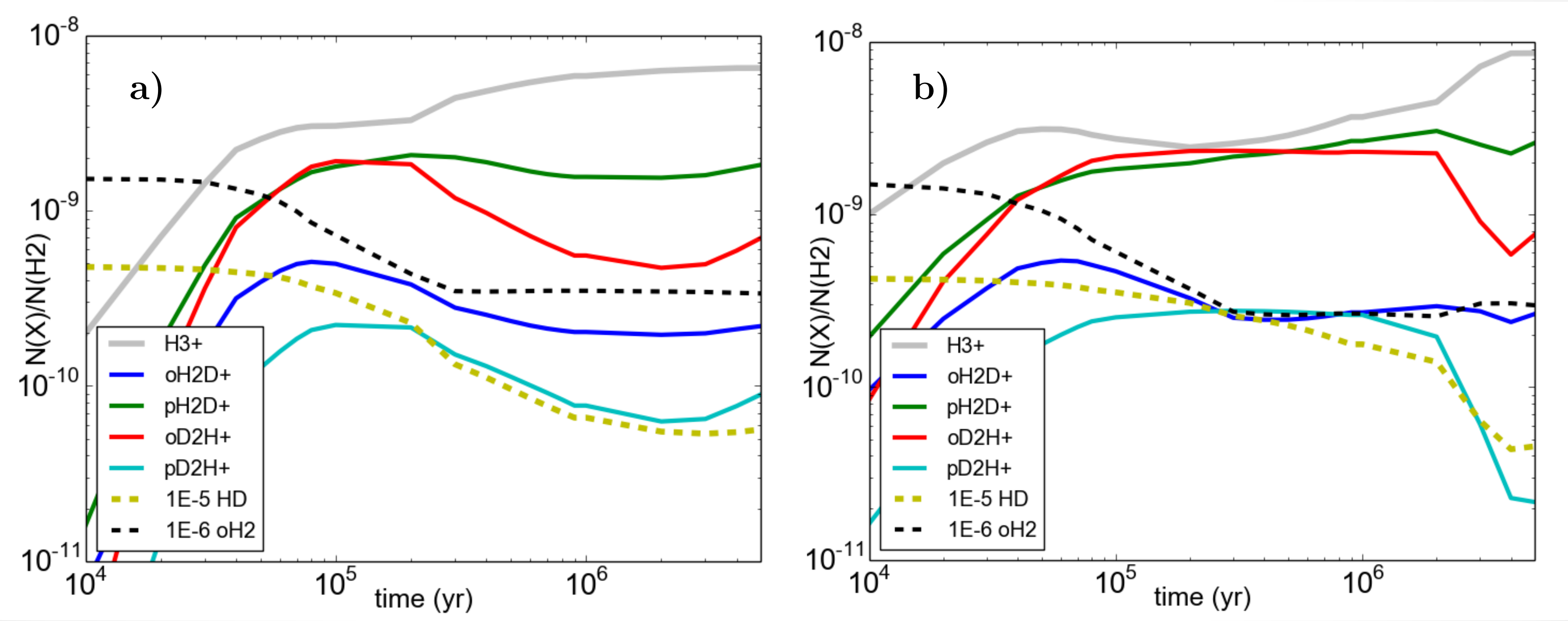
physical structure of the model core
+ ambient cloud

abundances of selected species at
$t = 5 \times 10^5$ yr

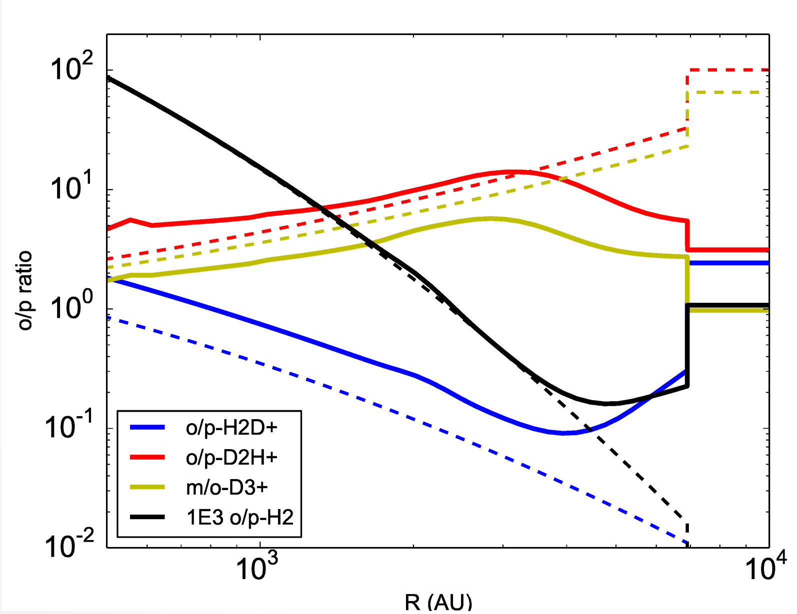




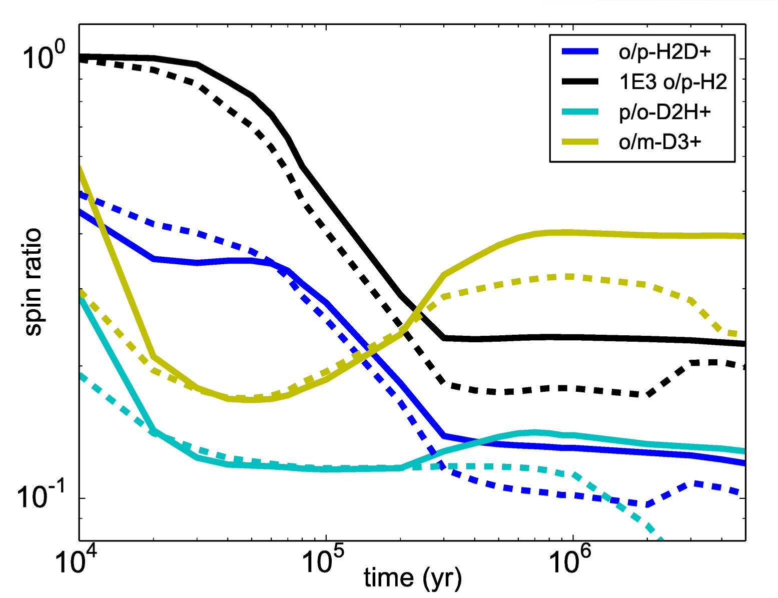
the ambient cloud is a bit denser than in the previous paper (temperature was varied too) initial abundances (obviously) make a difference to the time evolution



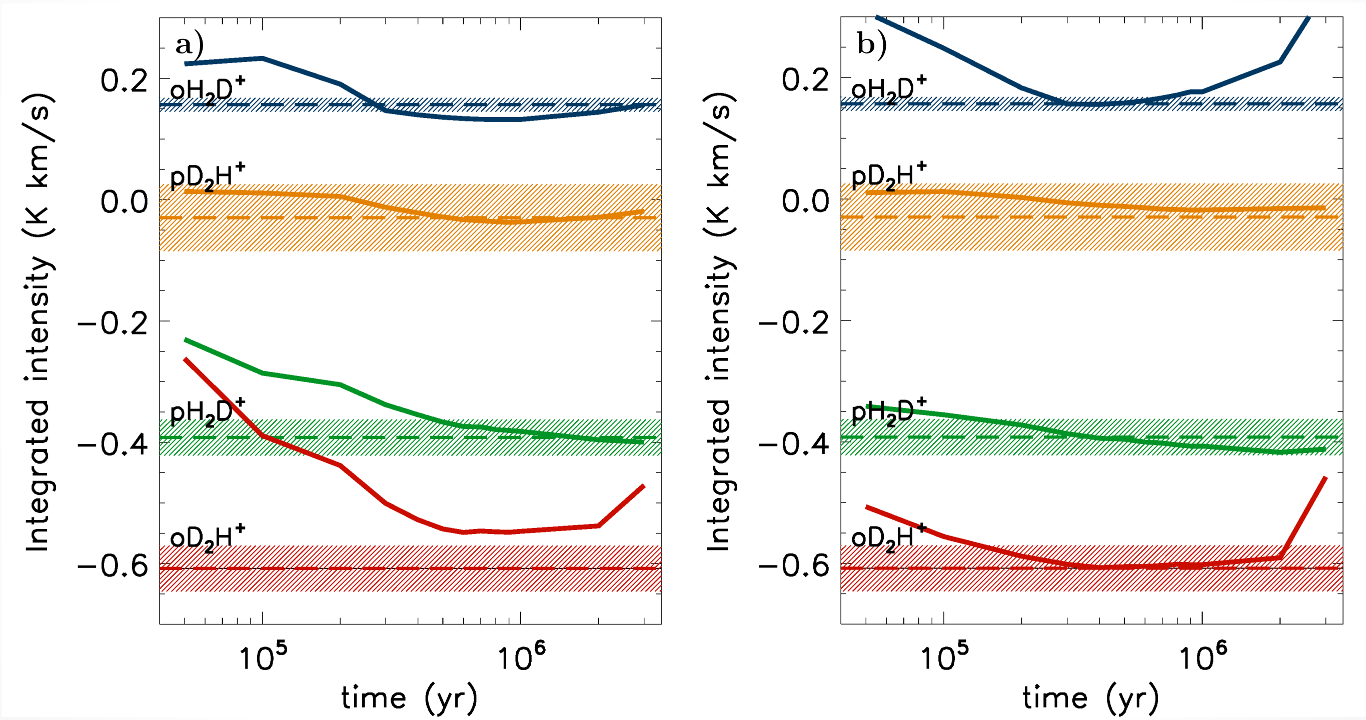
o/p ratios at t = $5x10^5$ yr



average o/p ratios



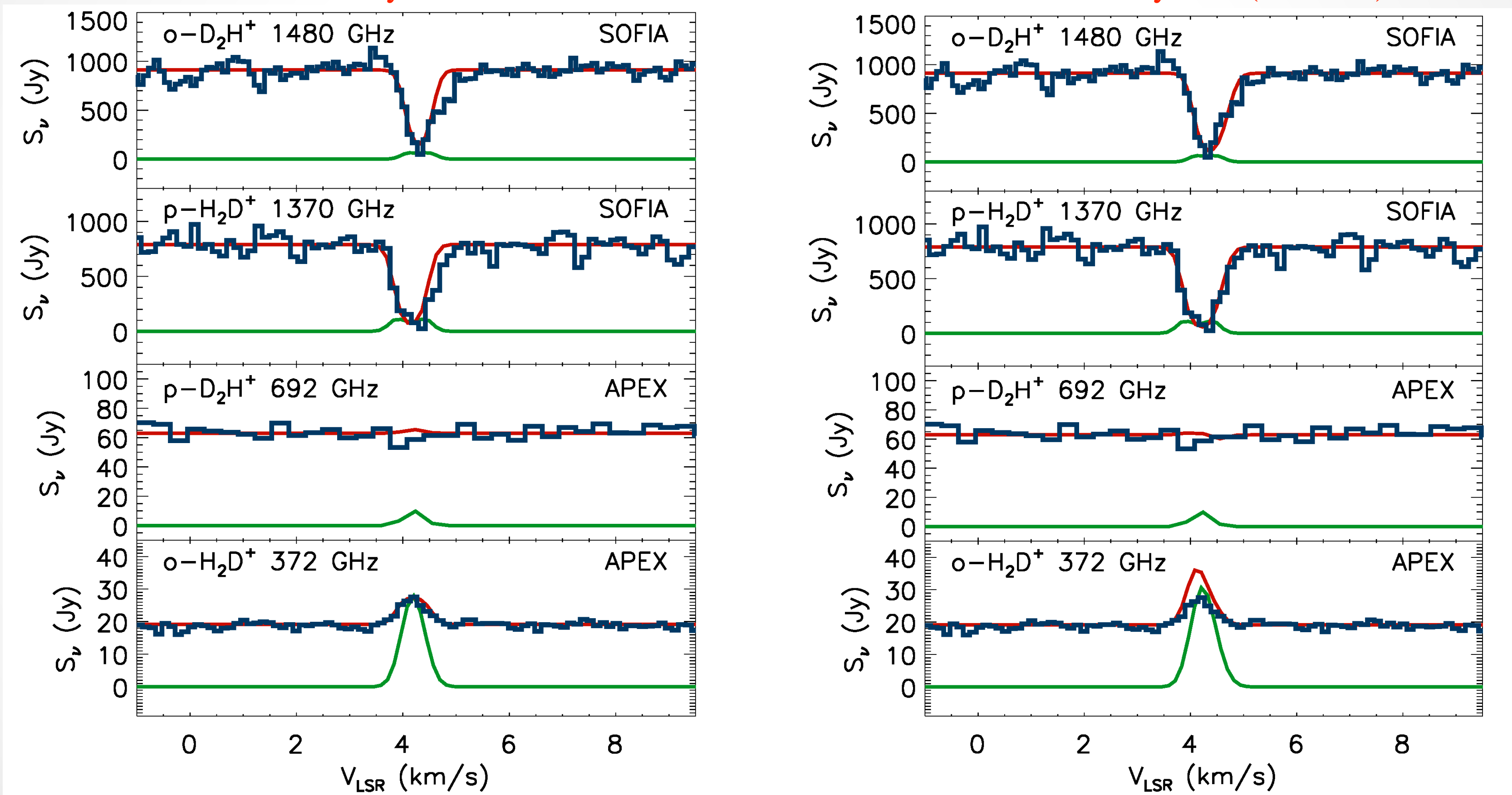
abundances not in steady state!



Spin states of H_2D^+ and D_2H^+ as chemical age tracers

observed + modeled spectra, Harju et al. (2017)

no velocity shift | with velocity shift (0.2 km/s)



best-fit chemical age is refined to $5x10^5+5x10^5$ ($\pm 2x10^5$) yr, i.e., still of the order of 10^6 yr in total

- the dominant reaction that influences the H_2D^+ o/p ratio is

$$\mathrm{pH_2D^+} + \mathrm{oH_2} \underset{\mathrm{k_1^-}}{\overset{\mathrm{k_1^+}}{\rightleftharpoons}} \mathrm{oH_2D^+} + \mathrm{pH_2}$$

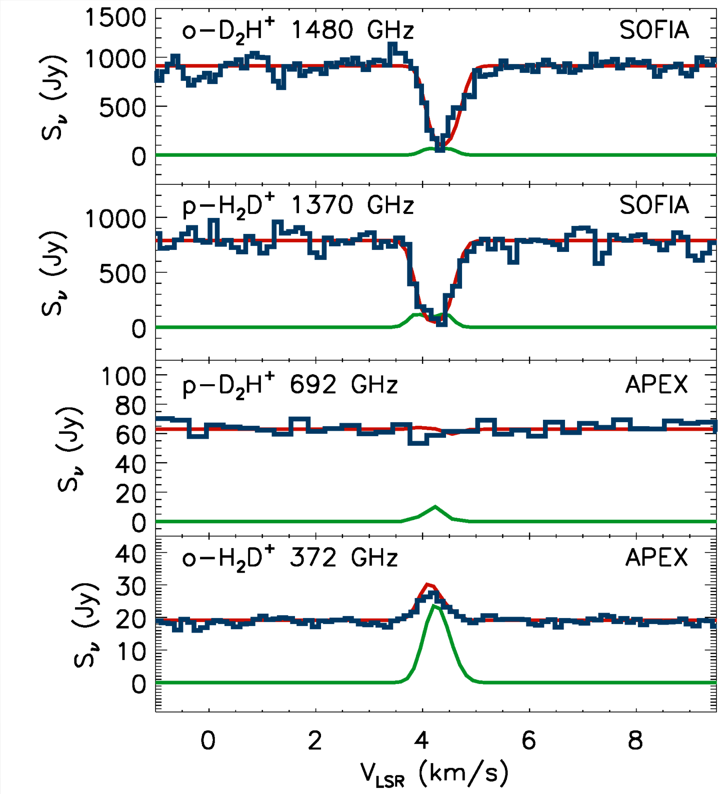
- an in-depth analysis of the reaction rates revealed that

$$k_1^+/k_1^- \sim 2.25\ \exp(87.7/T)$$

while the equilibrium constant is

$$K_1(T) \equiv \frac{k_1^+}{k_1^-} = \frac{Q_{\mathrm{oH_2D^+}}(T)}{Q_{\mathrm{pH_2D^+}}(T)} \frac{Q_{\mathrm{pH_2}}(T)}{Q_{\mathrm{oH_2}}(T)} \sim \exp(84.1/T)$$

hinting that ortho-H_2D^+ is overproduced in the model



- a simple test where the rate coefficient of the backward reaction is increased yields a much better agreement with the observations
- this implies that the effect of excited rotational states on the rate coefficients should not be ignored
- this makes sense also because H_2D^+ is detected in emission ubiquitously

Spin states of H_2D^+ and D_2H^+ as chemical age tracers

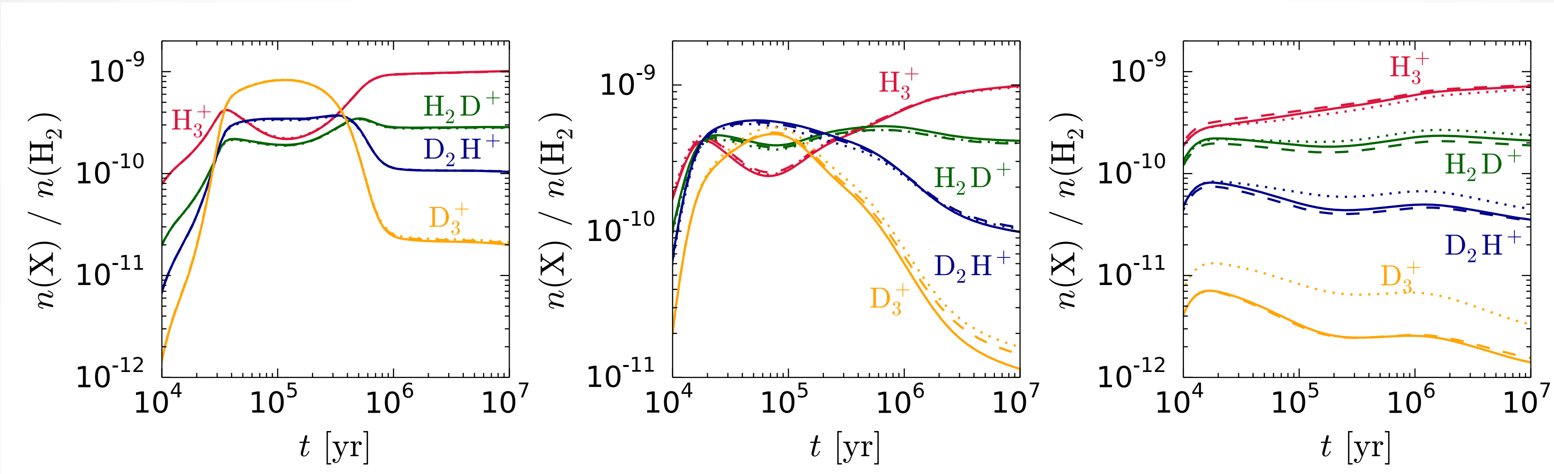
- upcoming publication on the effect of excited rotational states on the abundances of the H_3^+ isotopologs (Sipilä, Harju & Caselli subm.)

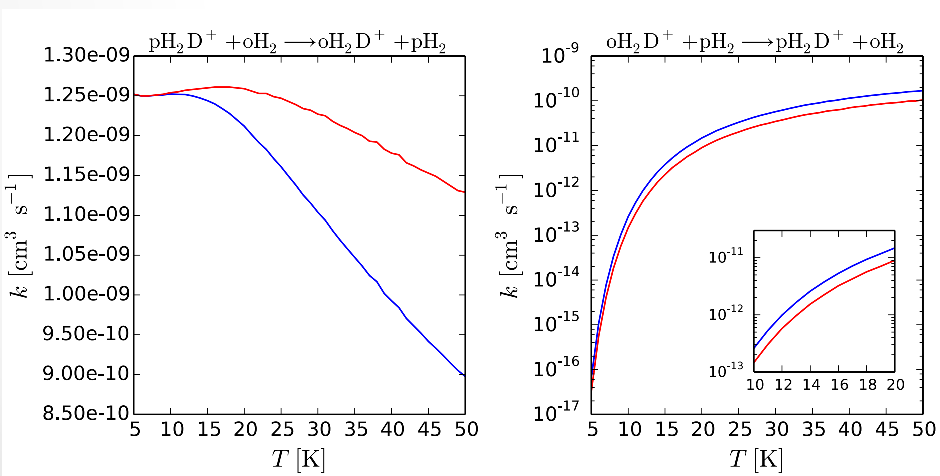
- we construct a new set of species-to-species rate coefficients based on the state-to-state rate coefficients calculated by Hugo et al. (2009)

- we find that the new model produces the kind of behavior for H_2D^+ and D_2H^+ that we expected based on the simple test in Harju et al. (2017)

- the new rates *decrease* deuteration at high density and for $T > 10$ K

abundances at $n(H_2) = 10^6$ cm^{-3}, T = 10 - 20 K





comparison of rate coefficients (blue: new, red: old)

Sipilä, Harju & Caselli (subm.)

- the spin states of H_2D^+ and D_2H^+ can be useful as tracers of the chemical age of cold and dense gas

- the main problem is the detection of p-H_2D^+ and o-D_2H^+

- a survey during *SOFIA* Cycle 4 produced no detections of p-H_2D^+ (sources too warm?); we are continuing the search in Cycle 5

- ongoing and future work: species-to-species rate coefficients for the H_3^+ + H_2 system, spin-state chemistry in hydrodynamical simulations, ALMA observations of deuterated ammonia...