Deuterium in Water Ice

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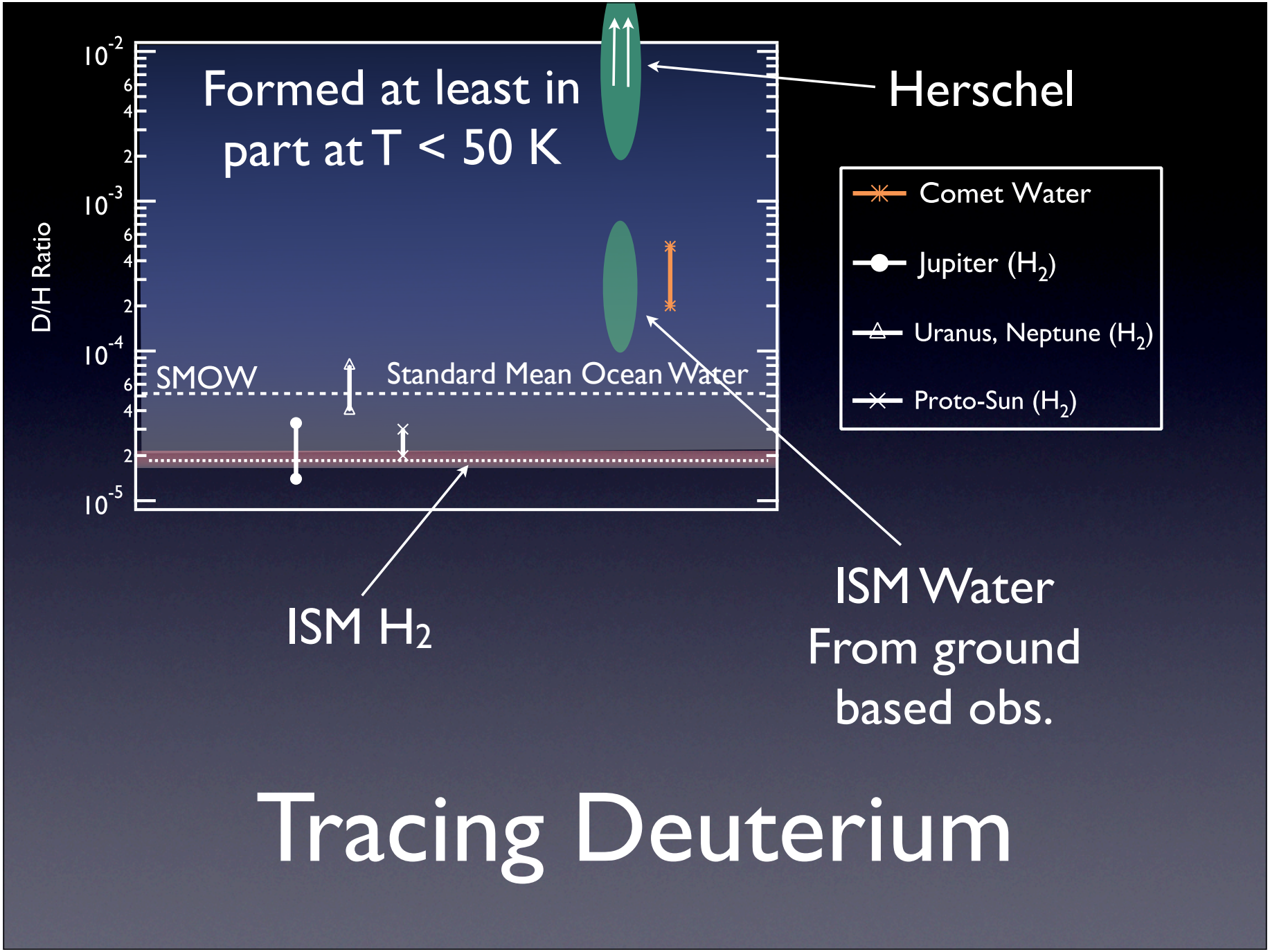
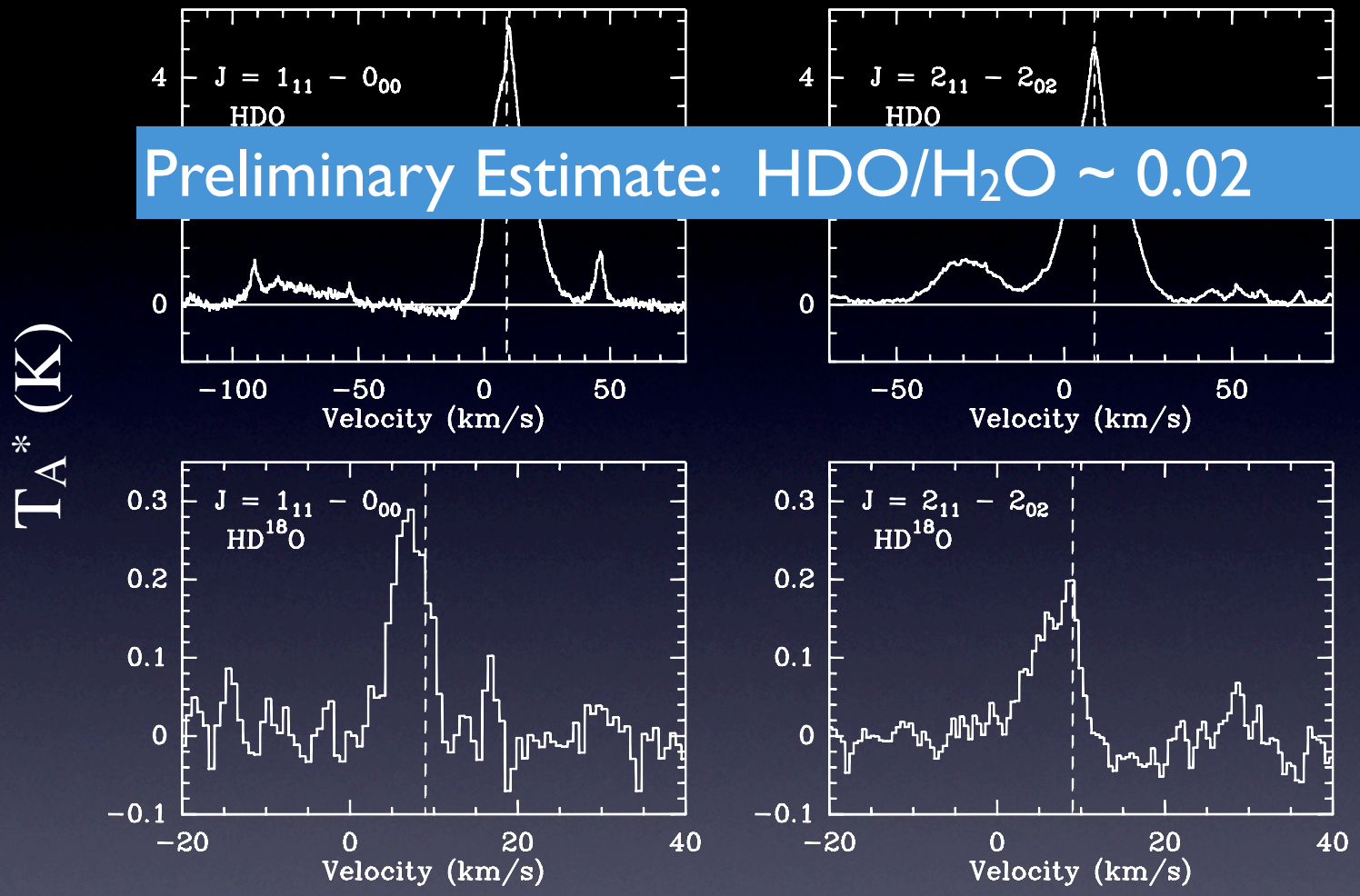
Deuterium Fractionation

- Comic interstellar ratio of $[HD]/[H_2] \sim 3 \times 10^{-5}$, which sets the initial condition in molecular clouds.

- When a molecule is "fractionated" at low temperatures (< 50 K), H is replaced by D because of its lower ground energy, resulting in $[xD]/[xH] >> [HD]/[H_2]$.



Tracing Deuterium

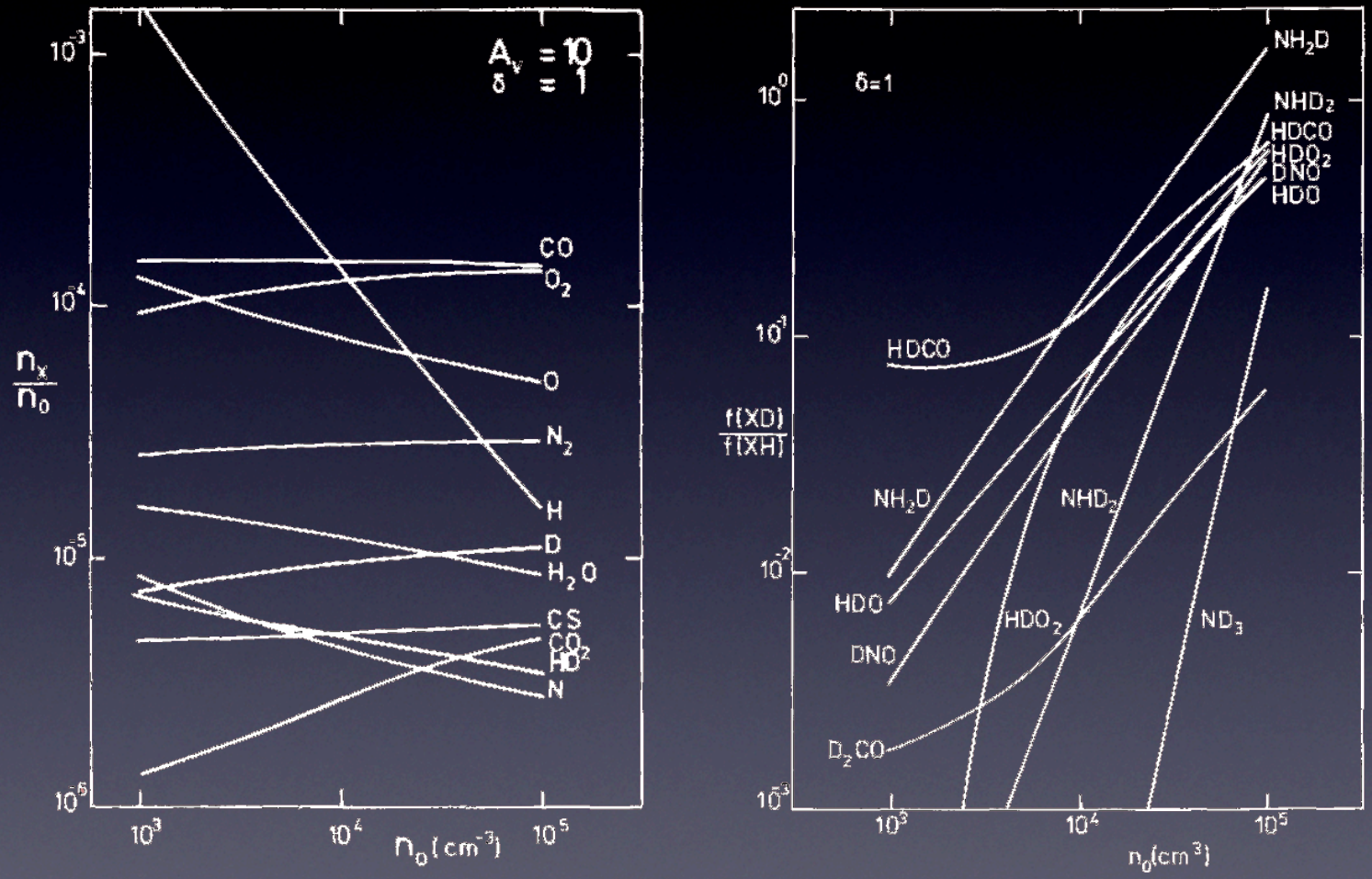


Detection of $HD^{18}O$

Issues

- There is a significant diversity of [HDO]/[H_2O] from < 10^{-4} (Gensheimer et al. 1996; Jorgensen & van Dishoeck 2010) to > 0.1 (Liu et al. 2011) in the star forming regions.
  - This diversity may be intrinsic to the conditions under which ices form.
- If X(H_2O)=10^{-4} and [HDO]/[H_2O]=0.1, then X(HDO)=10^{-5}.
  - Significant amount of deuterium is possibly locked in ices.

High Concentration of Deuterated Molecules in a Grain Mantle



Tielens 1983

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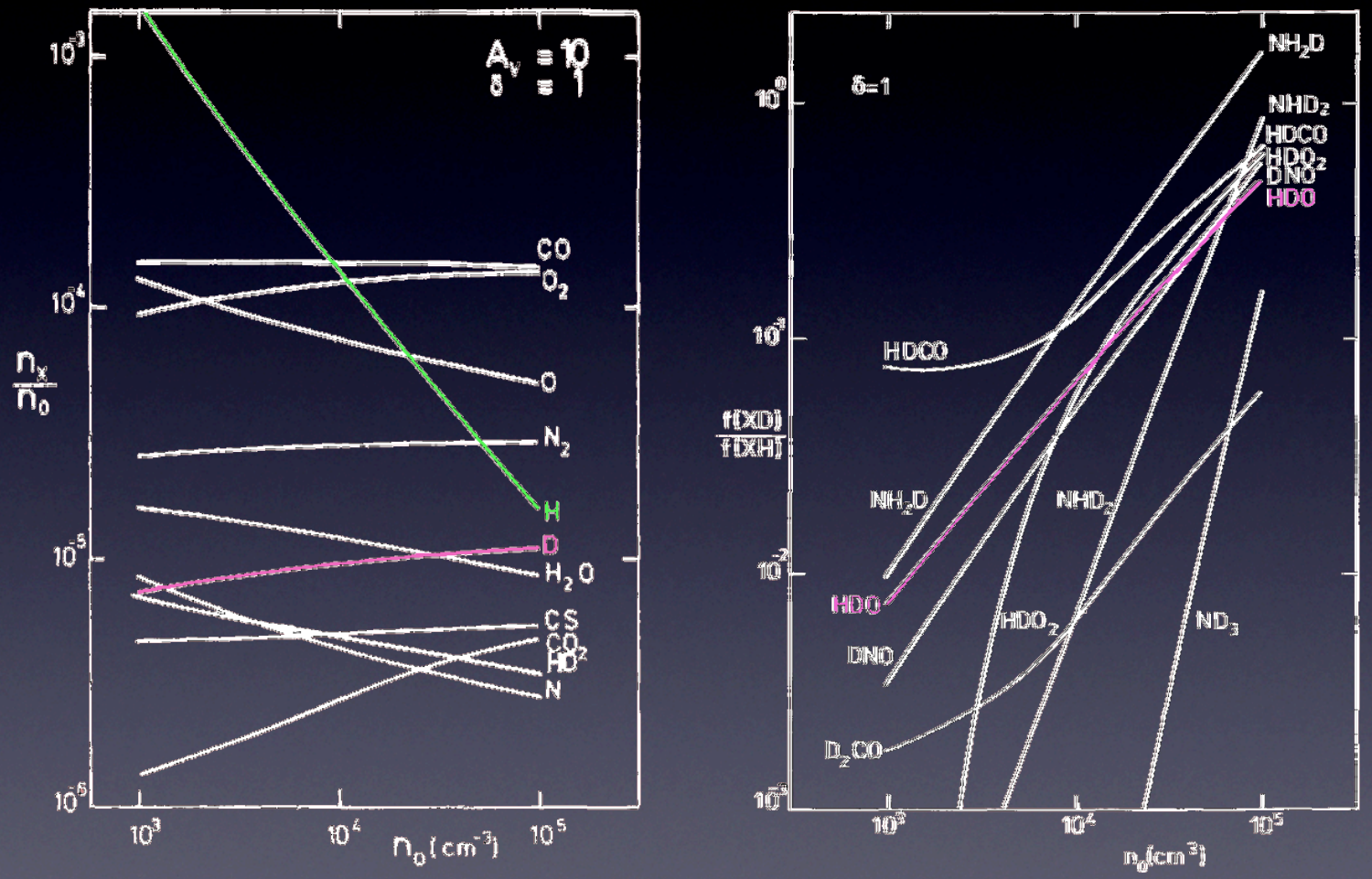


Tielens 1983

Deuterium Fractionations in the Gas

$$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2 + 230\ K$$

$$H_2D^+ + HD \rightleftharpoons D_2H^+ + H_2 + 180\ K$$

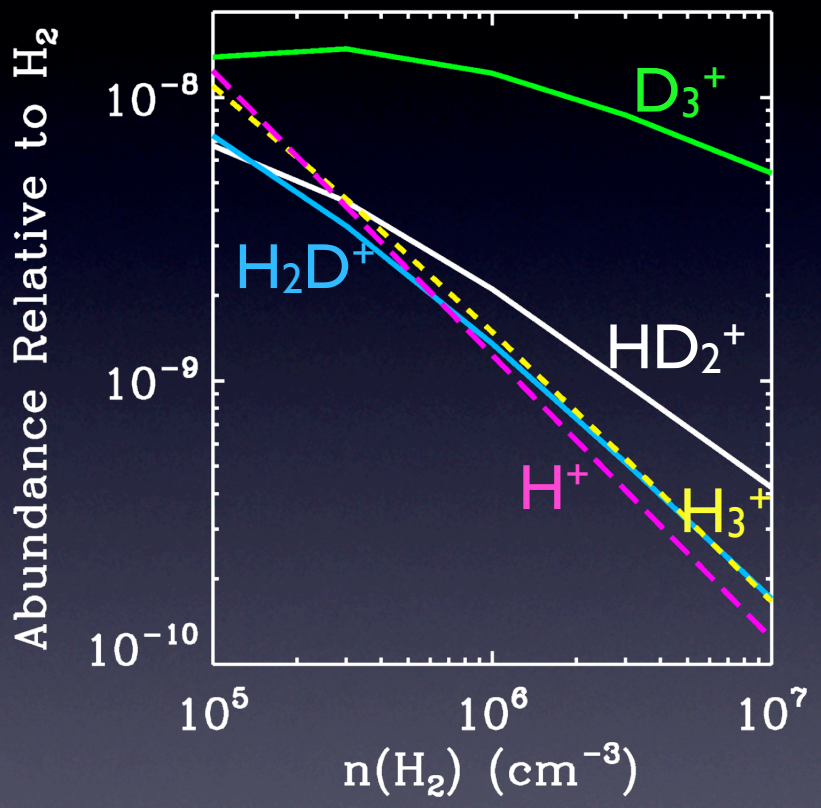
$$D_2H^+ + HD \rightleftharpoons D_3^+ + H_2 + 230\ K$$

- are active at low temperatures resulting in an excess of D atoms relative to H atoms in the gas.
- depend on the ortho-to-para (o/p) ratio of H_2 (Gerlich et al. 2002) and also on the relative abundances of the high and low energy spin isomers of each of the reactants (H_3^+, H_2D^+, D_2H^+, and D_3^+; Flower et al. 2004; Hugo et al. 2009).

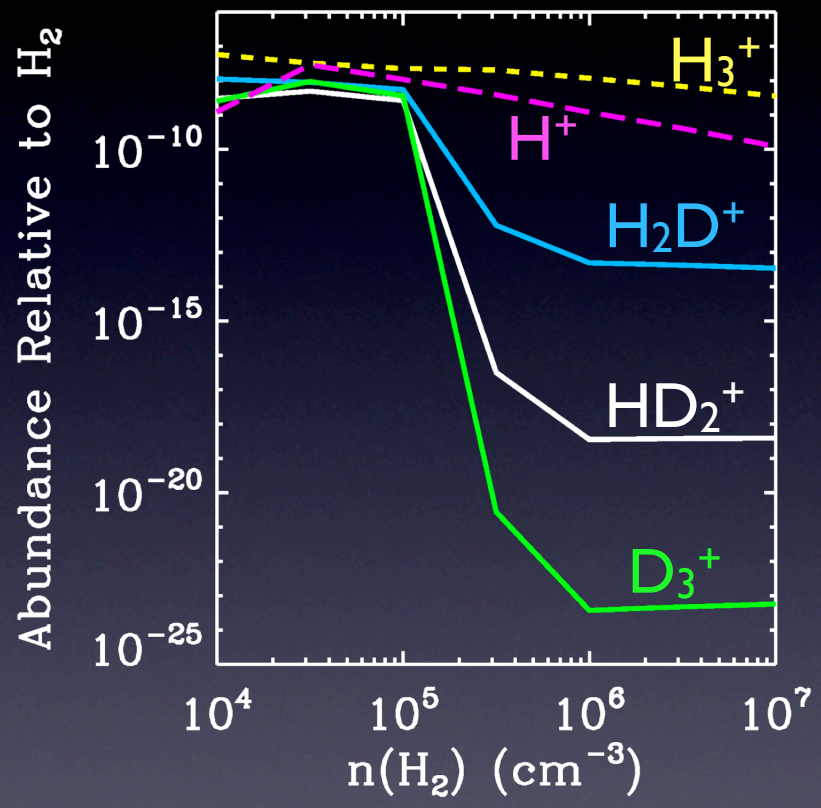
This work

- Aims to explore the deuterium fractionation implanted within ices in the context of a cloud and its dependence on the gas temperature and the o/p ratio of H_2.
- Adopts the state to state rate coefficients for each reaction calculated by Hugo et al. (2009).
- Assumes the equilibrium values of the o/p ratio for a given temperature except for H_2.

Results I



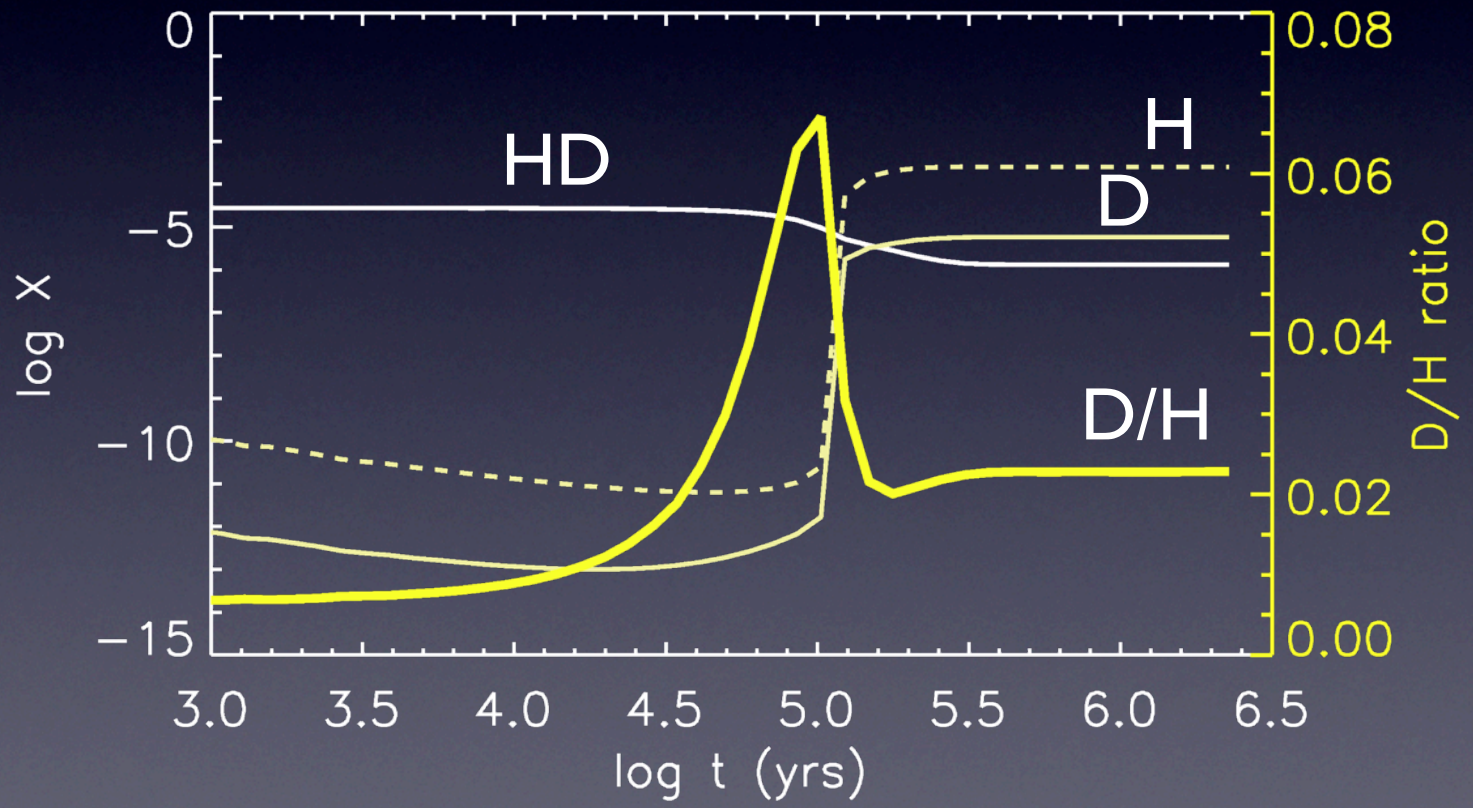
"without" surface chemistry of water



"with" surface chemistry of water

Results II

Time dependence in the model with
T=10 K, $n(H_2)=10^5$ cm $^{-3}$, $o/p(H_2)$ $=7x10^{-5}$



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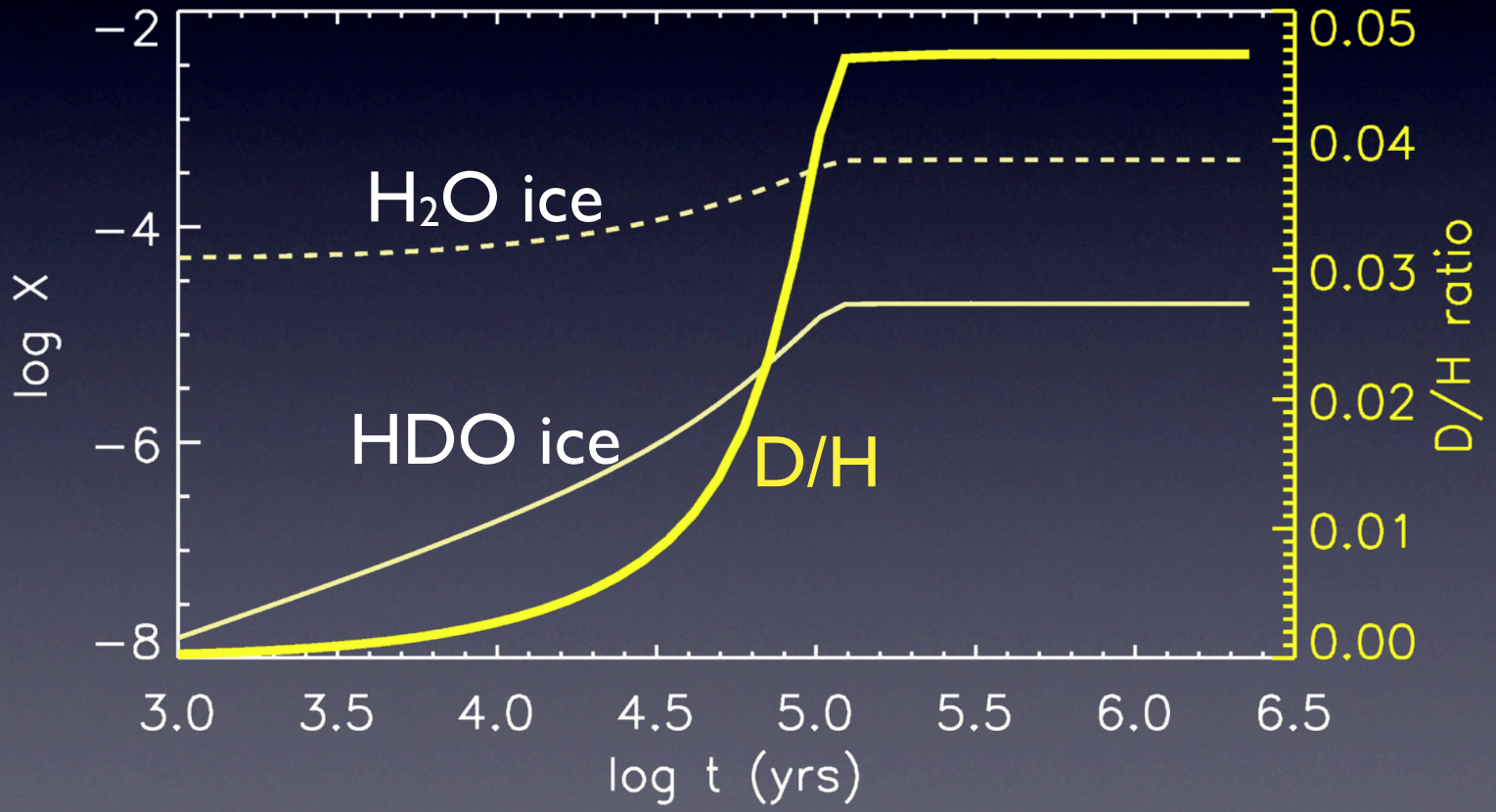
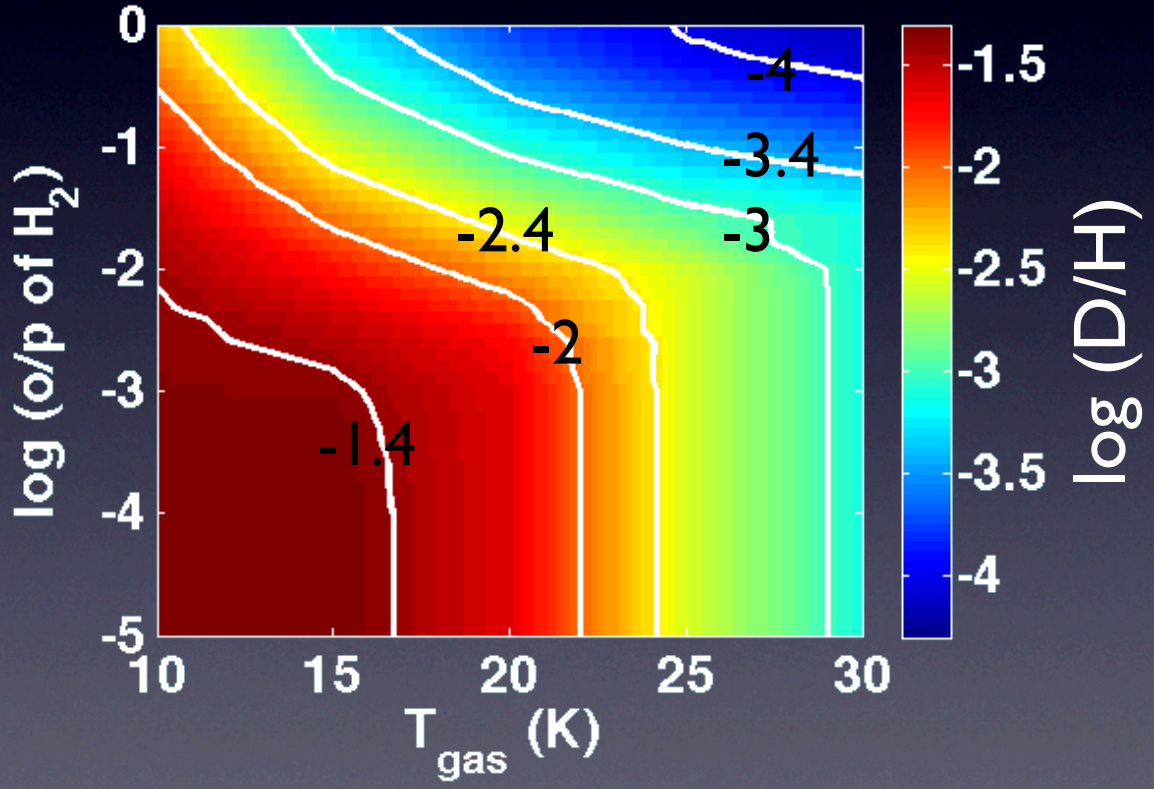


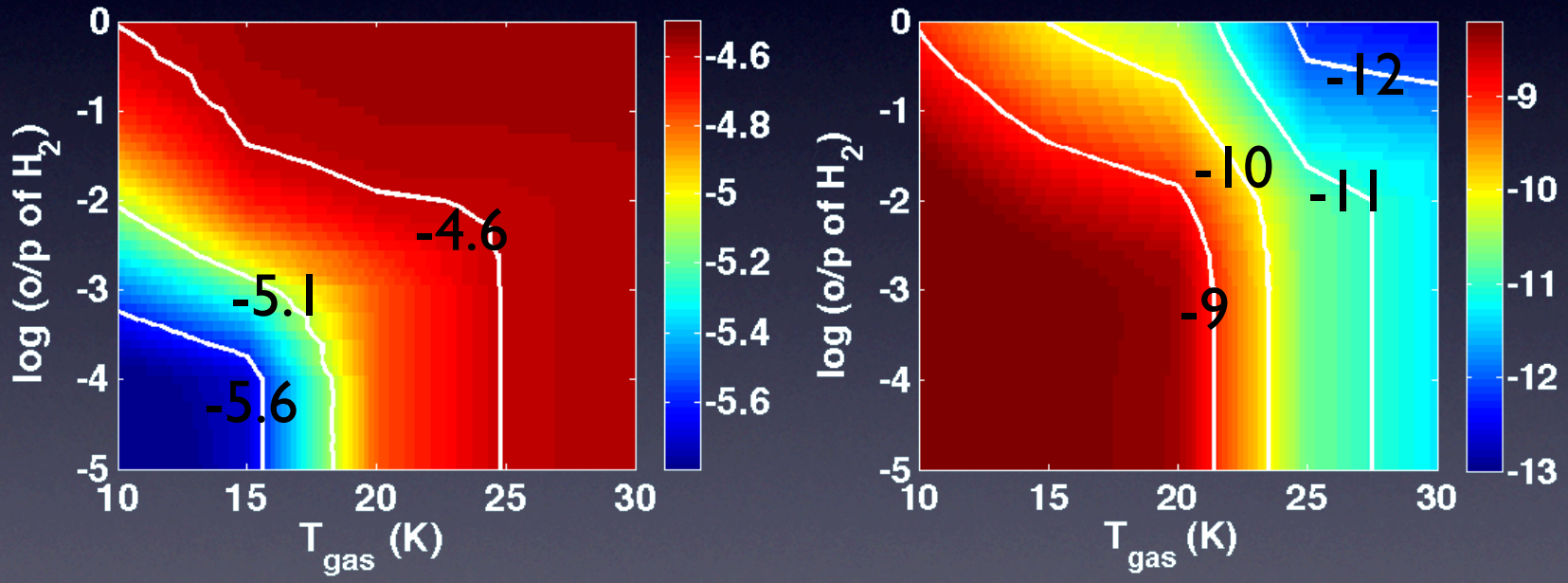
Results III

The dependence of D/H of water on T and o/p(H_2) at t=3x10^5 yrs



Results III

X(HD) and X(H_2D^+) vs. T and o/p(H_2)
at t=3x10^5 yrs

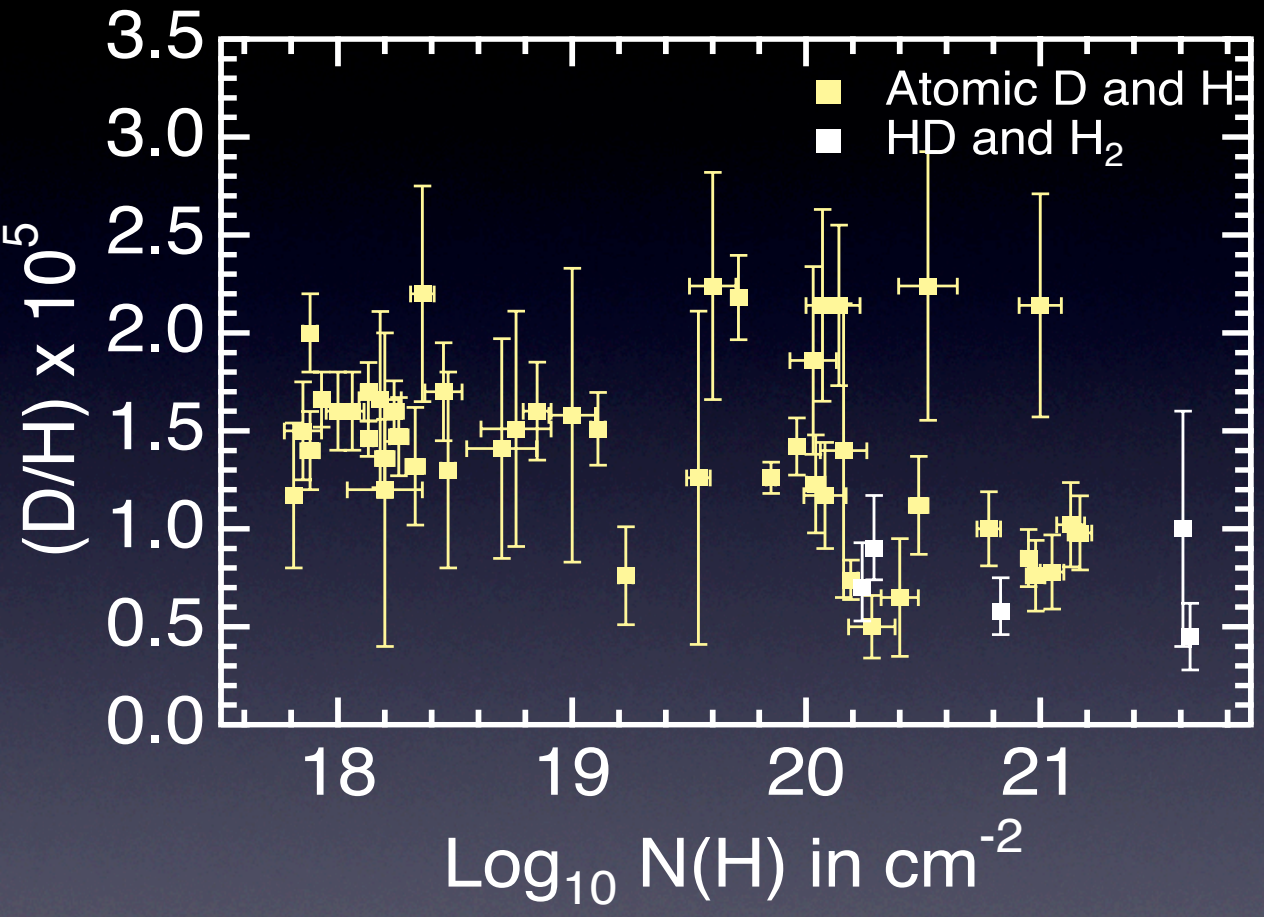


log (X)

Summary

- Elevated D/H ratios are being found through observations of water vapor in star forming regions.
- Deuterium fractionation can increase the relative abundance of deuterium atoms in the gas, resulting in the high concentration of deuterated water in grain surface.
  - The relative fractions of spin isomers can significantly alter the deuterium fractionations in the gas and in ices.
  - The implantation of deuterium into ices can trap a significant fraction of the cosmic deuterium, which has implications for the resulting gas-phase chemistry.
- Stars that form in warm (> 20 K) gas should have ices with lower D/H ratios than those that form from cold (10 K) gas.

Depletion of D and HD from Gas



from atomic D & H (Friedman et al. 2006)

from HD & H_2 (Neufeld et al. 2006)