



MAX PLANCK INSTITUTE
FOR EXTRATERRESTRIAL PHYSICS

**Deuterium chemistry in the ISM, and how ALMA Band 2 will
enhance our knowledge of it**

Olli Sipilä

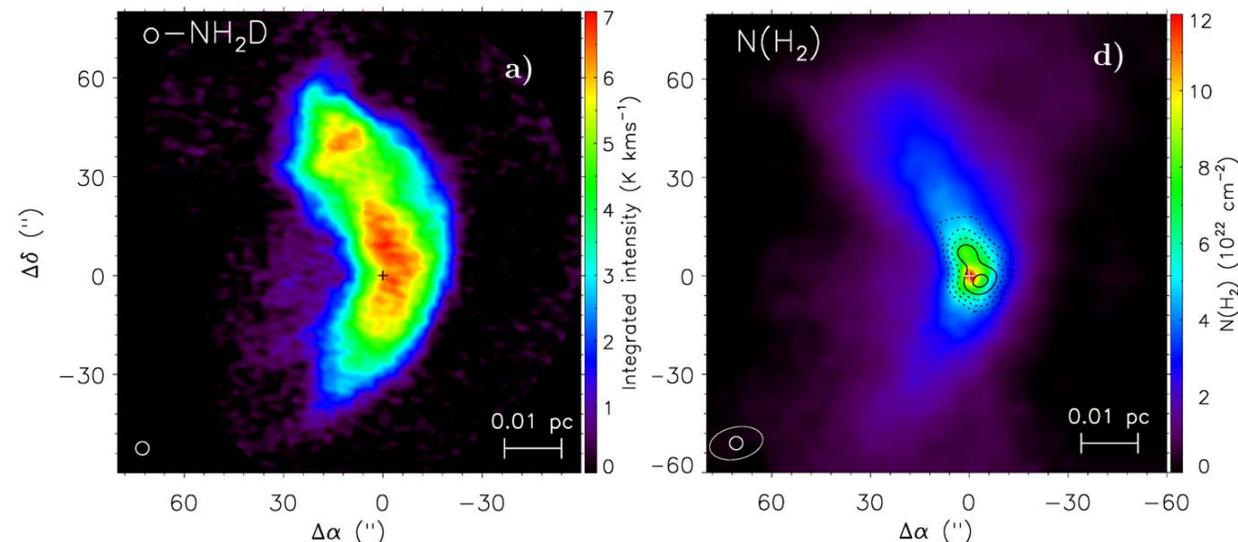
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Max Planck Institute for Extraterrestrial Physics, Garching, Germany*

Deuterated molecules are excellent tracers of physical conditions in the ISM

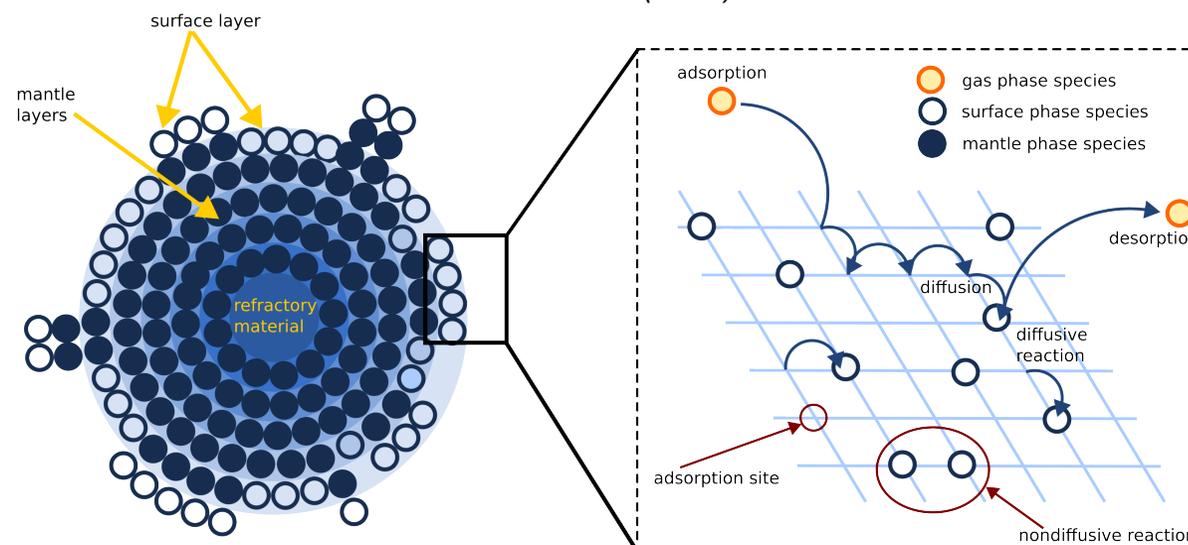
In dense cores, CO is heavily depleted and deuterated species start increasing in abundance via:

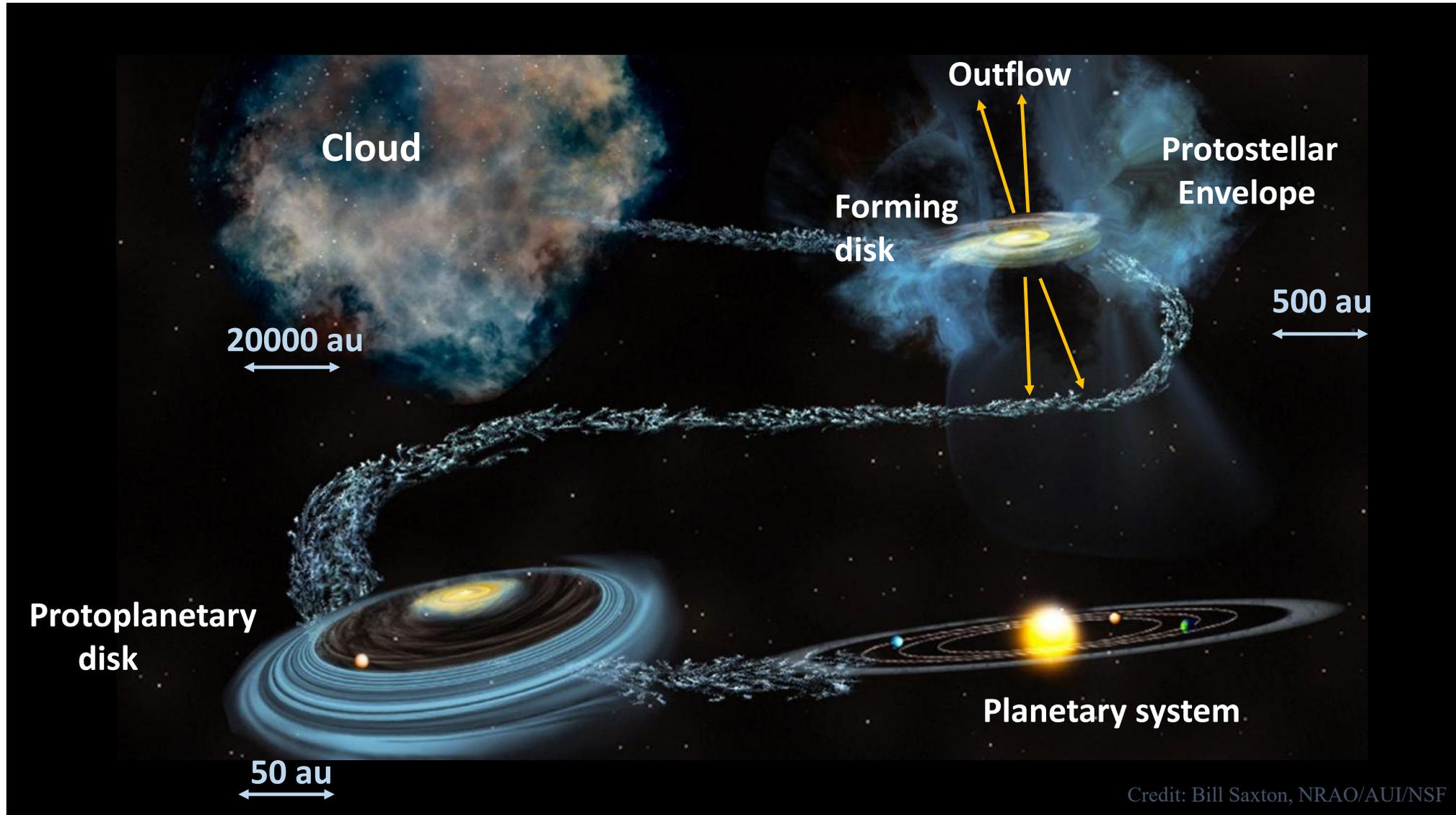


The dissociative recombination of $\text{H}_2\text{D}^+/\text{D}_2\text{H}^+/\text{D}_3^+$ with electrons releases atomic D that can end up on grains



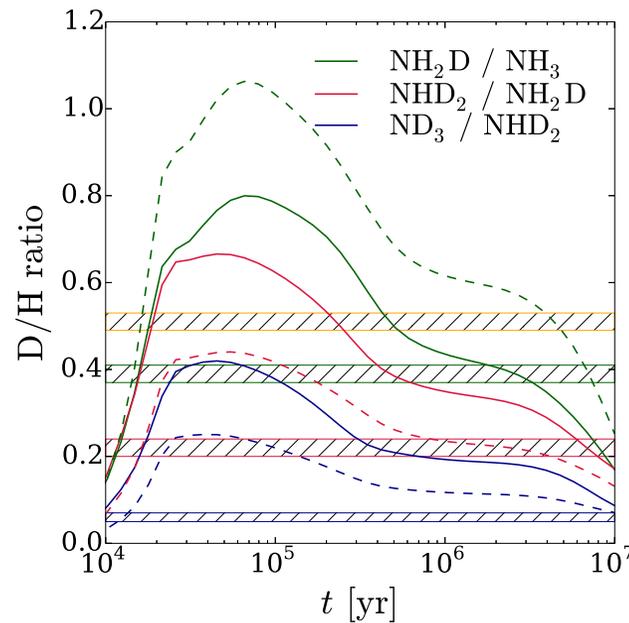
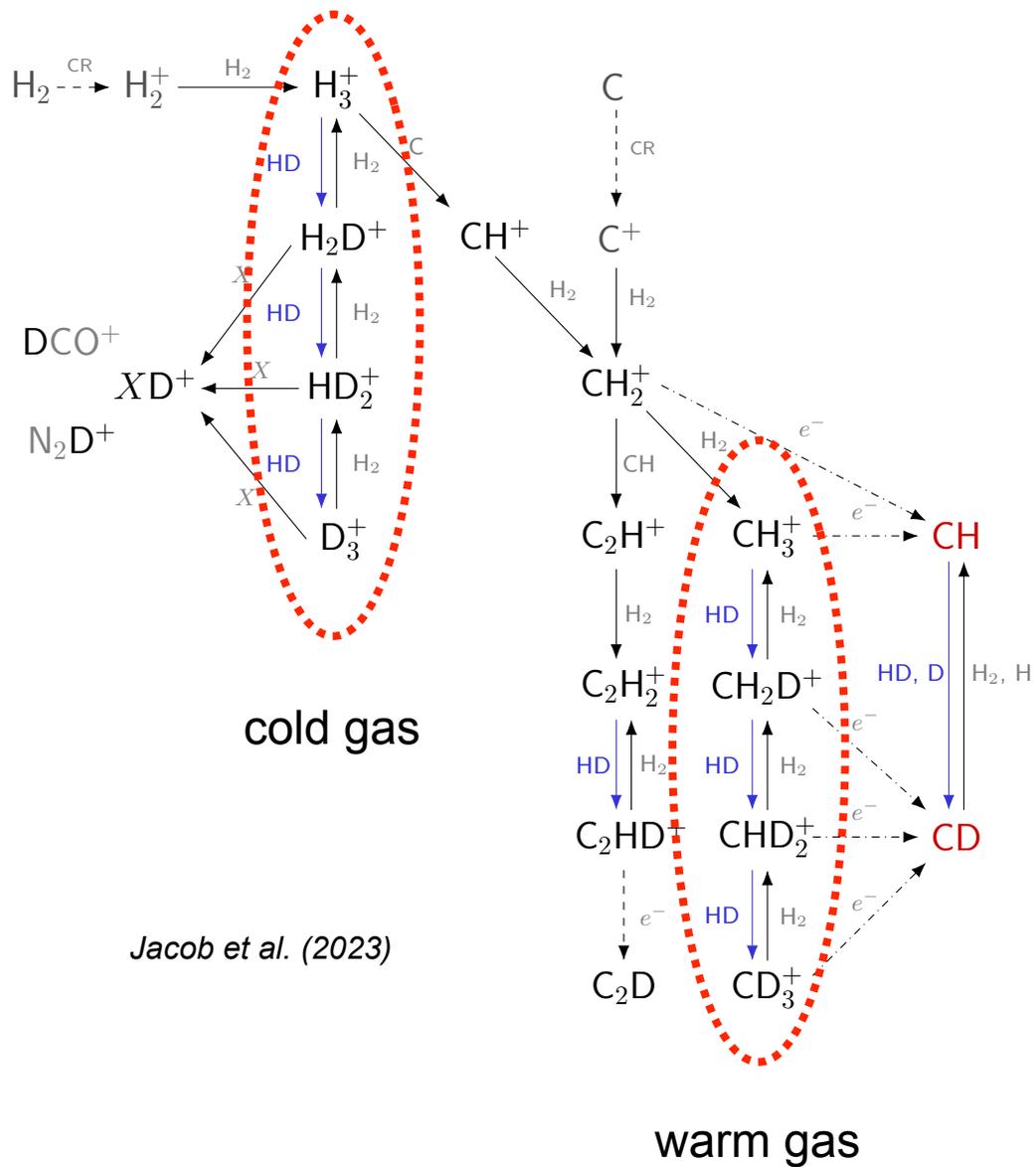
Yamamoto (2016)





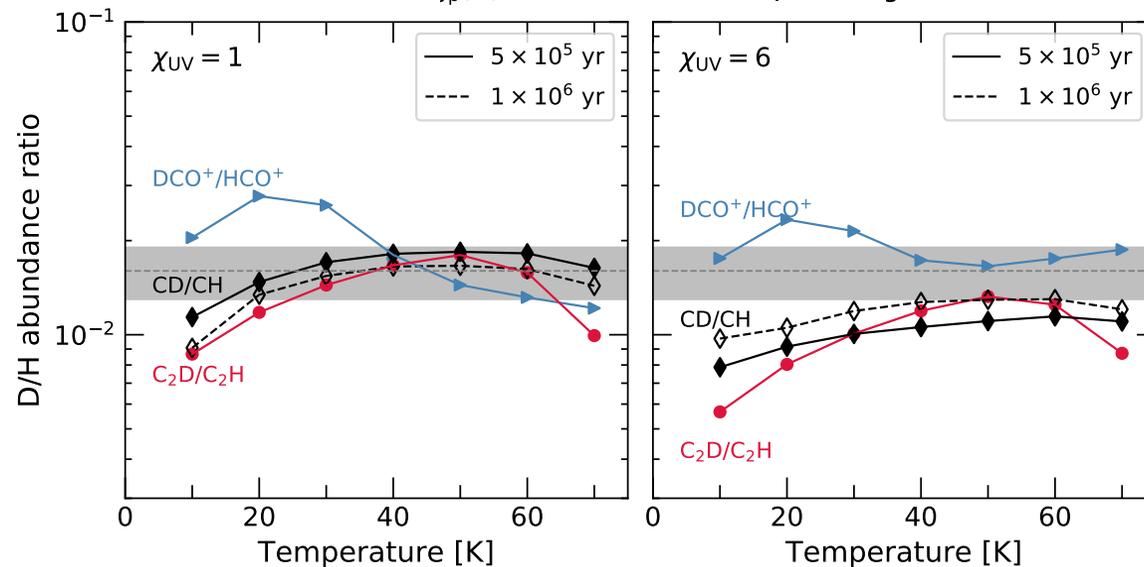
Credit: Bill Saxton, NRAO/AUI/NSF

Clouds: deuteration in the gas phase



Sipilä et al. (2019)

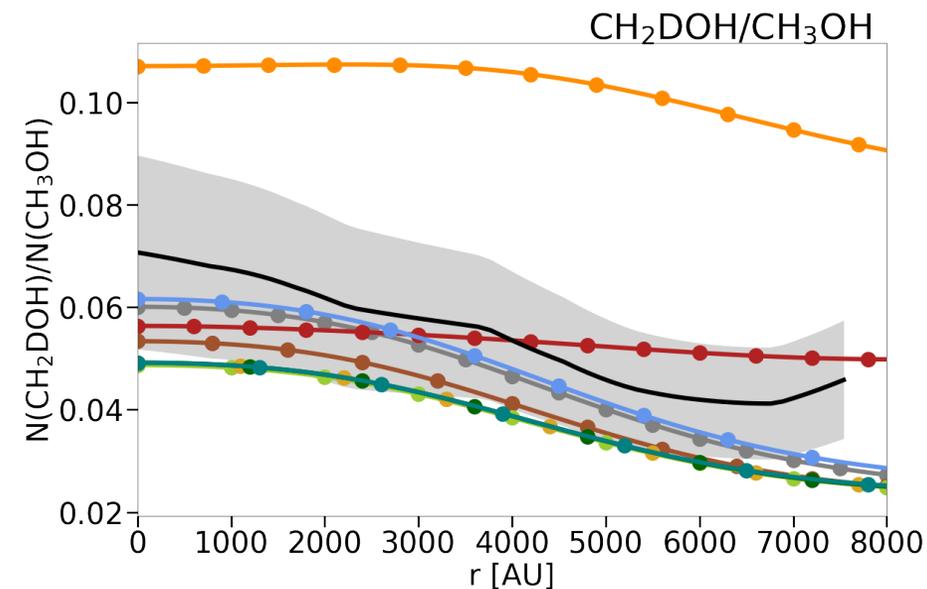
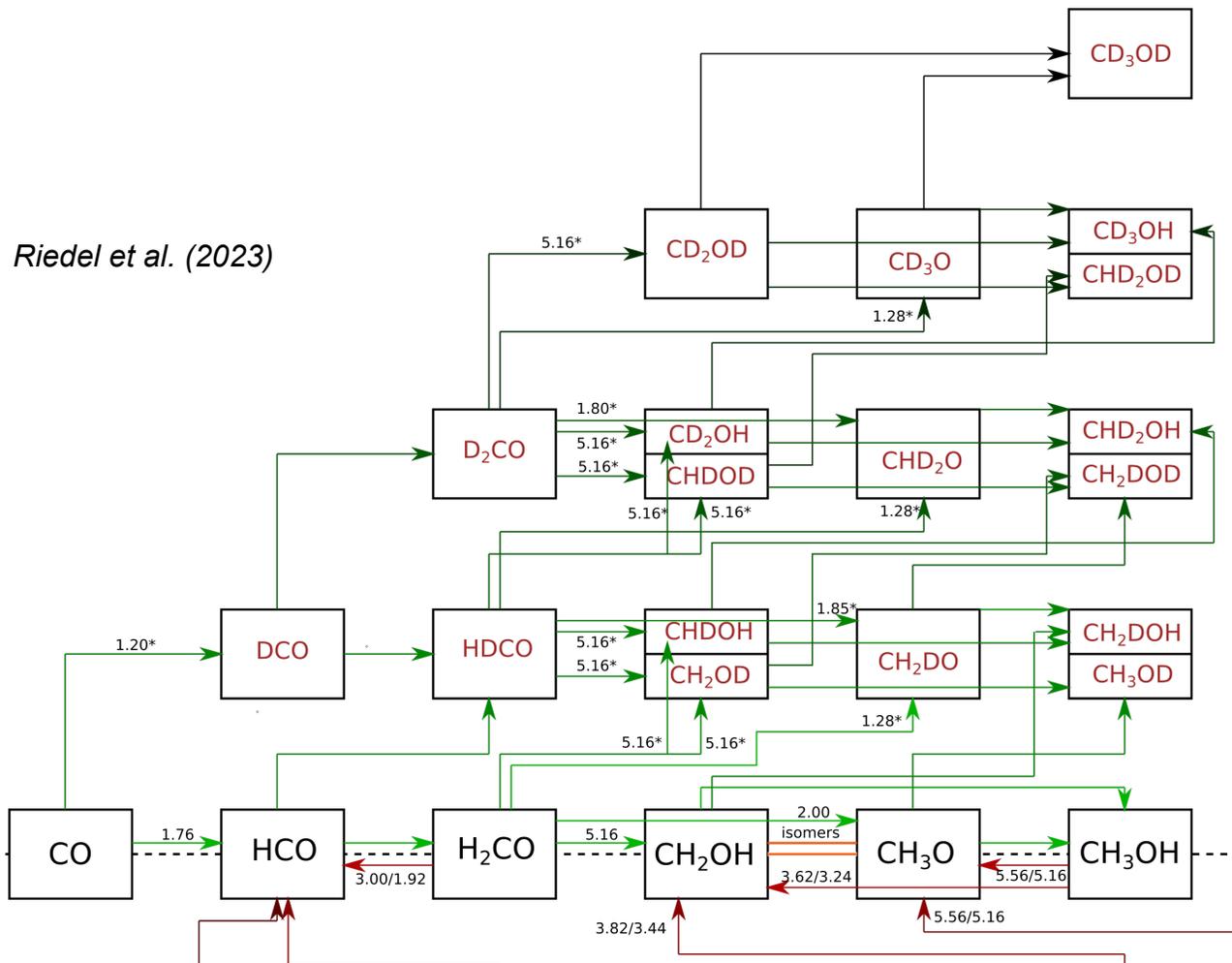
$\zeta_p(\text{H}) = 1.3 \times 10^{-17} \text{ s}^{-1}$, $A_v = 4 \text{ mag}$



Jacob et al. (2023)

Clouds: deuteration of COMs (on grains)

Riedel et al. (2023)

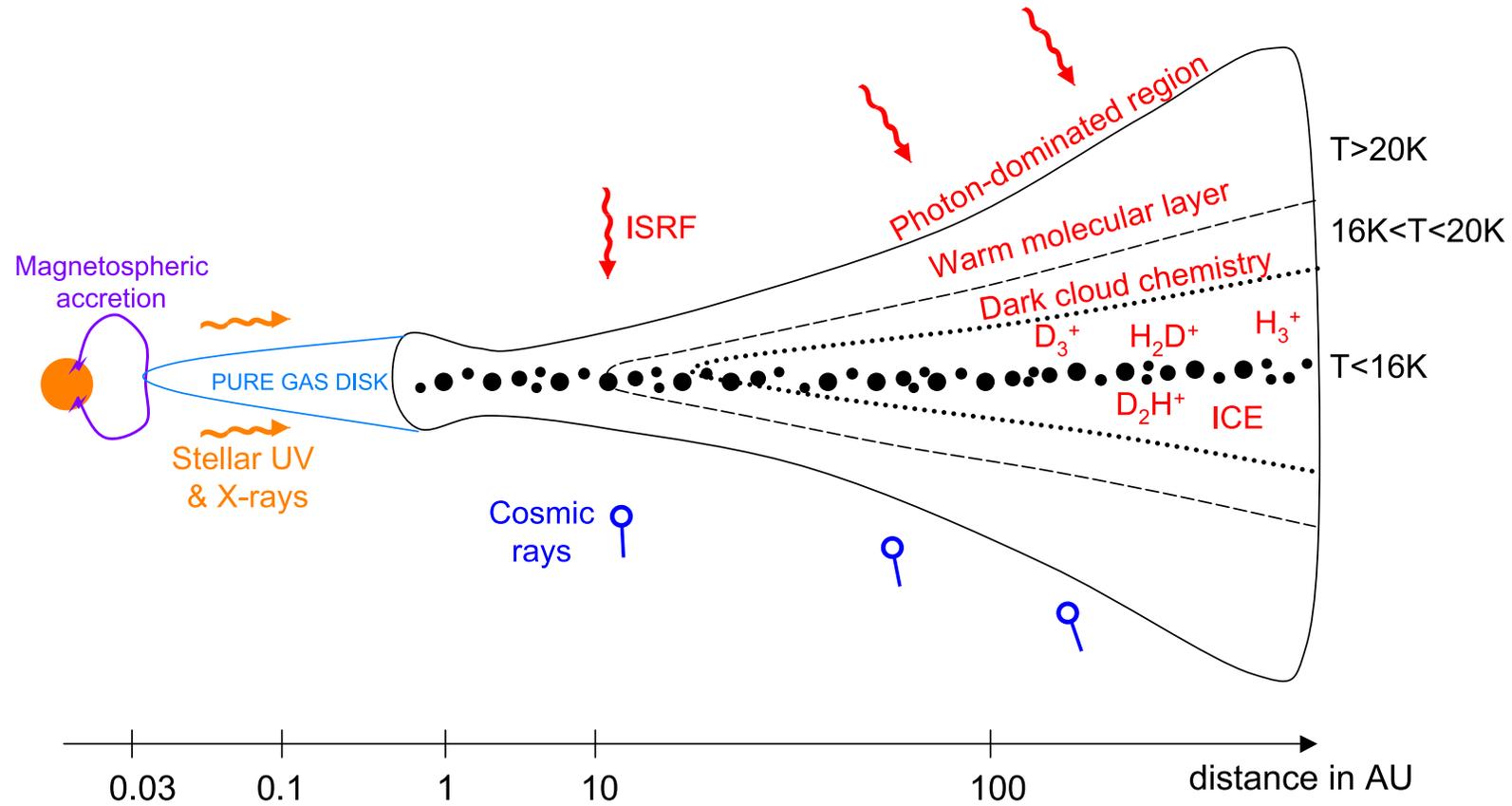


Riedel et al. (2025)

Stay tuned for Riedel et al. (in prep.)

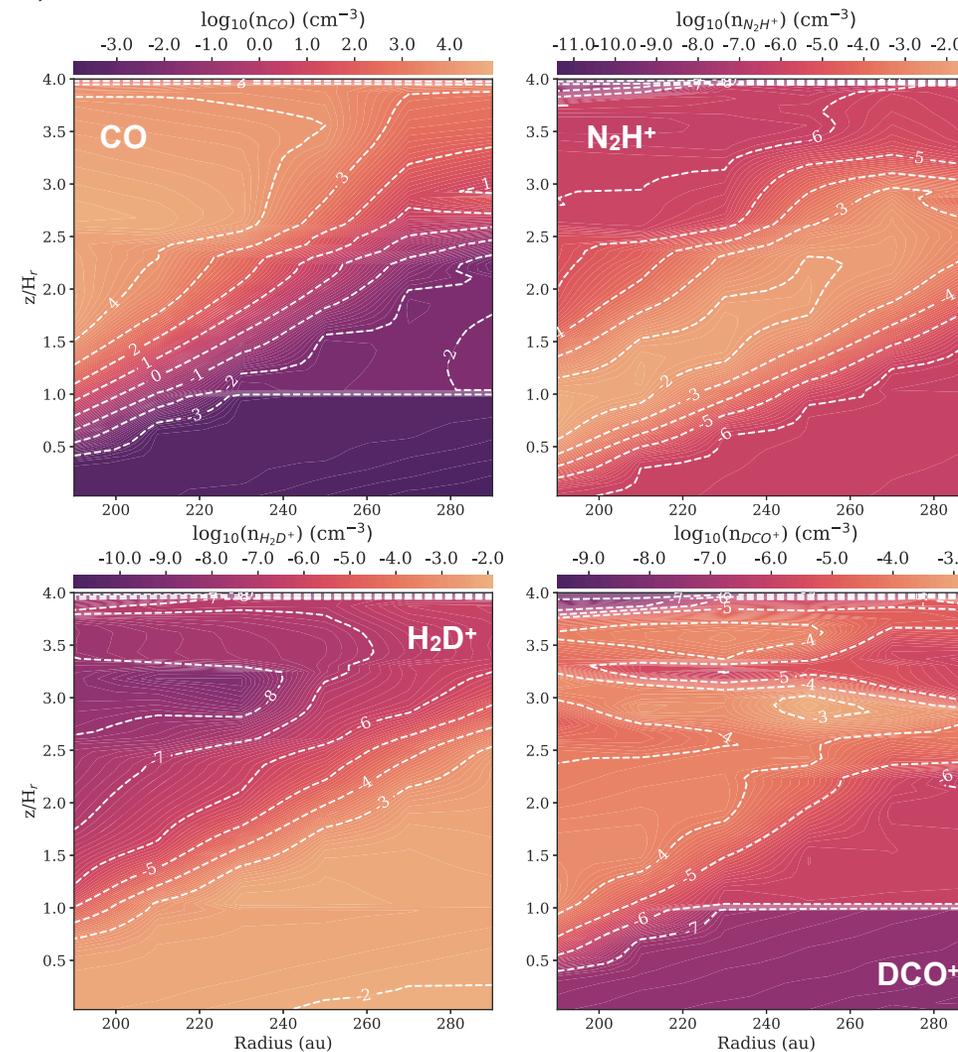
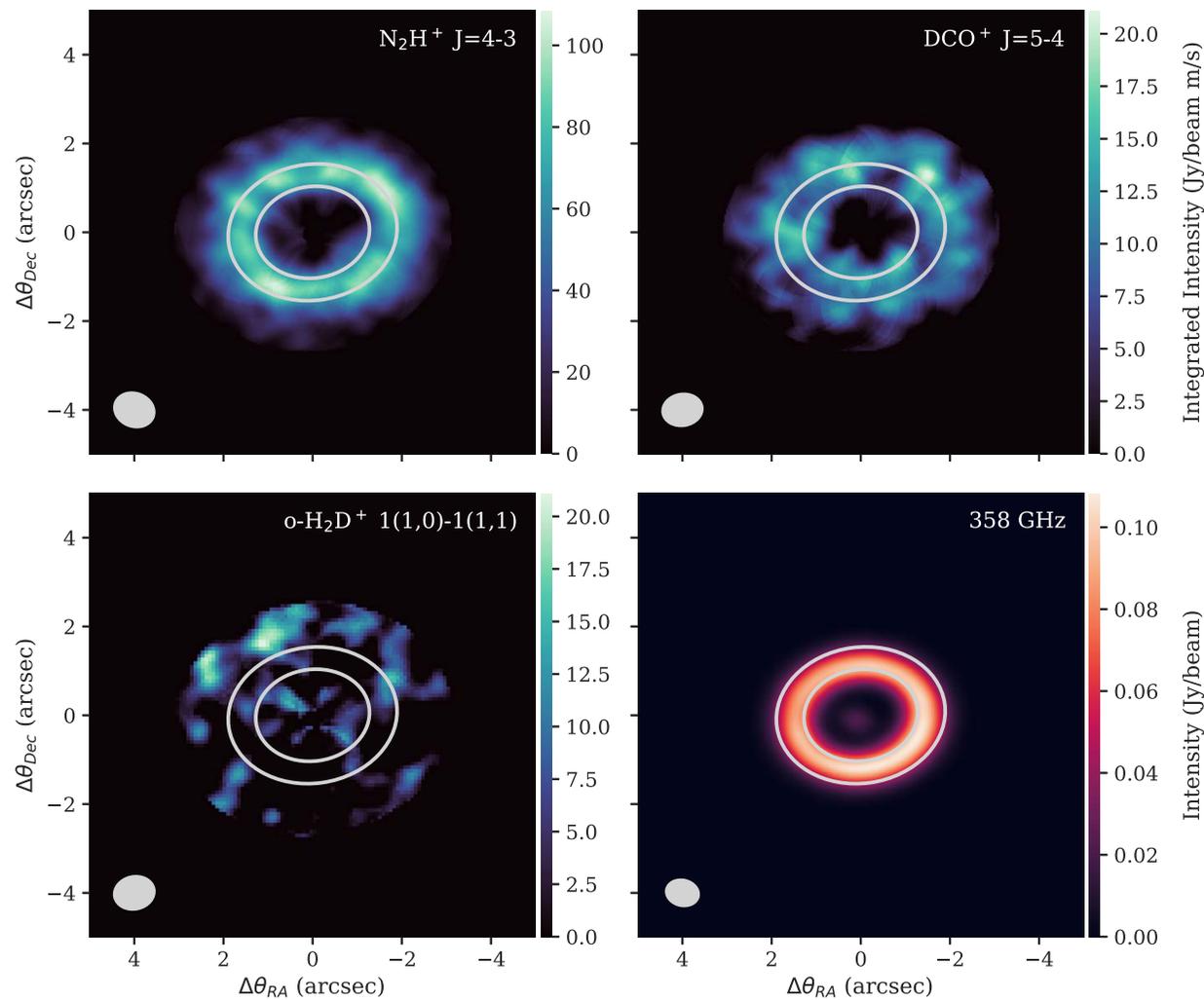
Deuteration in disks

Caselli & Ceccarelli (2012)



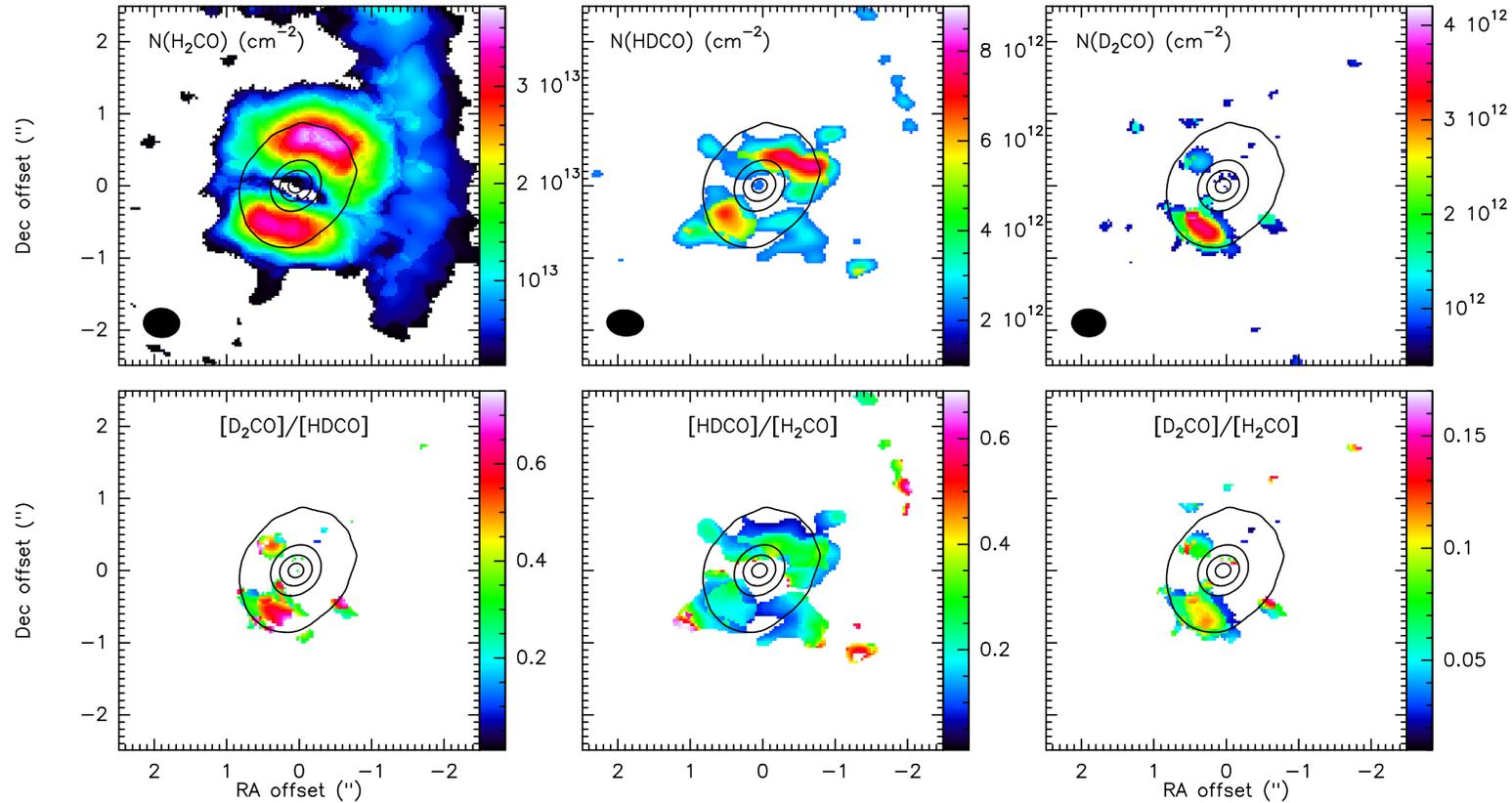
Deuteration in disks: observations & models

Kashyap et al. (2024)



Deuteration in disks: gas-phase vs. grain-surface chemistry

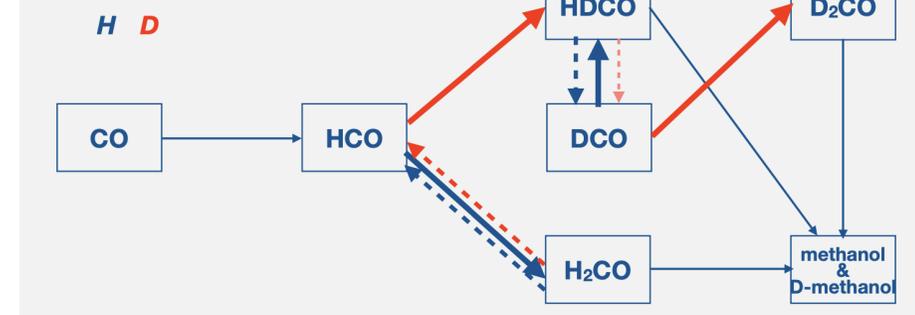
Podio et al. (2024)



Gas-phase

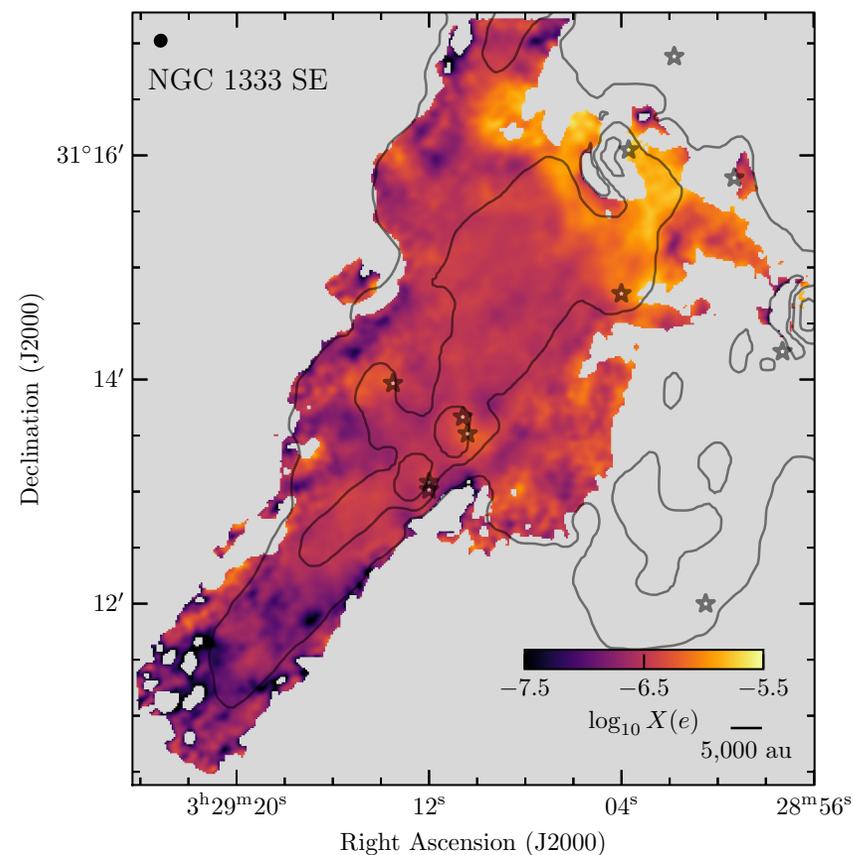
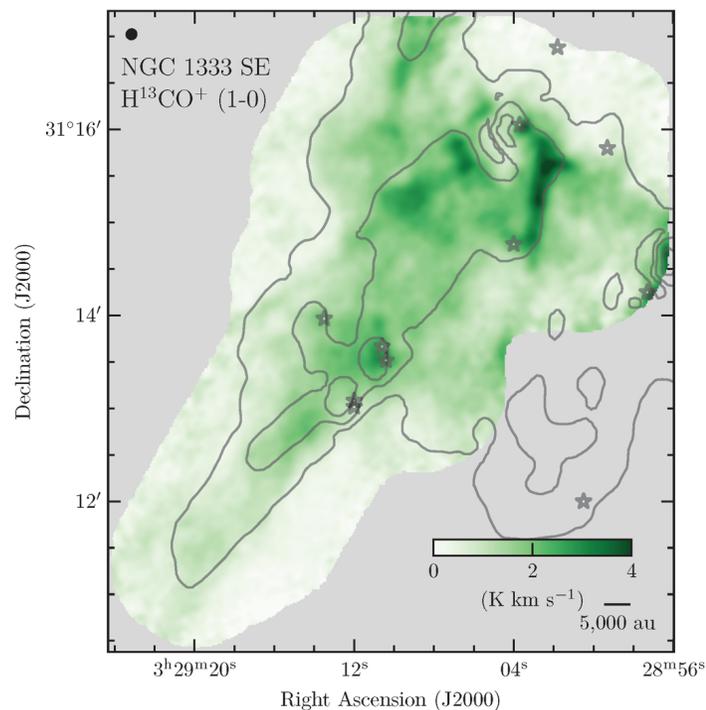
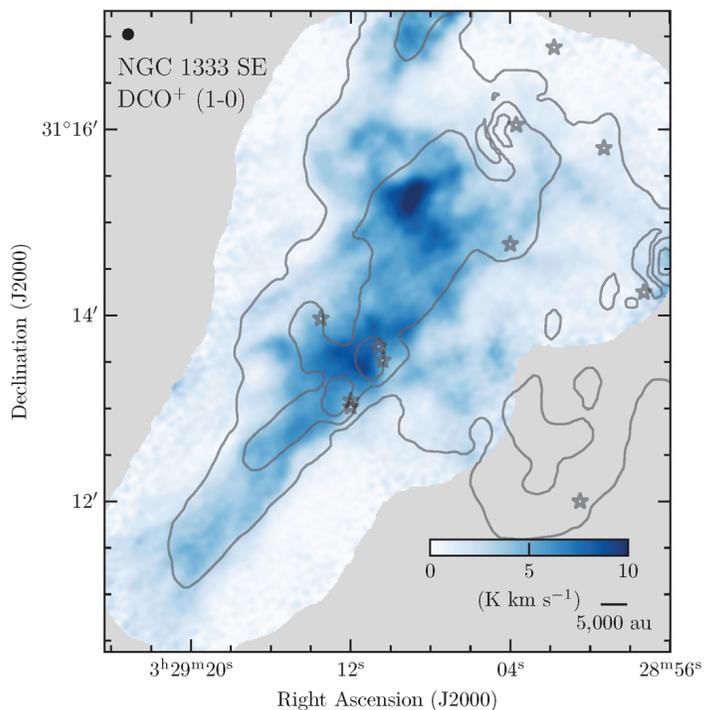


Grain-surface



Observational use cases for deuteration: probe of the physical characteristics of clouds

Pineda et al. (2024)



$R_D = \text{DCO}^+/\text{HCO}^+$

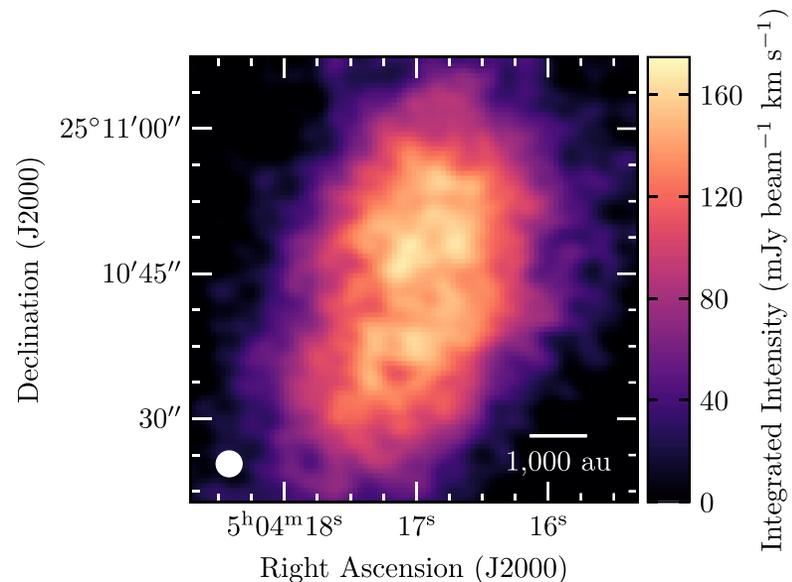
$$X(e) = \frac{2.7 \times 10^{-8}}{R_D} - \frac{1.2 \times 10^{-6}}{f_D},$$

$$\zeta(\text{H}_2) = \left[7.5 \times 10^{-4} X(e) + \frac{4.6 \times 10^{-10}}{f_D} \right] X(e) n(\text{H}_2) R_H$$

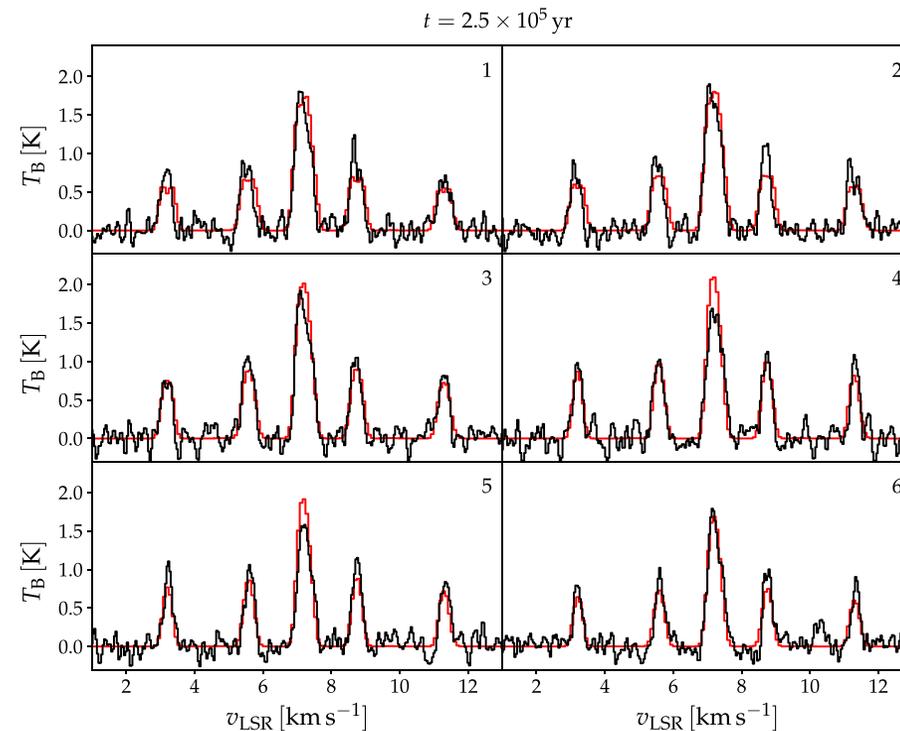
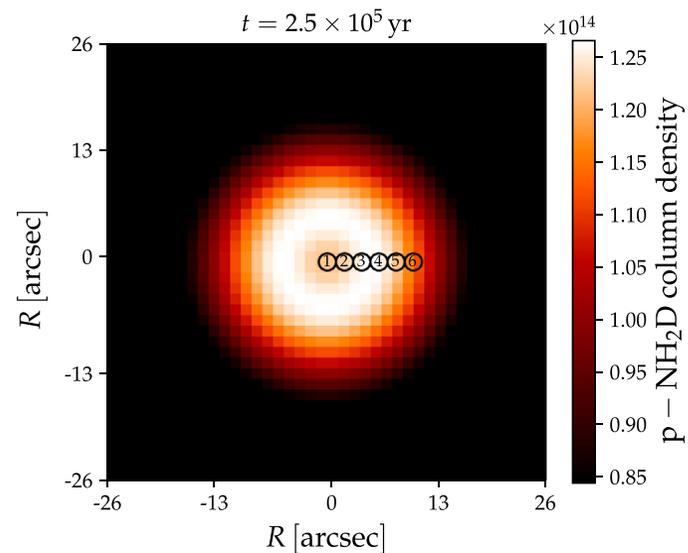
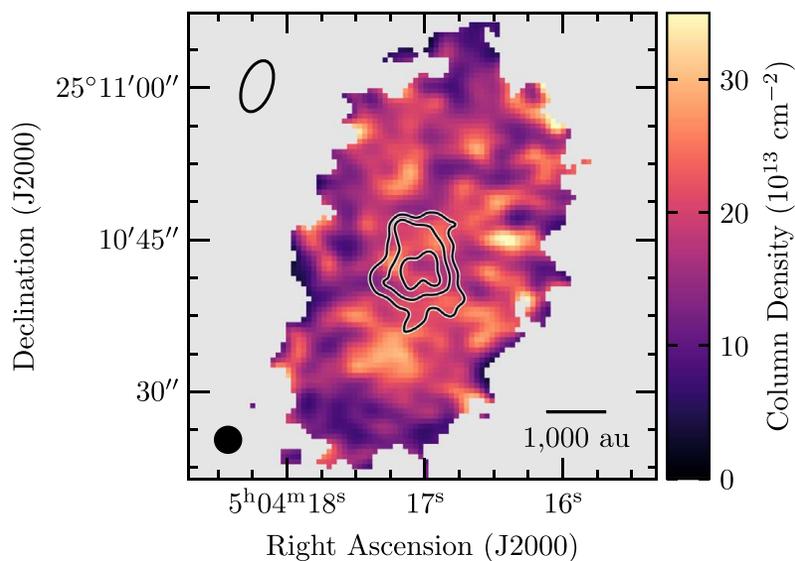
$R_H = \text{HCO}^+/\text{12CO}$

Stay tuned for Socci et al. (in prep.)

Observational use cases for deuteration: tracing dense core centers

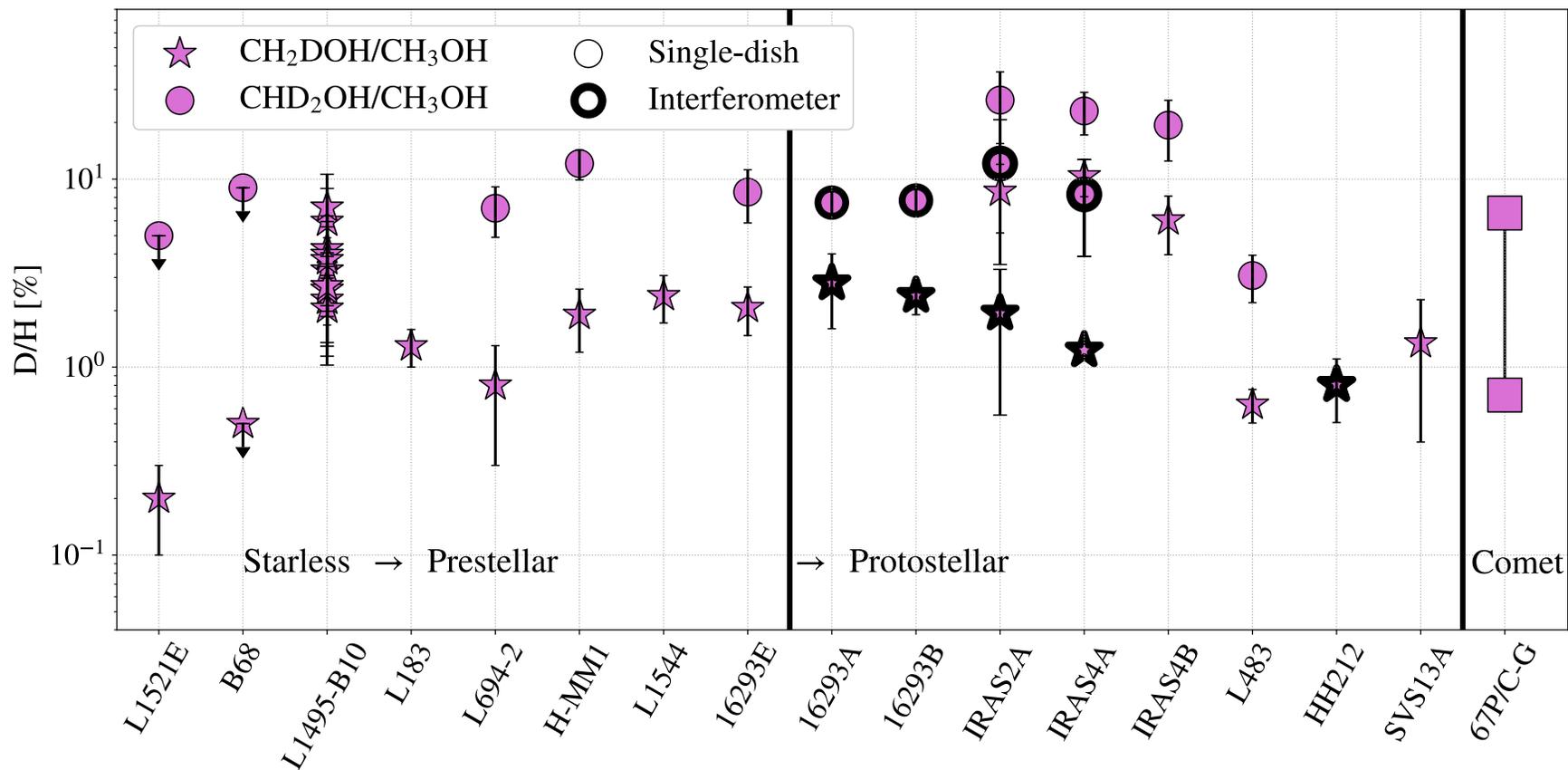


Caselli, Pineda, Sipilä et al. (2022)



Observational use cases for deuteration: chemical inheritance from clouds to disks

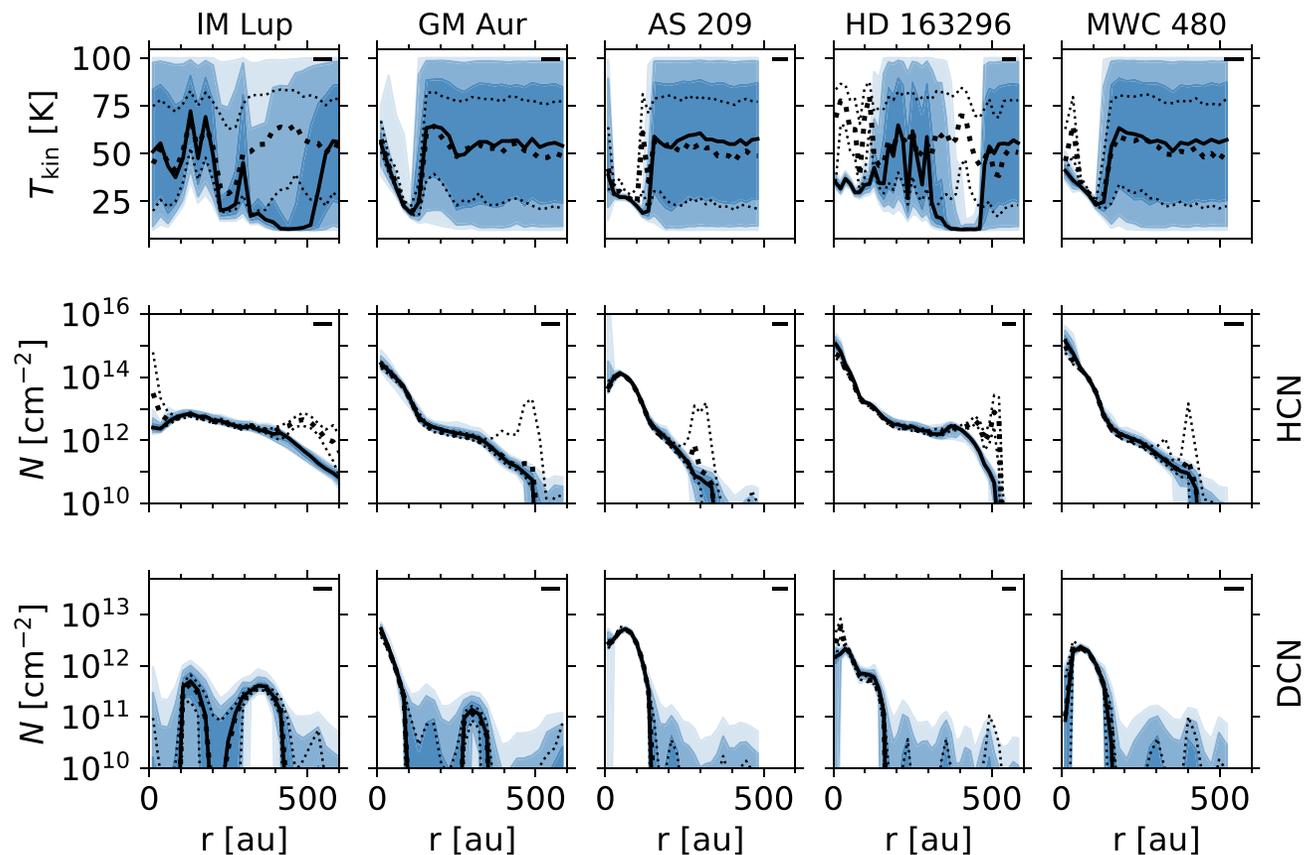
Scibelli et al. (2025)



Observational use cases for deuteration: probe of disk properties



Cataldi et al. (2021)



other possibilities:

- tracing snow lines
- estimation of ionization degree, linewidths (turbulence level?)
- (multiply-deuterated species)

estimation of T_{gas} with multi-line analysis (HCN & DCN)

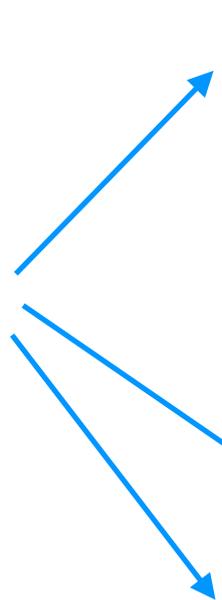
What kind of information can ALMA Band 2 provide us, in relation to current knowledge?



Friesen et al. (2018)

Molecule	Transition	Rest Frequency (GHz)
o-CH ₂ D ⁺	1 _{1,0} - 1 _{1,1}	67.273
p-NHD ₂	1 _{1,1} - 1 _{0,1}	67.842
D ¹³ CO ⁺	1 - 0	70.733
DCO ⁺	1 - 0	72.0393
D ¹³ CN	1 - 0	71.175
DCN	1 - 0	72.415
CCD	1 - 0	72.108
DN ¹³ C	1 - 0	73.368
DNC	1 - 0	76.306
N ₂ D ⁺	1 - 0	77.109
HDO	1 _{1,0} - 1 _{1,1}	80.6
o-NH ₂ D	1 _{1,1} - 1 _{0,1}	85.928
p-NH ₂ D	1 _{1,1} - 1 _{0,1}	110.15
CH ₂ DOH	<i>Multiple</i>	67 - 95

cold deuteration tracers



warm deuteration tracers

Some open questions in simulations of deuteration



1. How do deuteration reactions actually proceed? (**ammonia**)
2. What is the role of the environment in D fractionation? (**multiple species**)
3. To what extent do grain-surface reactions influence gas-phase abundances? (**COMs, H₂CO**)
- (4. Can deuterated species be used as reliable chemical clocks?) (**multiple species**)

CONCLUSIONS

Deuterated molecules are excellent tracers of physical conditions in clouds and disks

They facilitate studies of chemical inheritance across the star formation process, while also acting as proxies of important quantities such as the ionization fraction

ALMA Band 2 observations will provide more information of the distributions of key deuterated molecules in varying physical conditions, which also helps to improve chemical models