# Physical and Chemical Drivers of Deuteration in Protoplanetary Disks

**Ilse Cleeves**

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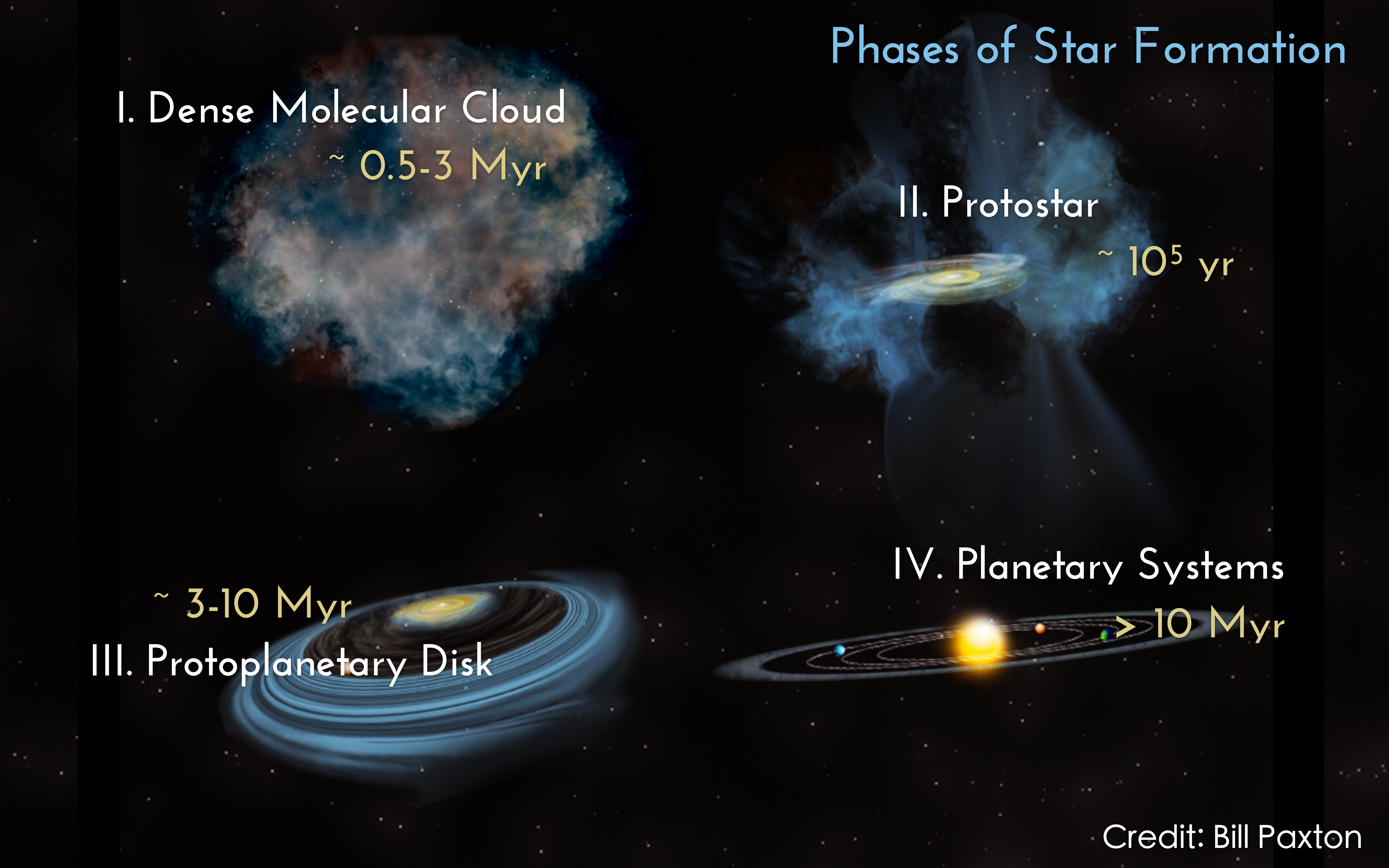
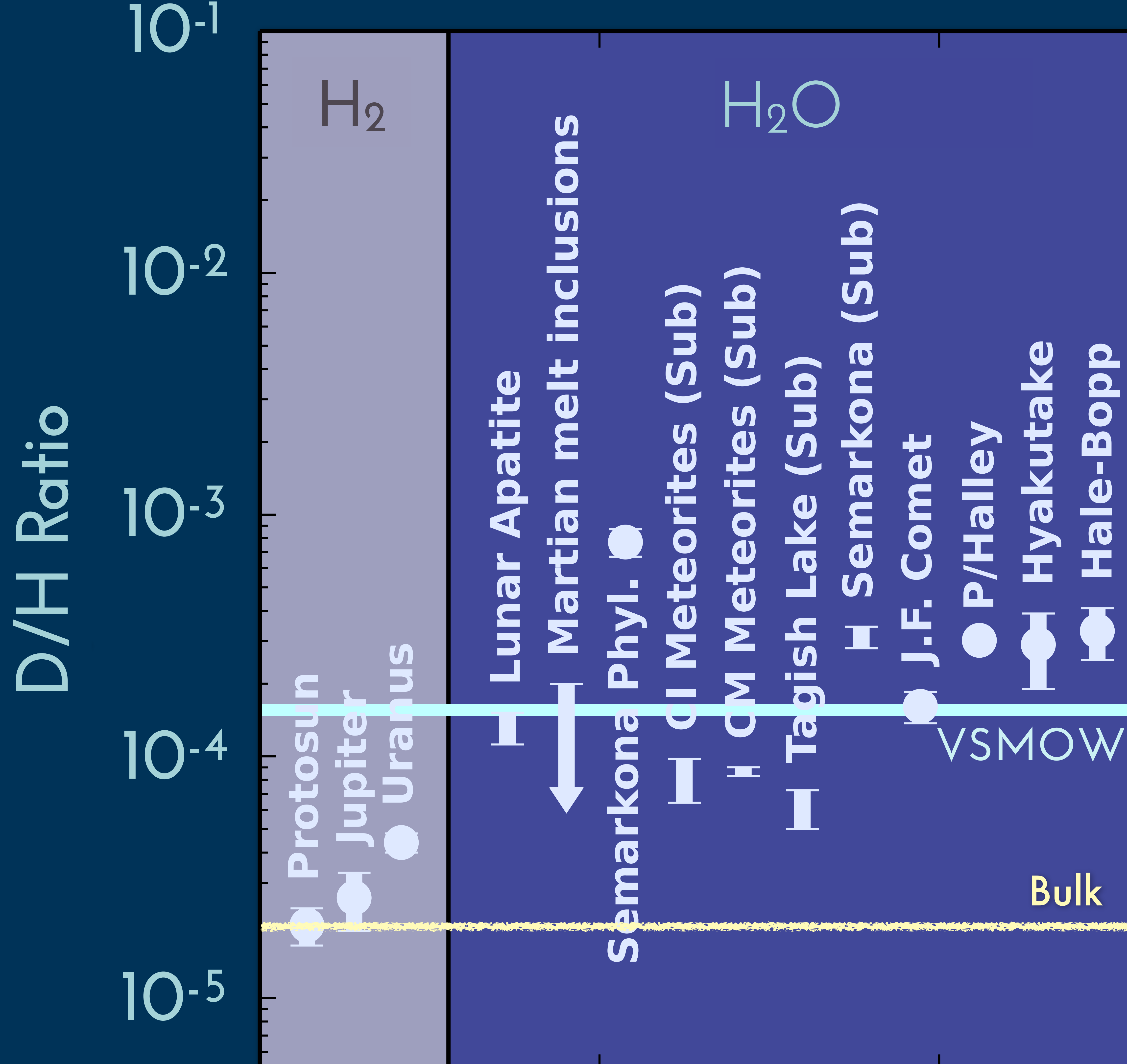
1) University of Michigan, 2) Carnegie DTM, 3) Harvard-Smithsonian CfA, 4) University of Exeter


Phases of Star Formation
I. Dense Molecular Cloud
~ 0.5-3 Myr
II. Protostar
~ 10⁵ yr
~ 3-10 Myr
III. Protoplanetary Disk
IV. Planetary Systems
> 10 Myr
Credit: Bill Paxton




Plot references collected in Cleeves et al. 2014

Water throughout a diversity of solar system bodies has characteristically high $HDO/H_2O$.

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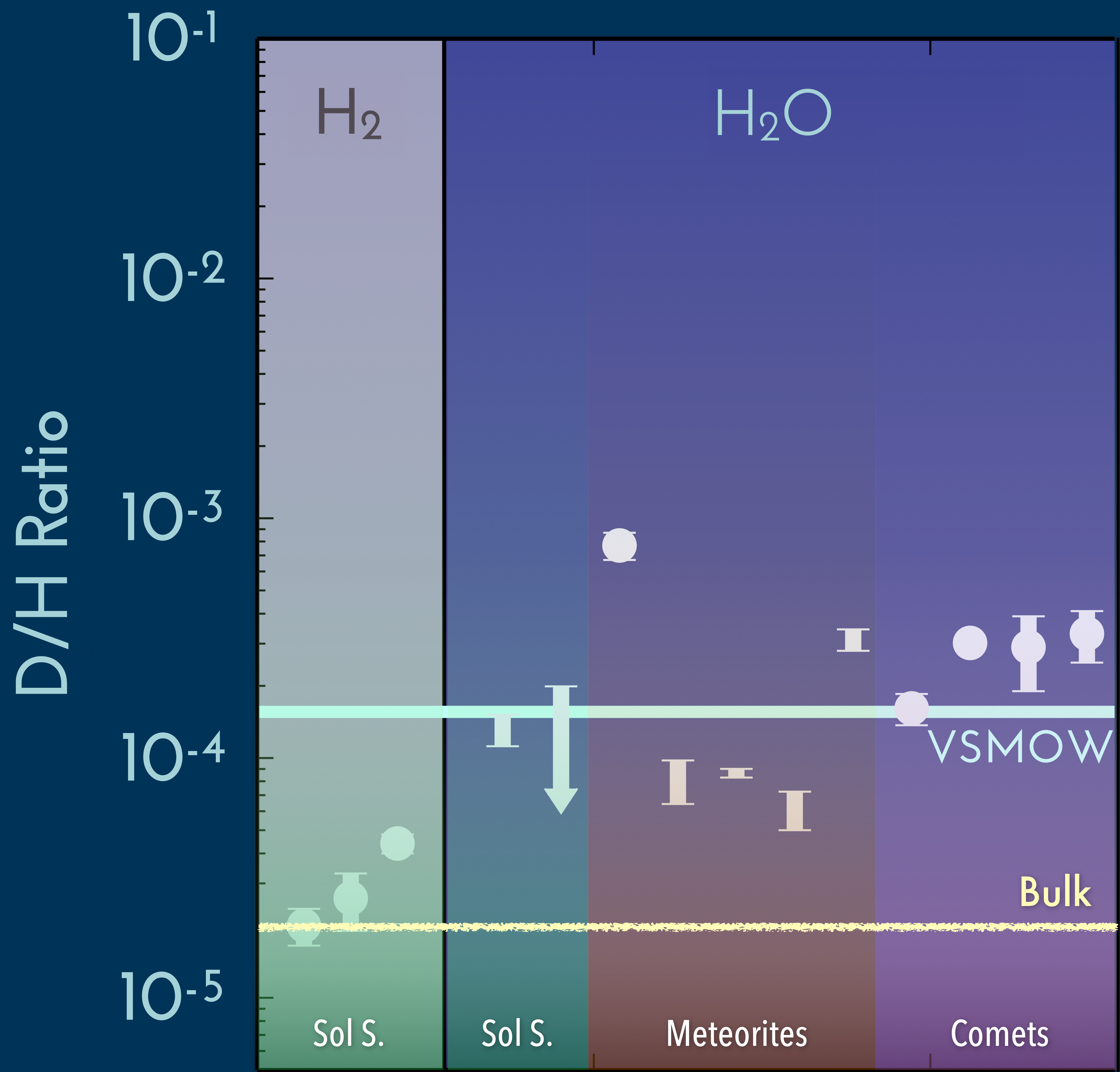


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Factors of ~3-20 excess $HDO/H_2O$

We know water formed in a relatively cold environment.

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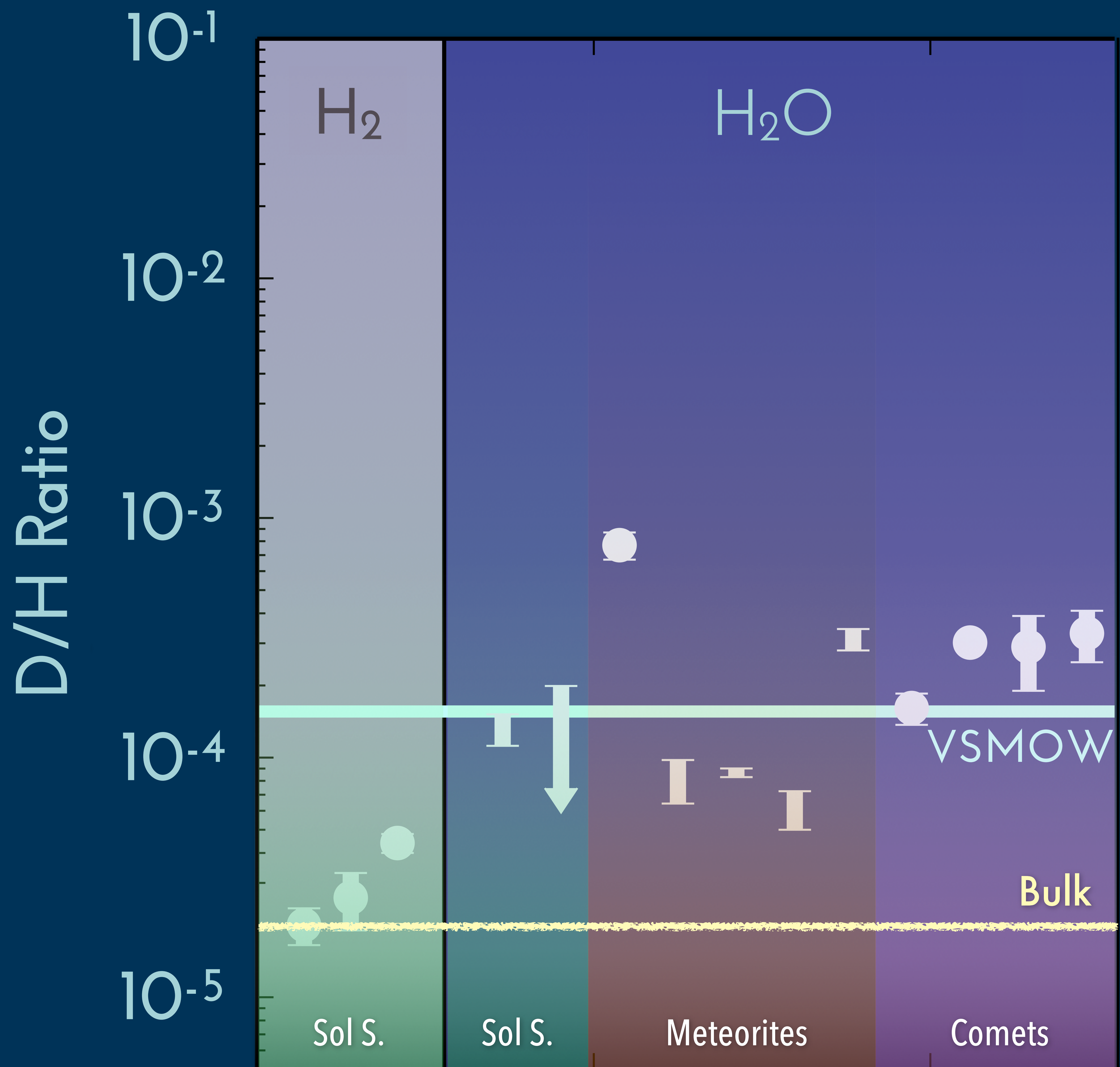


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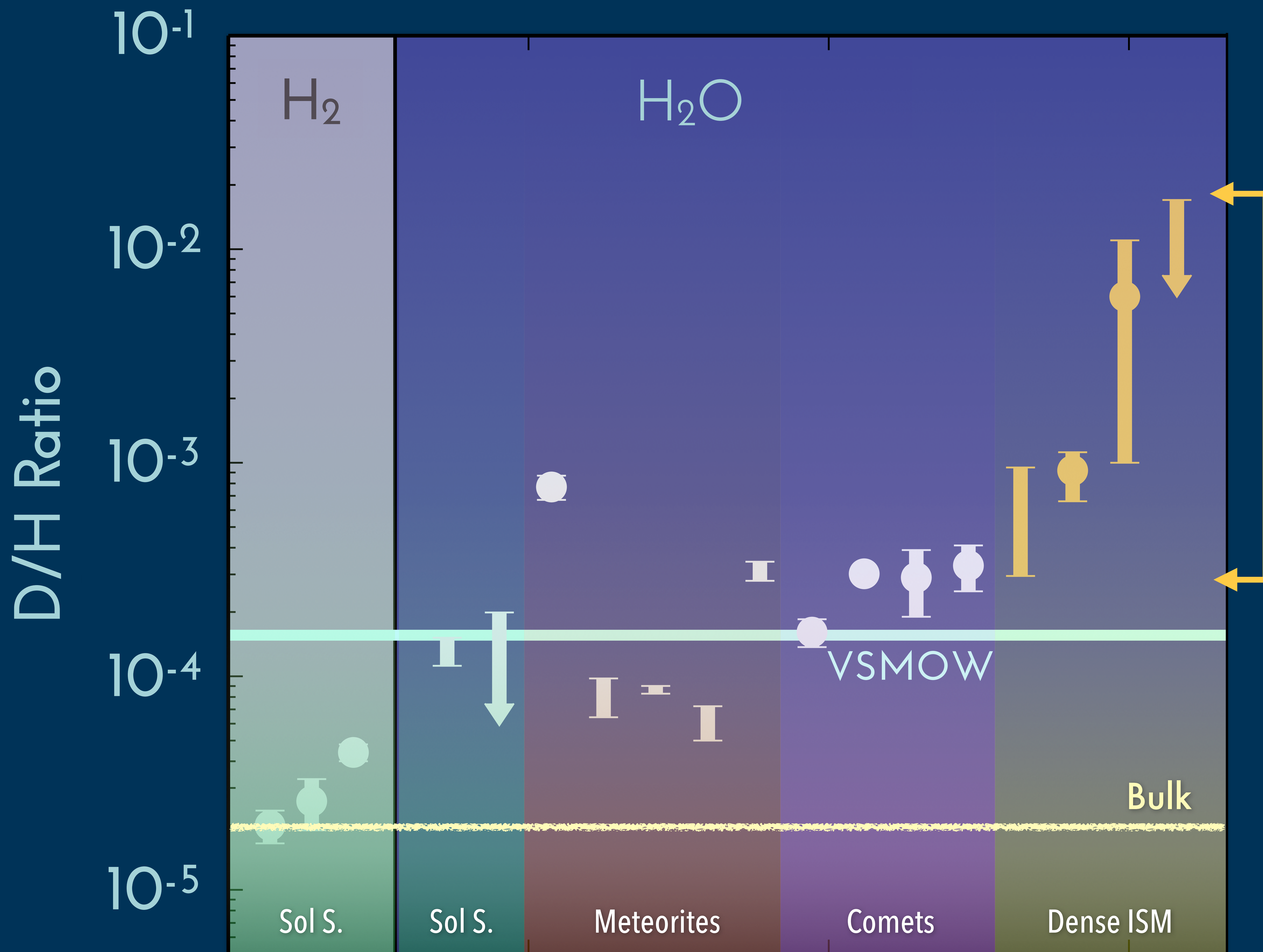


Primordial ices in the envelopes of protostars exhibit a high level of D/H.

ISM: Persson+2014, 2012, Coutens+2012, Parise 2003.

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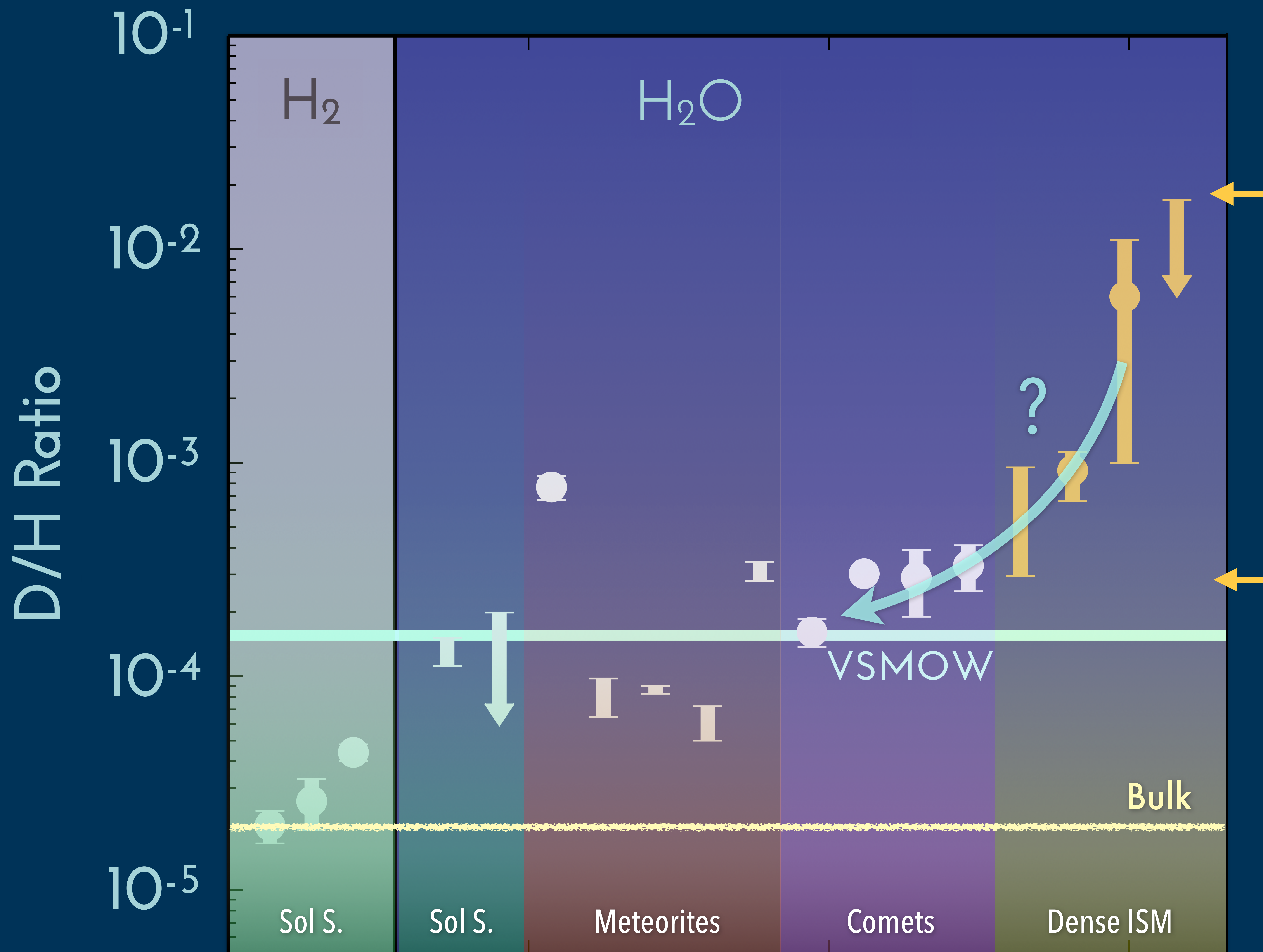


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Are these early stages (the primordial ISM ices) chemically linked?

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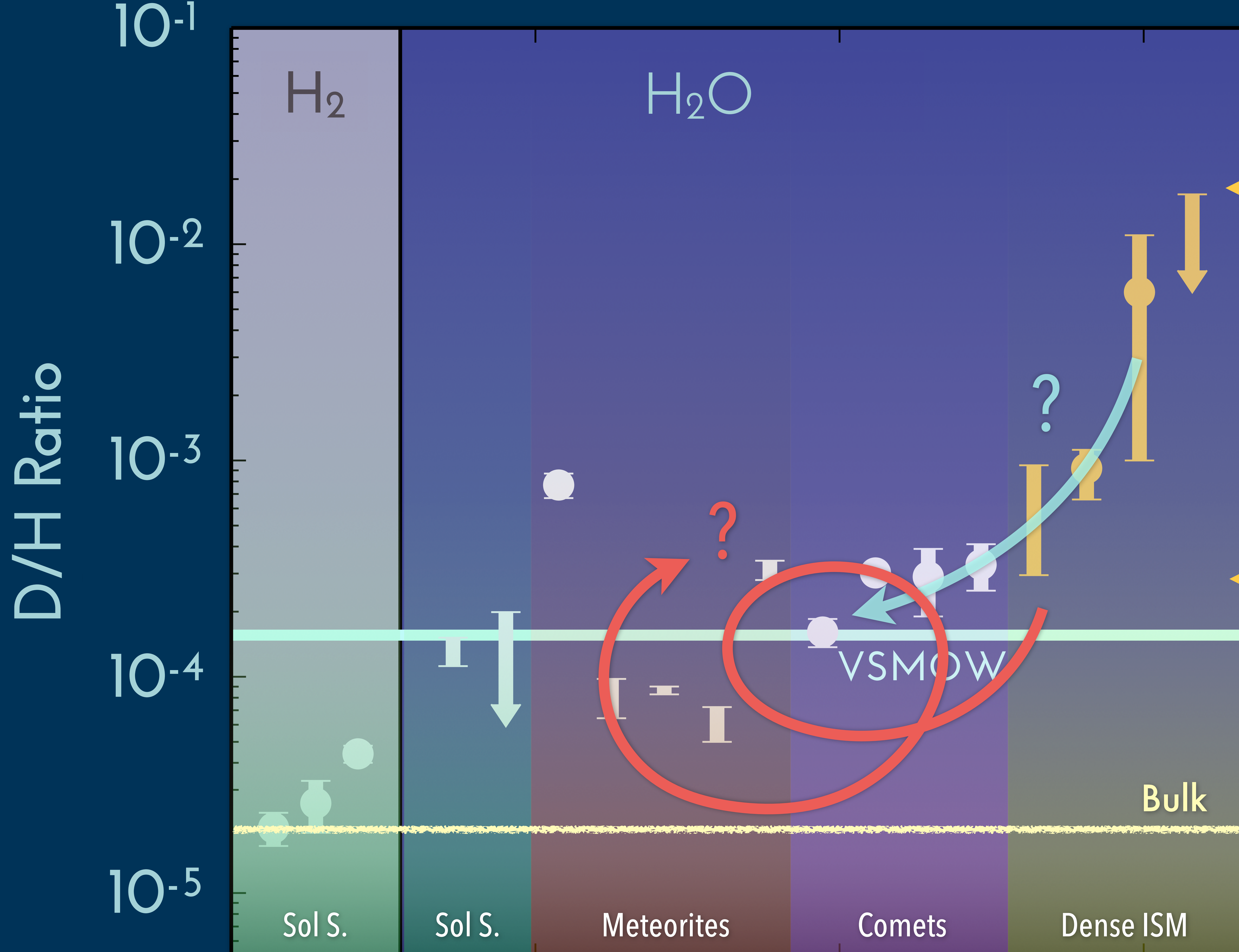


Primordial ices in the envelopes of protostars exhibit a high level of D/H.

Are these early stages (the primordial ISM ices) chemically linked?

What is the role of disk processing?

ISM: Persson+2014, 2012, Coutens+2012, Parise 2003.

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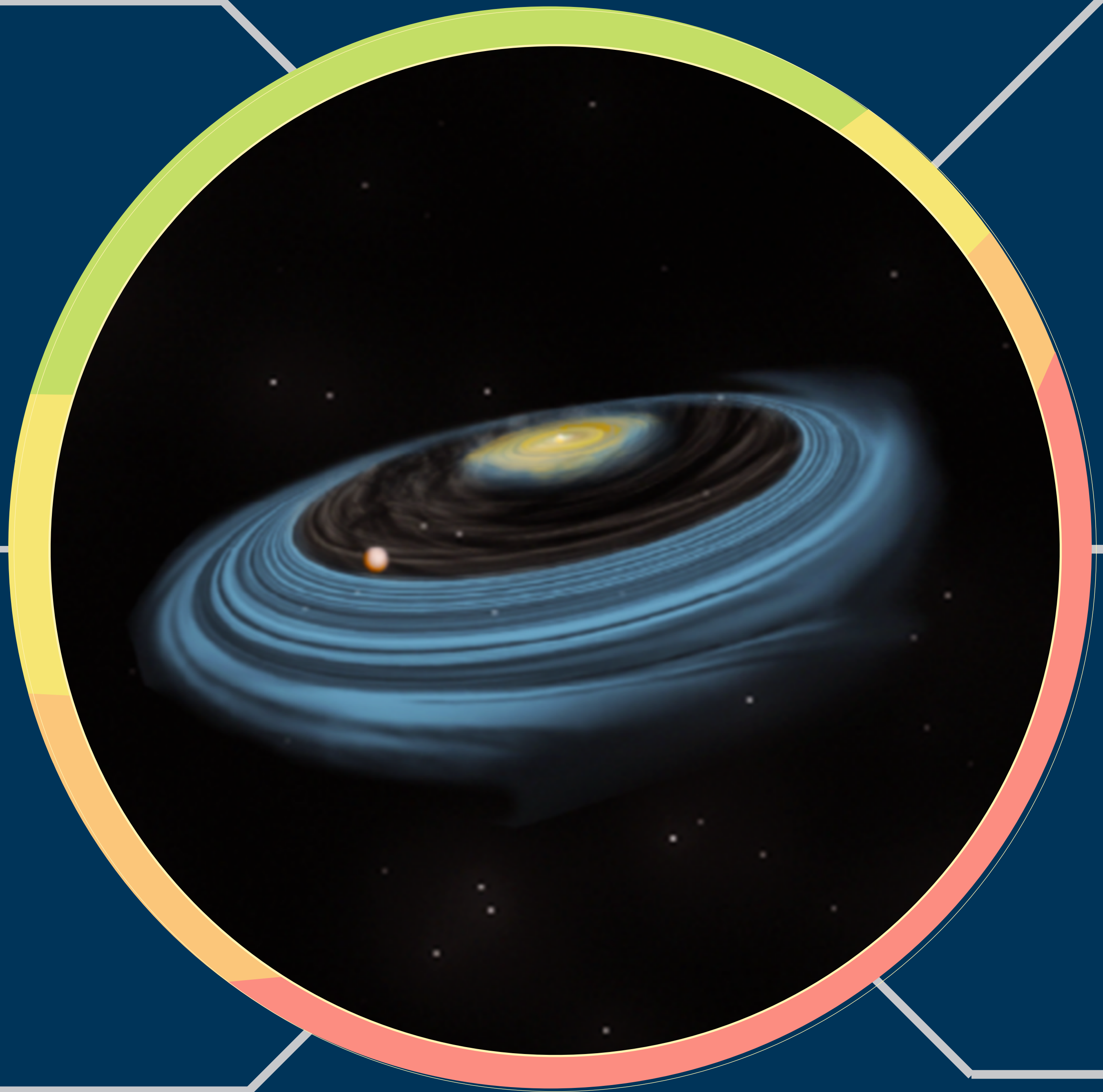
# Talk Overview

1) Key Ingredients For Disk Deuterium Chemistry

2) What Are The Disk Initial Conditions?

3) Effect Of Gas Viscous Evolution, Turbulence, And Mixing



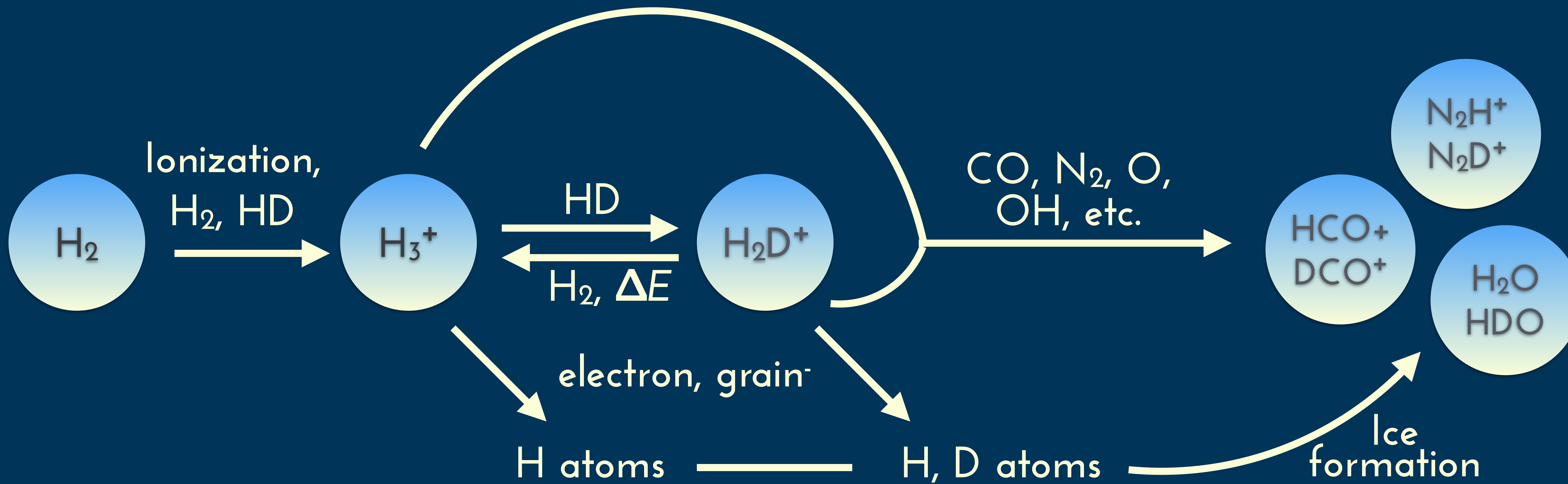
4) The Late Phase Redistribution Of Ices

5) Not All Roads Lead To Rome: Variations In Fractionation Pathways

6) Moving Towards A Comprehensive Picture Of Disk Deuterium Chemistry

# 1) Key ingredients for disk deuterium chemistry

# 1) Key Ingredients for High Molecular D/H




Supports fractionation
up to T < 50 K

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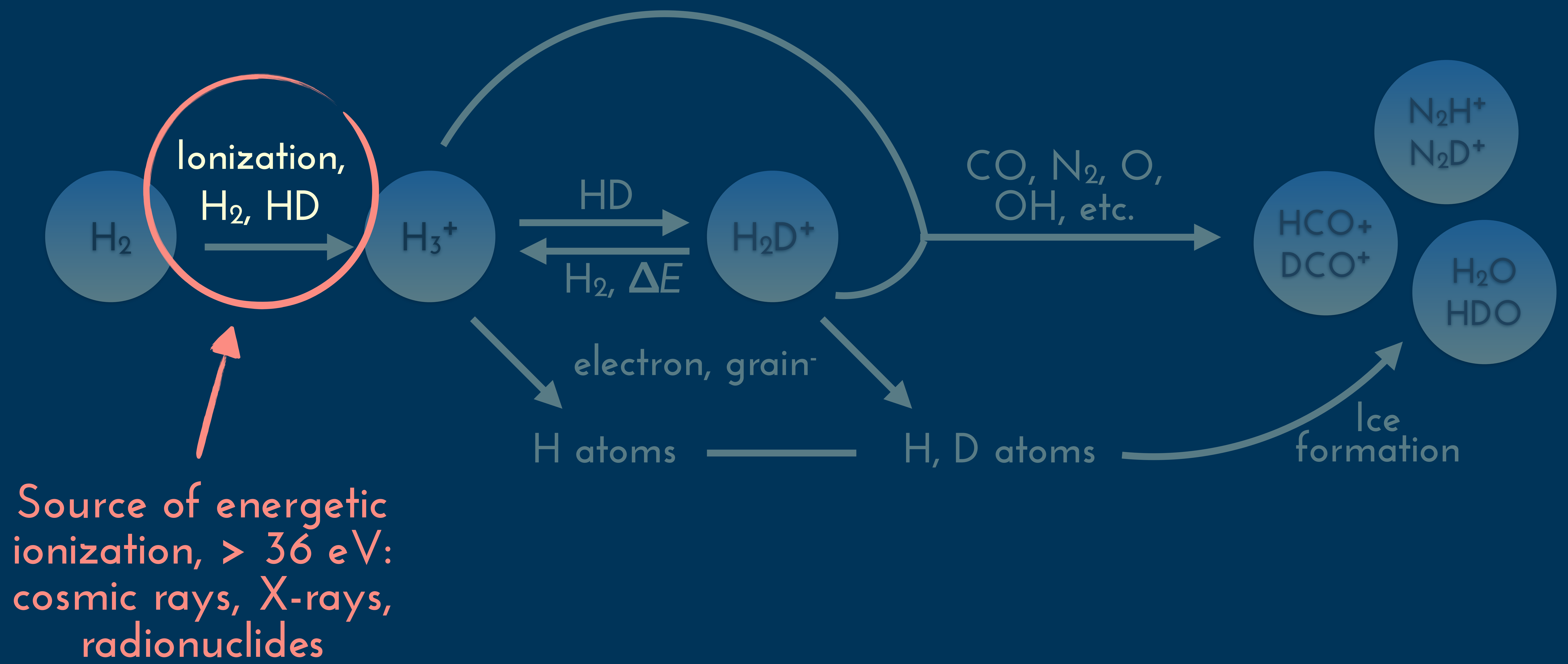

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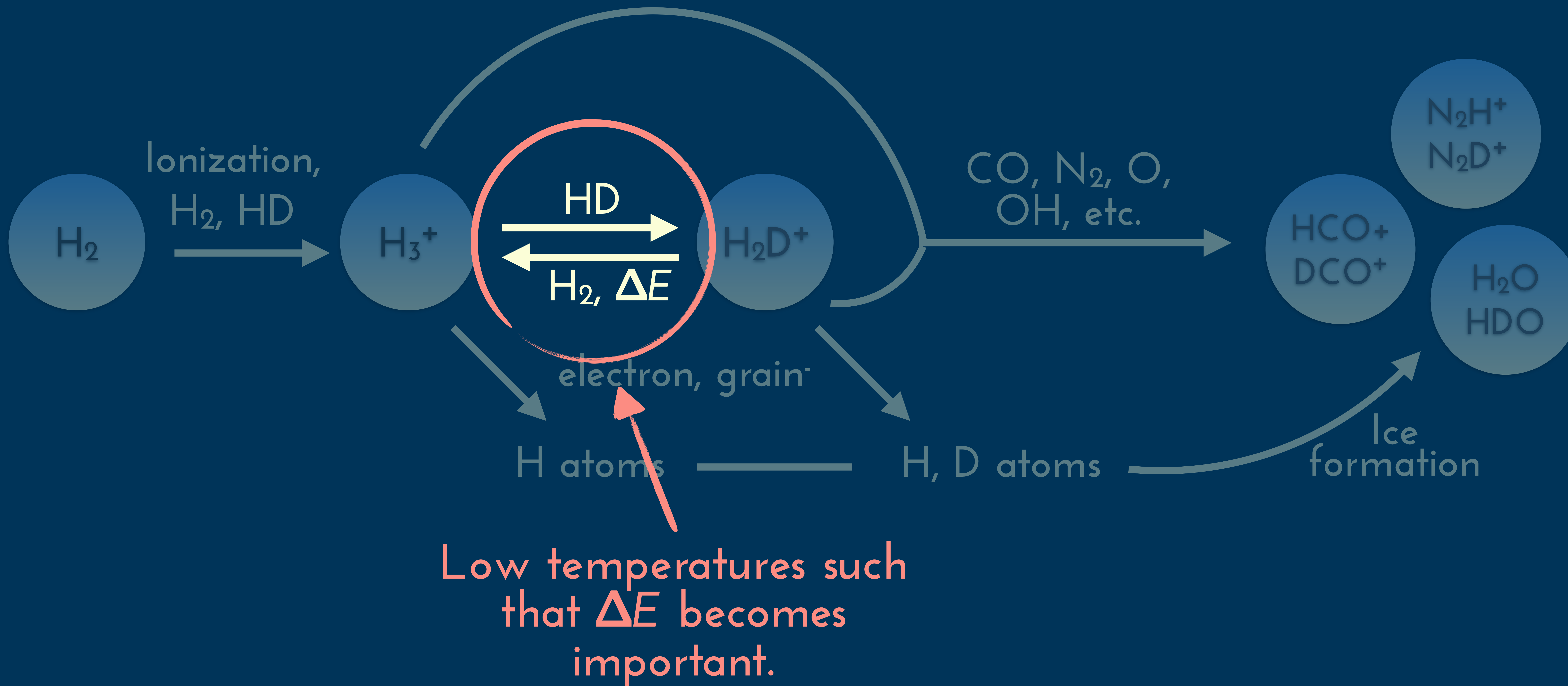


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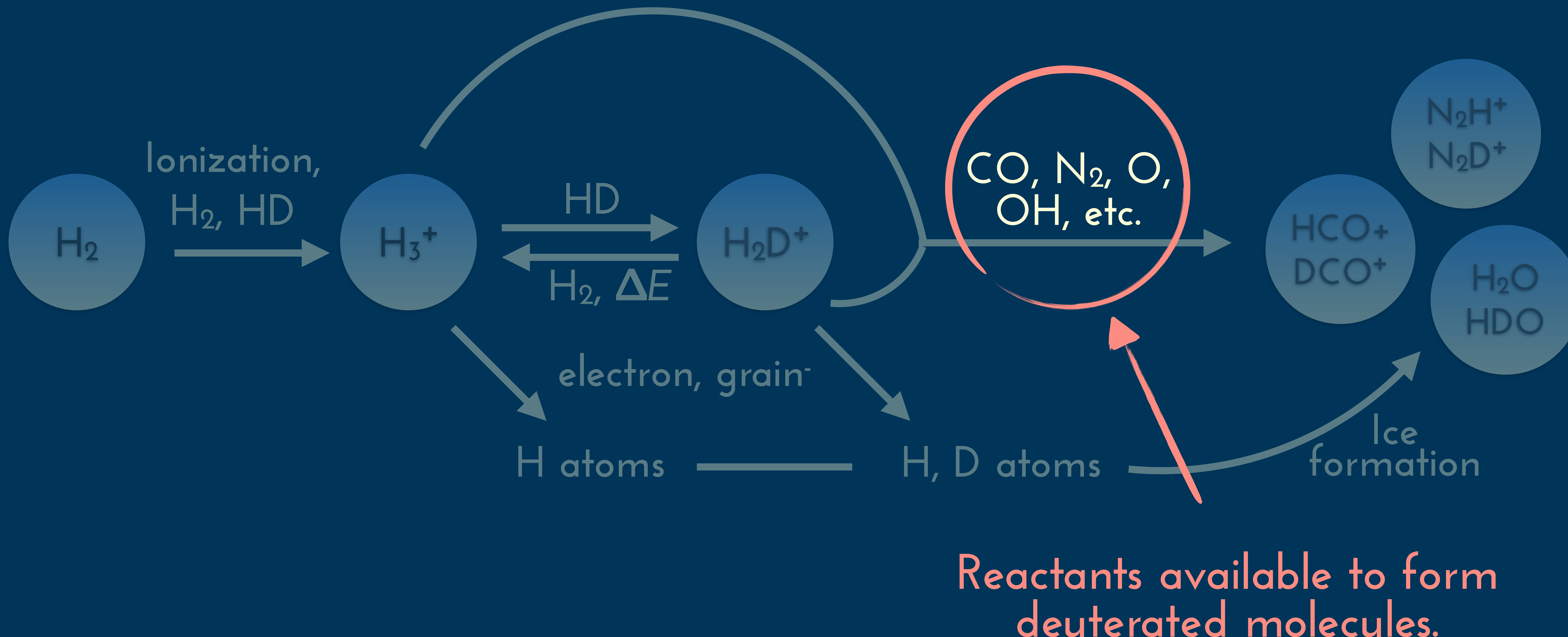

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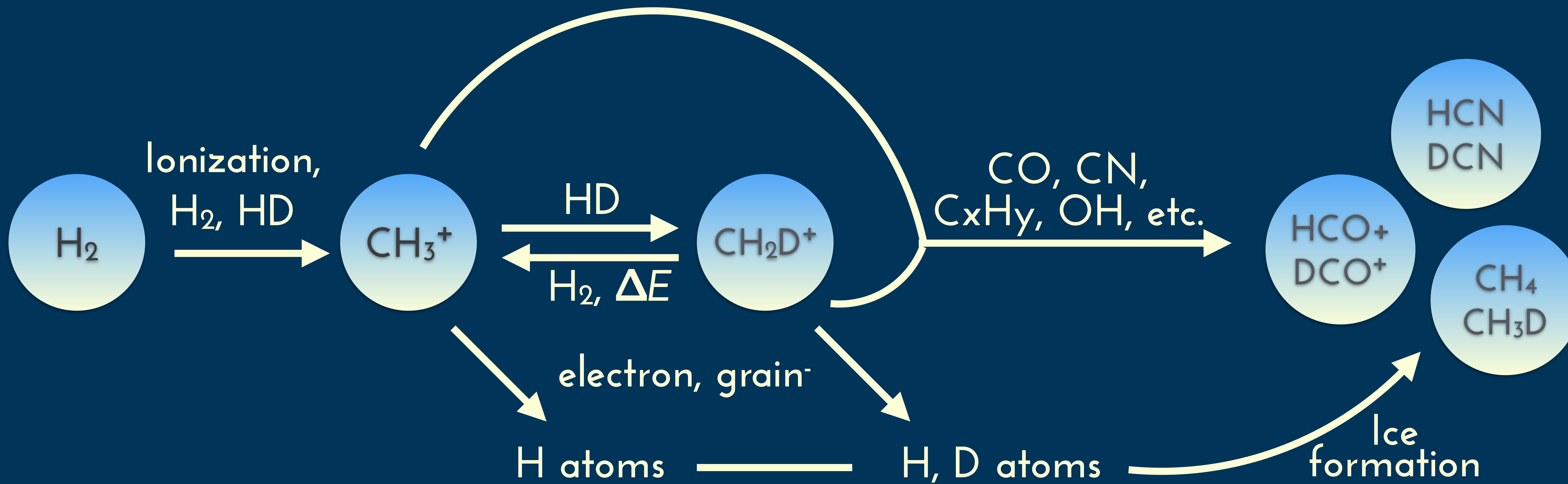
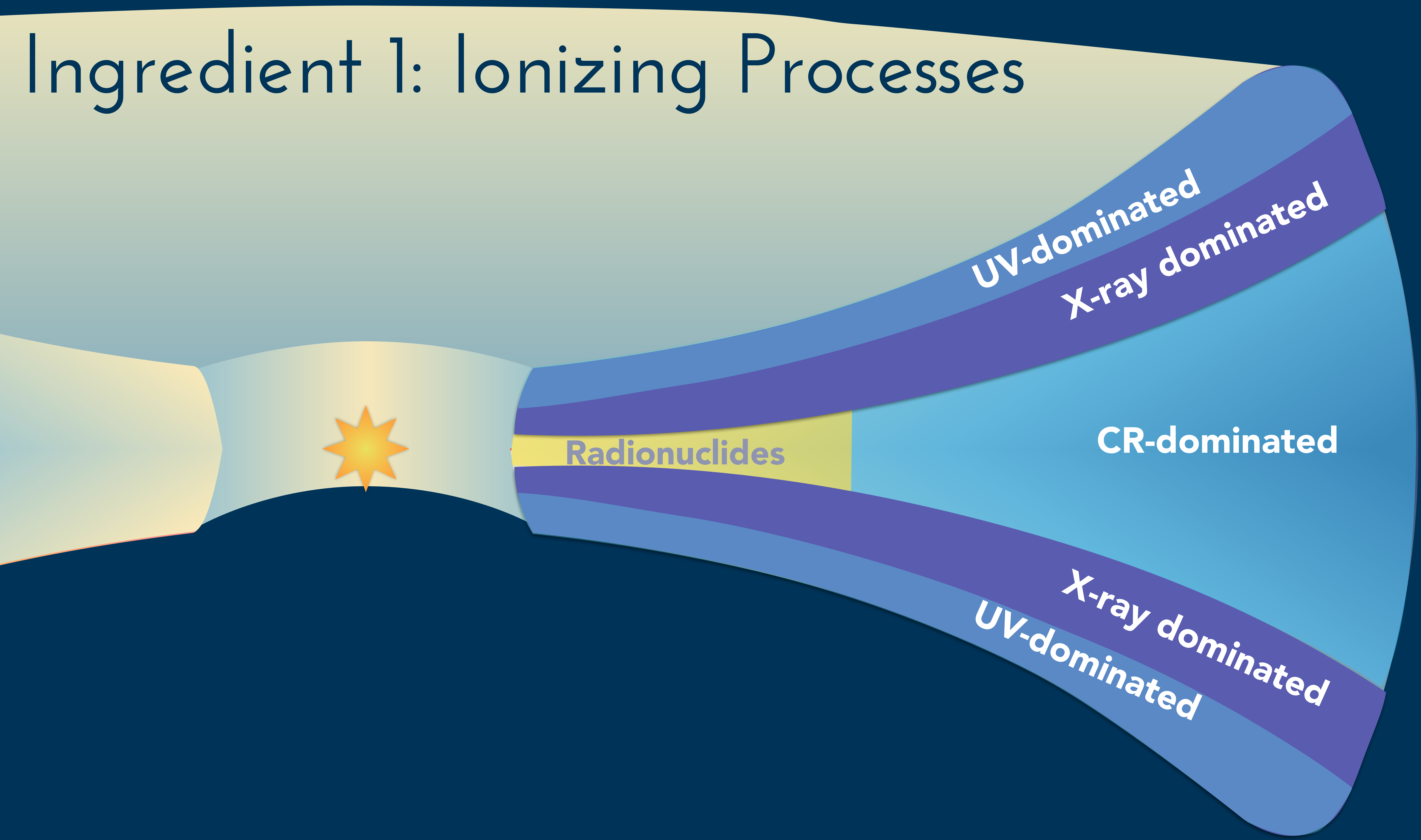



Carbon pathways support fractionation up to T < 100 K, see Roueff et al. 2013

# Ingredient 1: Ionizing Processes

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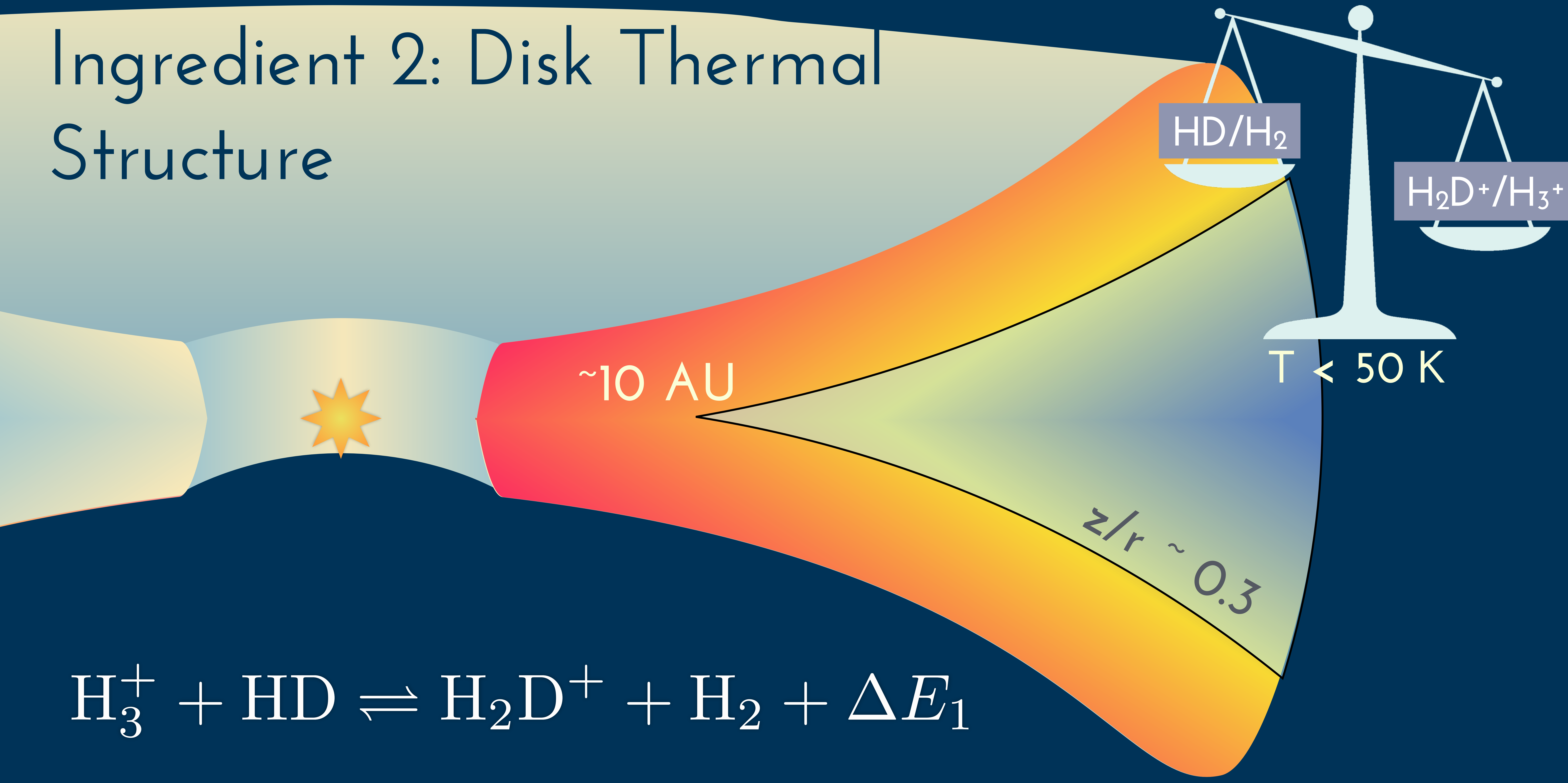
# Ingredient 2: Disk Thermal Structure




$$H_3^+ + HD \rightleftharpoons H_2D^+ + H_2 + \Delta E_1$$

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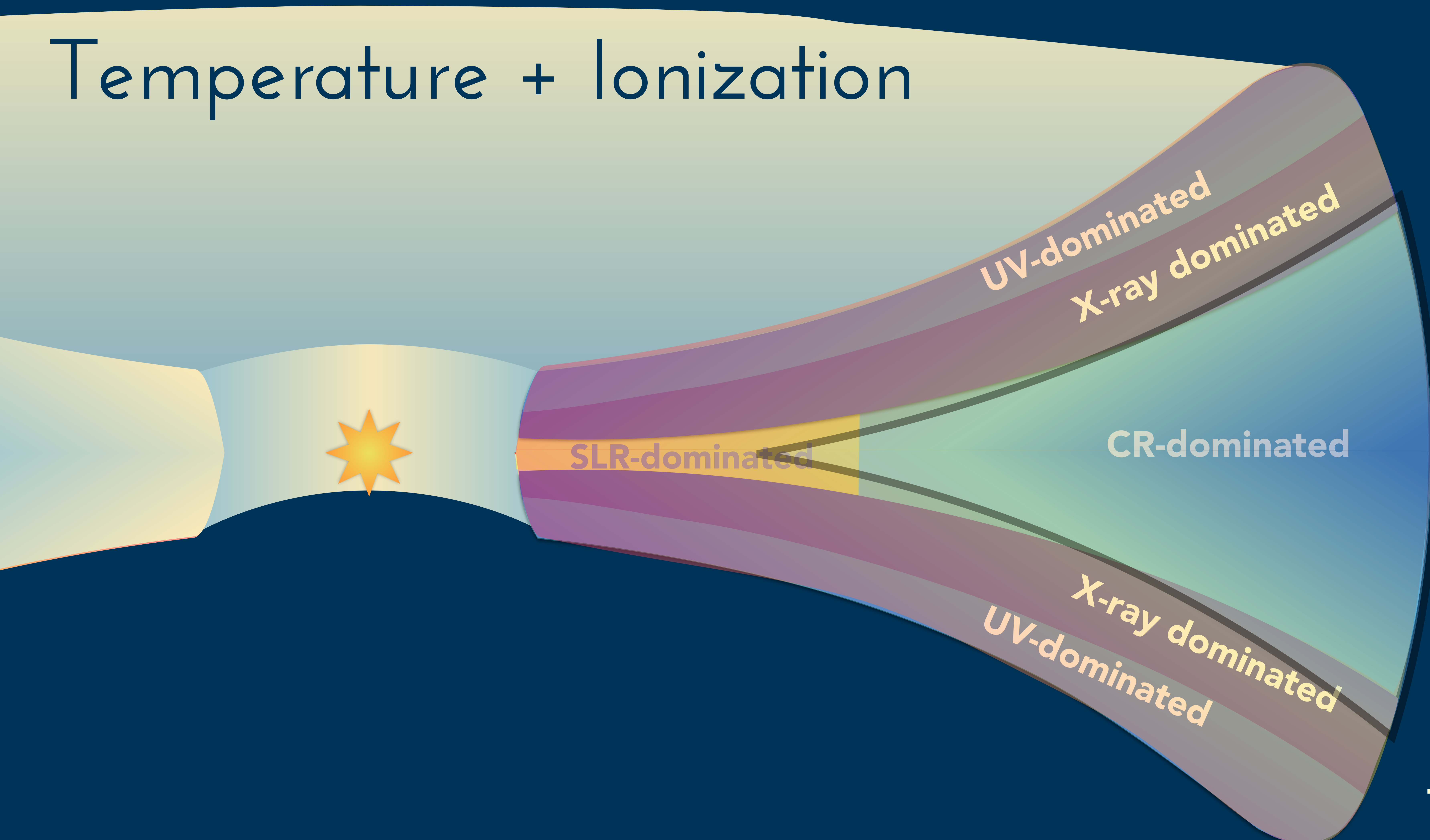
# Temperature + Ionization




Cool (<50 K) regions of the disk are also in the region most sensitive to CRs.

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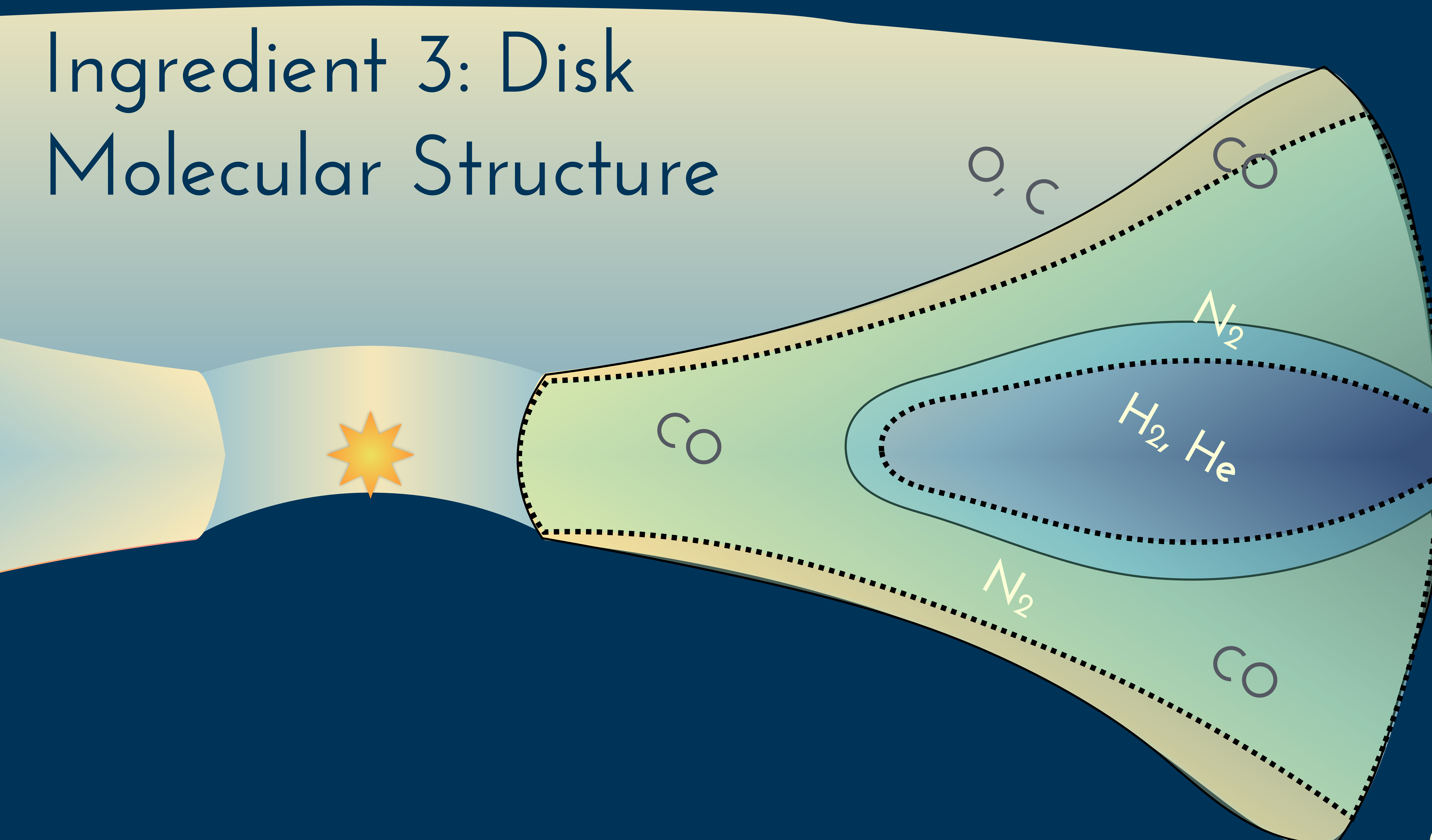
# Ingredient 3: Disk Molecular Structure




Need reactive species to transfer D to, CO, $N_2$, O, …

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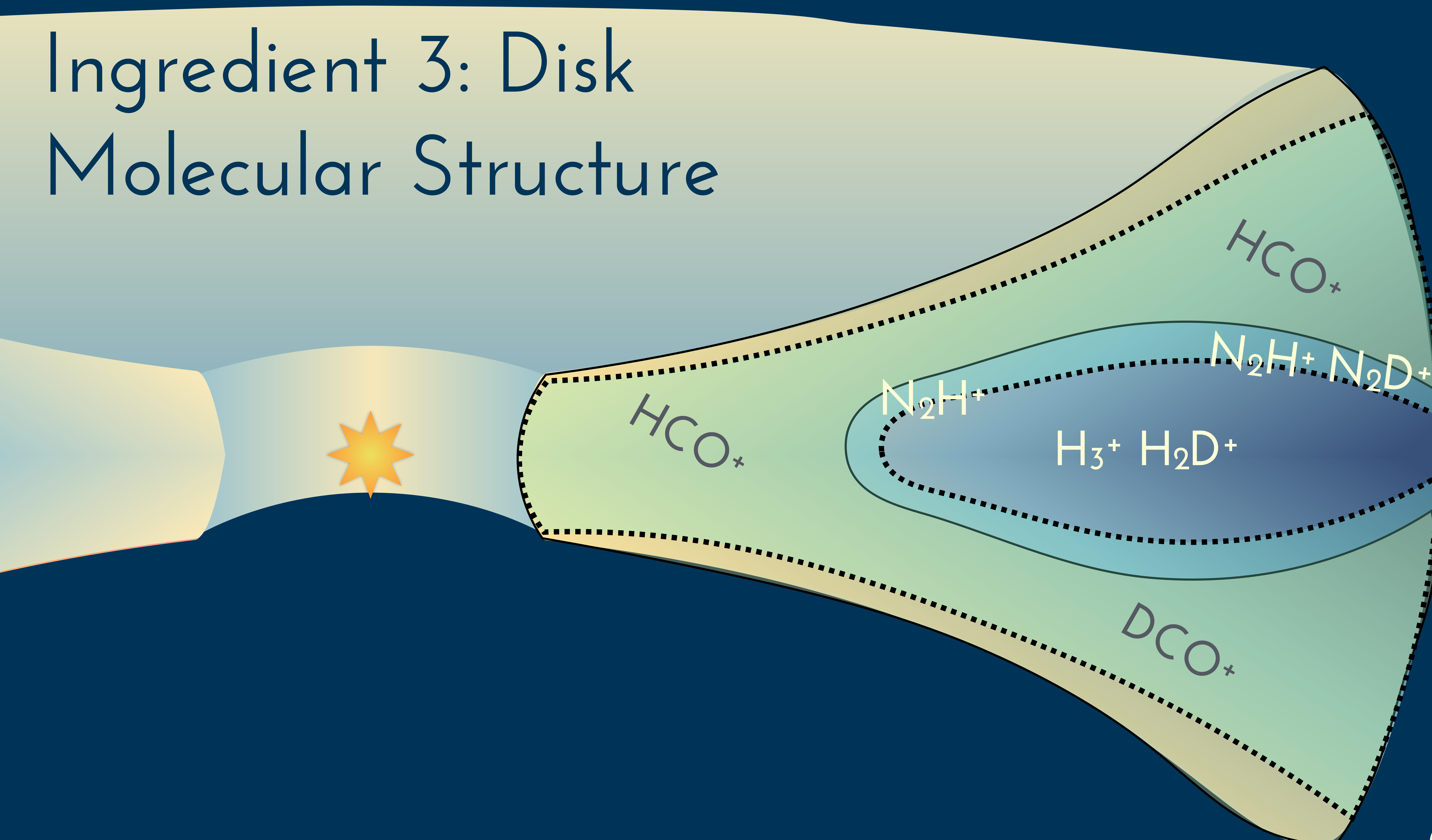
# Ingredient 3: Disk Molecular Structure




Need reactive species to transfer D to, CO, $N_2$, O, ...

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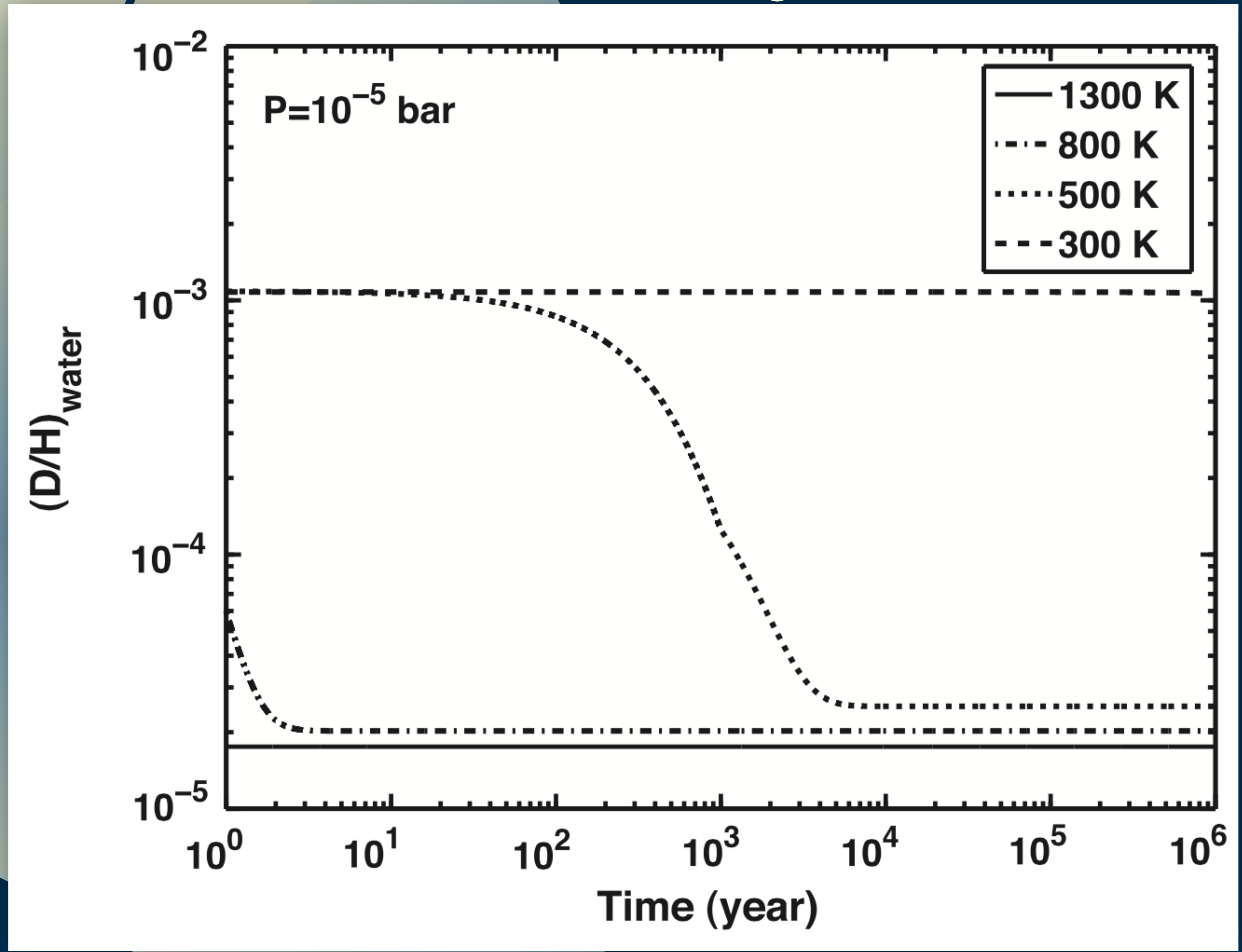
# Hot-Phase Deuterium Chemistry

Yang et al. 2013




The hot inner disk also can fractionate through neutral neutral isotopic exchange.

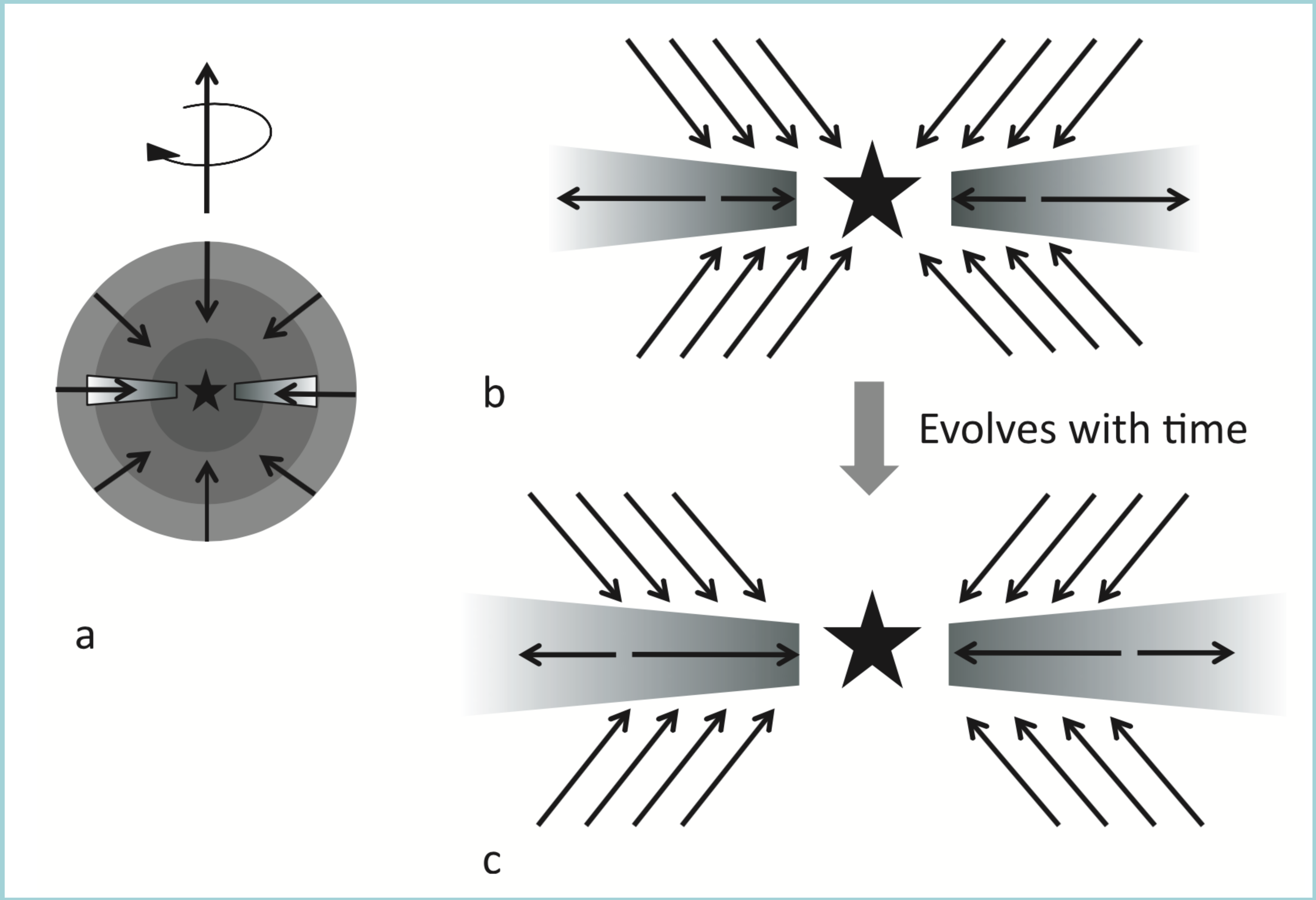
e.g., $H_2O + HD \leftrightarrow HDO + H_2$

$D + OH \leftrightarrow H + OD$ (e.g. Thi et al 2010)

e.g., Drouart 1999, Mousis 2000, Hersant et al. 2001, Thi et al 2010

# 2) Disk Initial Conditions?

# 2) What are the initial disk chemical conditions?




Yang and Ciesla 2012

- Mass of the envelope? Initial angular momentum?
- Thermal history of infalling material? Shocks? Is it symmetric or streamers?
- Subsequent viscous +disk+stellar evolution?

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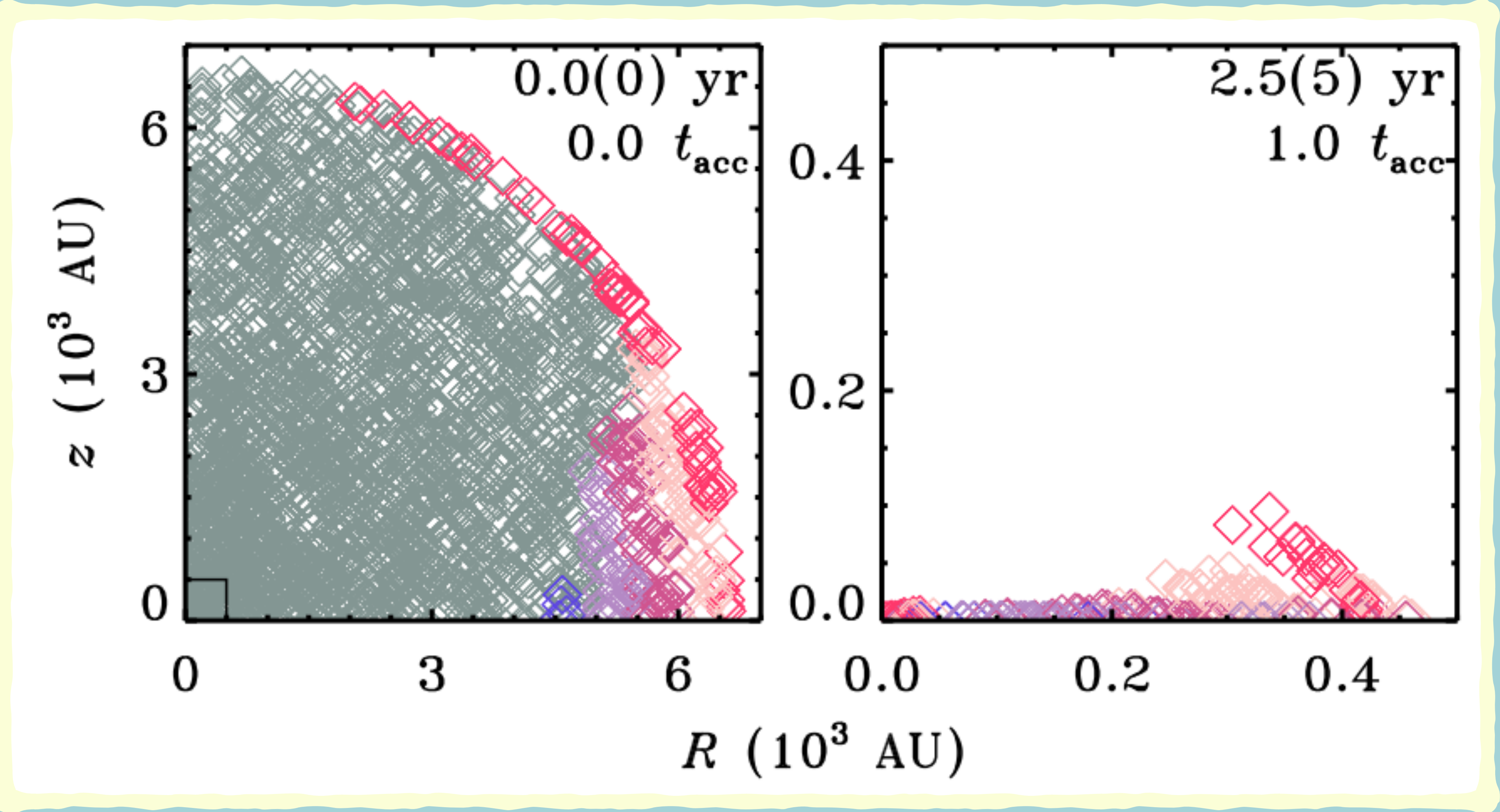
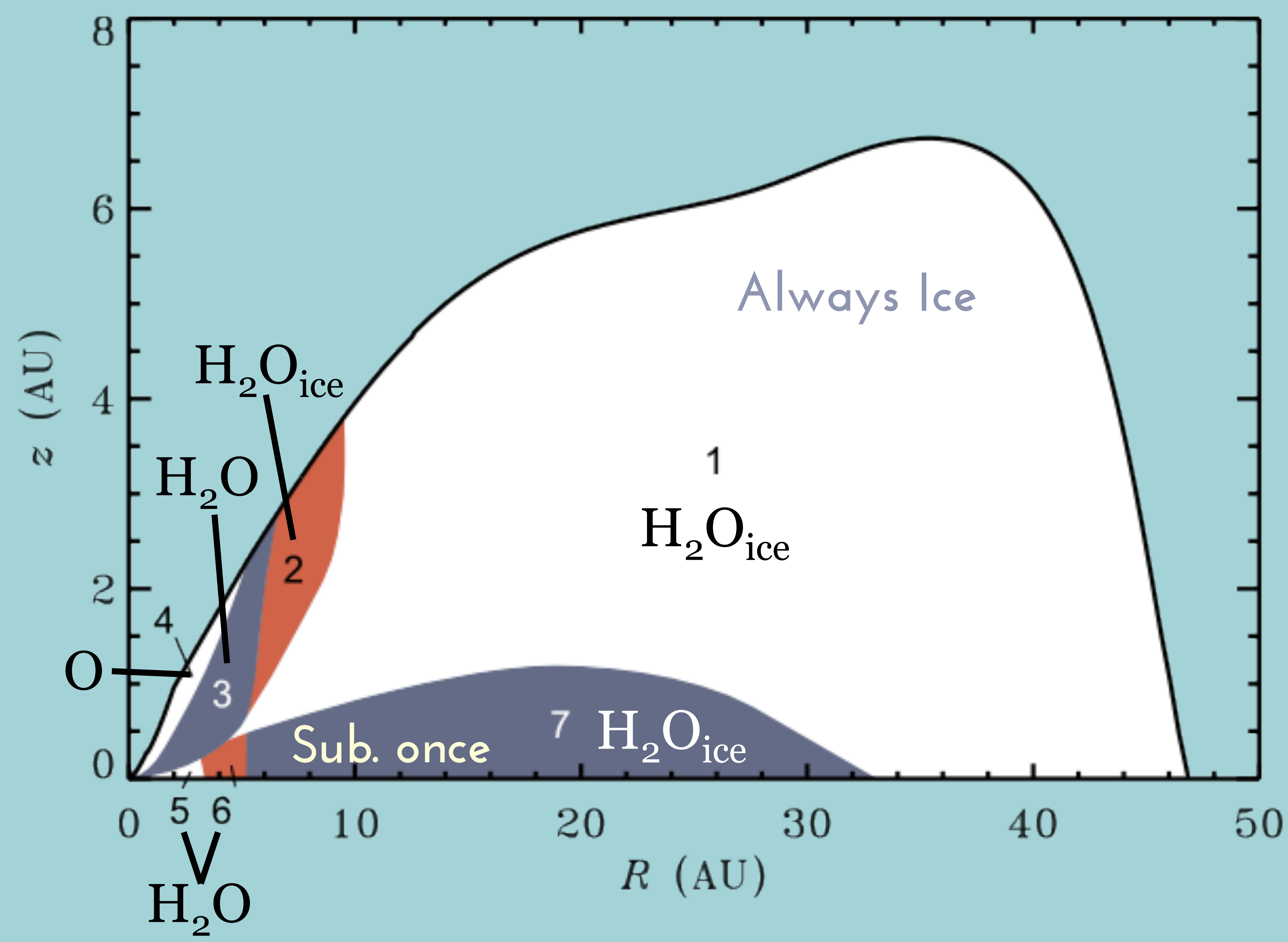



Visser, van Dishoeck, Doty & Dullemond 2009



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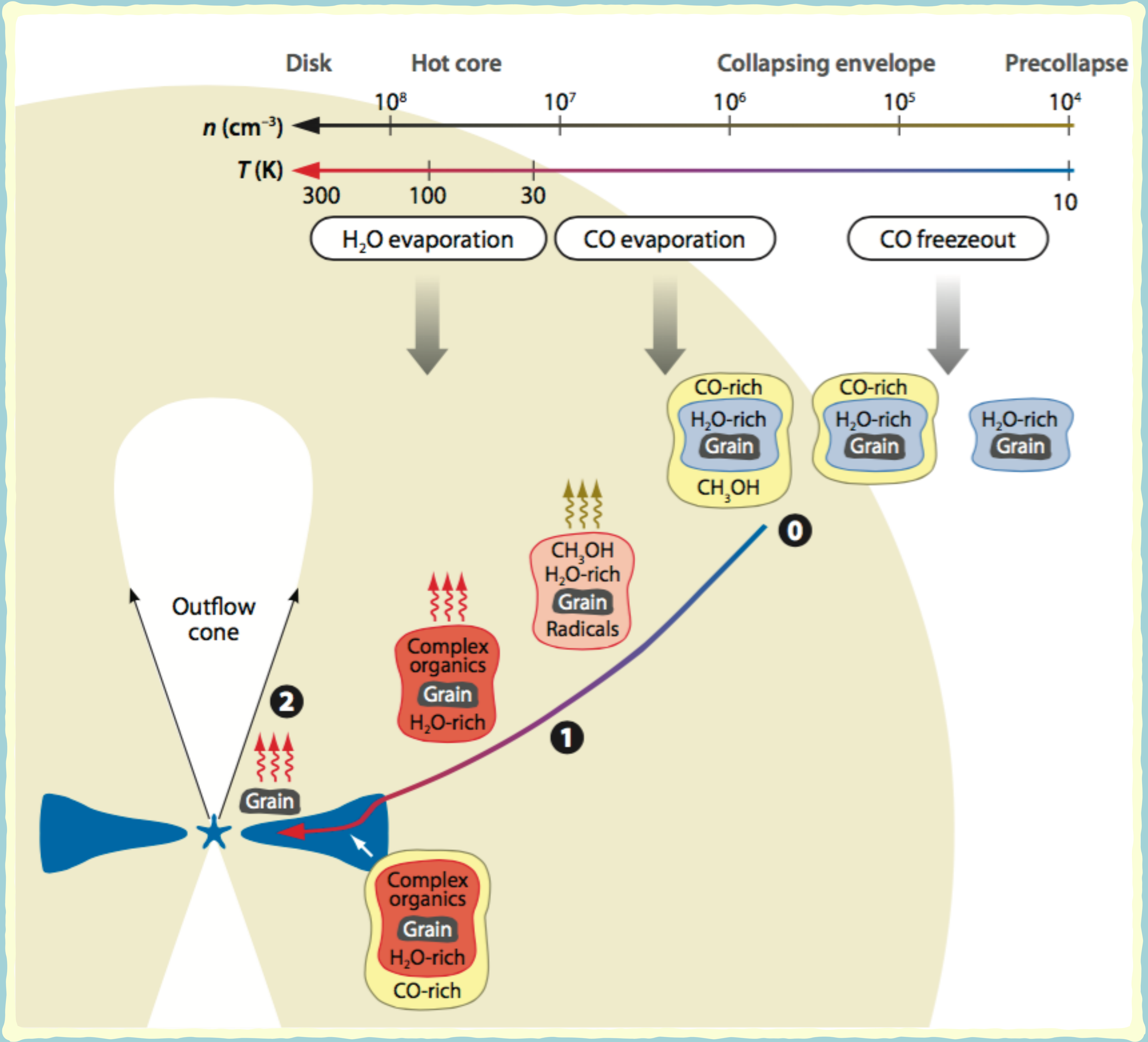
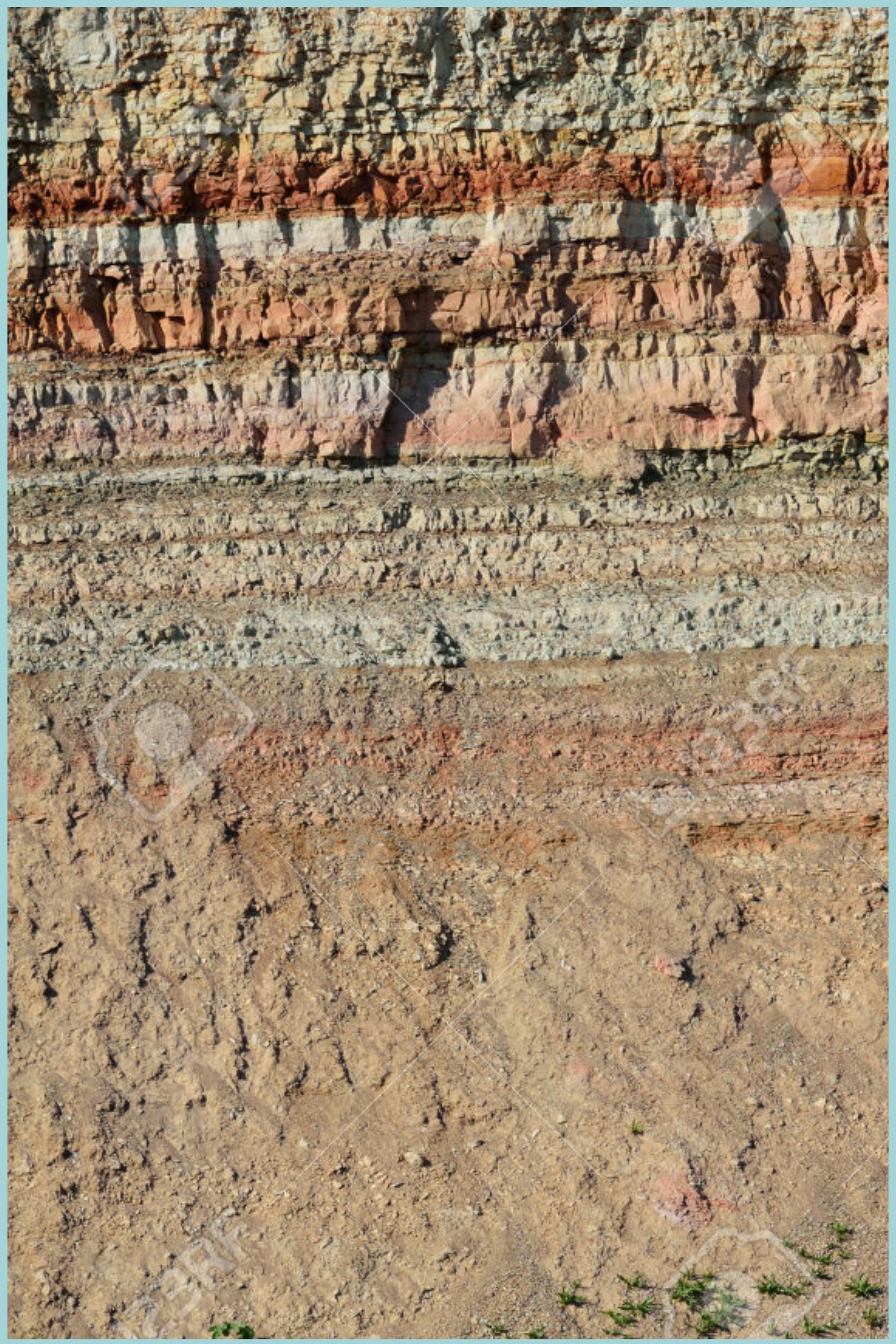
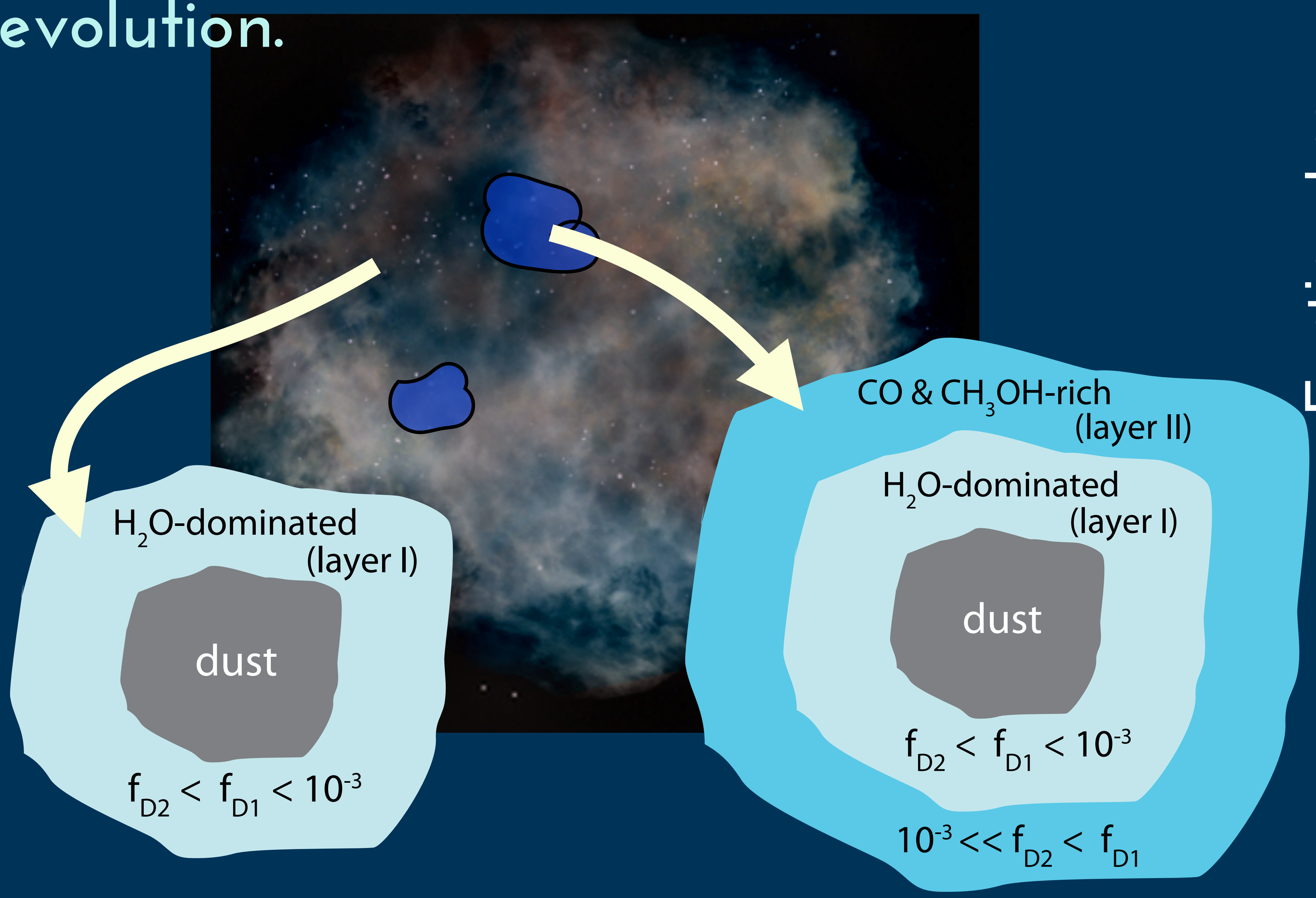


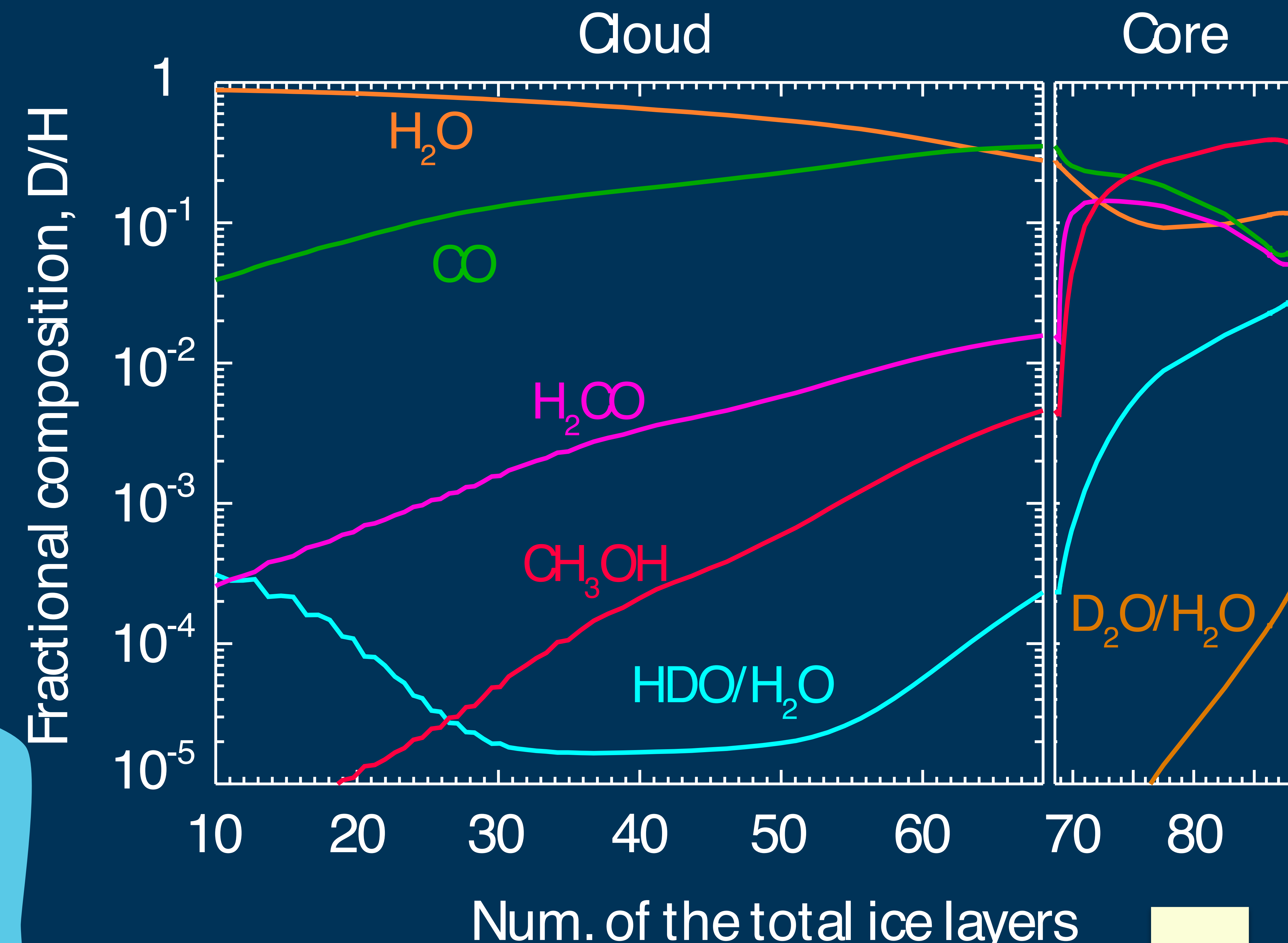



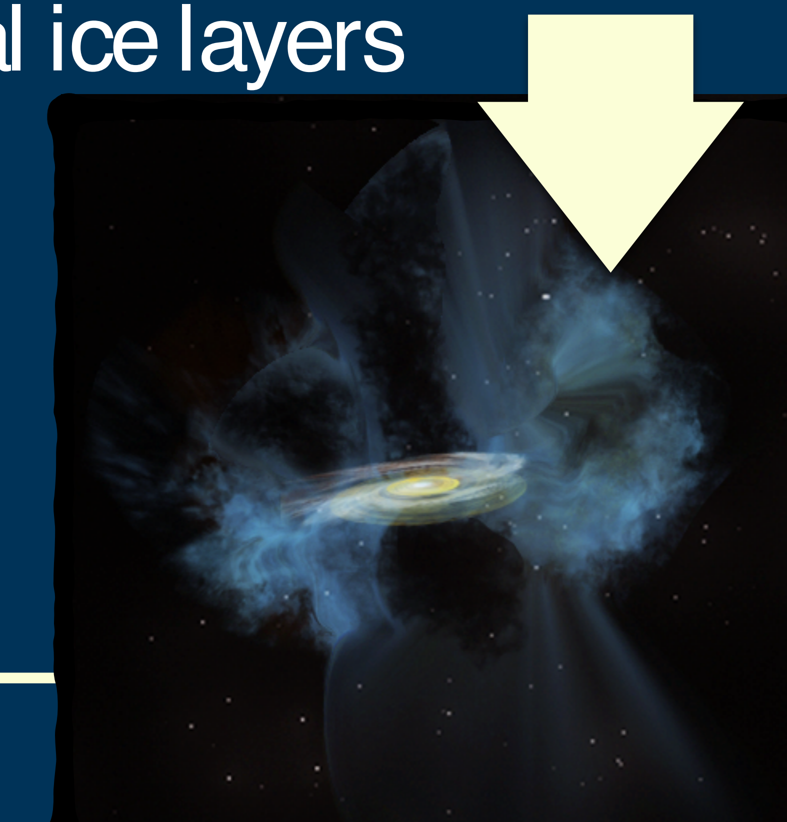
Herbst & van Dishoeck 2009

# 2) What are the initial disk chemical conditions?

By modeling $D_2O/HDO$, $HDO/H_2O$ and using layered ice model the Furuya +2015 models can explain water's early evolution.



Furuya, Aikawa et al. 2015, and Furuya, van Dishoeck, & Aikawa 2015

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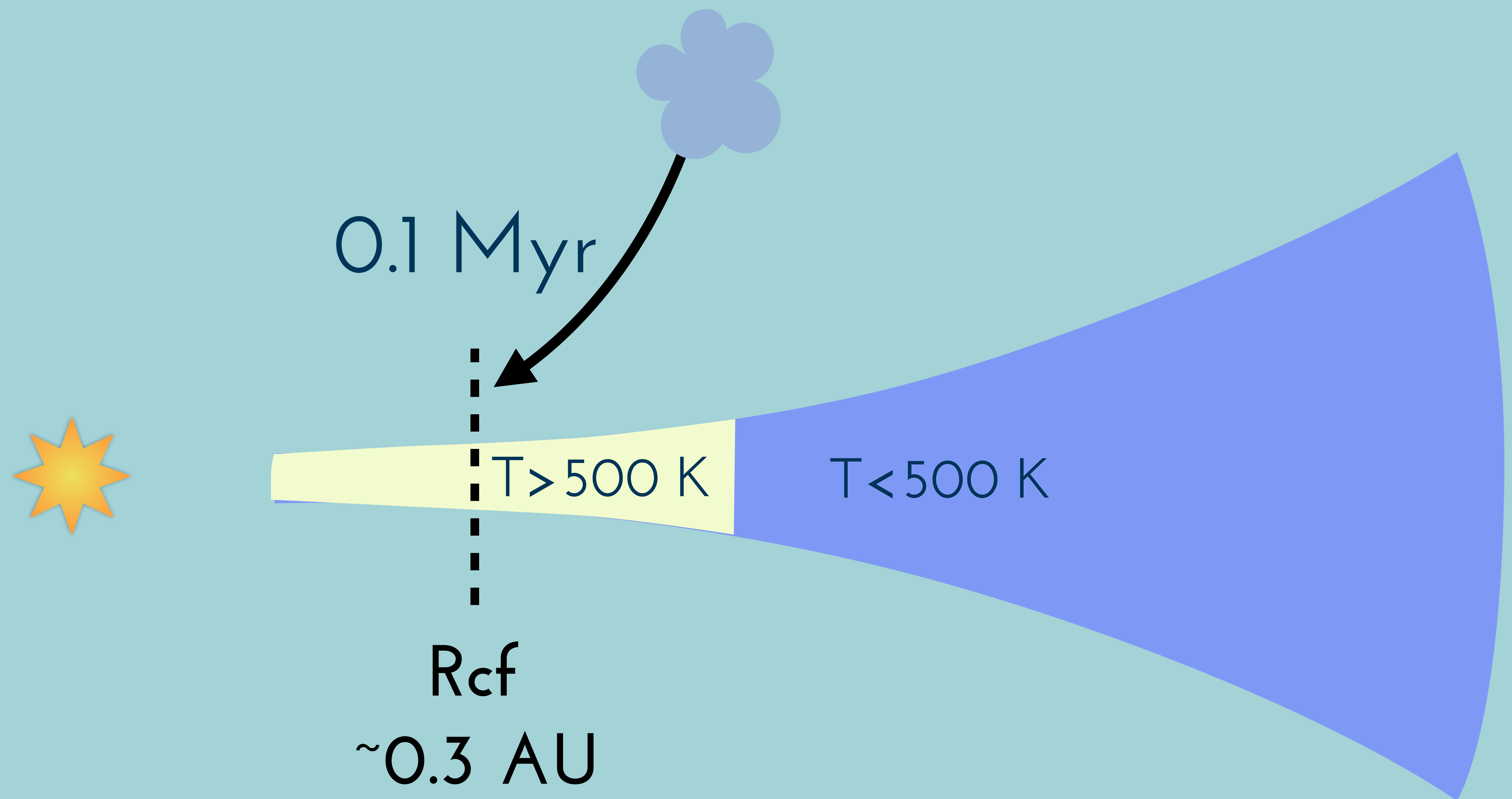


Low angular momentum

Initial Cloud Angular Momentum is Key

Yang and Ciesla 2012, Yang, Ciesla, Alexander 2013

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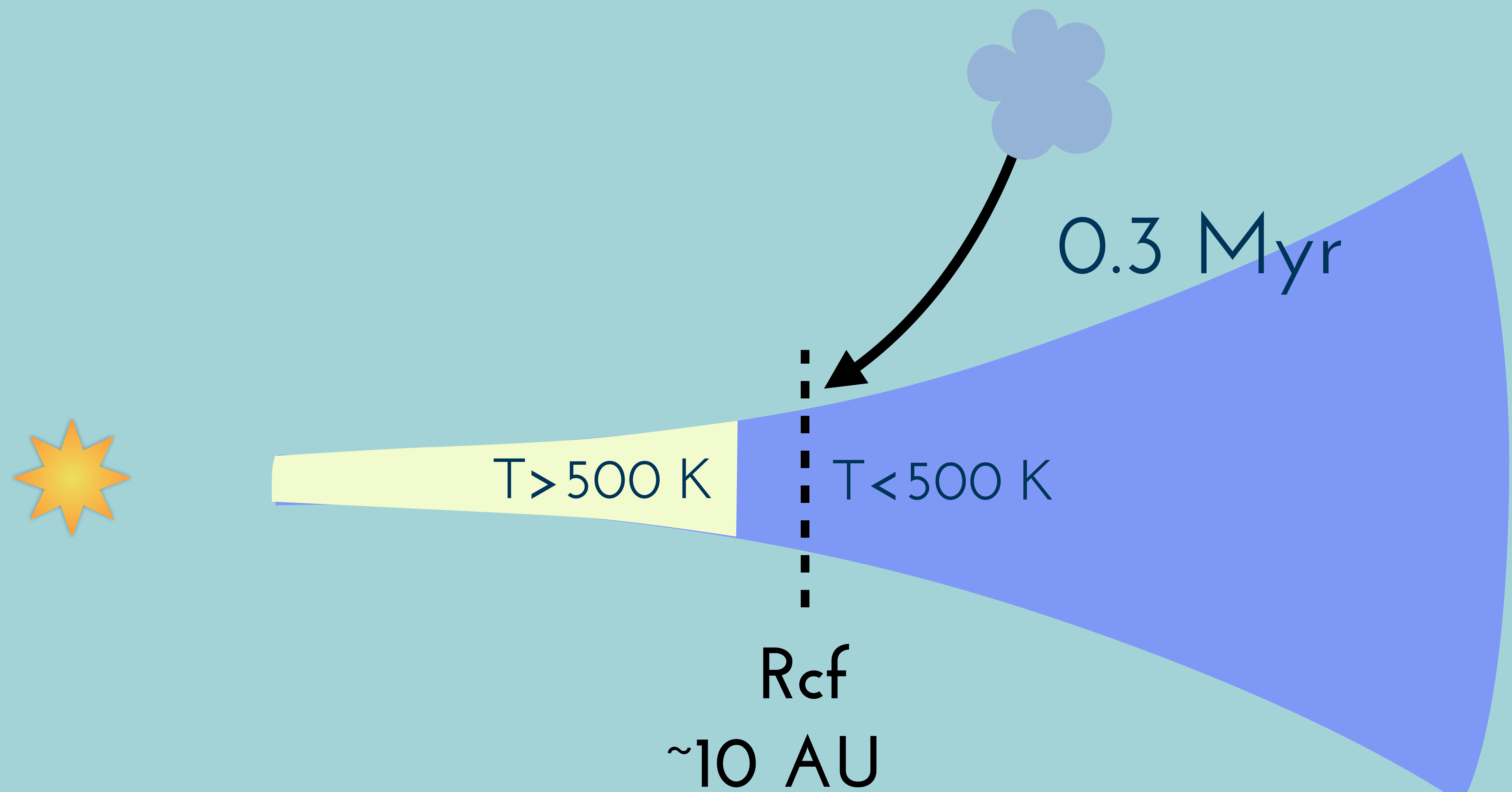


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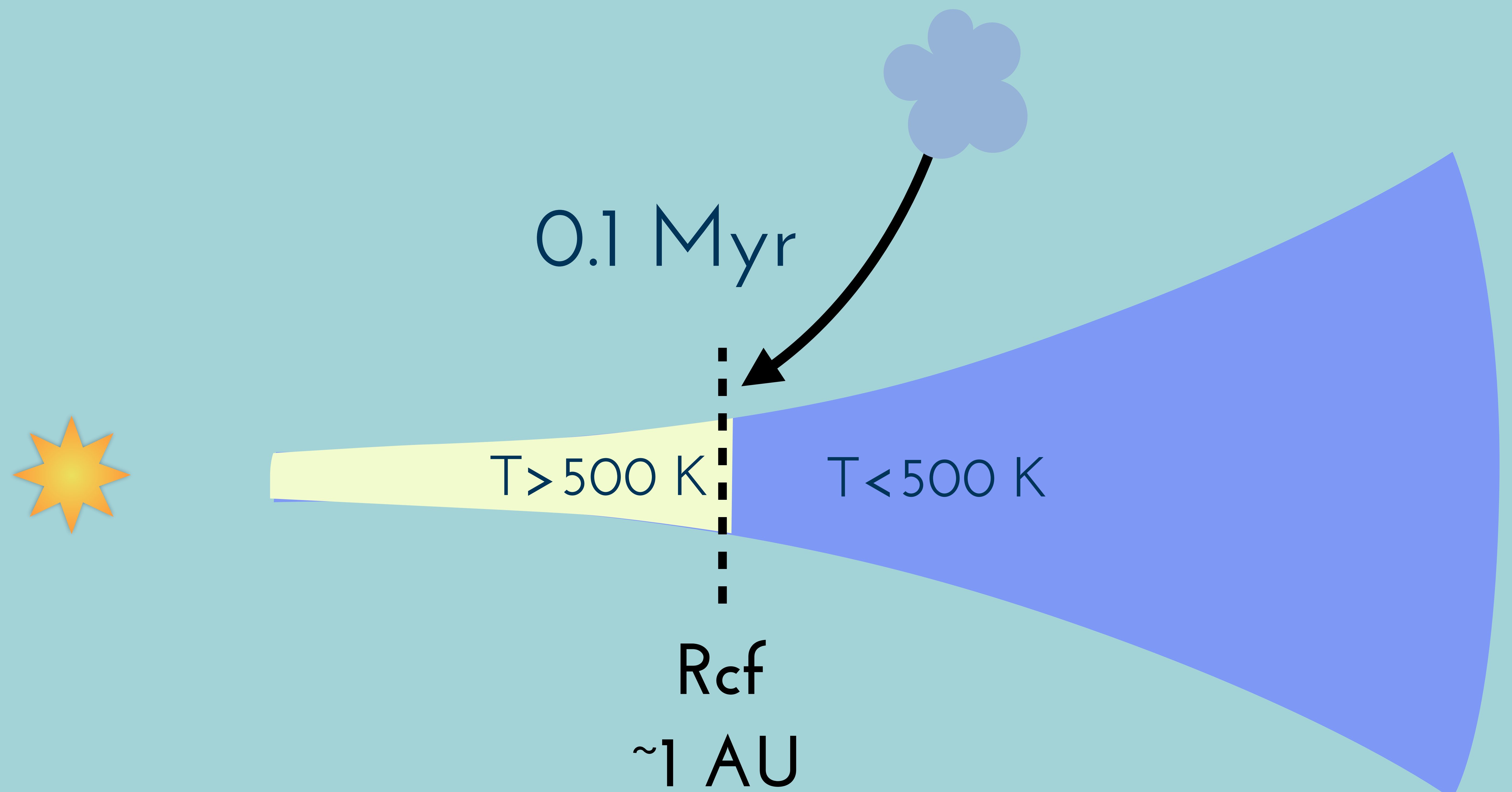


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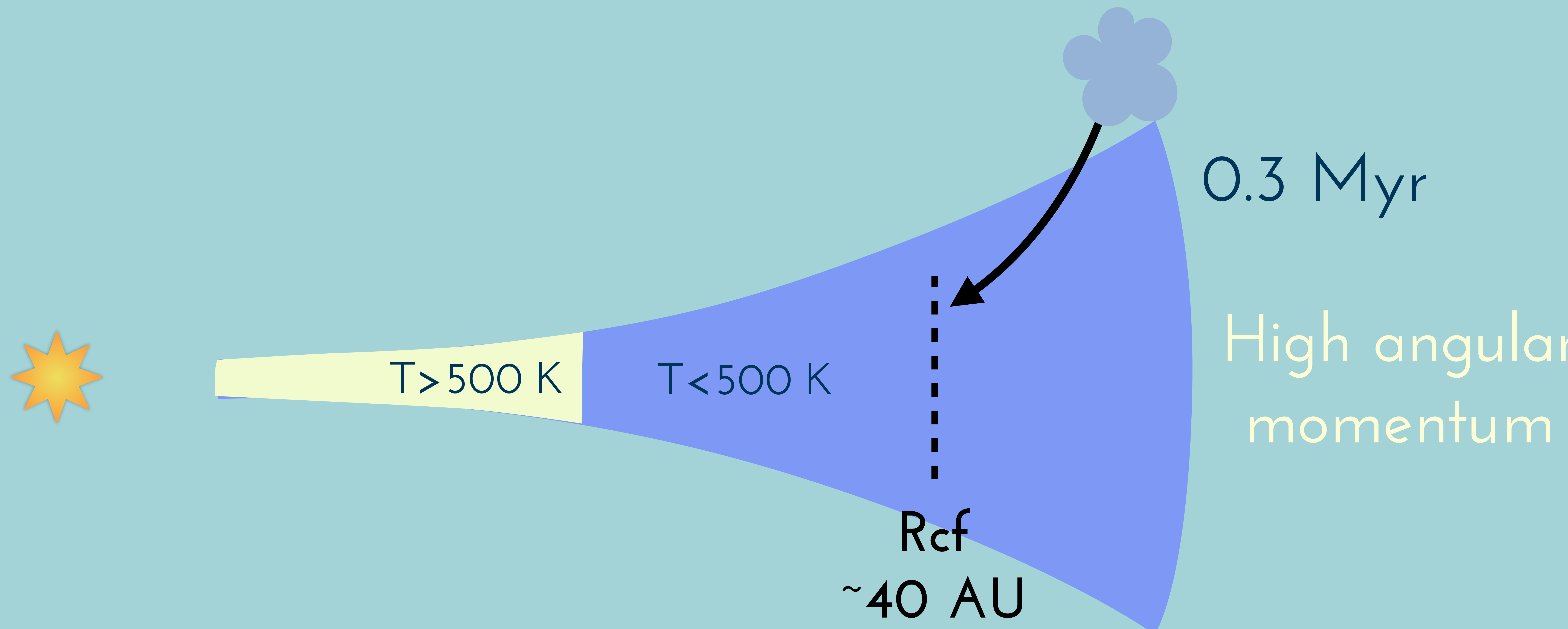


Initial Cloud Angular Momentum is Key

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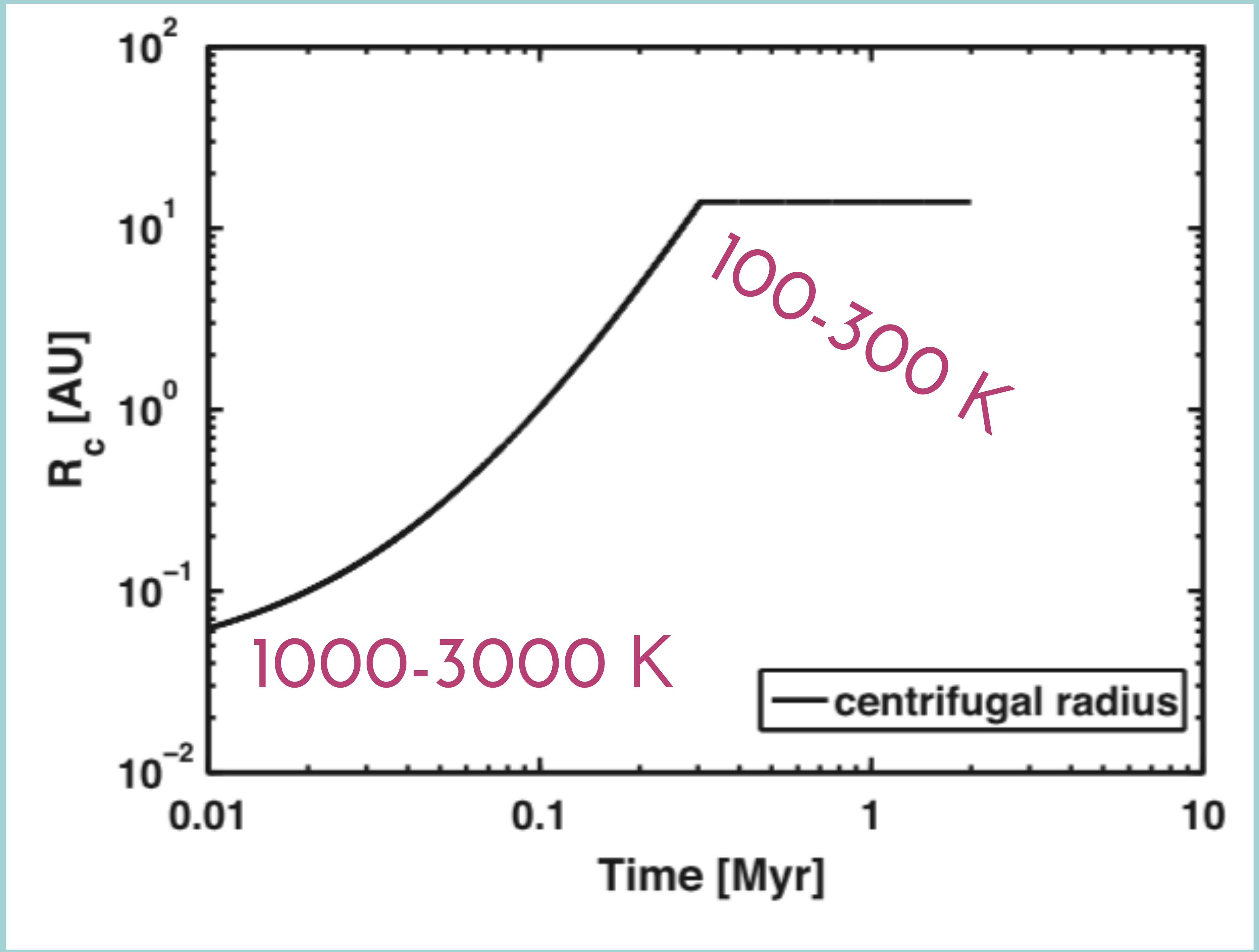
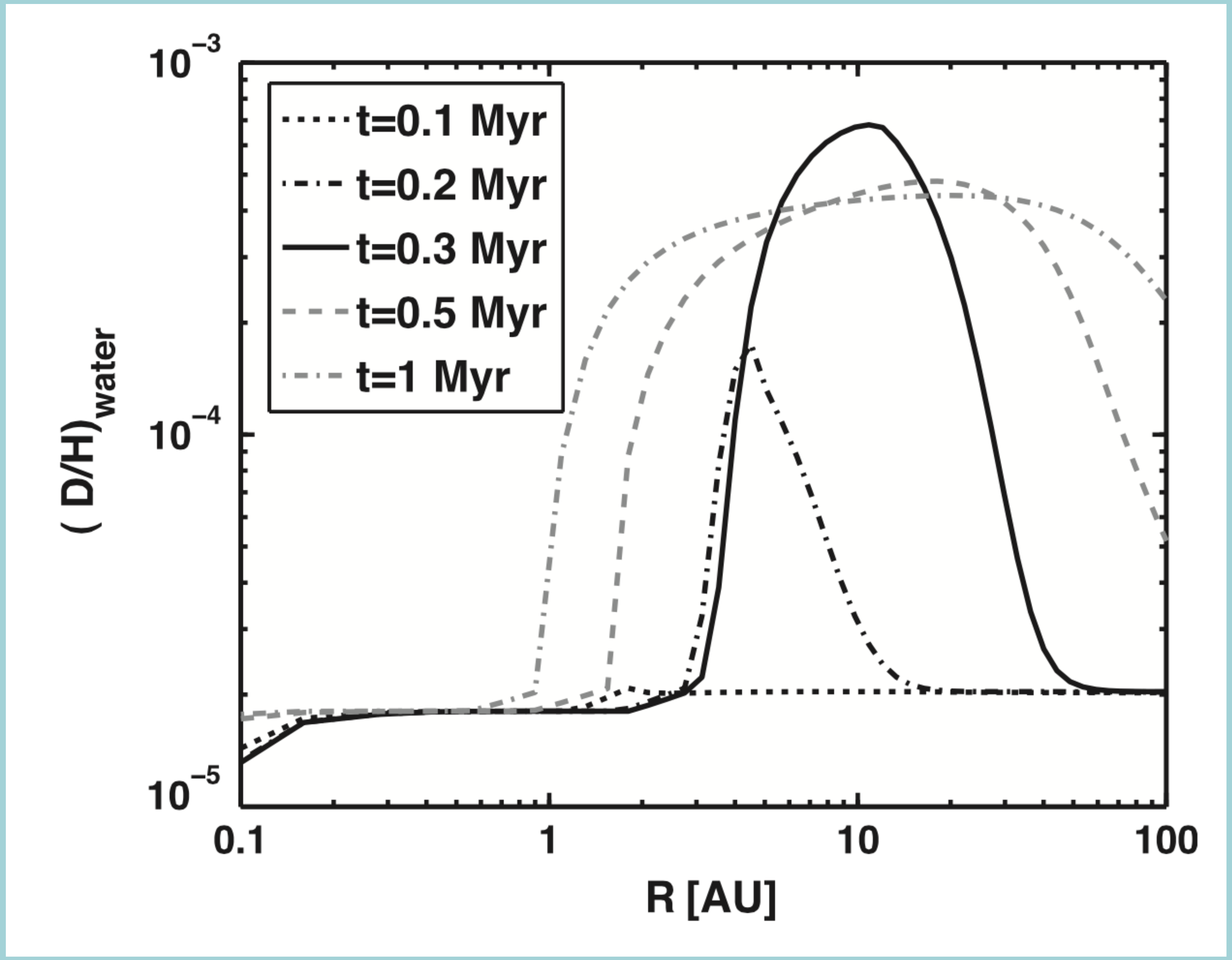
# 2) What are the initial disk chemical conditions?

- $w_{cloud} = 10^{-14}$ s$^{-1}$ typical is $10^{-15}$ - $10^{-13}$ s$^{-1}$

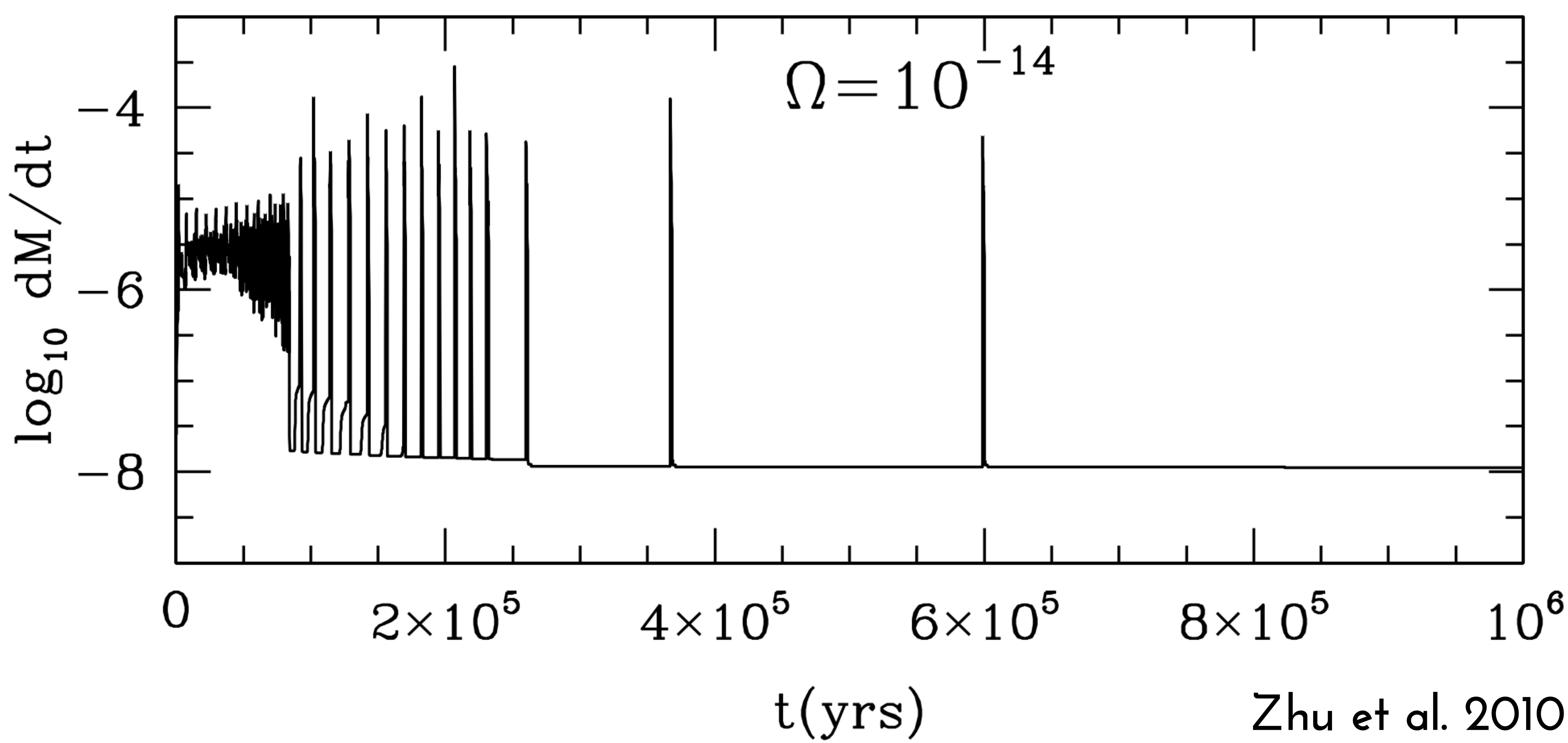



Yang, Ciesla, Alexander 2013

# 2) What are the initial disk chemical conditions?

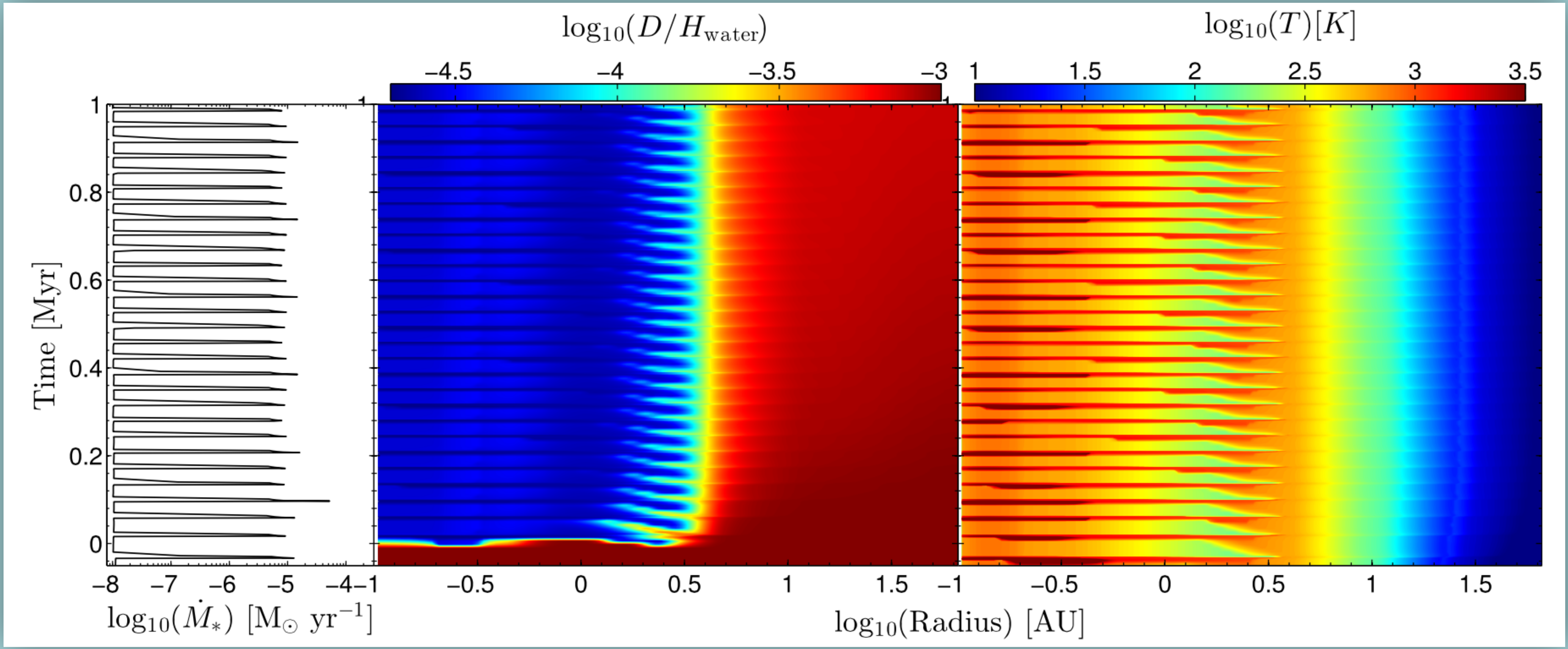
## Violent disk processing through young stellar outbursts?




Zhu et al. 2010

# 2) What are the initial disk chemical conditions?

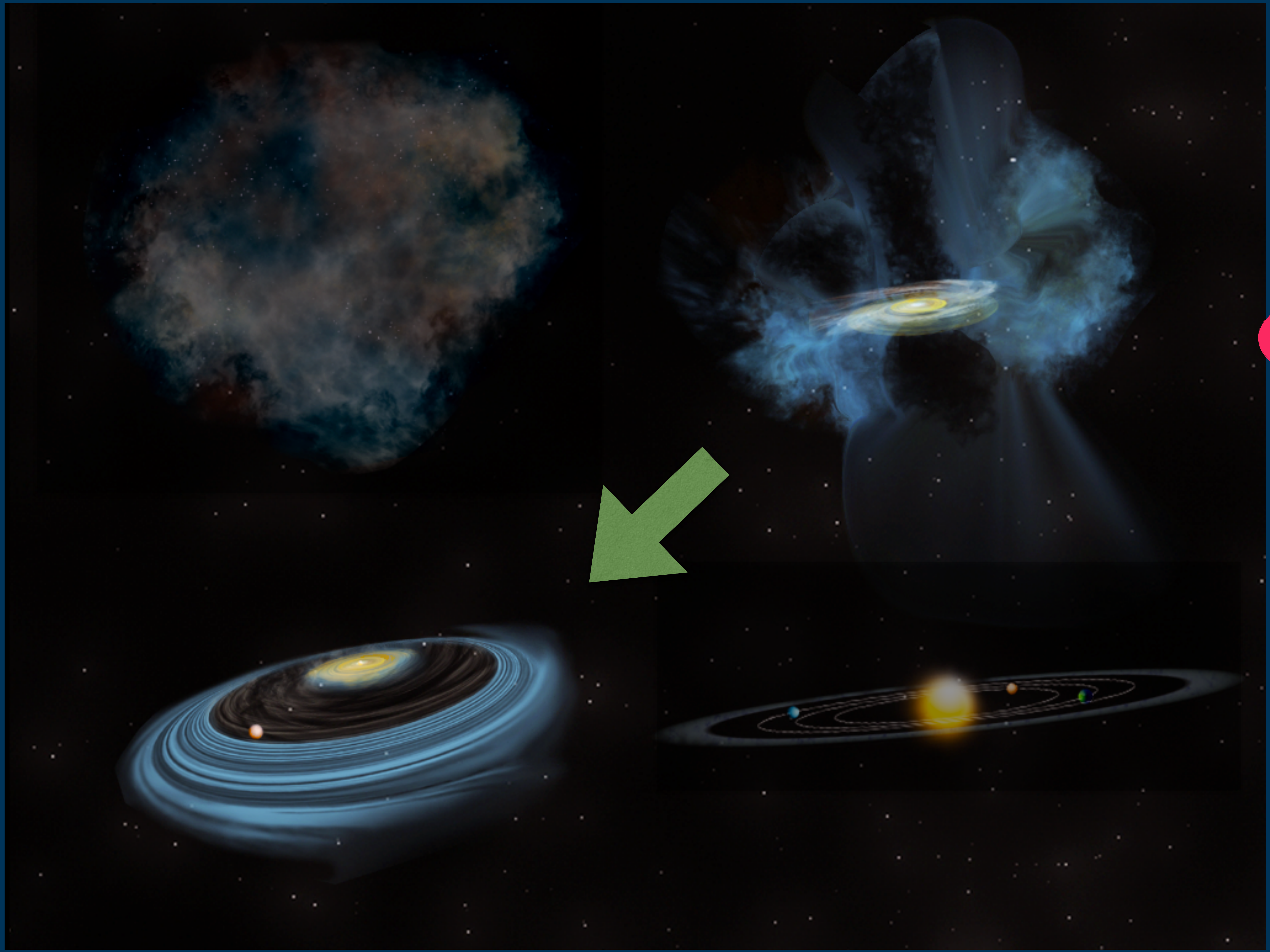
## Violent disk processing through young stellar outbursts?




Owen and Jacquet 2015

# 3) Impact of Gas Disk Evolution

# Post protostellar gas kinematics

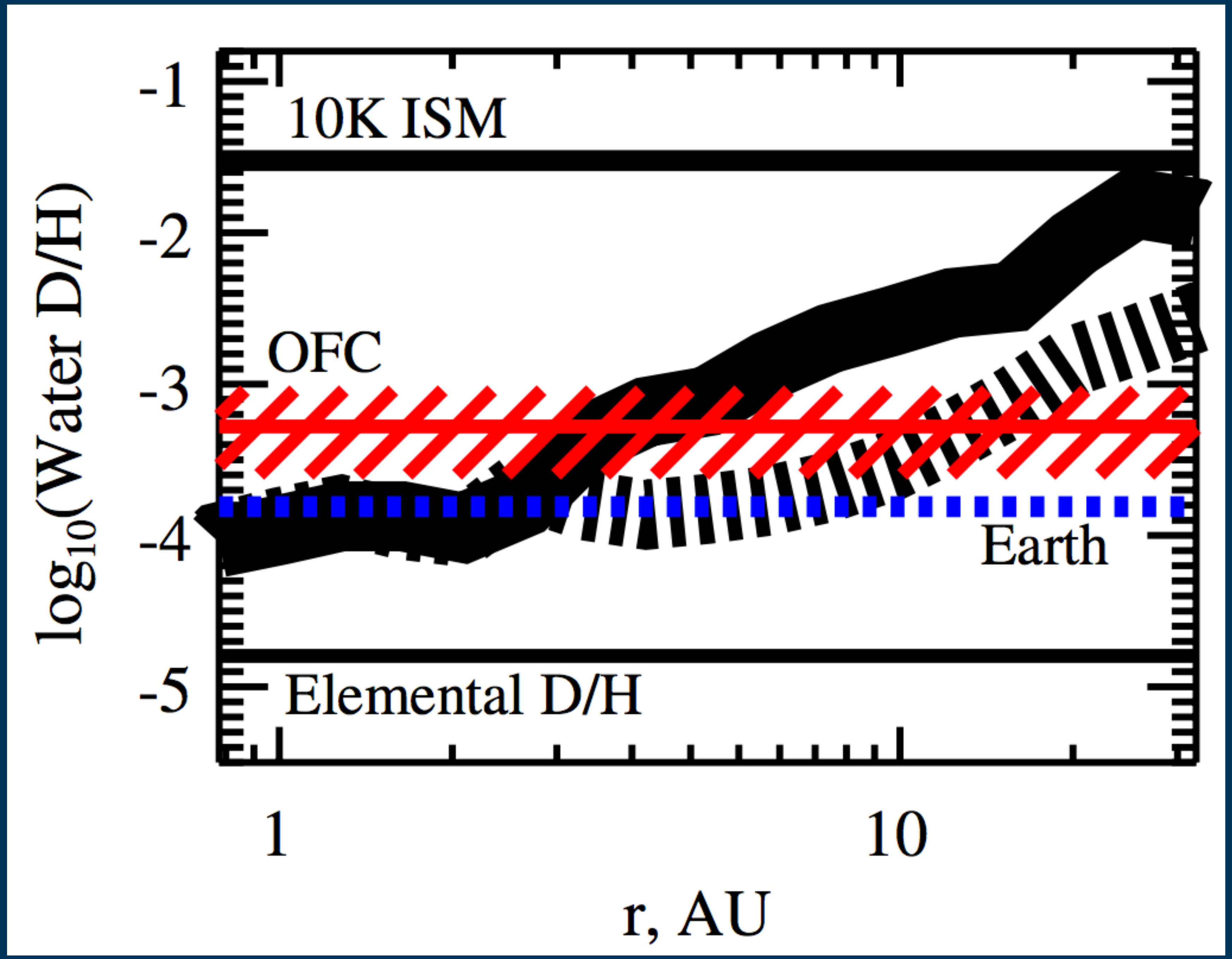


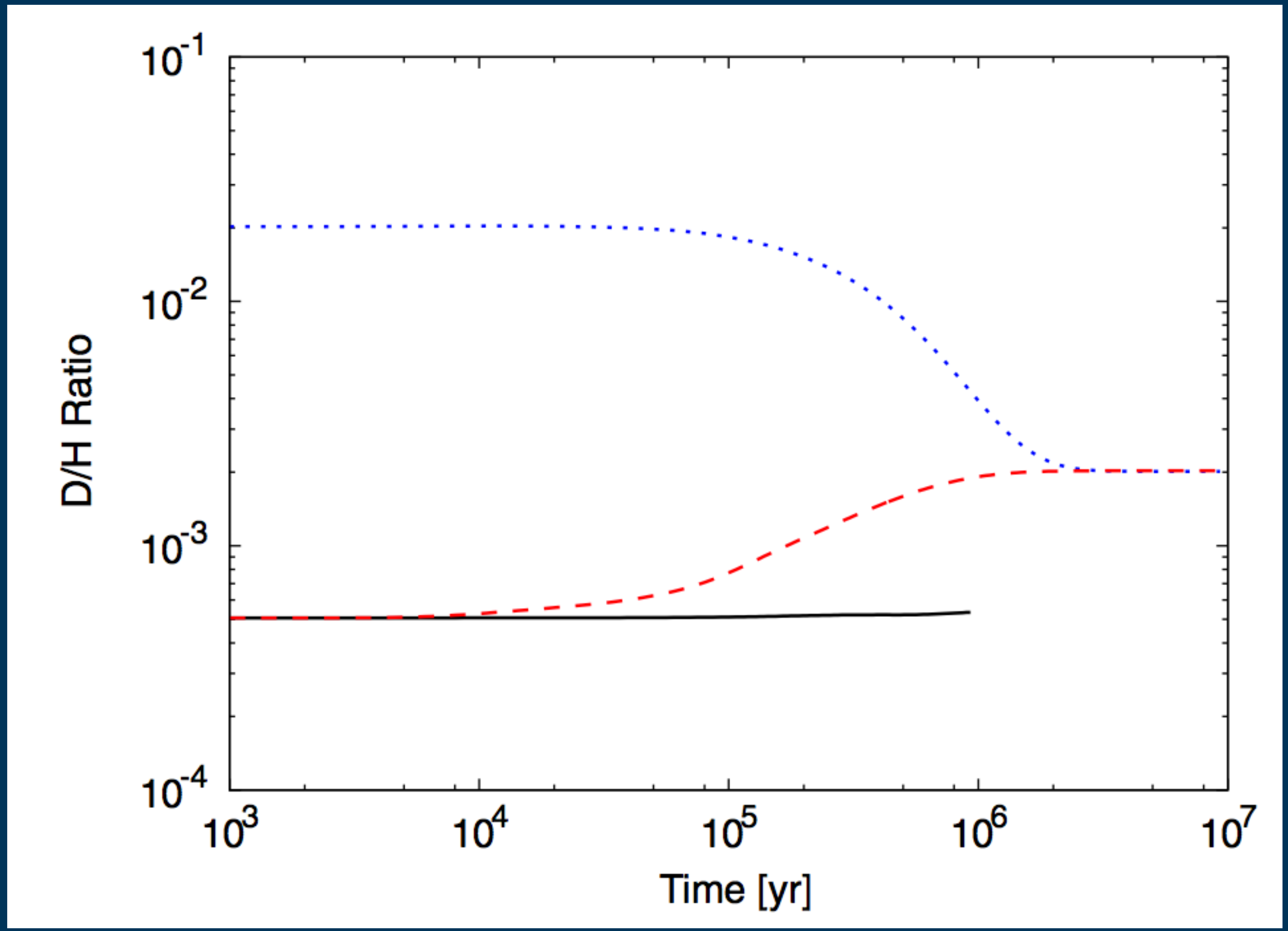
- Keplerian Motion + Thermal Pressure Support
- Turbulence?
- Viscous Evolution/ Accretion?
- Winds? Photoevap. or MHD?

# 3) The role of mixing/turbulent evolution?

- Mixing: The jury is still out.
- Theory demonstrates mixing can both produce significant D/H enhancements in water and decrease D/H (Albertsson et al. 2015 and Furuya et al. 2013).
- May also operate on other deuterated species, including organics.

# 3) The role of mixing/turbulent evolution?

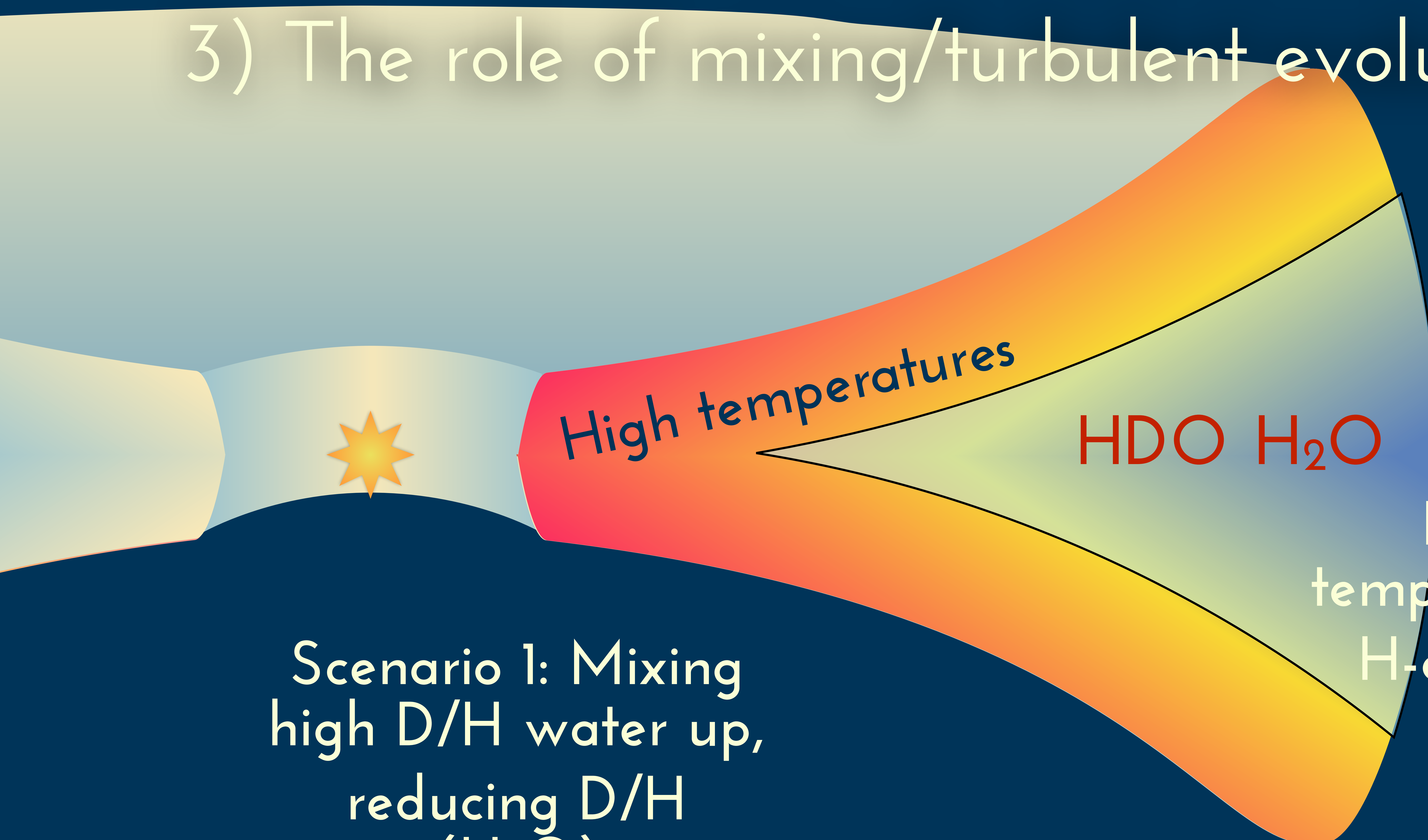



"Turbulent mixing slowly transports some of the water ice into warmer or irradiated regions where it desorbs and is quickly defractionated by ion-molecule and dissociative recombination processes in the gas phase." - Albertsson et al. 2014

"Still, transport of oxygen affects water and deuterated water chemistry; atomic oxygen is transported from the surface to the deeper region and (re)forms $H_2O$ and HDO ices. " - Furuya et al 2013

# 3) The role of mixing/turbulent evolution?




Scenario 1: Mixing high D/H water up, reducing D/H ($H_2O$)

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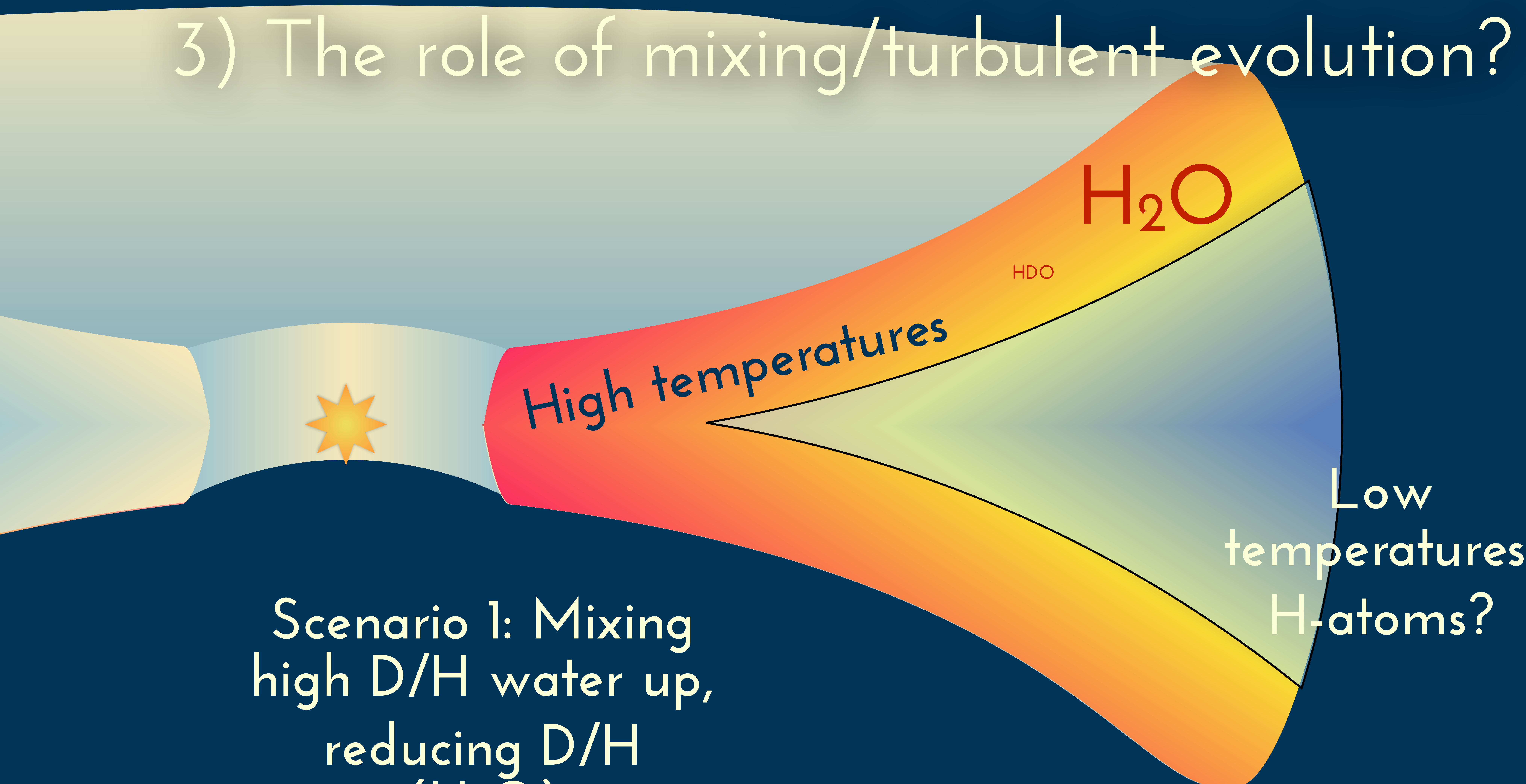


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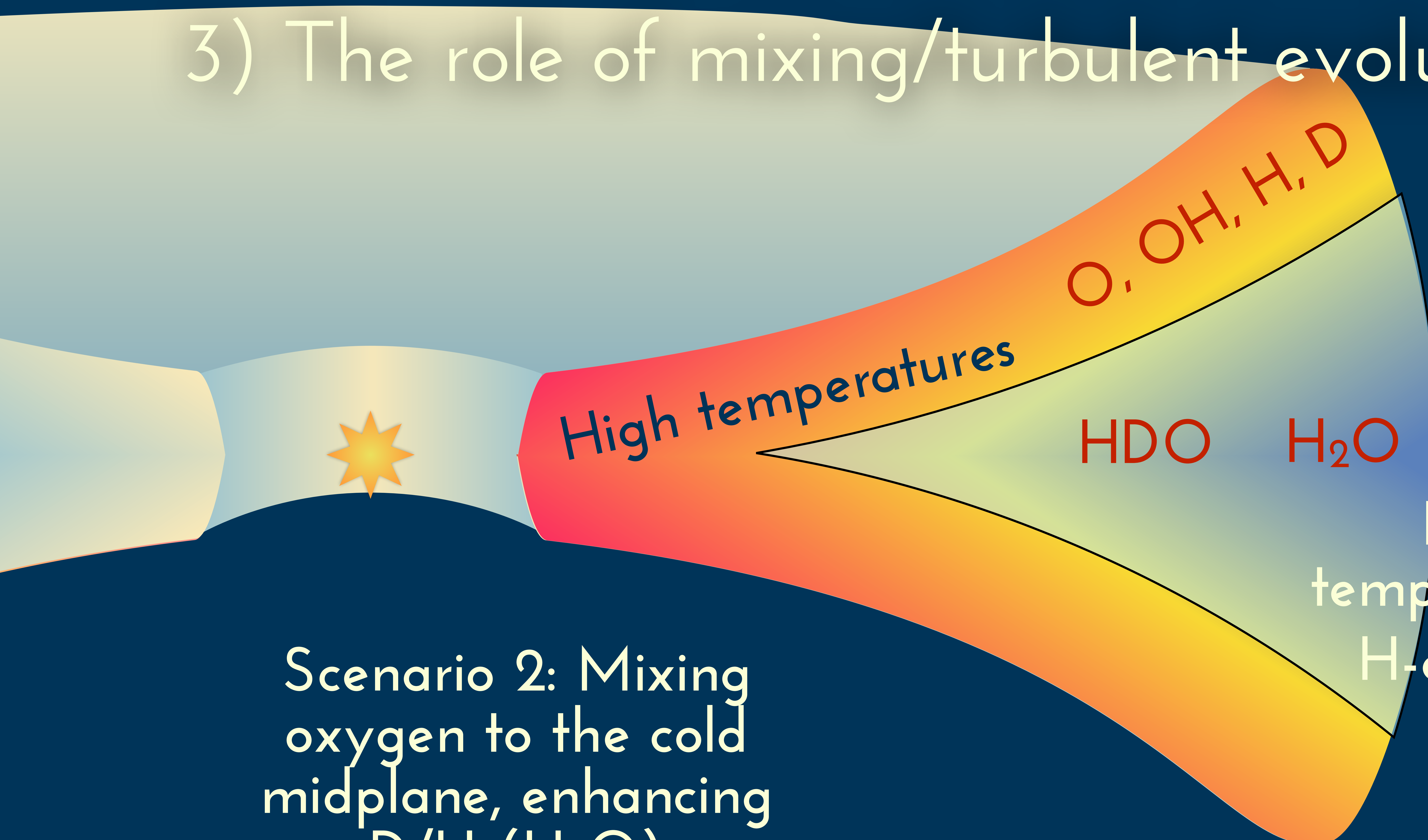


Scenario 2: Mixing oxygen to the cold midplane, enhancing D/H ($H_2O$)

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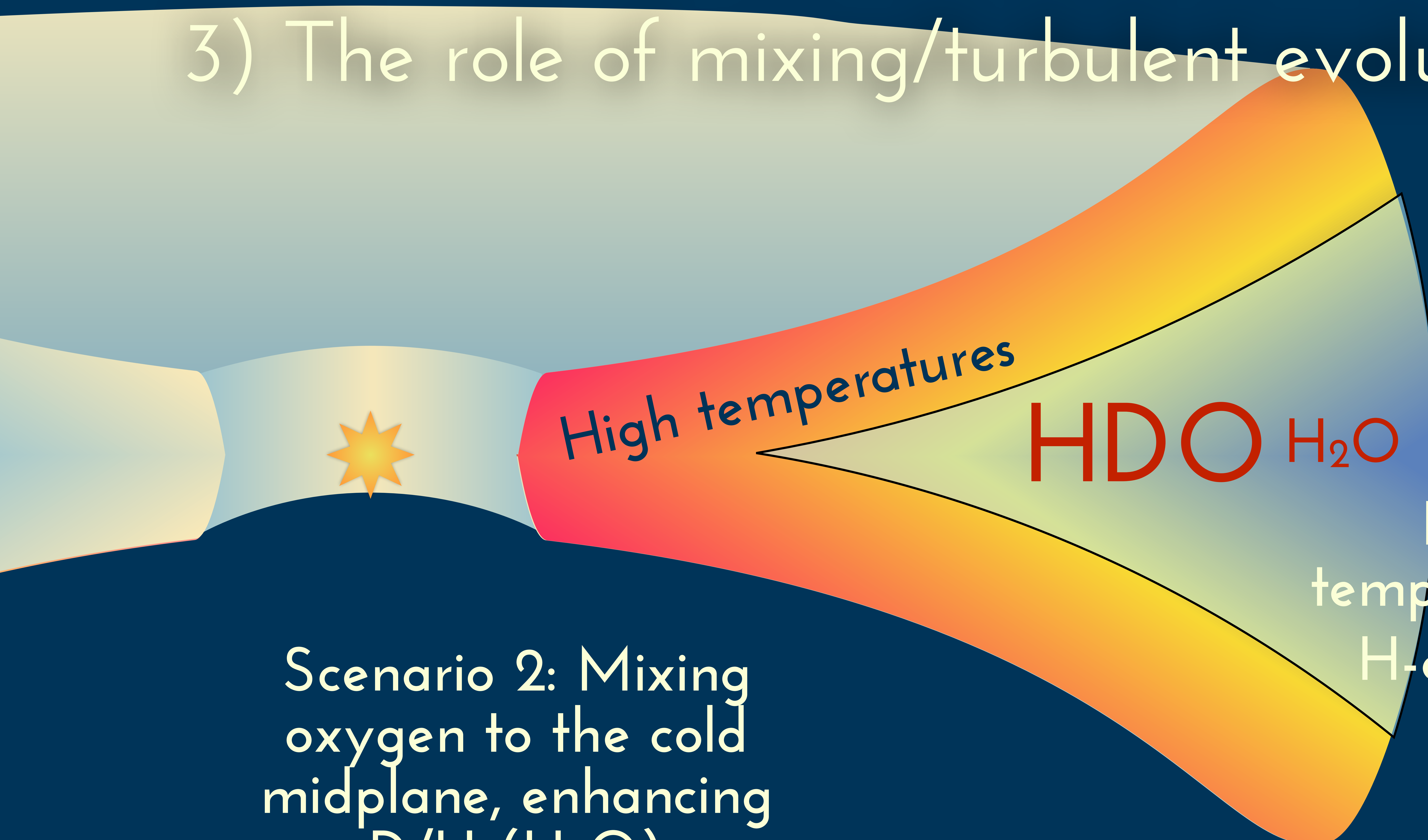


Scenario 2: Mixing oxygen to the cold midplane, enhancing D/H ($H_2O$)

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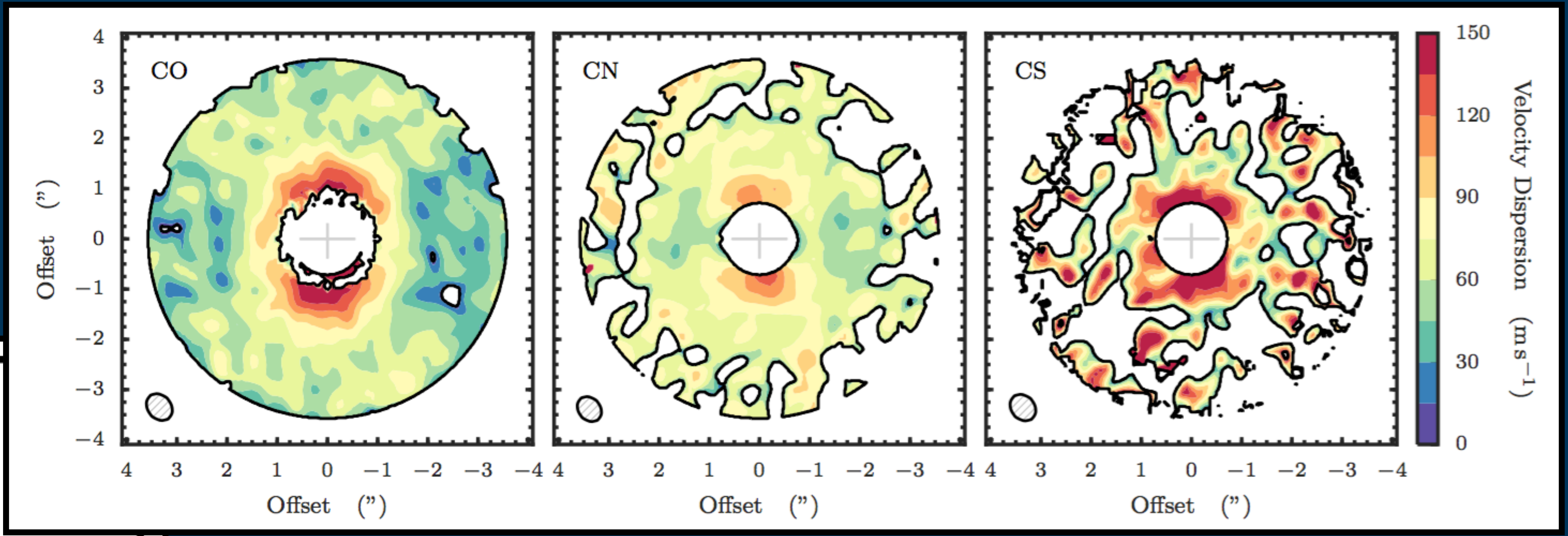
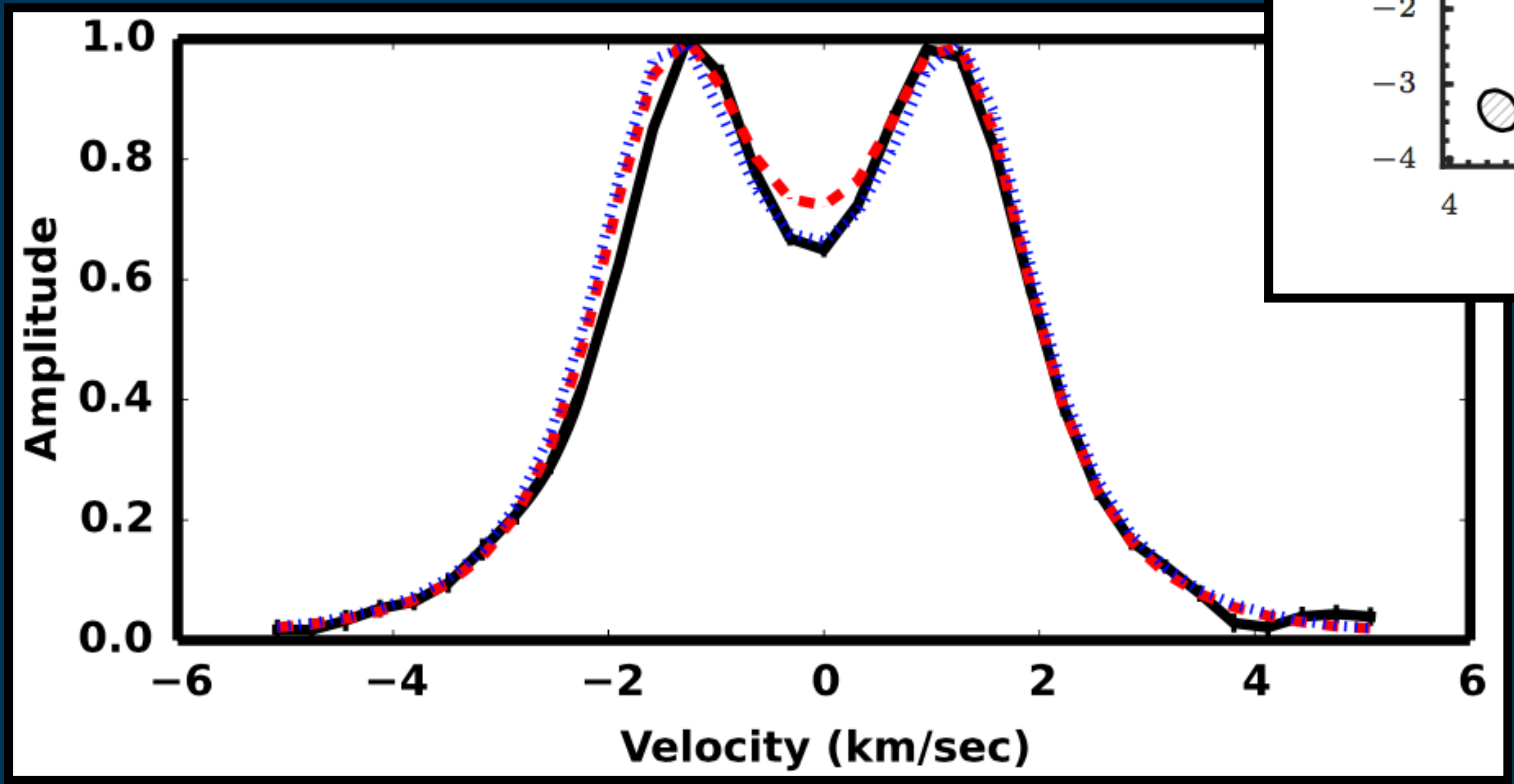
# 3) The role of mixing/turbulent evolution?

- ✴ Need more constraints on disk turbulence, e.g., Hughes+2011, Guilloteau+2012, Teague+2015, Flaherty+2015 ($\alpha < 9 \times 10^{-4}$).




CO 2-1, Flaherty+2015

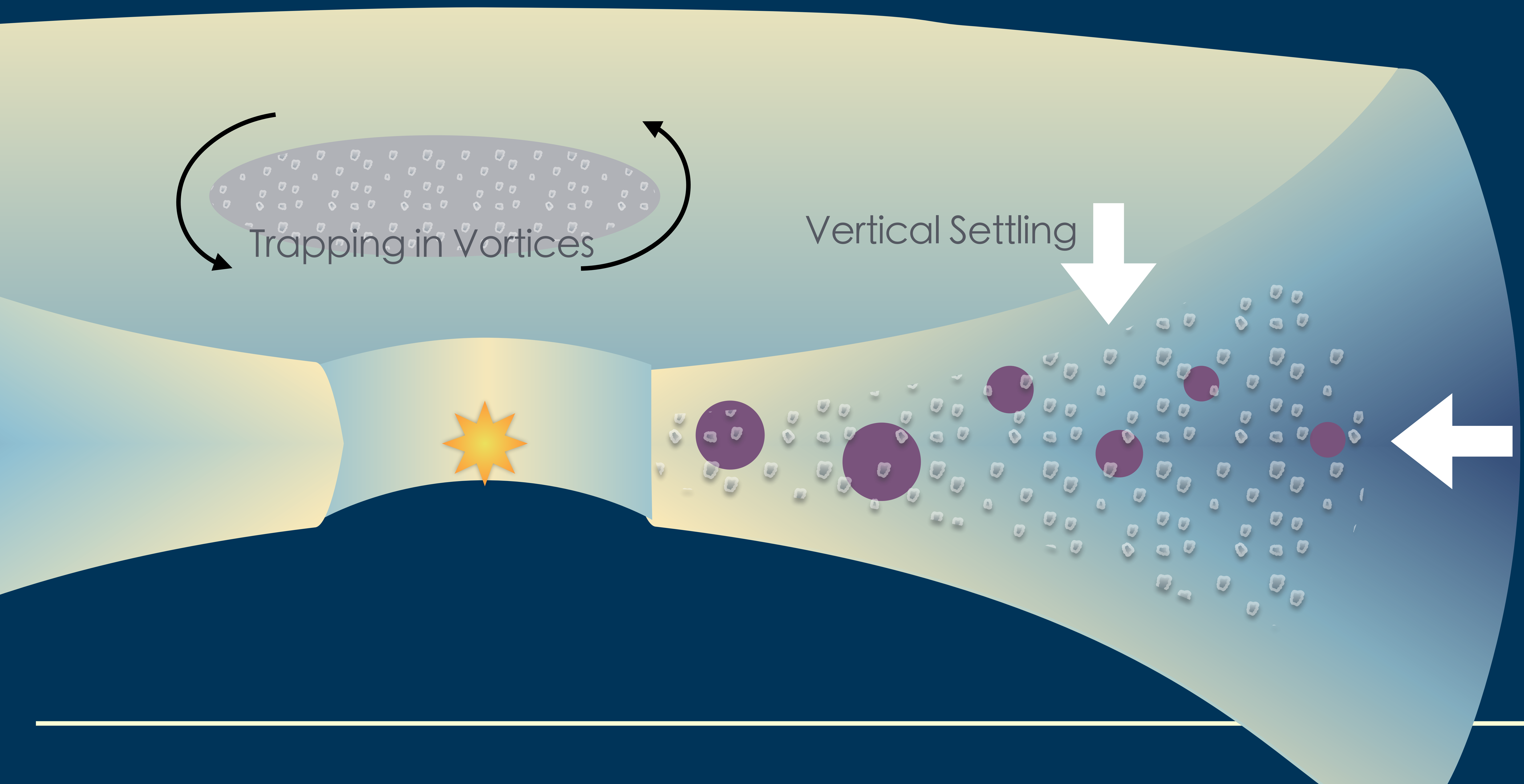
"CO and CN displayed a near constant $v_{turb}$ ~ 0.2 cs. However, the analysis of the possible sources of errors shows that these numbers should most likely be interpreted as upper limits."

Teague+2016

# 4) Differential Evolution of Solids and Ice

# 4) Differential Evolution of Solids

- Redistributes volatiles carried in the ices (Hogerheijde+2010, Bergin +2016, Du+2015, 2016, sub.). Changes the C/O ratio (e.g., Piso+2015).

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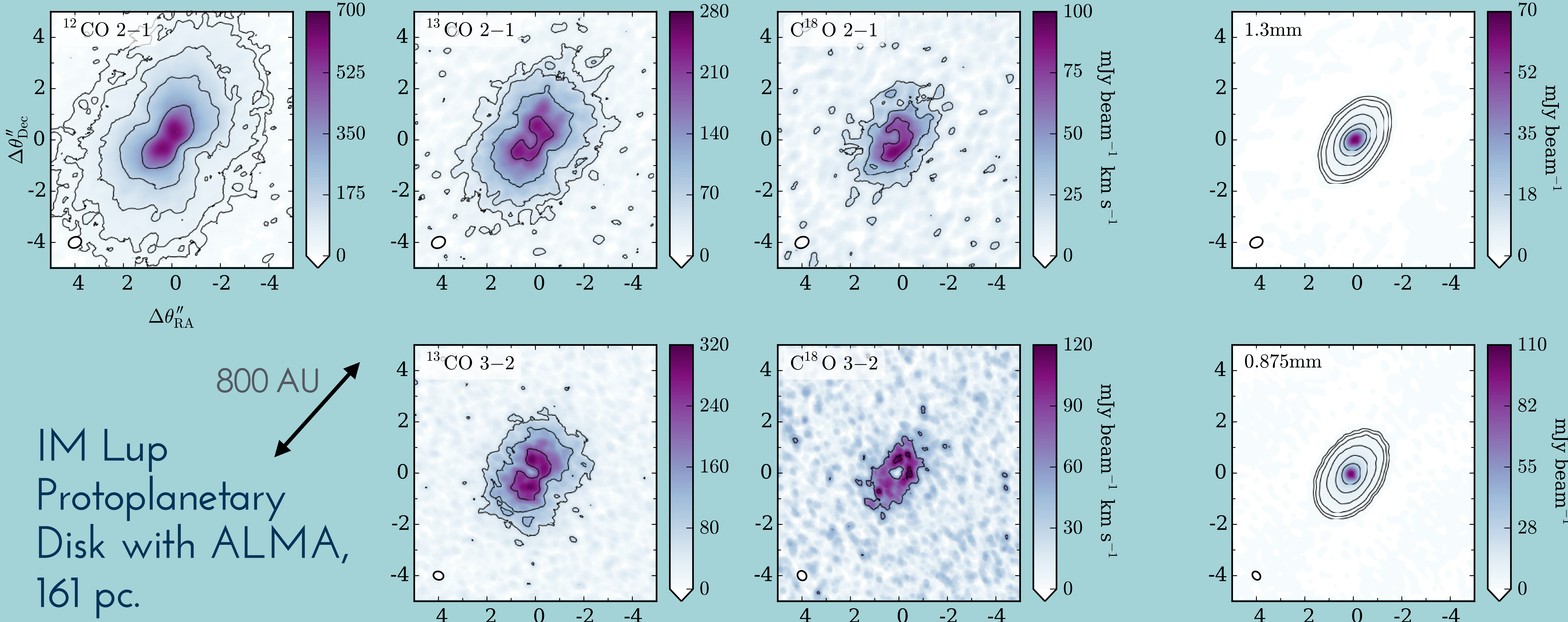
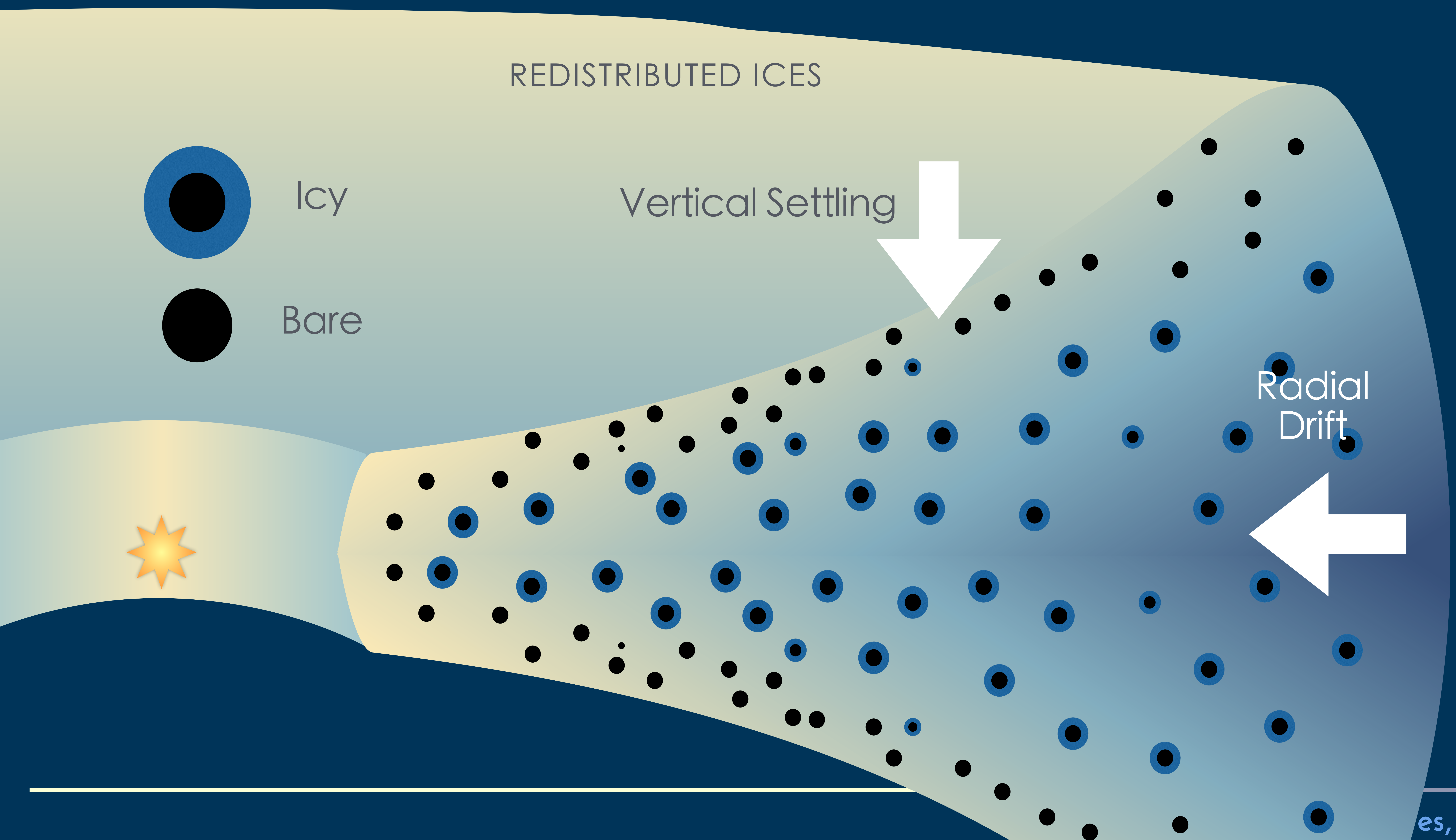
# 4) Differential Evolution of Solids



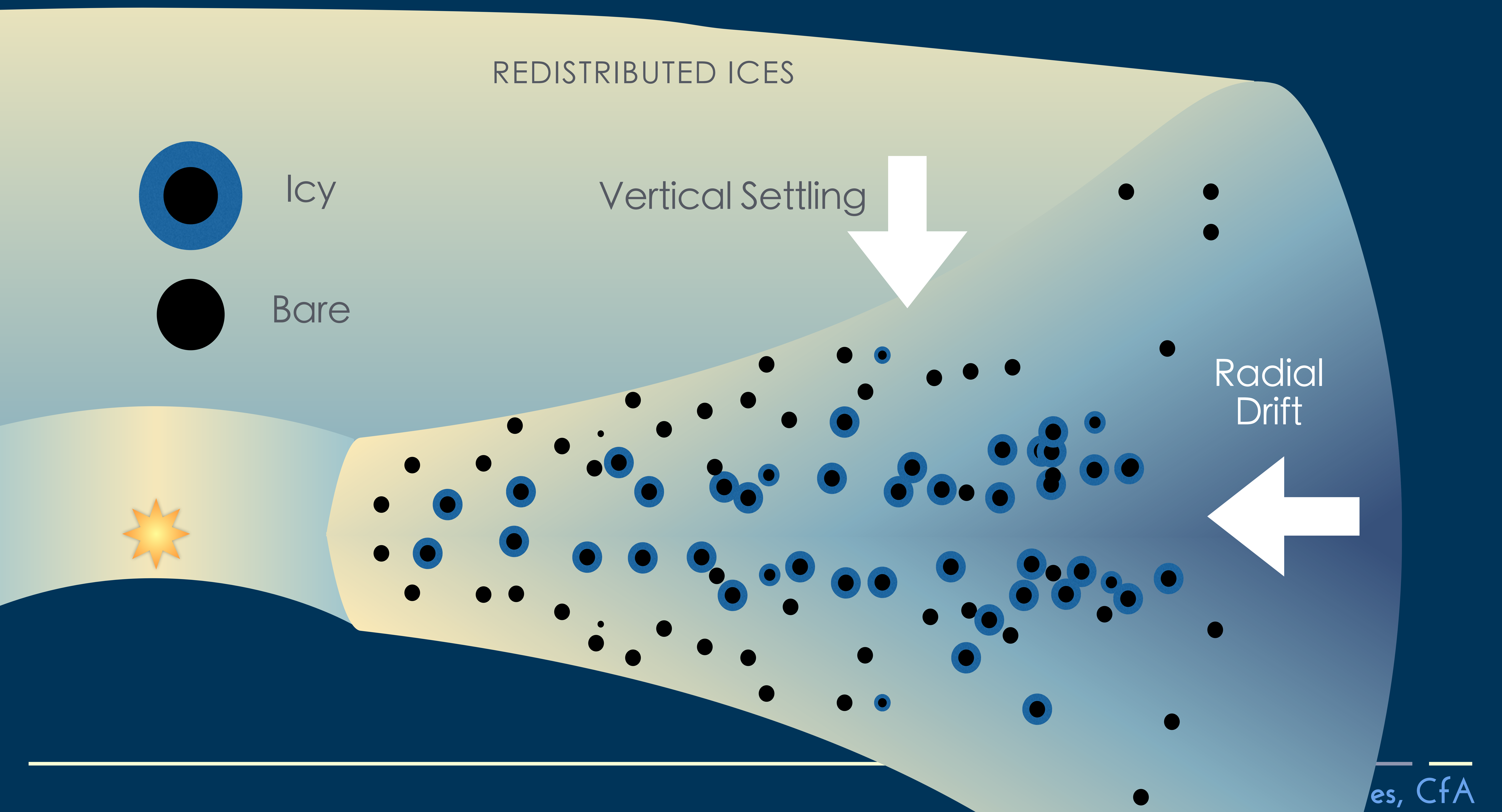

800 AU

IM Lup Protoplanetary Disk with ALMA, 161 pc.

Panic et al. 2009, Cleeves et al. 2016c


REDISTRIBUTED ICES
Icy
Bare
Vertical Settling
Radial
Drift

es, CfA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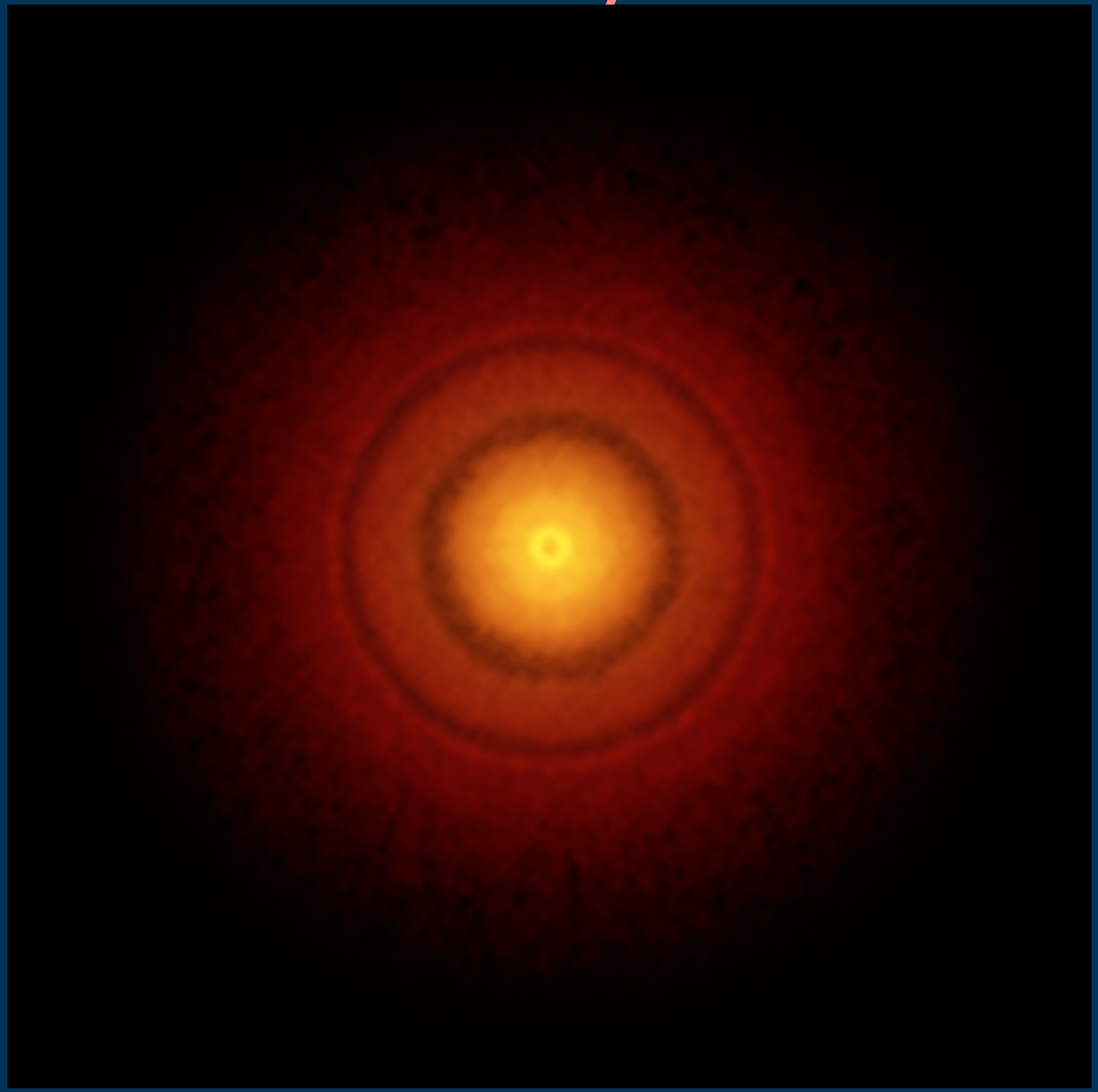
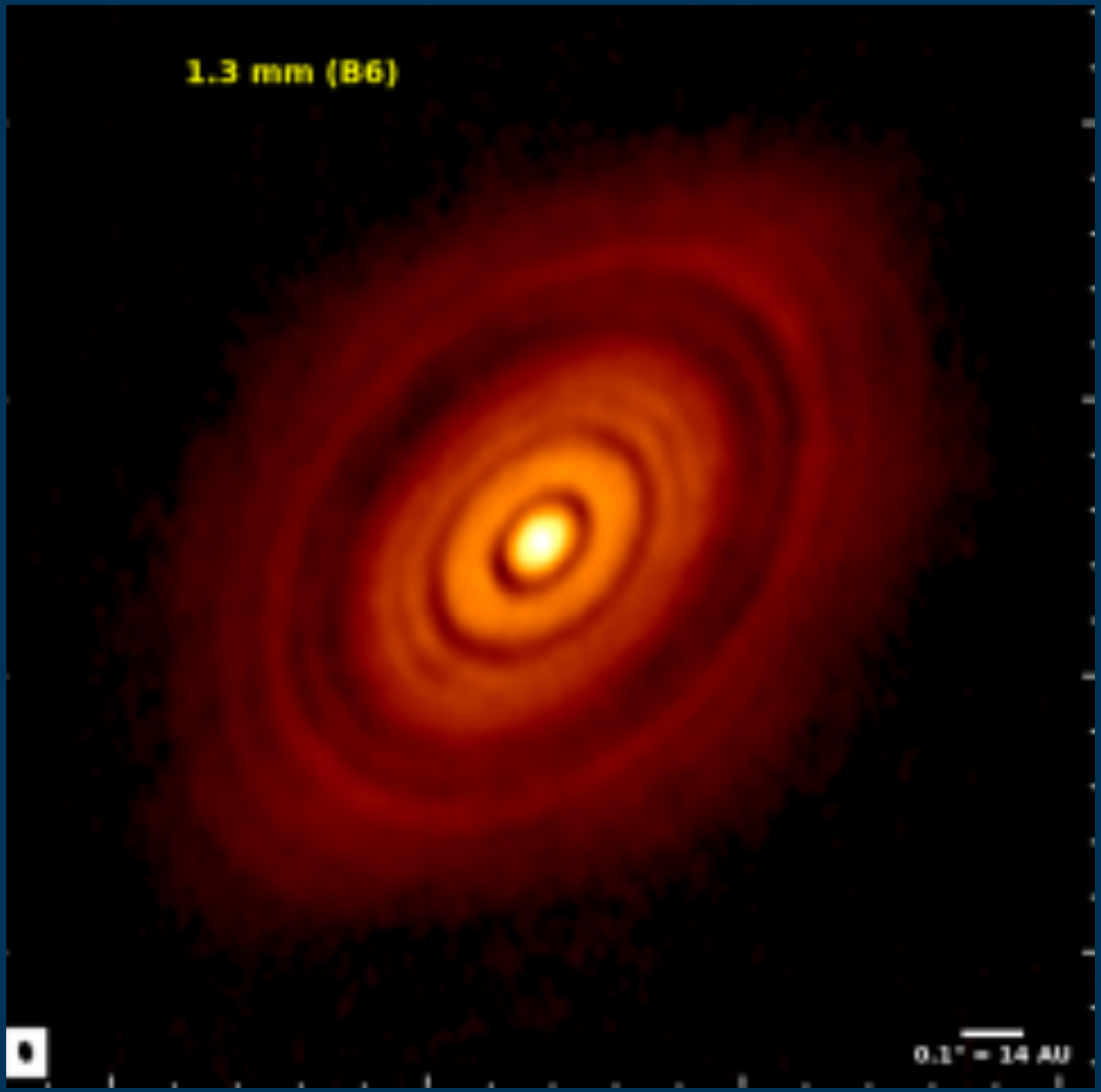
# 4) Differential Evolution of Solids

TW Hya



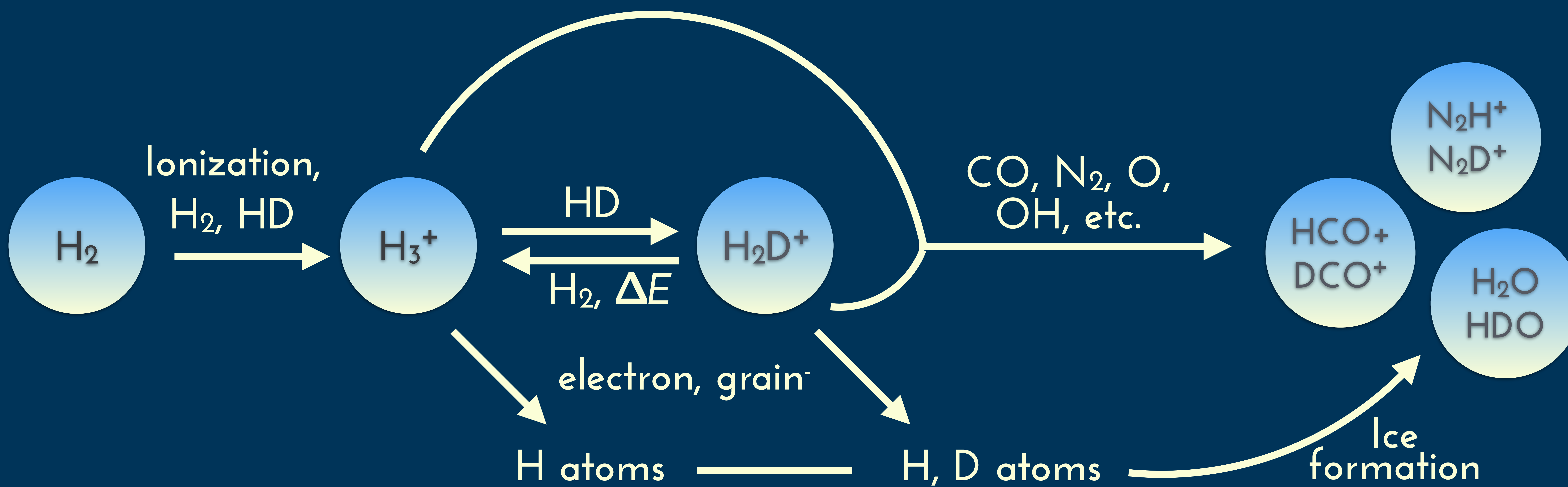
HL Tau




Perhaps halted by substructure, formation of rings?

# 5) Baseline Models of Water and Simple Organic Deuteration: Variations in Deuteration Pathways

# 1) Key Ingredients for High Molecular HDO/$H_2O$




Supports fractionation
up to T < 50 K

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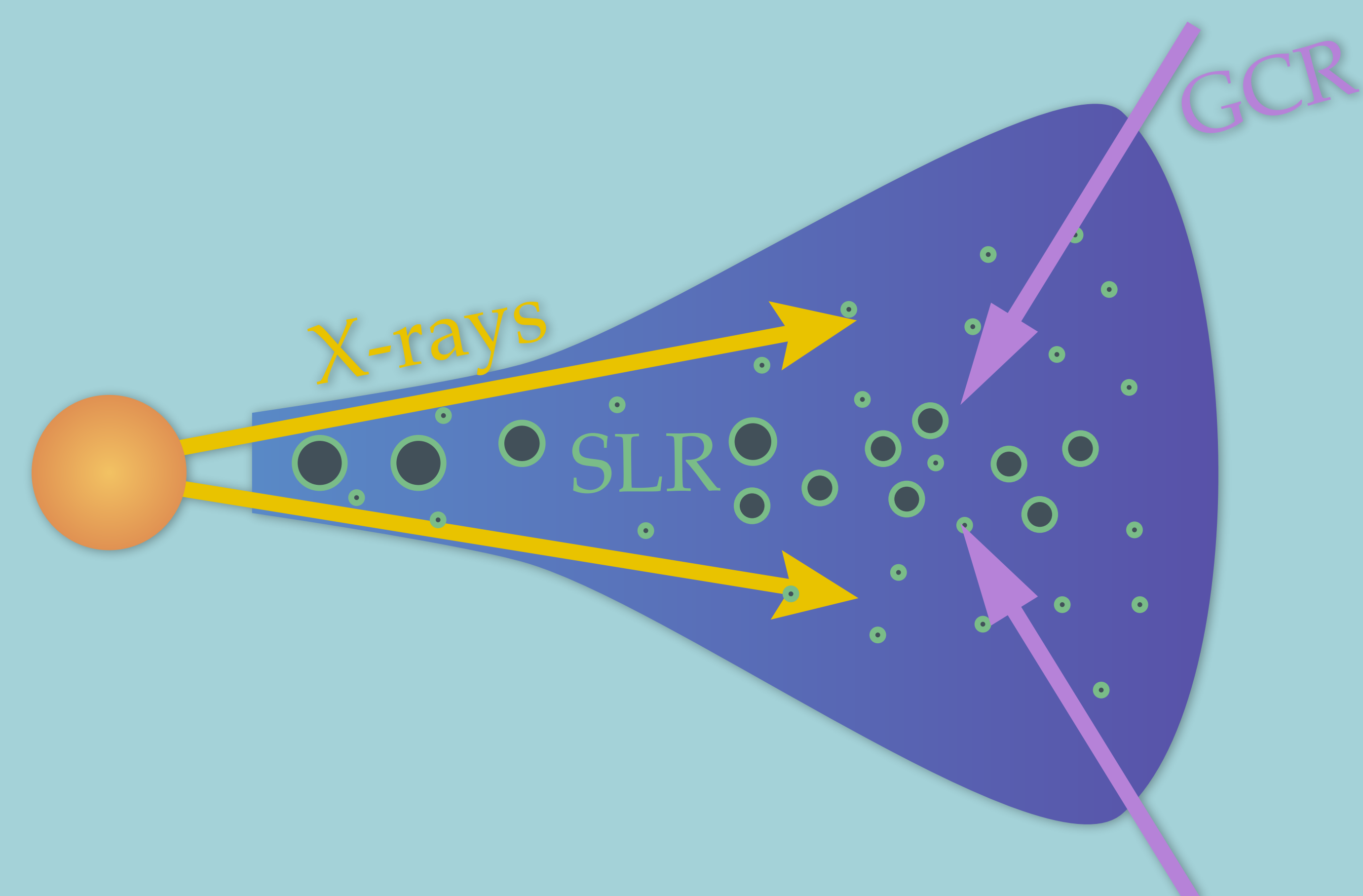
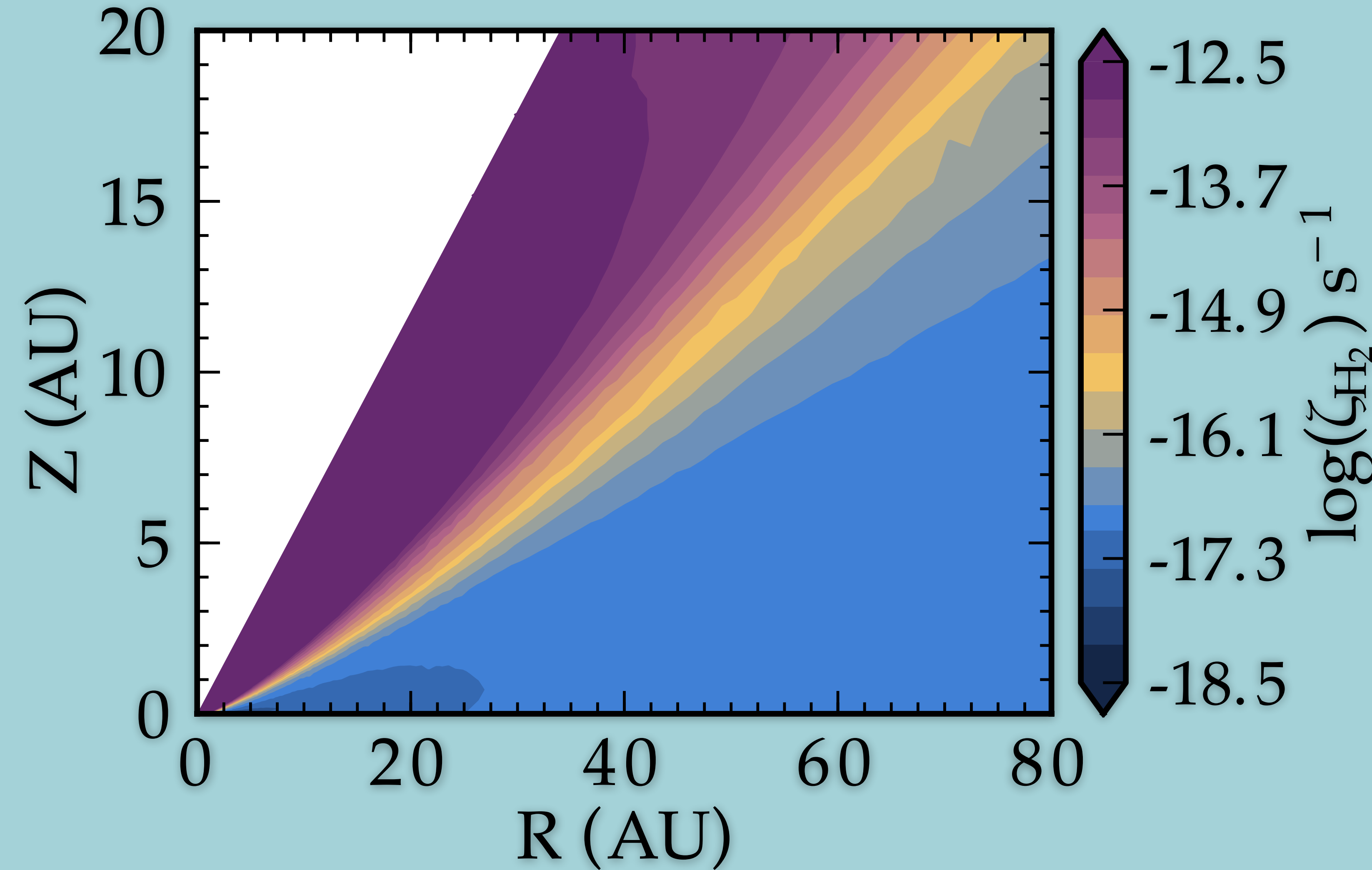
Starting out with $HDO/H_2O = HD/H_2$, how much does cold water formation in the disk contribute to elevated $HDO/H_2O$?

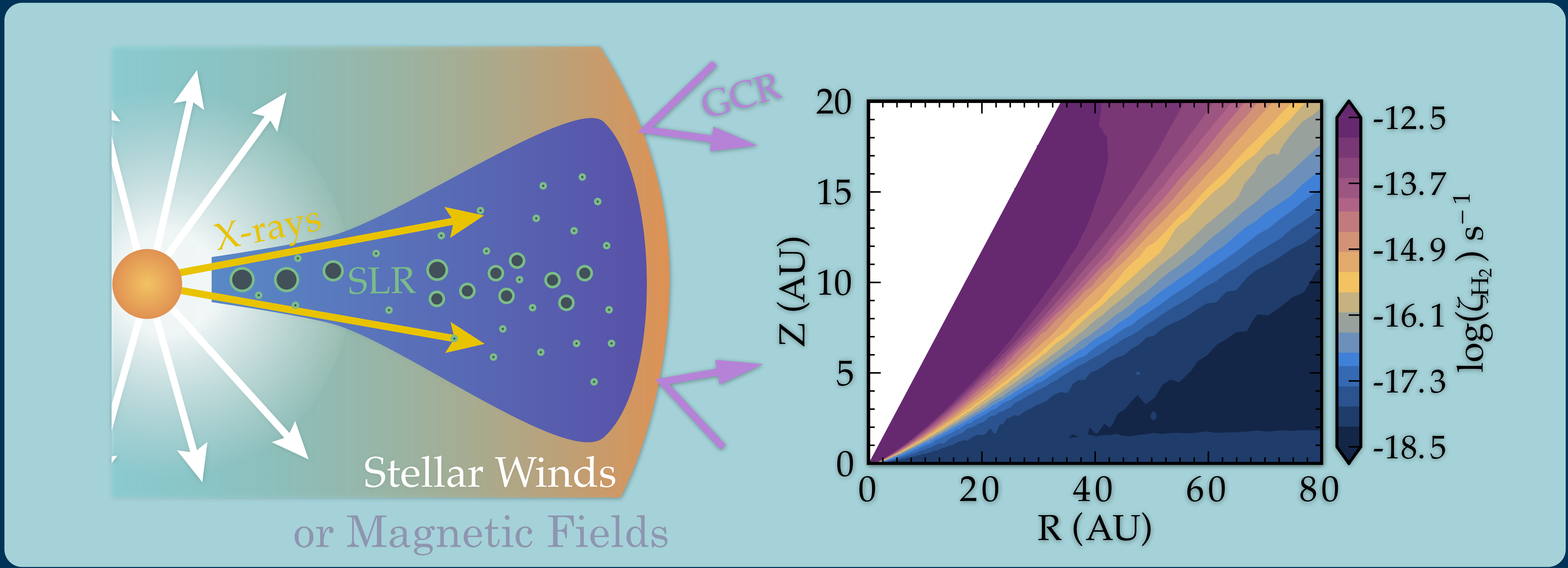
# The Classical Picture of Disk Ionization




Glassgold 1997, 2000, 2001 (and more), Igea & Glassgold 1999, Umebayashi+1989, 2009, Ilgner & Nelson 2006a/b, 2008.

# An Updated Picture of Disk Ionization




Cleeves et al. 2015 measured a significantly subinterstellar CR ionization rate in TW Hya (> 100x reduced).

High densities + low ionization rates → very low ion fraction in the cold gas where deuterium enrichment is otherwise facilitated..

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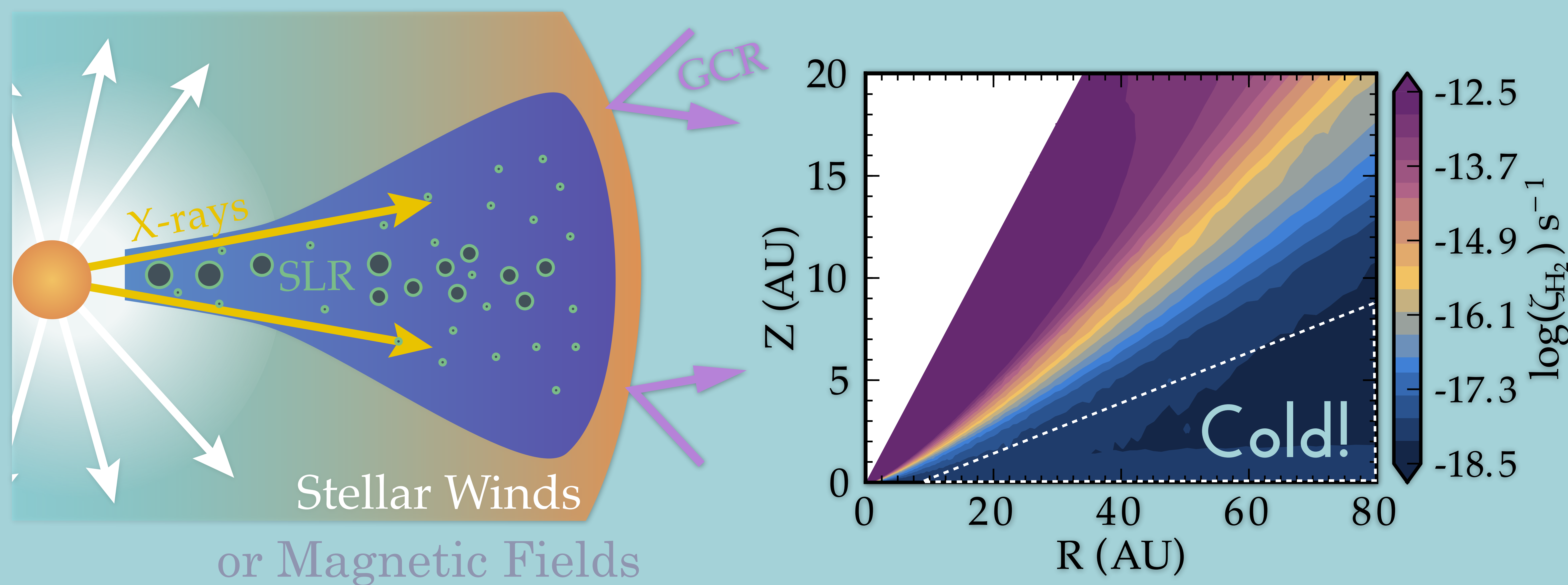
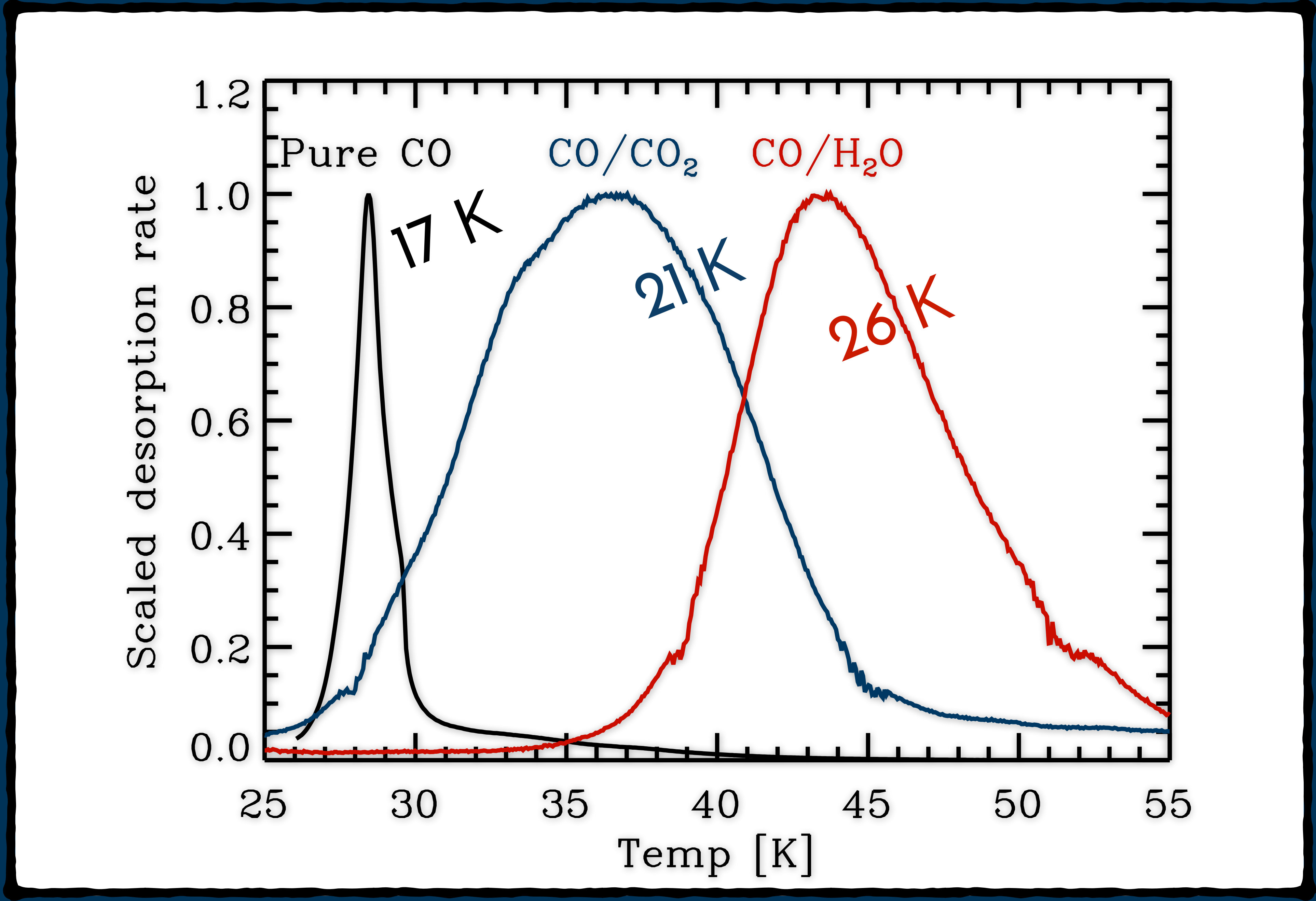



Cleeves et al. 2015 measured a significantly subinterstellar CR ionization rate in TW Hya (> 100x reduced).

High densities + low ionization rates → very low ion fraction in the cold gas where deuterium enrichment is otherwise facilitated..

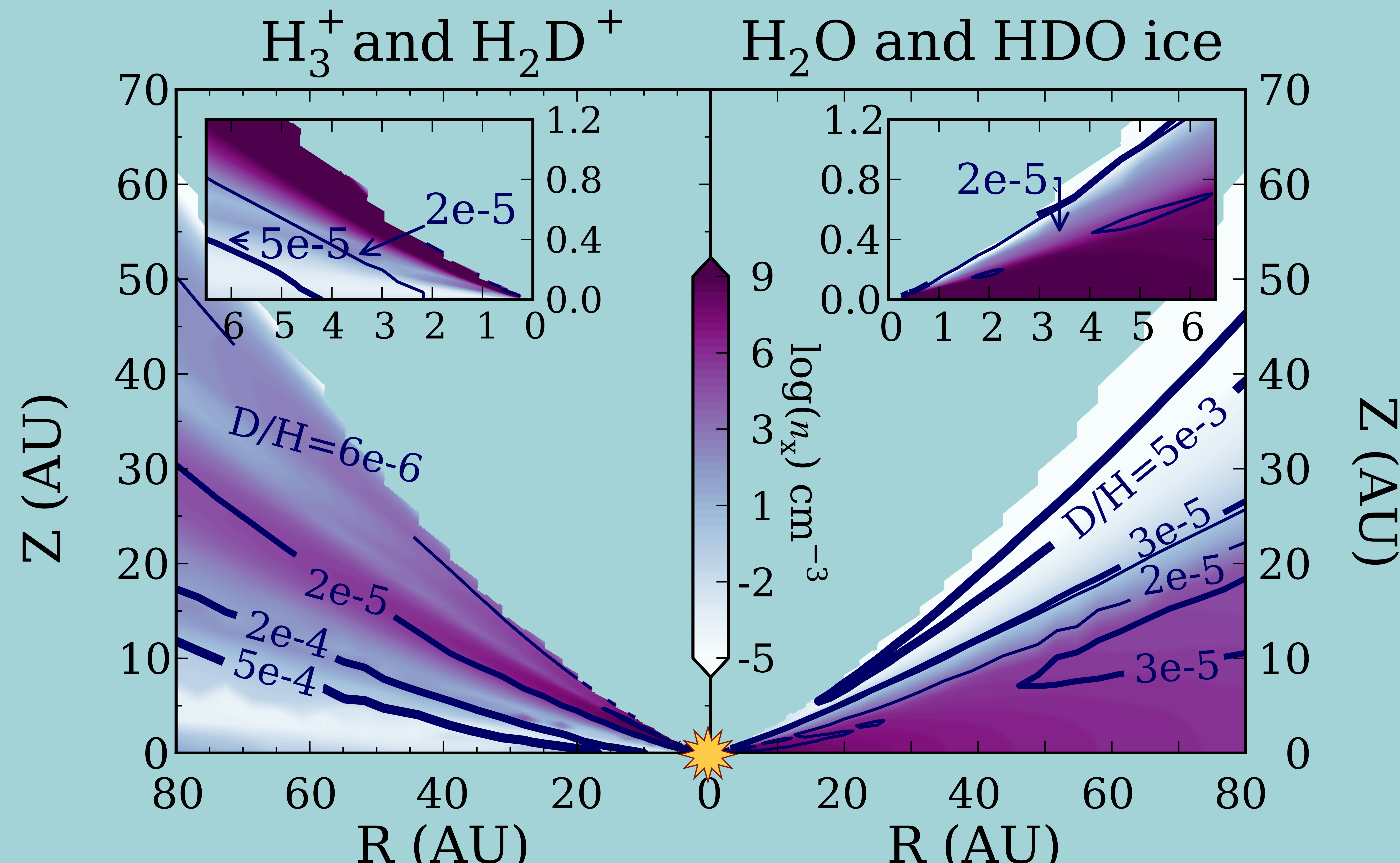
# Chemical Model

- Mini-deuterium chemical network designed to robustly predict HDO abundances.
  - 6268 reactions, 600 species.
- $H_2/HD/D_2$ self-shielding (Wolcott-Green+2011)
- Simple grain-surface chemistry (Hasegawa, Herbst, Leung 1992),
- Thermal o/p ratios assumed for $H_2$ and $H_2D^+$ (Lee & Bergin 2015)
- Warm fractionation reactions of Thi+2010.




And updated lab data on CO binding energies for oxygen-regulation.

# HDO/$H_2O$ Results (1 Myr)




Contour lines = D/H

Filled contours = total density $cm^{-3}$

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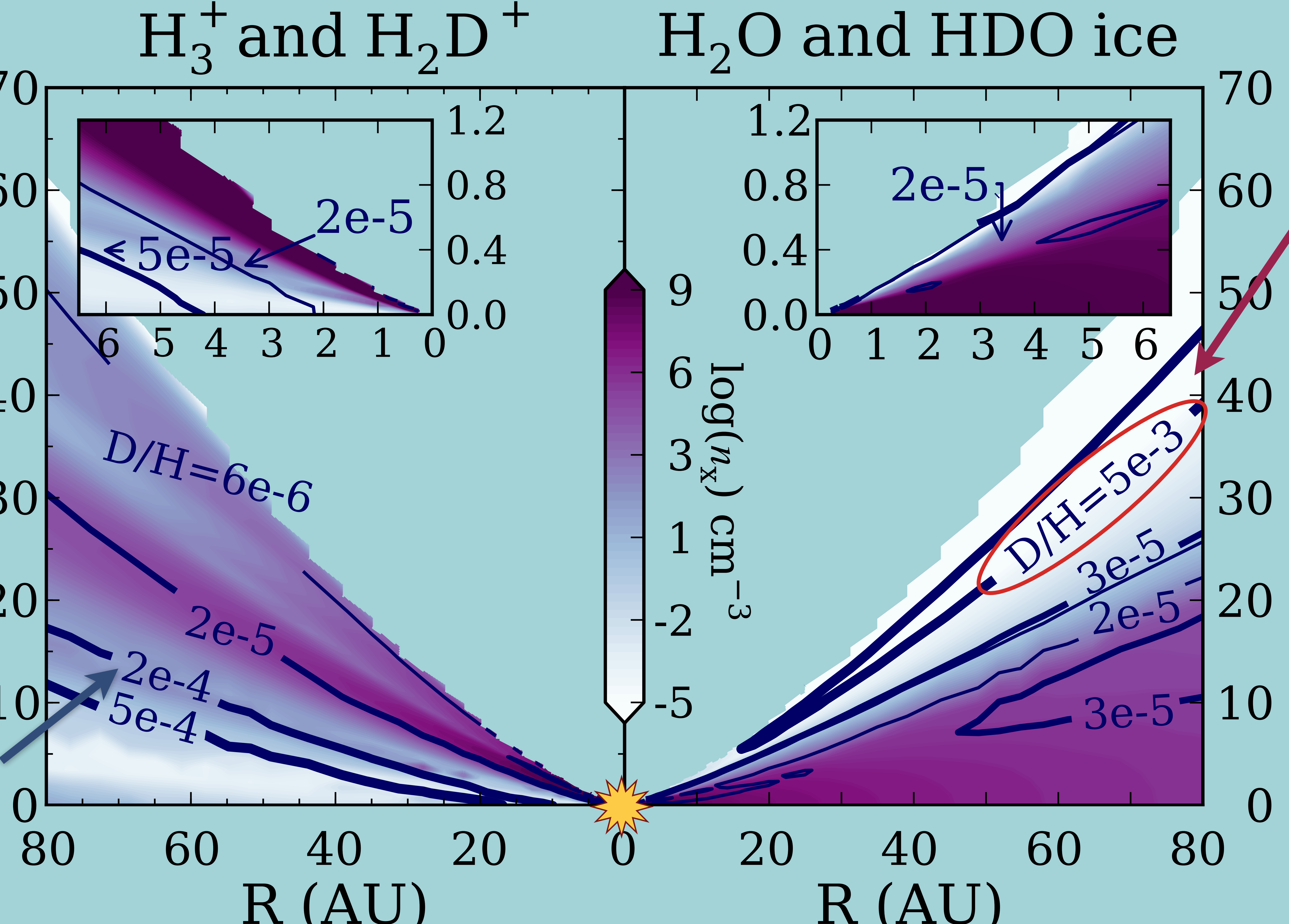
# HDO/$H_2O$ Results (1 Myr)




Differential self-shielding of HD vs H2 leads to high HDO/ $H_2O$, but in a very tenuous upper layer.

The ions have the highest D/H in the midplane but the lowest volume density.

Contour lines = D/H

Filled contours = total density cm$^{-3}$

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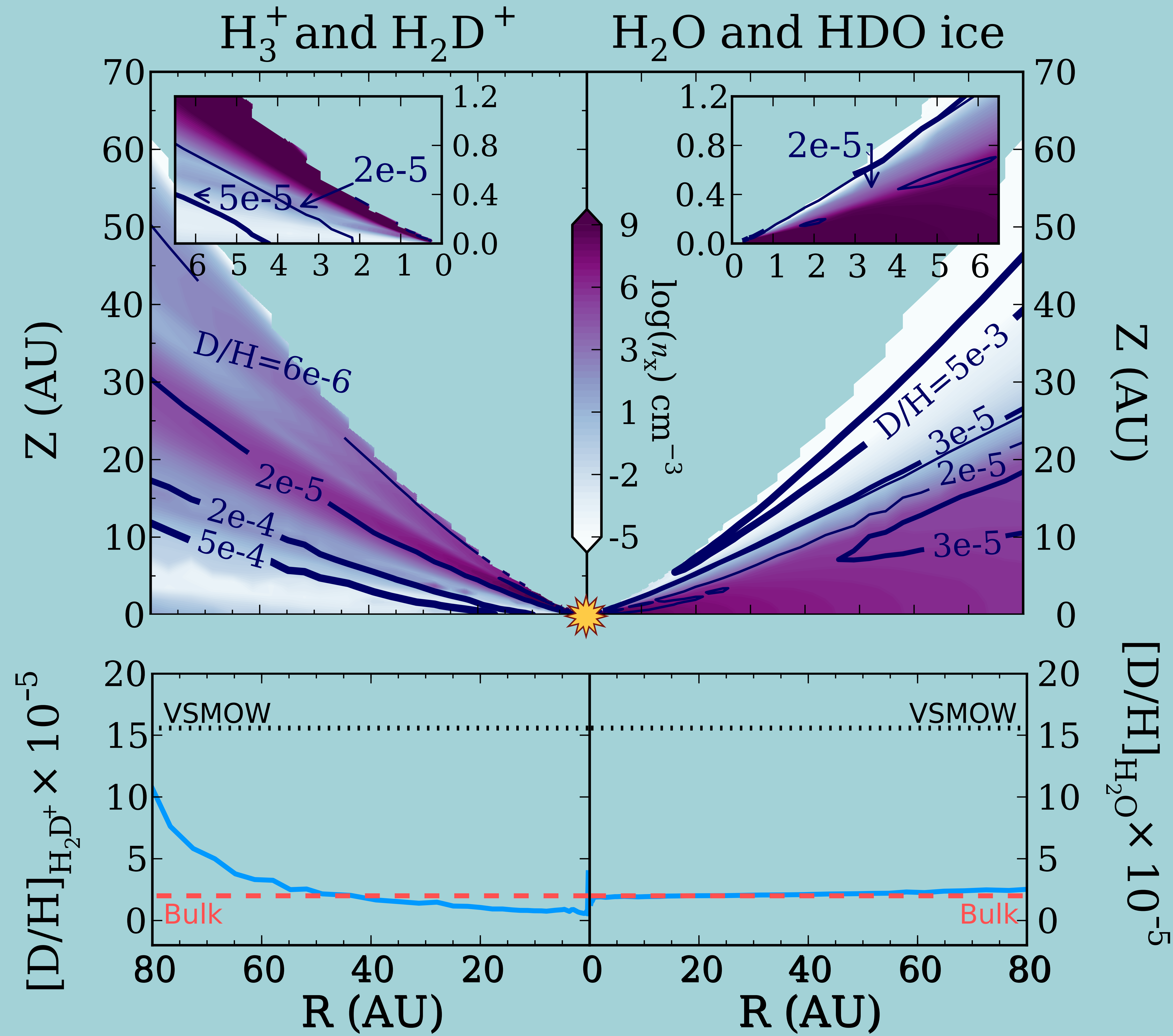
# HDO/$H_2O$ Results (1 Myr)



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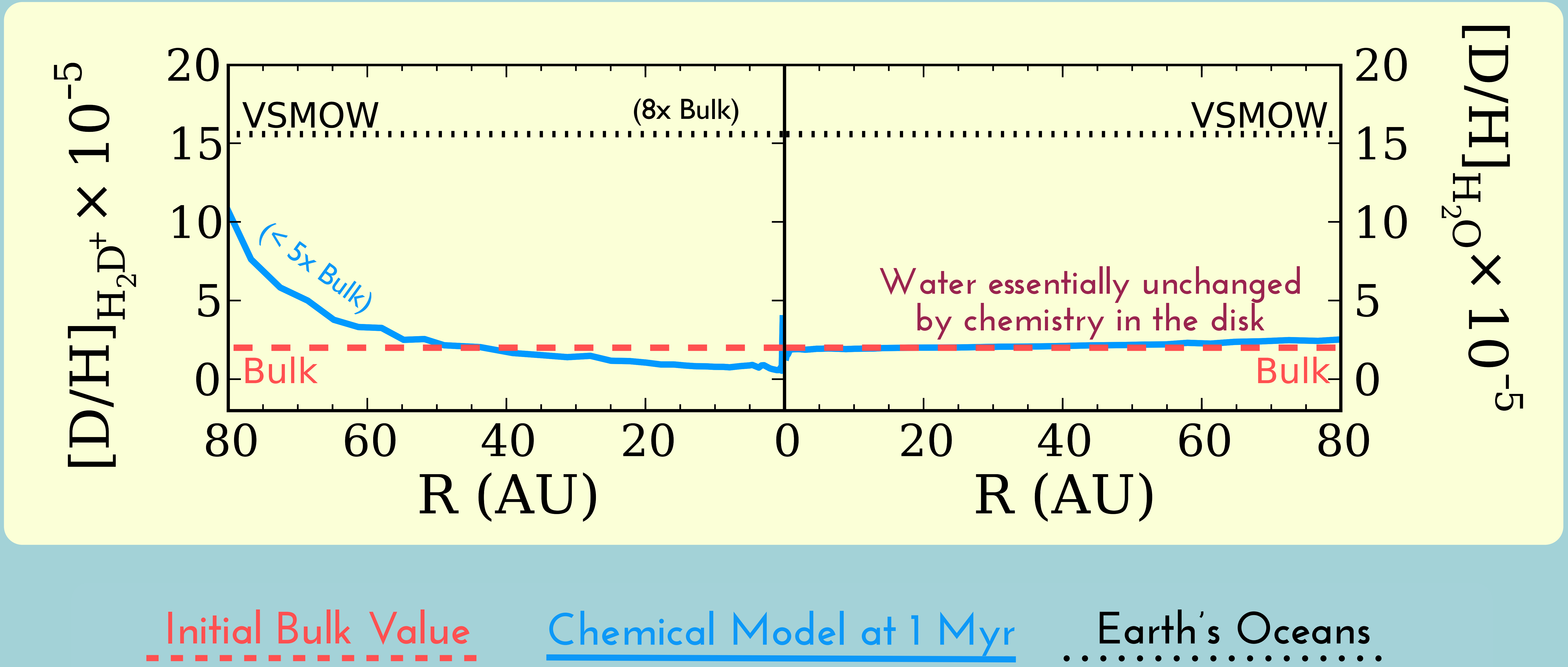
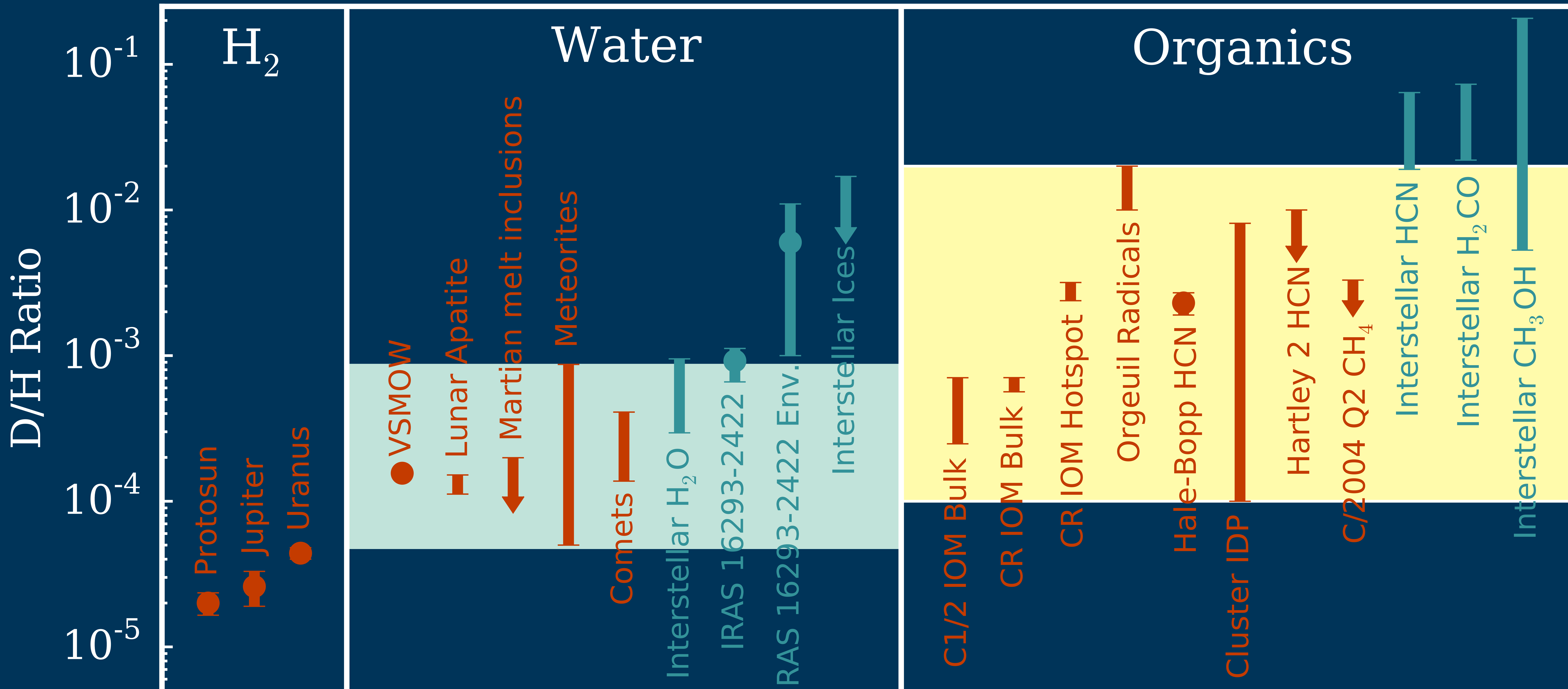


# Disk-Sourced Deuterium: Results

- ➡ Chemistry in a laminar disk is not a viable source origin for HDO, $H_2O$ or D/H($H_2O$) in the Solar System.
- ➡ These conditions require ISM heritage such that interstellar ices would be incorporated into comets, meteorites, and Earth's oceans (30-40%).
- ➡ But what else came along for the ride?

Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2014, Sci, 345, 1590.

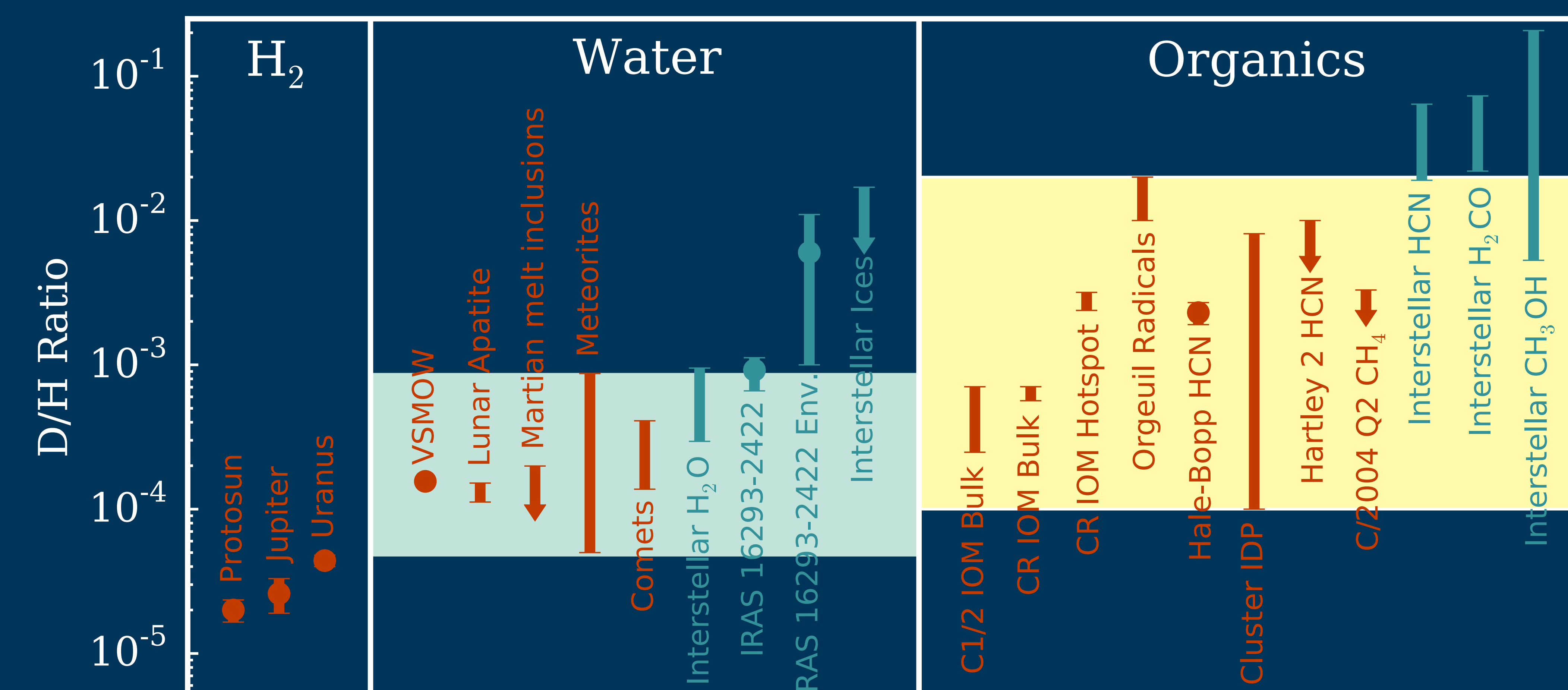
# D/H in Water vs. Organics




Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

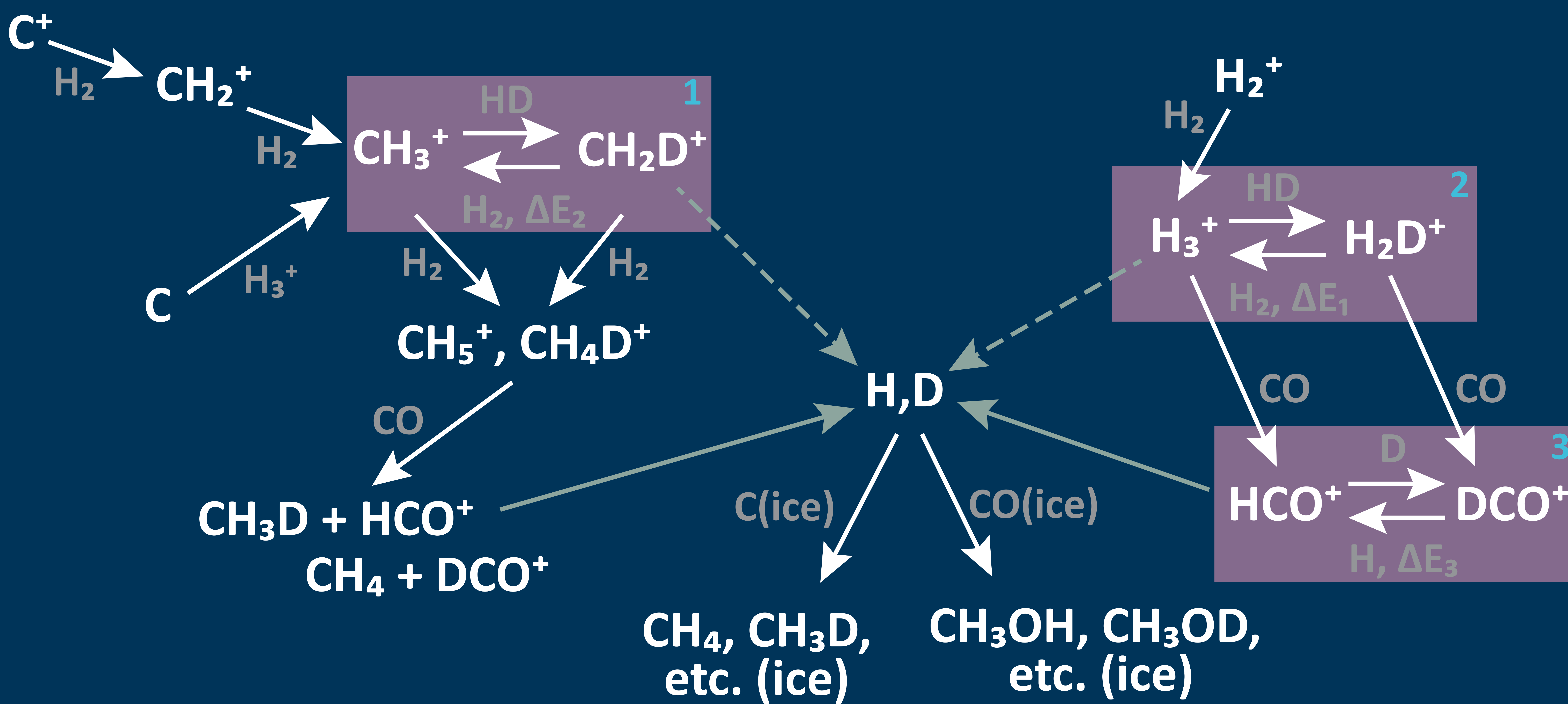
# D/H in Water vs. Organics

- Globally higher organic D/H than water. Perhaps due to:
  - $CH_3^+ + HD \rightleftarrows CH_2D^+ + H_2 + \Delta E$
  - Operates in the forward direction even at 80-100 K due to higher $\Delta E \sim 483\text{-}660$ K (Roueff+2013).
- Larger range in organic D/H = many reaction pathways?




Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

# Organic Fractionation Pathways




1) Roueff+2013, 2) Hugo+2009, 3) Adams&Smith 1985

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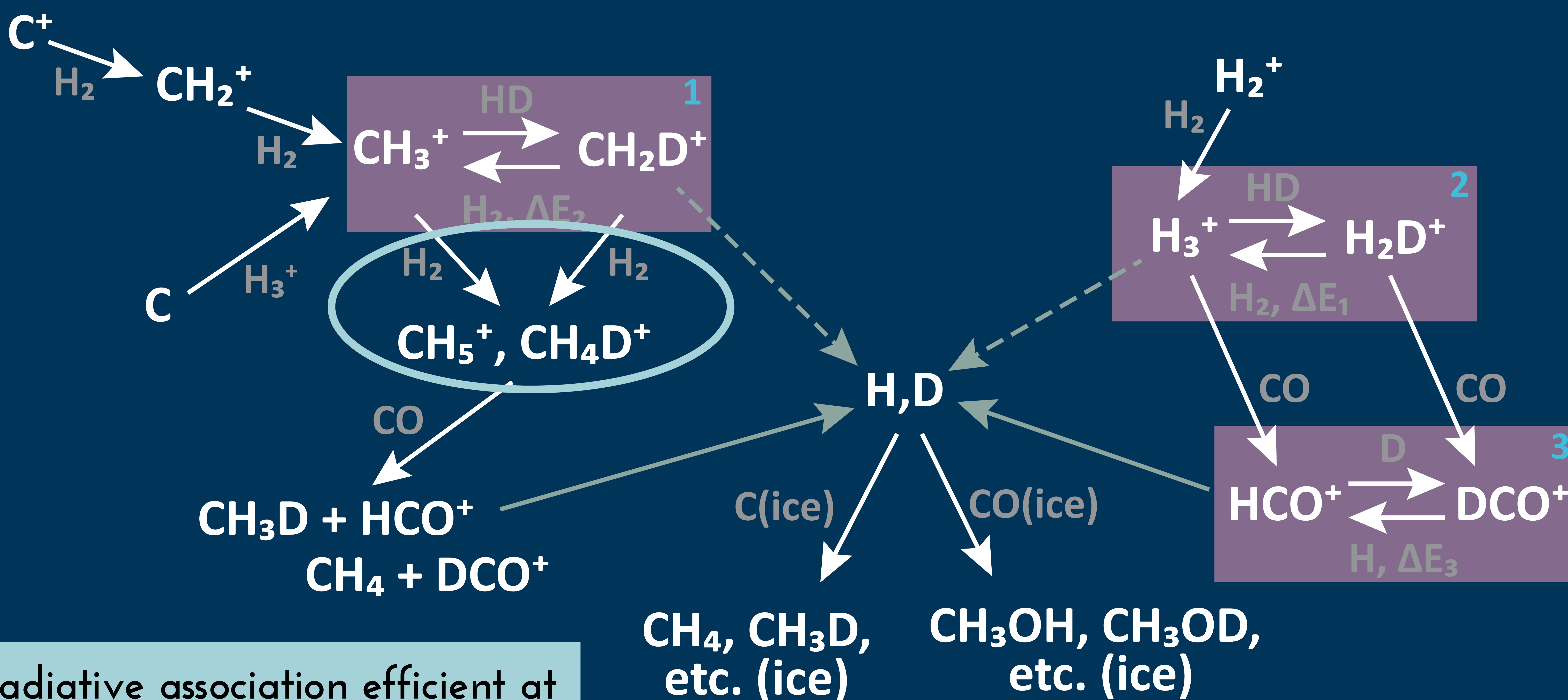
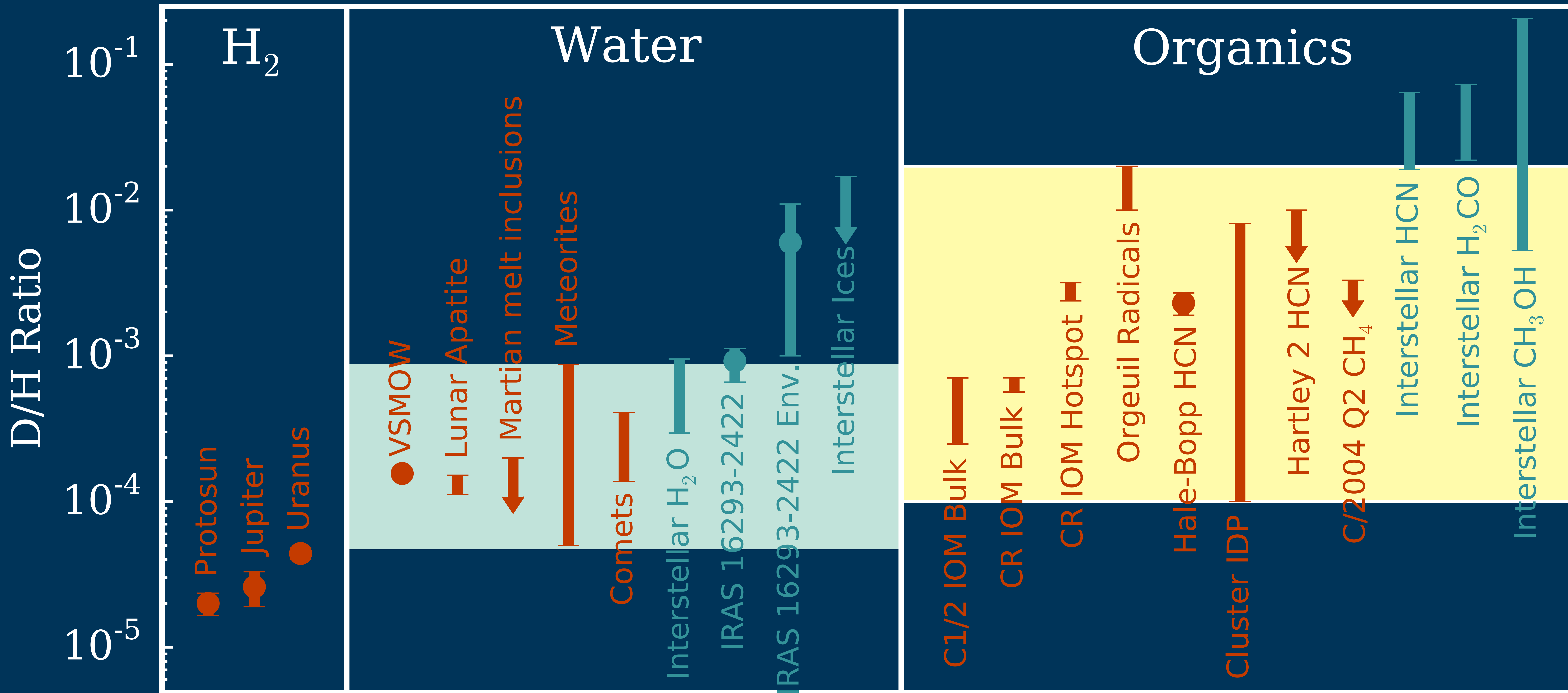



Radiative association efficient at disk-like densities, $10^9$-$10^{12}$ $cm^{-3}$

1) Roueff+2013, 2) Hugo+2009, 3) Adams&Smith 1985

# D/H in Water vs. Organics




Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

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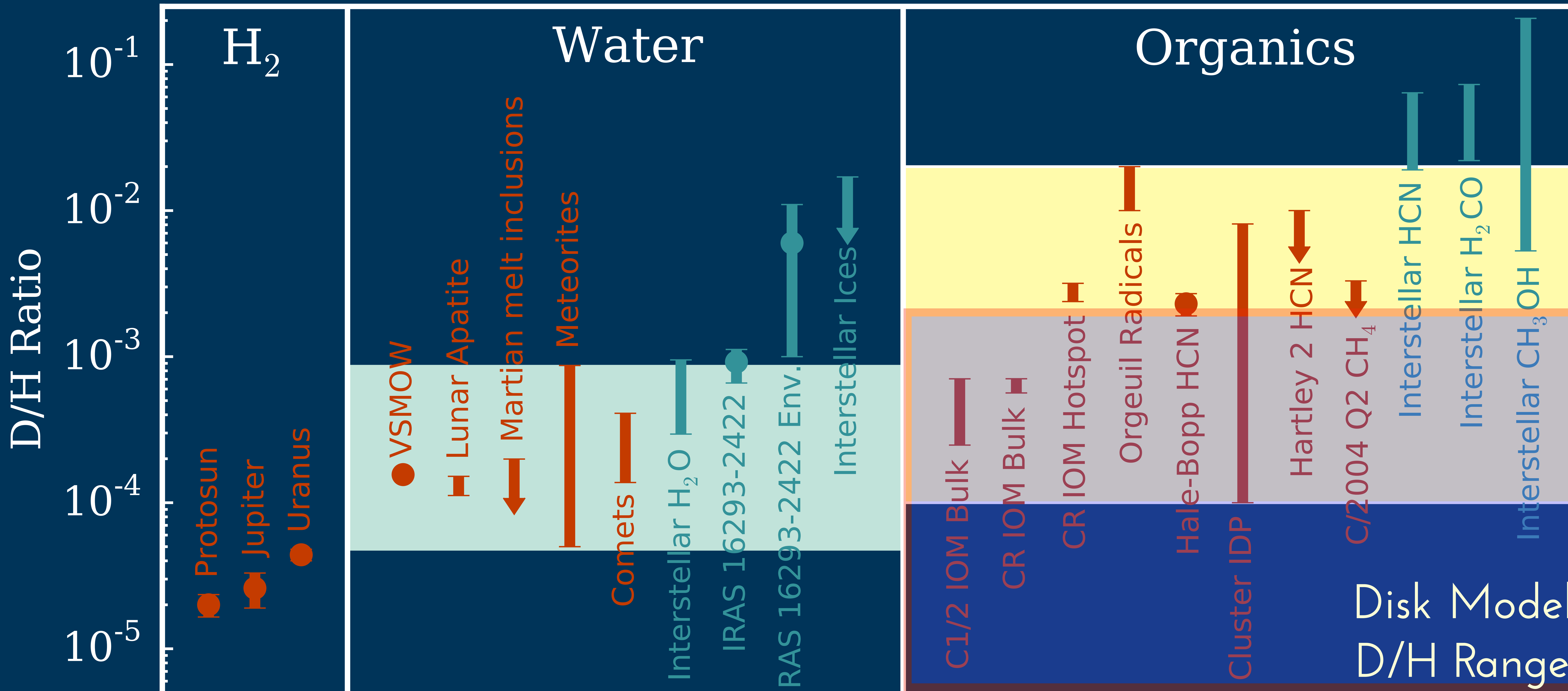
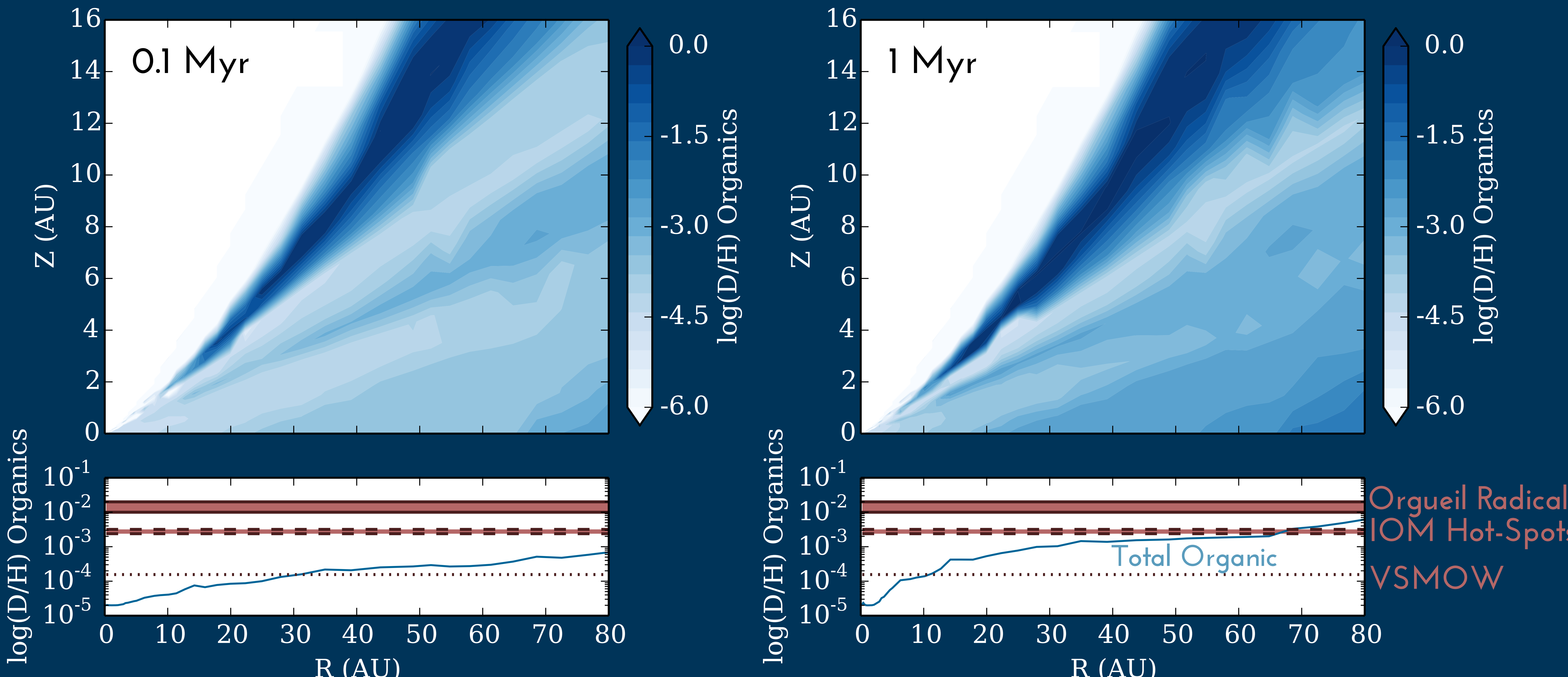



Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

# Global Organic D/H

Now with 15,000 reactions, 1000 species




Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

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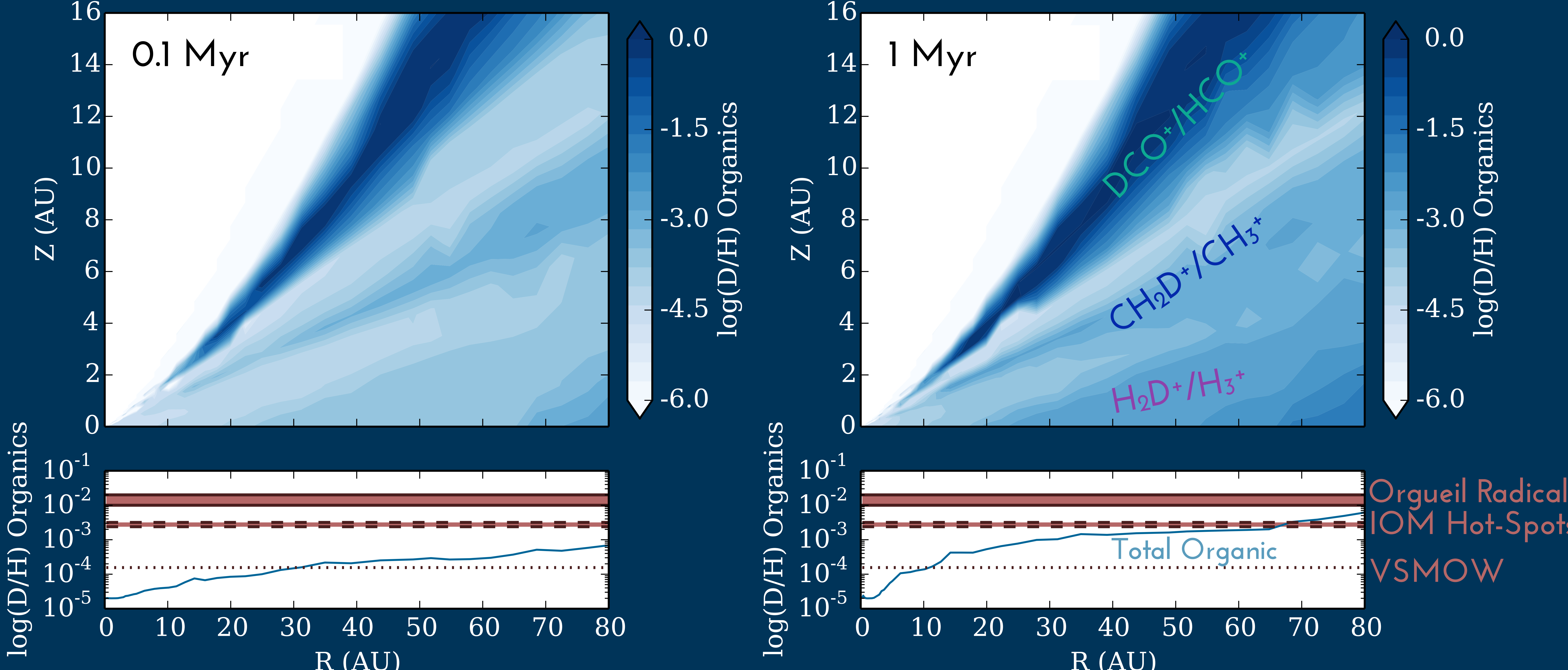


Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

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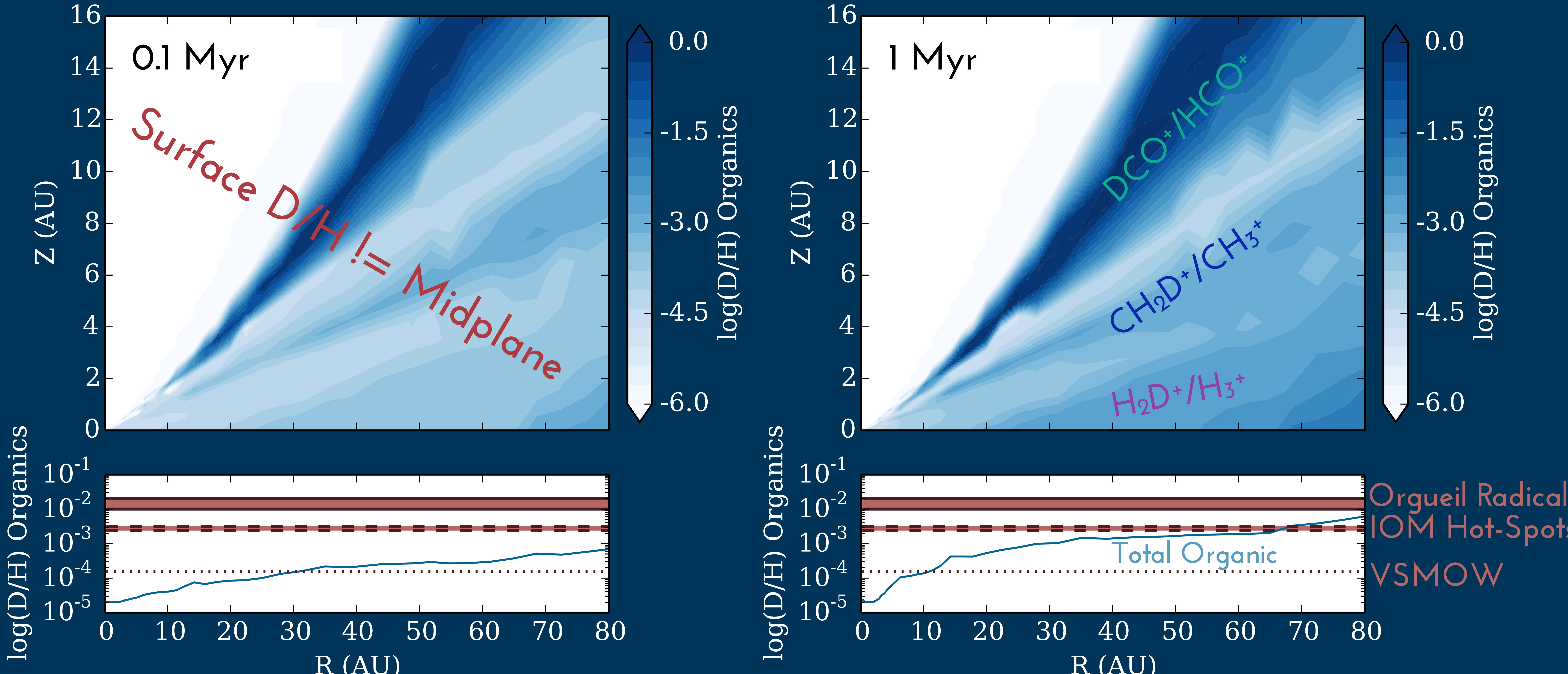
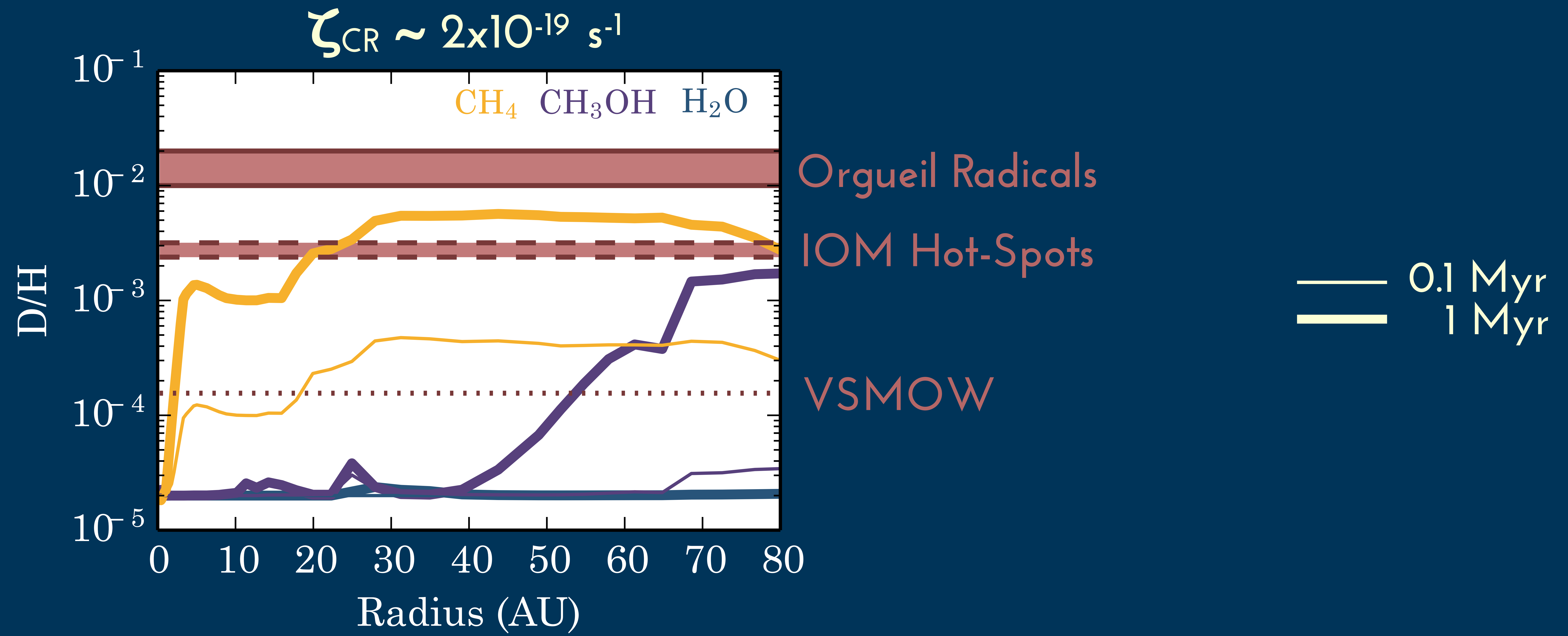



Cleeves, Bergin, Alexander, Du, Graninger, Öberg, Harries, 2016

# Midplane Organic Deuterium Fractionation



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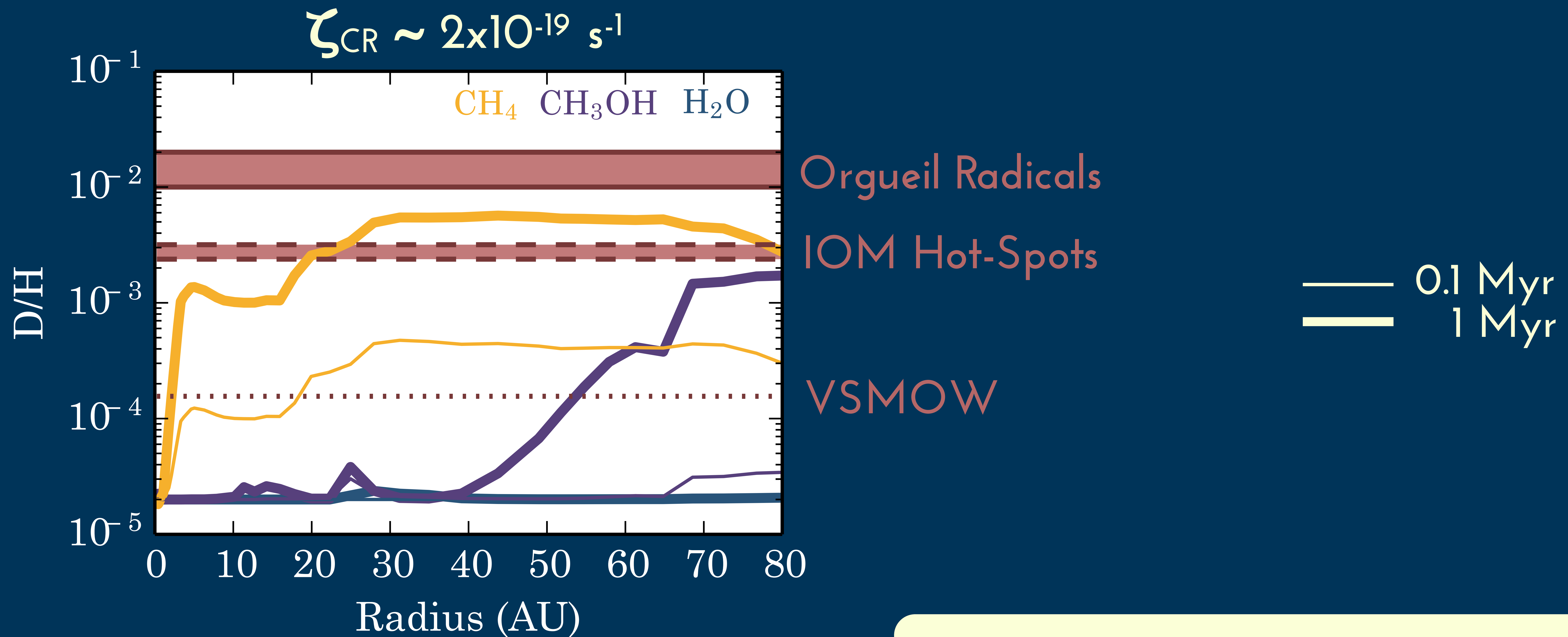
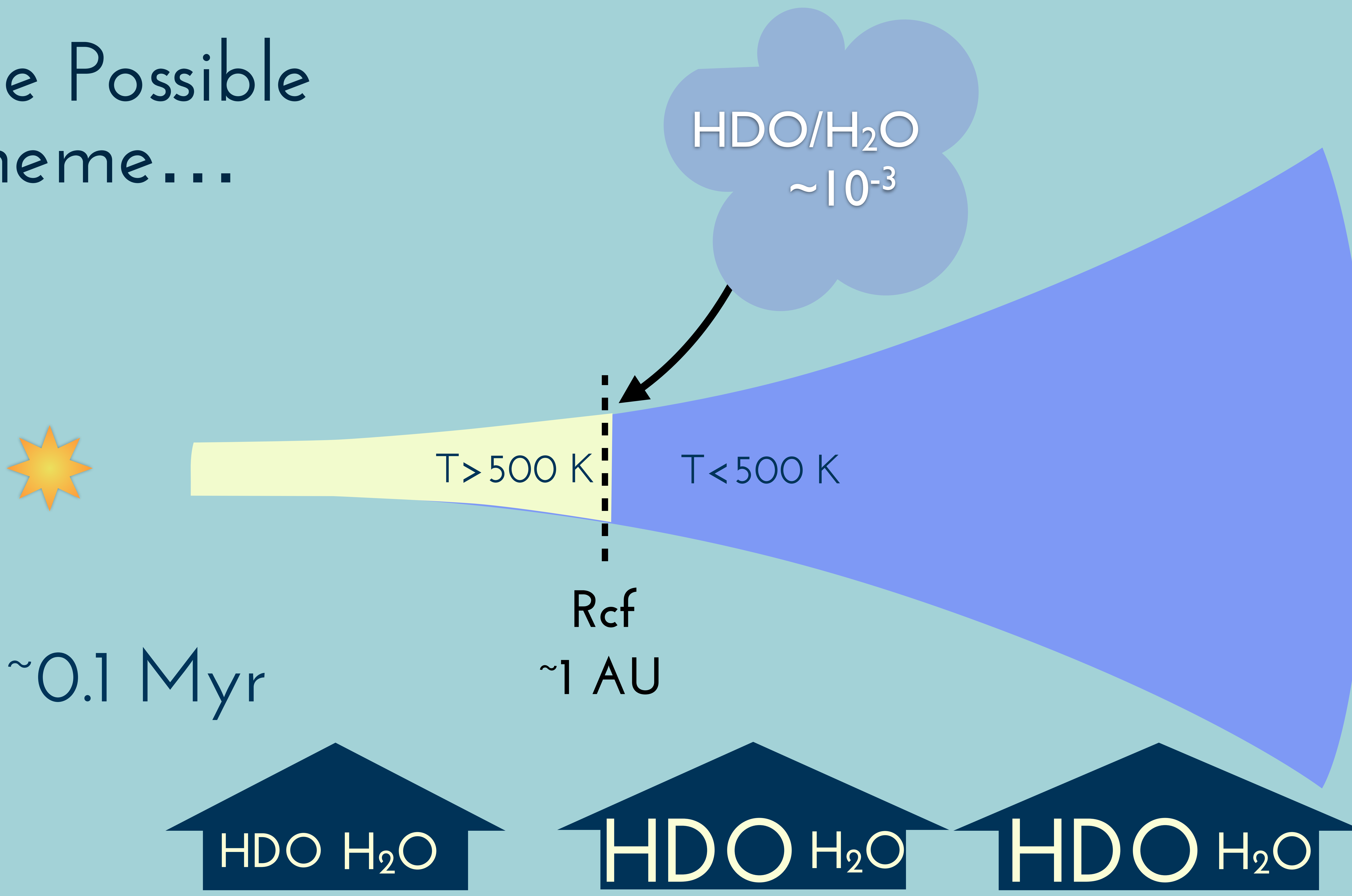



Interesting predictions for cometary D/H in $CH_3OH$?

# 6) So what's happening?

# One Possible Scheme…



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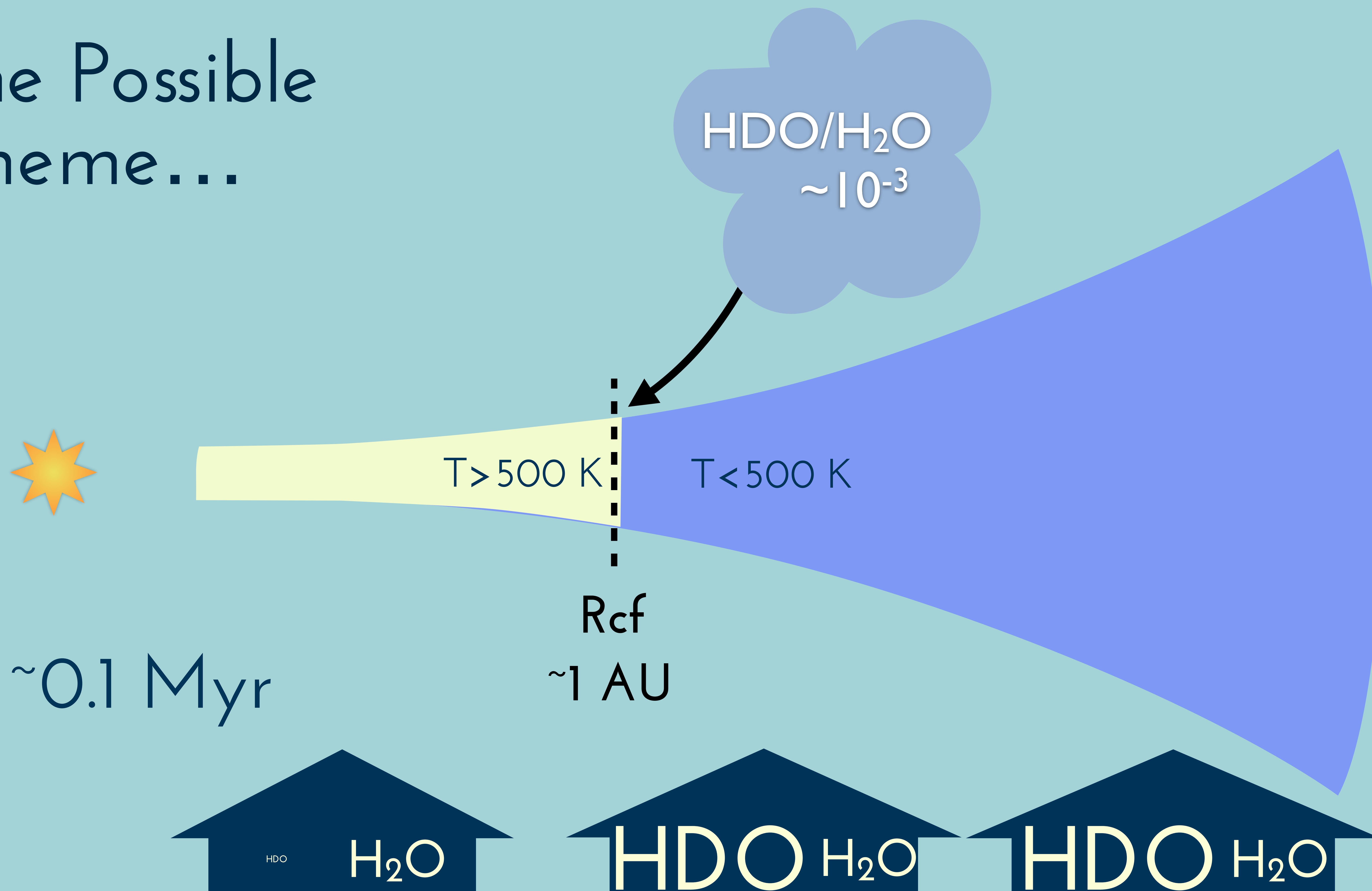


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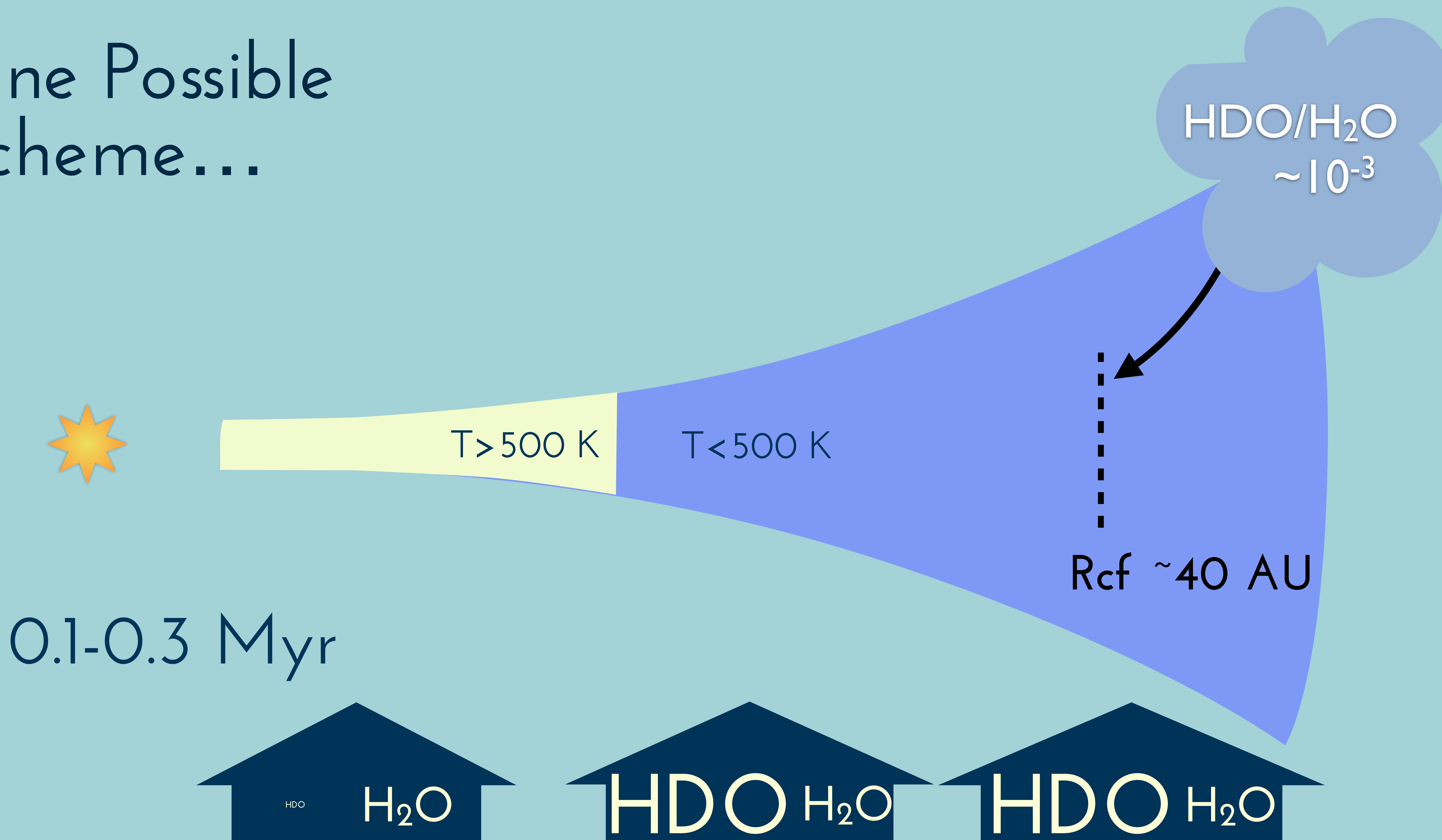


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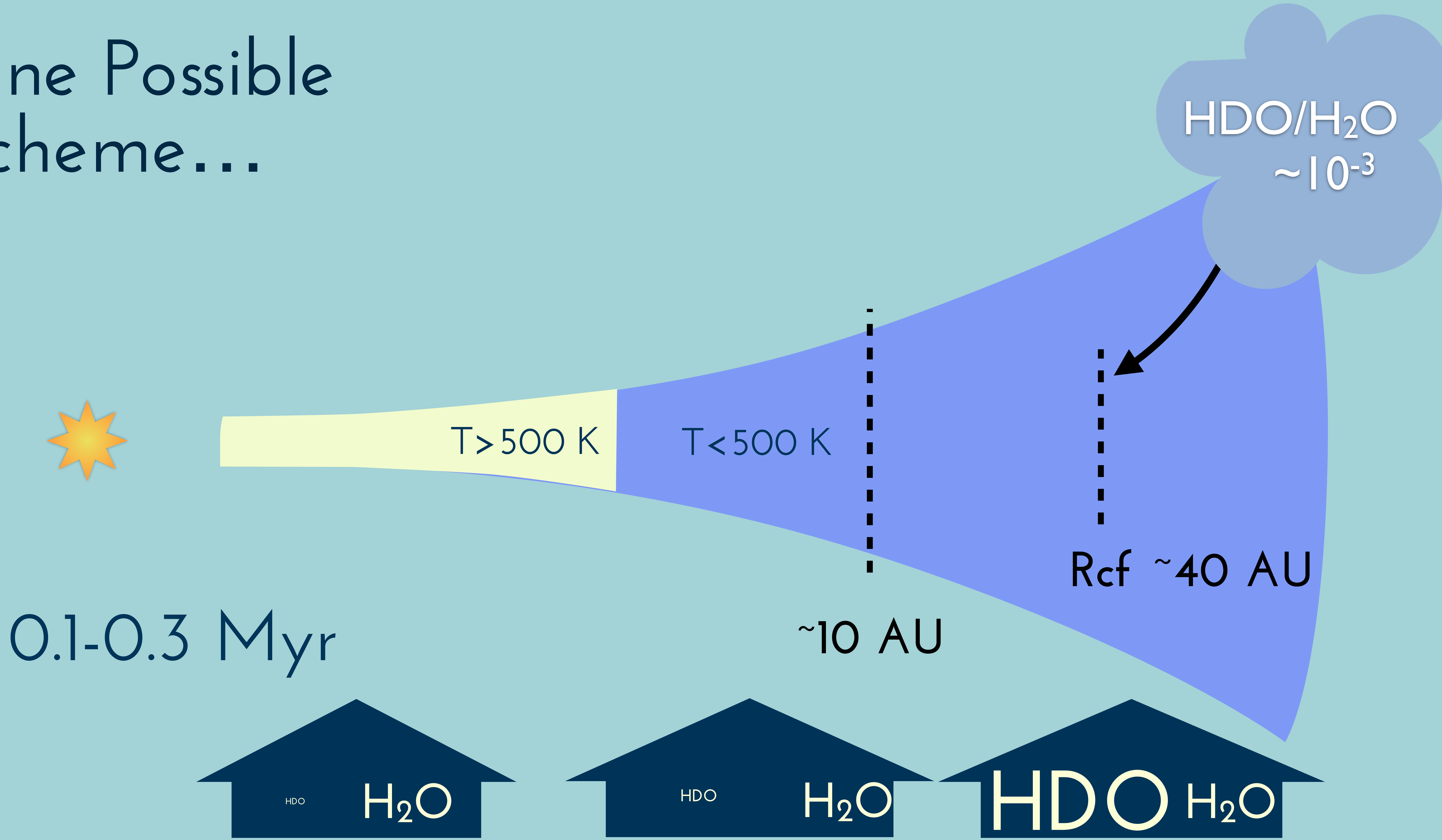

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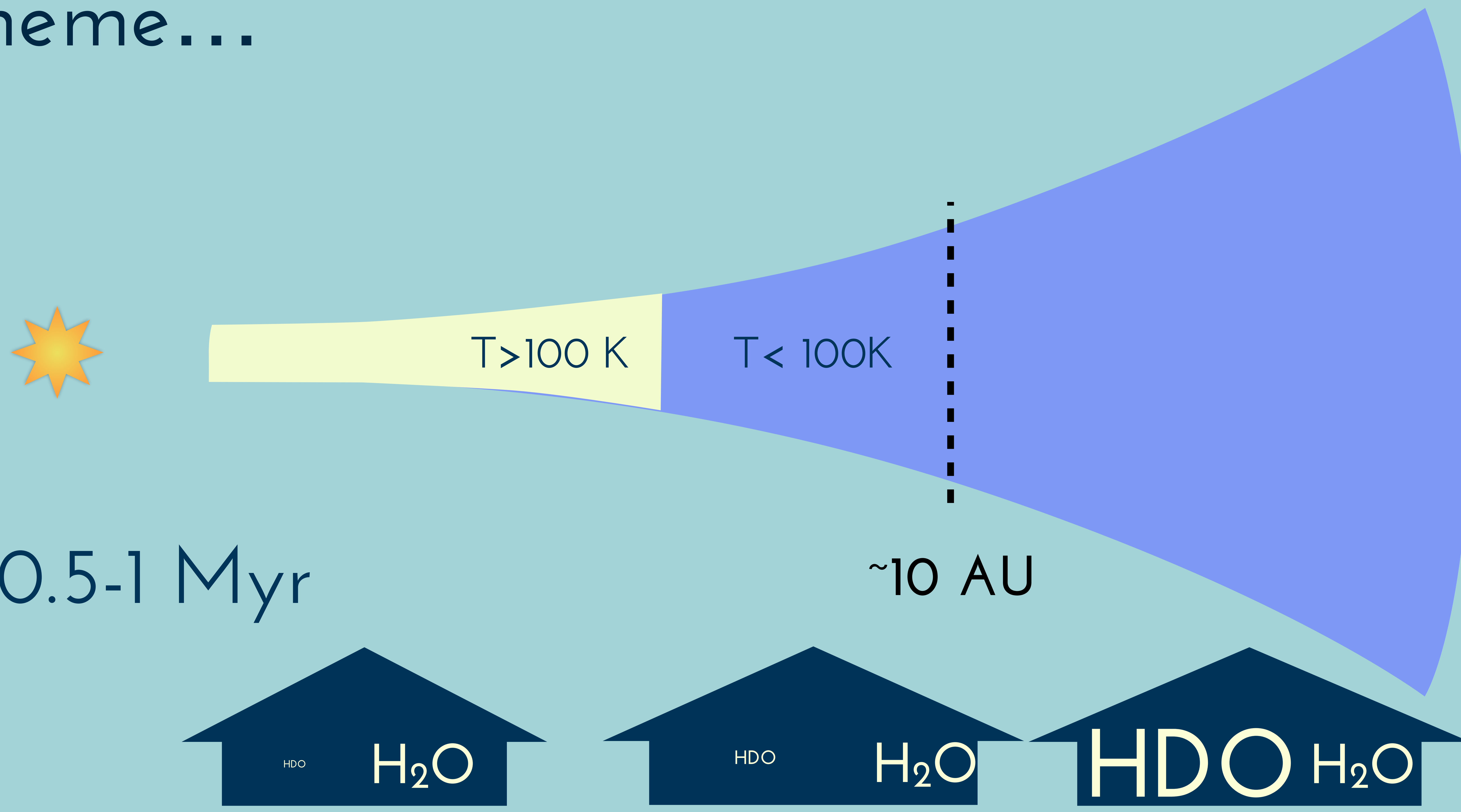


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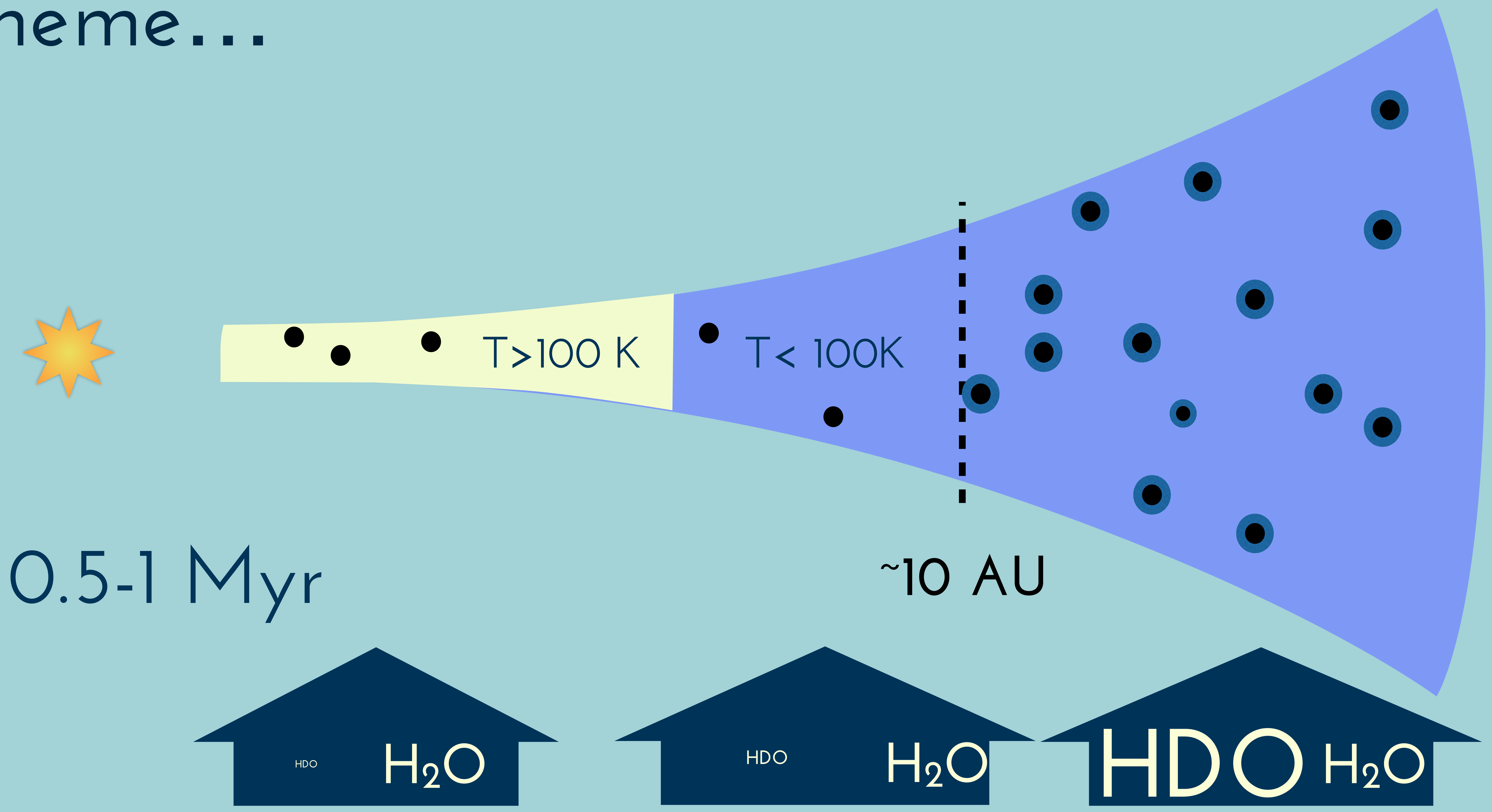


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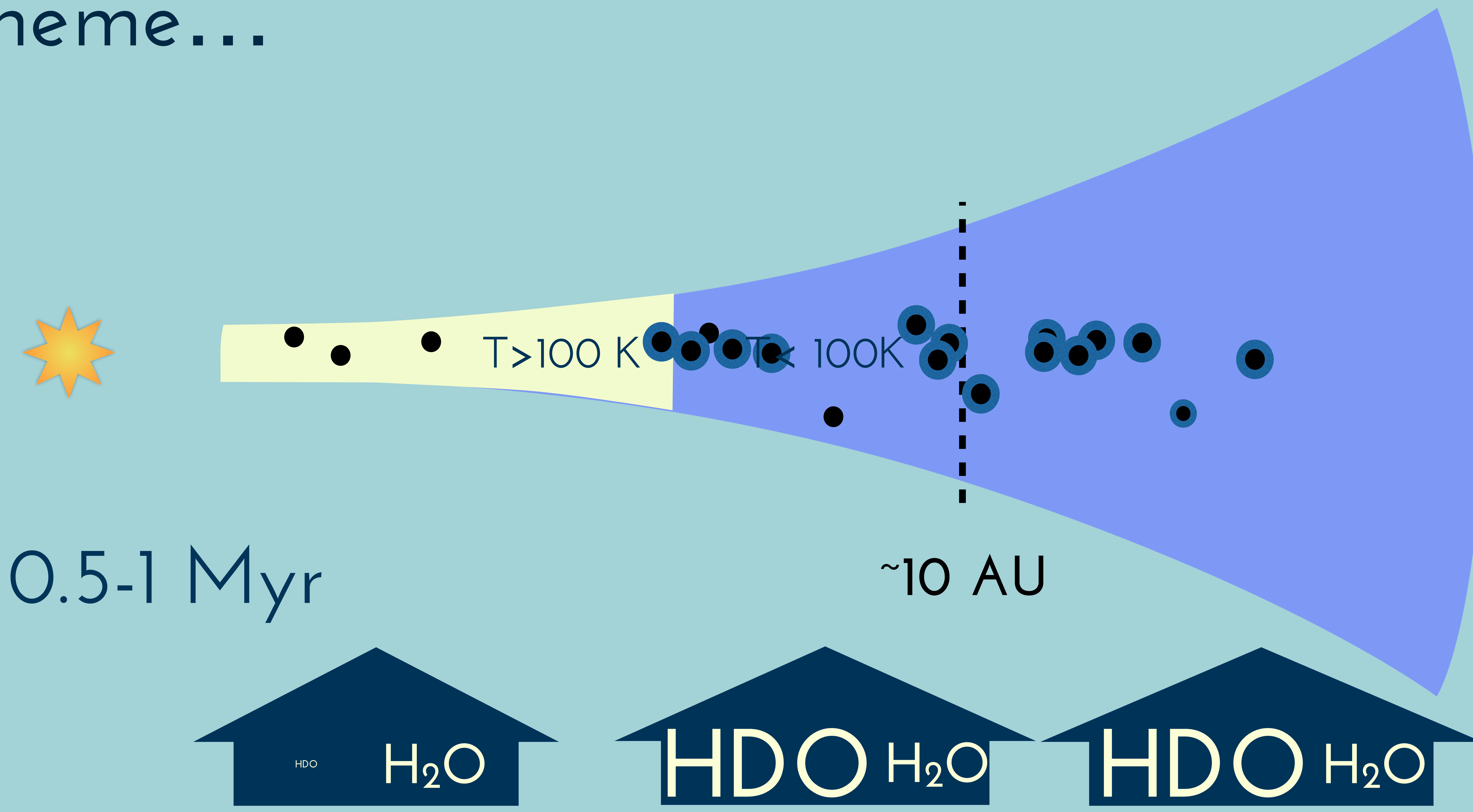


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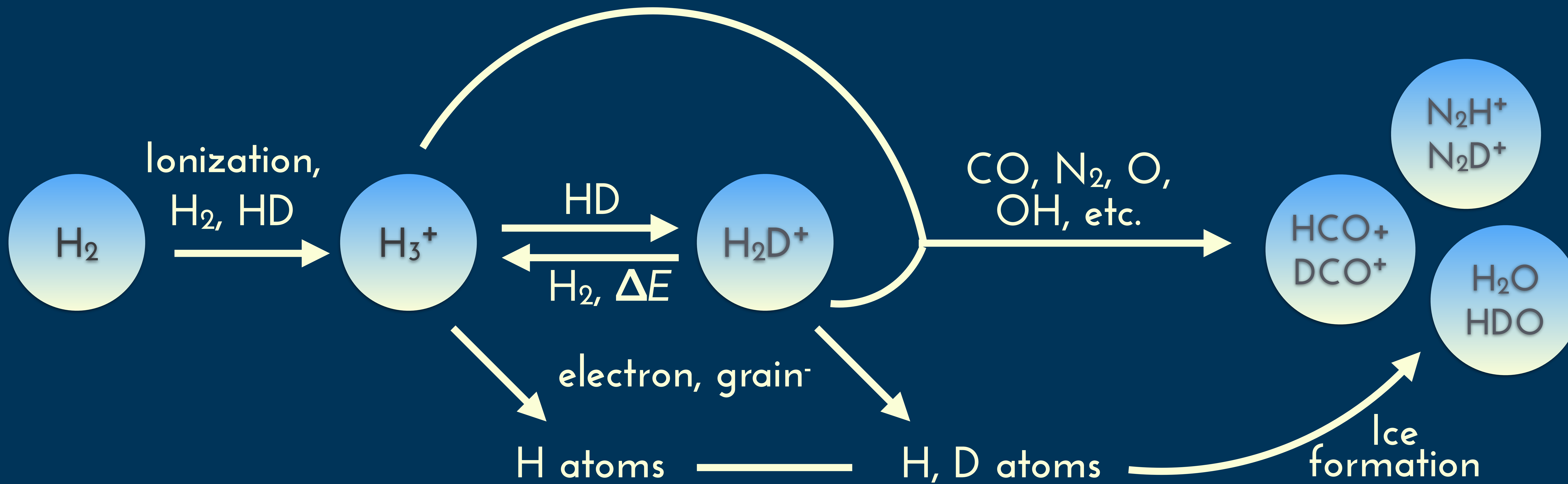
# Ingredients for Disk Deuterium Fractation



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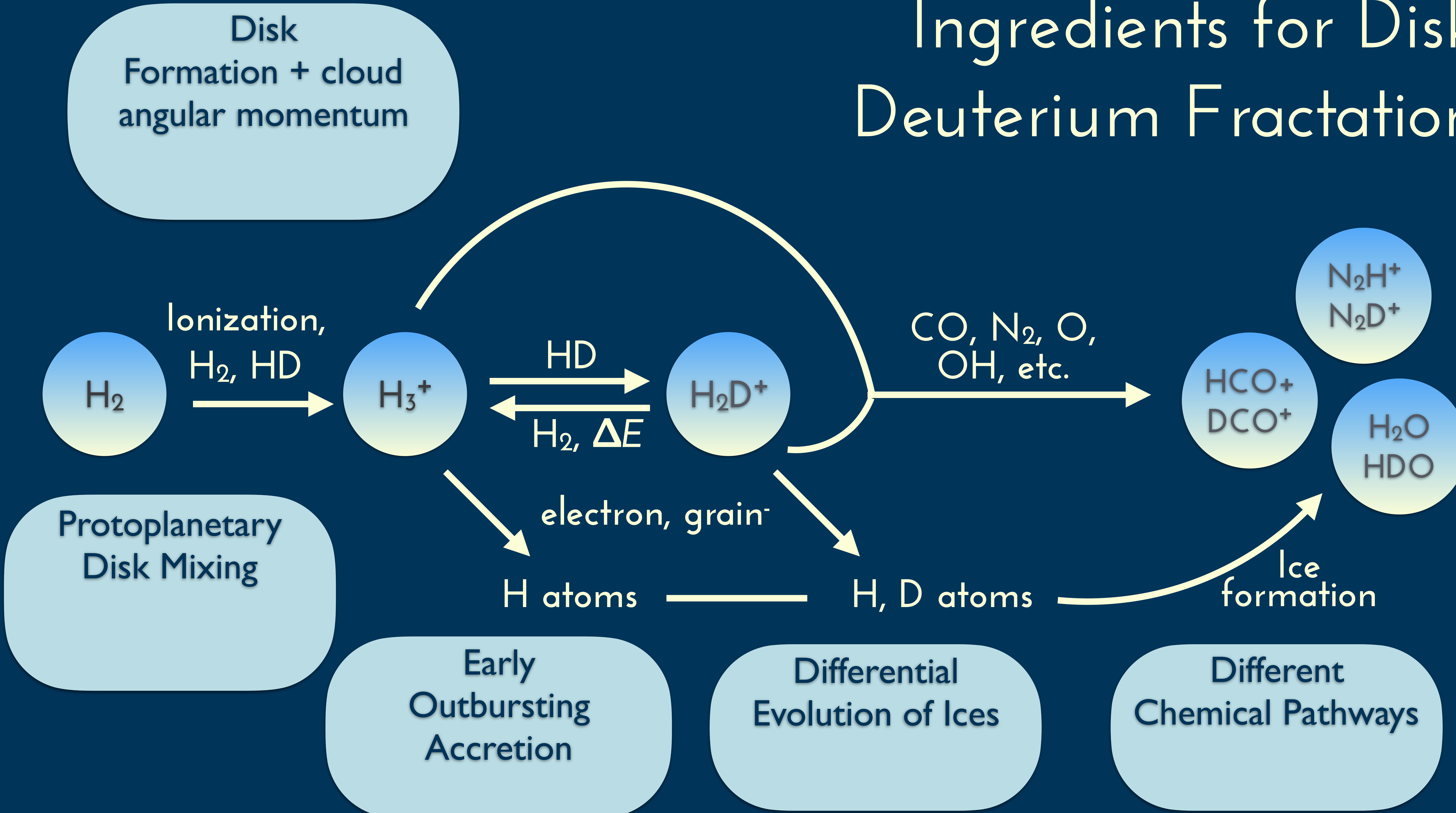


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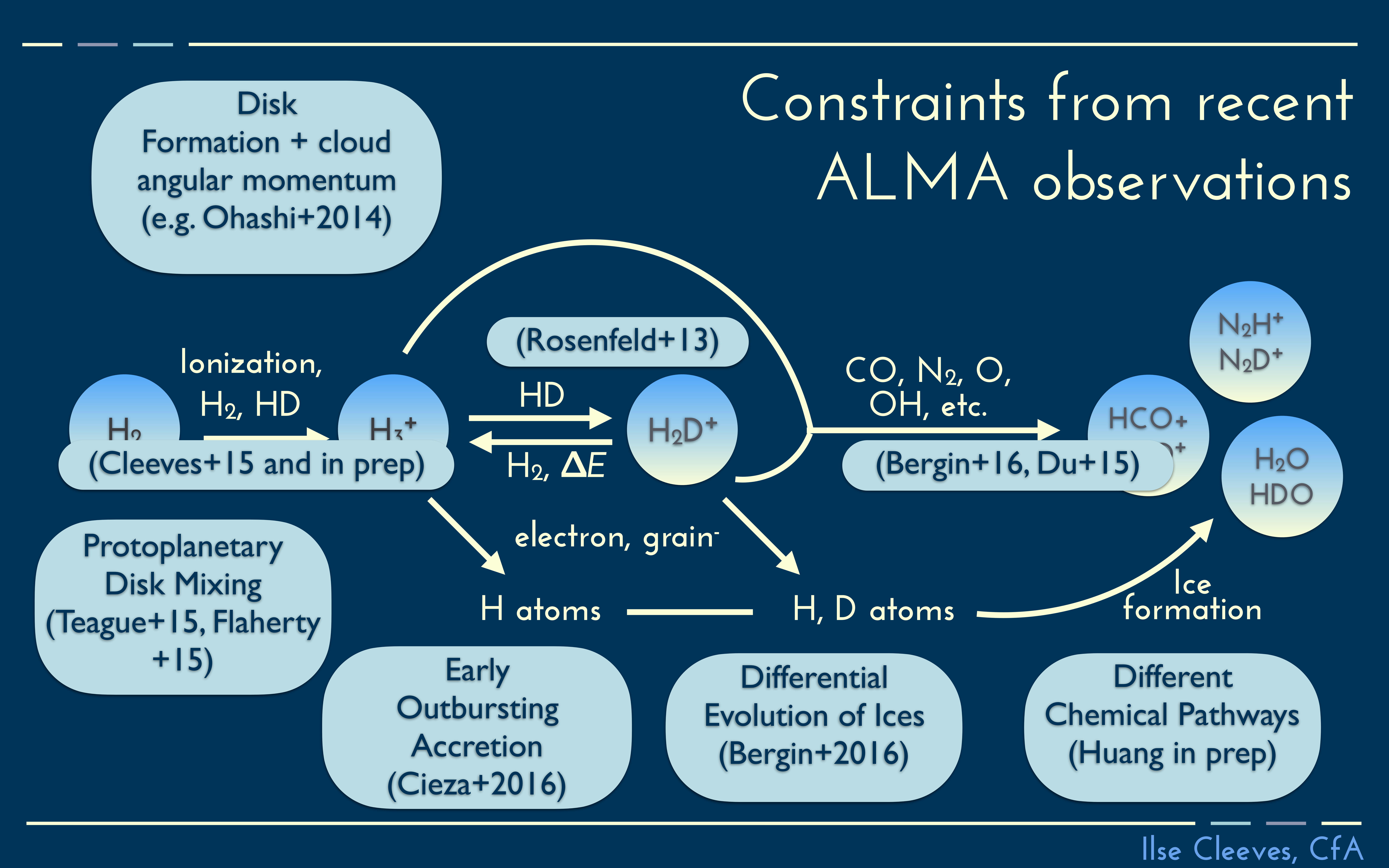

Constraints from recent ALMA observations
Disk Formation + cloud angular momentum (e.g. Ohashi+2014)
Ionization, $H_2$, HD
$H_2$
$H_3^+$
(Cleeves+15 and in prep)
(Rosenfeld+13)
HD
$H_2$, $\Delta E$
$H_2D^+$
CO, $N_2$, O, OH, etc.
$HCO^+$
(Bergin+16, Du+15)
$N_2H^+$
$N_2D^+$
$H_2O$
HDO
electron, grain$^-$
H atoms
H, D atoms
Ice formation
Protoplanetary Disk Mixing (Teague+15, Flaherty +15)
Early Outbursting Accretion (Cieza+2016)
Differential Evolution of Ices (Bergin+2016)
Different Chemical Pathways (Huang in prep)
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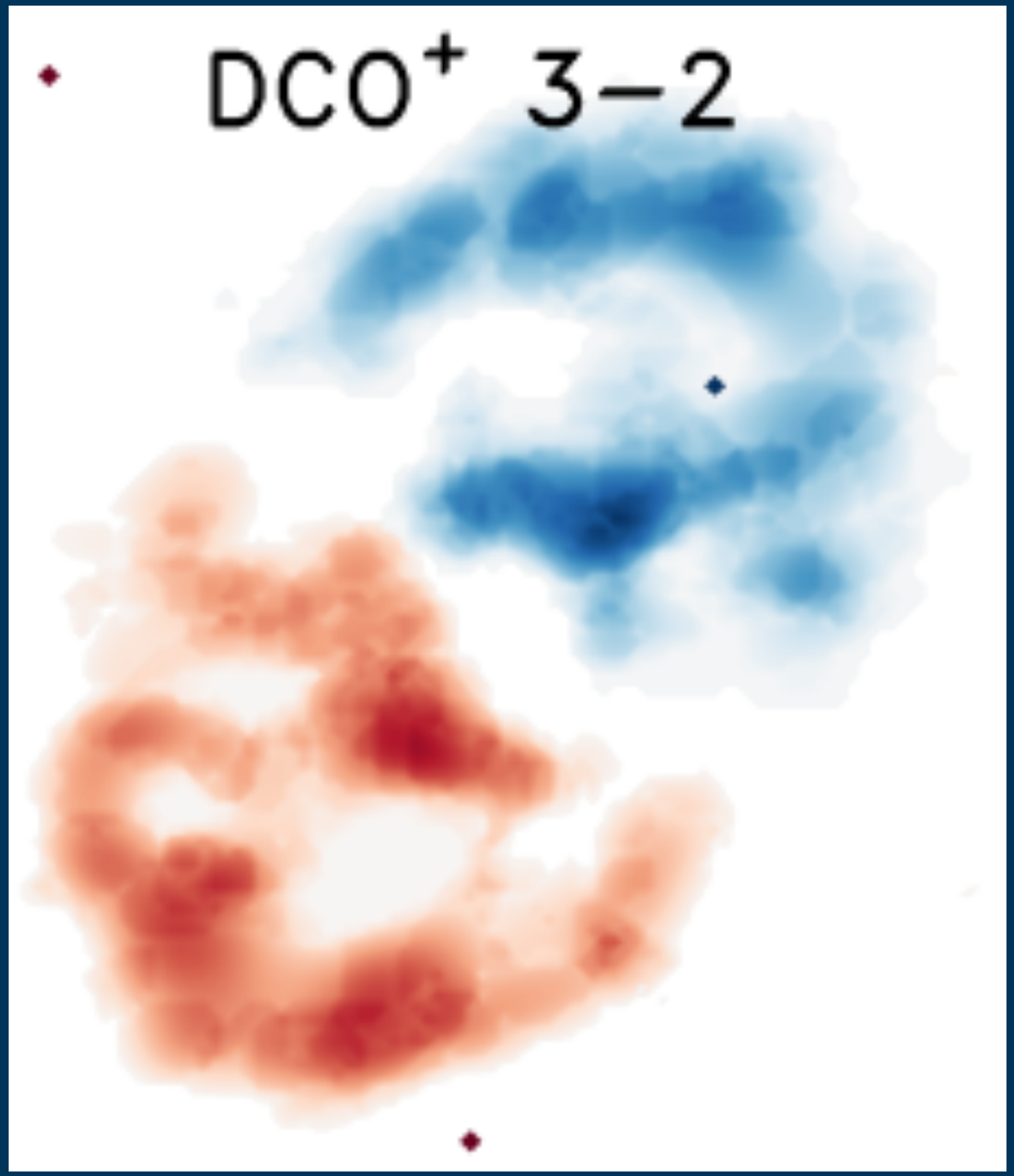
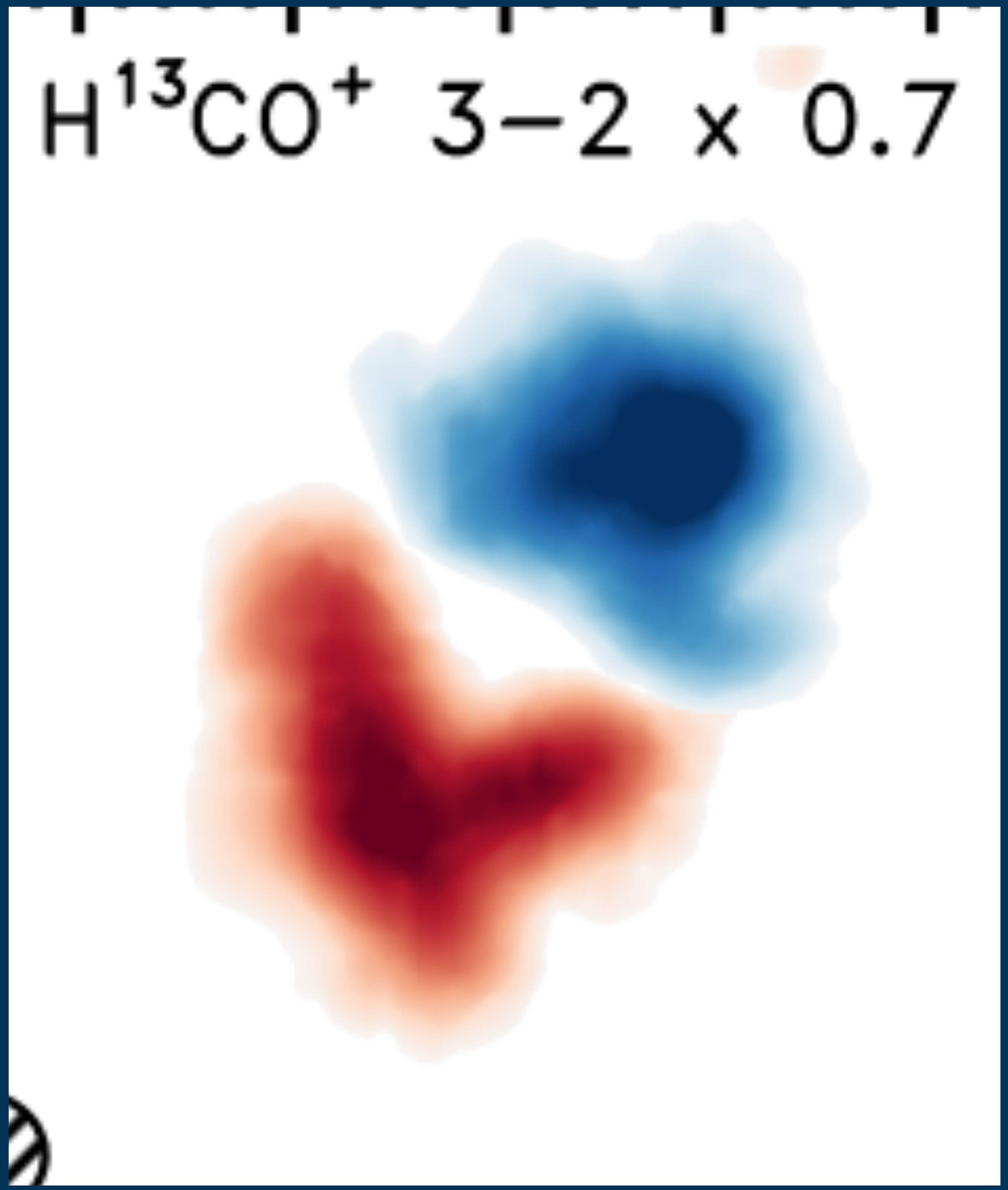
# But also many more puzzles!




Öberg et al 2015

# Summary

- The ionization, thermal, and chemical structure of protoplanetary disks impacts the deuterium chemistry, especially in the observable layers.
- The assembly of the disk from the cloud can change the initial D/H affected by to cloud angular momentum and early accretion outbursts.
- Mixing would be important for D/H (raising and lowering), but not clear if mixing is *active* in protoplanetary disks.
- Transport of solids is observed and likely efficient carrier of volatile ices.
- Organics more readily fractionated even in relatively warm gas due to high endothermicity of $CH_2D^+ + H_2$ compared to $H_2D^+ + H_2$.

Thank you!