

# The Chemistry of Protoplanetary Disks

Karin Öberg (Harvard University)

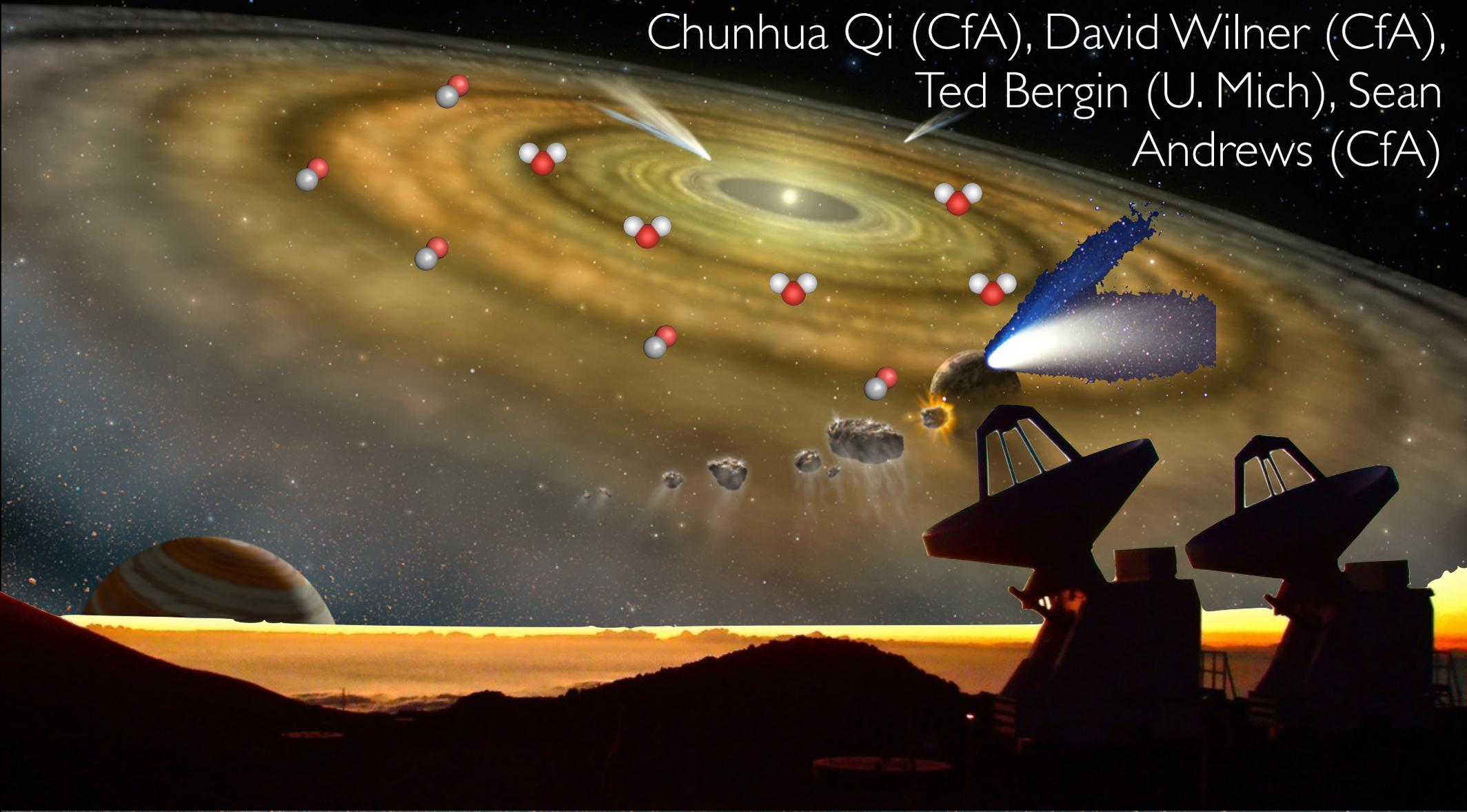
Chunhua Qi (CfA), David Wilner (CfA),  
Ted Bergin (U. Mich), Sean  
Andrews (CfA)



# The Chemistry of Protoplanetary Disks

Karin Öberg (Harvard University)

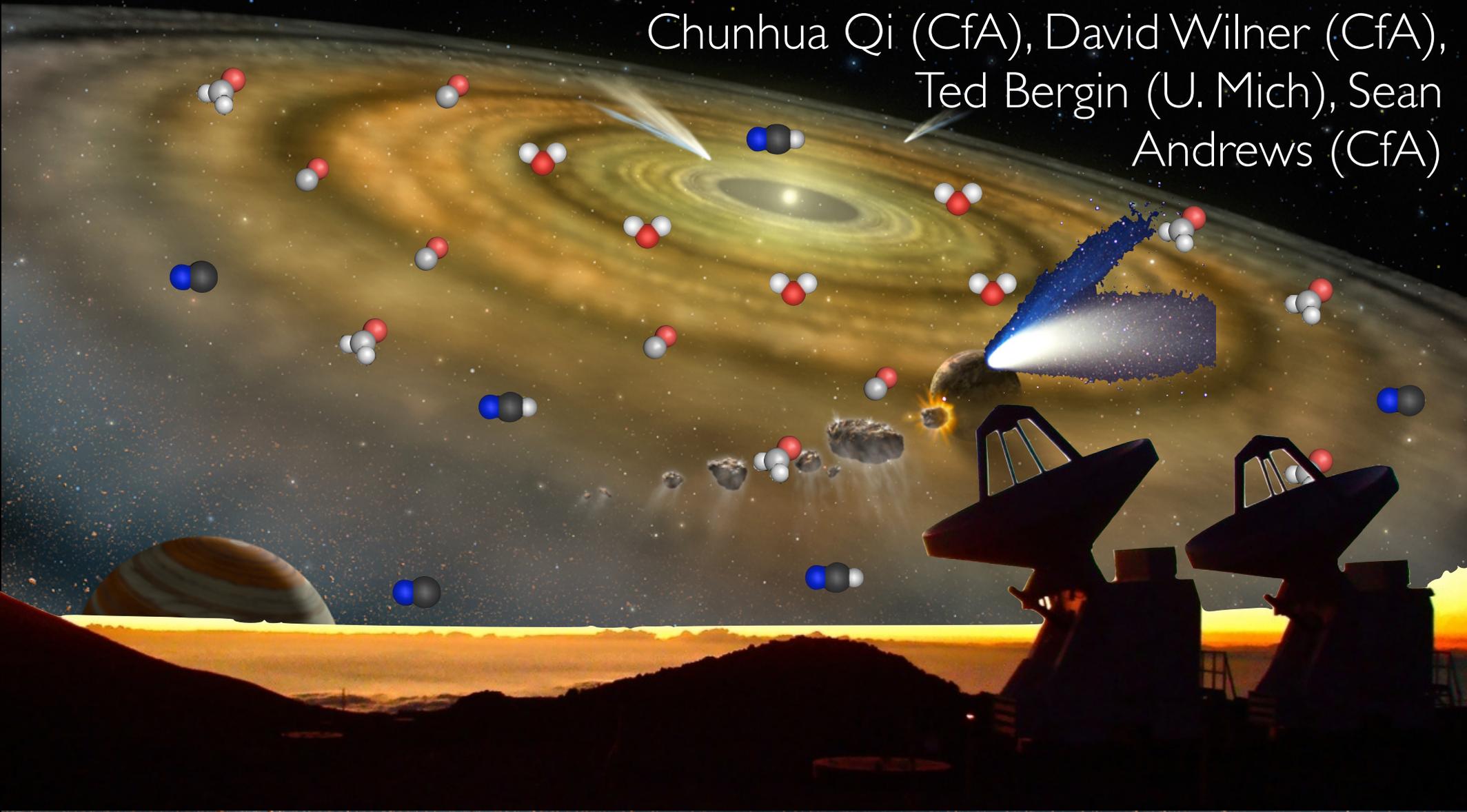
Chunhua Qi (CfA), David Wilner (CfA),  
Ted Bergin (U. Mich), Sean  
Andrews (CfA)



# The Chemistry of Protoplanetary Disks

Karin Öberg (Harvard University)

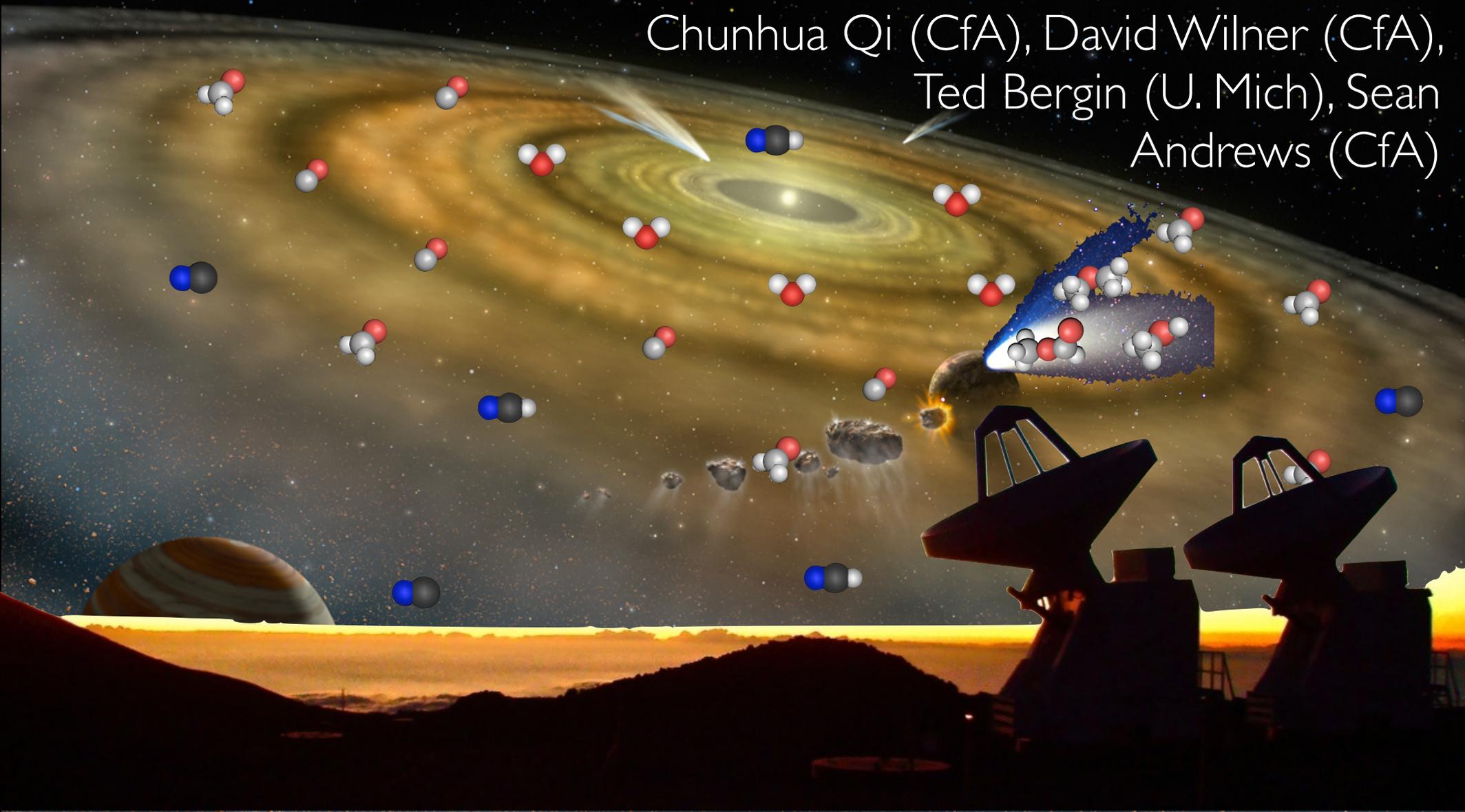
Chunhua Qi (CfA), David Wilner (CfA),  
Ted Bergin (U. Mich), Sean  
Andrews (CfA)



# The Chemistry of Protoplanetary Disks

Karin Öberg (Harvard University)

Chunhua Qi (CfA), David Wilner (CfA),  
Ted Bergin (U. Mich), Sean  
Andrews (CfA)



# Disk chemistry:

## Molecular probes and planetary volatiles

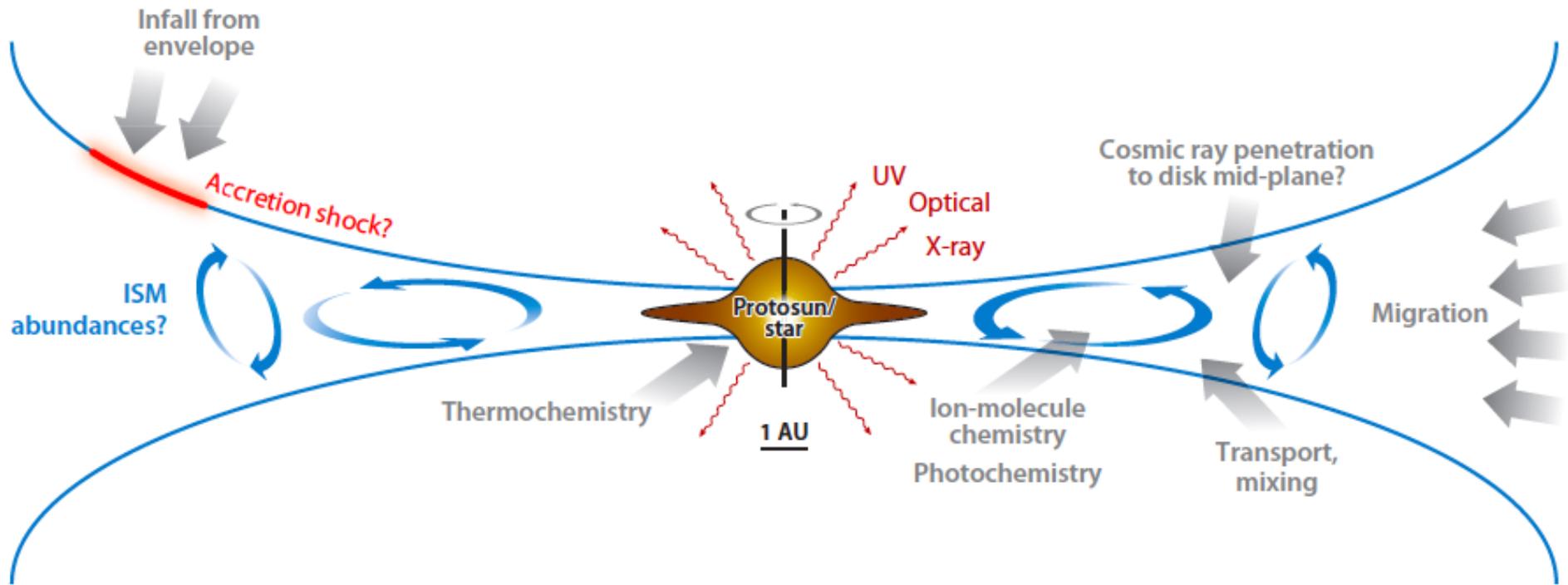
Chemistry regulates:

- what disk regions and processes a certain molecule probes, and
- the abundance, form, and composition of volatiles and organics in different planet forming regions.

Disk chemistry hot topics:

1. What is the relationship between CO and the total disk mass?
2. Where are the snowlines and how do they affect chemistry?
3. What does the terrestrial D/H ratio tell about water delivery?
4. How can ionization and radiation fields be constrained?

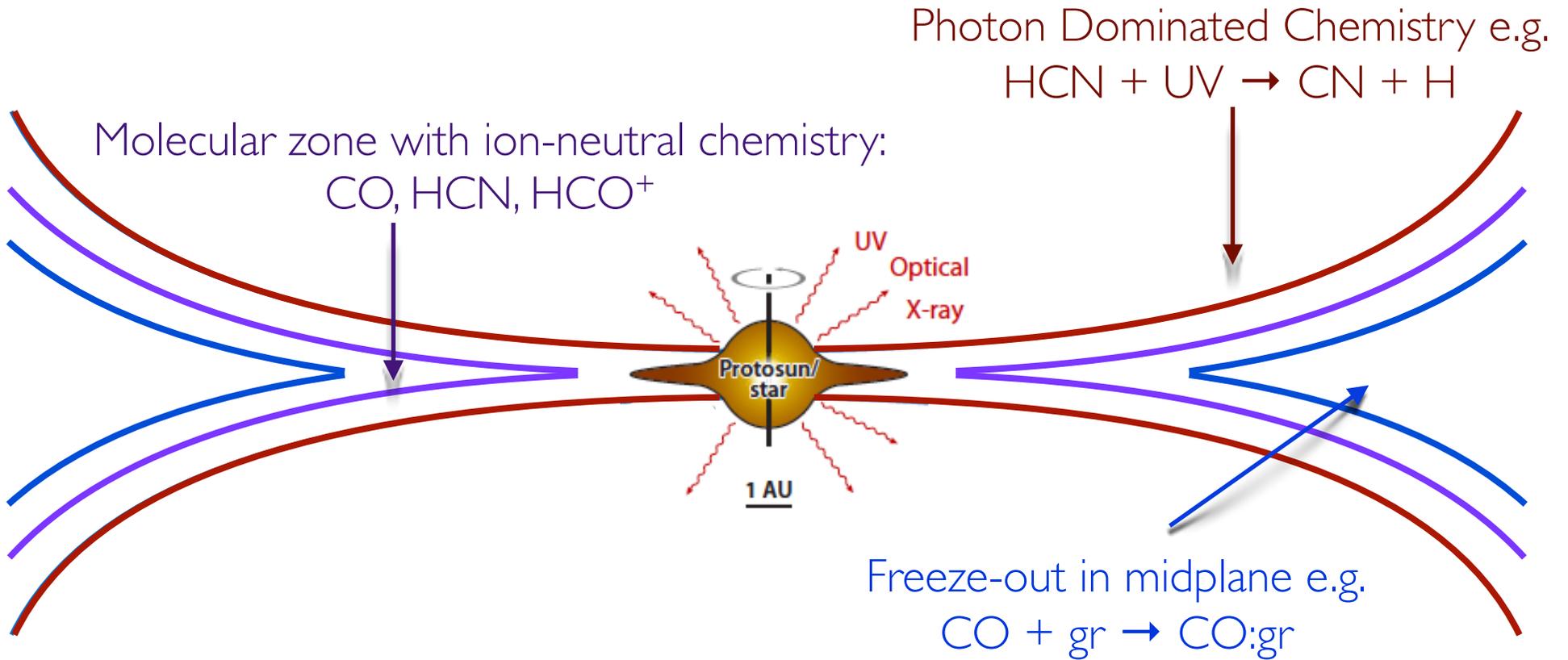
# Protoplanetary disks



Steep density and temperature gradients. Many different radiation environments.

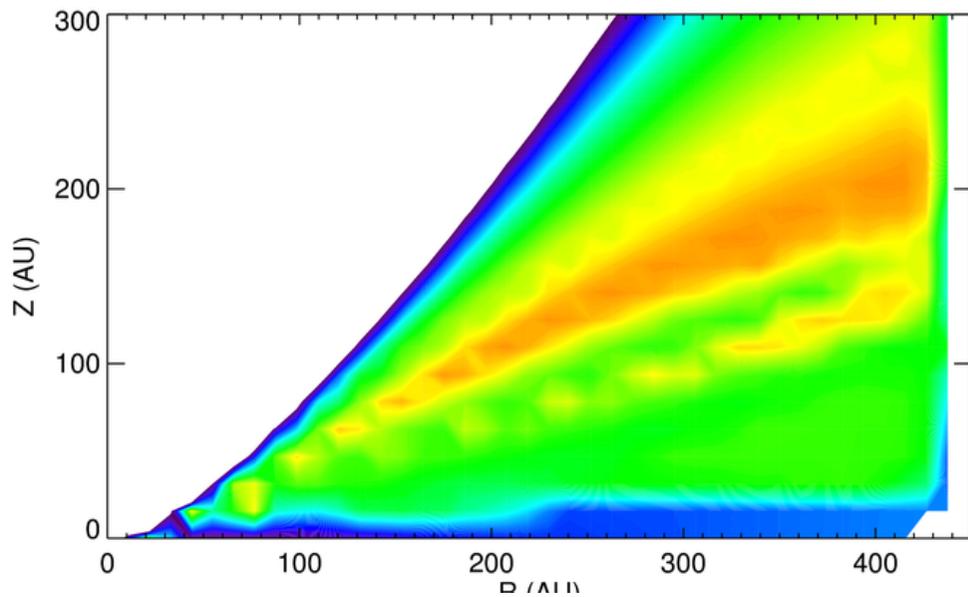
Need probes of these characteristics, and models on how they affect prebiotically relevant chemistry

# Protoplanetary disk chemistry

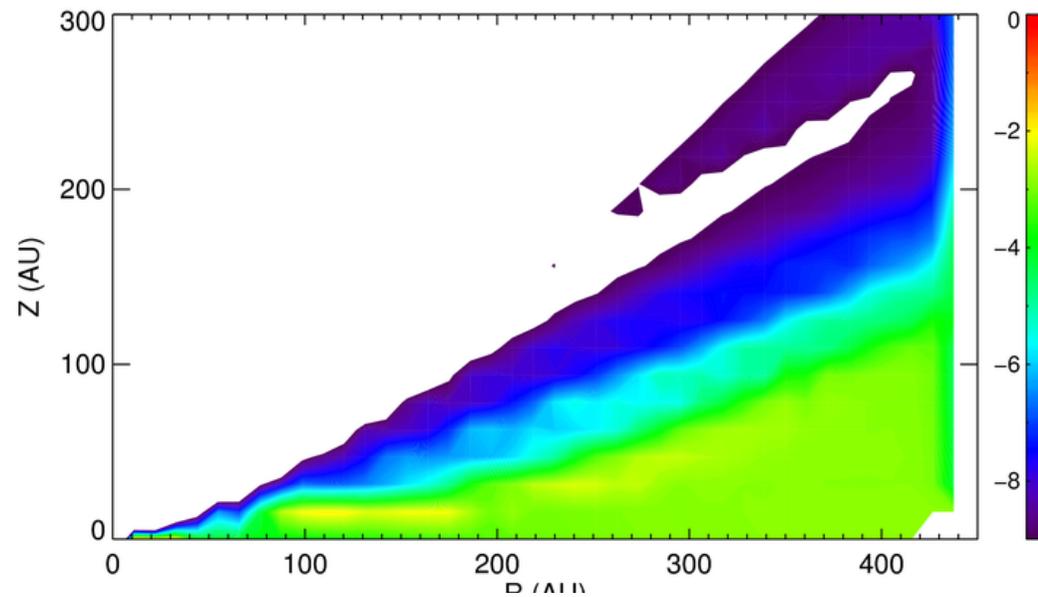


# Chemical layers

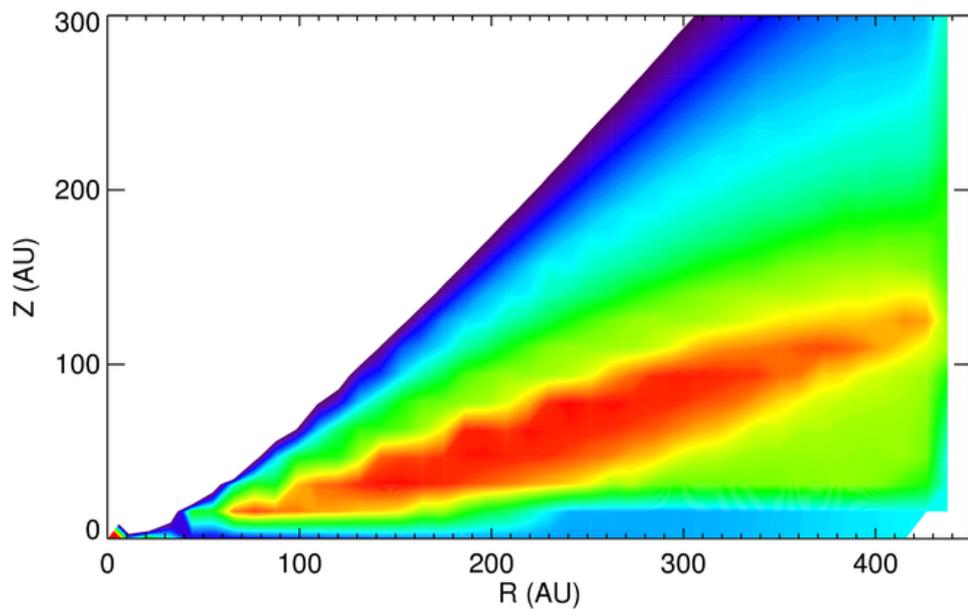
CN



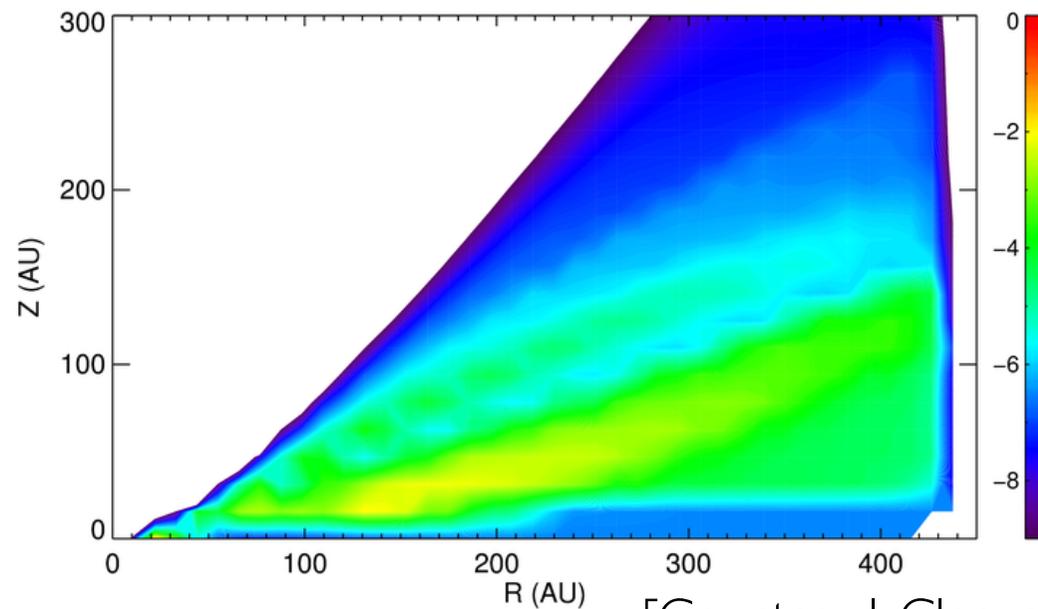
N<sub>2</sub>H<sup>+</sup>



HCN

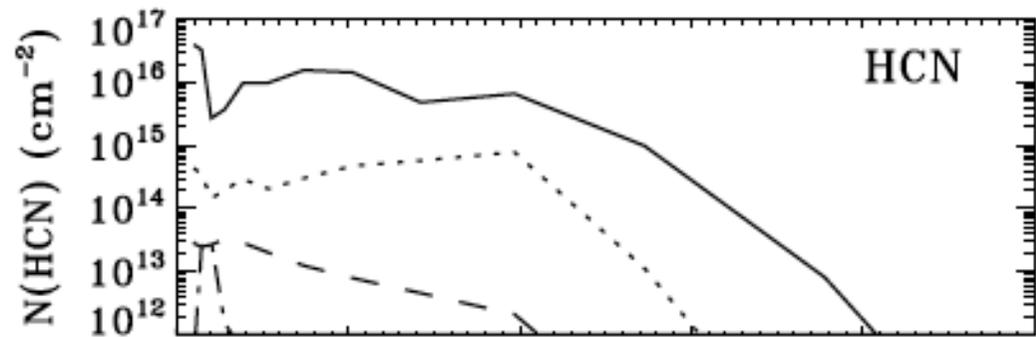


HCO<sup>+</sup>

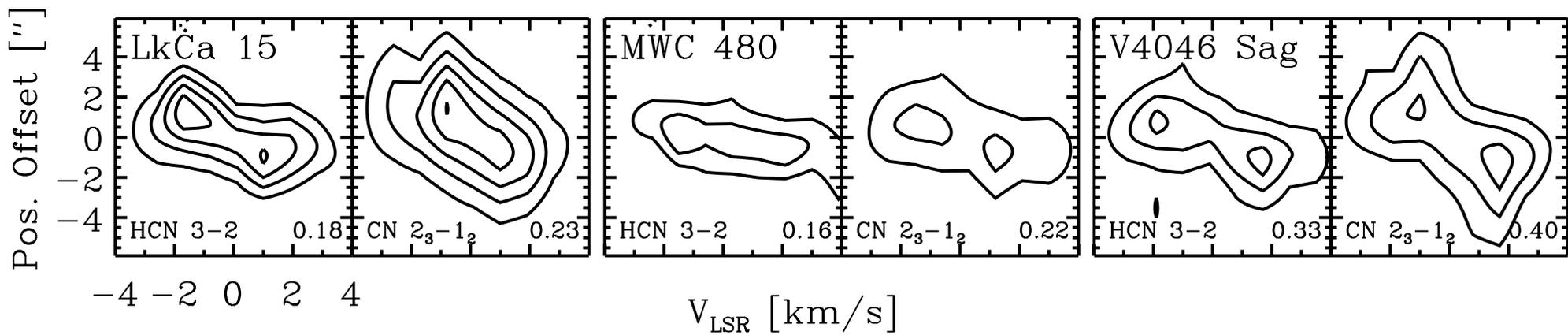
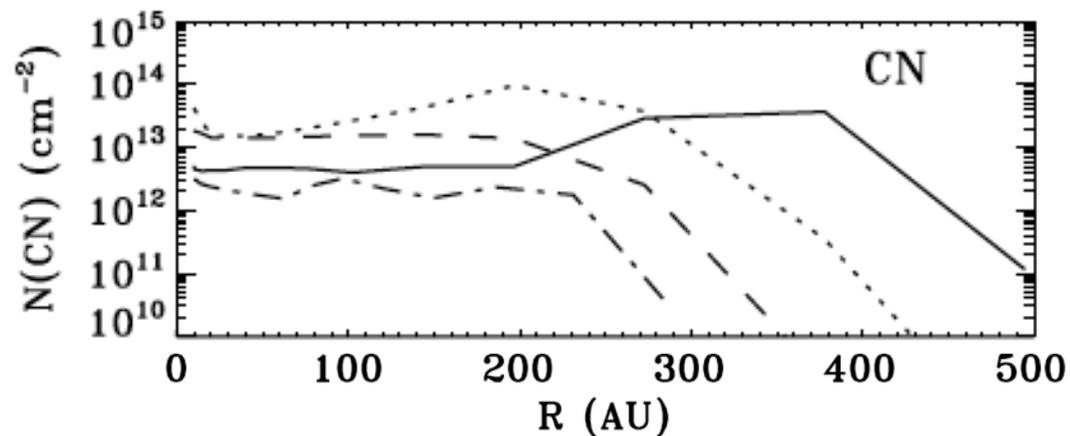


[Courtesy I. Cleeves]

# HCN vs. CN with SMA

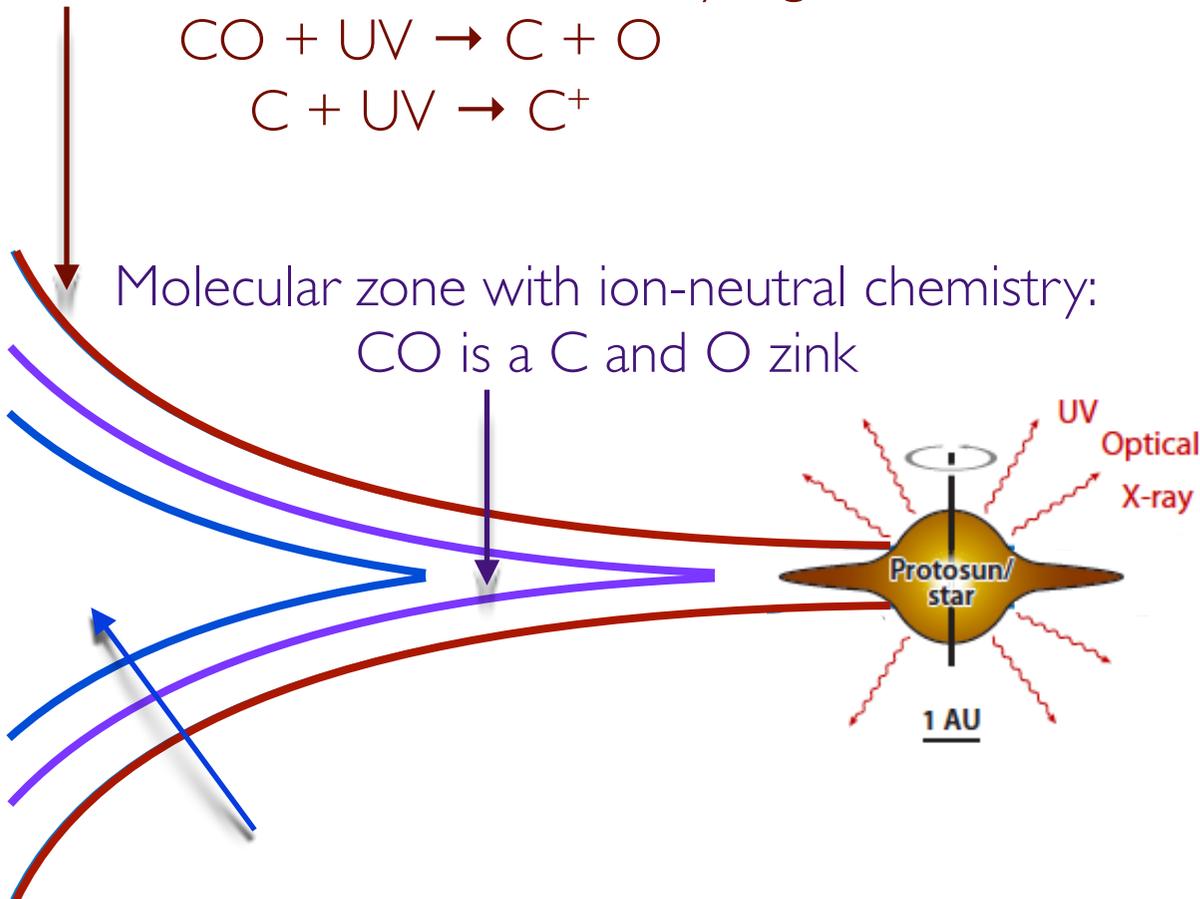


[Jonkheid et al. 2007]



# CO chemistry in disks

Photon Dominated Chemistry e.g.



Molecular zone with ion-neutral chemistry:  
CO is a C and O sink

Most common tracer of disk  
gas mass and distribution

Most abundant molecule —  
easy to observe

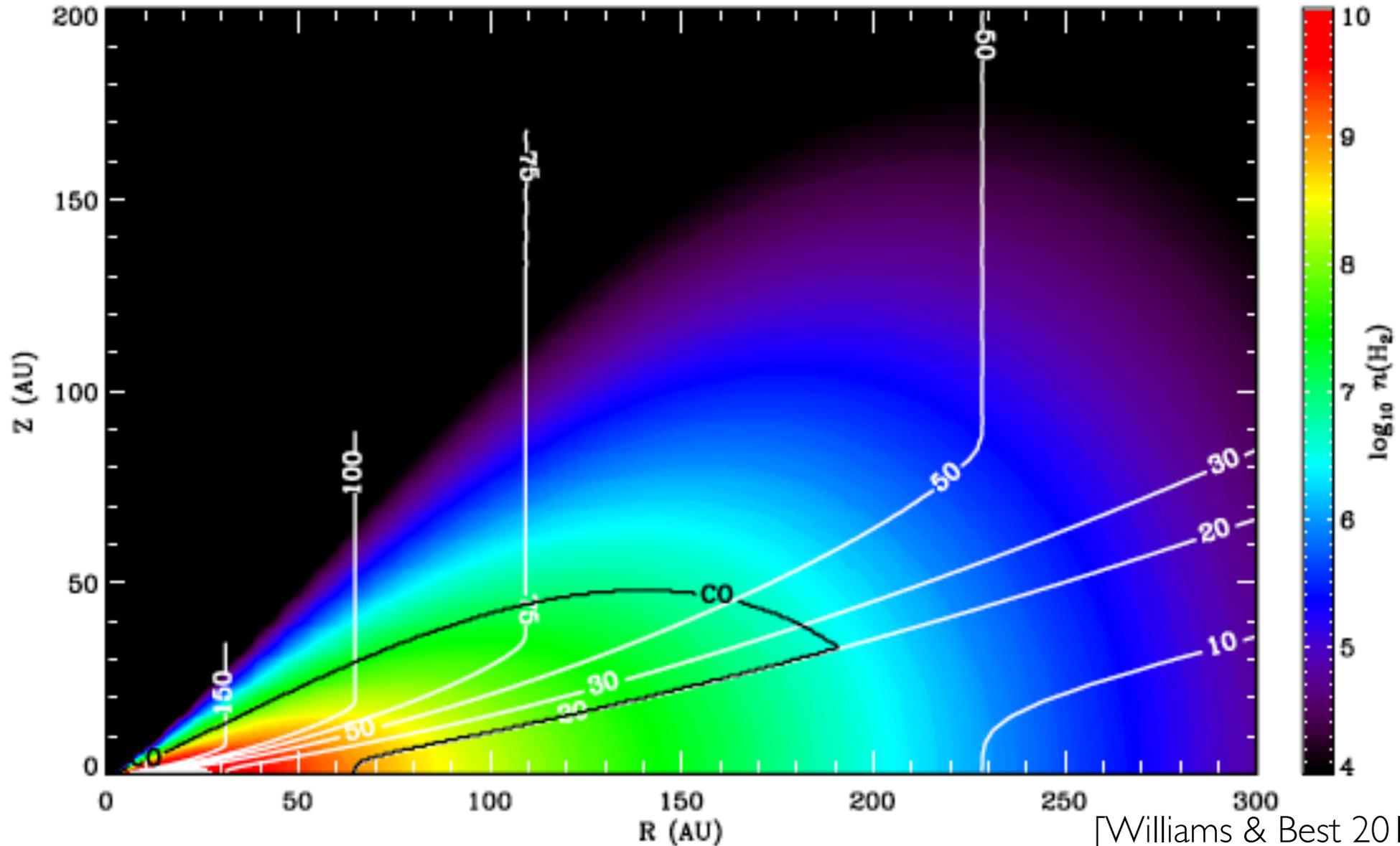
Relatively simple chemistry —  
easy to interpret?

Freeze-out in  $T < 20$  K midplane e.g.



# CO as a gas mass probe

Assume very simple CO chemistry



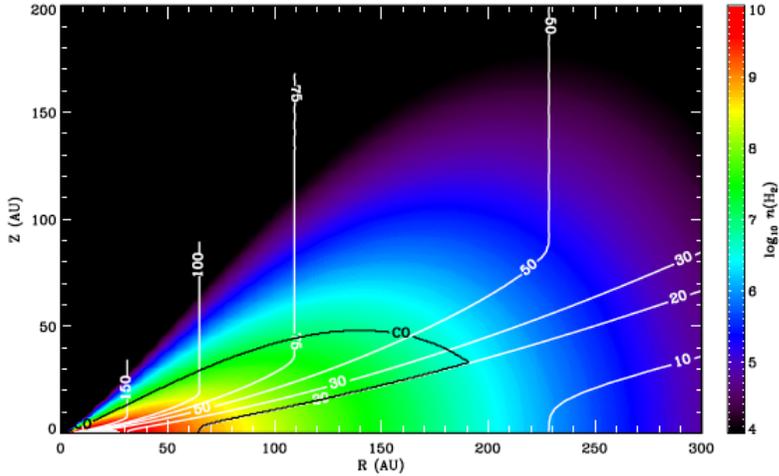
[Williams & Best 2014]

# CO as a gas mass probe

Assume very simple CO chemistry

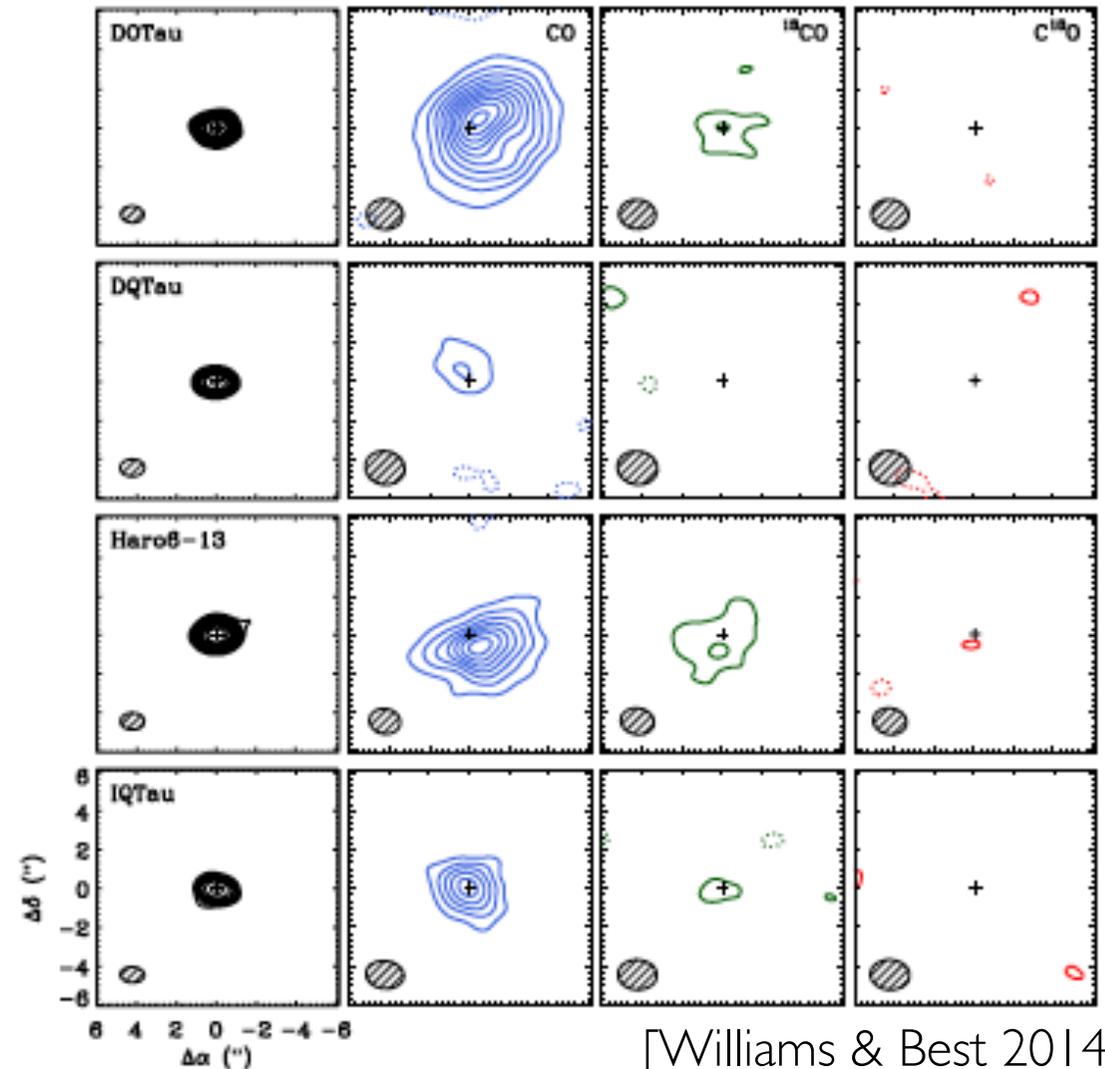
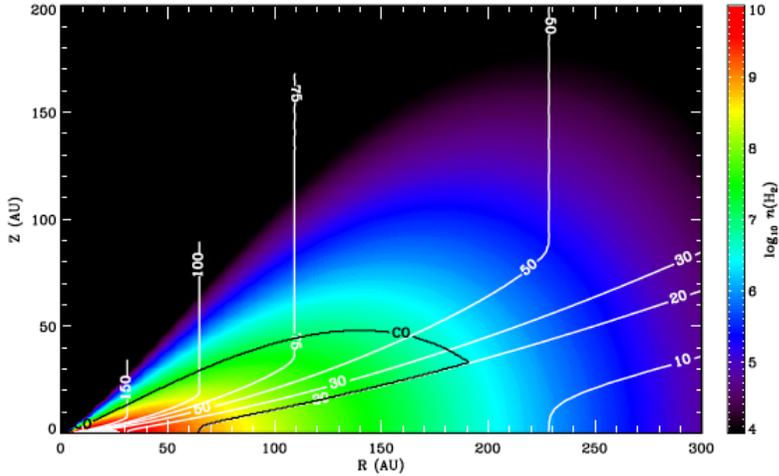
SMA observations of CO isotopologues

Obtain gas-poor disks



# CO as a gas mass probe

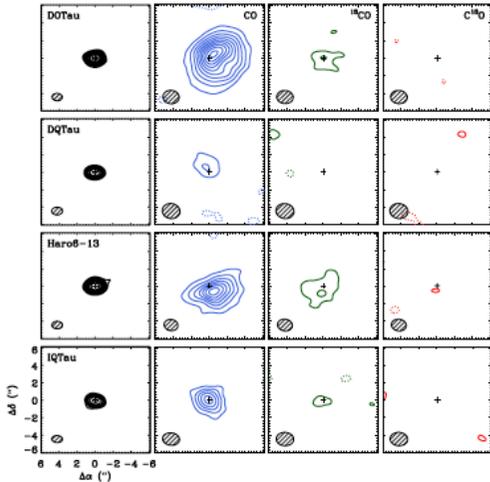
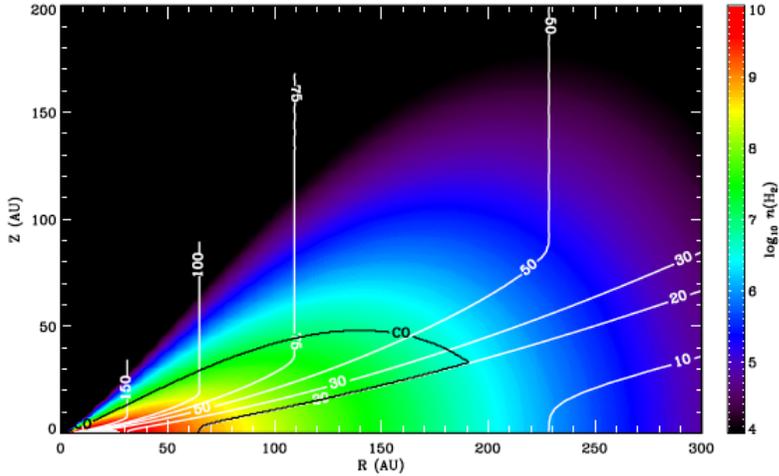
Assume very simple CO chemistry  
SMA observations of CO isotopologues  
Obtain gas-poor disks



[Williams & Best 2014]

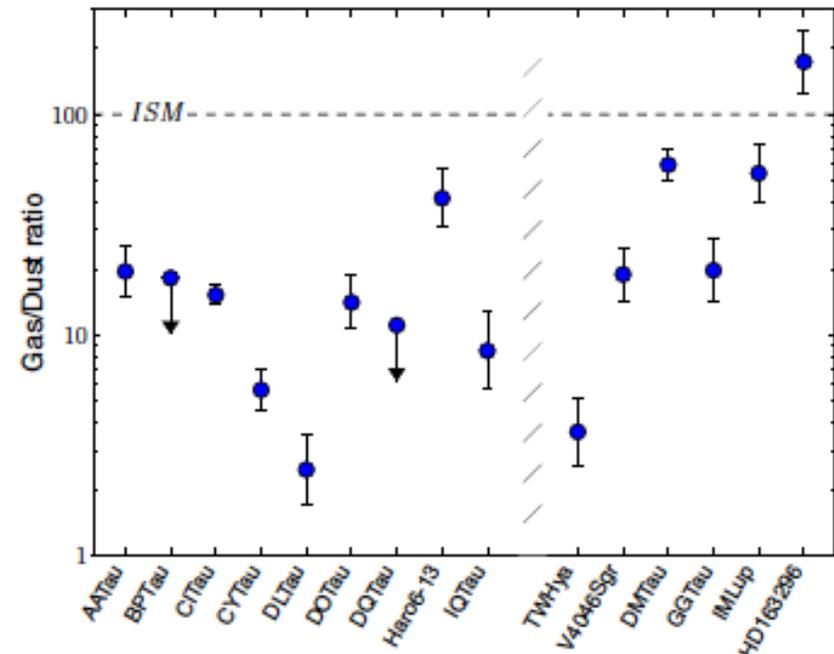
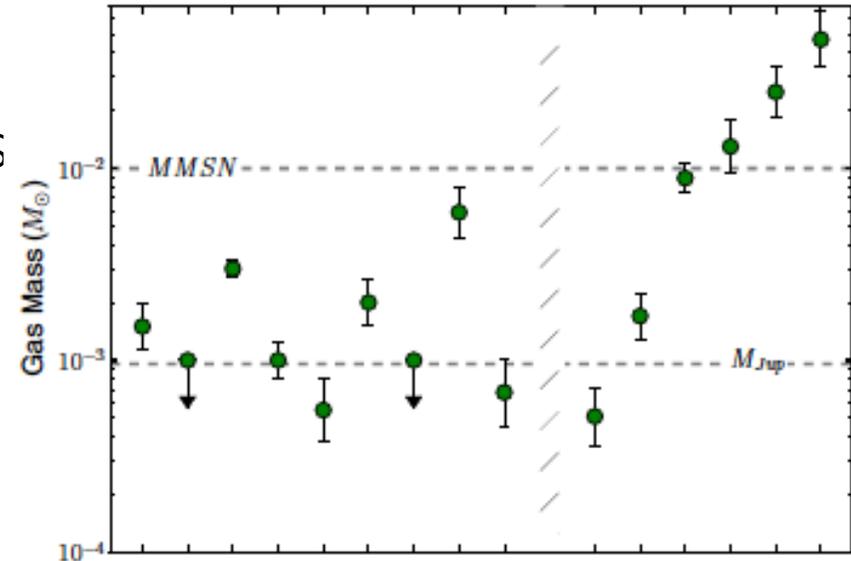
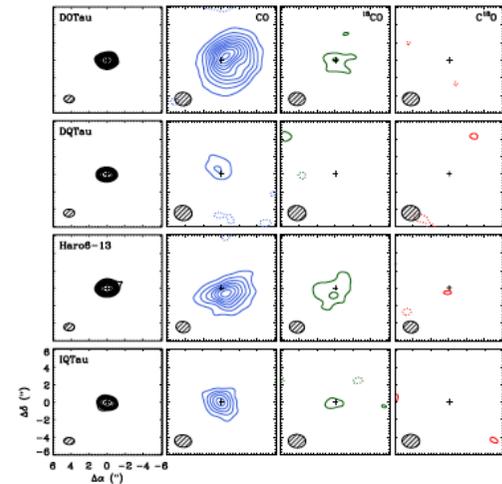
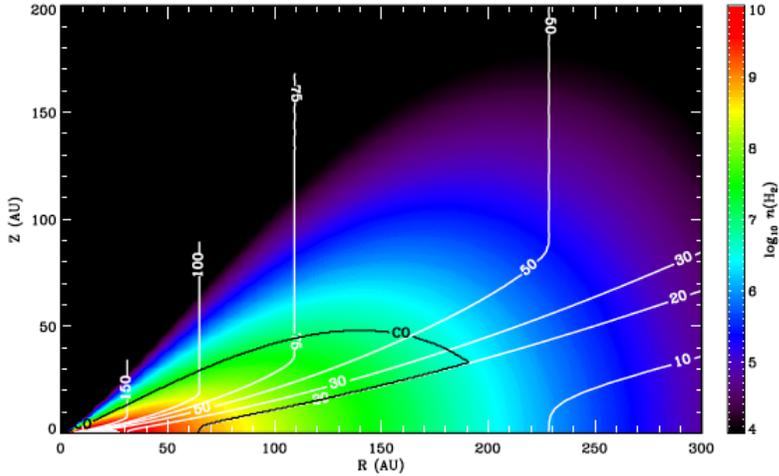
# CO as a gas mass probe

Assume very simple CO chemistry  
SMA observations of CO isotopologues  
Obtain gas-poor disks



# CO as a gas mass probe

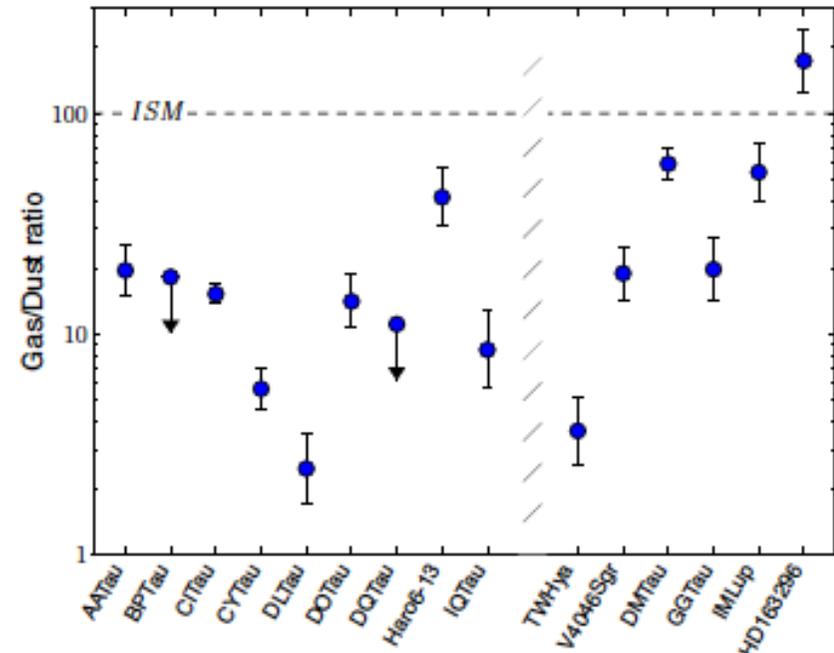
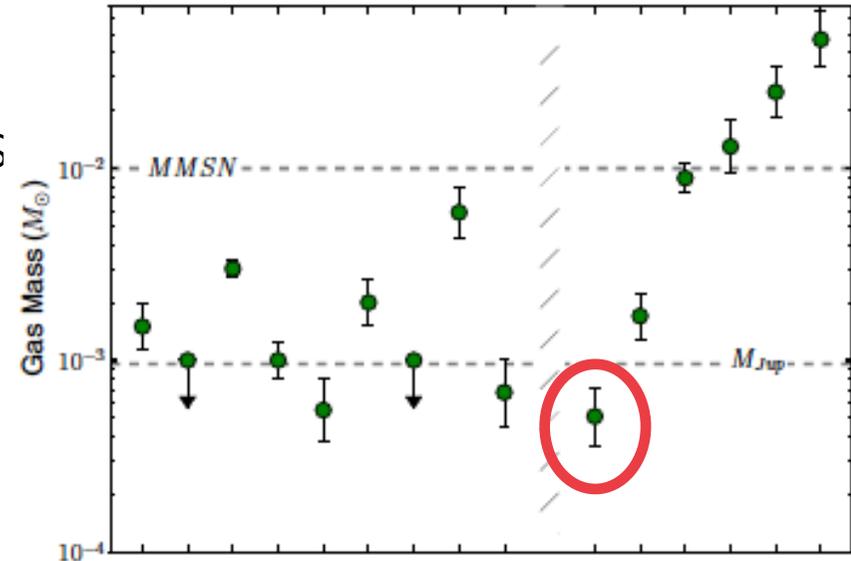
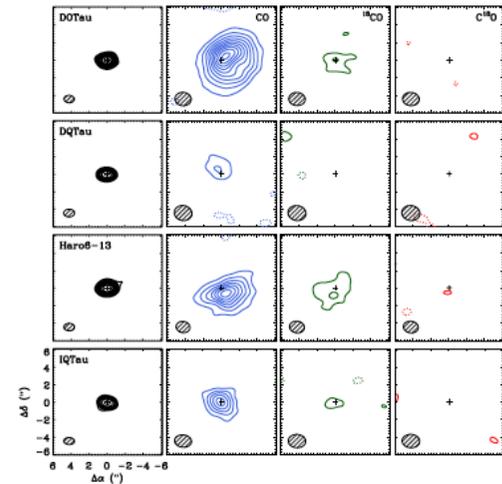
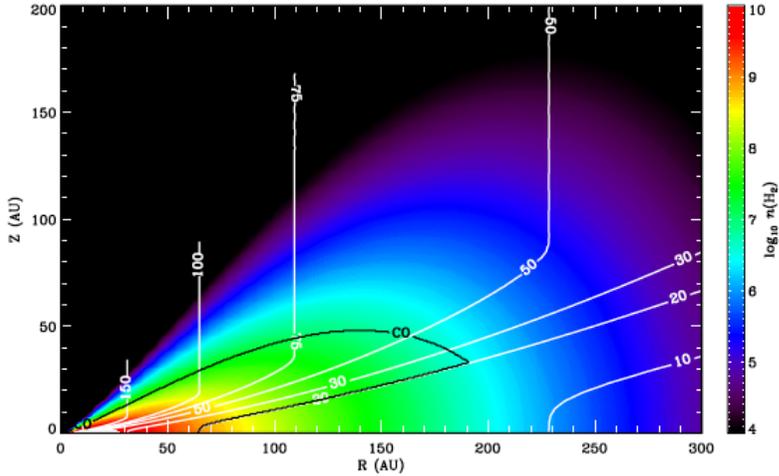
Assume very simple CO chemistry  
 SMA observations of CO isotopologues  
 Obtain gas-poor disks



[Williams & Best 2014]

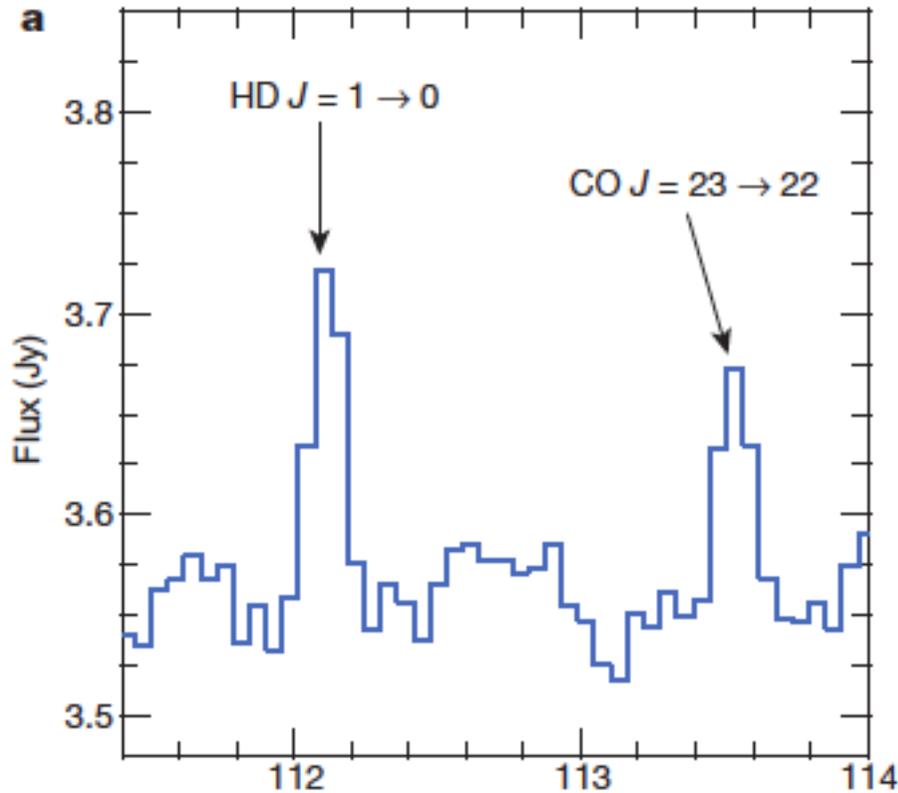
# CO as a gas mass probe

Assume very simple CO chemistry  
 SMA observations of CO isotopologues  
 Obtain gas-poor disks



[Williams & Best 2014]

# The CO chemistry revisited



X-rays  $\rightarrow$  He<sup>+</sup>  $\rightarrow$  CO dissociation  
in molecular layer  $\rightarrow$  C<sub>x</sub>H<sub>y</sub>

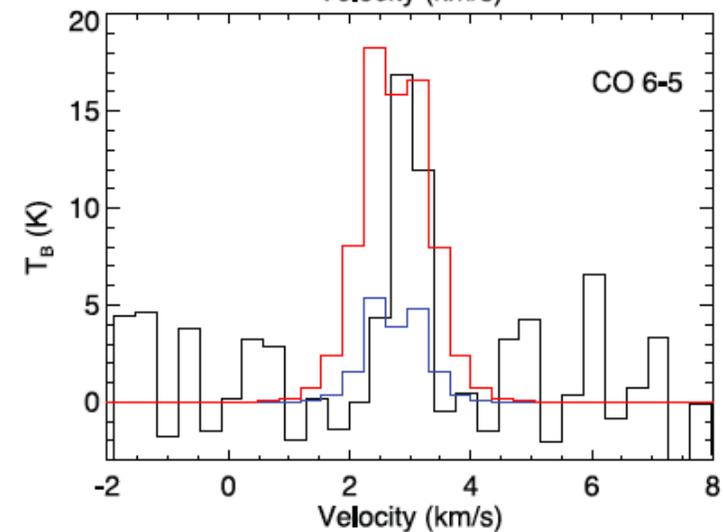
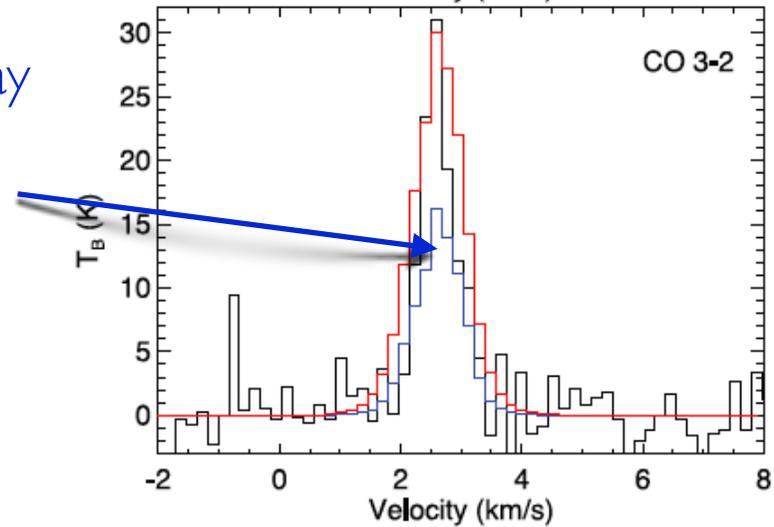
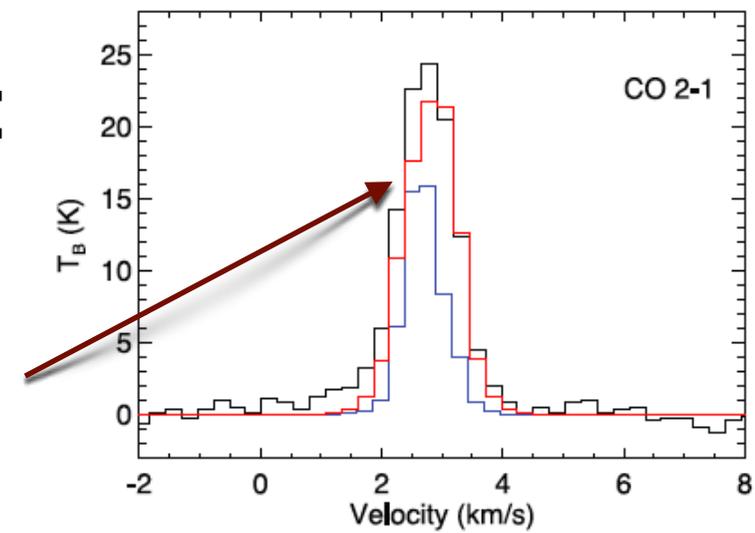
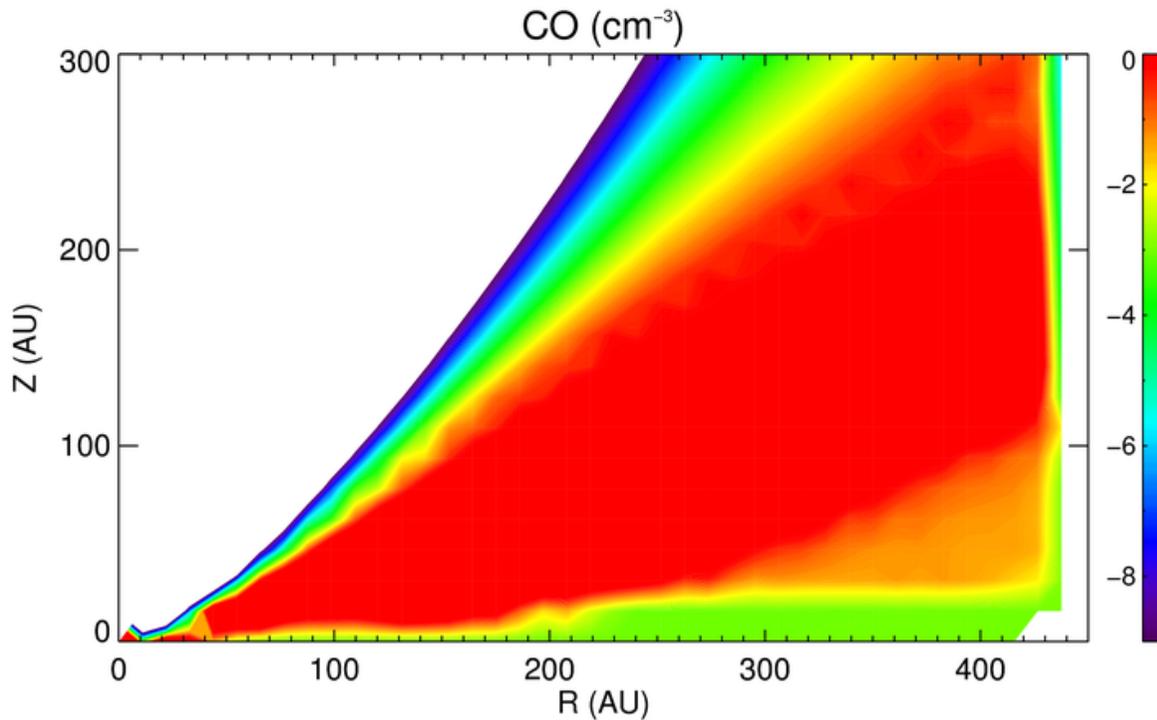
CO + gr  $\rightarrow$  CO:gr  $\rightarrow$  CO<sub>2</sub>:gr

Combining HD and SMA CO observations toward TW Hya yields an order of magnitude more gas  $\rightarrow$  Chemical CO depletion.

# CO as disk temperature probe: Super-heated layers

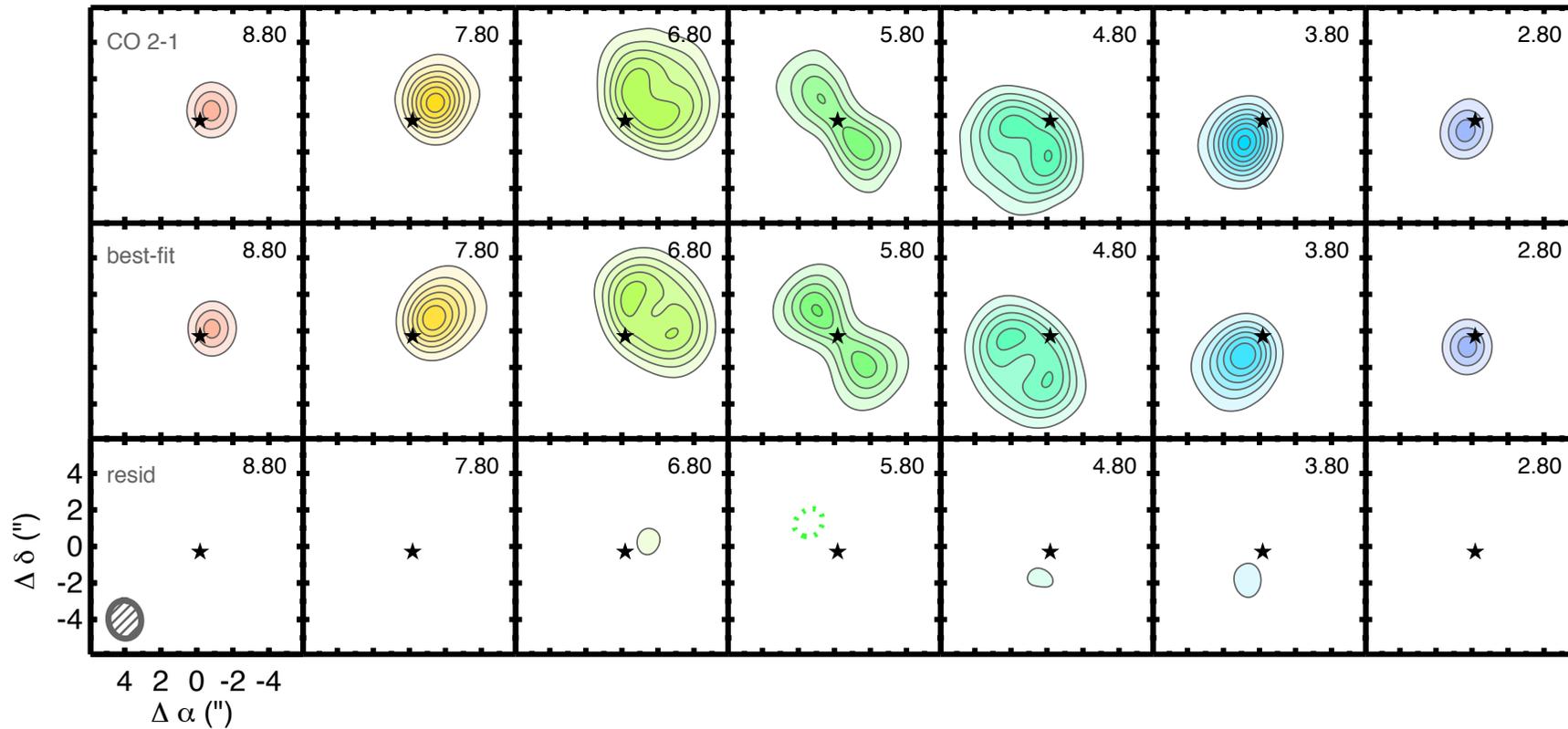
Model that includes  
X-ray heating

Model without X-ray  
heating

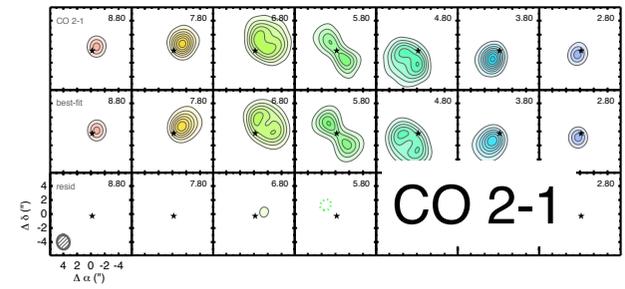


Multi-isotope/transition CO  
constraints: HD 163296

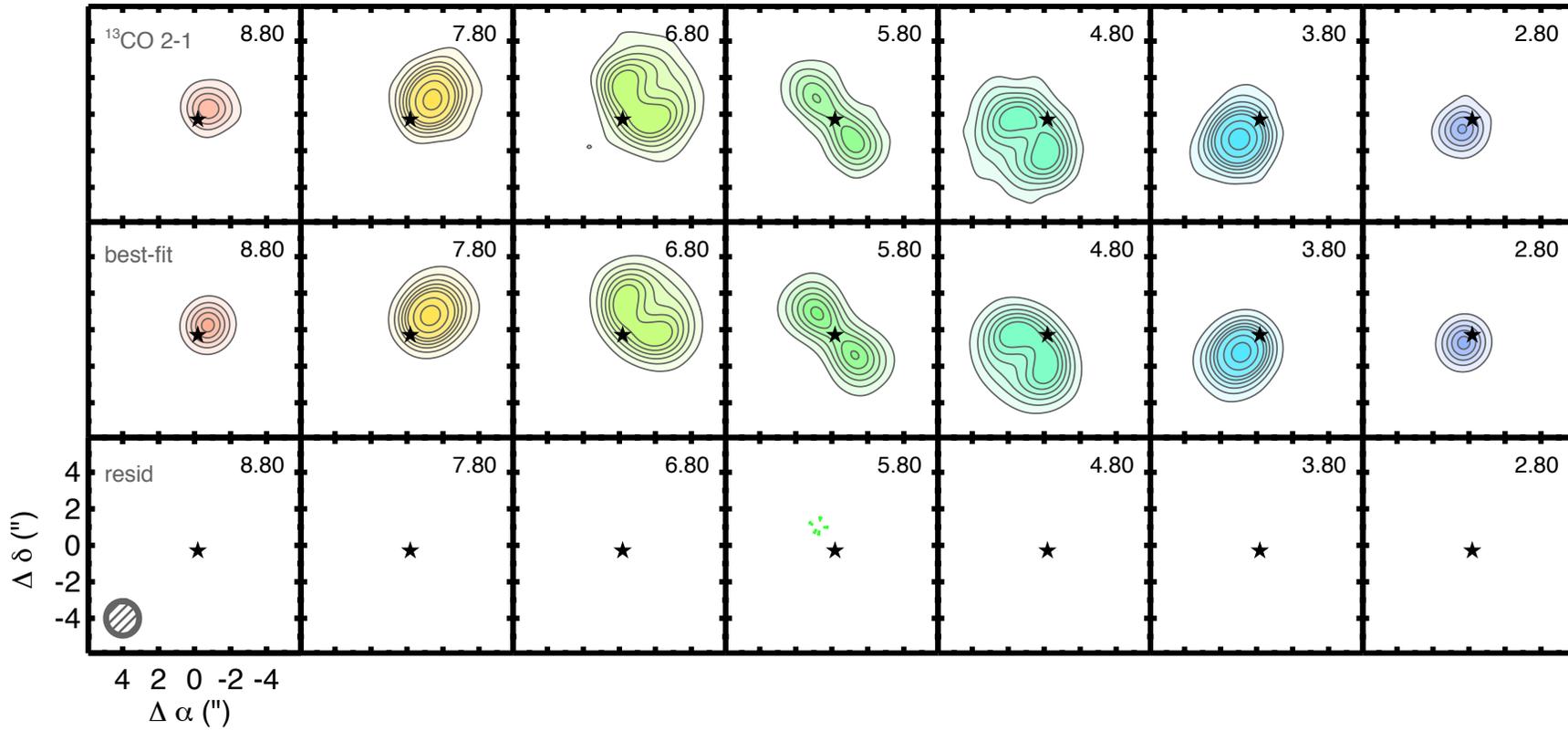
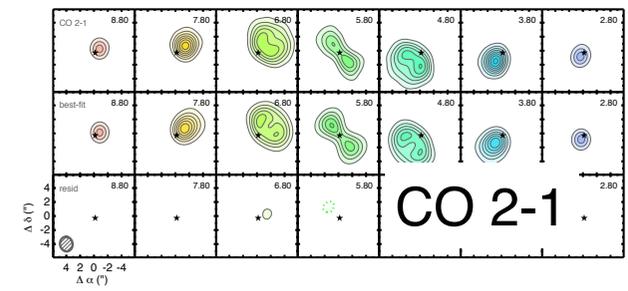
# Multi-isotope/transition CO constraints: HD 163296



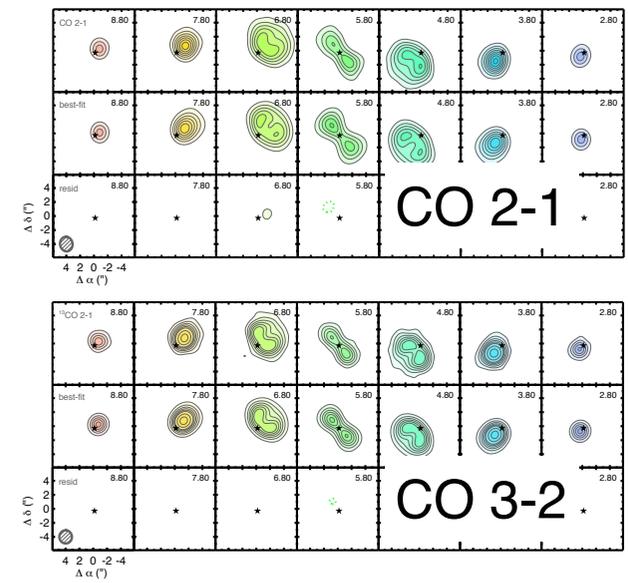
# Multi-isotope/transition CO constraints: HD 163296



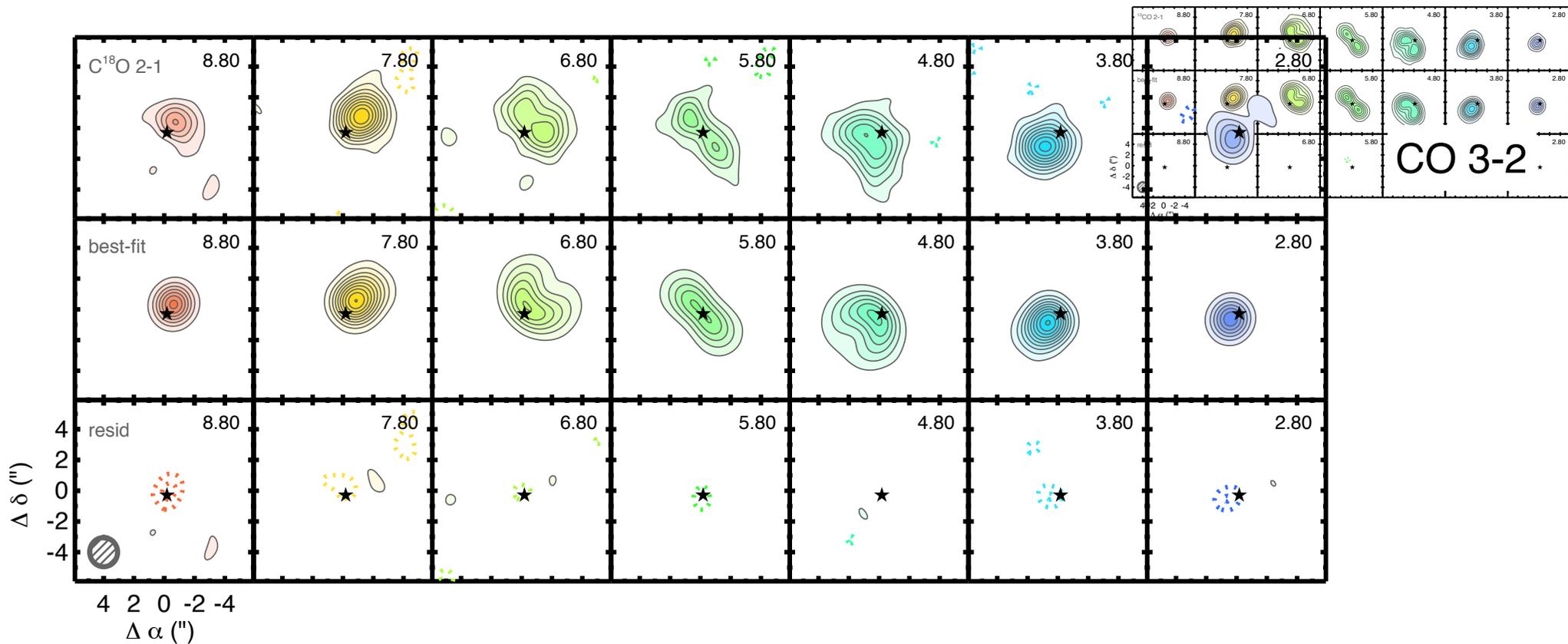
# Multi-isotope/transition CO constraints: HD 163296



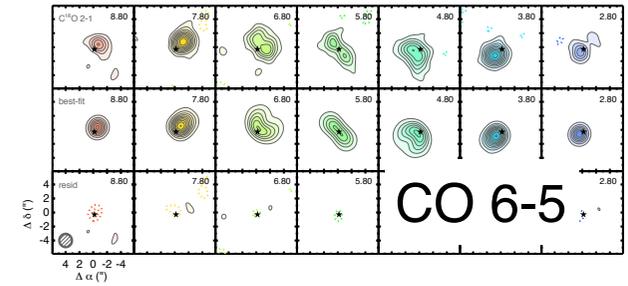
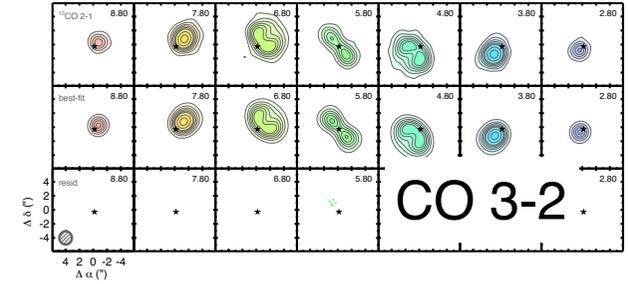
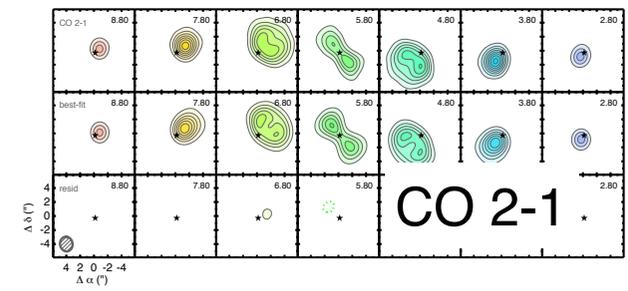
# Multi-isotope/transition CO constraints: HD 163296



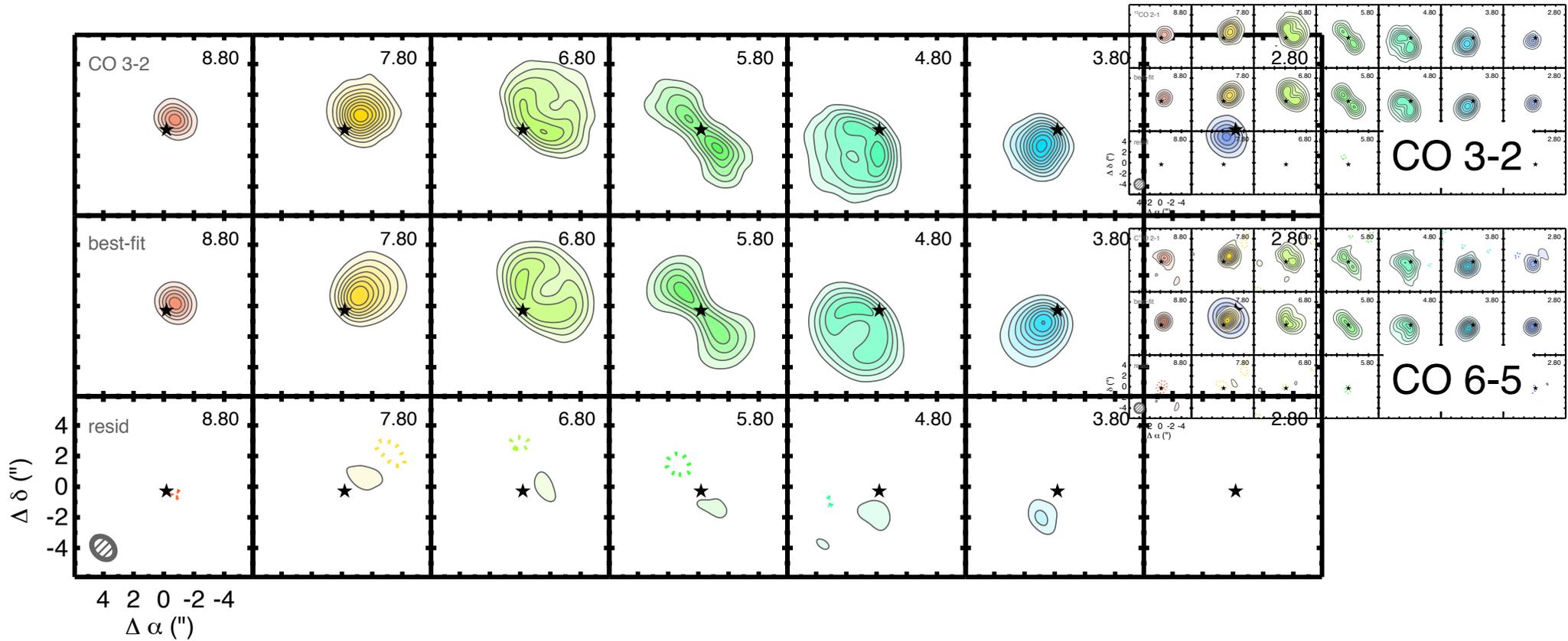
# Multi-isotope/transition CO constraints: HD 163296



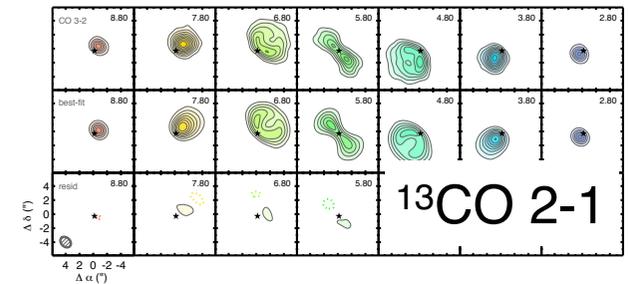
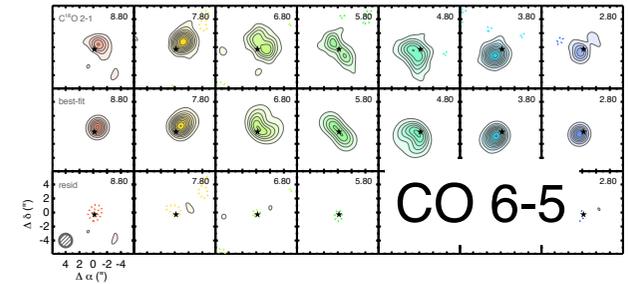
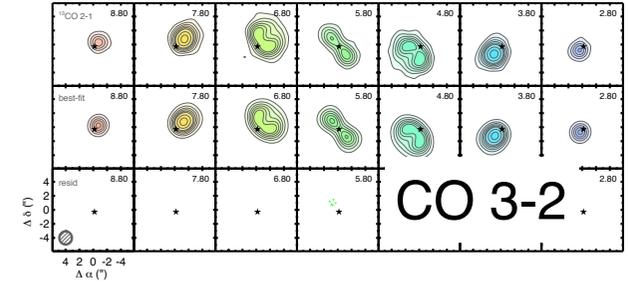
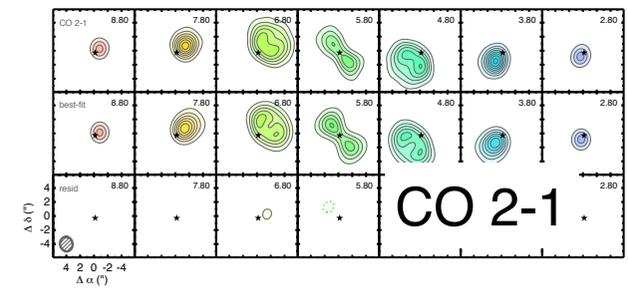
# Multi-isotope/transition CO constraints: HD 163296



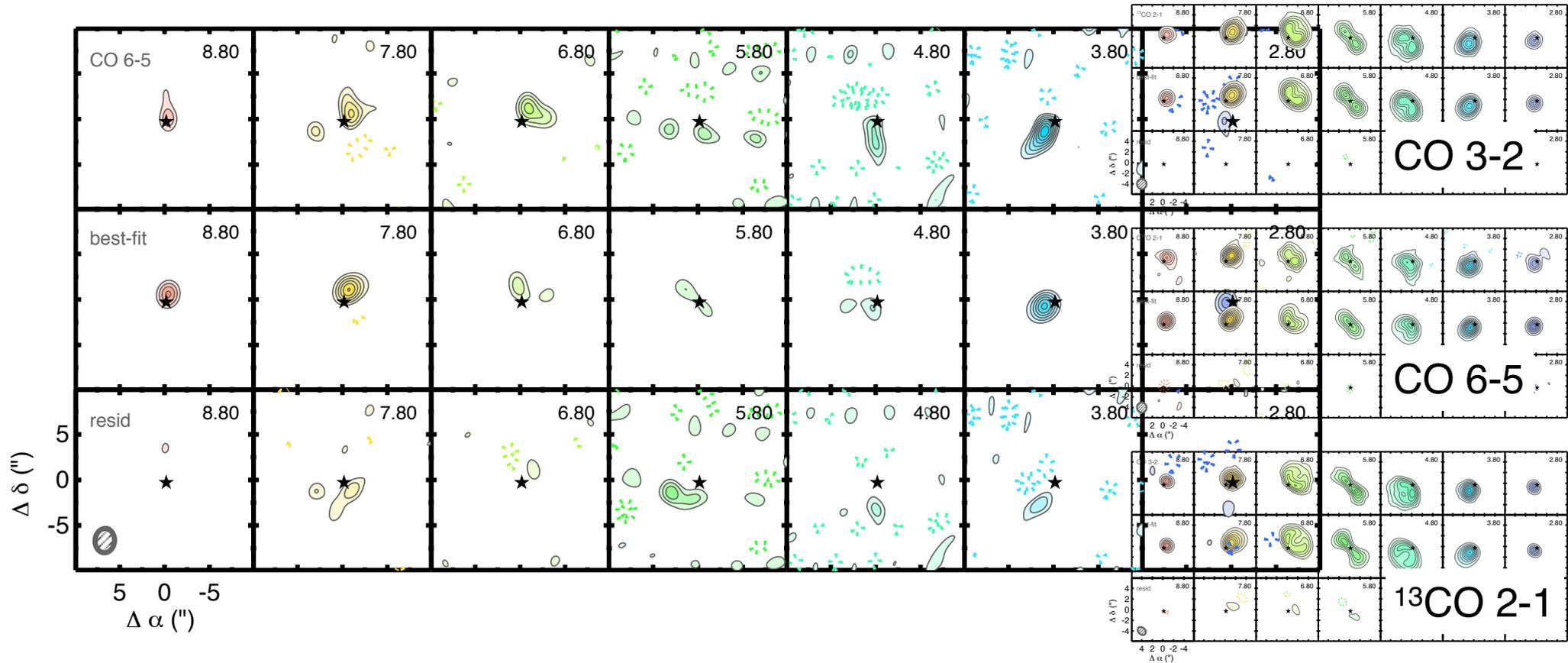
# Multi-isotope/transition CO constraints: HD 163296



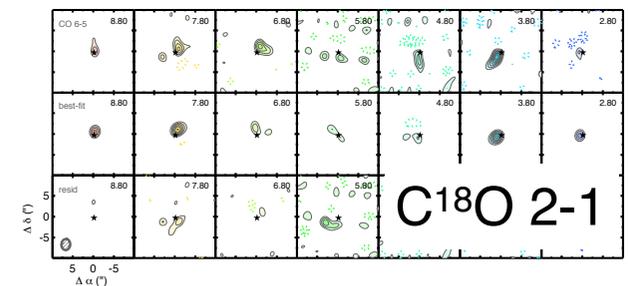
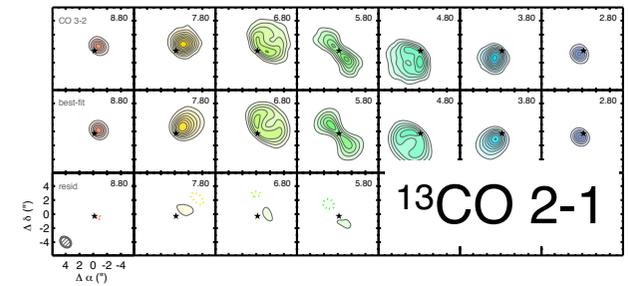
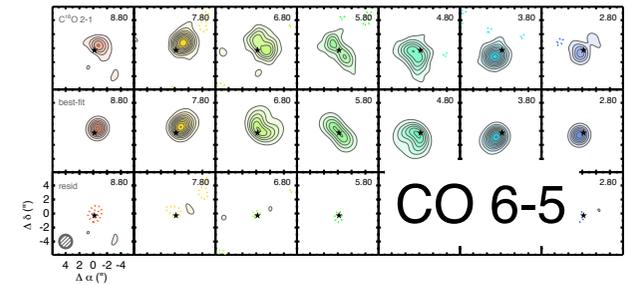
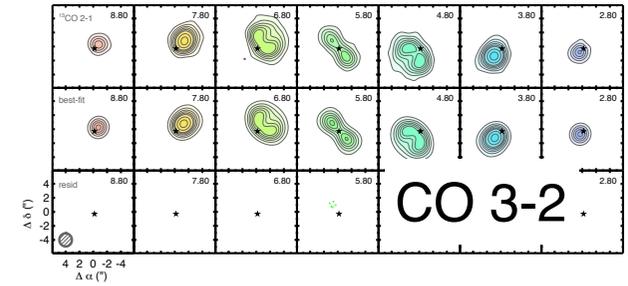
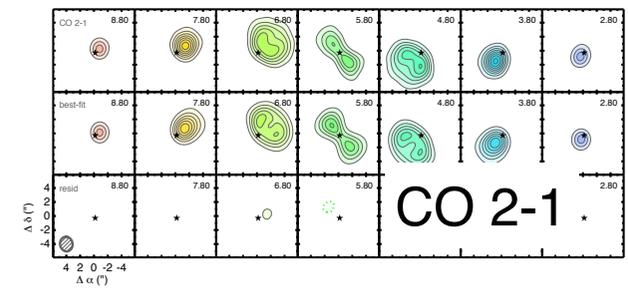
# Multi-isotope/transition CO constraints: HD 163296



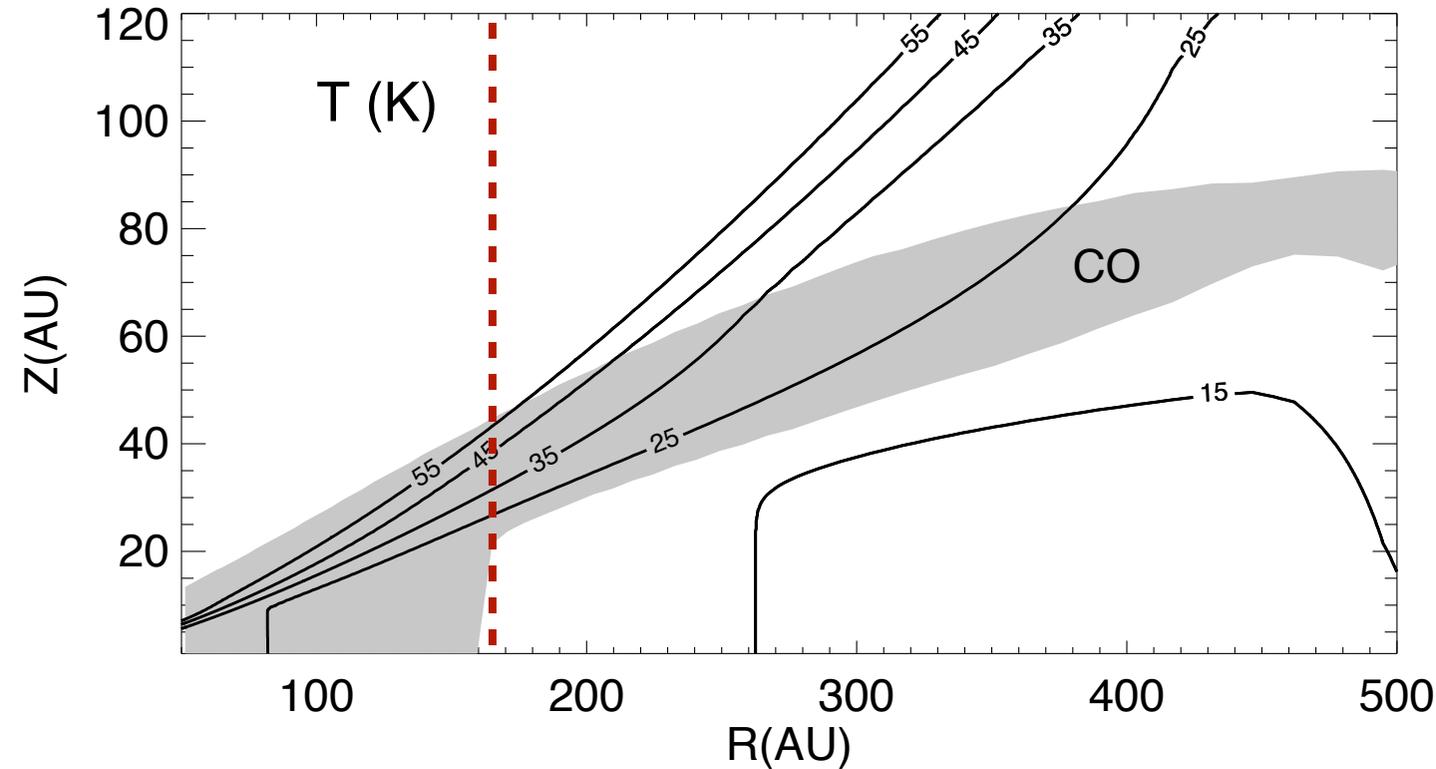
# Multi-isotope/transition CO constraints: HD 163296



# Multi-isotope/transition CO constraints: HD 163296

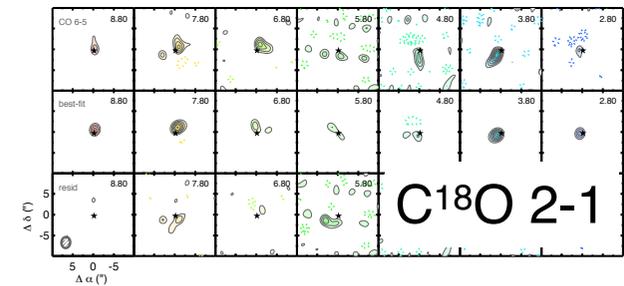
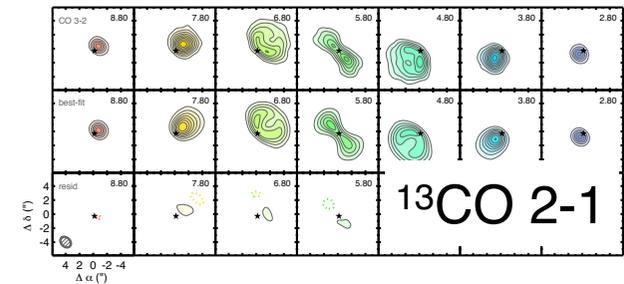
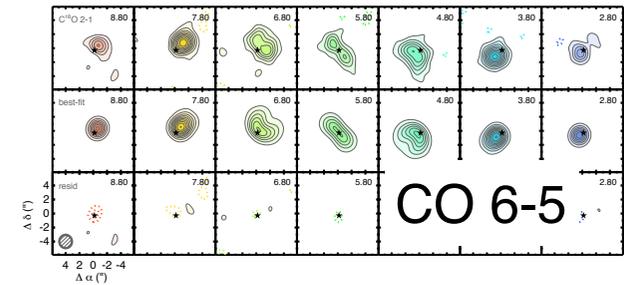
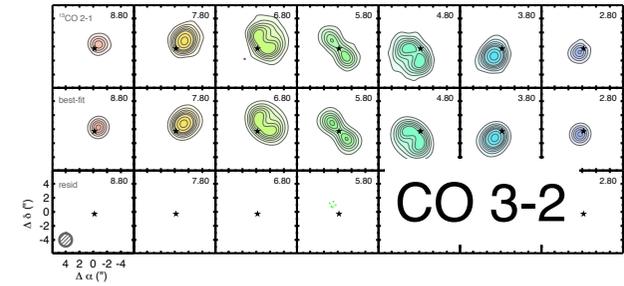
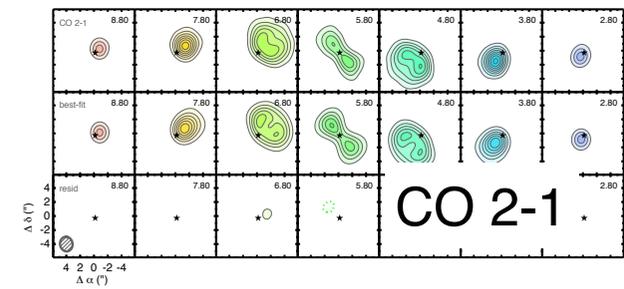


# Multi-isotope/transition CO constraints: HD 163296

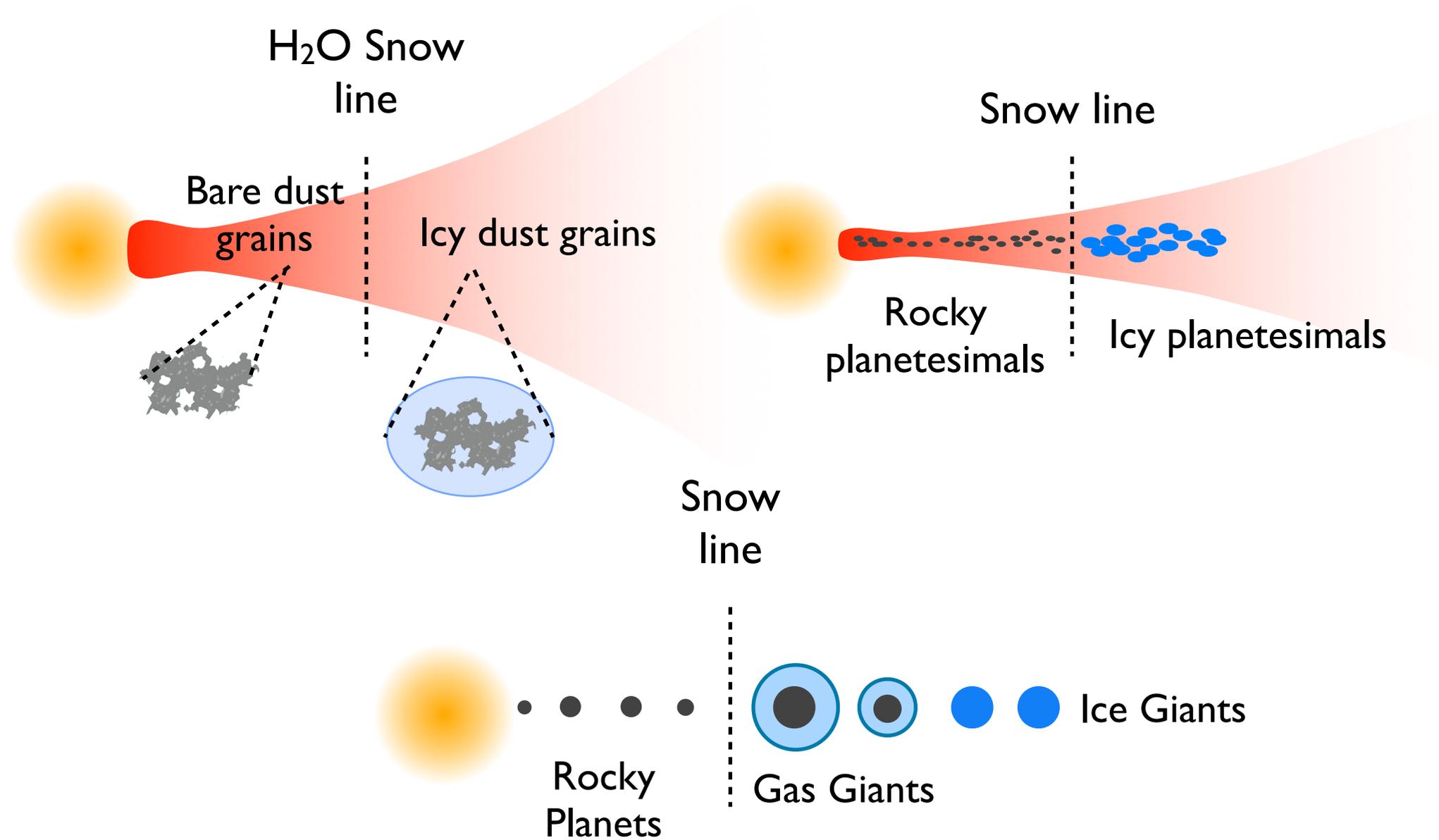


Multi-transitional/isotopologue CO data constrain gas temperature structure, and finds evidence for CO freeze-out outside of 170 AU, or below  $\sim 19$  K

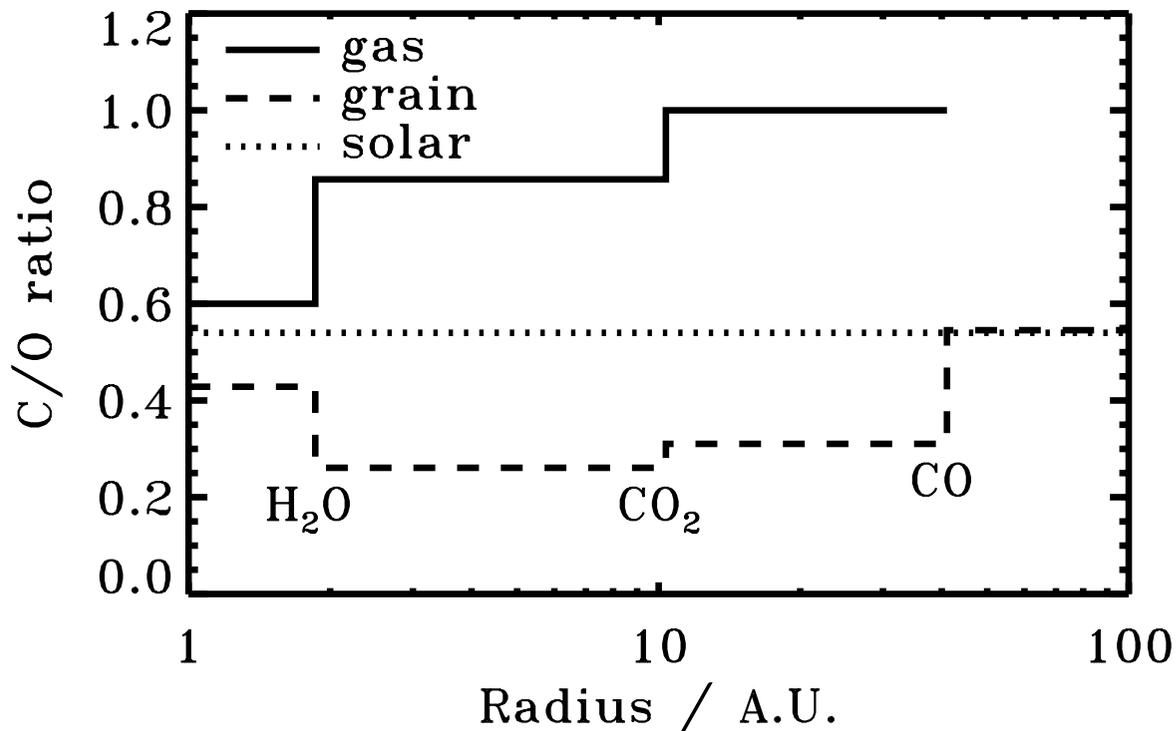
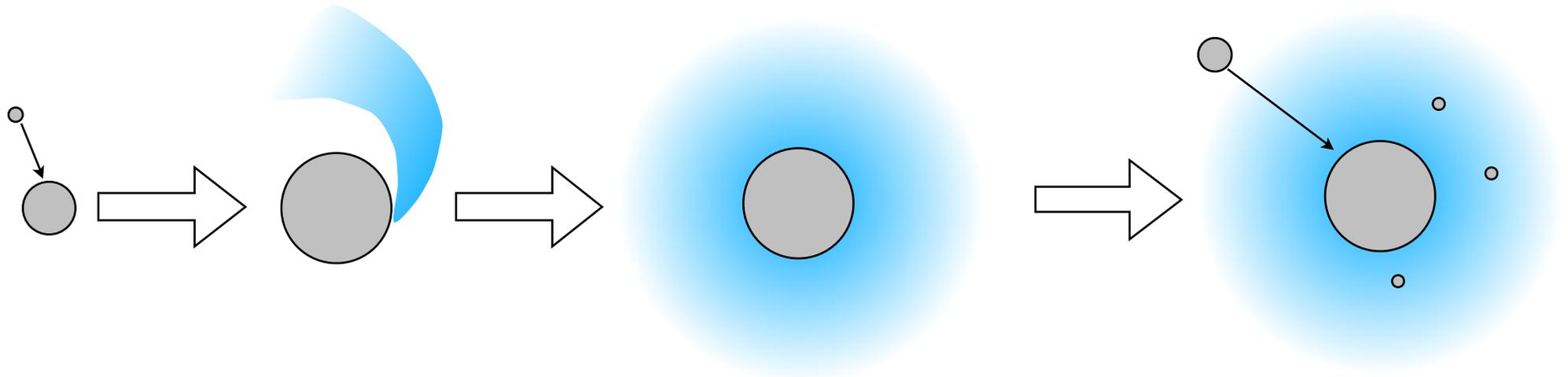
[Qi, d'Alessio et al. 2011]



# The water snowline in the Solar Nebula



# Condensation lines change the gas-phase and solid elemental ratios



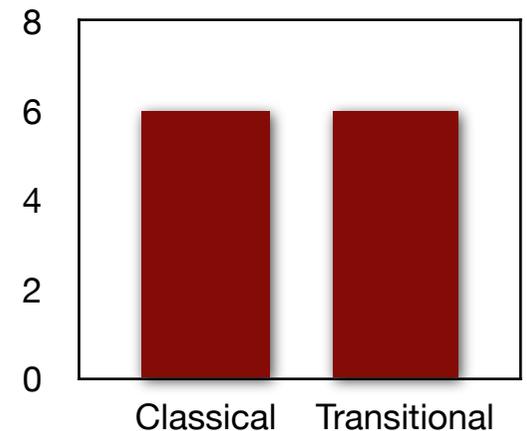
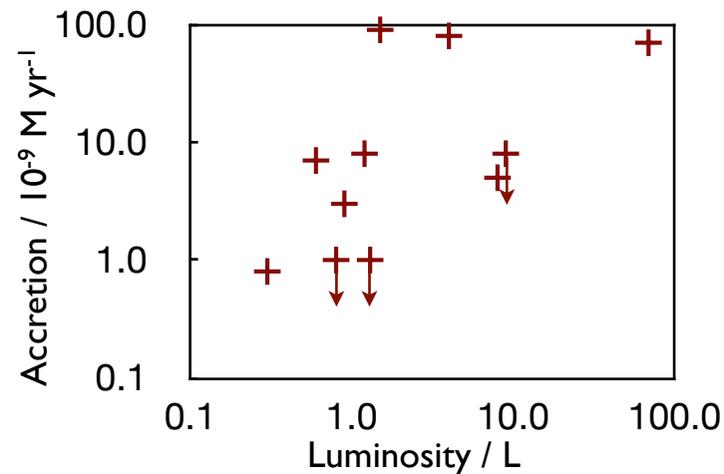
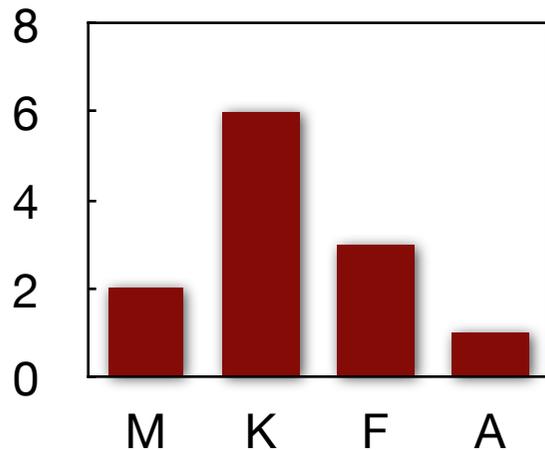
Assuming interstellar molecular abundances,  $C/O \sim 1$  between the  $CO_2$  and  $CO$  snowlines.

If a gas giant accretes the core from solids and envelope from gas,  $C/O \sim 1$  in the atmosphere, assuming no planetesimal pollution or core dredging.

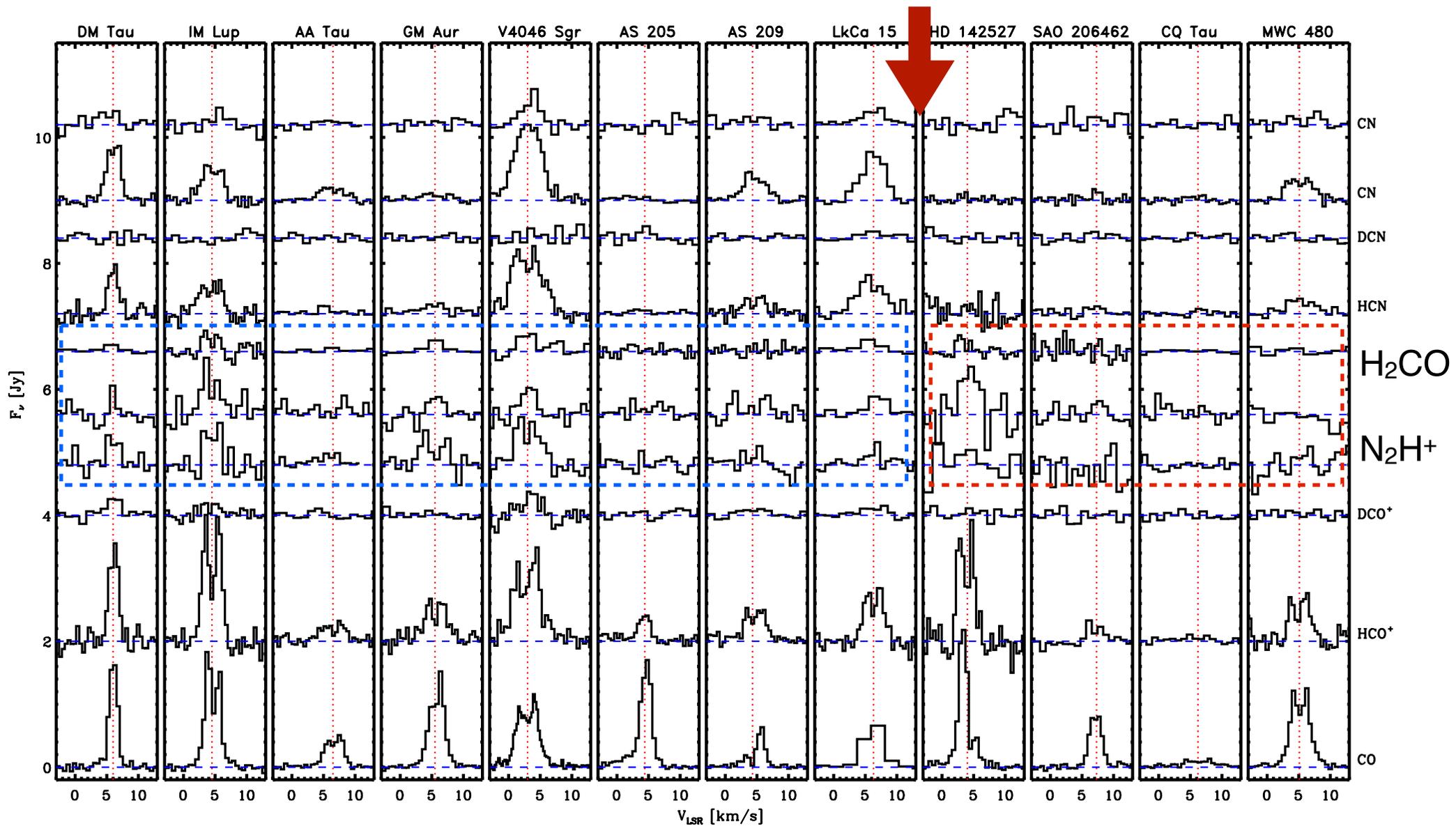
# Disk Imaging Survey of Chemistry with the SMA



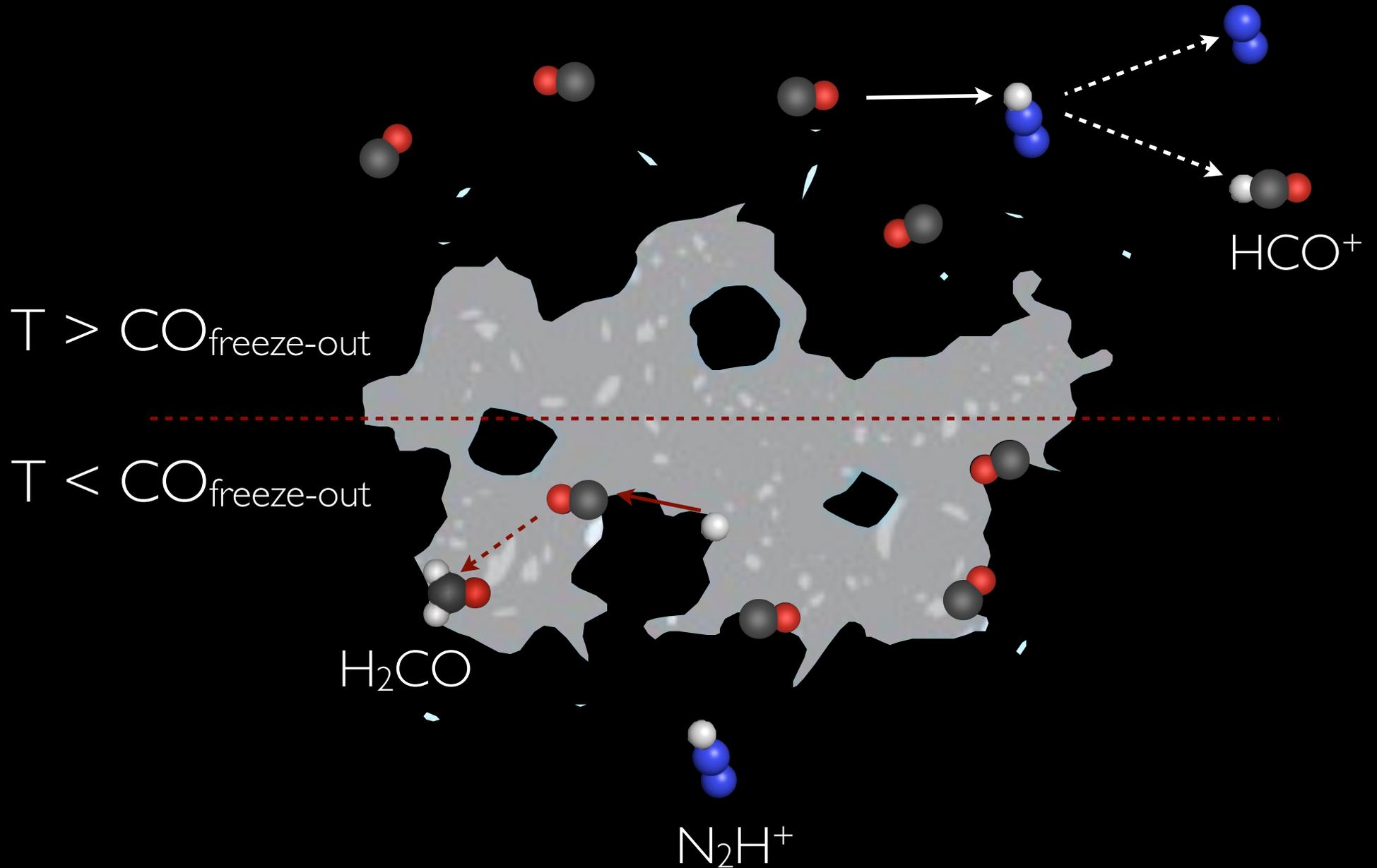
DISCS: spatially and spectrally resolved 10 molecular lines  
toward 12 protoplanetary disks in 20 tracks



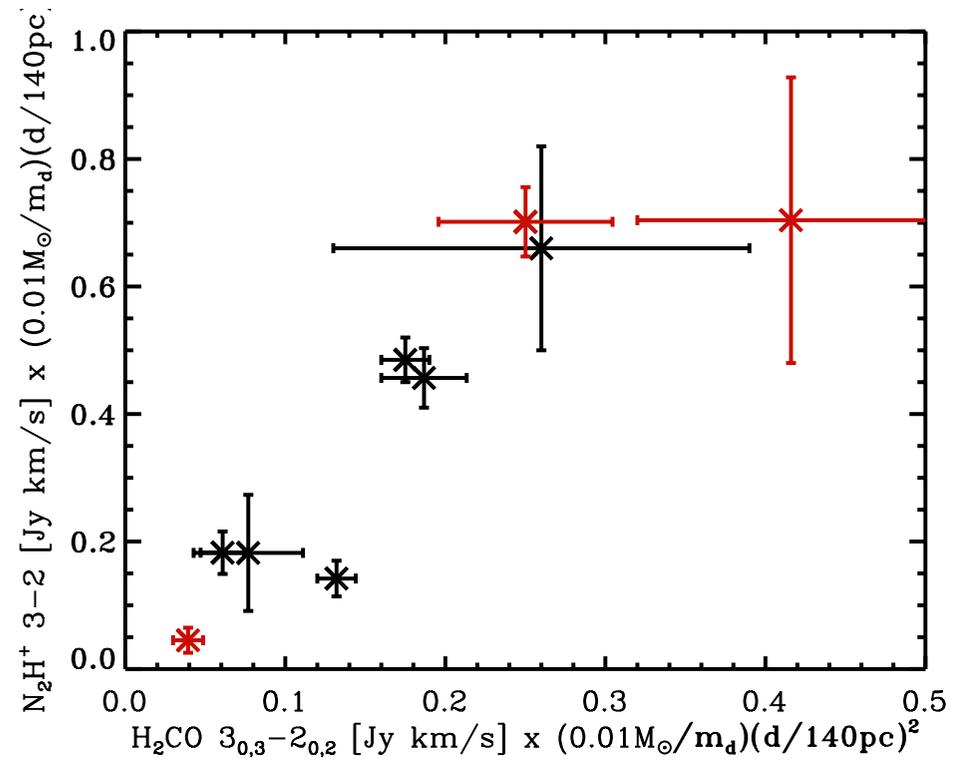
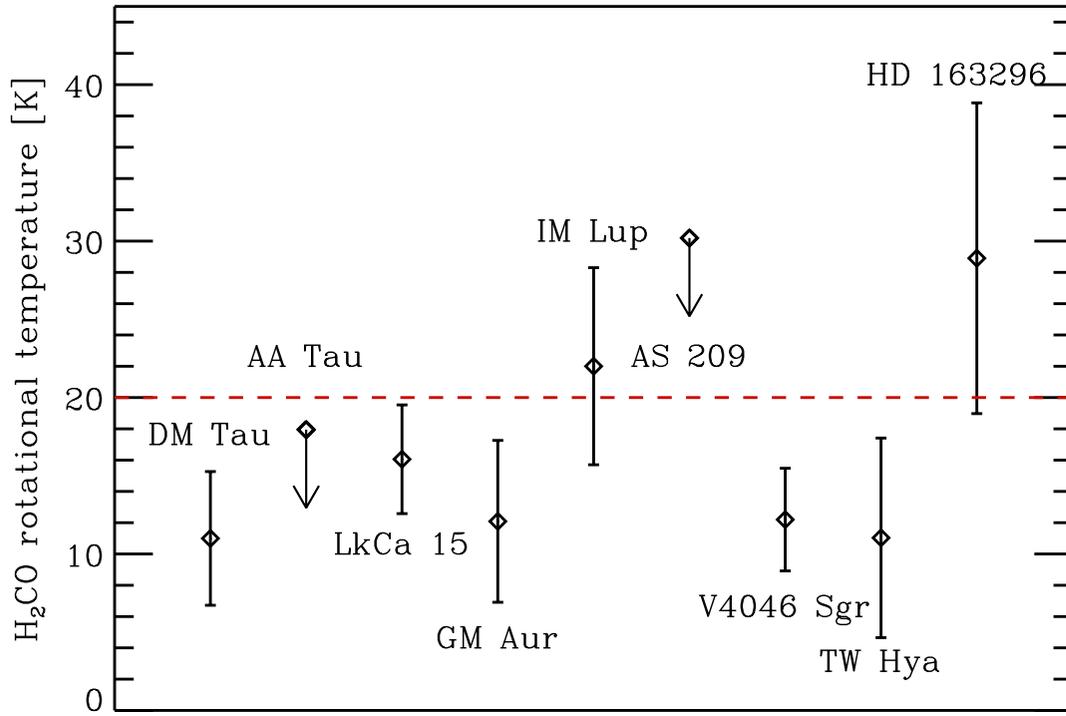
 DiSCS suggests that  $\text{H}_2\text{CO}$  and  $\text{N}_2\text{H}^+$  are more common in colder disks



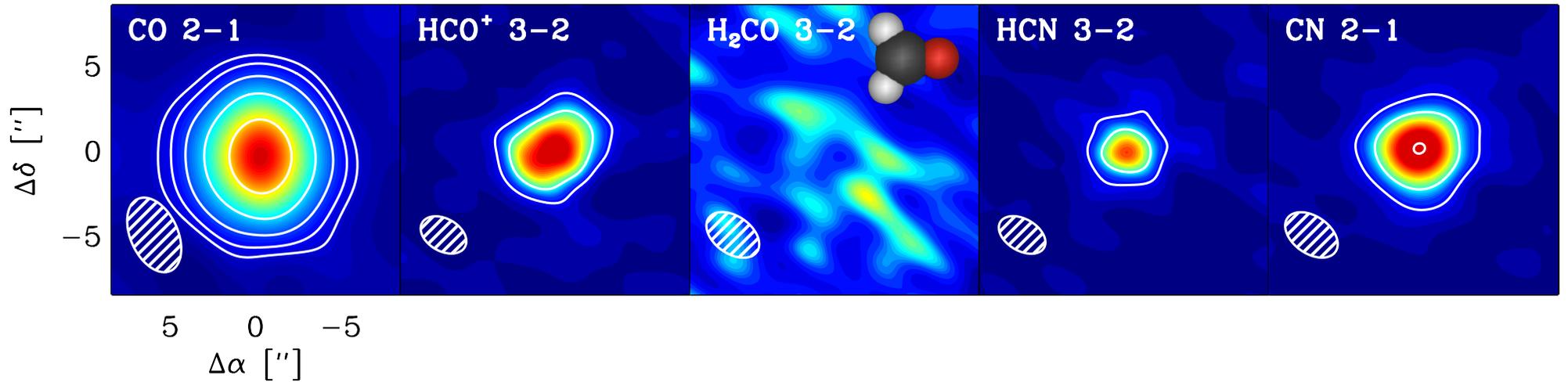
# Chemical effects of CO freeze-out



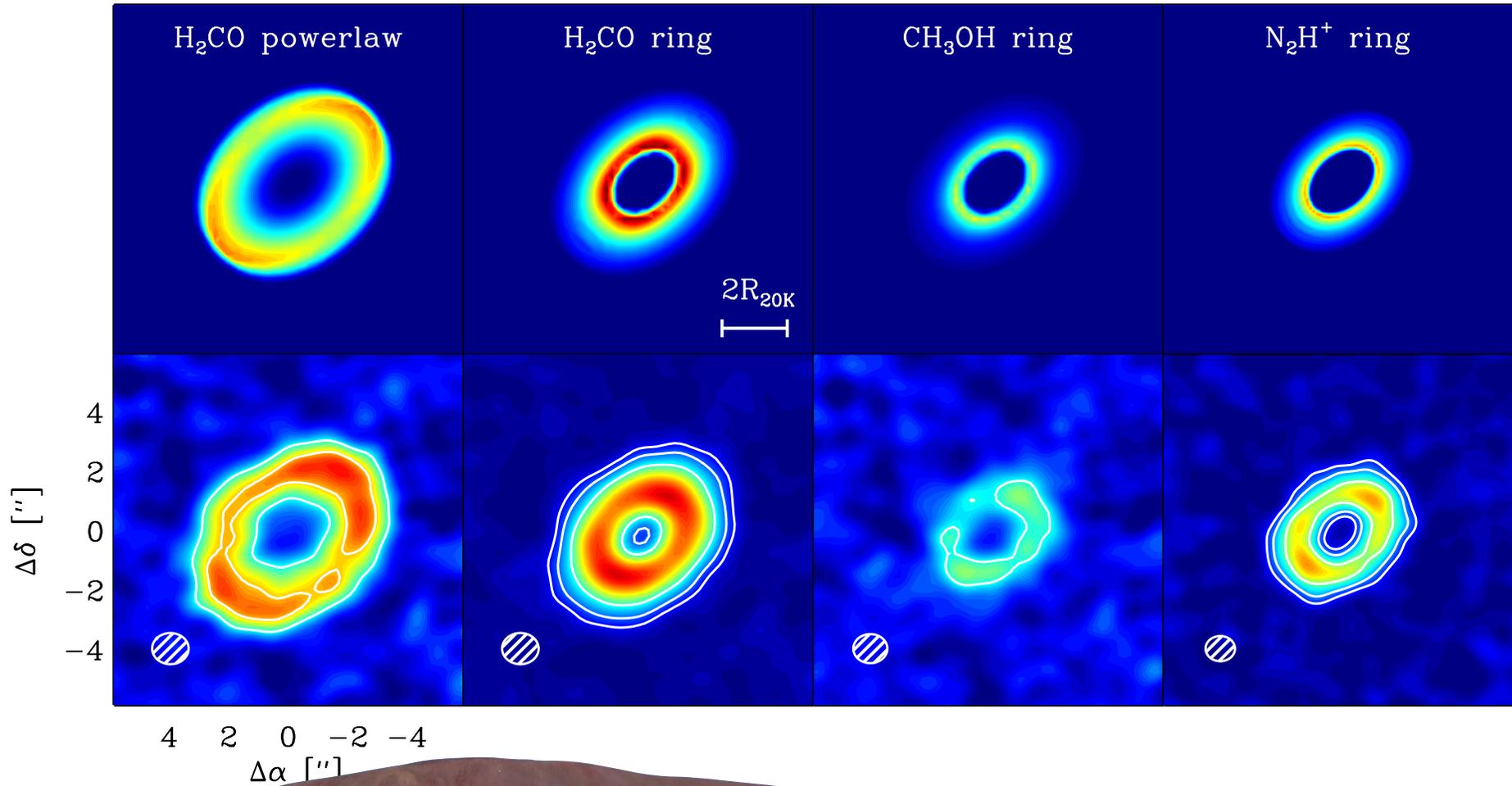
# $\text{N}_2\text{H}^+$ and $\text{H}_2\text{CO}$ in DiSCS



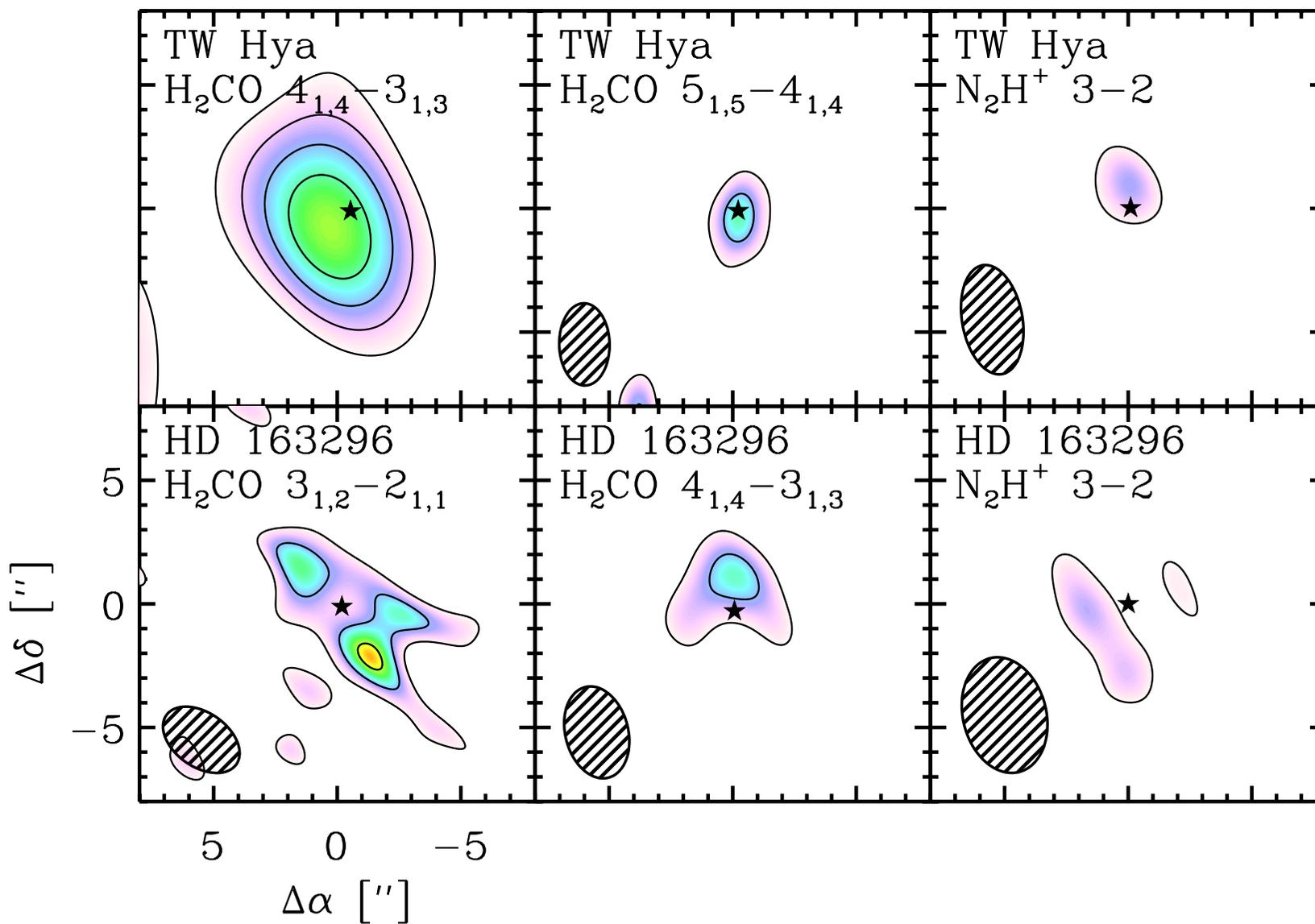
# H<sub>2</sub>CO and the CO snow line in HD 163296



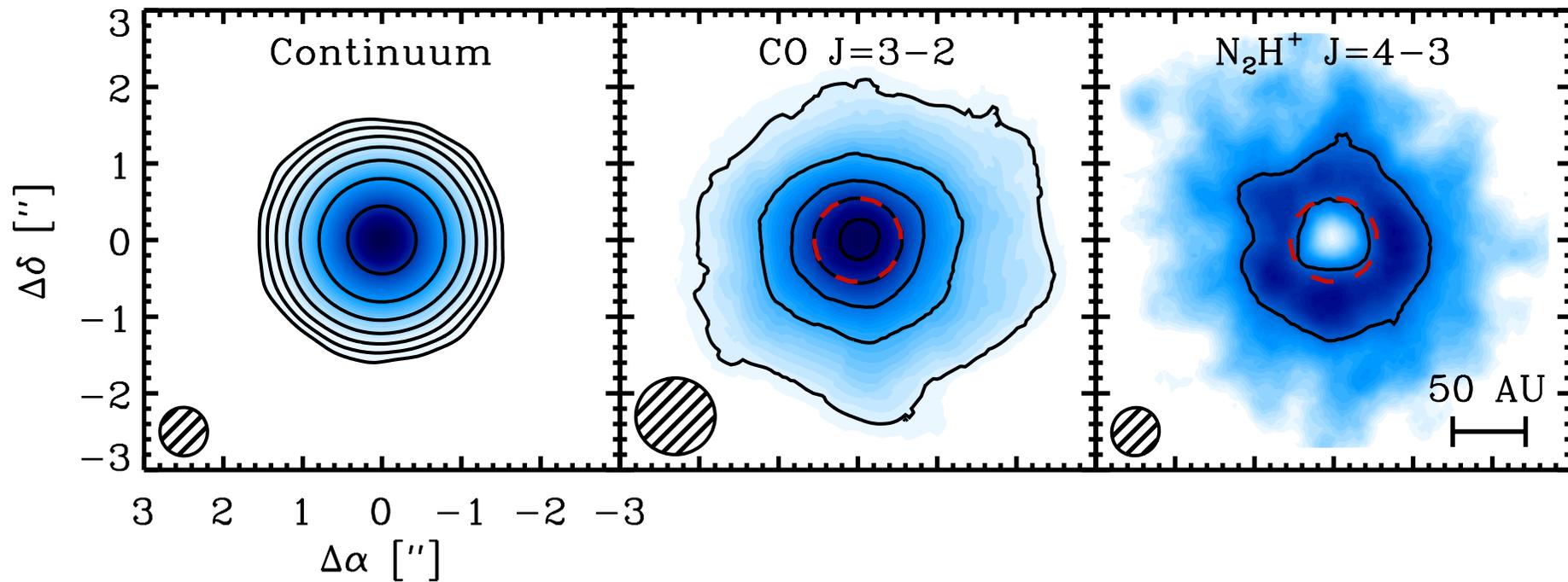
# ALMA Simulations: $\text{H}_2\text{CO}$ , $\text{CH}_3\text{OH}$ and $\text{N}_2\text{H}^+$



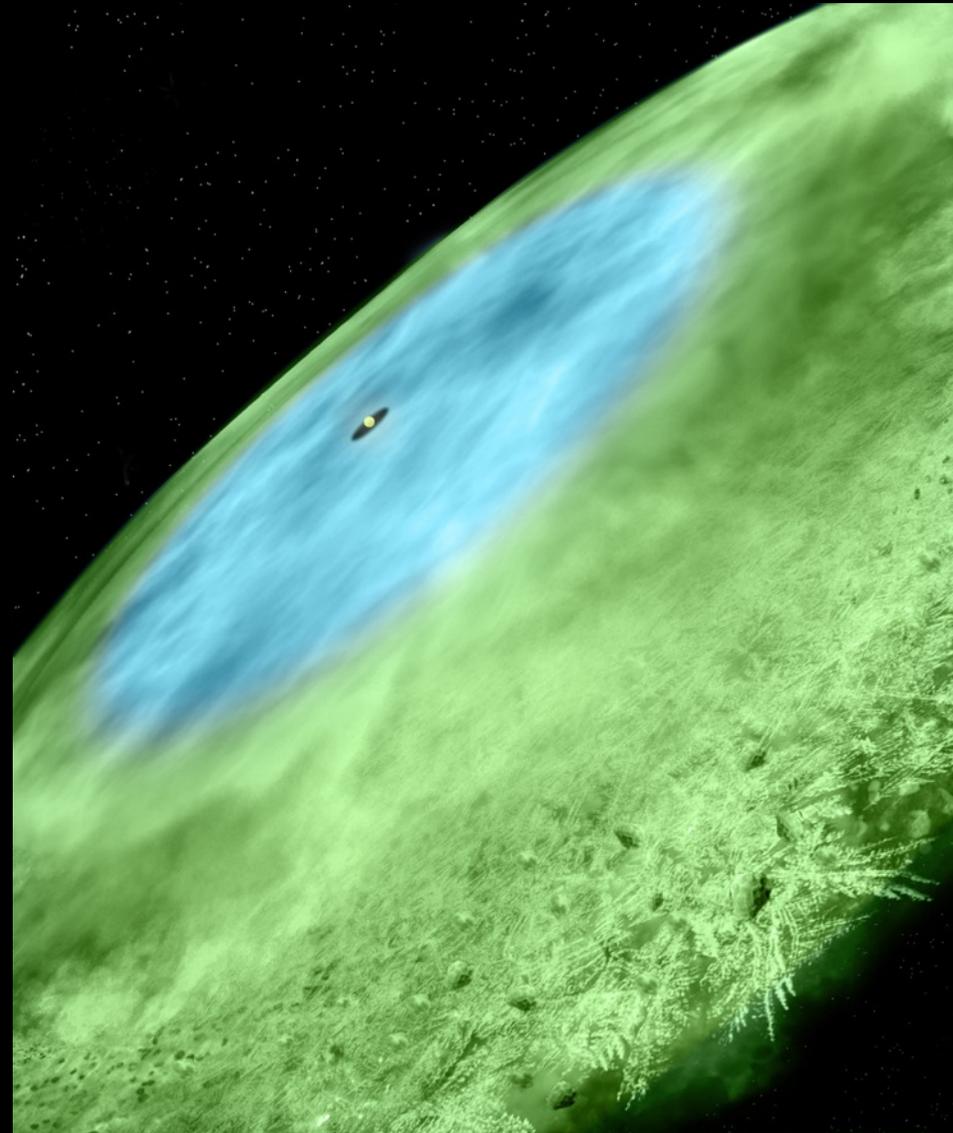
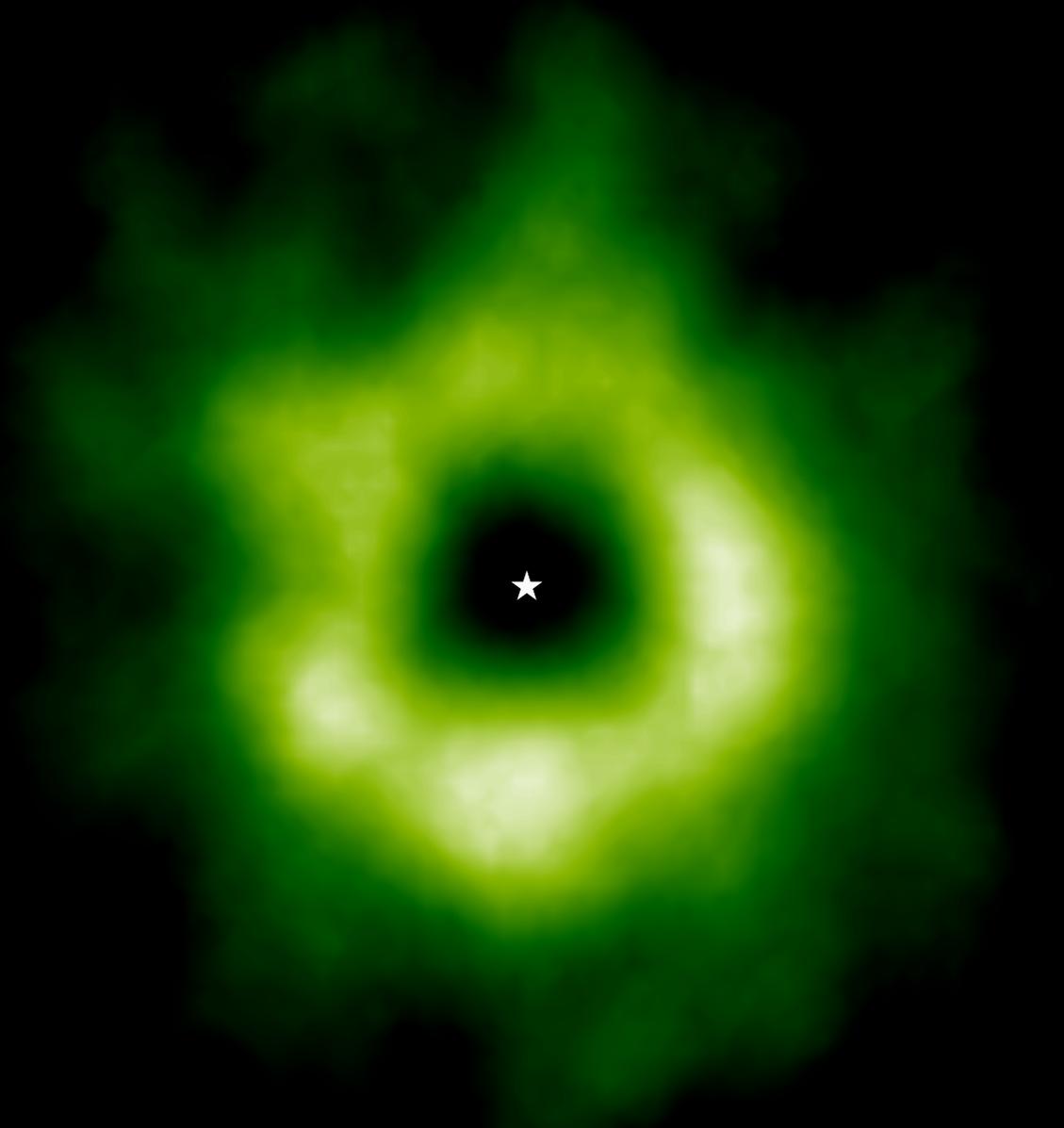
# $\text{N}_2\text{H}^+$ and $\text{H}_2\text{CO}$ toward TW Hya



# ALMA observations of the CO snowline



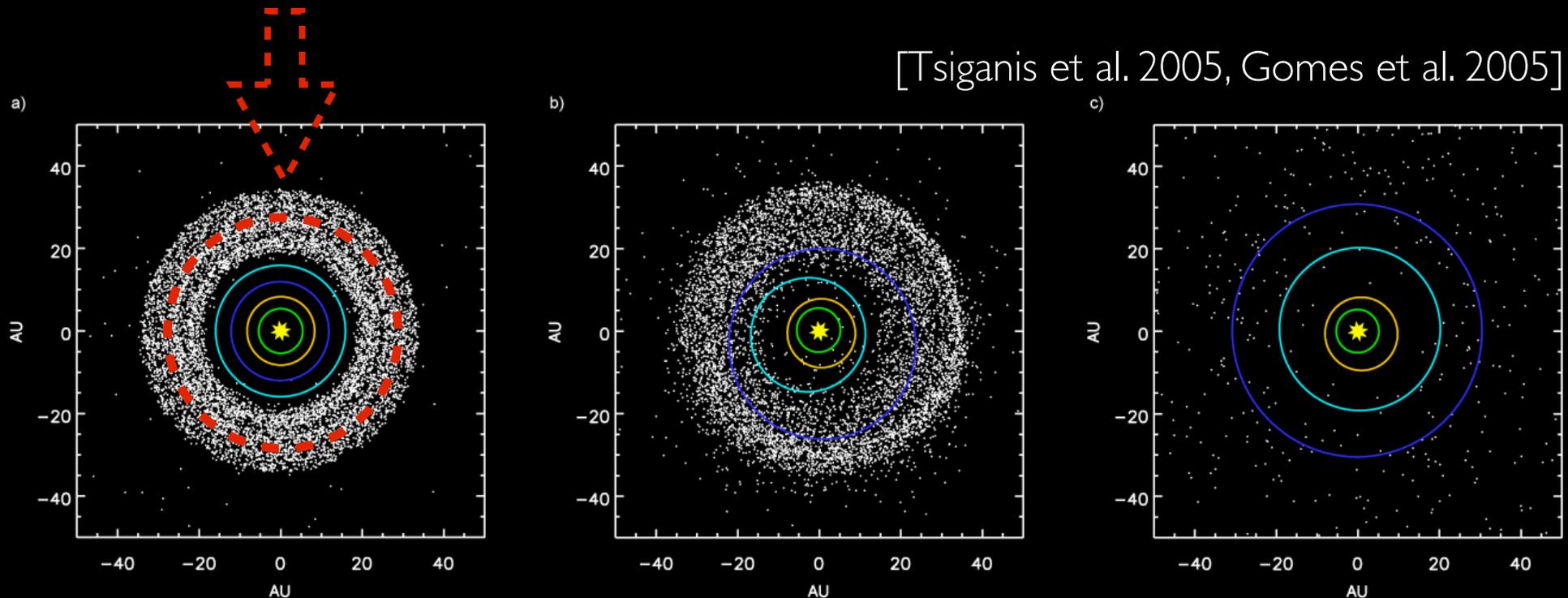
# Imaging the CO snowline



# CO snow line radius implications for the Solar System

CO snow line

[Tsiganis et al. 2005, Gomes et al. 2005]

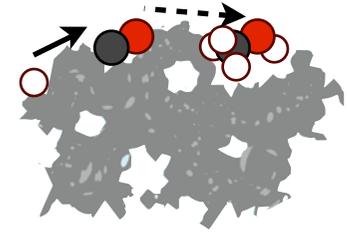


CO snow line is outside of Ice Giant formation zone according to Nice model

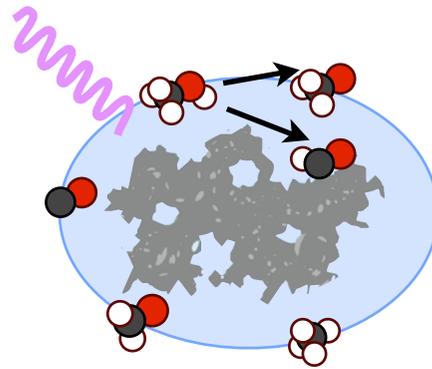
**Some** comets and Kuiper belt objects should have formed from CO-ice grains

# Ice Chemistry

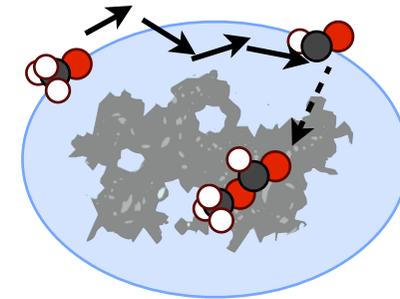
0. Grain surface atom addition reactions (10-20 K)



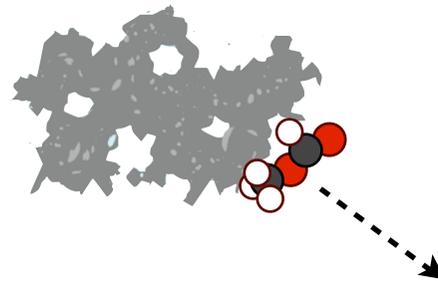
I. Ice dissociation (All T)



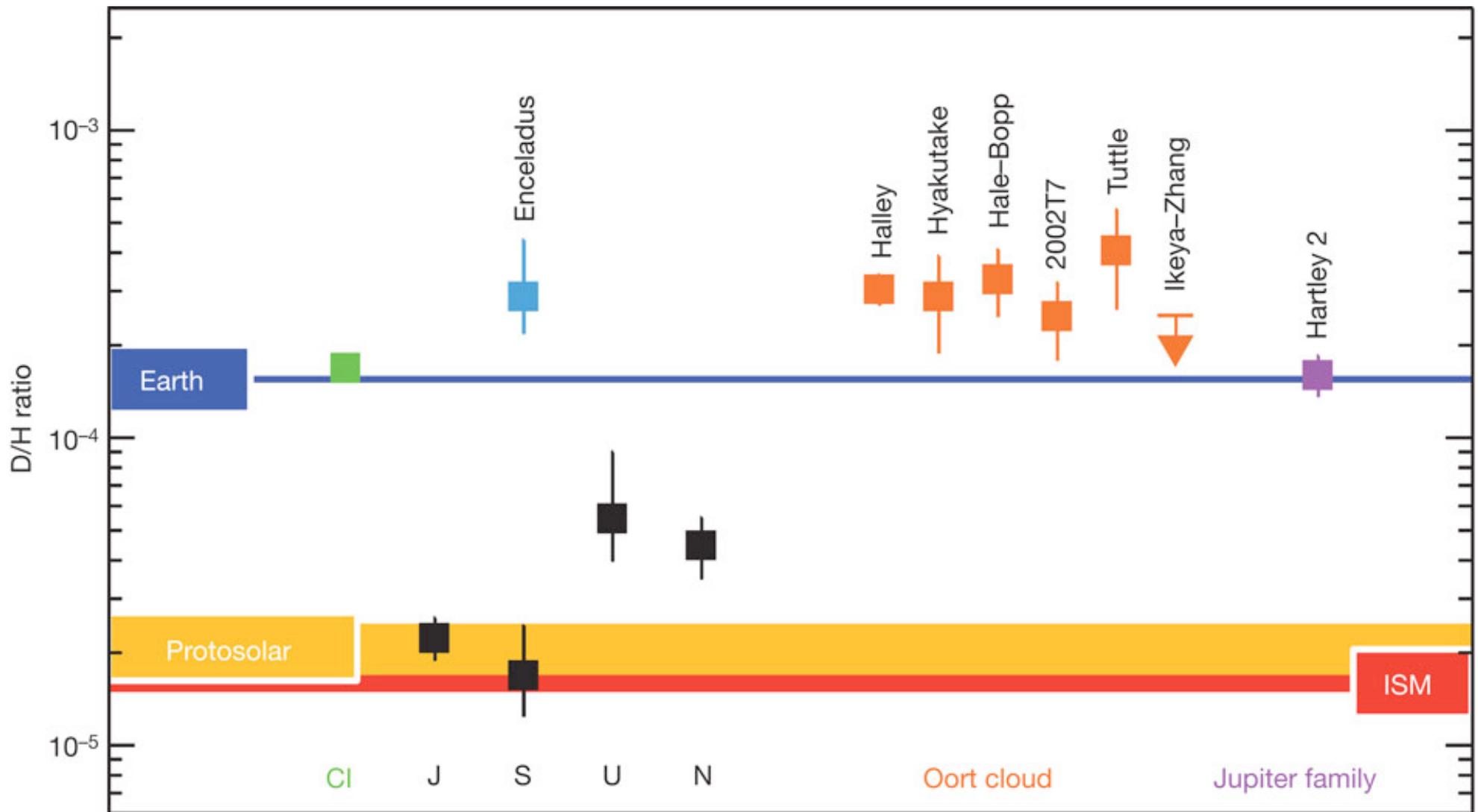
II. Radical diffusion + recombination (25+ K)



III. Ice desorption (30-200 K)

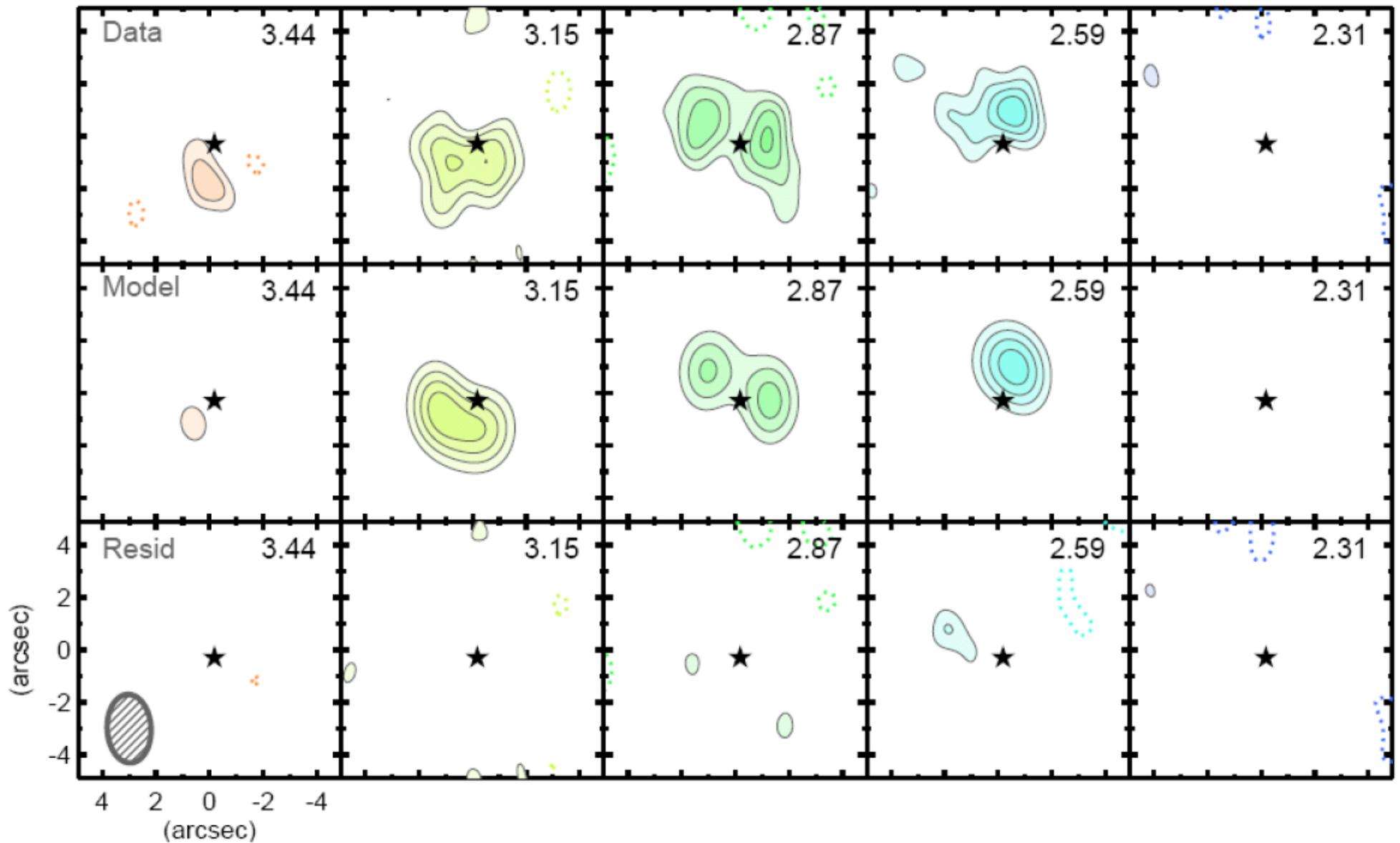


# Delivery of volatiles to Earth from Comets?

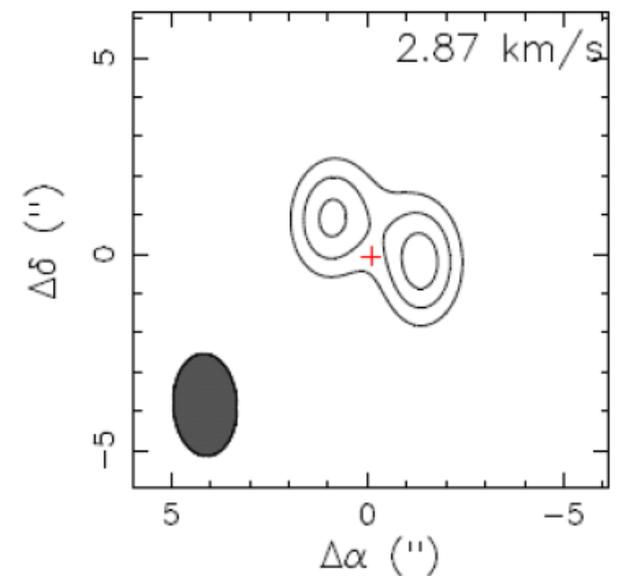
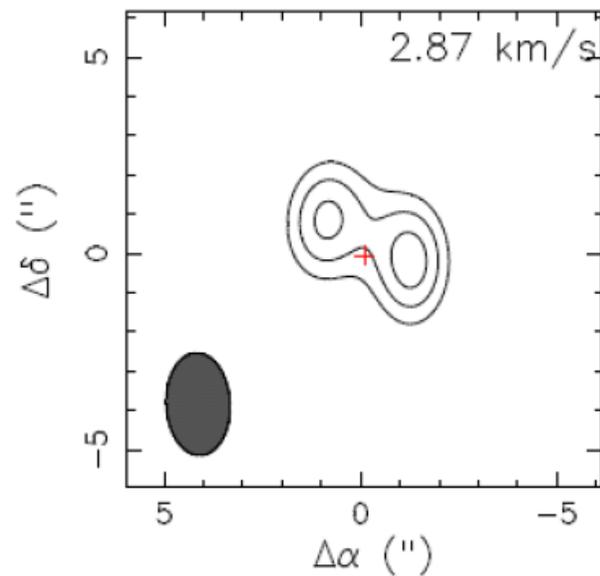
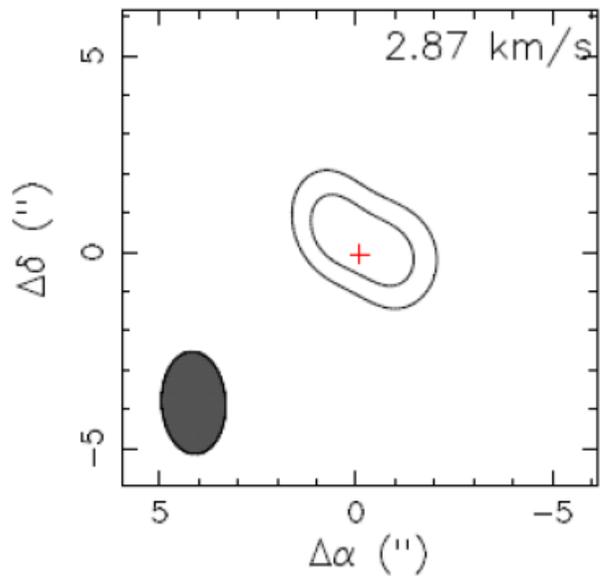
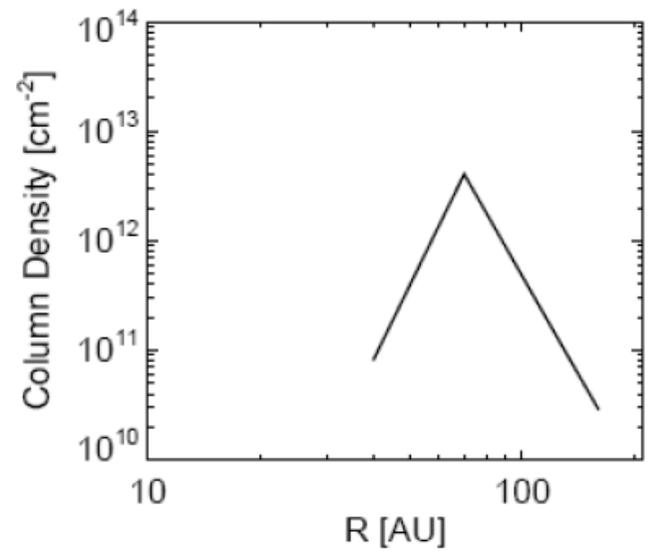
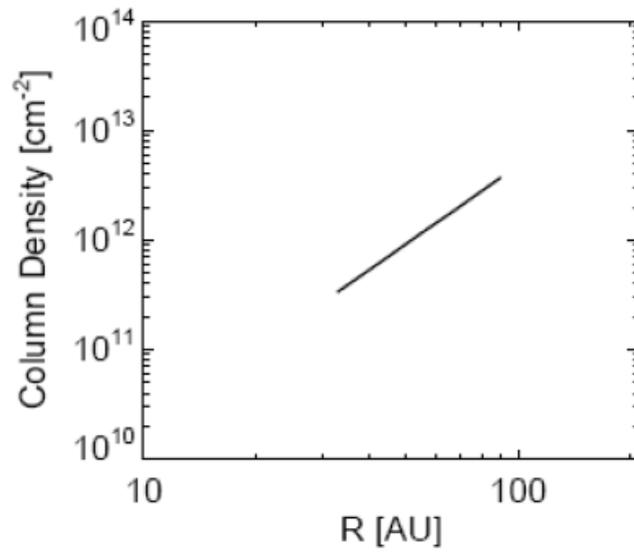
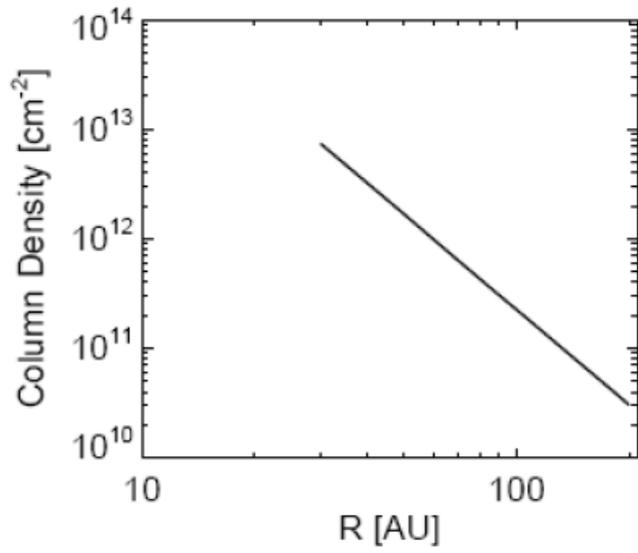


Deuterium enrichment expected at low temperatures because:  
 $XH + HD \leftrightarrow XD + H_2 \quad \Delta H < 0$ , but  $\Delta H$  is “small”

# DCO<sup>+</sup> toward TW Hya

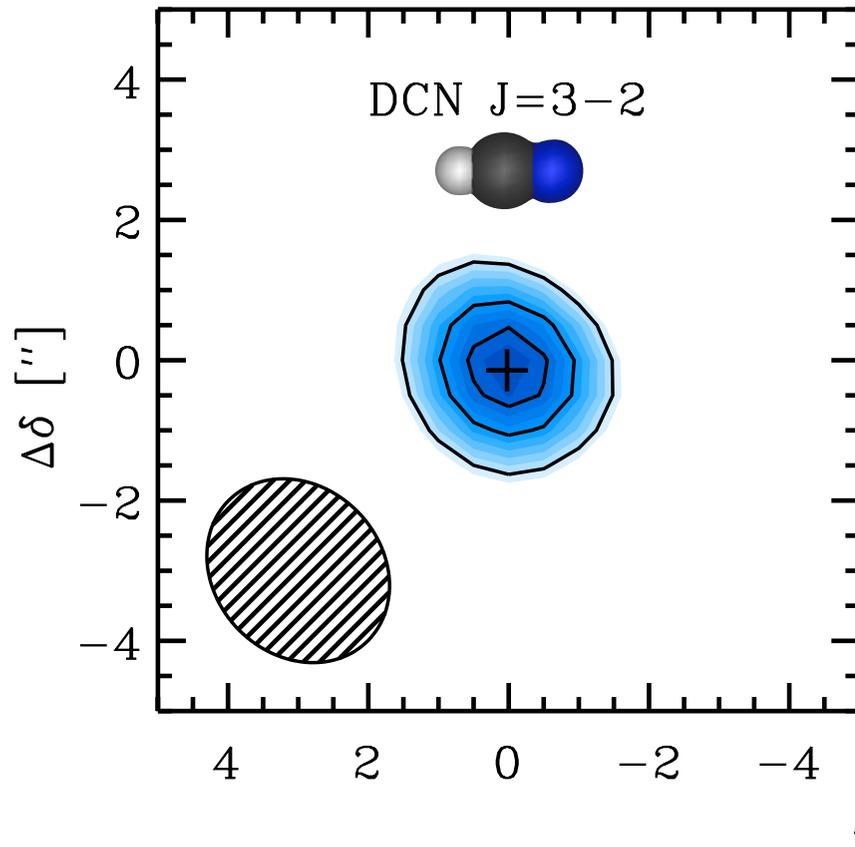


# A DCO<sup>+</sup> ring

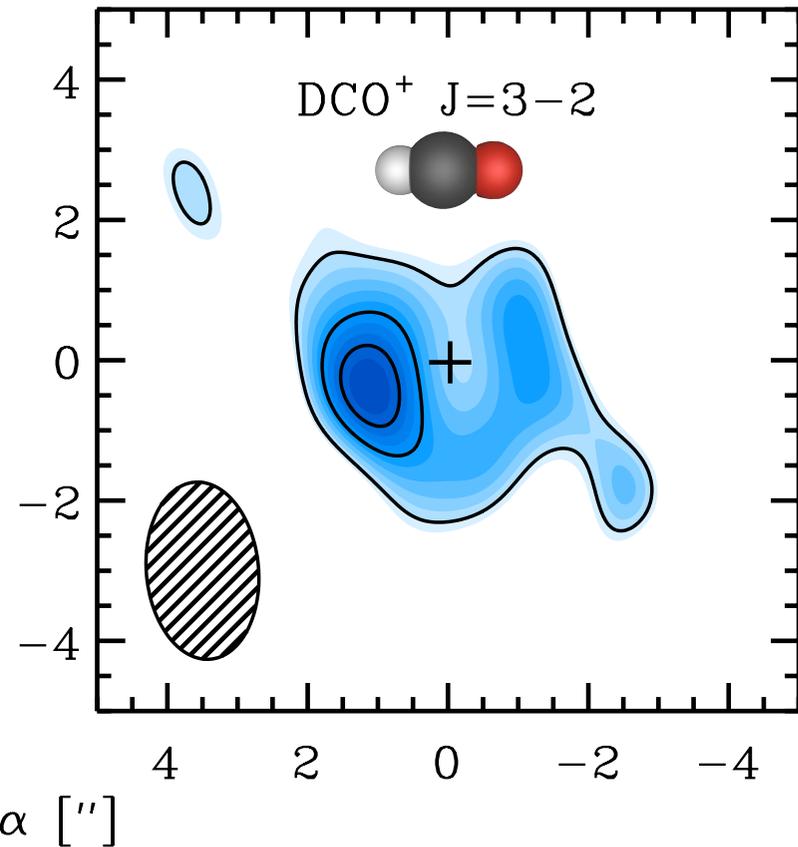


# Cold and warm deuterium fractionation pathways from SMA+ALMA

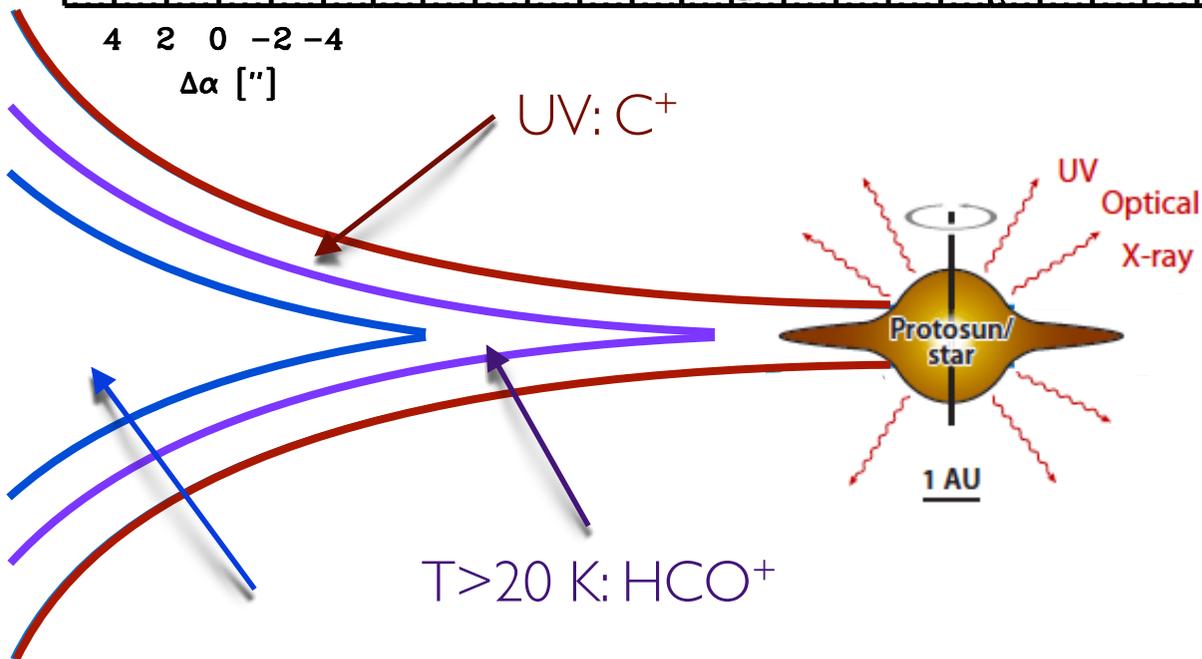
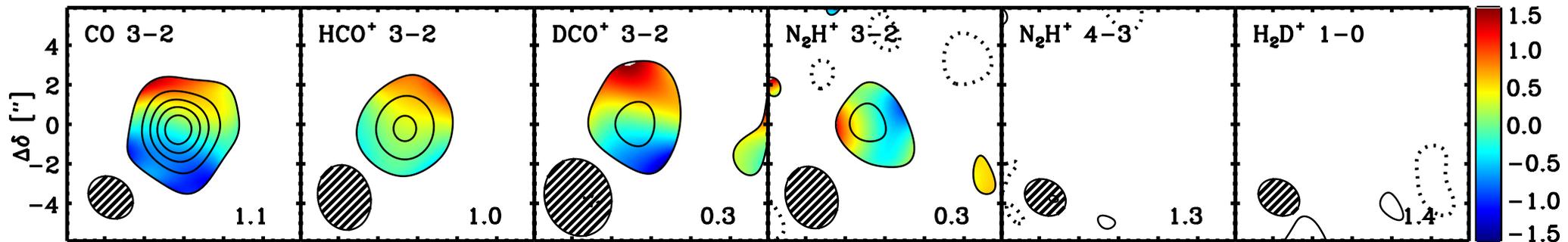
$\text{CH}_2\text{D}^+$   $T < 50$  K



$\text{H}_2\text{D}^+$   $T < 30$  K



# Ionization toward DM Tau

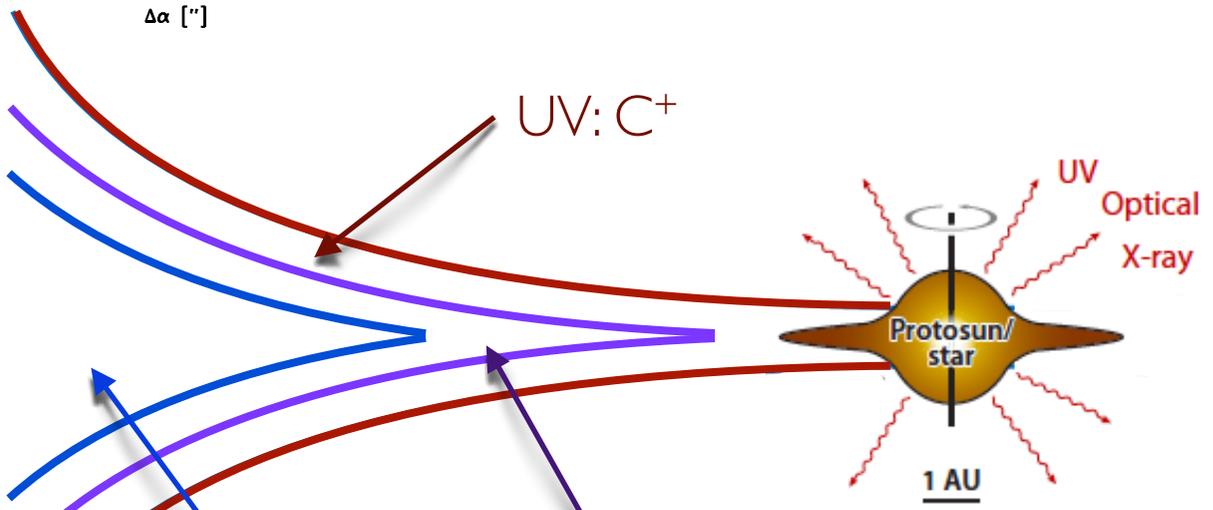
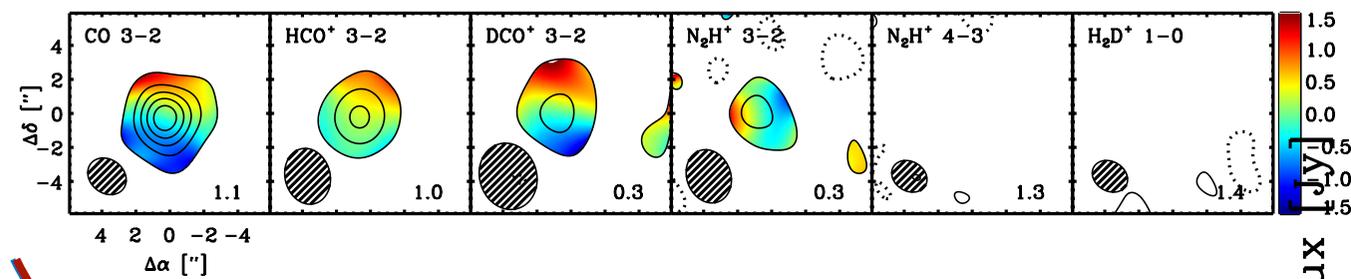


T < 20 K: CO + gr → CO:gr, N<sub>2</sub>H<sup>+</sup>, N<sub>2</sub>D<sup>+</sup>

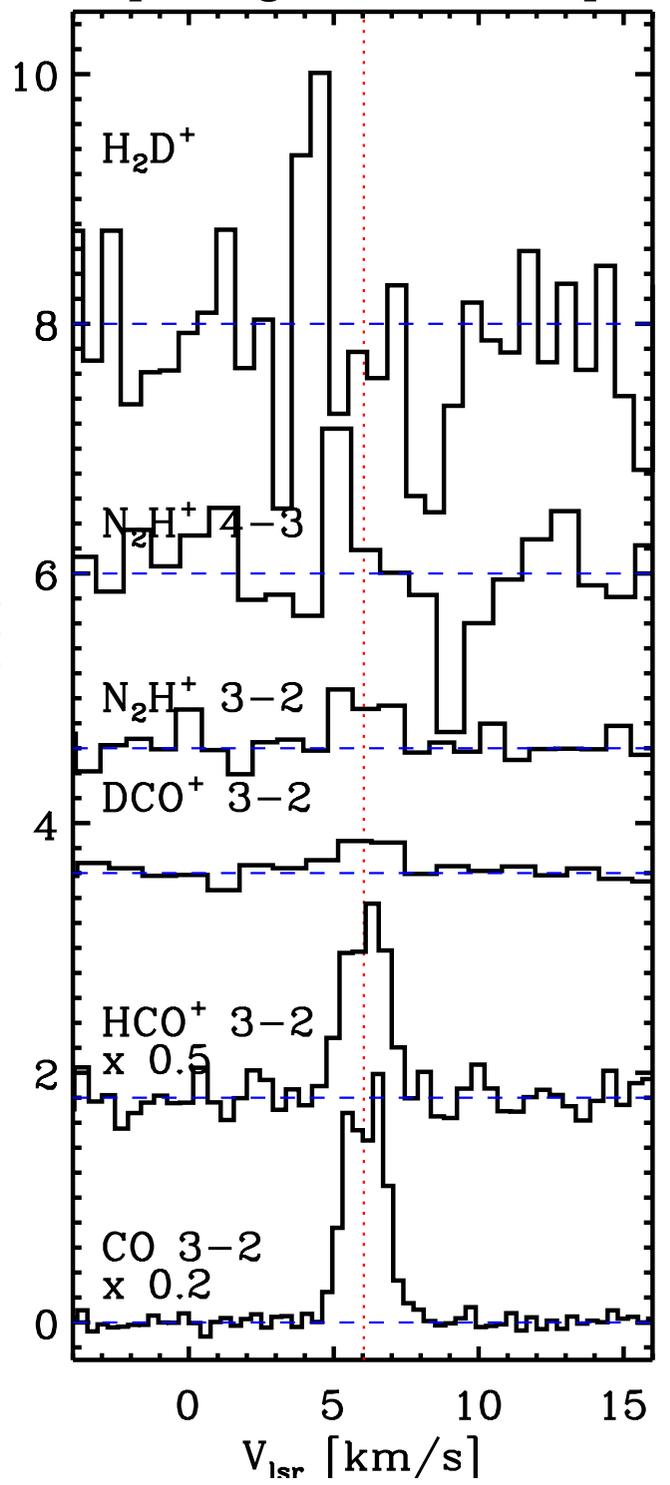
T < 16 K: N<sub>2</sub> + gr → N<sub>2</sub>:gr, H<sub>2</sub>D<sup>+</sup>

# Ionization toward DM Tau

[Öberg, Qi et al. 2011]



$T < 20 \text{ K: CO} + \text{gr} \rightarrow \text{CO:gr, N}_2\text{H}^+, \text{N}_2\text{D}^+$   
 $T < 16 \text{ K: N}_2 + \text{gr} \rightarrow \text{N}_2\text{:gr, H}_2\text{D}^+$



# The Chemistry of Protoplanetary Disks

CO observations have revealed a rich disk temperature structure, but its chemistry is causing trouble. The first snow line has been chemically imaged. SMA observations have challenged models on deuterium fractionation, UV chemistry and ionization — looking to ALMA for answers

