DTA Symposium
June 1-4, 2015 @ NAOJ

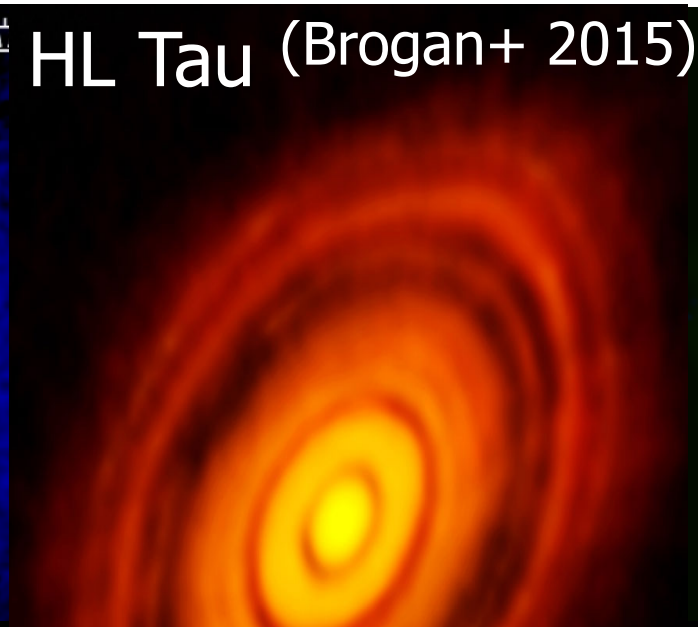
Chemical Processes in Protoplanetary Disks

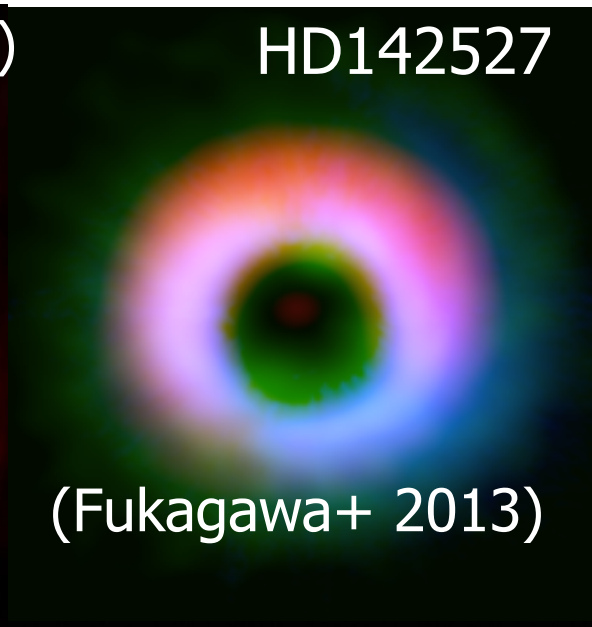
~ Water, Snowlines & Organic Molecules ~

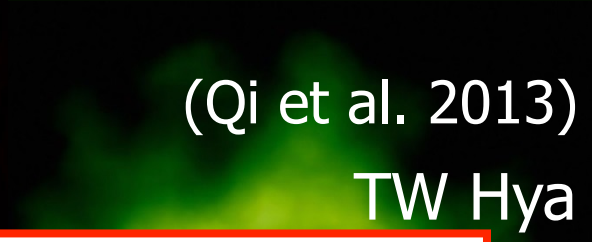
Hideko Nomura (TITECH)

§1 Introduction

Gas & Dust Observations in PPDs







Observationally diagnosing physical & chemical structure of planet-forming regions

Obs. of Gas in Protoplanetary Disks

UV H_2 Lyman-Werner band transitions

Optical

[OI] 6300A

NIR

H_2 v=1-0 S(1), S(0),
CO $\Delta v=2$, $\Delta v=1$, etc.

MIR

H_2 v=0-0 S(1), S(2), S(4)

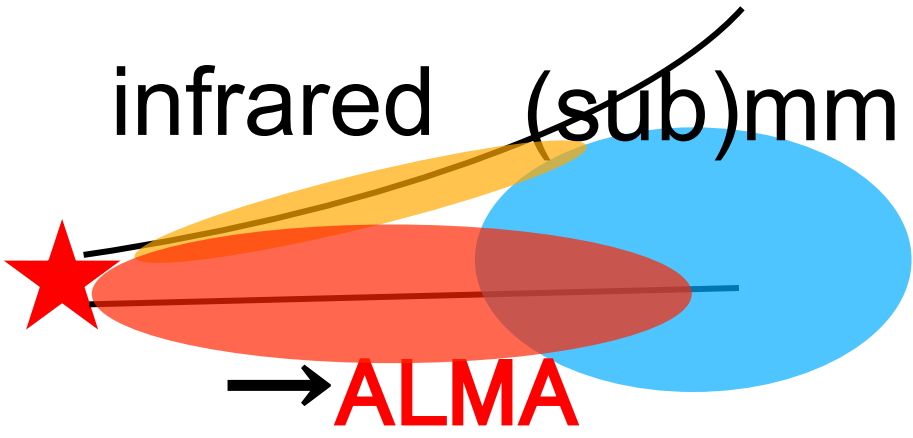
H_2O, OH, HCN, C_2H_2, CO_2
(Spitzer Space Telescope)

FIR

[OI] 63um, 145um,
CO, H_2O, CH^+, HD, etc.
(Herschel Space Observatory)

(sub)mm

^{12}CO, ^{13}CO, $C^{18}O$,
HCO^+, $H^{13}CO^+$, DCO^+,
C_2H, c-C_3H_2, H_2CO,
HCN, HNC, DCN, CN,
N_2H^+, HC_3N, CH_3CN,
CS, $C^{34}S$, etc.



Chemical Models of Protoplanetary Disks

Chemical reaction network + Physical model of PPDs

- Include physical processes :

  dust evolution & gas motion

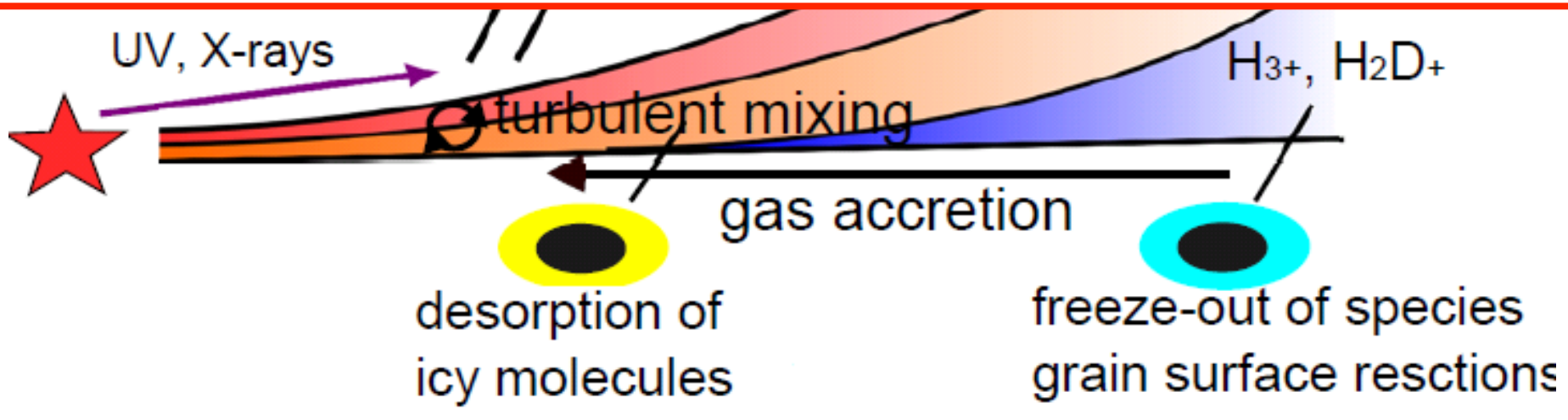
- Include various chemical reactions:

  dueterated species, grain surface chemistry, etc.

Comparison between model & obs.

→ Physical structure of PPDs &

Origin of materials in our Solar System



Contents

§1. Introduction

§2. Water & Snowlines in PPDs

- Detecting H_2O snowline in PPDs
- C/O ratio distribution in PPDs

~ Exoplanet formation process~

- Deuterated water

§3. Formation of Organic Molecules in PPDs

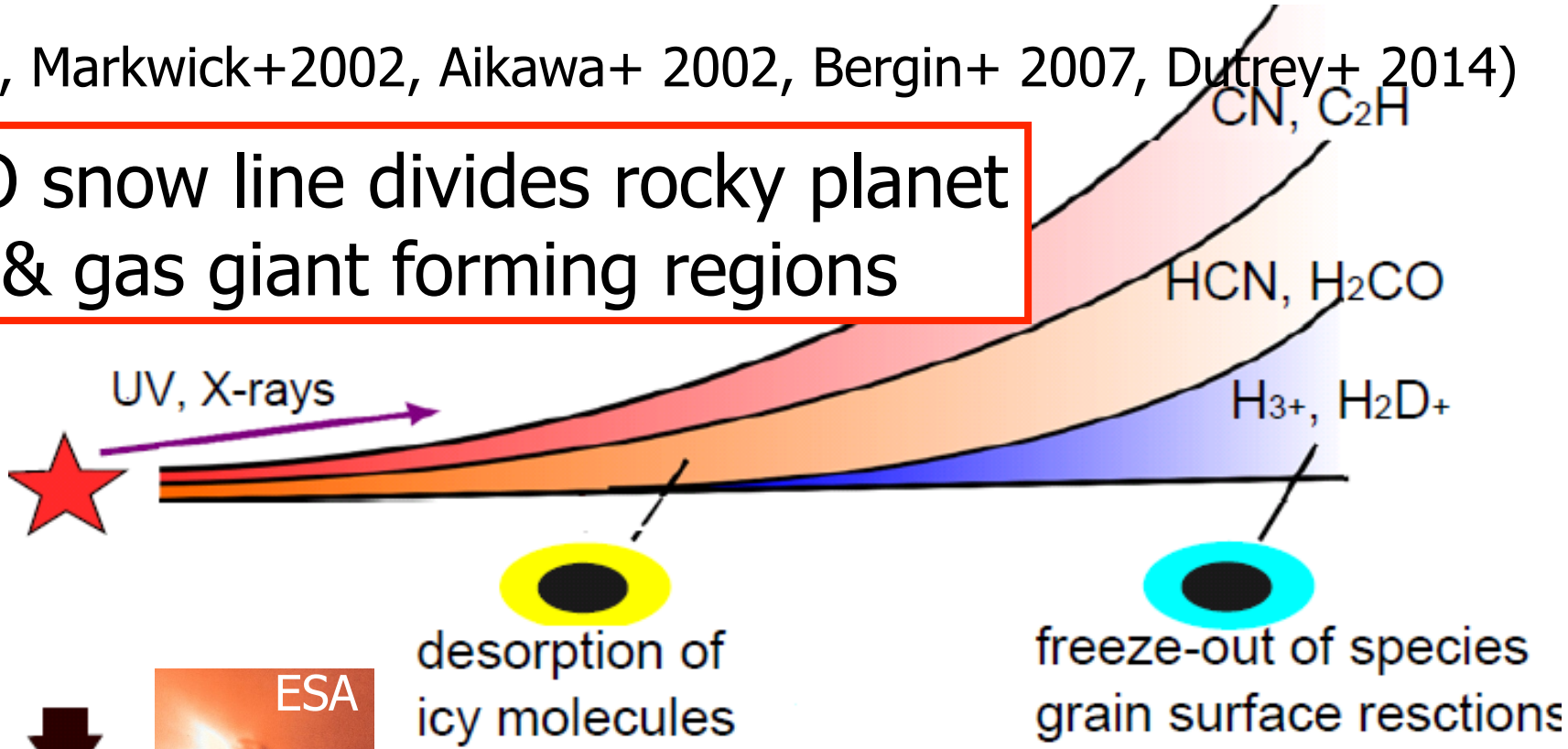
§4. Summary

§2
Water & Snowlines in Protoplanetary Disks

H_2O Snow Line & Planet Formation

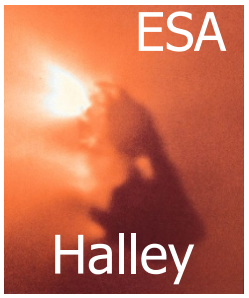
(e.g., Markwick+2002, Aikawa+ 2002, Bergin+ 2007, Dutrey+ 2014)

H_2O snow line divides rocky planet & gas giant forming regions



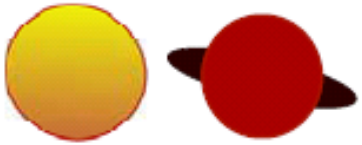
desorption of icy molecules

freeze-out of species grain surface resctions



H_2O, CO_2, CH_4, CH_3OH, H_2CO, NH_3, HCN, etc.

rocky planets



gas giants

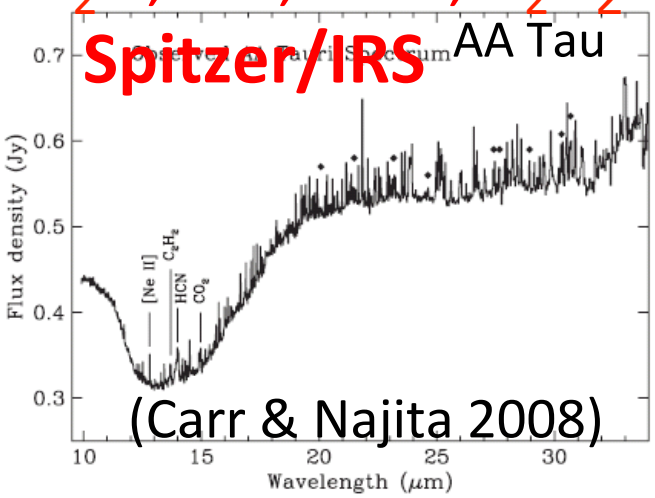
ice giants

H_2O snow line

Obs. of water lines from PPDs

H_2O, OH, HCN, C_2H_2

Spitzer/IRS

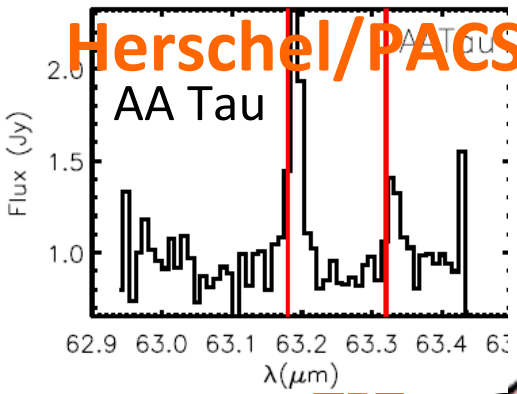


(Carr & Najita 2008)

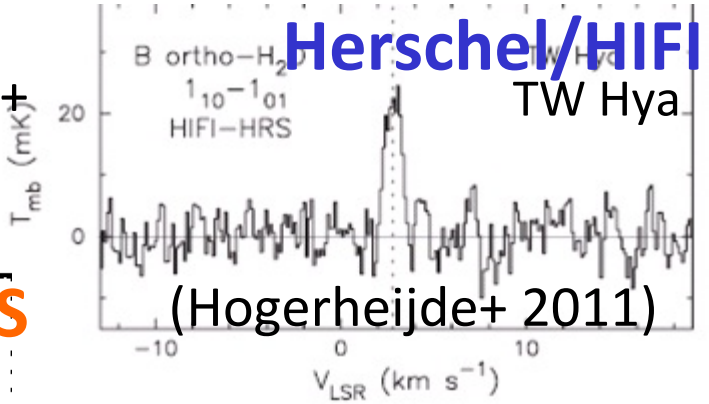
(Riviere-Marichalar+ 2012)

[OI] H_2O

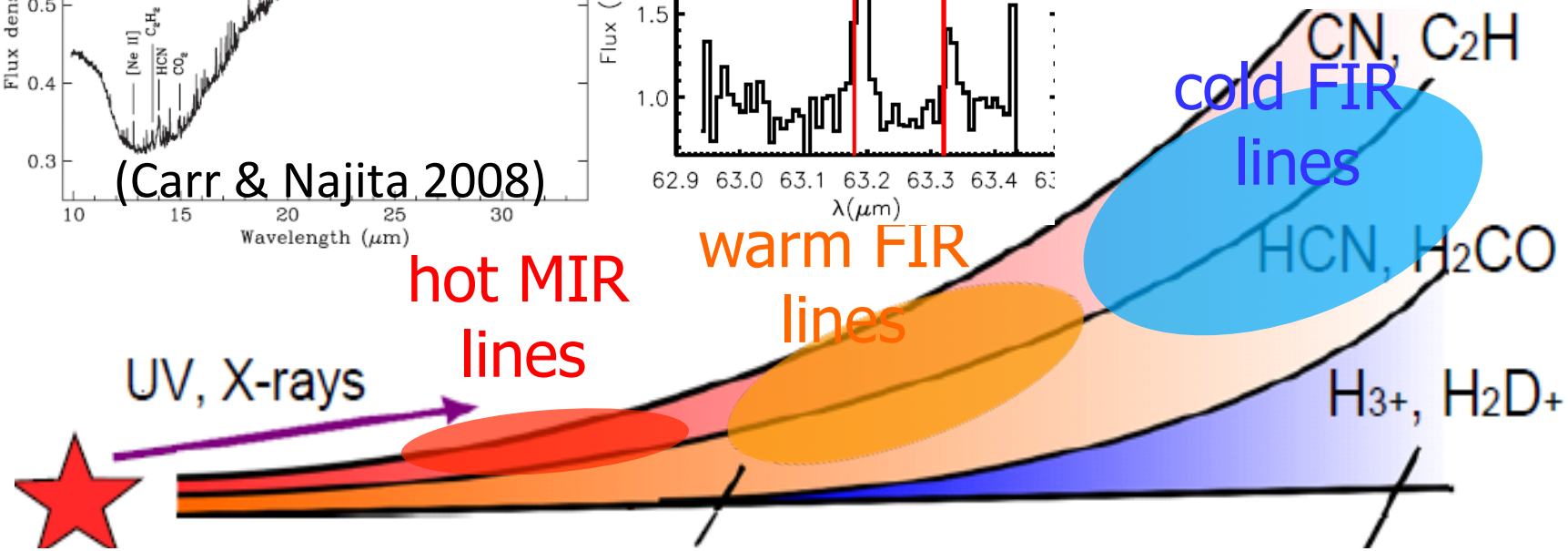
Herschel/PACS



Herschel/HIFI



(Hogerheijde+ 2011)

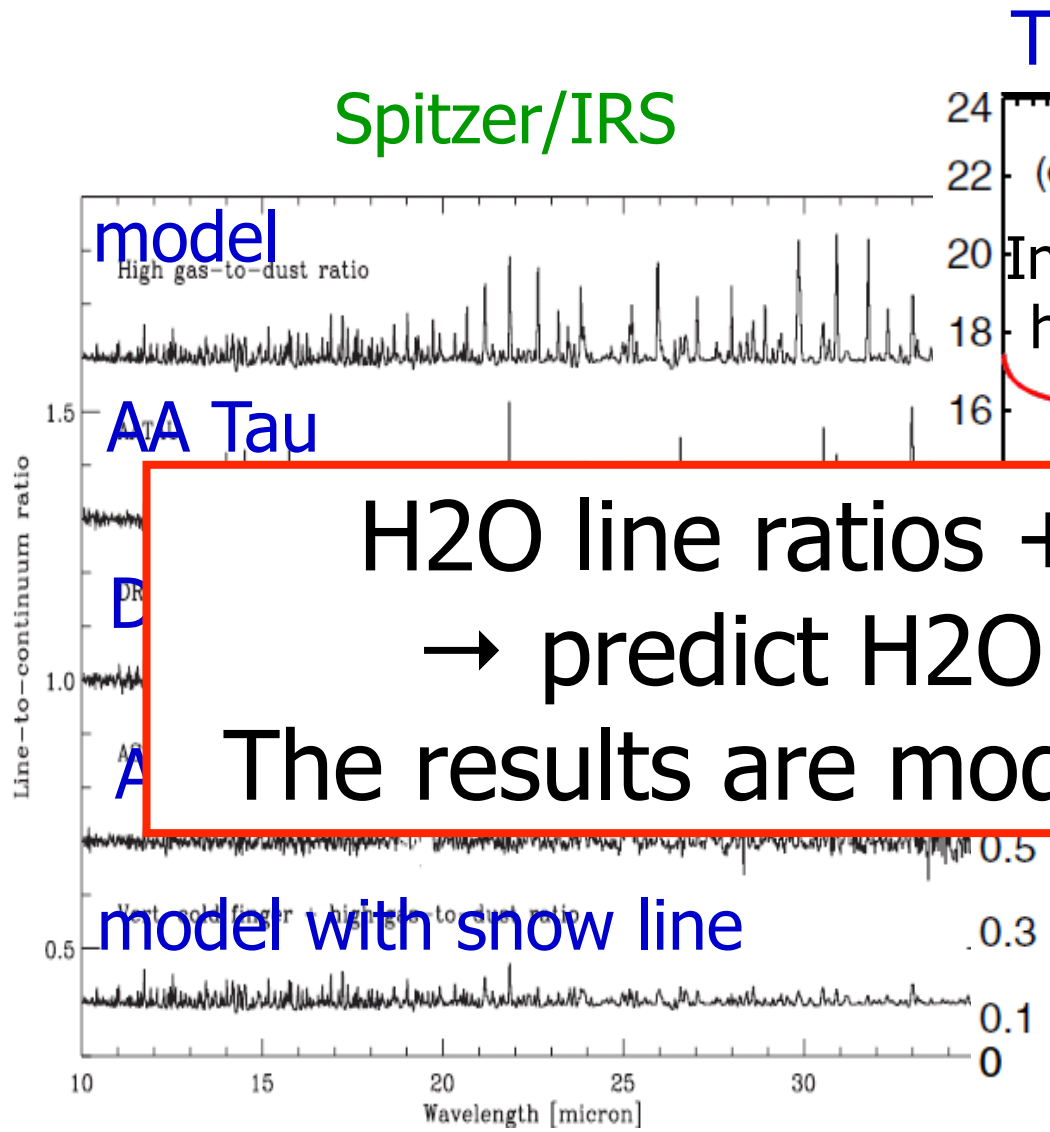


Spitzer hot H2O@10-35μm, TTSs: detect, HAEBEs: upper limits

Herschel warm H2O TTSs, HAEBEs: @55-180μm

Herschel cold H2O @267μm, 539μm, TW Hya, HD100546

H2O snow lines in PPDs

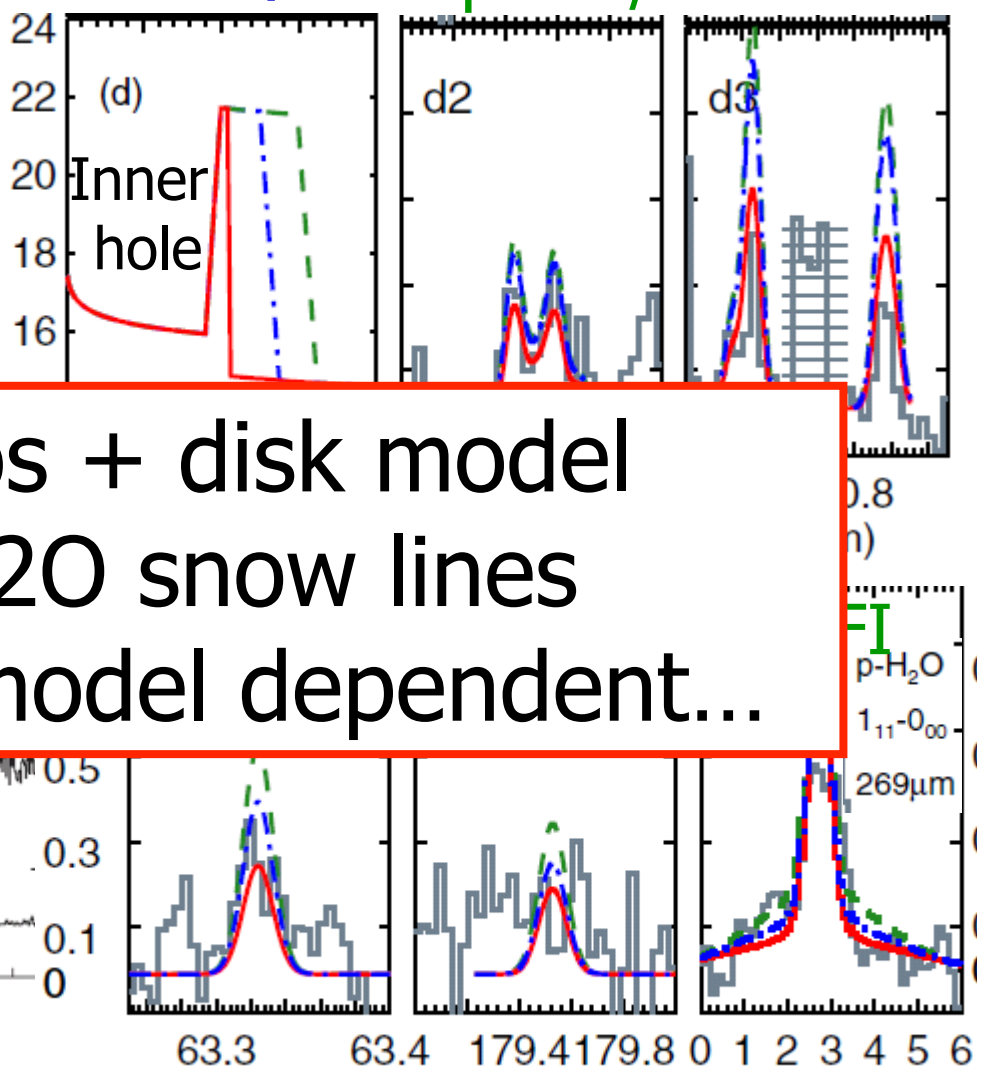


H_2O Snow line @ ~1AU

(Meijerink+ 2009)

TW Hya

Spitzer/IRS



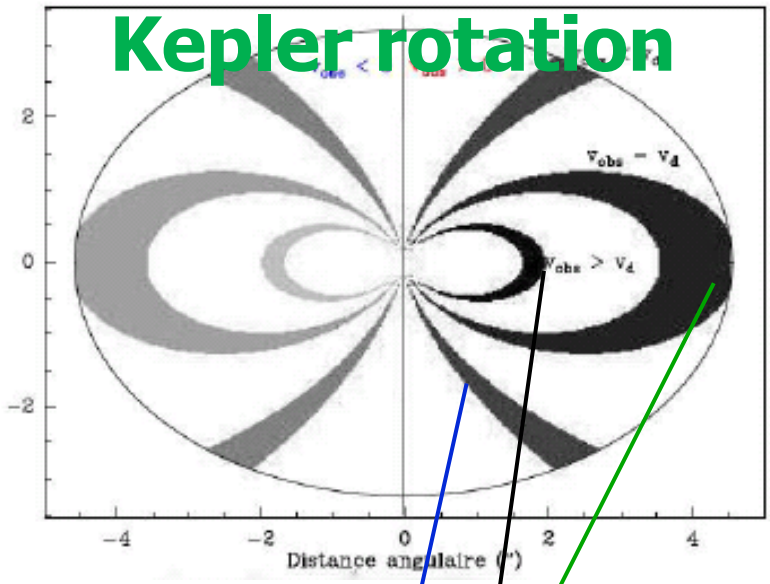
H2O line ratios + disk model
→ predict H2O snow lines
The results are model dependent…

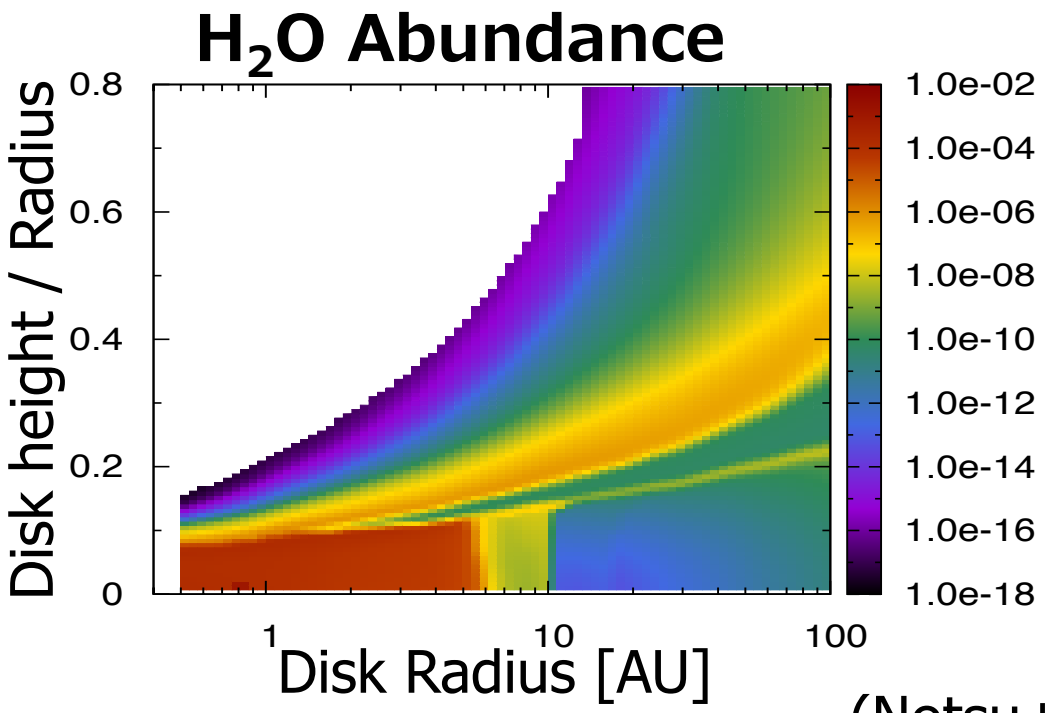
H_2O Snow line @ ~4AU

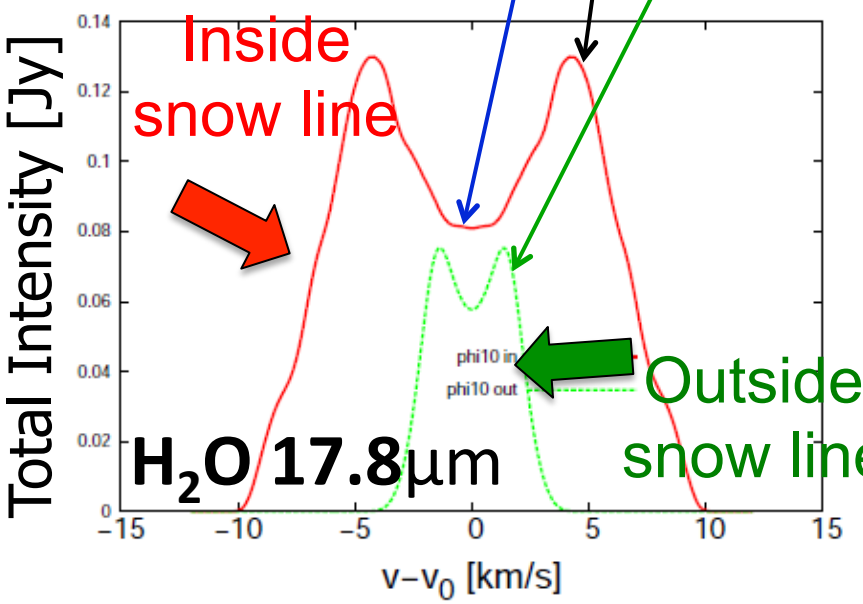
(Zhang+ 2013)

H_2O Snow Line by High-R. Obs.

H_2O snow line will be detected using high-R (R~100,000) spectroscopic observations (ALMA, TMT, SPICA, …)

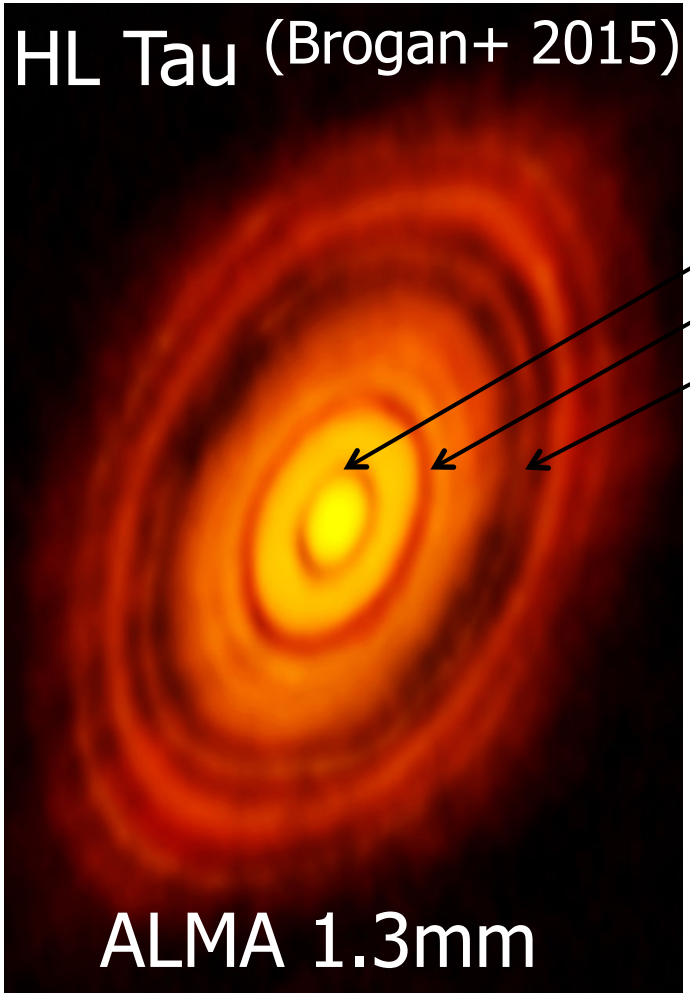


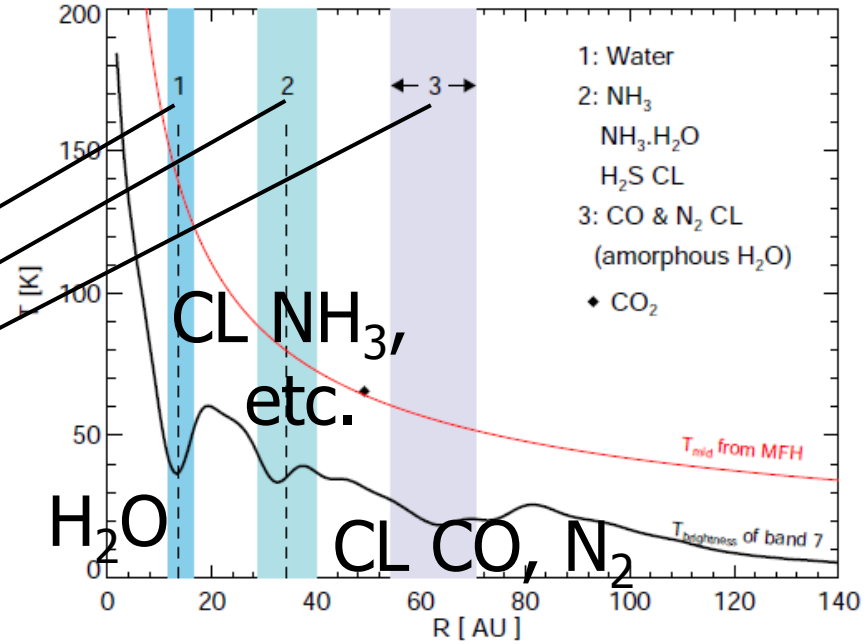




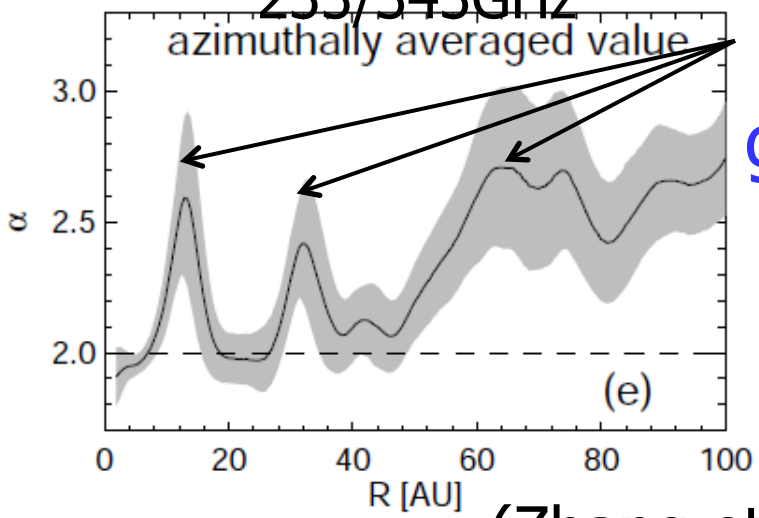
(Notsu+ in prep.)

Fast Pebble Growth @ Snow Lines?





233/343GHz azimuthally averaged value



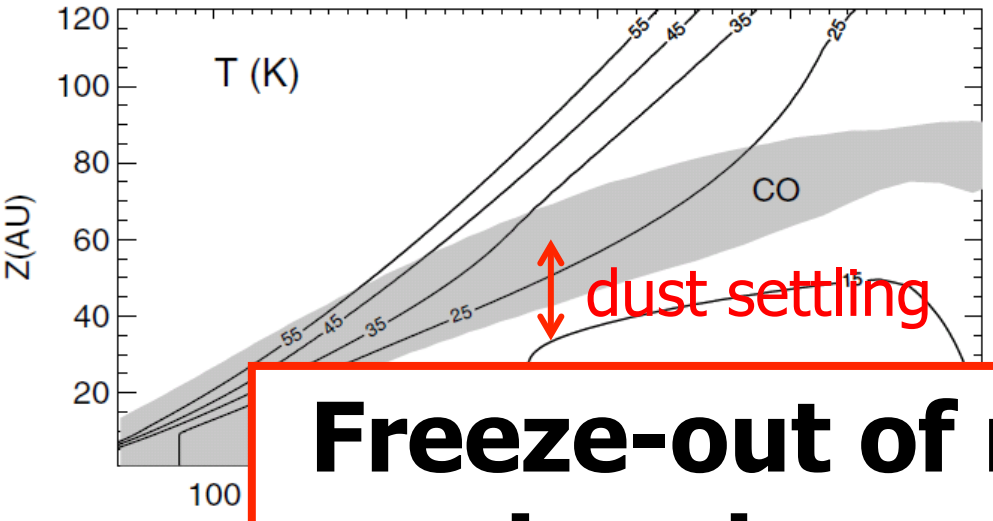
Grain growth?

Grain growth @ snow lines?

(Zhang et al. 2015)

CO Snow Line

HD163296



SMA

CO6-5@691GHz ^{13}CO2-1@220GHz

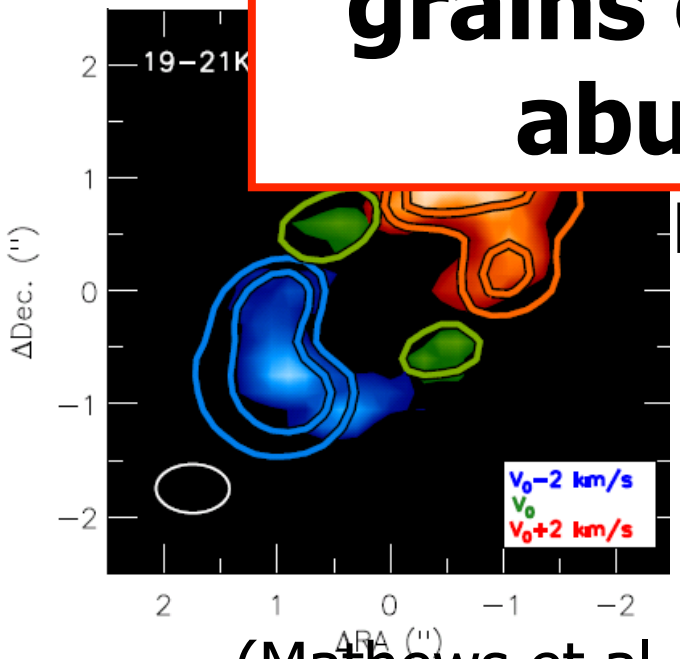
CO3-2@346GHz C^{18}O2-1@220GHz

CO2-1@231GHz C^{17}O3-2@337GHz

CO snow line @ R~155AU

011)

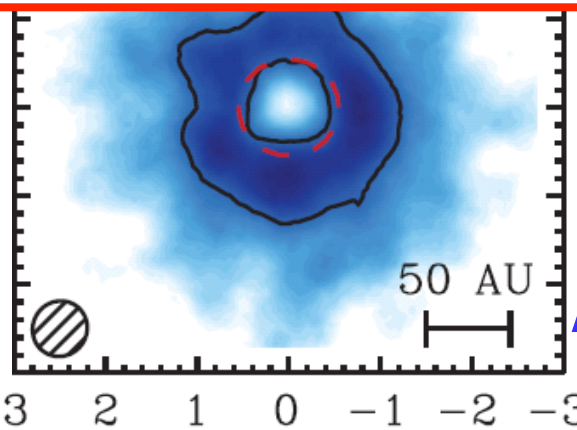
Freeze-out of molecules on grains changes elemental abundance in PPDs



DCO$^+$ 5-4

[DCO$^+$] /[HCO$^+$] =0.3

(Mathews et al. 2013)



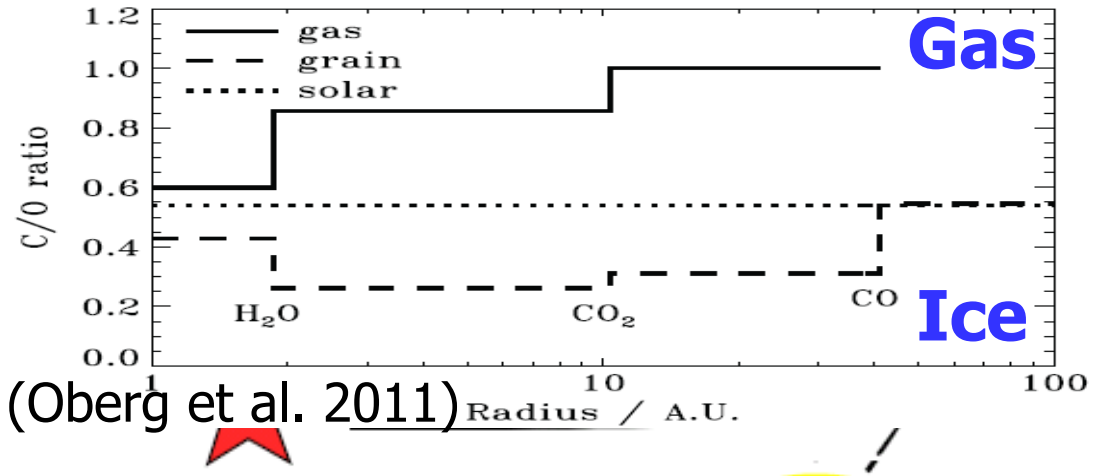
CO snow line @ R~30AU

Aikawa-san's talk

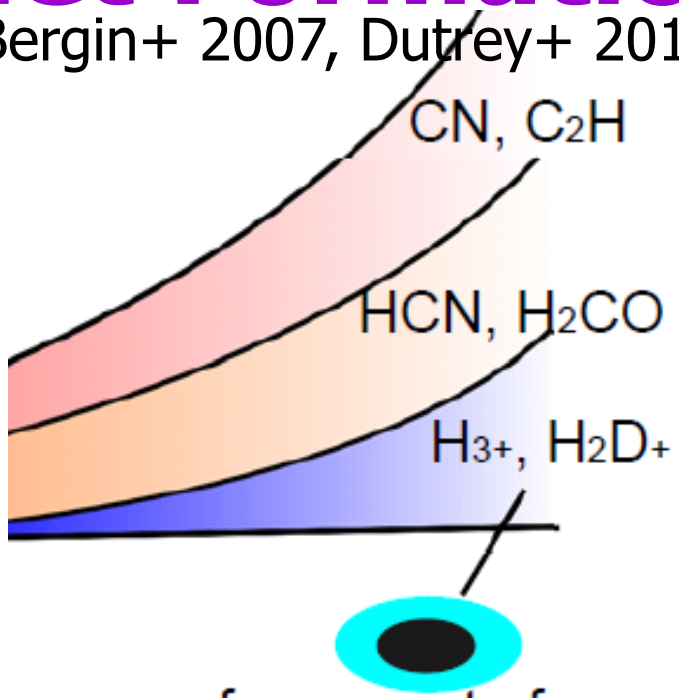
(Qi et al. 2013c)

Snow Lines & Planet Formation

(e.g., Markwick+2002, Aikawa+ 2002, Bergin+ 2007, Dutrey+ 2014)



(Oberg et al. 2011)



desorption of icy molecules

freeze-out of species grain surface resctions

C-rich in Ice

O-rich in Gas

O-rich in Ice

C-rich in Gas

rocky planets

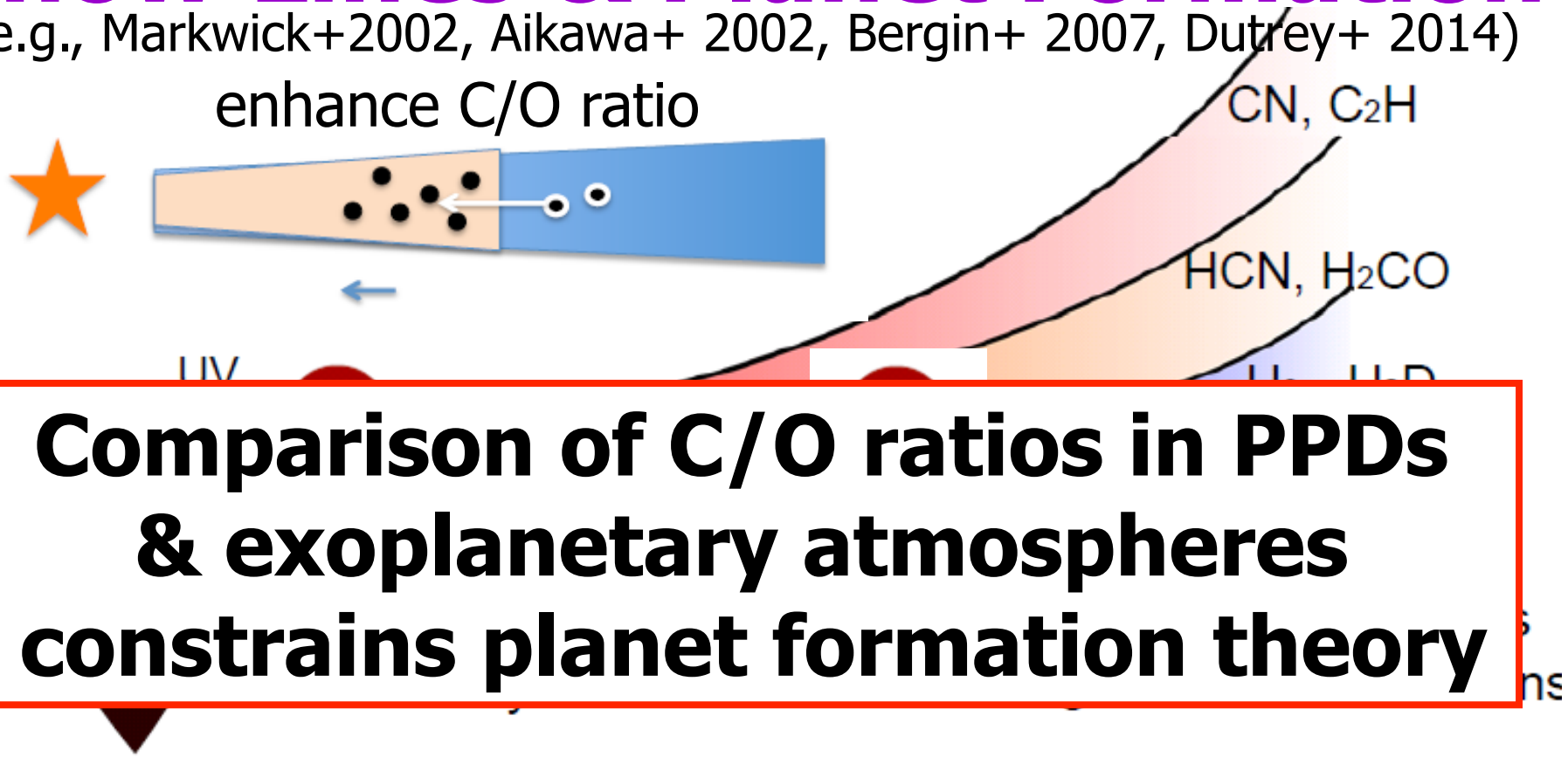
gas giants

ice giants

H_2O snow line

Snow Lines & Planet Formation

(e.g., Markwick+2002, Aikawa+ 2002, Bergin+ 2007, Dutrey+ 2014)



Comparison of C/O ratios in PPDs & exoplanetary atmospheres constrains planet formation theory

C-rich in Ice
O-rich in Gas

rocky planets

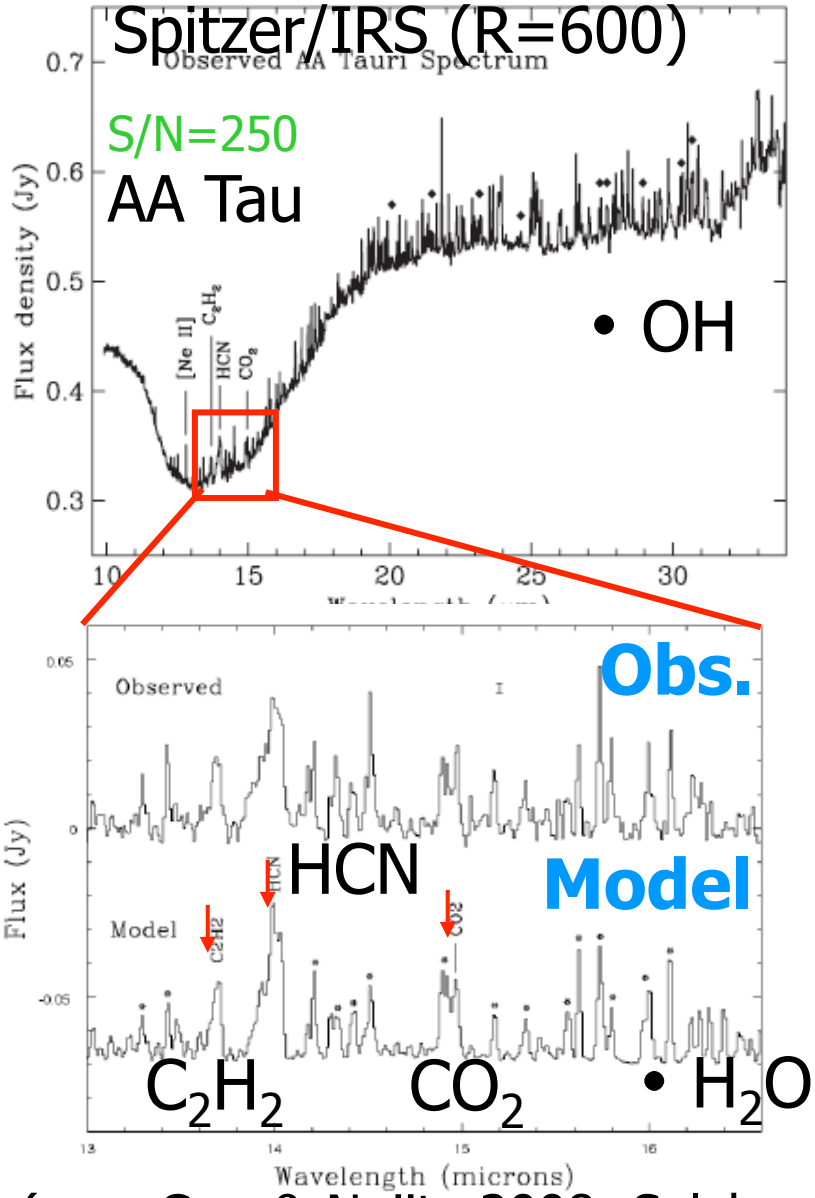
O-rich in Ice
C-rich in Gas

gas giants

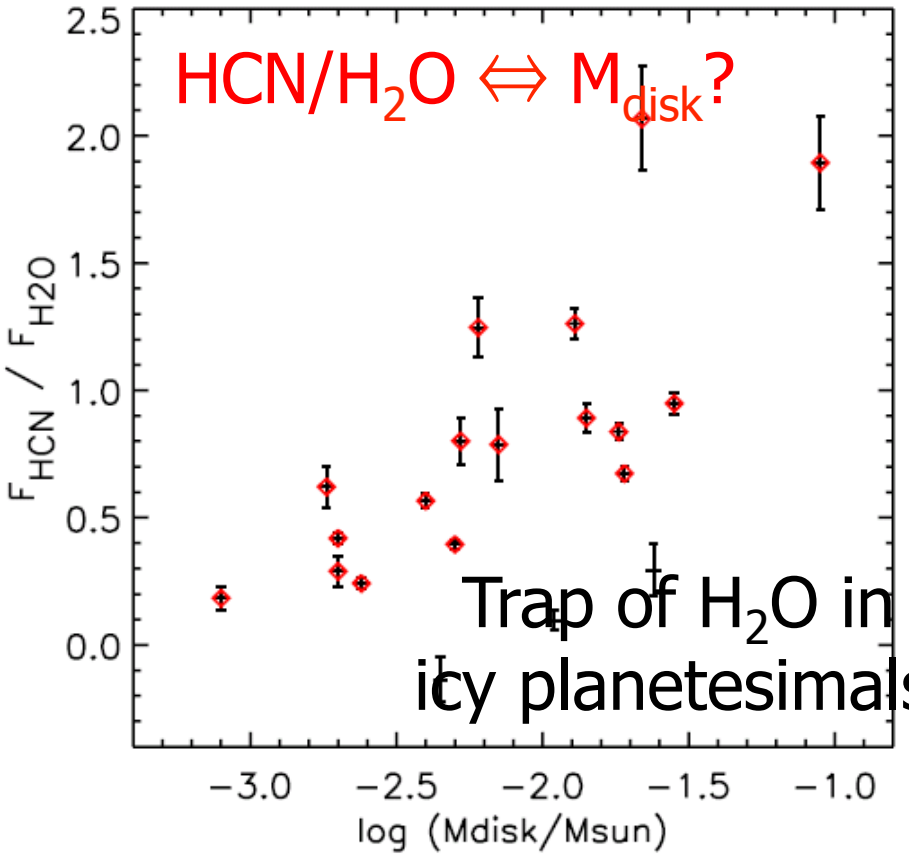
ice giants

H_2O snow line

Obs. of Water & Organic Molecules



(e.g., Carr & Najita 2008; Salyk+ 2008, 2011; Pontoppiddan+ 2010)



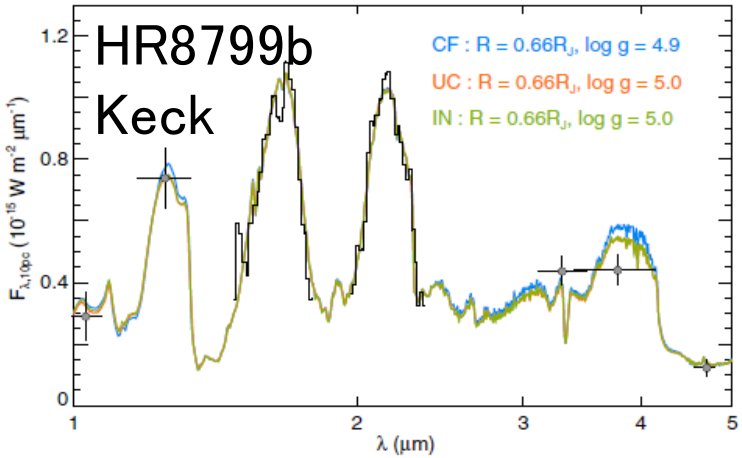
(Carr & Najita 2011, Najita+ 2013)

Infrared molecular lines could be tracer of C/O ratio distribution in PPDs

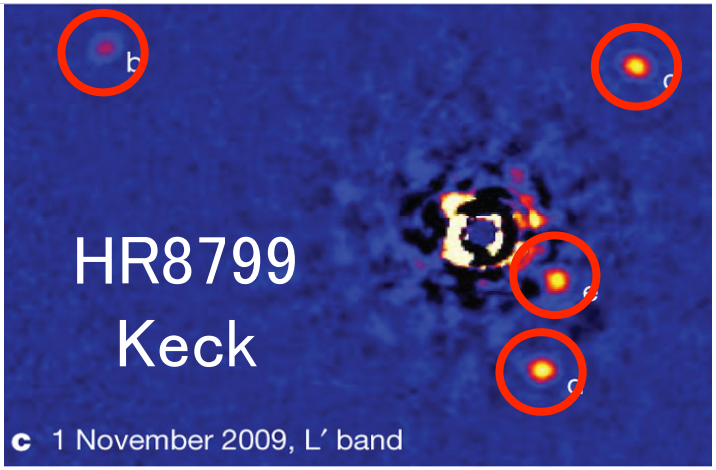
(JWST, TMT, SPICA, …)

Obs. of Exoplanetary Atmospheres

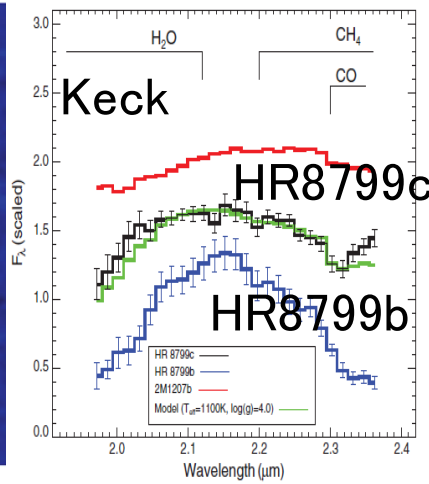
Directly Imaged Gas Giants



(Lee+ 2013, Barman+ 2011)

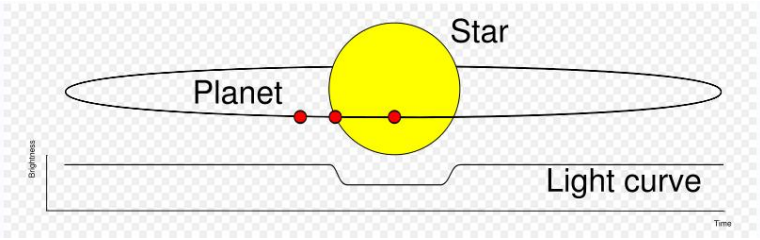


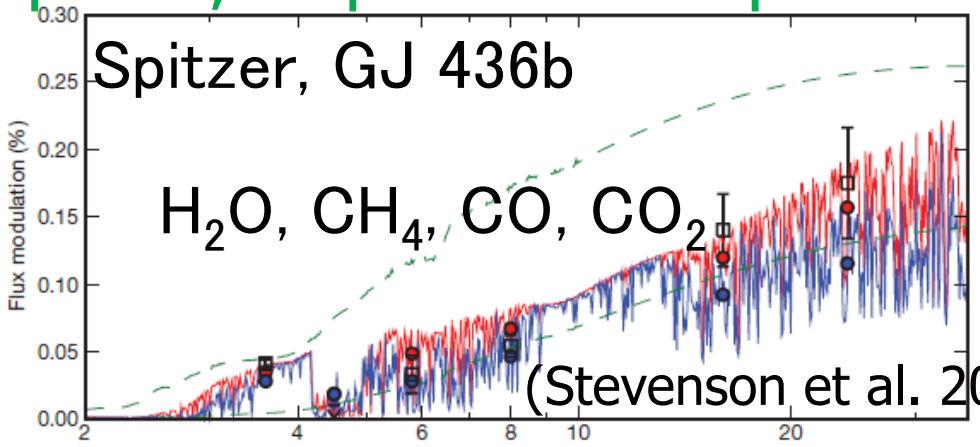
(Marois et al. 2008, 2010)



(Konopacky+ 2013)

Transiting Short Period Jupiters, Neptunes & Super-Earths





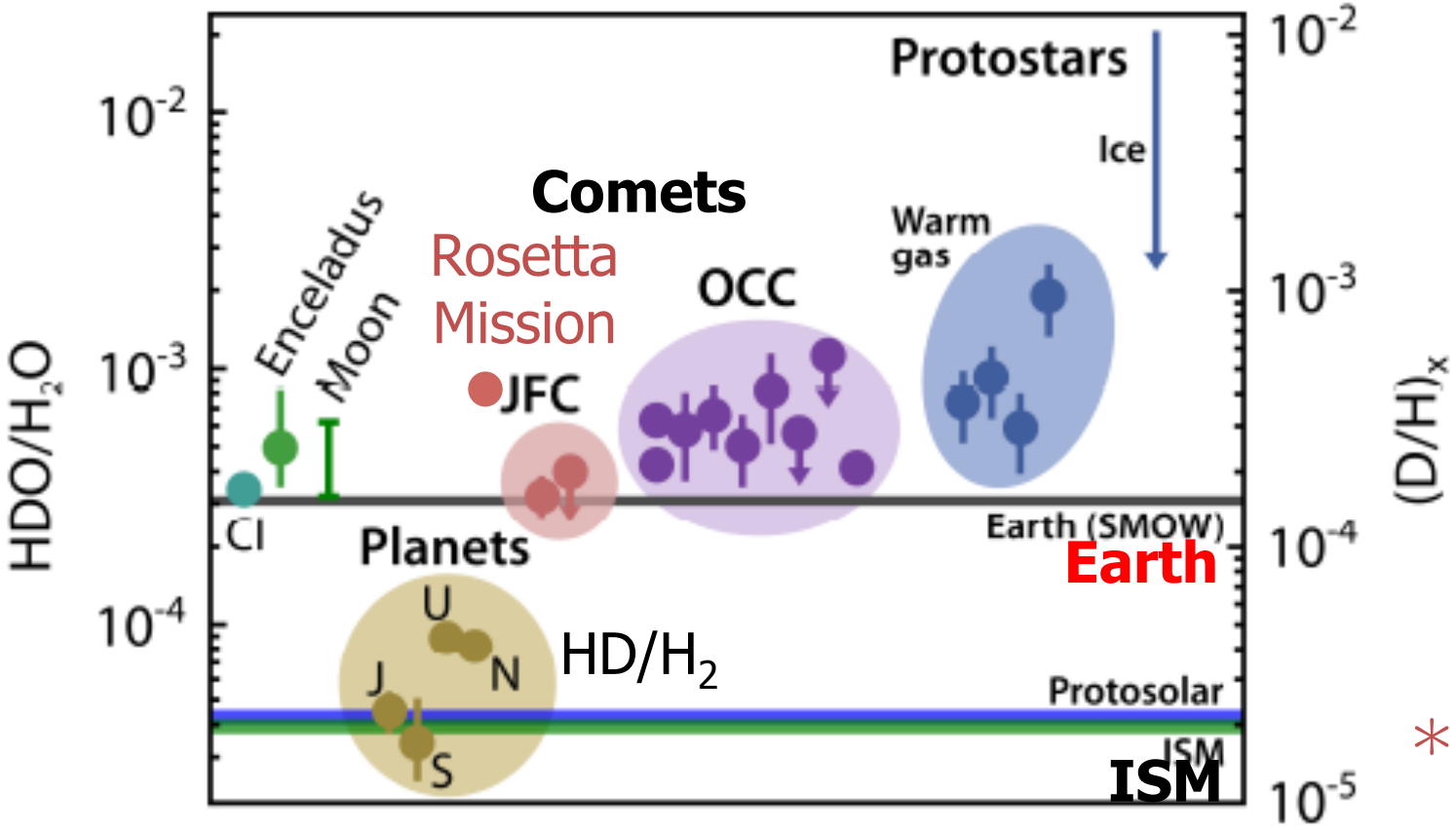
(Stevenson et al. 2010)

JWST, TMT, SPICA, …

Water & methane, etc. are found→ C/O ratios

→ constrain planet formation theory?

Deuterated Water



(van Dishoeck et al. 2014)

∗Rosetta Mission

(Altwegg+2015)

Obs. of Deuterated Species in PPDs

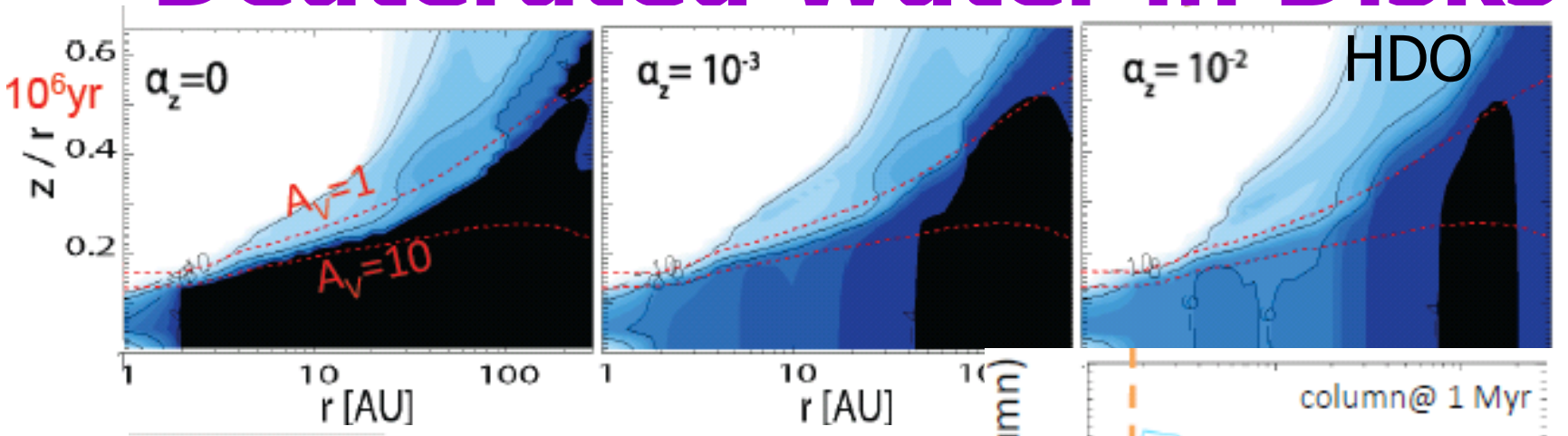
DCO^+ : TW Hya, DM Tau, LkCa 15, HD163296 D/H~0.02-0.3
(van Dishoeck+ 2003, Guilloteau+ 2006, Oberg+2010, Mathews+ 2013)

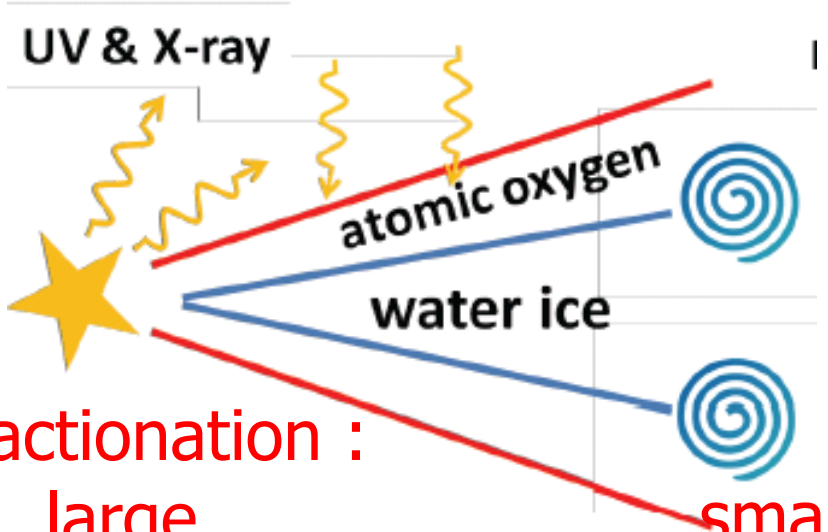
DCN : TW Hya, LkCa 15 (Qi+ 2008, Oberg+ 2010, 2012) ~0.02

HD : TW Hya (Bergin+ 2013) $\sim 10^{-5}$

HDO, H_2D^+ : non-detection (Guilloteau+ 2006, Chapillon+ 2011)

Deuterated Water in Disks





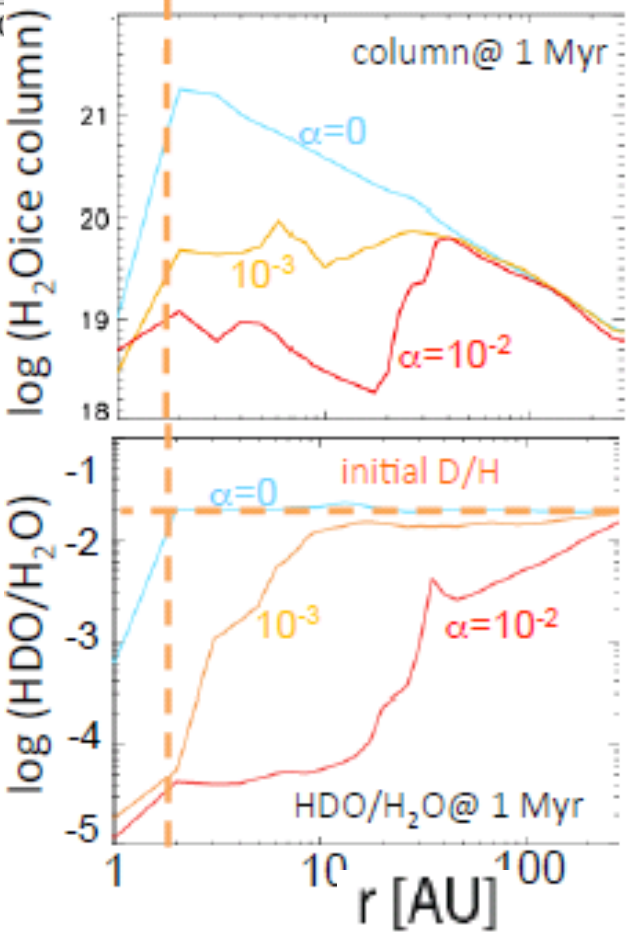
D fractionation :

large small

H_2O(ice) → O → H_2O(ice)

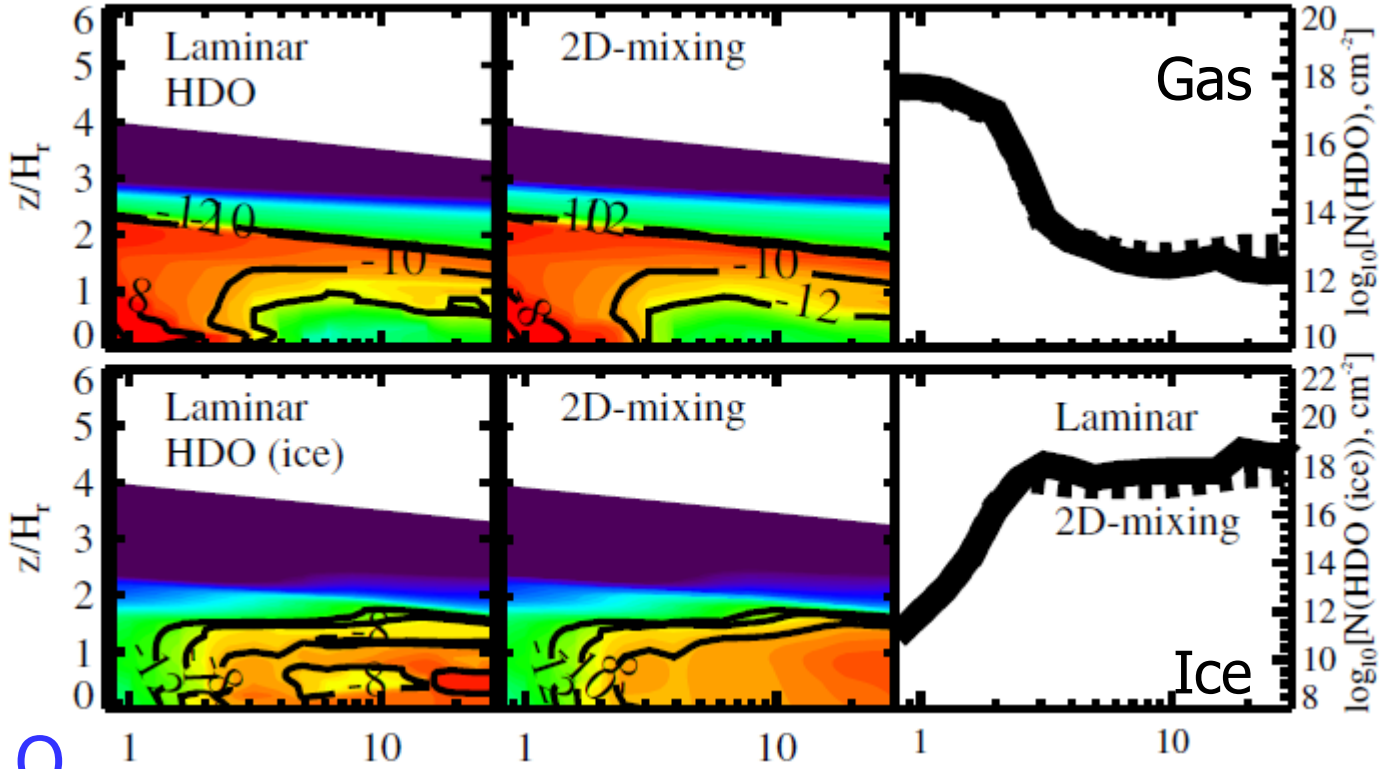
photodesorption
• dissociation
@ disk surface

adsorbed
on grains

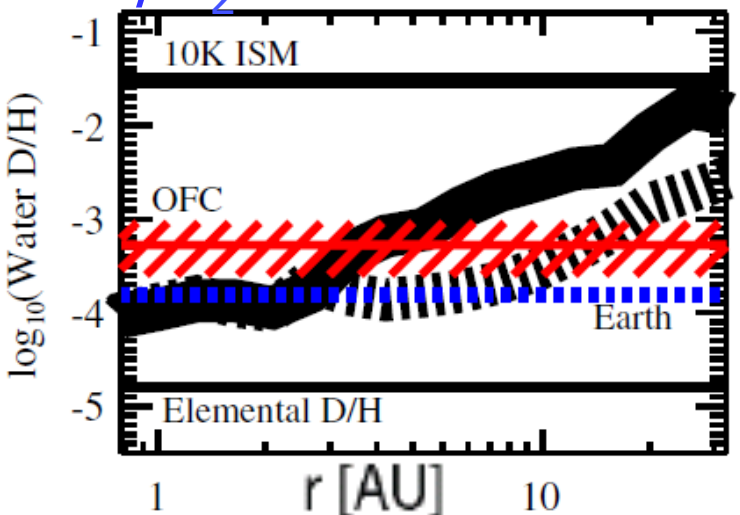


(Furuya+ 2013, Cleaves+ 2014)

Deuterated Water in Disks



HDO/H_2O



Laminar

2D mixing

OCC

Earth

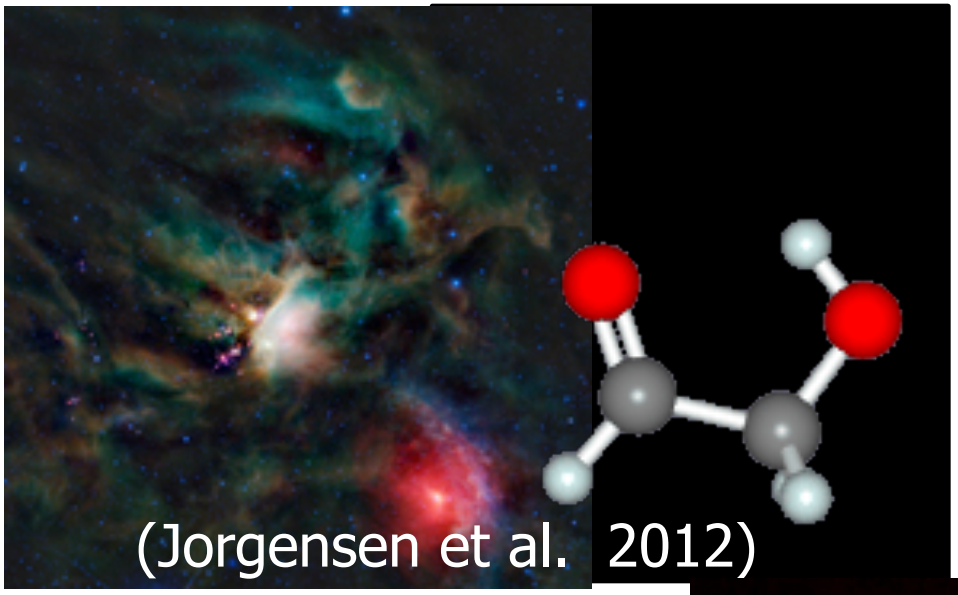
Deuterium fractionation is consistent with
- Earth @ ~1AU
- Comets @ ~10AU (2D mixing)

Obs. of HDO will test the models!

(Albertsson, Seminov & Henning 2014)

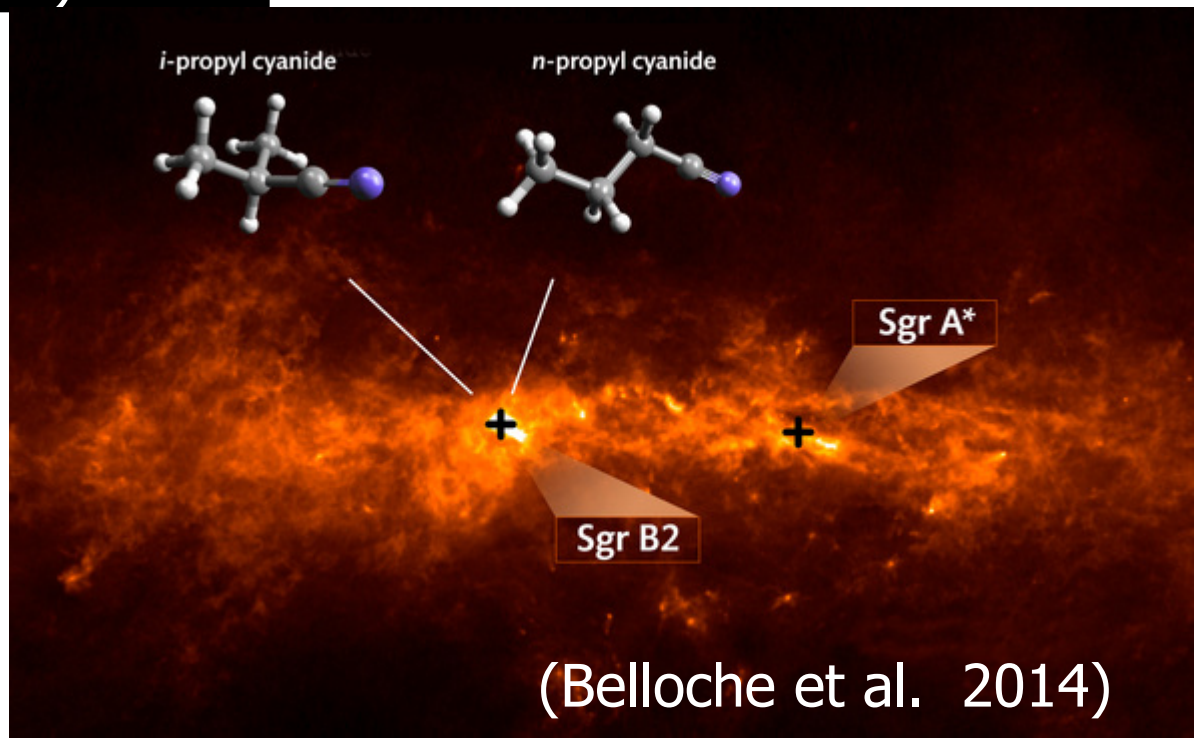
§3
Formation of Organic Molecules in Protoplanetary Disks

COMs Observations with ALMA



Glycolaldehyde around low mass star forming regions

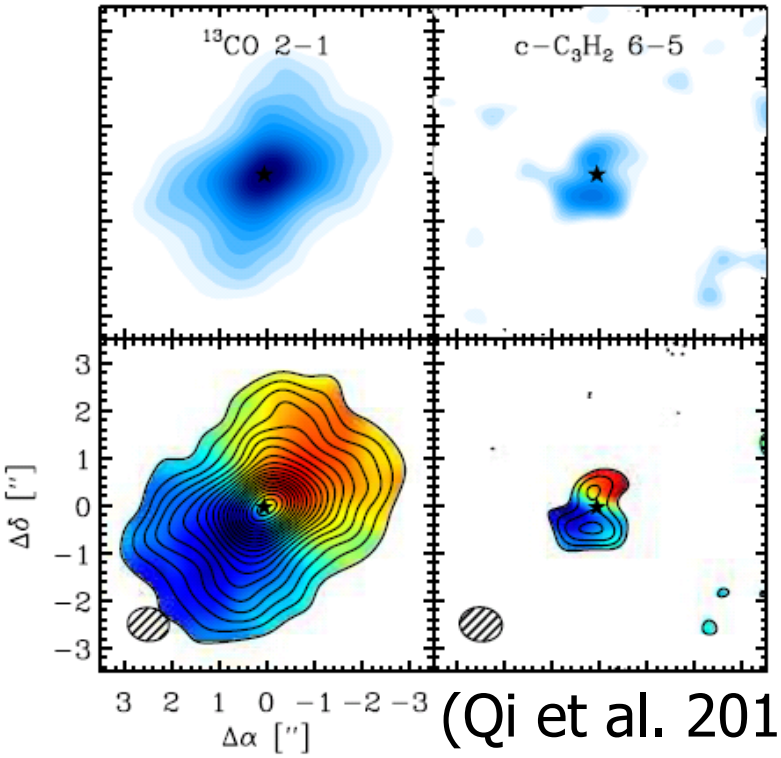
Iso-propyl cyanide around high mass star forming regions in Galactic center



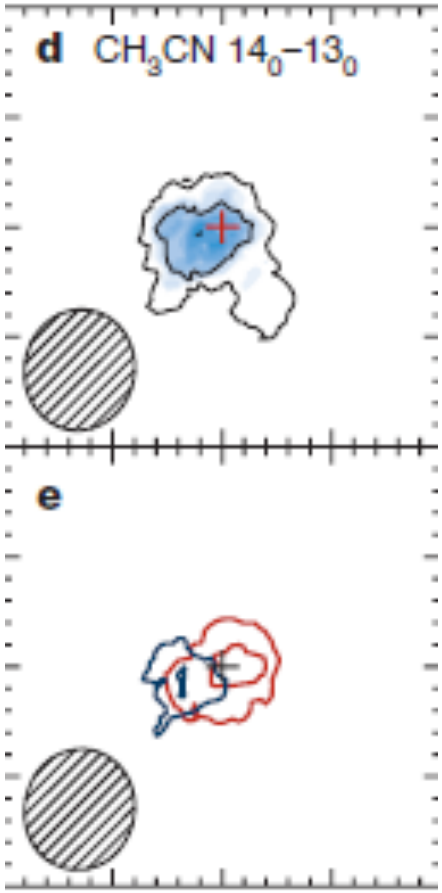
Complex Organic Molecules in Disks

HC_3N J=16-15, 12-11, 10-9 @ 146, 109, 91GHz
MWC480, LkCa15, GO Tau, IRAM 30m, PdBI
(Chapillon et al. 2012)

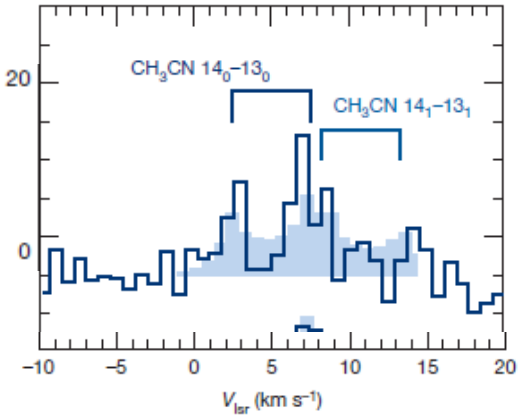
$c\text{-}C_3H_2$ J=6-5 @ 218GHz
HD163296, ALMA SV



(Qi et al. 2013b)



CH_3CN
14_0-13_0, 14_1-13_1,
@ 257GHz,
MWC480,
ALMA cycle 2



(Oberg et al. 2015)

→more complex mol. will be found by ALMA

Observed Interstellar Molecules

by ~1975 after ~1997

CH+	HCN	H2CO	HC3N	CH3OH	HC5N	HCOOCH3	HC7N
CS	HNC	H2CS	HCOOH	CH3CN	CH3CCH	CH3C3N	HC9N
CO	HCO	H2CN	CH2NH	CH3NC	CH3NH2	CH3COOH	HC11N
CN	OCS	HNCO	CH2CO	CH3SH	CH3CHO	CH2CHCHO	C2H5CN
C2	CH2	HNCS	NH2CN	NH2CHO	CH2CHCN	CH2OHCHO	CH3C4H
						H2C6	CH3C5N
					H4O		CH3OCH3
					CHOH		C2H5OH
					-		CH3CONH2
							CH3COCH3
							OHCH2CH2OH
							C2H5OCHO
		HCNH+	C4H-				C8H-
		C3N-					NH2CH2COOH?

Amino acids in comet @ STARDUST

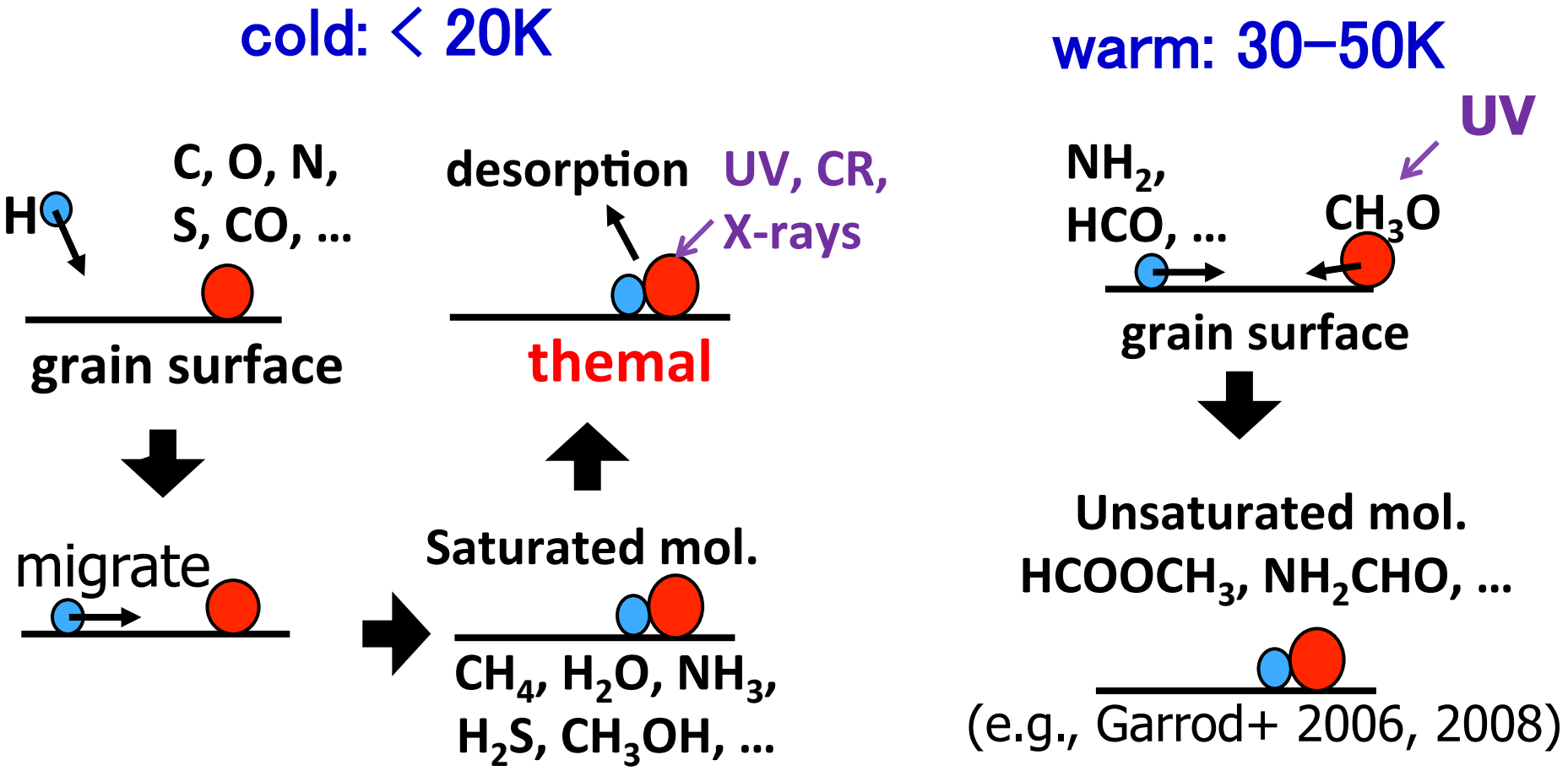
(Elsila et al. 2009)

Amino acids in meteorites ⇔ relation with interstellar molecules ?

amino acids ?

1970 ~10 species → 1980 ~50 → 1995 ~100 → 2015 ~180 species

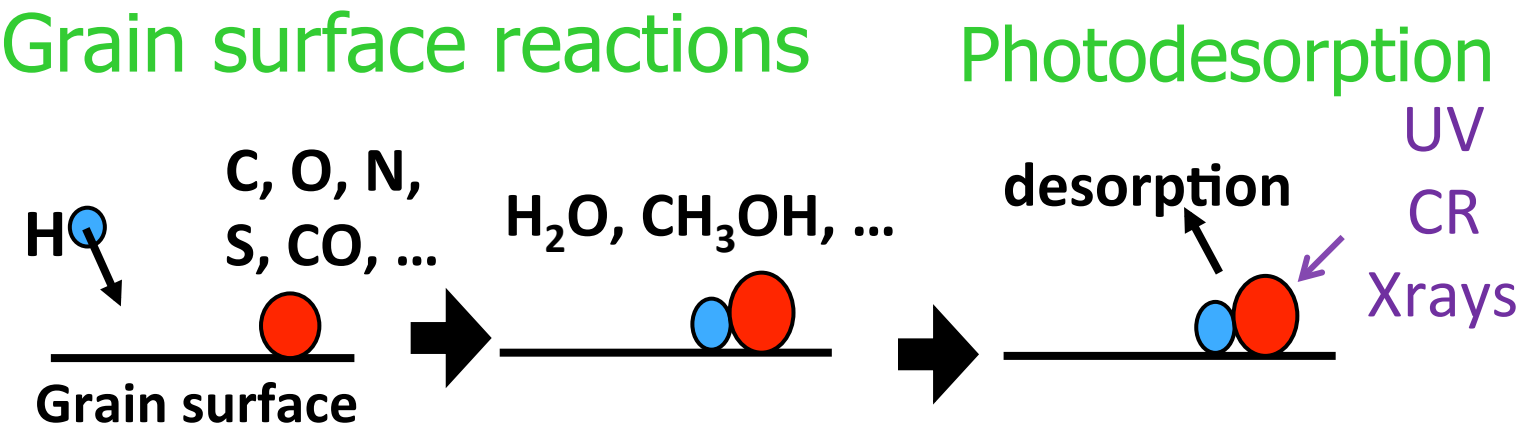
Complex Molecule Fomration on Grain Surface

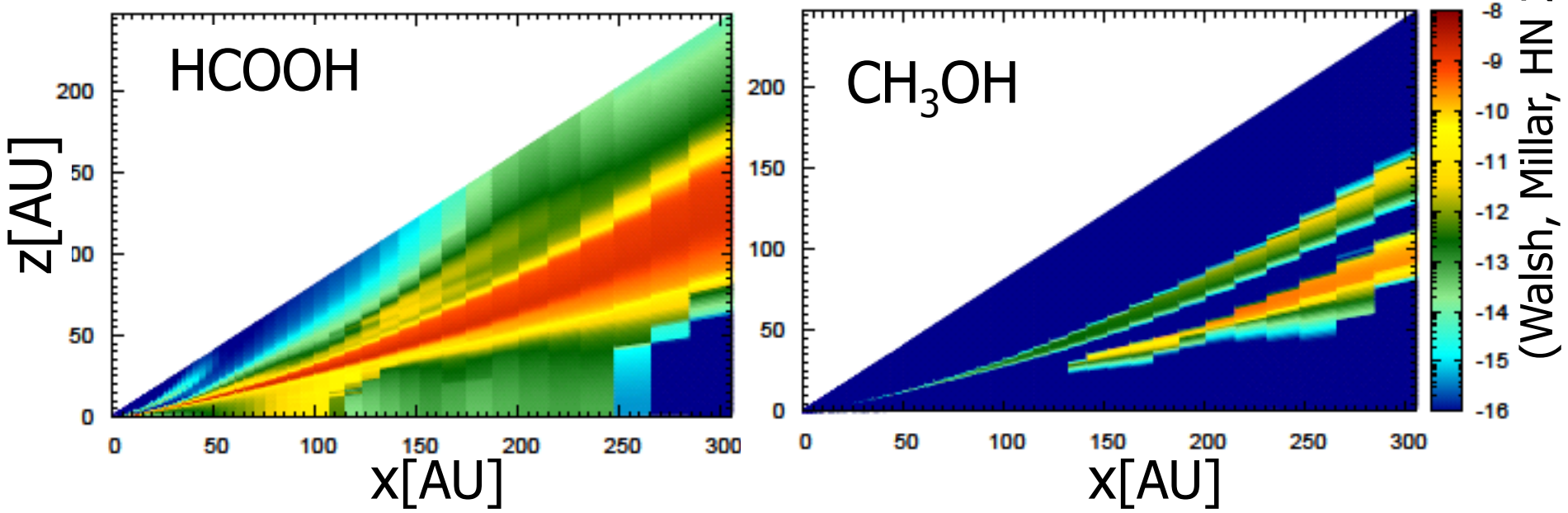


Complex molecules are formed on grains

More complex molecules on warm grains

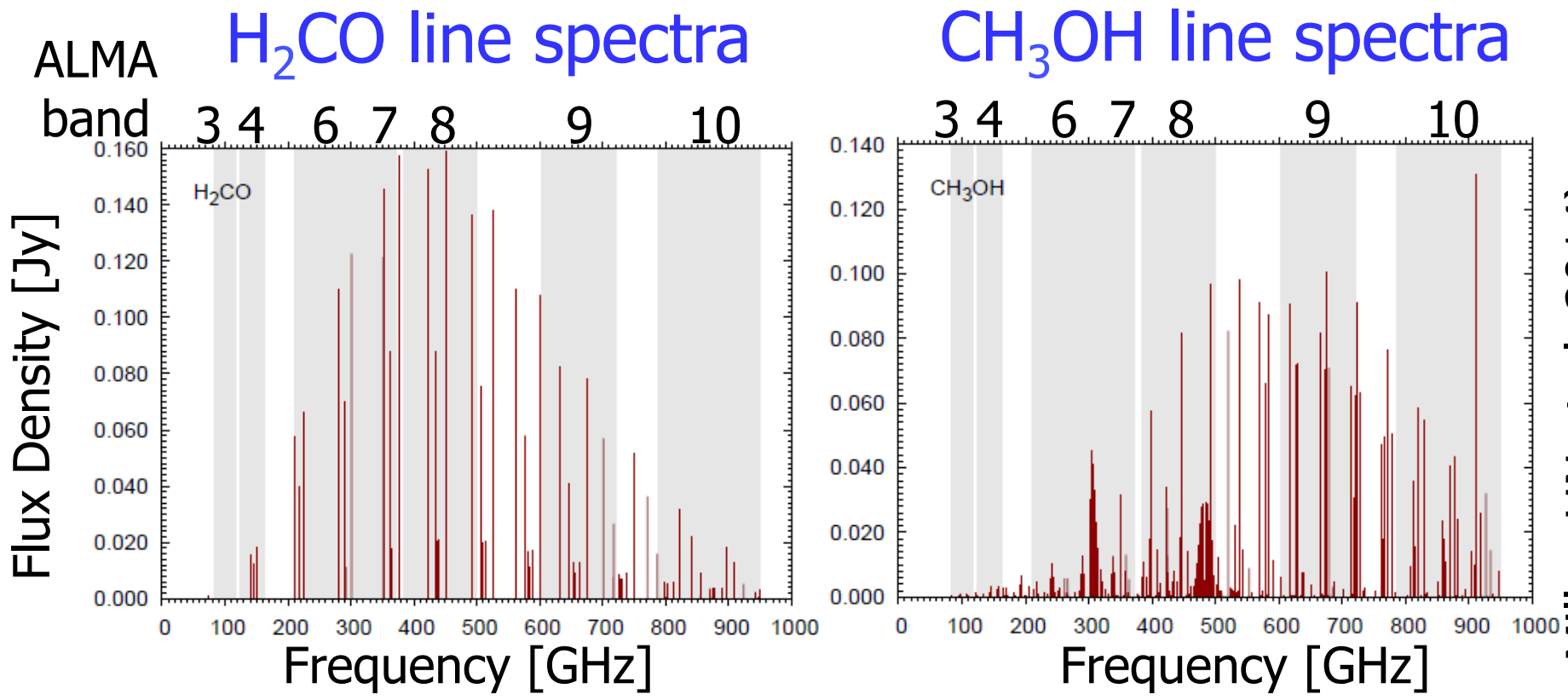
Modeling Complex Molecules in PPD





Observing complex mol. & grain surface reactions

Prediction of CH_3OH line fluxes (ALMA)



(Walsh, Millar, HN et al. 2014)

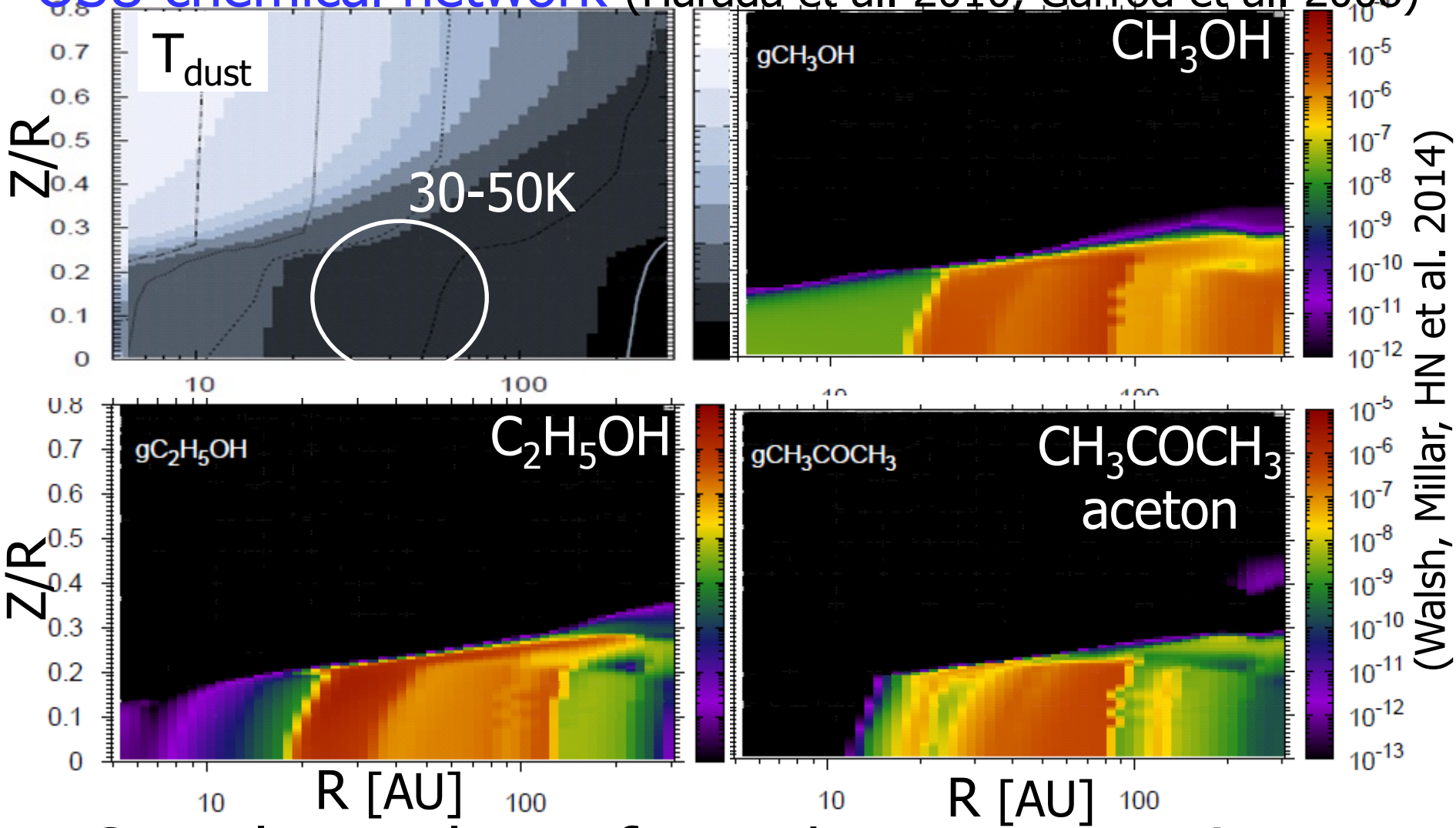
H_2CO line fluxes: consistent with observations

CH_3OH line fluxes: constrained by ALMA observations

→ Diagnosing grain surface reactions in PPDs

Complex Molecules on Warm Grains

OSU chemical network (Harada et al. 2010, Garrod et al. 2008)



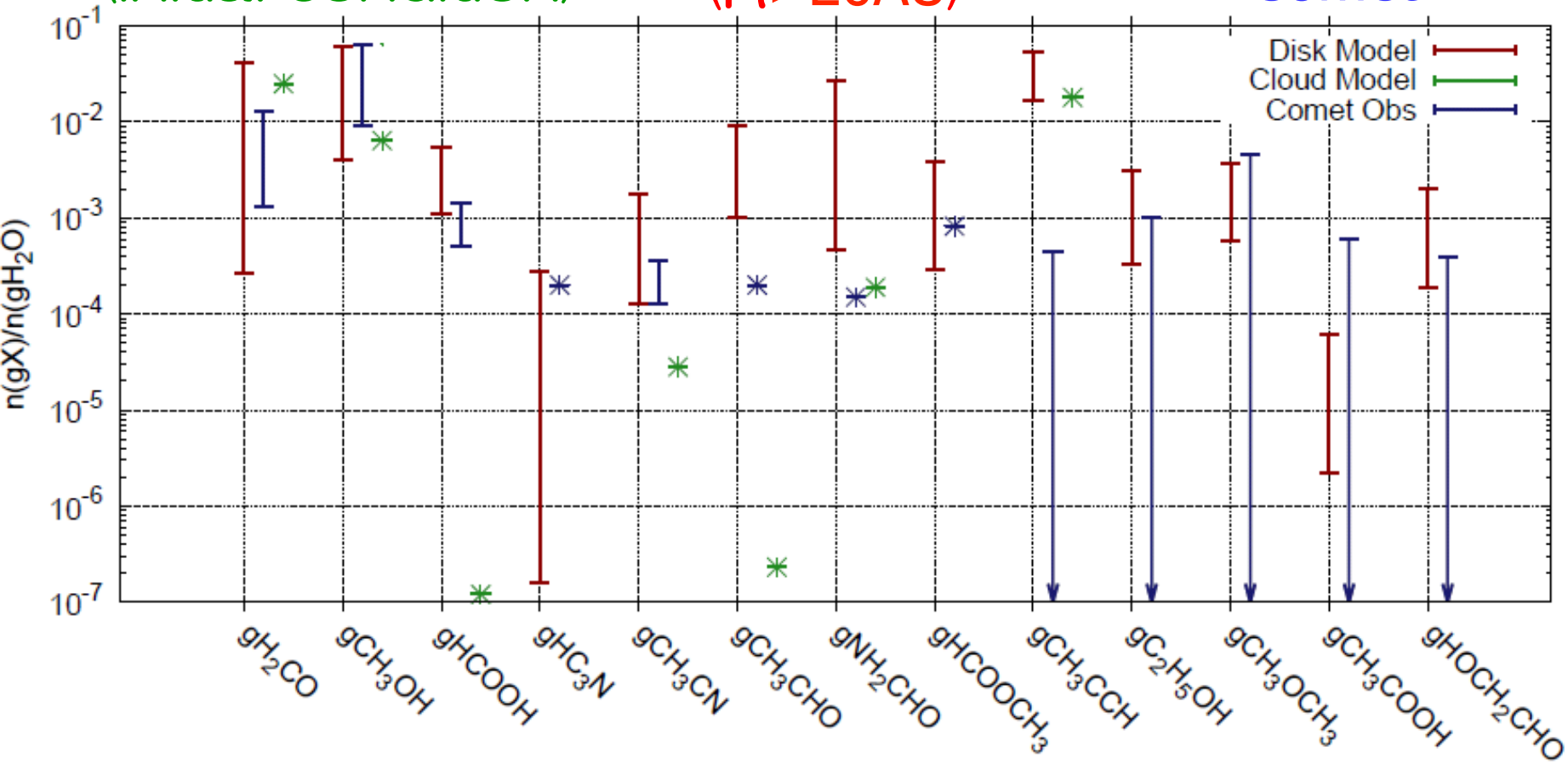
Complex mol. are formed on warm grains at T~30-35K(~50AU) = cometary region

Comparison with Obs. tw. Comets

Mol. clouds (initial condition)

Model (ice) (R>20AU)

Obs. from Comet



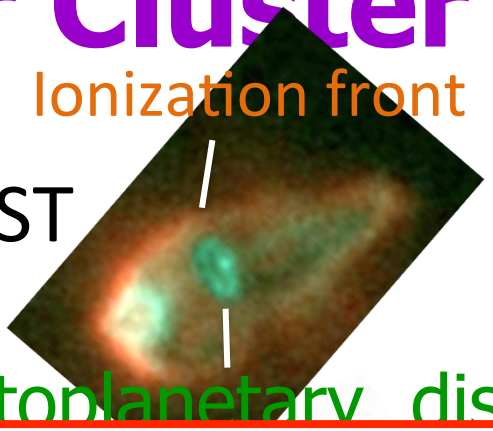
(Walsh, Millar, HN et al. 2014)

Complex molecules are formed on grains in disk

Obs. toward comets are consistent with PPD model

Disks in a Young Star Cluster

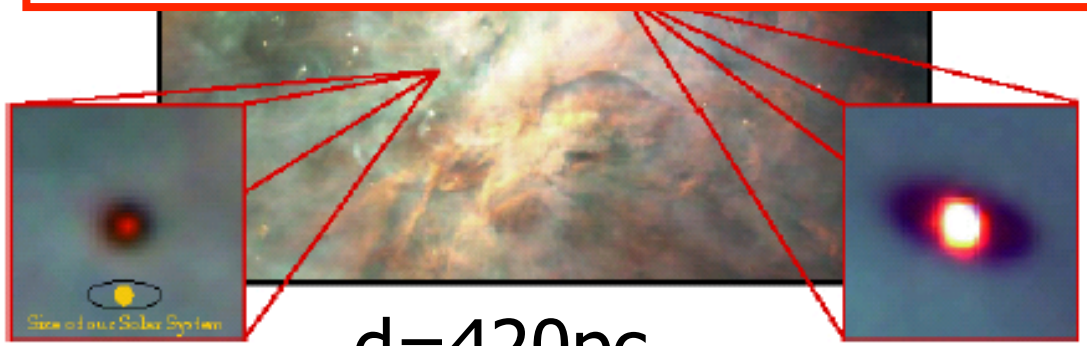
Trapezium cluster in Orion Nebula



Most stars are formed in young star clusters

↓ (e.g., Lada & Lada 2003)

Environmental effects in star clusters?



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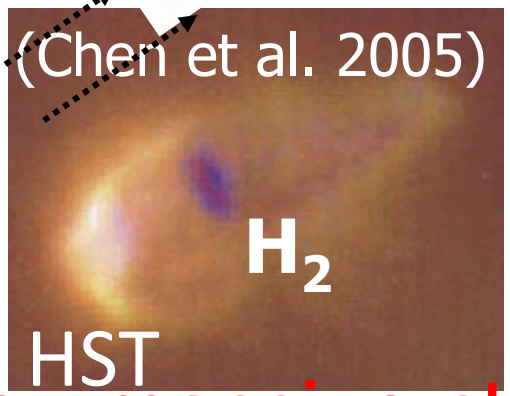
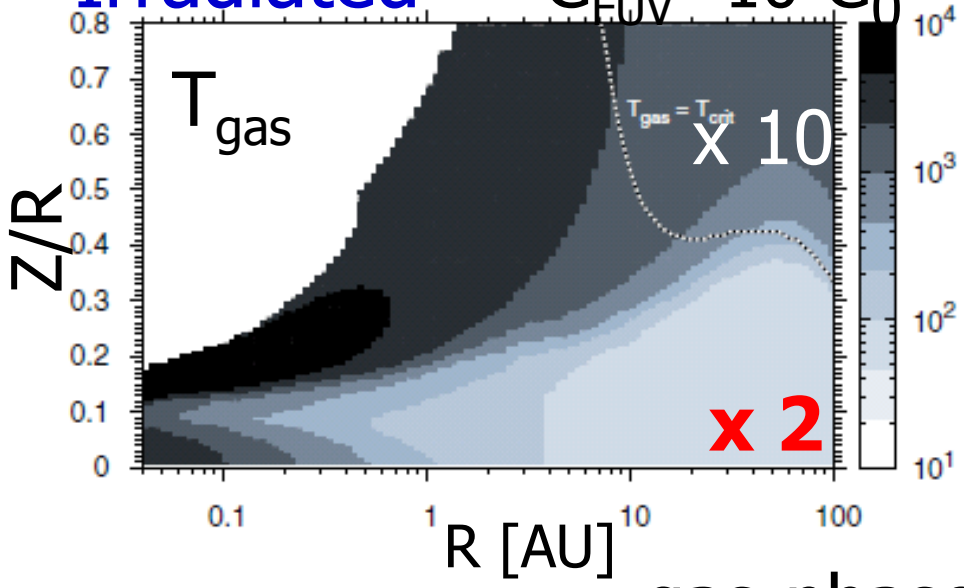
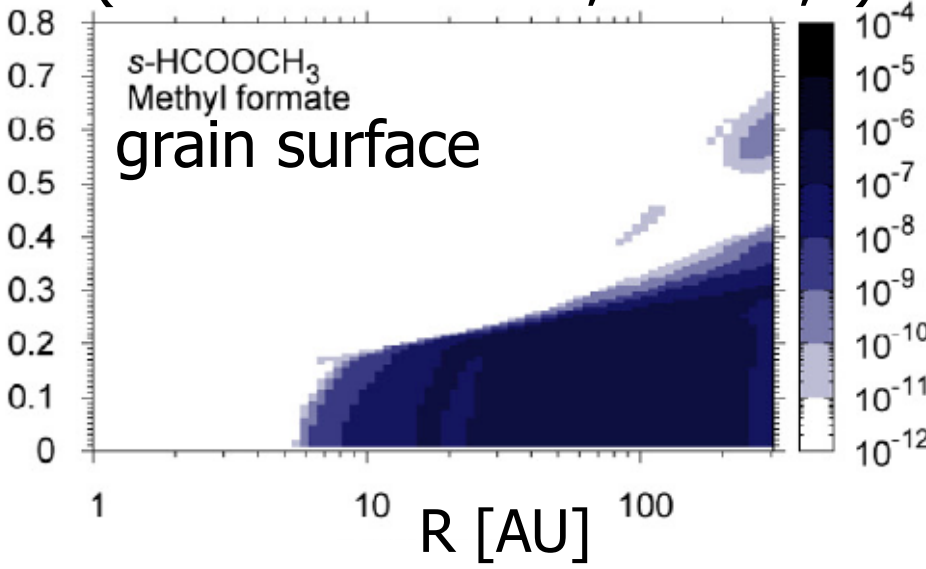


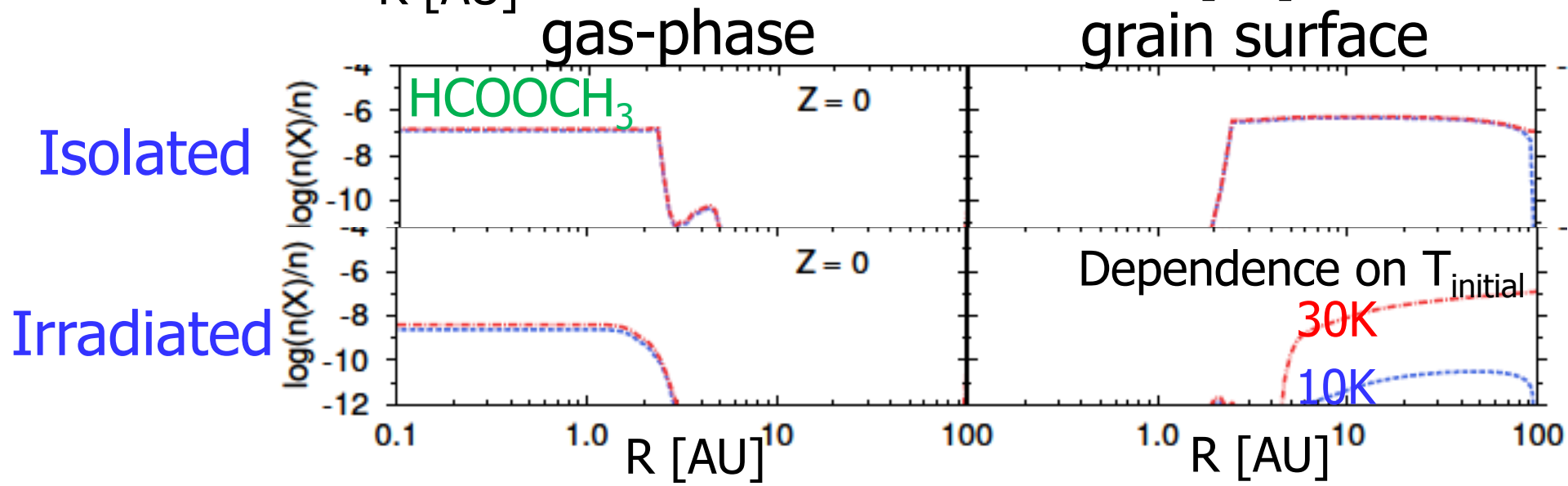
Effect of irradiation from nearby massive star on chemical structure in disks?

COMs : irradiated vs. isolated

Irradiated $G_{FUV}=10^6G_0$ (Walsh et al.2013, 2014a,b)







Irradiated: some COMs are not formed efficiently

Summary

Water, snow lines & organic molecules in protoplanetary disks

H_2O snow line in PPDs will be detected using high-R spectroscopic observations

Comparison of C/O ratios in PPDs & exoplanetary atmospheres constrains planet formation theory

Obs. of deuterated molecules constrain disk model

Obs. of complex molecules in PPDs & comets constrain formation process of COMs in PPDs

Carbon Fractionation in Disks

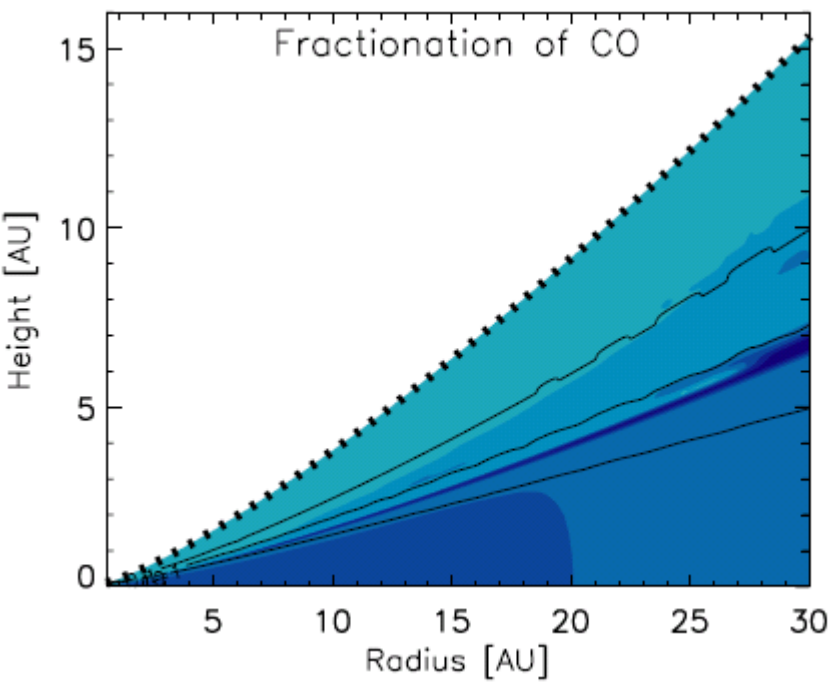
- Fractionation due to self-sheilding

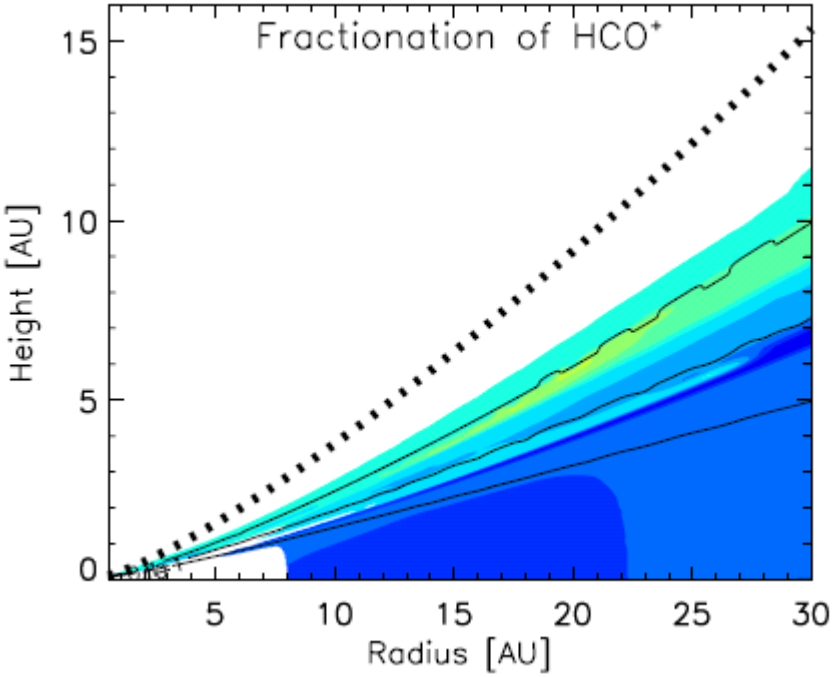
surface: $^{12}C^{16}O \rightarrow {}^{13}CO \rightarrow C^{18}O \rightarrow C^{17}O \rightarrow \ldots$:midplane

- Fractionation due to chemistry

$$^{13}C^{+} + {}^{12}CO \rightleftharpoons {}^{13}CO + {}^{12}C^{+} + \Delta E, \qquad \Delta E = 35K$$

$$H^{12}CO^{+} + {}^{13}CO \rightleftharpoons H^{13}CO^{+} + {}^{12}CO + \Delta E, \qquad \Delta E = 9K$$





(Woods & Willacy 2009)

Fractionation may depend on temperature