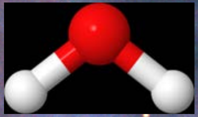
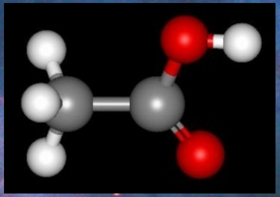
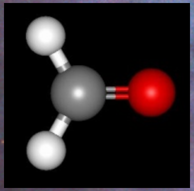
Molecules from clouds to stars and planets

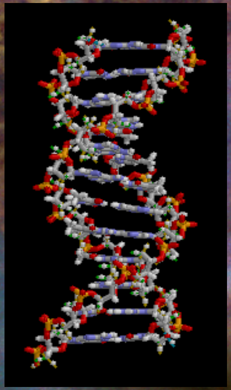






Ewine F. van Dishoeck
Leiden Observatory/ MPE

NASA/HST
Carina nevel



Thanks to many students, postdocs, colleagues

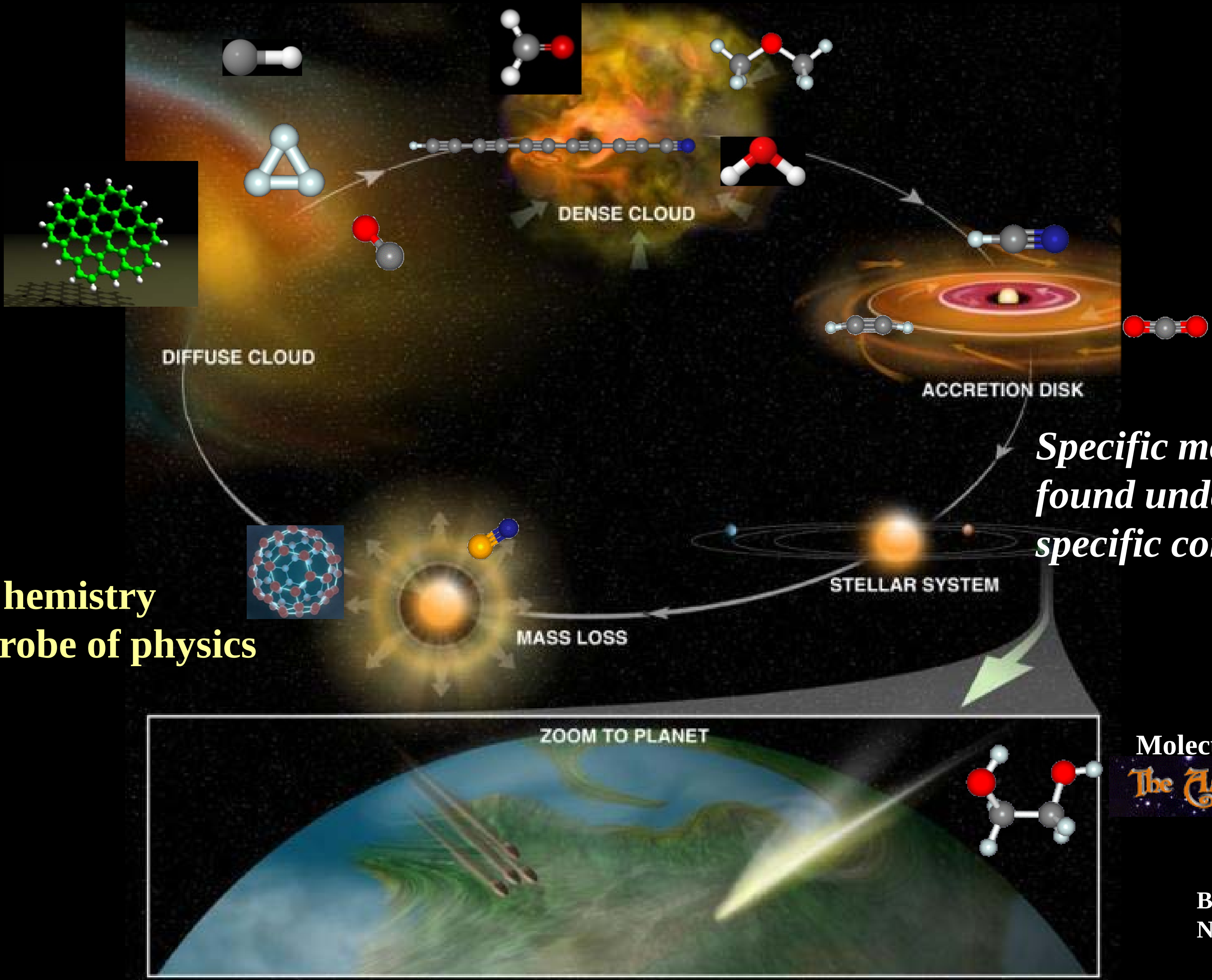
CSH lunchtalk Bern, 19 October 2017

erc European Research Council

NWO Nederlandse Organisatie voor Wetenschappelijk Onderzoek

NOVA

From clouds to stars and planets



Specific molecules found under specific conditions

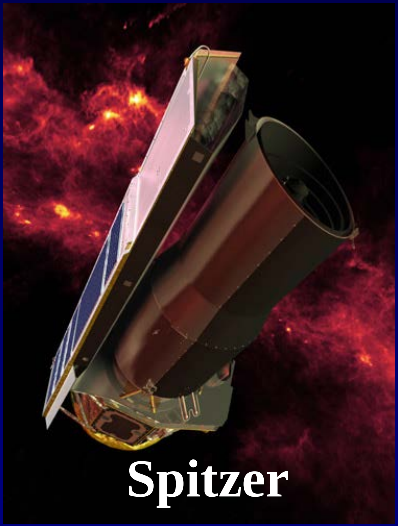
- Chemistry
- Probe of physics

Molecule images: The Astrochymist

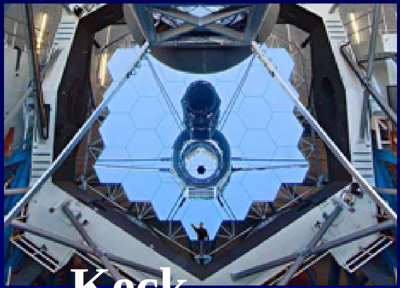
B. Saxton
NRAO

Fantastic facilities for astrochemistry

Herschel



Spitzer



Keck

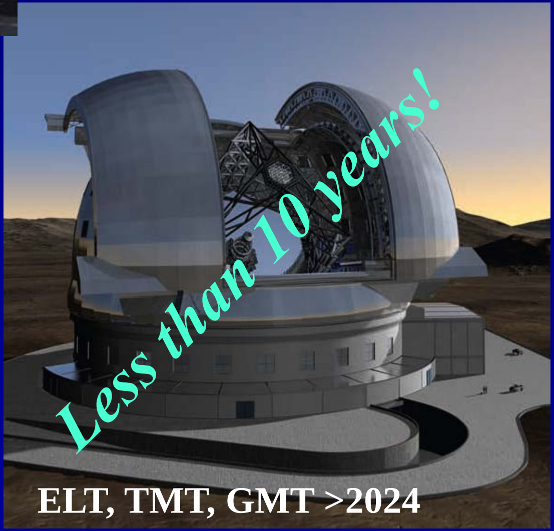
VLT

SOFIA

Rosetta

JWST

To be launched in 2019!

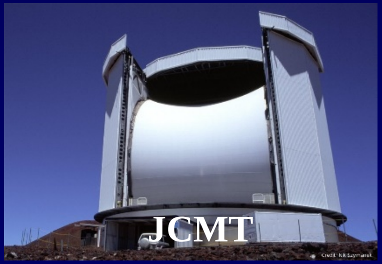


ELT, TMT, GMT >2024

Less than 10 years!

ALMA: *the* astrochemistry machine

ESO/NRAO/NAOJ



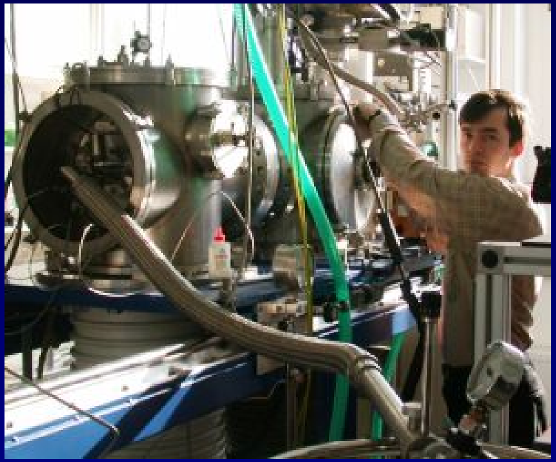
NOEMA, CARMA,
SMA

Lots of astrochemistry still based on single-dish data

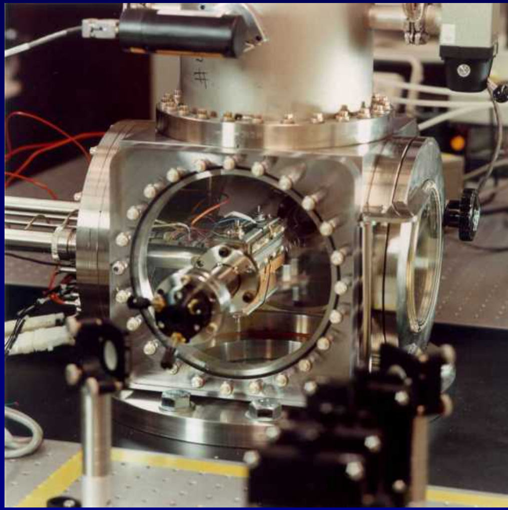
Fantastic new experiments and new groups!

Spectroscopy

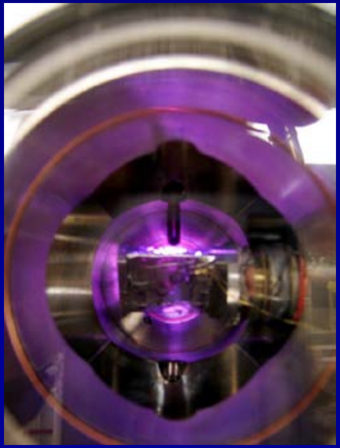
He droplets



Cavity Ringdown Spectroscopy



UV plasma



UHV surface science

Crossed beam experiments

Outline

- **Introduction**
- **Water from clouds to disks**
  - **Also O_2, HDO/H_2O**
- **Protoplanetary disks**
  - **Does chemical evolution matter?**
  - **JWST prospects**

See reviews by Herbst & vD 2009, Caselli & Ceccarelli 2012, Tielens 2013 special issue of Chemical Reviews 2013, van Dishoeck 2014, 2017

Most molecules are found in dark clouds shielded from UV

HST Carina nebula

- Collision time: once per month at 10^4 cm^{-3}
- Chemistry dominated by two-body processes: kinetics, not TE
- Three-body processes at $>10^{12}$ cm^{-3}

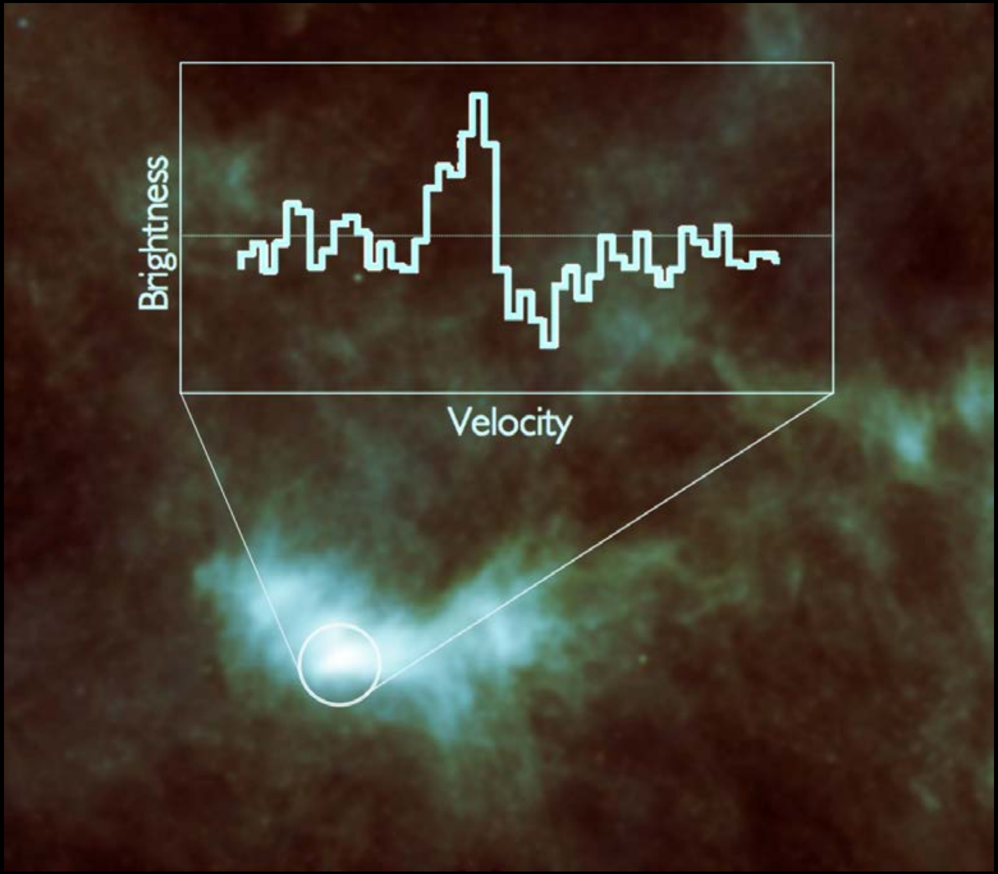
II. Water from clouds to disks

*Hersche*l WISH team, Ringberg, January 2013

www.strw.leidenuniv.nl/WISH

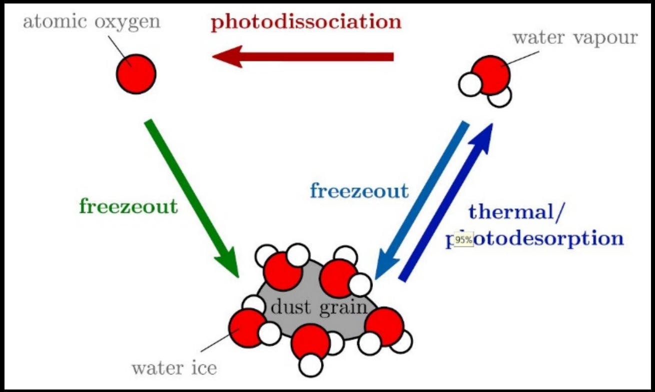
~70 papers, van Dishoeck et al. 2011, PASP
Bergin & van Dishoeck 2012, van Dishoeck et al. 2013, Chem. Rev. , 2014, Protostars & Planets VI

Detection of cold water reservoir



L1544 prestellar core
H_2O 557 GHz HIFI

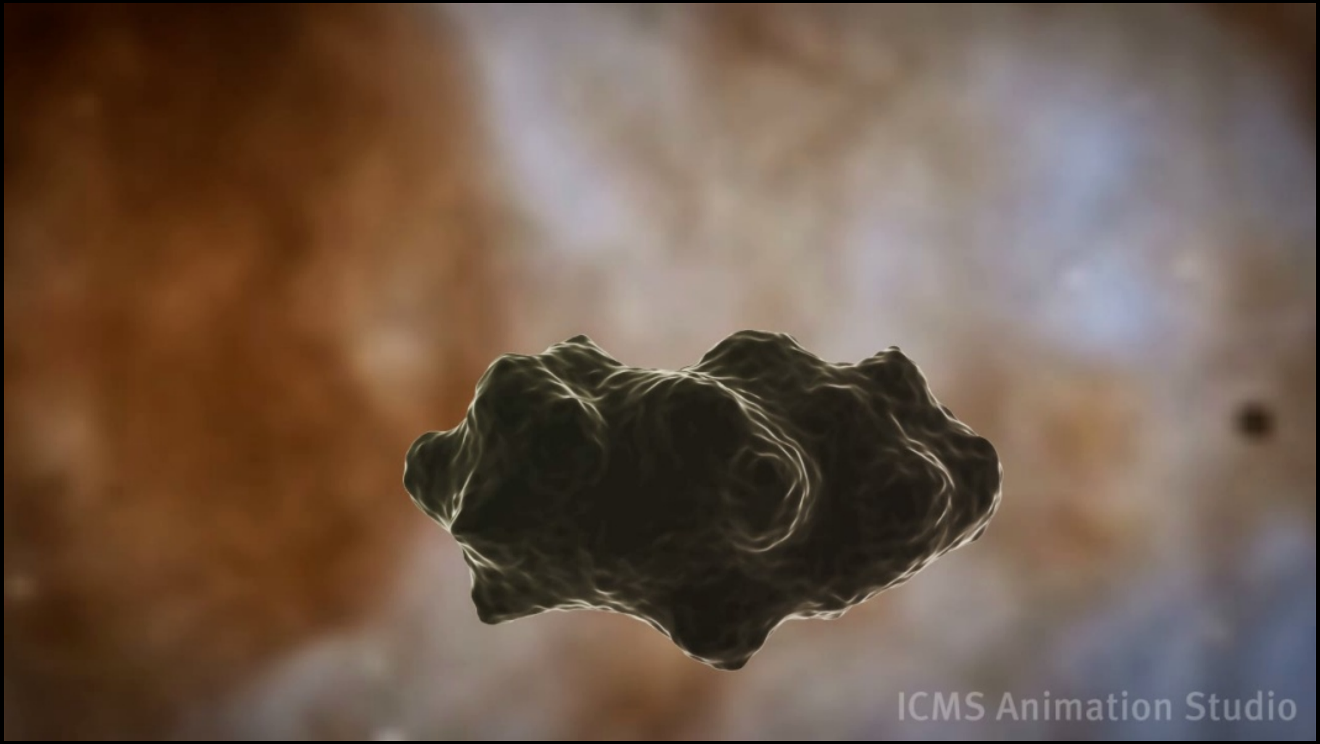
~1 million oceans of water ice



Caselli et al. 2012
Schmalz et al. 2014
Mottram et al. 2014

Signal consistent with simple ice chemistry

Bulk of water is formed on grains

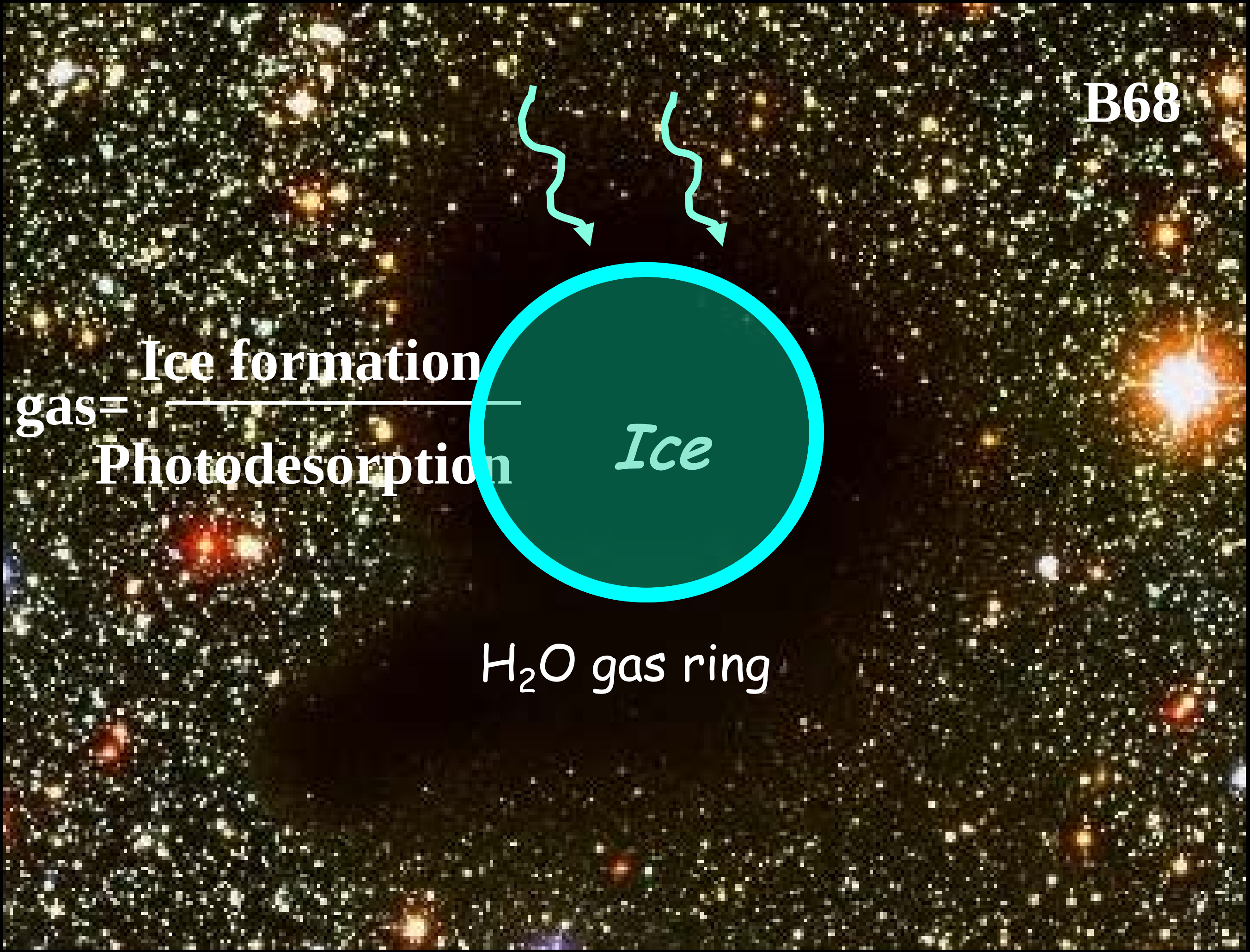


Ice formation starts in clouds with $A_V > 1$ mag

Based on laboratory data
Cuppen et al. 2010

Movie posted at www.strw.leidenuniv.nl/WISH

Where is water formed?



$$H_2O\ \text{gas} = \frac{\text{Ice formation}}{\text{Photodesorption}}$$

Alves et al. 2001
Caselli et al. 2012
Schmalzl et al. 2014

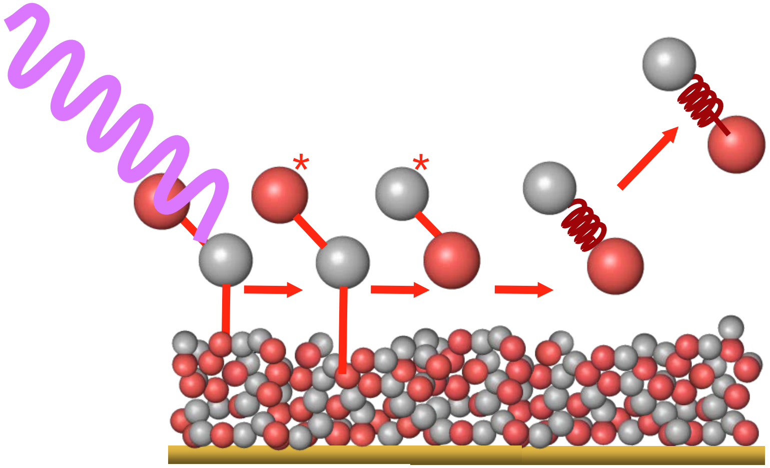
$n = 2.10^4 - 5.10^6\ \text{cm}^{-3}$, $T = 10$ K

Layer of water gas where ice is photodesorbed

Getting molecules off the grains at low T: photodesorption

- Typical efficiencies of 10^{-3} per incident photon

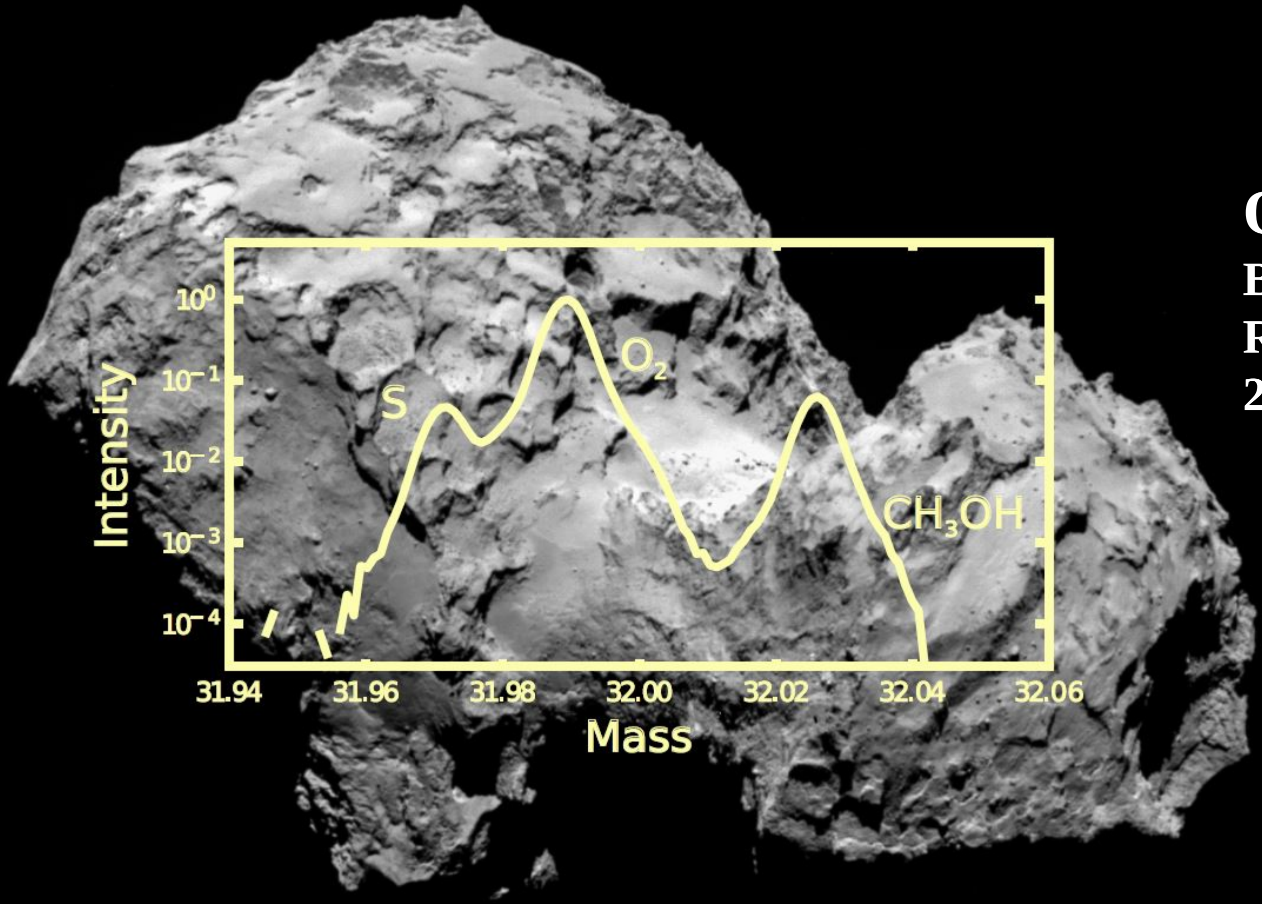
Direct vs kick-out mechanism



Öberg et al. 2007, 2009,
Paardekoper+ 2016, Bertin+ 2016
van Hemert, Takahashi & vD 2014.

Andersson, Kroes, vD 2006
Arasa et al. 2010, 2011, 2015

Abundant O_2 in comets!

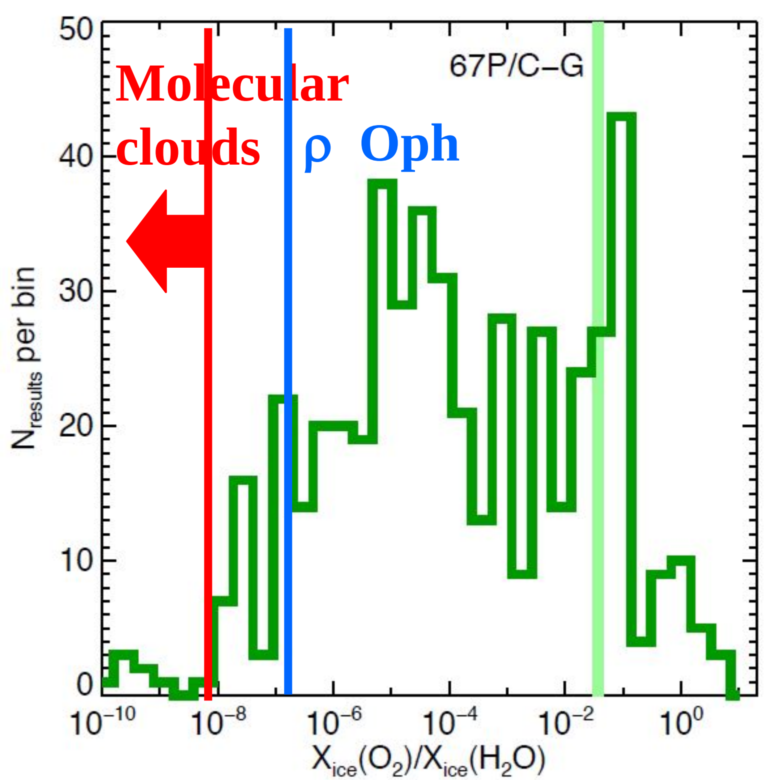


O_2/H_2O~4%

Bieler et al.
Rubin et al.
2015

- **O_2 not detected in molecular clouds, except ρ Oph A and Orion**
  (Goldsmith et al. 2011, Liseau et al. 2012)

The puzzling O_2 story



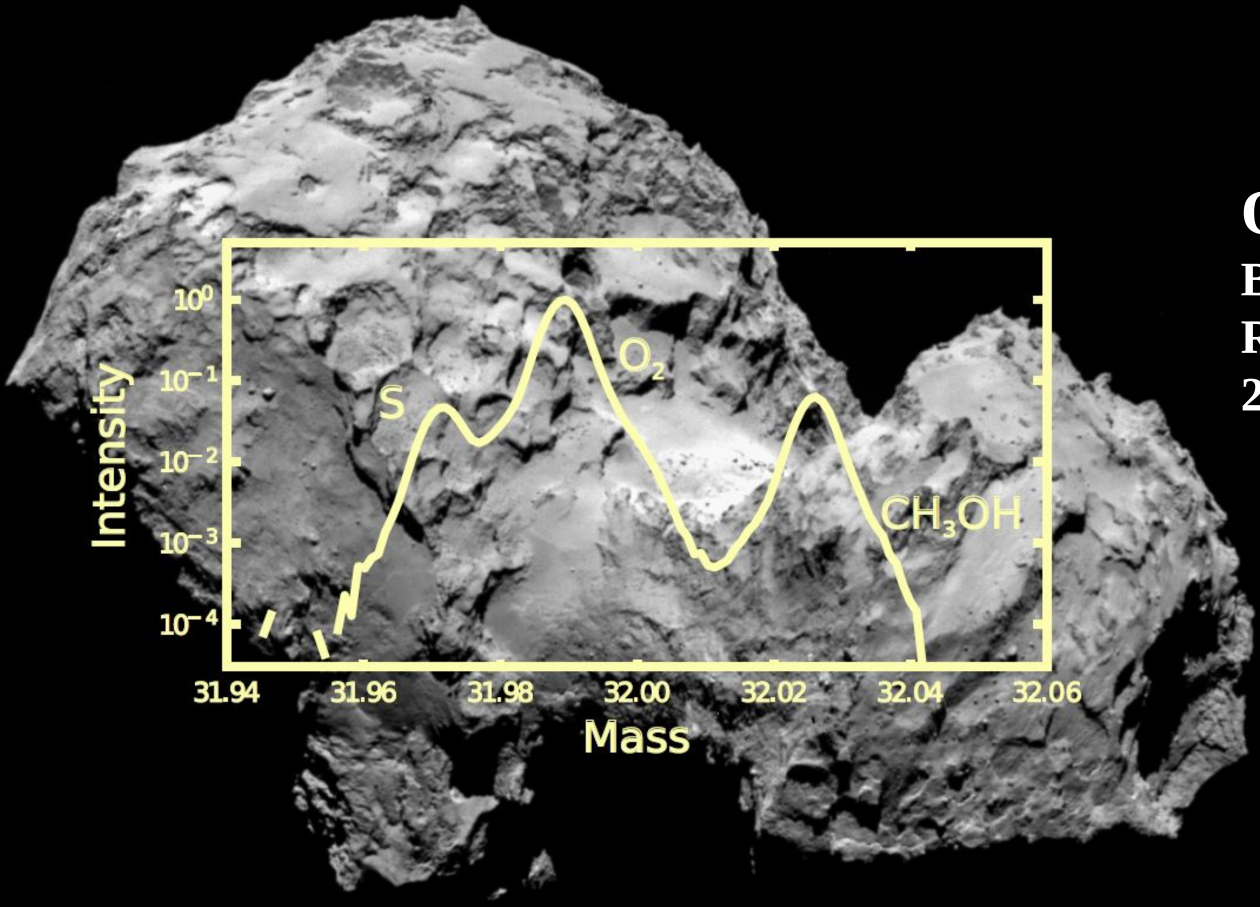
Comets:
High O_2
Low HO_2, H_2O_2, O_3

Molecular clouds:
Low O_2
HO_2, H_2O_2 detected

Taquet et al. 2016

- **Run large set of models for different parameters**
- **Only a very small set of models reproduces 67P values**
- **Requires warm cloud (20-30 K), high *n*, low CR ion rate ζ**

Abundant O_2 in comets!



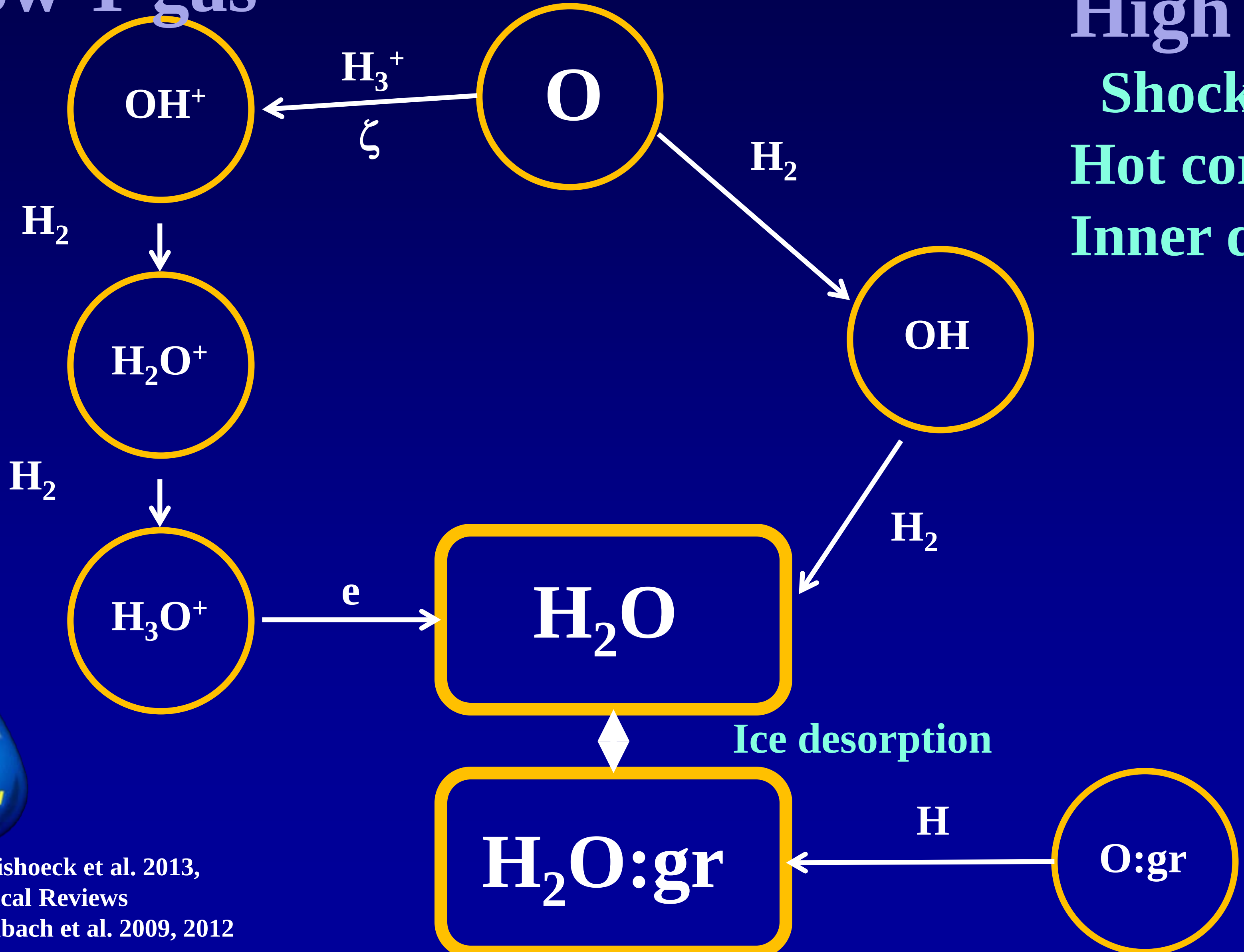
O_2/H_2O~4%

Bieler et al.
Rubin et al.
2015

Needs low
H/O
Taquet et al.
2016

High abundance of O_2 suggests our solar system was formed in a dense warmish cloud (20-30 K vs 10 K)

Water formation routes



Low T gas

High T

Shocks

Hot cores

Inner disks

O

H_3^+

ζ

OH^+

H_2

H_2O^+

H_2

H_3O^+

e

H_2

OH

H_2

H_2O

Ice desorption

Ice

$H_2O{:}gr$

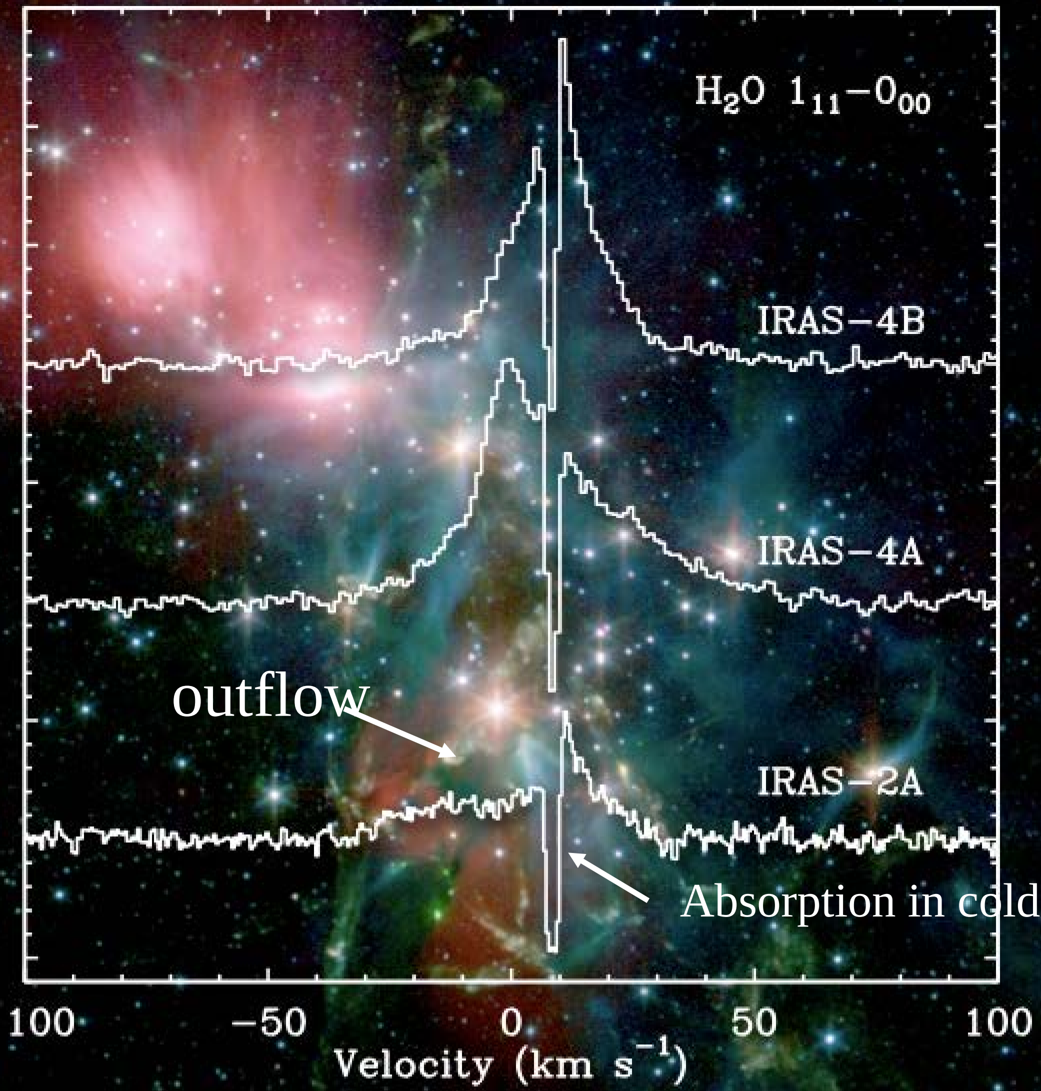
H

$O{:}gr$

Van Dishoeck et al. 2013,
Chemical Reviews
Hollenbach et al. 2009, 2012

Water in low-mass protostars

L~20 L_{Sun}
D~750 lyr



outflow

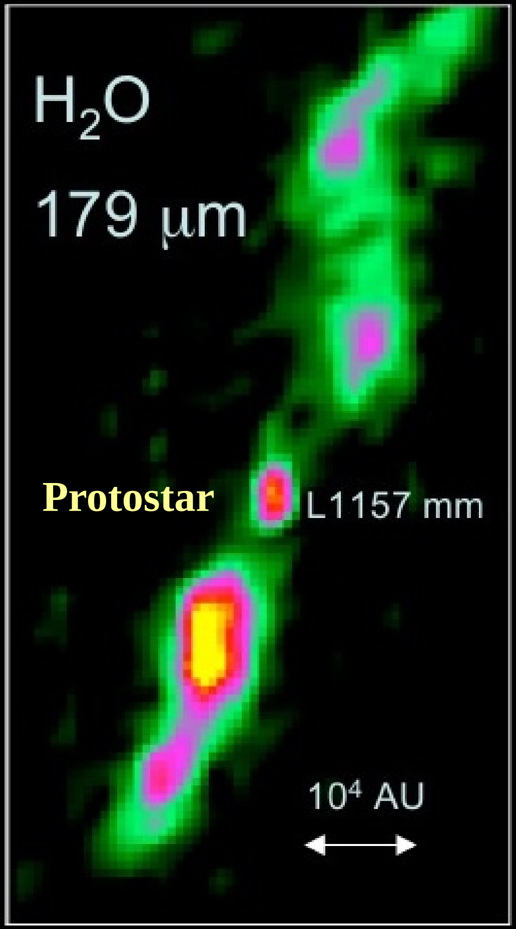
Absorption in cold outer envelope

NGC 1333
p-H_2O
ground-state
Line: 1 THz

Broad lines: outflow dominates, even for $H_2^{18}O$

Kristensen, et al. 2010, 2012
Mottram et al. 2014, 2017

Imaging water outflows



Nisini et al. 2010, 2014

Water traces ‘hot spots’ where shocks dump energy into cloud
But this water is lost to space, not included in forming solar systems

How much water is flowing?

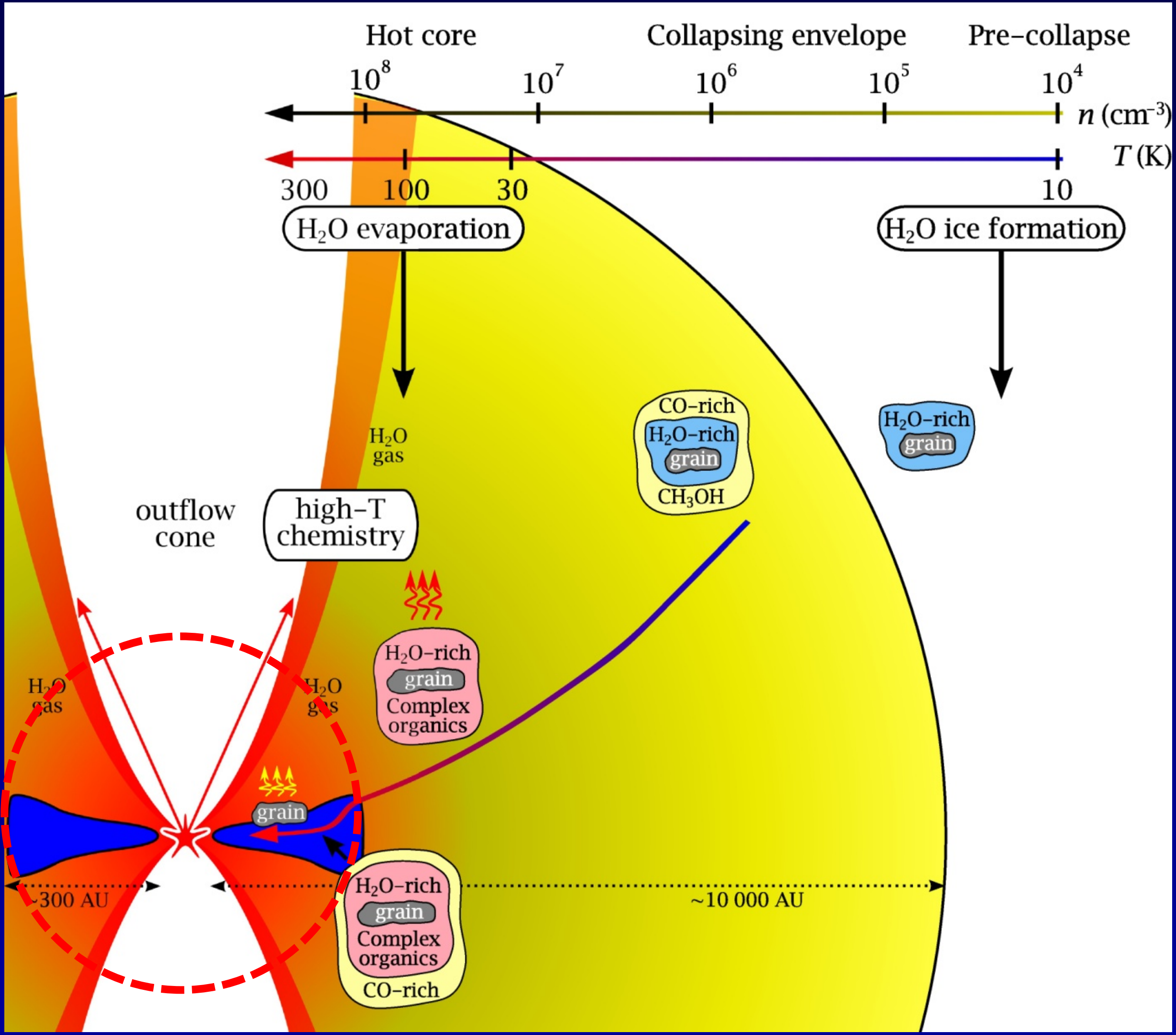
2330 m^3/s

Iguacu falls

One protostar = 10^9 Cataratas!
would fill up all of Earth's oceans in 5000 yr

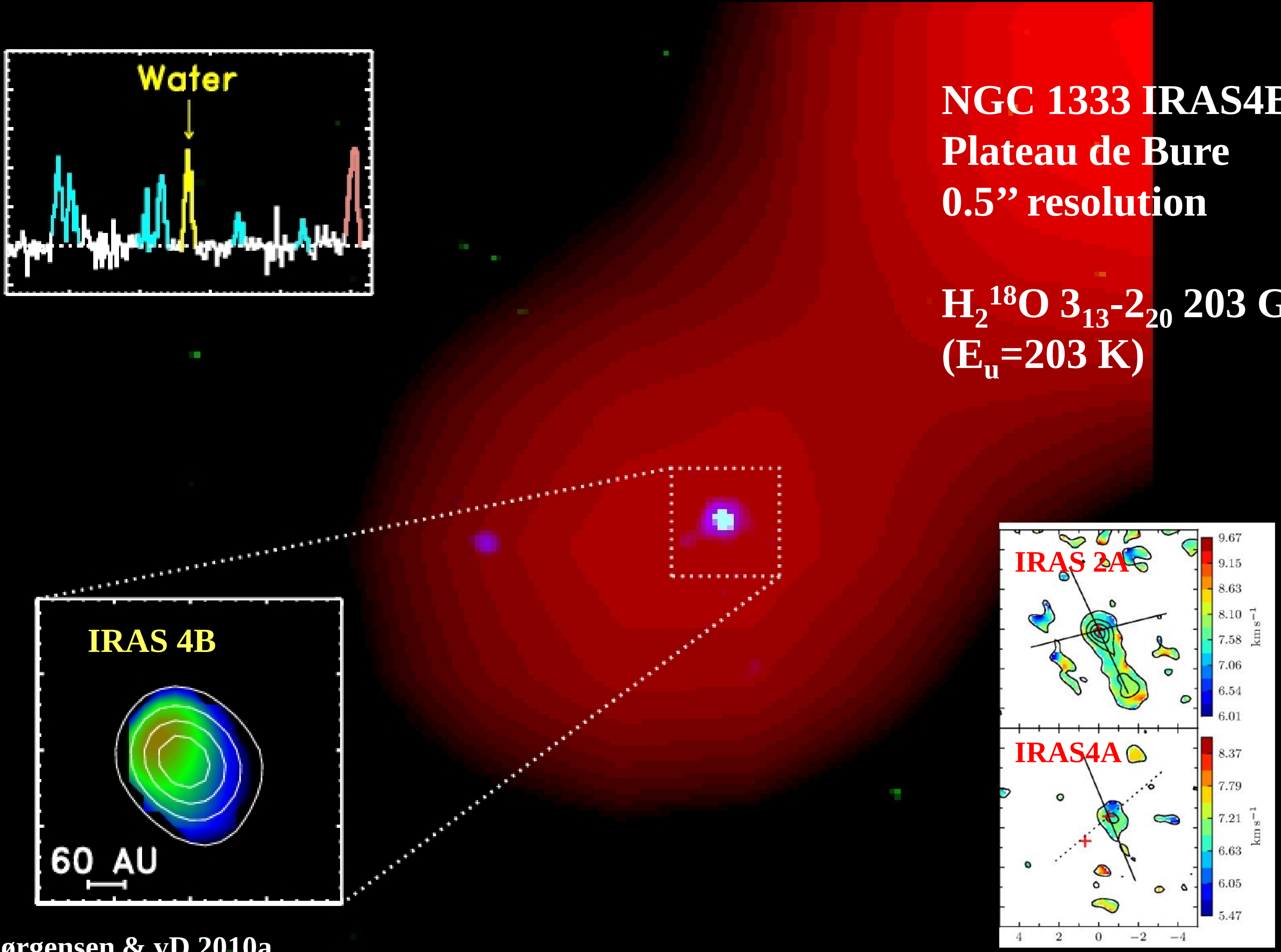
High rate of water production!

Follow water trail from cores to disk



Visser et al. 2009
Herbst & vD 2009

Hot water on solar system scales



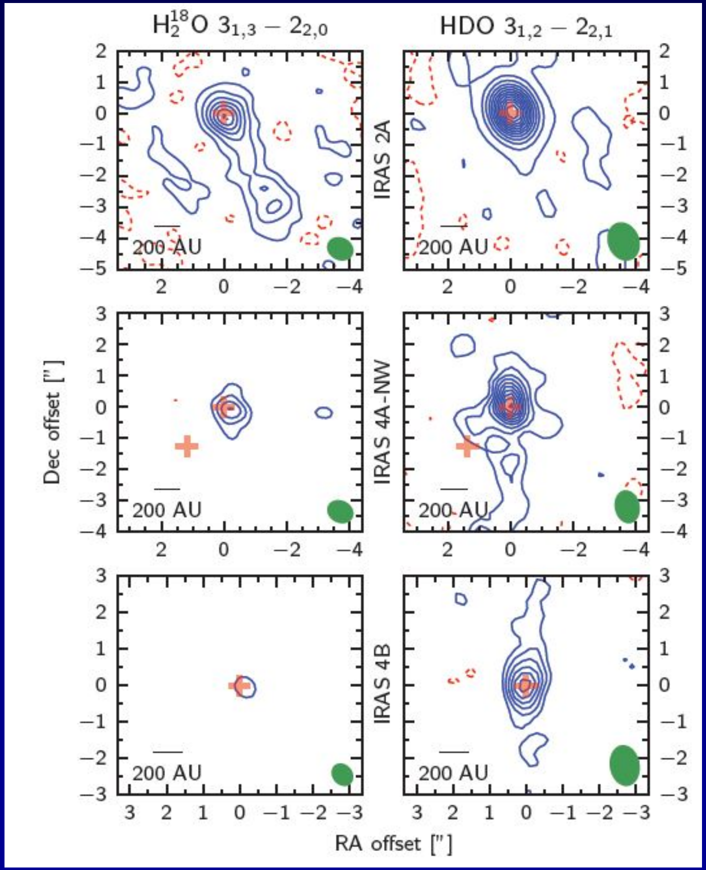
NGC 1333 IRAS4B
Plateau de Bure
0.5” resolution

$H_2{}^{18}O\ 3_{13}$-2_{20} 203 GHz
(E_u=203 K)

Jørgensen & vD 2010a
Persson et al. 2012, 2013

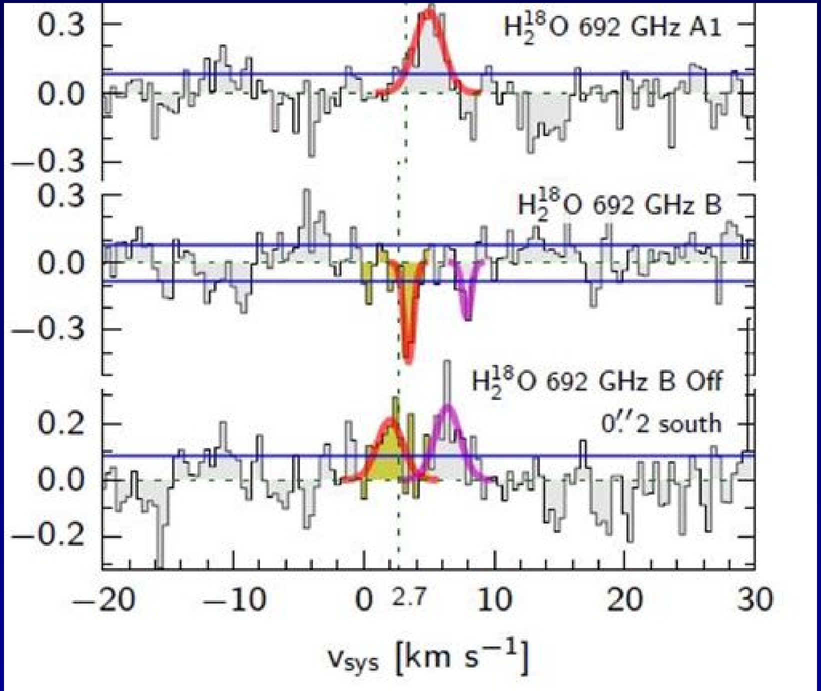
Hot water detected, but not all oxygen in water $<10^{-4}$

HDO/H_2O solar system scales



Persson et al. 2012, 2014, NOEMA
Jorgensen & van Dishoeck 2010a,b

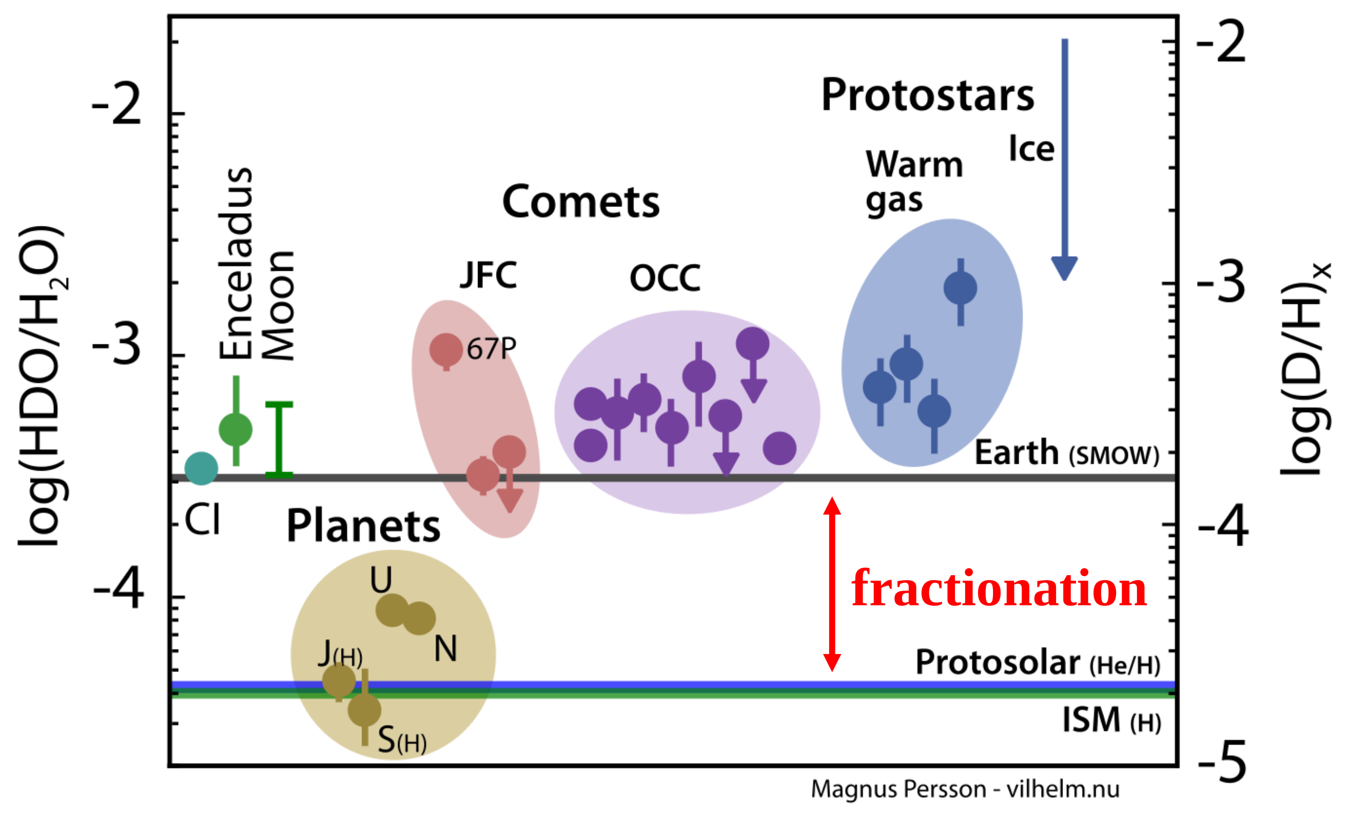
Young warm 'disks'



Persson et al. 2013, ALMA

HDO/H_2O~10^{-3}

HDO/H_2O as tracer history solar system



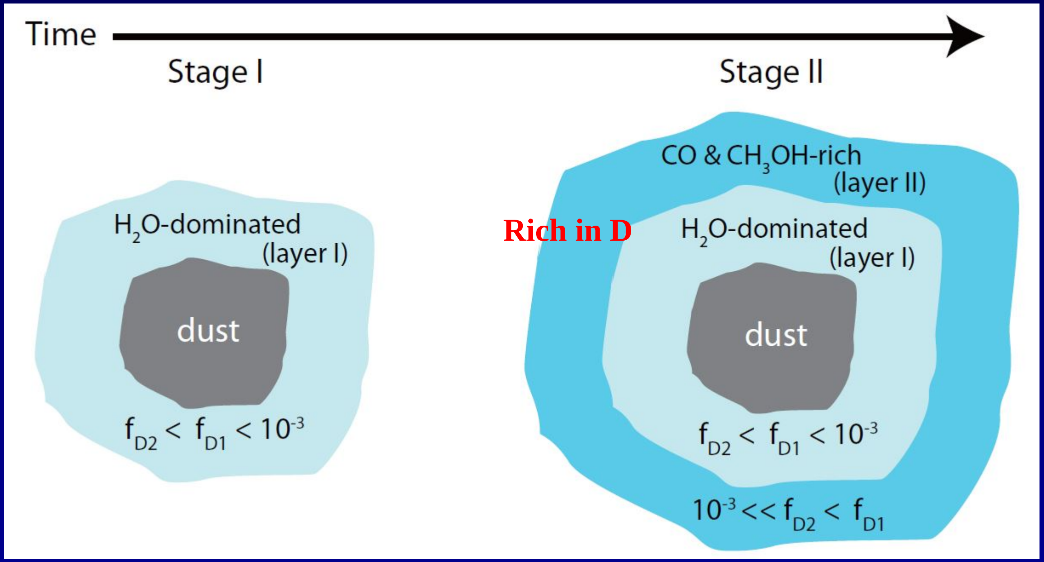
Persson et al. 2014

Bockelée-Morvan et al. 2014
Ceccarelli et al. 2014
Altwegg et al. 2014
vD et al. 2014

Similarity cometary and protostellar envelopes consistent with HDO/H_2O set in clouds and icy grains preserved upon disk and planetesimal formation

Doubly deuterated water in hot cores

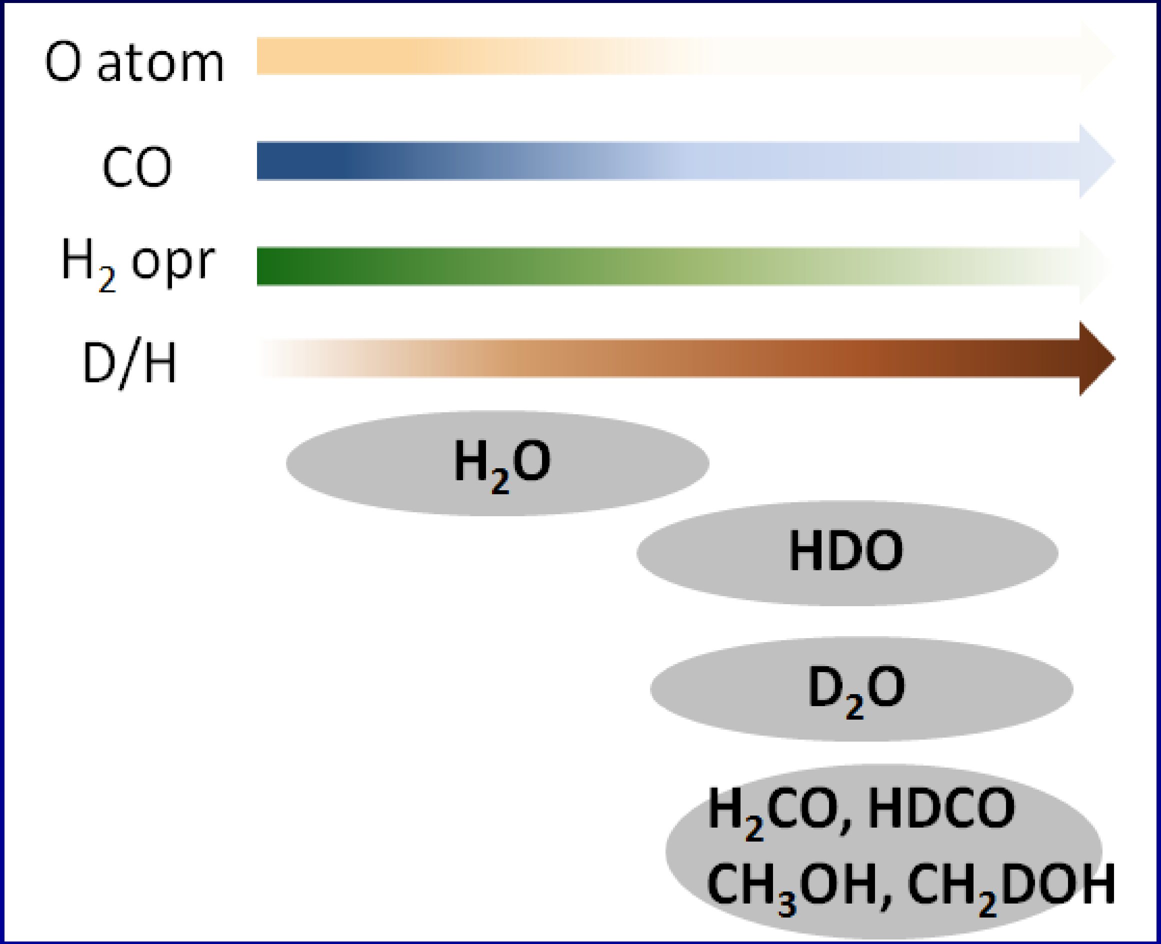
$$D_2O/HDO >> HDO/H_2O$$



Furuya et al. 2016, Coutens et al. 2014, Dartois et al. 2003

- **Most of H_2O formed in molecular clouds**
- **Most of HDO and D_2O formed in dense cores during heavy freeze out**
- **Consistent with ROSINA 67P results! (Altwegg et al. 2017)**

Deuteration sequence



O atom

CO

H_2 opr

D/H

H_2O

HDO

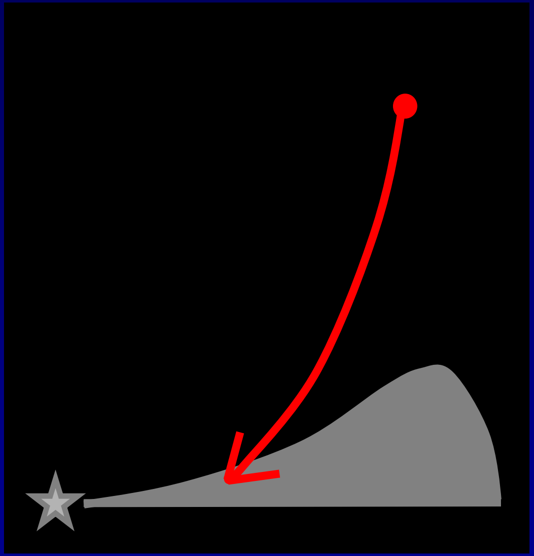
D_2O

H_2CO, HDCO

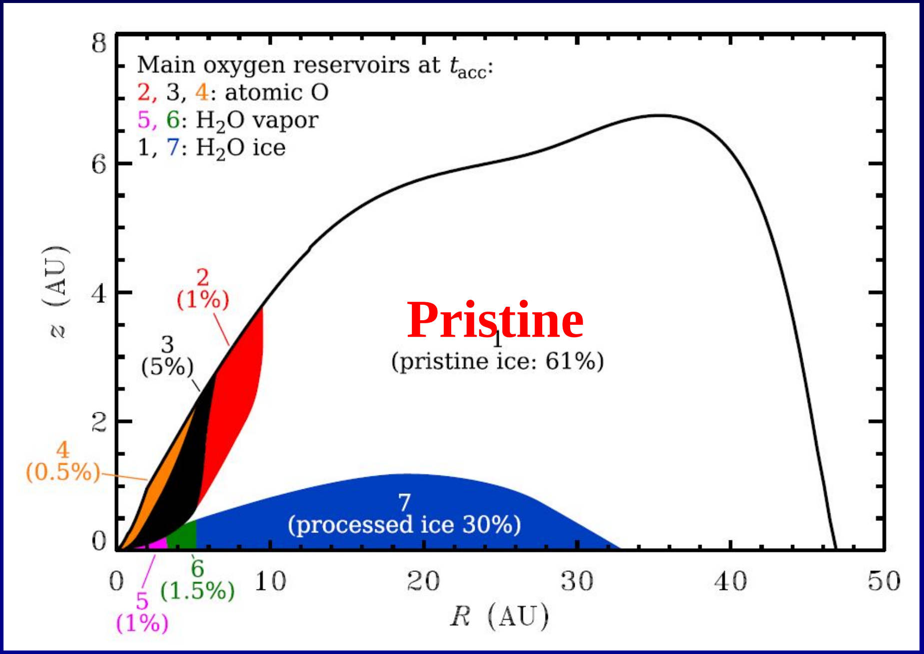
CH_3OH, CH_2DOH

Furuya et al. 2016
Taquet et al. 2012, 2014

‘Reset’ vs ‘Inheritance’



History of water in disk

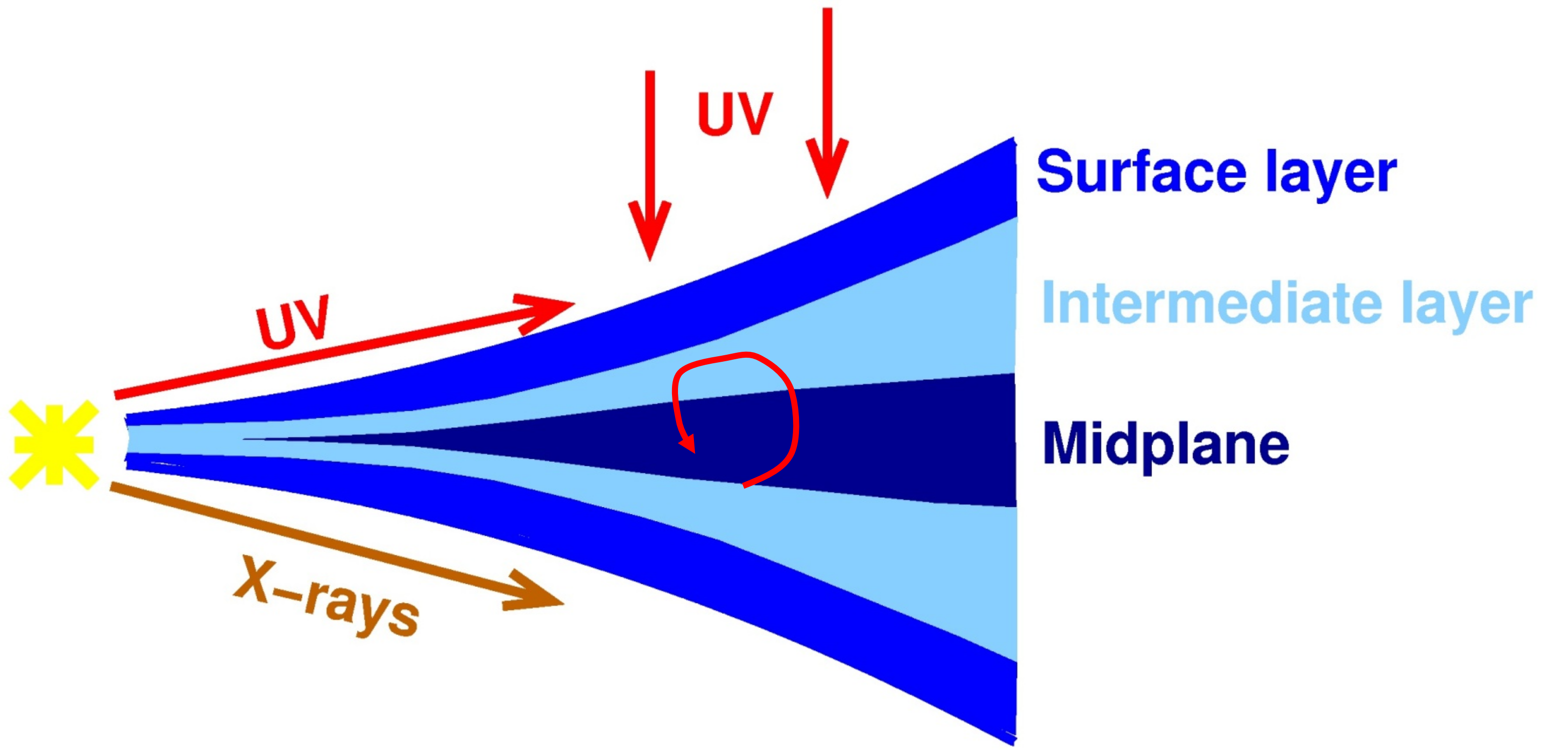


Visser et al. 2009, 2011
Drozdovskaya et al. 2014

- **Start at collapse phase, follow up to end of embedded phase**
- **Follow individual trajectories as they fall into disk**
- **Each trajectory has different *n*, *T*, UV (*t*)** (Ciesla & Sandford 2012)
- **Disk evolves and spreads**

III. Chemistry in disks

- Surface layer: molecules dissociated by UV photons
- Warm intermediate layer: molecules not much depleted, rich chemistry
- Cold midplane: molecules heavily frozen out

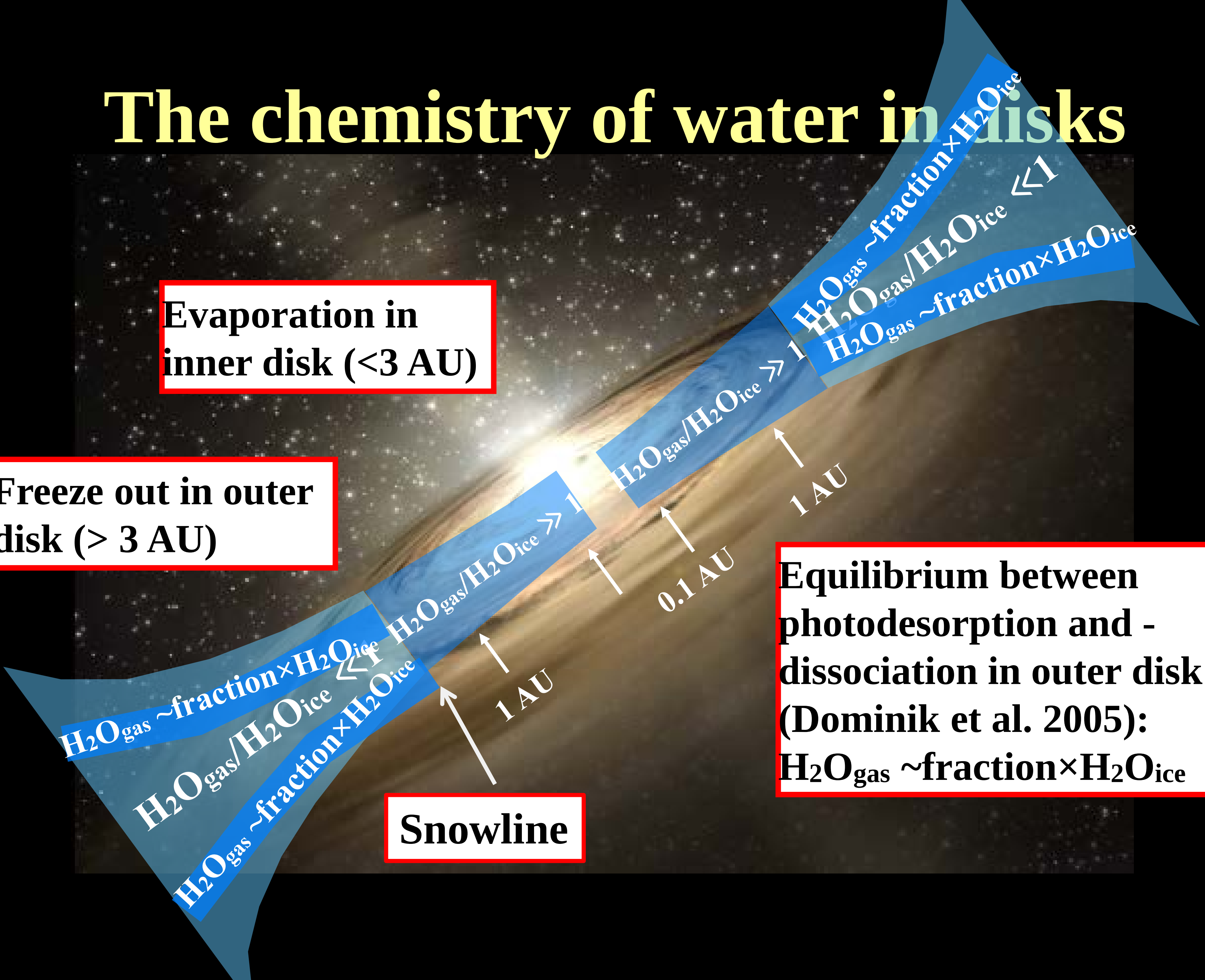


Q: How to trace midplane?

Aikawa & Herbst 1999
Aikawa et al. 2002
Van Zadelhoff et al. 2003
Fogel et al. 2010

Willacy & Langer 2000
Markwick et al. 2002
Henning & Semenov 2013
Woitke et al. 2009
Bruderer et al. 2012
+ many groups

The chemistry of water in disks



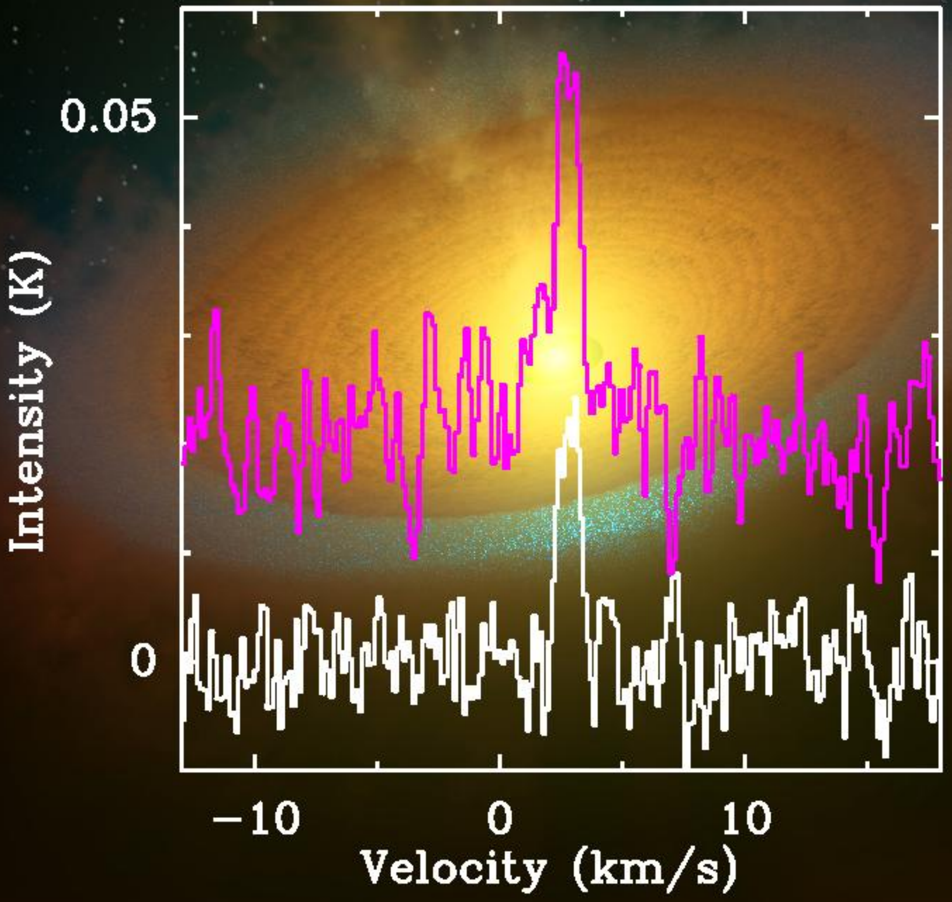
Evaporation in inner disk (<3 AU)

Freeze out in outer disk (> 3 AU)

Equilibrium between photodesorption and -dissociation in outer disk (Dominik et al. 2005): H_2O_{gas} ~fraction×H_2O_{ice}

Snowline

Detection cold water reservoir in disks



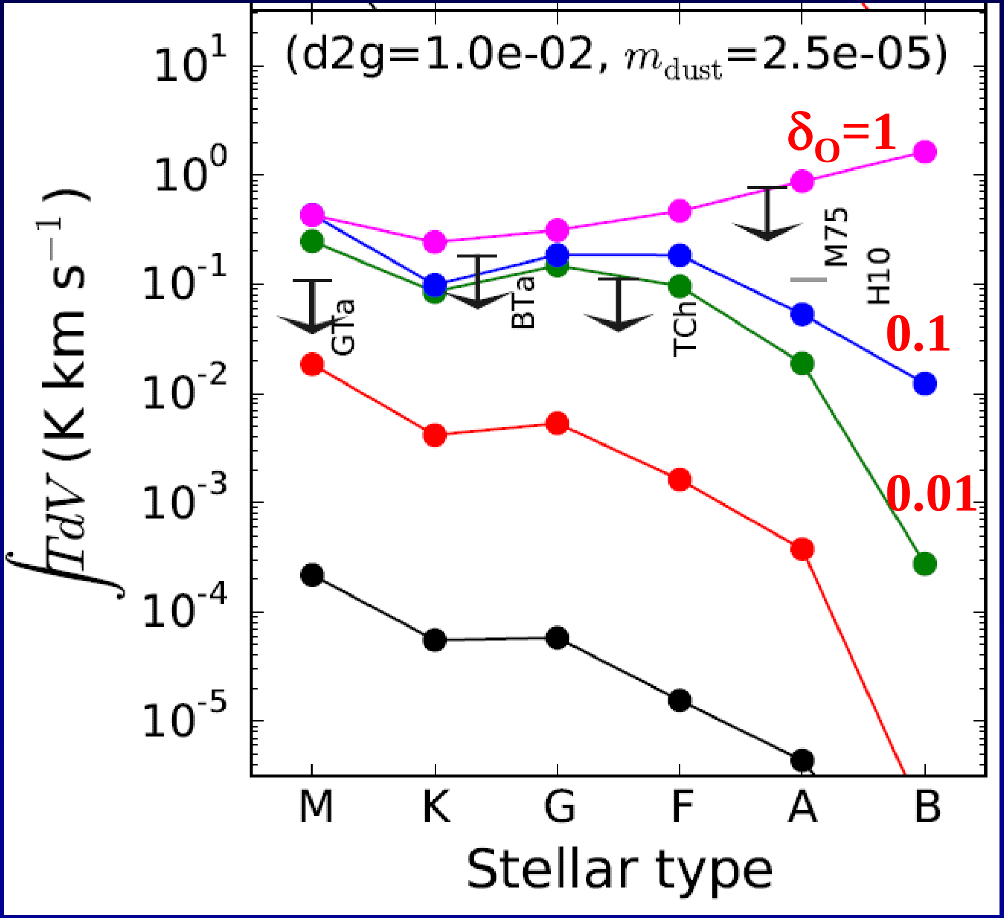
p-H_2O 1_{11}-0_{00}
1113 GHz

o-H_2O 1_{10}-1_{01}
557 GHz

Hogerheijde et al. 2011
Bergin et al. 2010

Signals point to presence of 6000 oceans of water ice

Weak water lines in disks

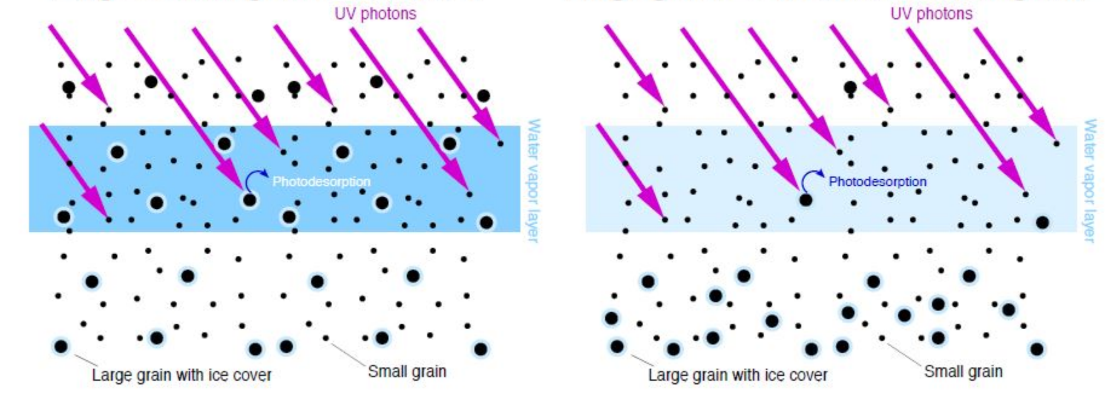


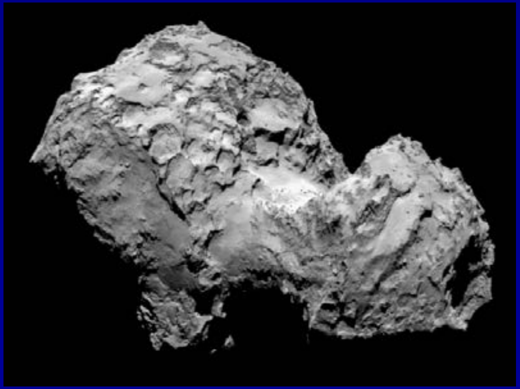
Du et al. 2017, 2015
Bergin et al. 2010

- Can only be fit by models with volatile oxygen reduced by factor of 10-100

Absence of cold gaseous water

- Water sequestered in large bodies early
  - Settling of mm-sized grains, planetesimal formation
- Water follows mm grains
  - Moved inward due to radial drift

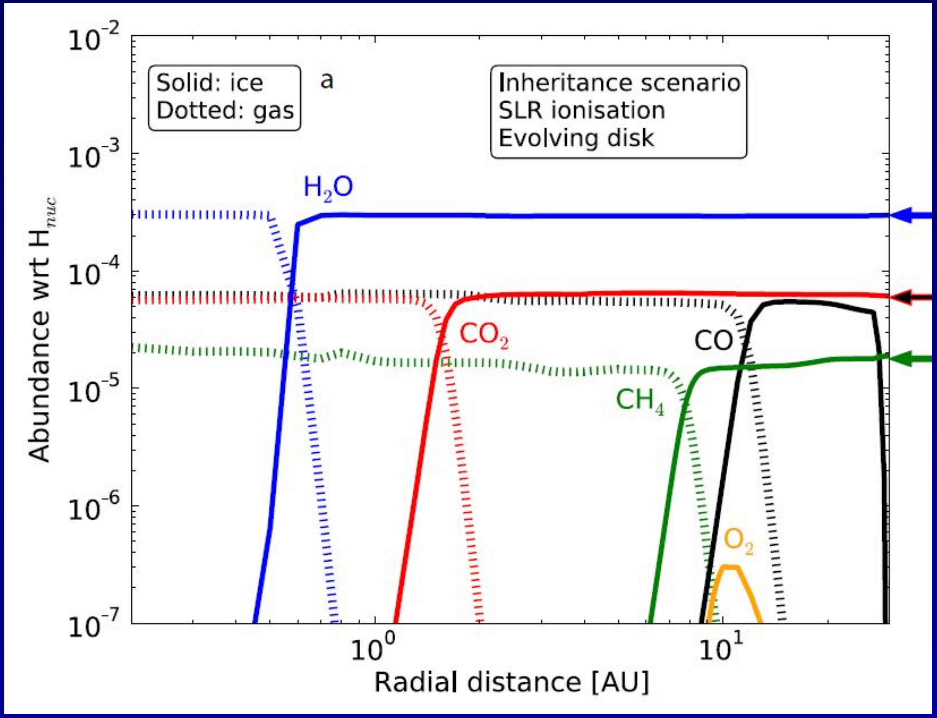


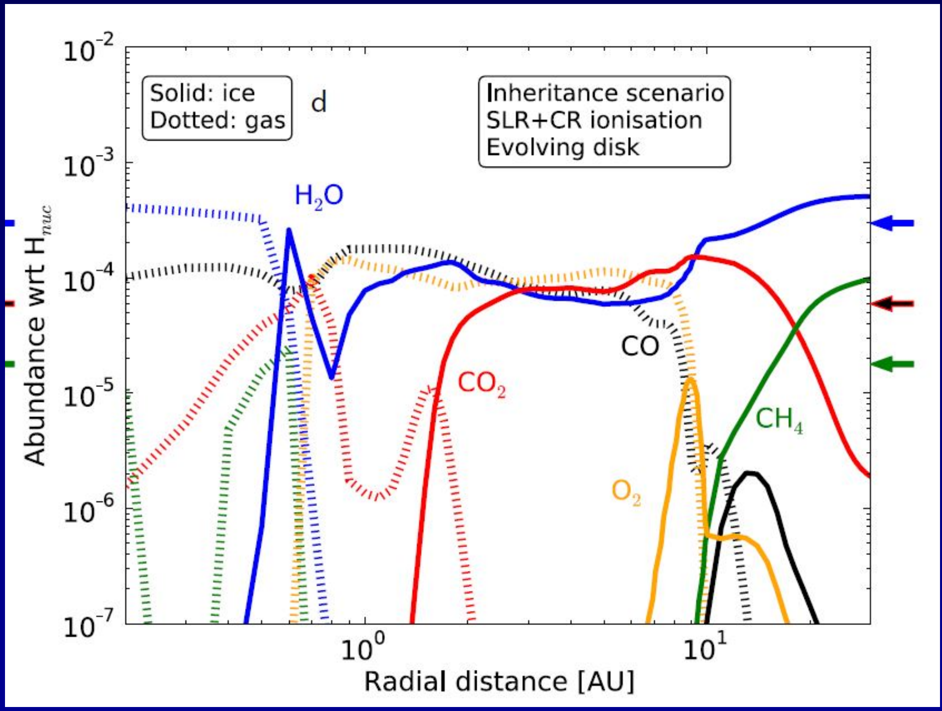


Bergin et al. 2010, Du et al. 2015, Kama et al. 2016

Does chemistry matter?

Only if ionization high enough



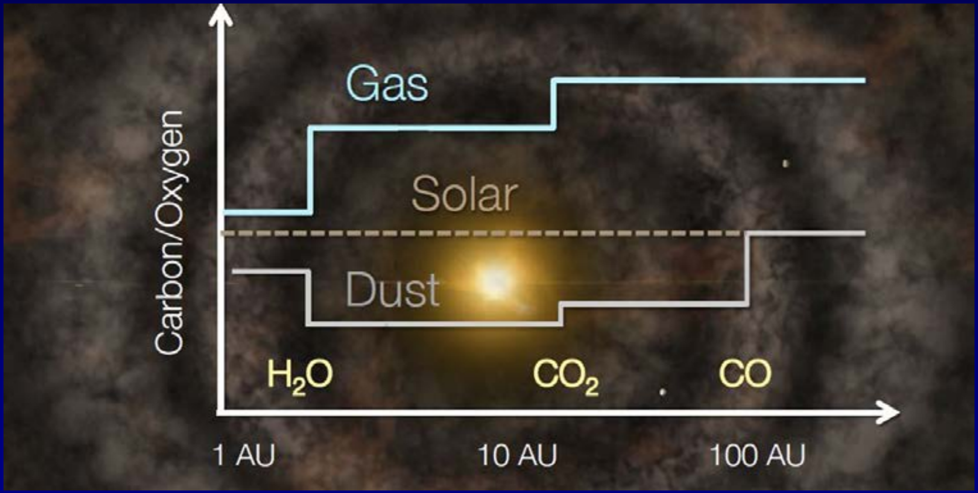


SLR=short-lived radionuclides

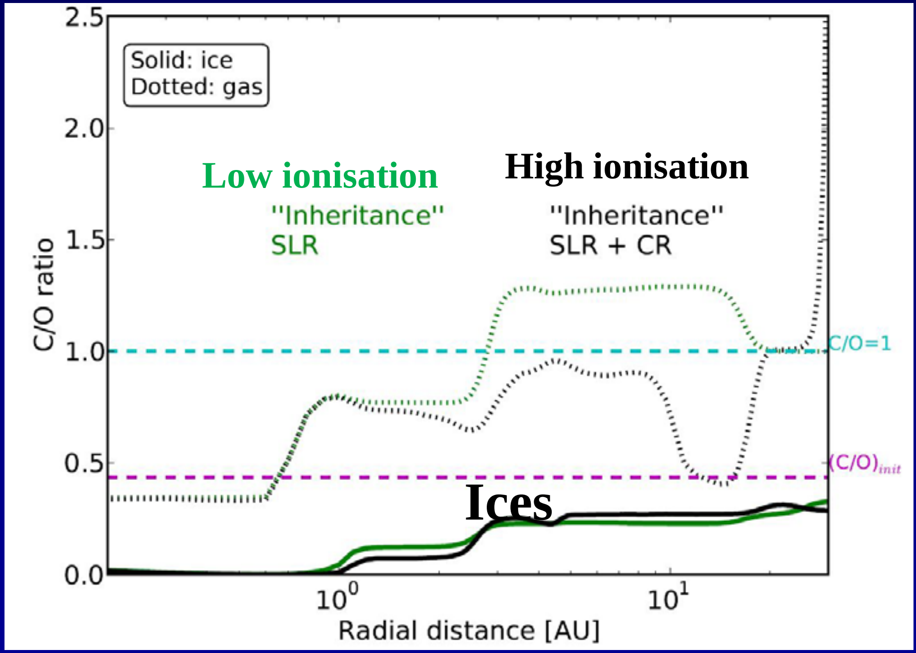
Eistrup et al. 2016, 2017

- Use Alibert+ disk models
- Inheritance (molecular) vs Reset (atomic) abundances
- High versus low ionization

Does midplane chemistry matter?



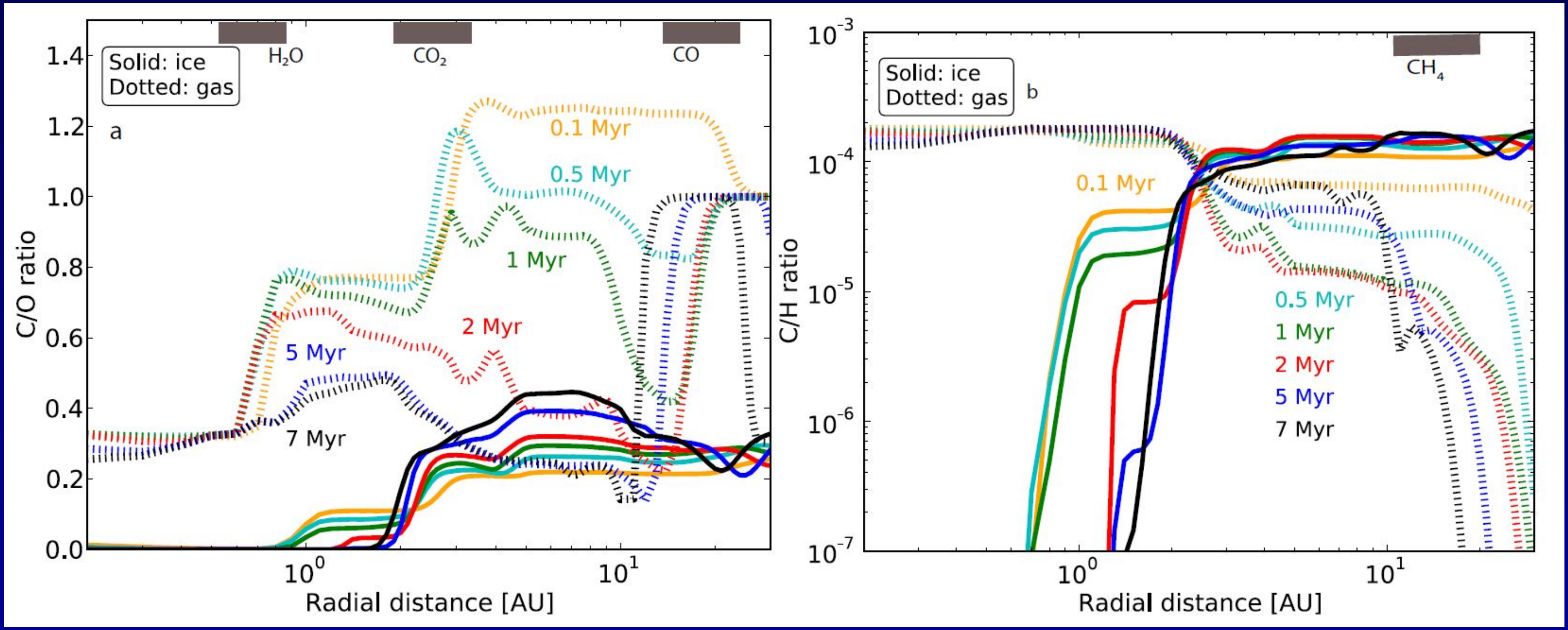
Öberg et al. 2011



Eistrup, Walsh, vD
2016, 2017

- Chemistry affects C/O in gas if high ionisation
- Importance depends whether planets accrete heavy elements from gas or ice

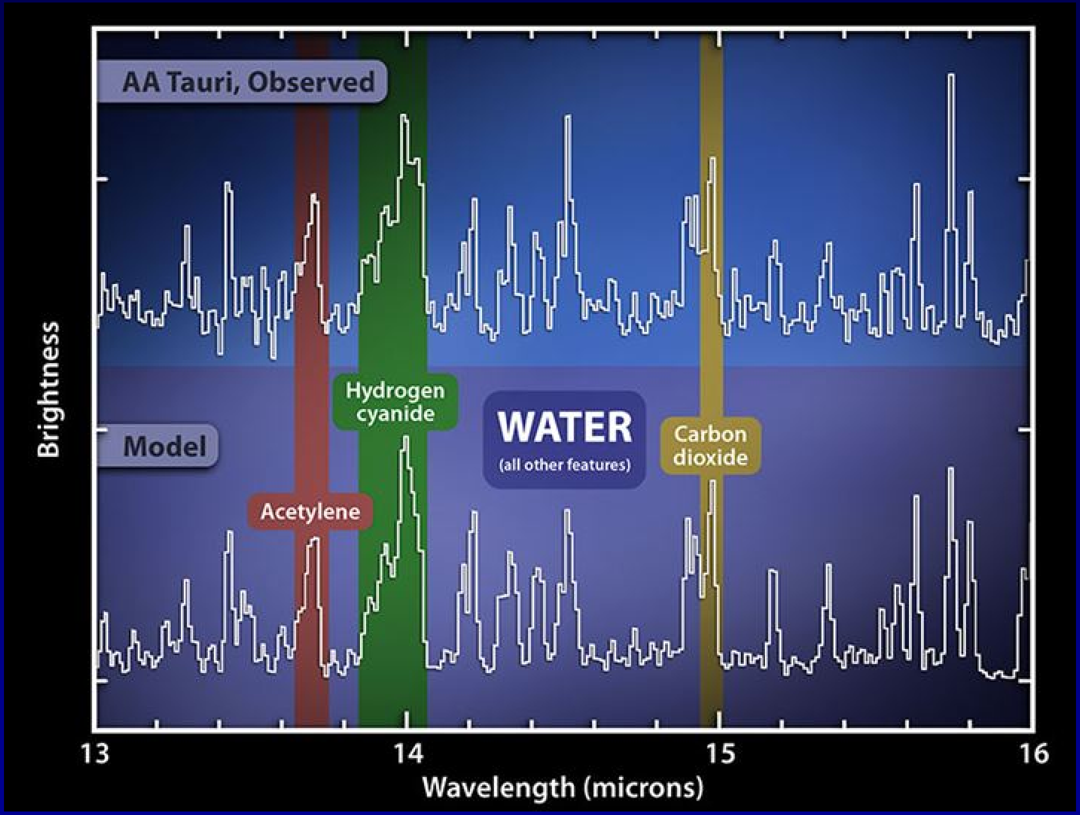
C/O ratio in evolving disk



Eistrup et al. 2017

- **C/O and C/H in gas high only at early times beyond water ice line**

Inner disk (<1 AU): hot chemistry

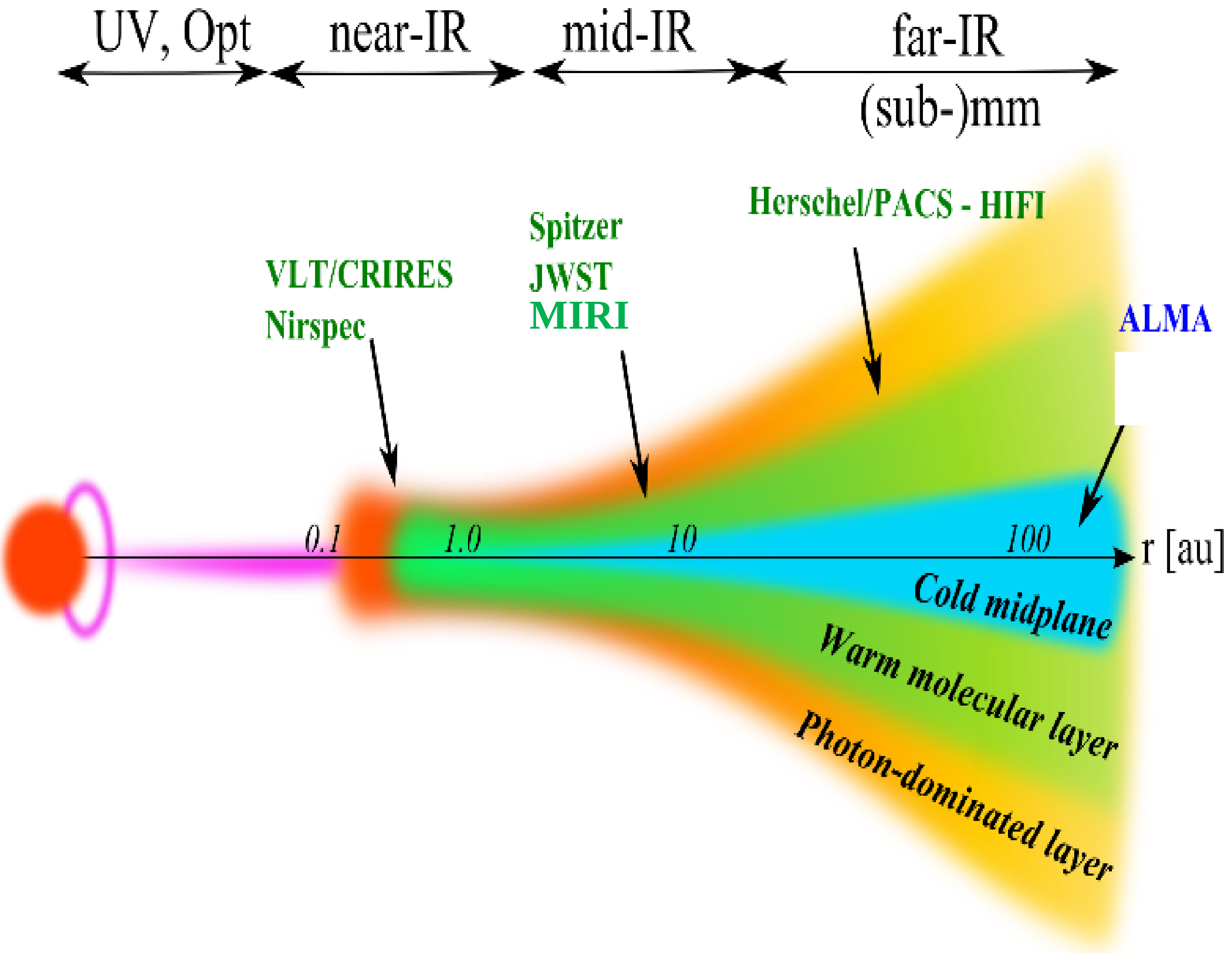


Note low line / continuum ratio at R~600

Carr & Najita 2008, Salyk et al. 2008, 2010, Lahuis et al. 2006, Pontoppidan et al. 2014

- **High temperature (300-1000 K) chemistry** **(e.g., Walsh et al. 2015)**

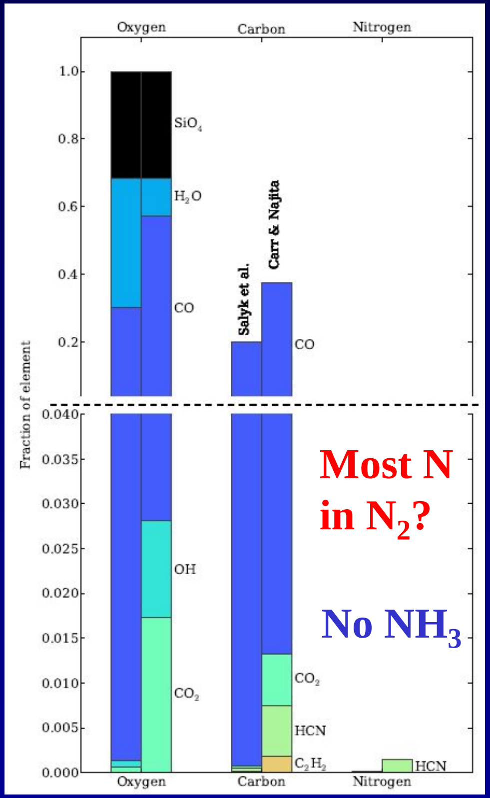
Probing protoplanetary disks



D. Fedele

ALMA measures the bulk of the gas and dust in disks and can observe bulk of molecules

C, N and O budget



Most N in N_2?

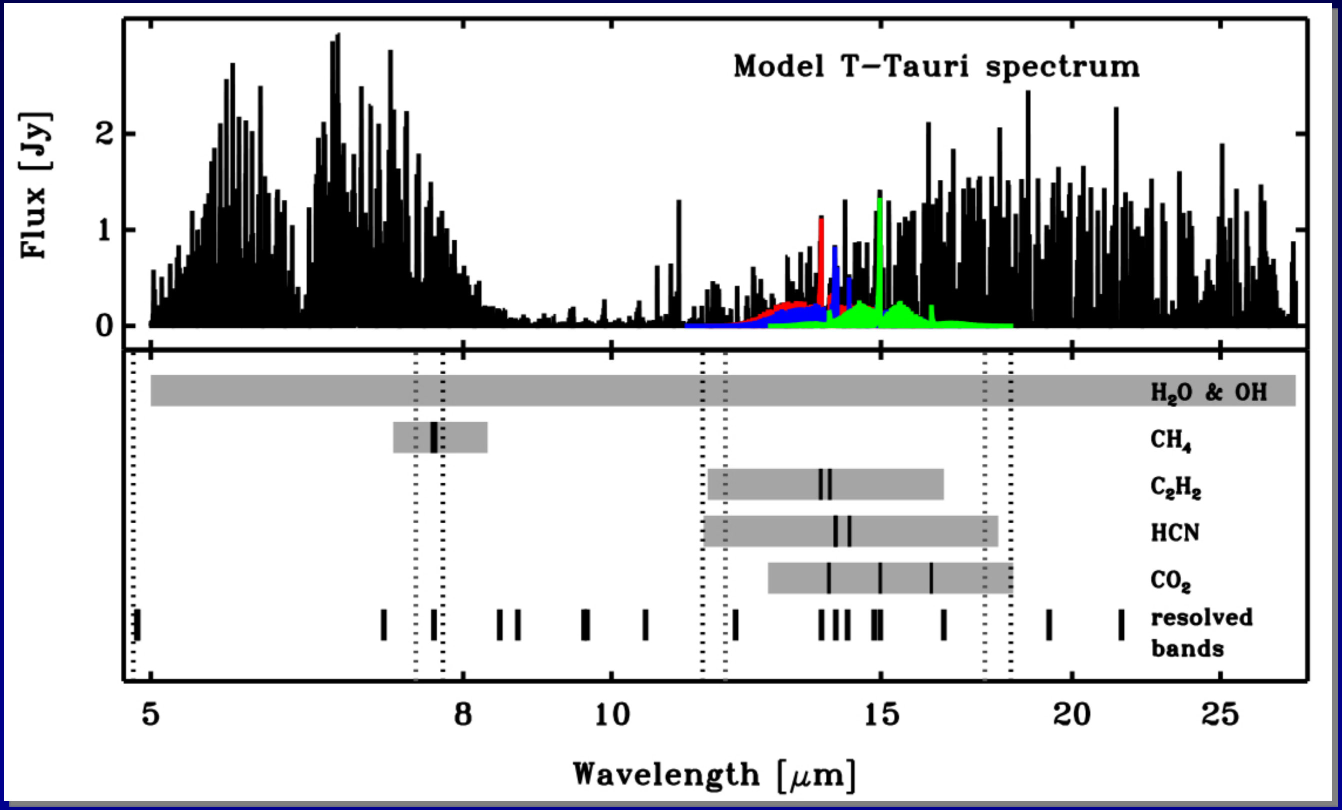
No NH_3

Pontoppidan et al. 2014

- Where are carbon and nitrogen?

JWST-MIRI will greatly improve sensitvity + spectral resolution

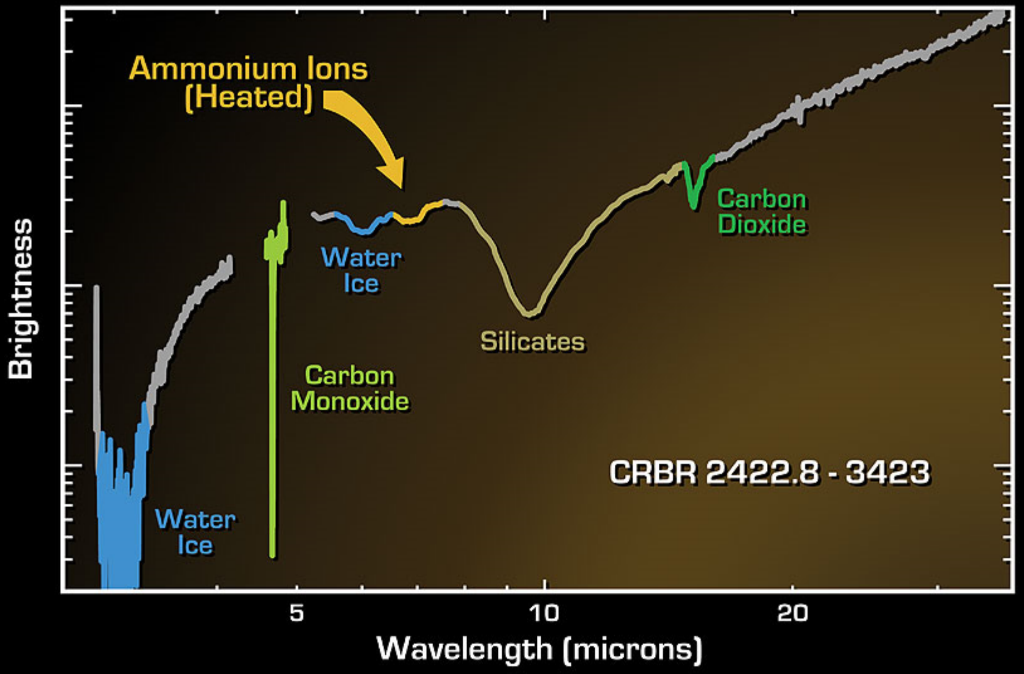
Model disk spectra JWST



Lahuis,
Bosman et al. 2017

- Chemical inventory inner disk: consistent with solar abundances? Similar to more evolved disks? Evidence for planetesimal formation and drift?
- CH_4 and NH_3 can now be observed!

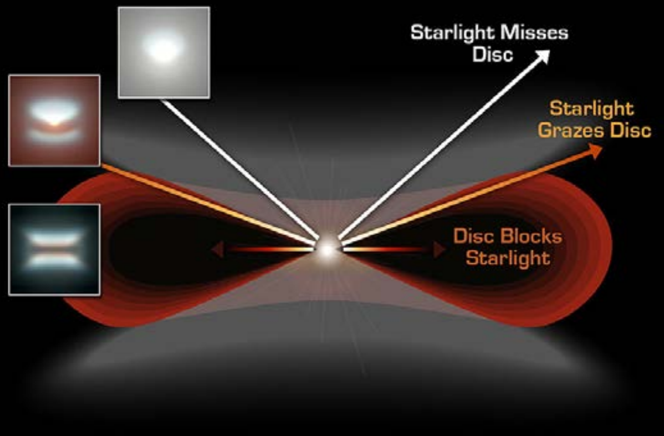
Ices in edge-on disks



Ices in a Protoplanetary Disc

NASA / JPL-Caltech / K. Pontoppidan (Leiden Observatory)

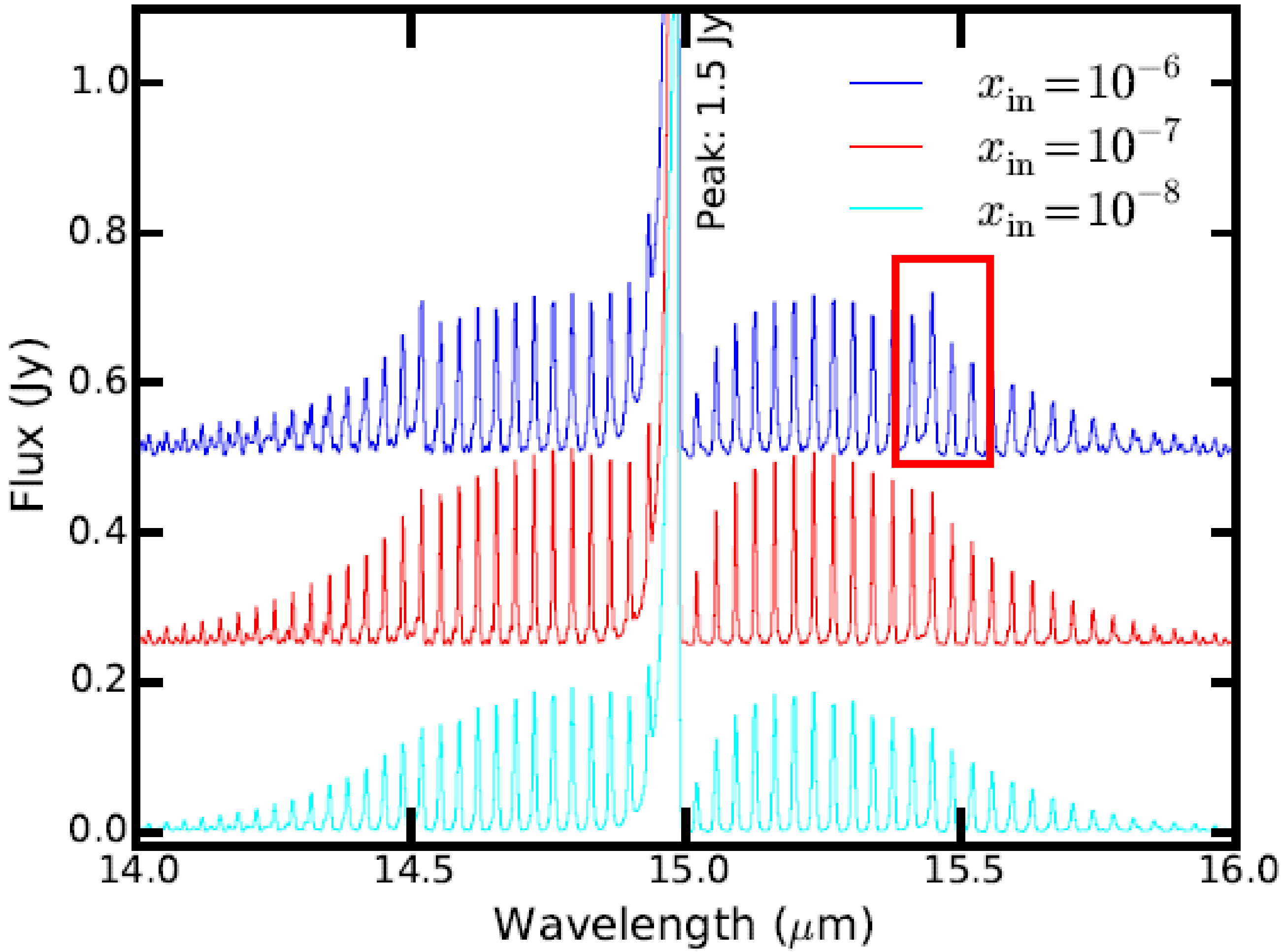
Spitzer Space Telescope • IRS
ESO • VLT–ISAAC
ssc2004-20c



Measure CO_2, CH_4 ice in disks for the first time; O_2 search

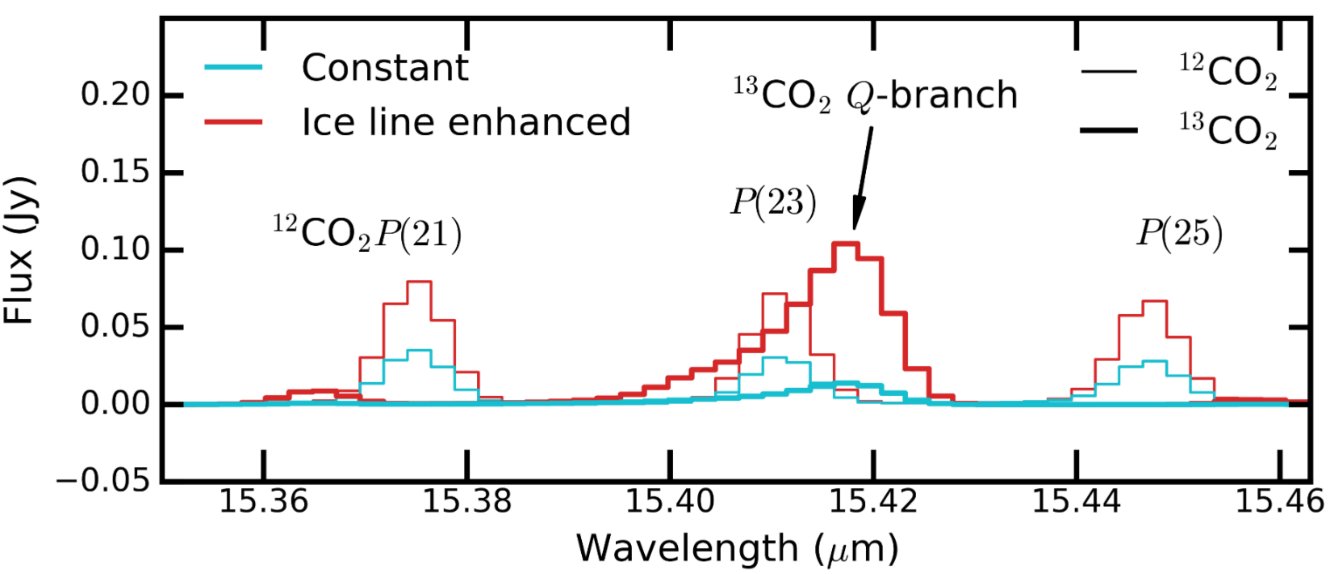
Pontoppidan et al. 2005

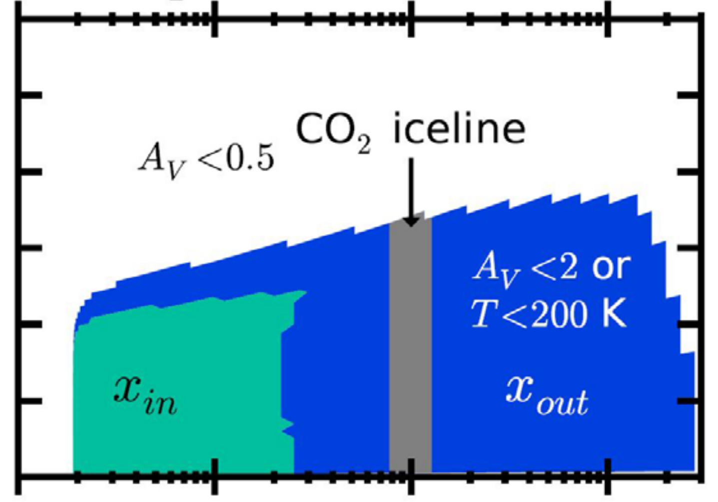
CO_2 spectrum



- Effect of different abundances difficult to see in spectra

Sublimating planetesimals at icelines



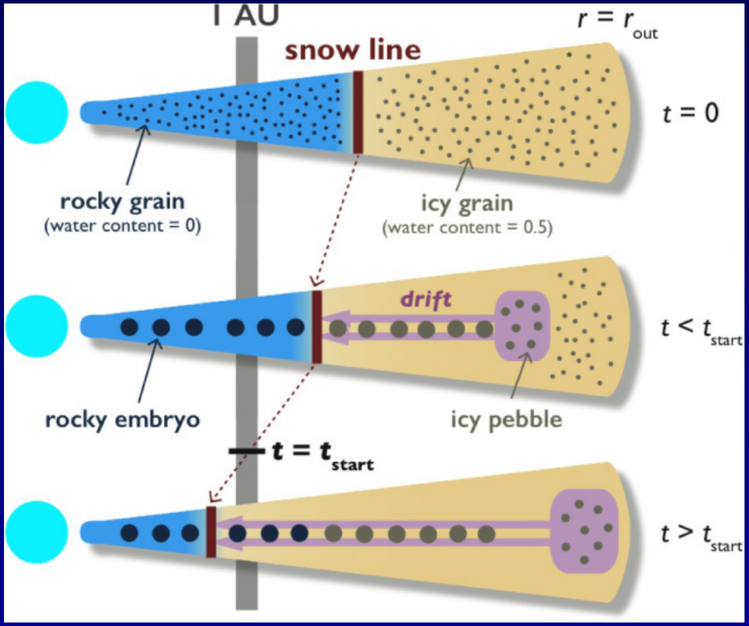


Bosman et al. 2017, 2018

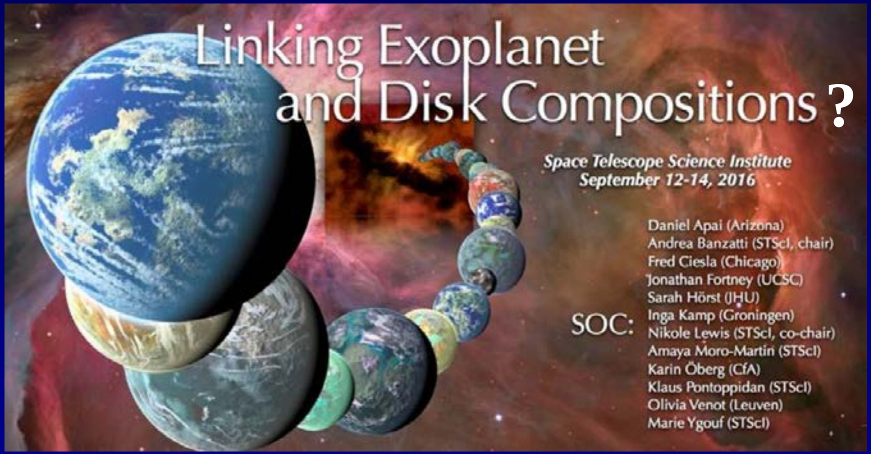
JWST can see this enhancement through $^{13}CO_2$

Can we link planetary atmosphere composition with its formation location / history?

Key question: are most heavy elements accreted from gas or ice?



Sato et al. 2016, Modasini et al. 2016



Linking Exoplanet and Disk Compositions ?

Space Telescope Science Institute
September 12-14, 2016

SOC:
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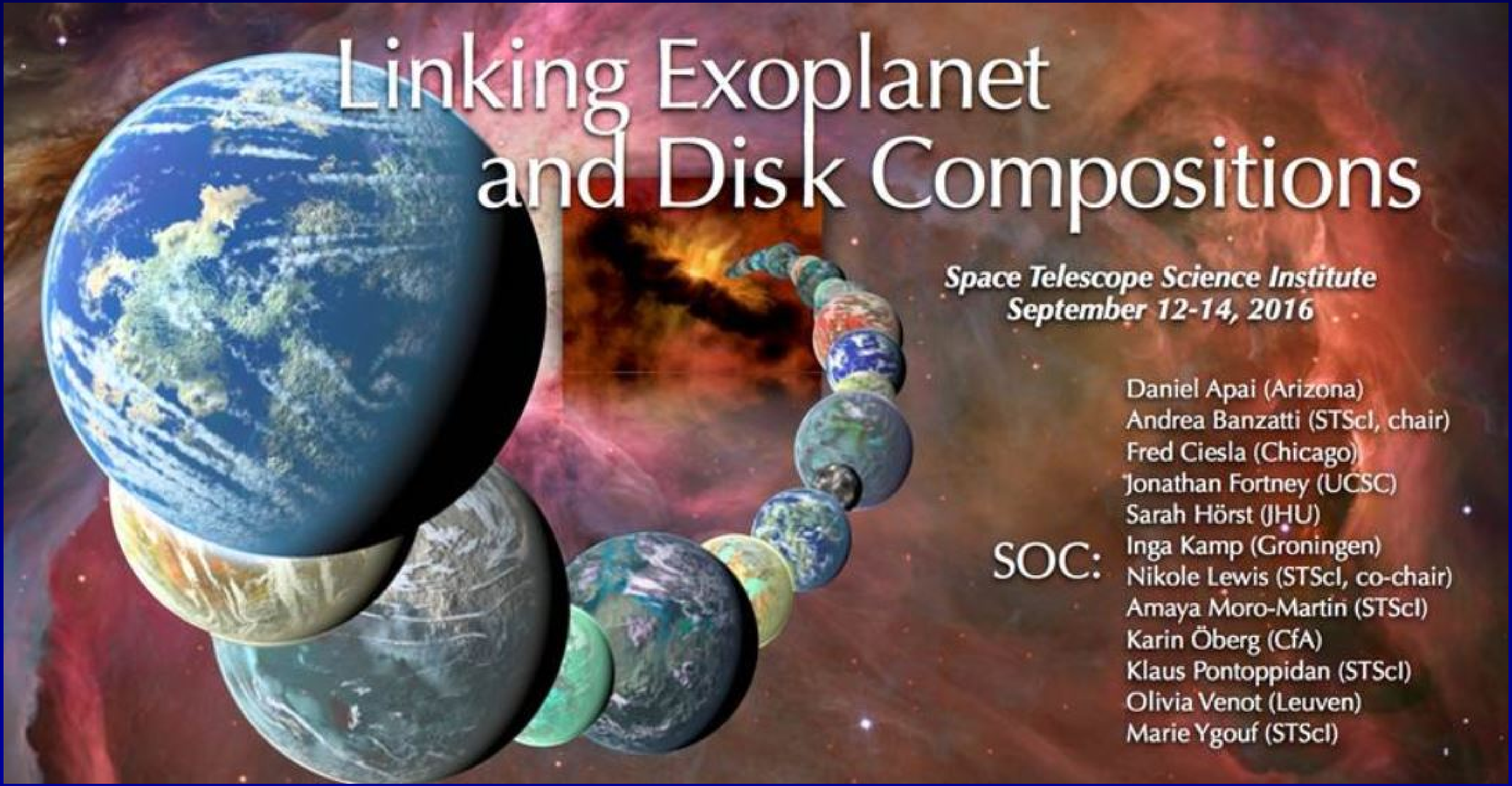
Klaus Pontoppidan (STScI)
Olivia Venot (Leuven)
Marie Ygouf (STScI)

Consider also:

- Radial drift pebbles, dust traps, diffusive mixing
- Migration planets
- Reset chemistry in inner disk (inside snow lines)
- Reset chemistry in planetary atmospheres→ preserve C/O, C/N?

The next step



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