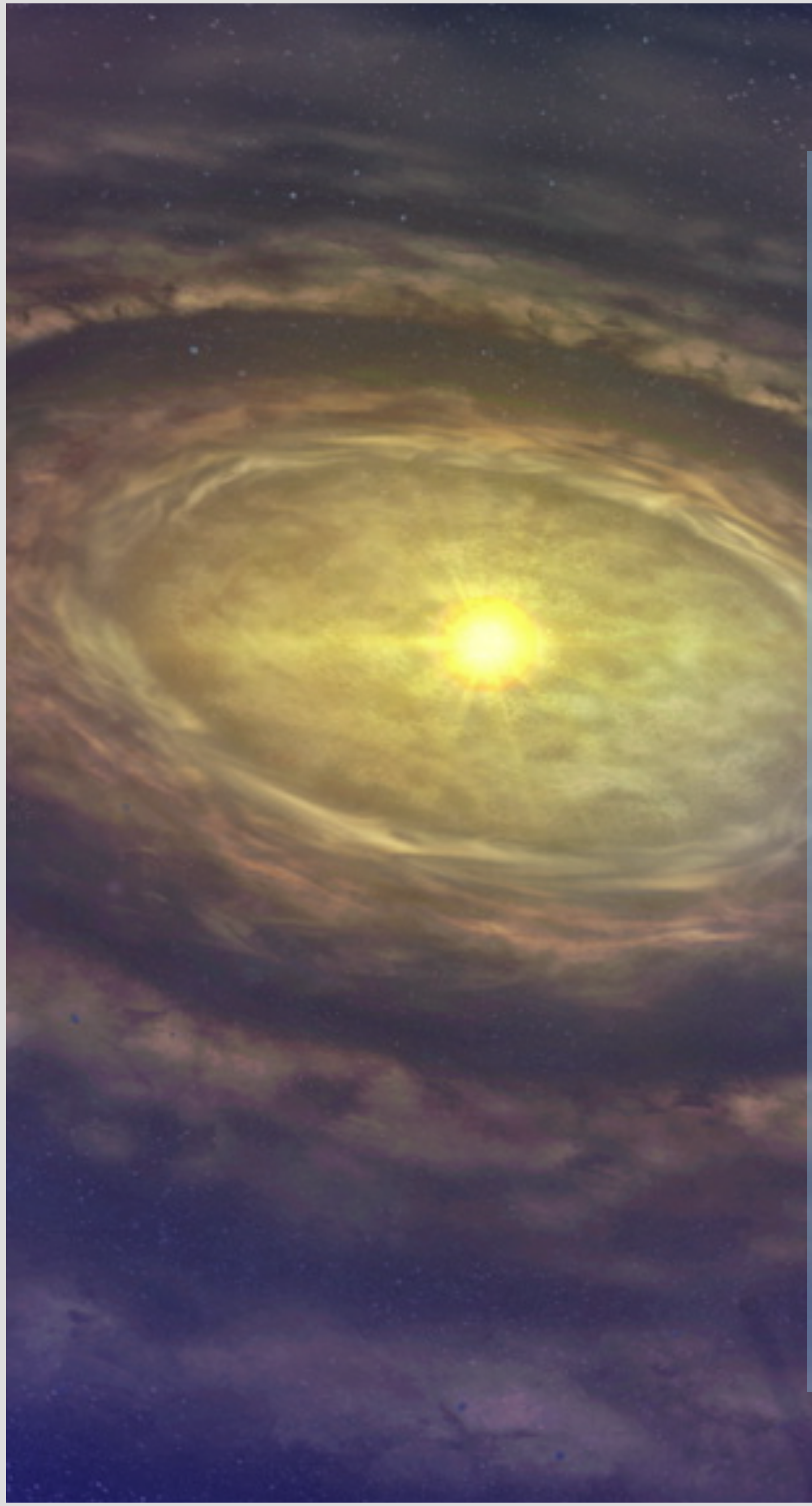


OBSERVING THE CHEMISTRY OF PLANET FORMATION

Ilse Cleeves
Assistant Professor, University of Virginia
July 26, 2019

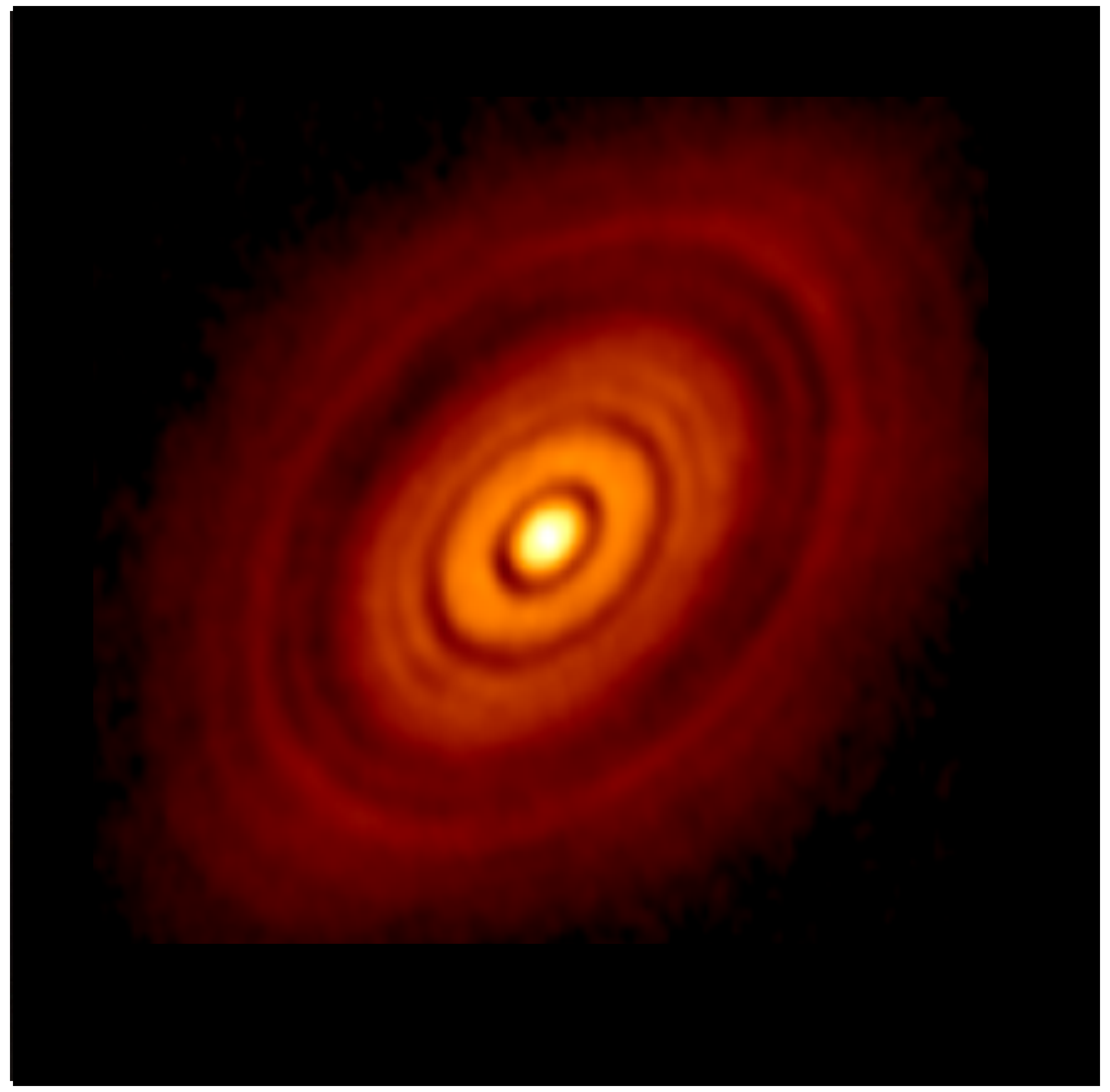
Edwin Bergin, Karin Oberg, David Wilner, Ryan Loomis, Jane Huang, Sean Andrews, Vivi Guzman

DISK COMPOSITION

The protoplanetary disks' compositions initially set by the parent molecular cloud, some amount of reprocessing as the central star(s) form

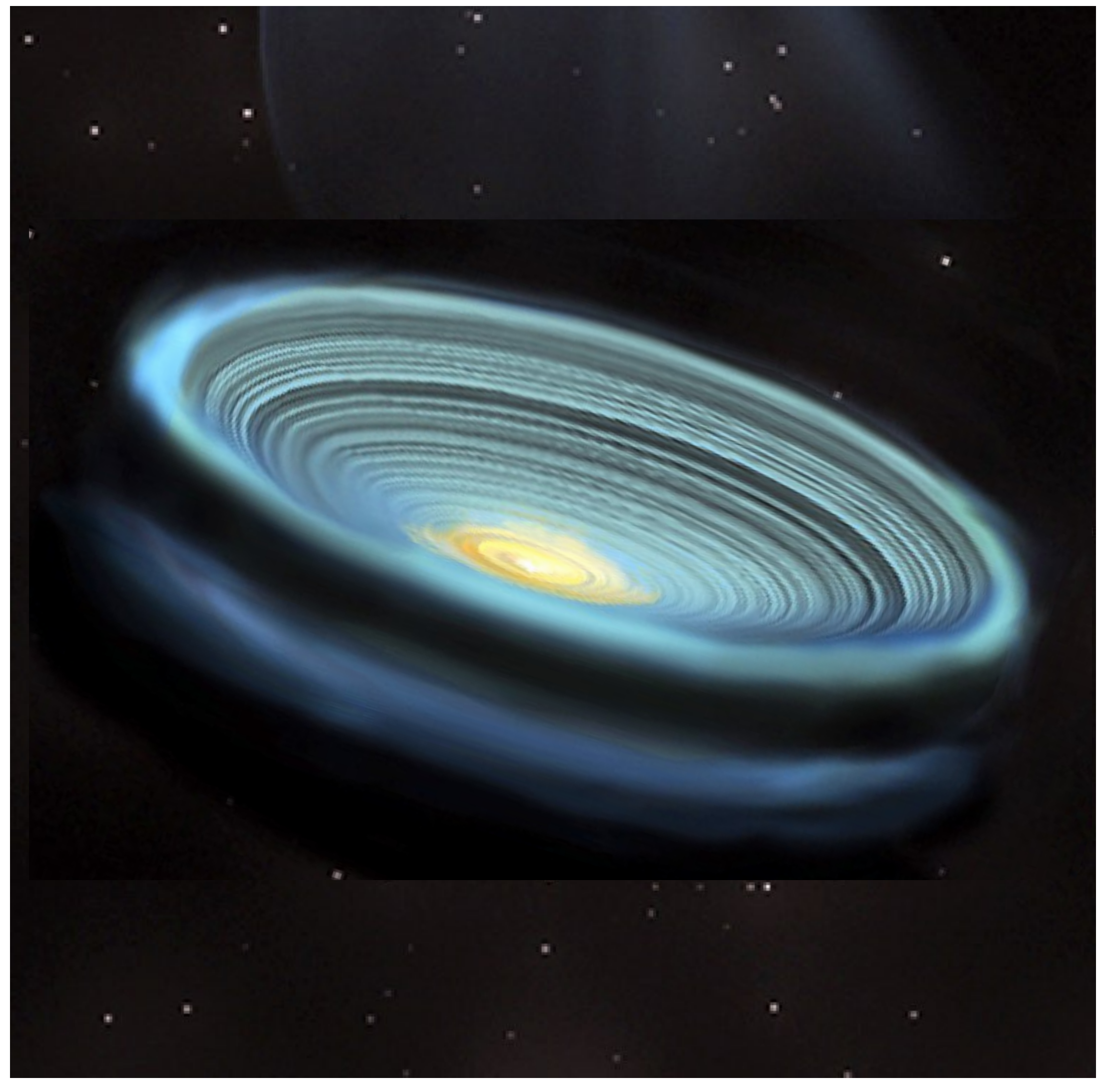
~10s of Myr

Cloud



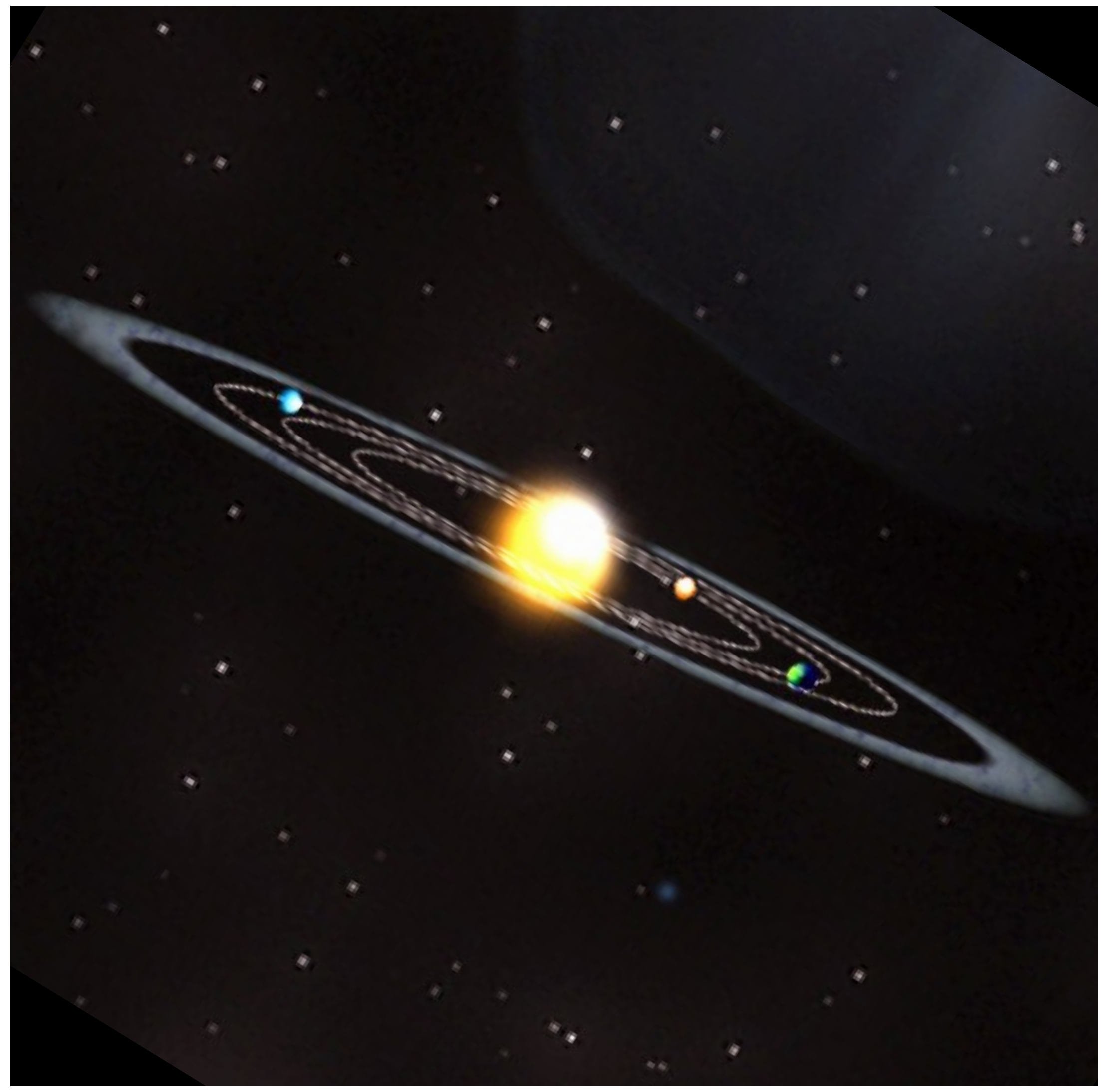
~100s of kyr

Protostar



~1-20 Myr

Protoplanetary Disk

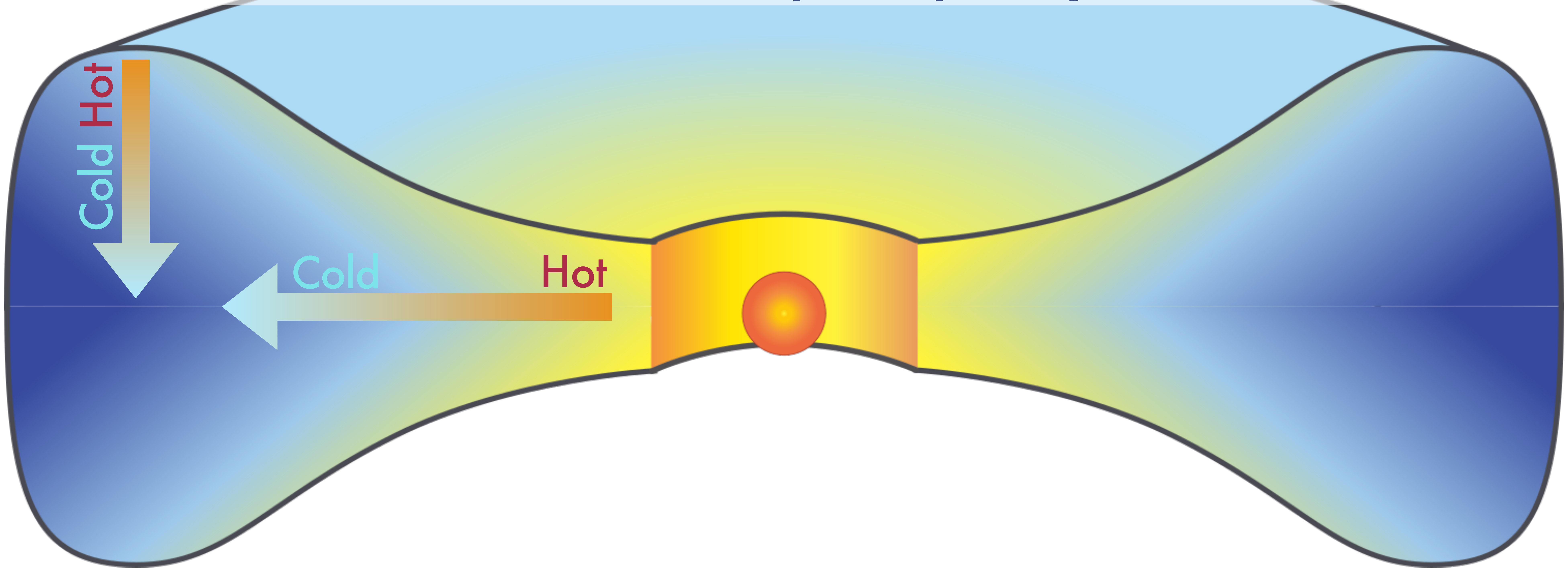


> Myr - Gyr

Debris disk, planetary system.

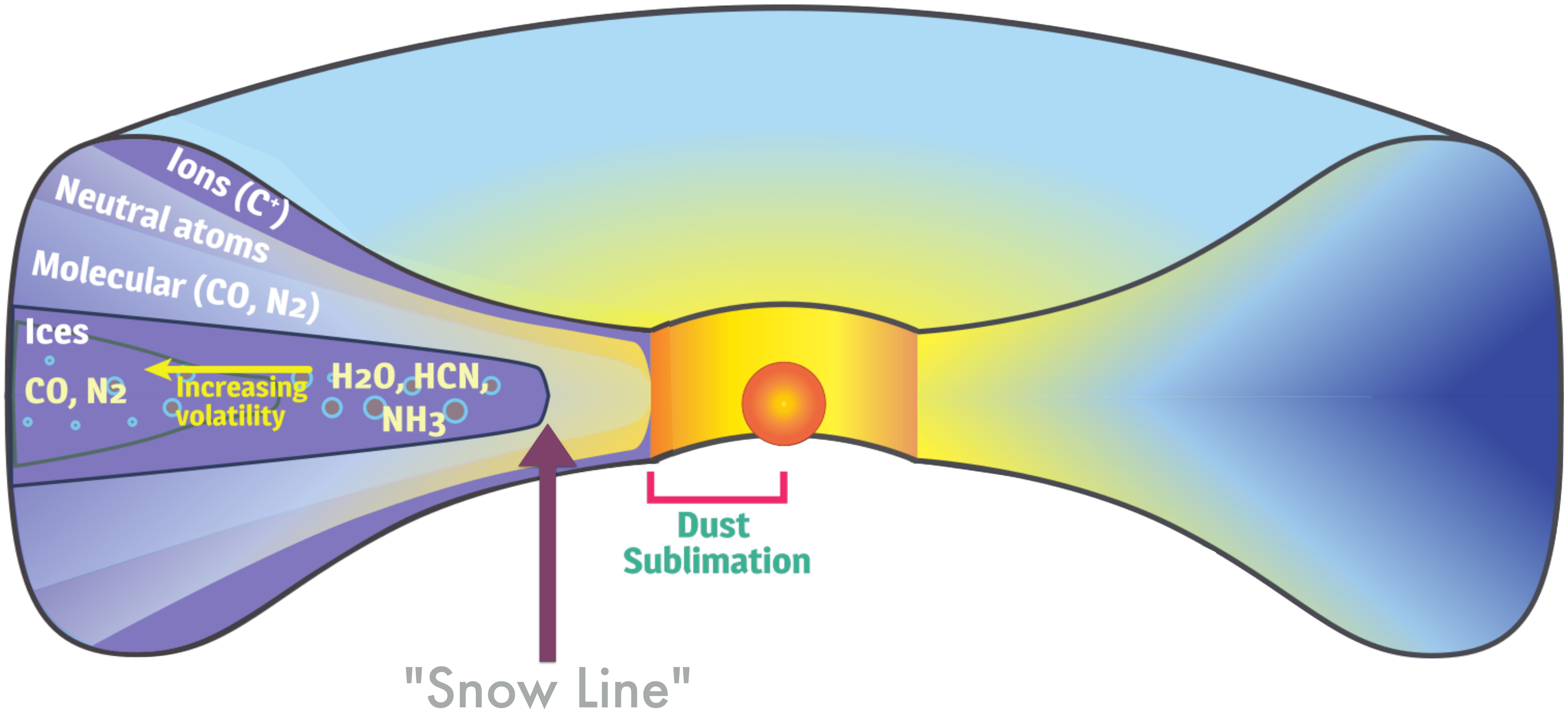
THE SIMPLE PICTURE

Disk composition initially ~molecular-cloud like, now irradiated by the young star



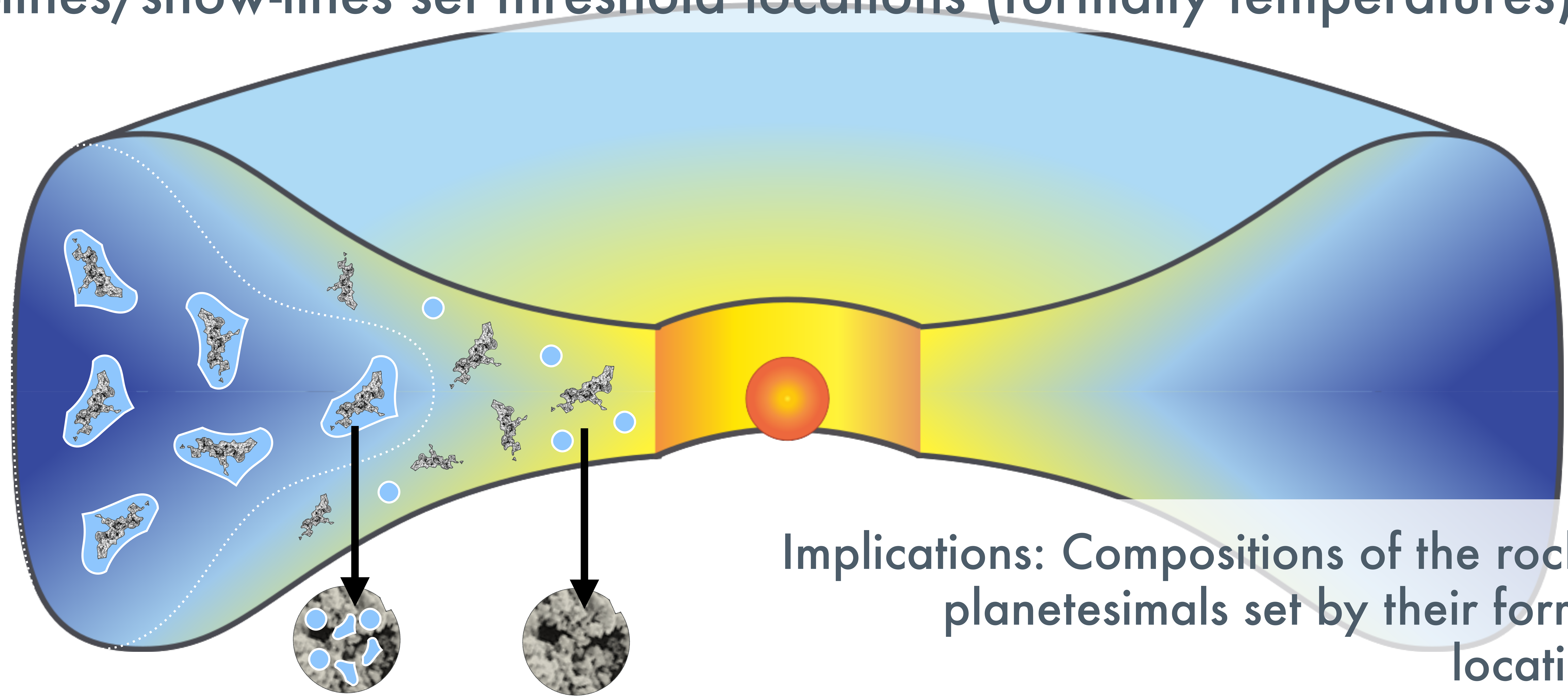
Dust opacity sets the thermal structure and shields the disk from stellar radiation, such as UV and X-rays

DISK GAS COMPOSITION



SNOW LINES AND PLANET(ESIMALS)

Frost-lines/snow-lines set threshold locations (formally temperatures)

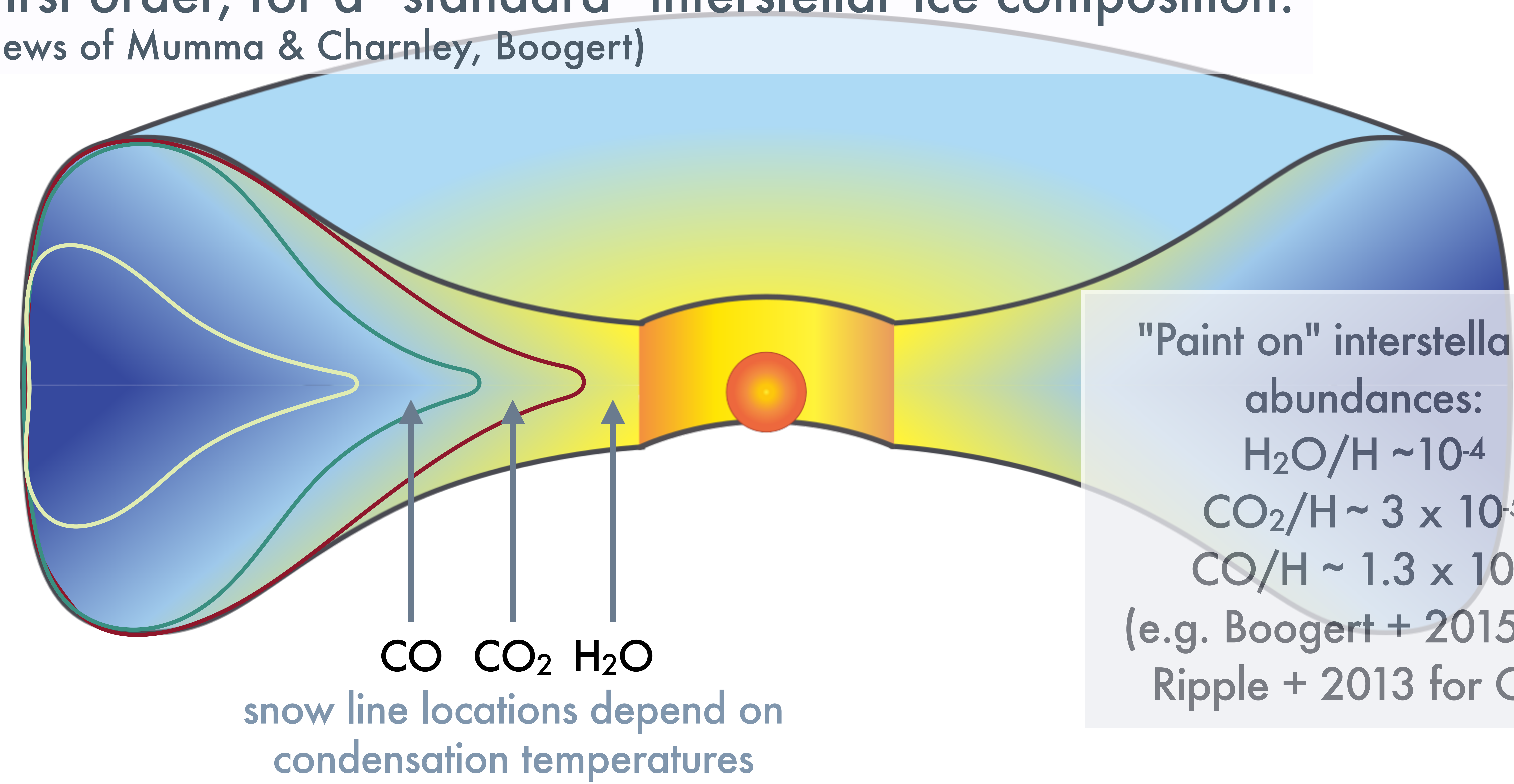


Implications: Compositions of the rocky/icy planetesimals set by their formation locations**

** if formed by core-accretion(Pollack+96)

DISK SNOW LINES

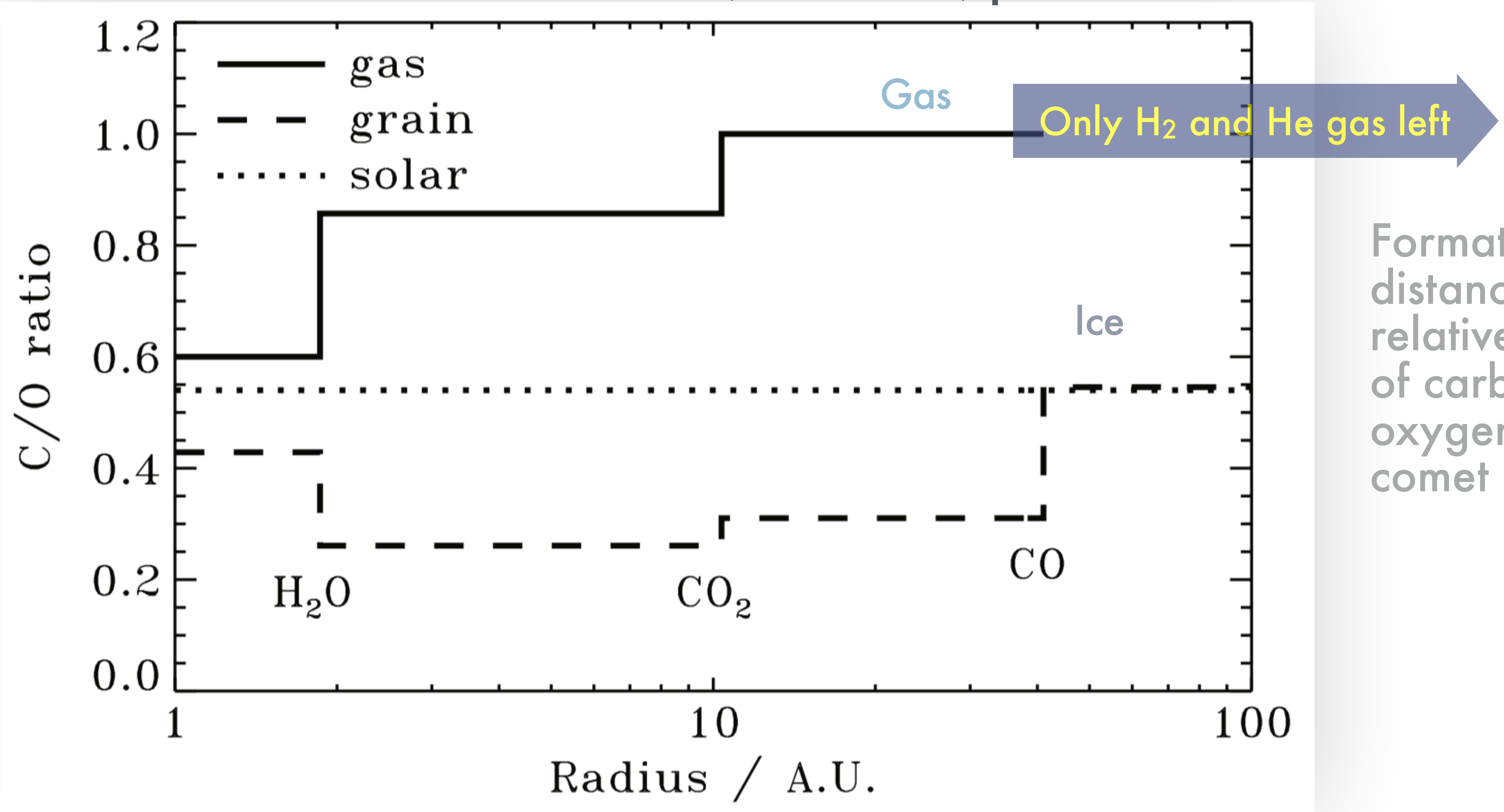
To first order, for a "standard" interstellar ice composition:
(Reviews of Mumma & Charnley, Boogert)



"Paint on" interstellar ice abundances:
$H_2O/H \sim 10^{-4}$
$CO_2/H \sim 3 \times 10^{-5}$
$CO/H \sim 1.3 \times 10^{-4}$
(e.g. Boogert + 2015 and Ripple + 2013 for CO)

SNOW LINES AND PLANETS

Baseline expectation: freeze-out changes the chemical environment from which comets, asteroids, planets accrete



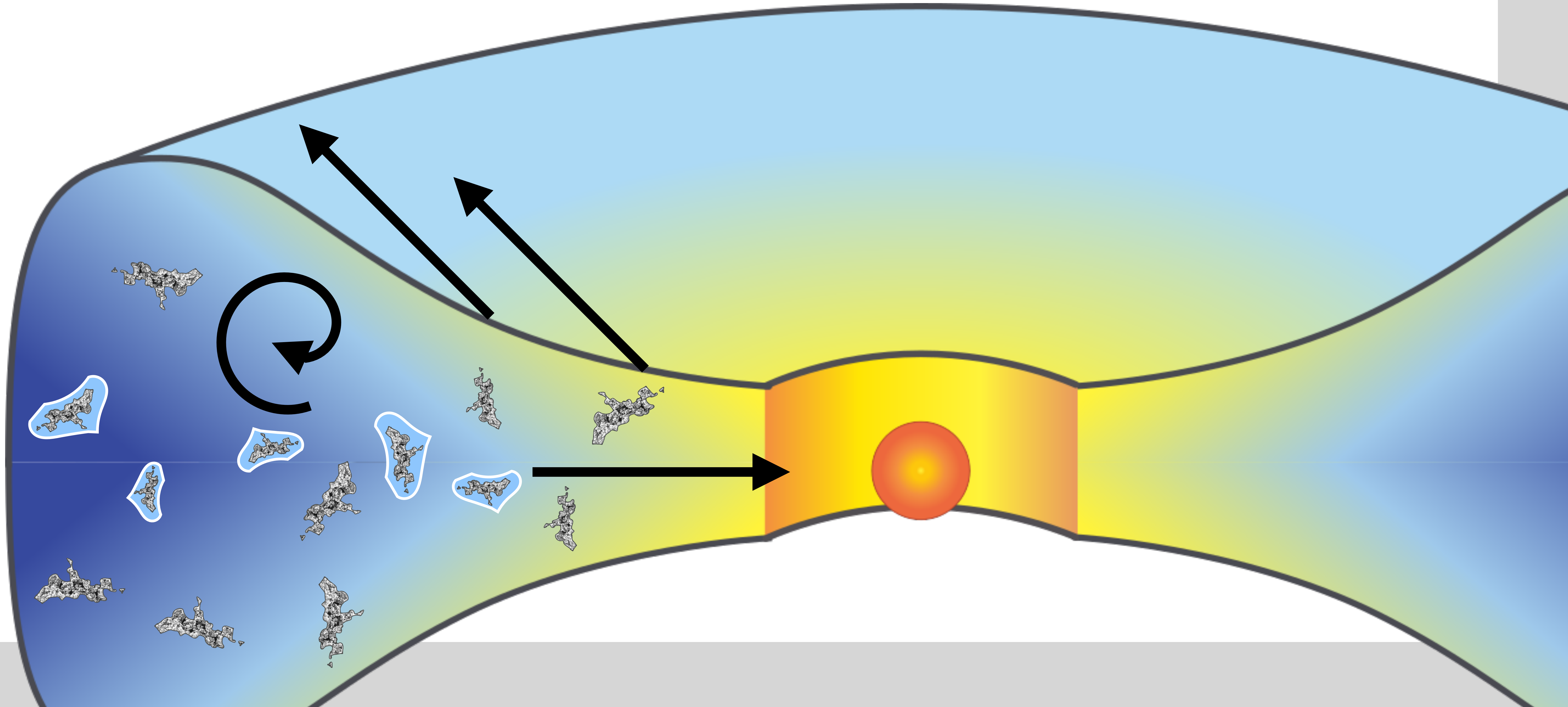
Formation distance changes relative amount of carbon to oxygen in your comet

Assuming interstellar composition (Öberg, Murray-Clay and Bergin 2011)

DISK CHEMICAL PROCESSING

Nice picture, but some caveats...
Disks are expected to be actively chemically evolving over ~0.1 to Myr+ time scales

- Winds (removal of light species)
- Gas transport and mixing (dredge up ices from the midplane, or send UV processed material downward)
- Galactic chemical evolution...?
- Ice transport on the surfaces of growing/fragmenting dust grains
- What are "interstellar abundances?"



DISK CHEMICAL PROCESSING

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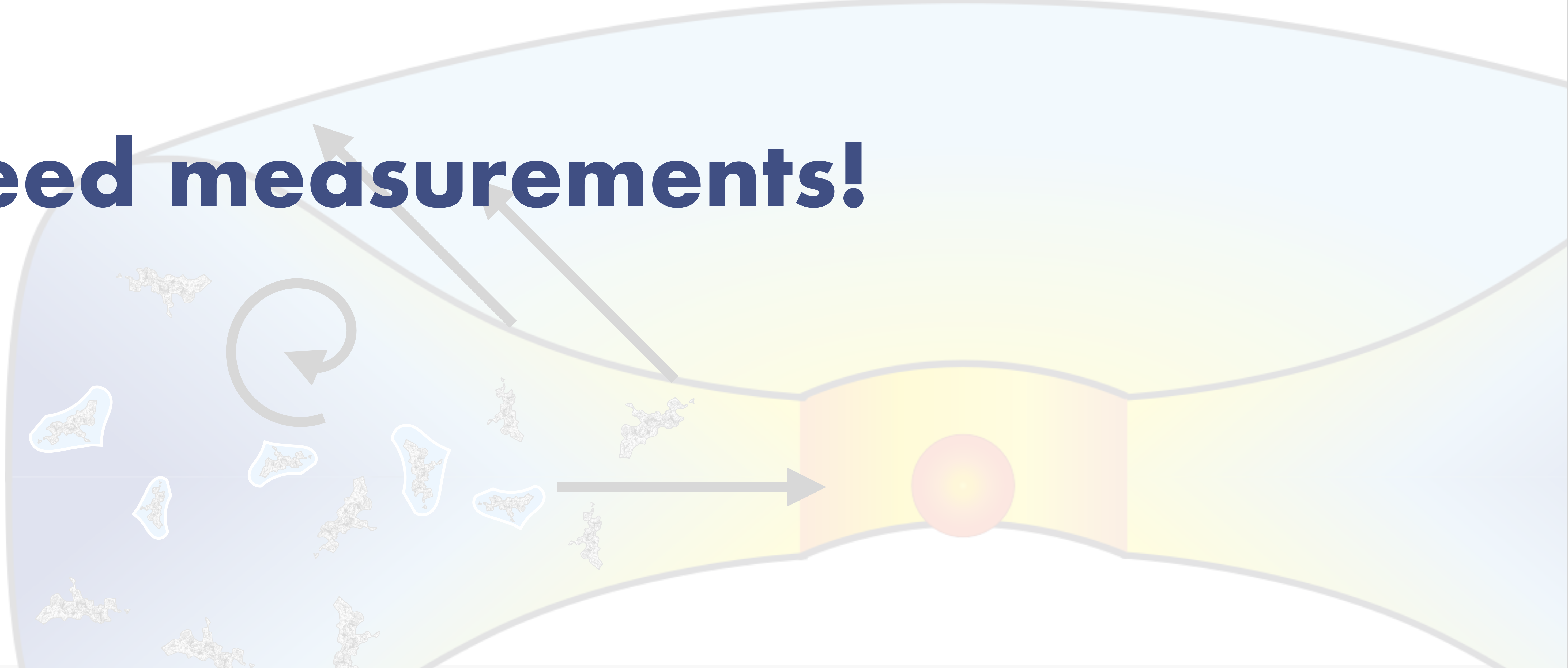
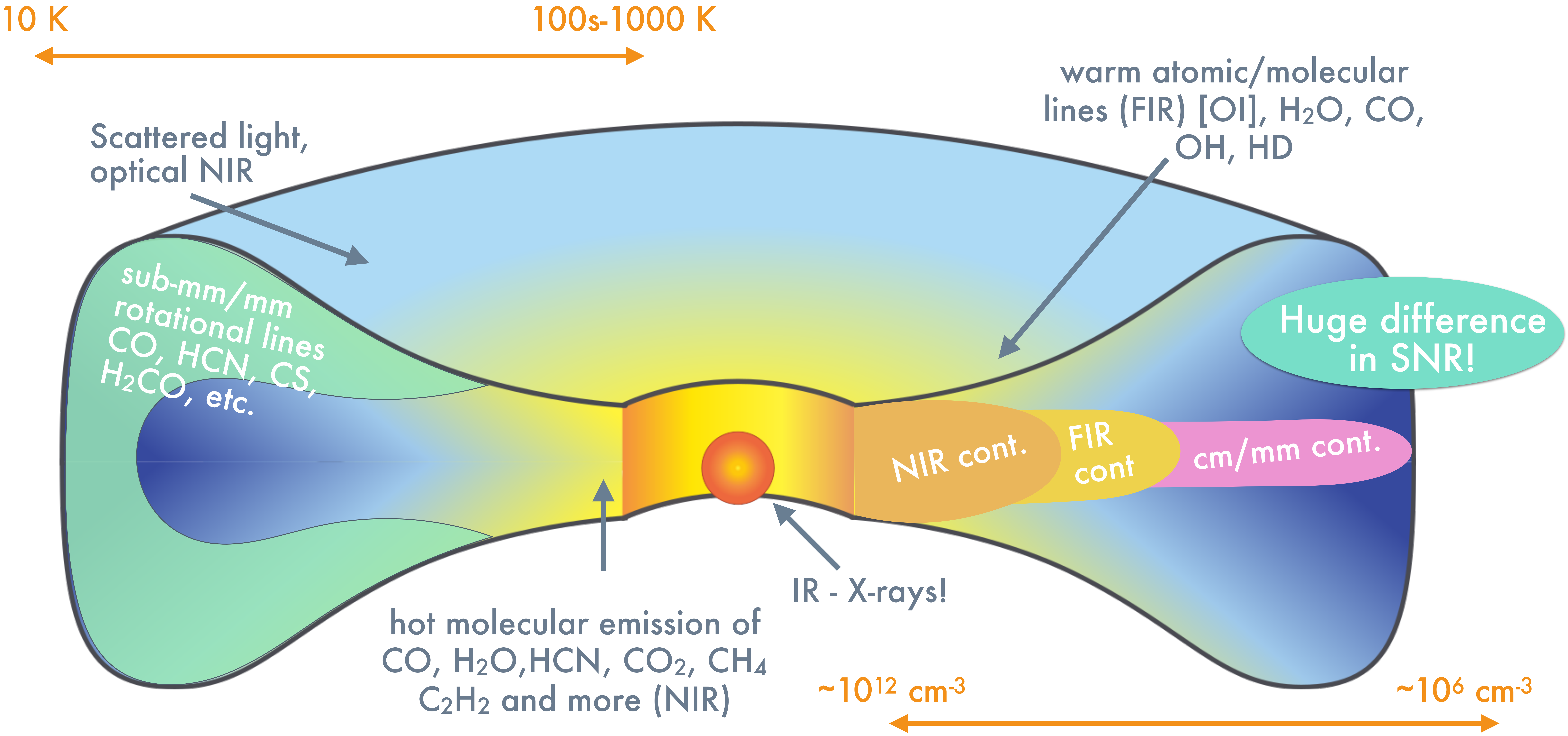
So what are the typical disk compositions?

We need measurements!

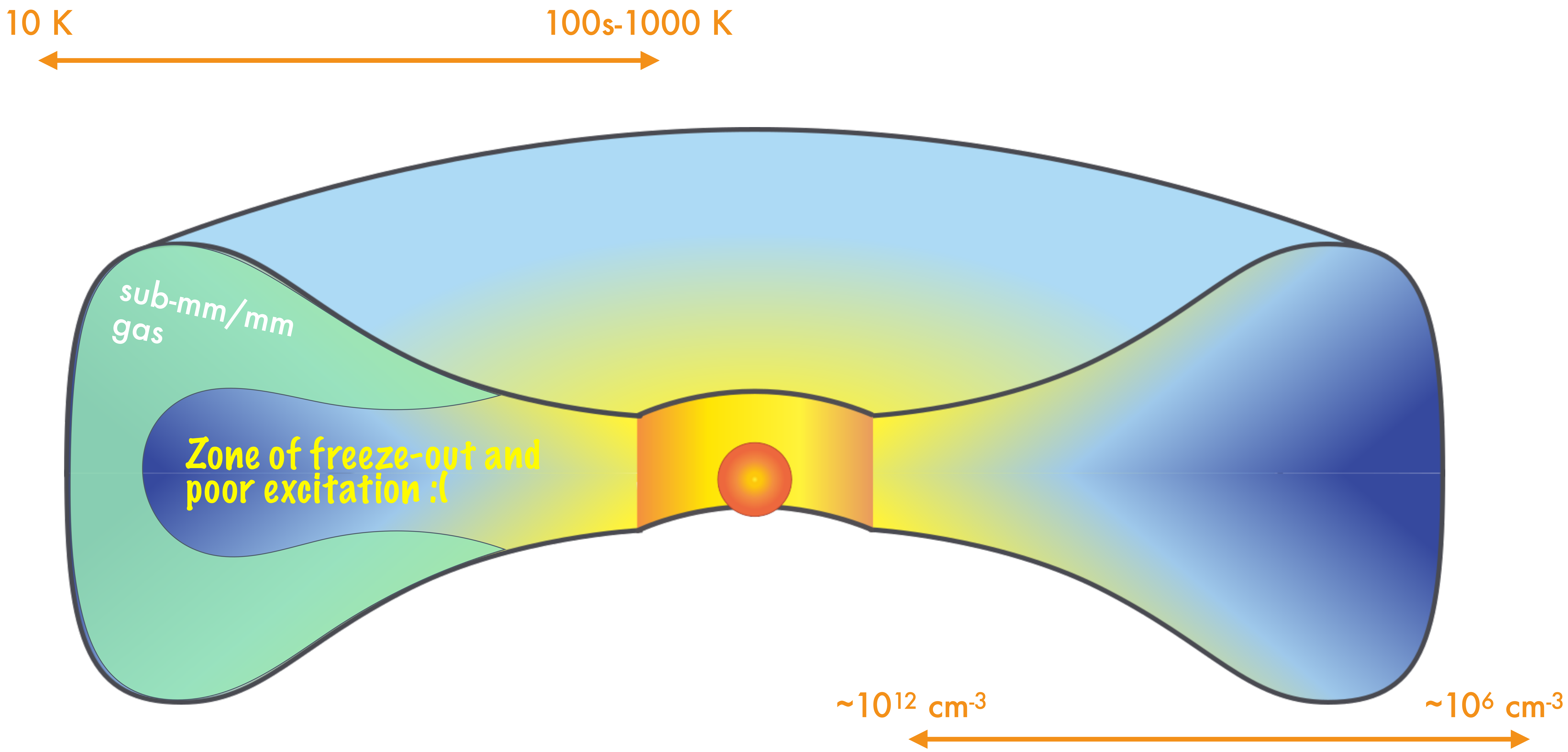


OBSERVATIONAL WINDOWS

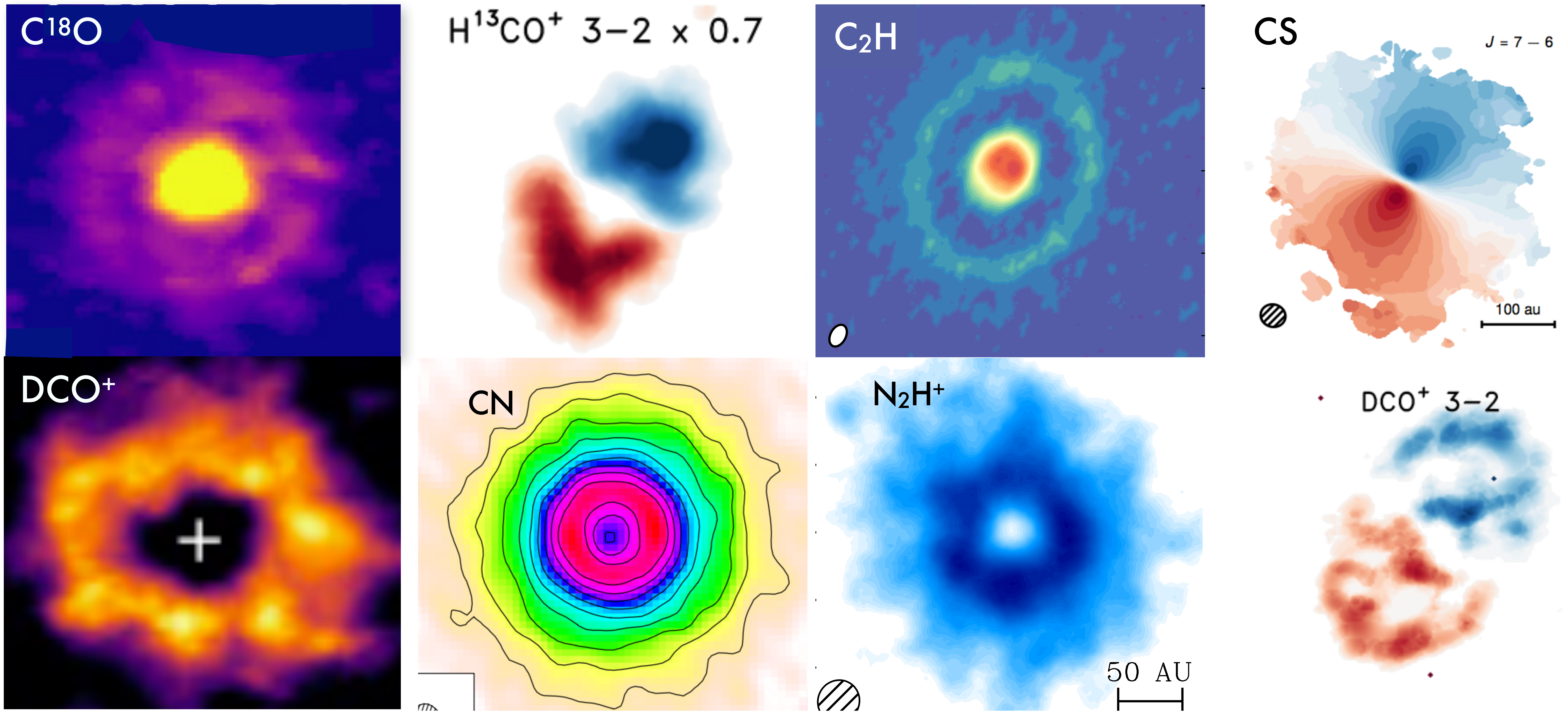


Credit: Melissa Hoffman

MIDPLANE VOLATILES HARDER TO OBSERVE



DISK GAS OBSERVATIONS WITH ALMA



Schwarz+2016, Öberg+2015, Bergin, Du, Cleeves+2016, Teague+2016, 2018, Huang+2017, Qi/Öberg+2013
(Stay tuned for the MAPS Large Program: PI: Oberg)

DISK GAS OBSERVATIONS WITH ALMA

ALMA TW Hya Rosetta Project

ALMA Cycle 4-6: Spatially resolved spectroscopic survey of TW Hya at 10-15 AU resolution. Mapping key molecules/isotopes.

PI: Cleeves

Co-Is: E. Bergin, K. Oberg, G. Blake, C.Walsh, M. Kama, V. Guzman, E. van Dishoeck, M. Hogerheijde, J. Huang, R. Loomis, D.Wilner, C. Qi

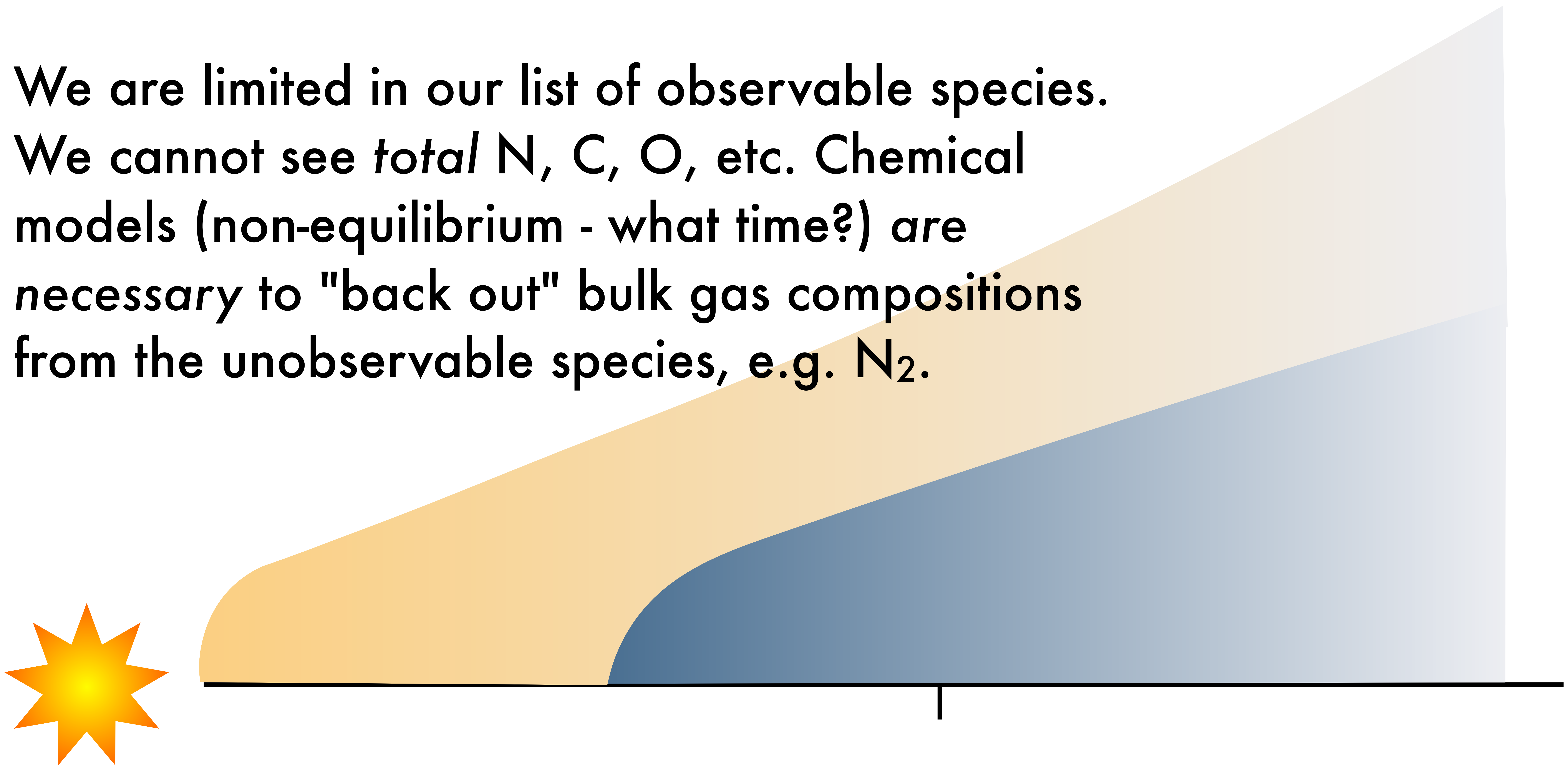
Band 6 Spectral Setting 1	
DCO^+ $3-2$	216.113
DCN $3-2$	217.239
H_2CO $3_{0,3}-2_{0,2}$	218.476
H_2CO $3_{2,1}-2_{2,0}$	218.222
H_2CO $3_{2,2}-2_{2,1}$	218.760
$C^{18}O$ $2-1$	219.560
CO $2-1$	230.538
^{13}CS $5-4$	231.221
N_2D^+ $3-2$	231.322

Band 6 Spectral Setting 2:	
^{13}CS $6-5$	277.455
N_2H^+ $3-2$	279.512
DCO^+ $4-3$	288.144
$C^{34}S$ $6-5$	289.209
DCN $4-3$	289.645
^{34}SO 6_7-5_6	290.562
H_2CO $4_{0,4}-3_{0,3}$	290.623
H_2CO $4_{3,2}-3_{3,1}$	291.380
H_2CO $4_{3,1}-3_{3,0}$	291.384

Band 7 Spectral Setting 4:	
CN $3-2$	340.249
$HC^{18}O^+$ $4-3$	340.631
SO 8_8-7_7	340.714
$^{34}SO_2$ $5_{3,3}-4_{2,2}$	342.209
CS $7-6$	342.883
SO_2 $5_{3,3}-4_{2,2}$	351.296
SO_2 $14_{4,10}-14_{3,11}$	351.873
$H_2^{13}CO$ $5_{0,5}-4_{0,4}$	353.812
HCN $4-3$	354.505
HDCO $10_{1,9}-10_{0,10}$	355.075
$H_2^{13}CO$ $5_{3,3}-4_{3,2}$	355.191

FROM SPECIFIC MOLECULES TO BULK?

We are limited in our list of observable species. We cannot see *total* N, C, O, etc. Chemical models (non-equilibrium - what time?) *are necessary* to "back out" bulk gas compositions from the unobservable species, e.g. N_2.



MOLECULAR "TOOLBOX"

To connect to possible planetesimals, want to measure and ideally *map total* C/O in a disk and N/O as well. Our simple molecular "toolbox" includes:

Outer Disk

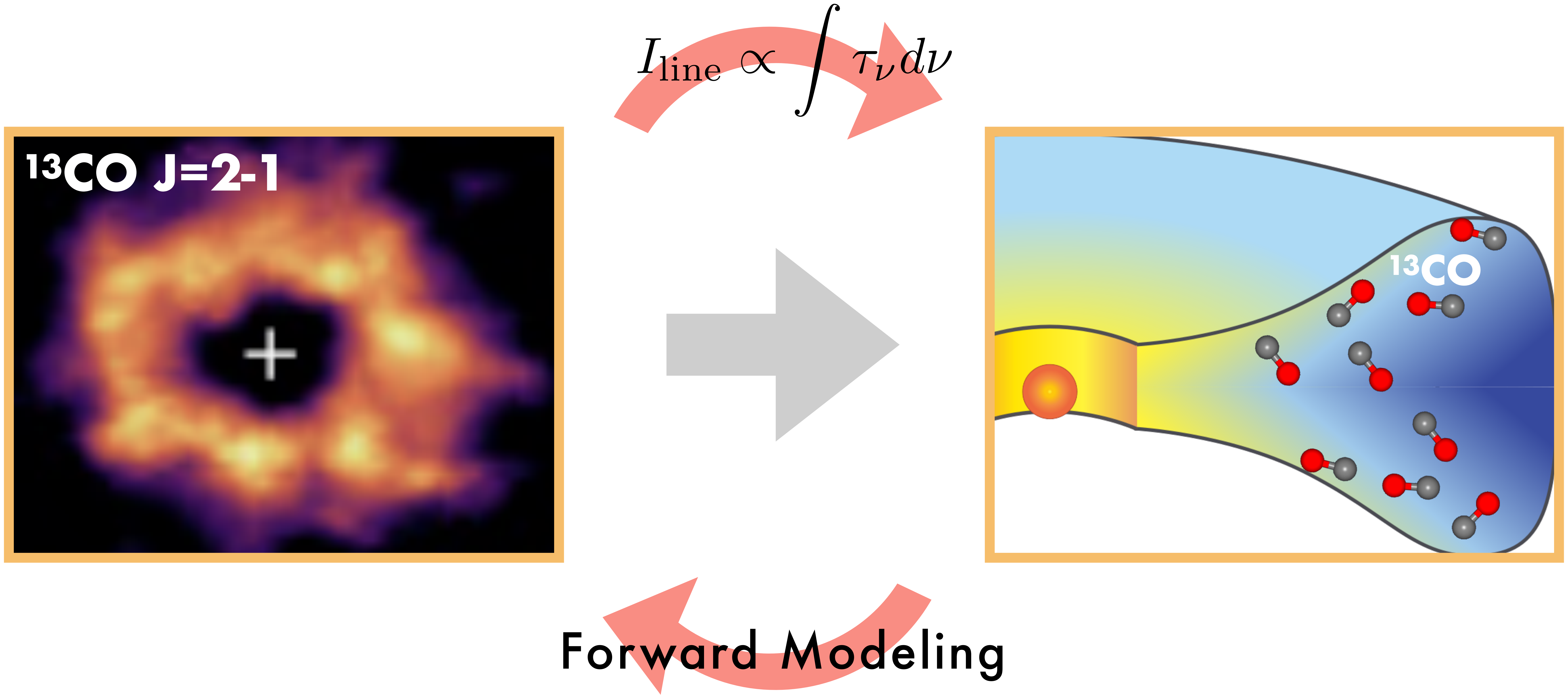
- **CO** and optically thin isotopologues.
- **C_2H, C_3H_2:** (Disks: Du et al. 2015, Bergin+2016, Cleeves et al 2018)
- **N_2H^+**: N_2 tracer, CO-ice tracer (but also ionization fraction).
- **HCO^+** - X-ray chemistry
- **HCN:** N-tracer, less dependent on disk physics, depends on C/H.
- **CS:** Sulfur tracer.

Inner Disk (Spitzer, JWST, CRIRES, IGRINS)

- **H_2O, C_2H_2, HCN, CO, CO_2**

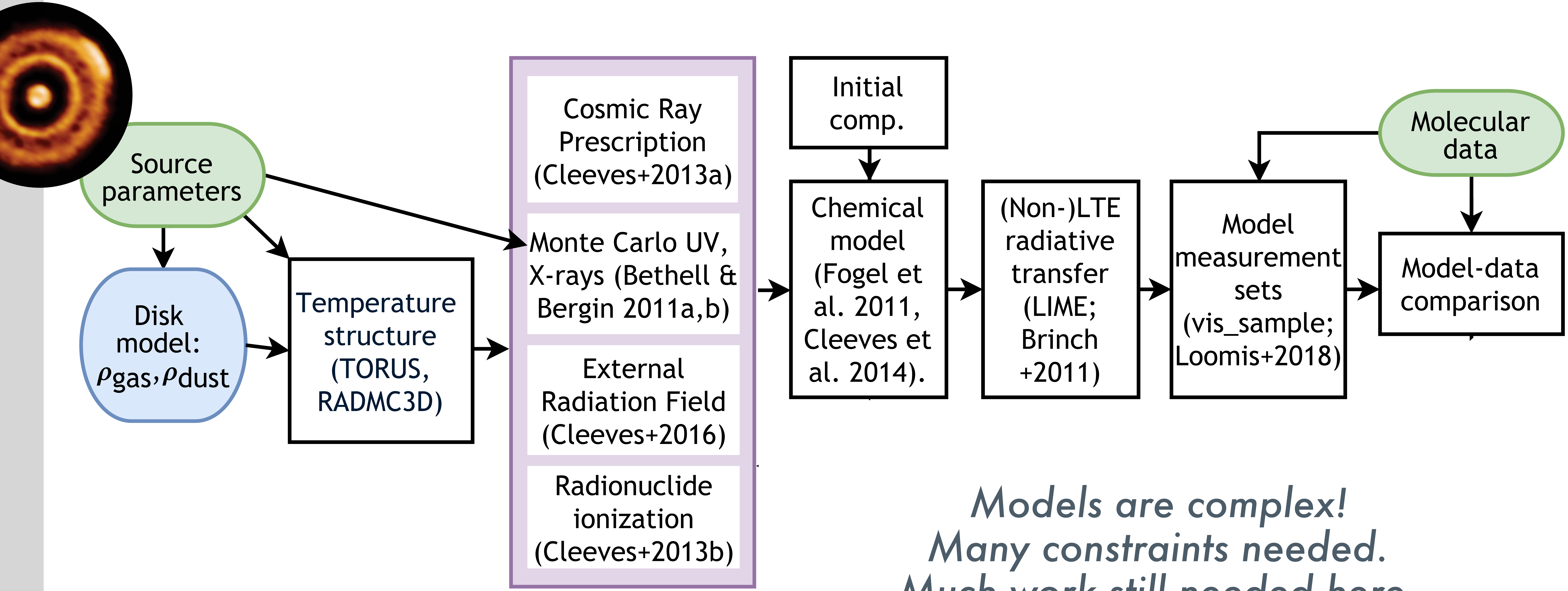
See also McGuire 2018, ApJS

APPROACHES TO RETRIEVING GAS COMPOSITIONS



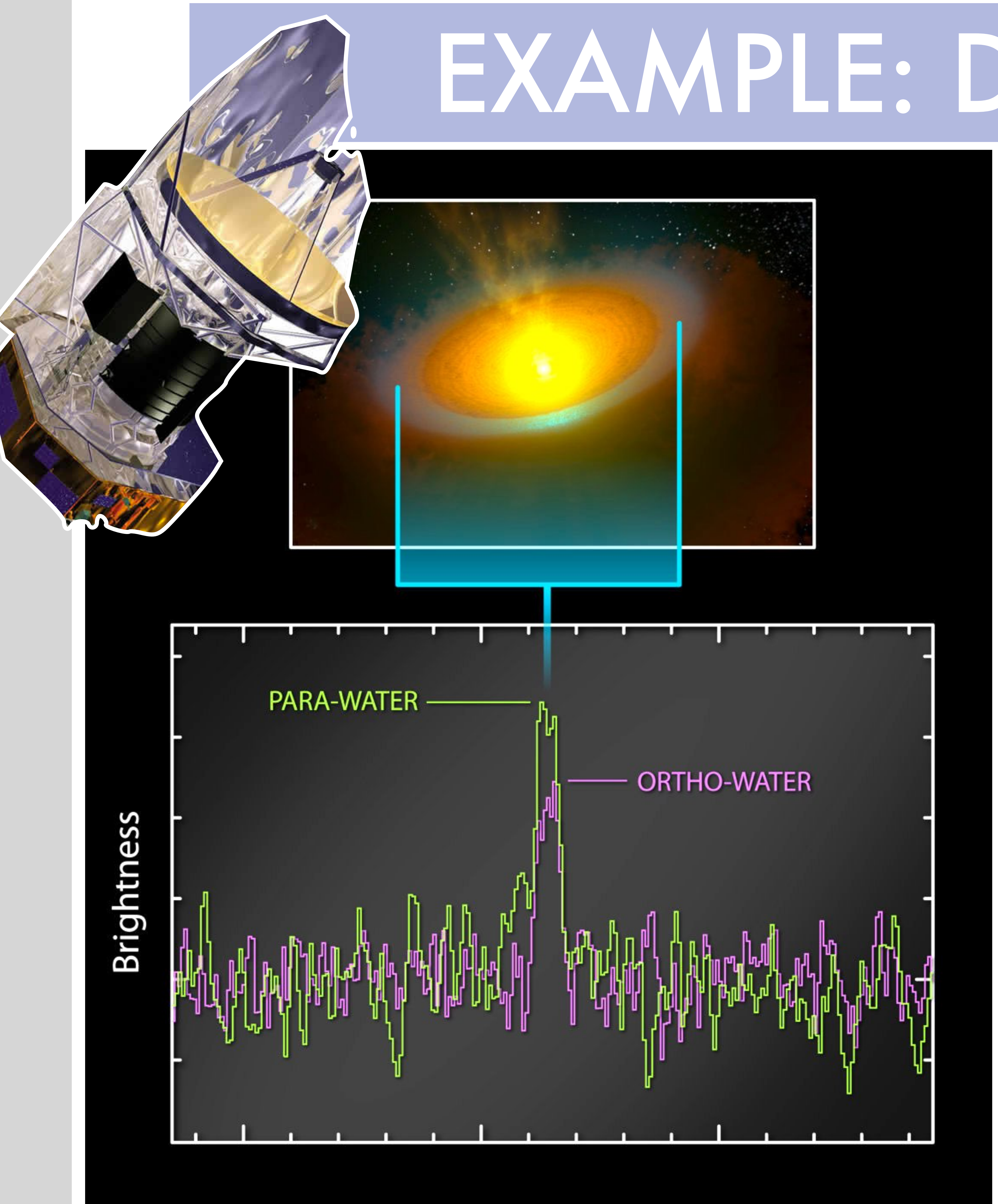
Forward modeling: Useful in constraining spatial abundance maps, testing out what reactions are important, and what are physical drivers behind the chemistry...

INFERRING BULK COMPOSITIONS: MODELING

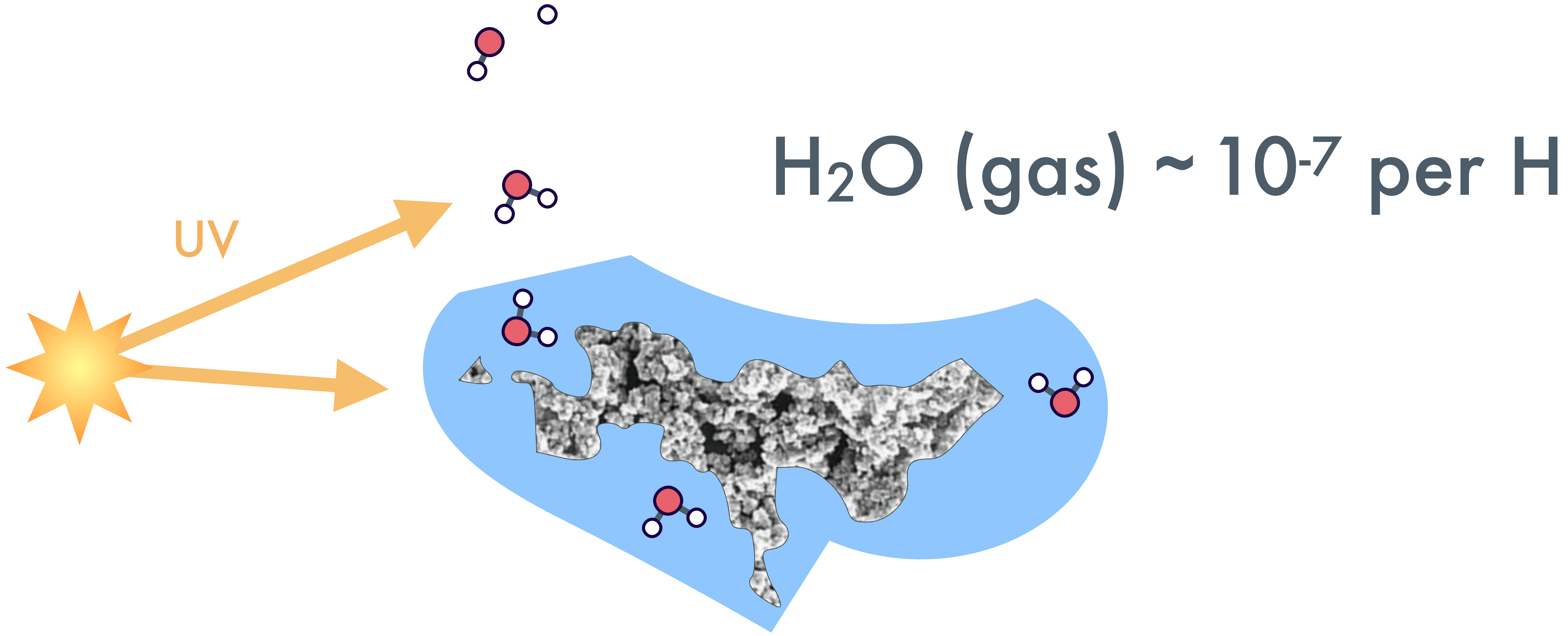


Models are complex!
Many constraints needed.
Much work still needed here.

EXAMPLE: DISK H_2O WITH *HERSCHEL*

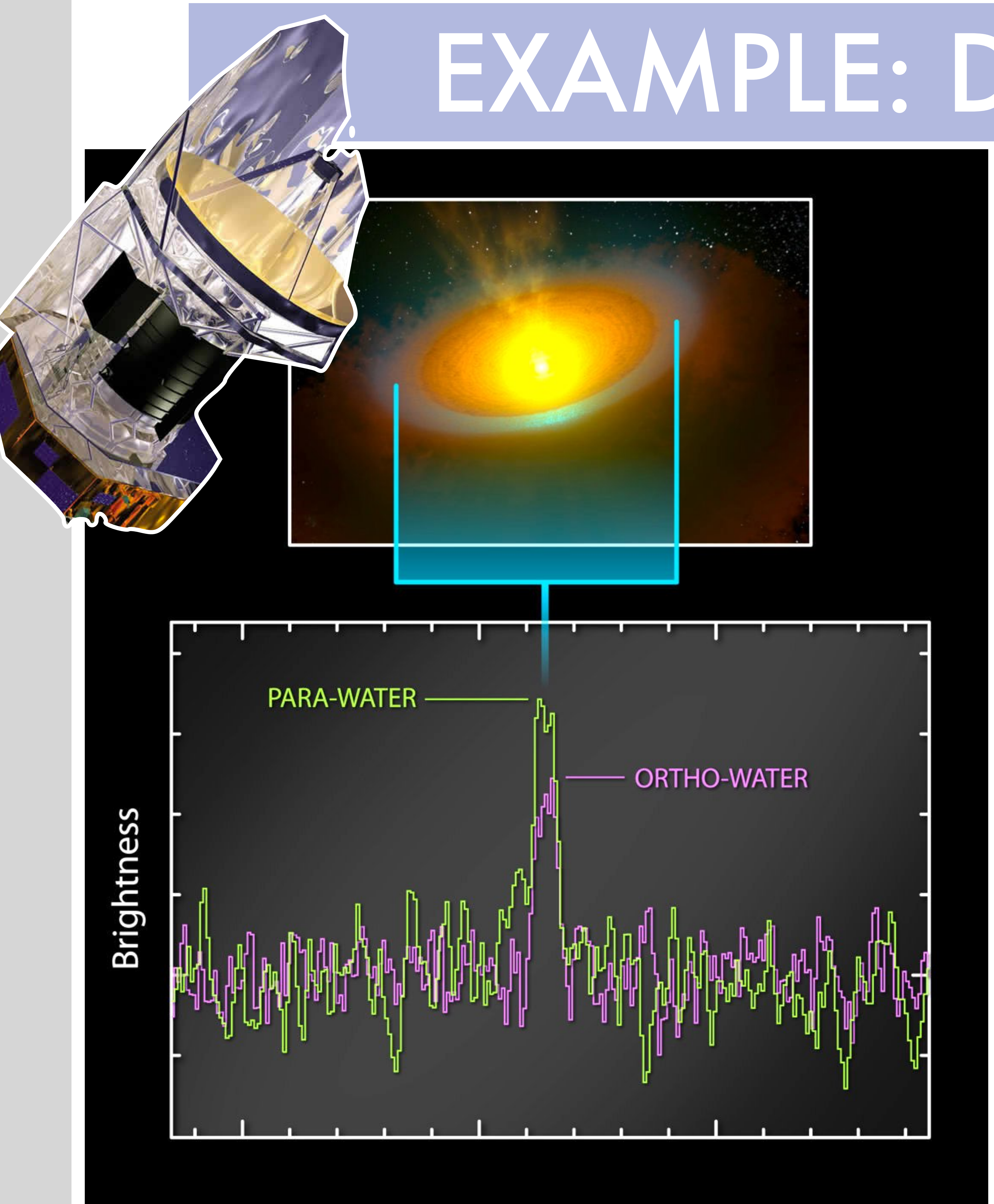


HIFI Spectroscopic Signatures of Water Vapor in TW Hydrae Disk
ESA/NASA/JPL-Caltech/M. Hogerheijde (Leiden Observatory)



- TW Hya, ~40-80x low in H_2O vapor (Hogerheijde+2010, Bergin+2013).
- DM Tau, ≲50x (Bergin et al. 2010 + rev. mass).
- See also *Herschel* H_2O survey (Du et al. 2017).

EXAMPLE: DISK H_2O WITH *HERSCHEL*



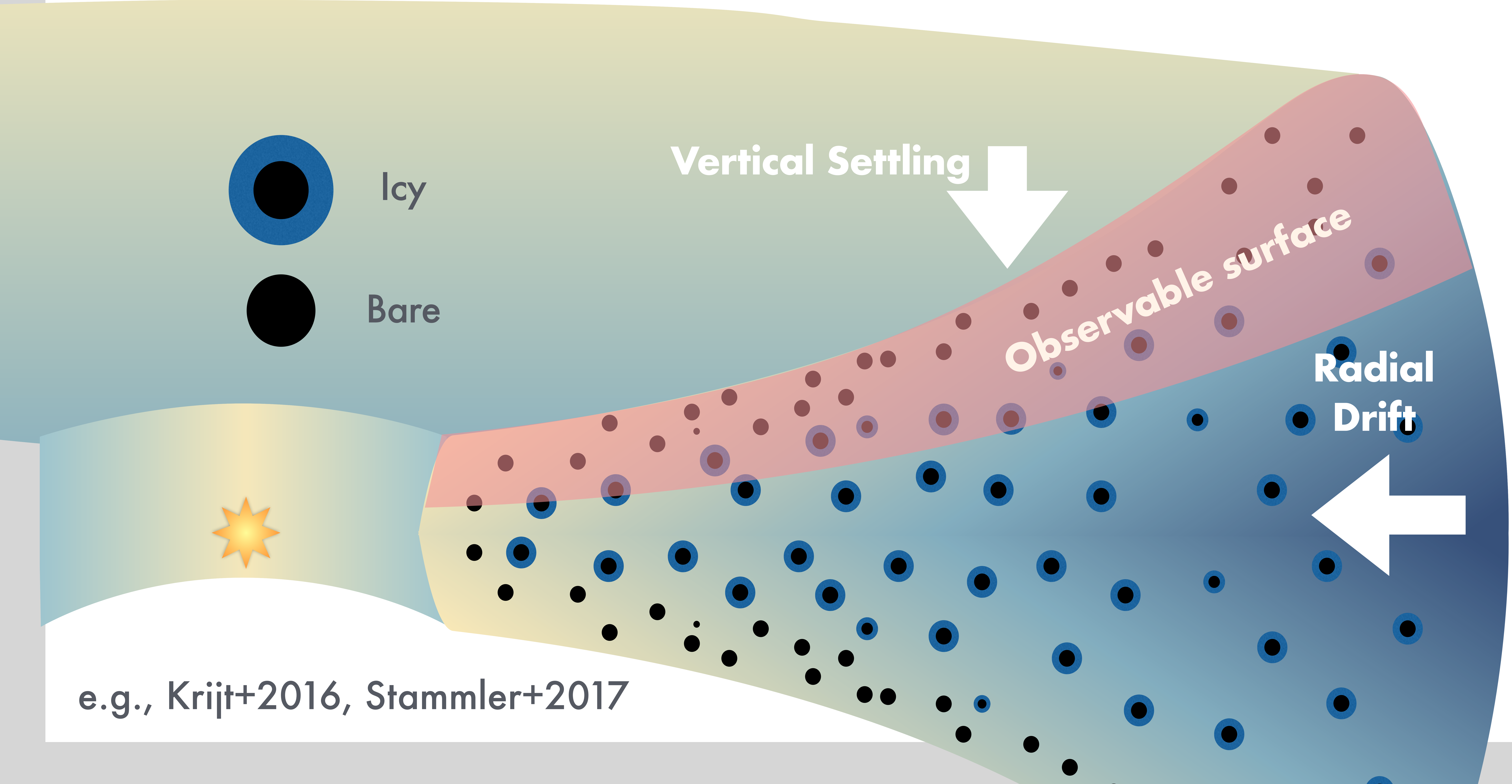
HIFI Spectroscopic Signatures of Water Vapor in TW Hydrae Disk
ESA/NASA/JPL-Caltech/M. Hogerheijde (Leiden Observatory)

Emission significantly (1 - 2 orders of magnitude) weaker than Fogel+2011 models predicted.

The mystery of missing water ice?

- Is water gone, or is gas gone?
- Or are the physical structures and models used to interpret the data faulty? (Kamp+2013)
- Could be that the ices are "coated" preventing desorption?
- Could it also be that the disk surface dust is just "dry"?

CO-EVOLVING DUST & CHEMISTRY

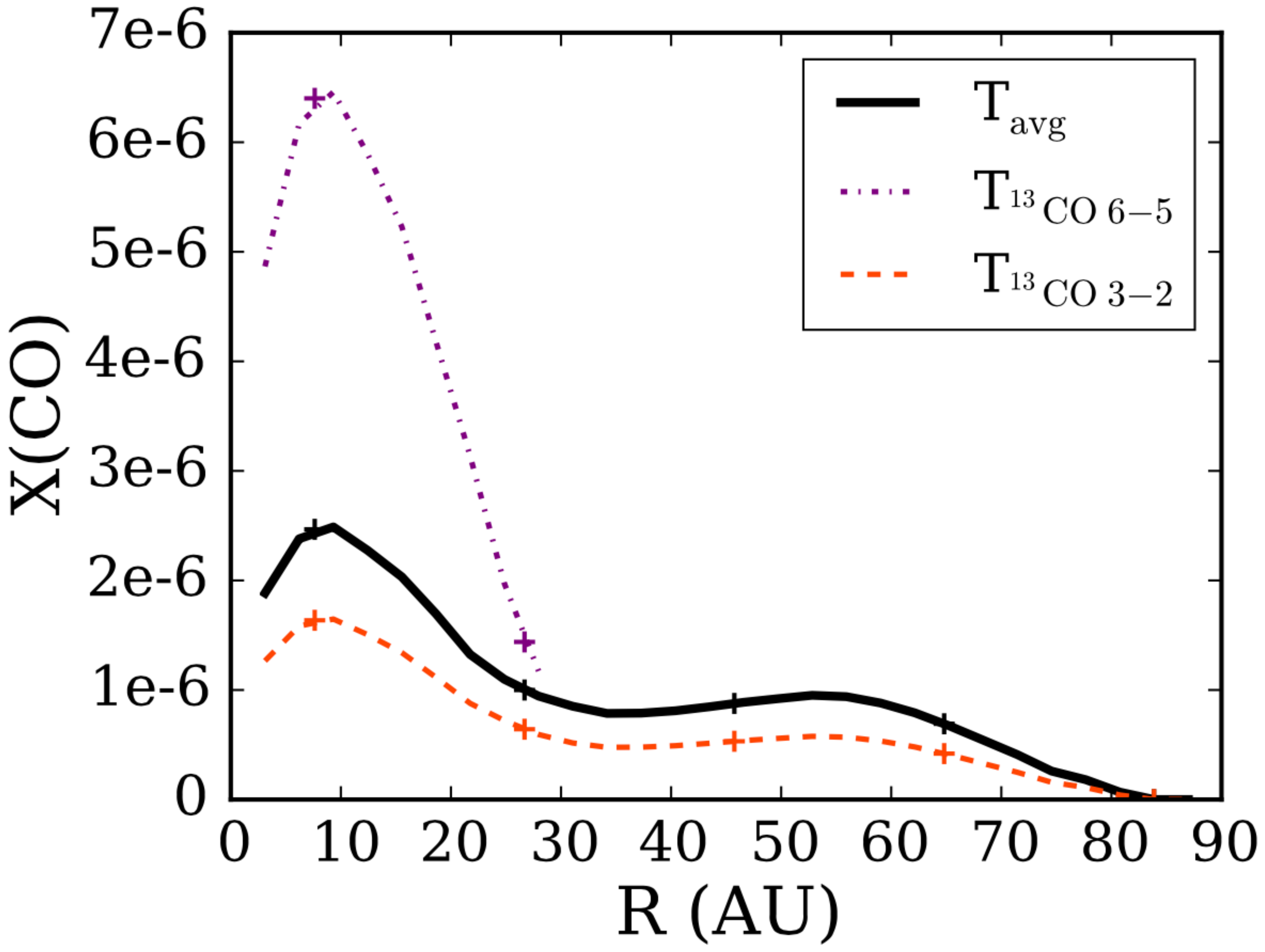


e.g., Krijt+2016, Stammler+2017

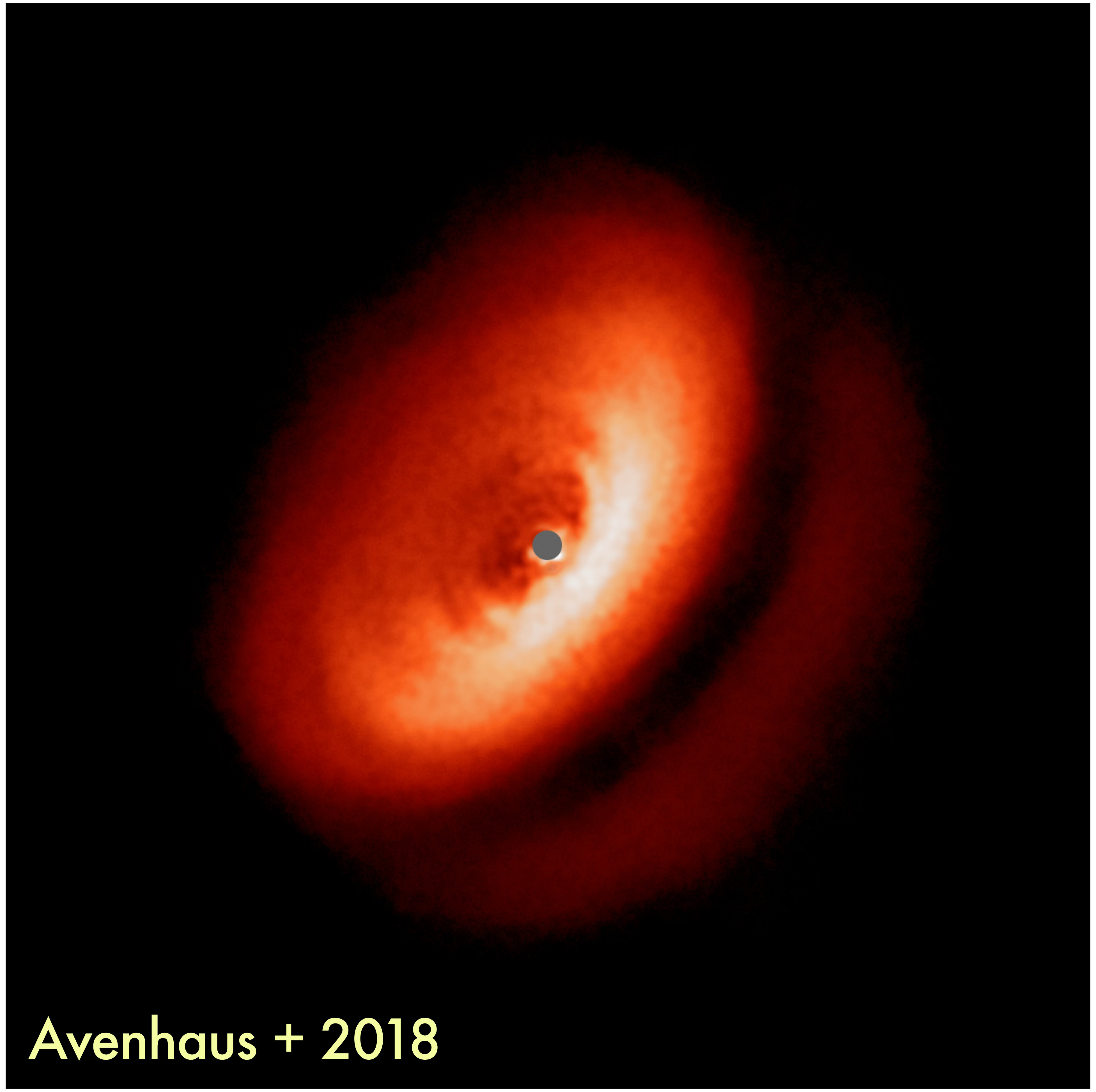
ALMA: CO ALSO VERY FAINT

Schwarz et al. 2016 modeled the temperature and abundance profile of TW Hya's CO using multi-line ^{13}CO and $C^{18}O$ resolved observations.

See also Yu+2018, Favre+13, Cleeves+15, Megan's talk, and Anna's talk.



WHAT ABOUT NITROGEN? CASE OF IM LUP



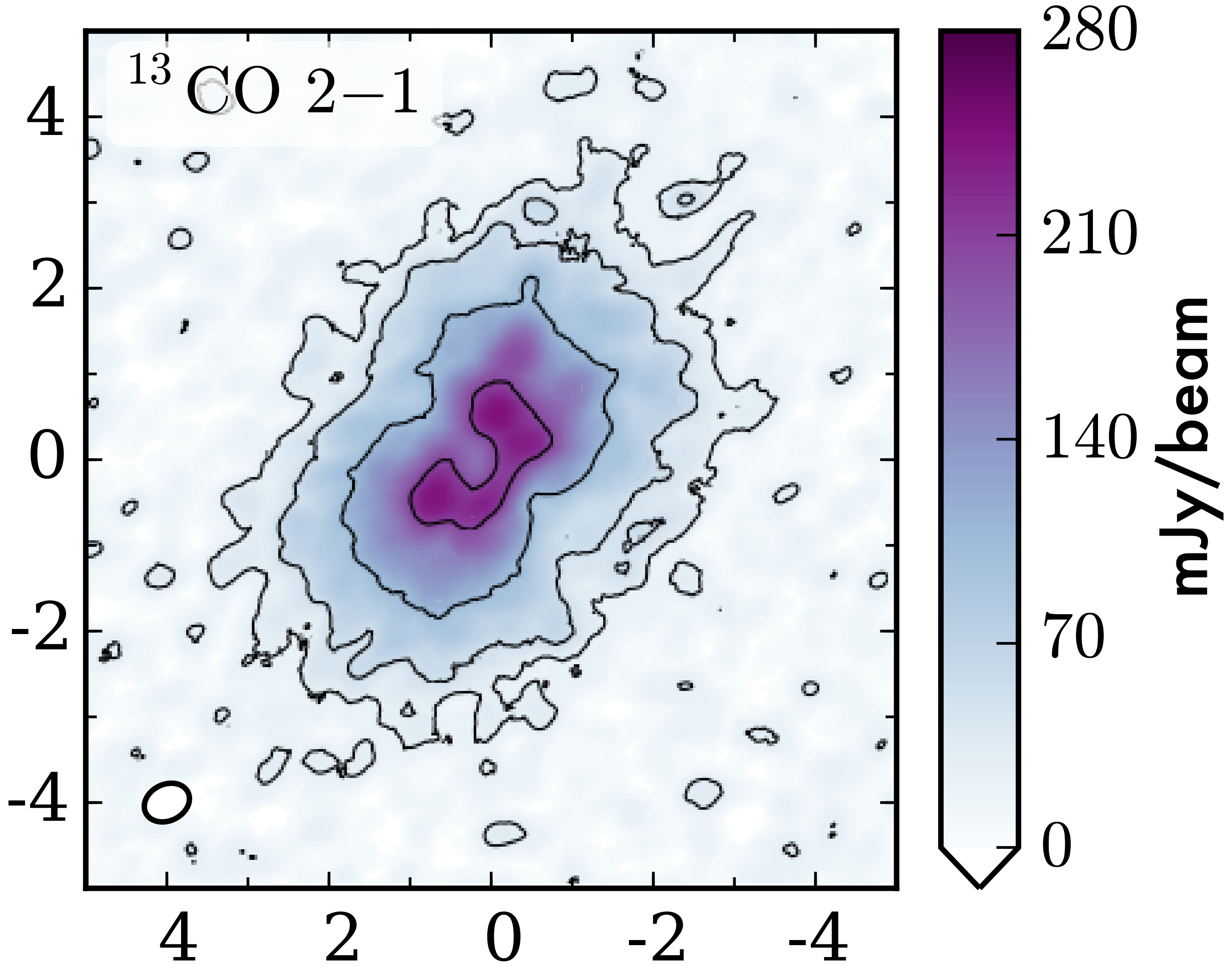
IM LUP

- Distance: 160 pc (Gaia)
- Stellar Mass: 1.0 M_{sun} (2.5 R_{sun})
- Age ~ 0.5-1 Myr (Mawet + 2012), late K/early M star.
- Extremely well studied, e.g., Pinte+2008, Panic+2009, Cleeves+2015

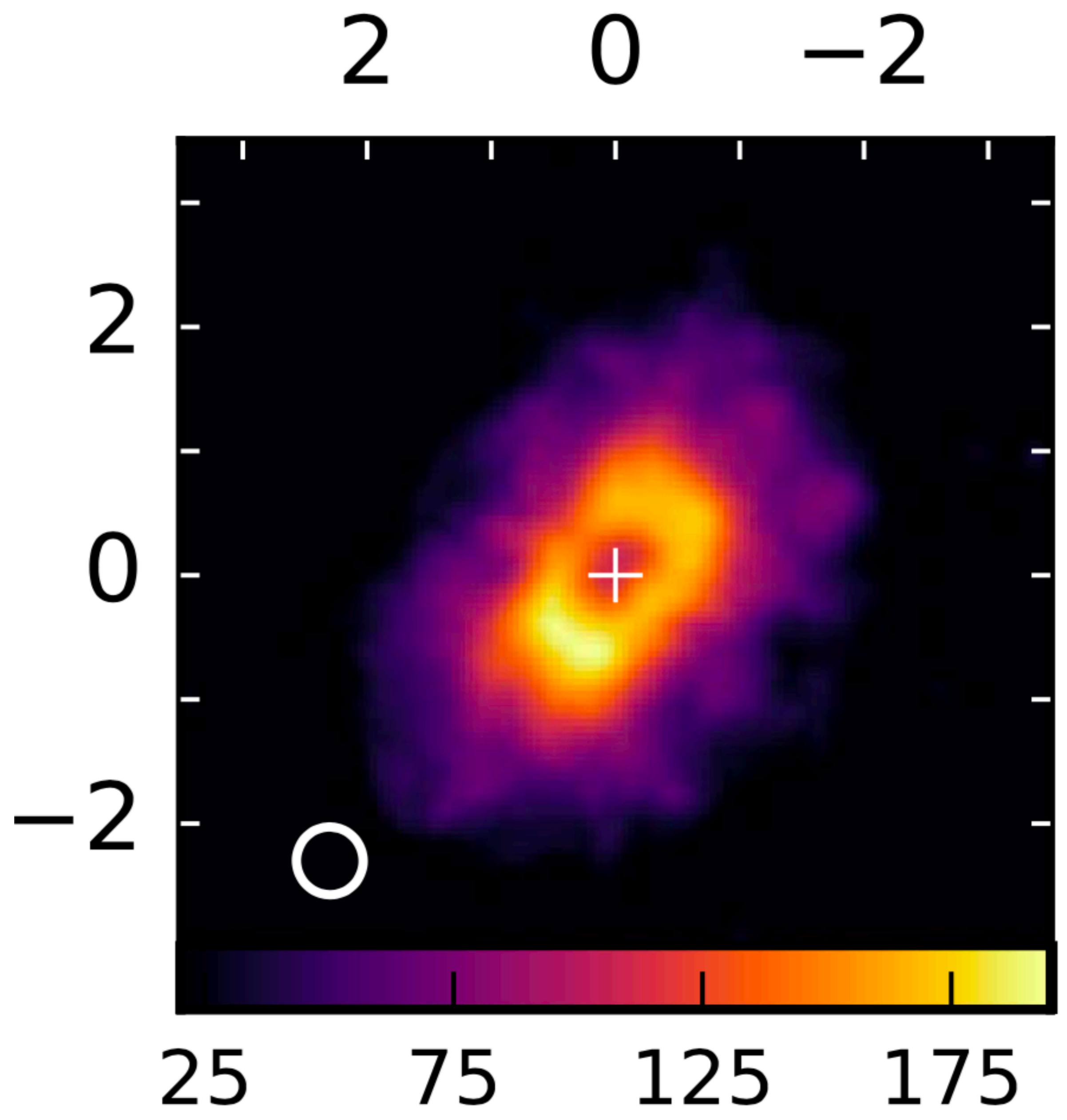
Widely observed! Our ALMA data:

- CO/$C^{18}O$/^{13}CO, J=3-2, 2-1, **C_2H N=3-2**, HCN J=4-3, $H^{13}CN$ J=4-3

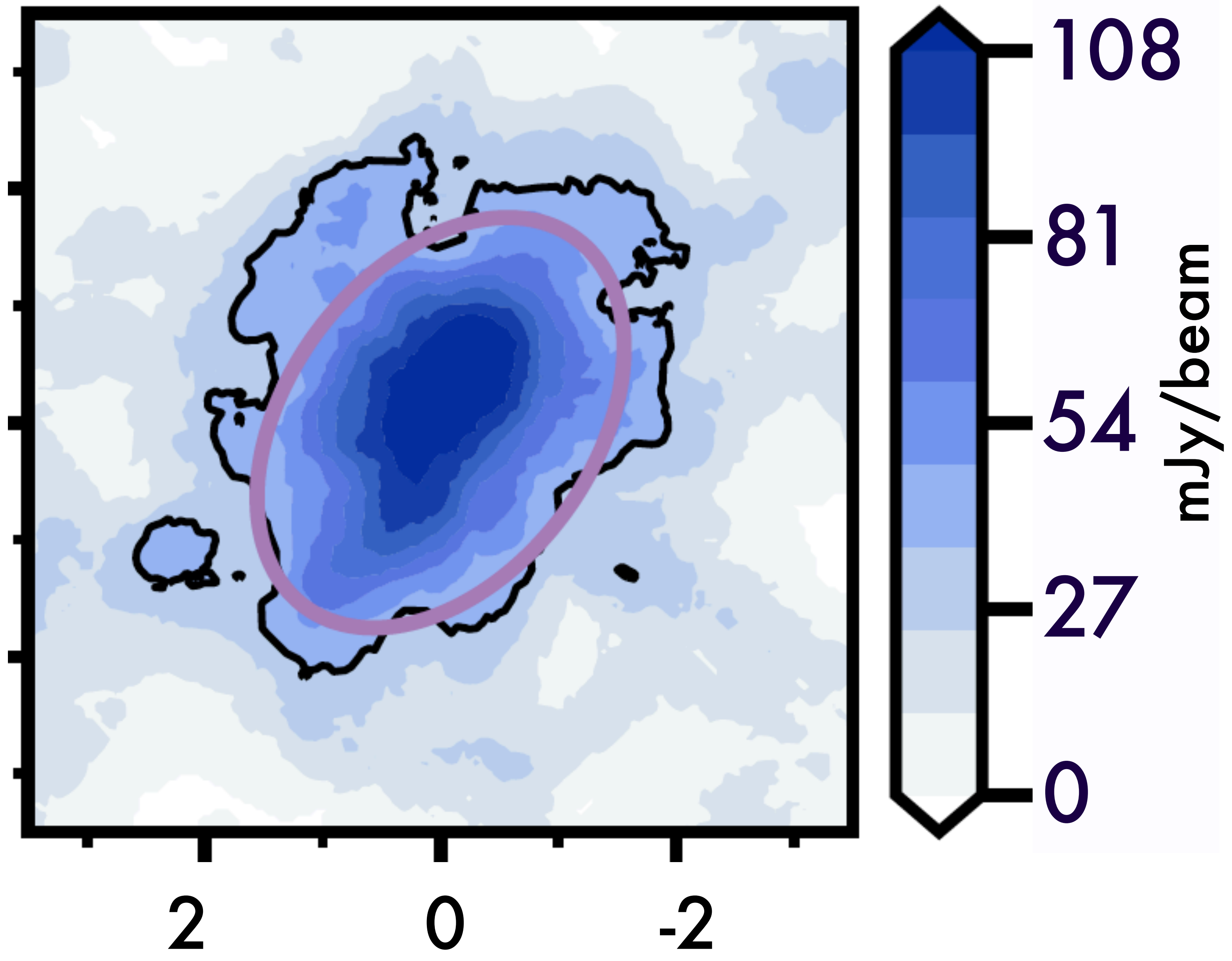
CONSTRAINING C, O, AND N IN IM LUP



CO + isotopologues in multiple rotational lines (J=2-1, 3-2) (Cleeves+2016)



HCN J=3-2
$H^{13}CN$ J=3-2 *not detected*



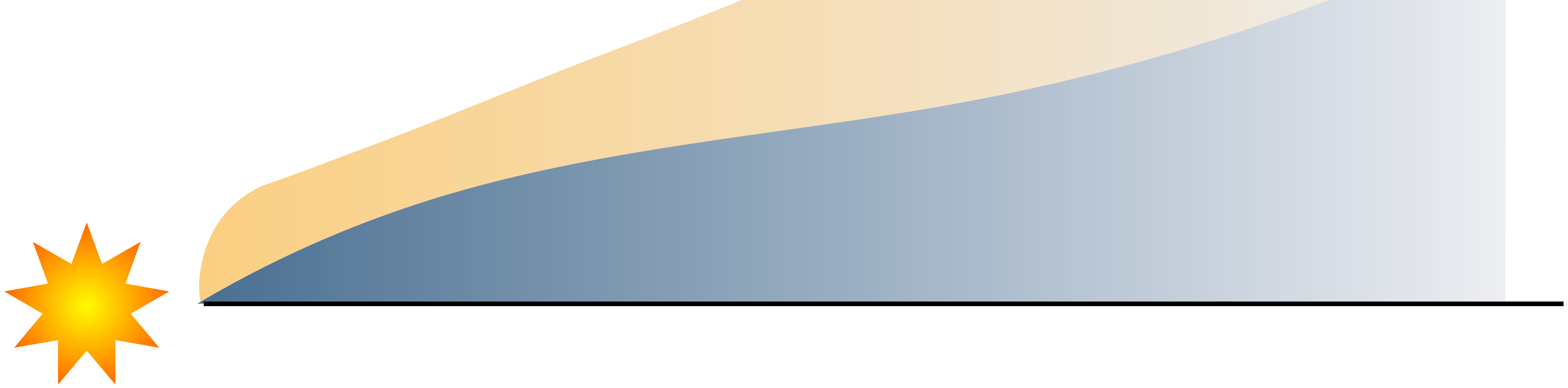
C_2H N=3-2, multiple HFS

Cleeves et al. 2018

CONSTRAINING ELEMENTAL ABUNDANCES

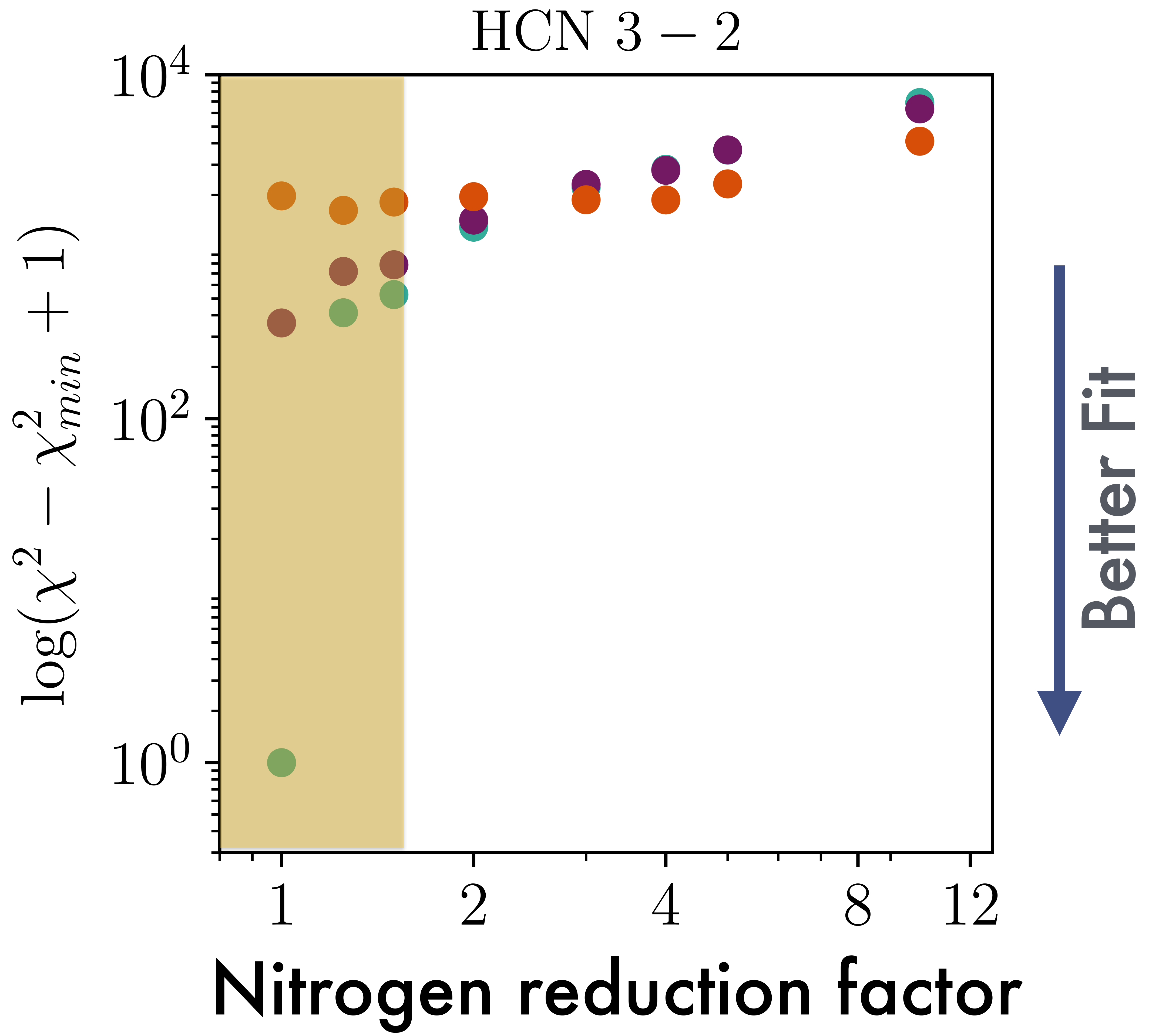
Process: fix the physical structure and CO abundance from Cleeves+2016, and vary the remaining oxygen content to fit C_2H, and the nitrogen content to fit HCN.

Also consider a range of cosmic ray ionization rates.



Cleeves et al. 2018

CONSTRAINING C, O, AND N IN IM LUP



Colors: CR ionization rate

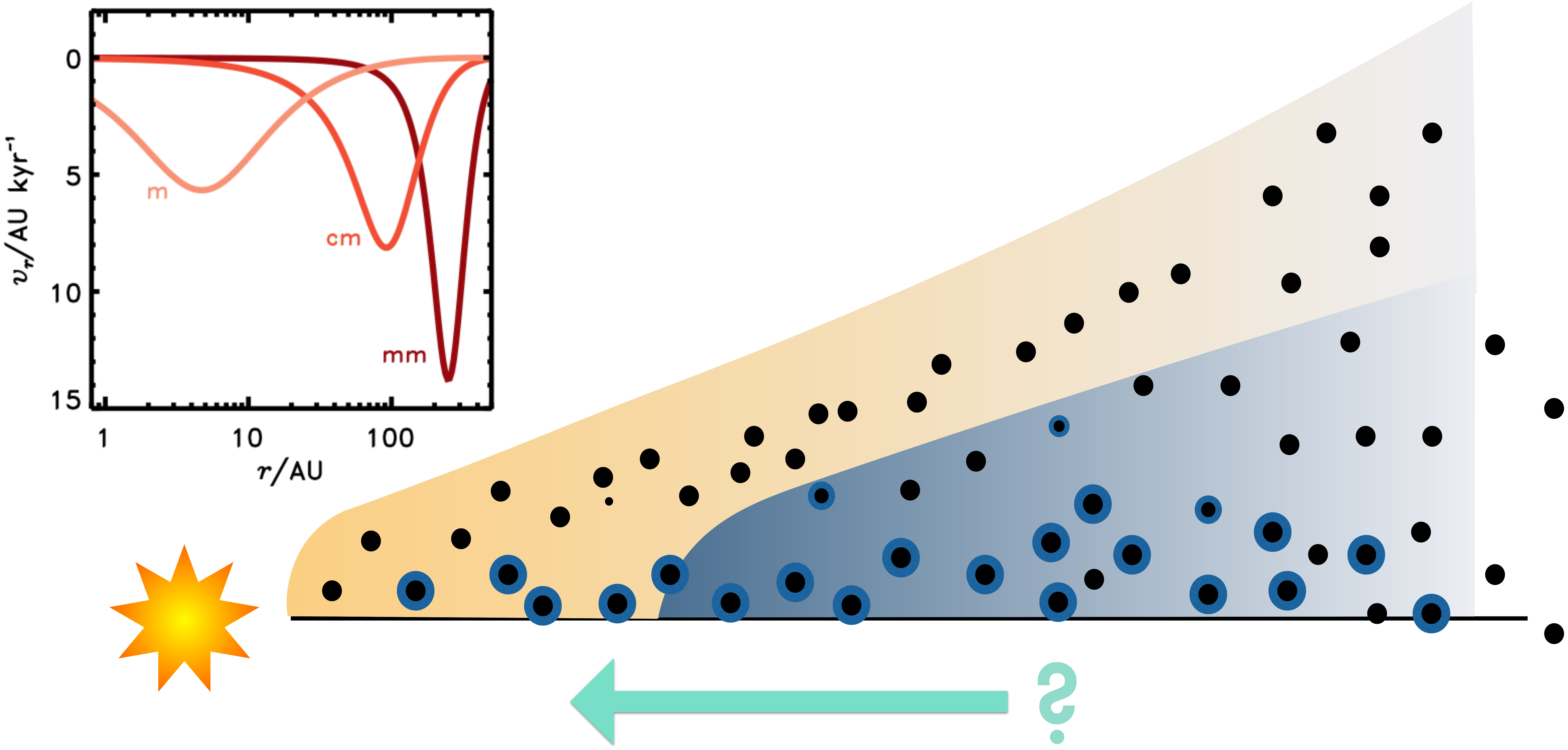
RESULTS:

Super-solar C/O ratio favored in the upper layers. Implies oxygen in the surface is lower than ISM by a factor of 50x, CO by 20x

Nitrogen gas essentially *interstellar* in the surface of the disk, minimal processing

Cleeves et al. 2018

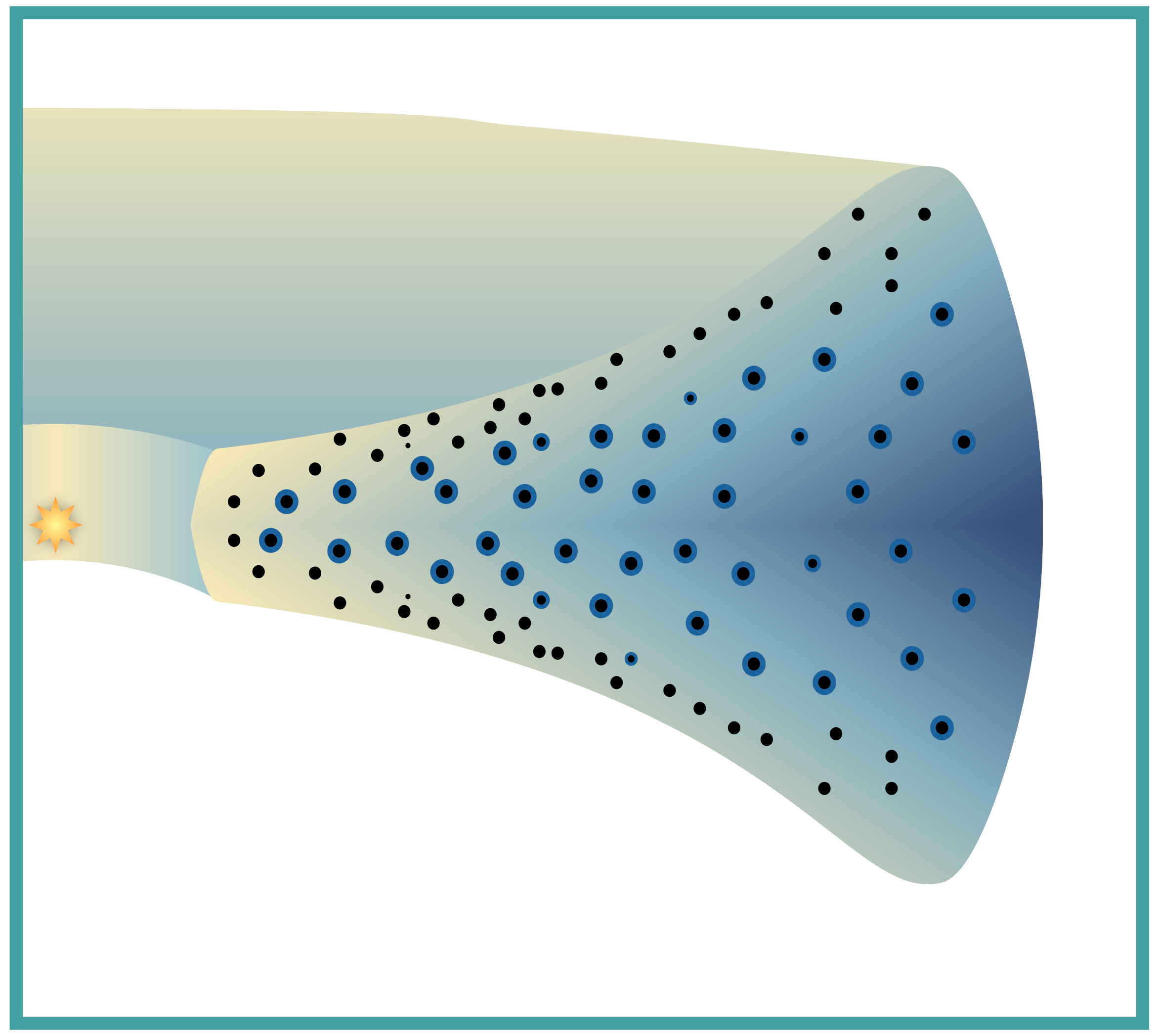
WHERE DO THE VOLATILES END UP?



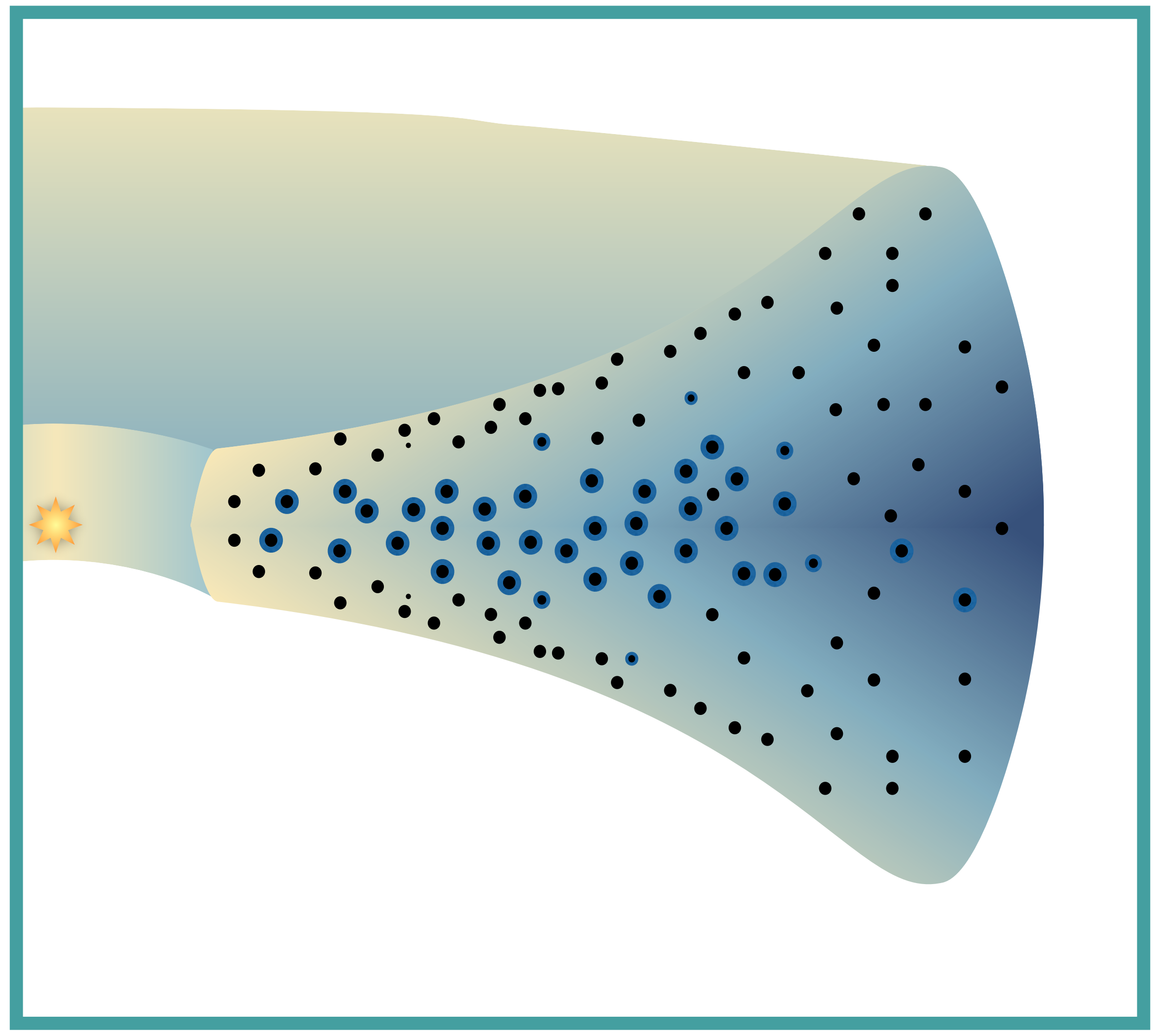
Andrews & Birnstiel (Handbook of Exop)

IMPLICATIONS FOR FORMING PLANETS

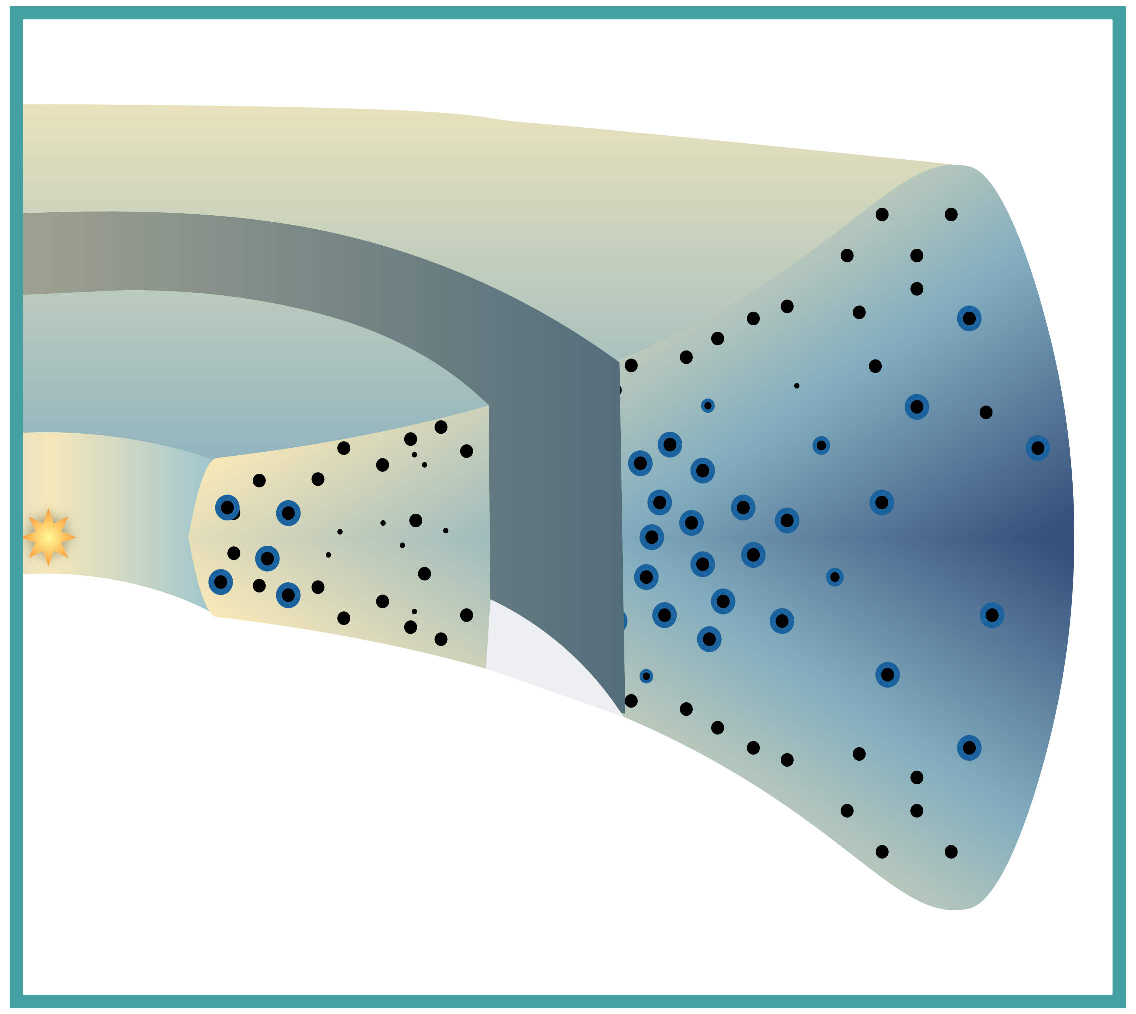
Volatile accretion onto forming planets will have radial and time dependence (see also Morbidelli's talk)



ISM-like



Volatile rich inner disk, poor outer disk

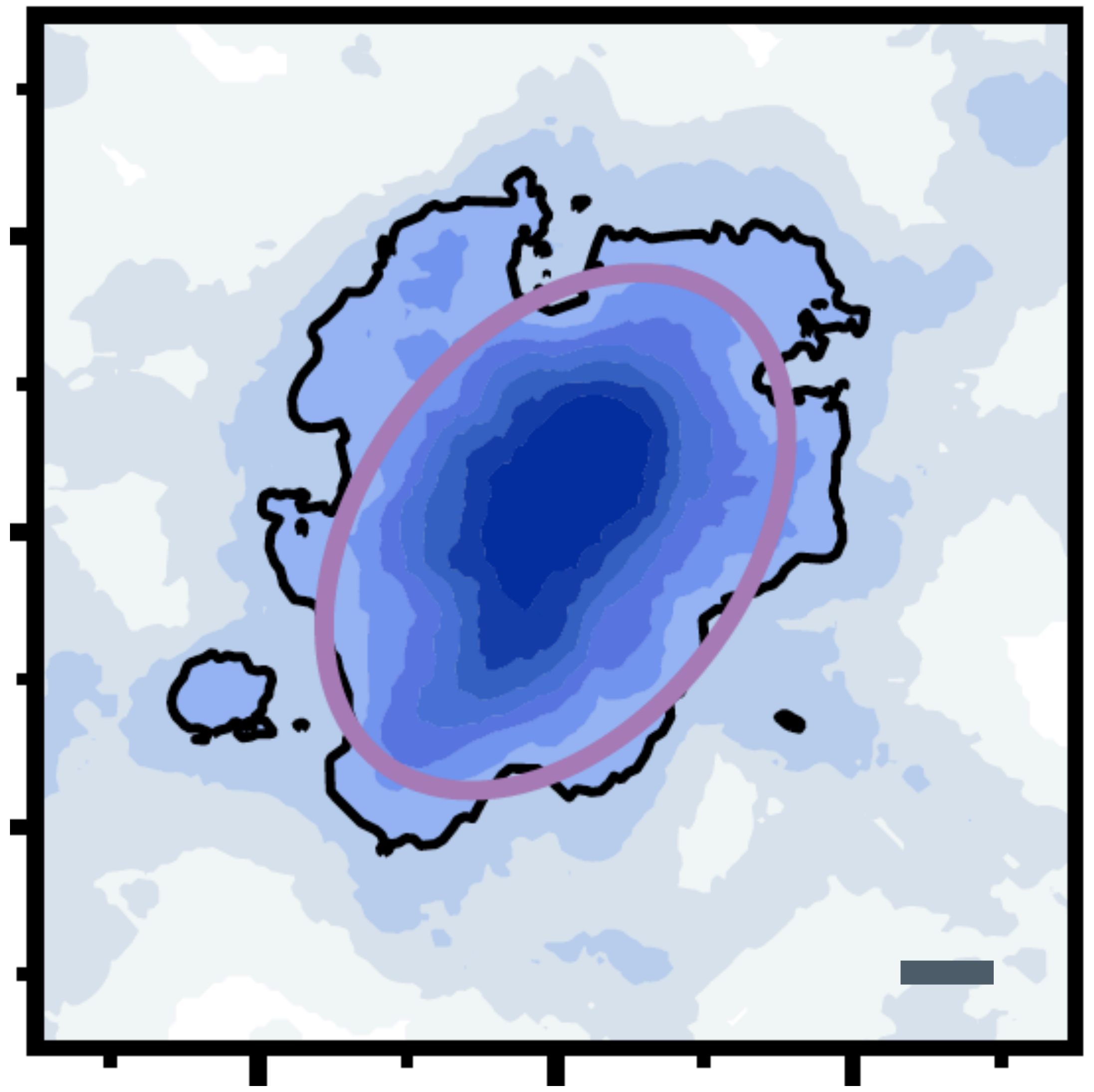


Radially dependent

May also imprint onto stellar spectrum (Kama+2015)

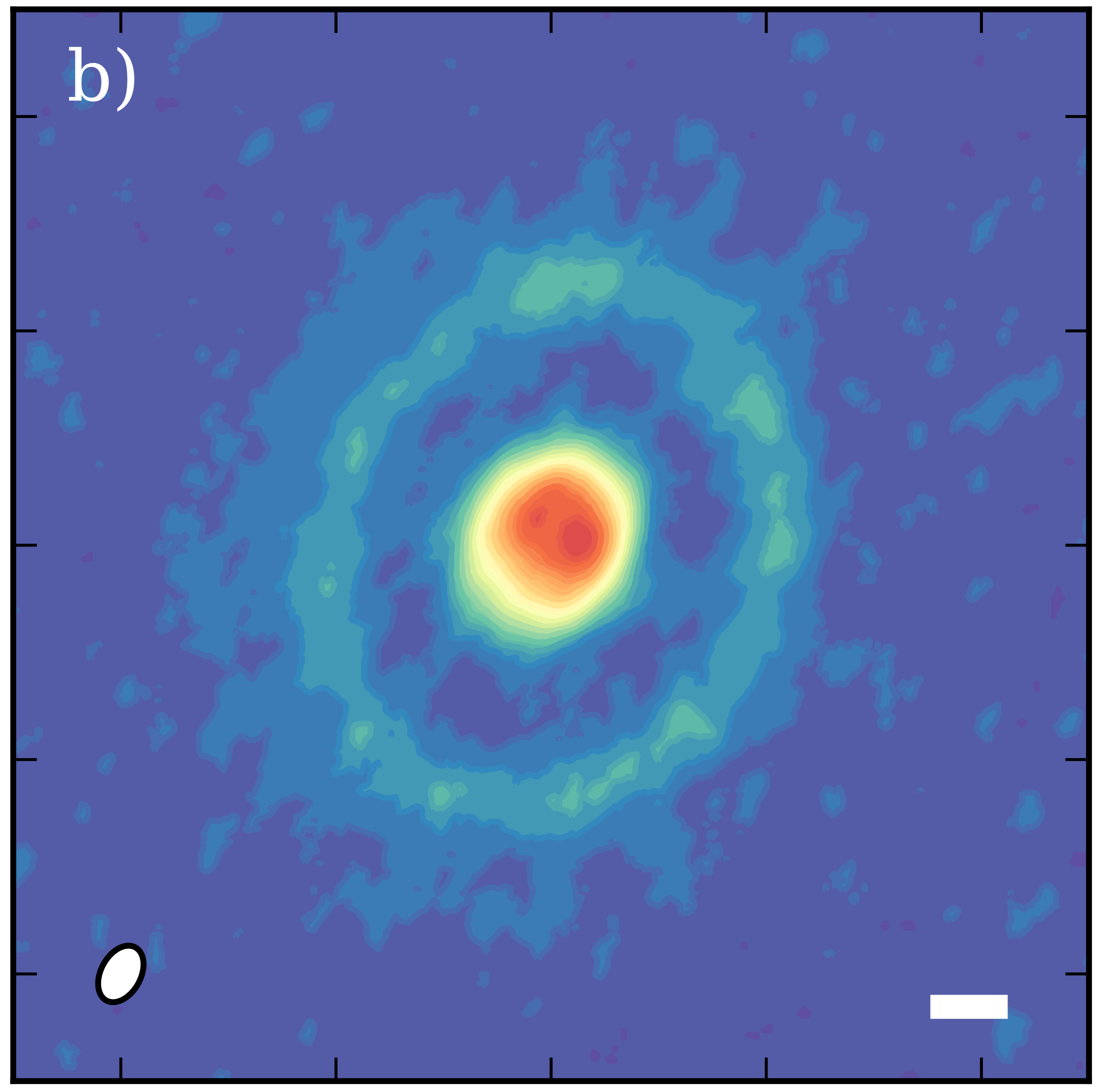
NEED A LARGER SAMPLE

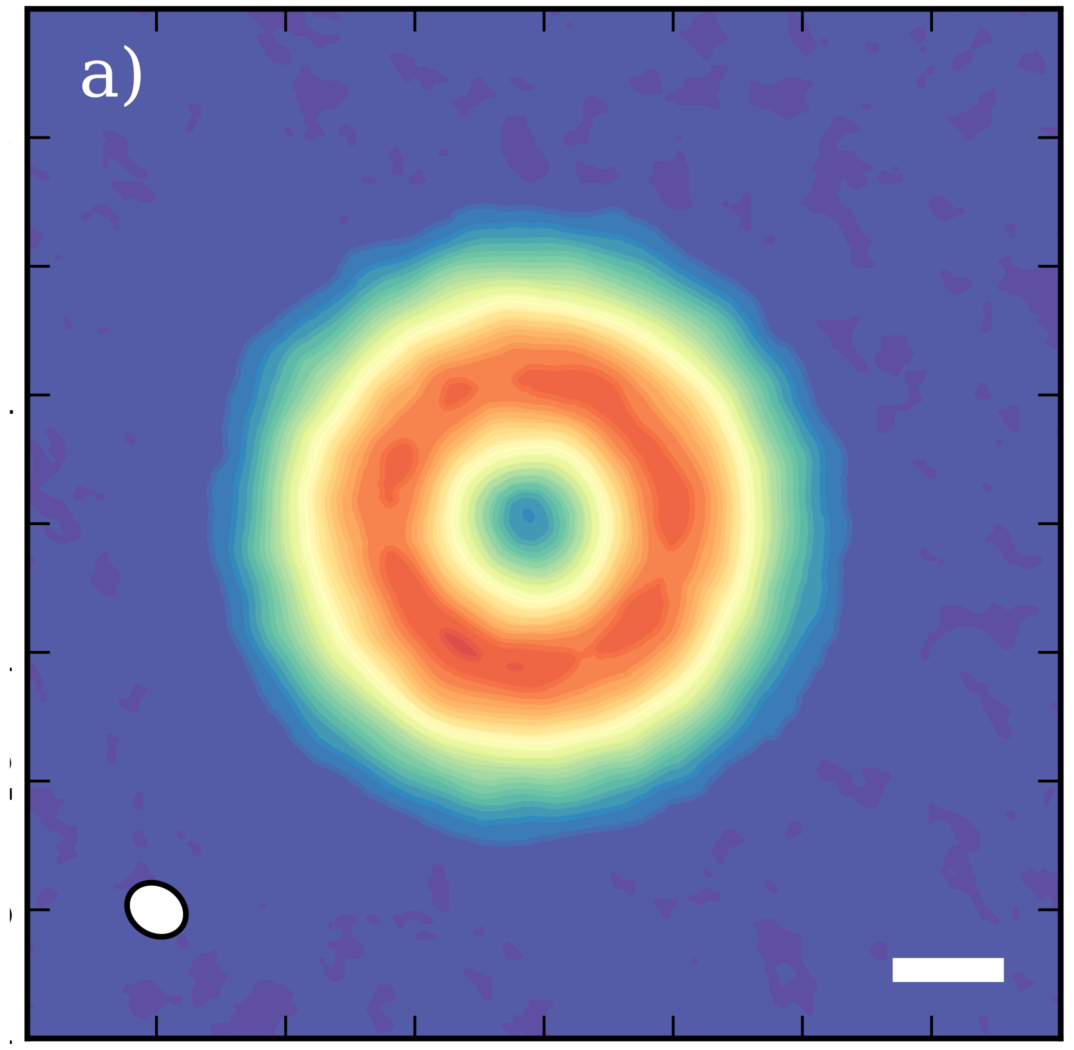
C_2H observations in a larger sample of disks, covering an age spread



IM Lup ~0.5-1 Myr
(Mawet+2016)

~1-4 Myr; (DM Tau)





TW Hya ~5-10 Myr
(Donaldson+2016)

Young → Old

100 au scale bar

SUMMARY

- Disk chemistry and physics are intractable.
- With sub-mm gas observations, finding evidence for deviations from interstellar chemistry in a handful of bright disks!

But many open questions…

- What disk composition is normal (and when/where)? Still small number statistics…
- How much was preserved from the molecular cloud? Isotope ratios?
- Models needed to overcome surface vs. midplane bias
- Cloud-to-cloud variations? Differing amounts of C, N, O, etc?
- Role of stellar environment, binarity?
- Timescale of planet formation? *What* chemistry matters?
- If volatile depletion is common, where does it go? Testable with inner disk chemistry with JWST