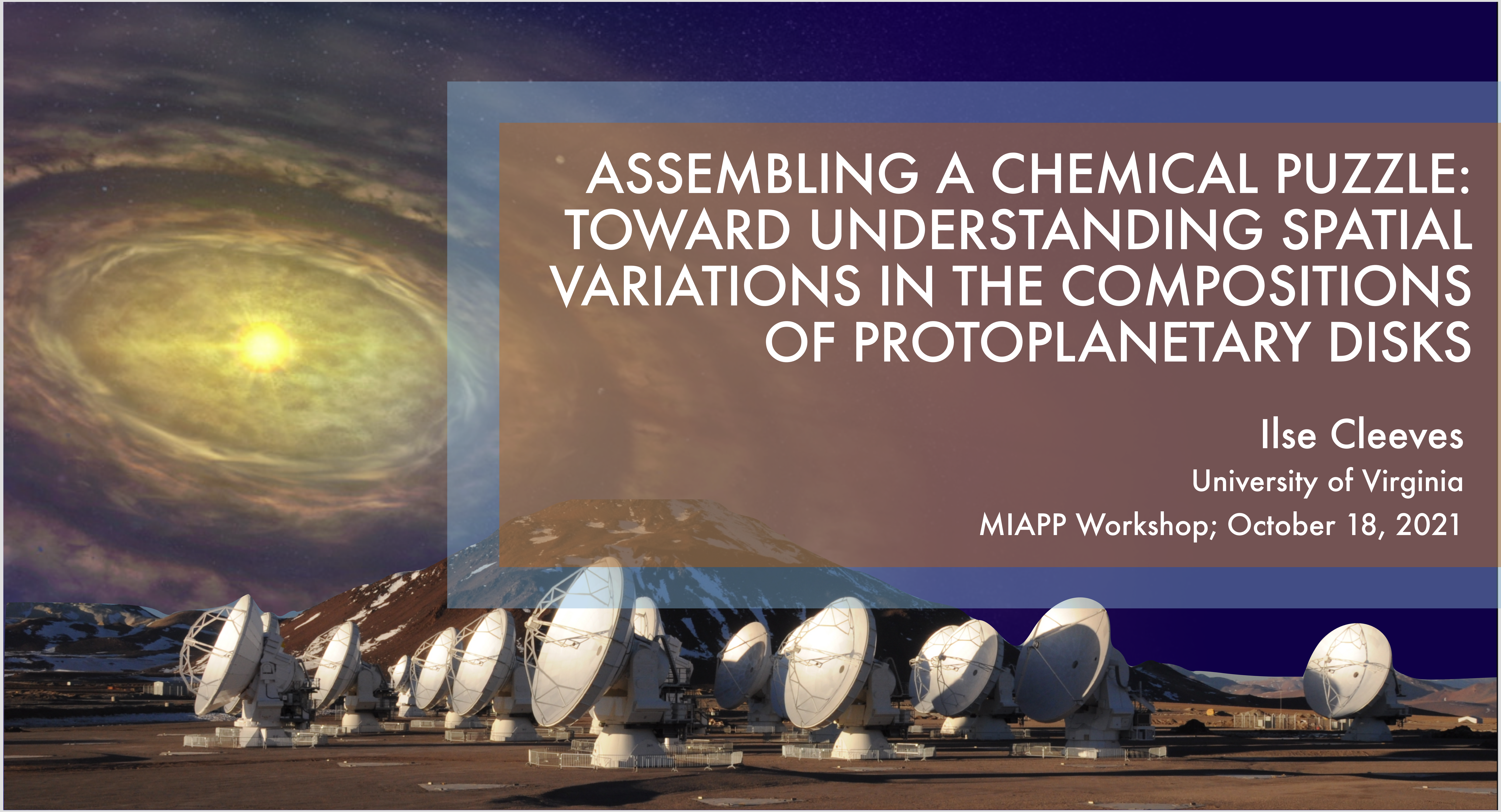


ASSEMBLING A CHEMICAL PUZZLE: TOWARD UNDERSTANDING SPATIAL VARIATIONS IN THE COMPOSITIONS OF PROTOPLANETARY DISKS

Ilse Cleeves
University of Virginia

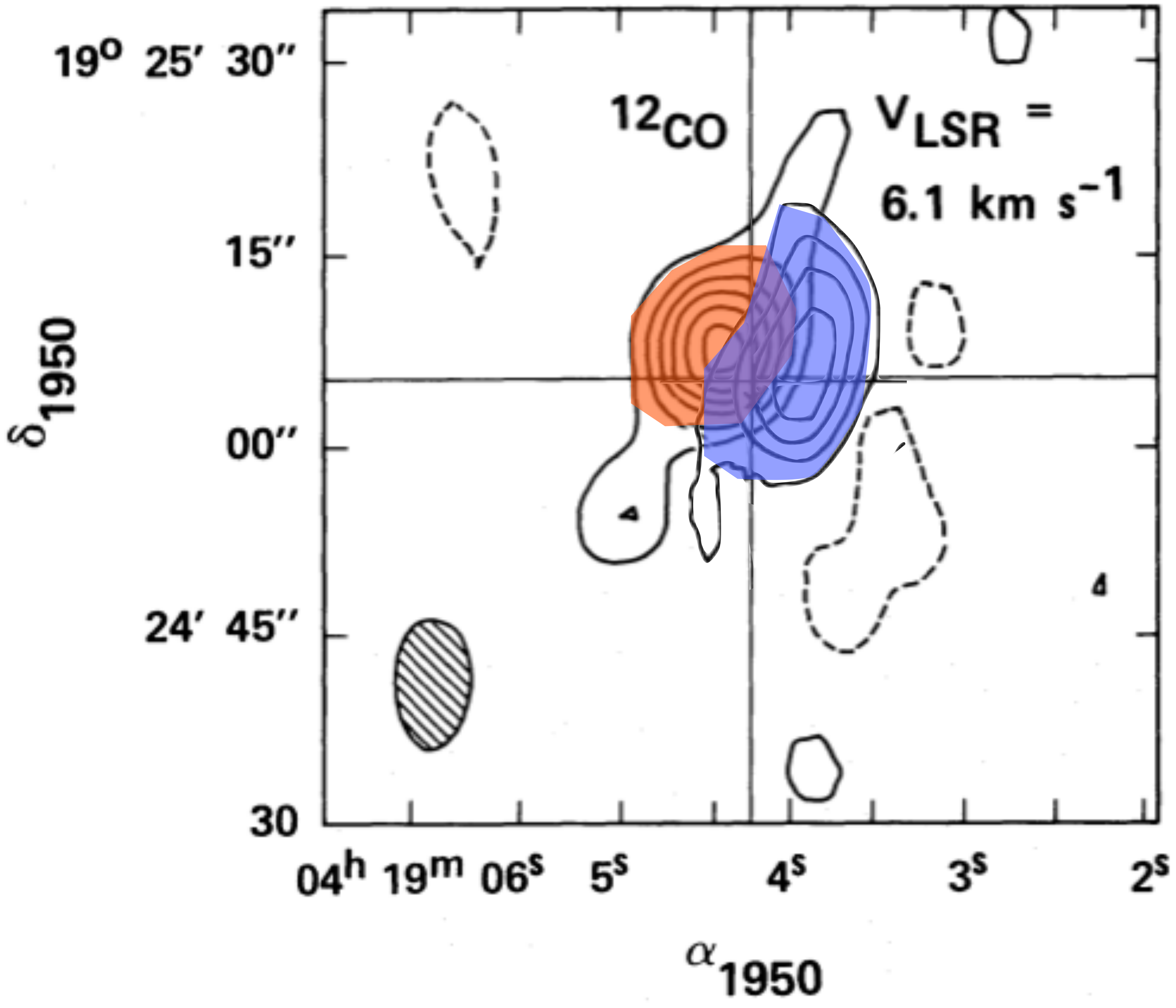
MIAPP Workshop; October 18, 2021

Image Credit: University of Copenhagen/Lars Buchhave, W. Garnier, ALMA (ESO/NAOJ/NRAO)

WHAT DO WE WANT TO KNOW?

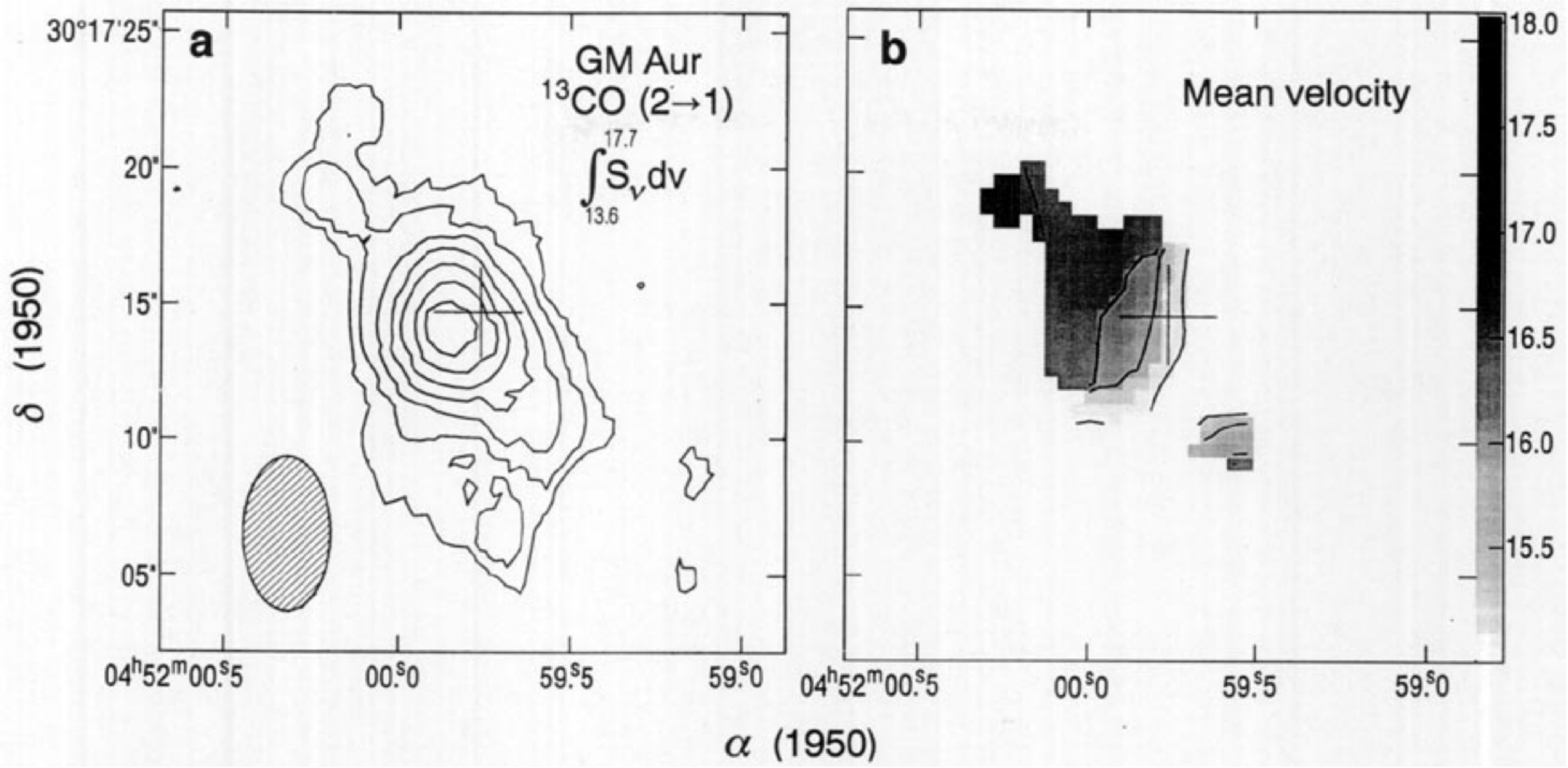
I. What's the *spatial distribution* of *bulk* molecular gas?
II. What is the *composition* of planet forming gas/solids?
III. What spatial constraints on disk *physics* do gas observations provide?

RESOLVING PLANET FORMATION: 1987



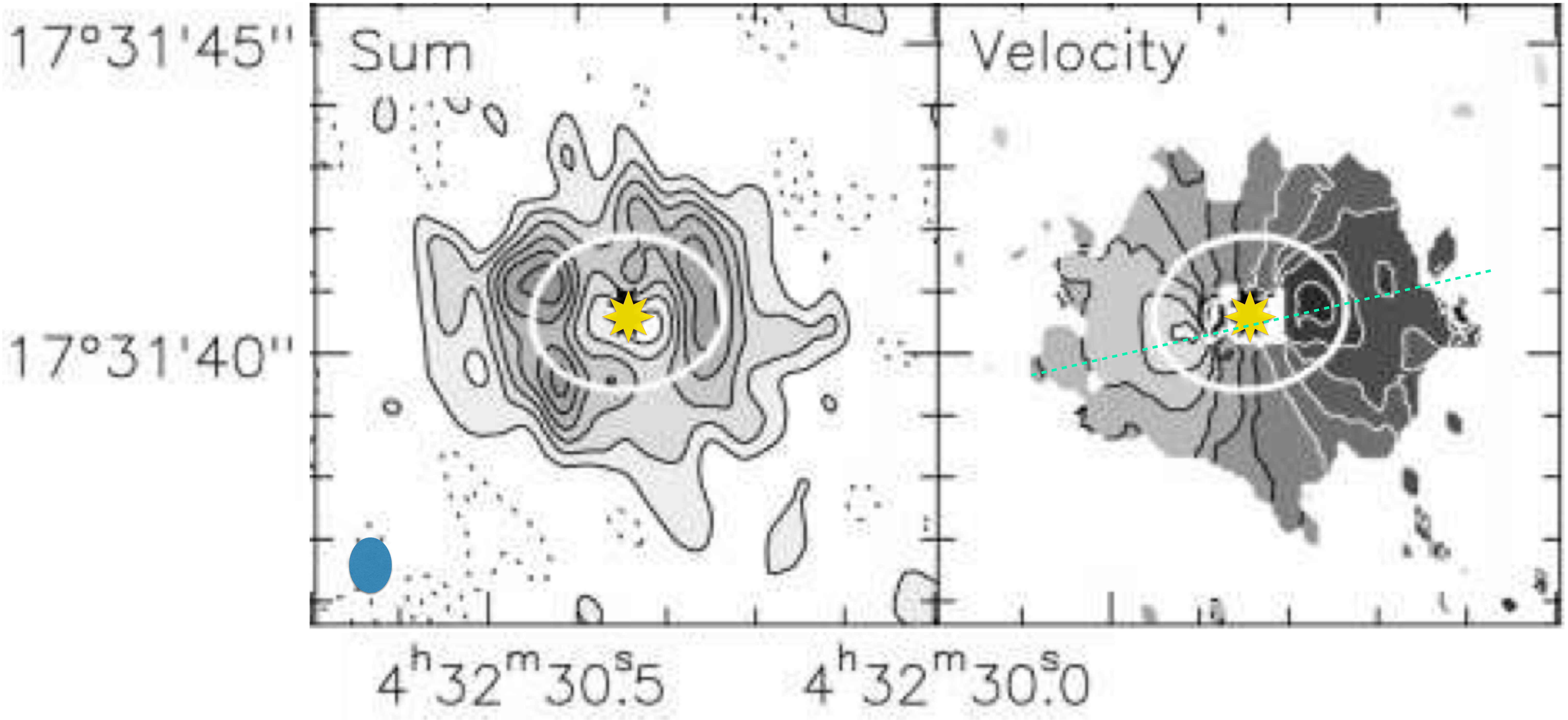
T Tau
CO 1-0
Weintraub,
Zuckerman,
Masson 1987

RESOLVING PLANET FORMATION: 1993



GM Aur
^{13}CO 2-1
Koerner, Sargent,
and Beckwith 1993

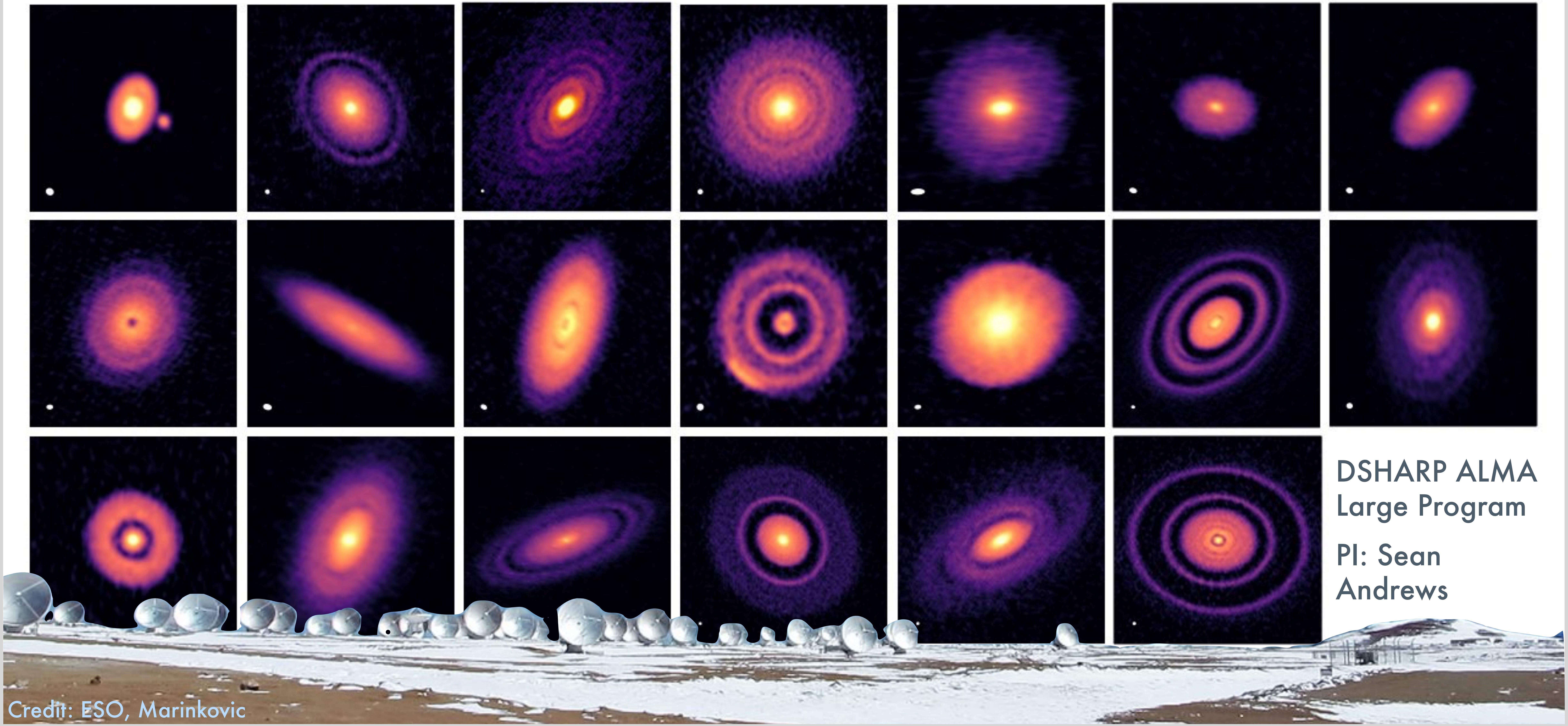
RESOLVING PLANET FORMATION: 1999



GG Tau
^{13}CO 2-1
Guilloteau, Dutrey, and Simon 1999

Facility: Plateau de Bure Interferometer (PdBI)

IMAGING DISKS WITH ALMA



DSHARP ALMA Large Program

PI: Sean Andrews

Credit: ESO, Marinkovic

IMAGING DISKS WITH ALMA

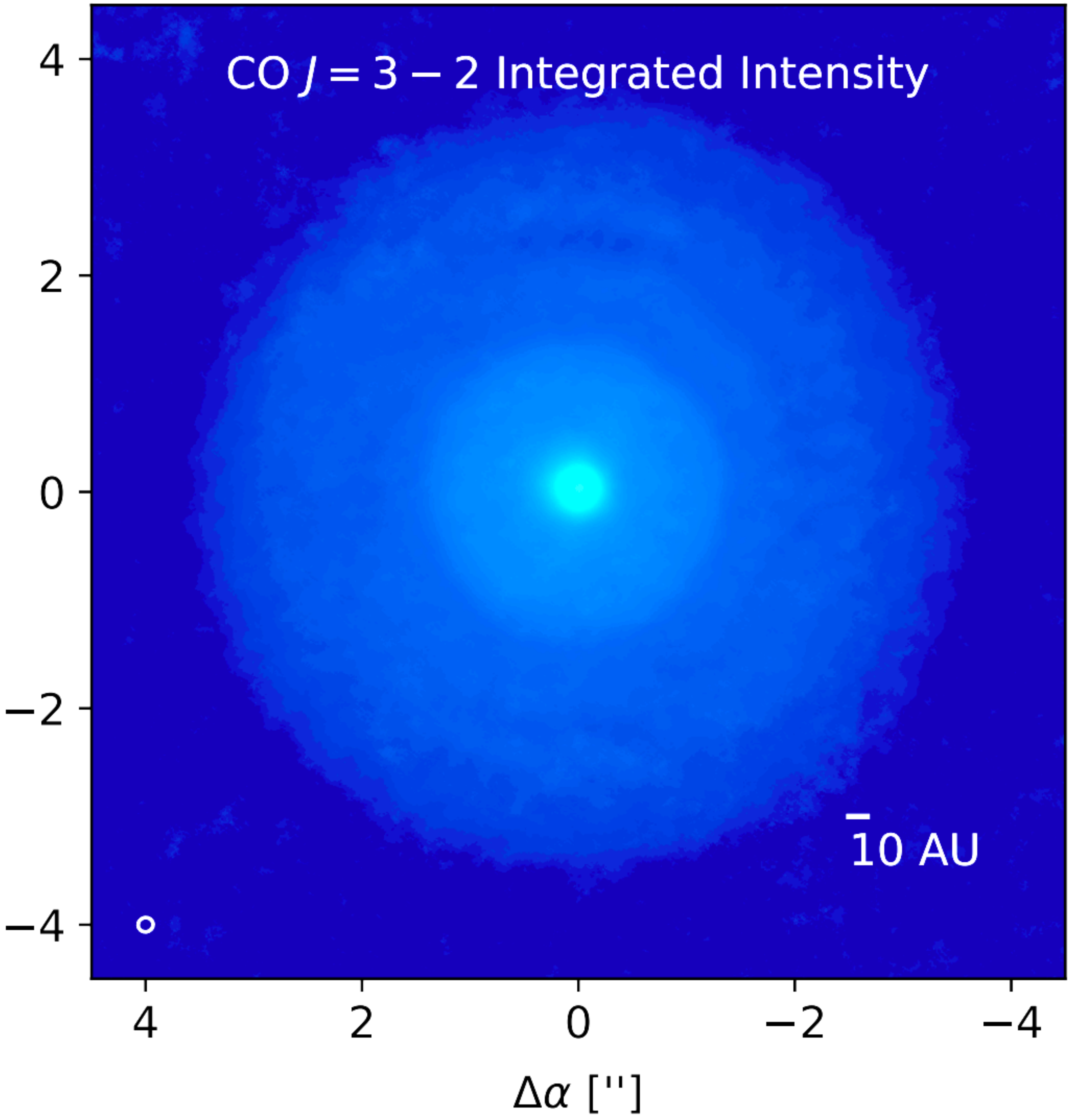
DSHARP ALMA Large Program

PI: Sean Andrews

Credit: ESO, Marinkovic

GAS, THE 99%, IS HARD

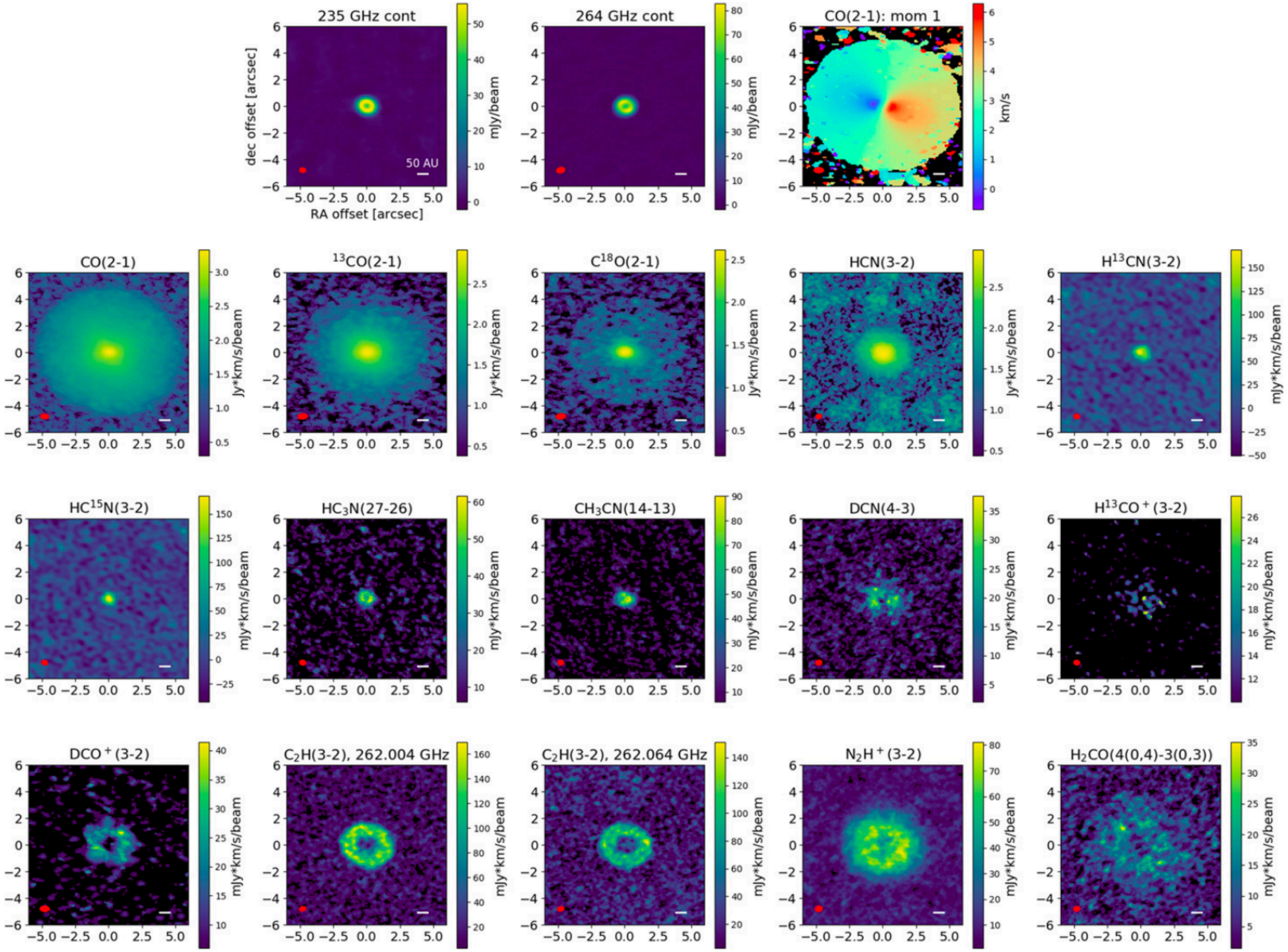
Synthesized beam of 2.2 × 1.5 AU!



Huang et al. 2018, combined data from many different programs: *total integration* 12 hours and 38 minutes

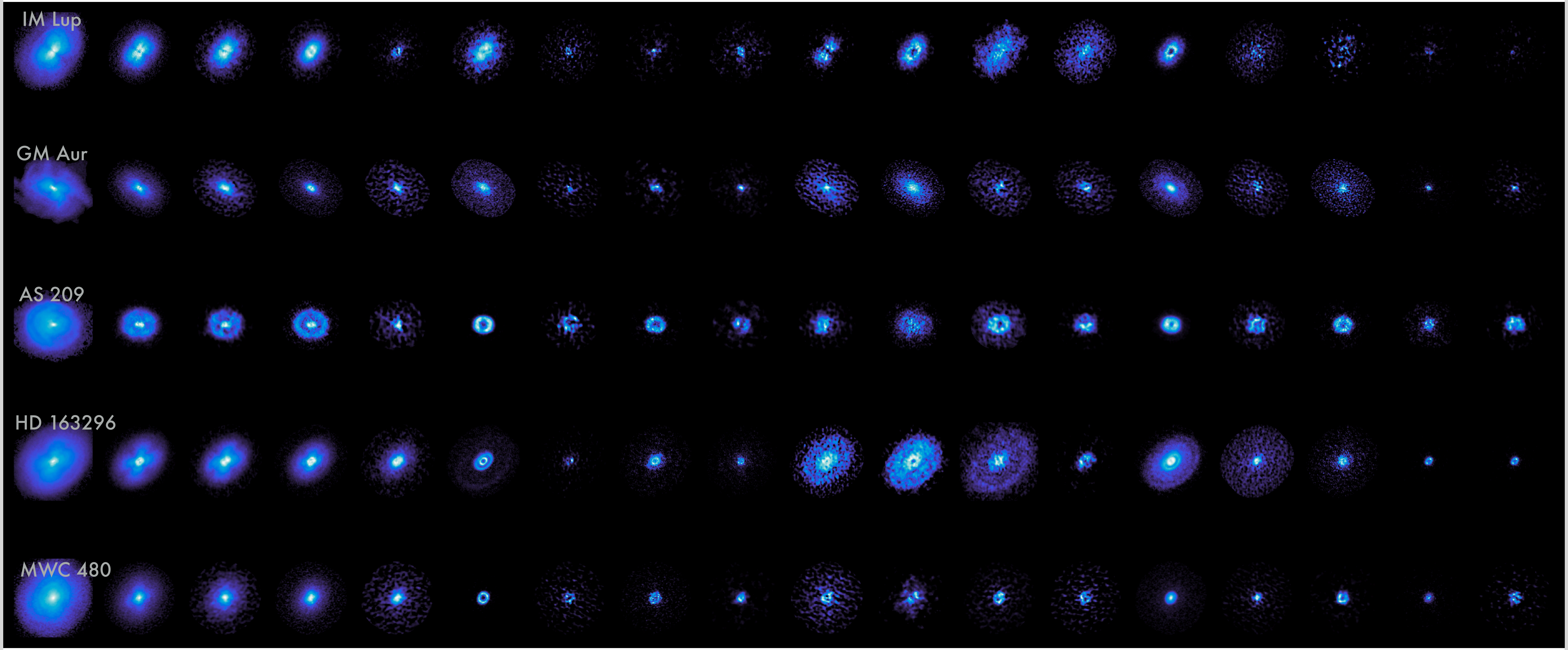
Background TW Hya CO 3-2 with the SMA
Andrews, Wilner, Hughes + 2012

RESOLVED CHEMISTRY BEYOND CO



Kastner et al. 2018; V4046 Sgr

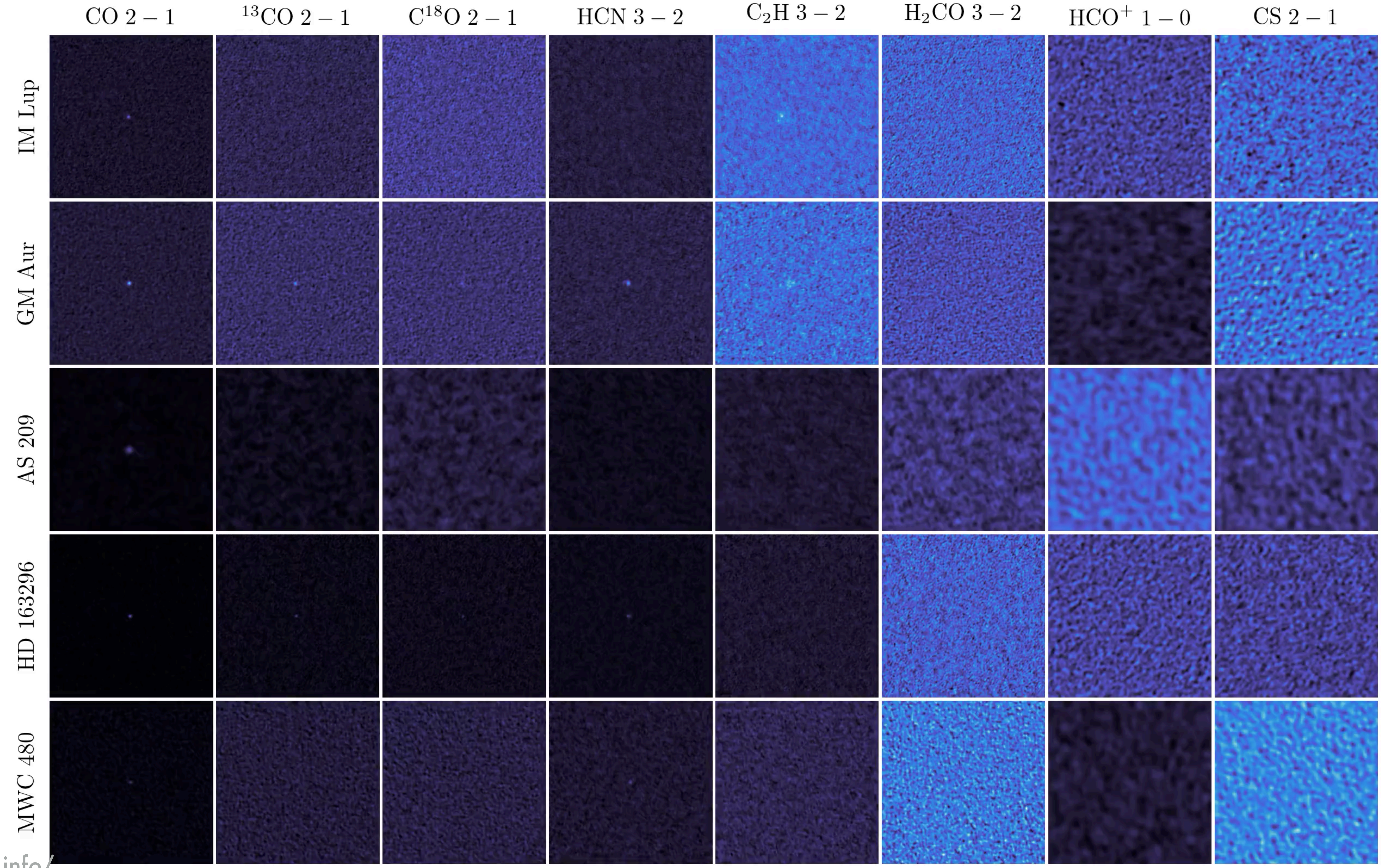
RESOLVED CHEMISTRY BEYOND CO



http://alma-maps.info/

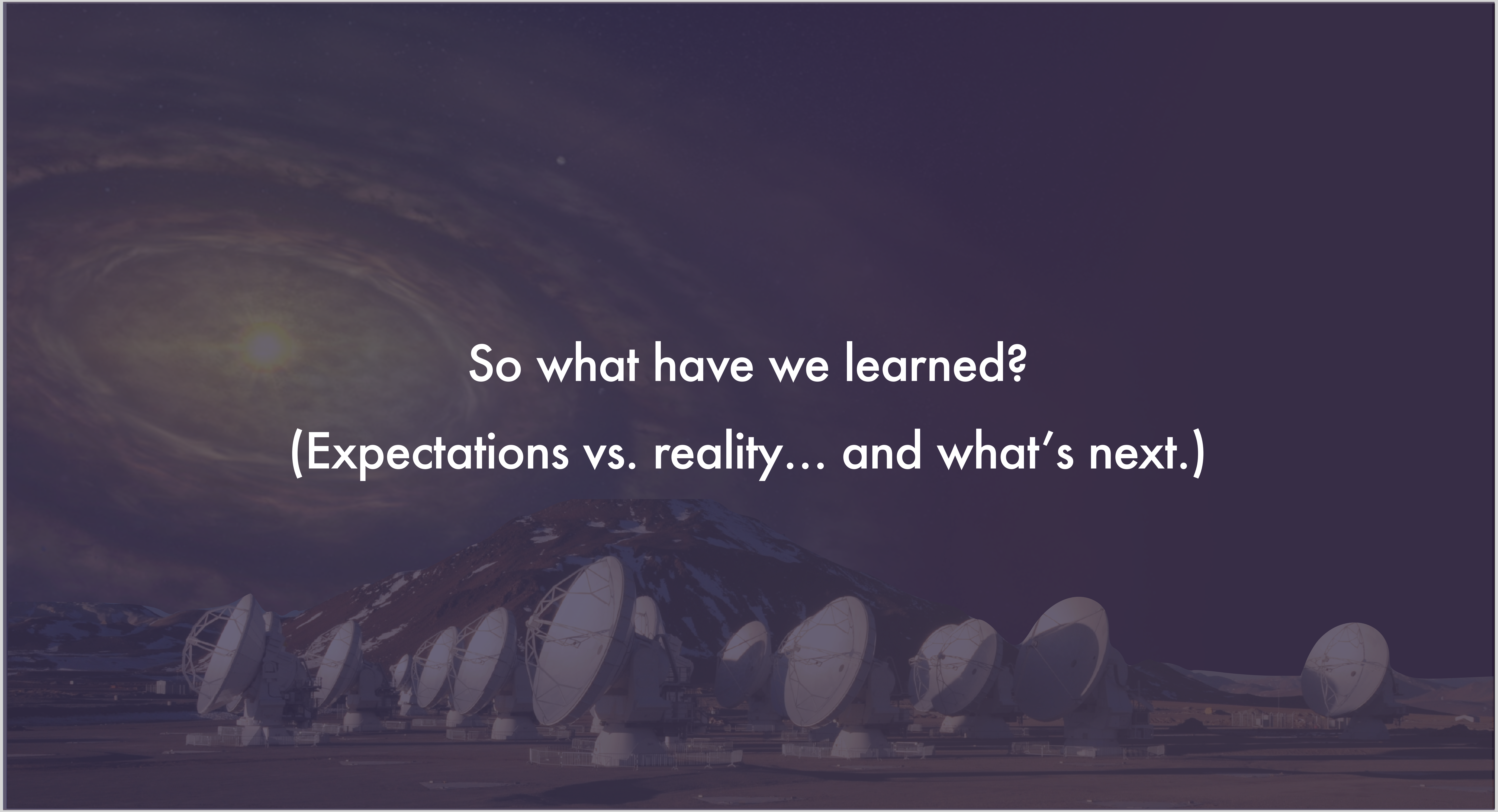
Fig Credit: C. Law

INCLUDING KINEMATICS…!



http://alma-maps.info/

Fig Credit: I. Czekala



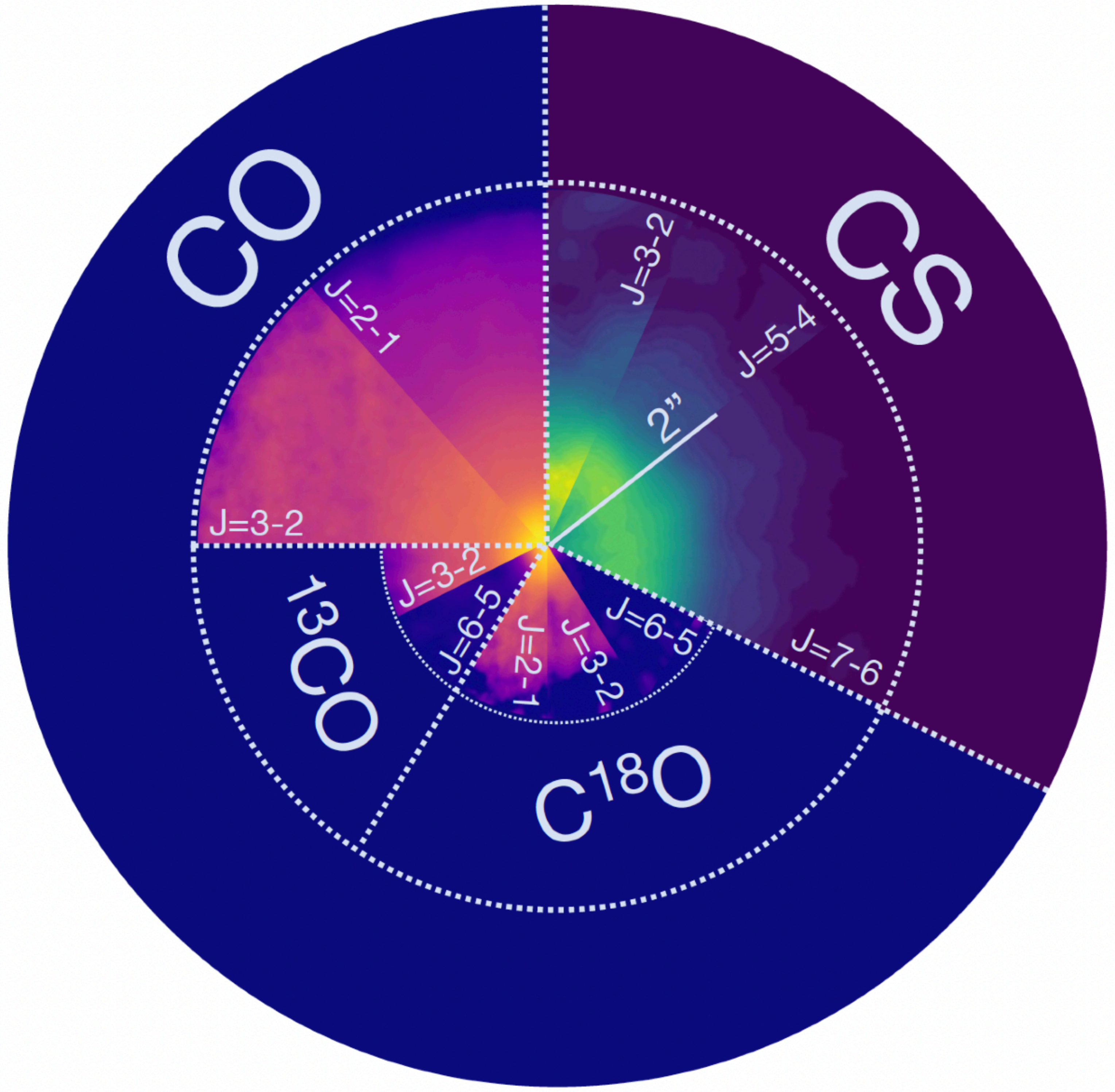
So what have we learned?

(Expectations vs. reality… and what’s next.)

Image Credit: University of Copenhagen/Lars Buchhave, W. Garnier, ALMA (ESO/NAOJ/NRAO)

I. GAS STRUCTURE

Do substructures identified in submillimeter dust observations or scattered light correspond to features in the observable gas?



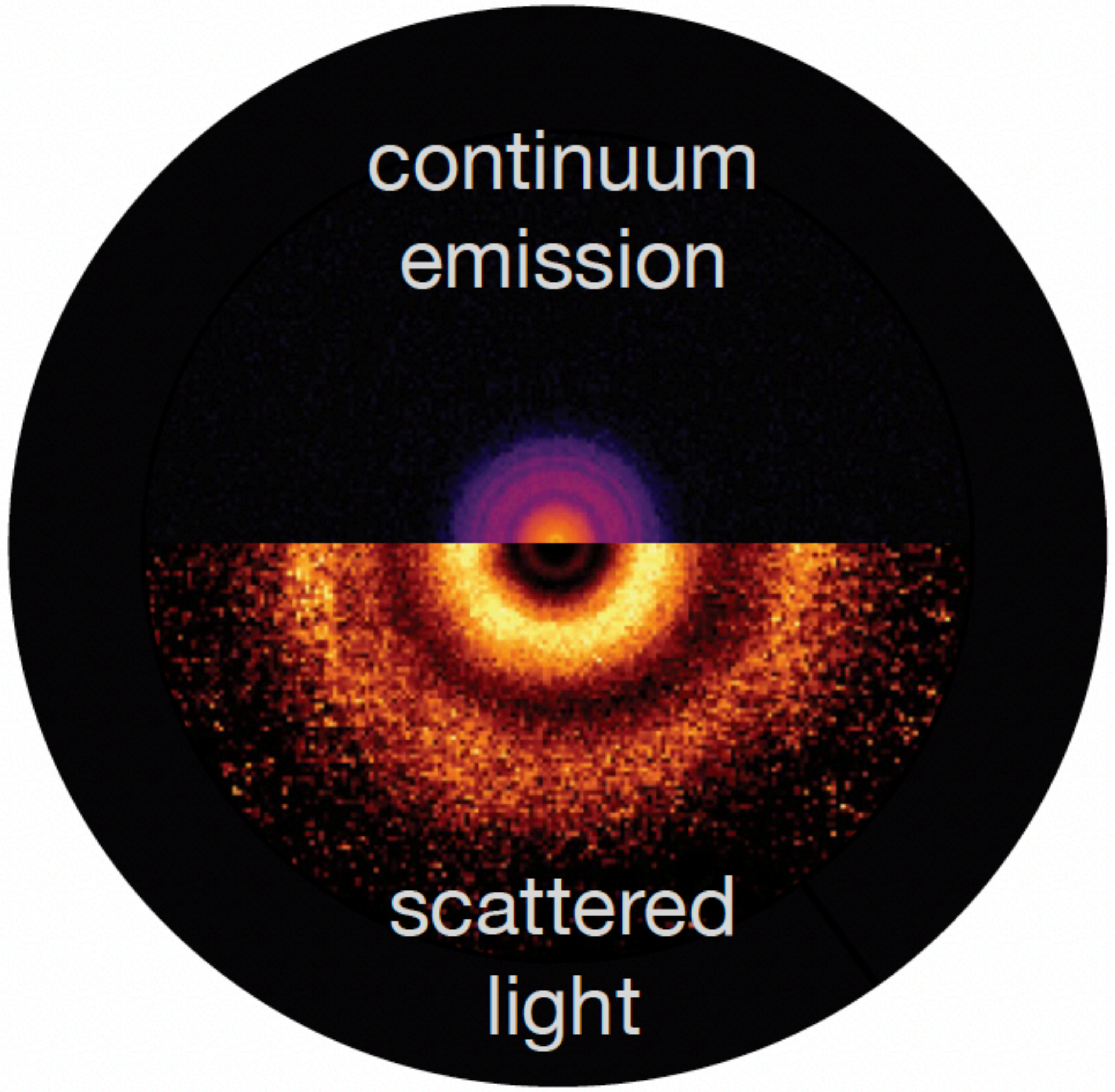
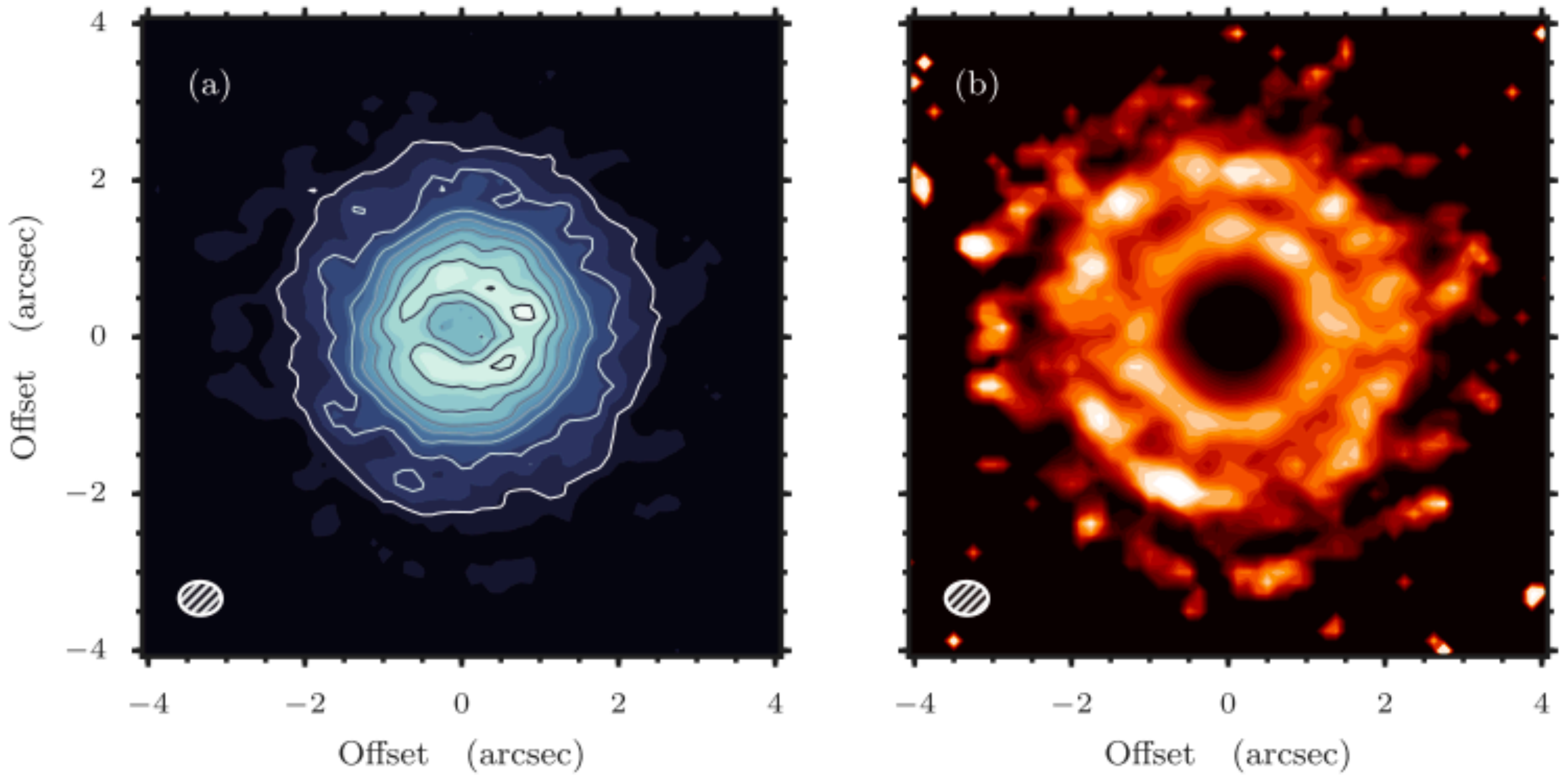


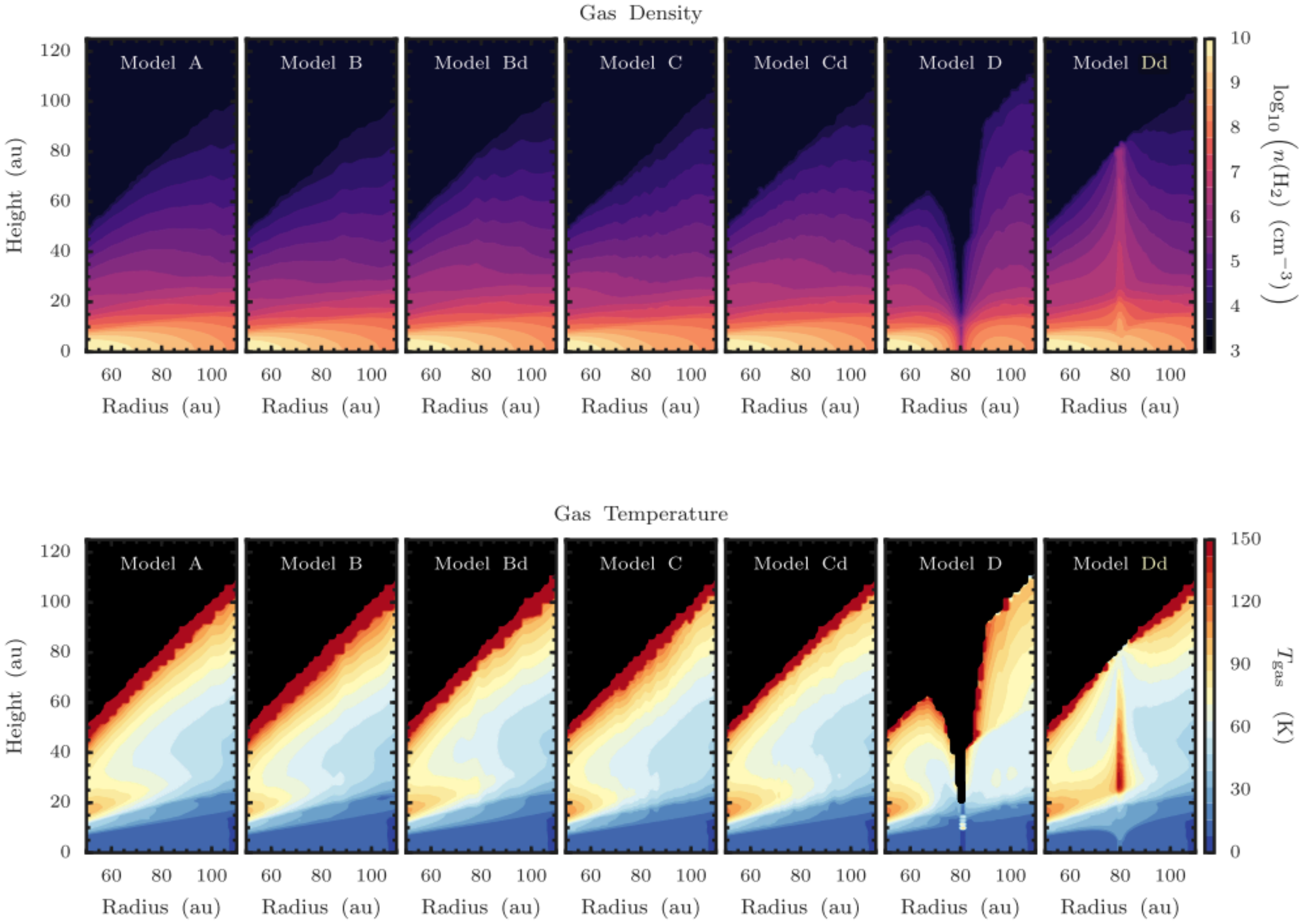
Fig Credit: Miotello (PPVII chapter)

I. GAS STRUCTURE: EXPECTATIONS

- **Naive picture:** If H_2 is disappearing, then all gas should drop as well, and so we should see similar patterns in all molecular tracers observed.
- **More sophisticated:** the changing conditions in gaps (temperature, radiation field, change in dust surface area) may result in a different gap-chemistry if the gaps are not 100% gas-poor.

CS 5-4 IN TW HYA

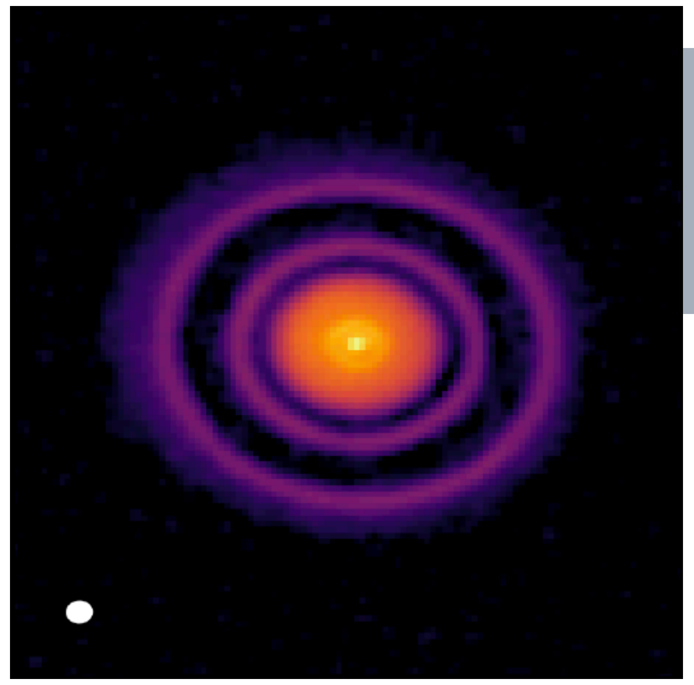




Teague+17 examined a variety of gap morphologies (dust depletion with or without gas depletion), created thermochemical structures, and post-processed with an astrochemical code.

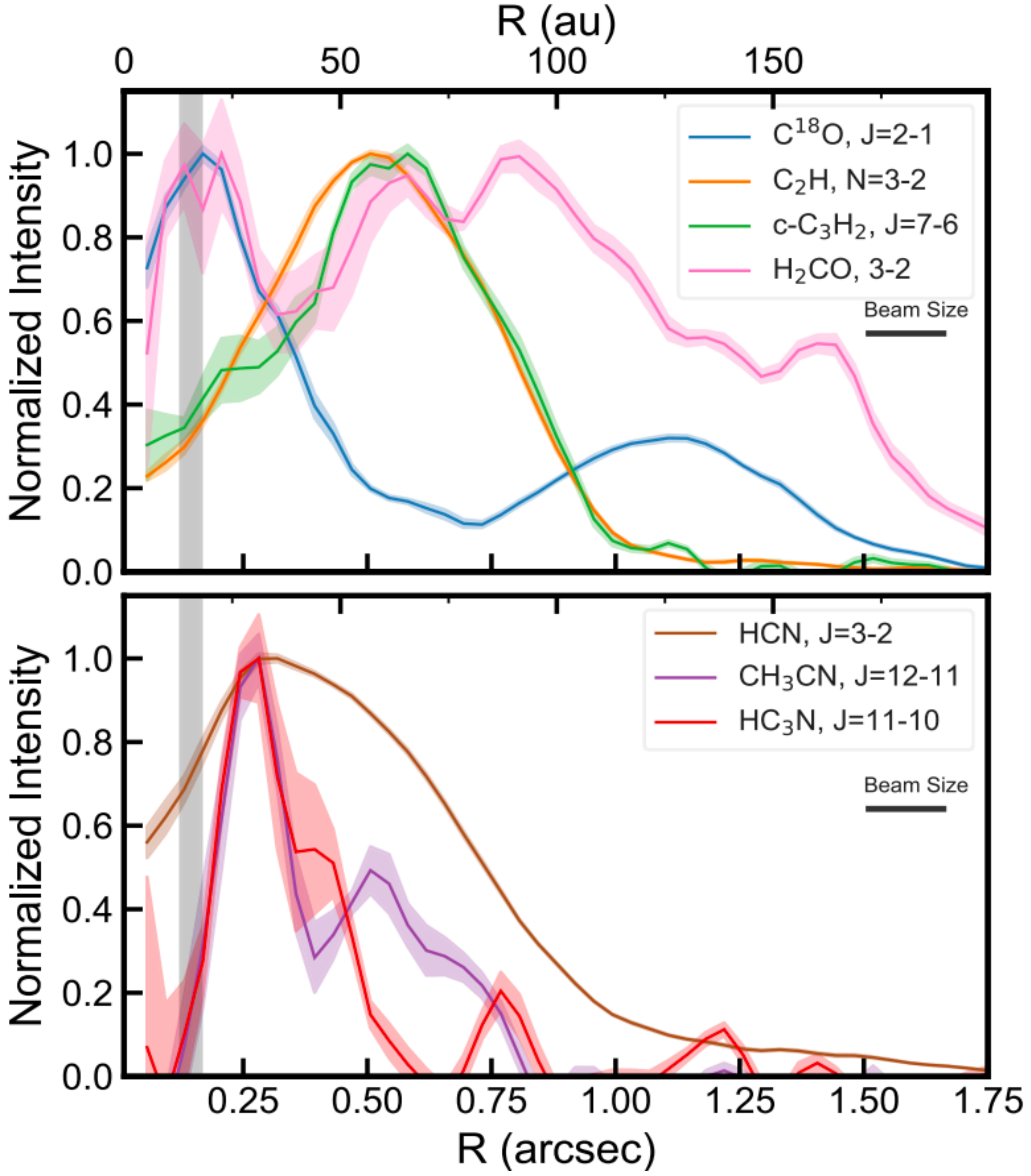
Required a moderately gas and dust poor gap.

Teague et al. 2017

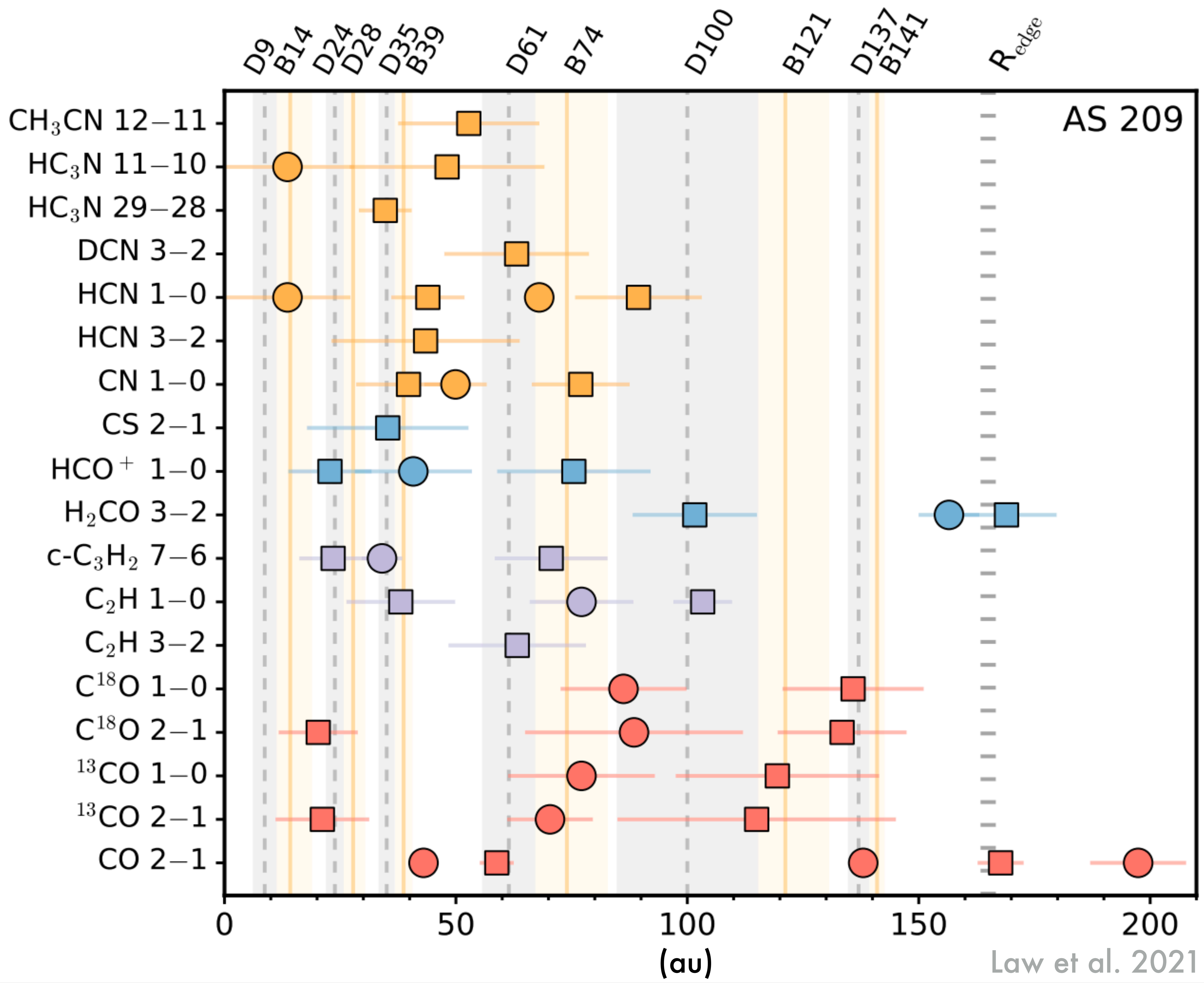


AS 209 WITH MAPS

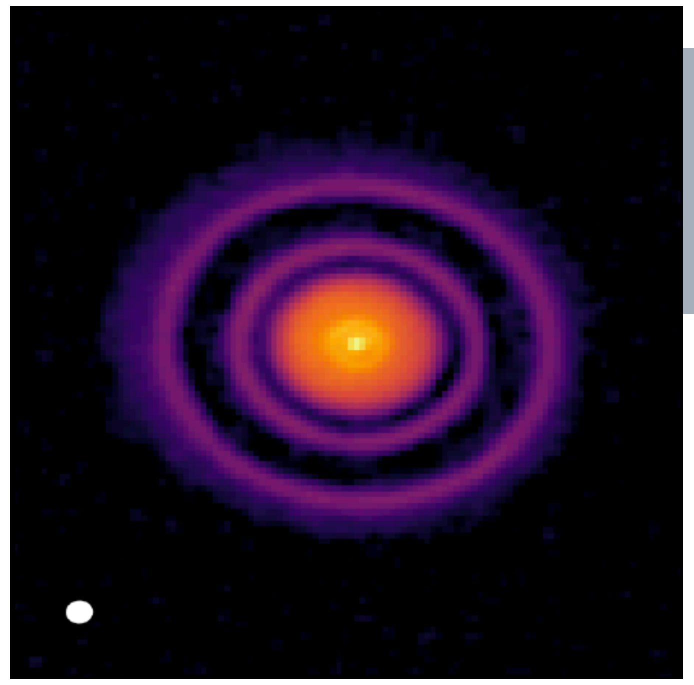
Sometimes the pattern is less clear. For example, C_2H peaking inside dust/$C^{18}O$ gap in AS 209 as seen and modeled in Alarcon+21.



Alarcon et al. 2021



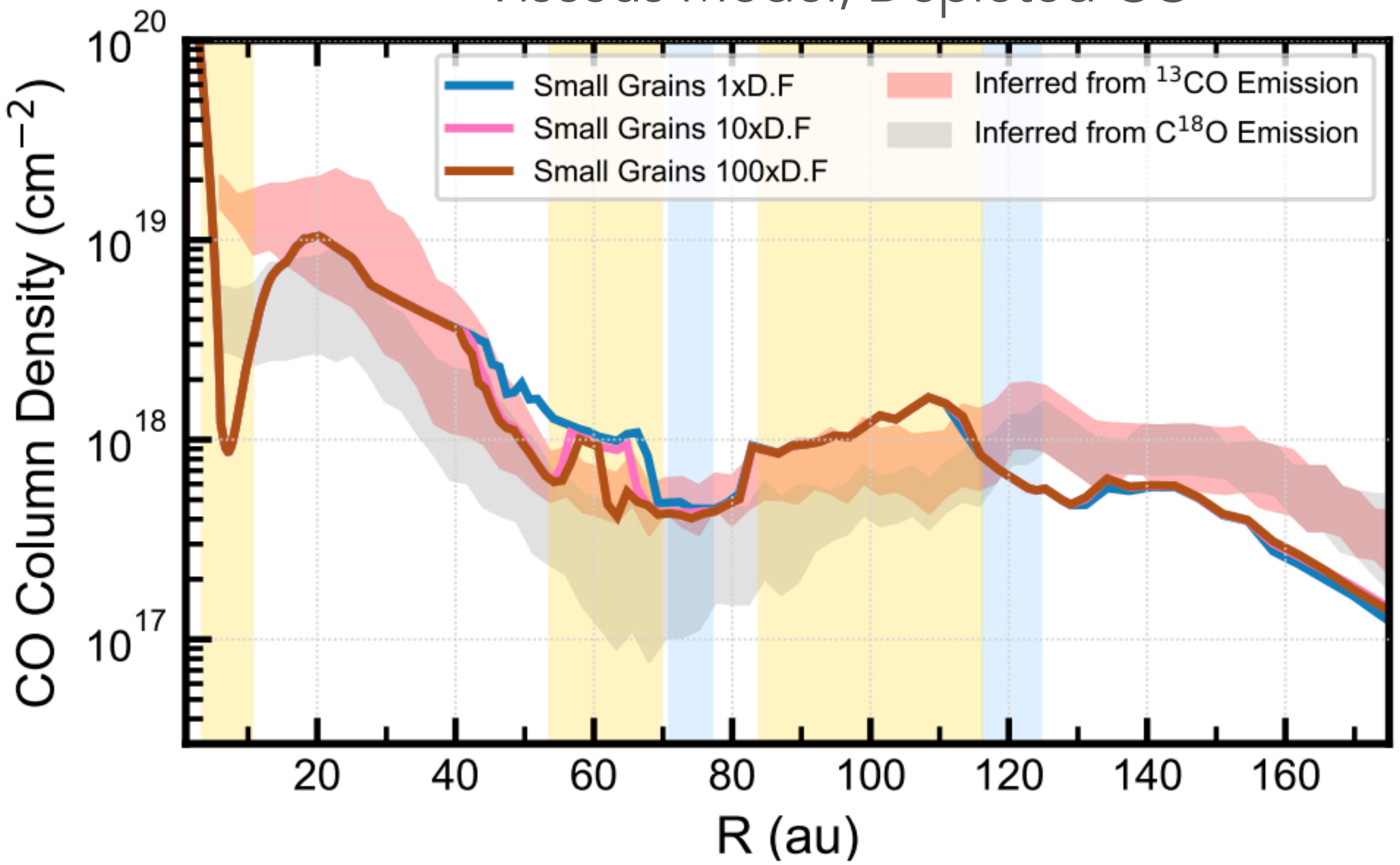
Law et al. 2021



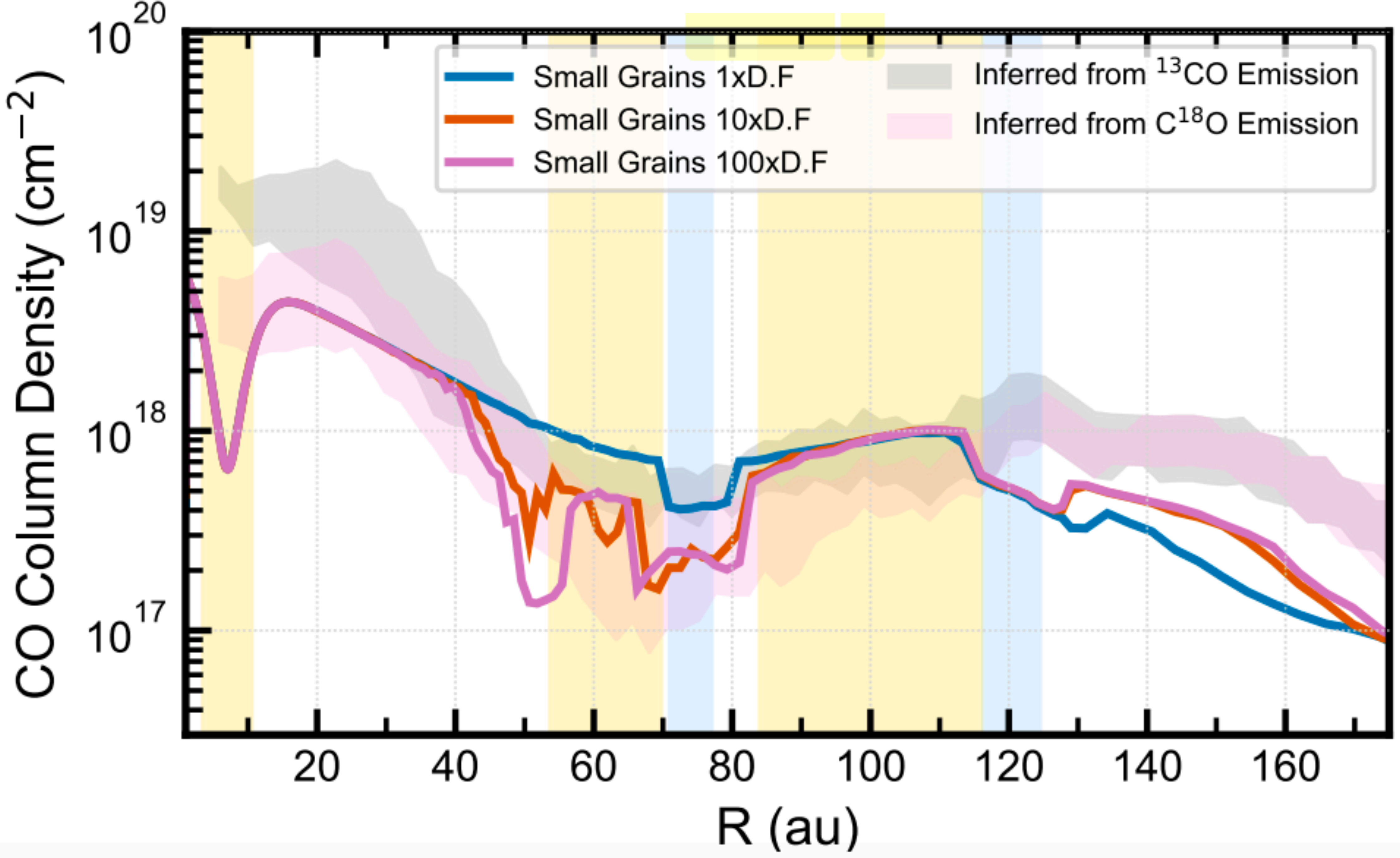
AS 209 WITH MAPS

Alarcon et al. 2021

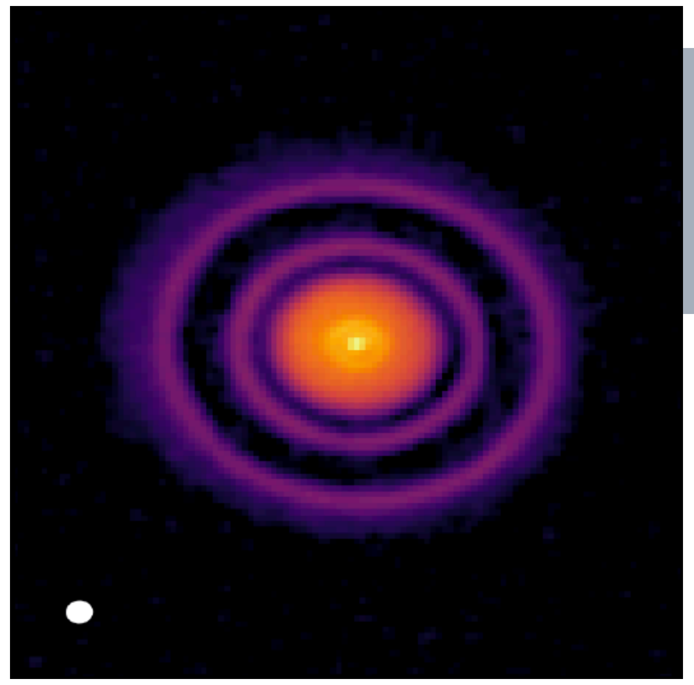
Viscous Model, Depleted CO



Gas deficit, normal CO.



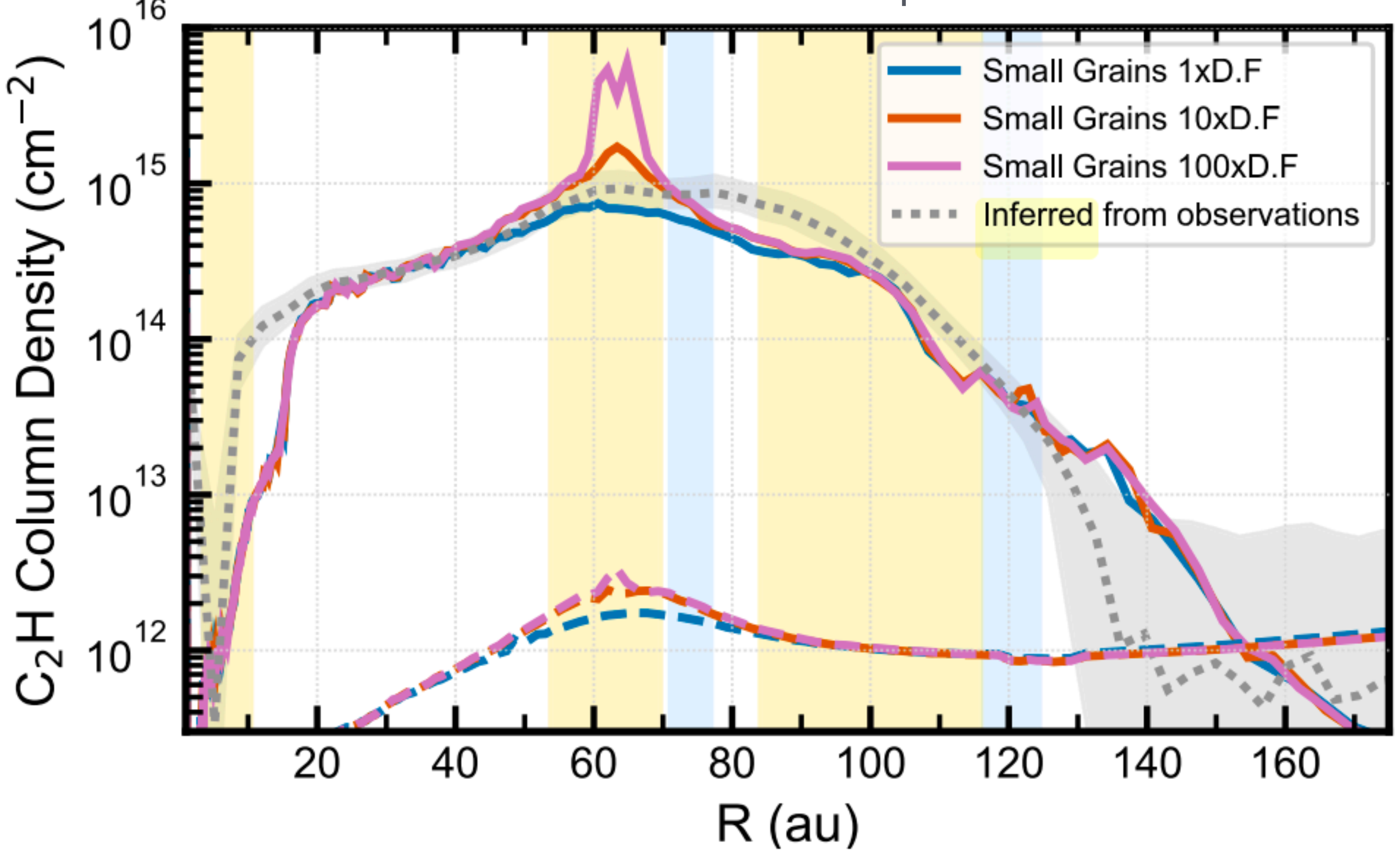
Small differences for H_2 or CO abundance decreases but within the errors. What about the C_2H enhancement?



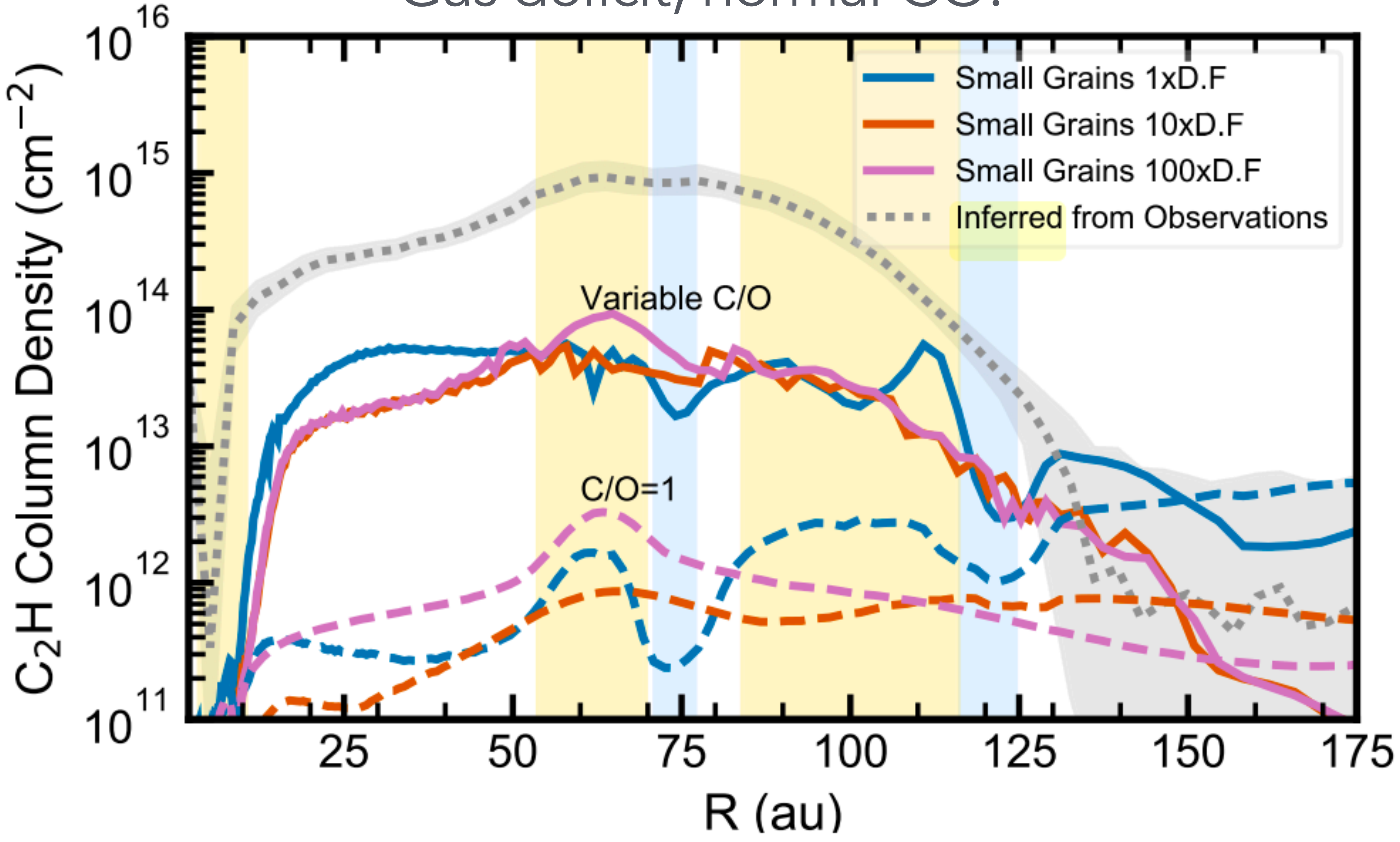
AS 209 WITH MAPS

Alarcon et al. 2021

Viscous Model, Depleted CO



Gas deficit, normal CO.



Highly super-solar C/O (2) and depleted CO abundance preferred over a gas deficit (right) to explain the radial morphologies.

I. GAS STRUCTURE: REALITY?

Many more examples in the literature (e.g., van der Marel+16 for transition disks, Huang+18 for TW Hya's CO, and Kastner+18 for circumbinary disk structure in V4046 Sgr).

In some cases seeing CO "enhancements" or N_2H^+ disappearing outside of the mm pebble disk unrelated to a gap. Possibly due to enhanced external photodesorption and/or thermal desorption? (e.g., Cleeves 2016)

Can we confirm with other photochemistry tracers? (e.g., CN; Cazzoletti+17)

Bottom line: CO is chemically active. Not sufficient alone to trace gas surface density perturbations, but what is?

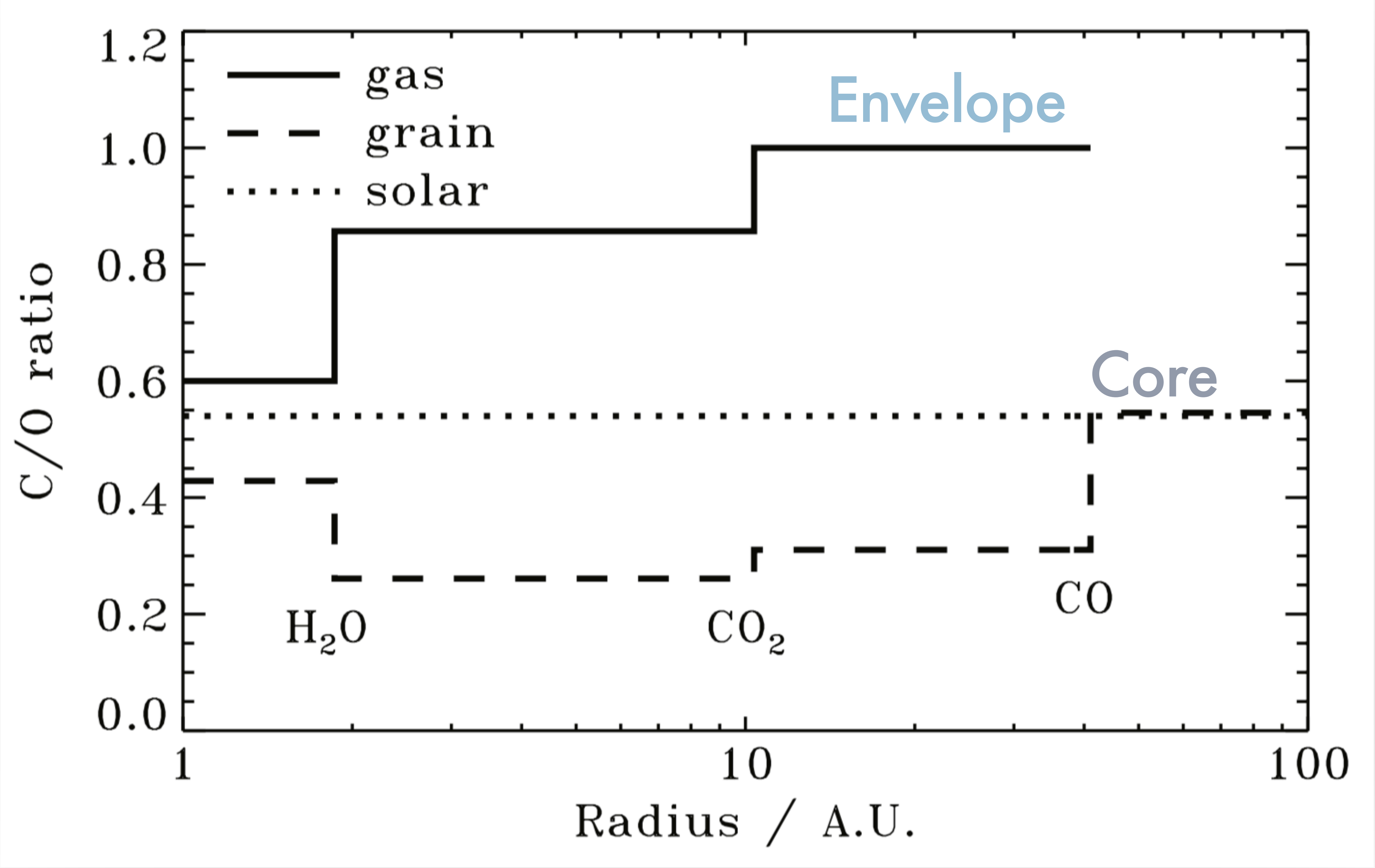
II. RADIAL CHEMICAL STRUCTURE

Many open questions… but just a few to focus on:

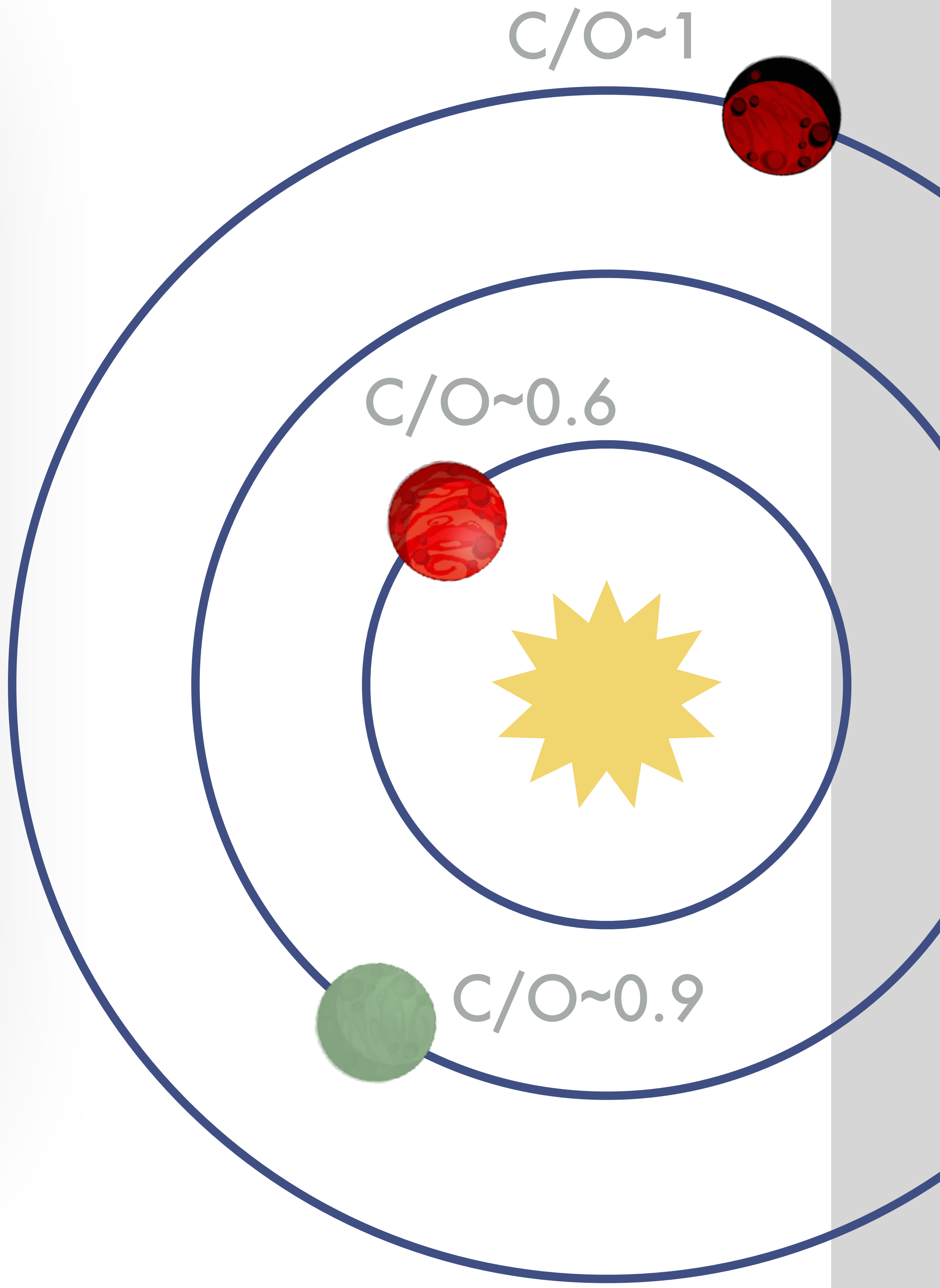
1. How do observed molecules translate into planet compositions? Can we link abundance ratios (C/O), or perhaps even bulk abundances to planet outcomes?
2. What do isotopic ratios tell us about the history of protoplanetary chemistry?
3. What can we learn from solid-phase? (Will come back later)

ABUNDANCES AND RATIOS

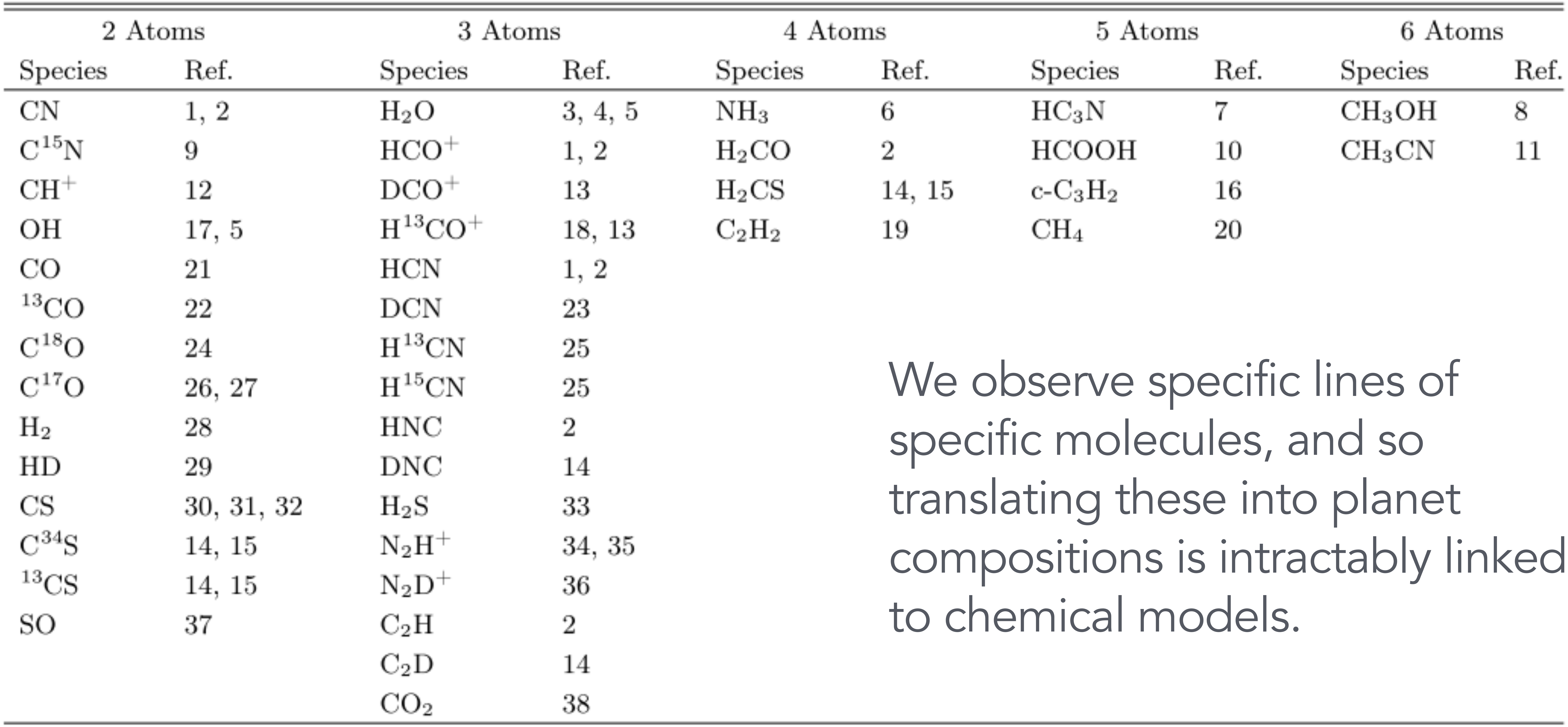
C/O has been an exciting topic as it is measurable in some exoplanet atmospheres. C/O expected to vary across disks due to chemically varying conditions.



Öberg, Murray-Clay and Bergin 2011



WE HAVE A NARROW WINDOW IN TO DISK CHEMISTRY



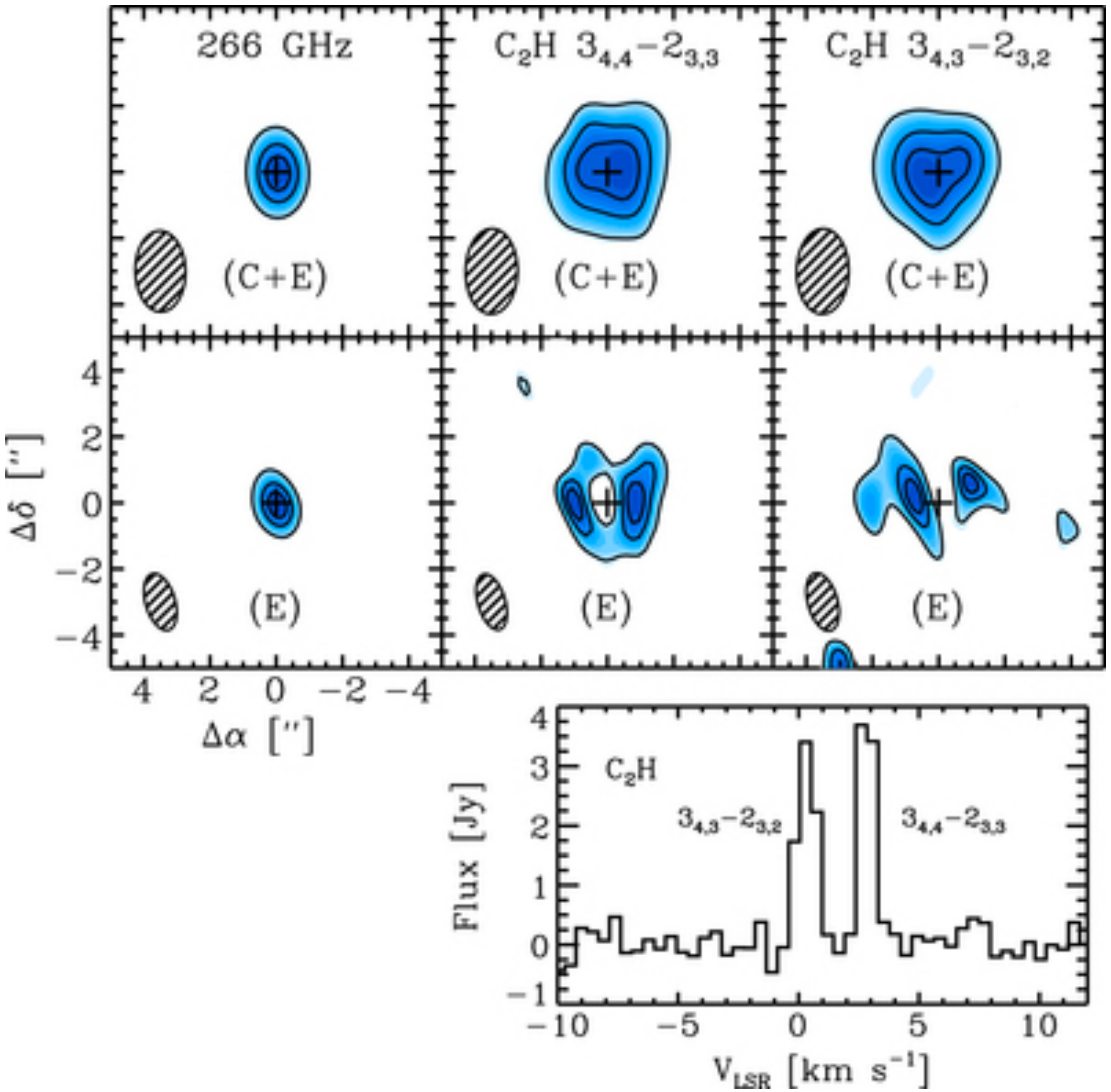
2 Atoms		3 Atoms		4 Atoms		5 Atoms		6 Atoms	
Species	Ref.	Species	Ref.	Species	Ref.	Species	Ref.	Species	Ref.
CN	1, 2	H_2O	3, 4, 5	NH_3	6	HC_3N	7	CH_3OH	8
$C^{15}N$	9	HCO^+	1, 2	H_2CO	2	HCOOH	10	CH_3CN	11
CH^+	12	DCO^+	13	H_2CS	14, 15	$c\text{-}C_3H_2$	16		
OH	17, 5	$H^{13}CO^+$	18, 13	C_2H_2	19	CH_4	20		
CO	21	HCN	1, 2						
^{13}CO	22	DCN	23						
$C^{18}O$	24	$H^{13}CN$	25						
$C^{17}O$	26, 27	$H^{15}CN$	25						
H_2	28	HNC	2						
HD	29	DNC	14						
CS	30, 31, 32	H_2S	33						
$C^{34}S$	14, 15	N_2H^+	34, 35						
^{13}CS	14, 15	N_2D^+	36						
SO	37	C_2H	2						
		C_2D	14						
		CO_2	38						

We observe specific lines of specific molecules, and so translating these into planet compositions is intractably linked to chemical models.

McGuire 2021, ApJS

MEASURING C/O IN DISKS: HYDROCARBONS

Hydrocarbons like C_2H and c-C_3H_2 are highly sensitive to C/O in the gas (Bergin et al. 2016). They were sufficiently bright that a ring of C_2H was even imaged prior to ALMA with the SMA (Kastner+2015)



C/O: BACKGROUND

- So what C/O is inferred?
- Recent results based upon observations of C_2H and c-C_3H_2 are finding disks on average have very high (>0.8) C/O ratios in their gas (Bergin+16, Cleeves+18, Miotello+19, Bosman+20,21, Alarcon+21).
- Well elevated above the elemental solar C/O value of 0.56.
- Even ~2 inside of the CO snowline (Bosman+21)

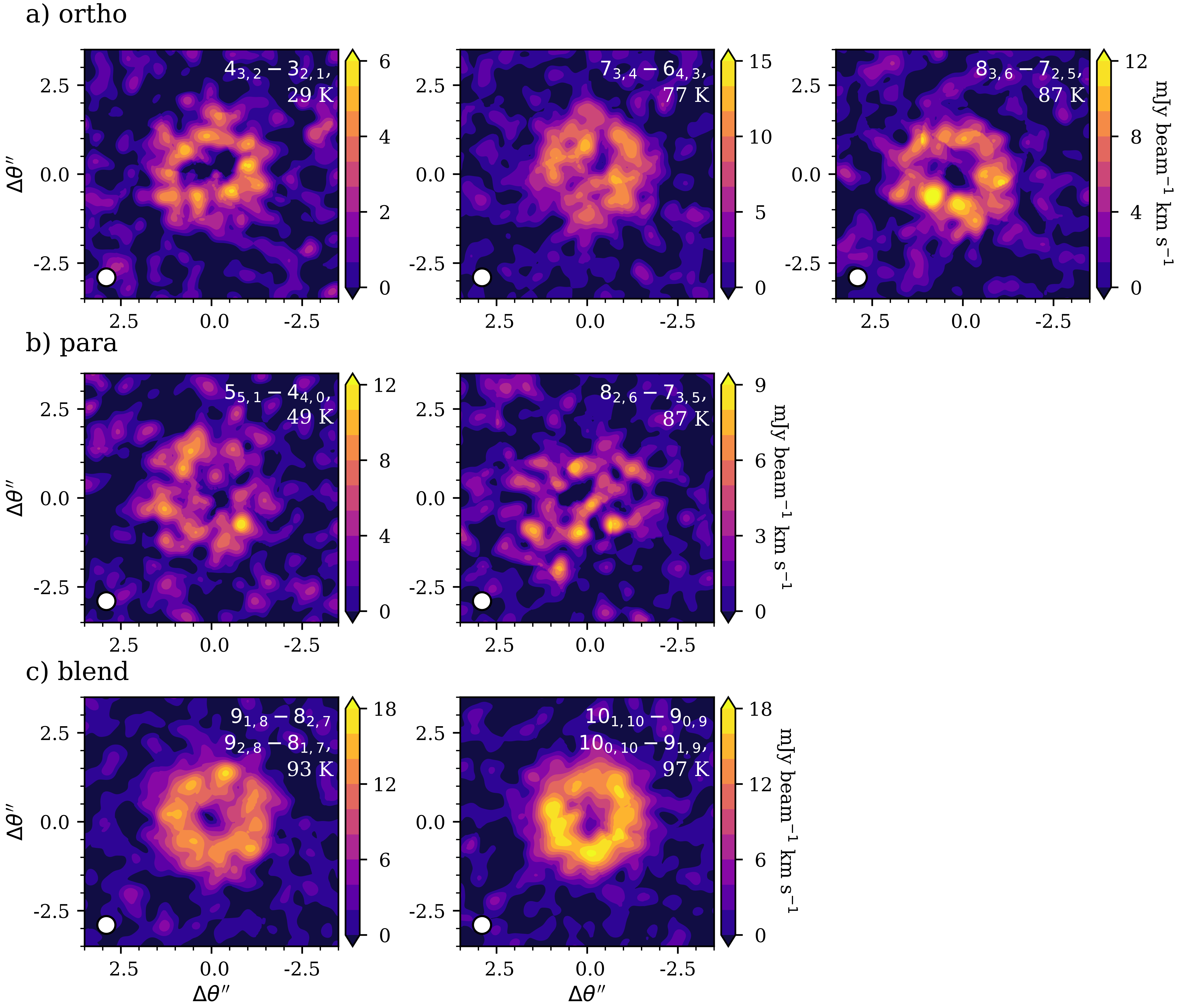
C/O: TW HYA c-C_3H_2

ALMA
TW HYA
ROSETTA
PROJECT

- Still observationally unclear what values of C/O are **typical** and **where** we measure the C/O ratio.
- As part of the TW Hya Rosetta Project, we obtained 7 lines of the sister molecule C_3H_2 (3 ortho, 2 para, 2 blends). Lines span upper state energies from 30 to 100 K! (Cleeves+21)
- Question: what layer do the hydrocarbons emit from?

C/O: TW HYA c-C_3H_2

ALMA
TW HYA
ROSETTA
PROJECT



Ortho

Para

Blend

C/O: TW HYA *c*-C_3H_2 RESULTS

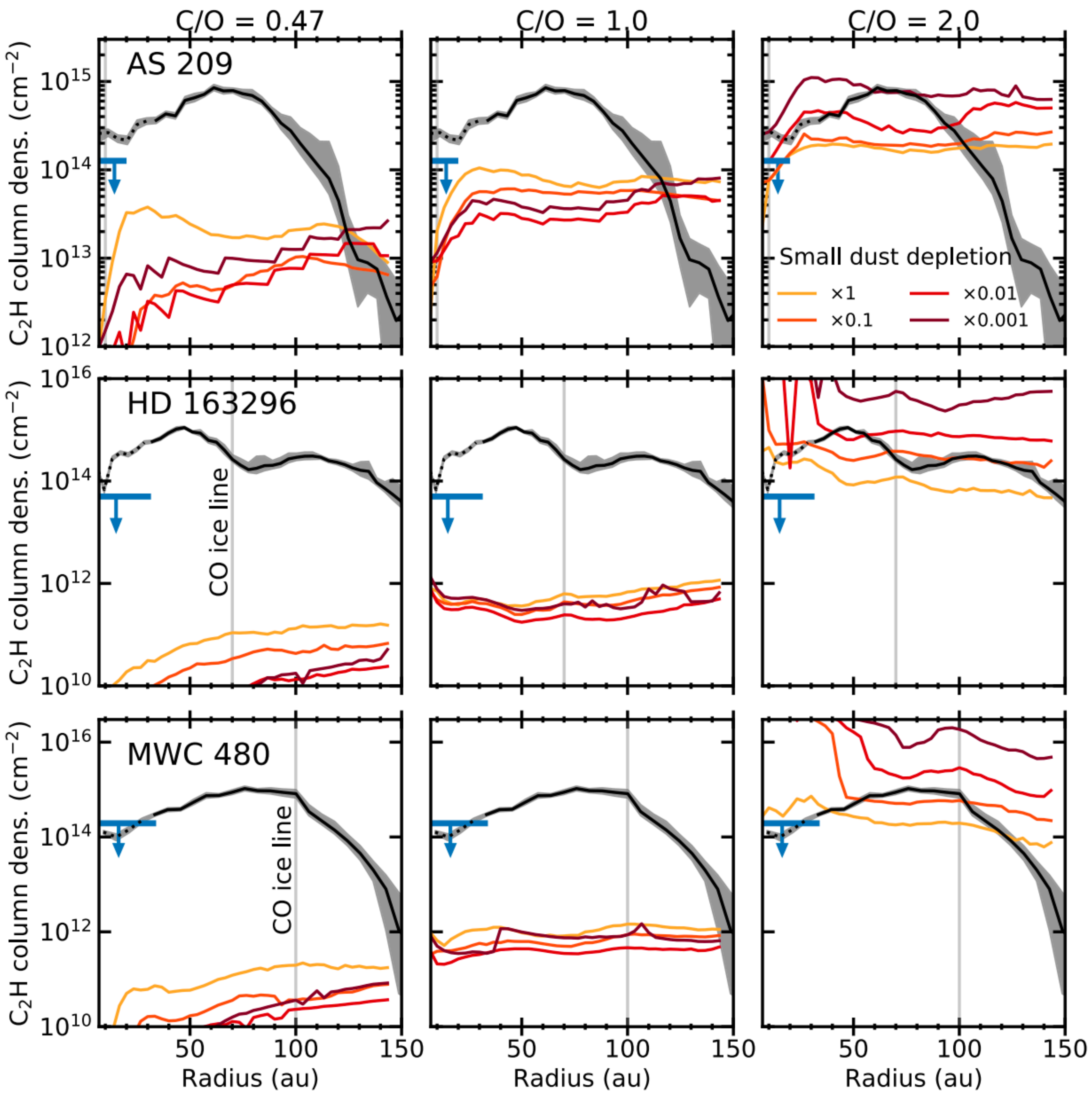
ALMA
TW HYA
ROSETTA
PROJECT

Findings of Cleeves+21 using slab models and non-LTE RT:

- Found C_3H_2 elevated *above* the midplane ($z/r > 0.2$, or >2x scale height)
- $o/p[C_3H_2] = 3$
- Emission thermalized ($n_{crit} \sim 1e7\ cm^{-3}$). Dense gas is present in the warm molecular layer between 25 and ~100 au!
- Abundance relative to C_2H matches chemical model predictions, *points to bottom up chemistry rather than top down.*

C/O RADIALLY

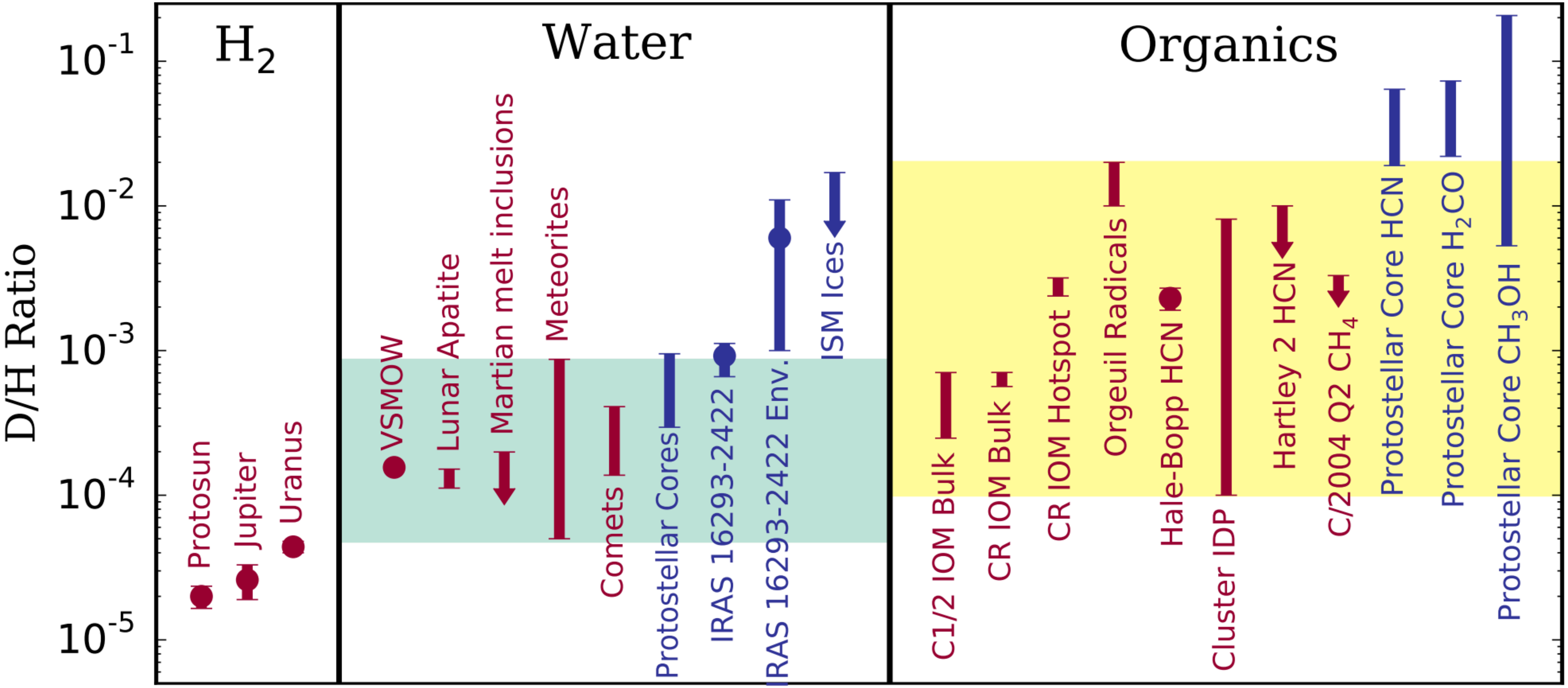
- Using source specific models, Bosman+2021 fit the radial behavior for three of the 5 MAPS disks.
- C/O preferentially high (2), though likely a single C/O value (bulk) is not able to reproduce AS 209 or MWC 480 (evidence of spatial C and O redistribution?)
- But these have been mainly detailed efforts around massive disks… what is typical? (e.g., Bergner+19, Miotello+19)



CONNECTING TO THE ISOTOPIC RECORD

- Where did the molecules that seeded our early planetary bodies *originally* form?
- Did we inherit anything from our star forming region or was the chemistry reset during our formation?
- **Isotopes** can 'tag' molecules with information about their formation environment (e.g., C, N, O, H).
- For example: Deuterium can become chemically enhanced, when molecules form at low (<50 K) temperatures. *Spatial gradients expected in disks.*

DEUTERATION IN THE SOLAR SYSTEM

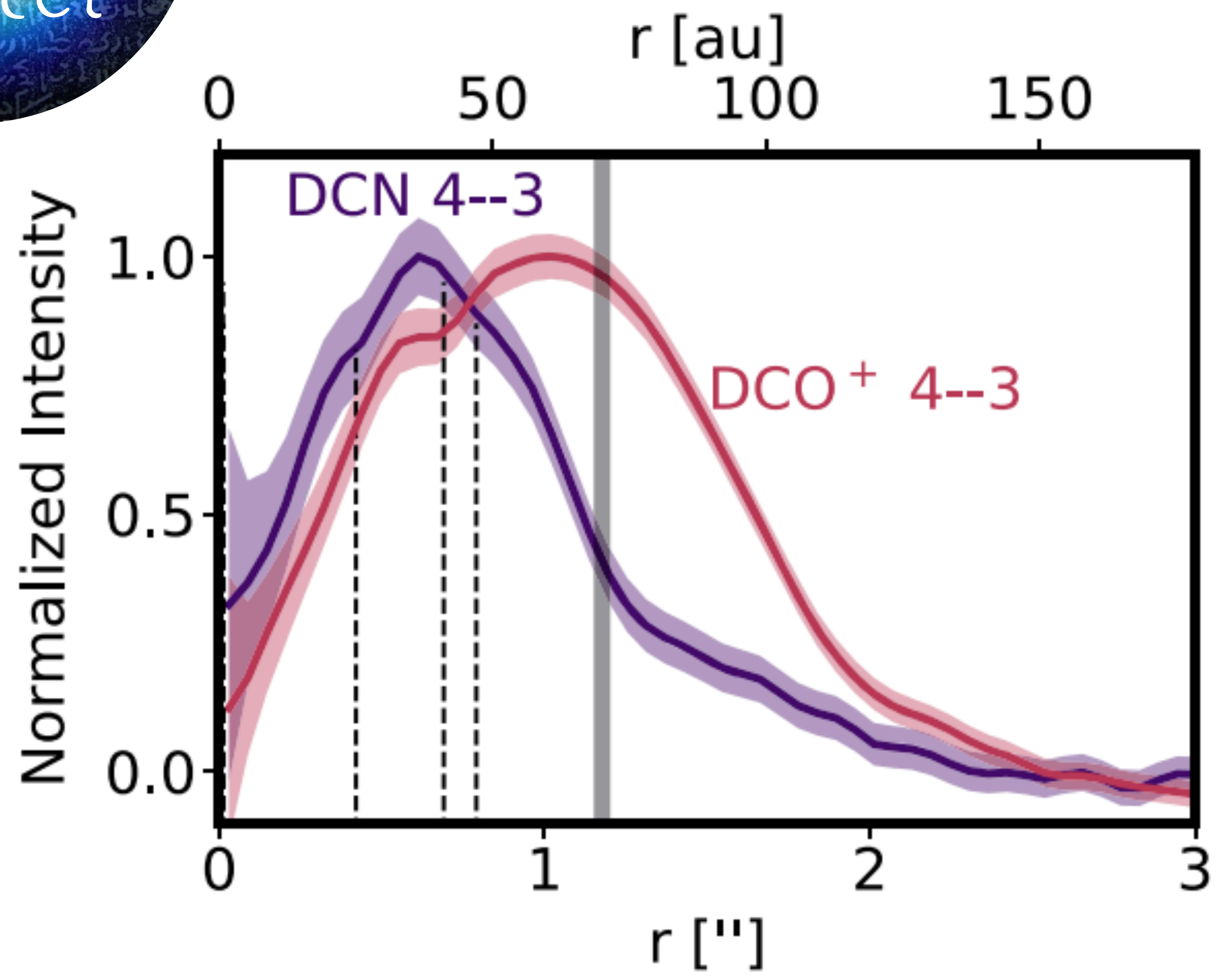


Cleeves et al. 2016

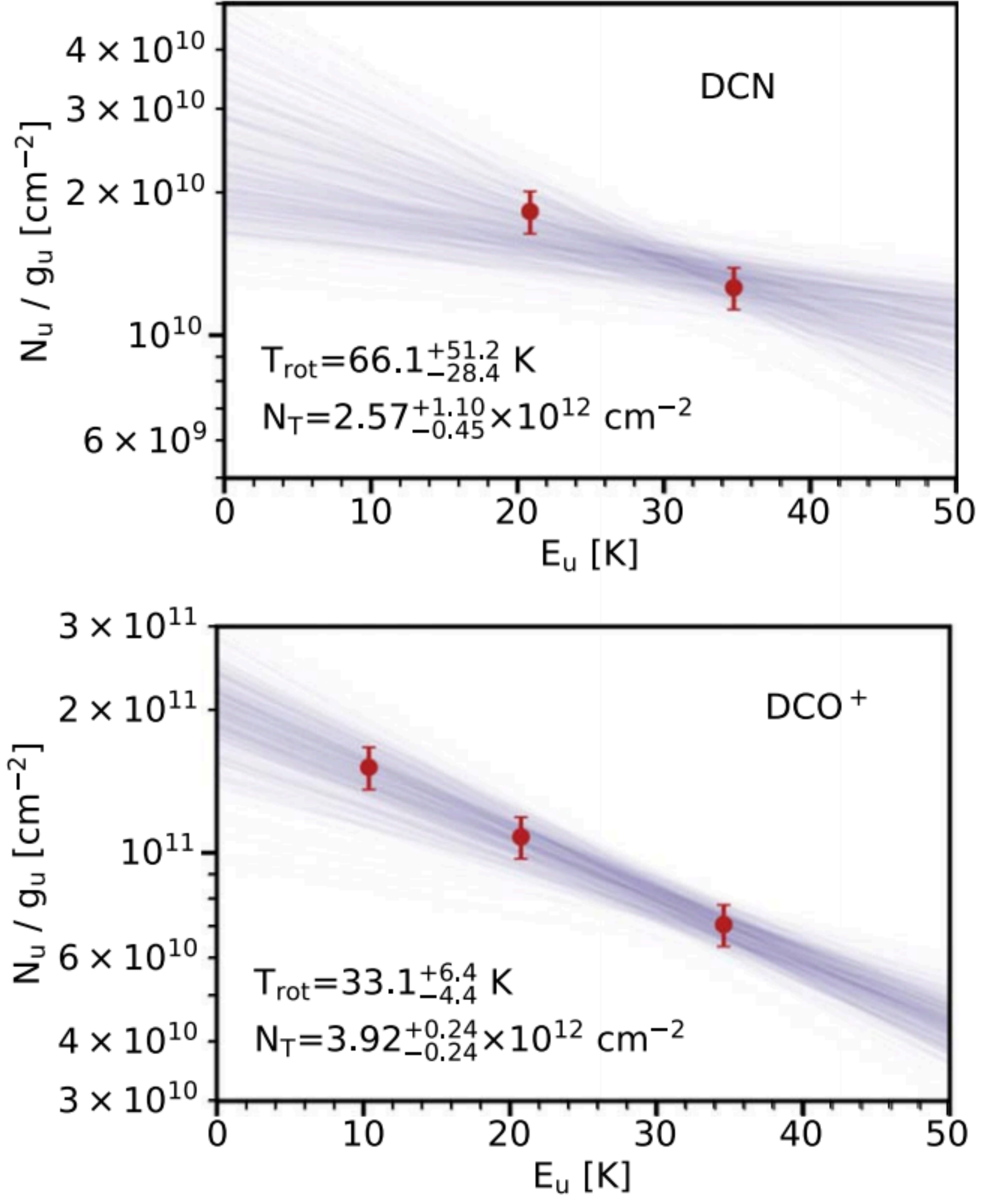
WARM DEUTERIUM CHEMISTRY?

ALMA TW HYA ROSETTA PROJECT

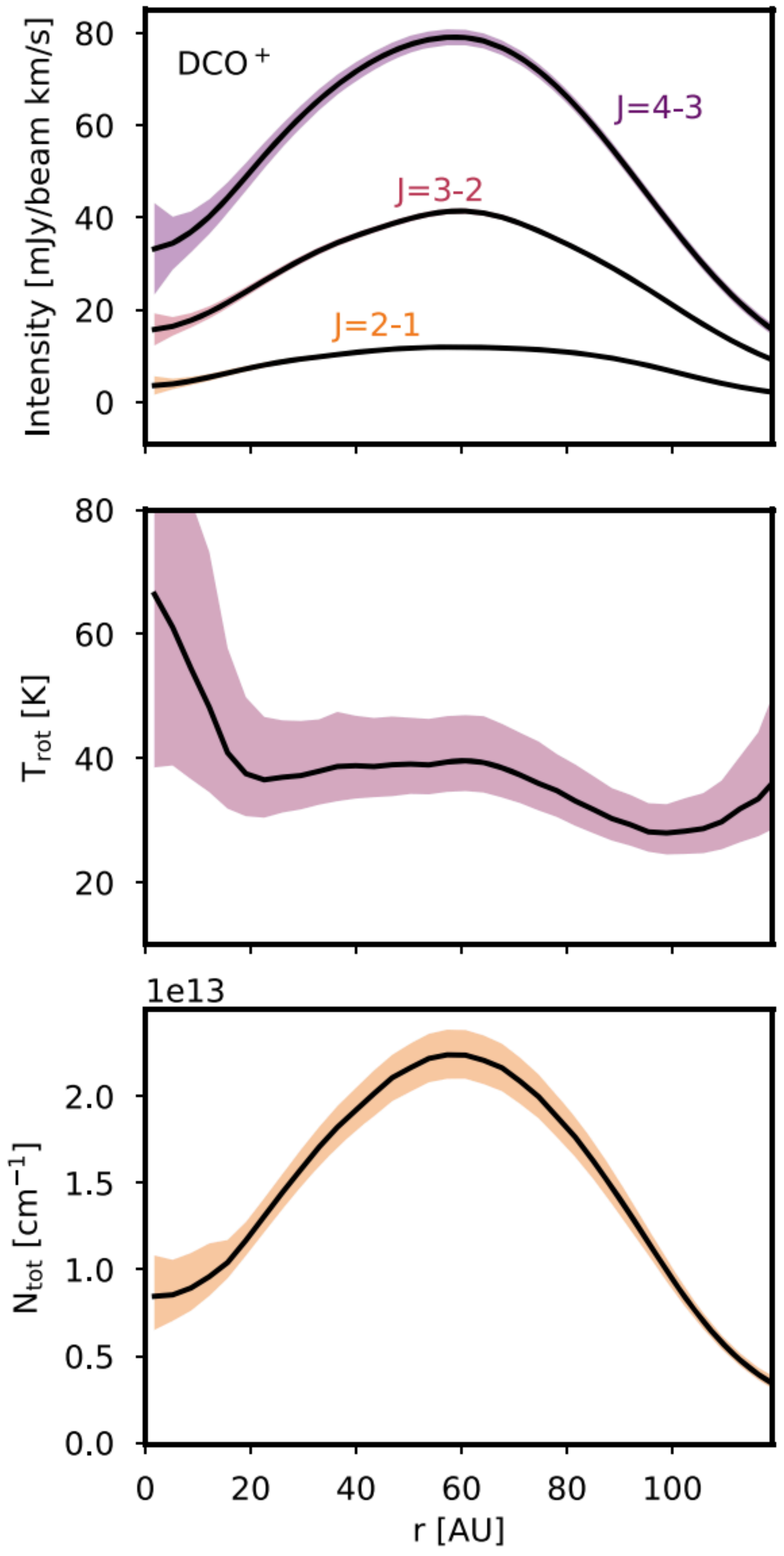
Radial Profile:



Rotational Diagram:

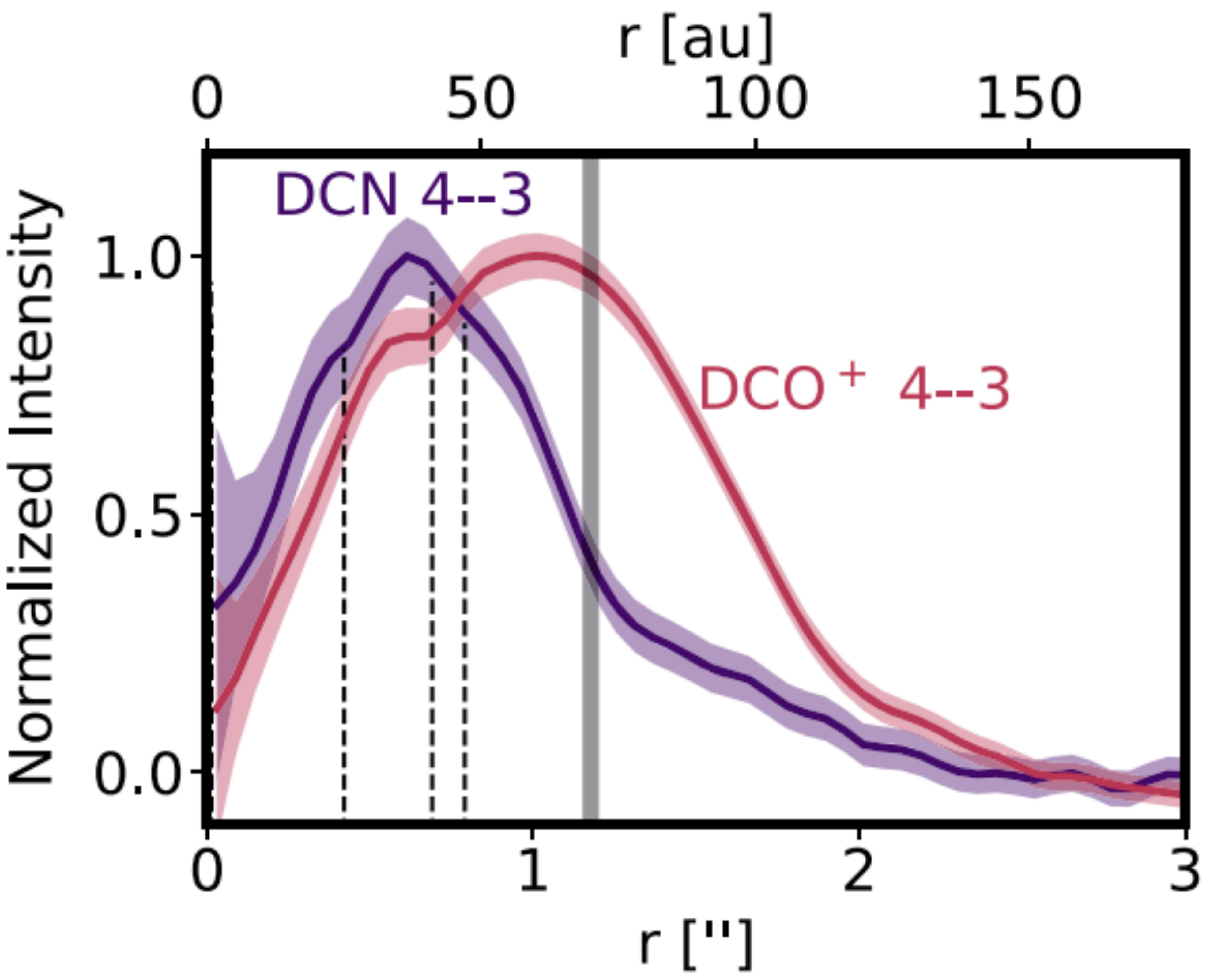


Resolved Rot. Diag:



Oberg and the Rosetta Collaboration, AJ 2021

OBSERVABLE DISK DEUTERIUM CHEMISTRY



Take Aways:

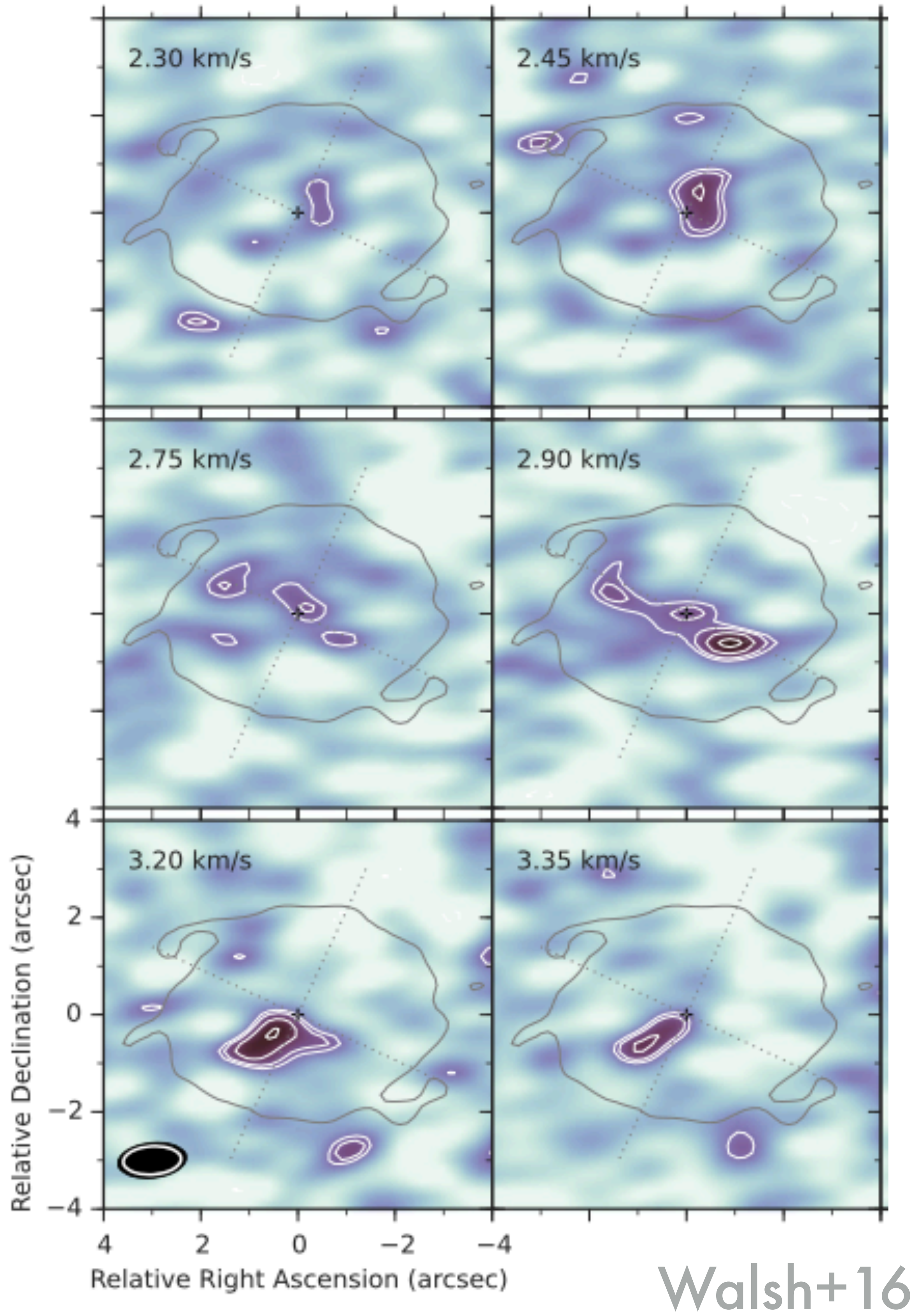
- ❖Not clearly seeing "cold deuteration" at work in this disk.
- ❖If bodies are forming in the cold mid-plane presently, would have to inherit any D-enrichments.
- ❖We're also not seeing D-fractionation in the inner disk (<25au), i.e., solar system scales?

See also Cataldi+21.

THE SEEDS OF ORGANICS

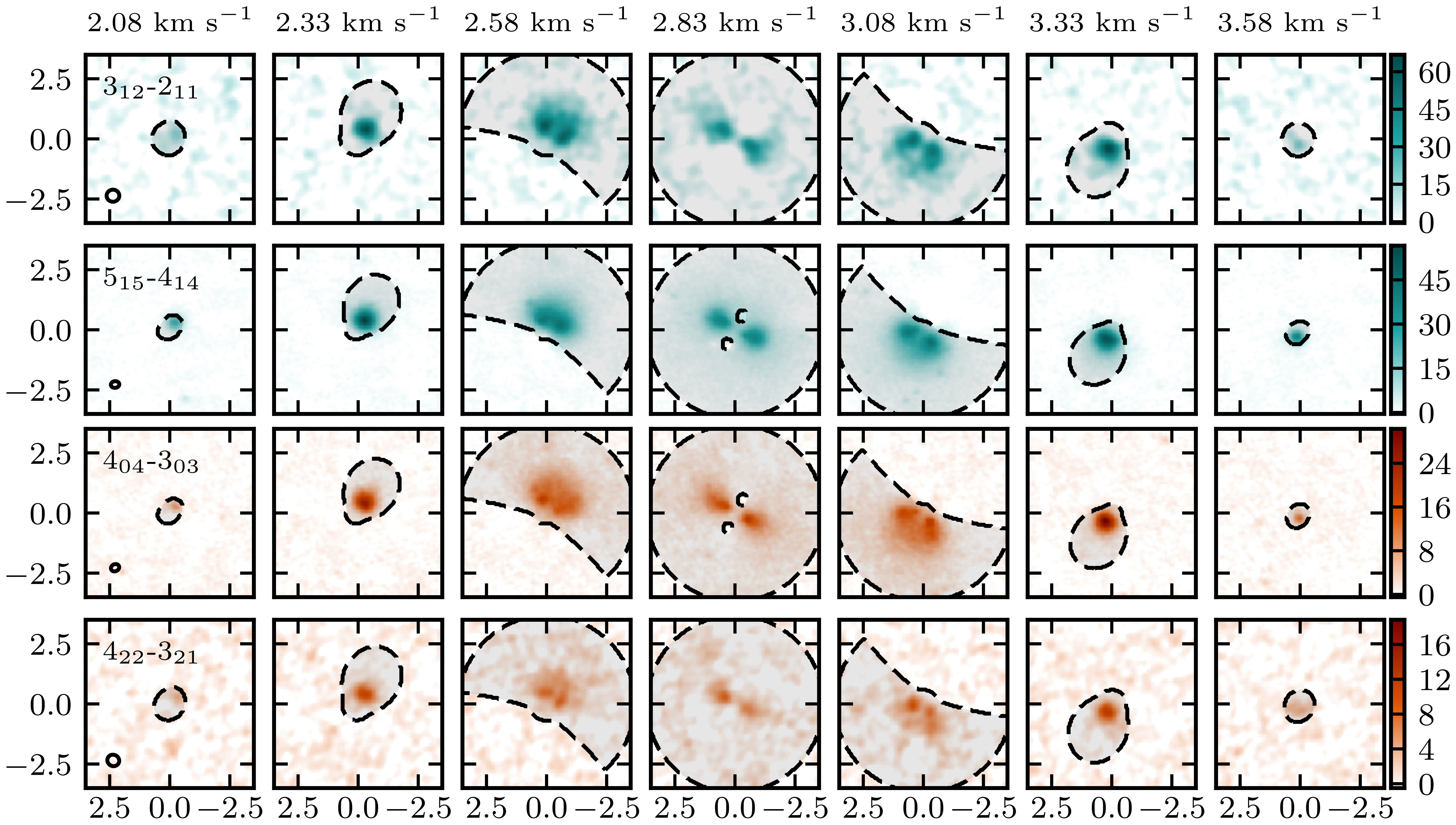
ALMA
TW HYA
ROSETTA
PROJECT

- Organic detections in disks are rare (hard! integrations of ~10 hours per source!)
- H_2CO is easier to detect and is a good organic starting point
- Questions about its formation - gas vs grain surface (see Loomis et al 2015)
- Jeroen Terwisscha van Scheltinga combined Rosetta + Archival ALMA data to pinpoint H_2CO origins.



Walsh+16

THE SEEDS OF ORGANICS



Note - Only showing a subset of the data.

THE SEEDS OF ORGANICS

ALMA
TW HYA
ROSETTA
PROJECT

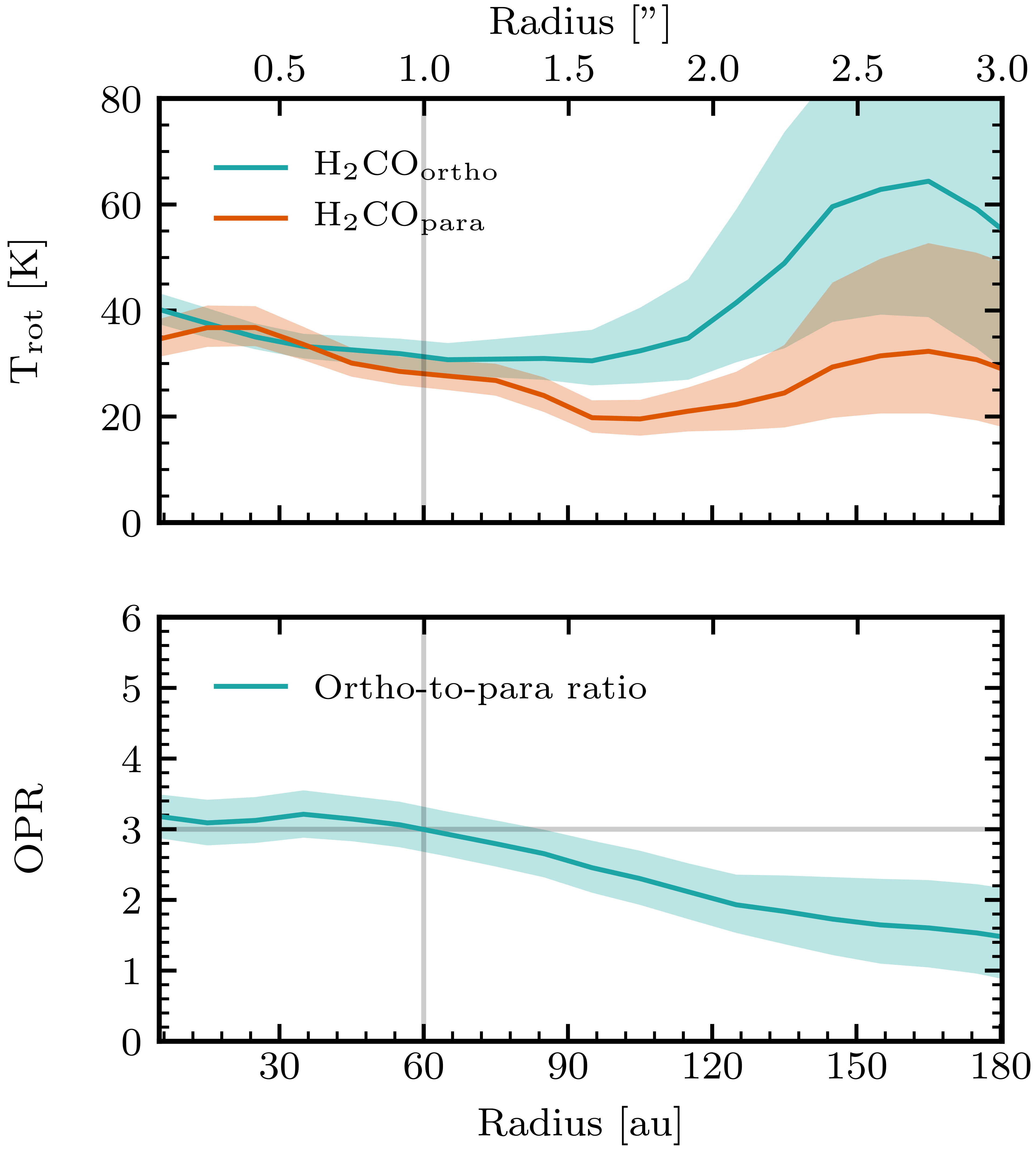
Temperature gradients (different?) in ortho and para.

Ortho/para column density ratio also changes with radius!

This hints that H_2CO is being formed in the gas phase (gas-grain symbiosis) in the disk surface. Experiments of o/p for water formation suggest o/p goes to three when formed as ice (Hama+18).

Rules out inheritance for observed H_2CO, but mid-plane could retain primordial ice.

See also Guzman+21 for the distributions of small organics in MAPS.



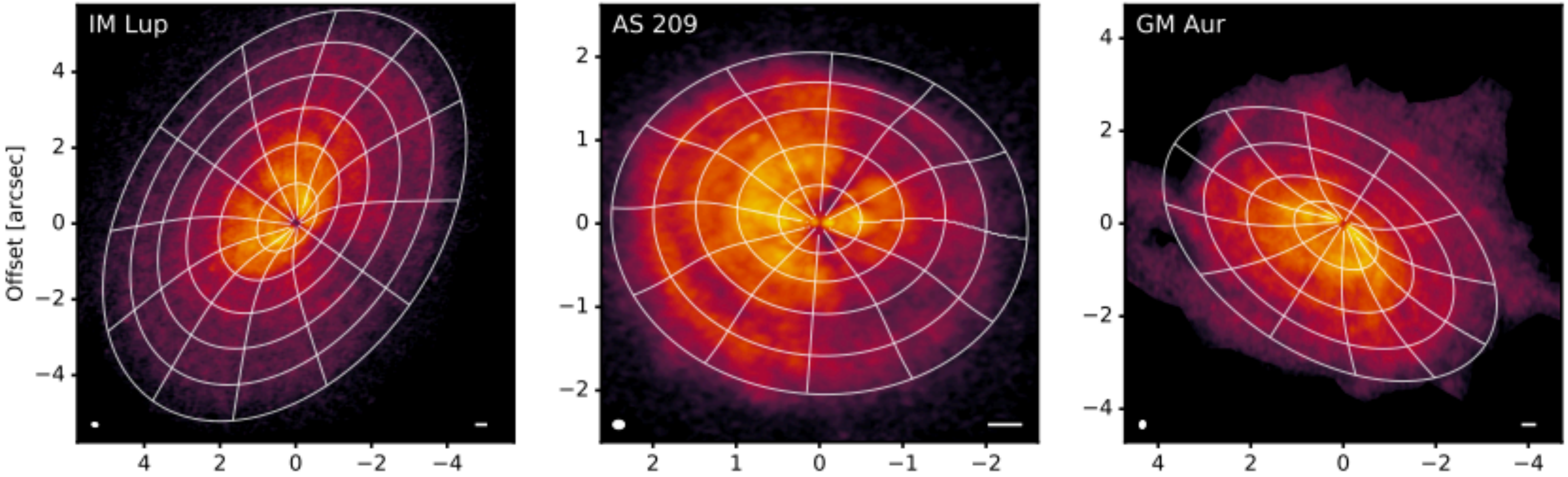
III. PHYSICAL CONDITIONS TRACED BY GAS

- Molecules are sensitive probes of disk physics. Presence/absence can tell you about the local conditions of the gas (radicals tracing UV field, ions for X-rays/CRs, etc.).
- Their emission properties (LTE or not, line ratios) can probe the densities and temperatures of the gas (see e.g., Guilloteau+16, Dutrey+17, Teague+17, 21, Loomis+18, Ruiz-Rodriguez+21)

Satoshi Kambayashi

III. PHYSICAL CONDITIONS TRACED BY GAS

For example, new constraints on temperature structure both empirically (with thick lines, deprojected surfaces, and channel maps) and using forward modeling.

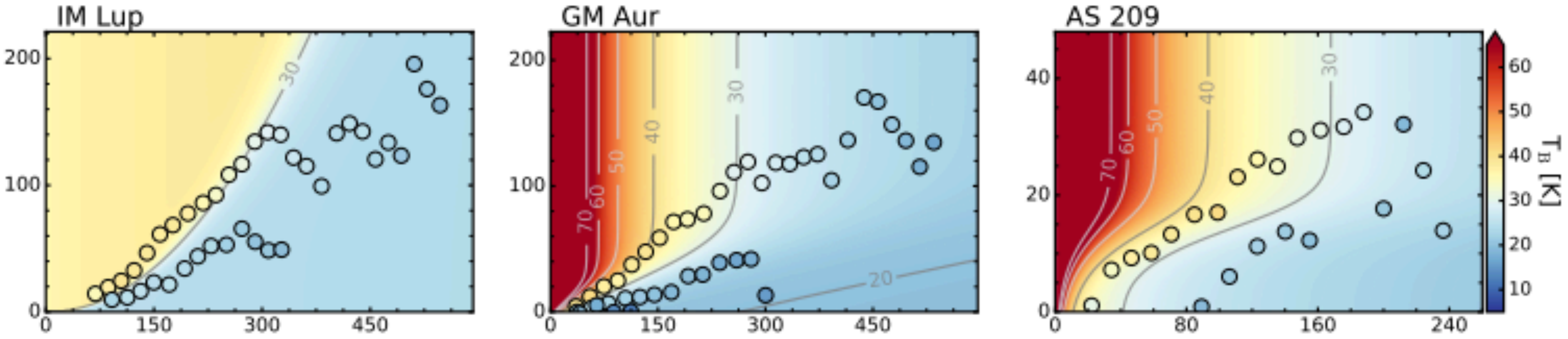


Law et al. 2021, MAPS IV

III. PHYSICAL CONDITIONS TRACED BY GAS

For example, new constraints on temperature structure both empirically (with thick lines, deprojected surfaces, and channel maps) and using forward modeling.

Derived Temperature Structures

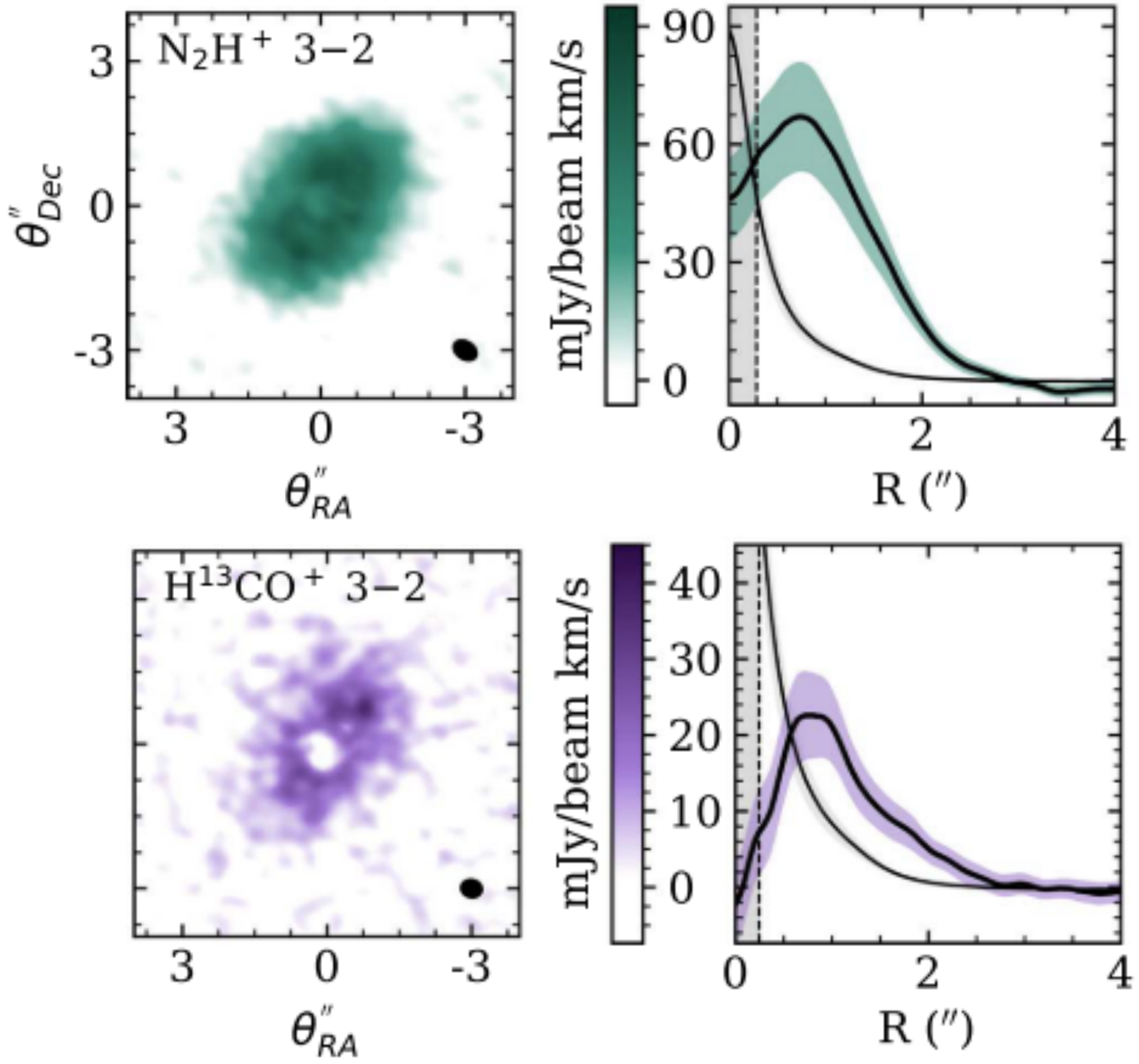


Law et al. 2021, MAPS IV

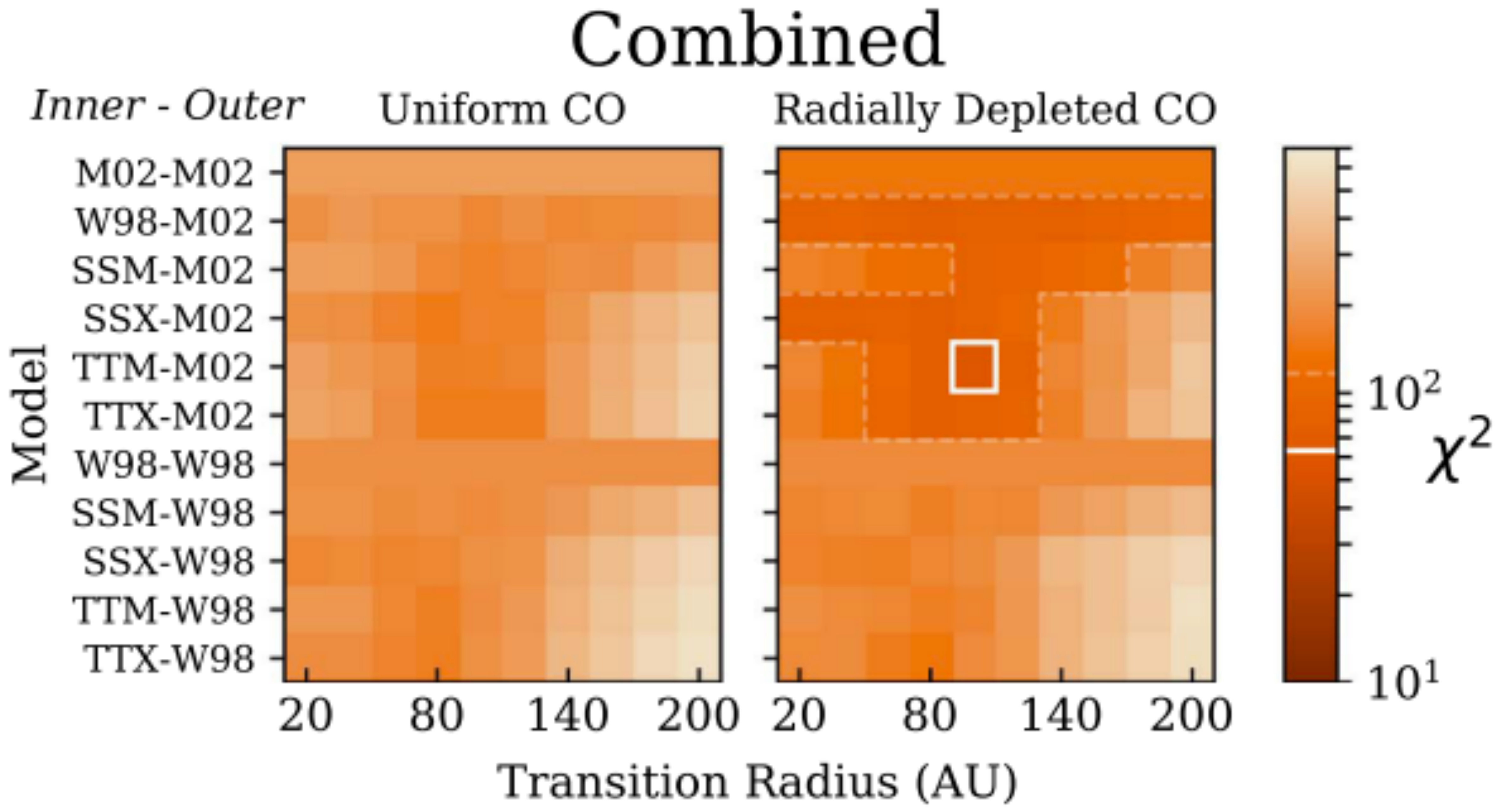
See also Calahan et al. 2020, 2021 for forward-modeled 2D temperature structures of TW Hya and HD163296.

III. PHYSICAL CONDITIONS TRACED BY GAS

New resolved ionization constraints for IM Lup (Seifert+21). Forward modeled from chemical simulations with different CR ionization rates.



Found that a single CR ionization rate could not describe the molecular ion data. Needed a different inner vs. outer value (with ~100 au as the transition).



We’ve learned a lot, but mostly to only a few sources…

How do we move forward?

Image Credit: University of Copenhagen/Lars Buchhave, W. Garnier, ALMA (ESO/NAOJ/NRAO)

I. GAS GAPS GOING FORWARD

- What is “enough” evidence to say there is a gap in gas?
- Multiple species with a deficit?
- Or do we also want to verify with chemical models? (i.e., predictions of some enhanced species)
- Or do we need to scrap chemistry and rely on local pressure measurements (but getting more observationally expensive)

II. PLANET FORMING CHEMISTRY

- Want to observe the planet-forming midplane, but seeing a lot of our tracers are mainly coming from the warm molecular layer (z/r between 0.1-0.4).
- Partially due to freeze-out and partially due to excitation combined with temperature gradients.
- Do we need more edge on disk studies (see Ruiz-Rodriguez+21)? Or more focus on the inner disk, where freeze-out is not a problem?
- What about the ice? (upcoming NASA SPHEREx and JWST! See also Ballering+21 and our upcoming JWST Cyc1 program!)
- Or do we focus efforts on Herbig disks that are warmer?

II. PLANET FORMING CHEMISTRY

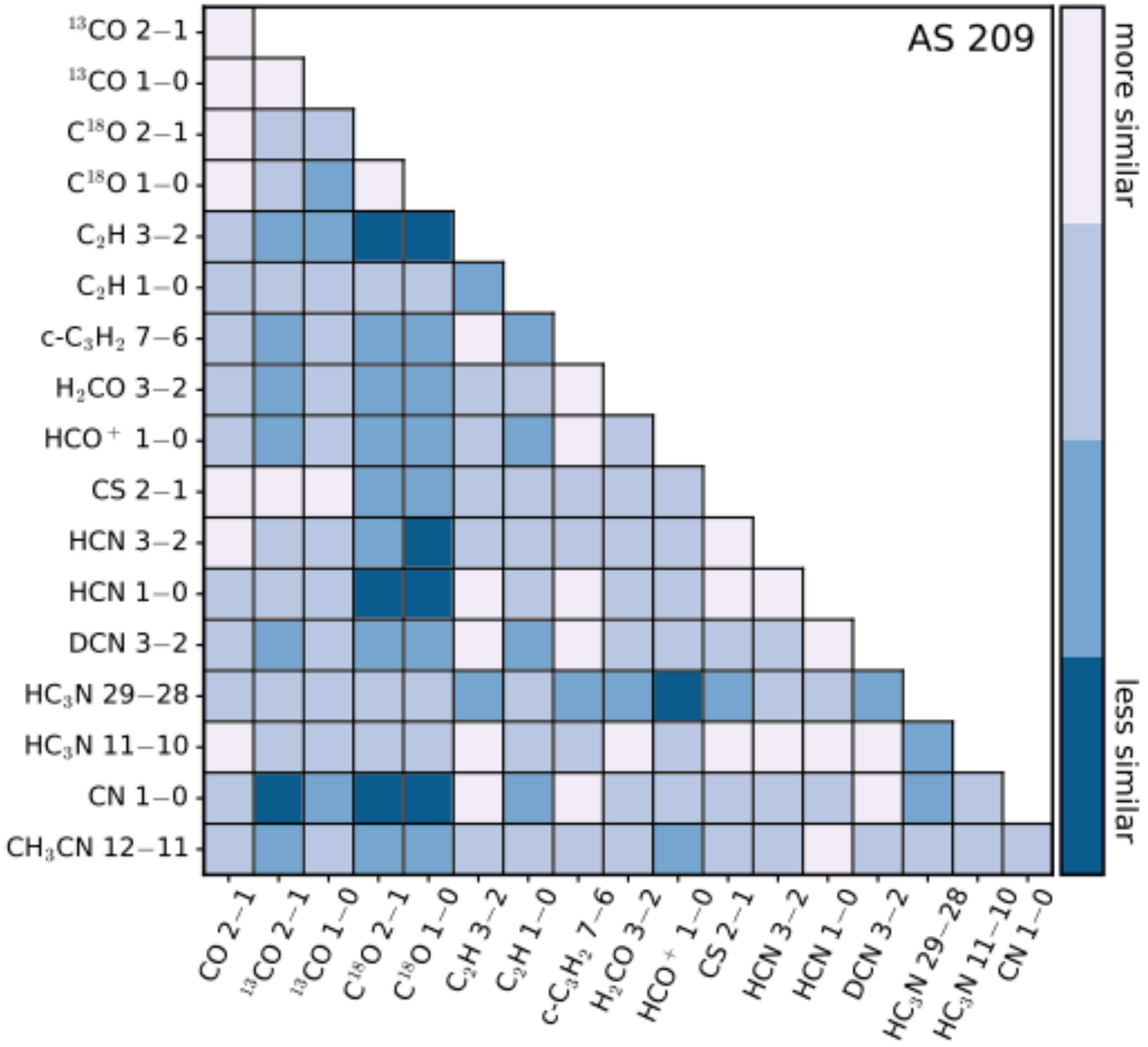
- Regardless, our limited molecular inventory means that a lot of questions we want answers to (C/O, isotope ratios) will be inescapably model dependent.
- Will be easier to determine trends in abundances/ratios like C/O than absolute values.
- For isotope ratios, how closely do the D/H in observed tracers (DCN, DCO^+) link to ratios measured in comets, etc?

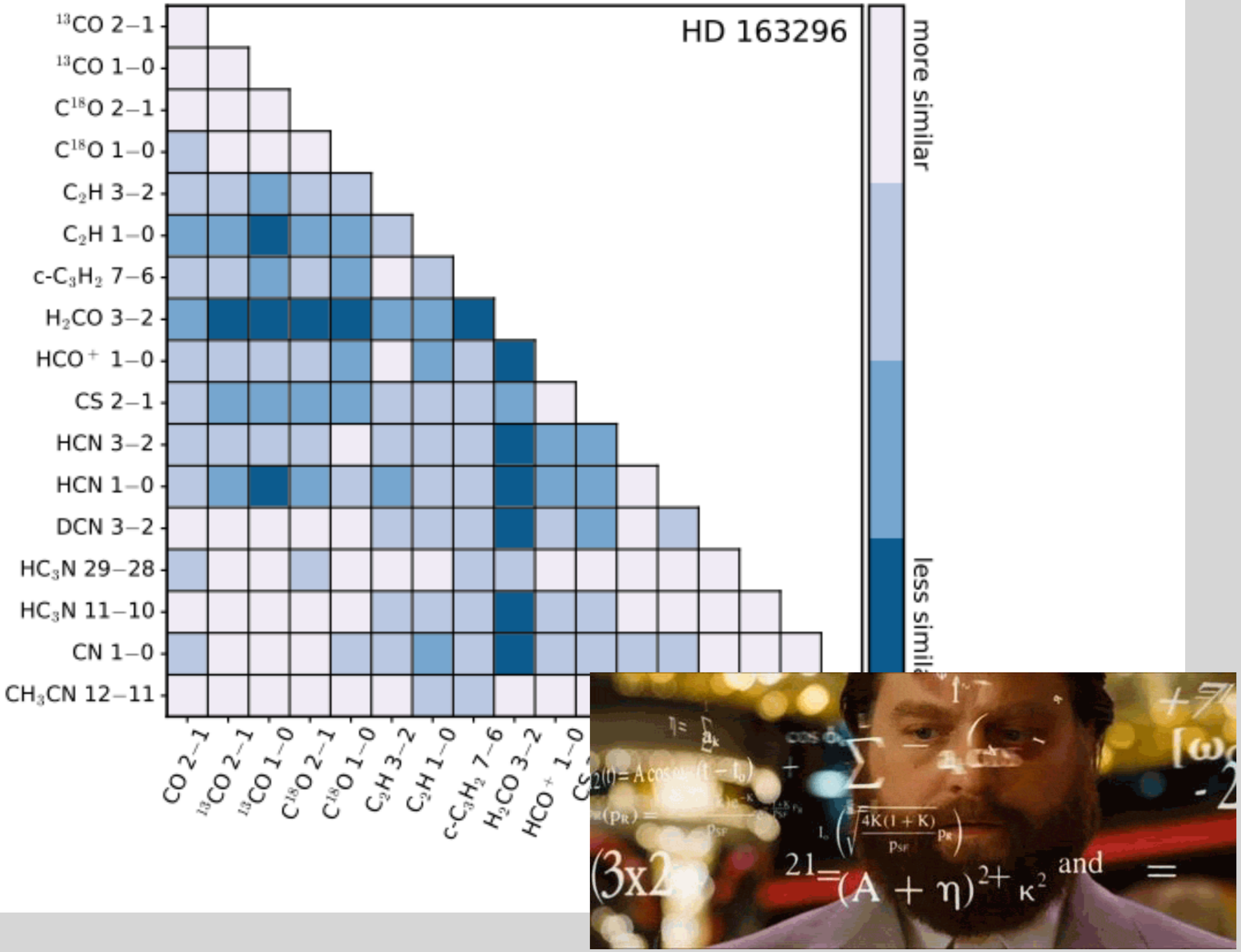
III. PHYSICS THROUGH GAS OBSERVATIONS

- **Chemically constrained physics:** Molecules are complicated *but* more lines are harder to model (and can give better constraints).
- **Emissively constrained physics**: More collision rate data please! Can't assume LTE especially as we go to larger molecules.
- Empirical methods are promising, but need to be tested with forward models. When we measure surface location, temperature, or density, how do the strong gradients present in disks bias these measurements?

BUT WHAT IF WE JUST LET THE DATA SPEAK?

Beautiful analysis in Law+21, MAPS III, comparing radial morphologies.





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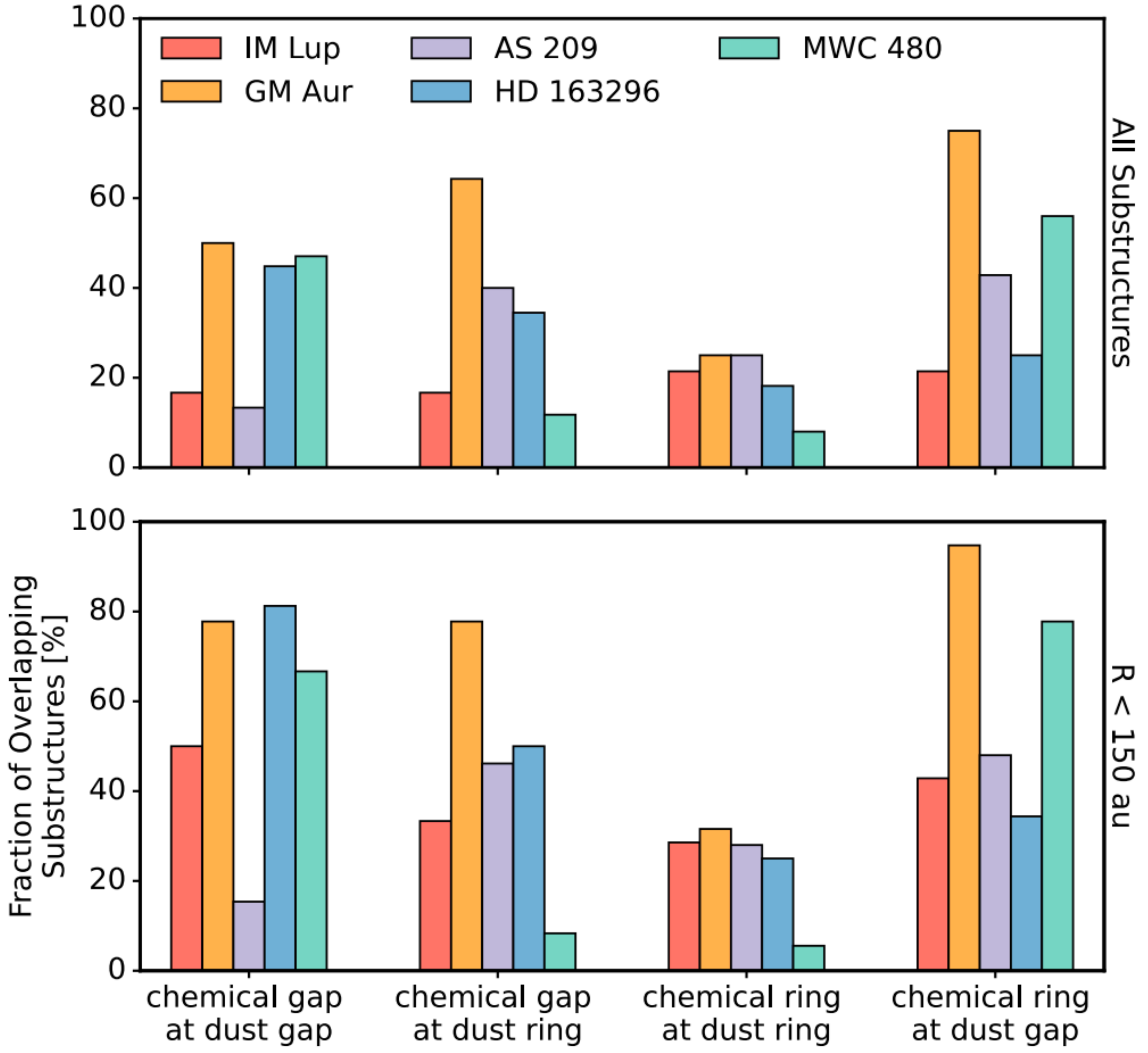
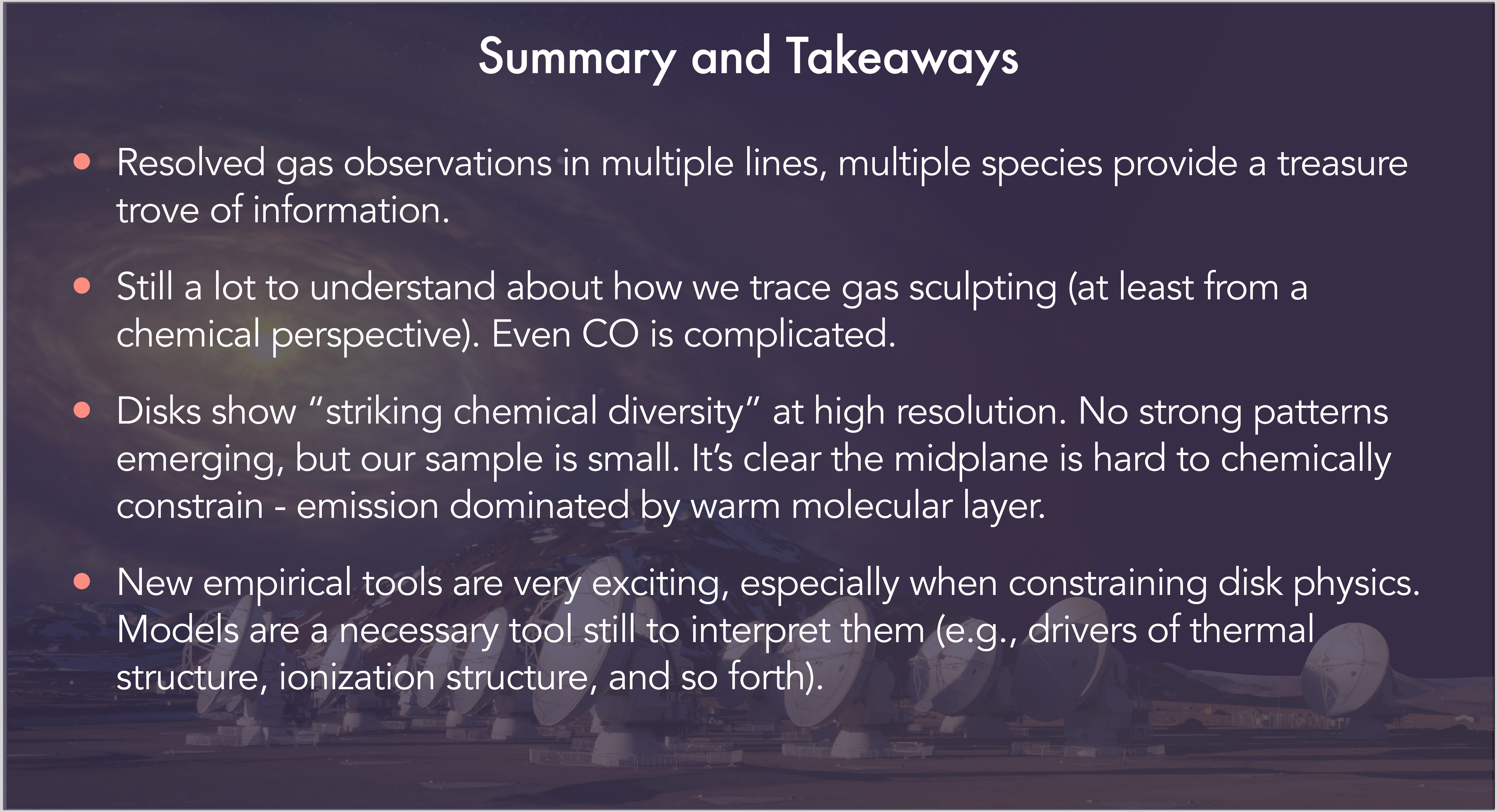


- Maybe some slightly *less* frequent association between co-spatial enhancements in dust and gas?
- No clear relationship with snowlines.

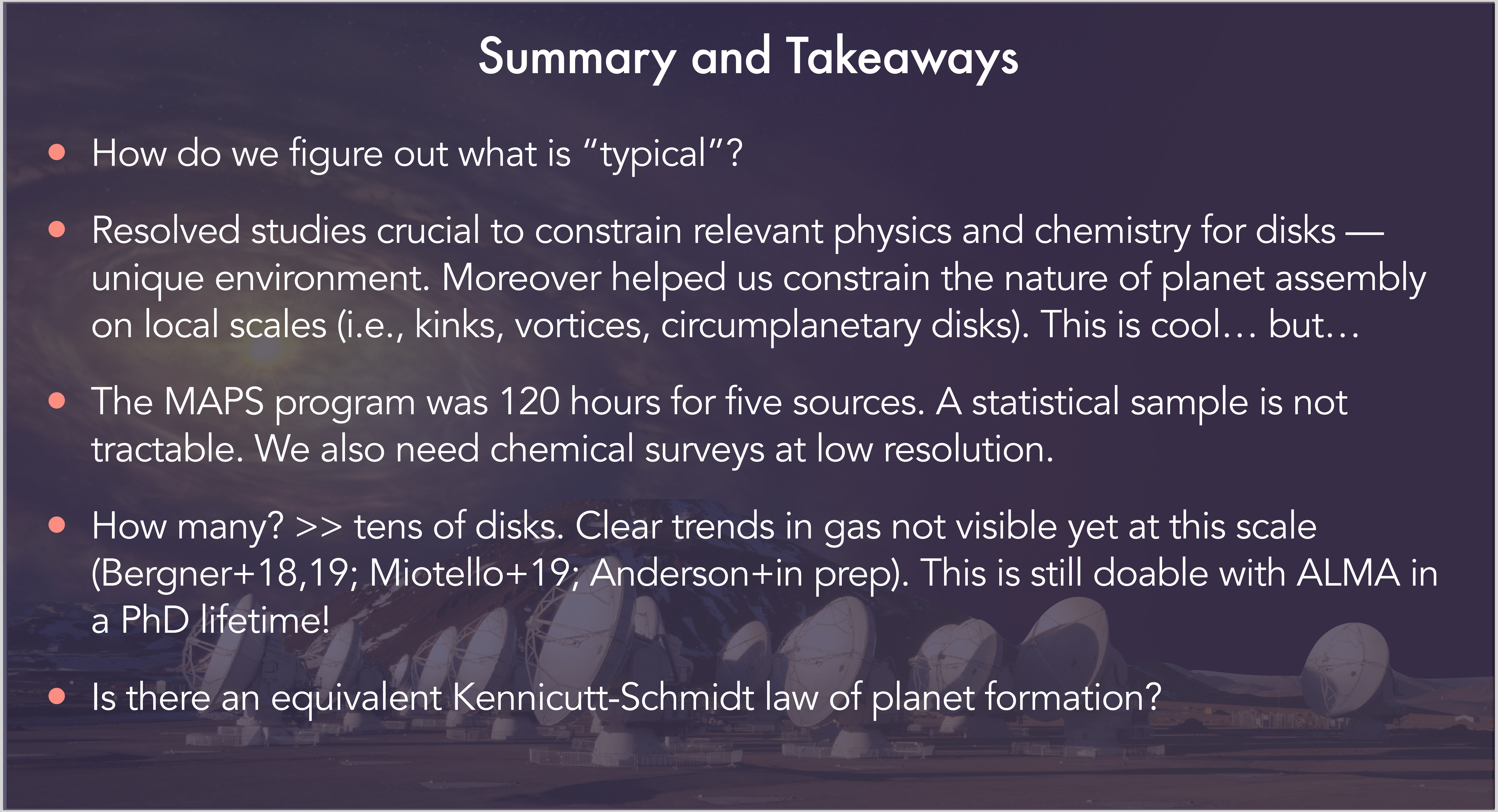
Summary and Takeaways



- Resolved gas observations in multiple lines, multiple species provide a treasure trove of information.
- Still a lot to understand about how we trace gas sculpting (at least from a chemical perspective). Even CO is complicated.
- Disks show “striking chemical diversity” at high resolution. No strong patterns emerging, but our sample is small. It’s clear the midplane is hard to chemically constrain - emission dominated by warm molecular layer.
- New empirical tools are very exciting, especially when constraining disk physics. Models are a necessary tool still to interpret them (e.g., drivers of thermal structure, ionization structure, and so forth).

Image Credit: University of Copenhagen/Lars Buchhave, W. Garnier, ALMA (ESO/NAOJ/NRAO)

Summary and Takeaways



- How do we figure out what is “typical”?
- Resolved studies crucial to constrain relevant physics and chemistry for disks — unique environment. Moreover helped us constrain the nature of planet assembly on local scales (i.e., kinks, vortices, circumplanetary disks). This is cool… but…
- The MAPS program was 120 hours for five sources. A statistical sample is not tractable. We also need chemical surveys at low resolution.
- How many? >> tens of disks. Clear trends in gas not visible yet at this scale (Bergner+18,19; Miotello+19; Anderson+in prep). This is still doable with ALMA in a PhD lifetime!
- Is there an equivalent Kennicutt-Schmidt law of planet formation?

Image Credit: University of Copenhagen/Lars Buchhave, W. Garnier, ALMA (ESO/NAOJ/NRAO)