Chemistry of protoplanetary disks in the ALMA/JWST era

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[Credit: Pat Rawlings / NASA]

IPAG

UGA Université Grenoble Alpes

iram Institut de Radioastronomie Millimétrique

anr agence nationale de la recherche

Outline

1. Why studying protoplanetary disk chemistry?
   => What for? How?

2. Can we probe the chemistry at planet-forming scales?
   => Which facilities? Which chemical tracers?

3. How does the disk's environment impact its chemistry and architecture?
   => Can we detect signatures of inheritance from the prestellar phase and/or chemical reprocessing within the disk?

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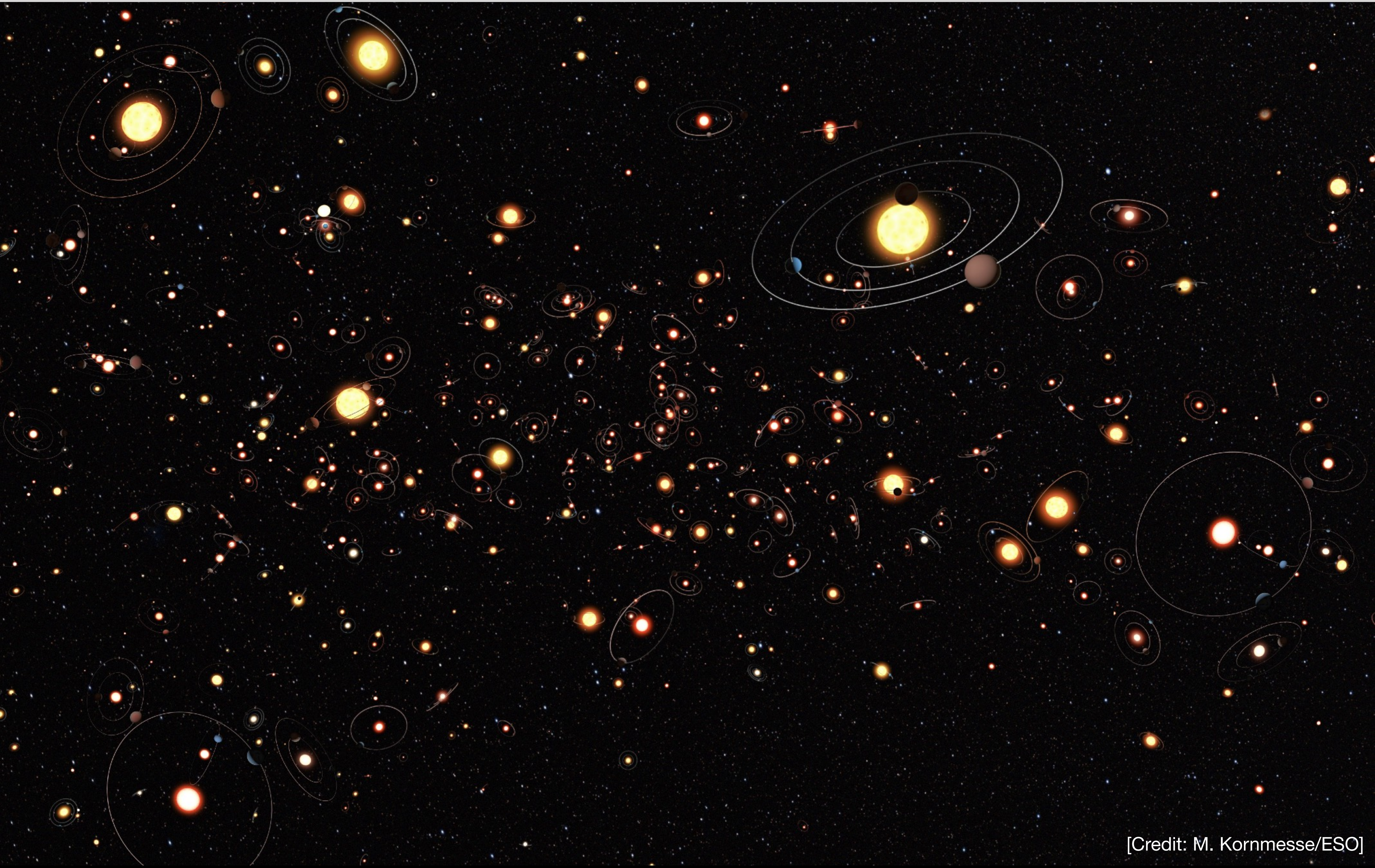
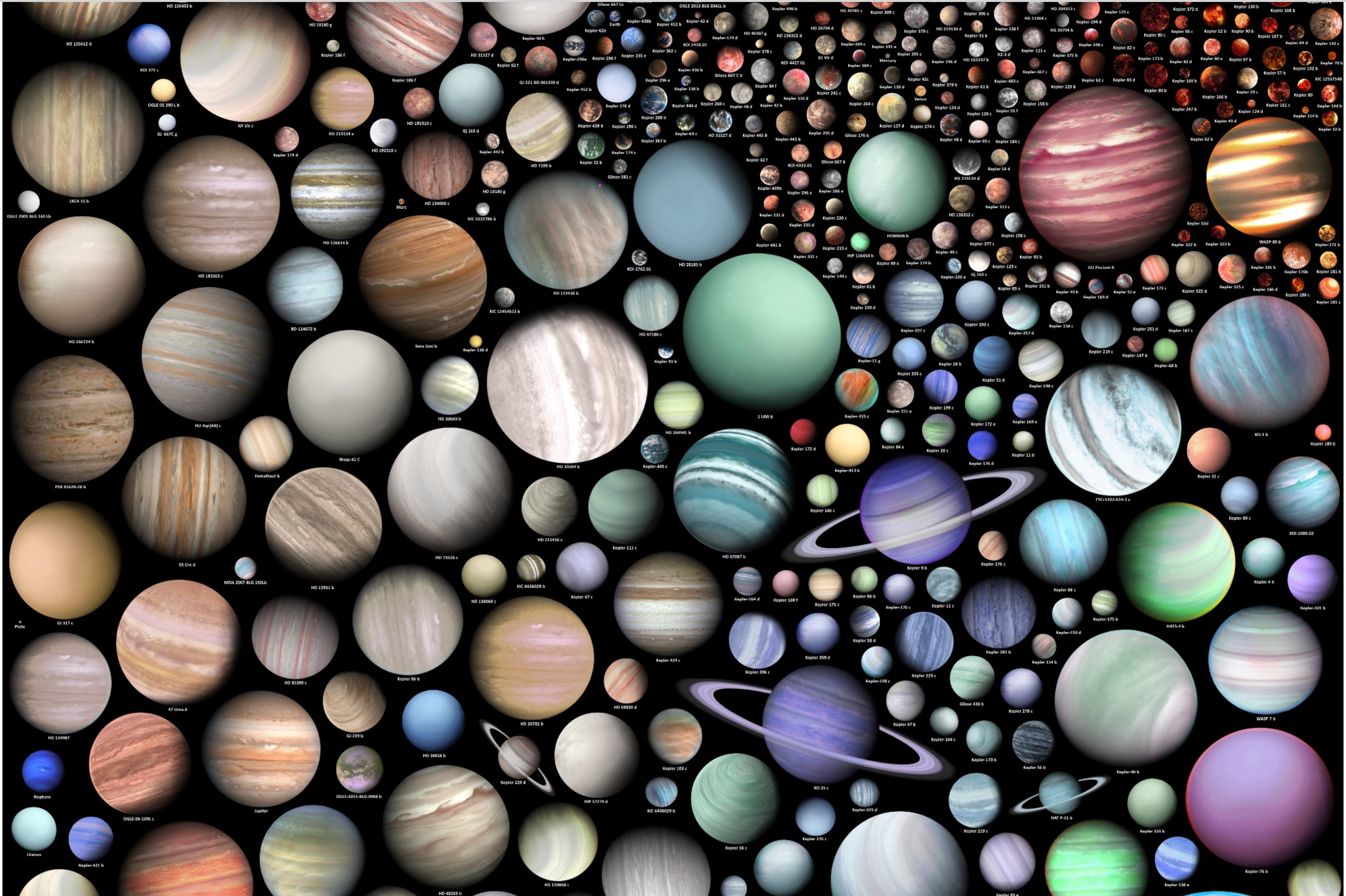
Most stars hosts his own planetary system



[Credit: M. Kornmesse/ESO]

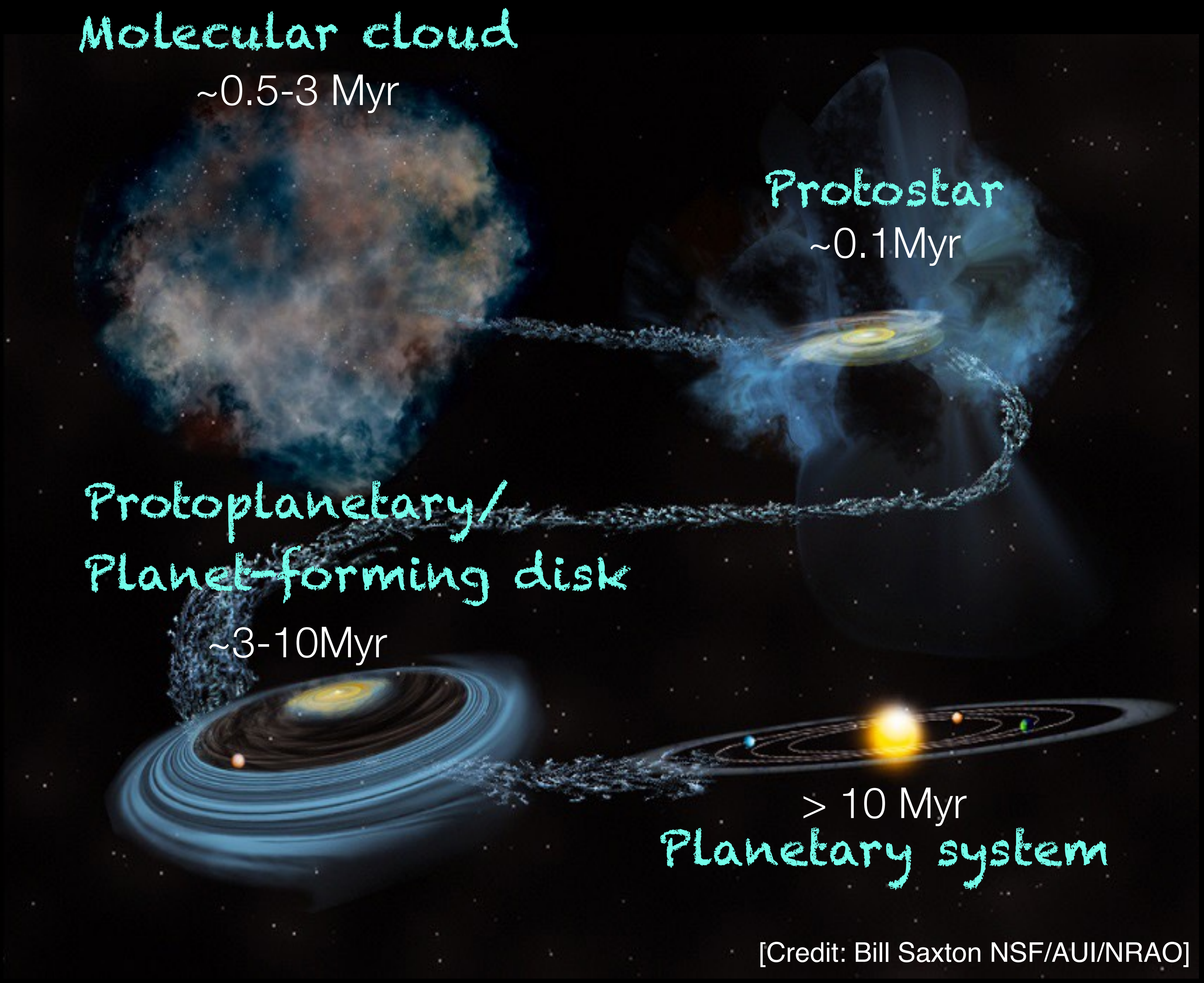
Planet bestiary

[Credit: M. Vargic]



Protoplanetary disks

- *Pivotal stage in evolution from interstellar molecular clouds to planetary systems.*



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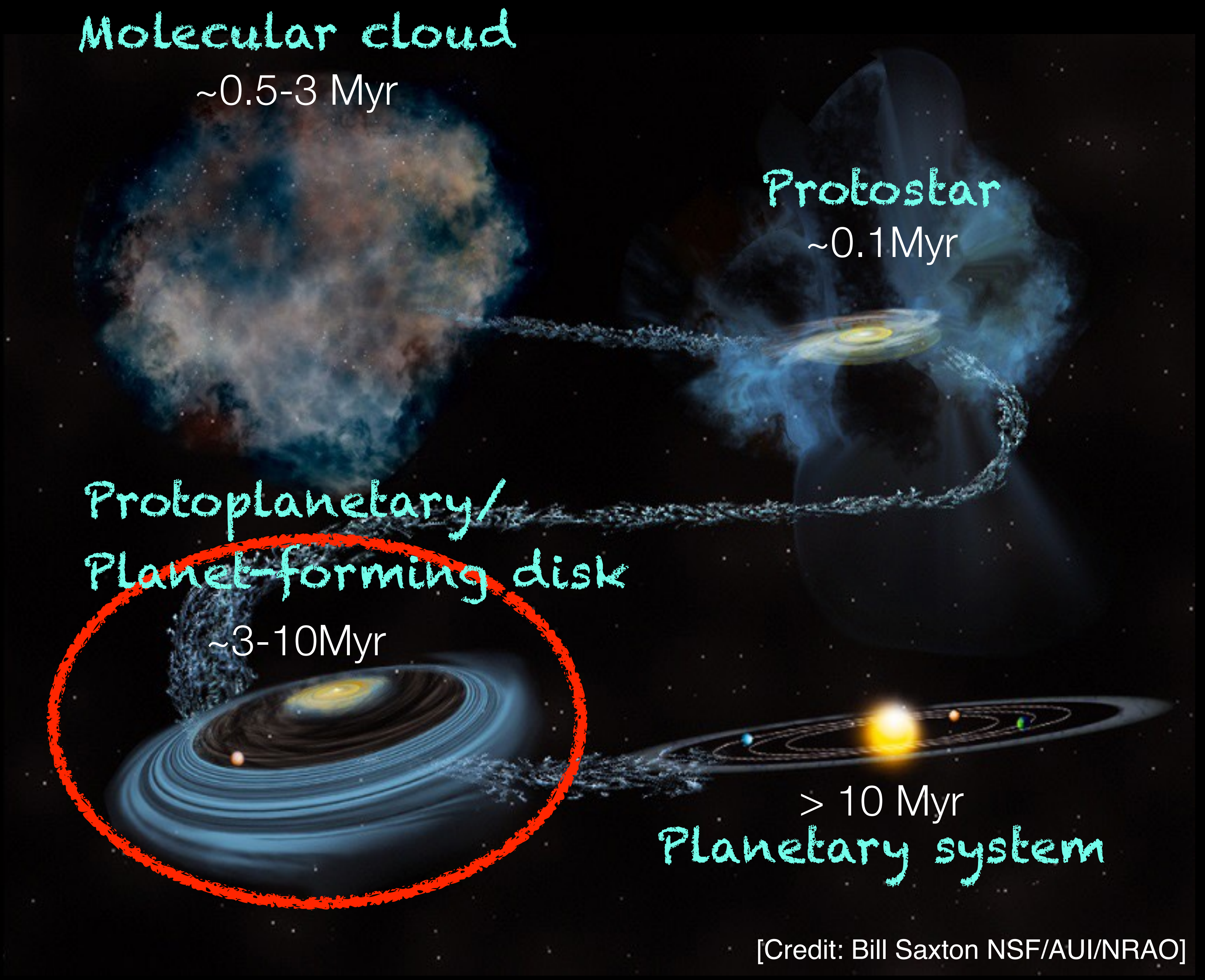

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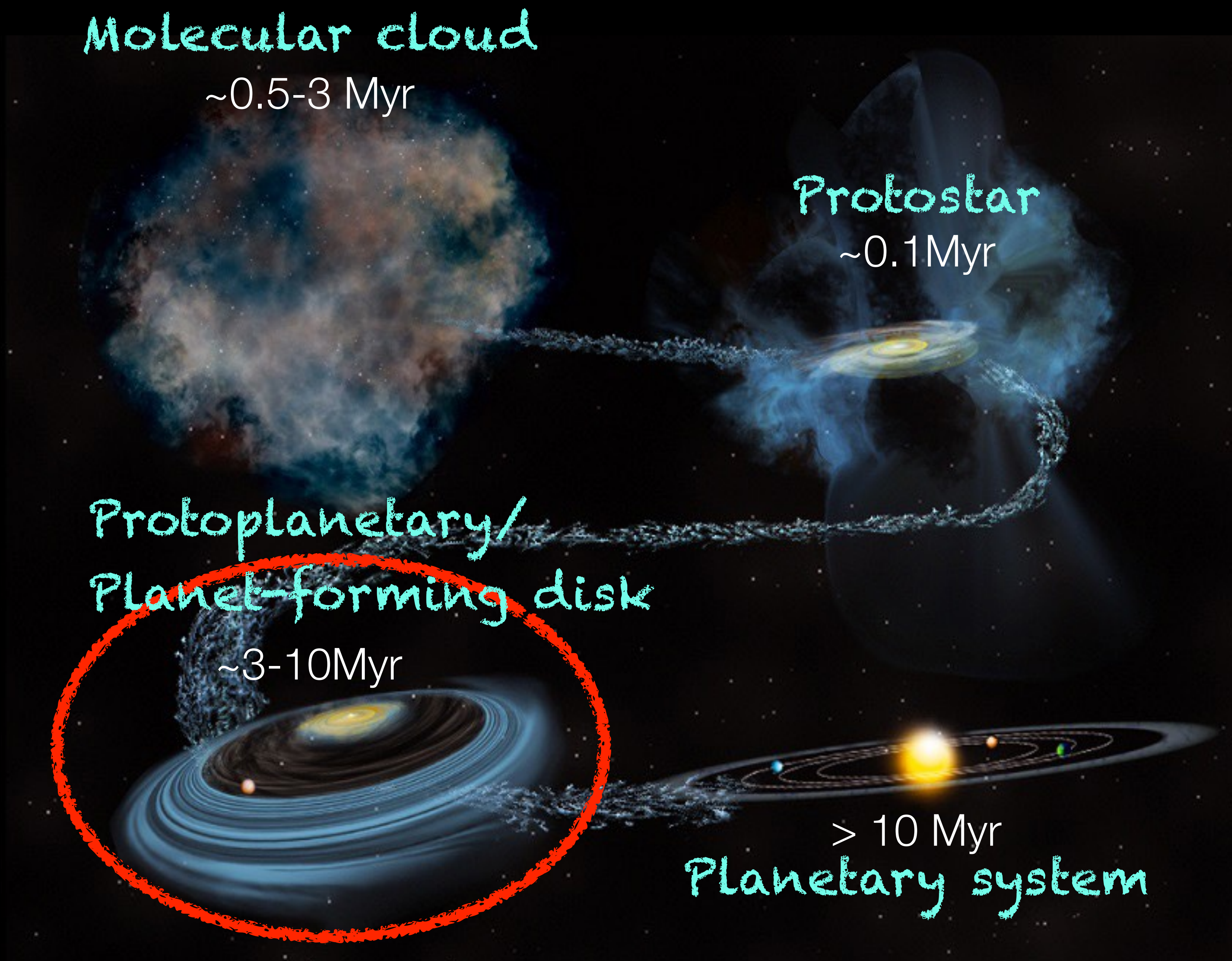

[Credit: Bill Saxton NSF/AUI/NRAO]

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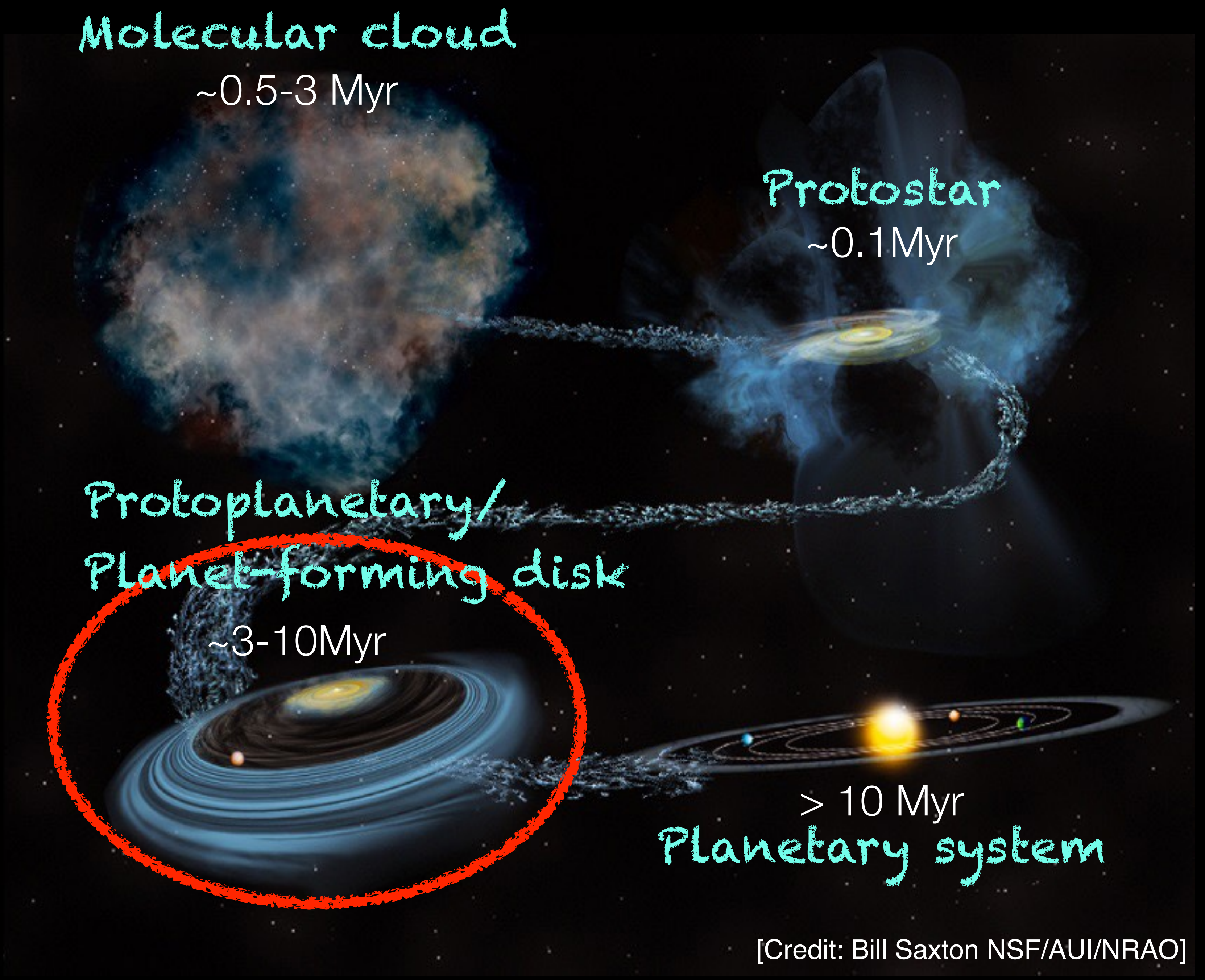

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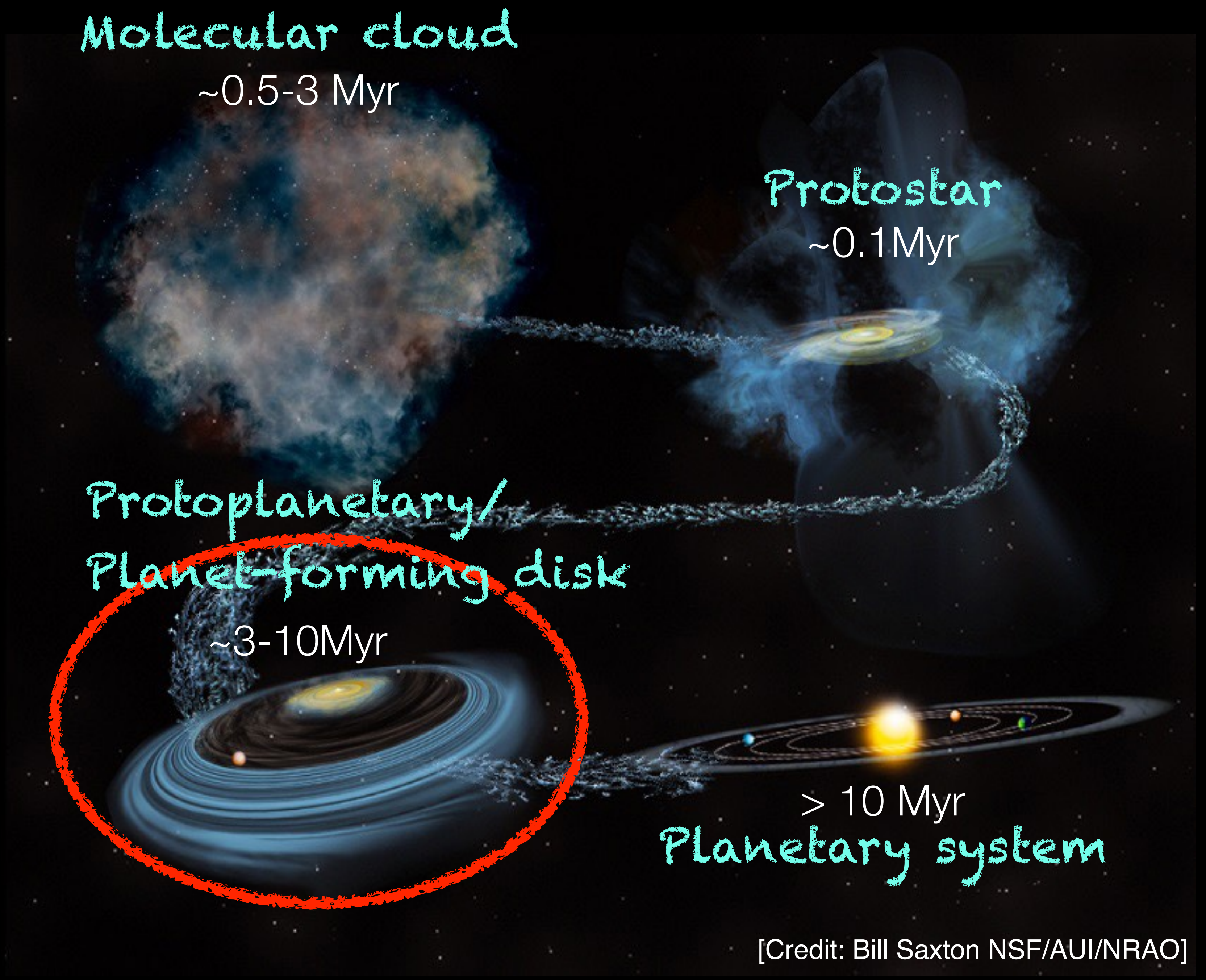
- *Formation, excitation & destruction of molecules?*
- *Are molecules preserved from their initial formation in molecular clouds?*
- *Chemical (re)processing during star & planet formation?*



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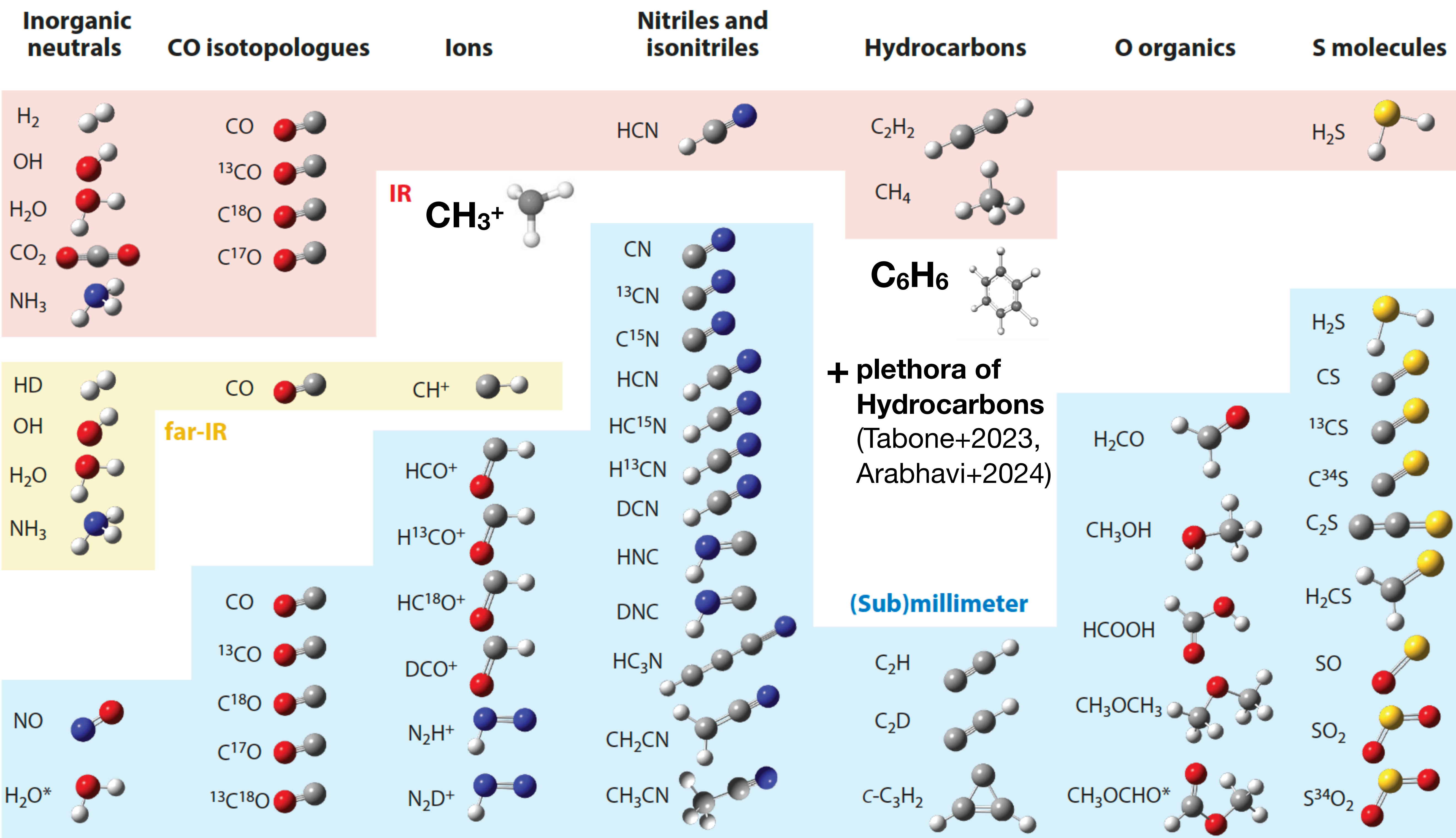
Observations

vs

Modeling

~40 molecules detected in disks



Adapted from Öberg, Facchini & Anderson 2023, ARA&A, 61, 287

=> $\gtrsim$10% of all the chemical species detected in Space so far ($\gtrsim$320)

~40 molecules detected in disks

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	> 6 atoms
CN	H_2O	NH_3	HC_3N	CH_3CN	CH_3OCH_3
CS	H_2S	H_2CO	HCOOH	CH_3OH	CH_3OCHO
SO	C_2S	H_2CS	$c\text{-}C_3H_2$	C_4H_2	C_6H_6
CO	SO_2	C_2H_2	CH_4		C_2H_6
CH^+	HCO^+	CH_3^+	CH_2CN		C_3H_4
OH	HCN	CH_3			
H_2	HNC				
NO	N_2H^+				
	C_2H				
	CO_2				

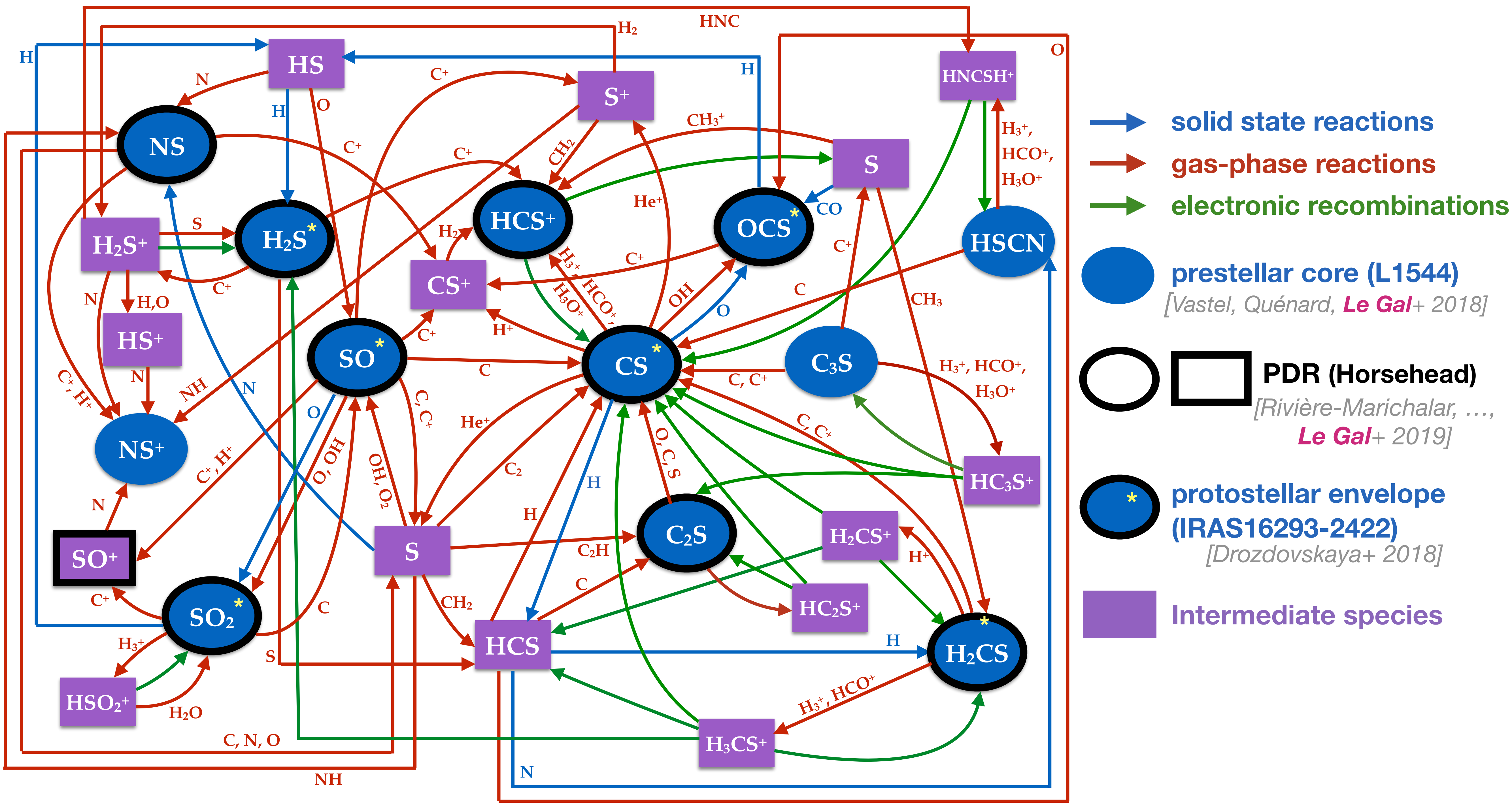
- $\gtrsim$10% of all the chemical species detected in Space so far ($\gtrsim$320)

6 S-molecules detected in disks

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	> 6 atoms
CN	H_2O	NH_3	HC_3N	CH_3CN	CH_3OCH_3
CS	H_2S	H_2CO	HCOOH	CH_3OH	CH_3OCHO
SO	C_2S	H_2CS	c-C_3H_2	C_4H_2	C_6H_6
CO	SO_2	C_2H_2	CH_4		C_2H_6
CH^+	HCO^+	CH_3^+	CH_2CN		C_3H_4
OH	HCN	CH_3			
H_2	HNC				
NO	N_2H^+				
	C_2H				
	CO_2				

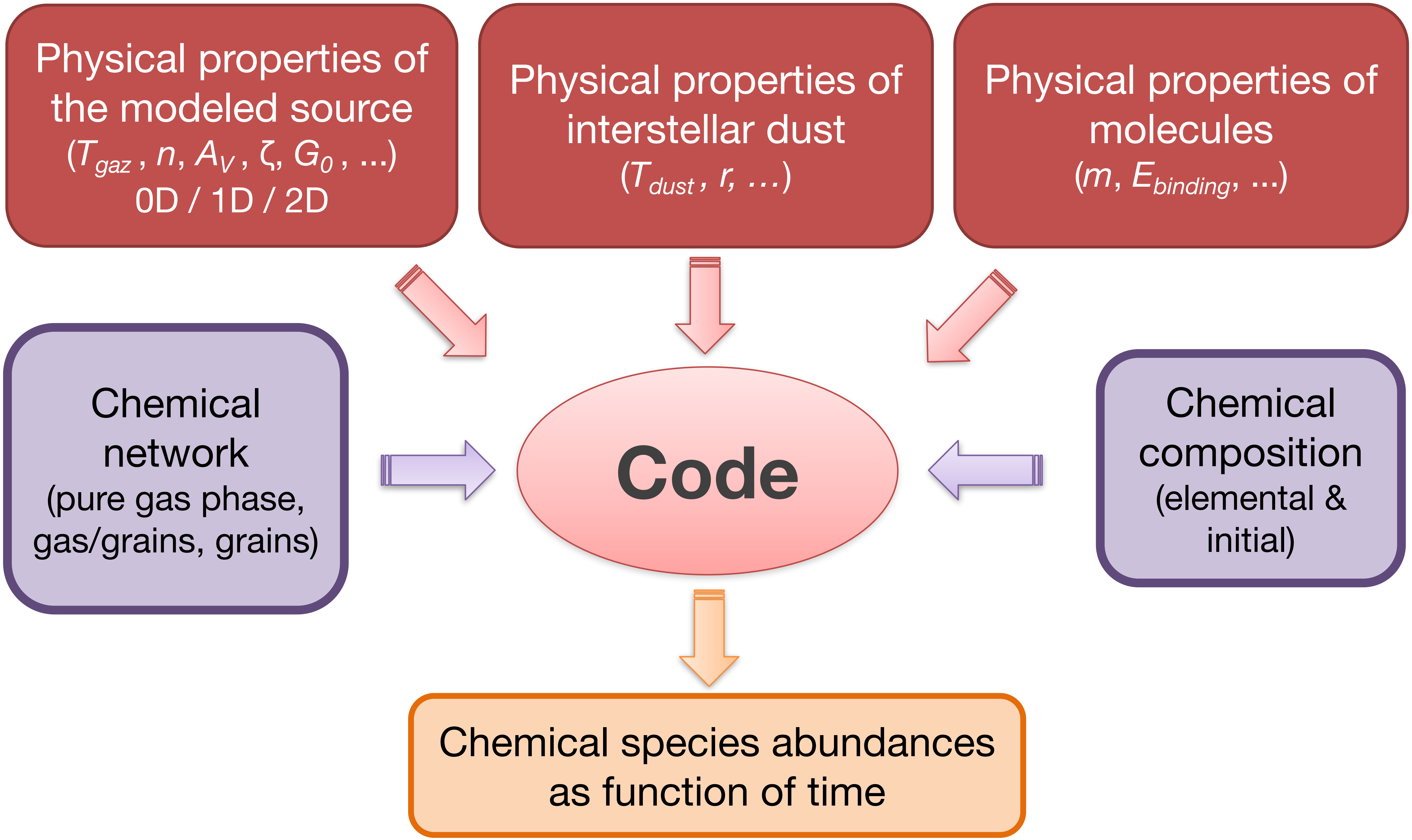
- Routinely observed in wide range of astrophysical objects:
  from extragalactic sources to our own Solar System
- Commonly used to probe the physical conditions (shock, infall, accretion, …)
- Key components in the formation of life building-blocks and in planet habitability
  [Chen et al. 2015, Ranjan et al. 2018, Ruf et al. 2019]

Schematic "simplified" view of the ISM sulfur chemical network

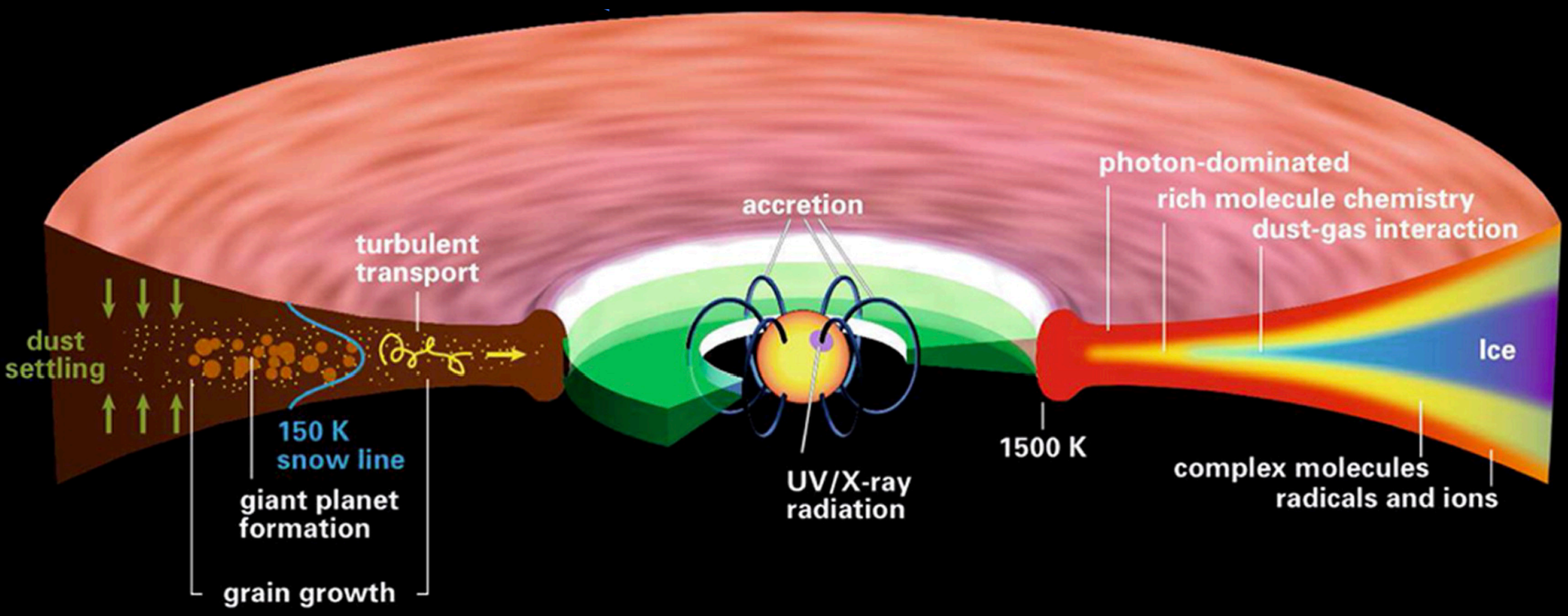


Adapted from: ***Vastel***, *Quénard*, ***Le Gal*** *et al. 2018, MNRAS, 478, 5514*

Astrochemical modeling



Protoplanetary disk structure



Henning & Semenov, Chemical Reviews, 113, 9016, 2013

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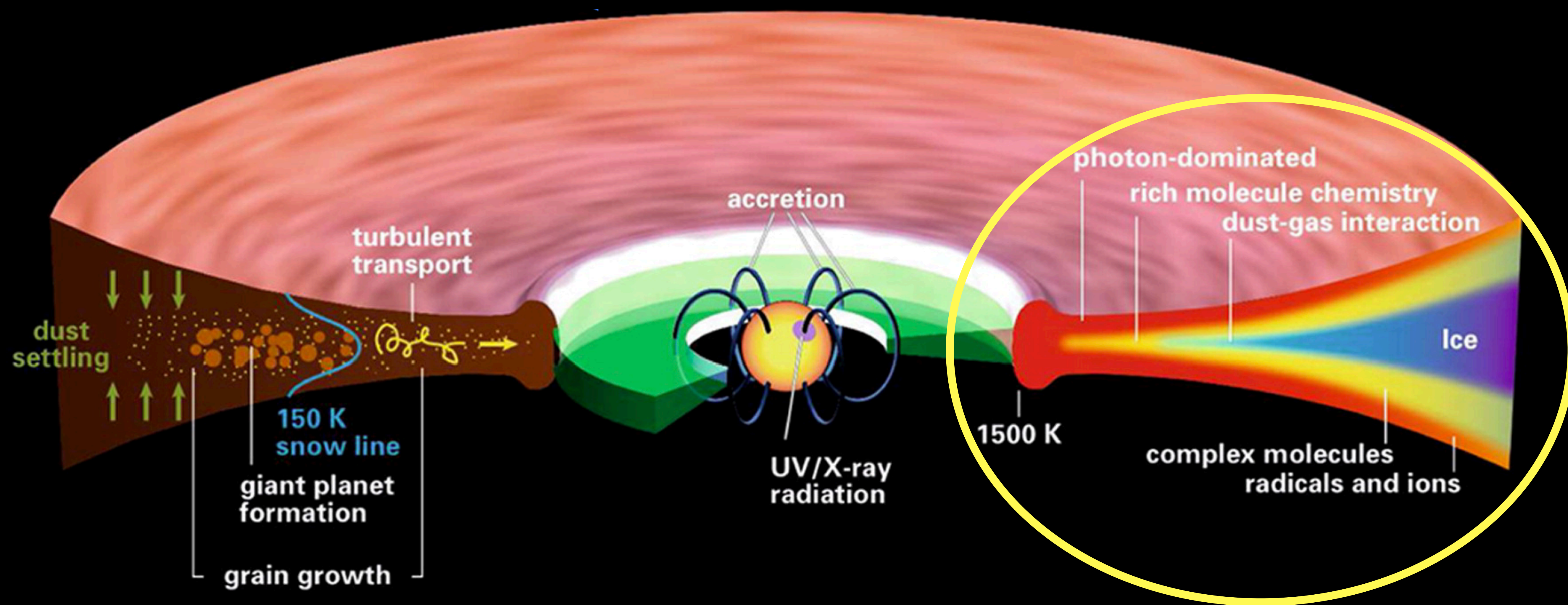

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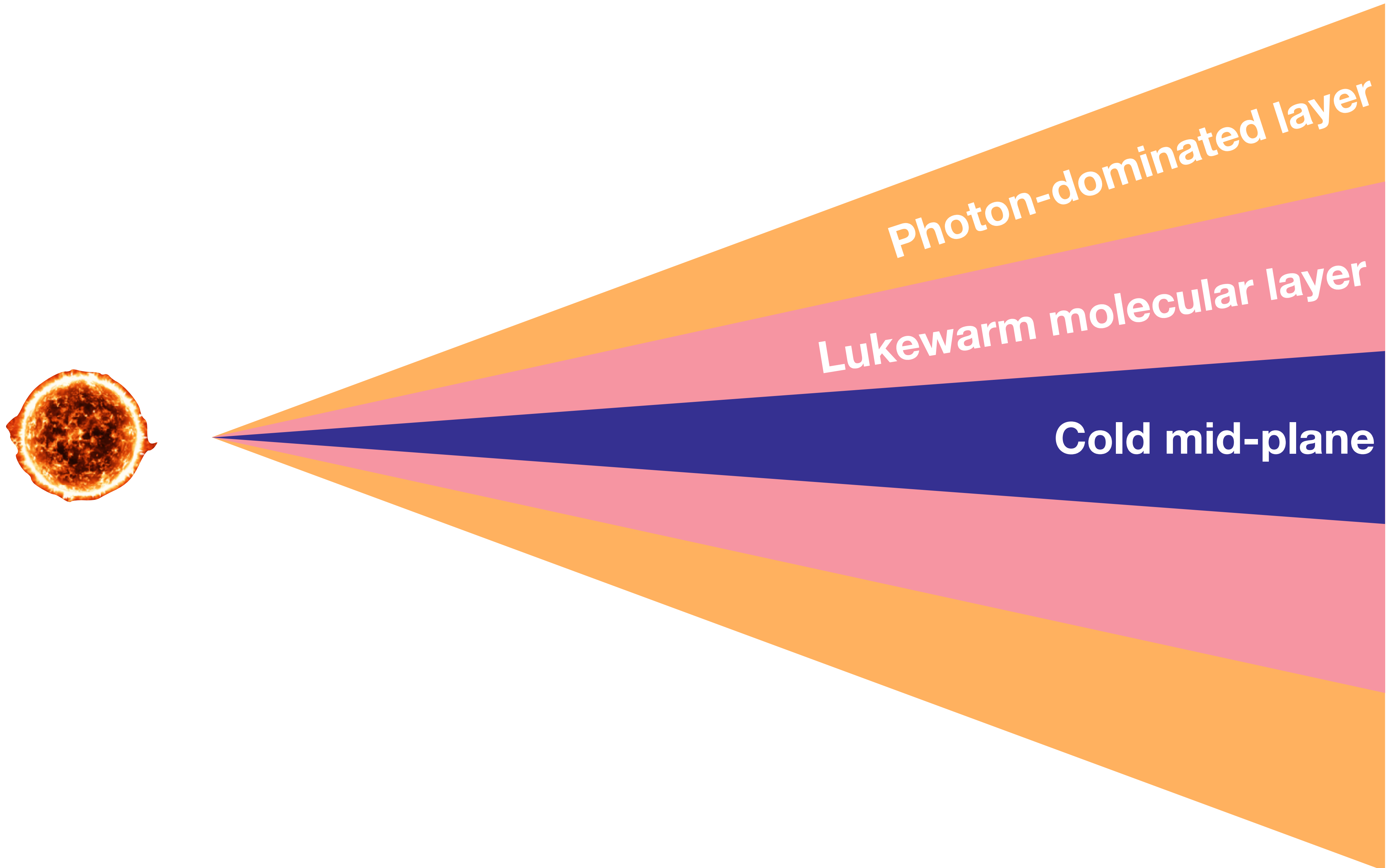

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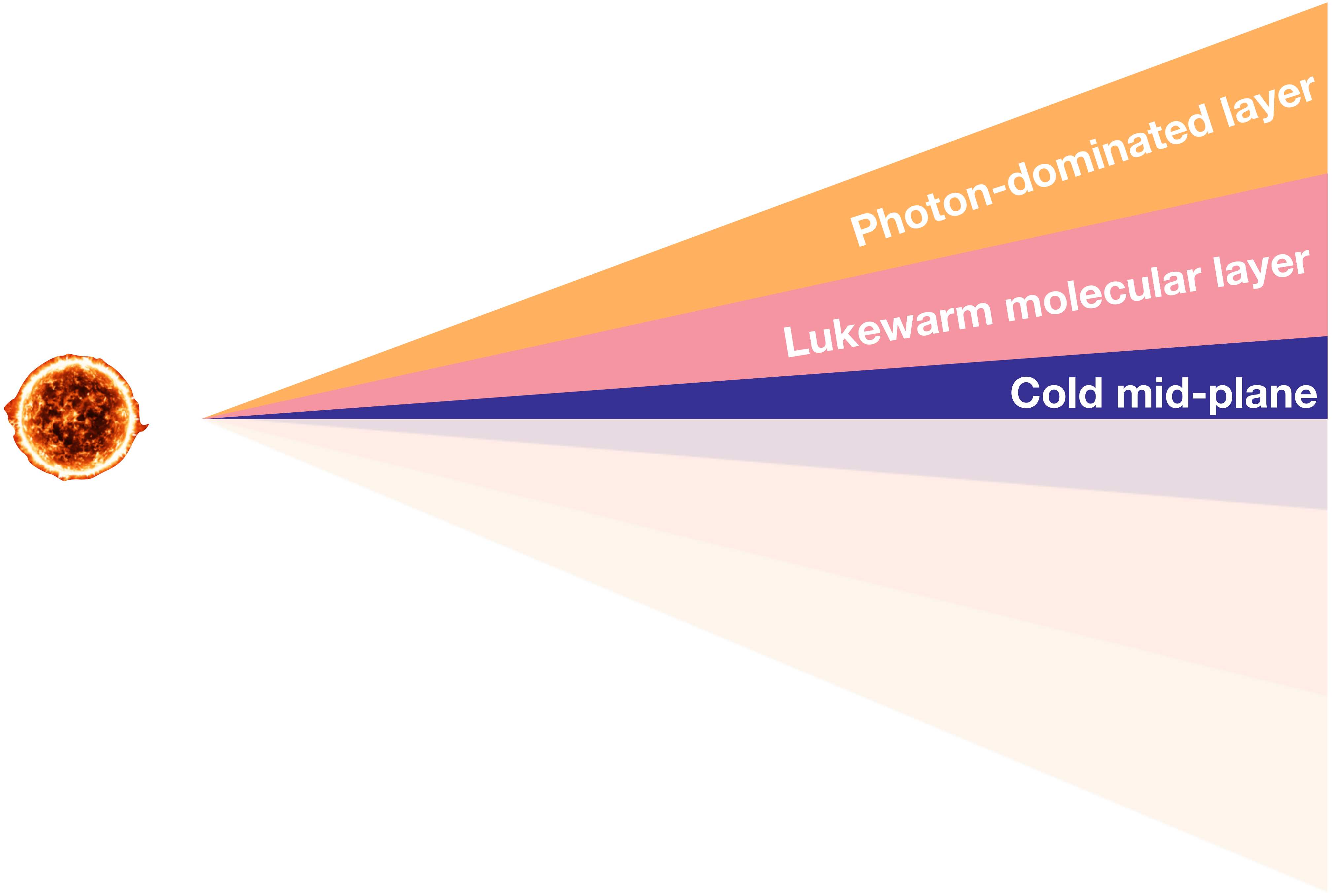

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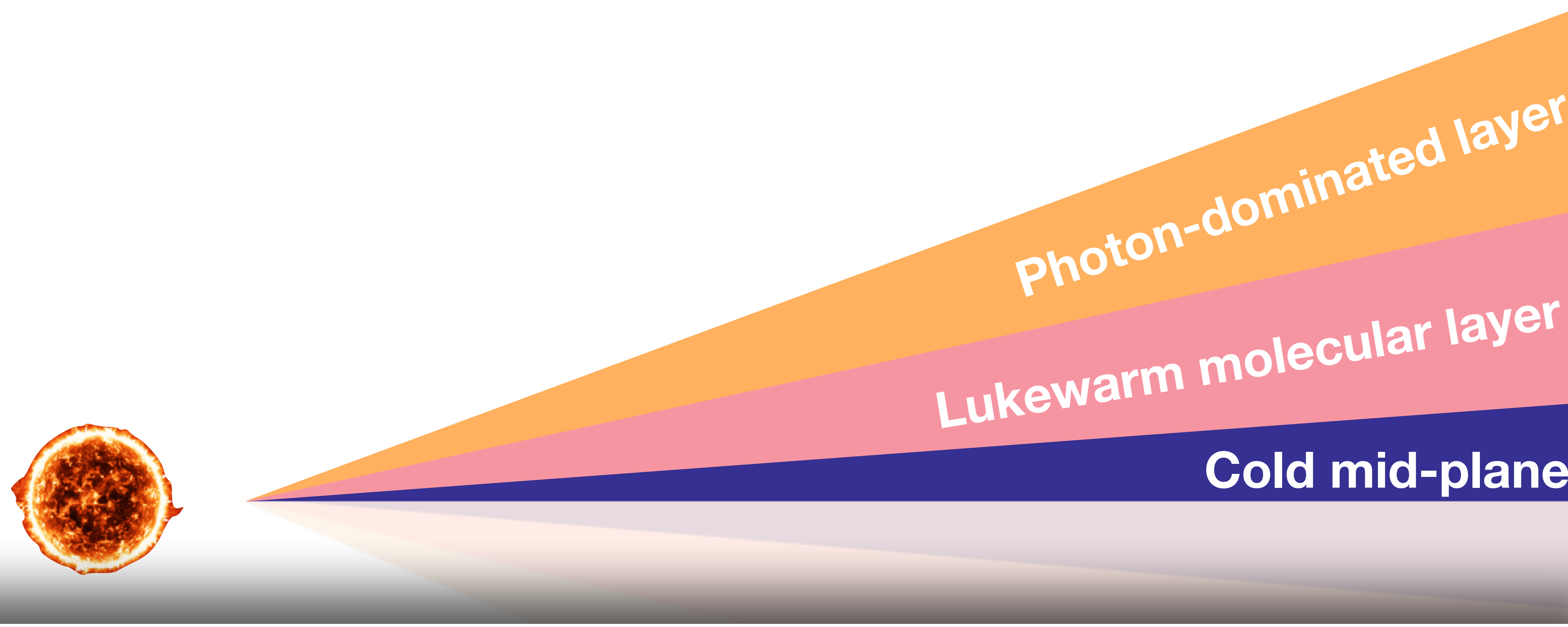
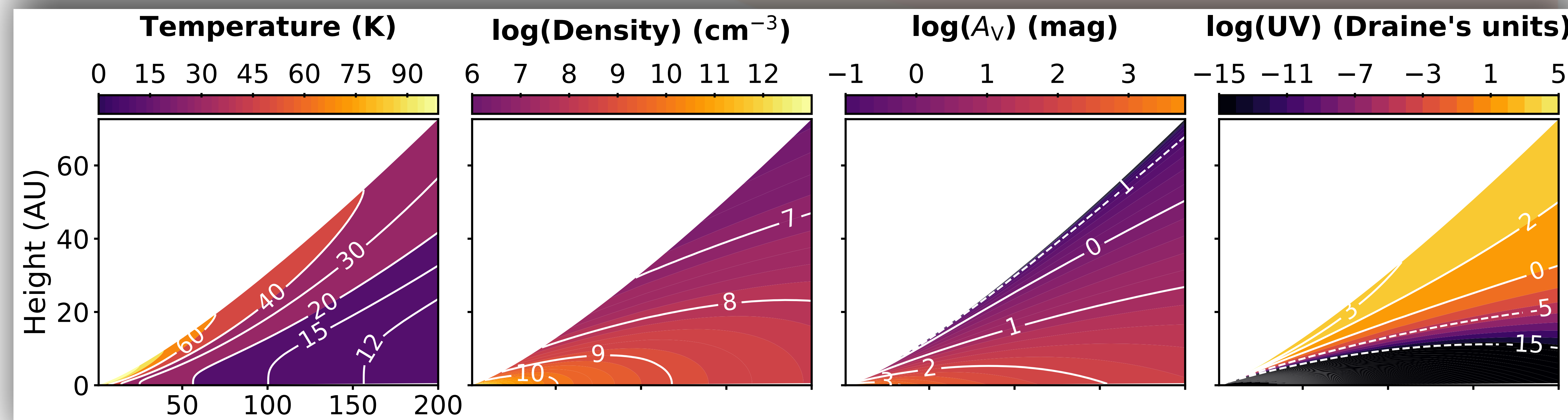
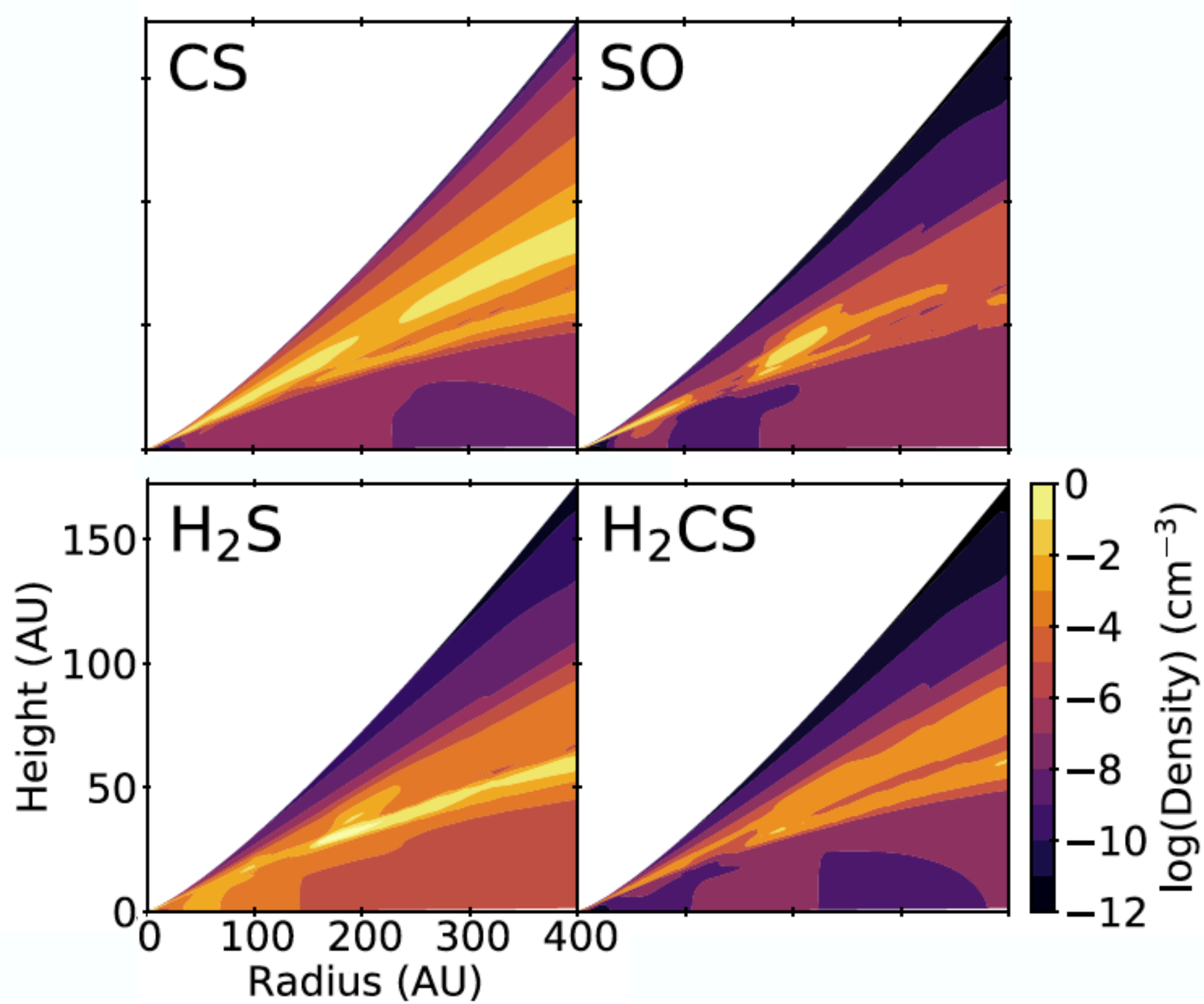




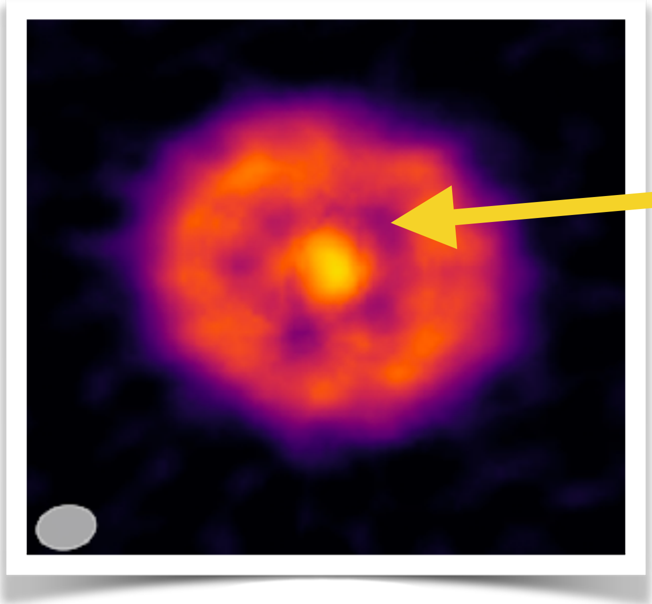
Le Gal et al. 2019a, ApJ, 876, 72

Disk chemistry modelling results



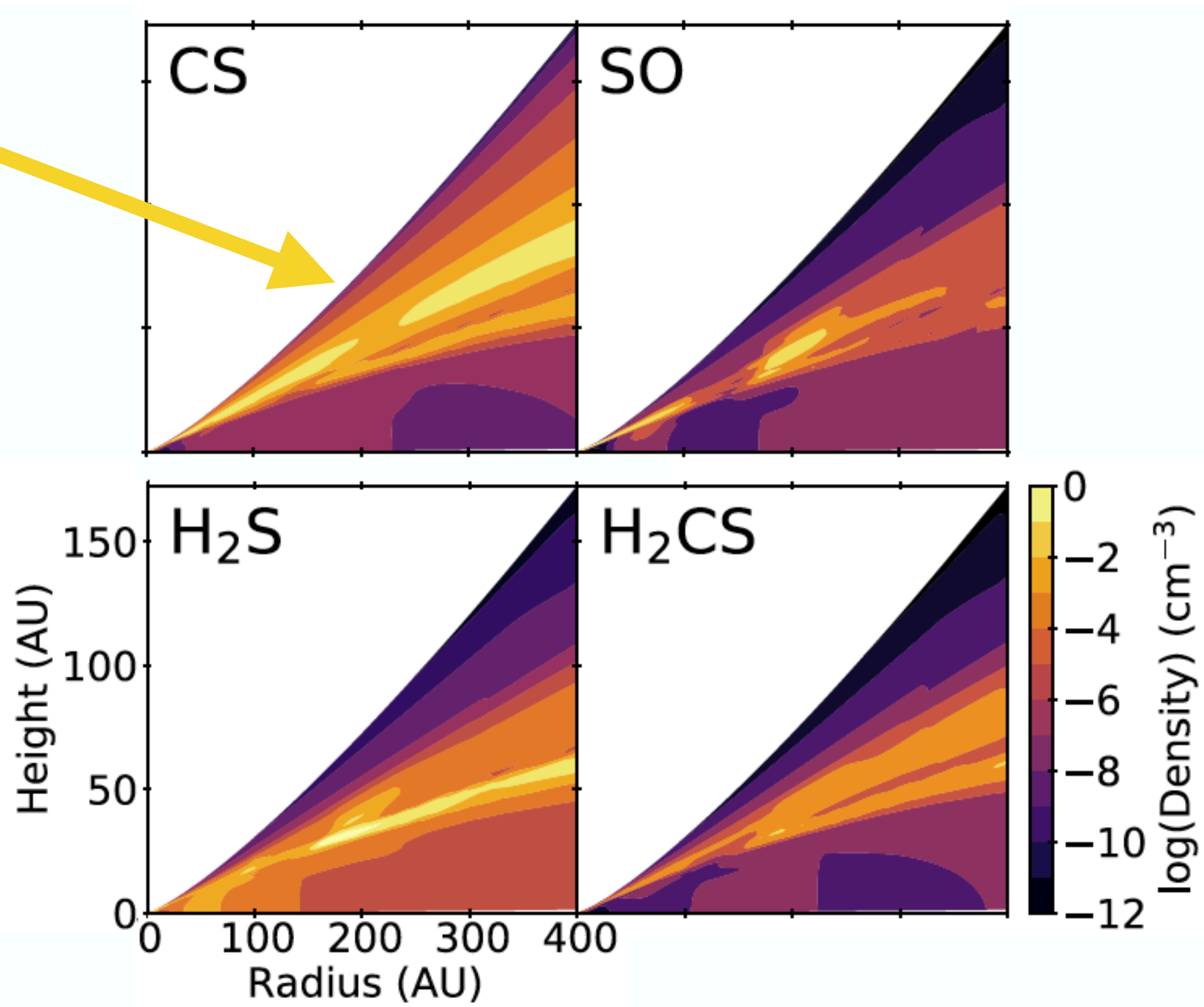
CS in disks: Observations *vs* models

ALMA observation of CS



gap

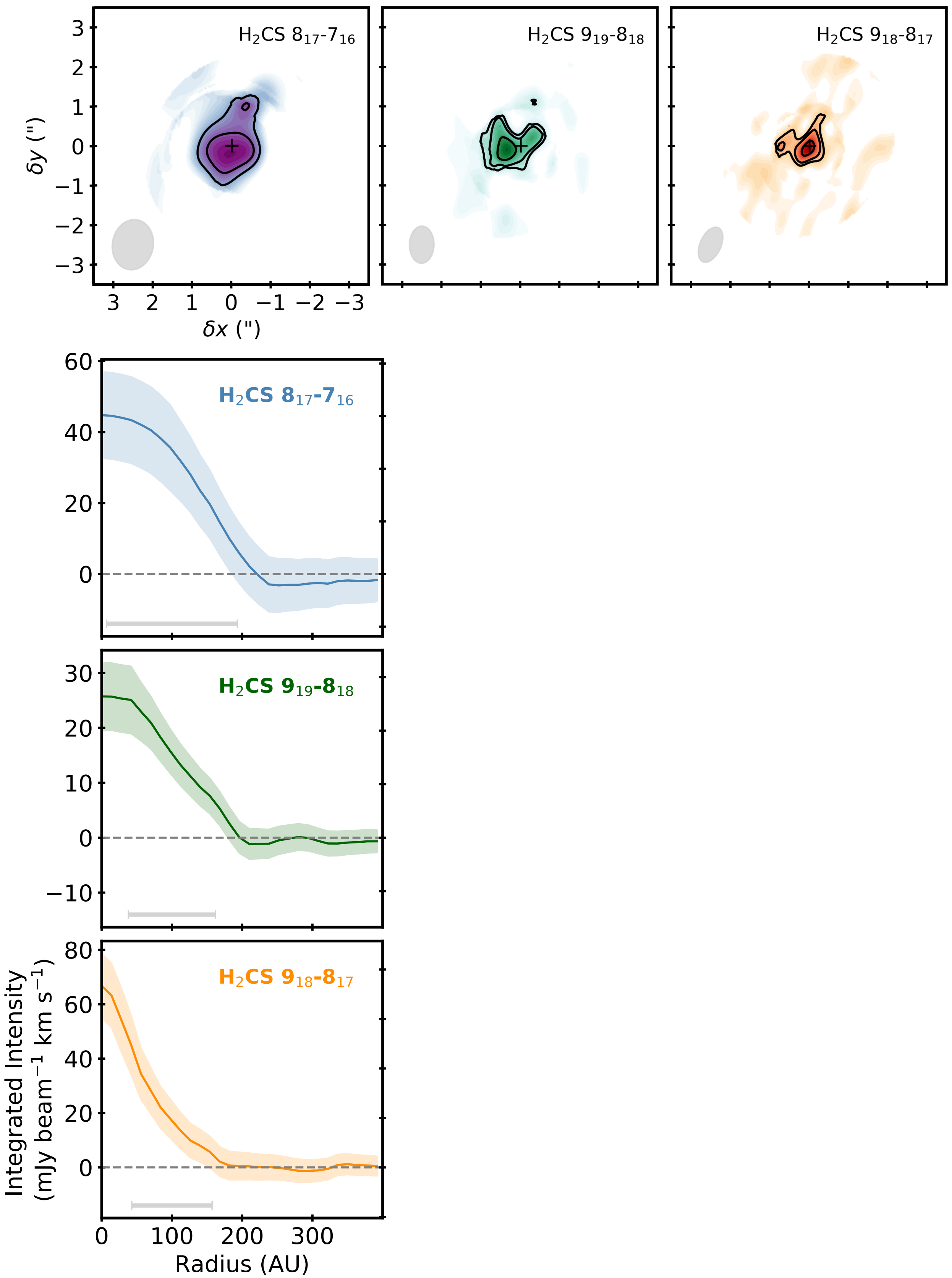
Modeling results



Understanding of the observed abundance & spatial structure of the most accessible sulfur molecule in disks, CS.

H_2CS in disks: Observations *vs* models

Detection of H_2CS in disks



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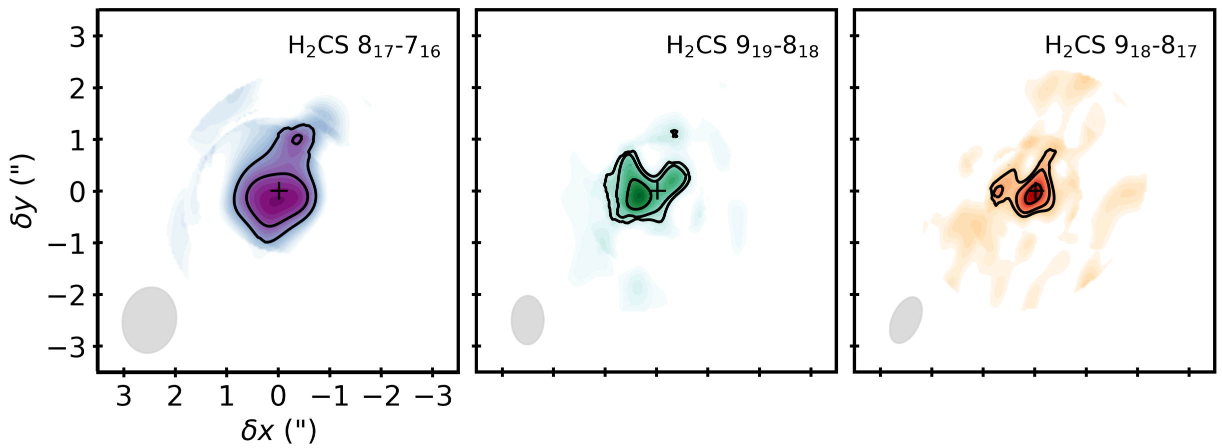

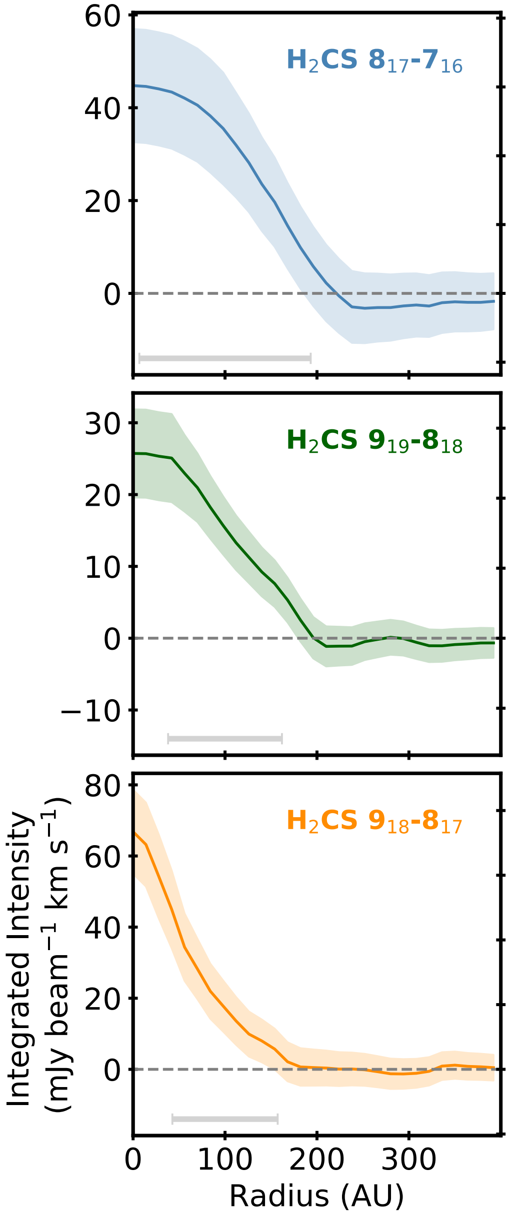

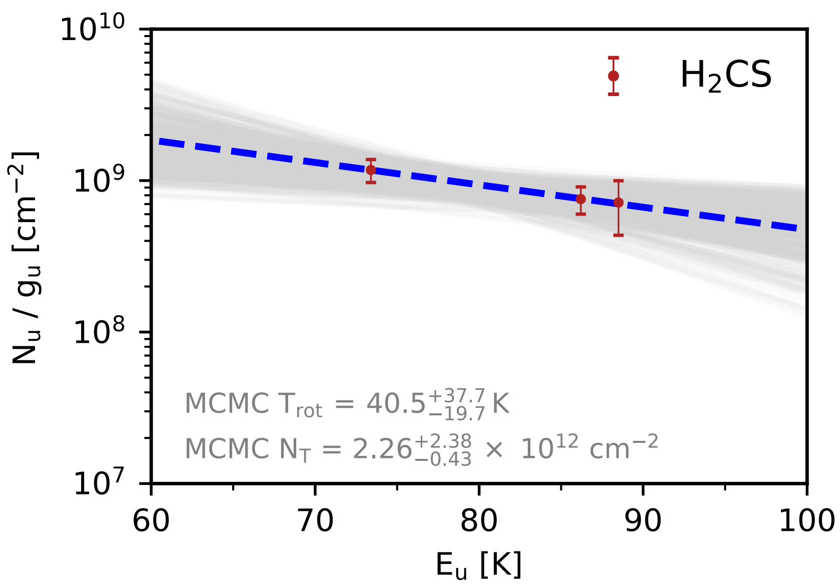

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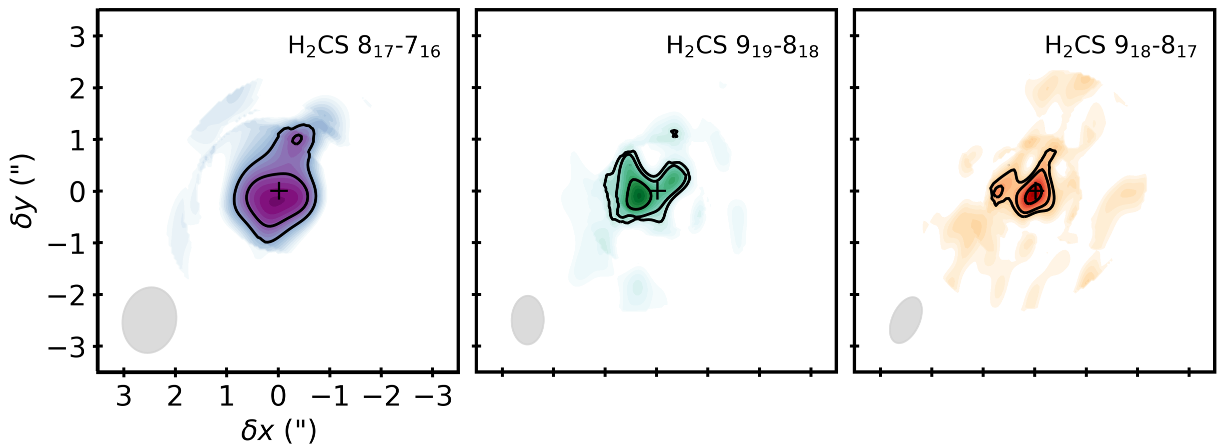

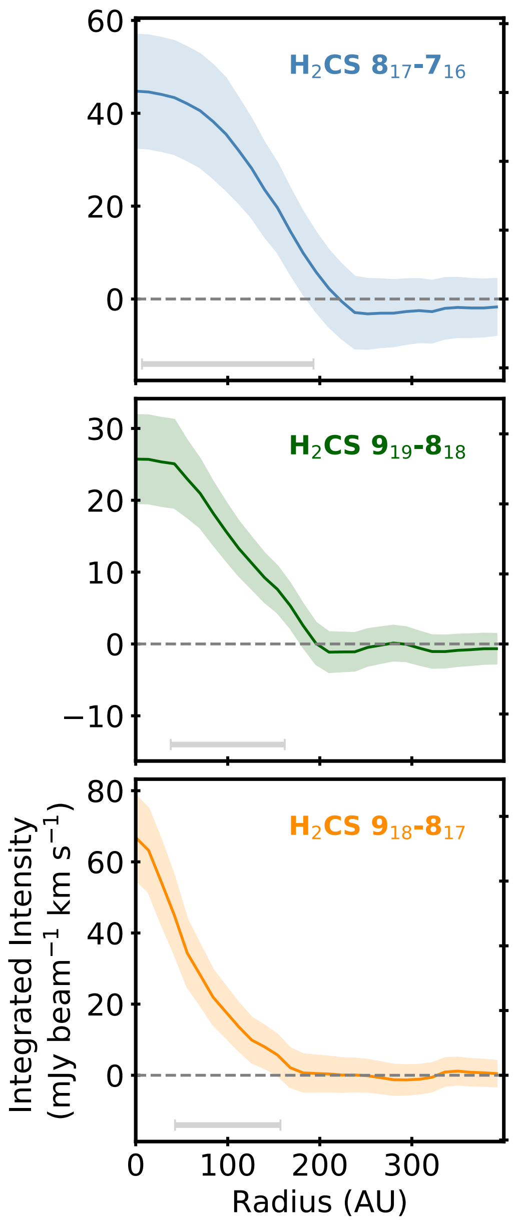

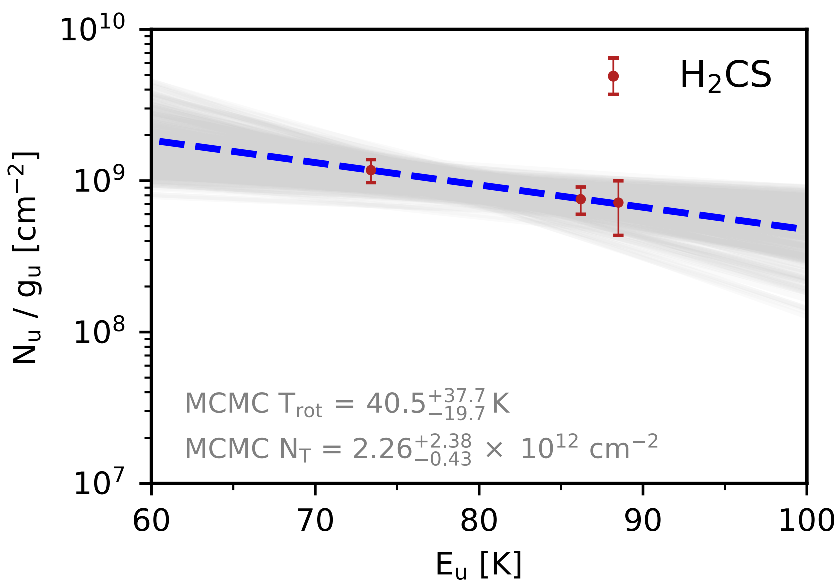

Key ratio: $H_2CS/CS \approx 2/3$

(vs $H_2S/CS \approx 1/20$)

→ **significant fraction** of the **disk S-reservoir** is **organic** (i.e. $C_xH_yS_z$)

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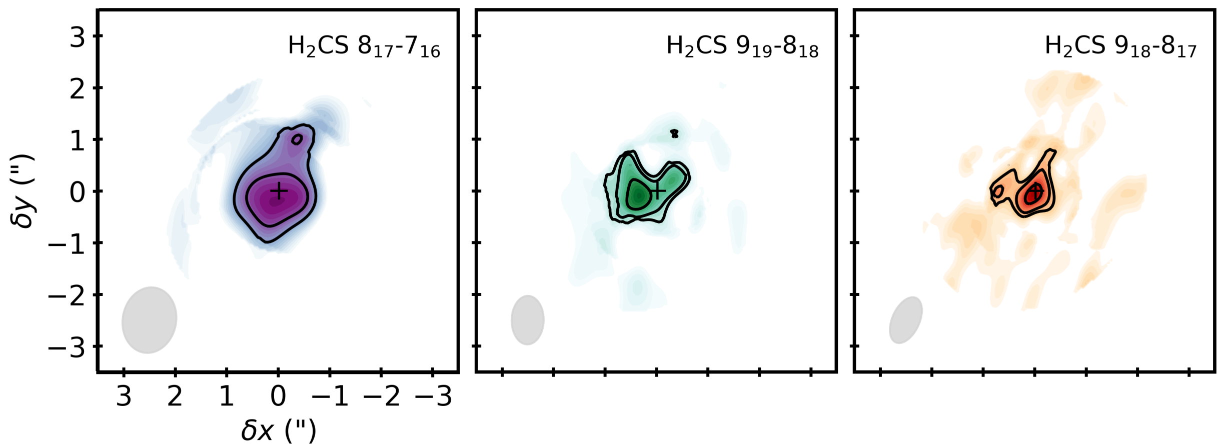

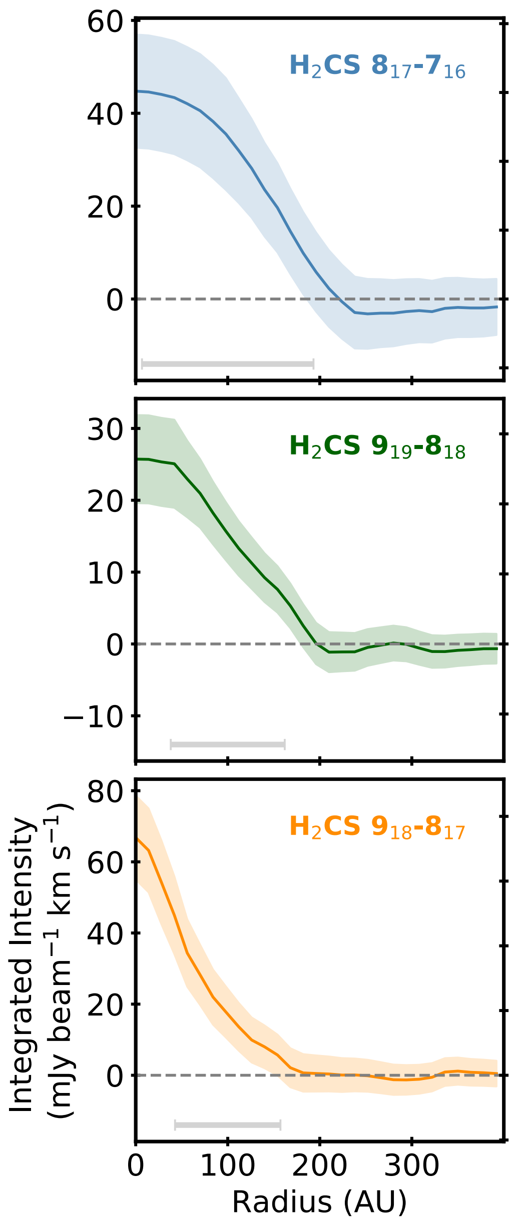

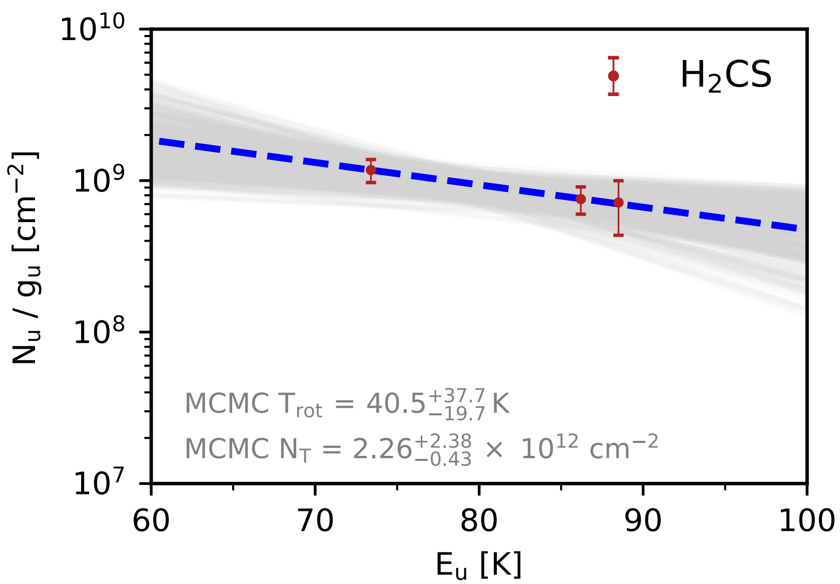

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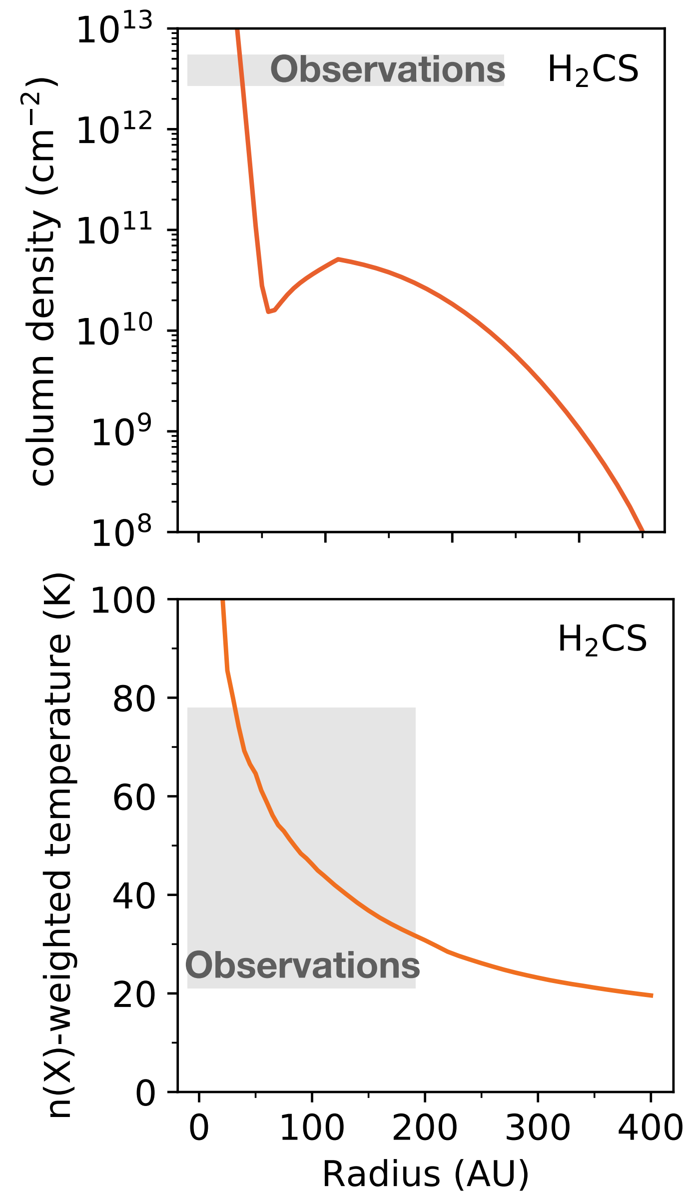
Modeling results vs observations



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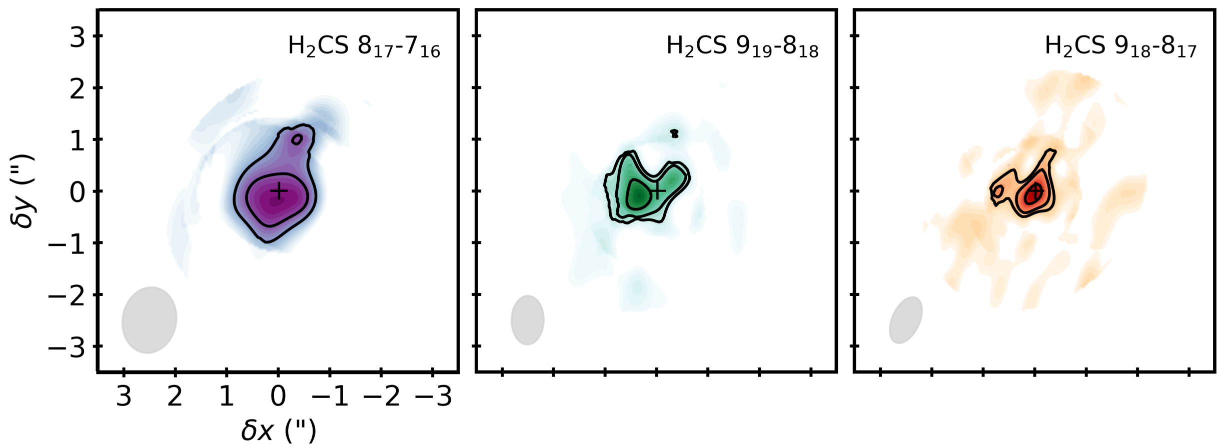

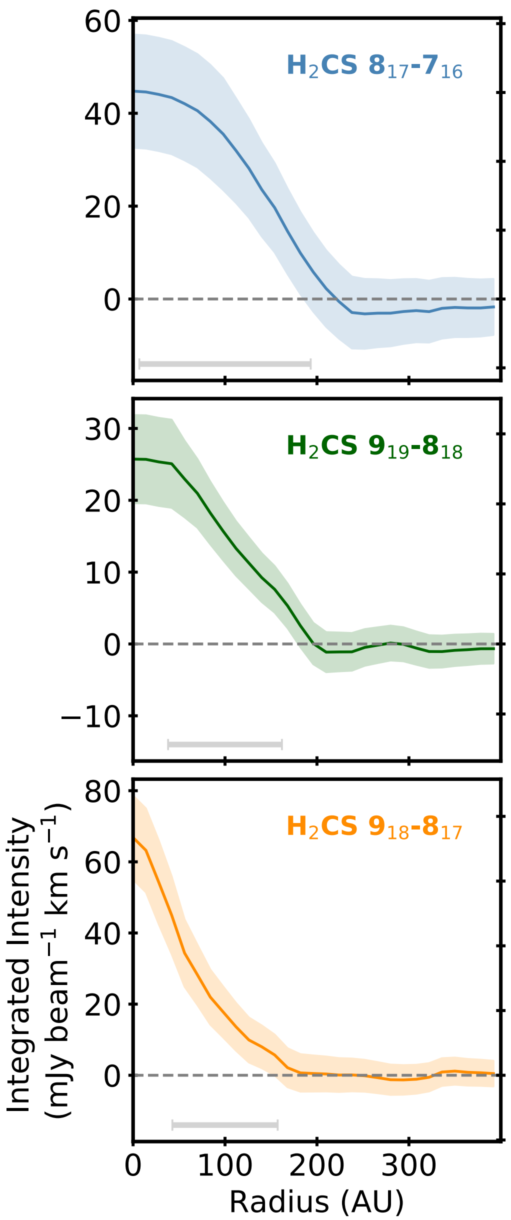

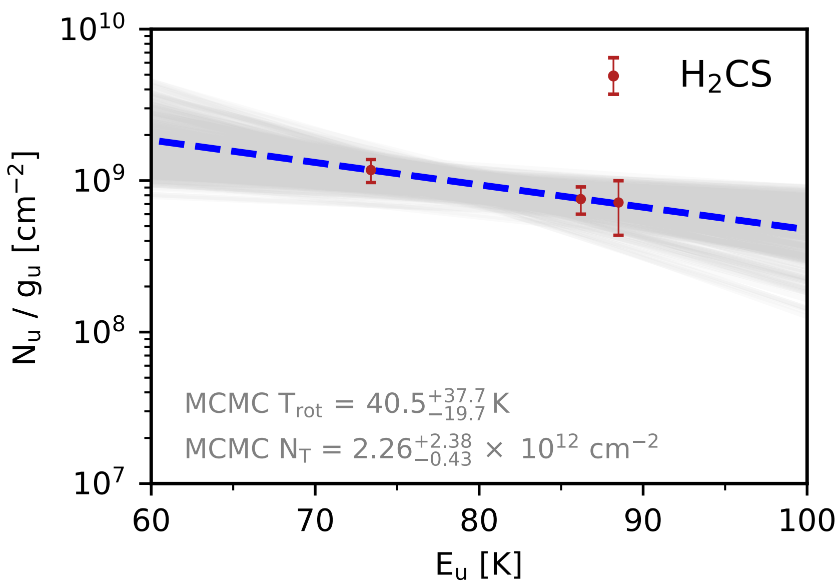

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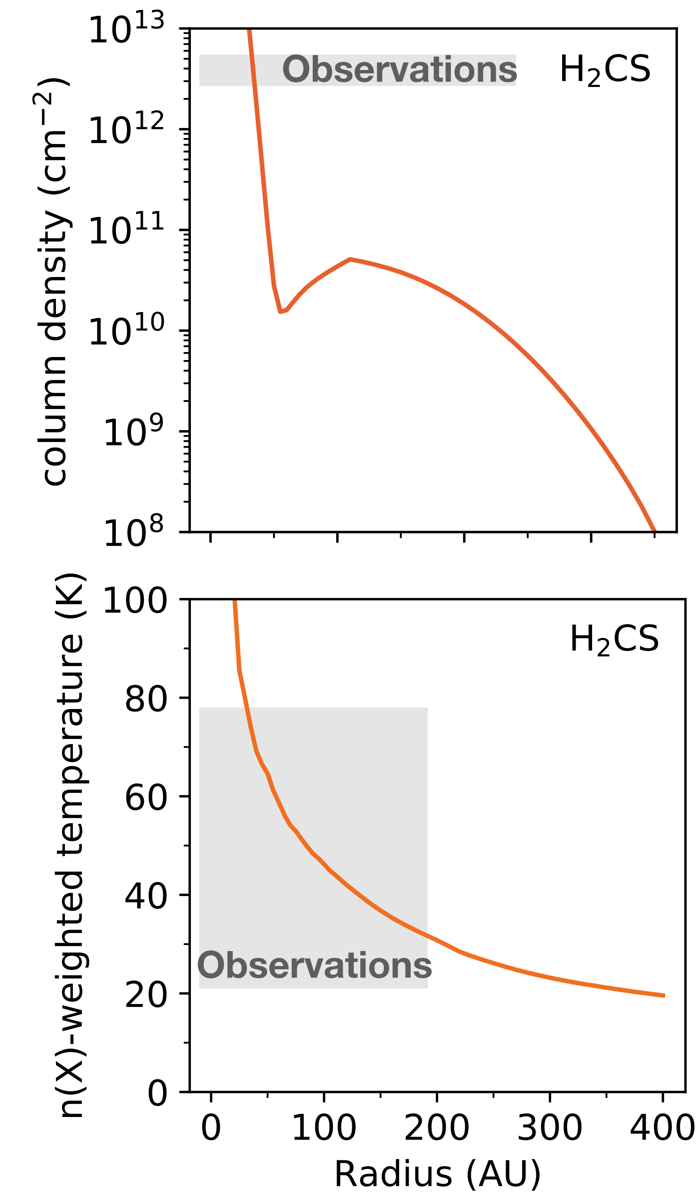
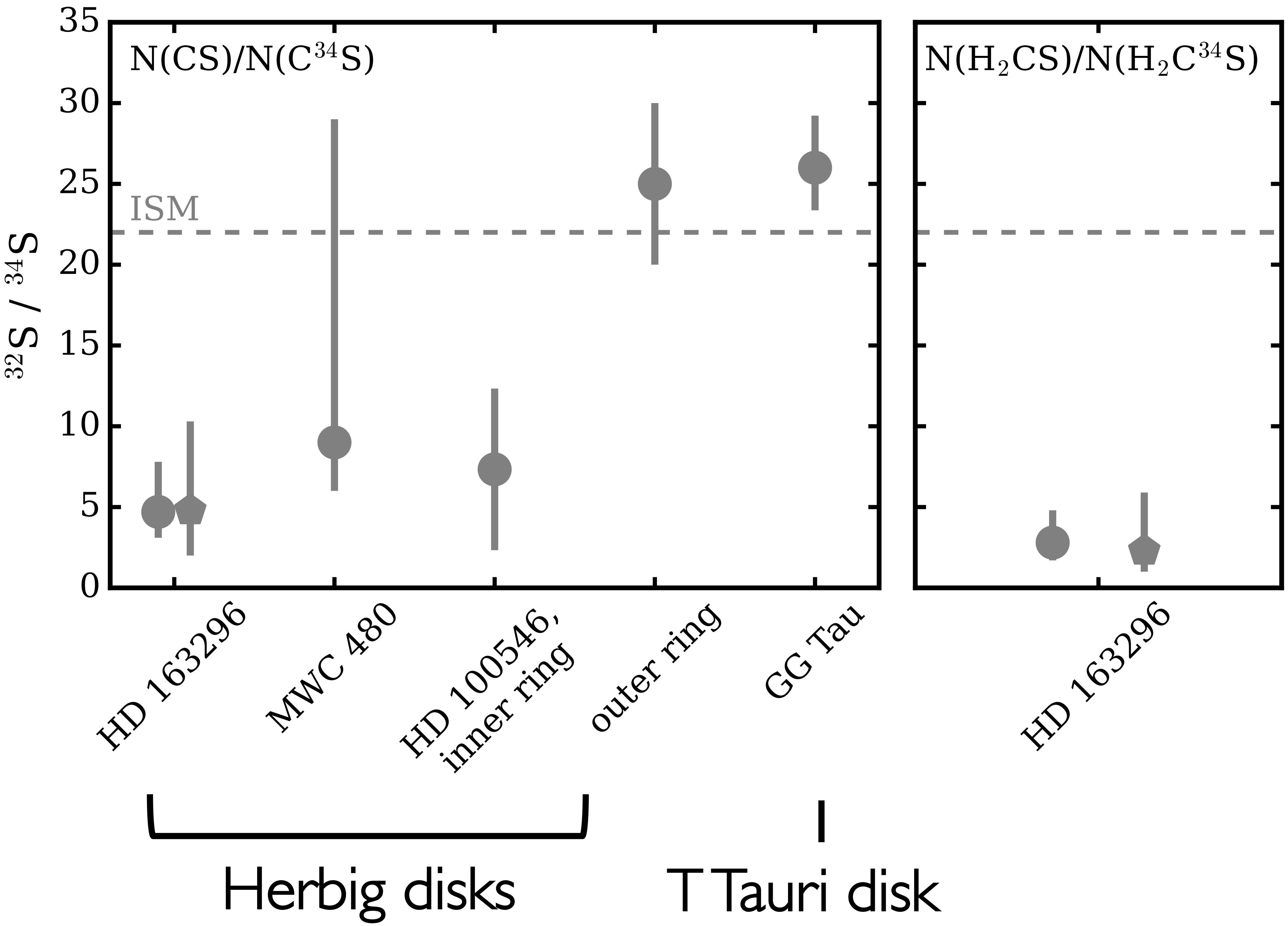


Models **underpredict H_2CS** by 1–2 orders of magnitude

→ need for refined sulfur chemistry models & new lab data!

*[**Le Gal** et al. 2019a, ApJ, 876, 72]*

Sulfur isotopic ratios in disks



*[Law, **Le Gal** et al. 2025, ApJ, 985, 84]*

MWC 480: Le Gal+2019, GG Tau: Phuong+2021 ; HD100546: Booth+2024 ; HD163296: Law+2025

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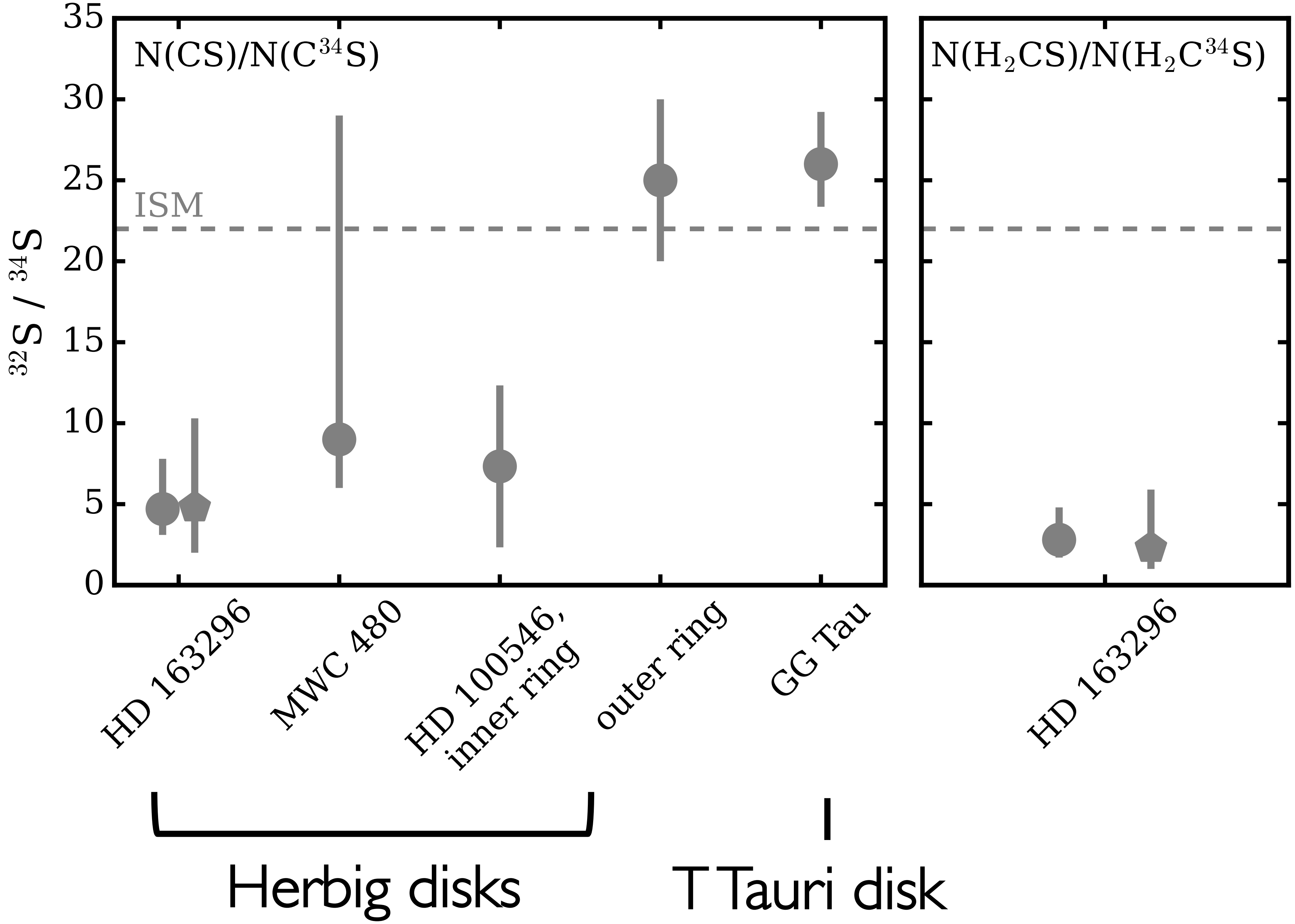

*[Law, **Le Gal** et al. 2025, ApJ, 985, 84]*

- **How does this imprint onto forming planet(s)?**
- **Do disks around Herbig stars show enhanced ^{34}S?**
- **Or inherited from an unusual molecular cloud when the disk formed?**
- **We need more multi-line observations of ^{34}S isotopologues in disks.**

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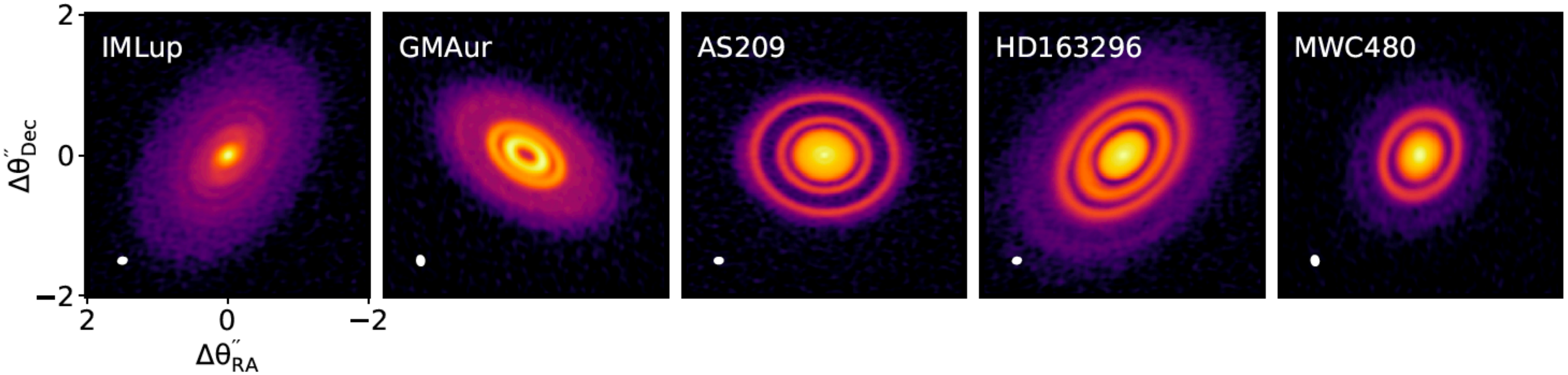
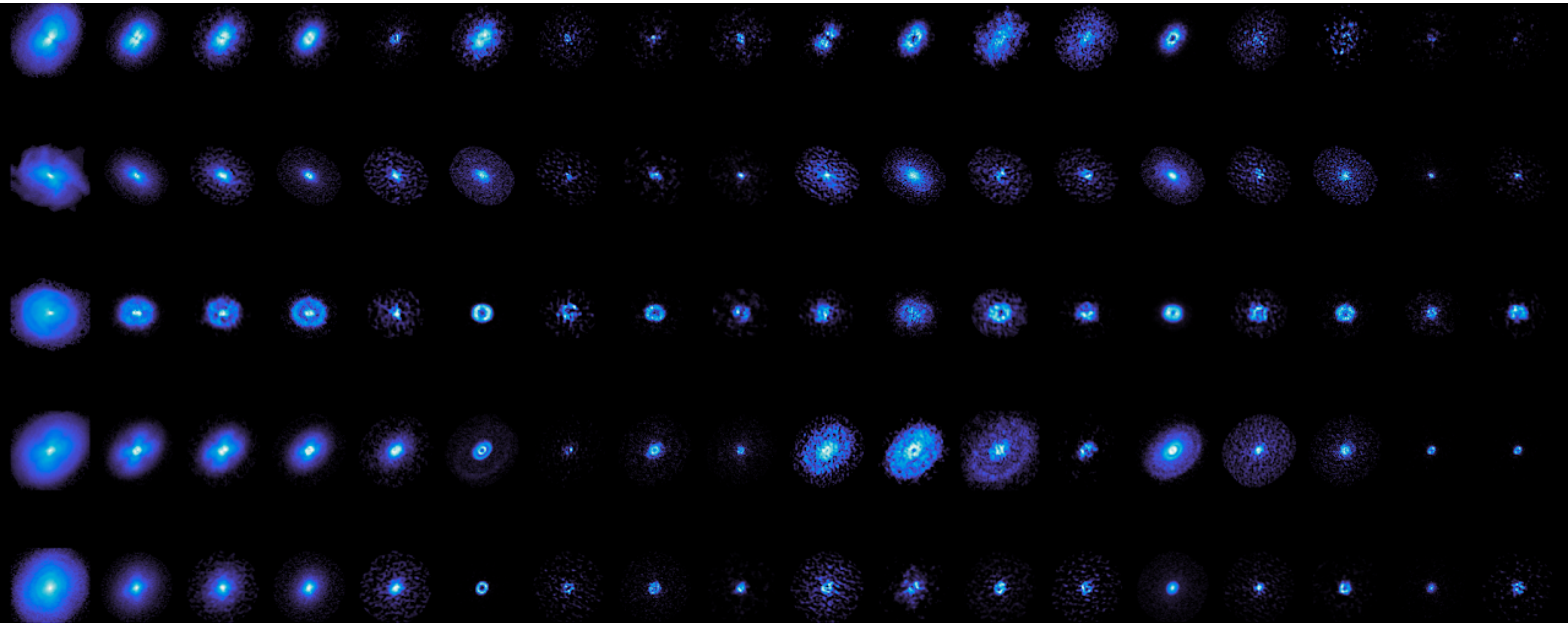
Molecules with **A**LMA at **P**lanet-forming **S**cales

http://alma-maps.info

[Öberg & MAPS collaboration, ApJS, 2021, 257, 1]





Team: 5 **co-PIs:** K. Öberg, Y. Aikawa, E. Bergin, V. Guzmán,C. Walsh + 39 **co-Is**

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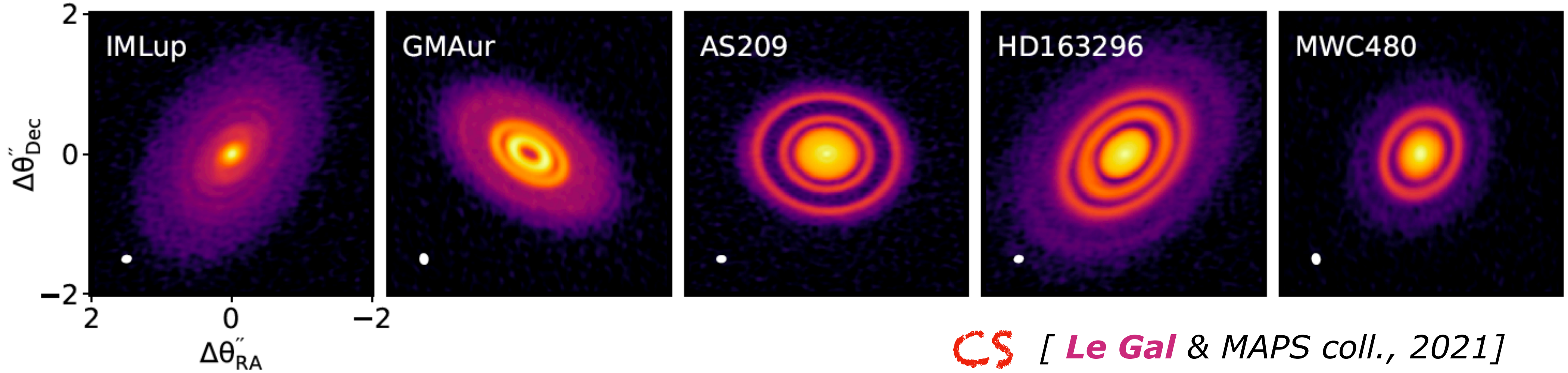
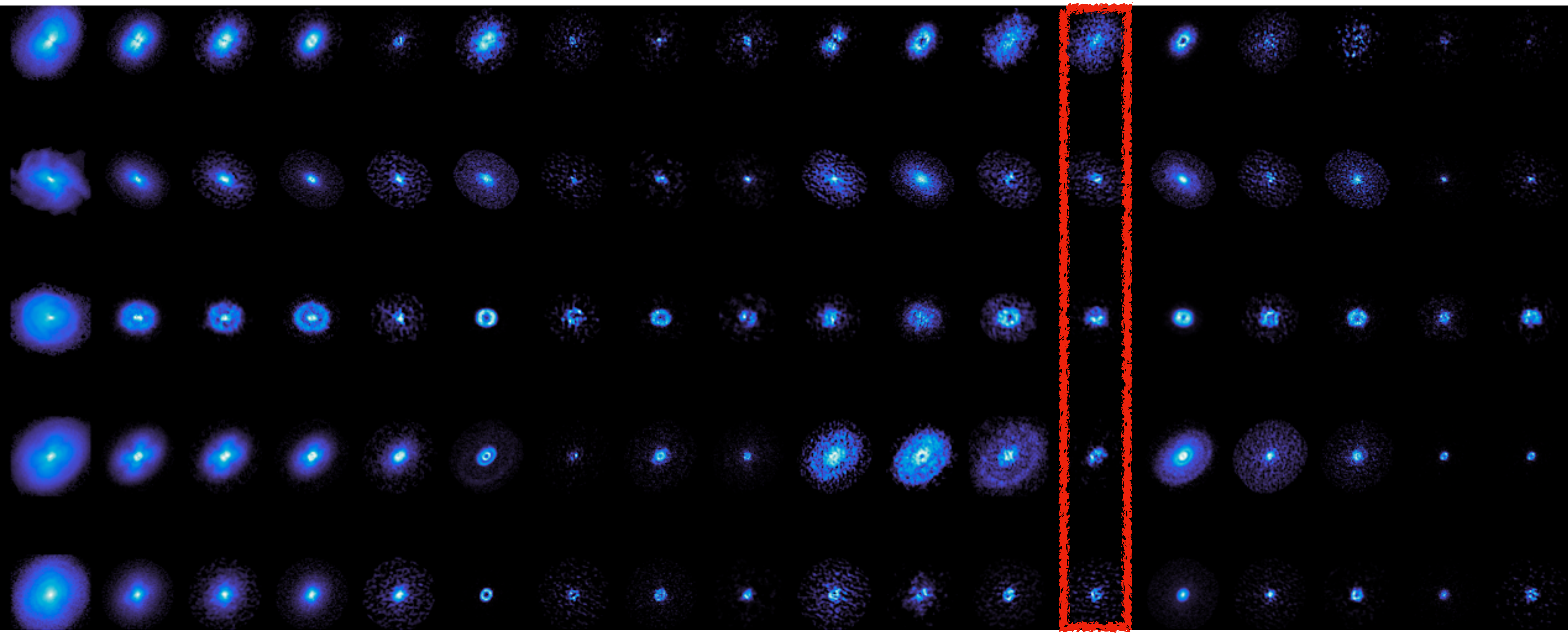


CS [**Le Gal** & MAPS coll., 2021]



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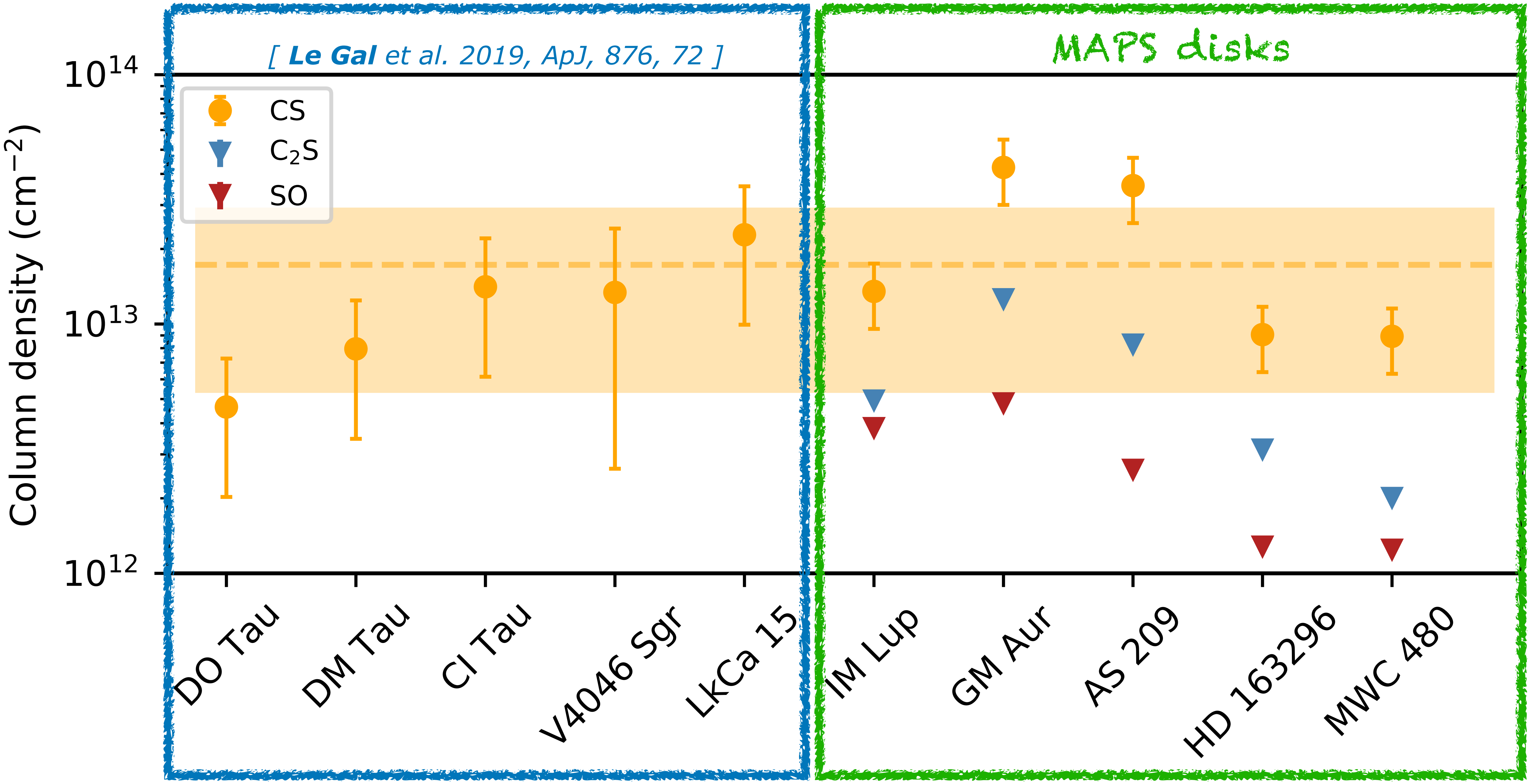
Disk-integrated column densities

*[**Le Gal** & MAPS collaboration, 2021, ApJS, 257, 12]*



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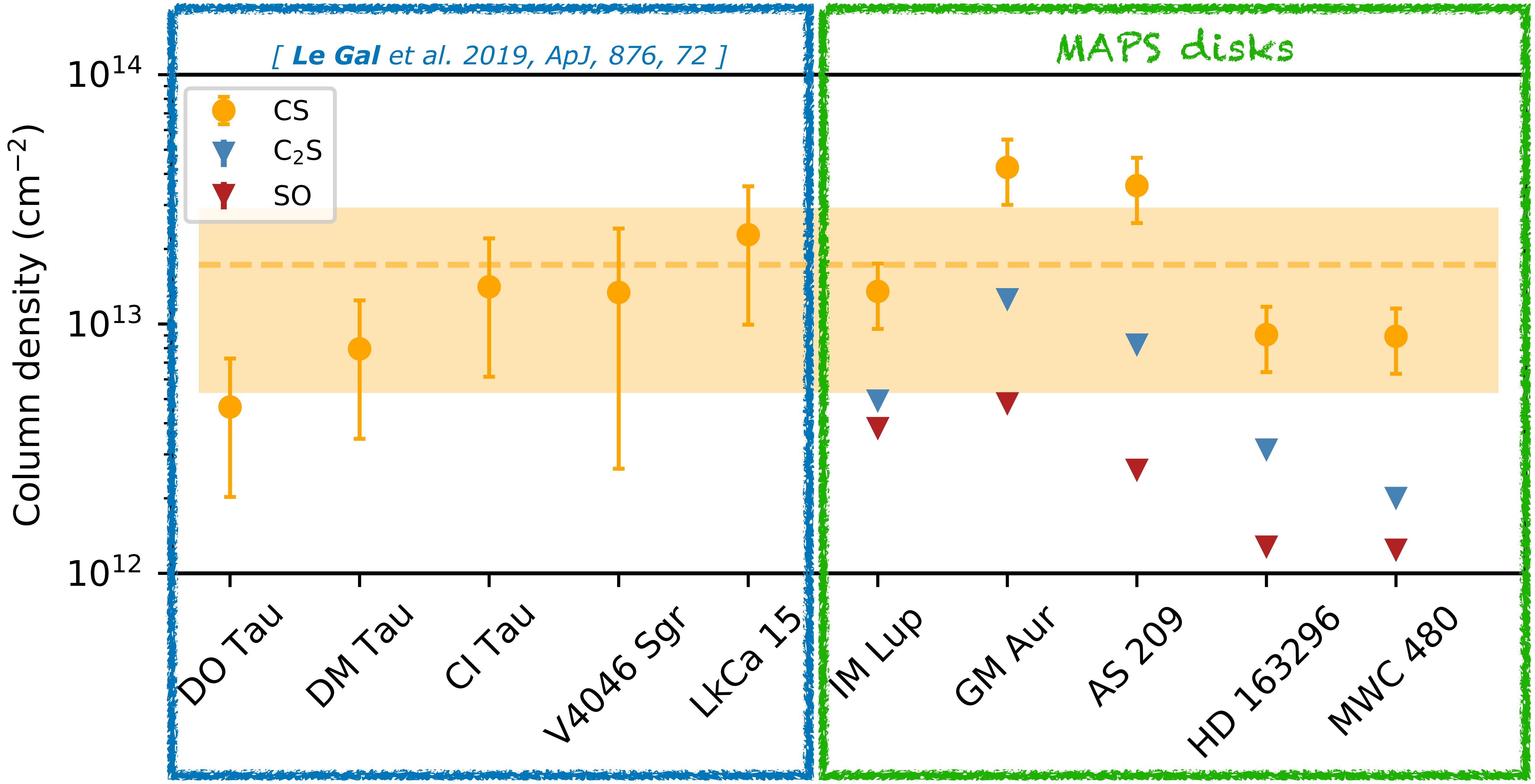
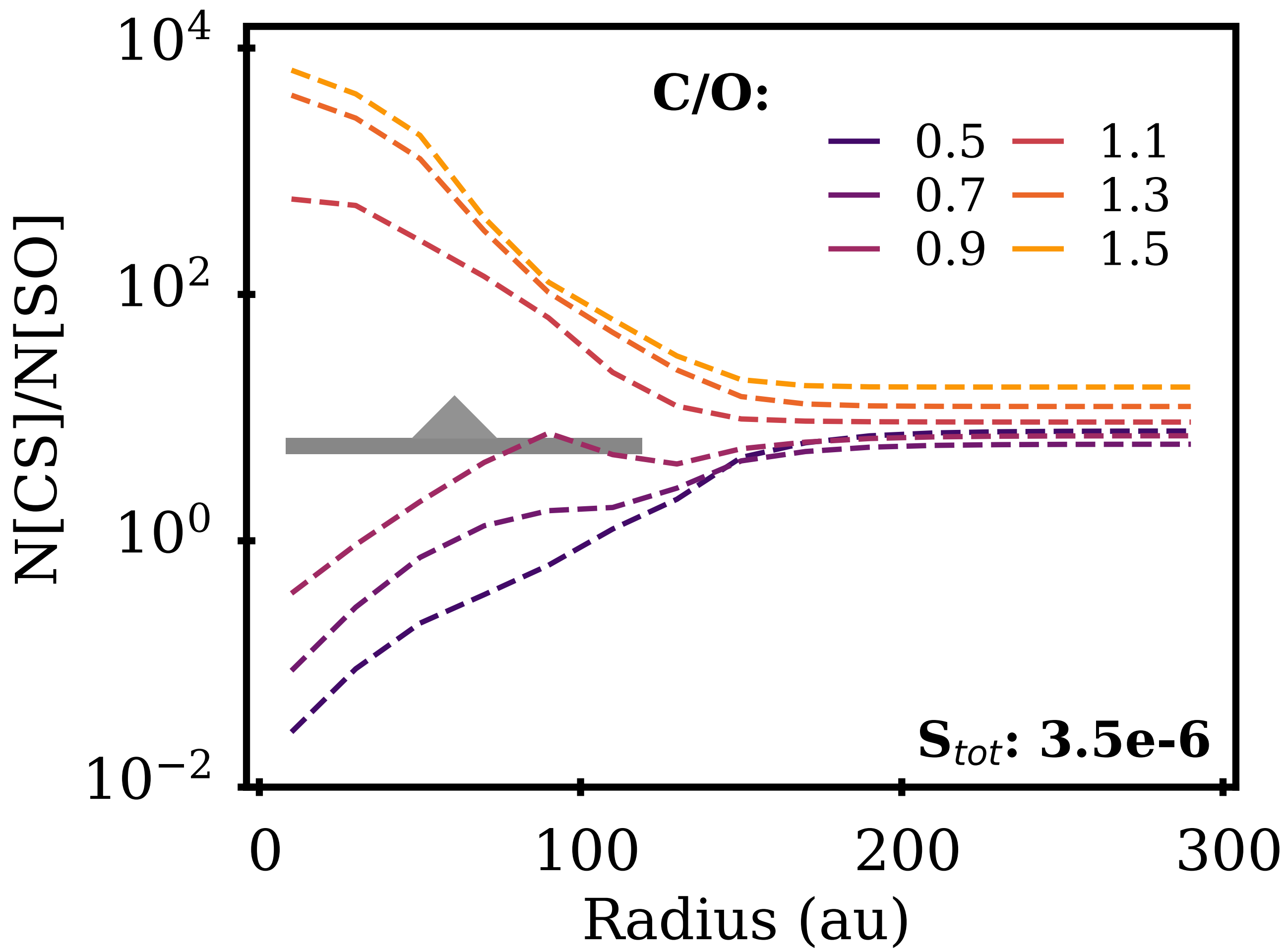


CS column density is rather flat in disks.

CS/SO probe for the C/O elemental ratio

Modeling results vs observations in MWC 480



=> CS/SO ratio is a promising probe for the C/O ratio in disks

[Bergin et al. 1997, Semenov et al. 2018]

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CS/SO probe for the C/O elemental ratio

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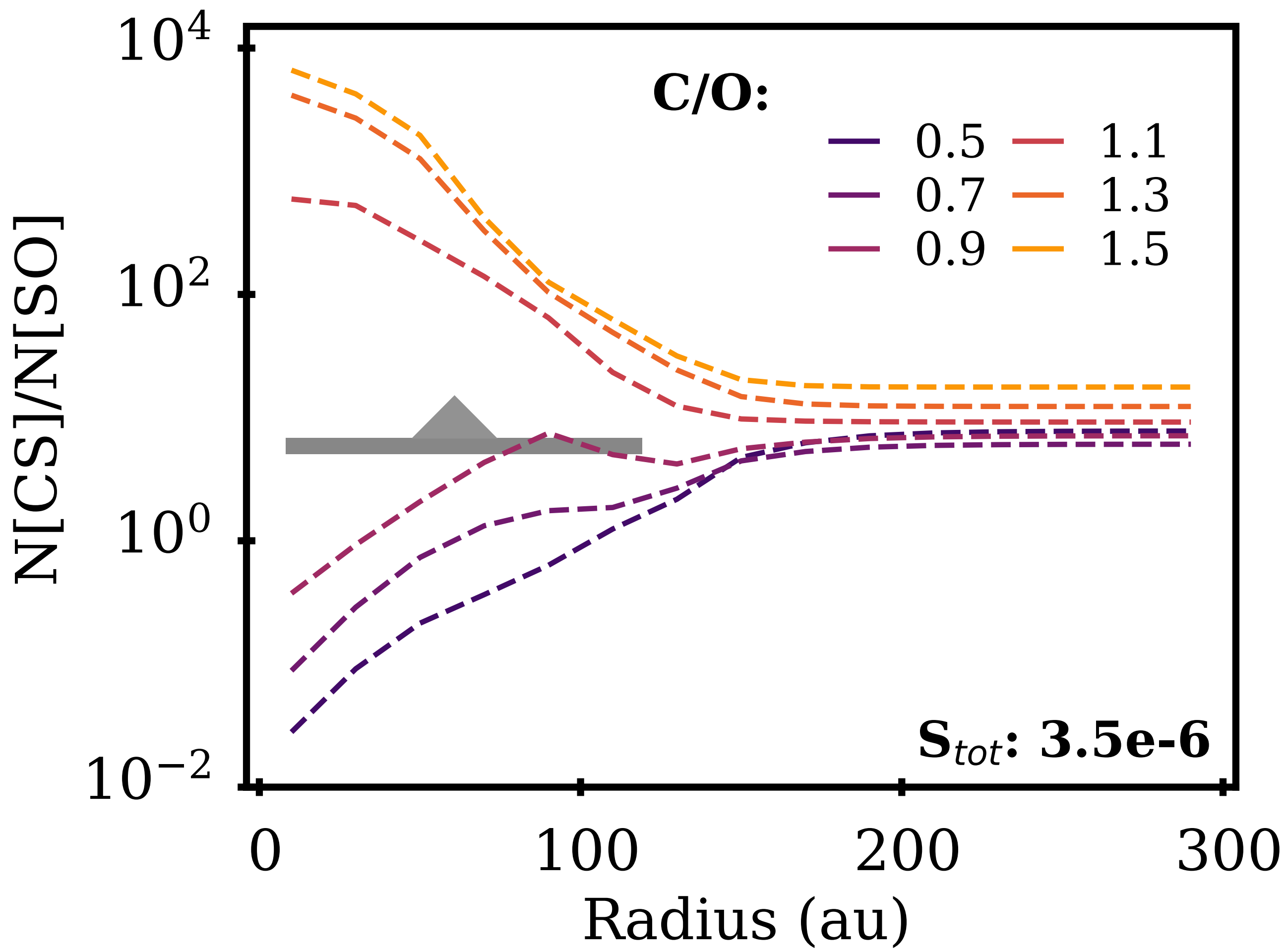

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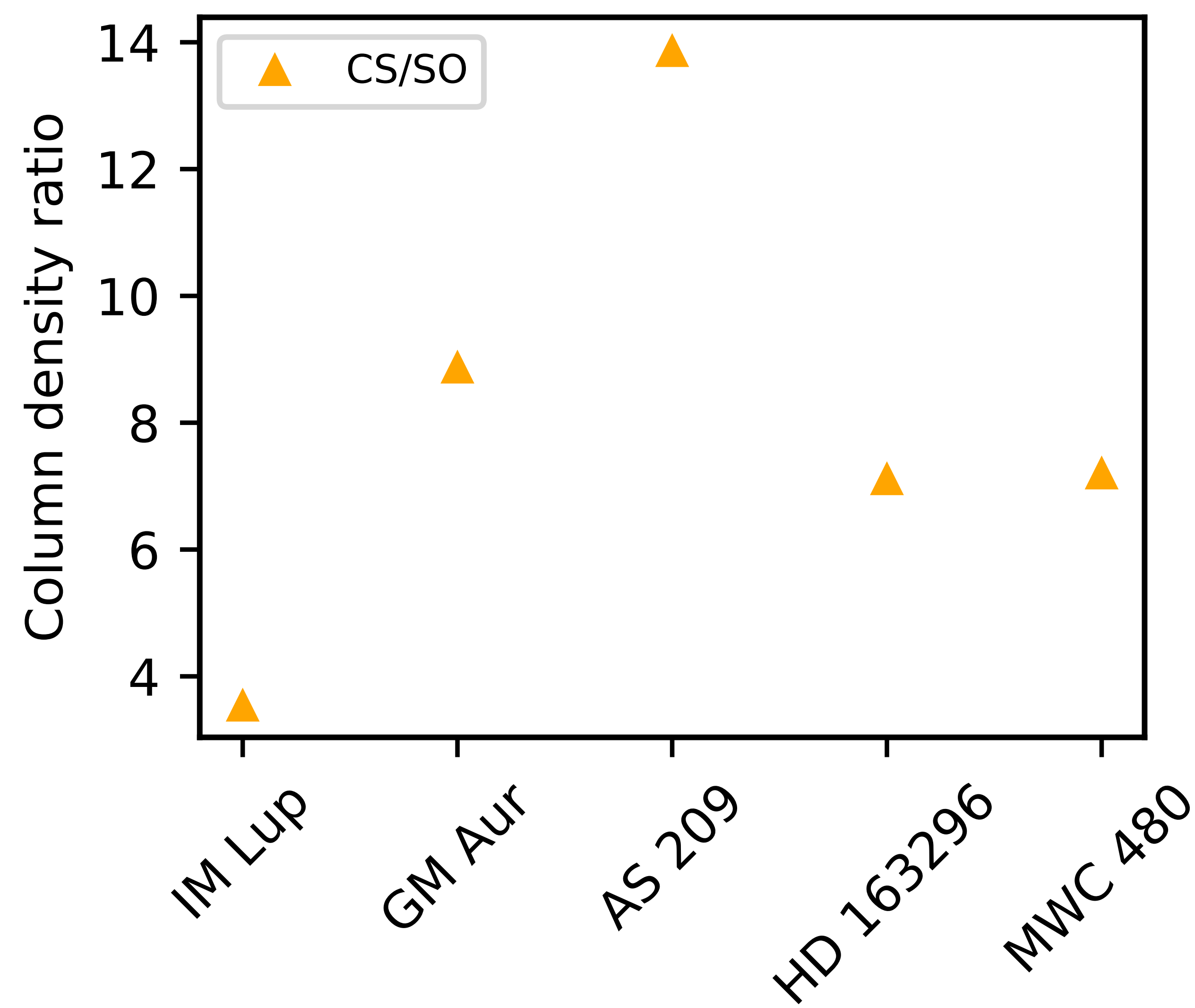
CS/SO observed in all five MAPS disks

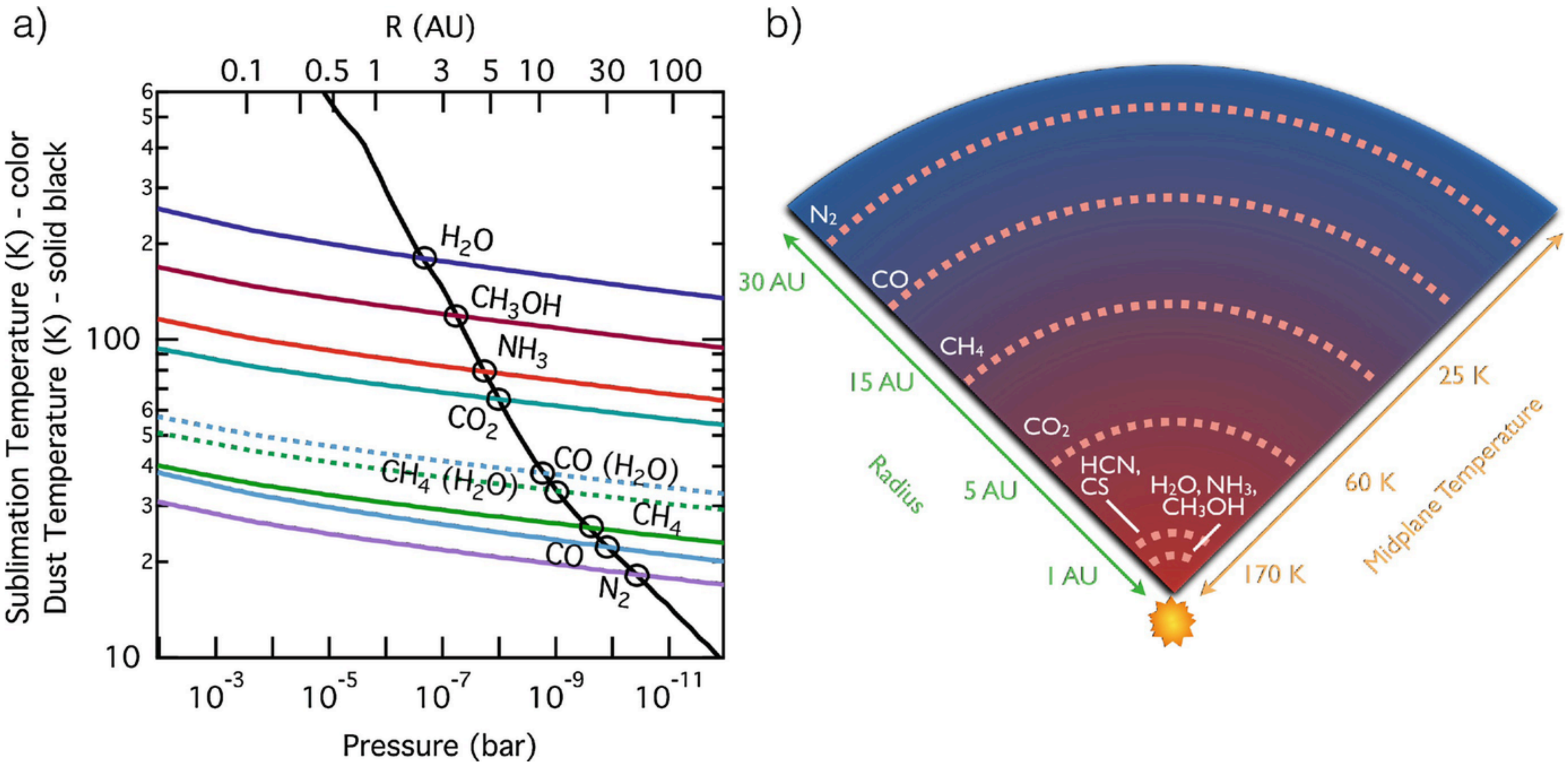


C/O ratio $\gtrsim$ 1 in most disks of our sample

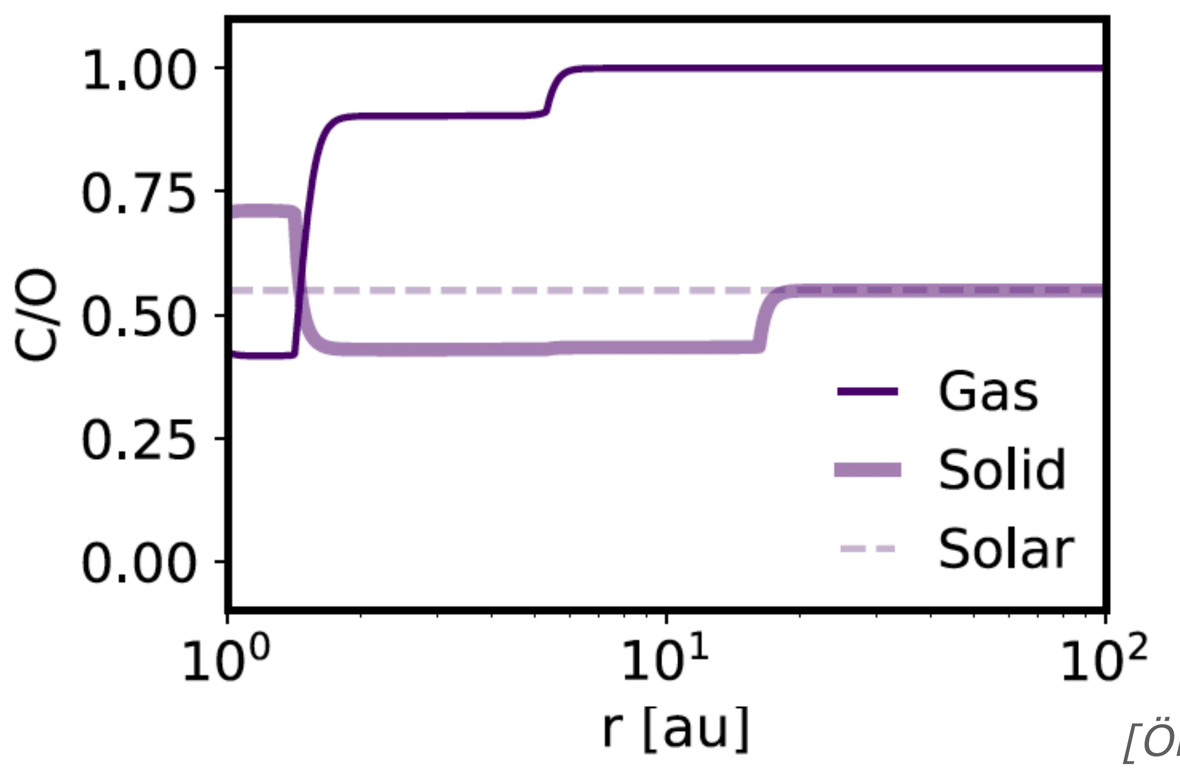
=> What does this telling us?

*[**Le Gal** & MAPS collaboration, 2021, ApJS, 257, 12]*

Why probing the C/O ratio?

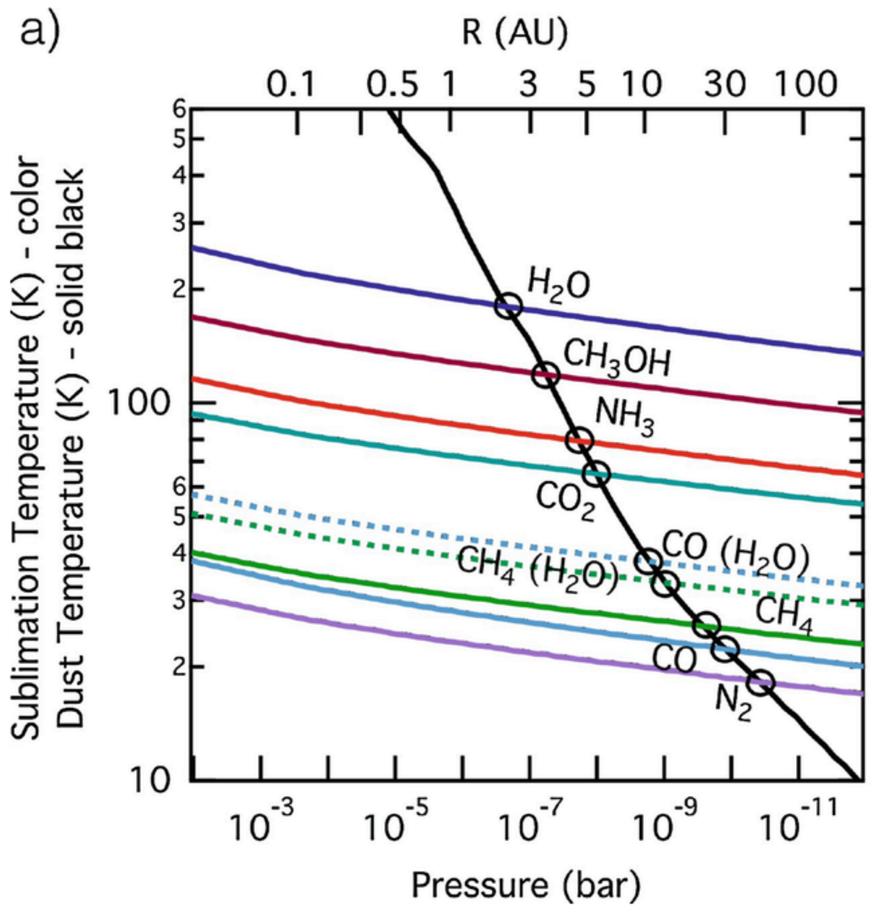


[Bergin & Cleeves 2018]



[Öberg & Bergin 2021]

Why probing the C/O ratio?



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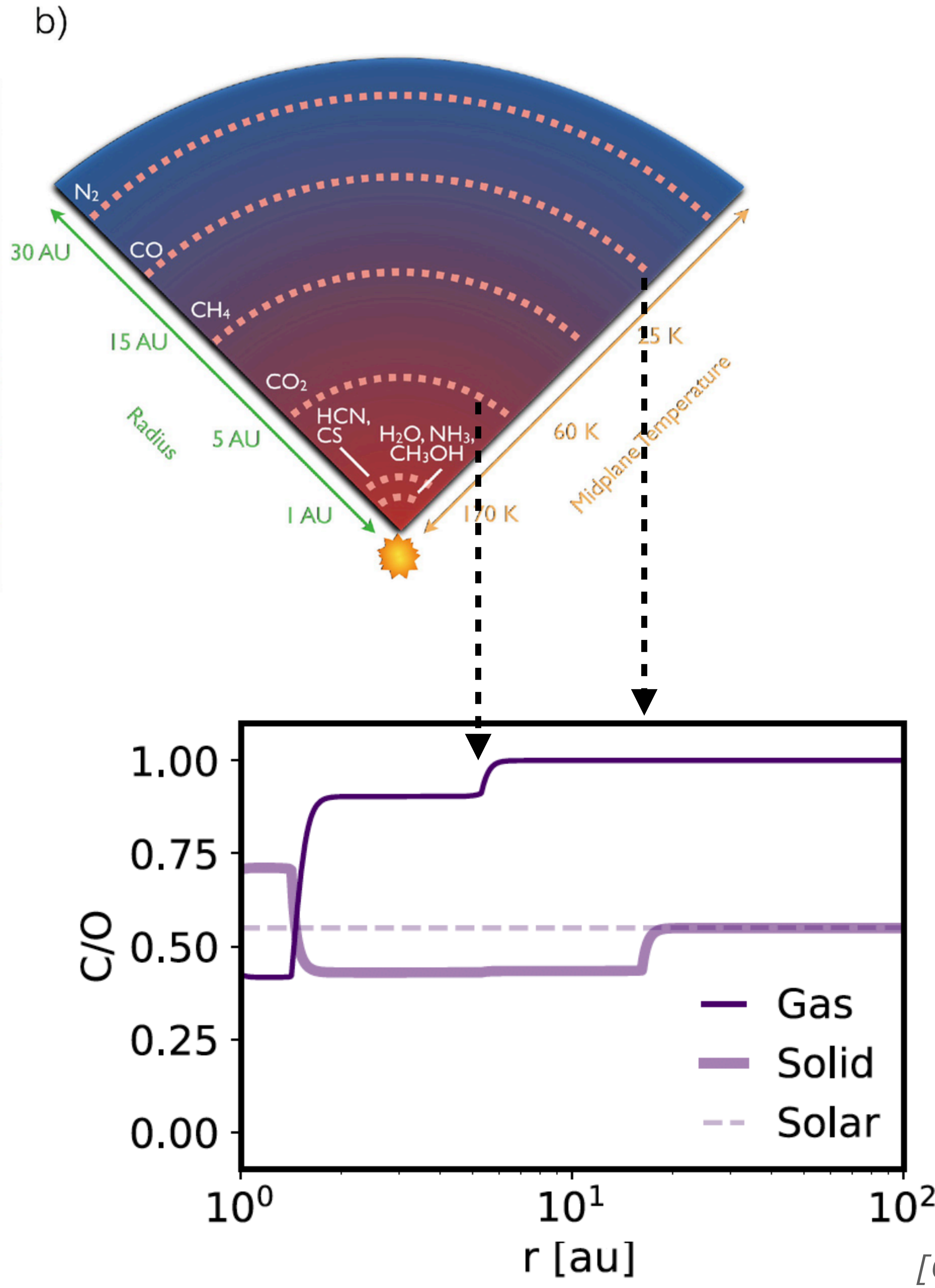
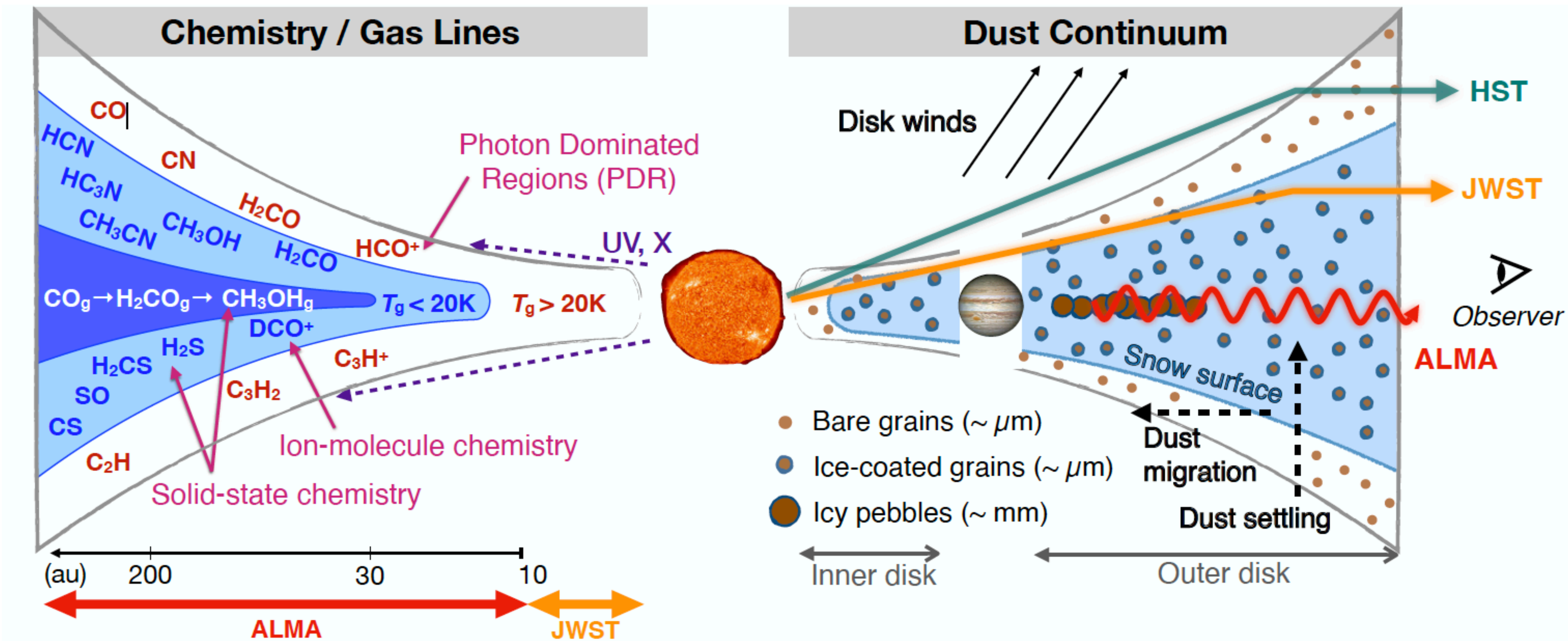


[Öberg & Bergin 2021]

Where do molecules reside vertically?

ALMA Large Program: **DiskStrat**

A comprehensive picture of chemical and vertical structures in protoplanetary disks



***PI: Le Gal** + **4co-PIs:** Ménard, Aikawa, Bergner, Espaillat*
*+ 34 **co-Is,** incl. **Maret** (Imaging Coordinator) & **Tanious** (Calibration Coordinator)*

ALMA-DiskStrat Sources

- 9 Edge-on-Disks:
  - already characterised in scattered-light by HST and JWST, mm continuum and CO emission and spanning a range of dust distributions, masses, thermal properties, and SFRs.
  - **all have guaranteed JWST observations**, which will provide complete datasets for a comprehensive picture of the full dust and gas vertical distribution from midplane (mm) to upper layers (NIR/scattered light).

Star	SFR	$M_\star (M_\odot)$	Dist. (pc)	Radius (")	Characteristics
TT	Tau	0.27	140	3.6	thick disk, jet, wind
TT	Tau	0.45	140	1.8	thick disk, jet & outflow
TT	Cha	1.0	190	0.7	thin disk, jet, binary system
TT	Cha	0.35	160	1.0	thick disk, jet, less incl. disk
TT	Cha	0.65	160	0.7	thin disk, jet & outflow
TT	Oph	1.2	147	1.3	thin disk, dust rings, wind
TT	Oph	0.58	120	2.1	thick disk, dust obs.
HAe	USco	–	145	0.9	thick disk, PAH, jet, binary system
HAe	–	2.5	250	5.0	thick disk, PAH, GoHam b

Outline

1. Why studying protoplanetary disk chemistry?
   => What for? How?

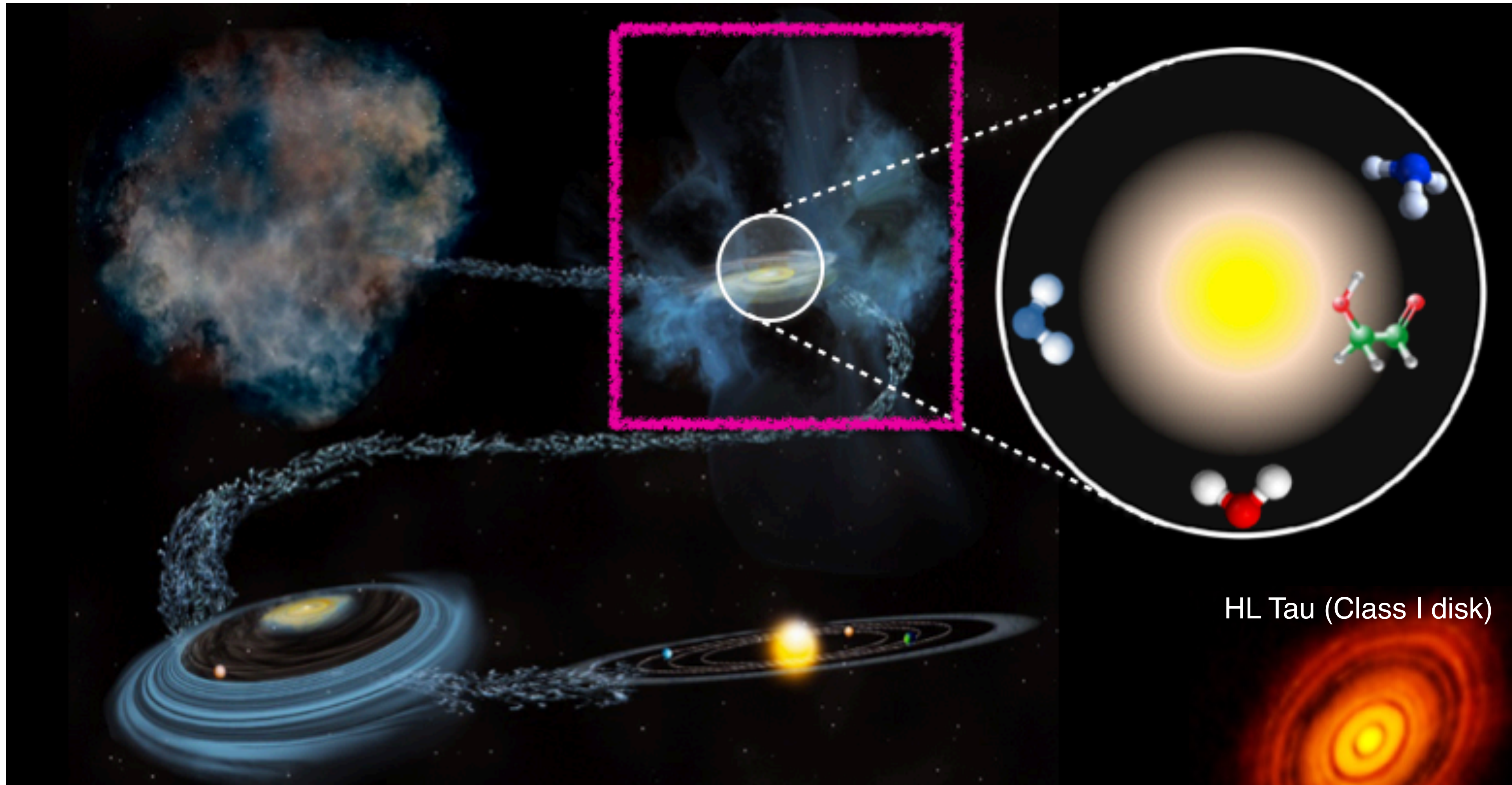
2. Can we probe the chemistry at planet-forming scales?
   => Which facilities? Which chemical tracers?

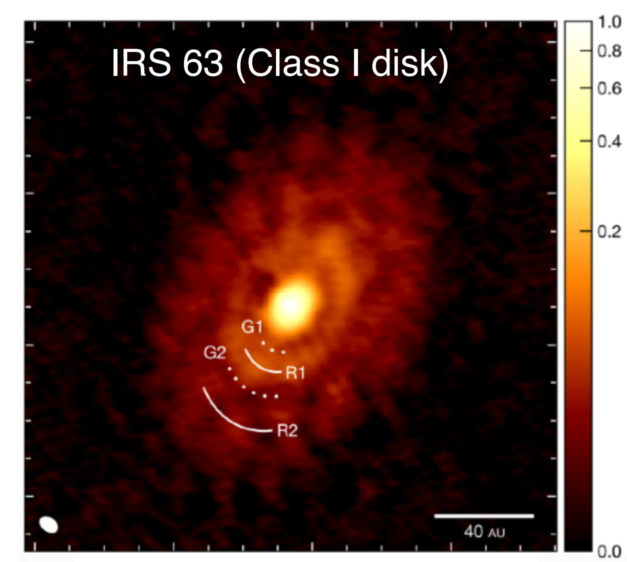
3. How does the disk's environment impact its chemistry and architecture?
   => Can we detect signatures of inheritance from the prestellar phase and/or chemical reprocessing within the disk?

Chemical exploration of Class I YSOs

- Several spectral surveys probed the chemistry of:
  (1) the earliest stages of star formation:
  - TIMASSS (Caux+2011),
  - PILS (Jorgensen+2016),
  - ASAI (Lefloch+2018),
  - SOLIS (Ceccarelli+2017),
  - FAUST (Codella+2021)

  (2) and of late planet-forming disks:
  - DISCS (Öberg+2010, 2011),
  - CID (Guilloteau+2016),
  - ALMA-MAPS (Öberg+2021)





Segura-cox+2020 (Nature)

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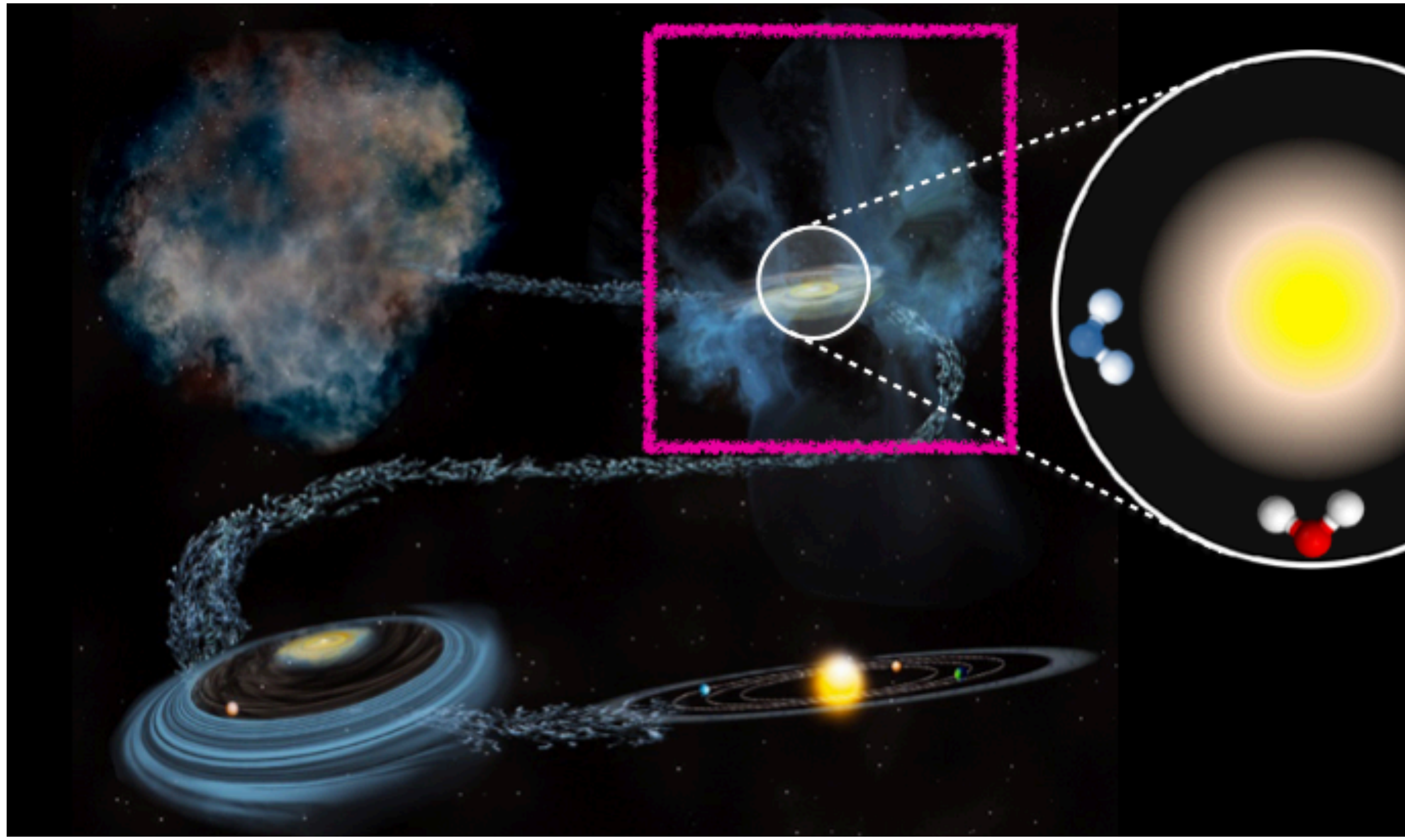


The CHEMYSO IRAM survey [PI: Le Gal]

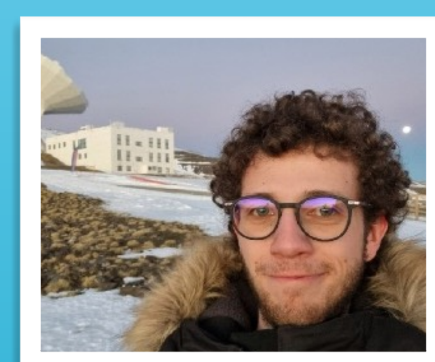
Source	R.A.[(a)] (J2000)	Dec.[(a)] (J2000)	T_{bol} (K)	$L_\star$[(b)] ($L_\odot$)	$M_{Env.}^{(b)}$ ($M_\odot$)	$M_{Disk}^{(b)}$ ($M_\odot$)	$M_{Disk}^{(b)}/M_{Env.}$	$R_{Env.}^{(b)}$ (au)	$R_{Disk}^{(b)}$ (au)	V_{LSR} (km/s)	Dist. (pc)
IRAS 04302+2247	04:33:16.501	22:53:20.400	122[(c)]	0.4	$0.017^{+0.006}_{-0.004}$	$0.114^{+0.019}_{-0.026}$	6.7	1086	244	5.5 [1]	161±3[(f)]
IRAS 04295+2251	04:32:32.055	22:57:26.670	270[(c)]	0.3	$0.037^{+0.008}_{-0.006}$	0.018±0.001	0.49	1081	127	5.3 [1]	161±3[(f)]
IRAS 04365+2535	04:39:35.194	25:41:44.730	164[(d)]	2.1	$0.071^{+0.035}_{-0.019}$	$0.030^{+0.002}_{-0.003}$	0.42	1829	143	6.6 [2]	140±4[(f)]
IRAS 04016+2610	04:04:43.071	26:18:56.390	226[(d)]	7.0	$0.023^{+0.010}_{-0.004}$	0.009±0.001	0.39	1446	497	6.8 [2]	∼140[(g)]
IRAS 04166+2706	04:19:42.627	27:13:38.430	75[(c)]	0.2	0.100±0.009	0.027±0.003	0.27	1209	180	6.7 [3]	160±3[(f)]
IRAS 04169+2702	04:19:58.449	27:09:57.070	133[(c)]	0.8	$0.055^{+0.004}_{-0.005}$	0.012±0.001	0.22	672	39	6.8 [2]	160±3[(f)]
IRAS 04181+2654A	04:21:11.469	27:01:09.400	346[(e)]	0.3	$1.234^{+0.688}_{-0.391}$	0.006±0.001	4.8e-3	> 20000	47	7.1 [1]	160±3[(f)]

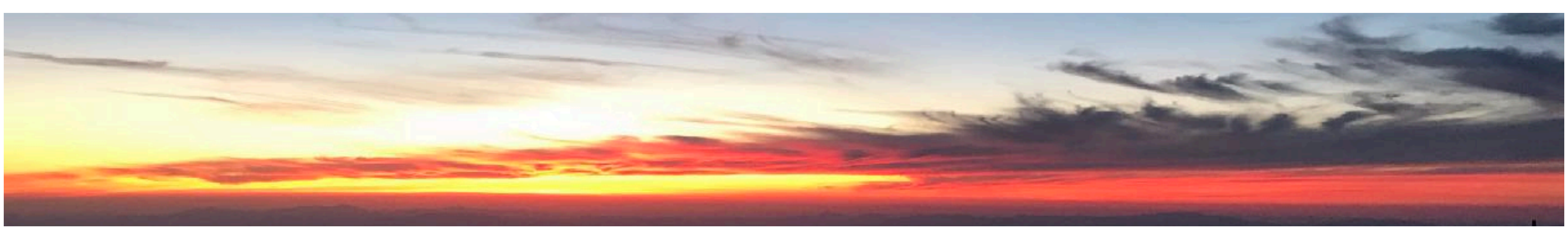
*[**Le Gal**, Öberg, Huang, Law, Ménard, Lefloch, Vastel, Lopez-Sepulcre, Favre, Bianchi, Ceccarelli et al. 2020, ApJ, 898,131]*
*[**Tanious**, **Le Gal**, Neri, Faure, Gupta, Law, Huang, Cuello, Williams, Ménard, 2024, A&A, 687,A92]*

First results of the CHEMYSO survey

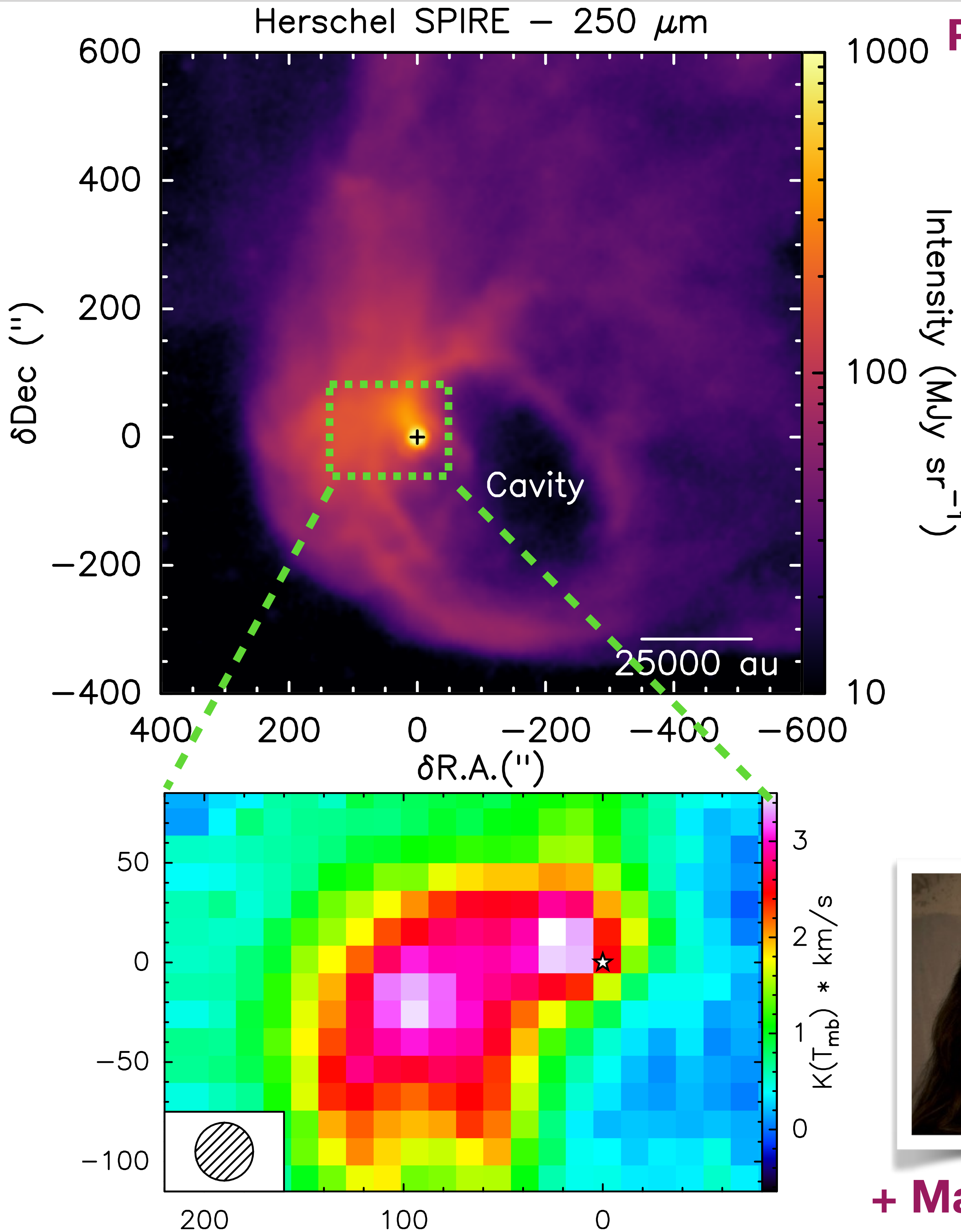
- ❖ Class I YSOs are molecule-rich! (*Le Gal et al. 2020*):
  - ▸ C, N, O, and S carriers (e.g. small cyanides, hydrocarbons, etc.) and variety of D, ^{13}C, ^{15}N, ^{18}O, ^{17}O and ^{34}S isotopologues
  - ▸ Other organics ($N_{atoms} > 3$) & COMs: H_2CO, C_3H_2, CH_3OH, HC_3N, CH_3CHO, *etc.*
- ❖ Detailed analysis: tracers of (i) dense cold gas, (i) shocked gas & dense ionized gas
- ❖ **Interferometric data required** to distinguish between YSO components
  => NOEMA data *(**Tanious**+2024, A&A & **Tanious**+2025 submitted),*

➜ **PHD of M. Tanious (2022-2025)**
(supervisors: R Le Gal & A. Faure)





Protostellar system environment



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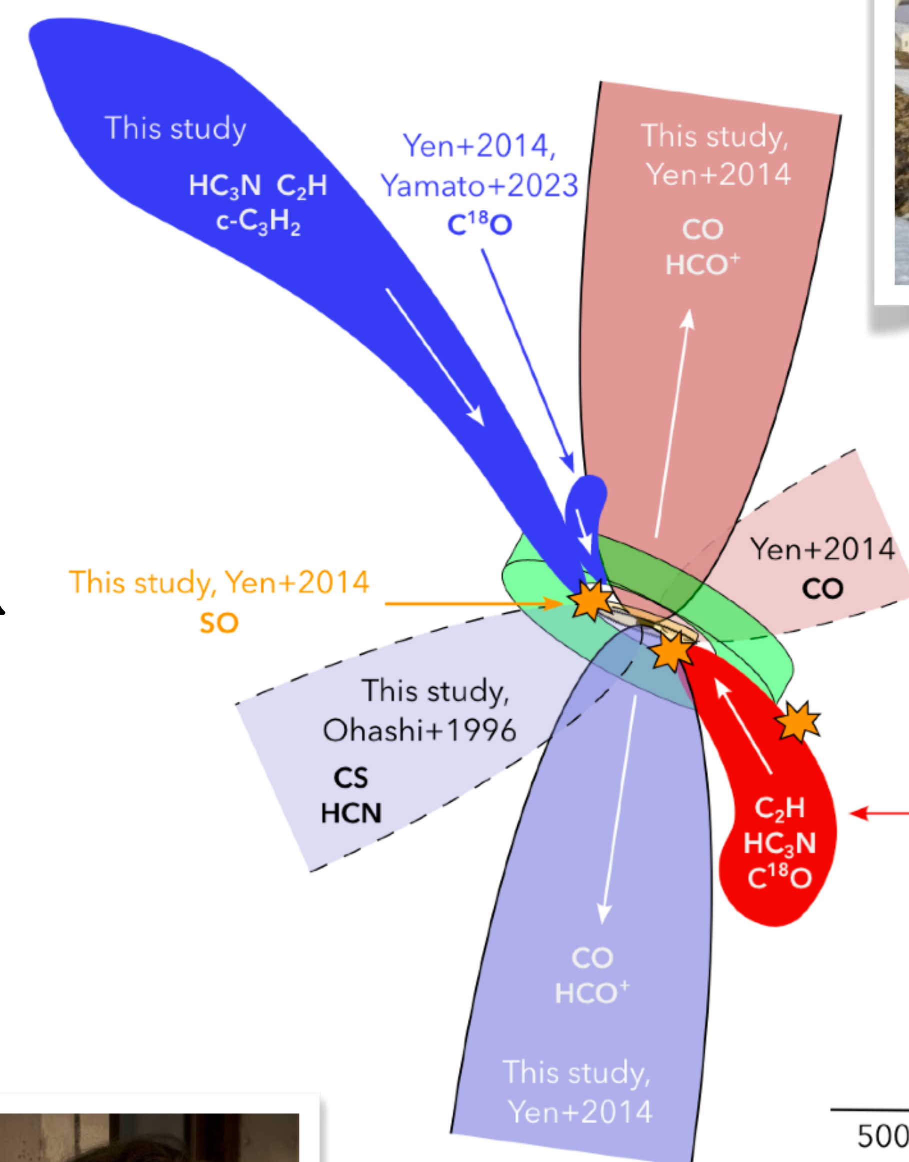
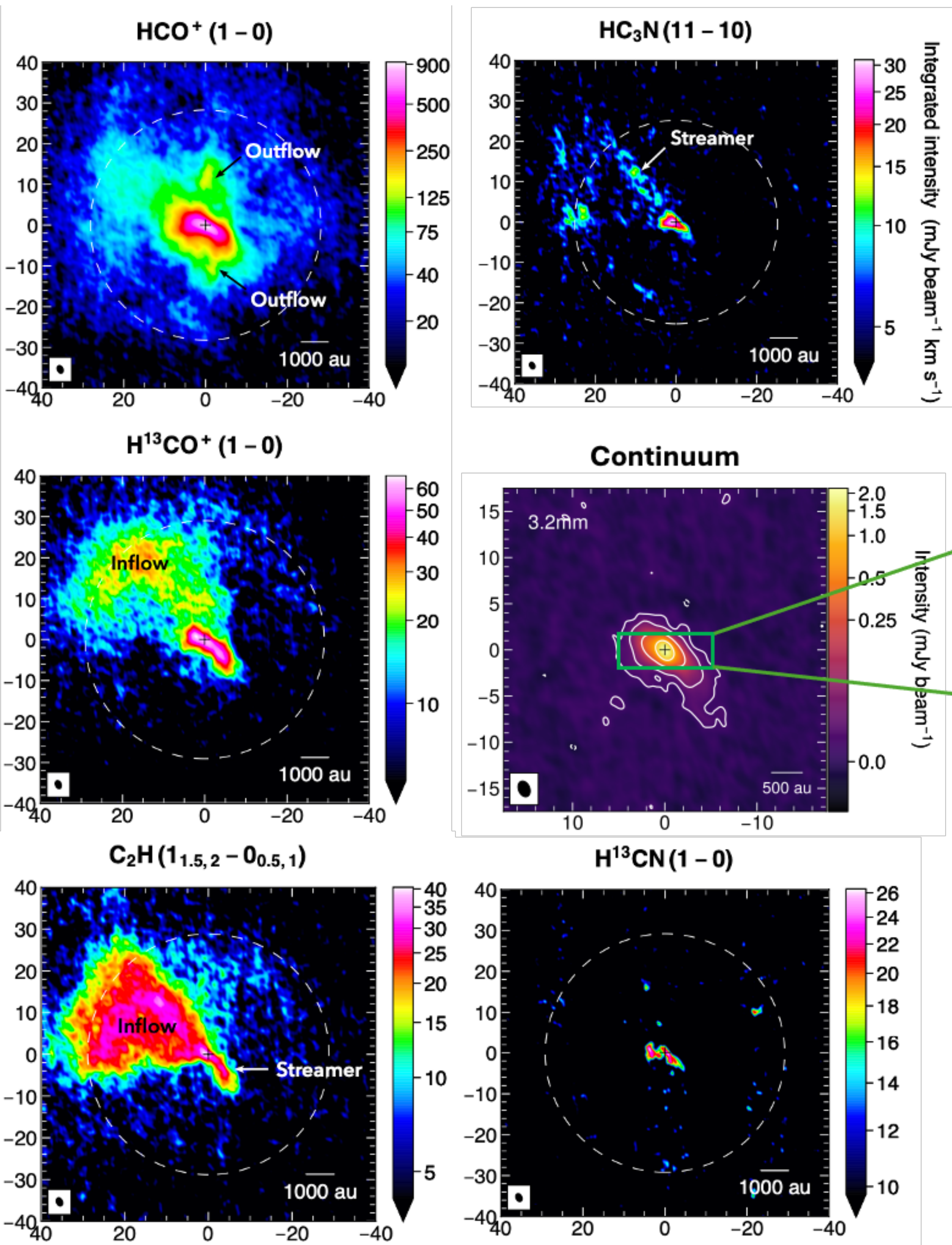


*[**Tanious+2024**, A&A*
*& **Tanious+2025** submitted]*

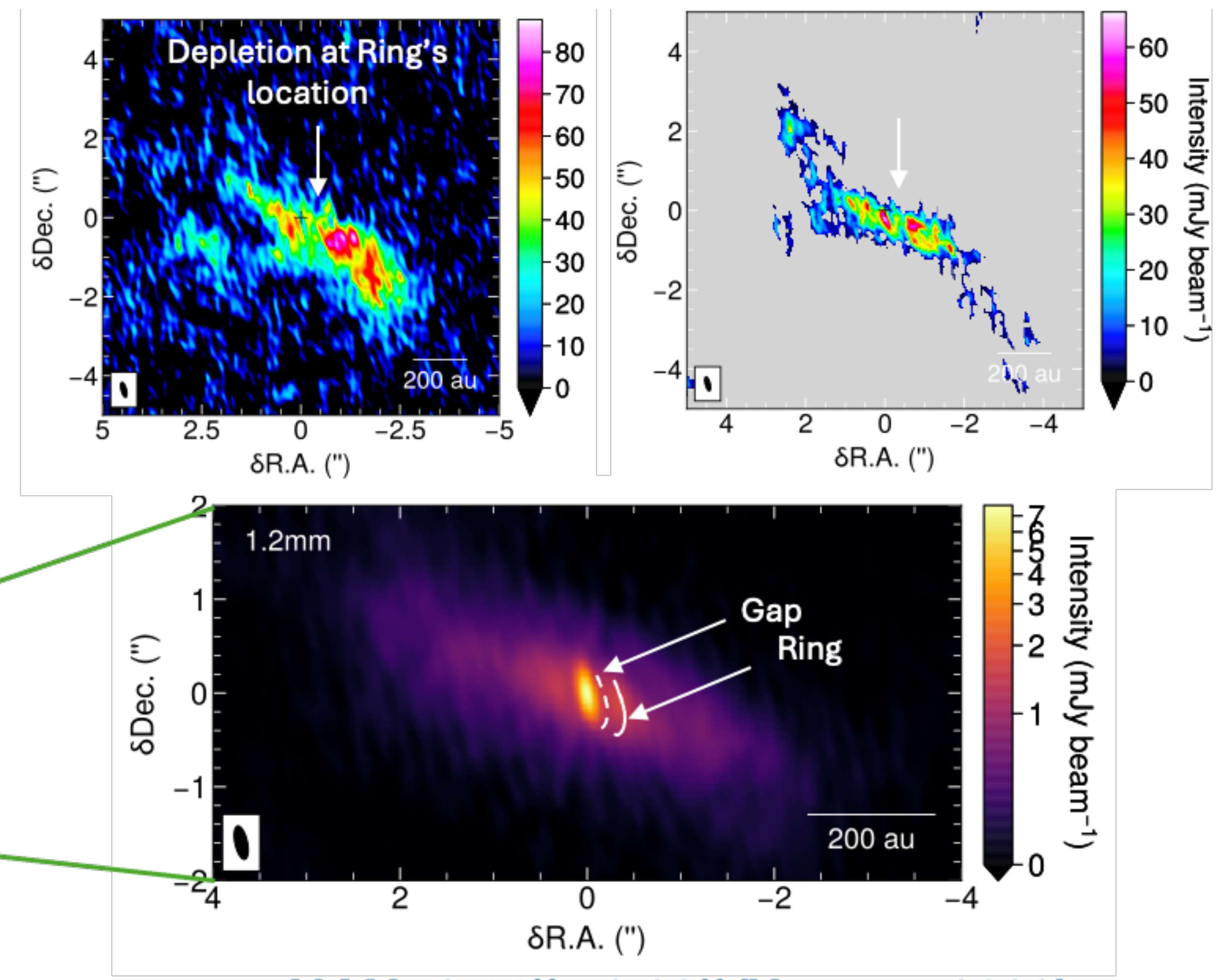
+ Master internship of C. Hoppe (2025)

Environmental influences on disk

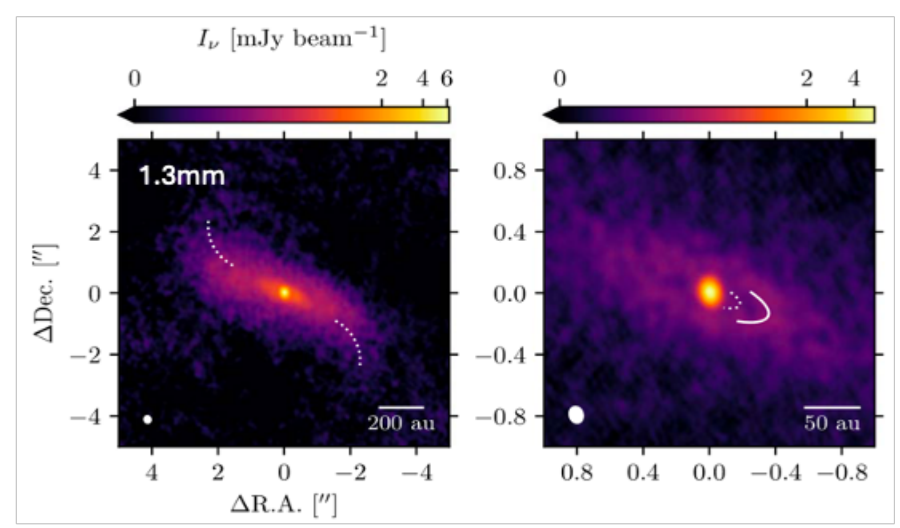
NOEMA+30m @ 3mm (Tanious et al. 2024)



NOEMA @ 1mm (A configuration, 0.36'' x 0.13'') in prep

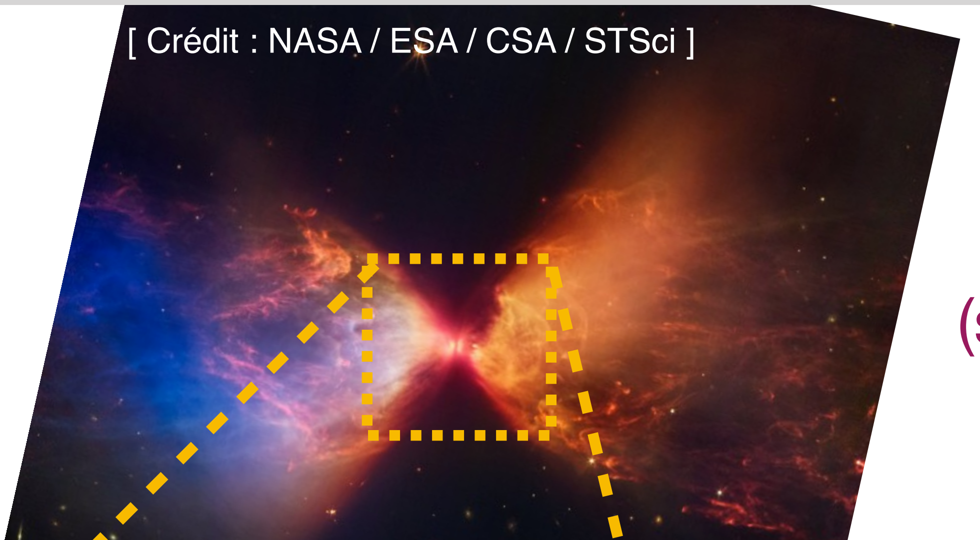


ALMA: 0.11'' x 0.08'' (Yamato+2023)

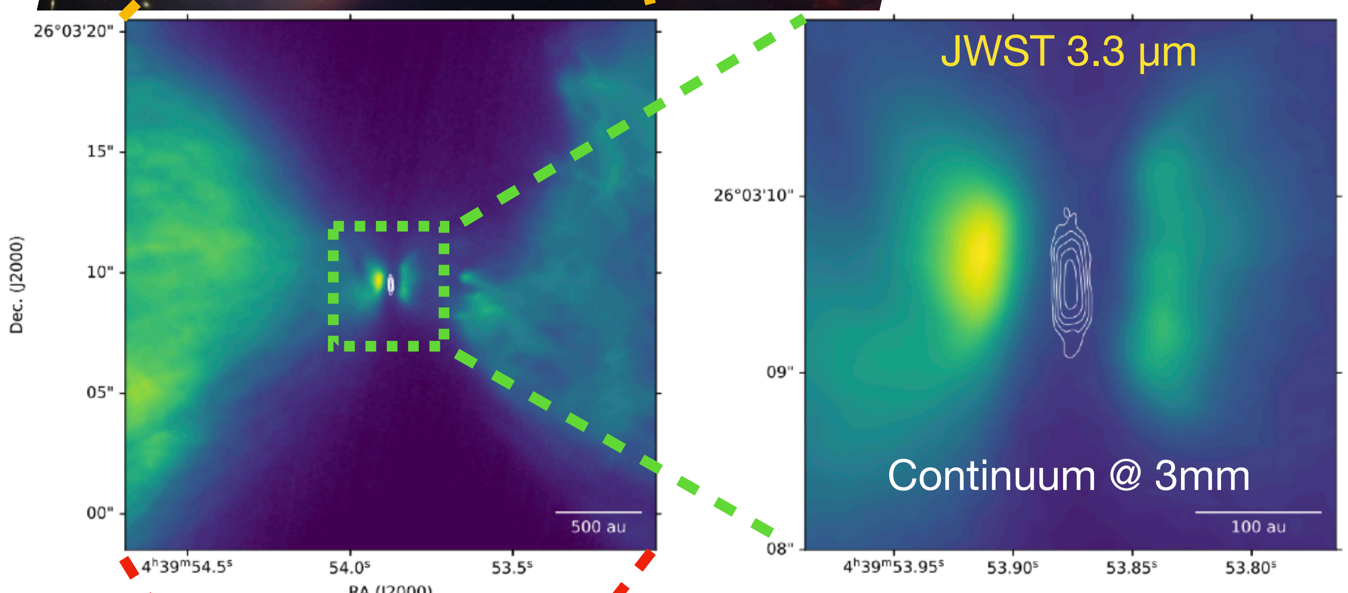


Environmental influences on disk

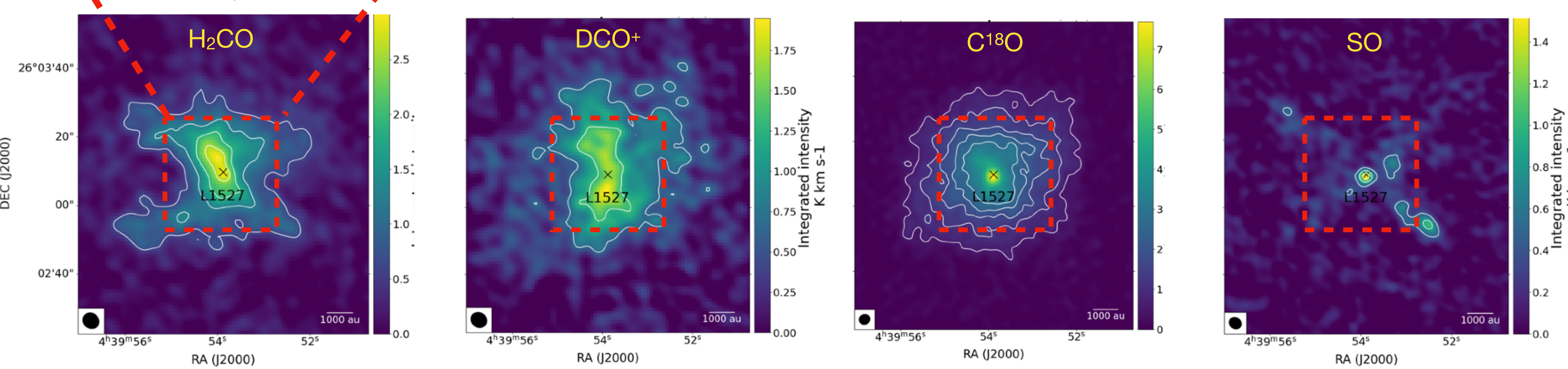
WORK IN PROGRESS

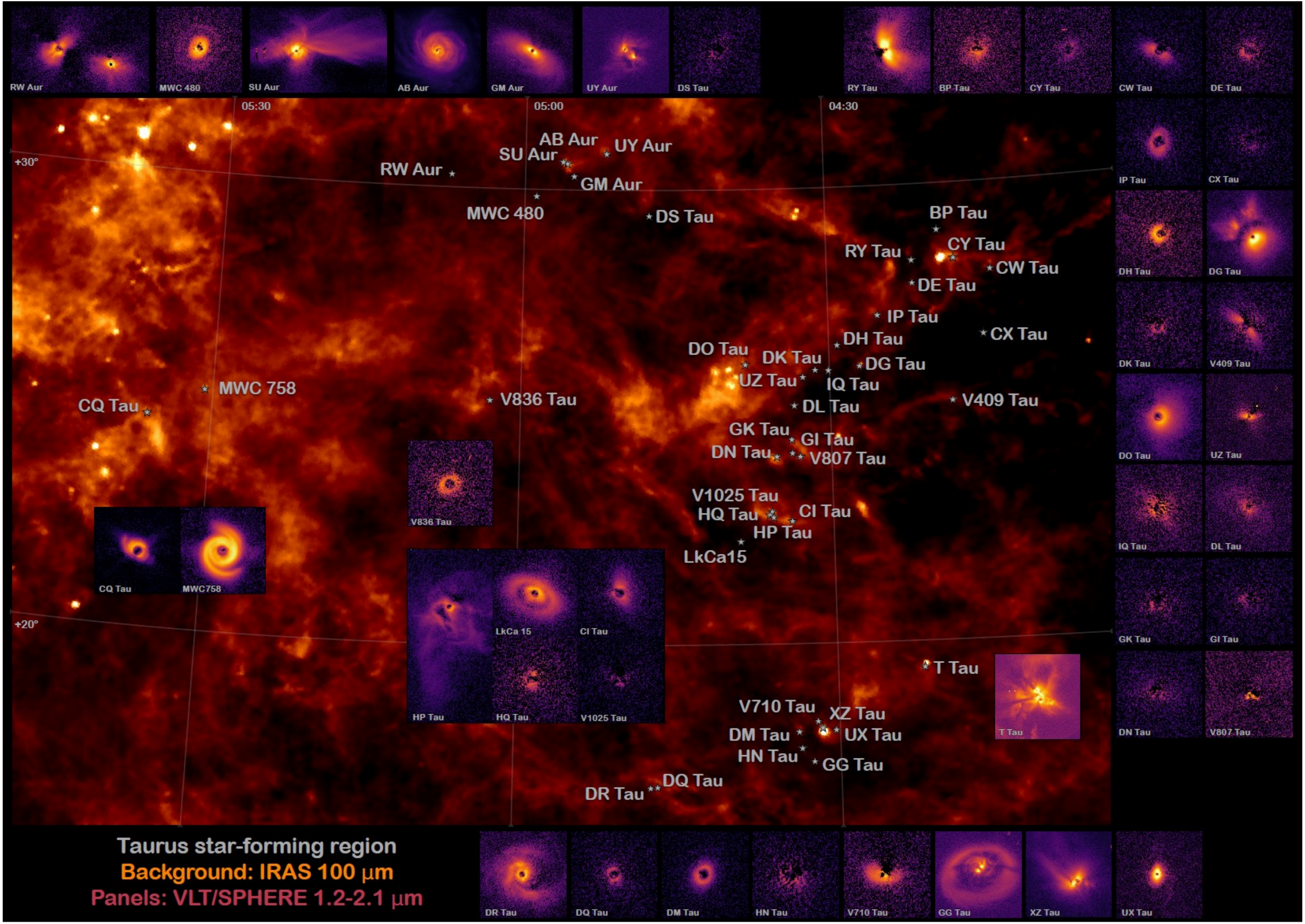


PHD of H. T'Kindt (2024-2027)
(supervised by S. Maret and R. Le Gal)



IRAM 30m + NOEMA project:
a chemical inventory of the gas infalling onto an emblematic nascent protoplanetary disk
—> check Hugo's Poster in S17





Planet-forming disks in Taurus observed by SPHERE
(Garufi, A., et al., 2024, A&A, 685, A53)

Summary and perspectives

- ➢ The latest high-resolution telescopes (e.g. JWST, ALMA and now NOEMA!) **allow detailed studies of the chemistry and structure of planet-forming disks:**
  - ✦ **Map** the vertical and radial molecular gas distributions (MAPS, exoALMA, DiskStrat)
  - ✦ **Key chemistry findings:** S**-reservoir in disks may be more organic than thought!**
  - ✦ **Search for new species in disks** predicted by models & obs. in ≠ astrophysical objects.
  - ✦ **Synergy with JWST (GTO & GO programs)** to probe the icy and warm gas disk composition

- ➢ **Astrochemical modelling to interpret observations** (chemical history & astrophysical probes)
  - ✦ **CS/SO** is a promising **probe for** the elemental **C/O ratio**
  - ✦ **C/O $\gtrsim$ 1 in most disks —> outer disk regions (?)**
  - ✦ **S/H** ratio : is sulfur partially released from clouds to disks?

- ➢ **Prospectives:**
  - ✦ Probe the **impact of large-scale environments on disk** structure and composition
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Hiring postdoc!

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