Tracing the chemical evolution of protoplanetary disks

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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. What about the environmental influence: How do large-scale conditions shape disk composition and architecture?
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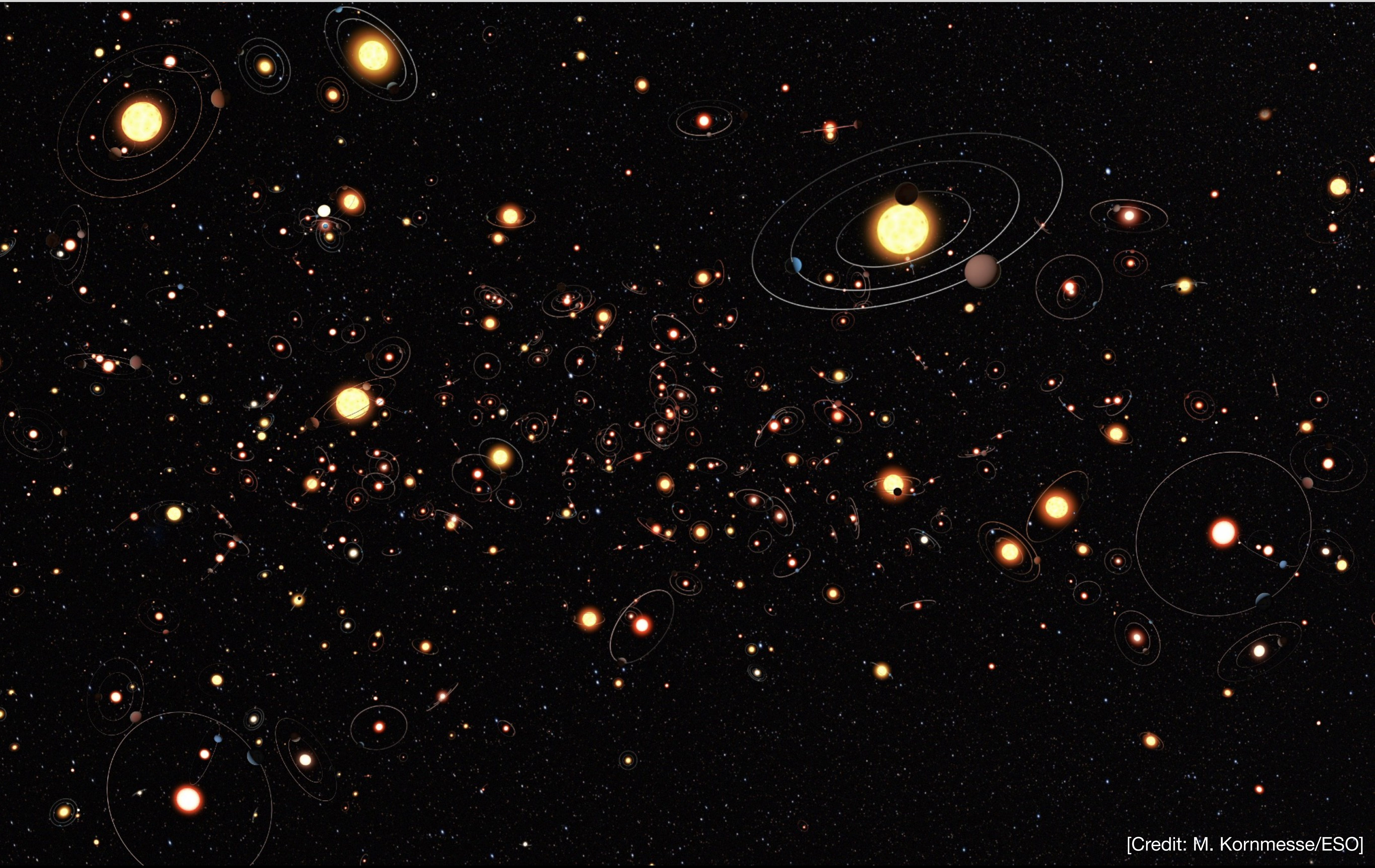
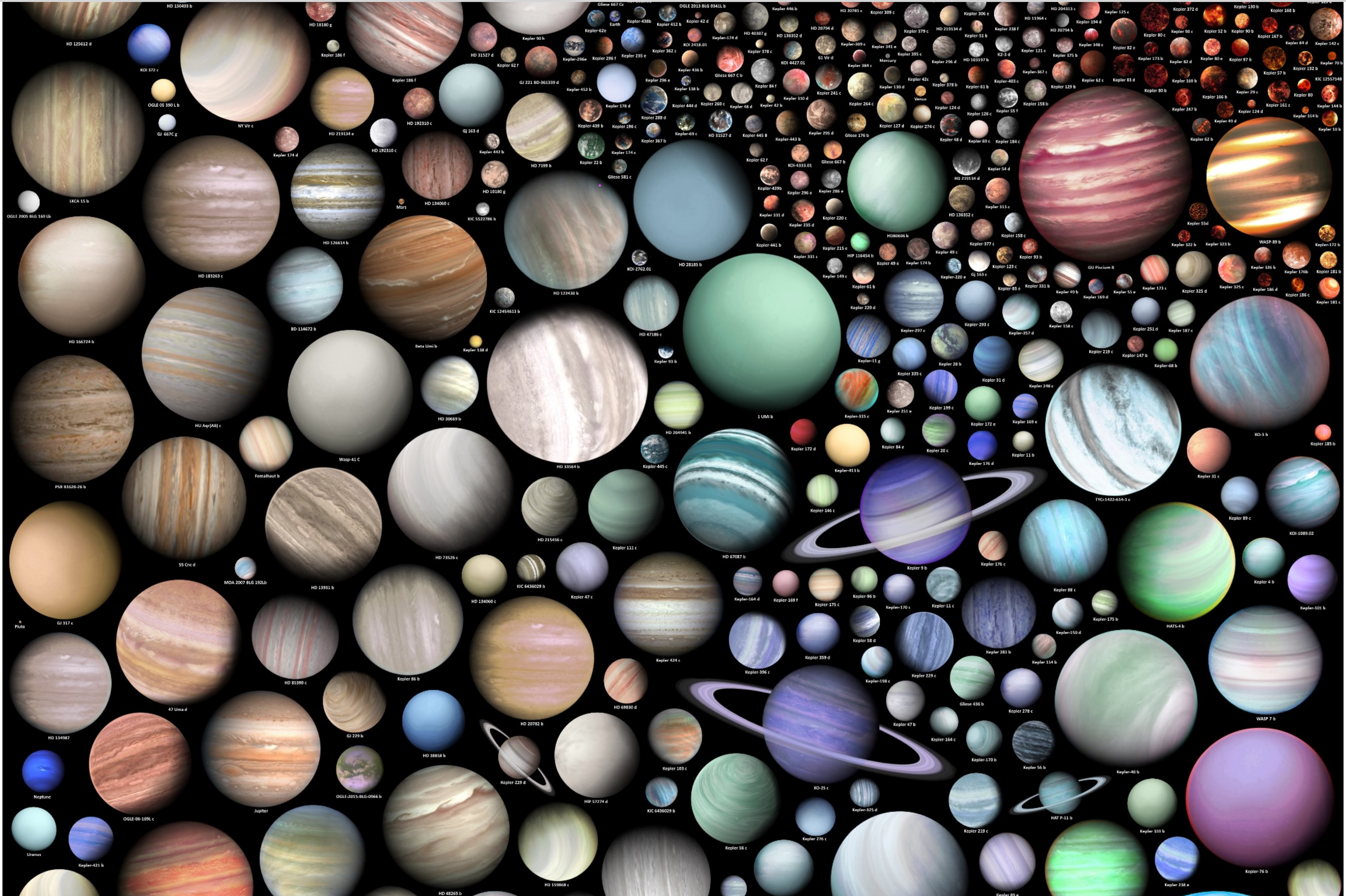
Most stars hosts his own planetary system



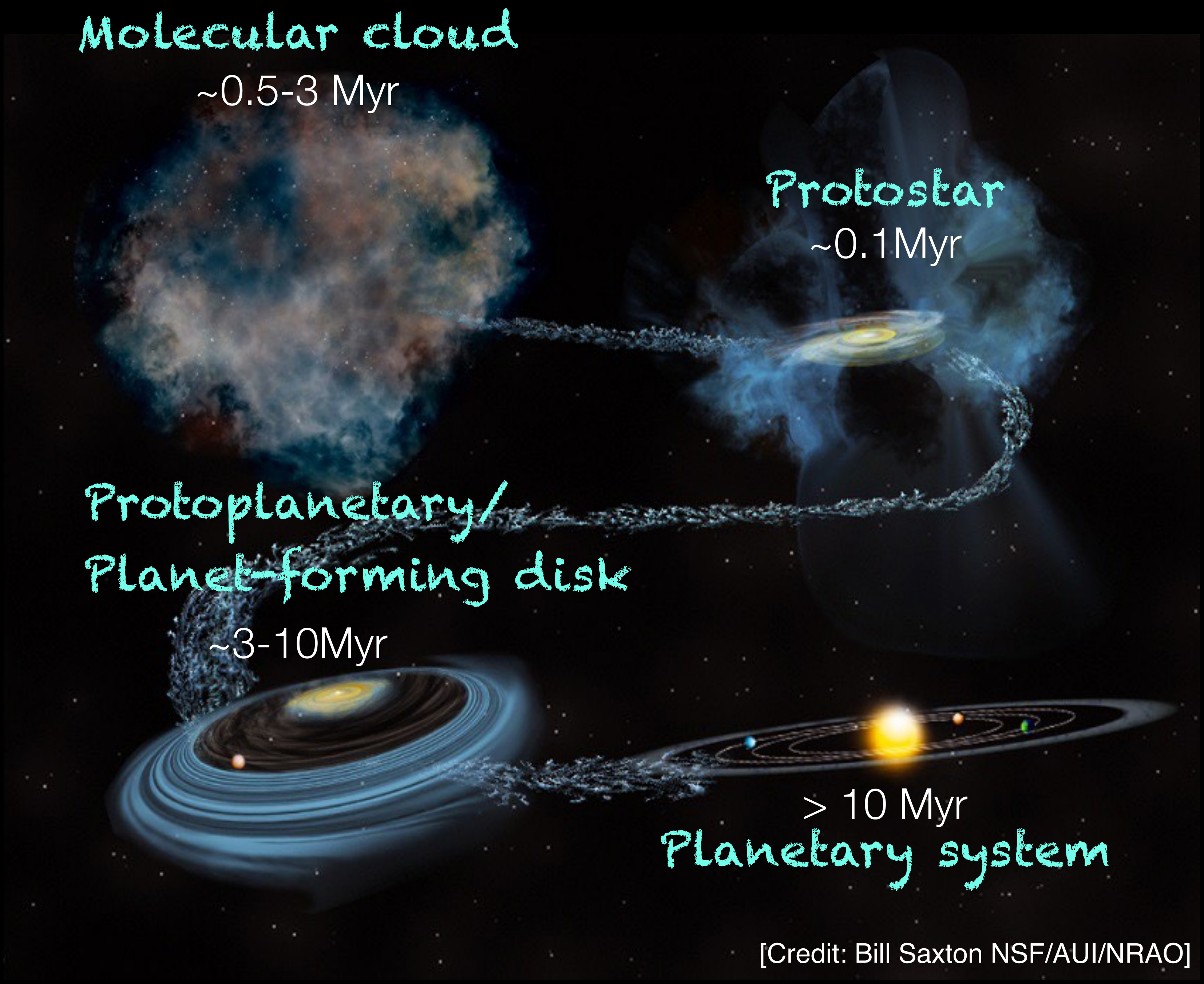
Planet bestiary

[Credit: M. Vargic]



Protoplanetary disks

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



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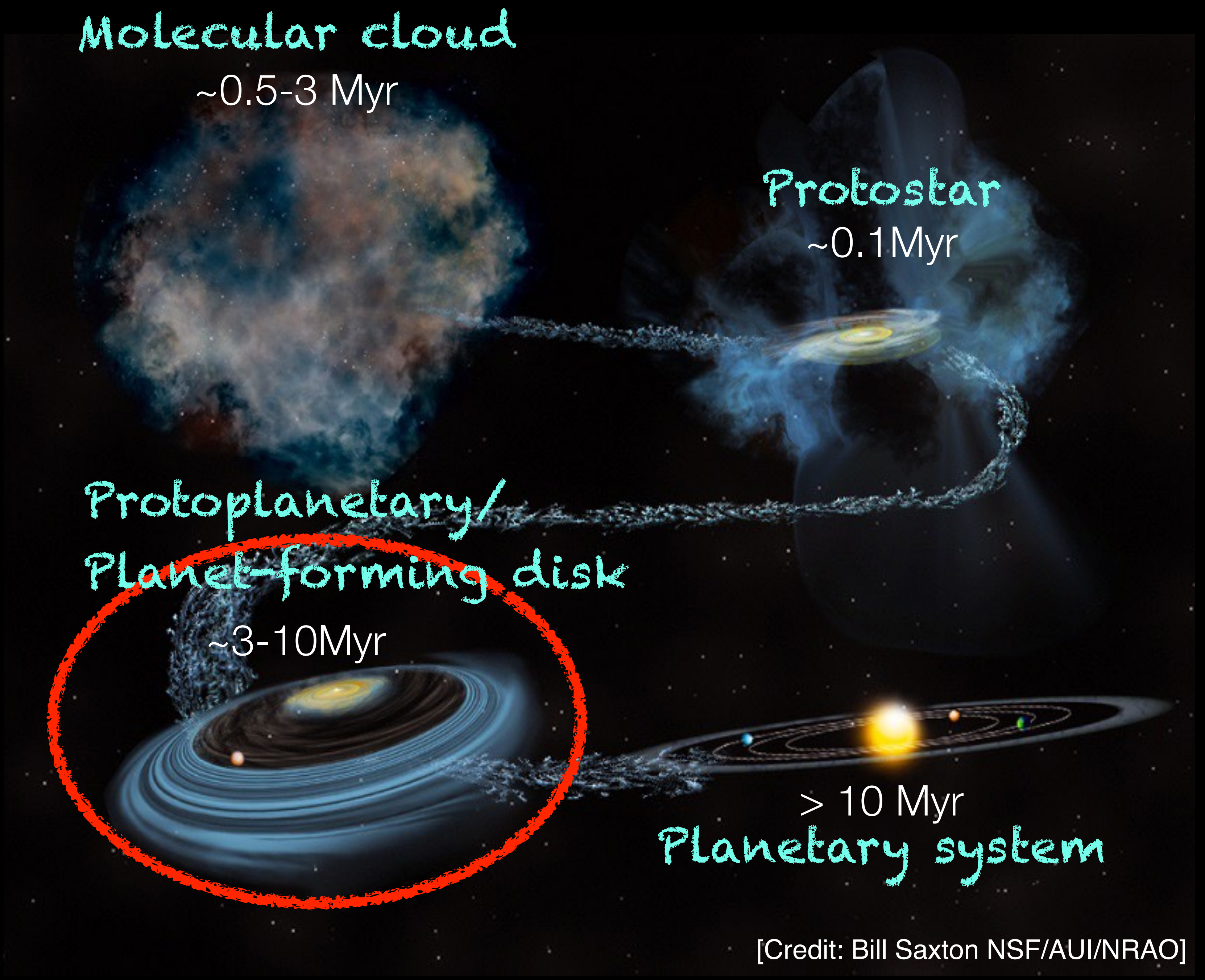

Chemistry in protoplanetary disks

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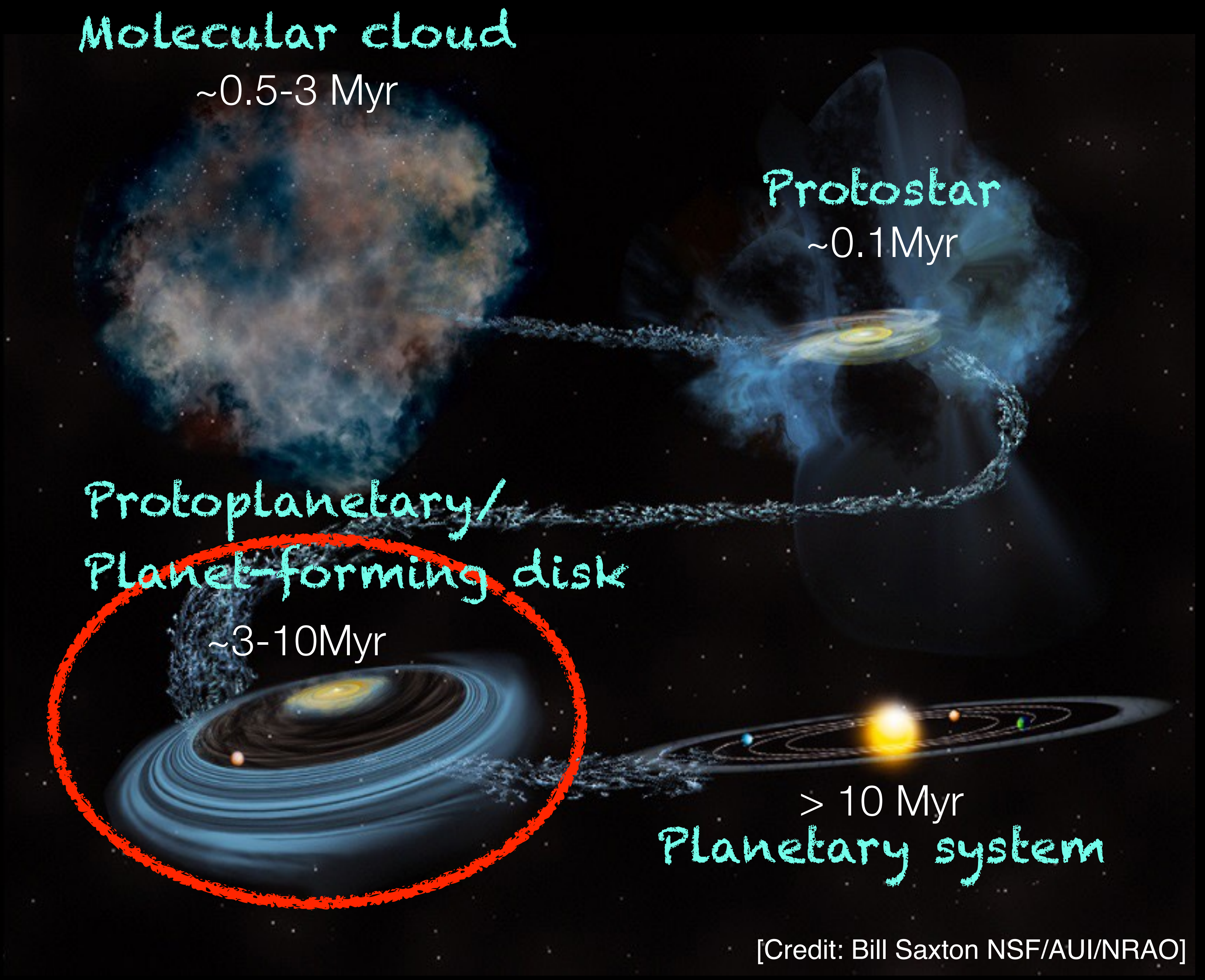
- *Formation, excitation & destruction of molecules?*



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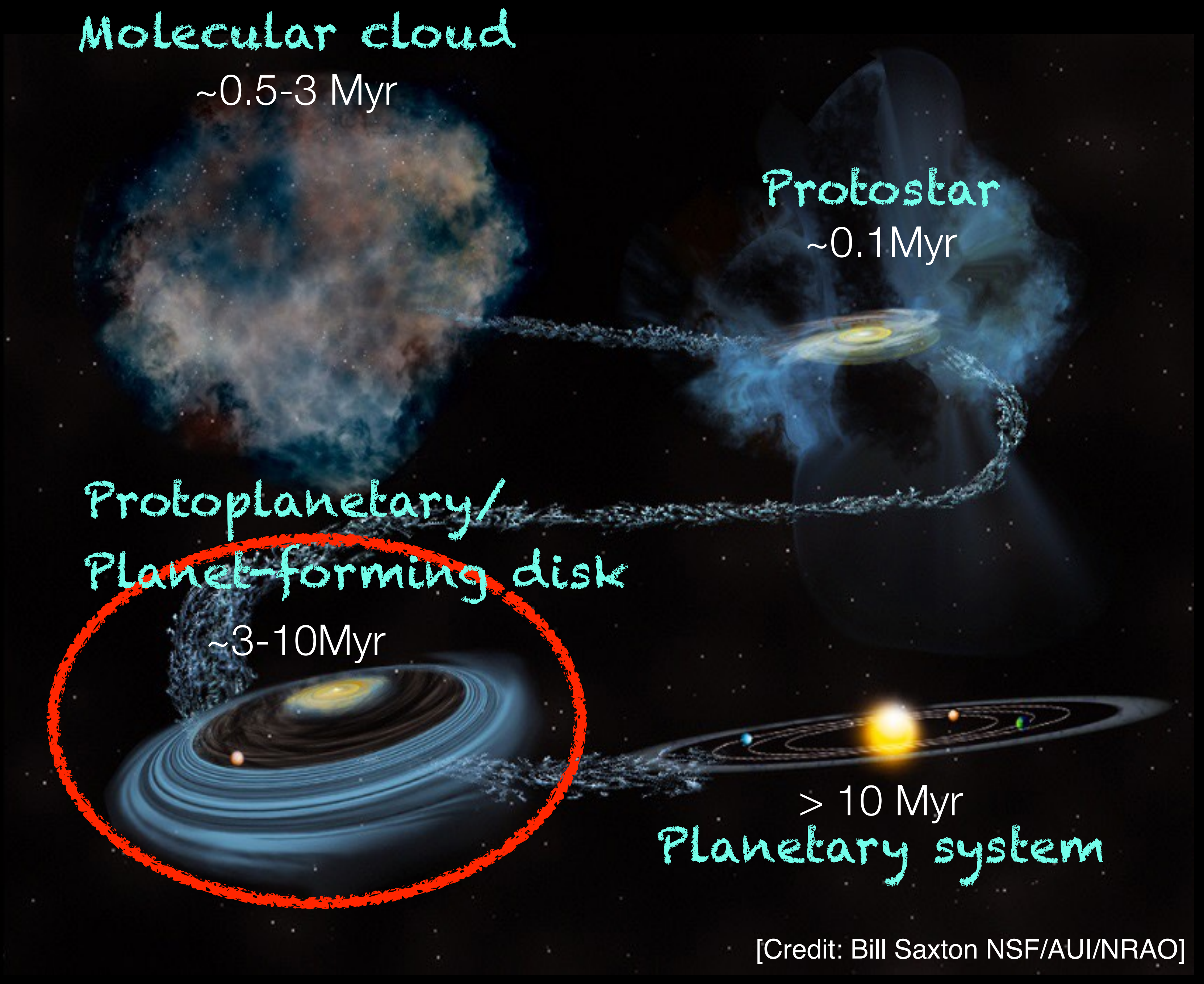

Chemistry in protoplanetary disks

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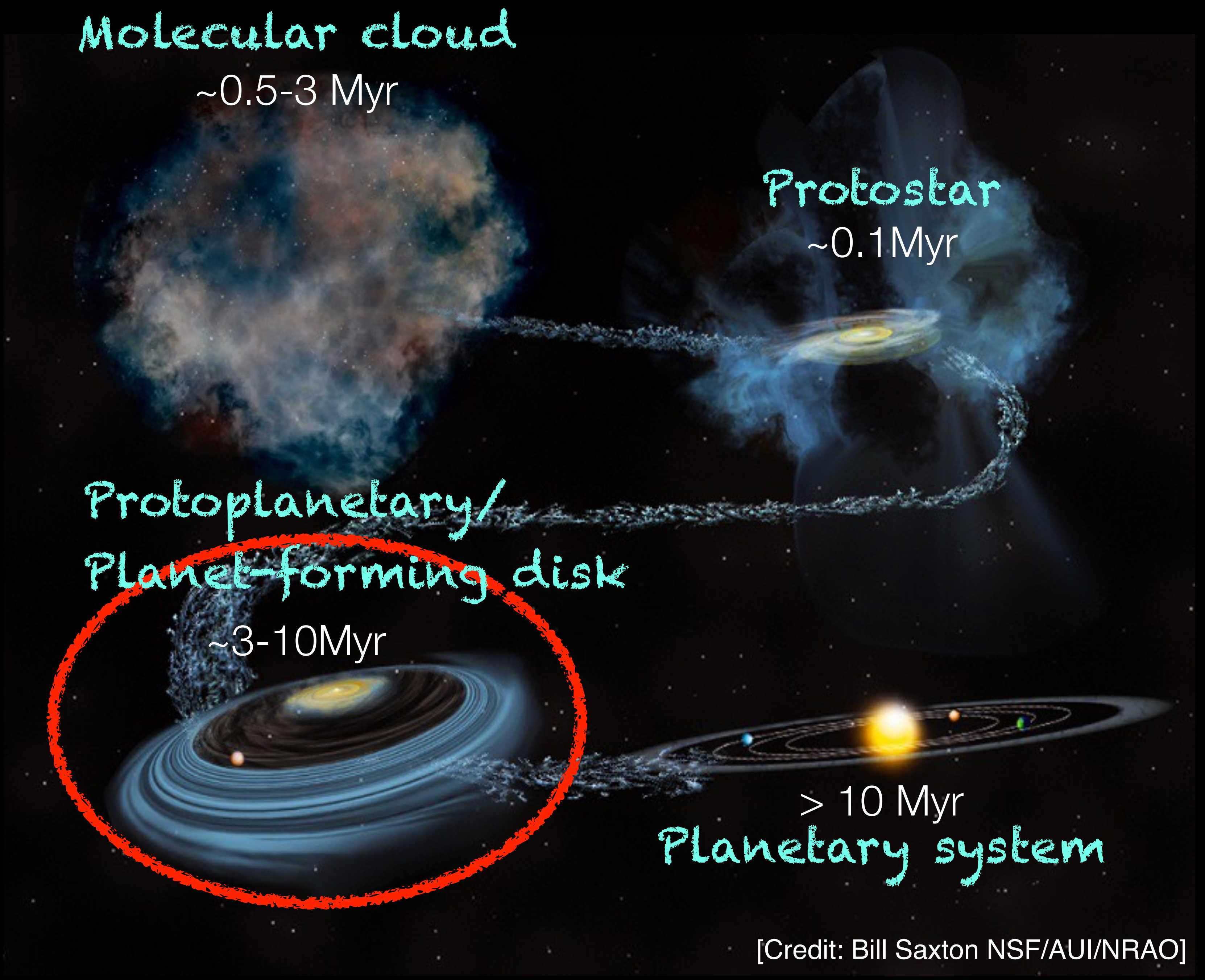
- *How does their chemical compositions and structures influence the future compositions of forming planets?*
- *Formation, excitation & destruction of molecules?*
- *Are molecules preserved from their initial formation in molecular clouds?*
- *Chemical (re)processing during star & planet formation?*



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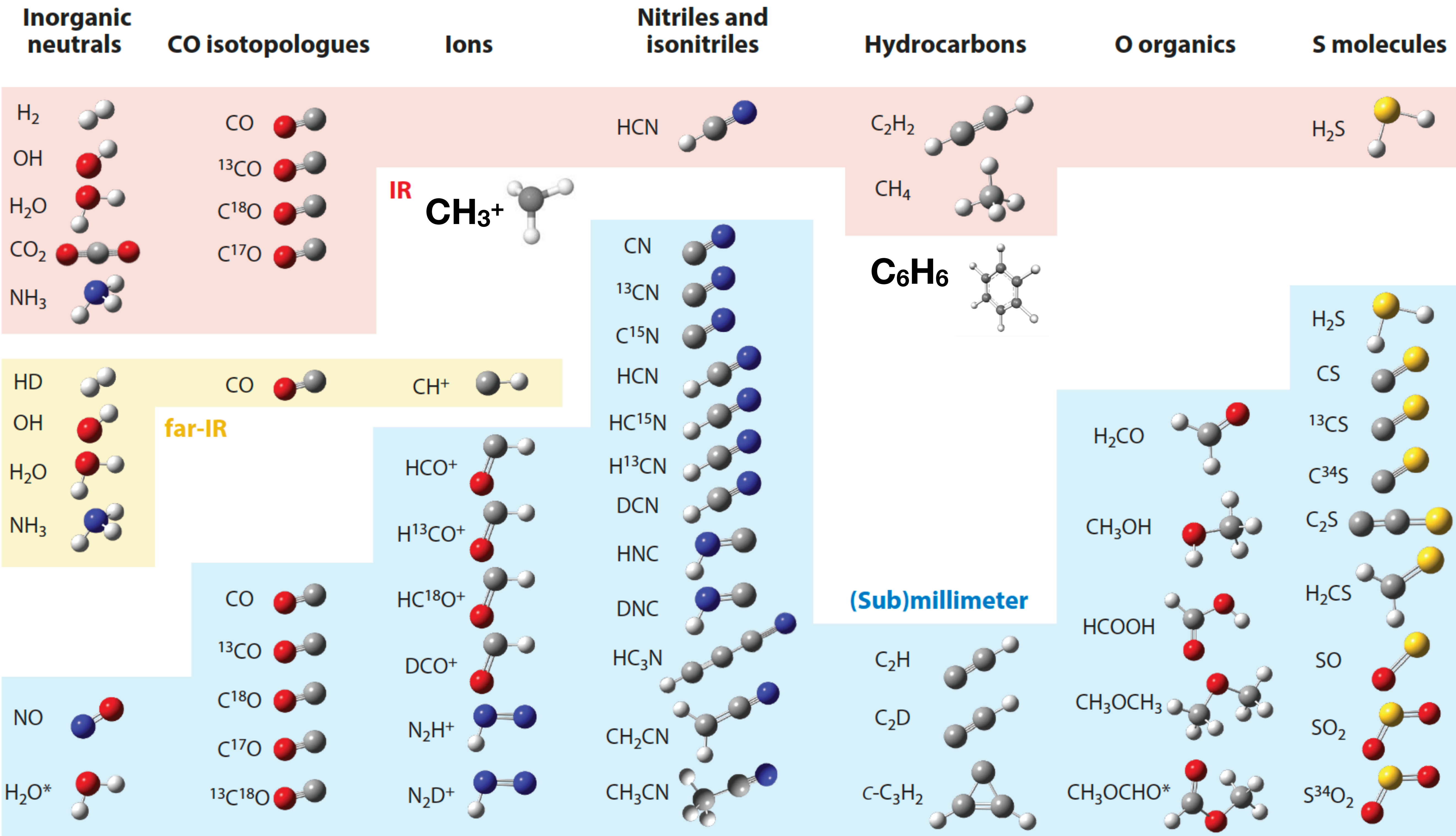
Observations

vs

Modeling

~30 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$300)

~30 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_6H_6
CO	SO_2	C_2H_2	CH_4		
CH^+	HCO^+	CH_3^+	CH_2CN		
OH	HCN				
H_2	HNC				
NO	N_2H^+				
	C_2H				
	CO_2				

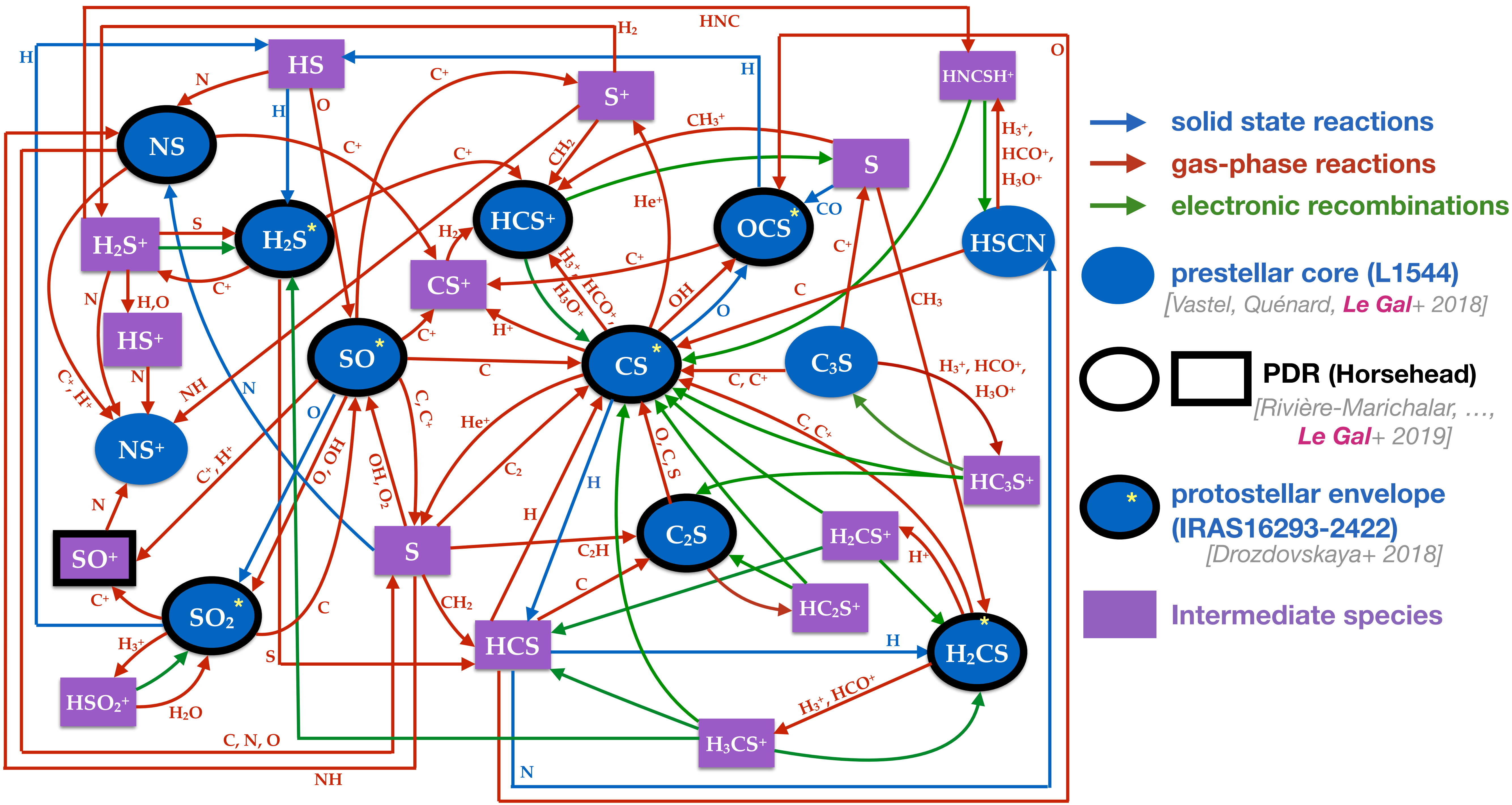
- $\gtrsim$10% of all the chemical species detected in Space so far ($\gtrsim$300)

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_6H_6
CO	SO_2	C_2H_2	CH_4		
CH^+	HCO^+	CH_3^+	CH_2CN		
OH	HCN				
H_2	HNC				
NO	N_2H^+				
	C_2H				
	CO_2				

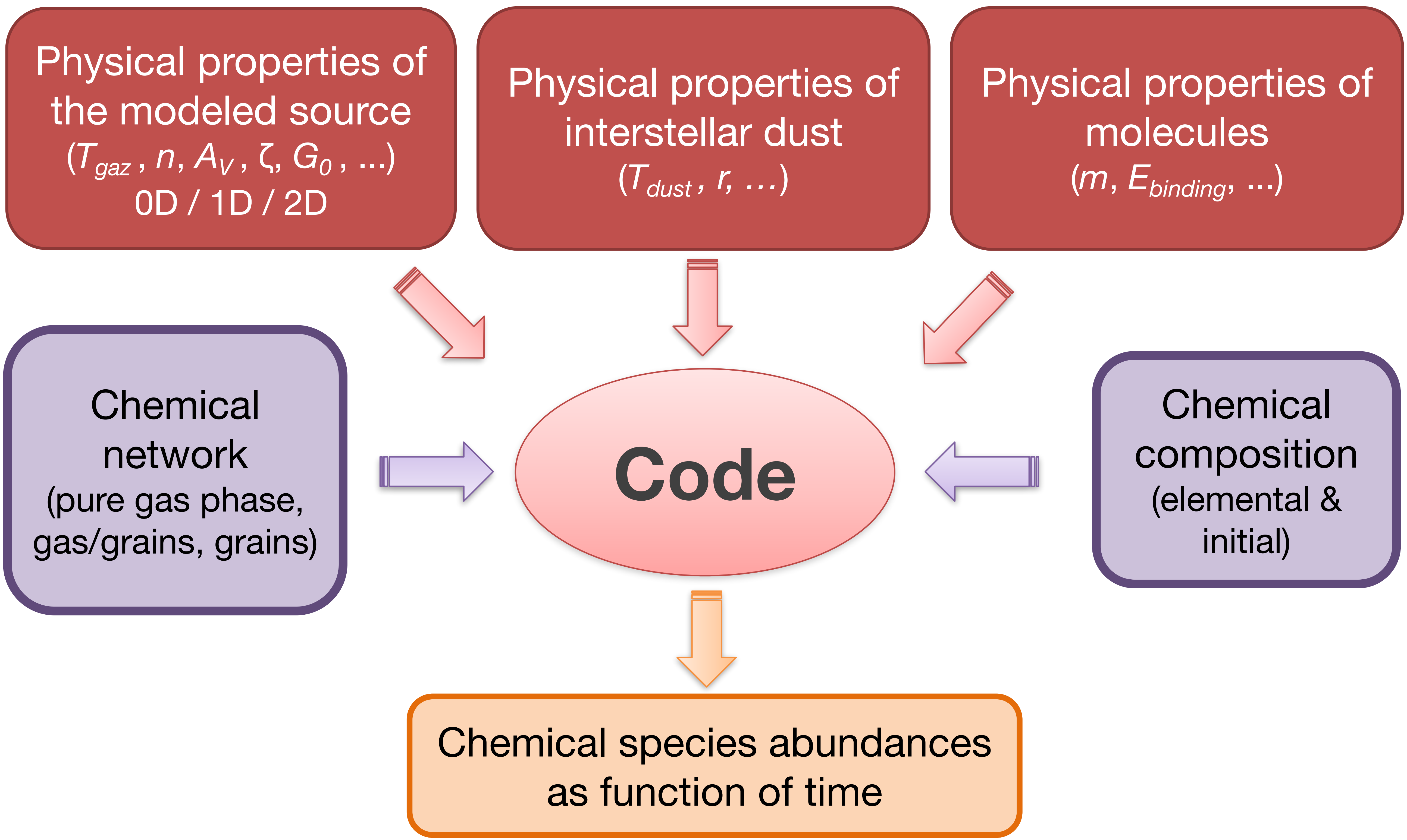
- Routinely observed in wide range of astrophysical objects: from extragalactic sources to our own Solar System
- Commonly used to probe the physical conditions (shock, infall, accretion, …)
- Key components in the formation of life building-blocks and in planet habitability *[Chen et al. 2015, Ranjan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

Schematic “simplified” view of the ISM sulfur chemical network

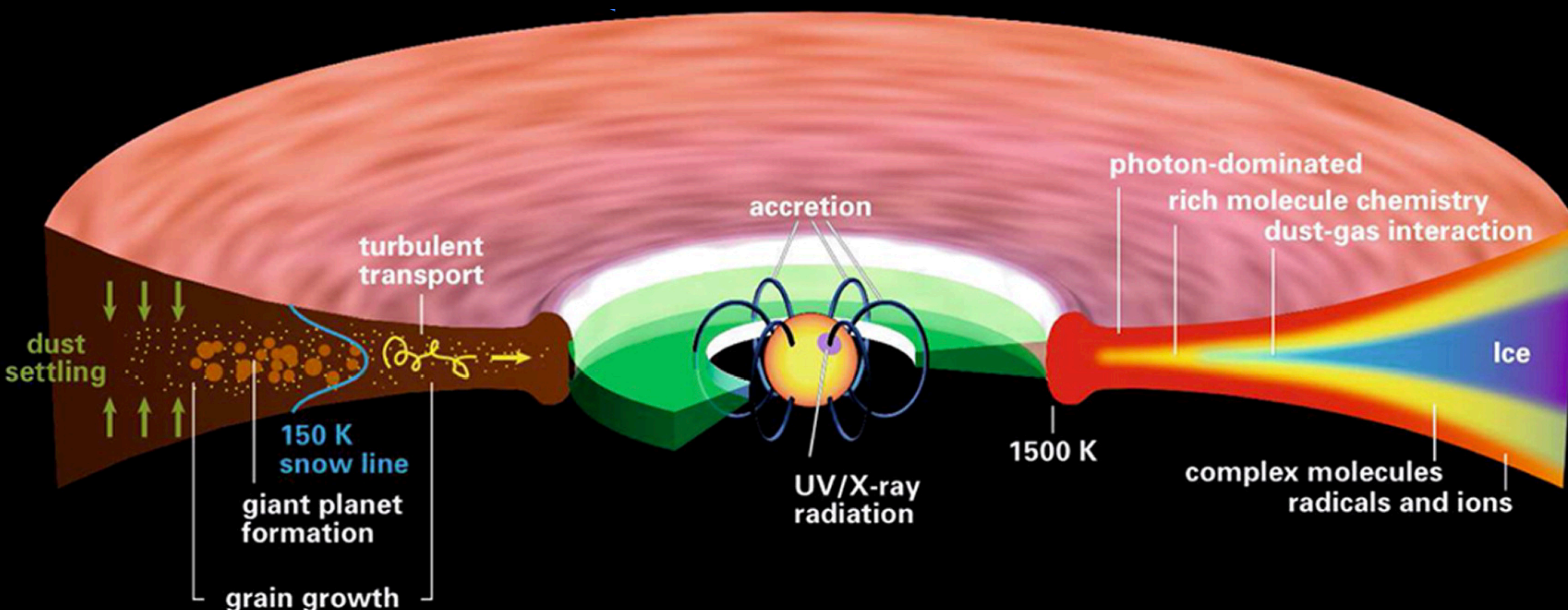


Adapted from: ***Vastel***, *Quénard*, ***Le Gal*** *et al. 2018, MNRAS, 478, 5514*

Astrochemical modeling



Protoplanetary disk structure



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

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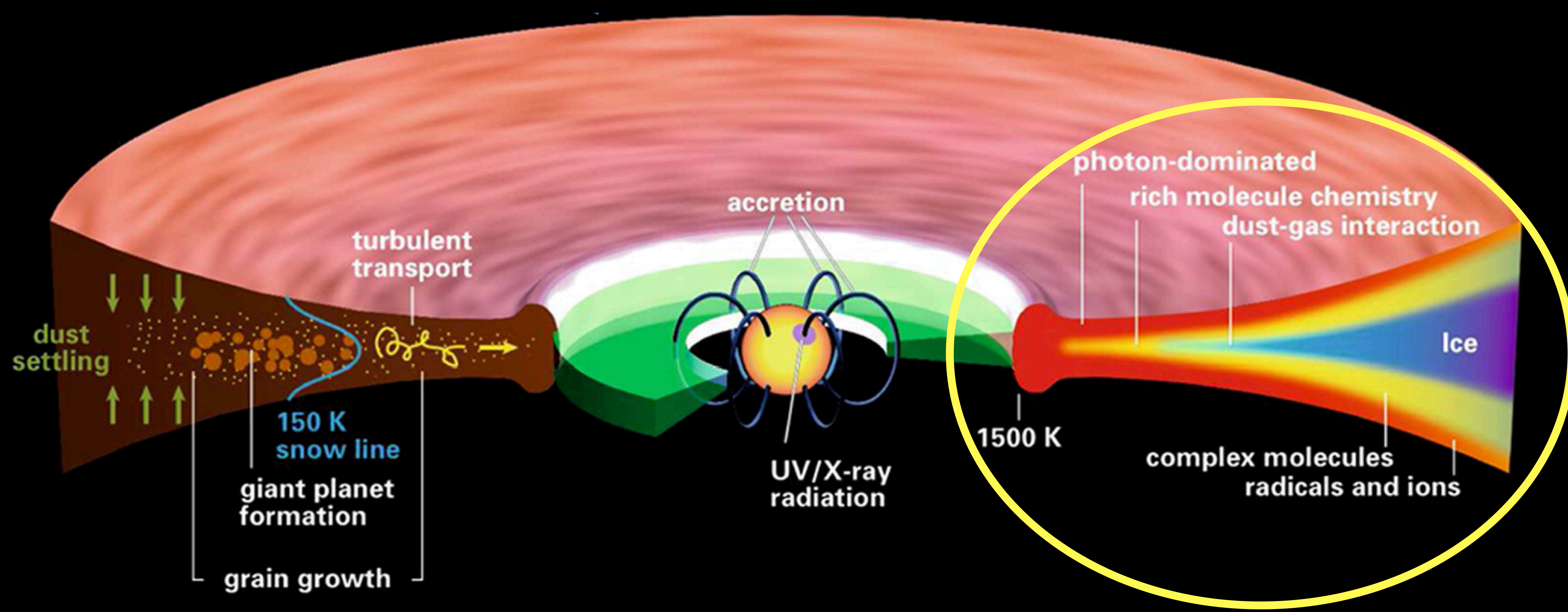

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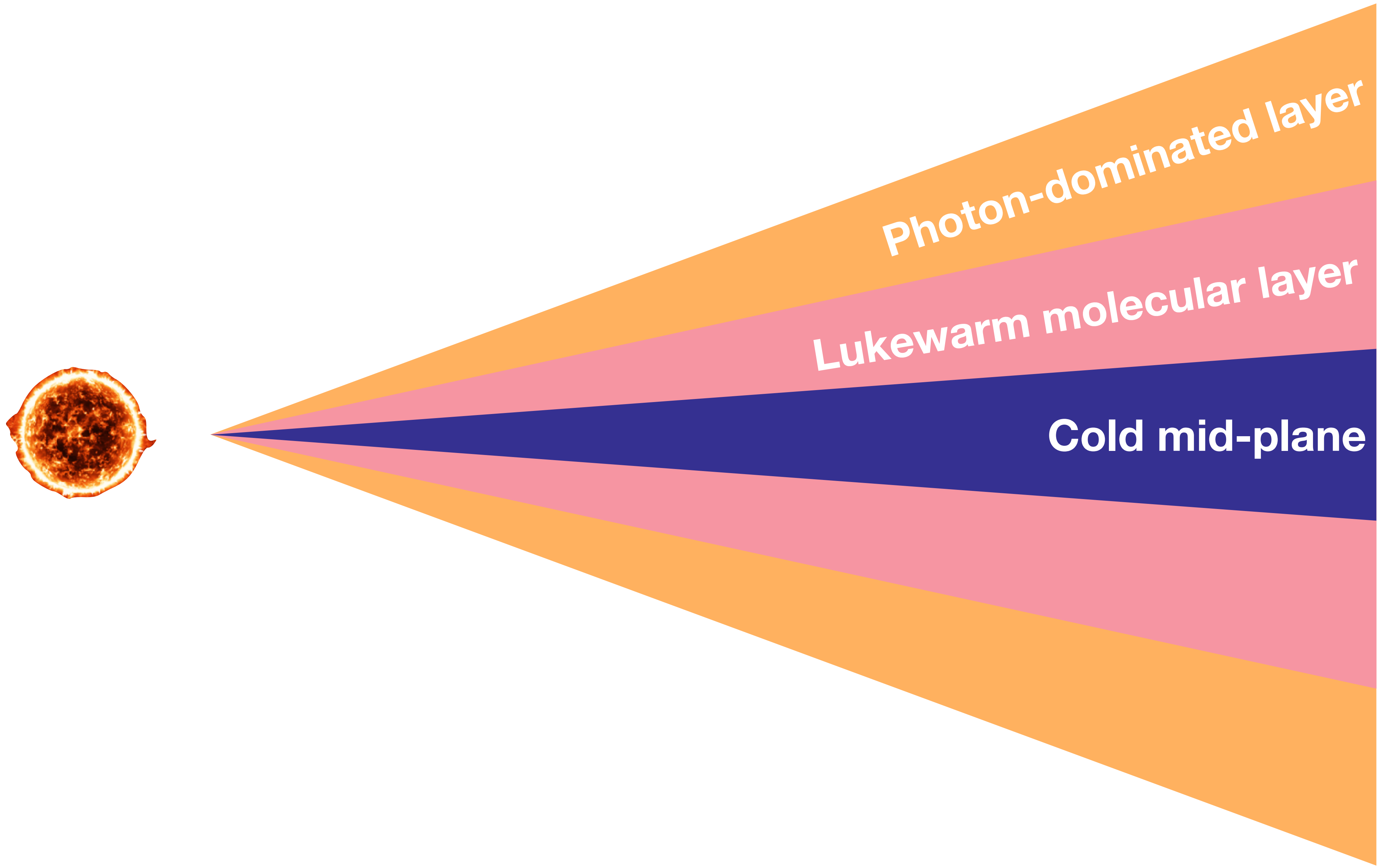

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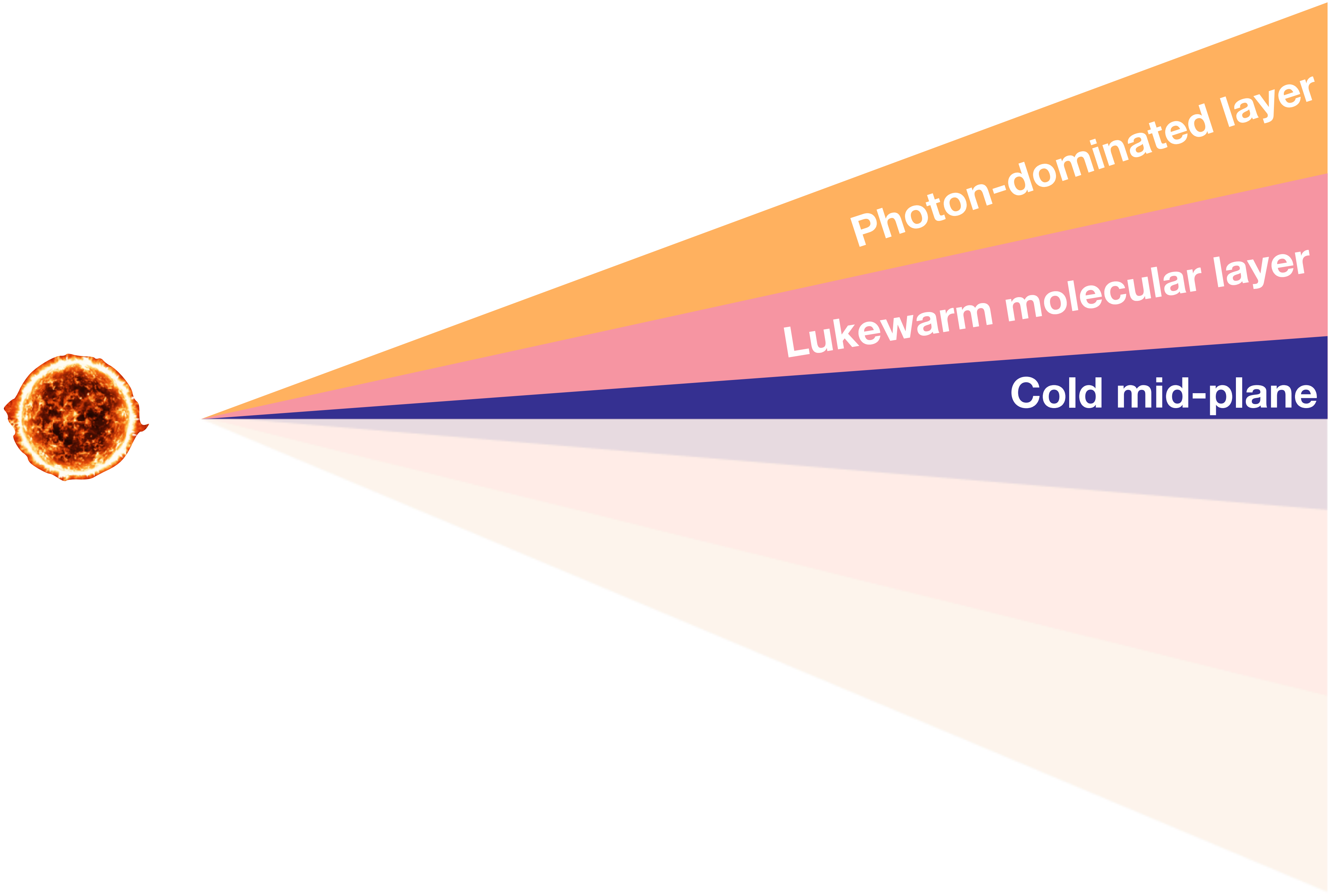

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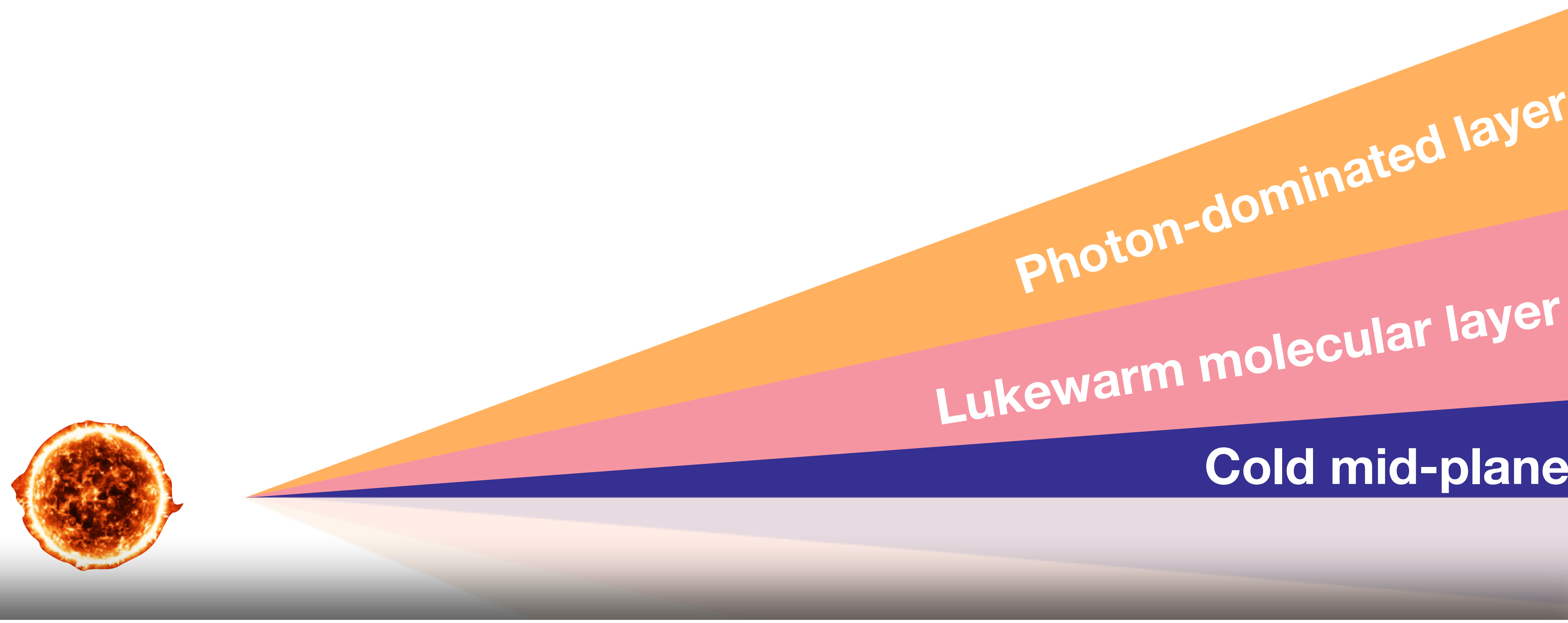
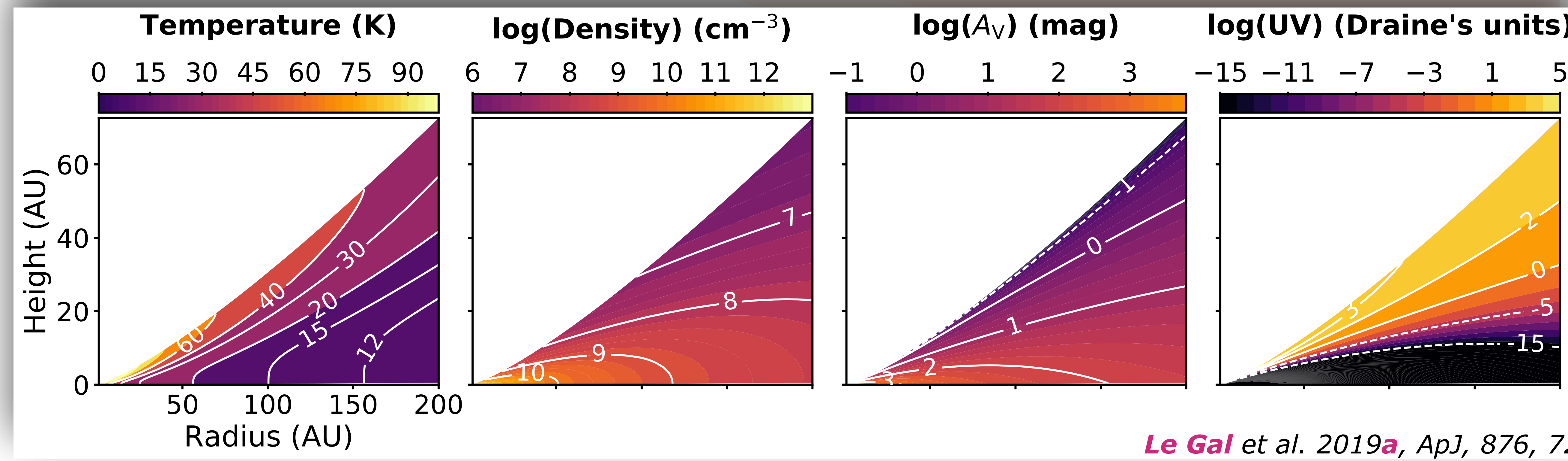
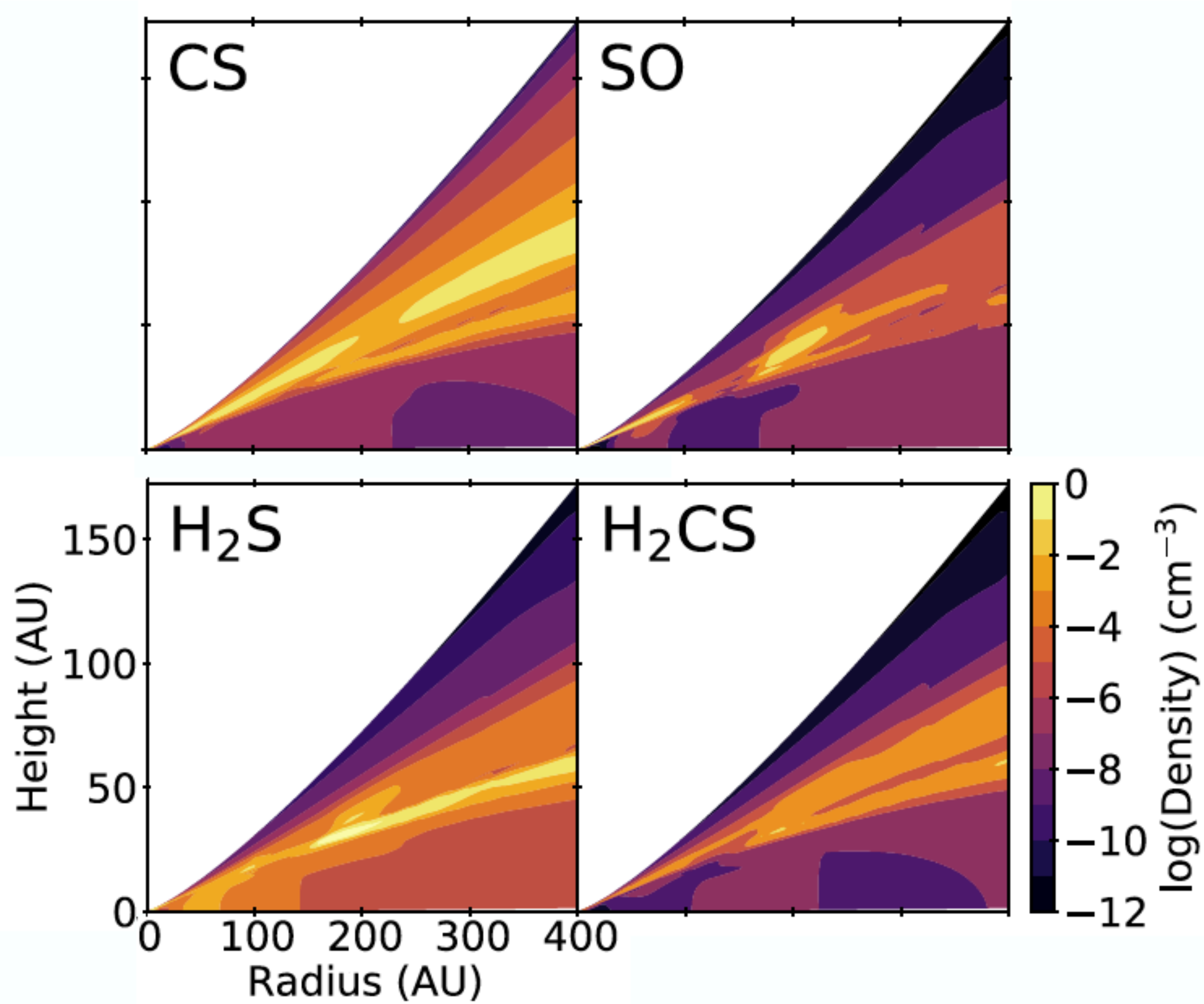




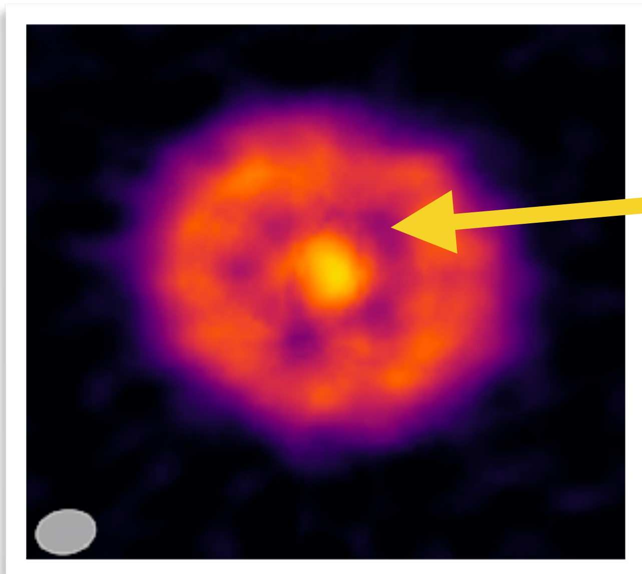
Le Gal et al. 2019a, ApJ, 876, 72

Disk chemistry modelling results



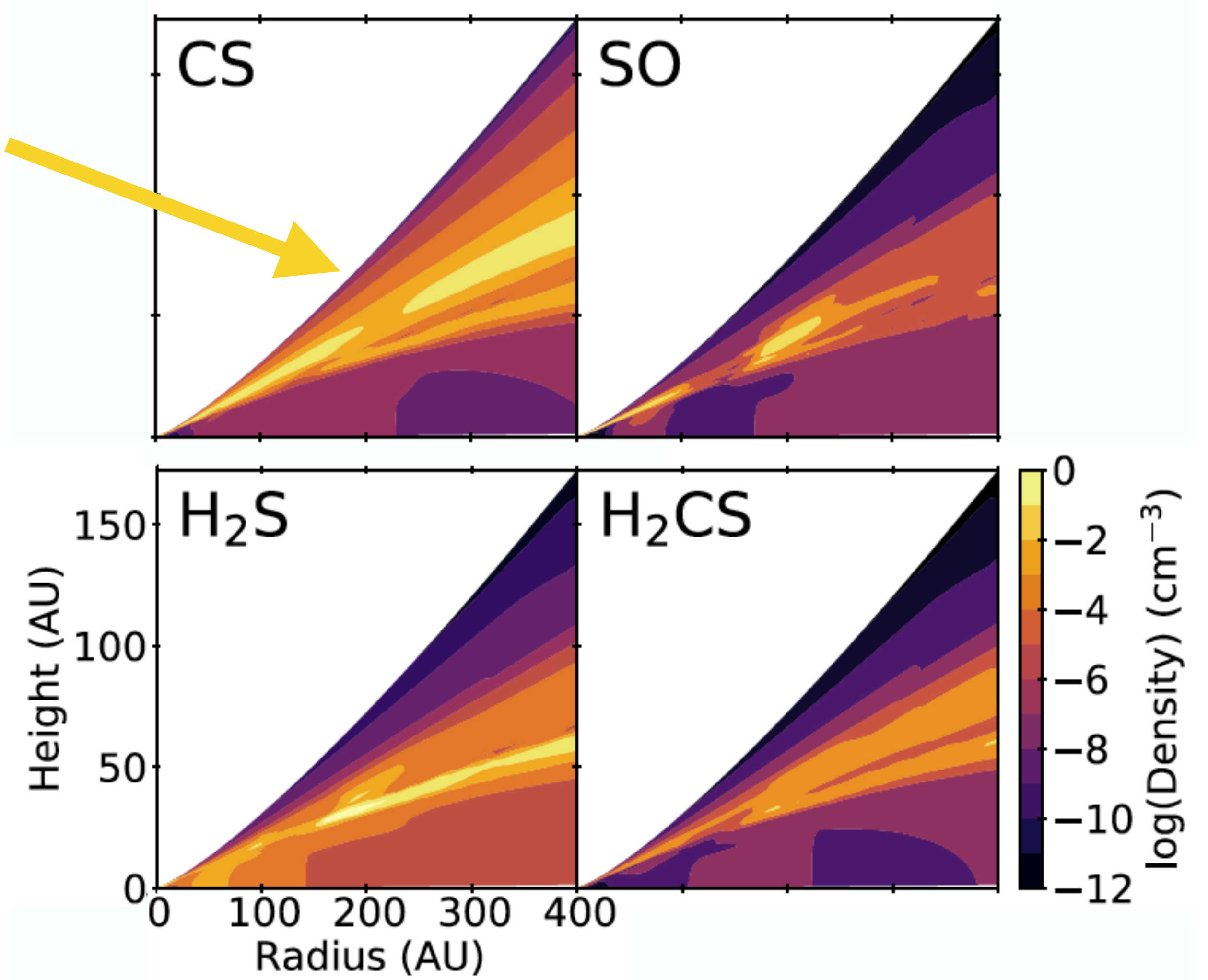
Models *versus* Observations: CS case

ALMA observation of CS



gap

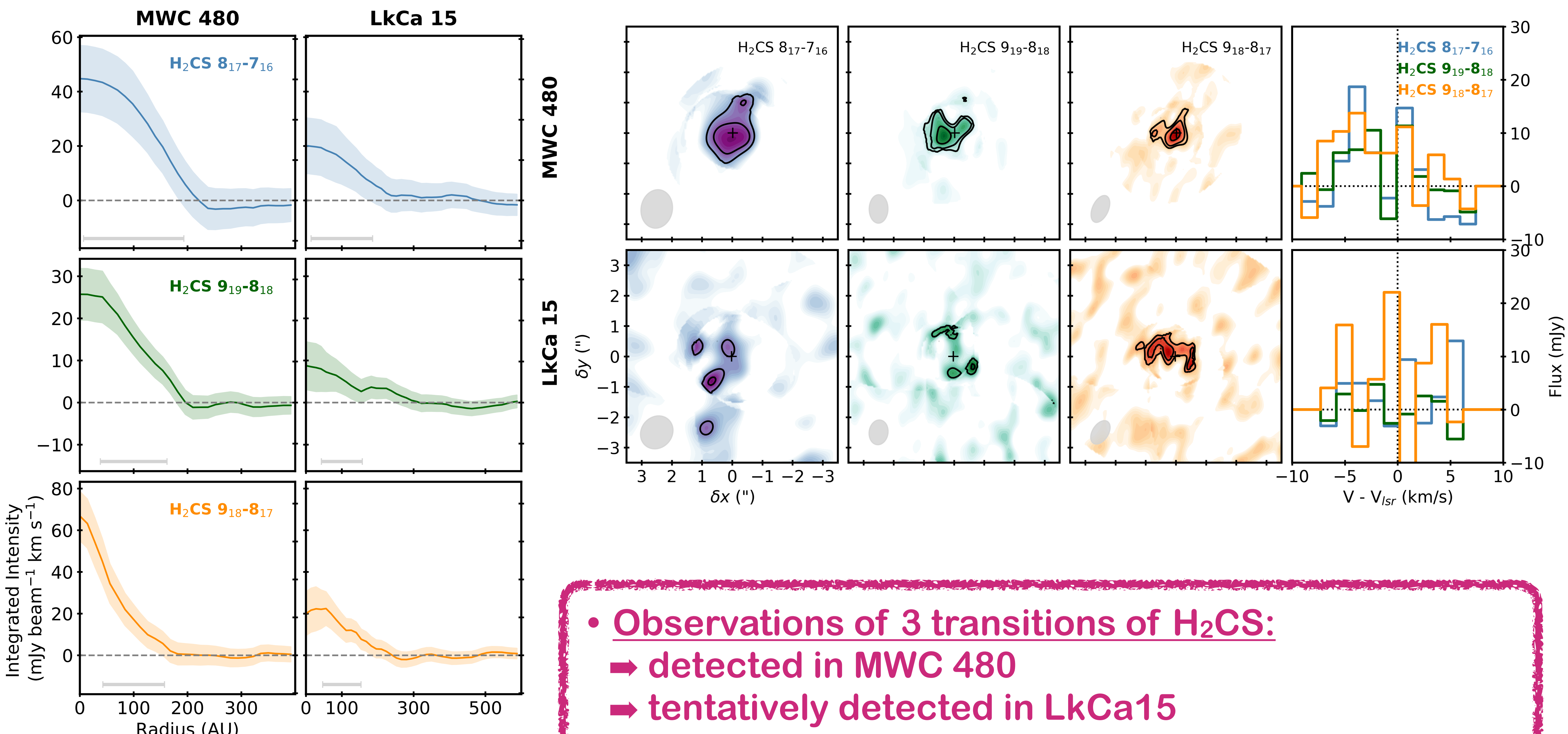
Modeling results



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

Detection of H_2CS in disks

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



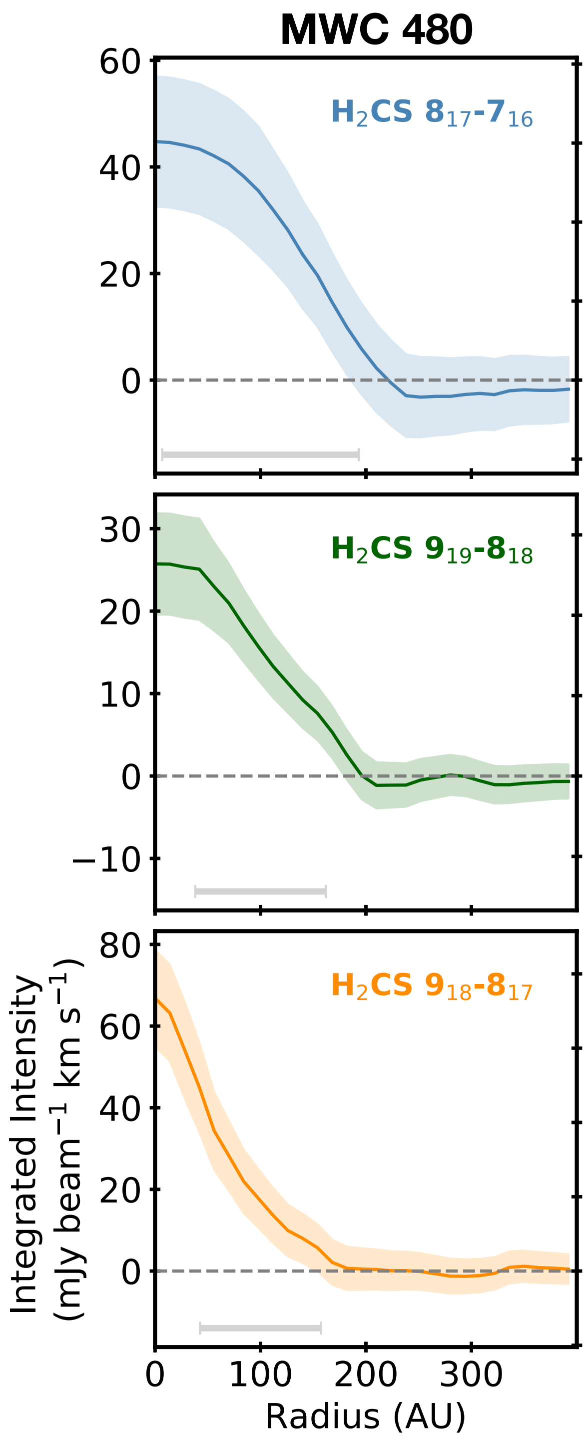
- **Observations of 3 transitions of H_2CS:**
  ➡ detected in MWC 480
  ➡ tentatively detected in LkCa15

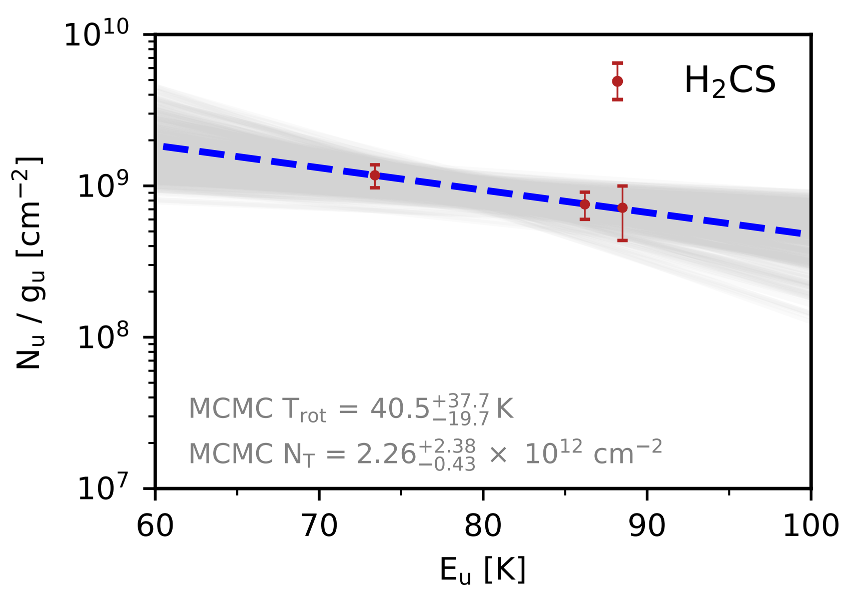
- **$H_2CS/CS \approx 2/3 >> H_2S/CS \approx 1/20$**
  ➡ part of the S-reservoir in disks is in organic form (i.e. $C_xH_yS_z$)

Observations *versus* models : H2CS case

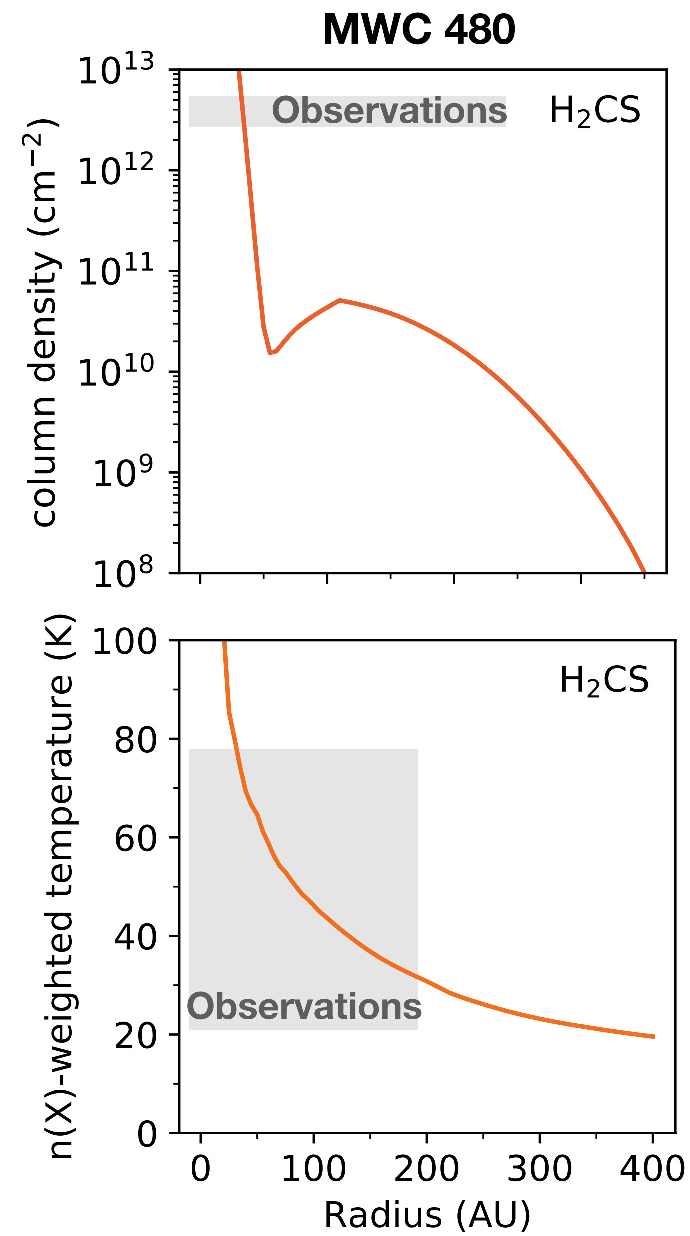
[**Le Gal** et al. 2019**a**, ApJ, 876, 72]

Observation analysis results



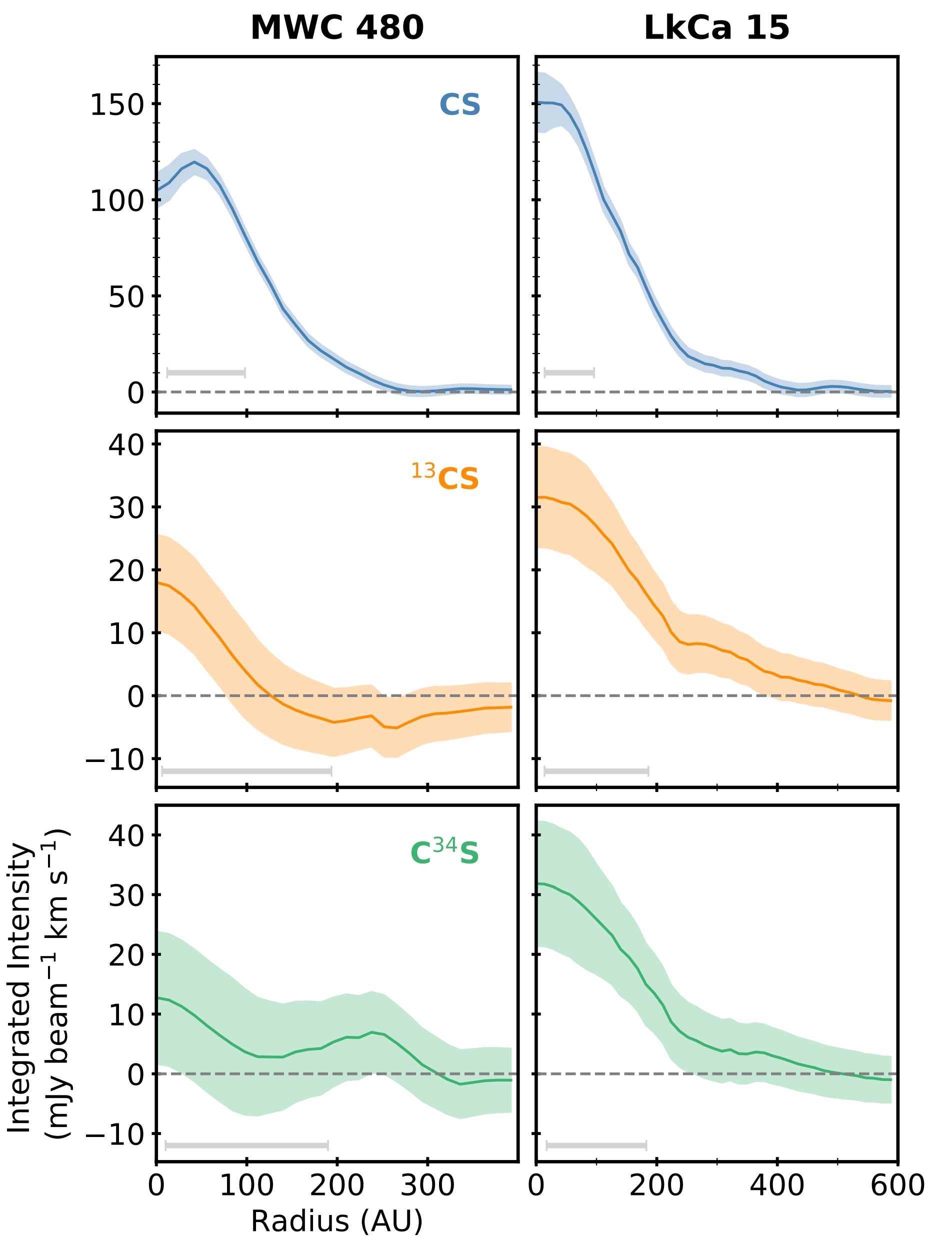


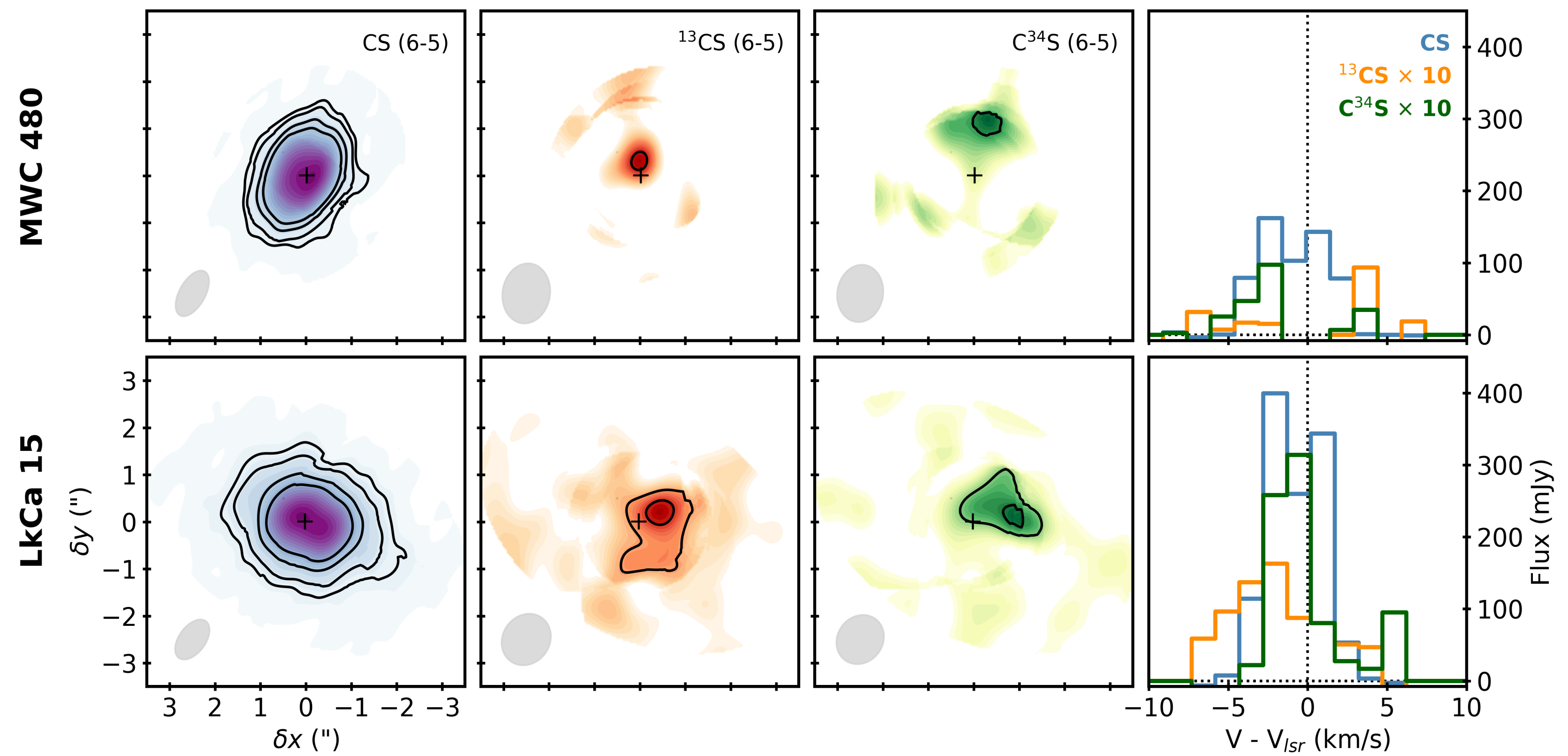
Modeling results vs observations



Under-prediction of H_2CS by 1– 2 orders of magnitude
=> further theoretical S-disk chemistry & experimental constraints!

Detection of CS isotopologues in disks





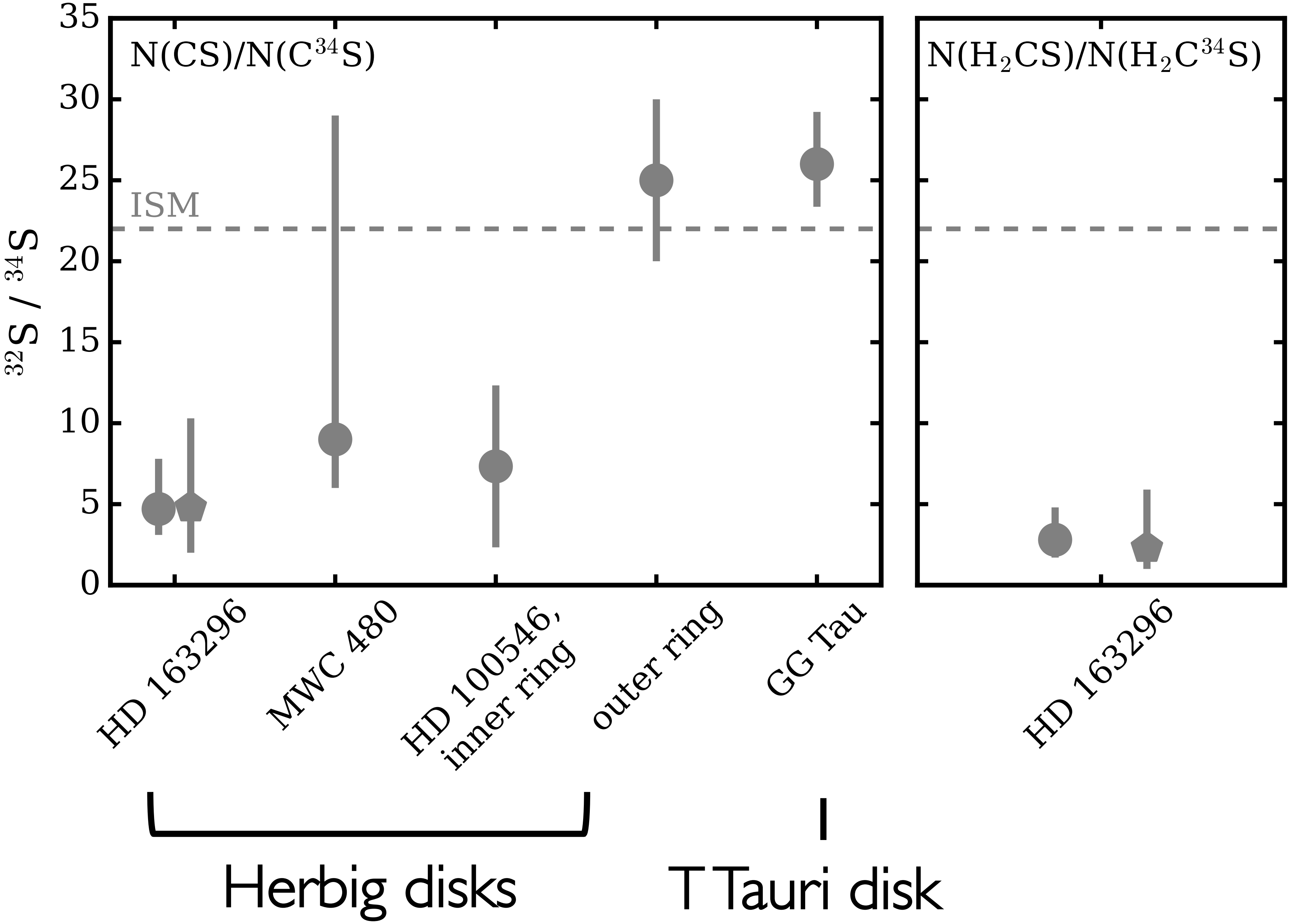
CS/^{13}CS & CS/C^{34}S << LISM ratios

=> (i) CS optically thick,
or (ii) ^{13}C & ^{34}S are enhanced in CS

=> Need multiple lines & higher SNR observations to disentangle these scenarios & address the fundamental question of chemical inheritance.

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

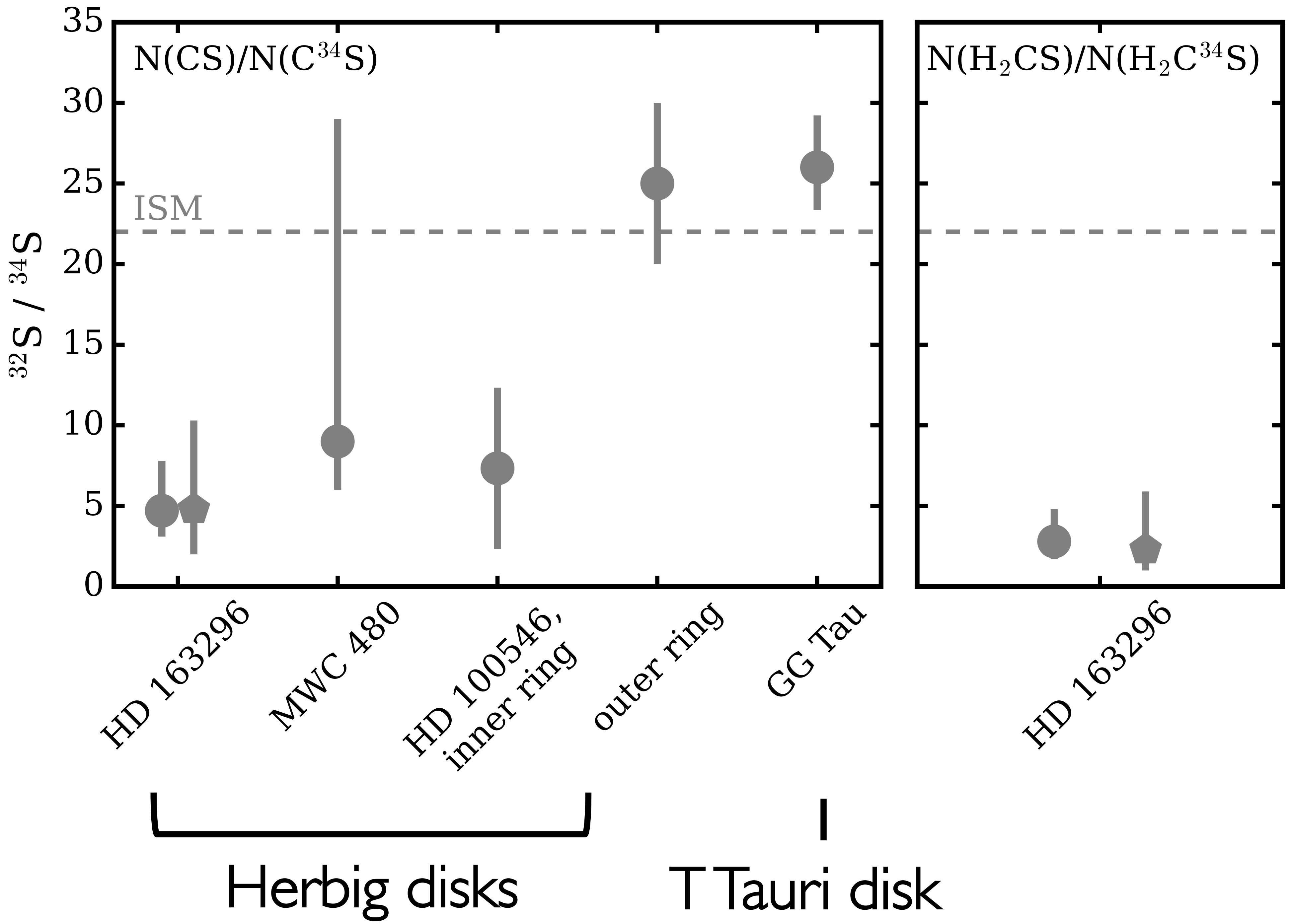
Sulfur isotopic ratios in disks



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

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

Sulfur isotopic ratios in disks



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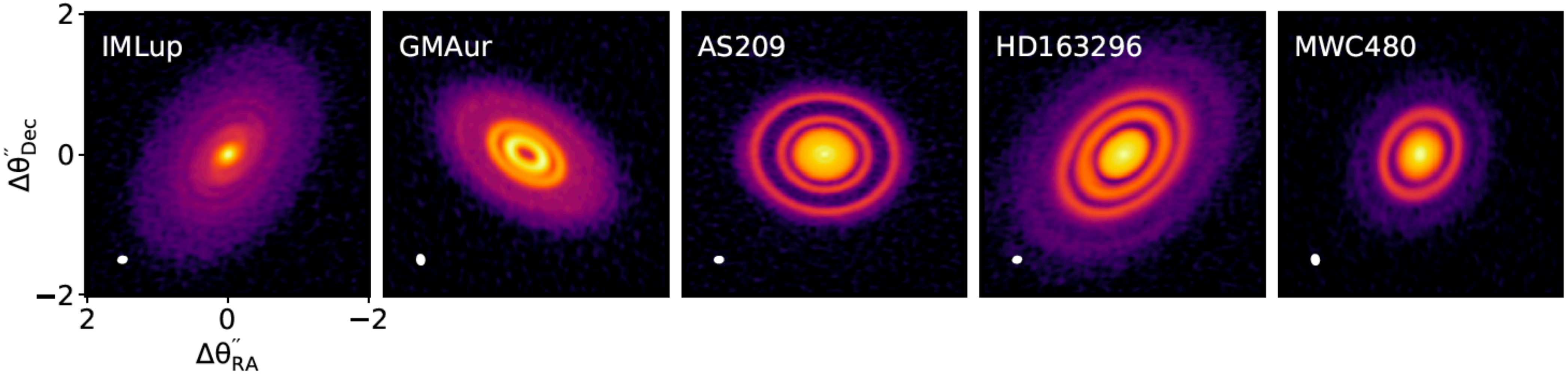
Molecules with **A**LMA at **P**lanet-forming **S**cales

http://alma-maps.info



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

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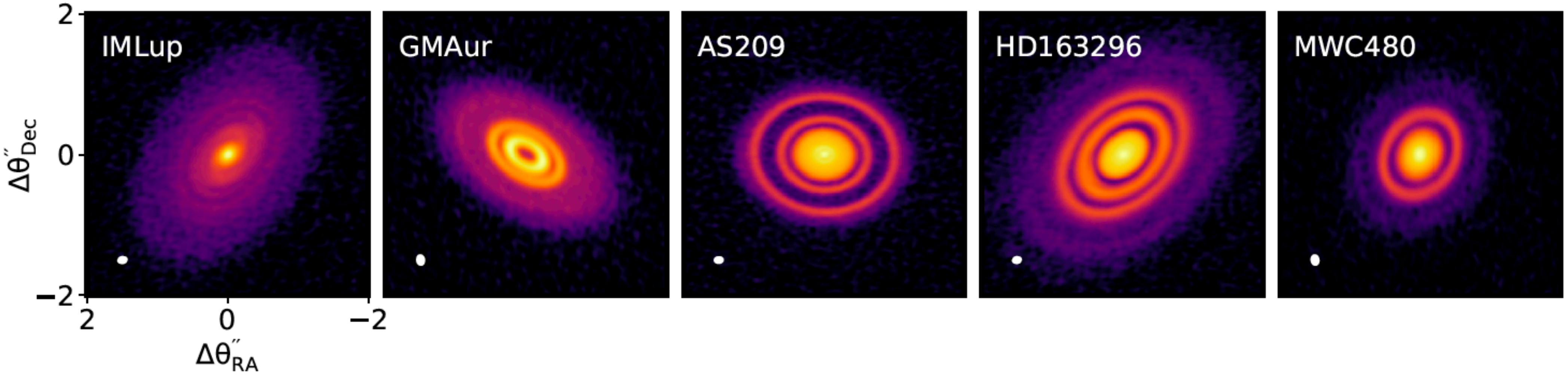

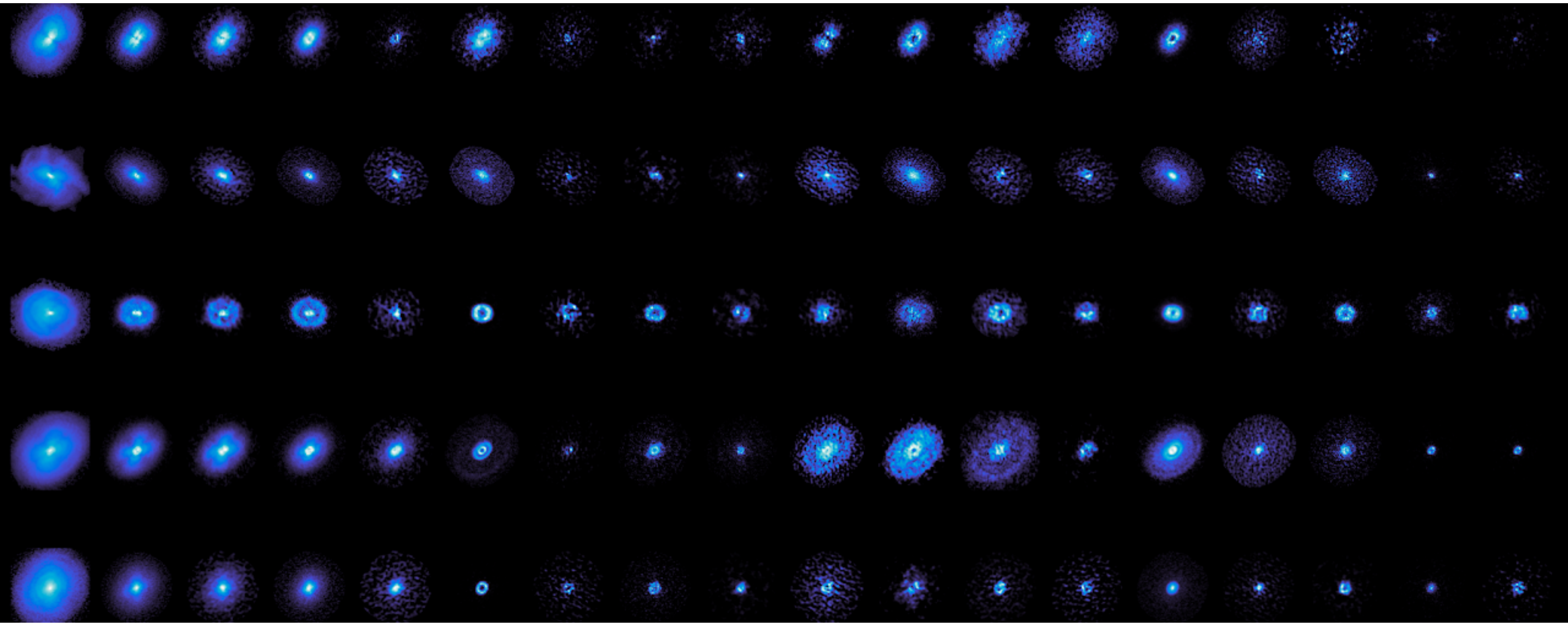

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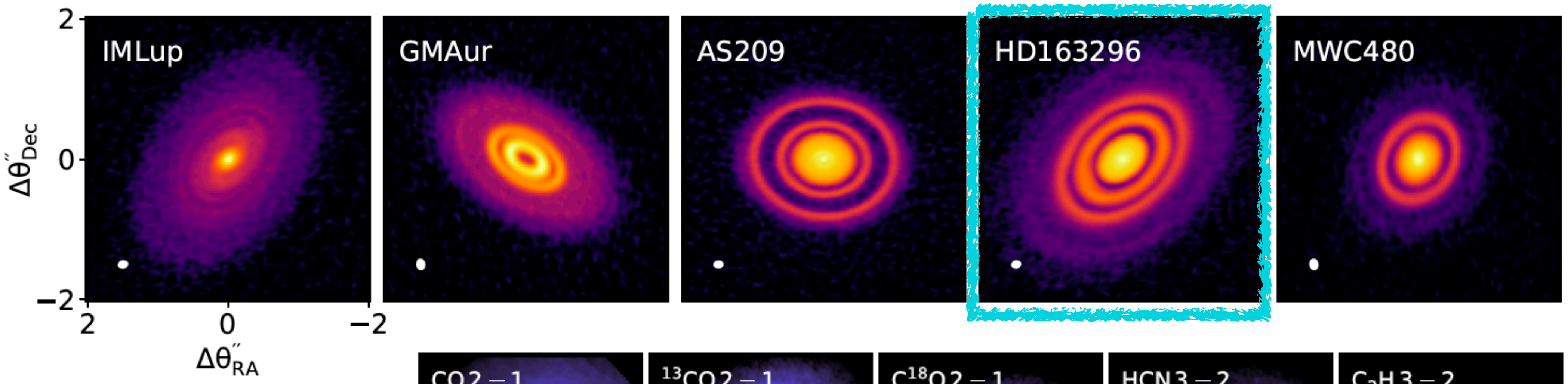

- 5 discs with signs of on-going planet formation
- 4 spectral settings across B3 & B6
- 20 species including CS

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

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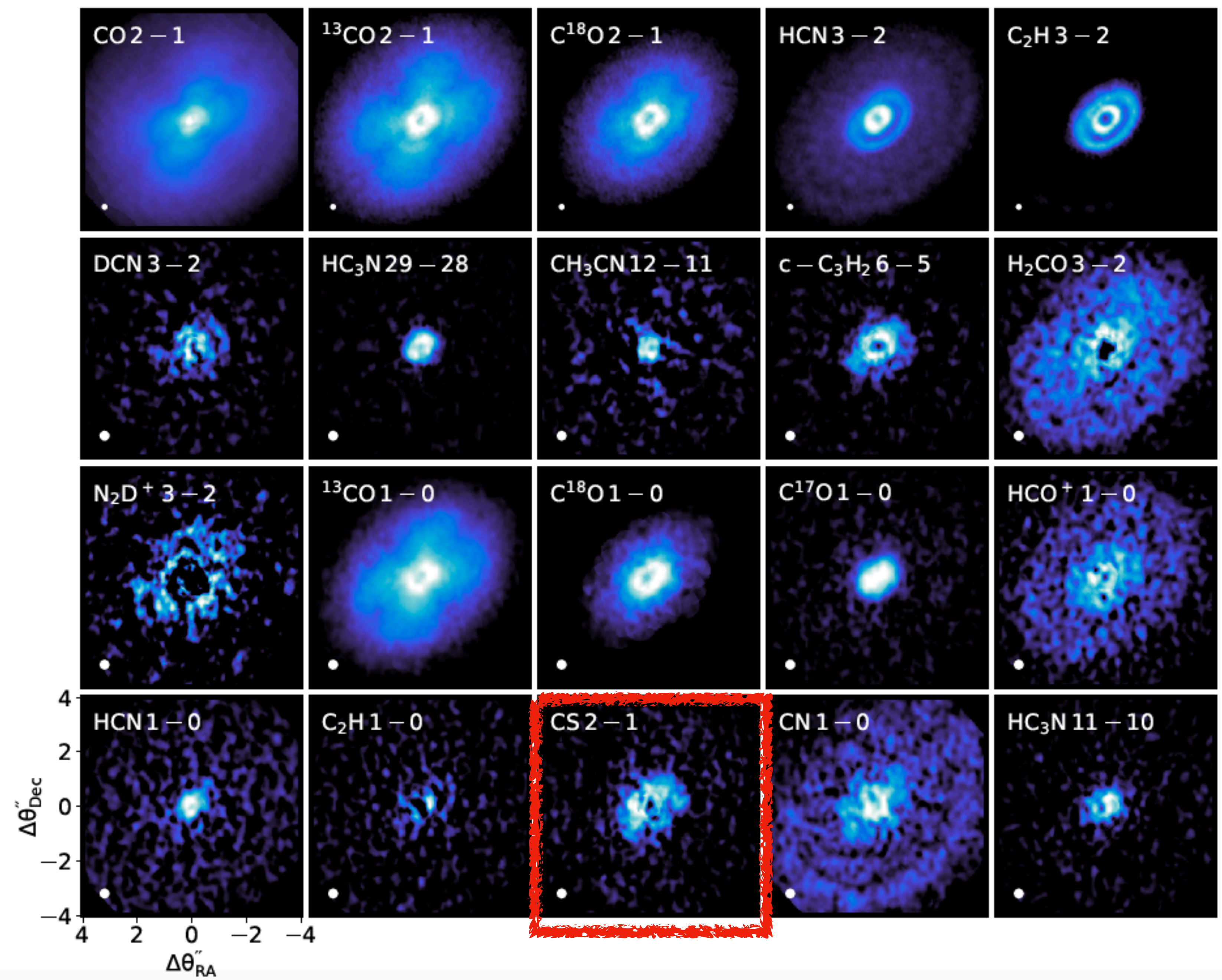
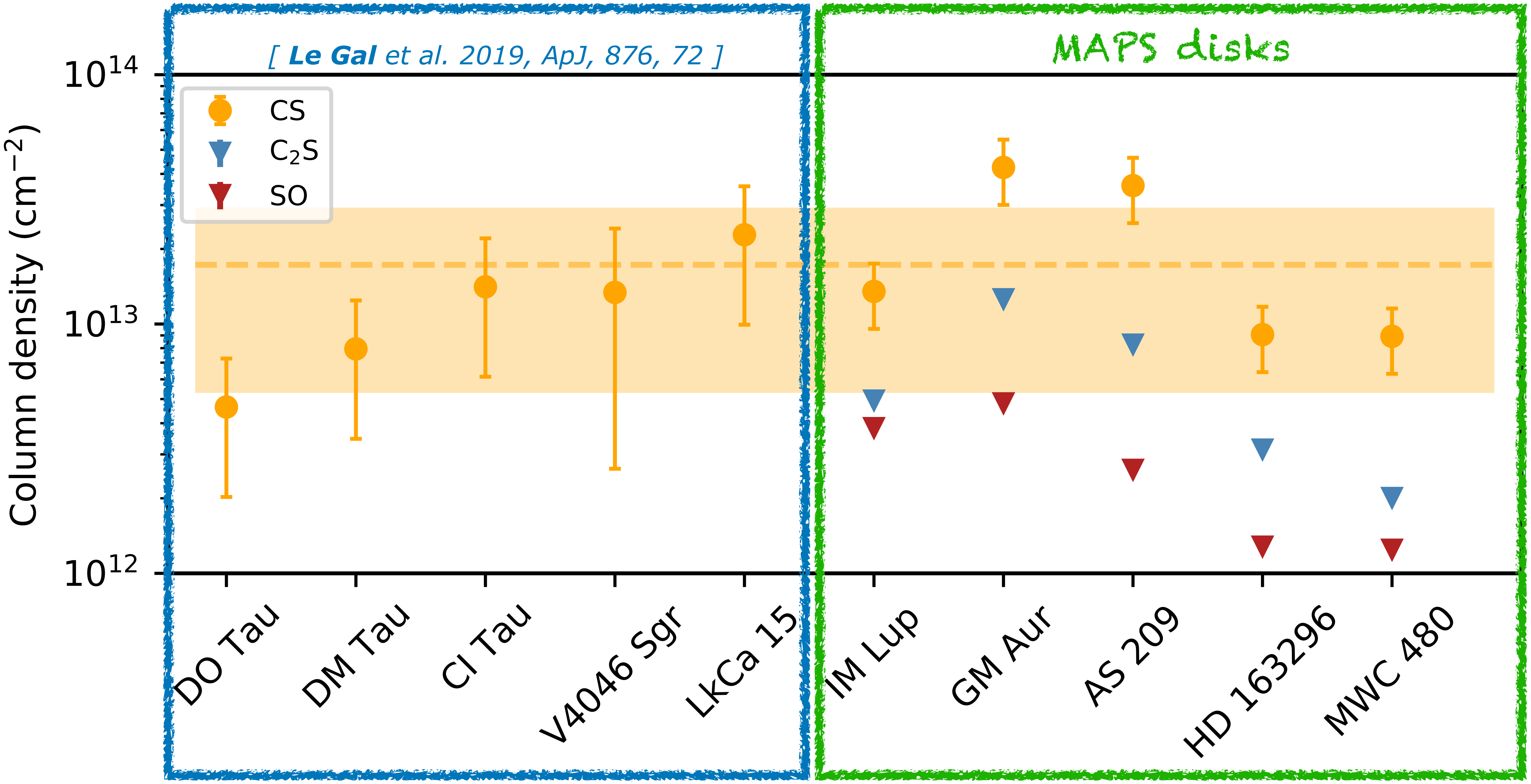


Disk-integrated column densities

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



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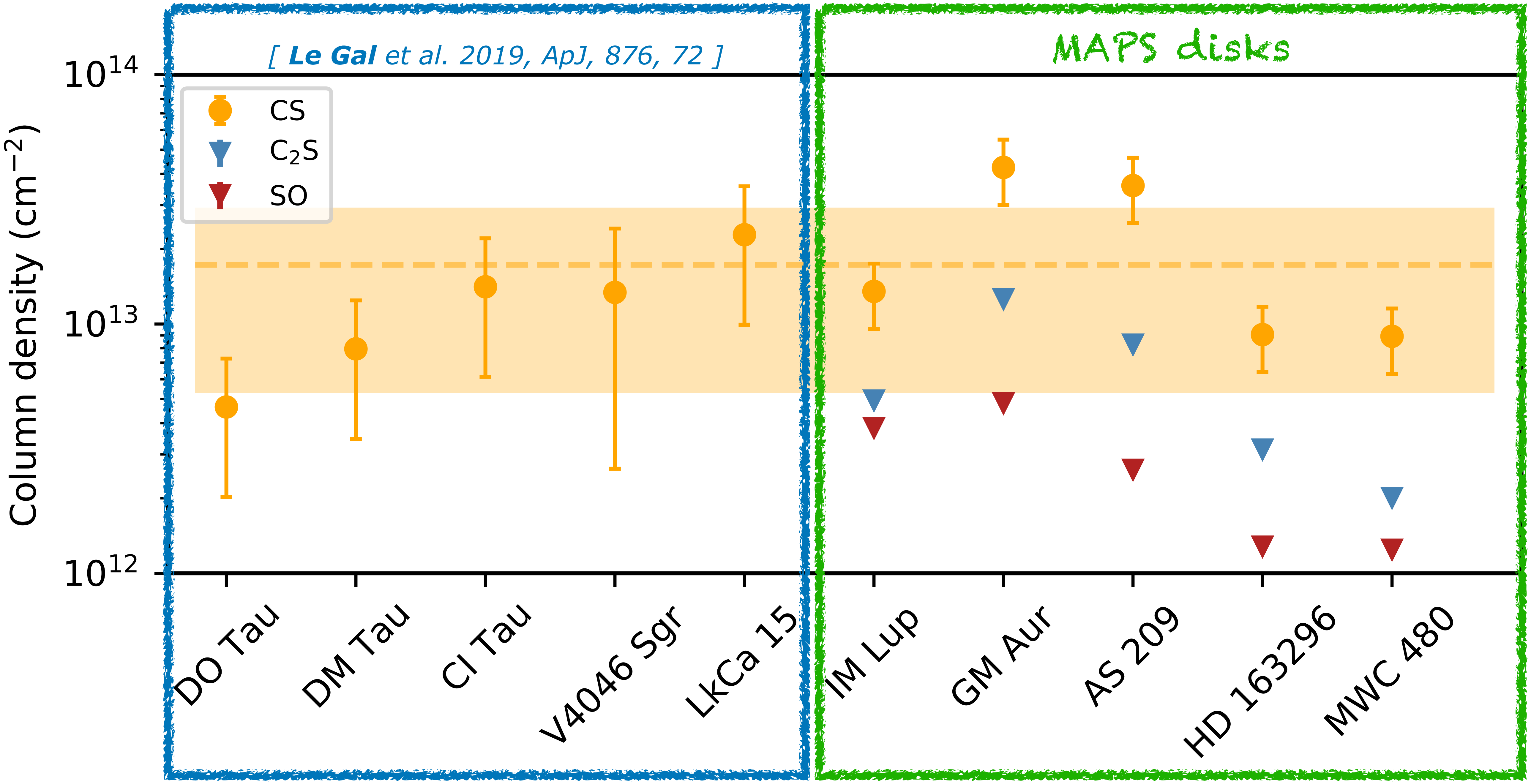
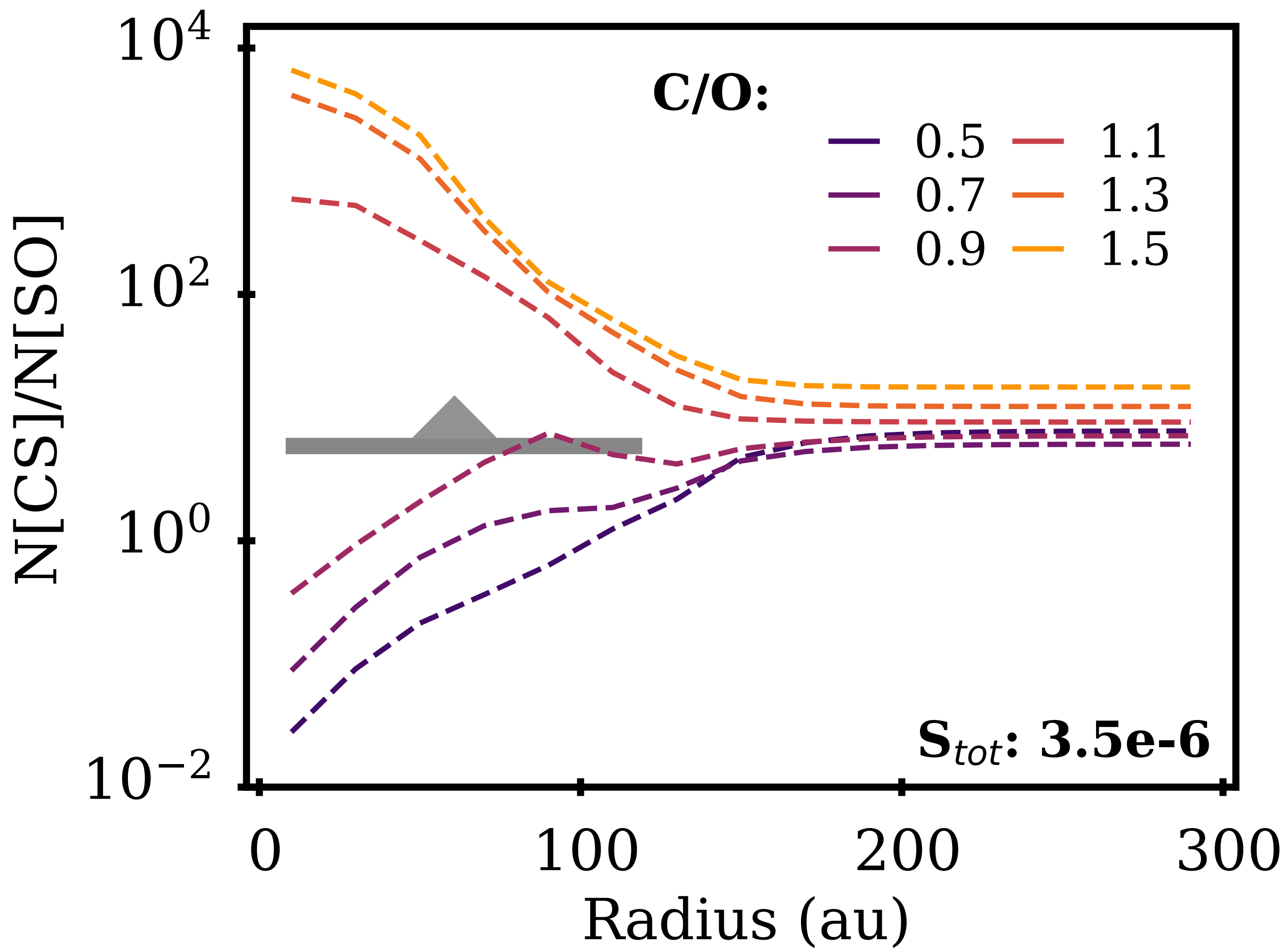


CS column density is rather flat in disks.

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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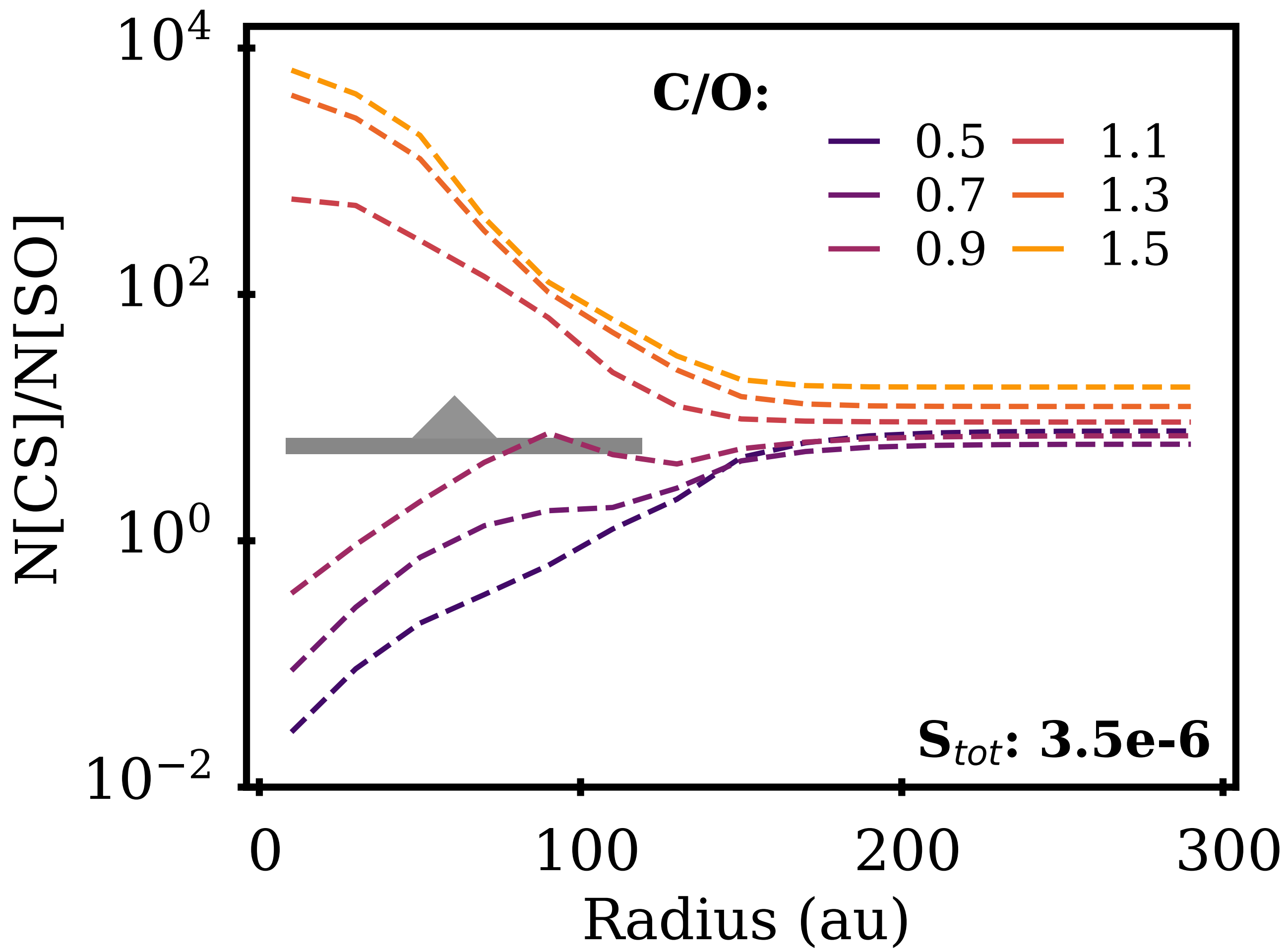
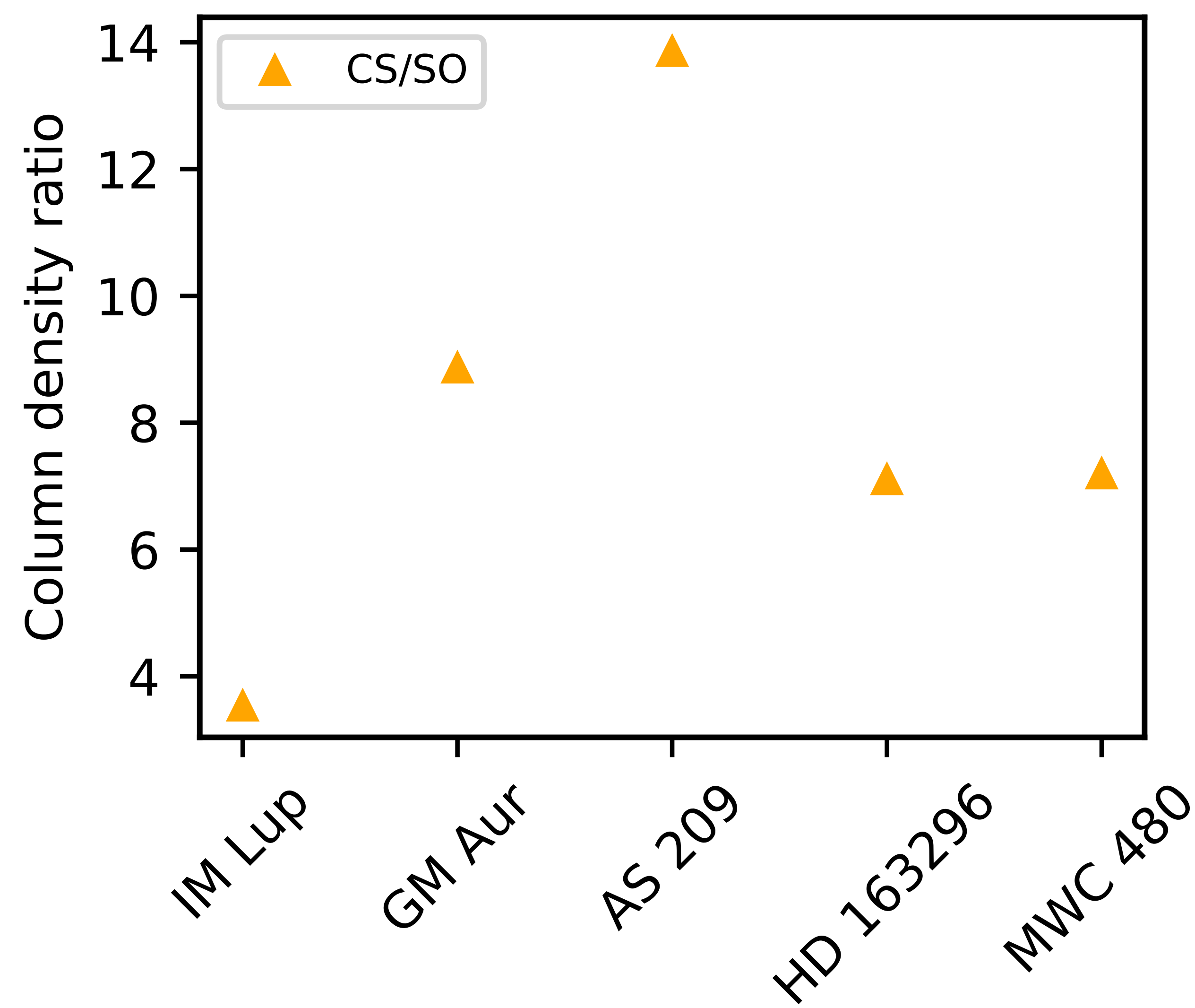


=> CS/SO ratio is a promising probe for the C/O ratio in disks.

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

CS/SO observed in all five MAPS disks

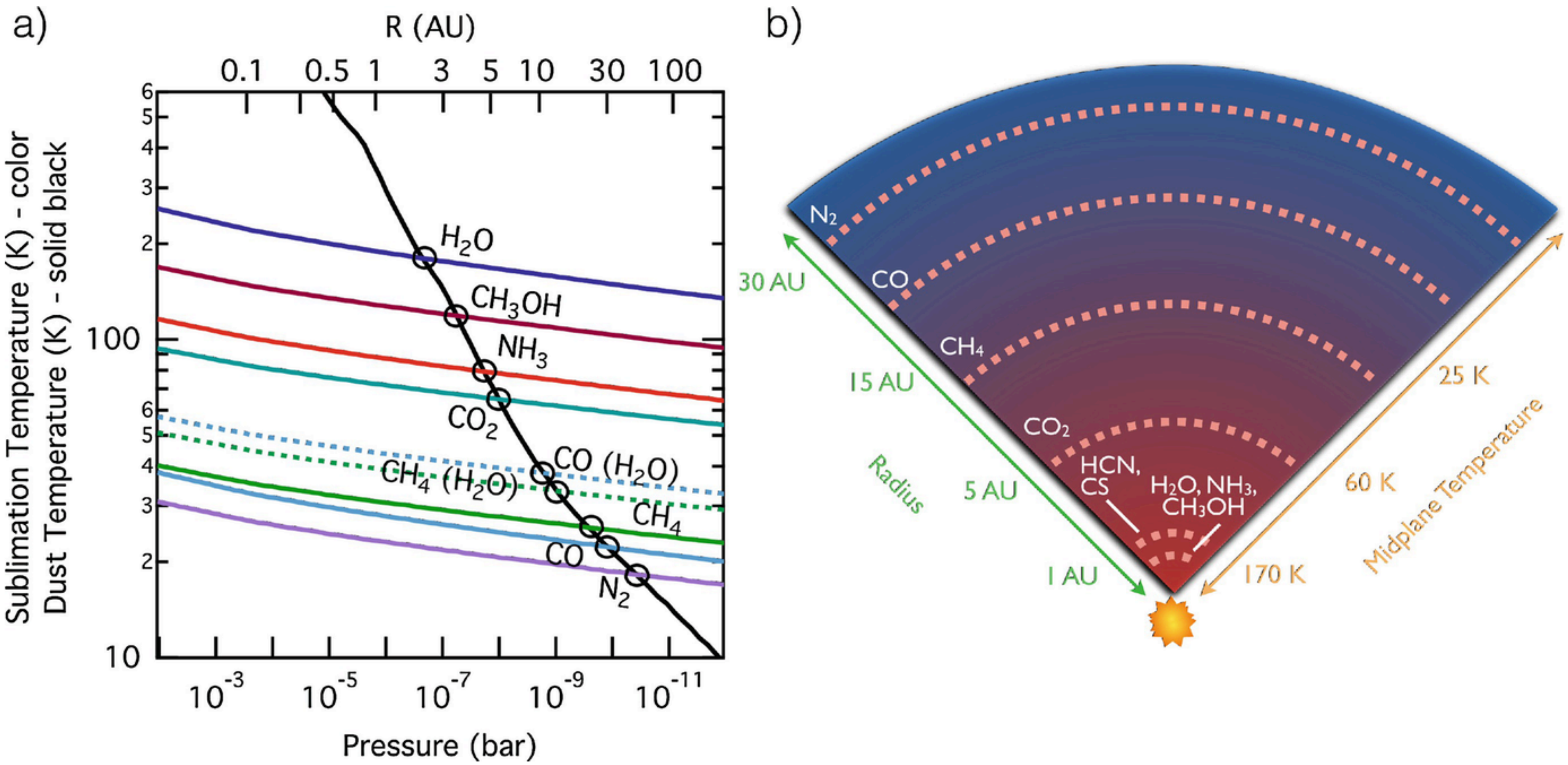


C/O ratio $\gtrsim$ 1 in most disks of our sample

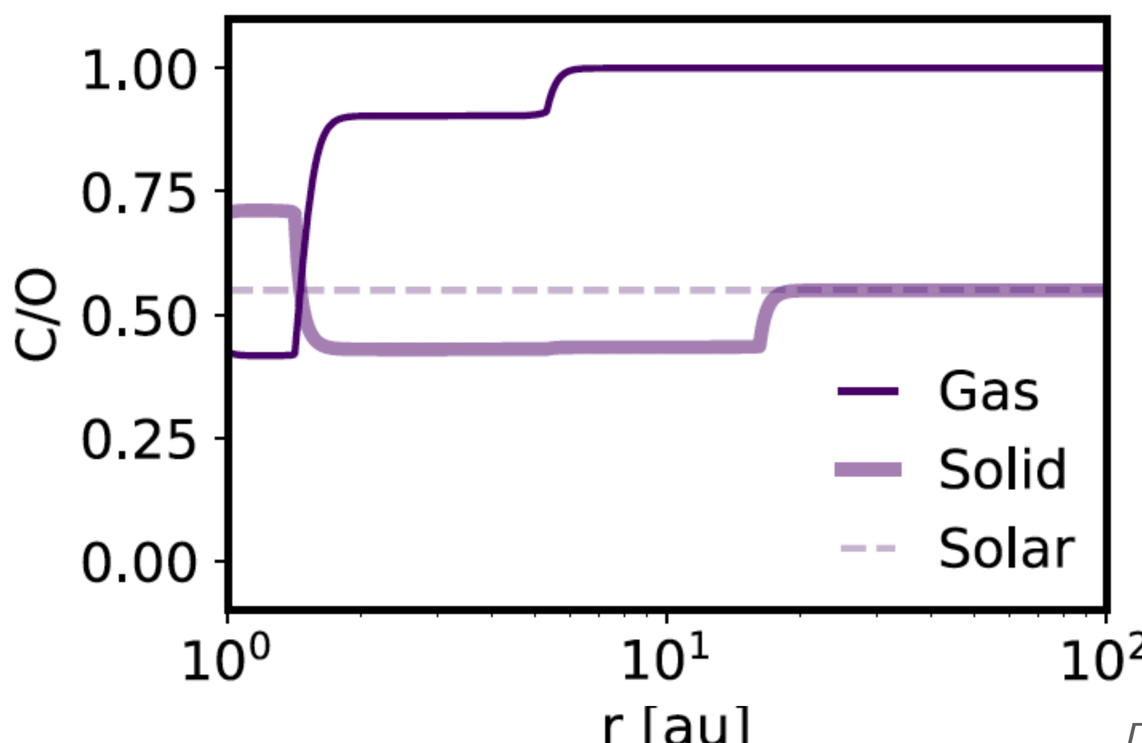
=> What does this telling us?

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

Why probing the C/O ratio?

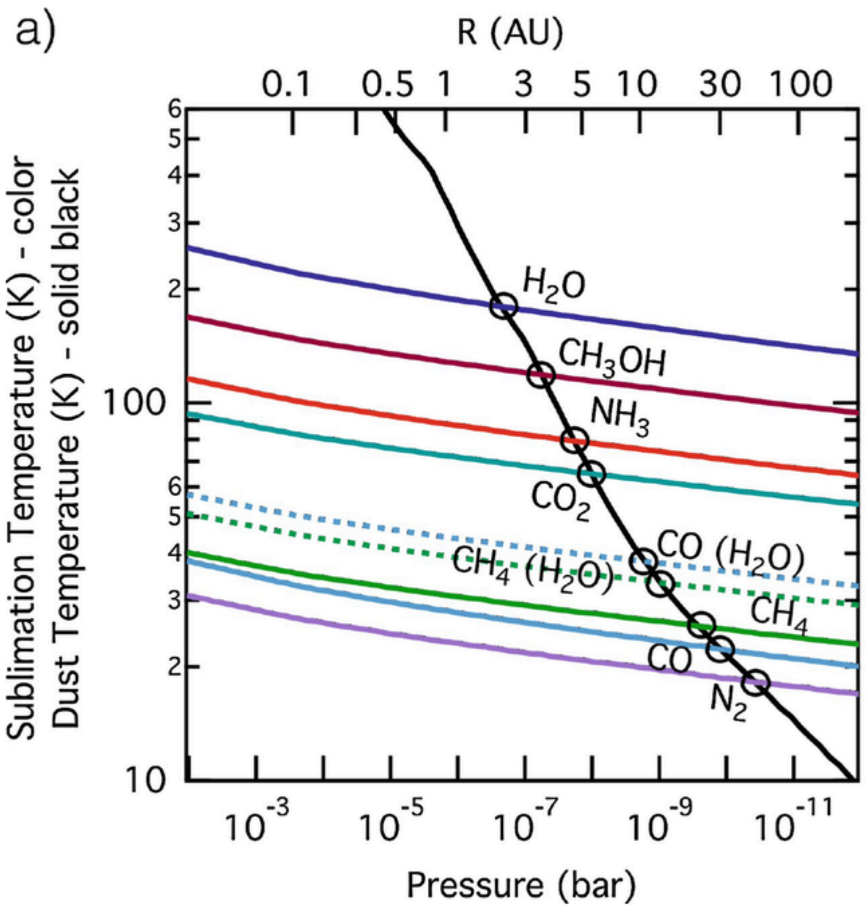


[Bergin & Cleeves 2018]



[Öberg & Bergin 2021]

Why probing the C/O ratio?



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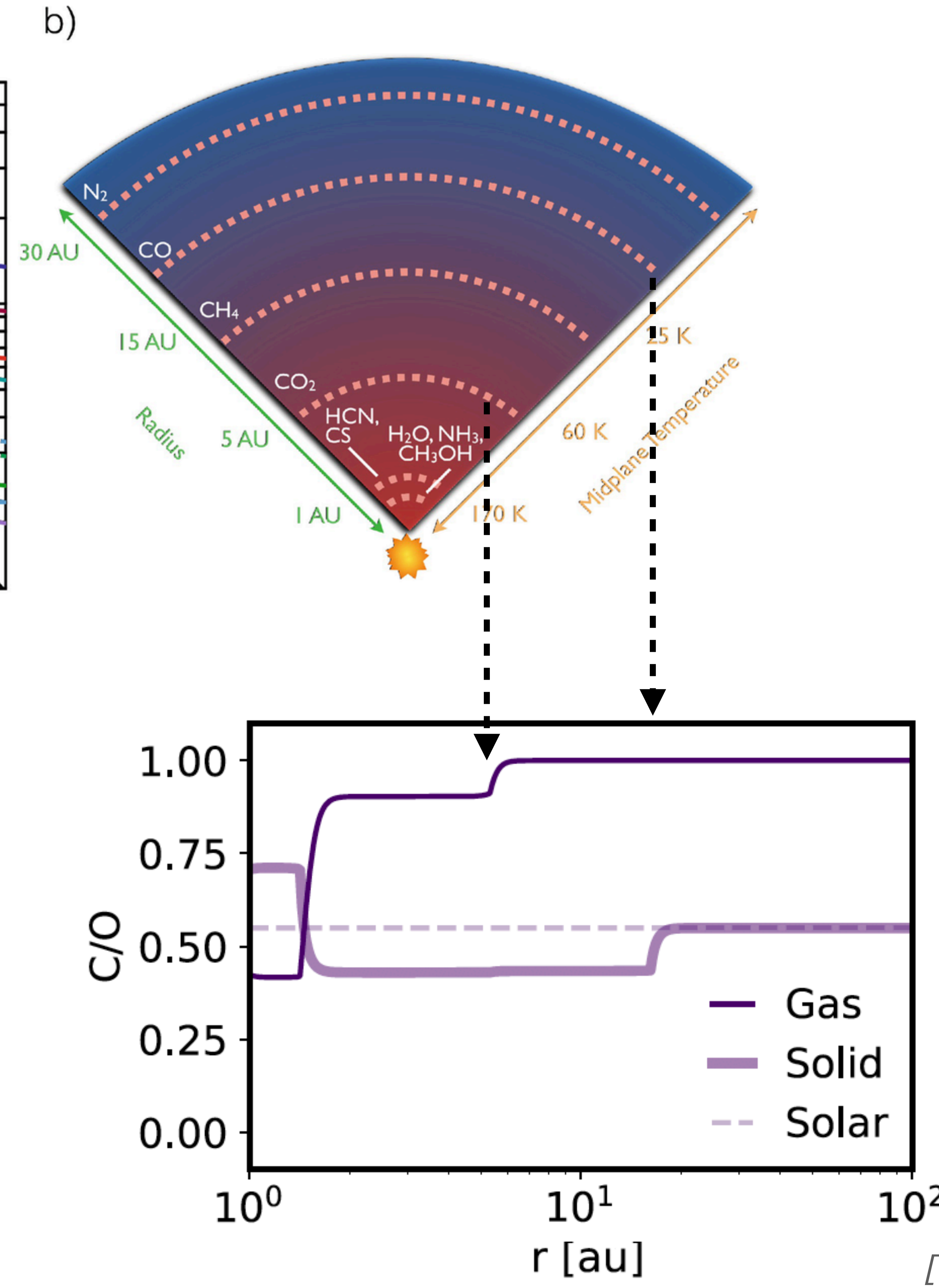
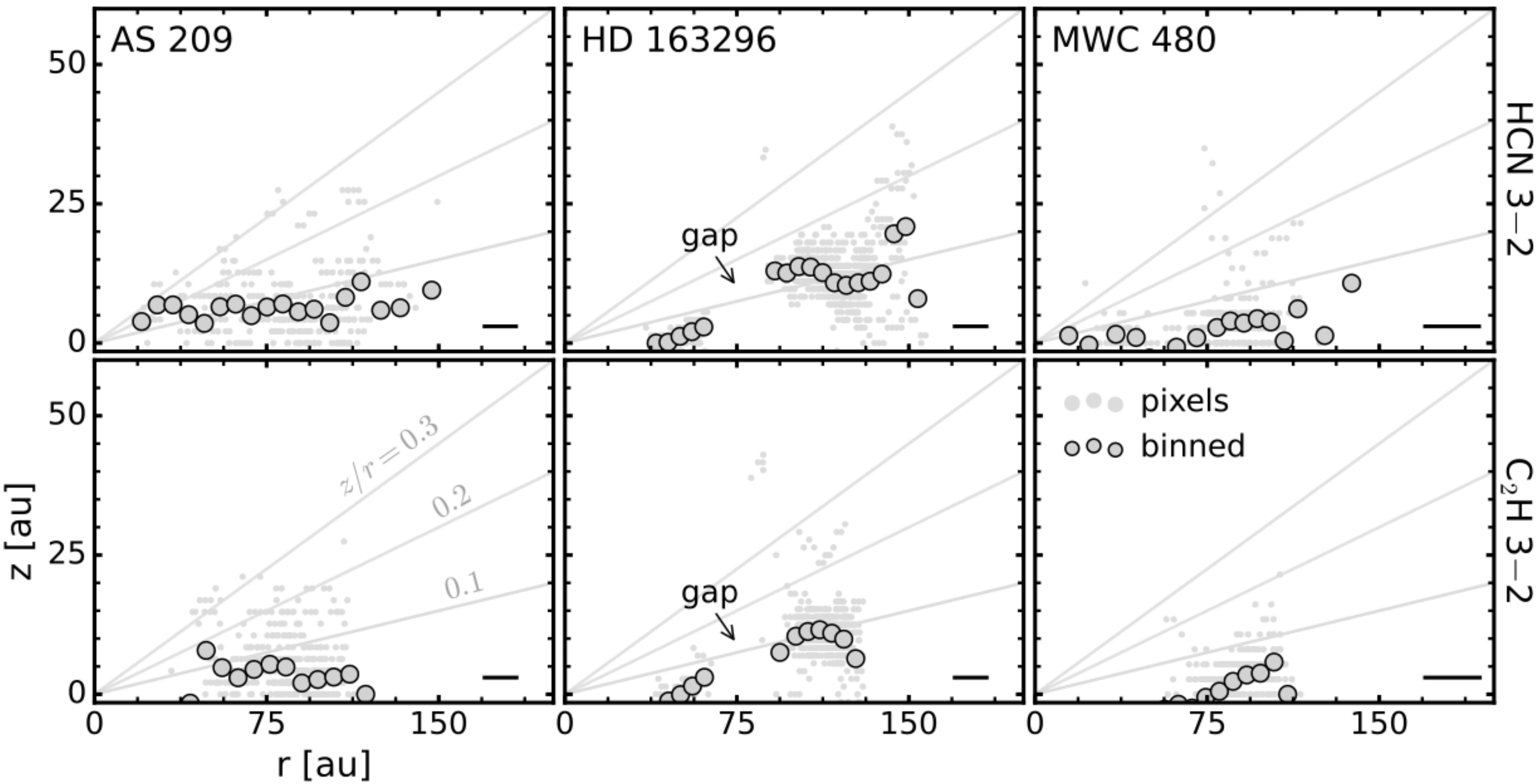


[Öberg & Bergin 2021]

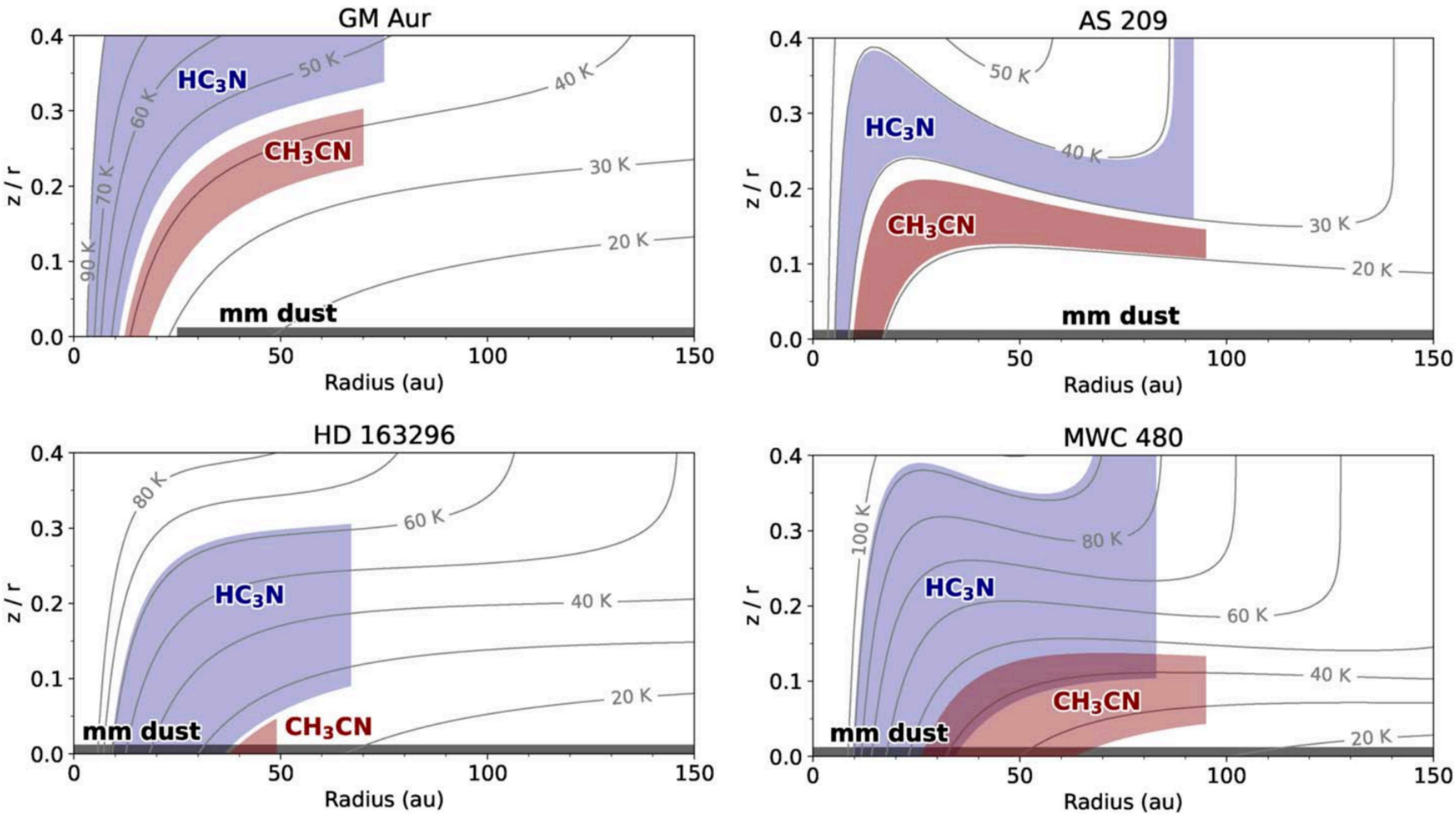
Where do molecules reside vertically?

Vertical disk chemical structure



[Law & MAPS collaboration, APJS, 257, 4]

MAPS largest organics: HC_3N & CH_3CN

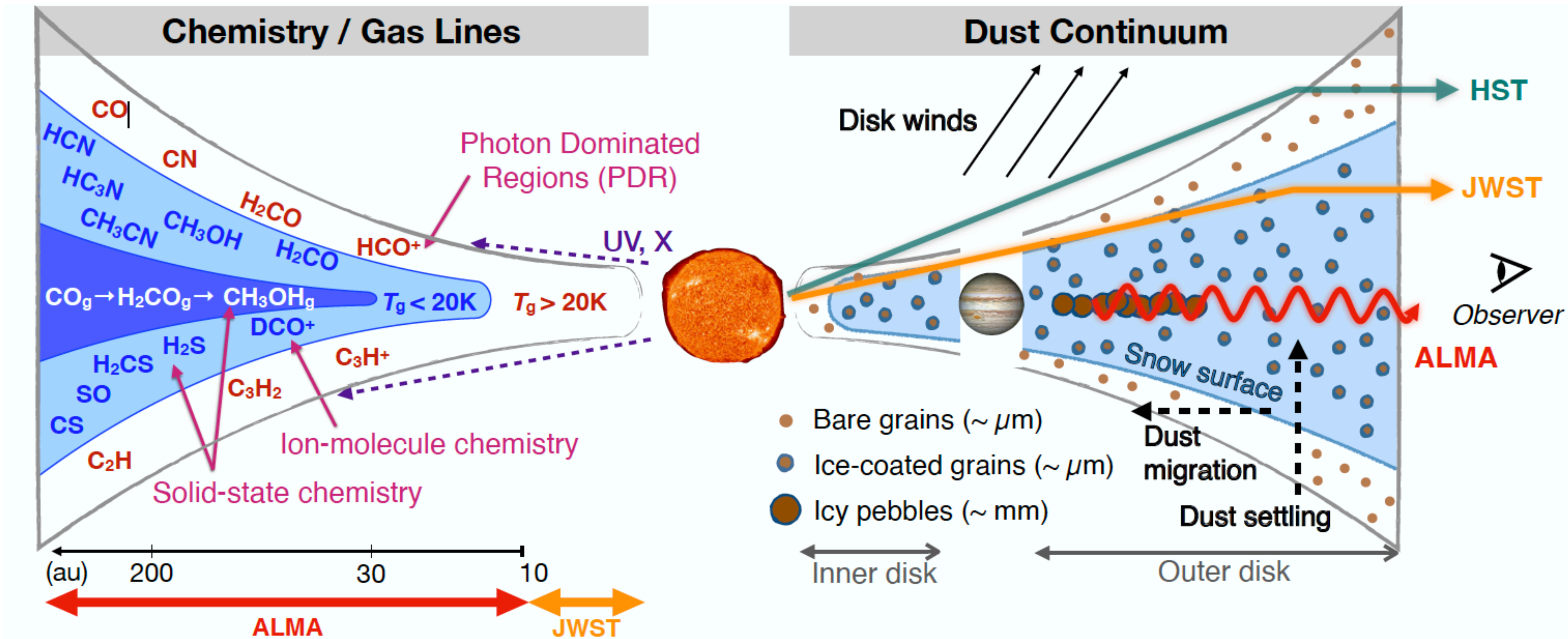


[Ilee & MAPS collaboration, APJS, 257, 9]

Can we get direct constraints?

ALMA Large Program: **DiskStrat**

A comprehensive picture of chemical and vertical structures in protoplanetary disks



Team: ***5 co-PIs: R. Le Gal****, F. Ménard, Y. Aikawa, J. Bergner, C. Espaillat* ***+*** *34* ***co-Is***

See also talk of ***S. Maret*** *(DiskStrat Imaging coordinator)*

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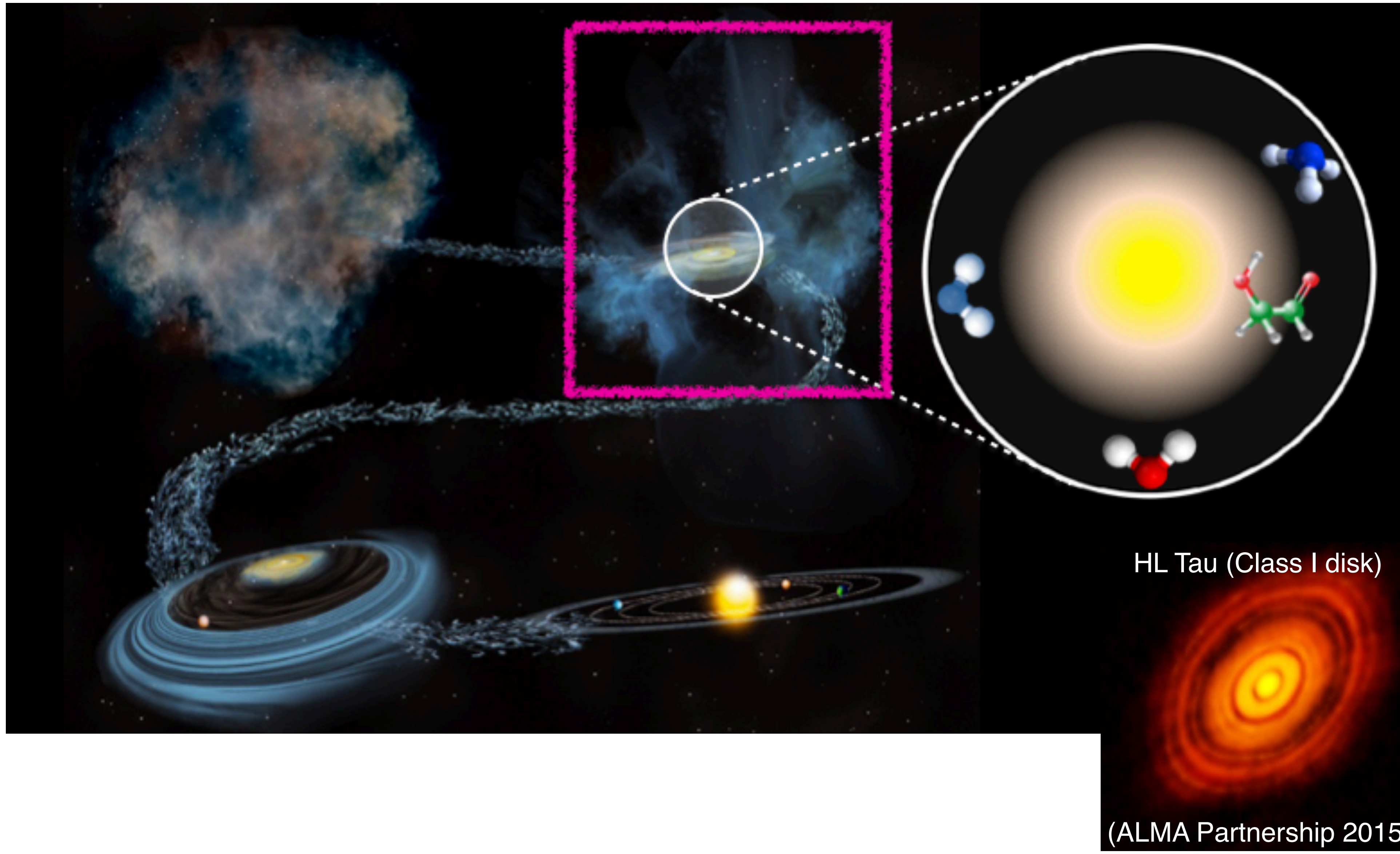
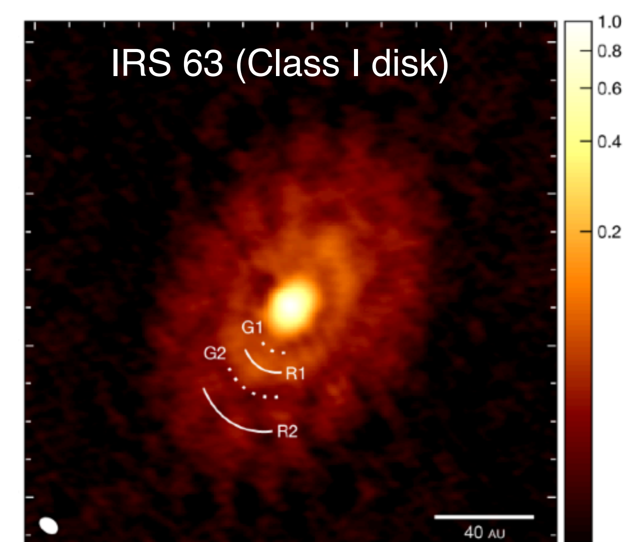
Chemical exploration of Class I YSOs

- 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)


HL Tau (Class I disk)
(ALMA Partnership 2015)



IRS 63 (Class I disk)

Segura-cox+2020 (Nature)

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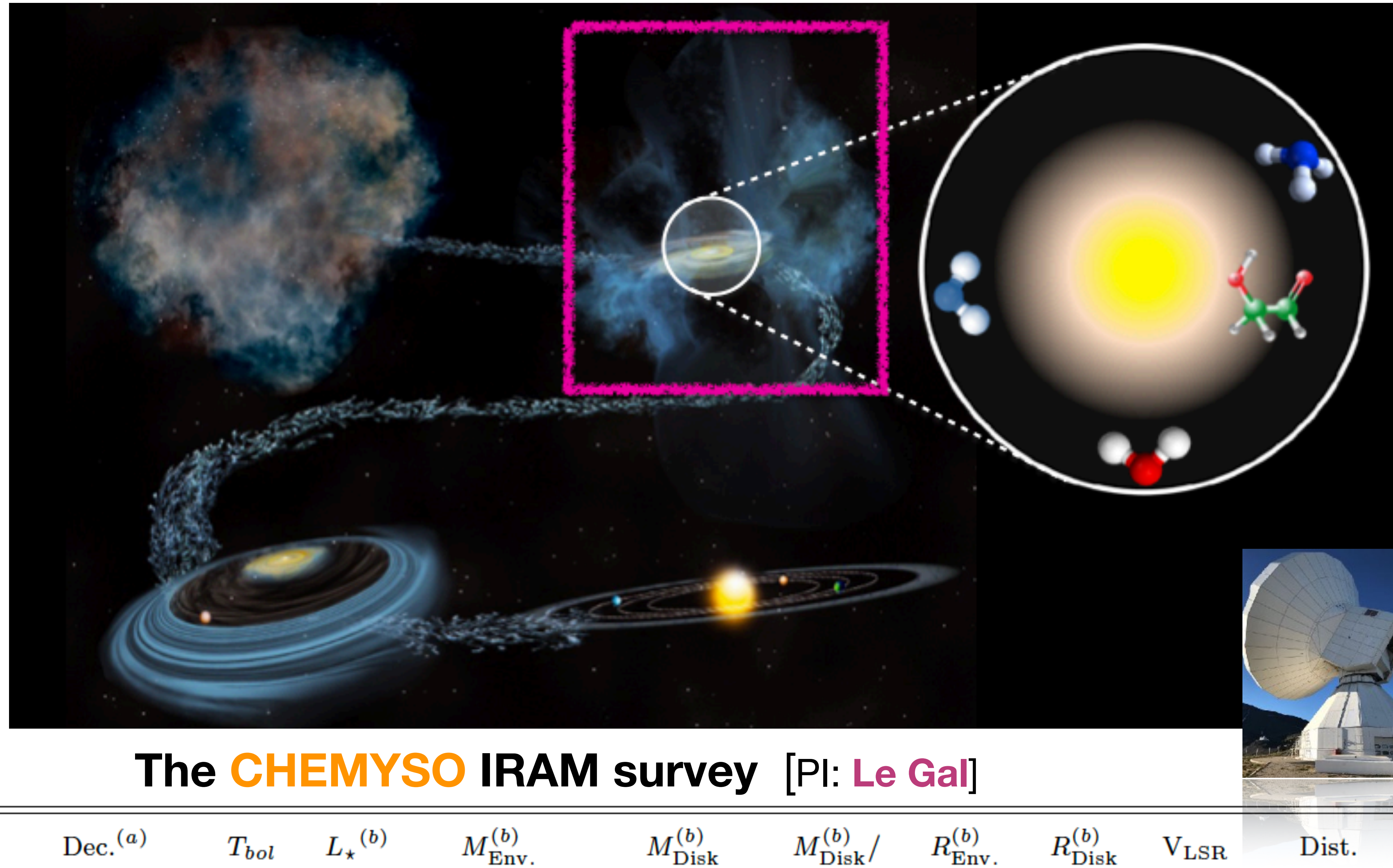
  - ALMA-MAPS (Öberg+2021)

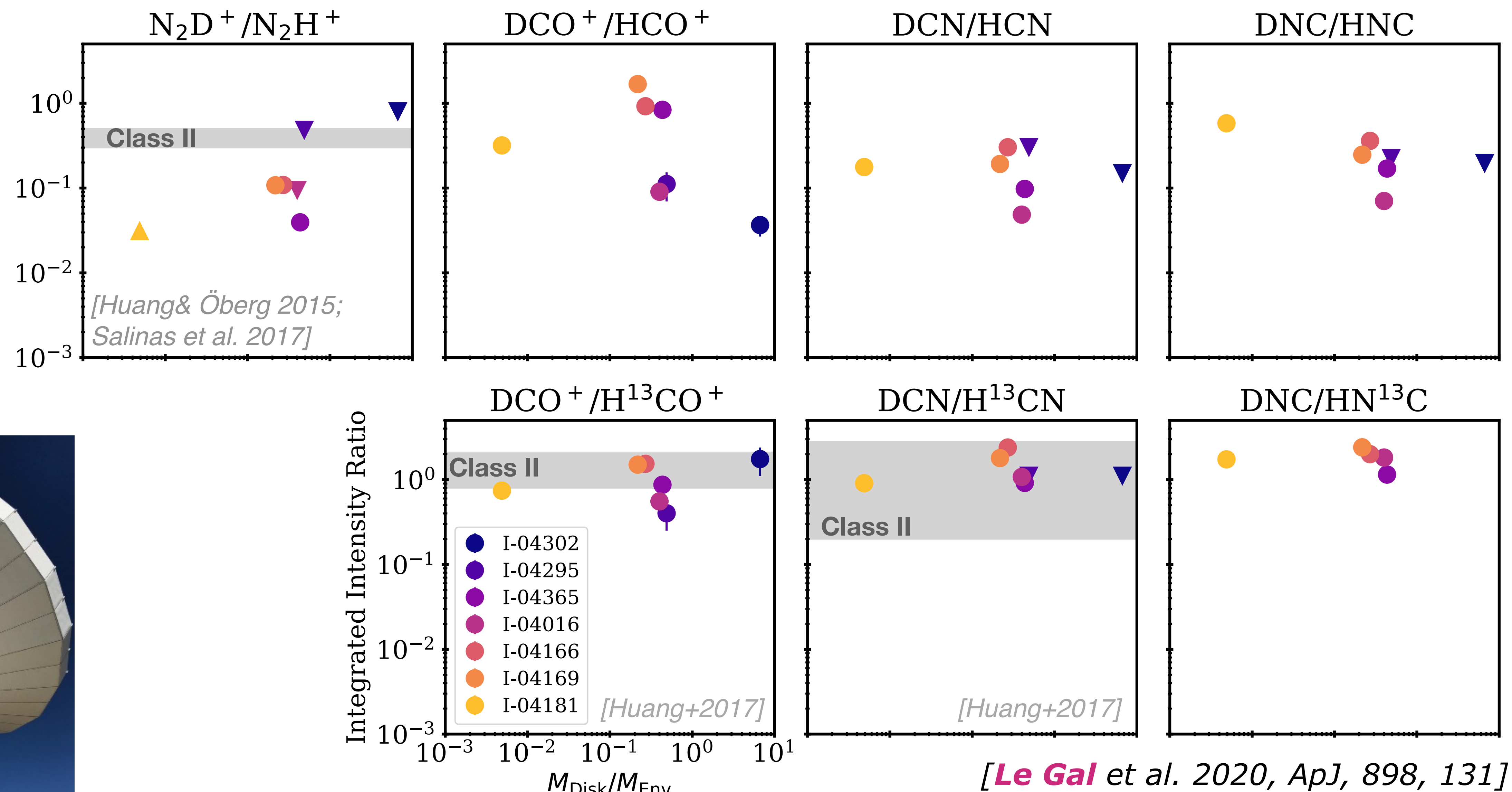


The CHEMYSO IRAM survey [PI: Le Gal]

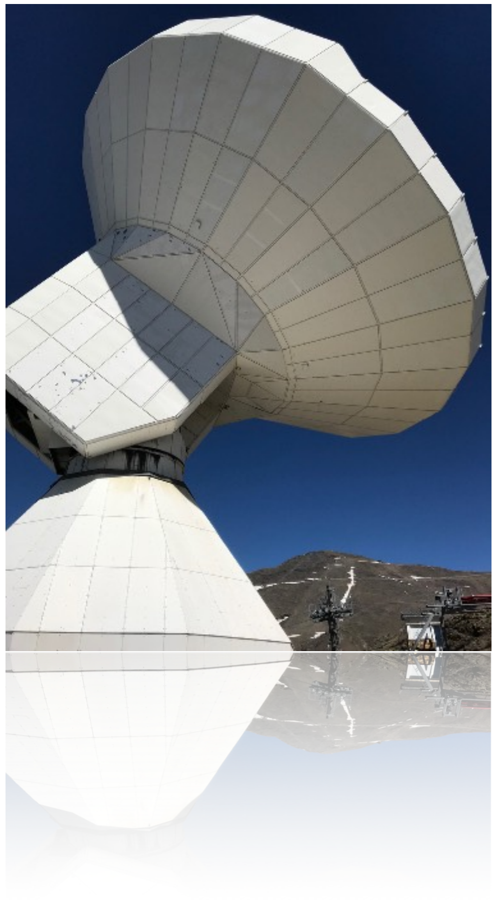
Source	R.A.[a] (J2000)	Dec.[a] (J2000)	T_{bol} (K)	$L_\star$[b] ($L_\odot$)	$M_{\rm Env.}$[b] ($M_\odot$)	$M_{\rm Disk}$[b] ($M_\odot$)	$M_{\rm Disk}$[b]/ $M_{\rm Env.}$	$R_{\rm Env.}$[b] (au)	$R_{\rm Disk}$[b] (au)	$V_{\rm LSR}$ (km/s)	Dist. (pc)
IRAS 04302+2247	04:33:16.501	22:53:20.400	122[c]	0.4	$0.017^{+0.006}_{-0.004}$	$0.114^{+0.019}_{-0.026}$	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]*

Probing chemical inheritance: are D/H ratios reliable tracers?



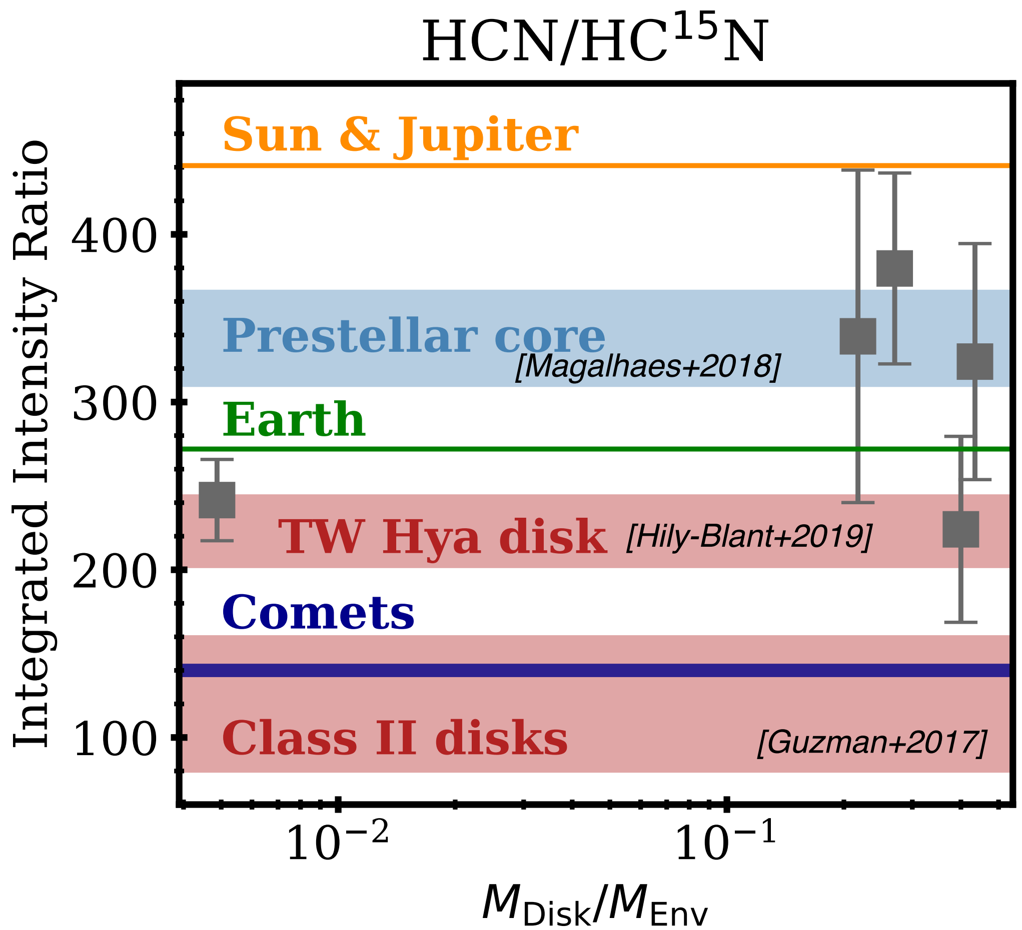
[*Le Gal* et al. 2020, ApJ, 898, 131]

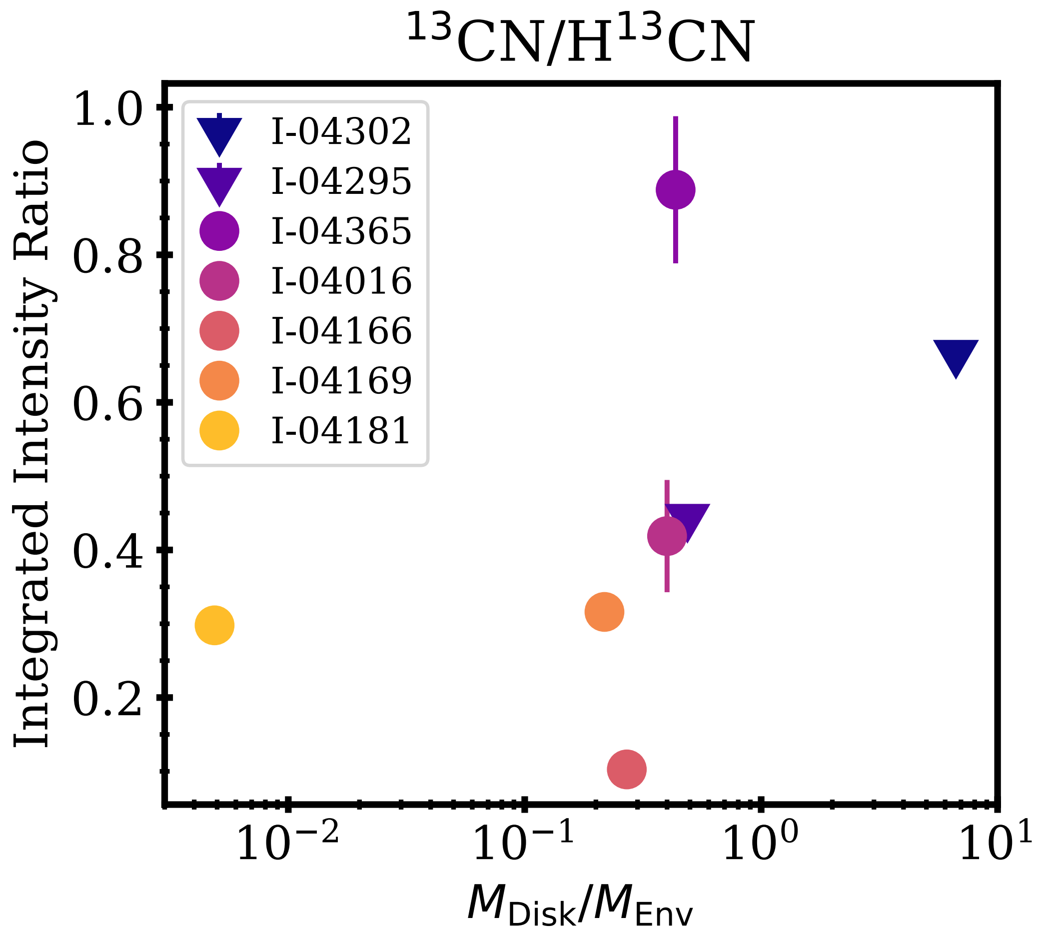


- Gas shows strong deuteration, though the brightest lines are affected by opacity
- N_2D^+ & ^{13}C isotopologues are optically thin, yielding relatively constant D/H ratio
- **Near-constant D/H ratio => similar thermal histories or thermal structures?**

Probing chemical reprocessing: is UV field a major driver?

*[**Le Gal** et al. 2020, ApJ, 898, 131]*



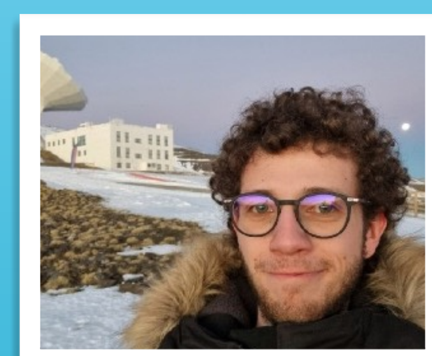


- **$HCN/HC^{15}N$**: span in evolutionary stage if the isotopic ratio is inherited
  or span in physical properties of our sample, if the ratio is reset *in situ*
- **CN/HCN**: highest in the second most luminous source of our sample

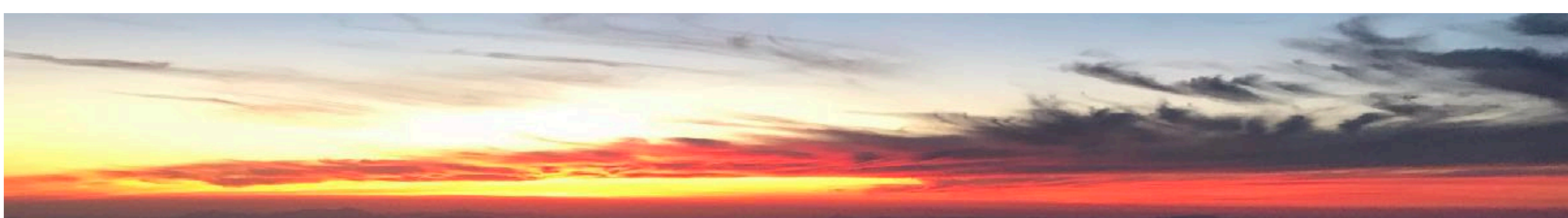
First results of the CHEMYSO survey

- ❖ Class I YSOs are molecule-rich! (at least for our 7 source sample…, *Le Gal et al. 2020*):
  - ▸ 30 small ($N_{atoms} \leq 3$) molecules detected: 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.*
- ❖ Statistical analysis: tracers of (i) dense cold gas, (i) shocked gas & dense ionized gas
- ❖ **Interferometric data required** to distinguish between envelope & disk chemistry => NOEMA data *(**Tanious**+2024, A&A + **Tanious**+2025 to be submitted),*

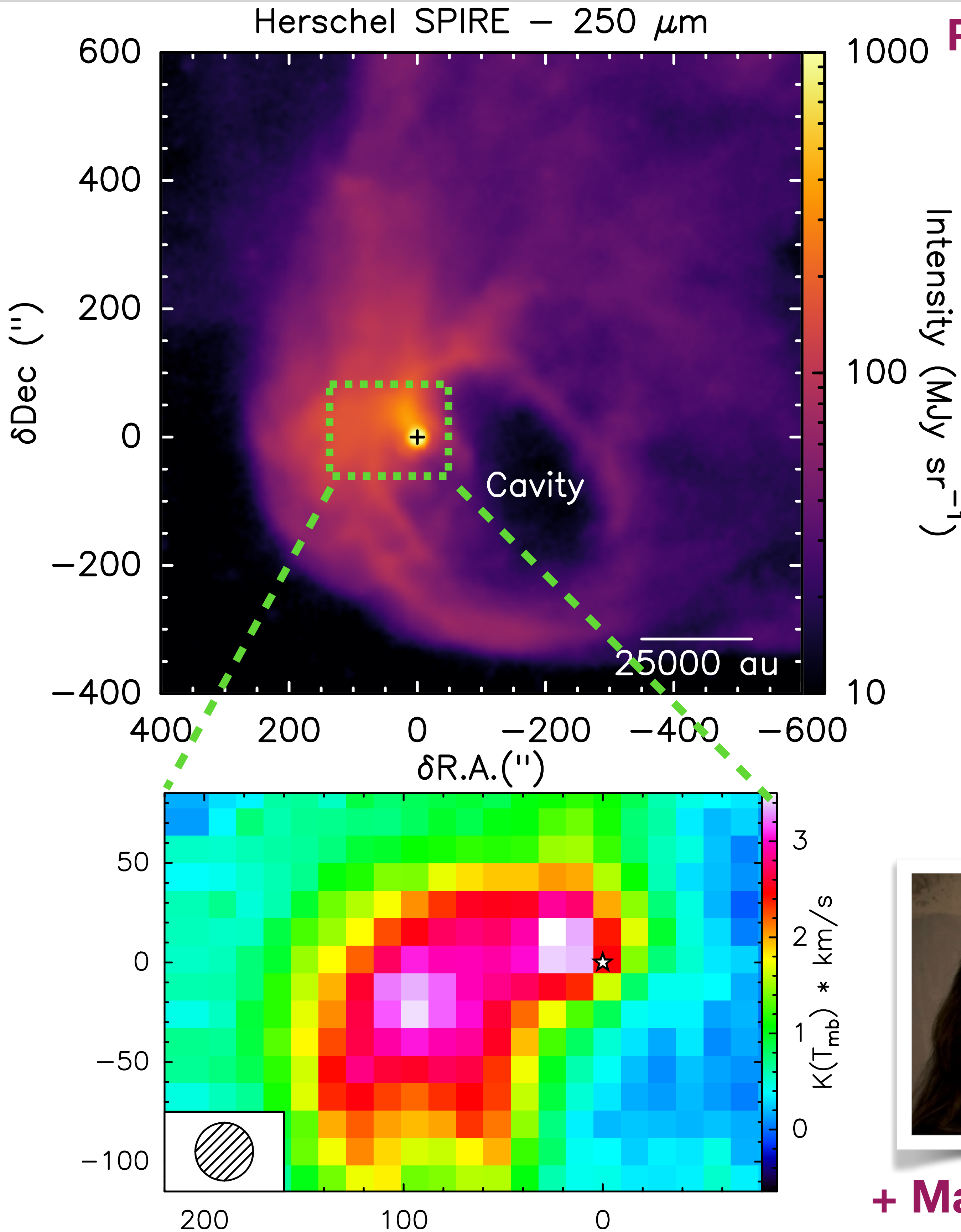
➡ **PHD of M. Tanious (2022-2025)**
(supervisors: R Le Gal & A. Faure)



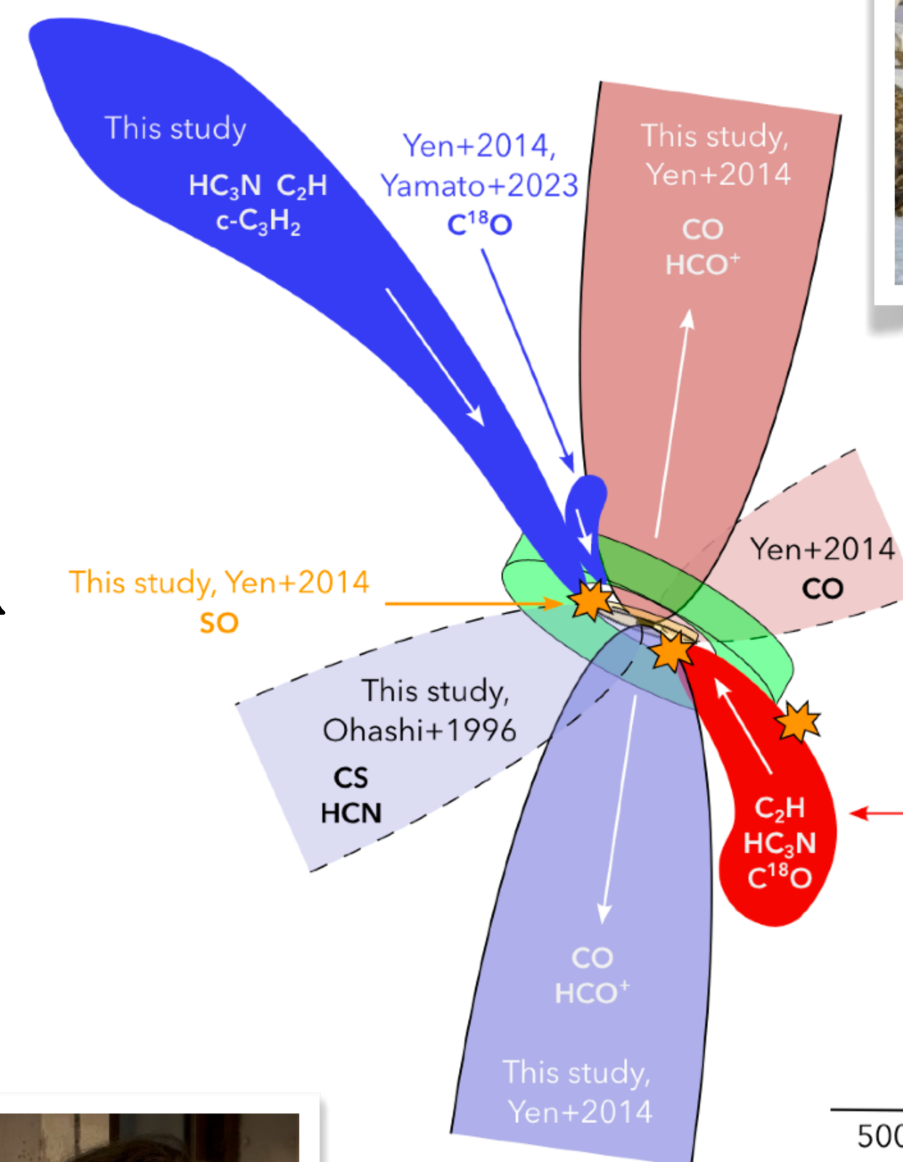
- ❖ Future plans: Extent the source sample & increase the statistics and demography



Protostellar system environment



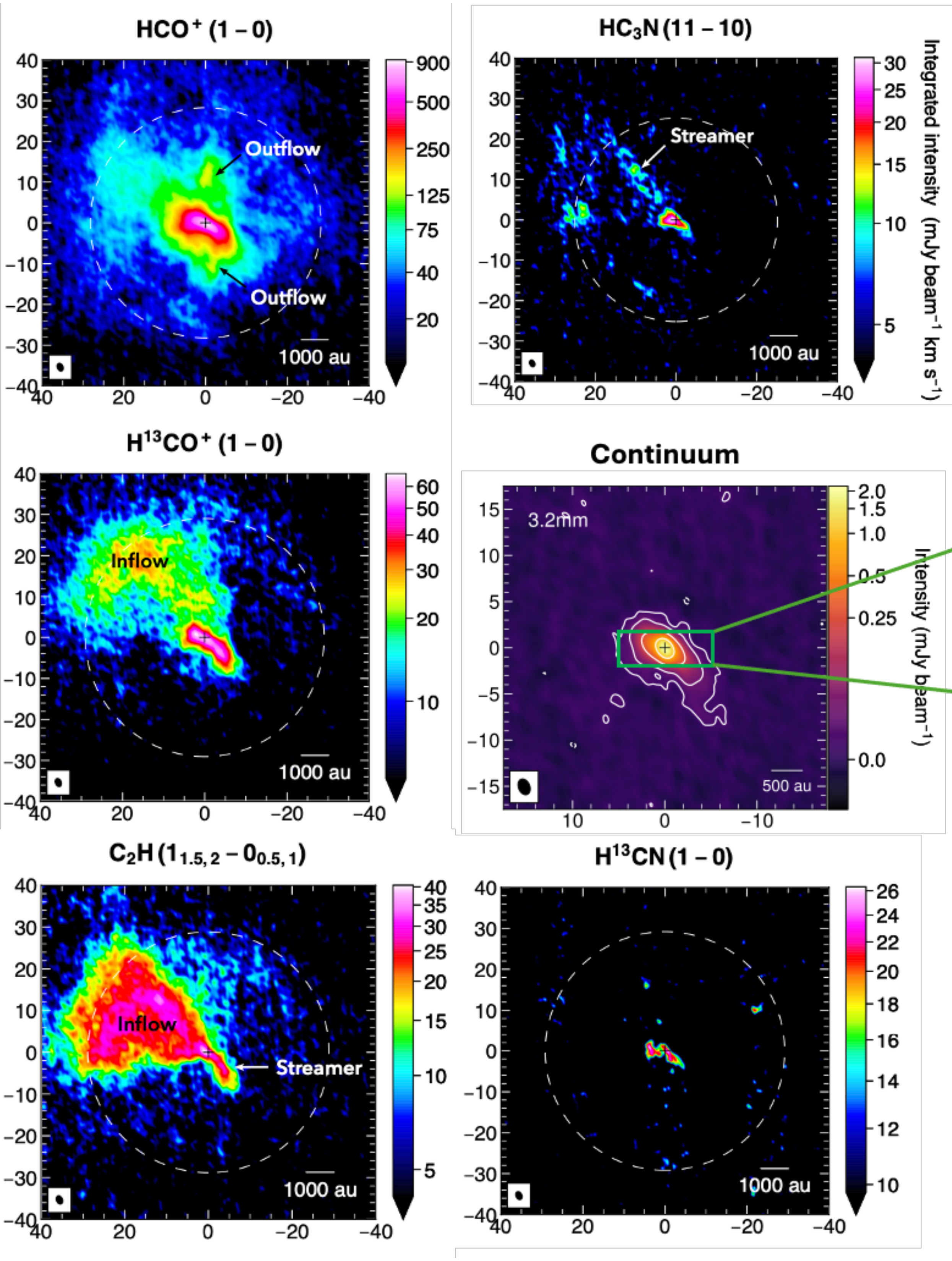
PHD of M. Tanious (2022-2025)



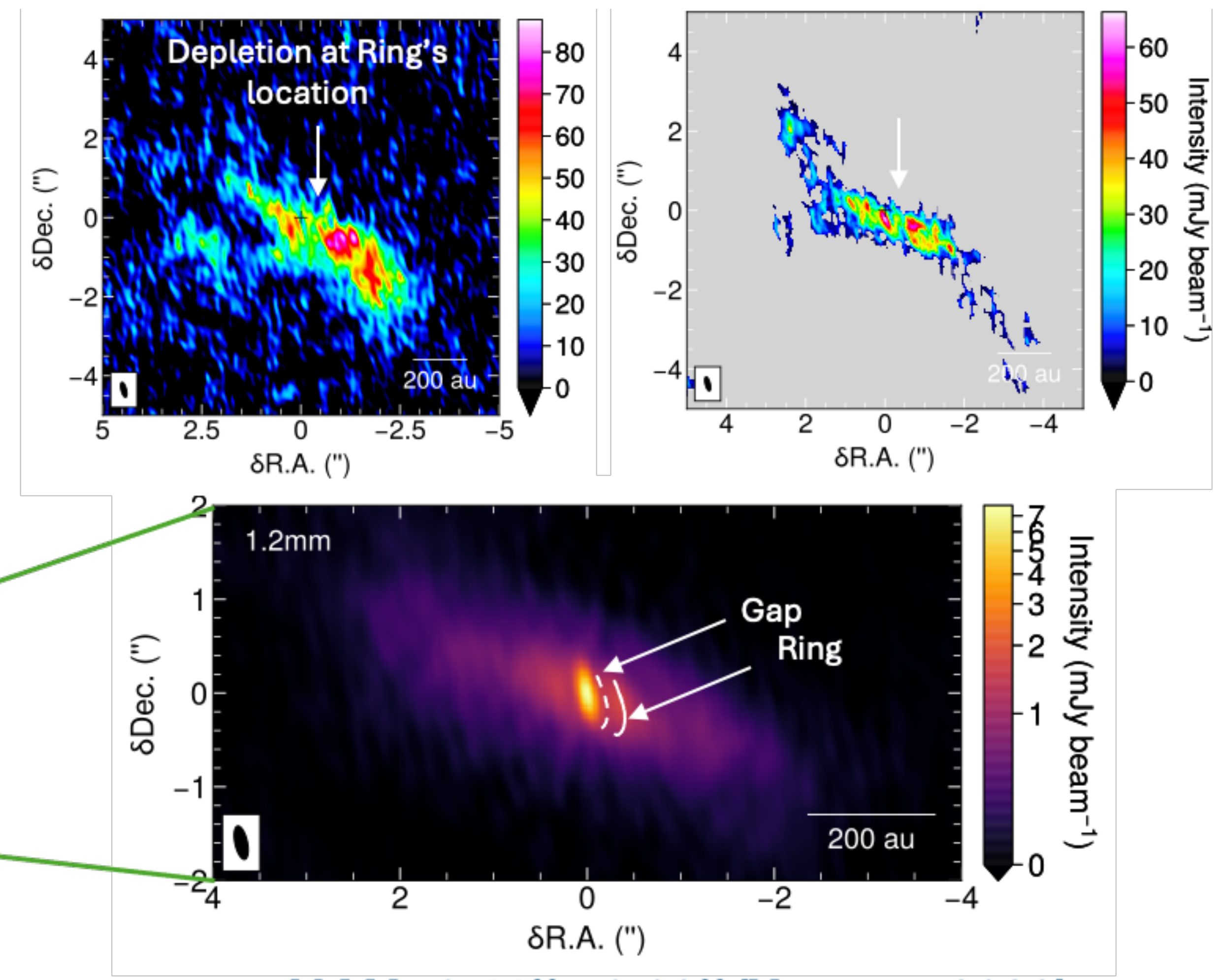
+ Master internship of C. Hoppe (2025)

Environmental influences on disk

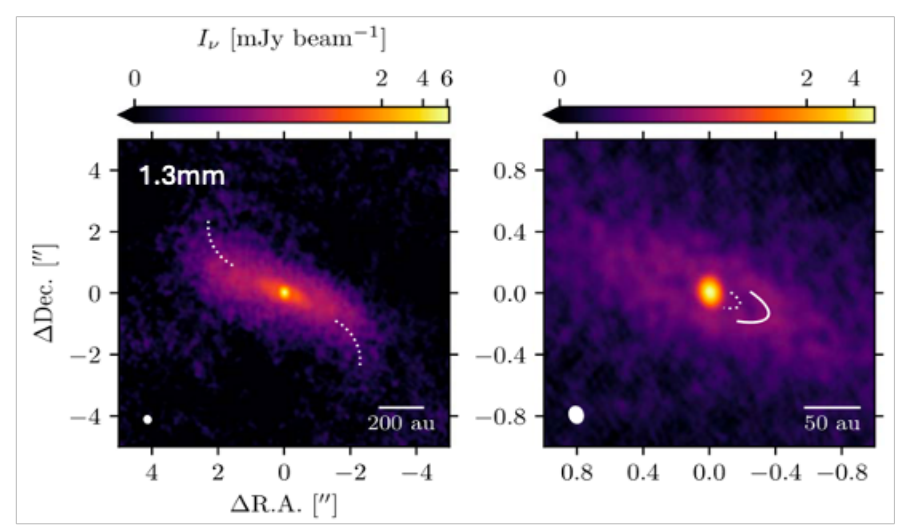
NOEMA+30m @ 3mm (Tanious et al. 2024)



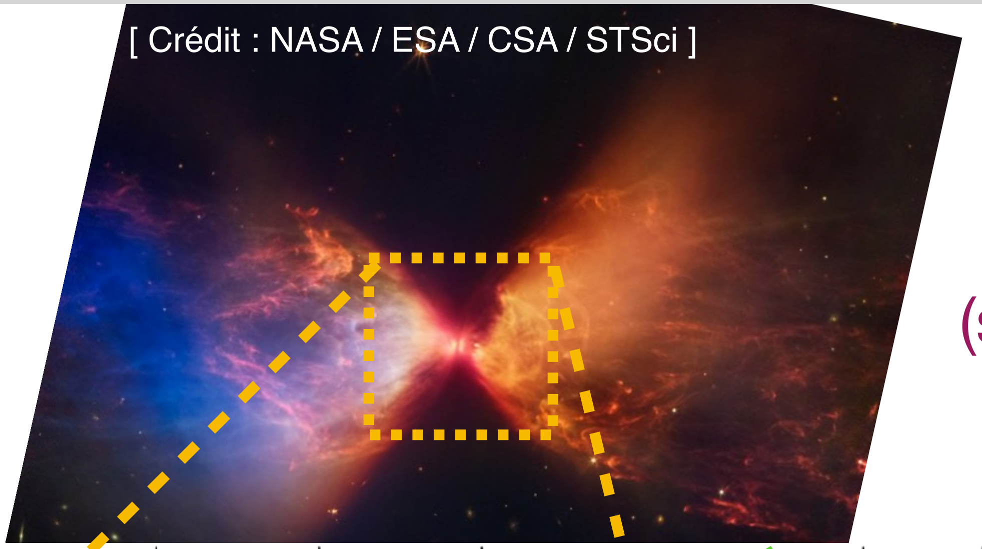
NOEMA @ 1mm (A configuration, 0.36'' x 0.13'') in prep



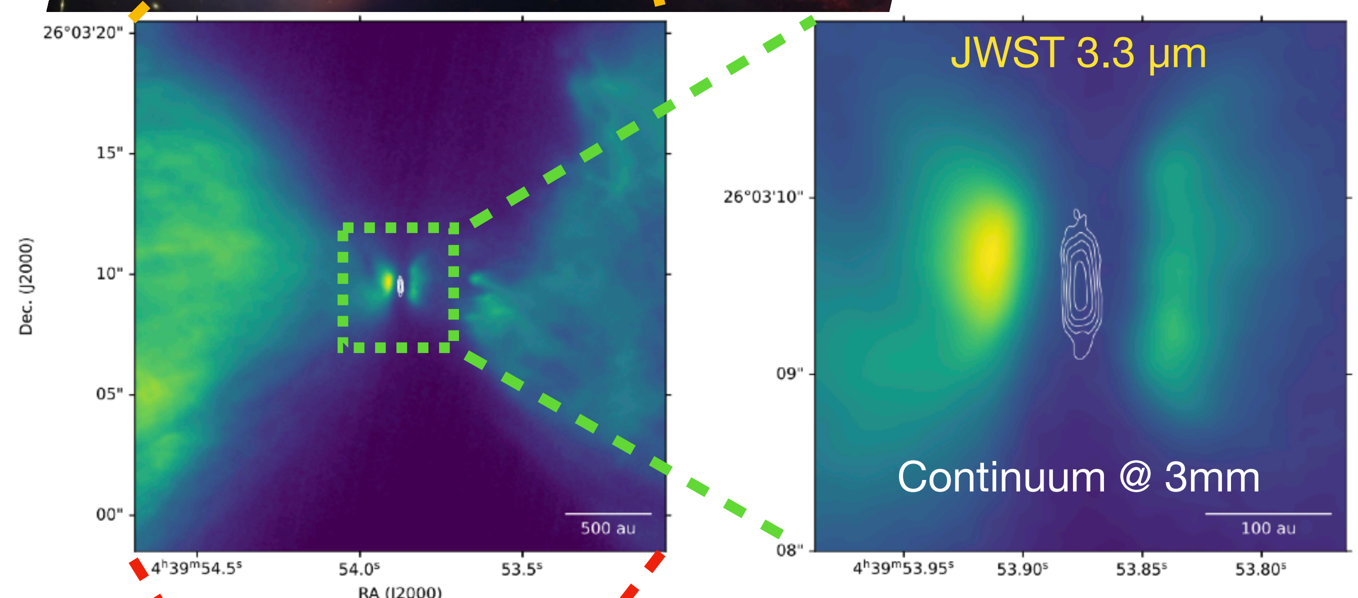
ALMA: 0.11'' x 0.08'' (Yamato+2023)



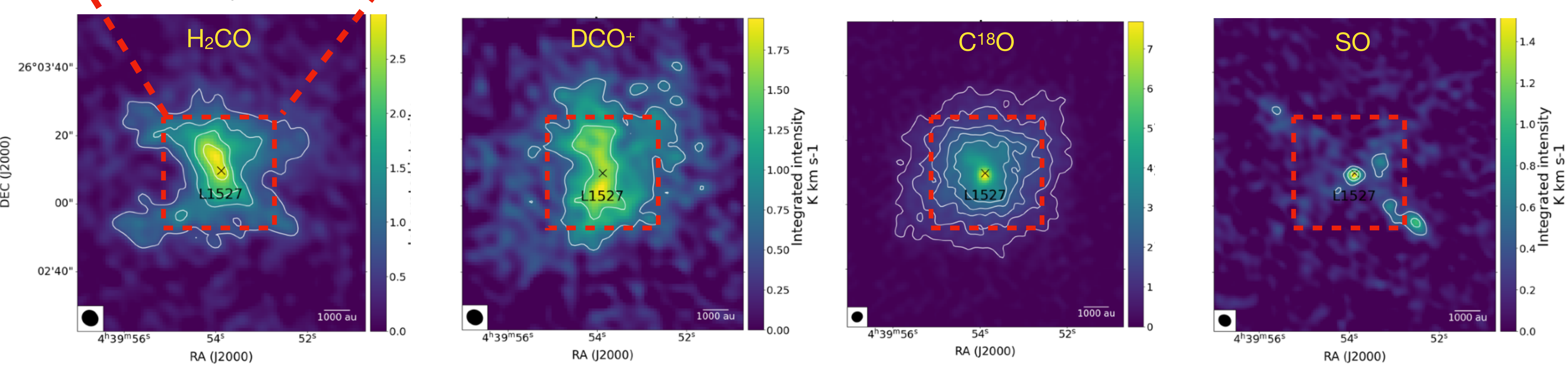
Environmental influences on disk

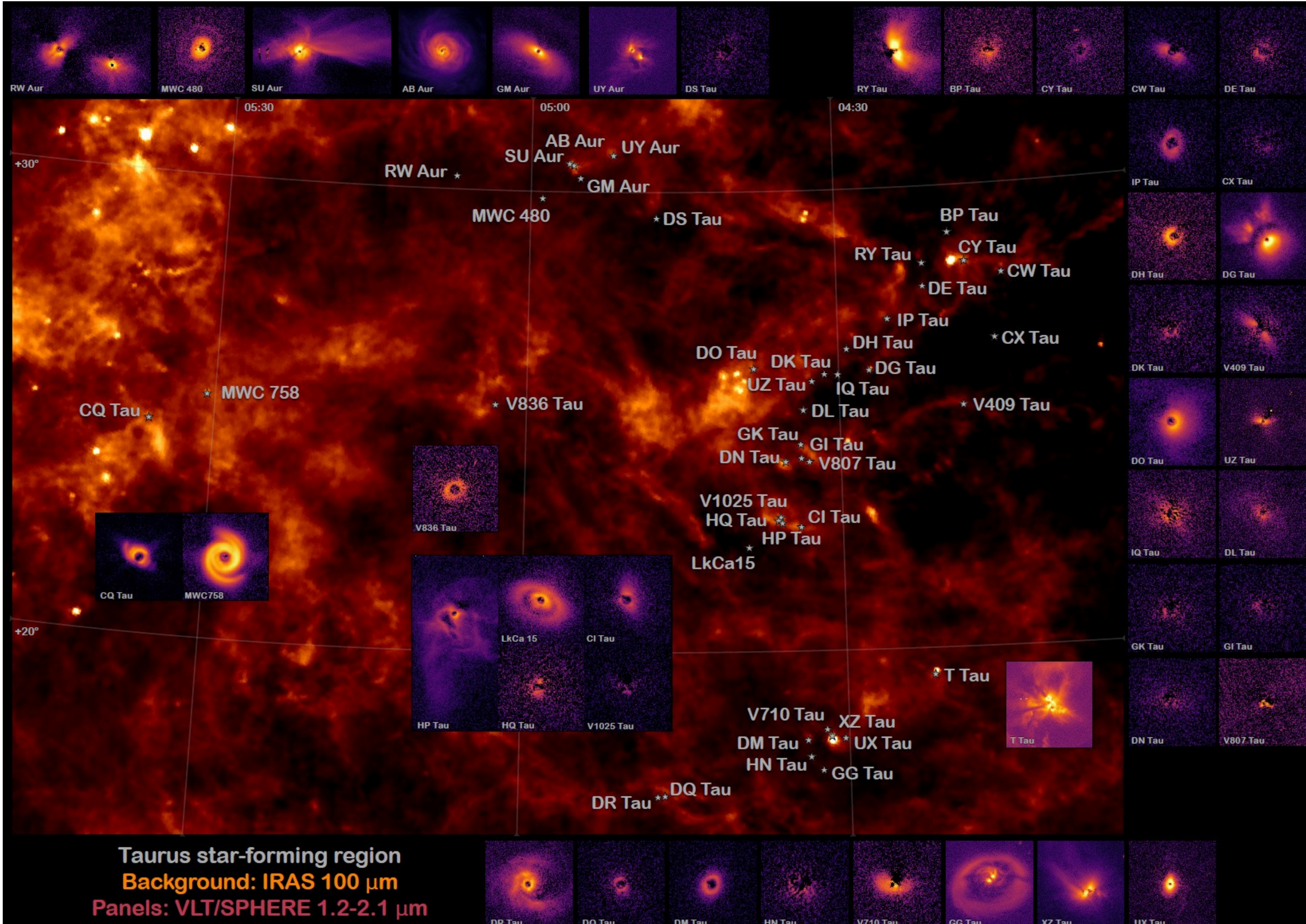


PHD of H. T'Kindt (2024-2027)
(supervised by S. Maret and R. Le Gal)



<u>IRAM 30m + NOEMA project:</u>
a chemical inventory of the gas infalling onto an emblematic nascent protoplanetary disk





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

Summary and perspectives

➢ The high spectral and spatial resolution of the last generation of telescopes (e.g. ALMA and now NOEMA!) **enables detailed studies of the chemical composition and structure of planet-forming disks:**

- ✦ **Map** the vertical and radial distributions of molecular gas, e.g. with CS, **the most readily detected S-bearing molecule in disks**
- ✦ $H_2CS/CS \sim 2/3$ => **S-reservoir in disks may be more organic than thought!**
- ✦ **Synergy with JWST** to probe both icy and warm gas components for a comprehensive view of disk chemistry

➢ **Synergies with the atLAST project:**

- ✦ Probe the **impact of large-scale environments on disk** structure and composition
- ✦ Perform **quick, wide-area sky mapping** to identify new disk targets
- ✦ Conduct **sensitive chemical surveys** as pathfinders for HR mapping, **targeting model-predicted species** & those detected in ≠ astrophysical objects

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