

# Tracing the icy path to form life

**Dr. Melissa K. McClure**

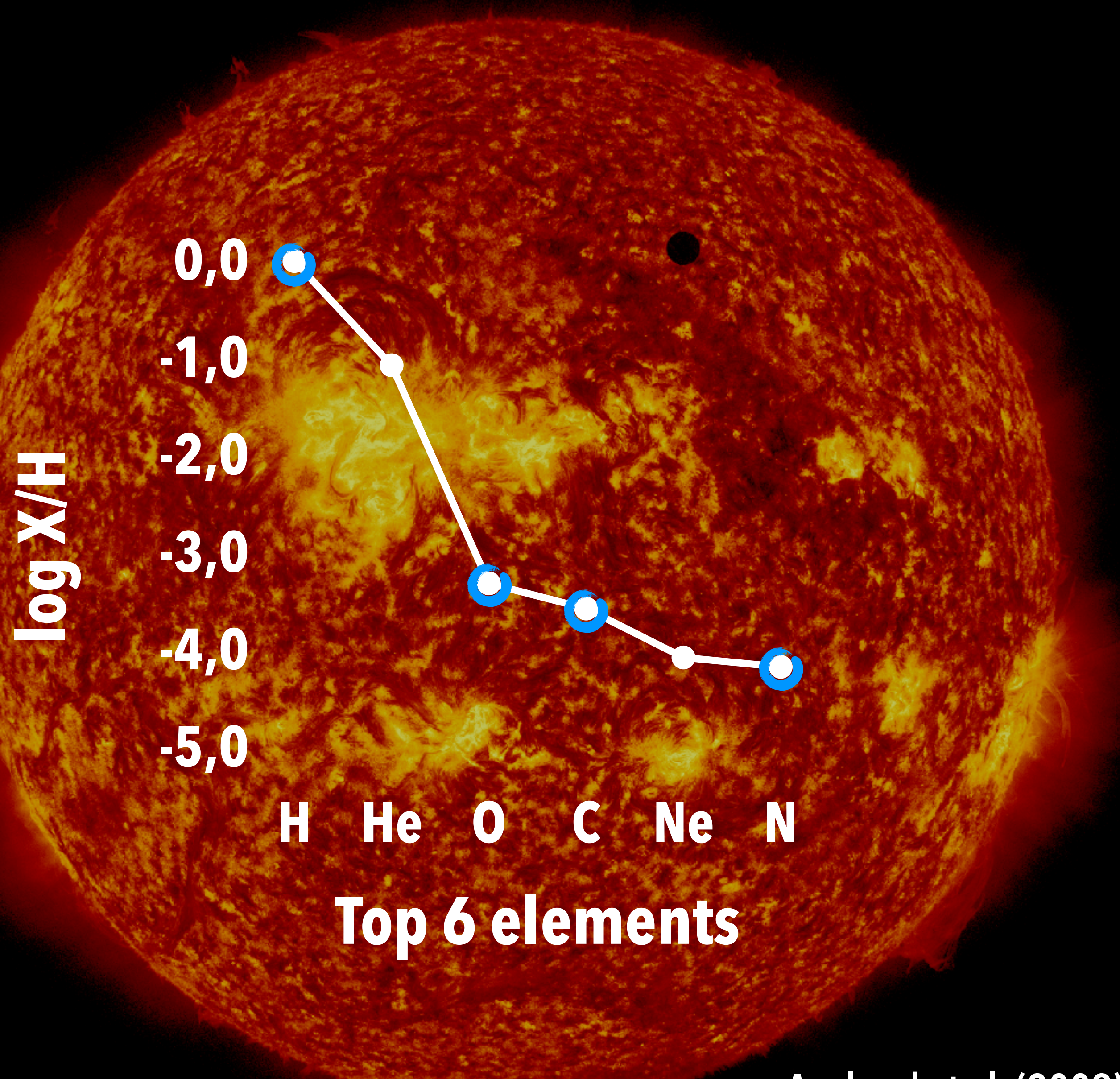
ASSISTANT PROFESSOR & VENI LAUREATE  
LEIDEN UNIVERSITY



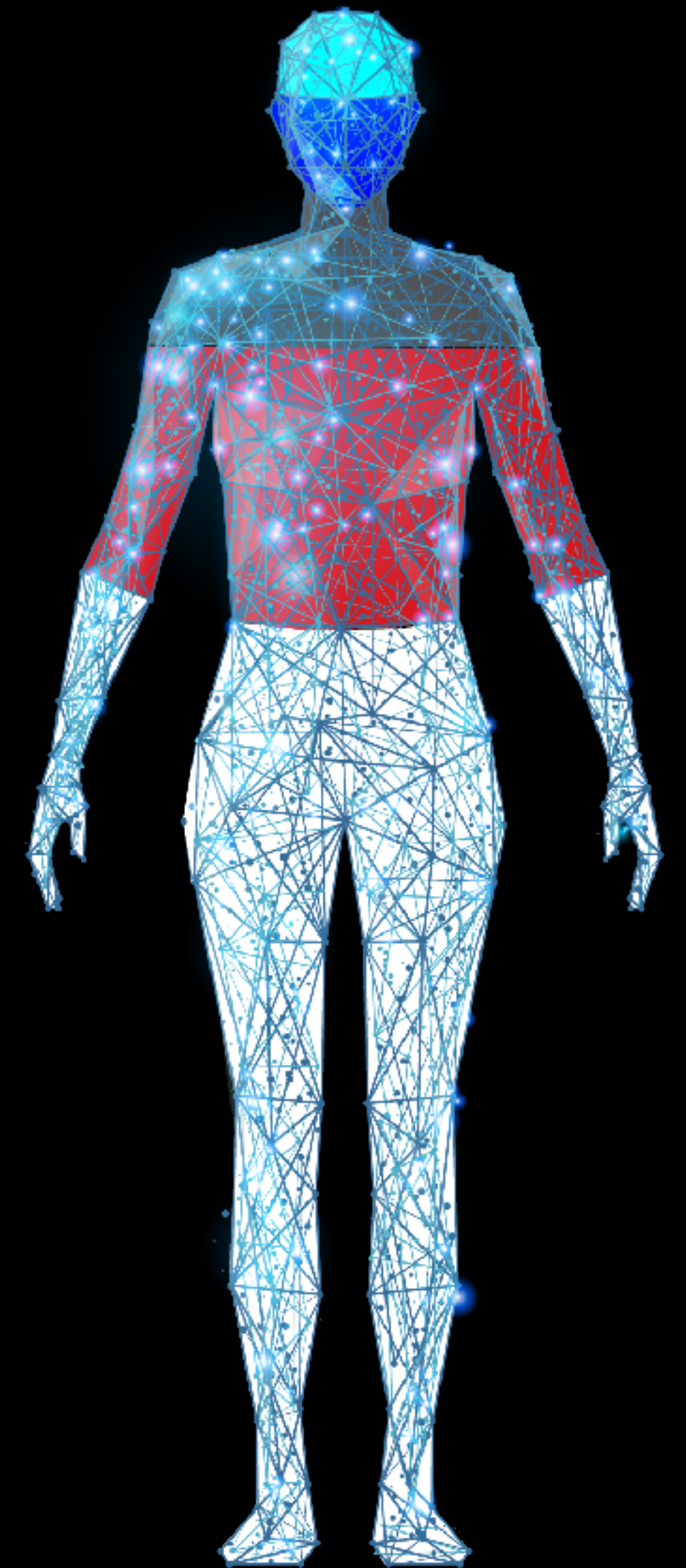
BUILDING THE SOFIA 2020-2025 INSTRUMENT ROADMAP

JUNE 23, 2020 EVERYWHERE, EARTH

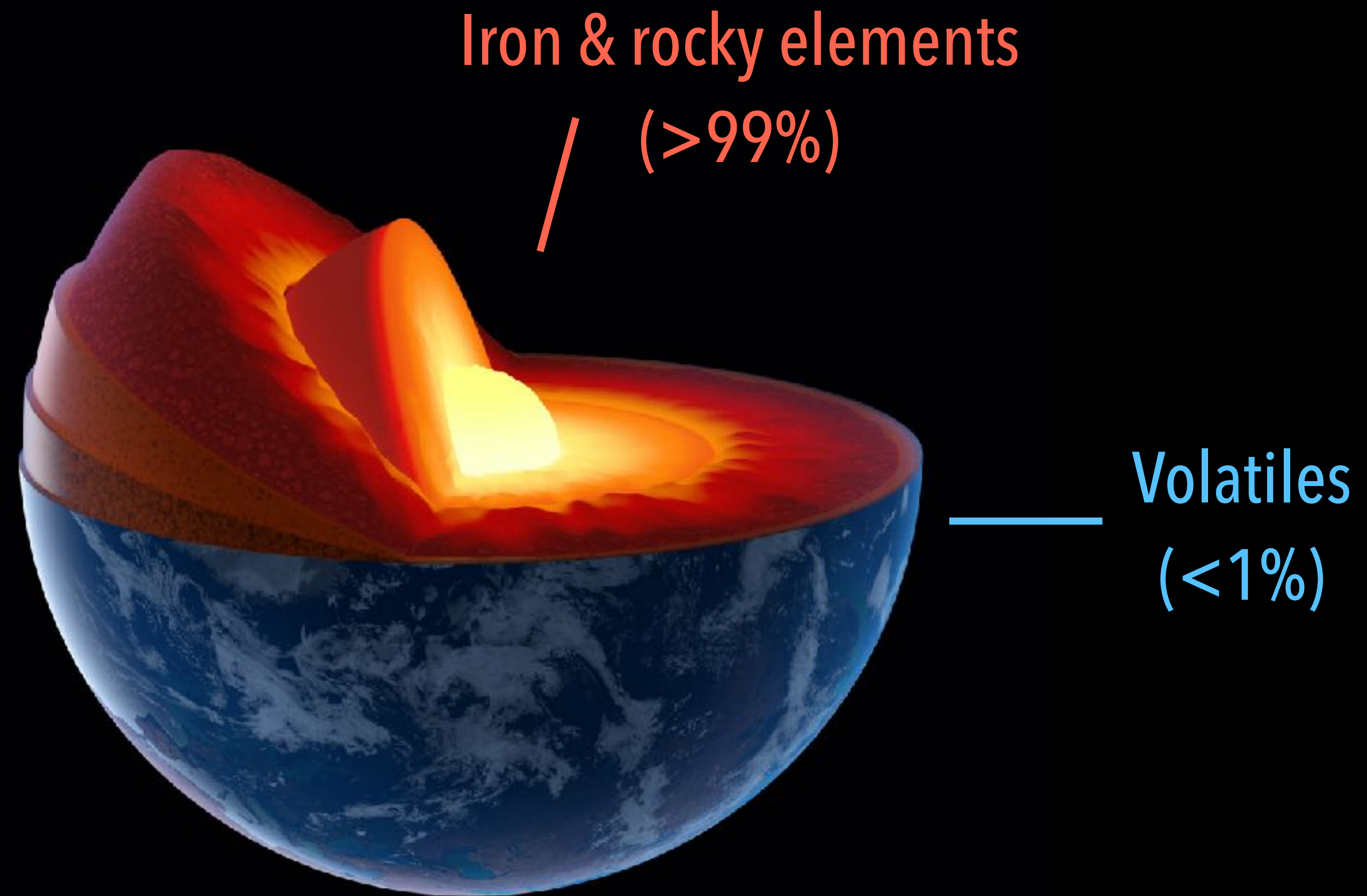
# Volatile elements dominate cosmo-, astro-, and bio-chemistry.



- ... (0.6%)
- N** (1.4%)
- C** (9.5%)
- O** (25.5%)
- H** (63%)



...but volatile elements are depleted on Earth.



**(Complex Organic Molecules: COMs  
carbon-based,  $\geq 6$  atoms)**

**(Simple ices)**

methanol

H<sub>2</sub>O

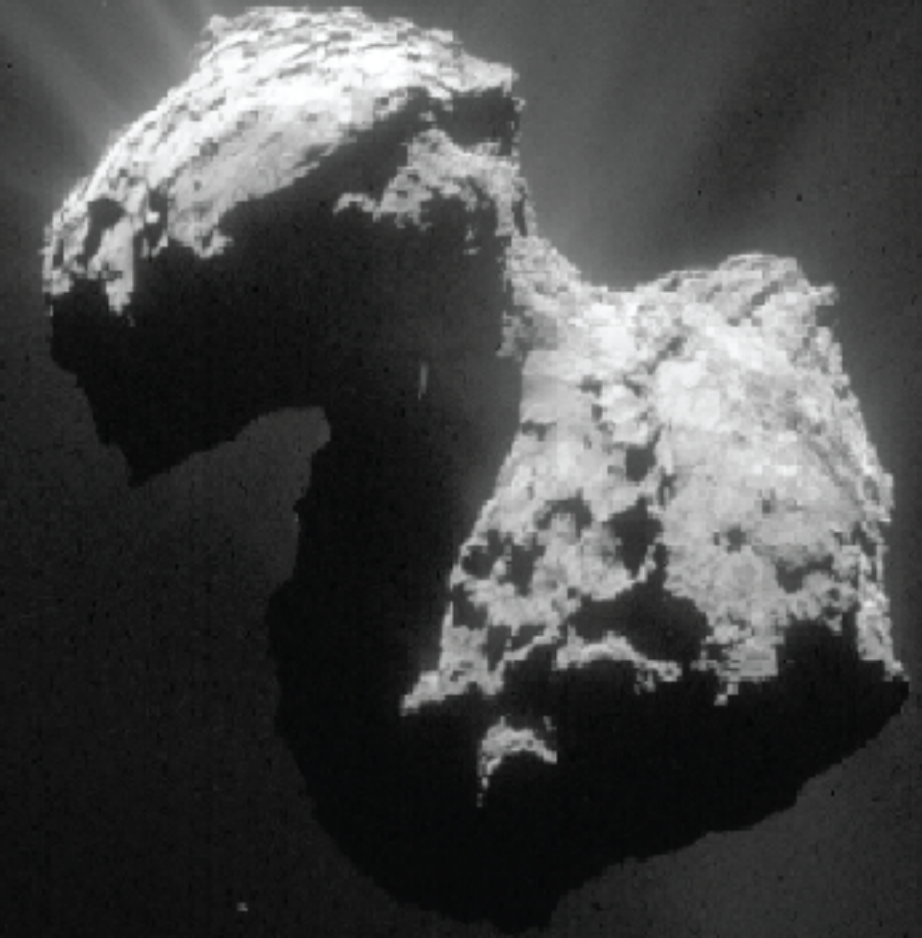
NH<sub>3</sub>

CO<sub>2</sub>

acetaldehyde

CH<sub>4</sub>

**Planetesimal impacts brought volatile organics to Earth...**  
*...and may have kick-started Earth's biochemistry.*



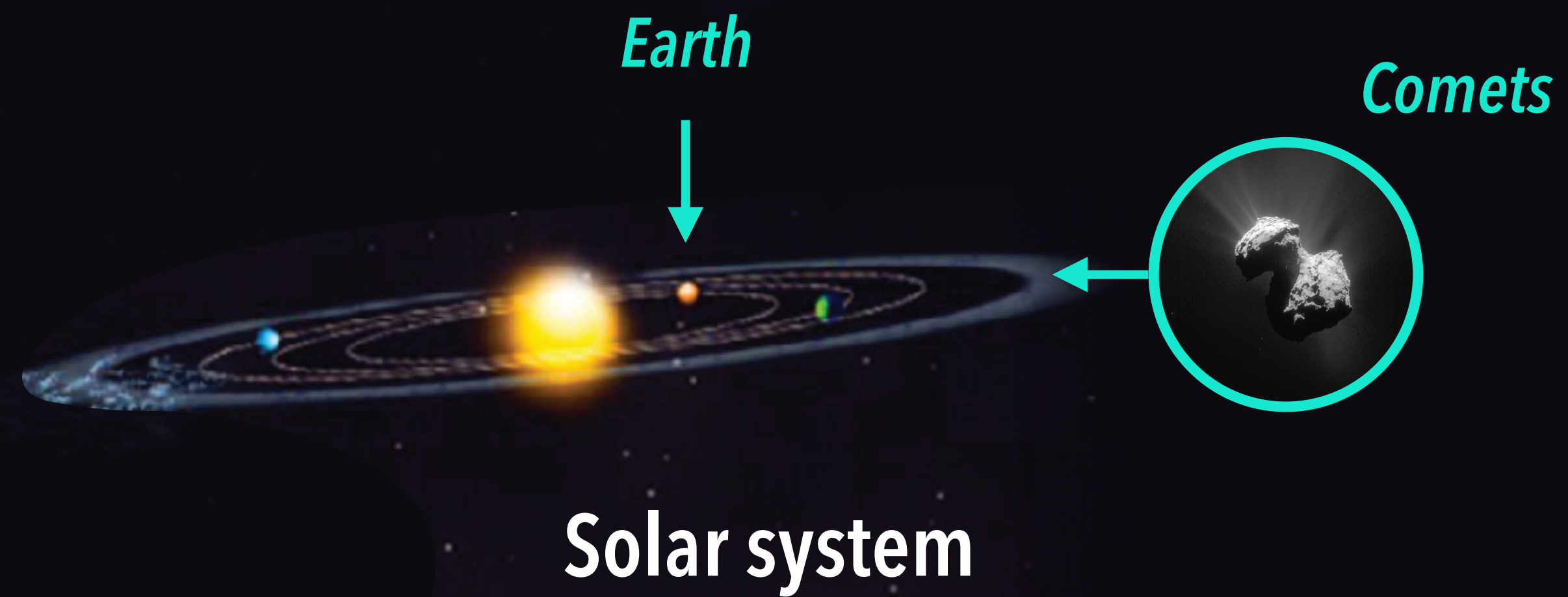
CO

ethanol

glycine  
**(biomolecule!)**

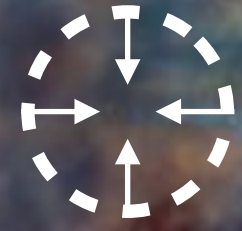
polycyclic aromatic  
hydrocarbons (PAHs)

**Planets and comets are leftover solid material from the star formation process.**



Dense, cold molecular cloud

Core



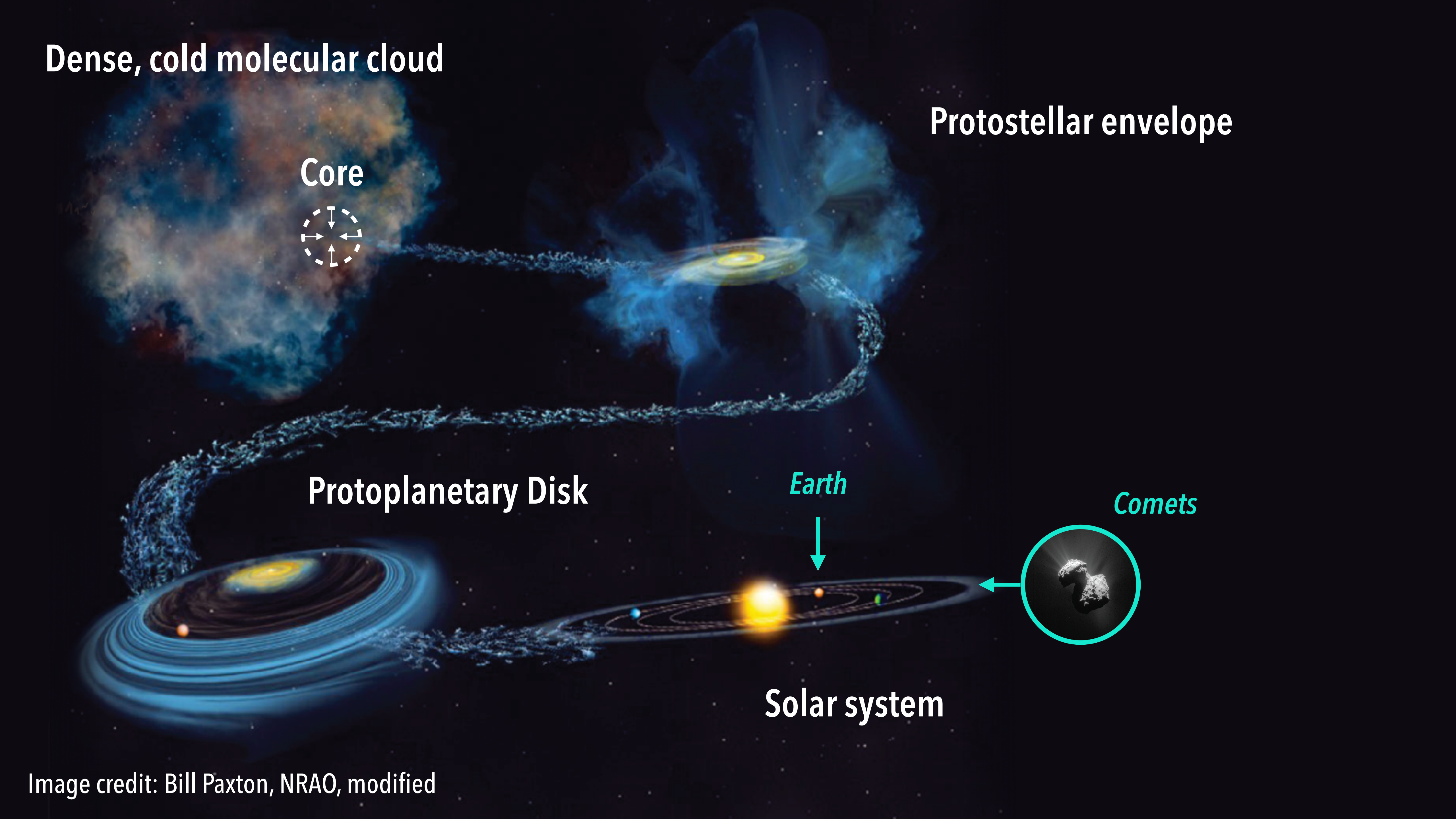
Protostellar envelope

Protoplanetary Disk

Earth

Comets



Solar system



# Big Picture

**If planets inherit ices & COMs from molecular clouds,  
then life may be universal, not unique to solar system.**

# Battle plan to probe ice evolution

#	Technique	Wavelengths	Science	Facility
1	Absorption spectroscopy	Near-, mid-Infrared	<ul style="list-style-type: none"> <li>● <b>Relative</b> abundances of all simple ices</li> <li>● COM detections</li> <li>● Thermal processing &amp; grain size signatures</li> </ul> 	JWST, SPHEREx
2	Thermal emission spectroscopy 	Far-infrared	<ul style="list-style-type: none"> <li>● <b>Absolute</b> abundance of ice(s) versus rocks</li> <li>● <b>Directly probe comet-forming regions (in disks)</b></li> <li>● Alternative COM detections?</li> </ul>	(OST, SPICA, formerly SOFIA HIRMES)
3	Scattered light imaging	Near-infrared	<ul style="list-style-type: none"> <li>● Spatially resolved ice distributions (compare with spiral arms/known exoplanets)</li> </ul>	(limited ground-based)



**#1**

Dense, cold molecular cloud

Hot



Cold

Hot

Cold

Protostellar envelope

Near-, mid-IR absorption spectroscopy

Protoplanetary Disk

Hot

Cold

log (flux)

Background star

Protostars

Edge-on  
disk

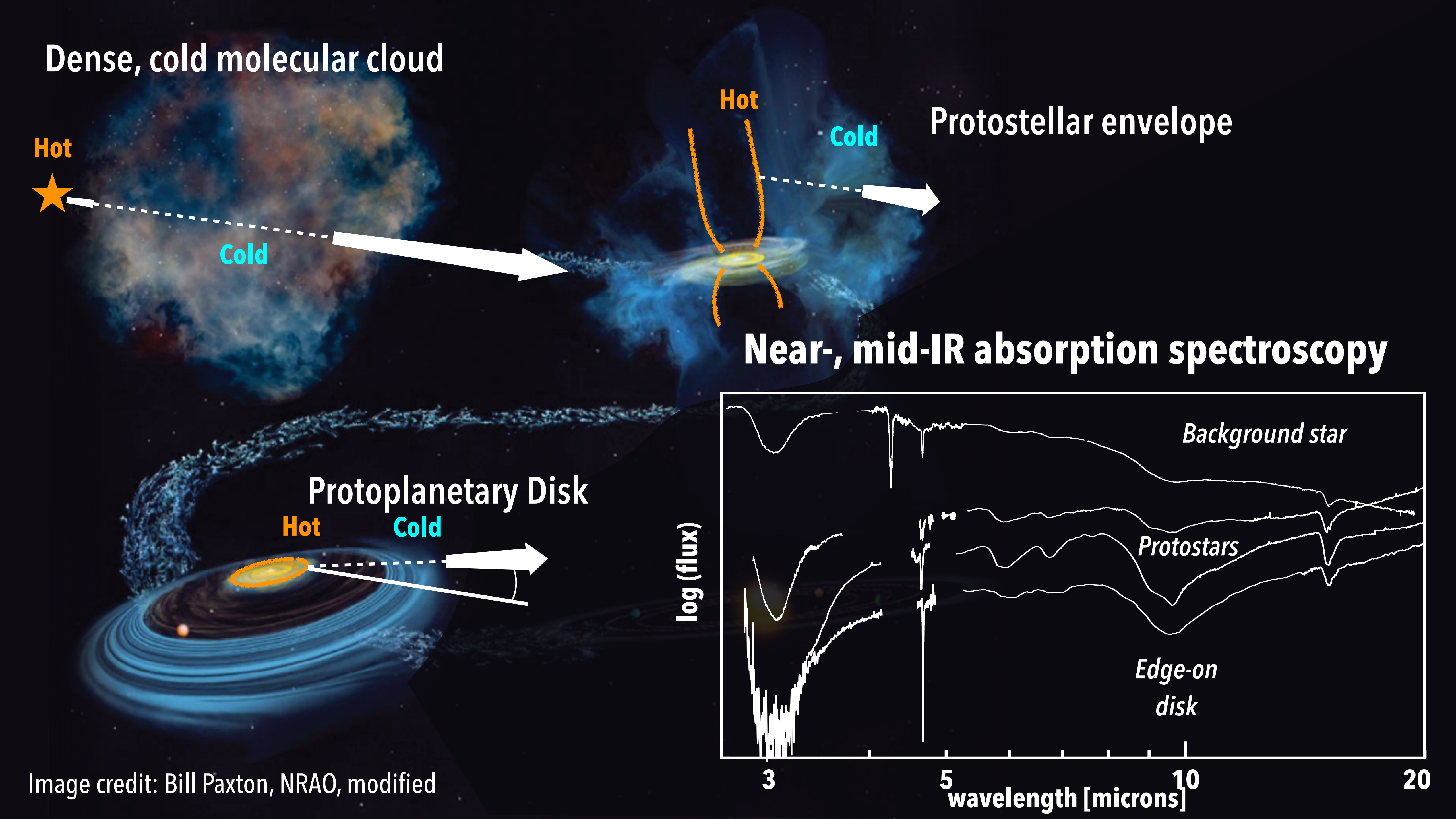
3

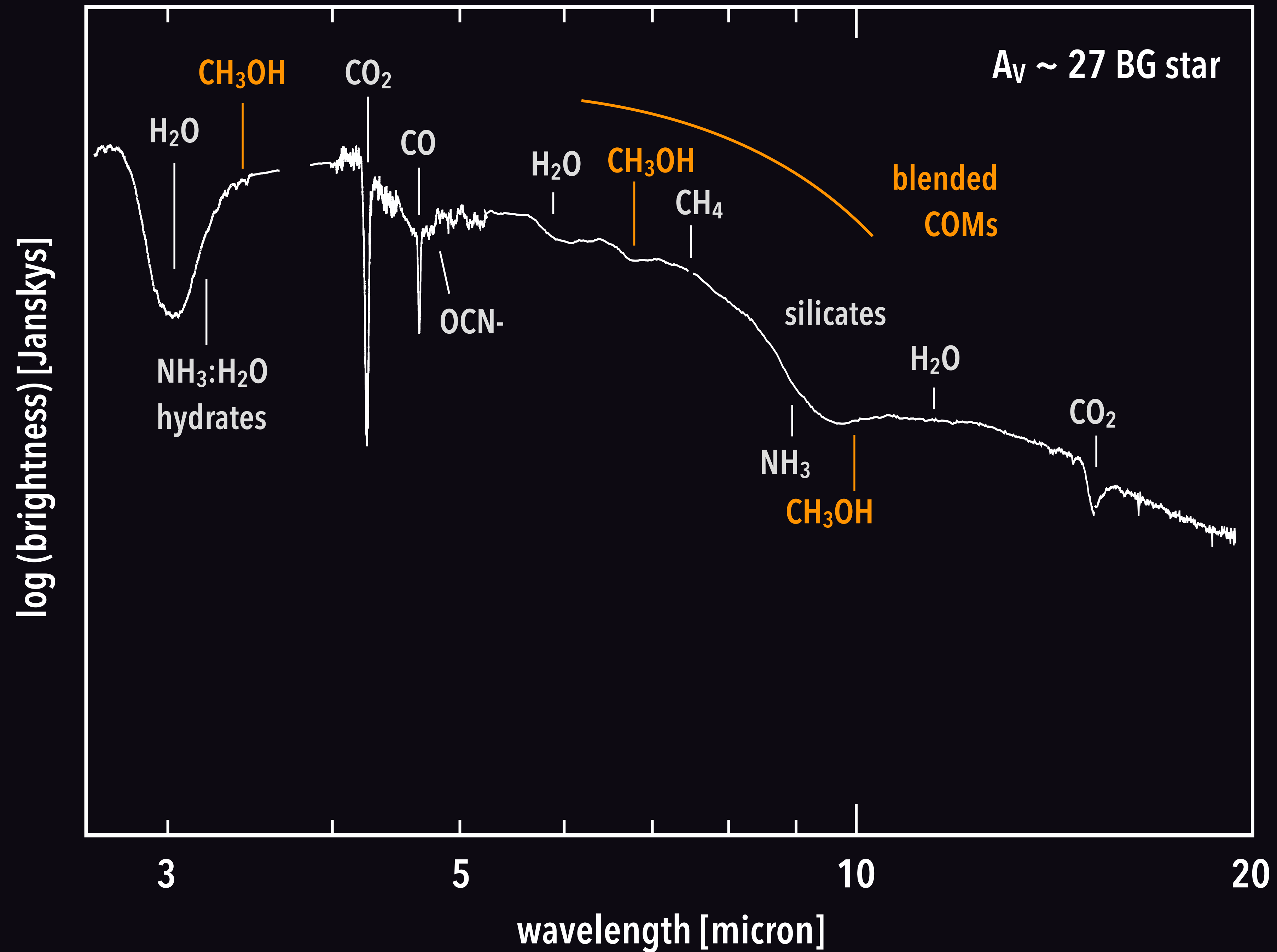
5

10

20

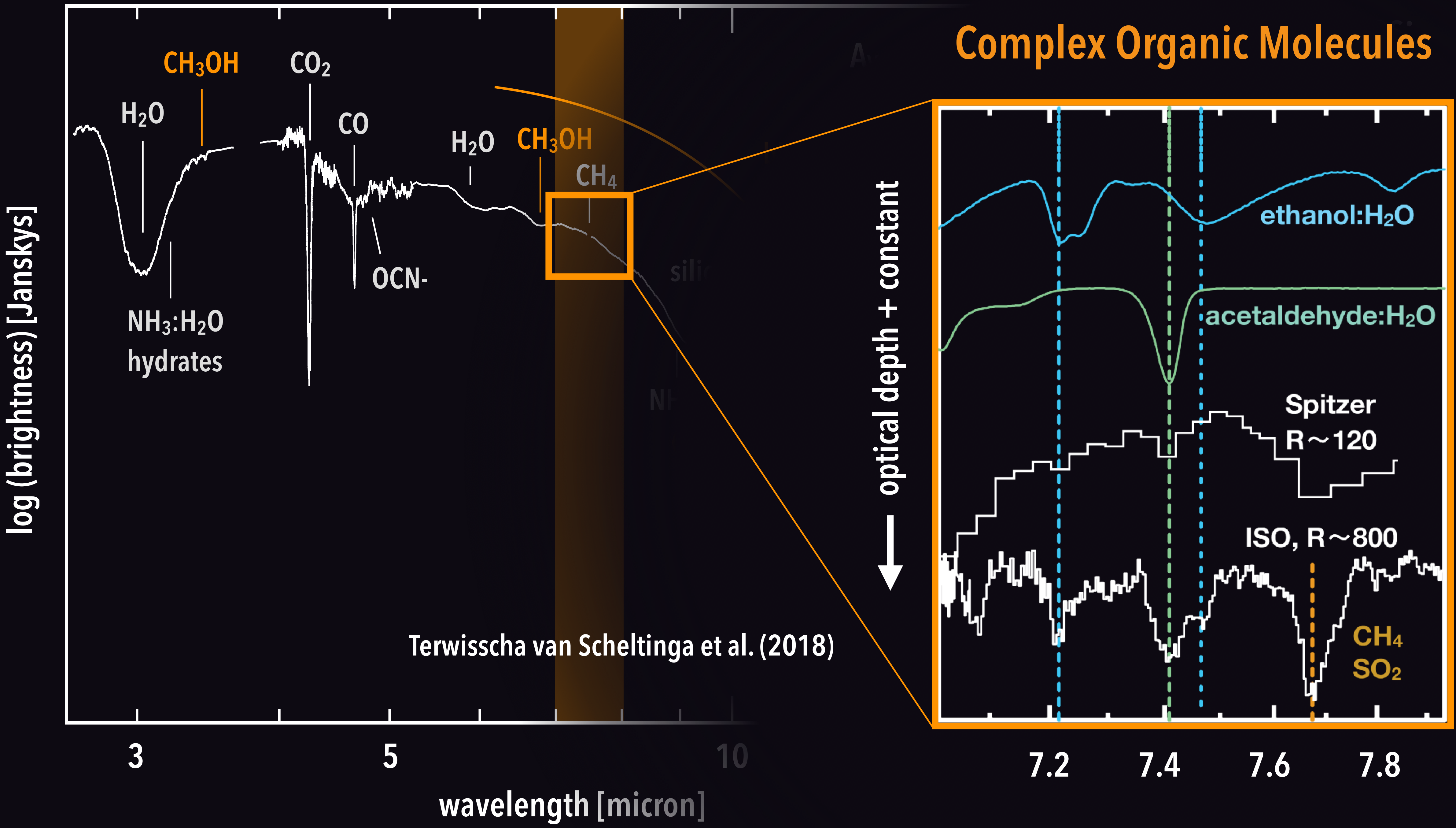
wavelength [microns]



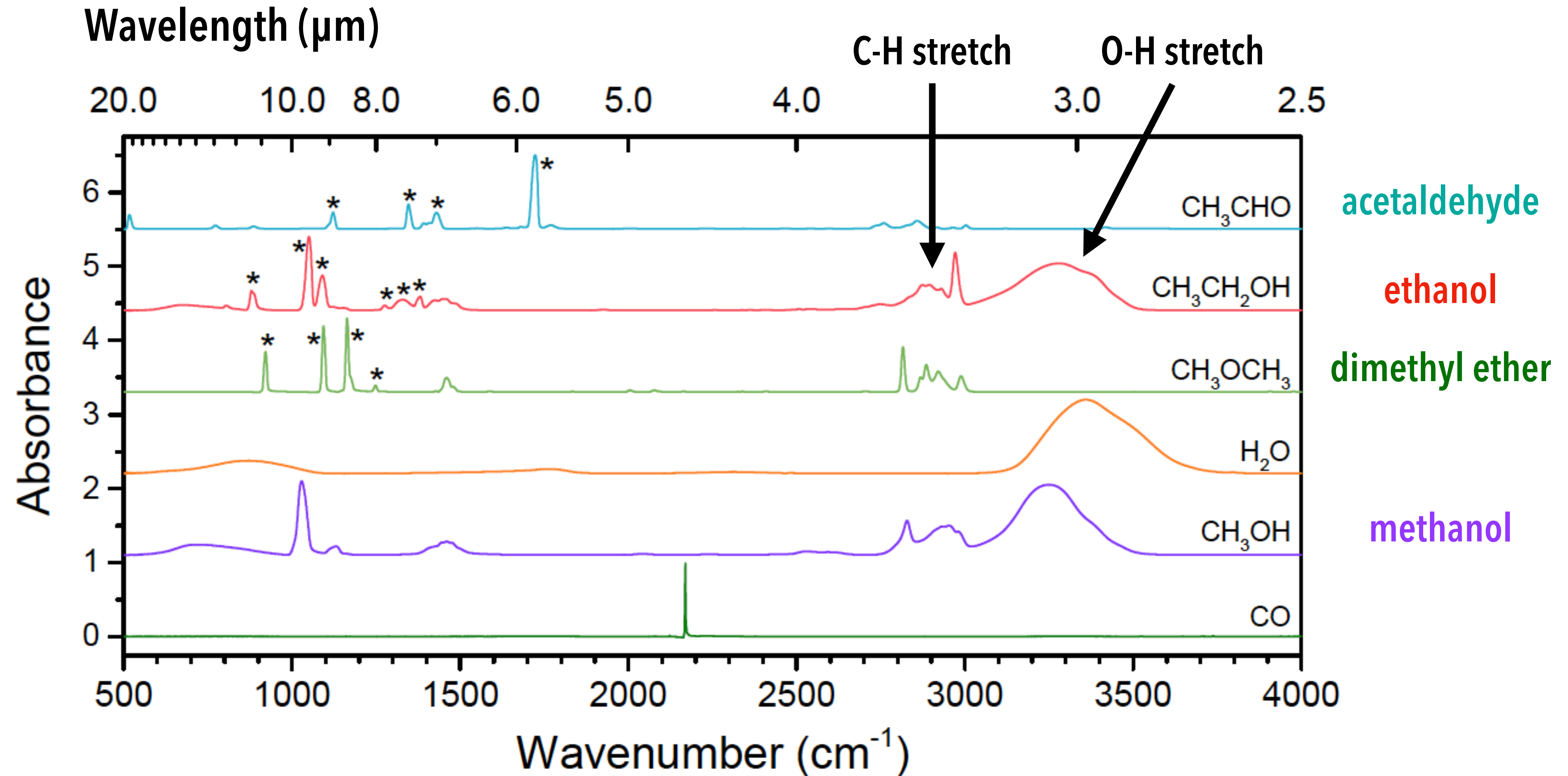


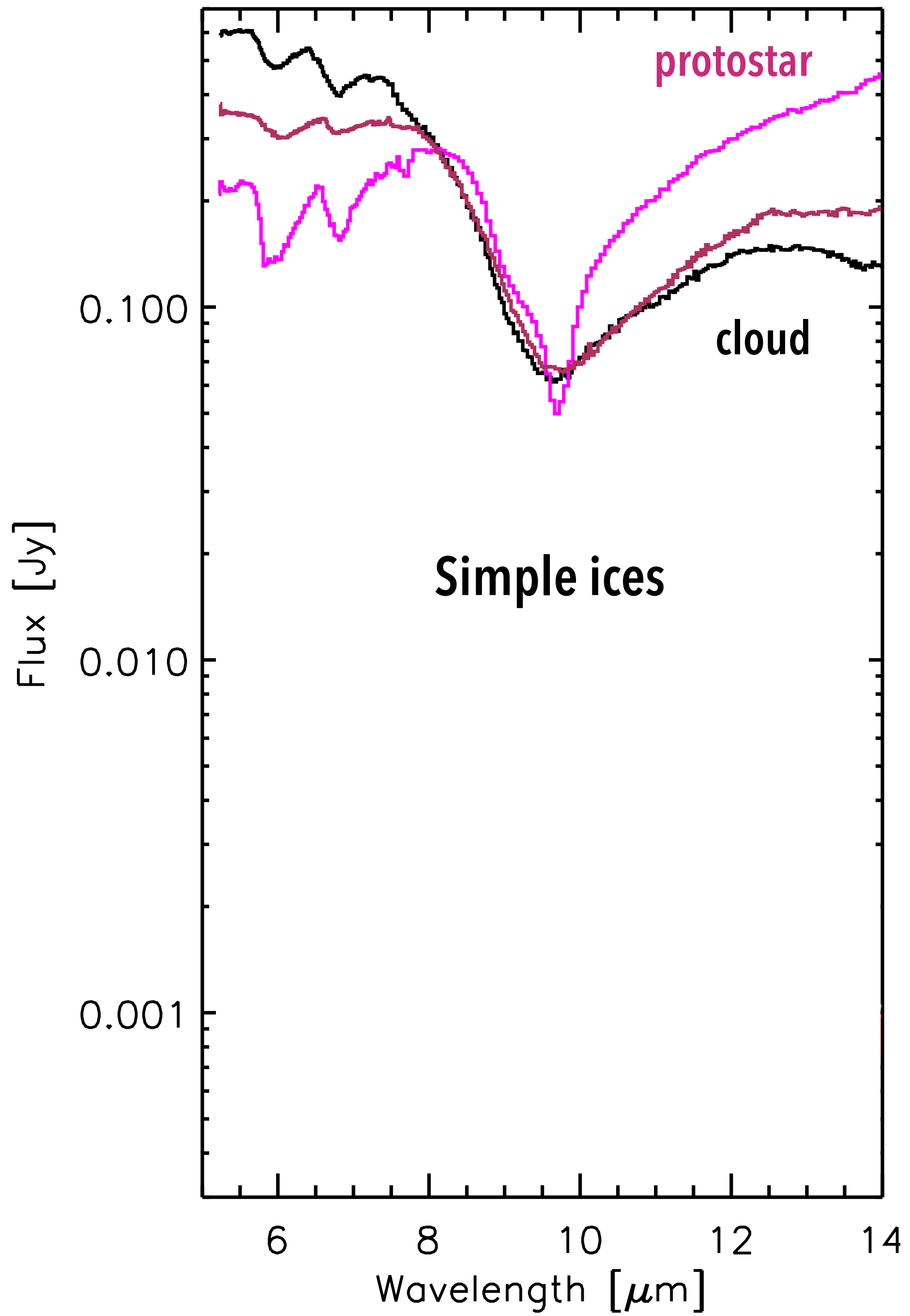
## Science cases

- 1) Relative abundances, 5 simple ice species, plus methanol
- 2) COM detection, I.D.

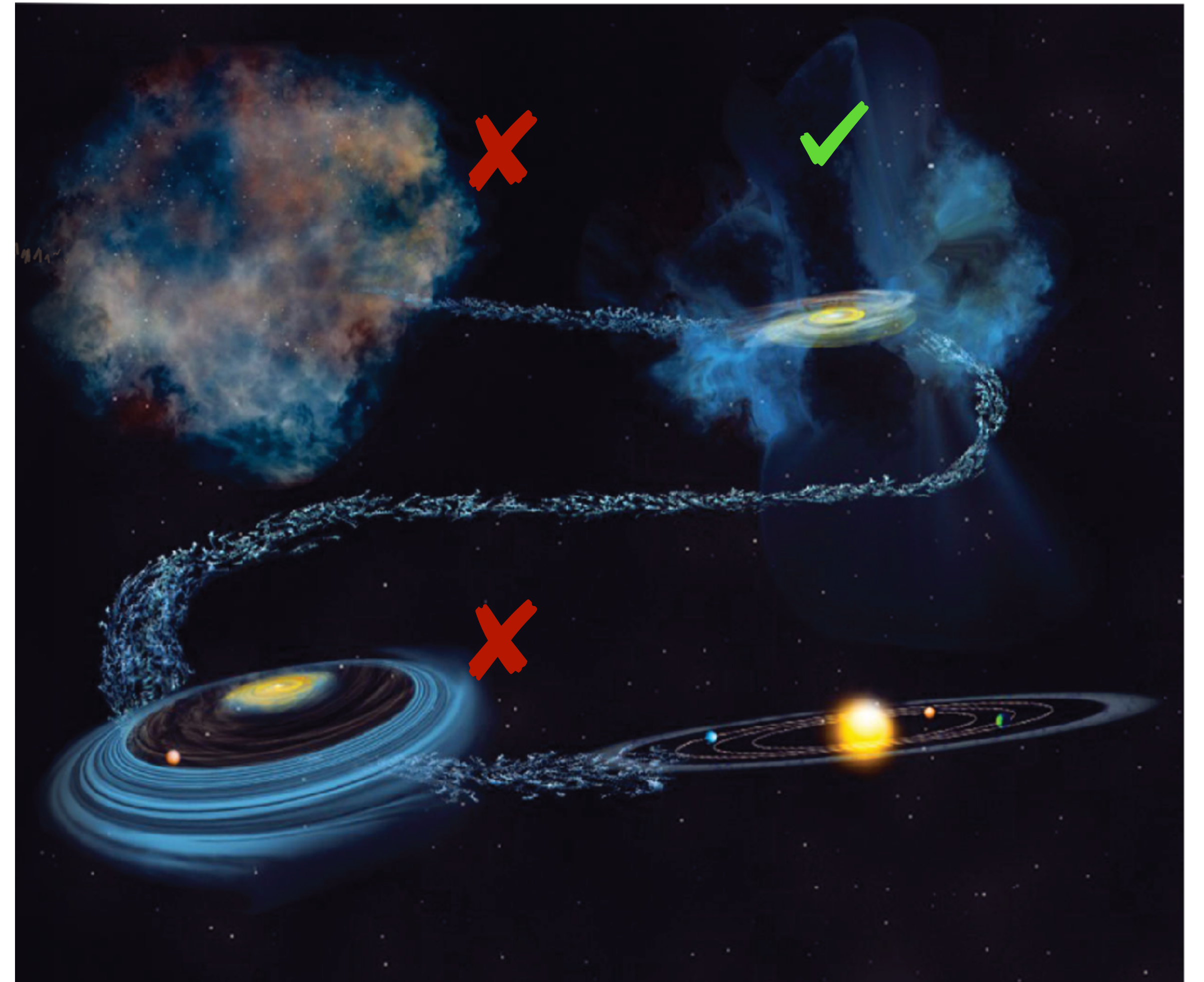


Lab spectra identify COMs via weaker features: at least 5 COMs should be ID'able.

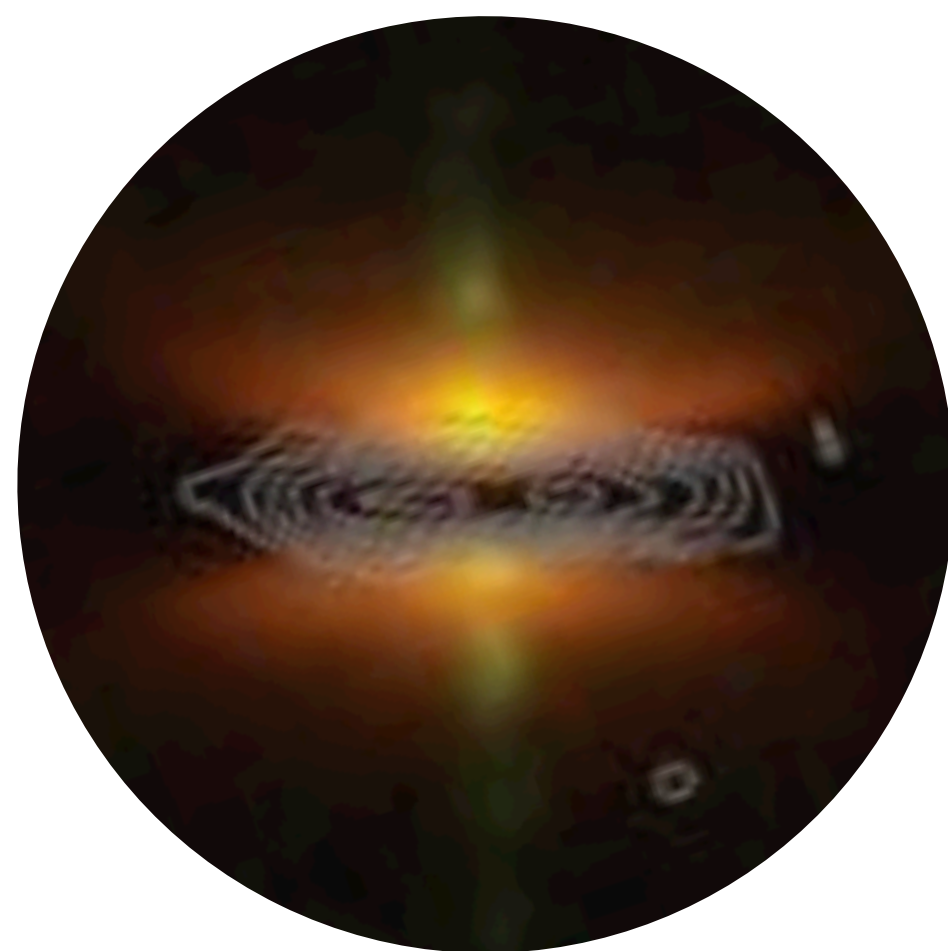
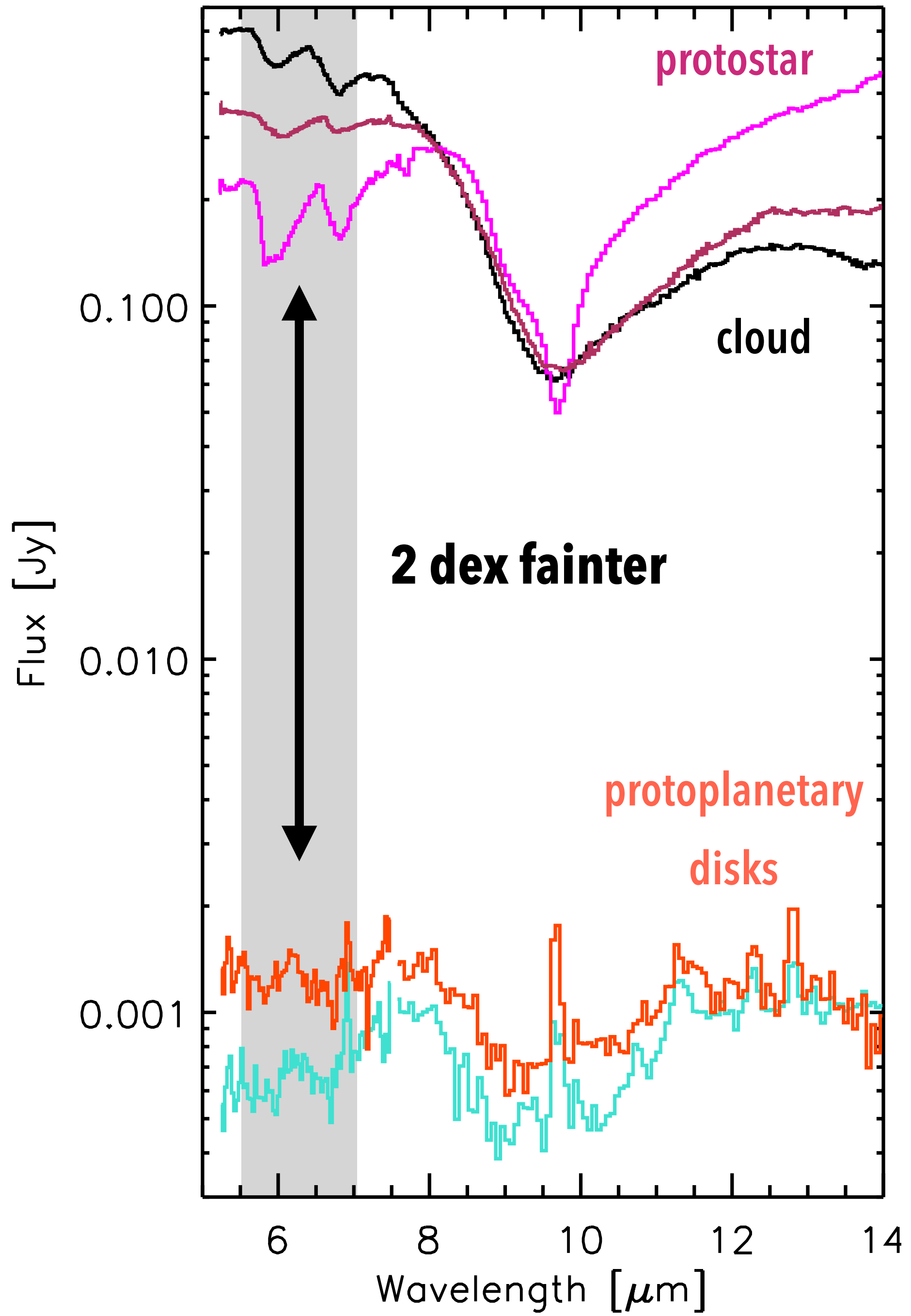


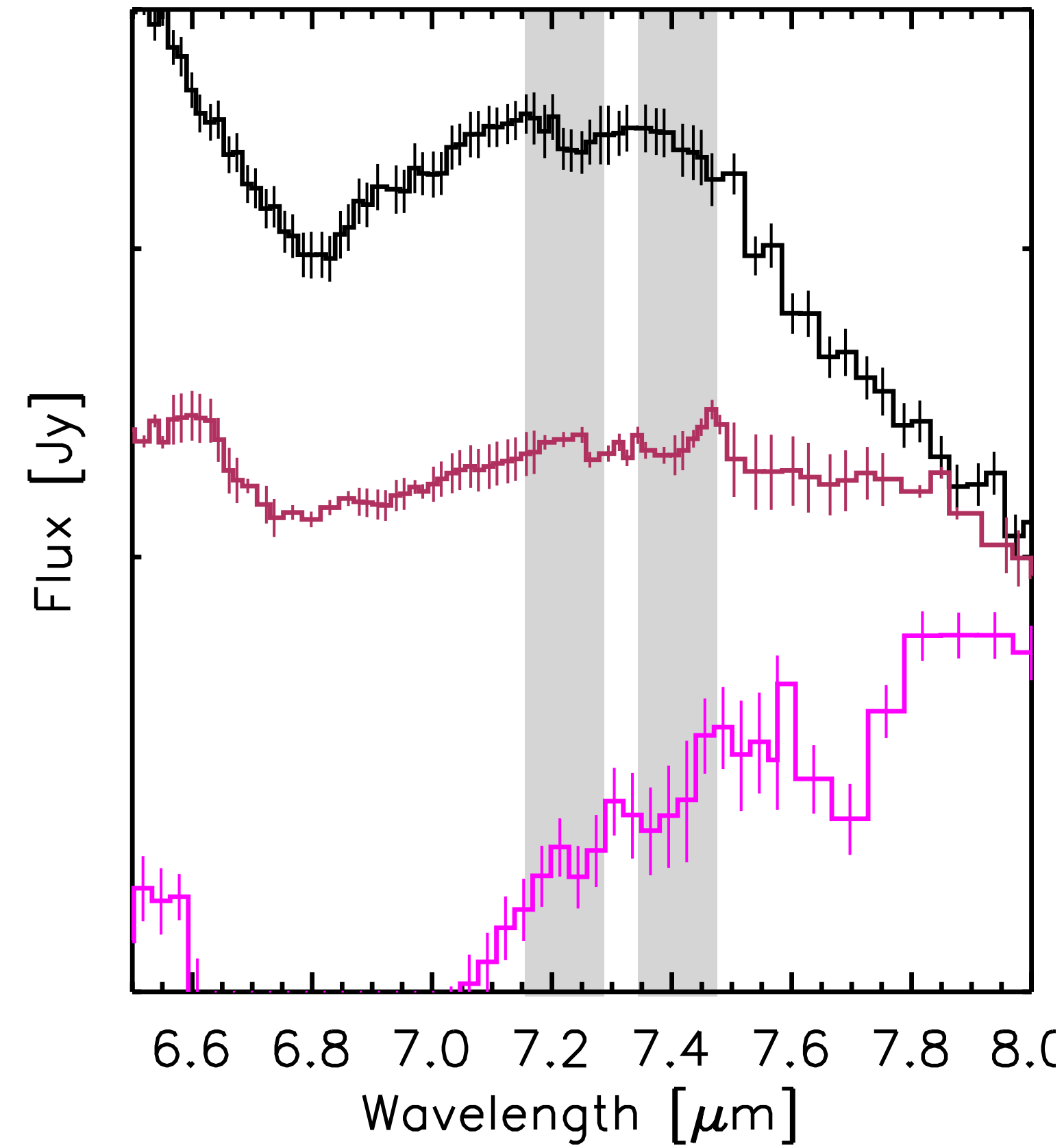
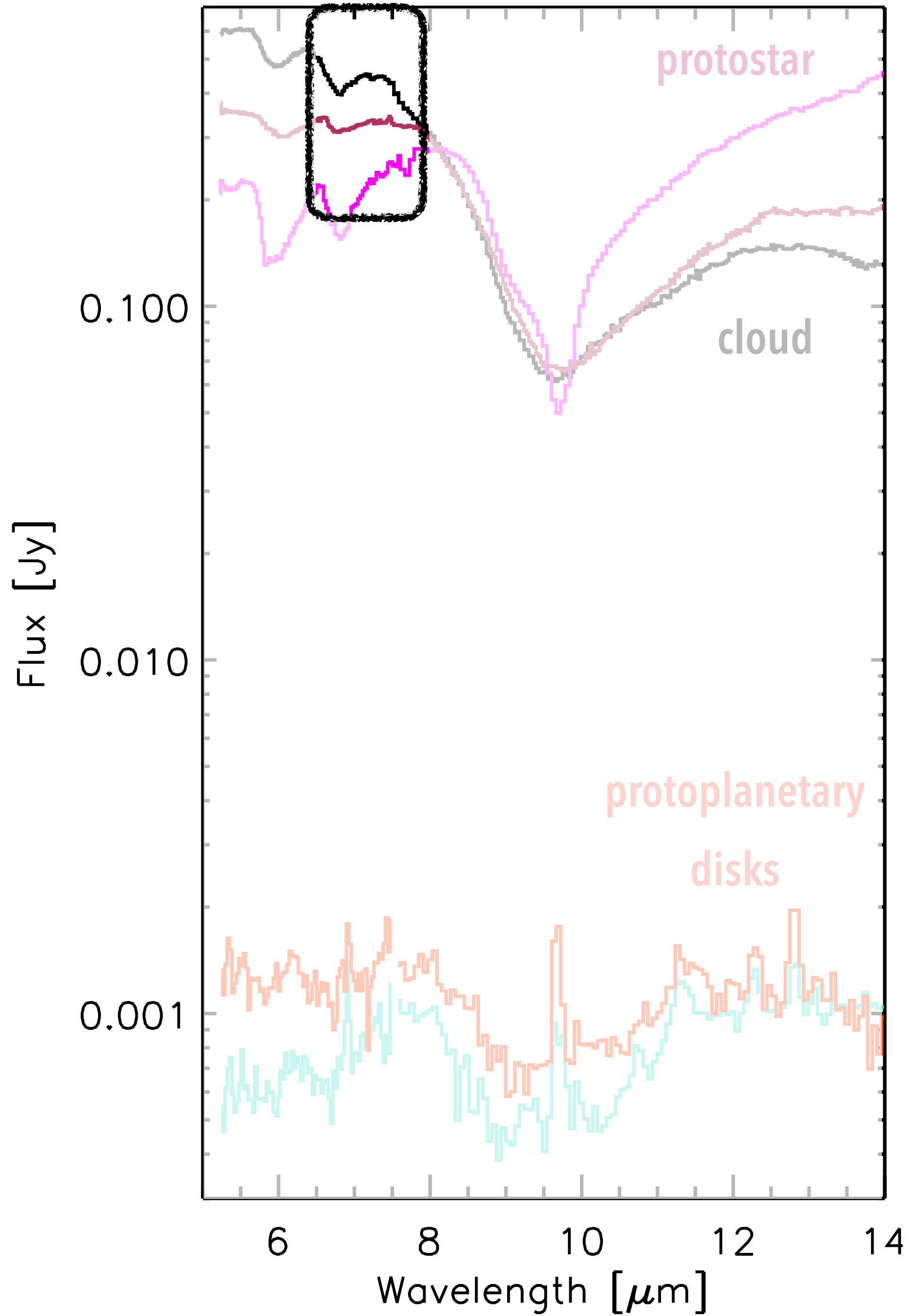


**Observations need to catch up to laboratory.**

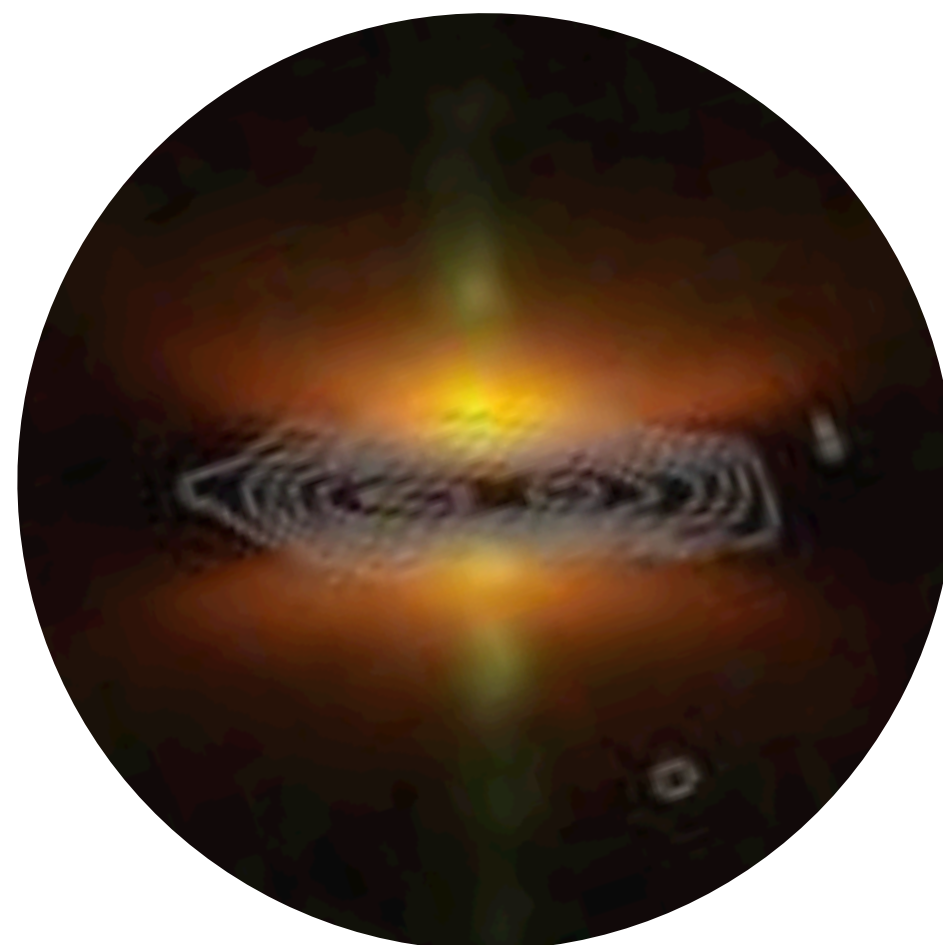


Chiar et al. (2007), McClure (2009), Boogert et al. (2010), (2015), Oberg et al. (2011)





**COMs ~ 1-3%  
of continuum**



**Require  $R > \sim 800$ , high  
sensitivity to characterize  
ices/COMs in disks.**





# IceAge JWST Early Release Science Program



PIs: McClure, Linnartz, Boogert

~25 member core team

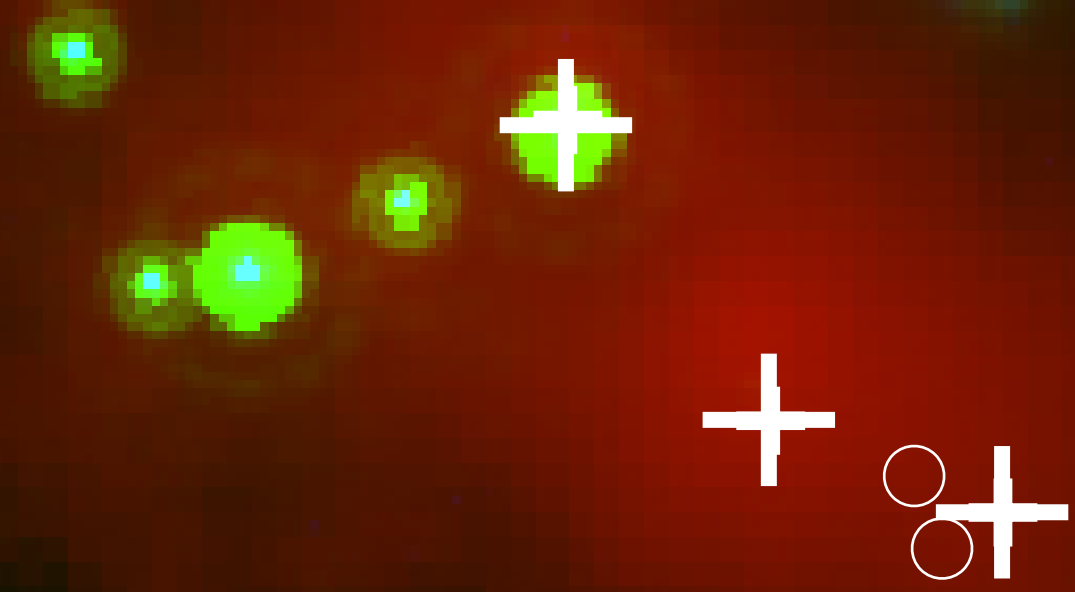
~25 scientific collaborators

Chameleon I: 160 pc (pre-GAIA)

IRAC 3.6  $\mu\text{m}$

MIPS 24  $\mu\text{m}$

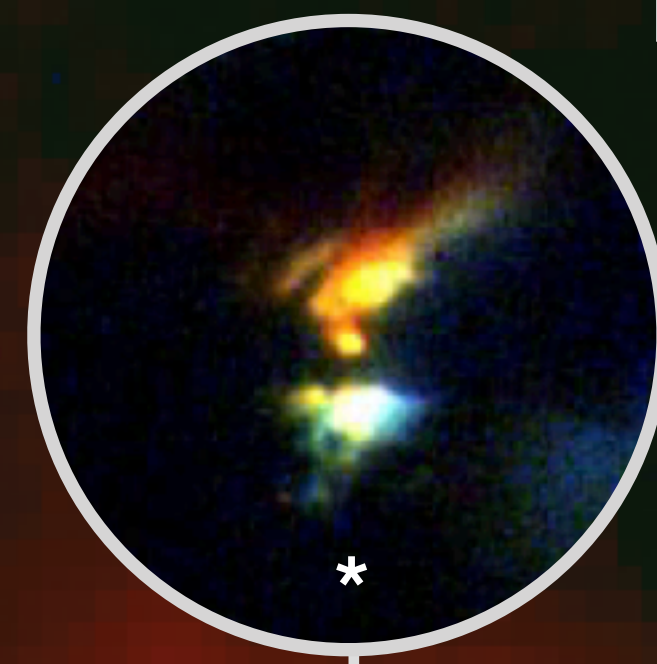
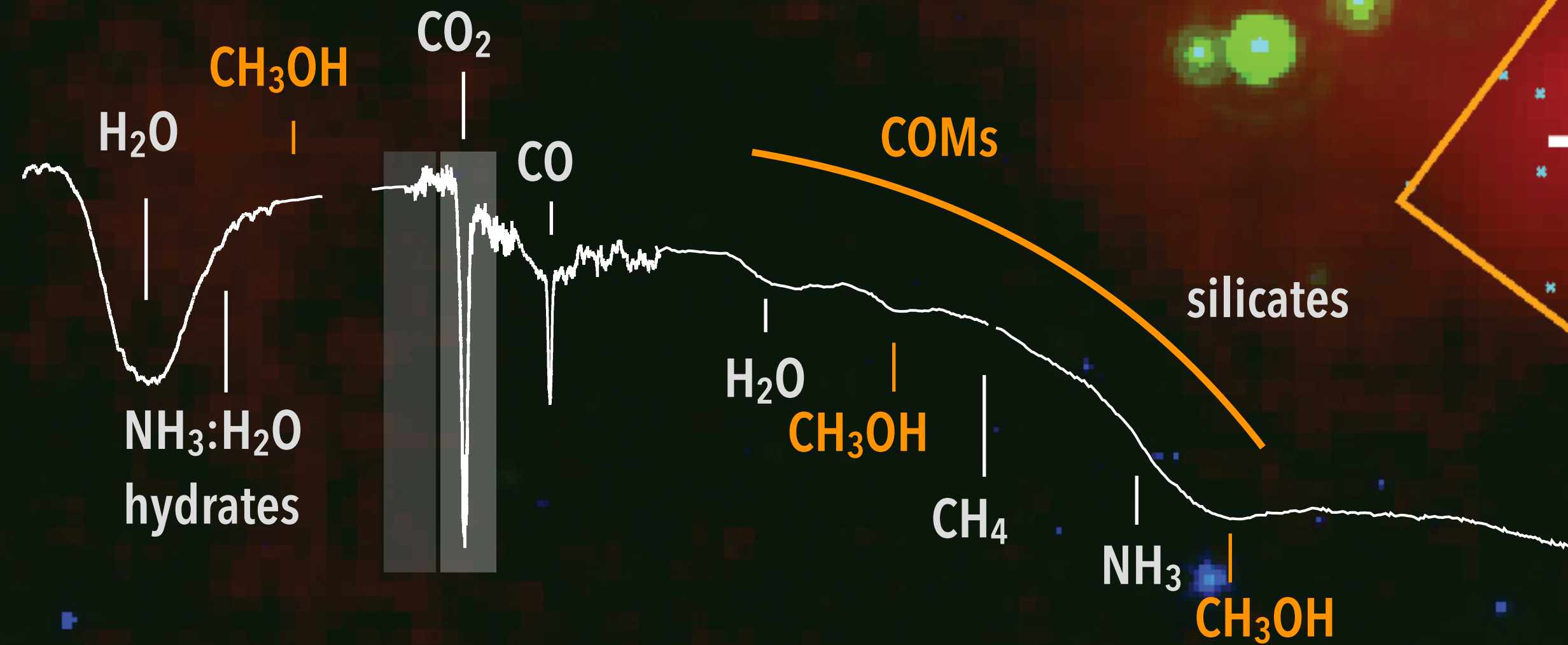
0.85 mm (Beloche et al. 2011)



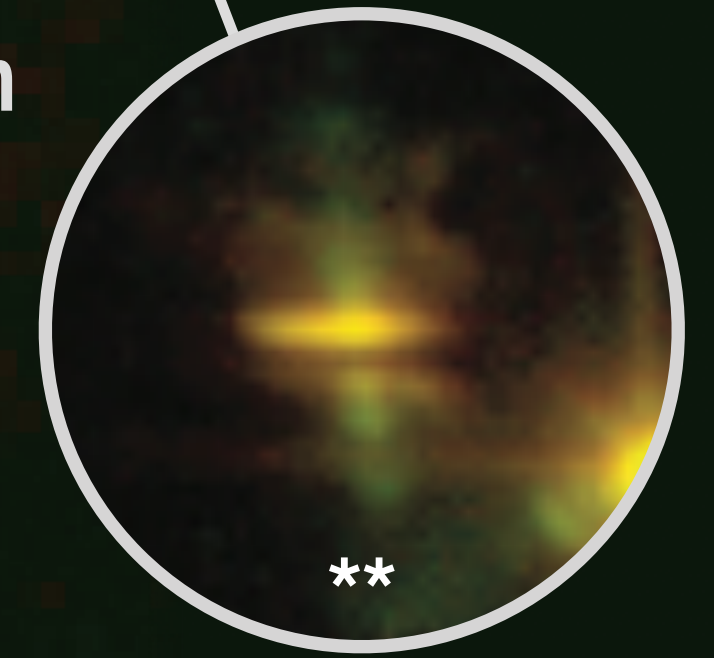


# IceAge JWST Early Release Science Program

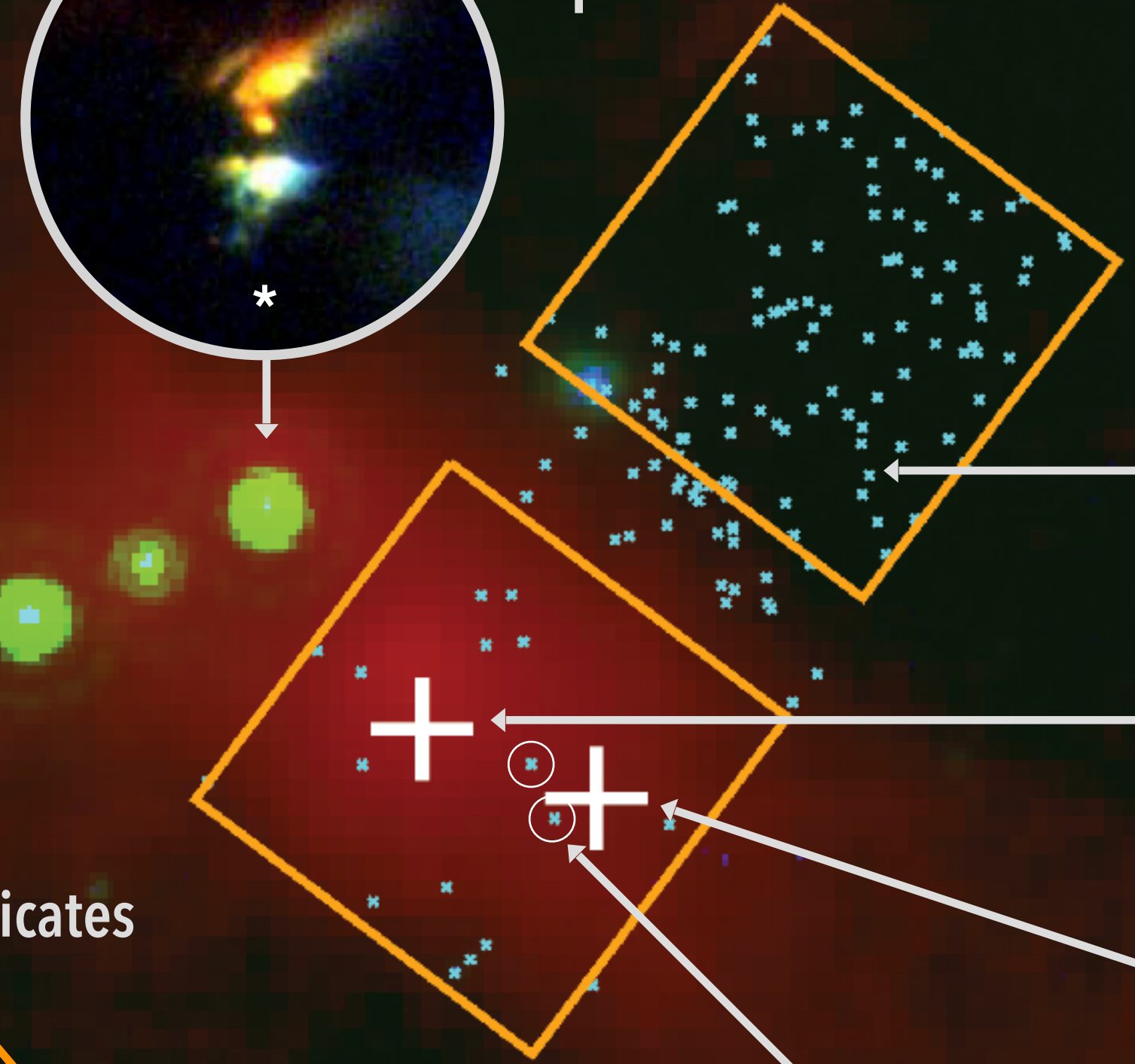
*But favorite bright objects saturate.  
FORCAST update?*



Edge-on Class I protostar



Edge-on disk



Known background stars

Class 0 protostar

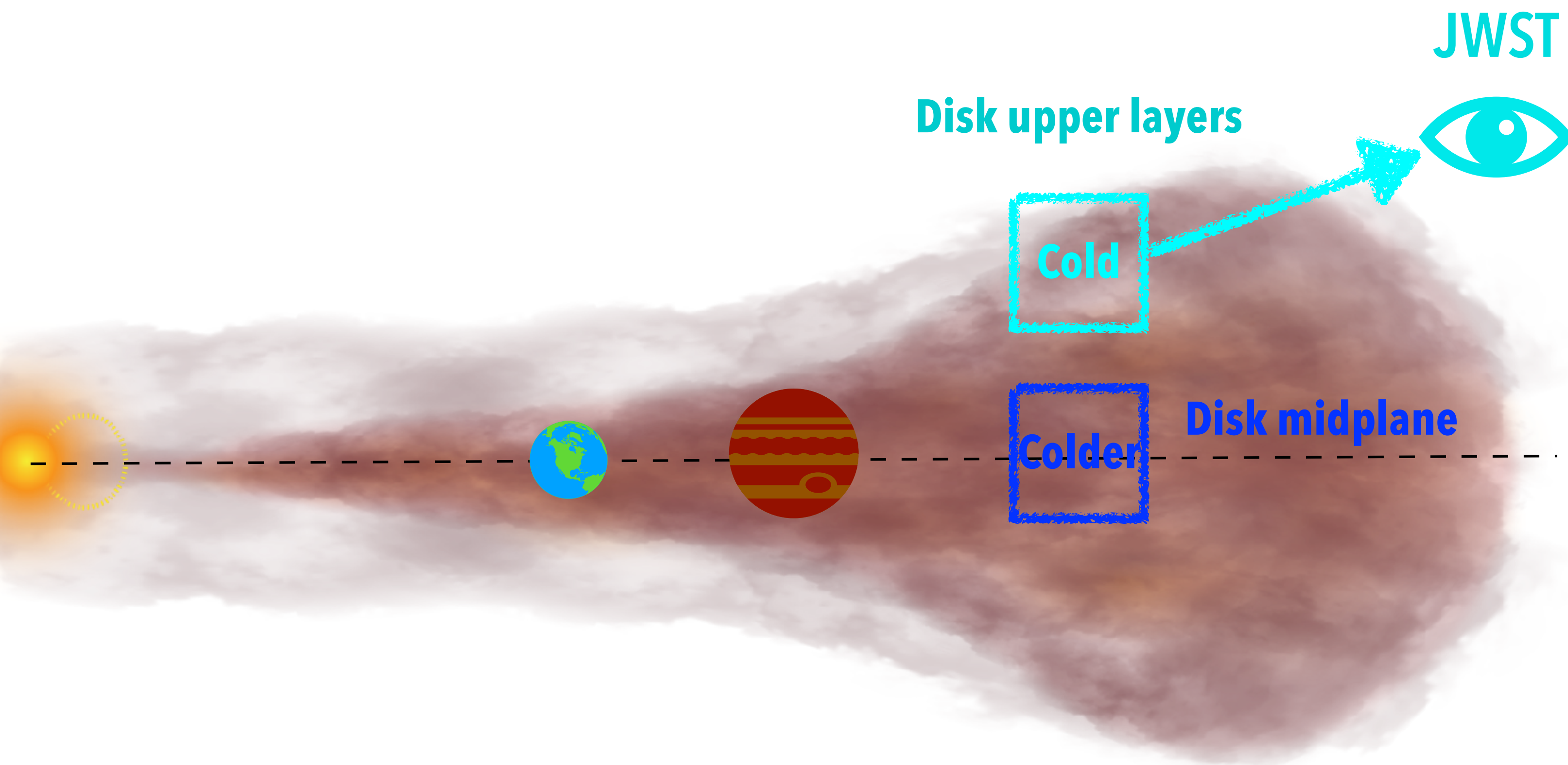
Pre-stellar core

$A_V \sim 60, 95$  background stars

BG stars: Persi et al (2001), K. Luhman, priv. comm.  
\*Persi et al. (2001), \*\*Stapelfeldt et al. (2013)

#2

# Far-infrared thermal emission measures midplane absolute ice abundances.

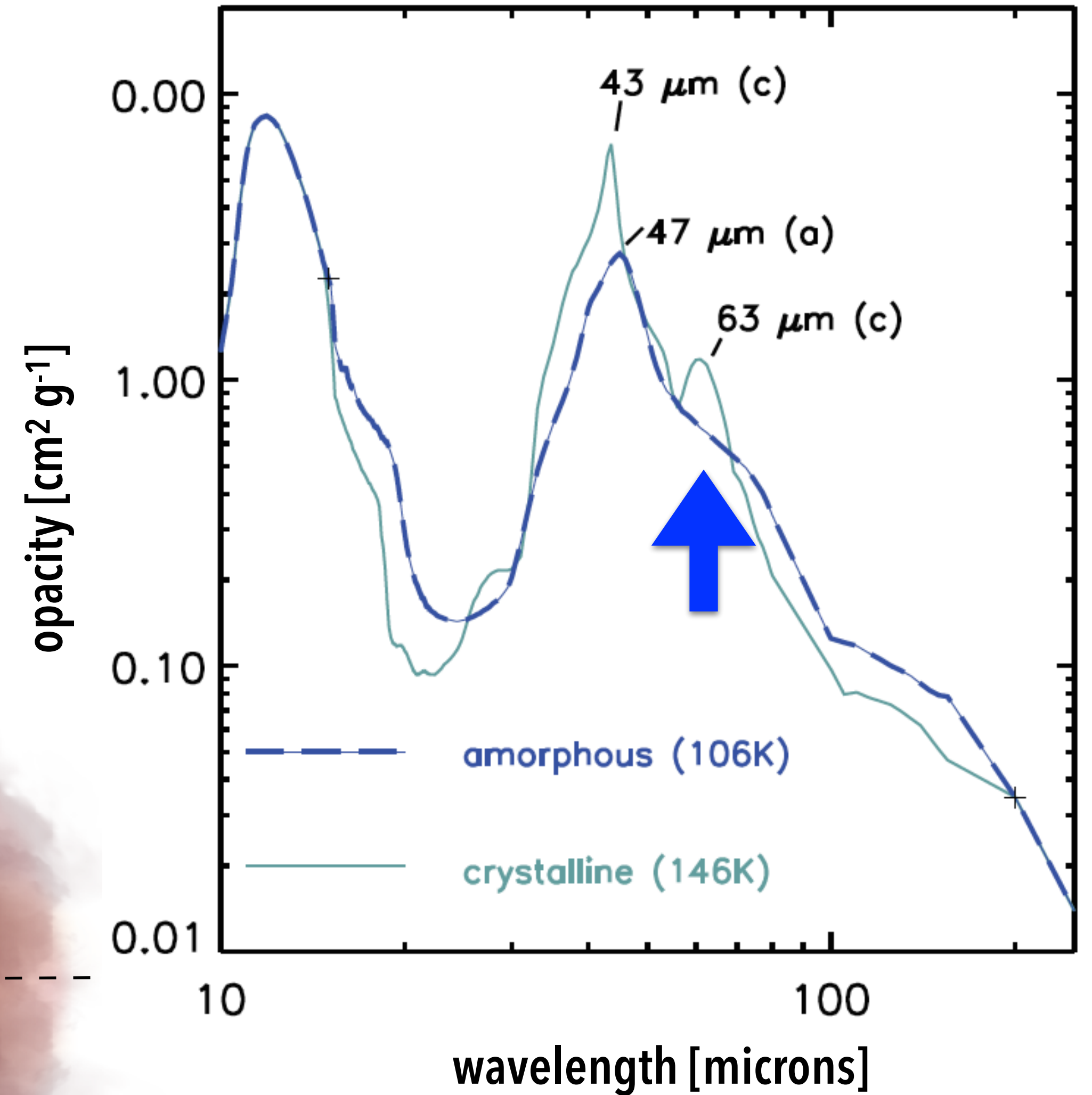
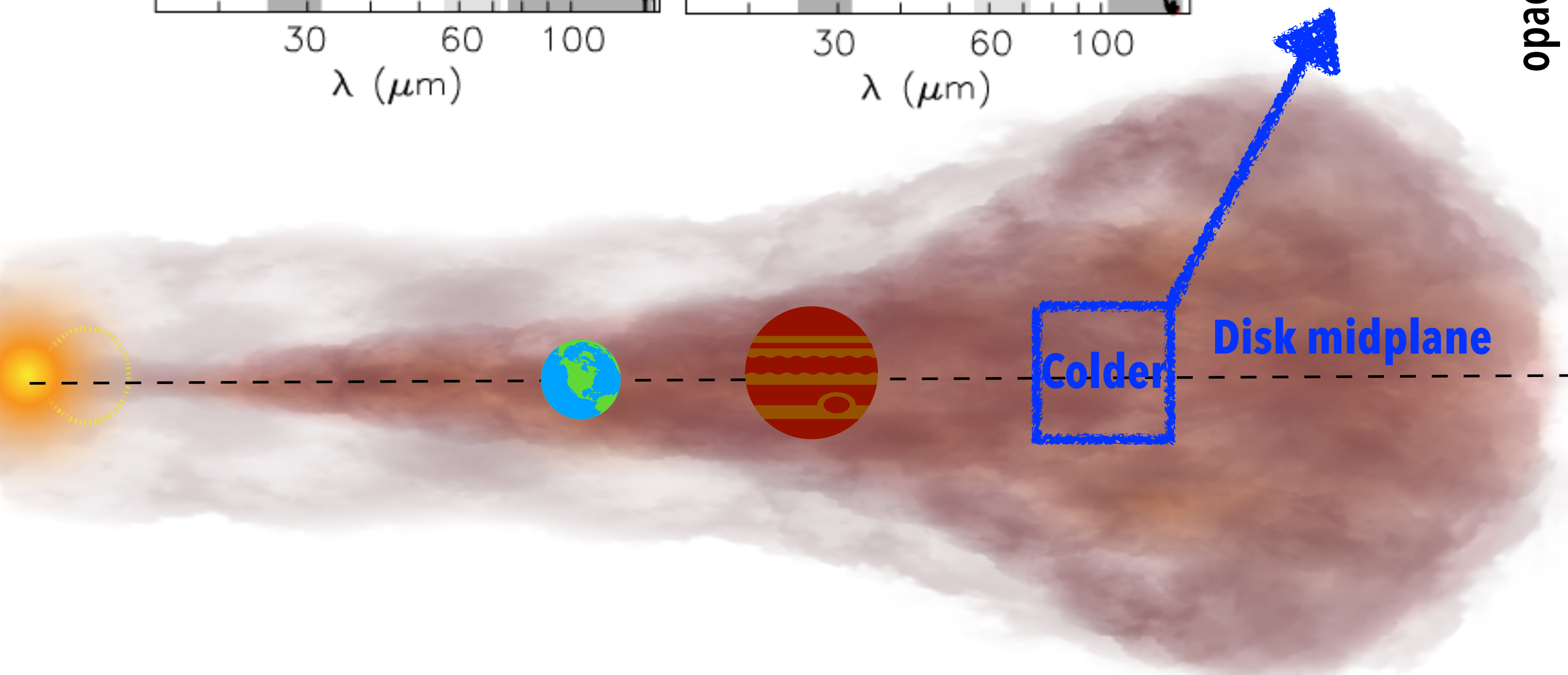
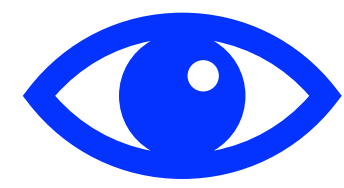
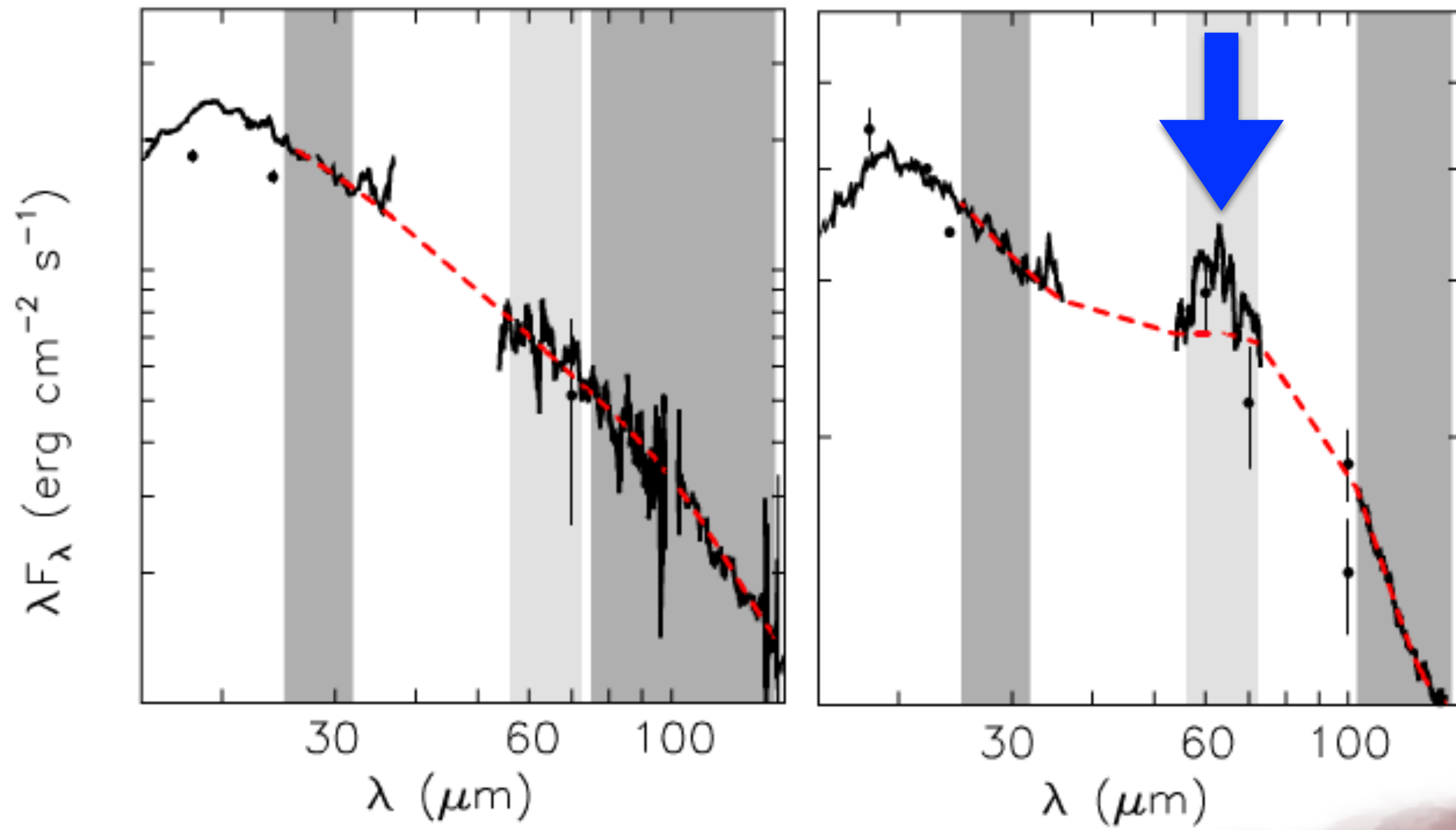


## JWST science cases

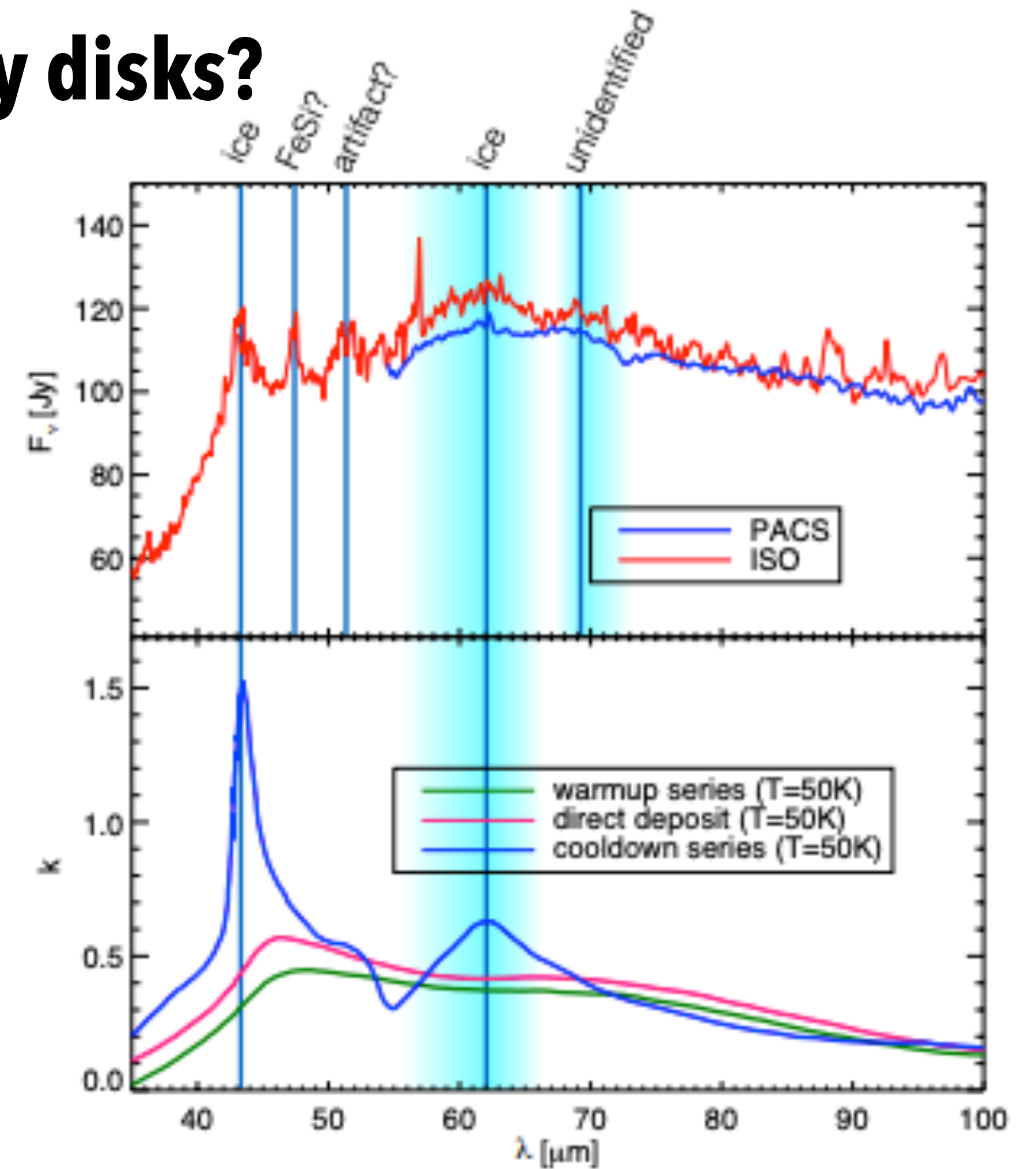
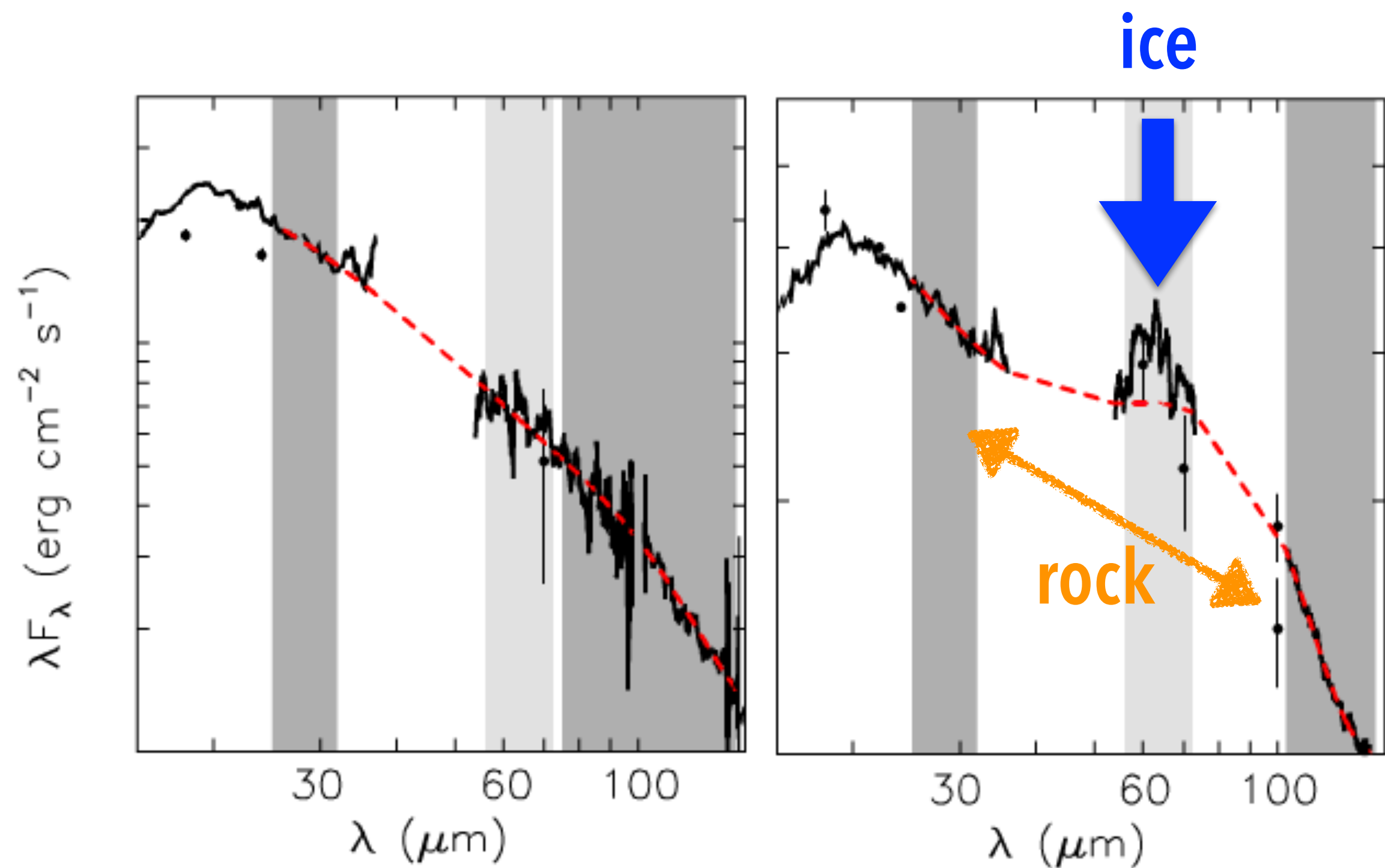
- 1) *Relative* abundances, 5 simple ice species, plus methanol
- 2) COM detection, I.D., 5 species

**But how to convert to absolute abundances (relative to rock)?**

# Far-infrared thermal emission measures midplane absolute ice abundances.



# Are water ice abundances reduced in protoplanetary disks?



Only 6% of sample show water ice.  
 3 low-mass disks, ice/rock ~ **0.5**

vs.

"Solar abundance" ice/rock ~ **1.6**  
 1 high-mass disk

McClure et al. (2012, 2015)

Min et al. (2016)

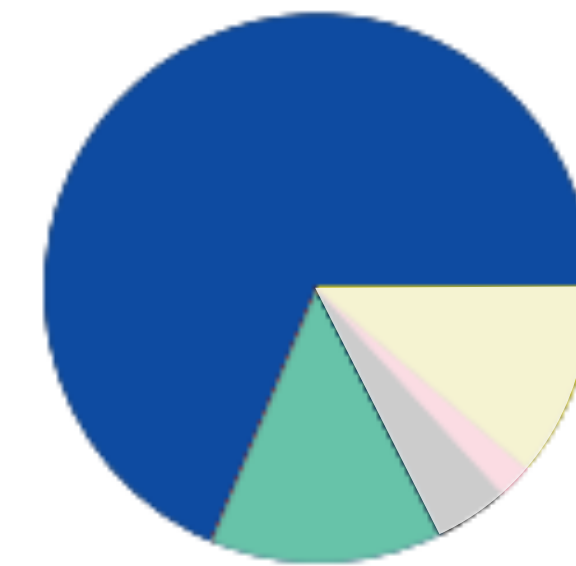
# Water ice/rock variations predicted by different initial conditions/chemistry.

Ice abundances >30 AU

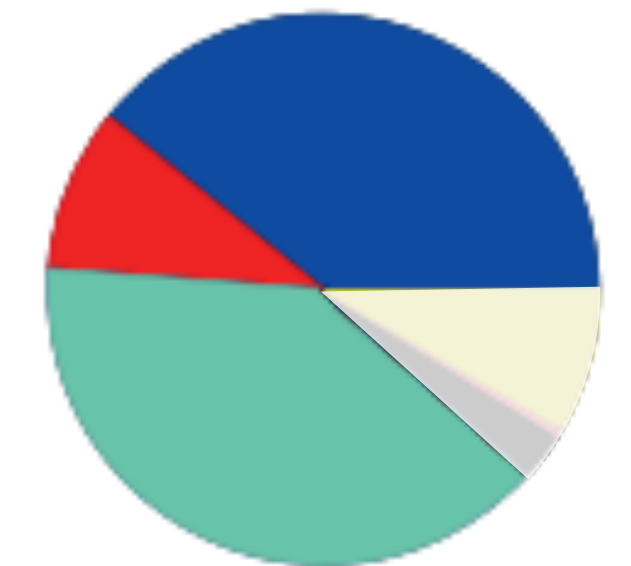
*Infall + viscous spread  
(inert grain interior)*

*Infall  
(active grain interior)*

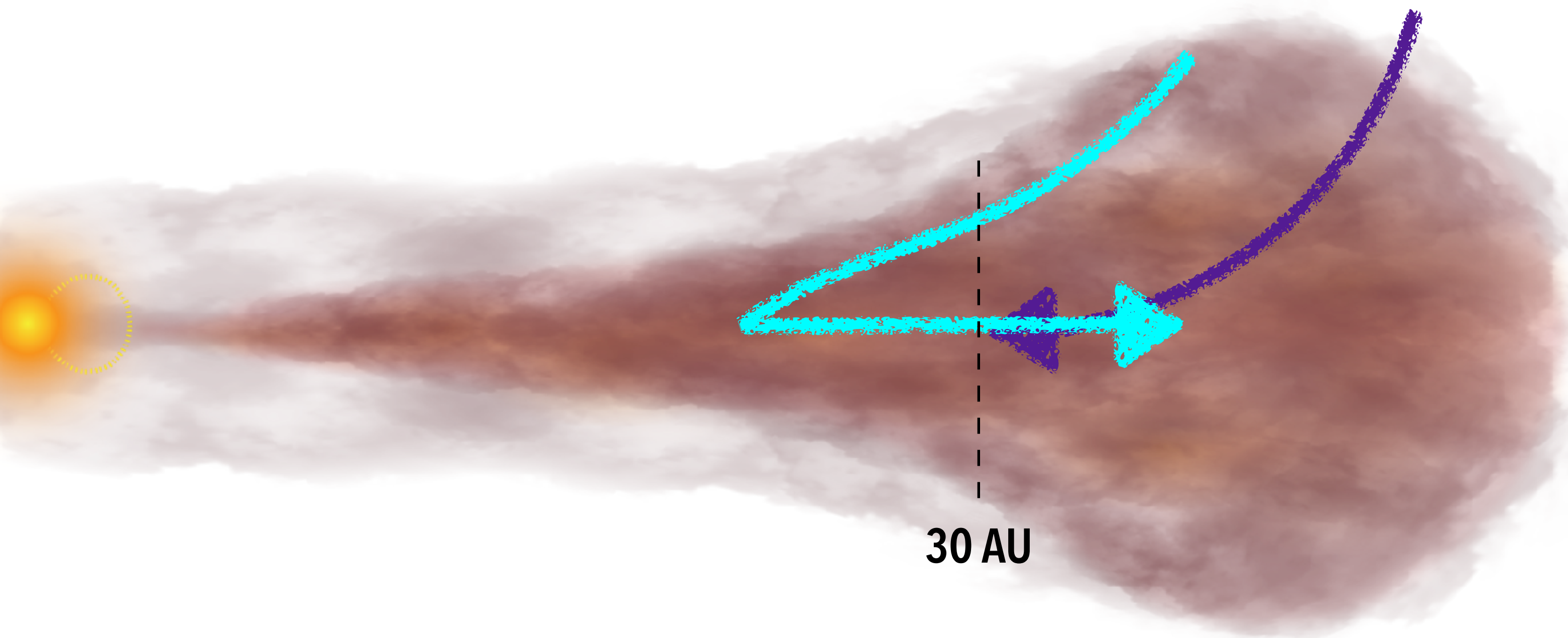
80-90% of midplane ice mass carried by 3 ice species.



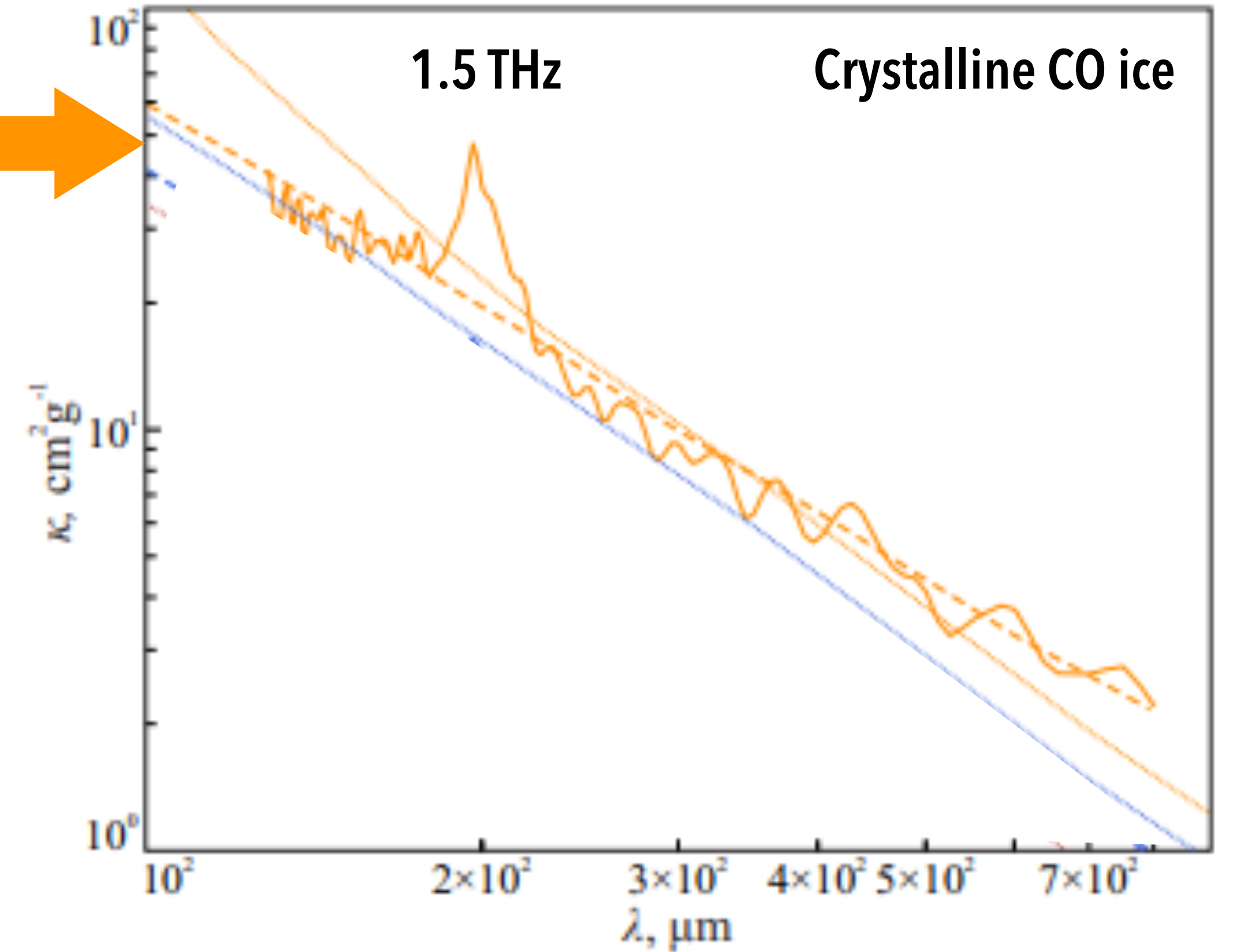
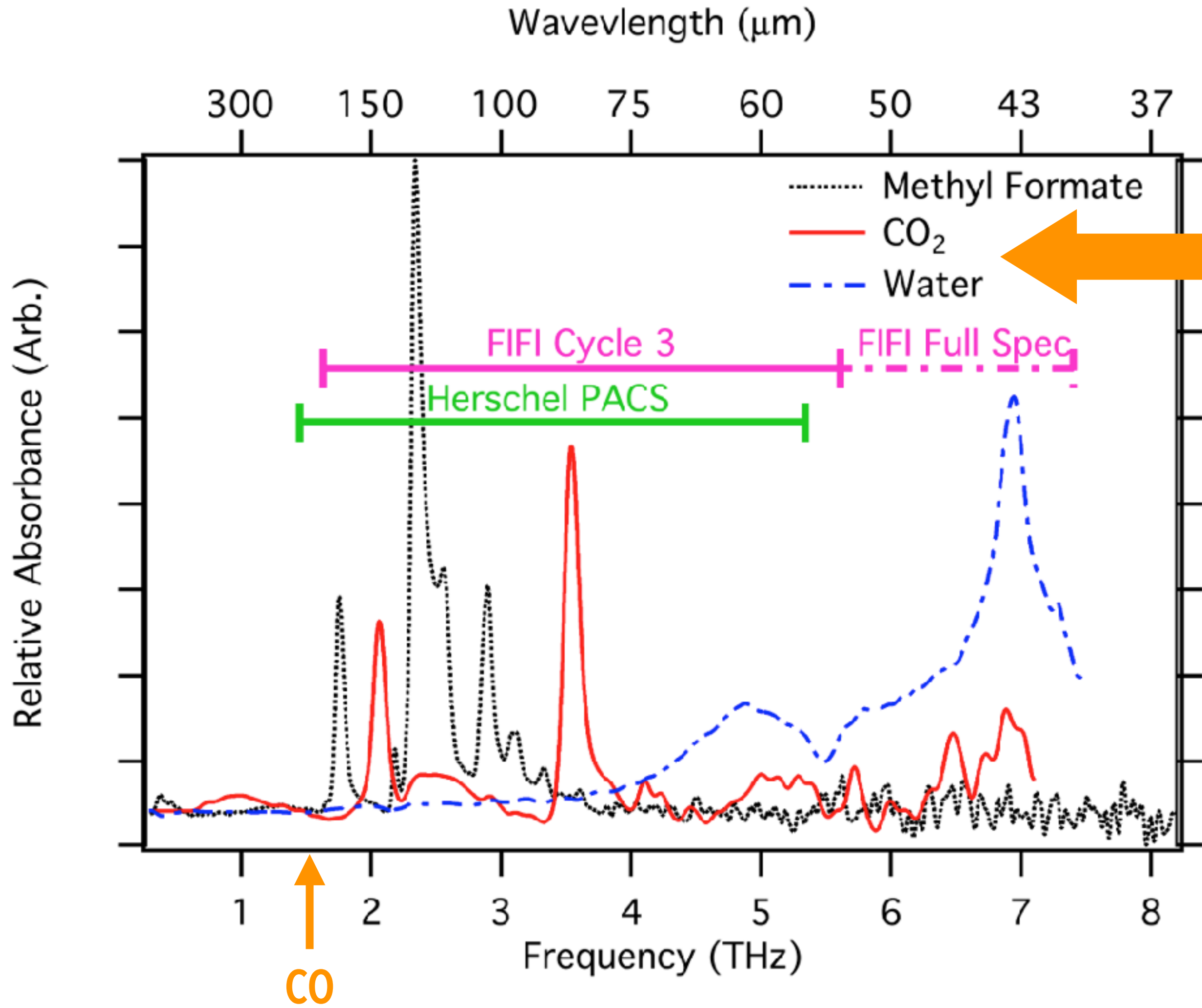
69% H<sub>2</sub>O  
14% CO<sub>2</sub>  
4% NH<sub>3</sub>  
2% CH<sub>3</sub>OH  
11% other



39% H<sub>2</sub>O  
10% CO  
39% CO<sub>2</sub>  
3% NH<sub>3</sub>  
8% other



# Far-Infrared hosts features from all of these 3 simple ices...

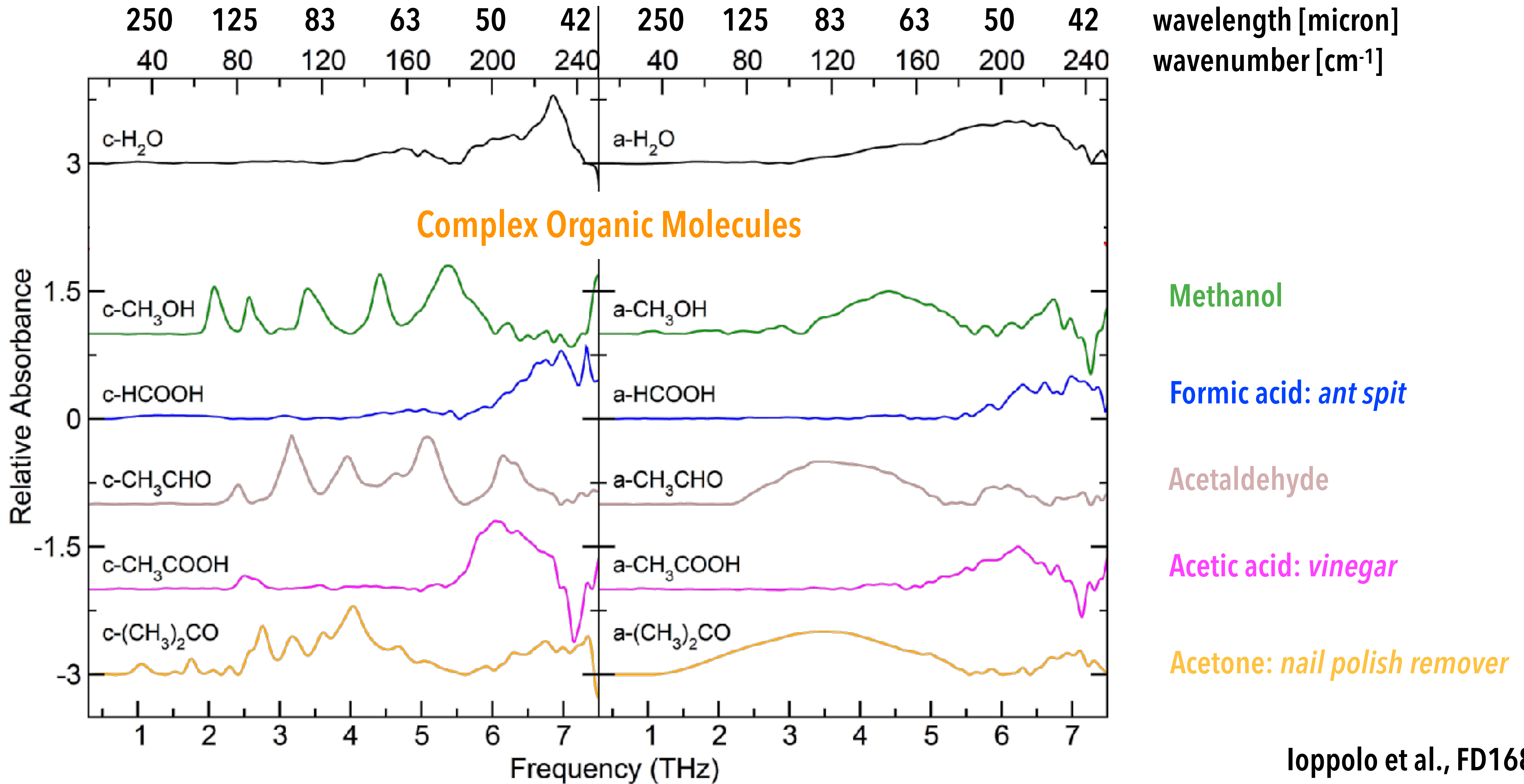


S. Ioppolo, private communication, McGuire, Ioppolo et al. (2016)

Giuliano et al. (2019)

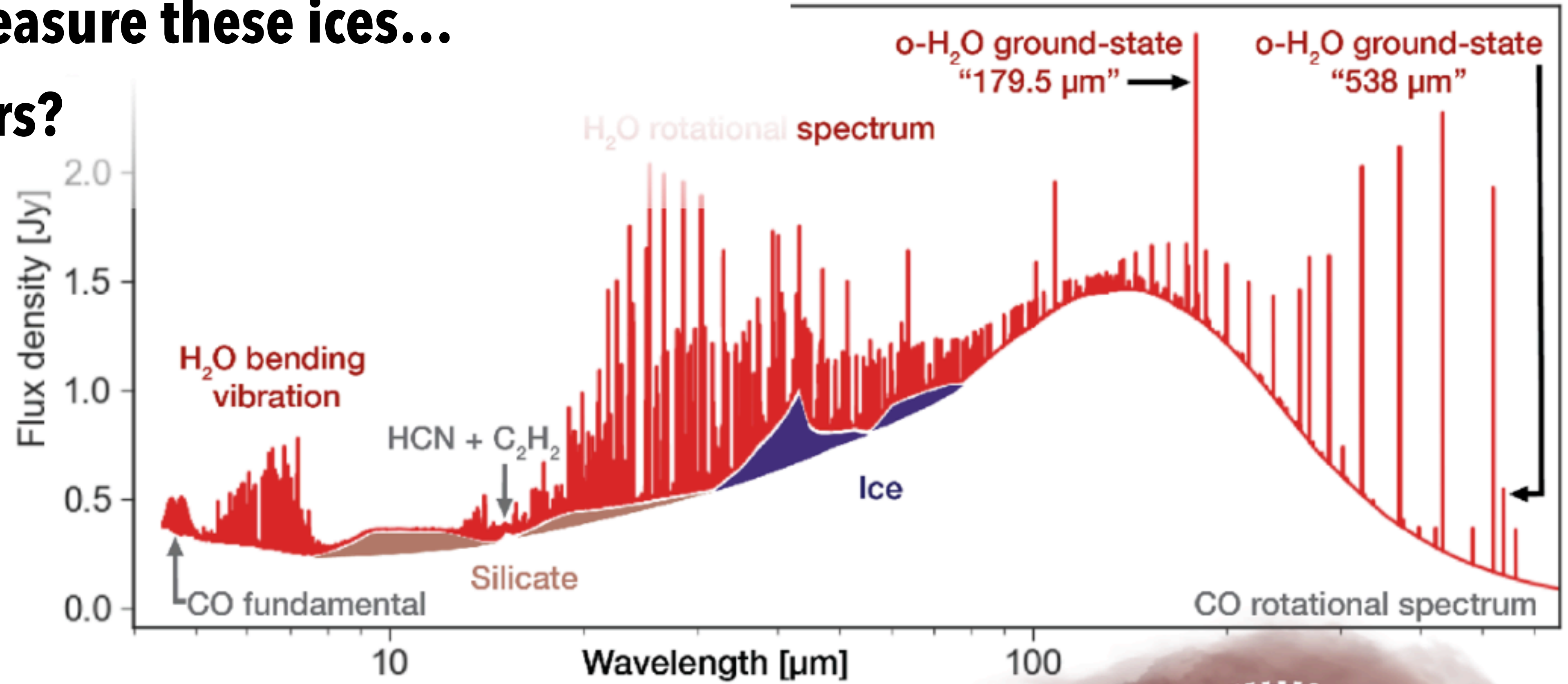


# ...and COM ices! Easier to separate than at mid-IR wavelengths (JWST).

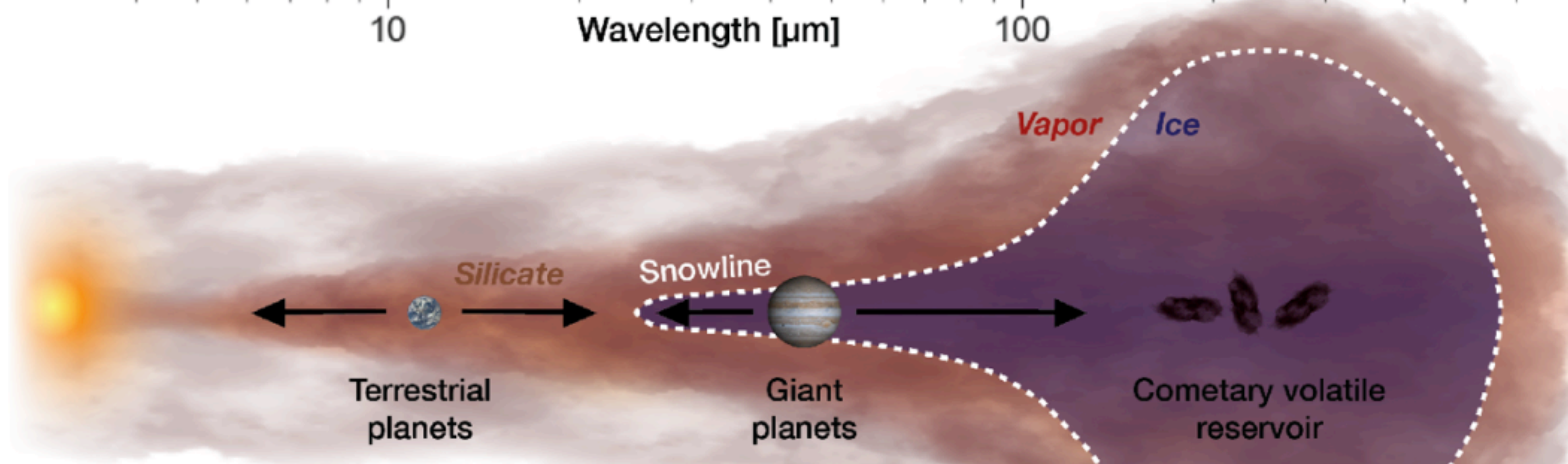


# OST/SPICA can measure these ices...

...but in >10 years?



Pontoppidan et al. (2019)  
OST white paper



# (Timely) far-IR ice abundances connect disk compositions with Solar System.



ESA

**Comet 67P:**

*Excess C-solids*

(Rubin et al. 2019)

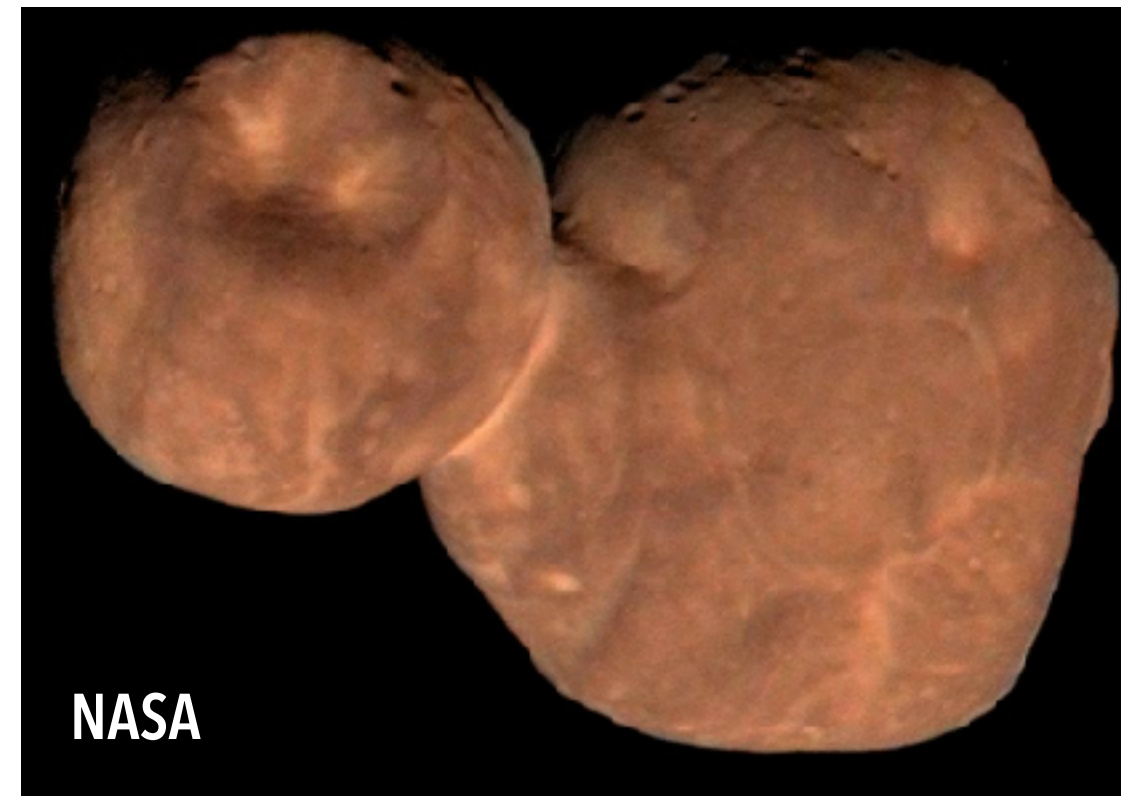


NASA

**C/2016 R2 (PanSTARRS):**

*Excess N<sub>2</sub>, low H<sub>2</sub>O*

(Opitom et al. 2019)

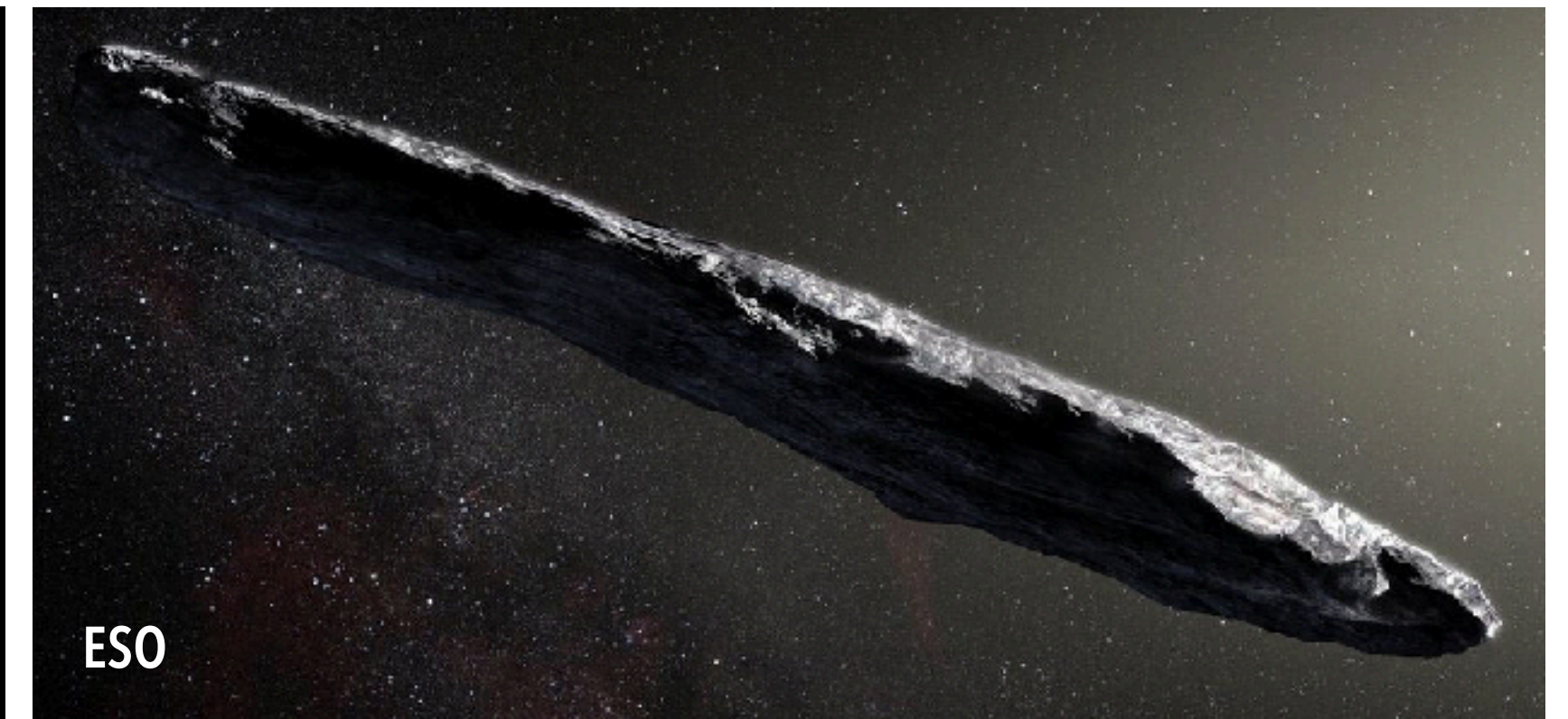


NASA

**KBO Arrokoth:**

*Low H<sub>2</sub>O, excess methanol*

(Grundy et al. 2020)

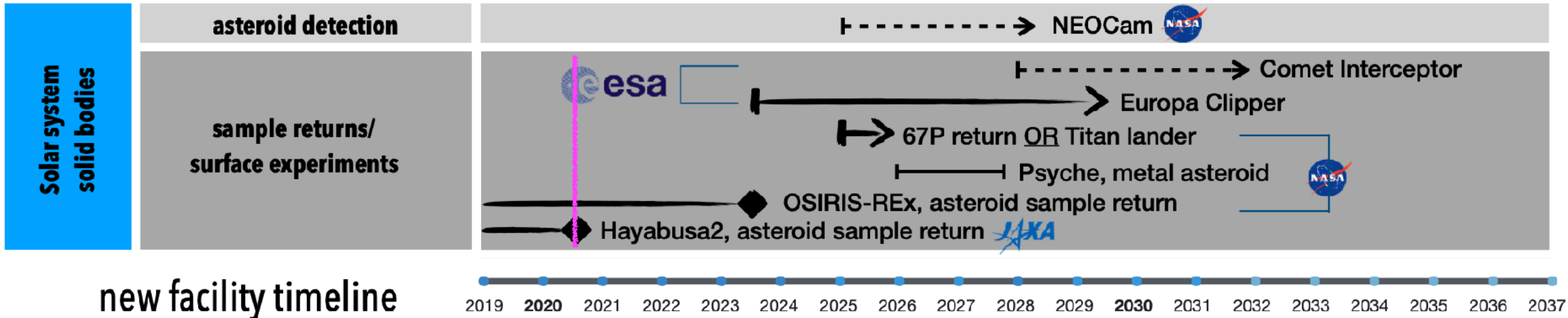


ESO

**Interstellar Oumuamua:**

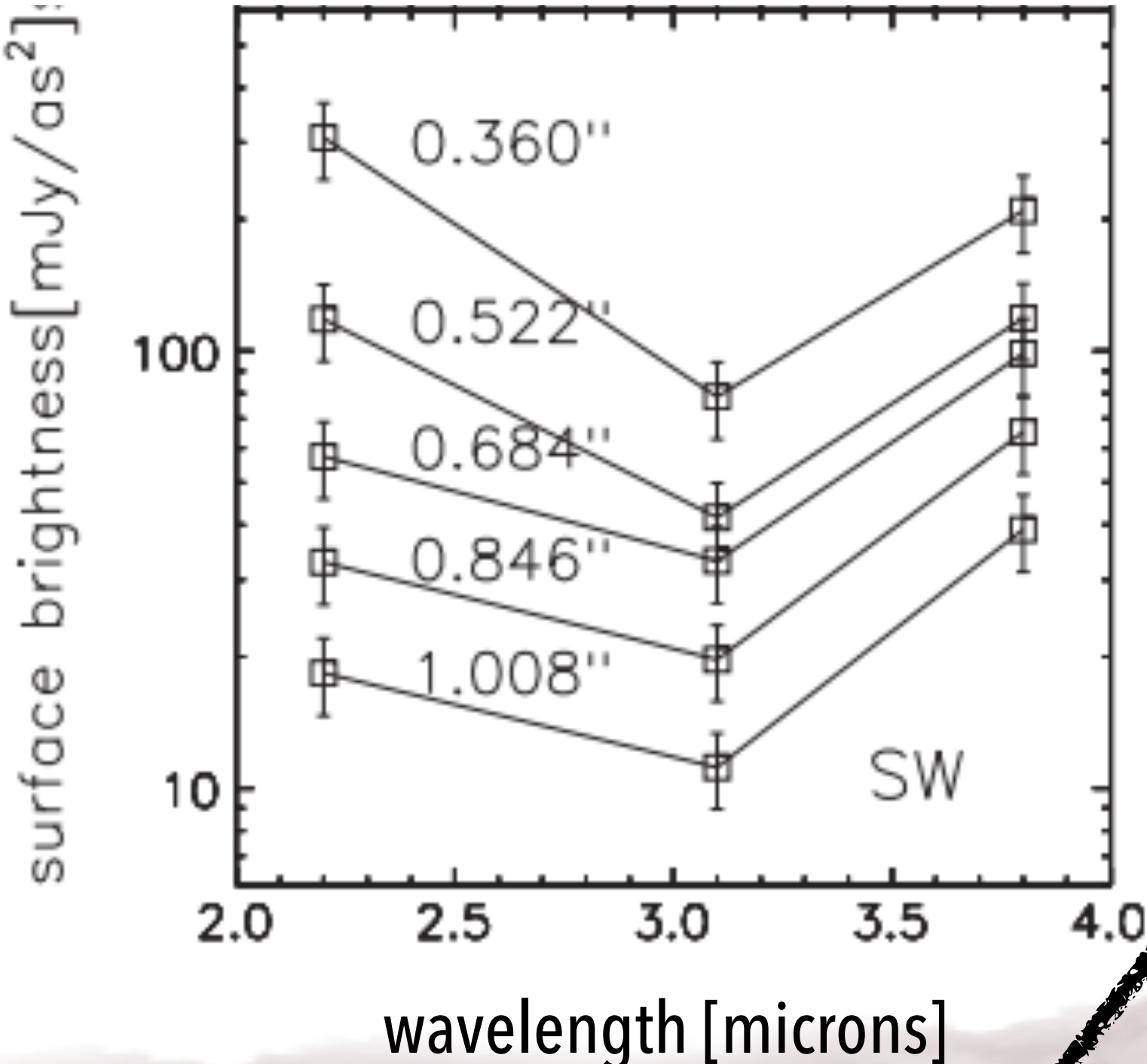
*Red colour: organics, ices?*

(Fitzsimmons et al. 2018)

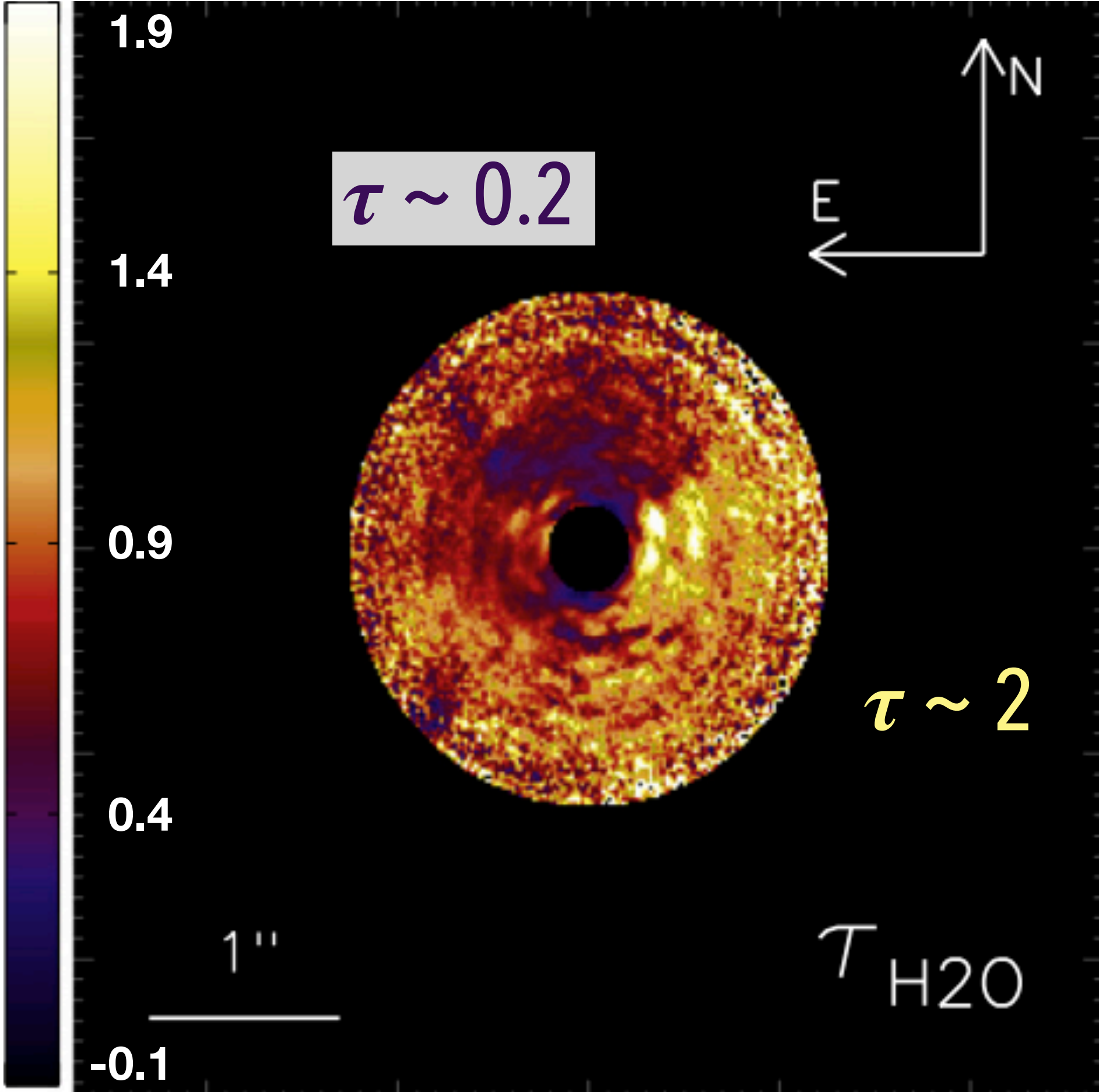
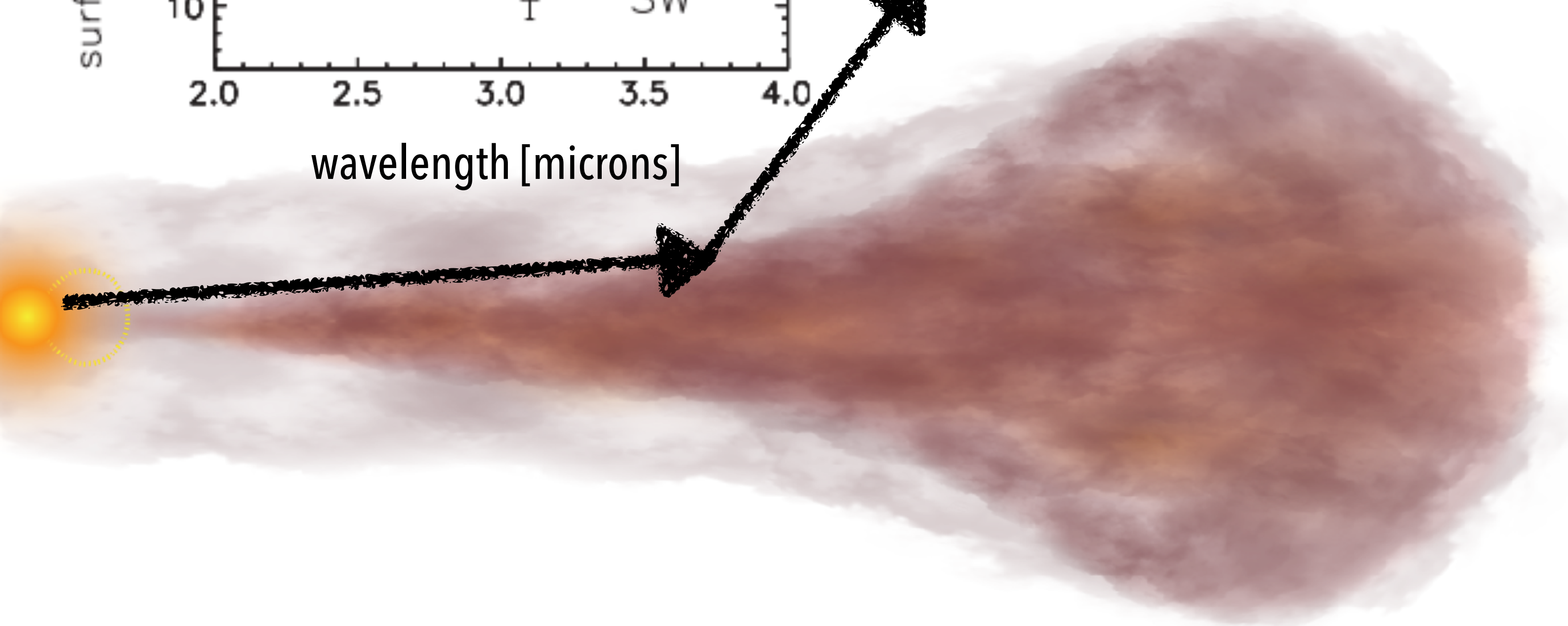
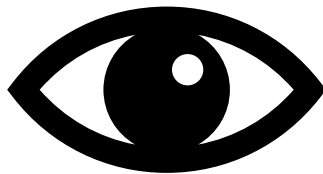


#3

# Near-IR scattered light imaging probes ice spatial distribution.

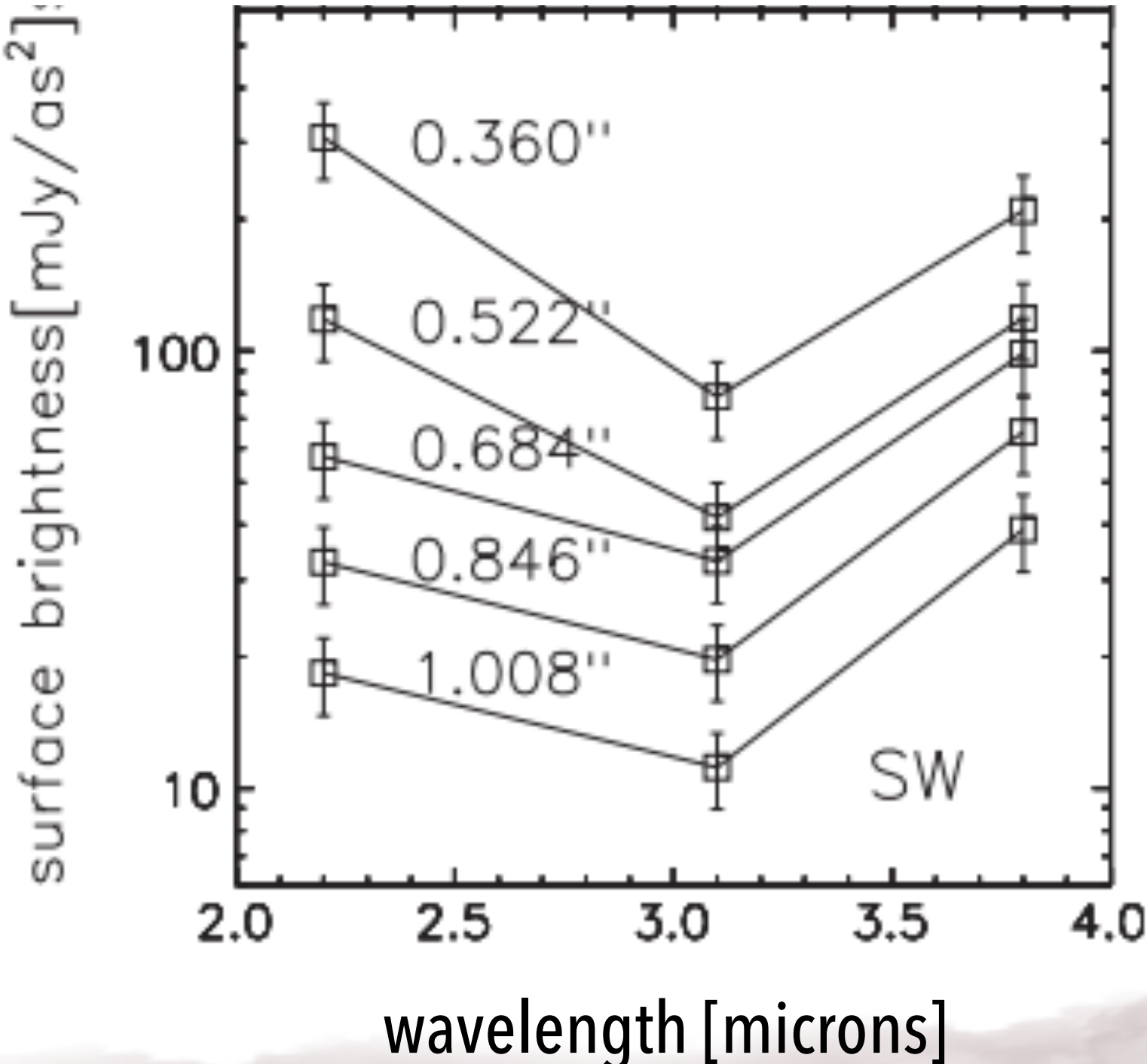


- Narrow-band imaging, continuum + H<sub>2</sub>O ice feature
- Stellar PSF removal

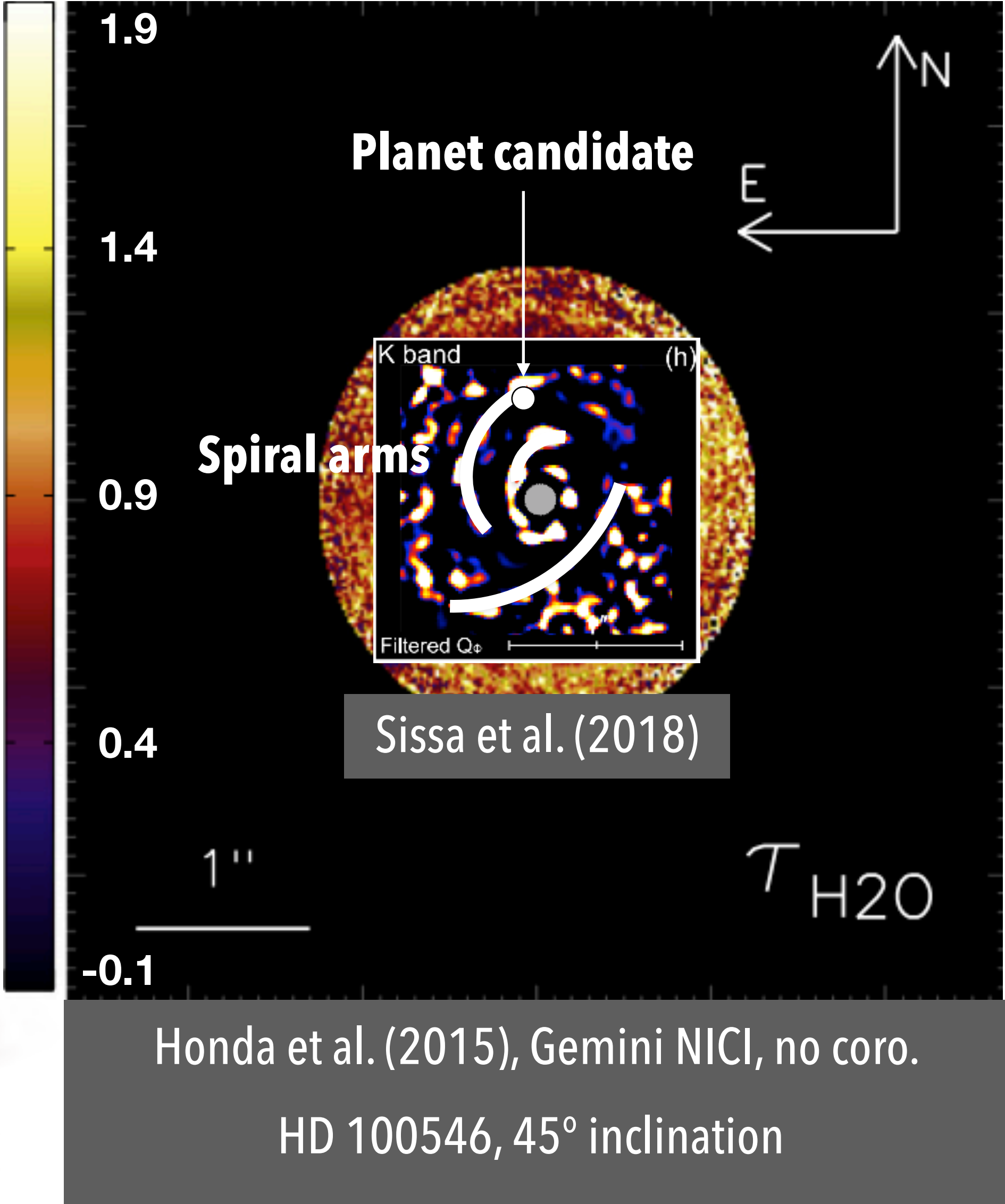
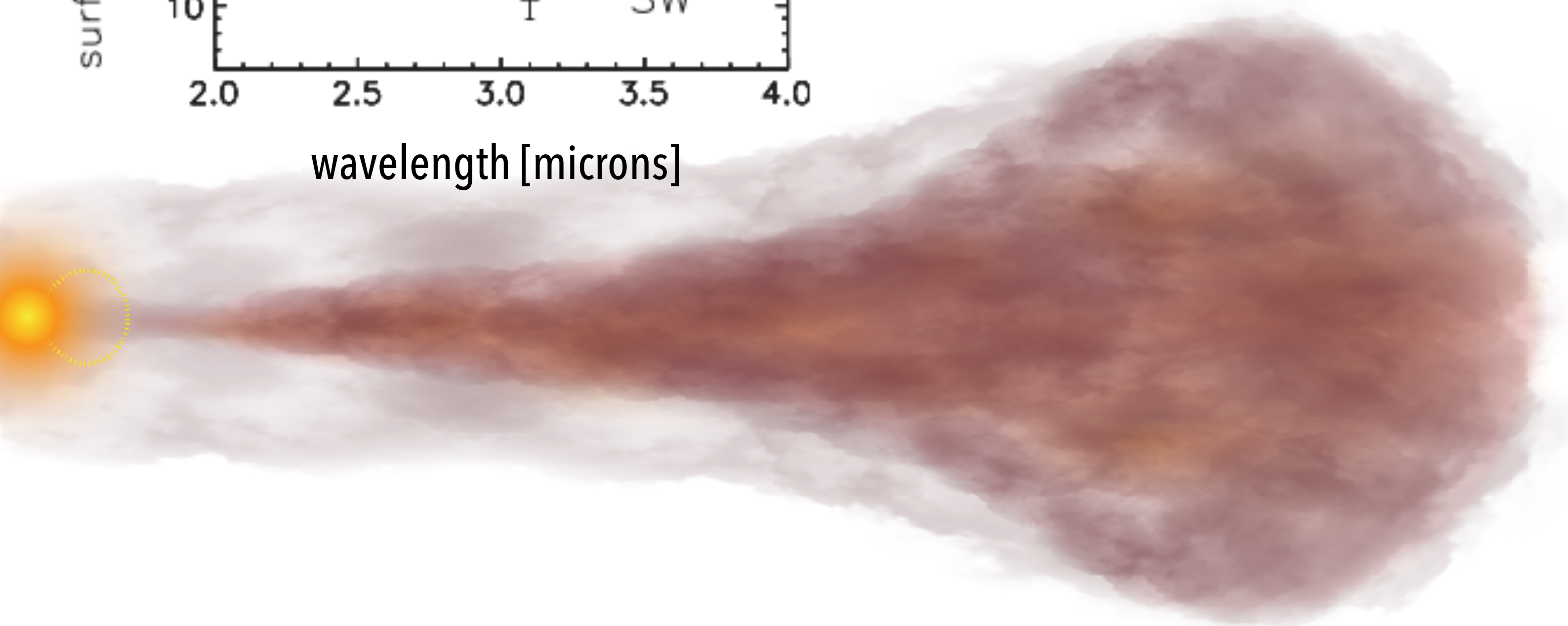


Honda et al. (2015), Gemini NIRC1, no coro.  
HD 100546, 45° inclination

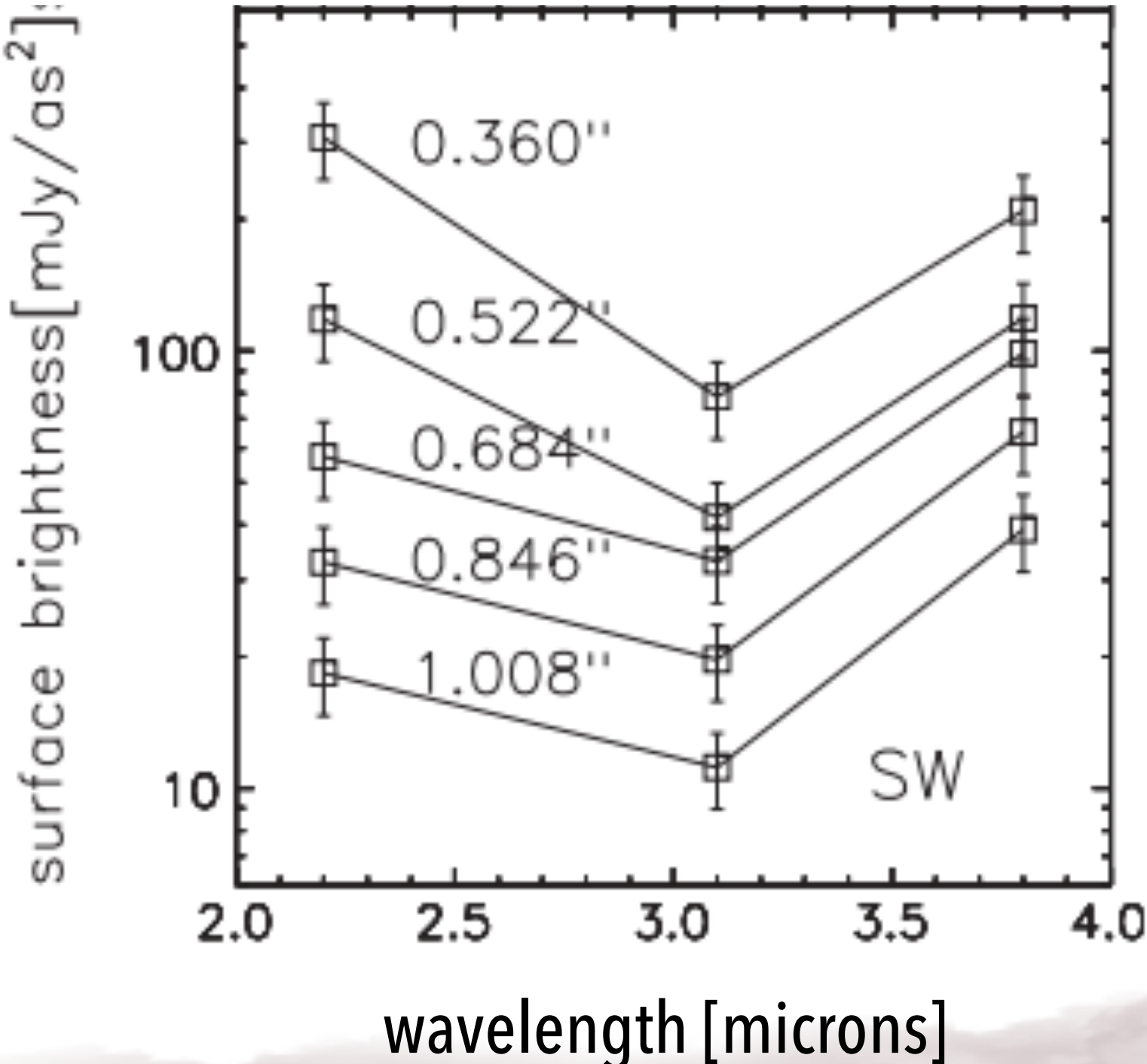
# Near-IR scattered light imaging probes ice spatial distribution.



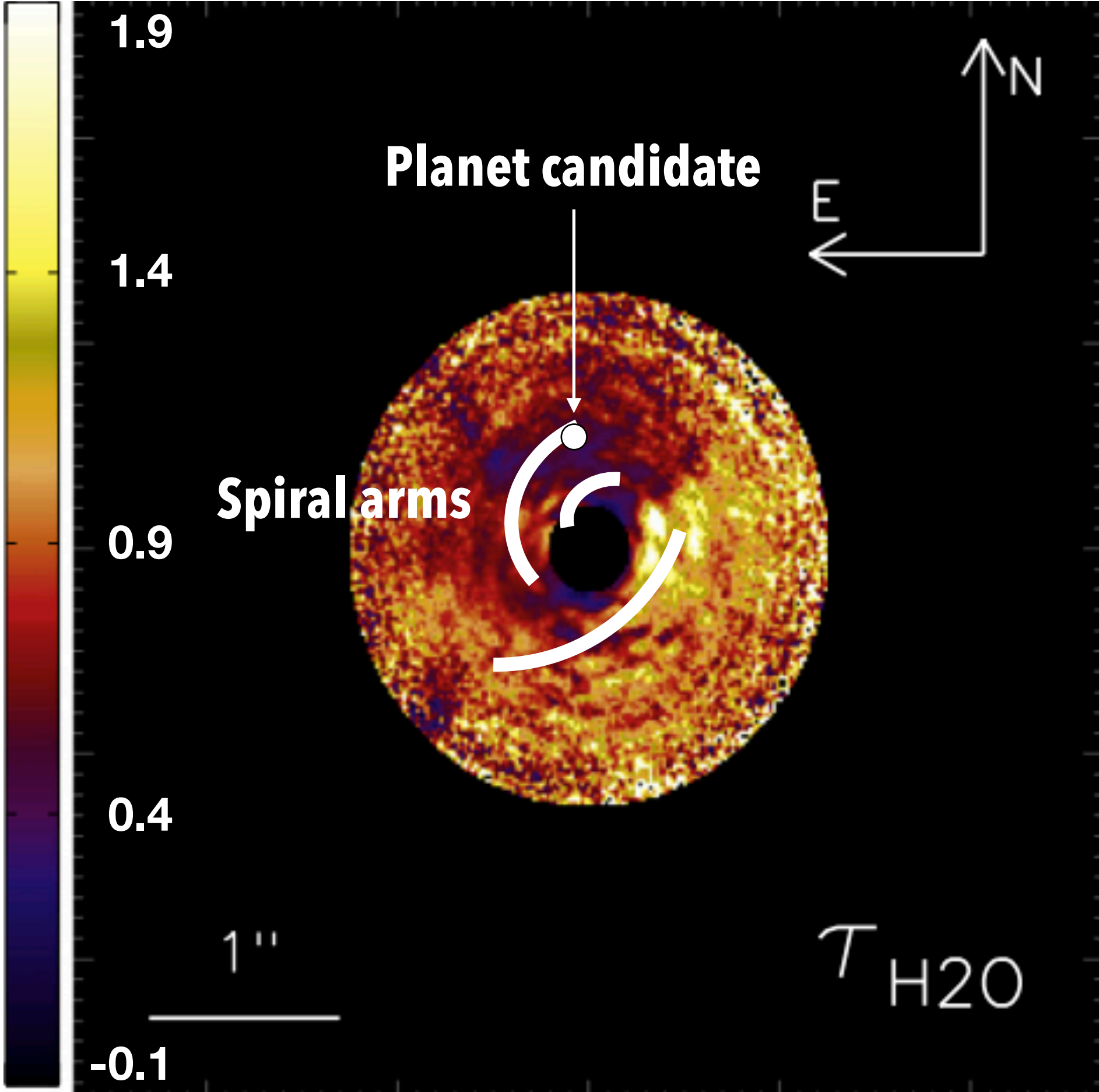
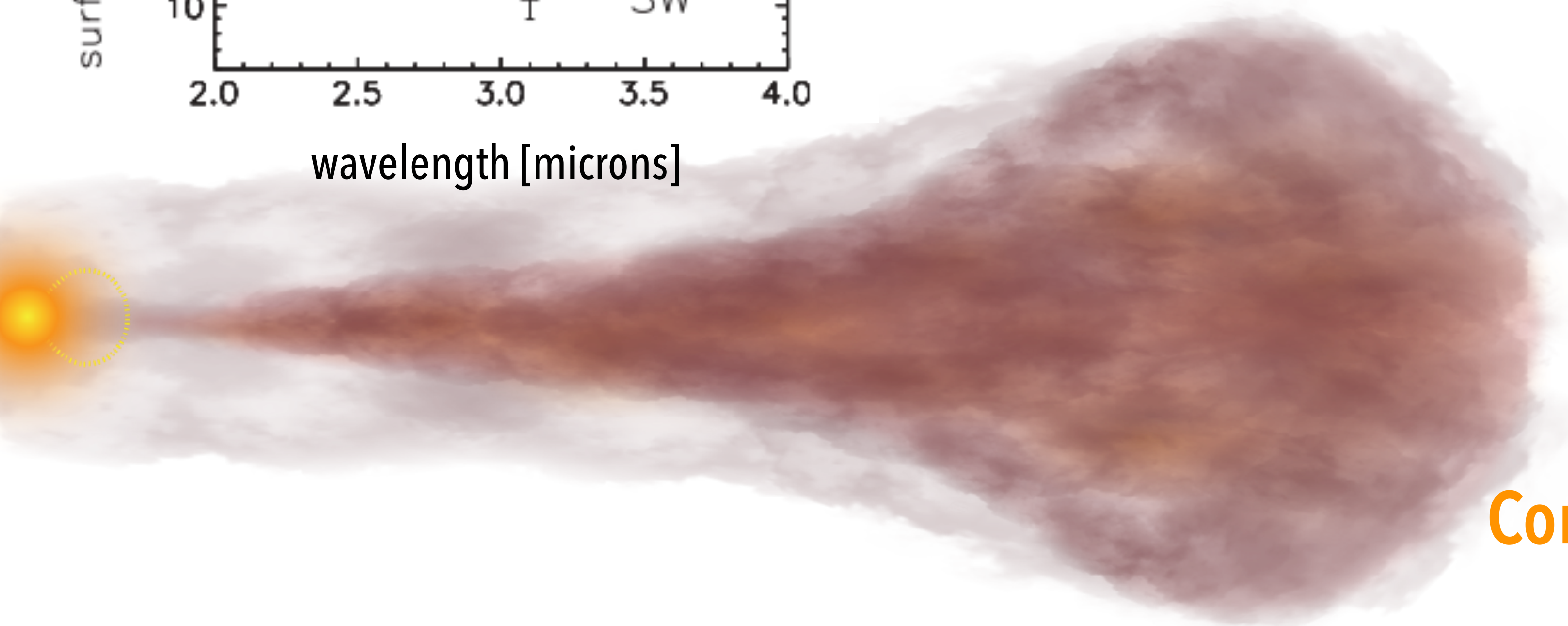
- Narrow-band imaging, continuum + H<sub>2</sub>O ice feature
- Stellar PSF removal



# Near-IR scattered light imaging probes ice spatial distribution.



- Narrow-band imaging, continuum + H<sub>2</sub>O ice feature
- Stellar PSF removal

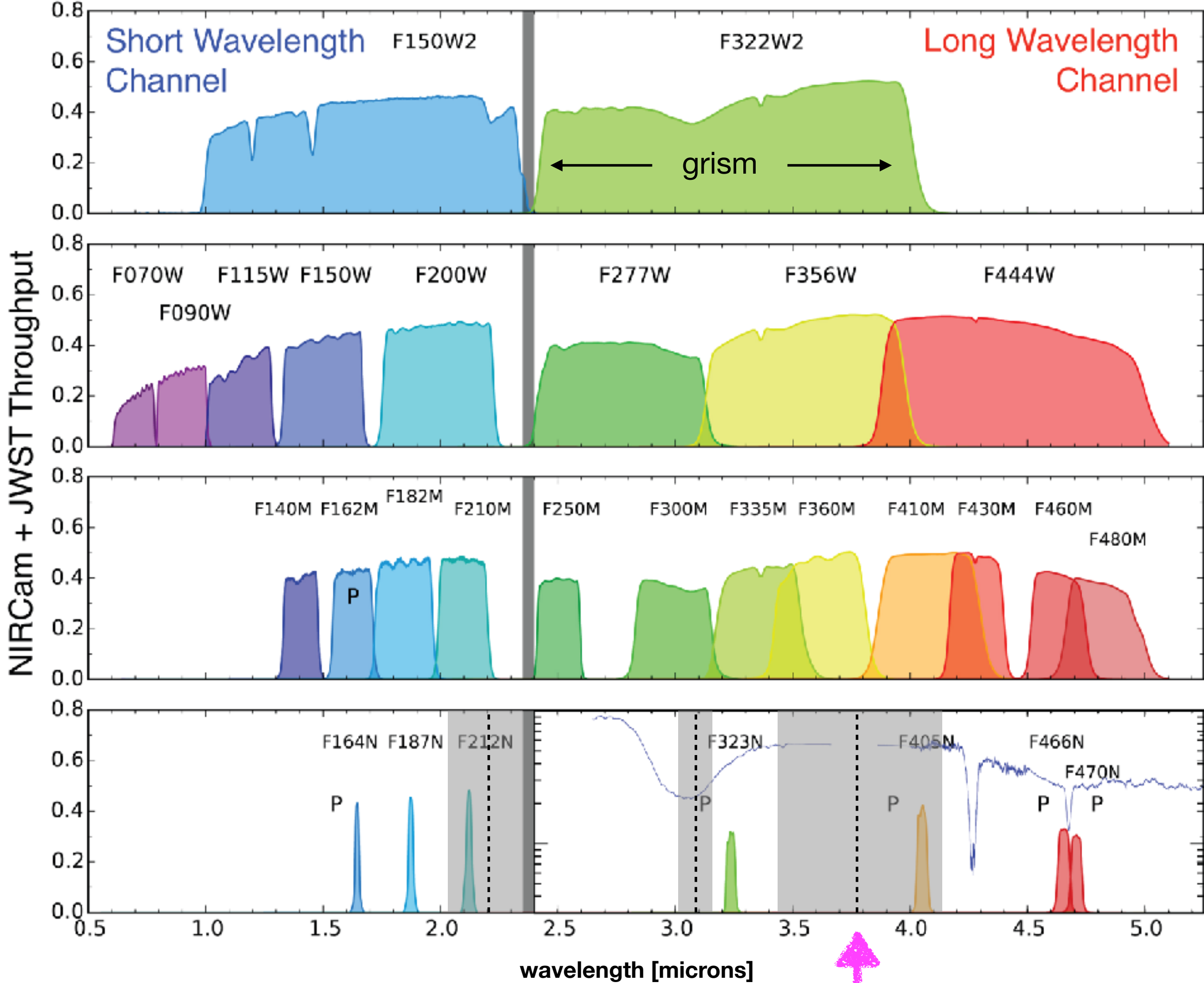


Honda et al. (2015), Gemini NIRC1, no coro.  
HD 100546, 45° inclination

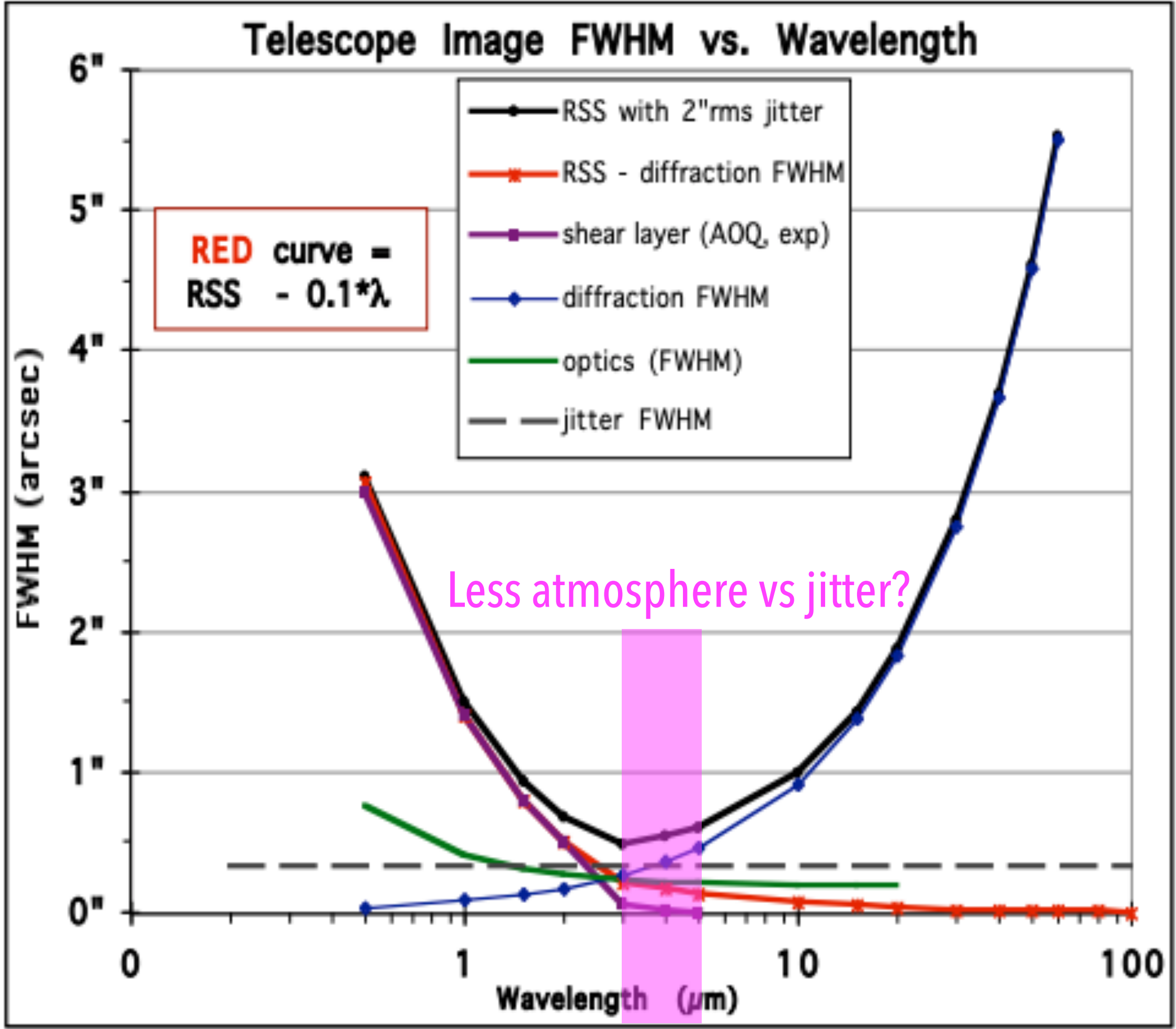
Composition of accreting exoplanet?

# JWST NIRCam lacks appropriate filters. NIRSpect IFU spaxels are 0."1: Room for SOFIA?

NIRCam Filters

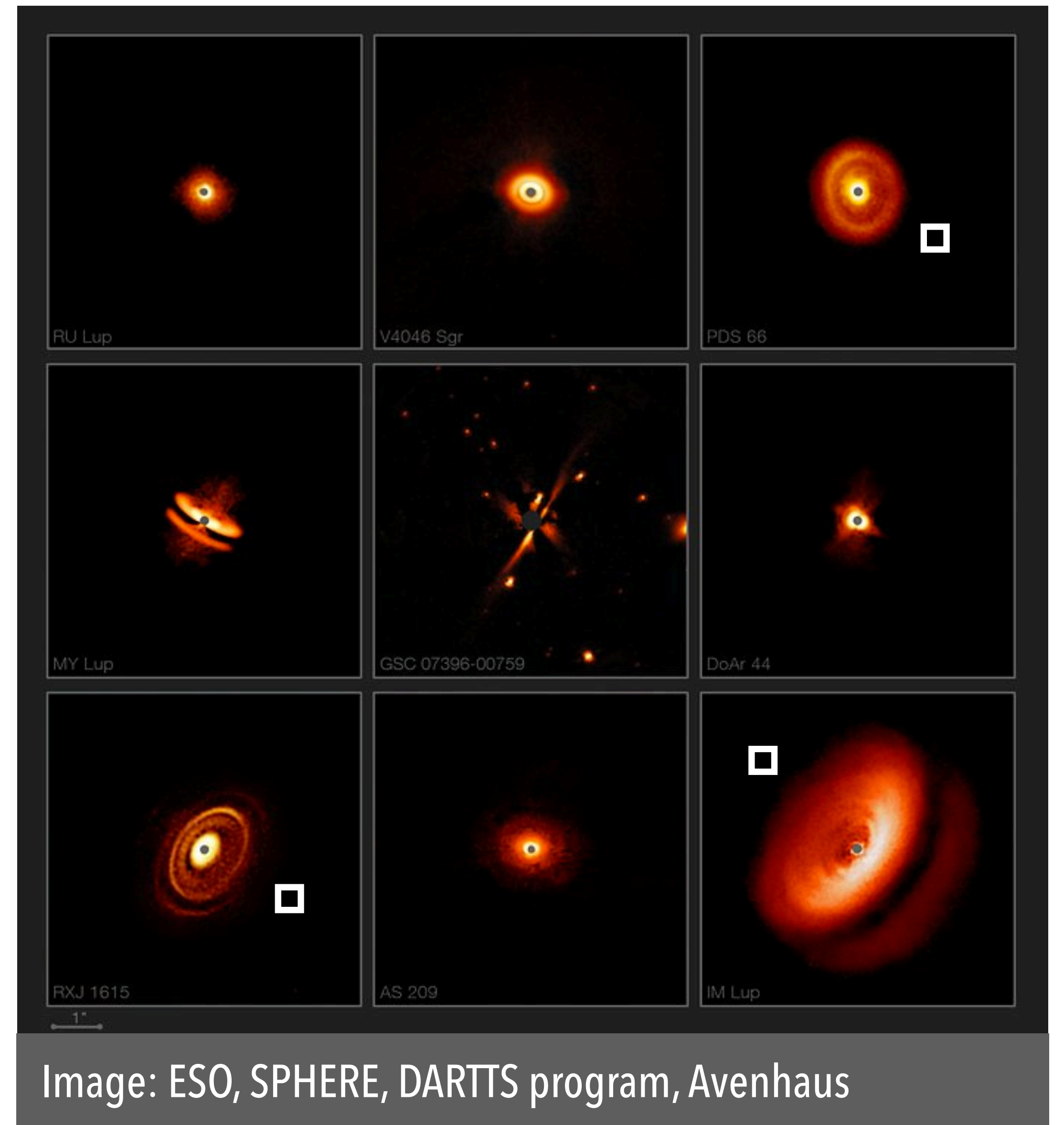
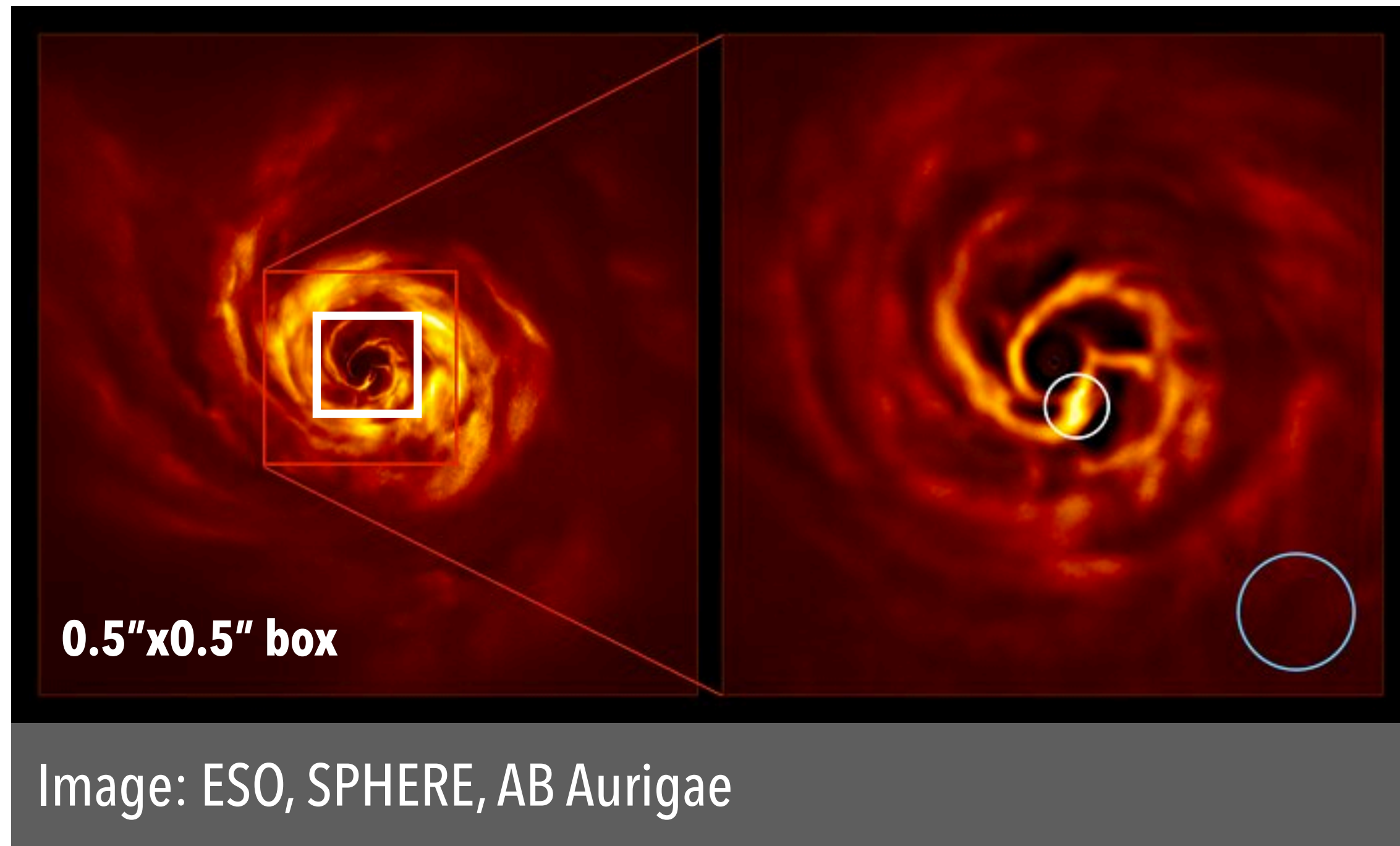


Gemini filters

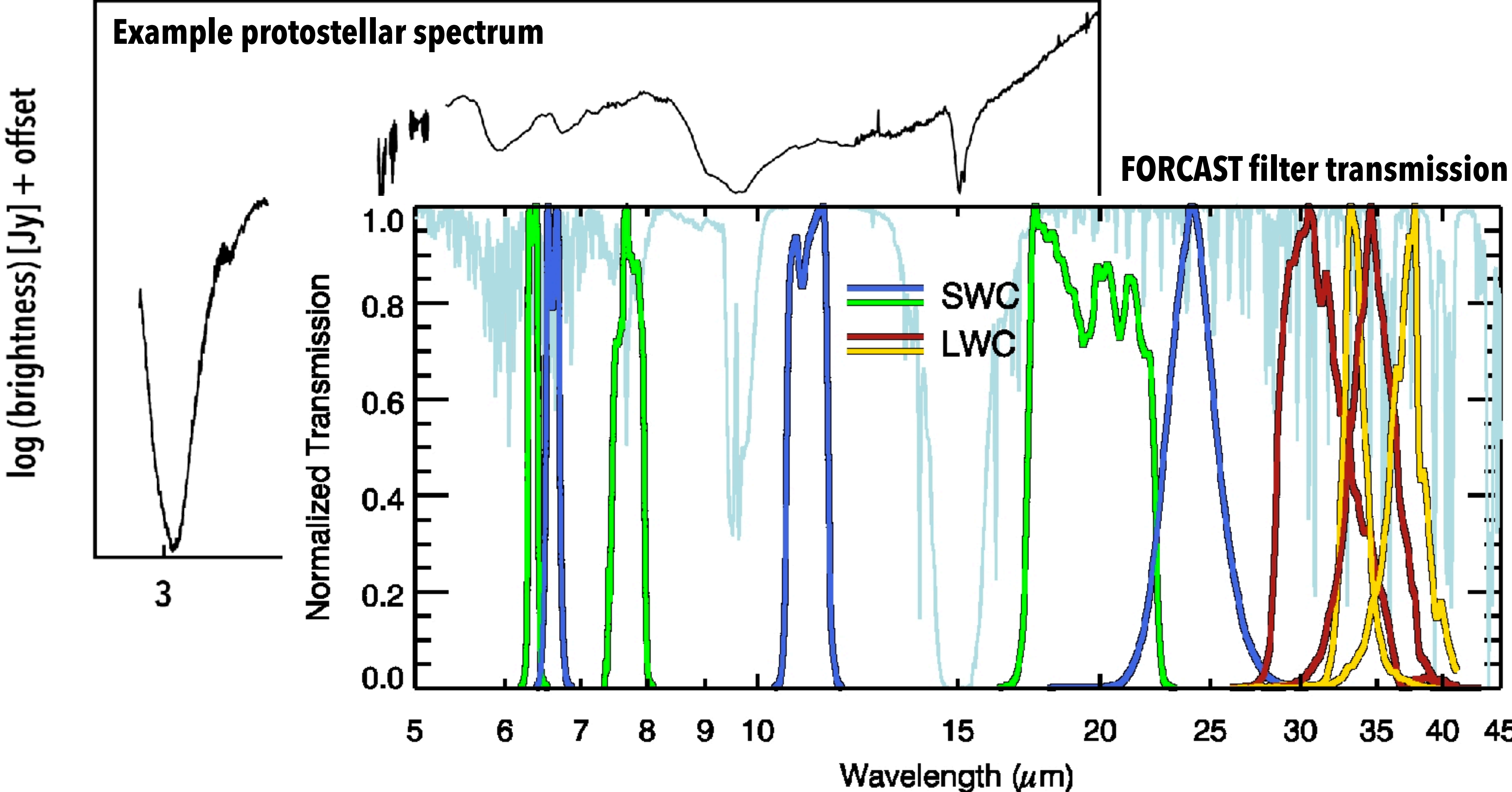




# Potential targets with large enough disks.



# Could additional narrow-band FORCAST filters provide similar measurements?



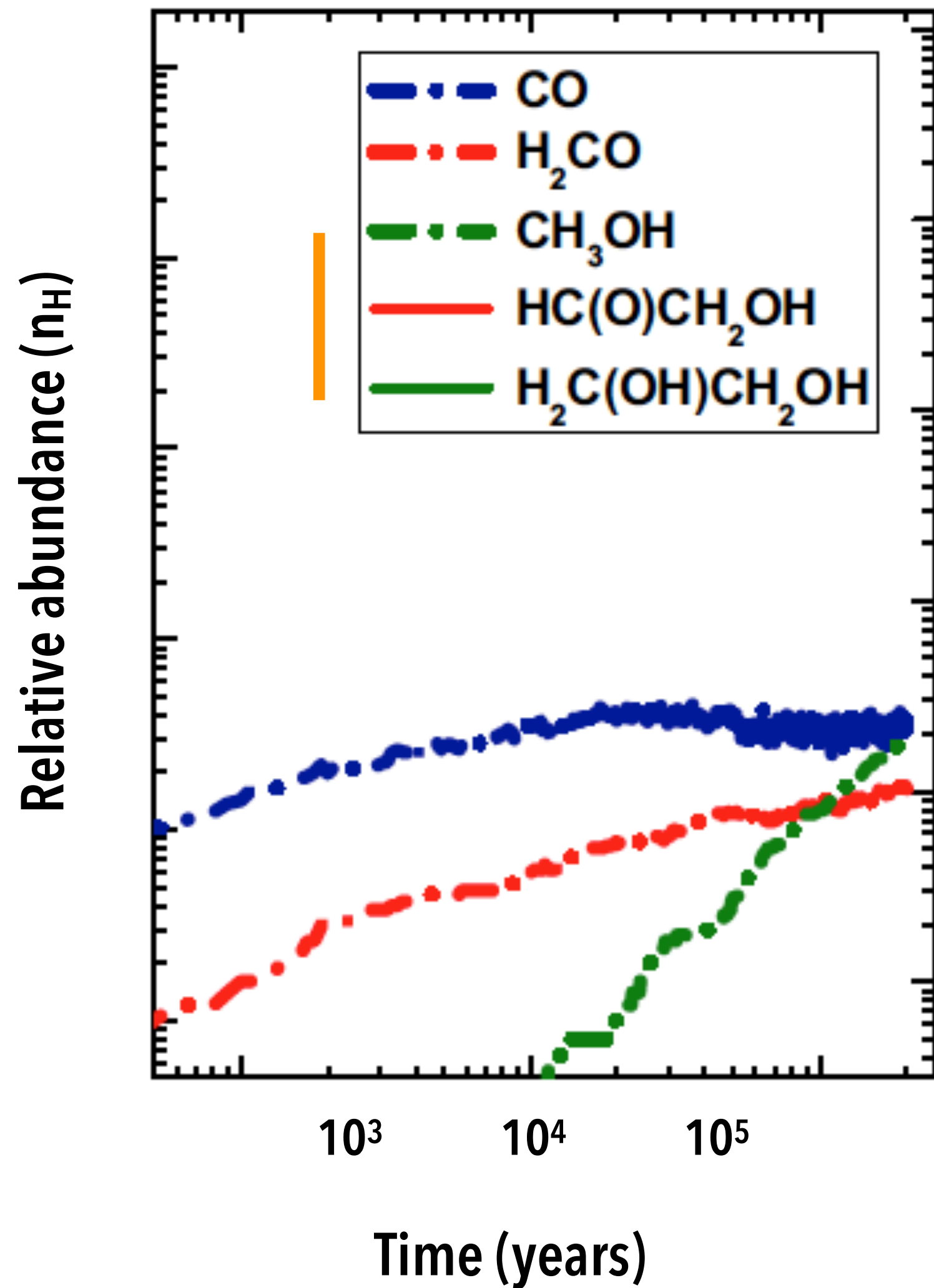
# Summary & Conclusions

- **JWST and Solar System missions will make enormous gains in next 5-10 years for the "Origins of life" community.**
- **Thermal ice spectroscopy is key to connect and capitalize on these results. Pre-OST/SPICA, we need a HIRMES-like instrument on SOFIA.**
- **There are potential upgrades to FORCAST imaging that could help, but they cannot replace HIRMES' utility for this science case.**

**Back-up slides...**

Diffuse cloud

$T=16.5\text{ K}$ ,  $n_{\text{H}}=1\text{ cm}^{-3}$



Lab experiments show COMs readily form under cloud-like conditions.



"simple" ices (methanol  $\sim$  CO)

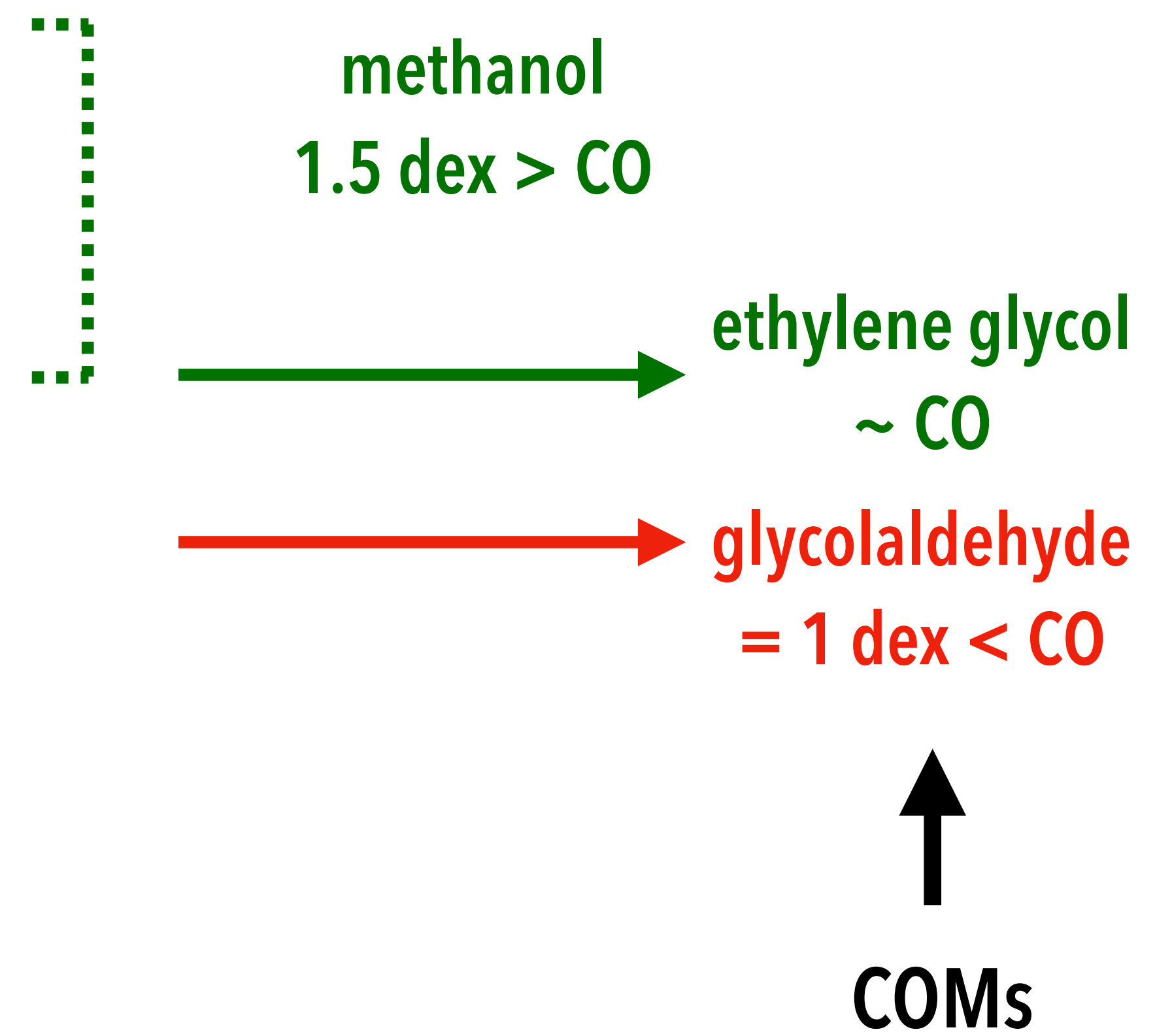
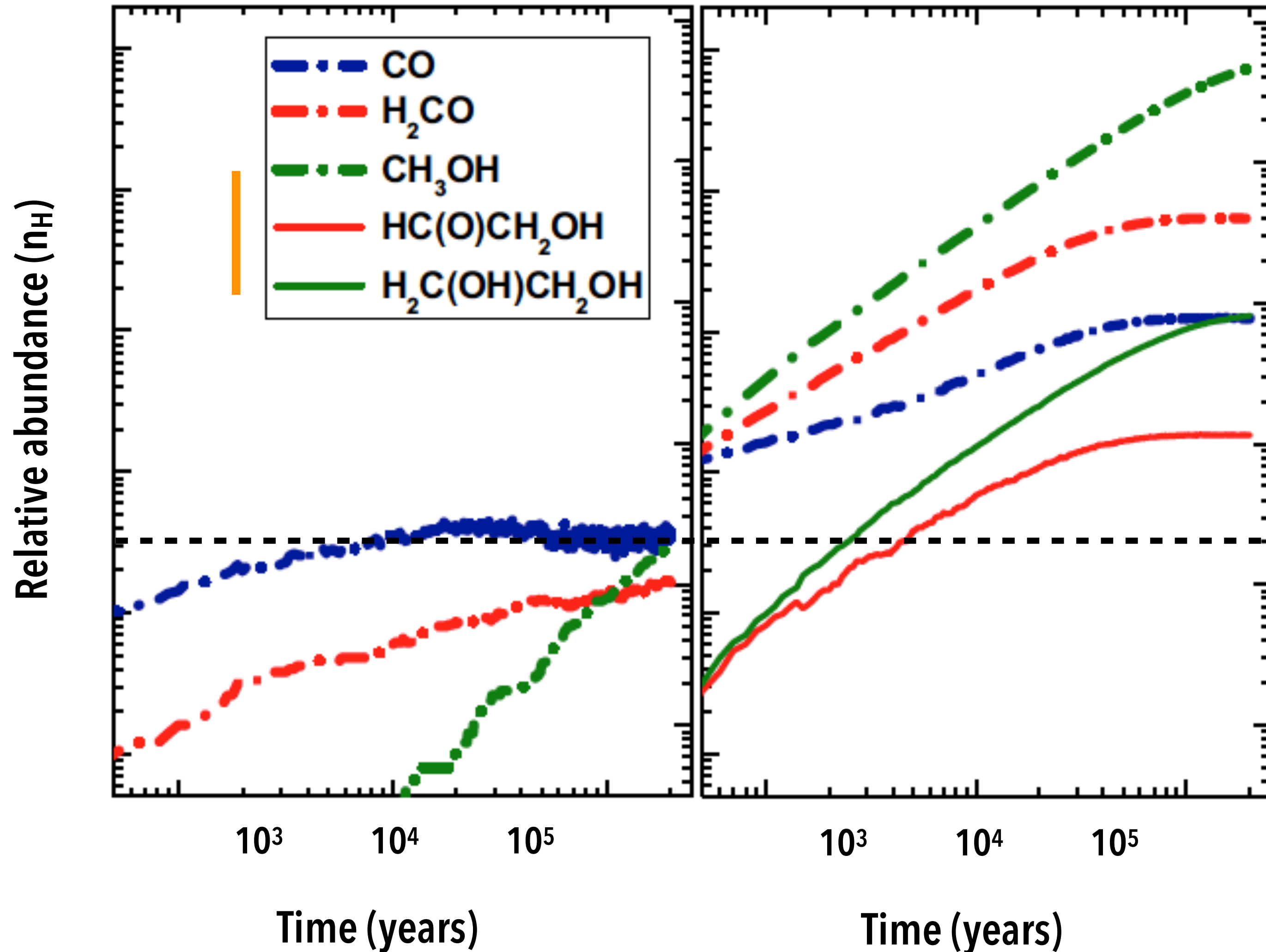
Diffuse cloud

$T=16.5\text{ K}, n_{\text{H}}=1\text{ cm}^{-3}$

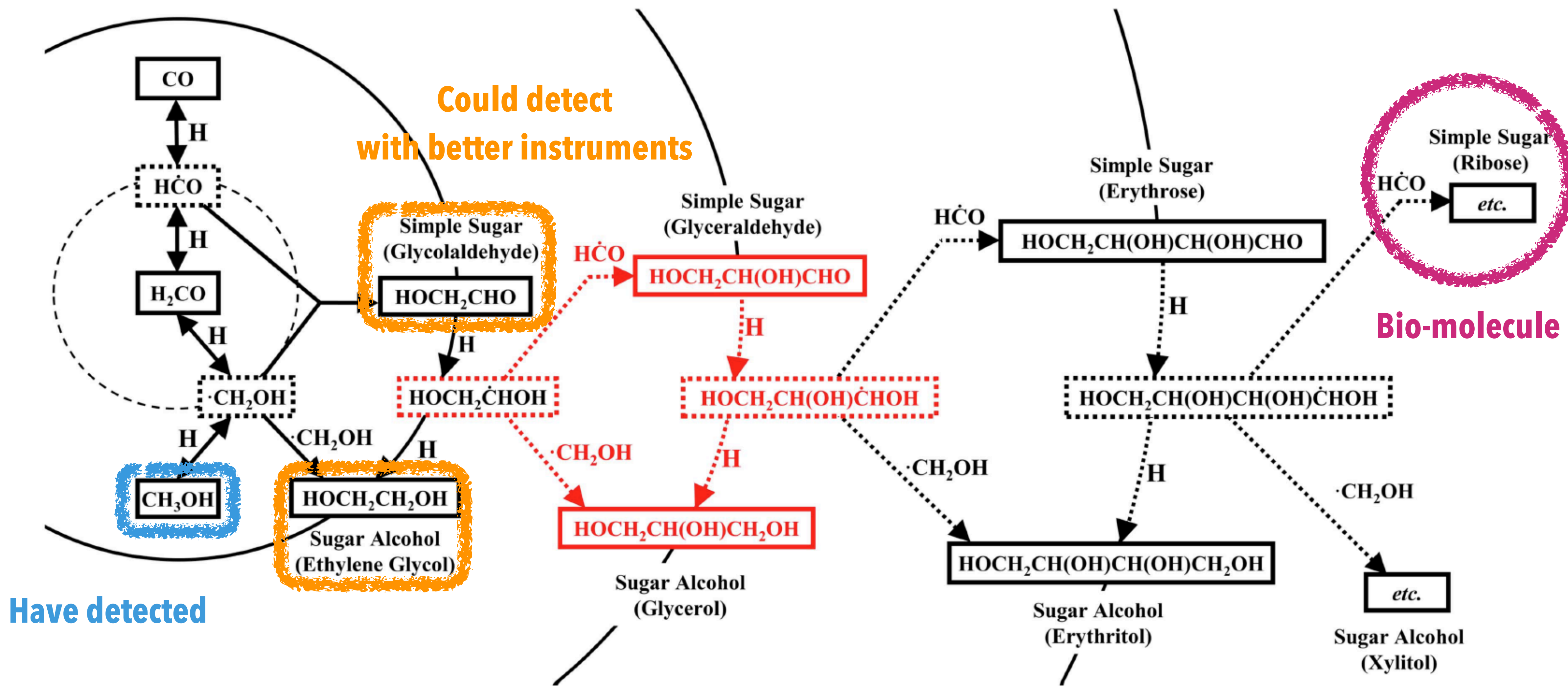
Dense core

$T=12\text{ K}, n_{\text{H}}=10\text{ cm}^{-3}$

Lab experiments show COMs readily form under cloud-like conditions.



# Forming simple sugars through atom-addition reactions in cold, dense cores.



High quality observations should identify at least 5 COMs in ices.

COM	formula	best ID features	References
methanol	CH <sub>3</sub> OH	3.9, 6.75, 9.74 μm	Boogert et al. (2015)
ethanol	CH <sub>3</sub> CH <sub>2</sub> OH	7.24, 11.36 μm	Terwisscha van Scheltinga et al. (2018)
acetaldehyde	CH <sub>3</sub> CHO	5.88, 7.427 μm	Terwisscha van Scheltinga et al. (2018)
dimethyl ether	CH <sub>3</sub> OCH <sub>3</sub>	8.011, 8.592 μm	Terwisscha van Scheltinga et al. (2018)
glycolaldehyde	HC(O)CH <sub>2</sub> OH	5.88, 7.14, 9.1 μm	Fedoseev et al. (2017)
ethylene glycol	H <sub>2</sub> C(OH)CH <sub>2</sub> OH	~9.1 – 10 μm	Fedoseev et al. (2017)



High quality observations should identify at least 5 COMs in ices.

COM	formula	best ID features	References
methanol	CH <sub>3</sub> OH	3.9, 6.75, 9.74 μm	Boogert et al. (2015)
ethanol	CH <sub>3</sub> CH <sub>2</sub> OH	7.24, 11.36 μm	Terwisscha van Scheltinga et al. (2018)
acetaldehyde	CH <sub>3</sub> CHO	5.88, 7.427 μm	Terwisscha van Scheltinga et al. (2018)
dimethyl ether	CH <sub>3</sub> OCH <sub>3</sub>	8.011, 8.592 μm	Terwisscha van Scheltinga et al. (2018)
glycolaldehyde	HC(O)CH <sub>2</sub> OH	5.88, 7.14, 9.1 μm	Fedoseev et al. (2017)
ethylene glycol	H <sub>2</sub> C(OH)CH <sub>2</sub> OH	~9.1 – 10 μm	Fedoseev et al. (2017)

**More COMs to come from  
Leiden Laboratory for Astrophysics**

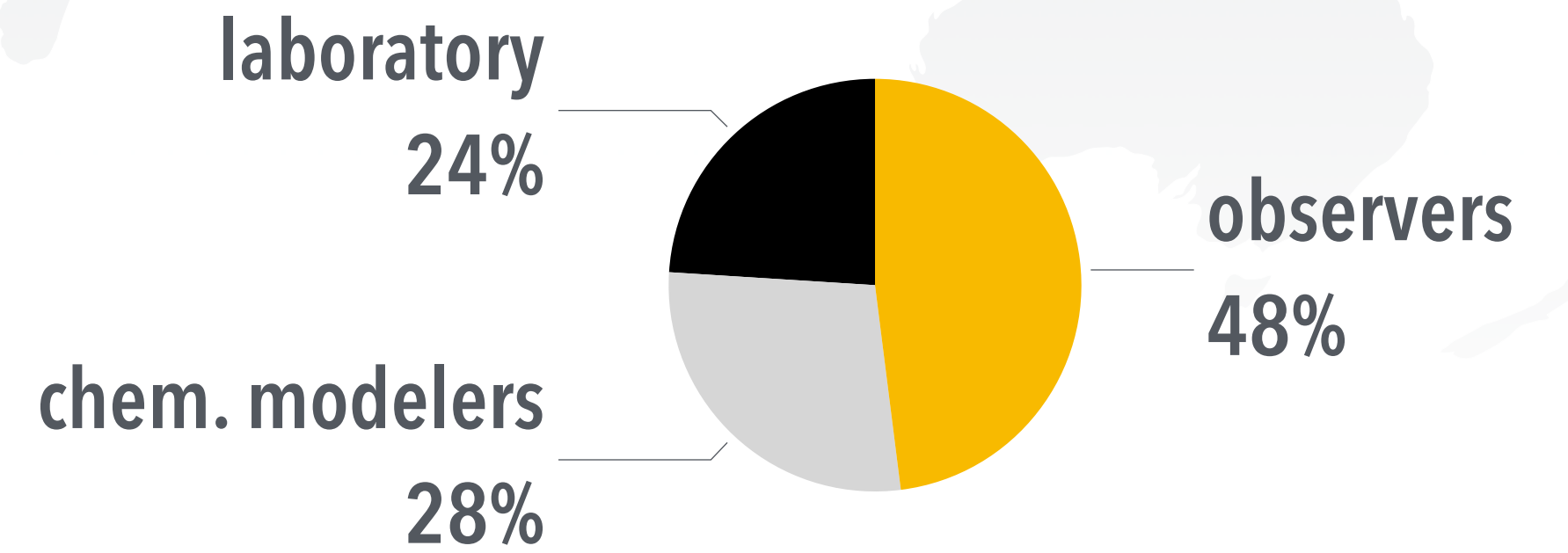


# JWST IceAge ERS Program (PI McClure)



## "Early Release Science"

- will be executed in the **first 5 months of observations**
- competitively selected (13 of 106 proposals)
- only 1 star formation proposal



# Feedback between observations, laboratory work, and chemical modeling is critical.

## 2. Models

## 1. Observations

*(JWST launches March 2021)*

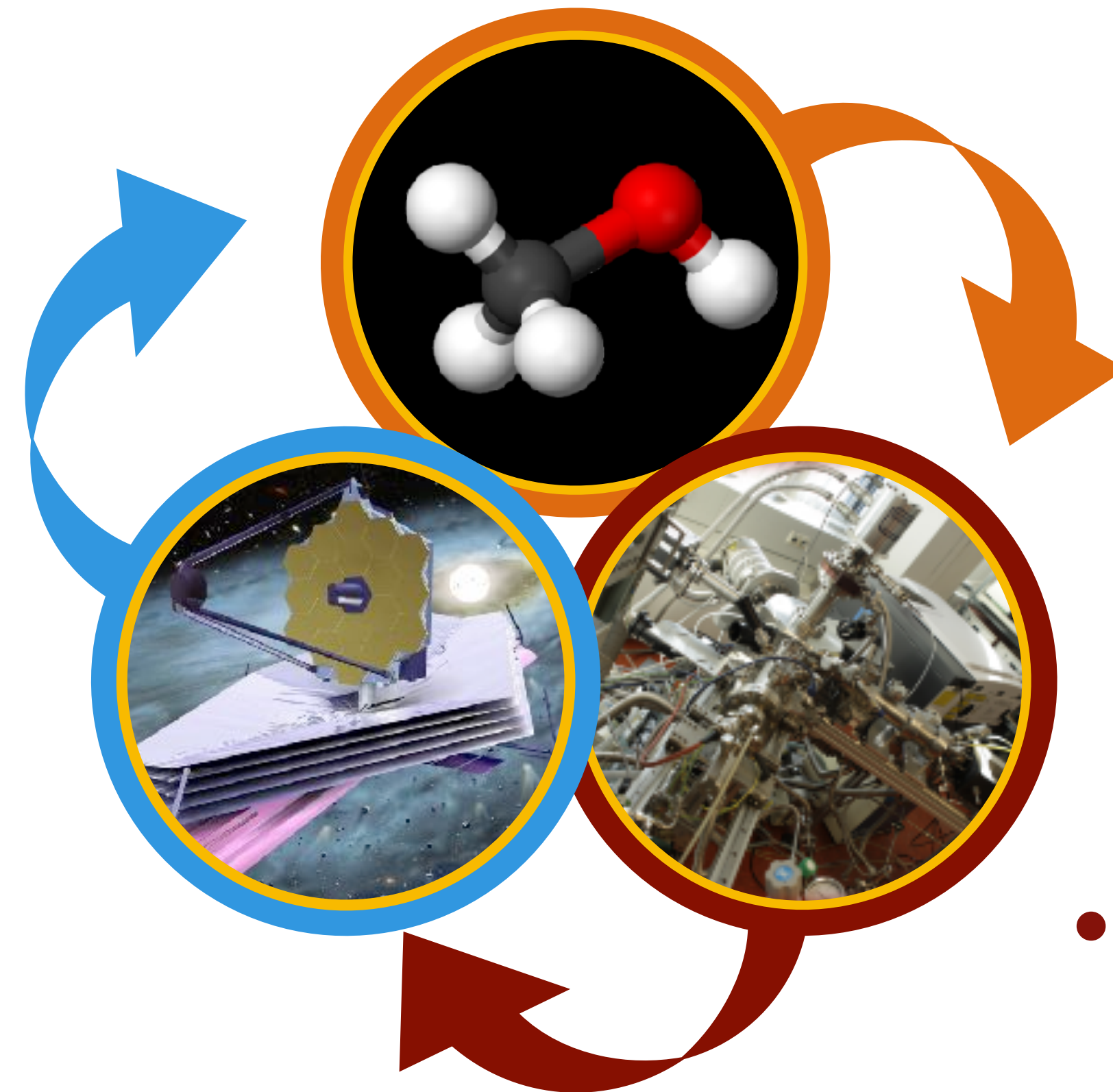
- dense core (#0)
- one disk (#2)



*Detect 5 simple ices  
+ 5 pre-biotic, icy COMs.*



*informs observational requirements*



- Physical conditions of individual regions  
+ laboratory absorbances/opacities



- Simple ice + COM abundances
- Object brightness vs wavelength

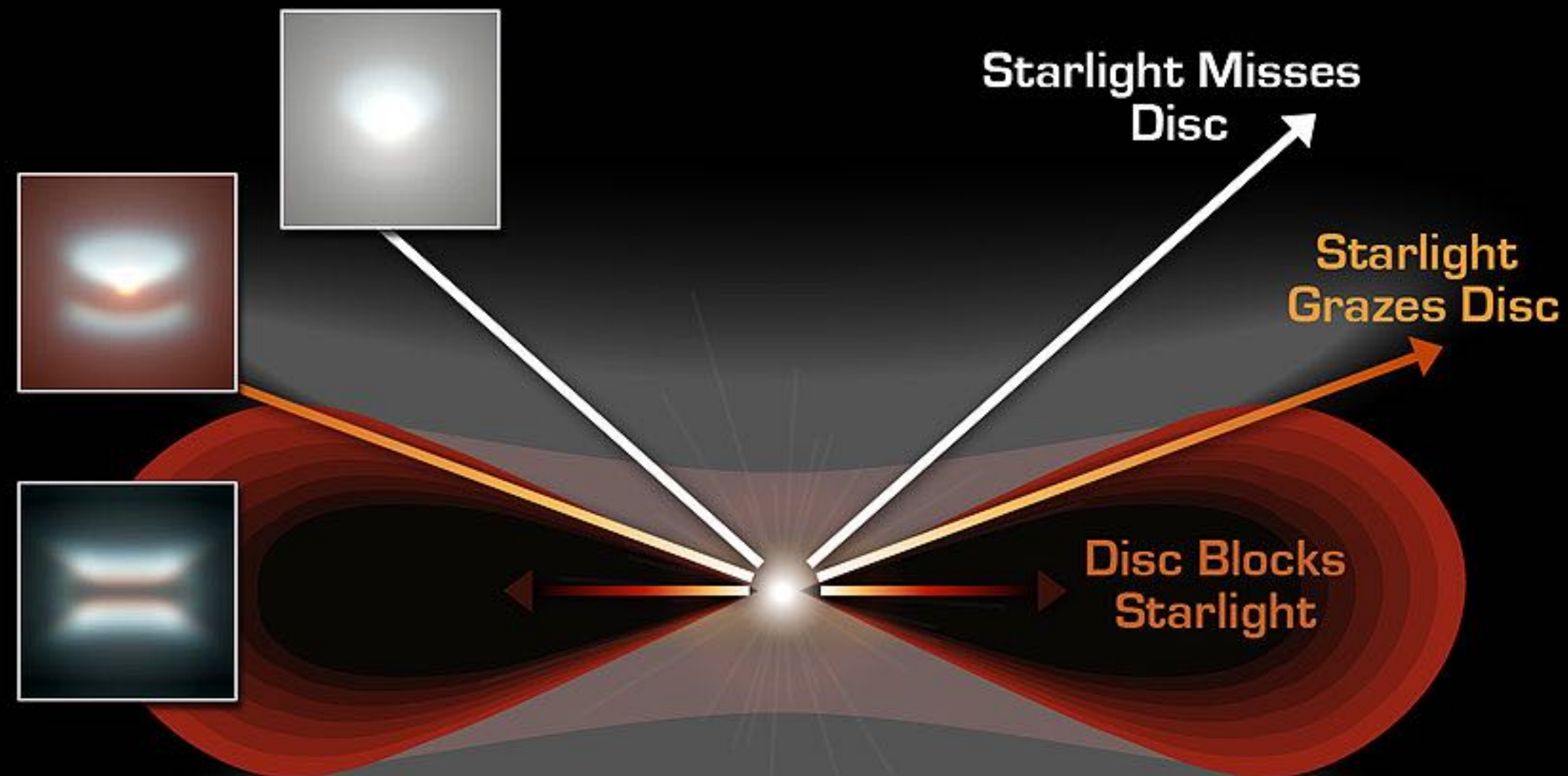
## 3. Laboratory Data

### Leiden Laboratory for Astrophysics

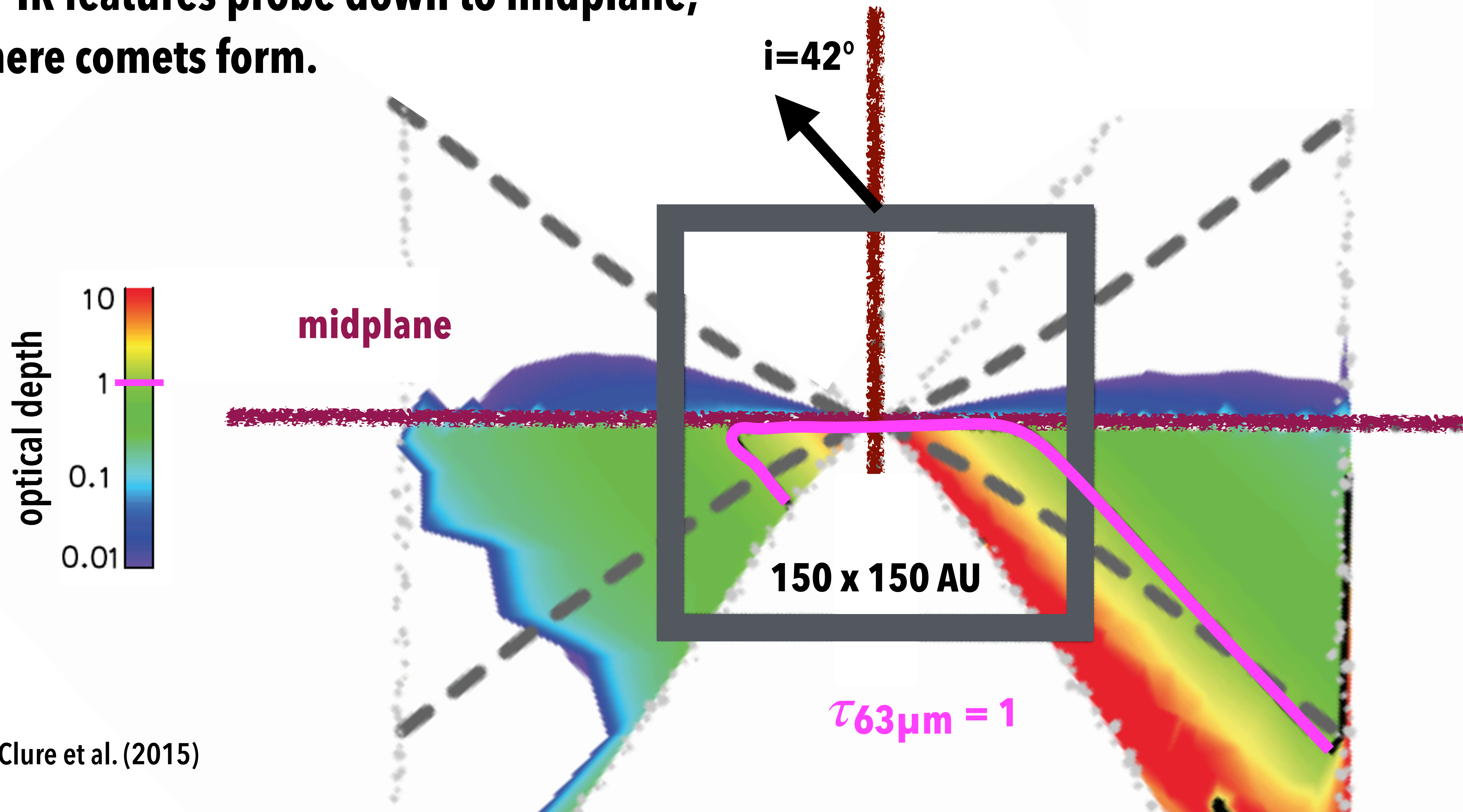
- Spectroscopy of simple ices, range of T, mixing ratios  
*(new: 2010 - present)*
- COM formation rates under cloud conditions
- Spectroscopy of COM ices (to identify in mid-infrared)

# JWST-MIRI EU Guaranteed Time Observations star formation program

Observations of 12 protostars & 4 edge-on disks (ices), 36 other disks, probe ice in different heights.



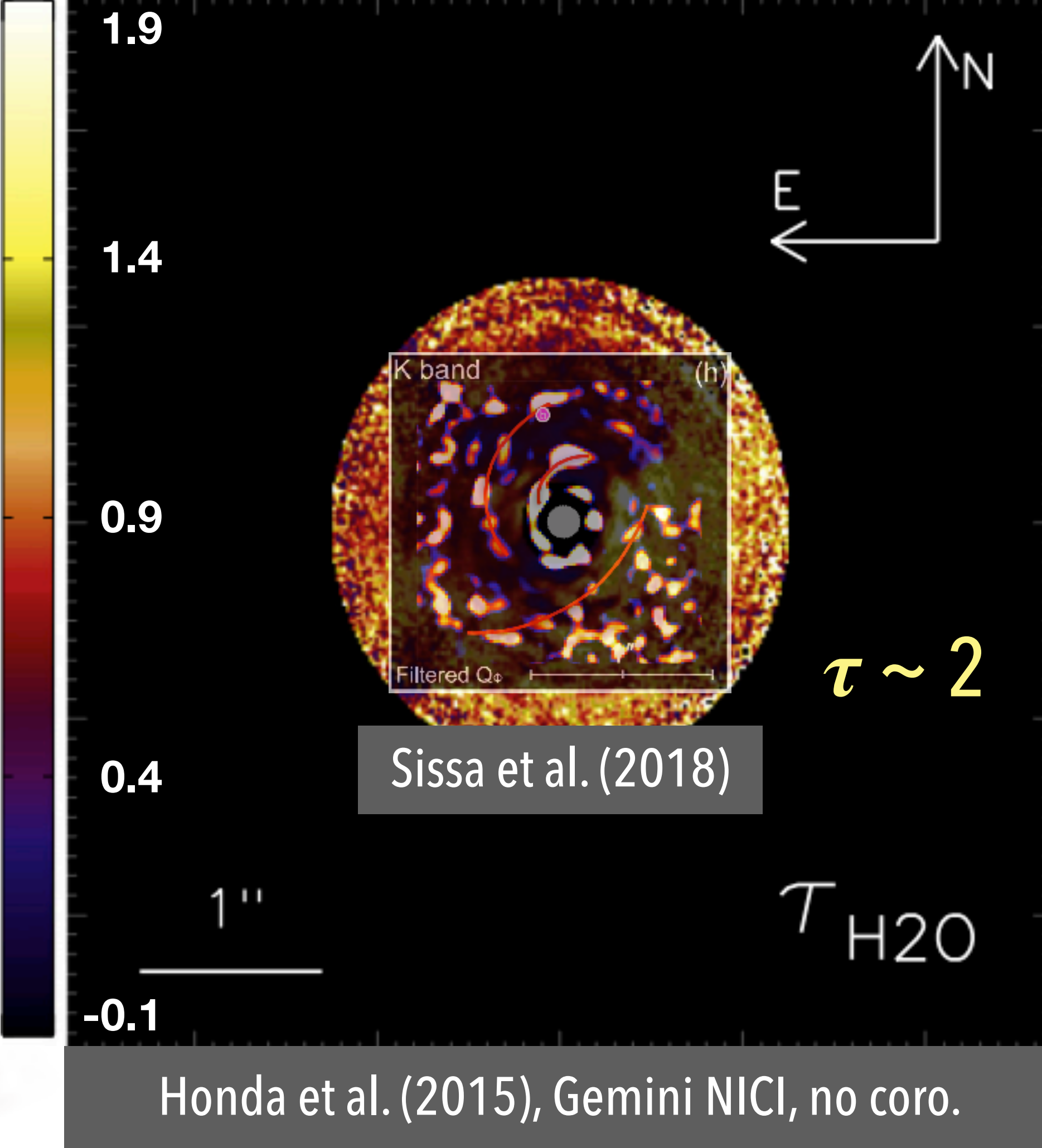
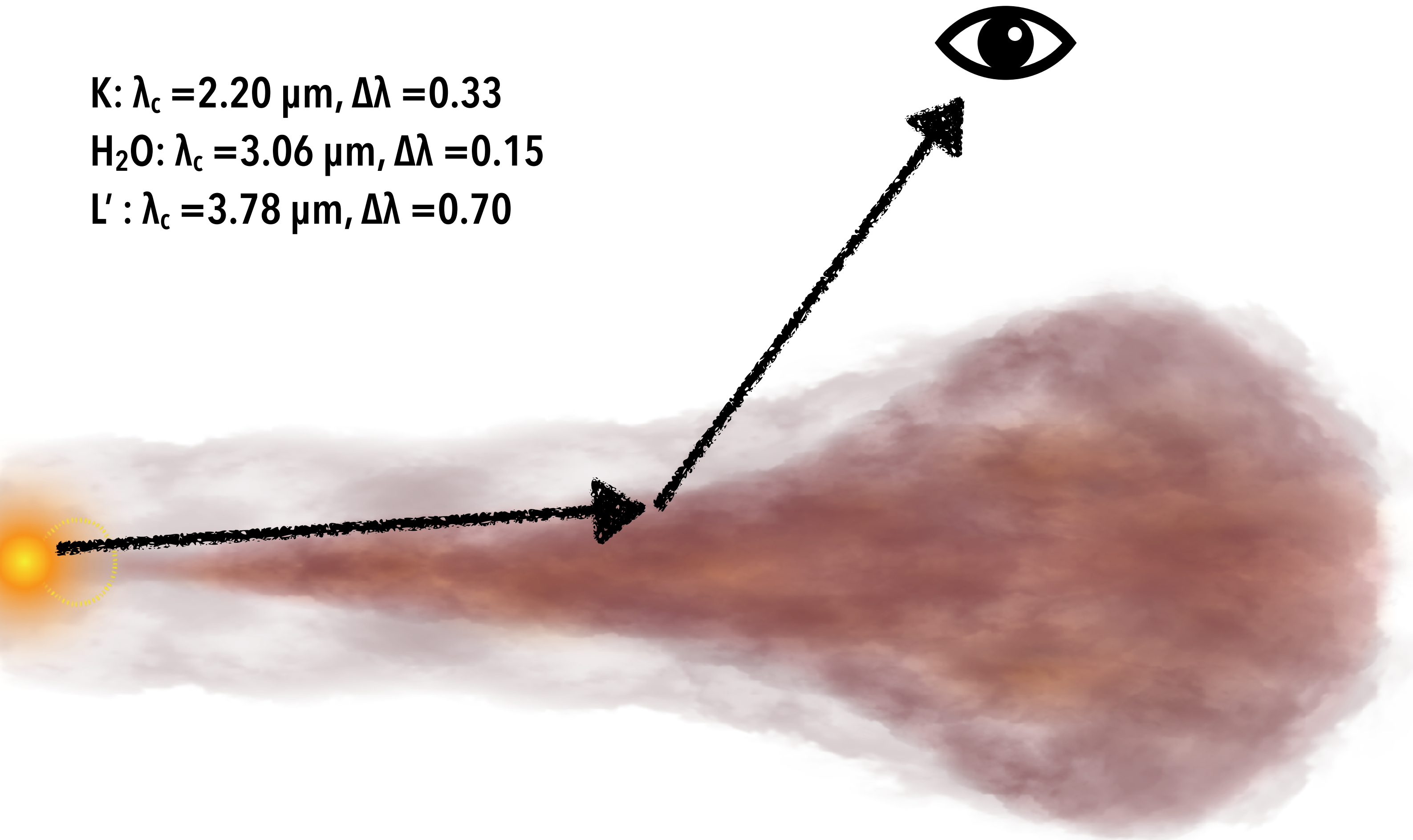
**Far-IR features probe down to midplane,  
where comets form.**



# Near-IR scattered light imaging connects ices to disk structure and exoplanets

Narrow-band AO-imaging in continuum + H<sub>2</sub>O ice feature  
Stellar PSF removal

K:  $\lambda_c = 2.20 \mu\text{m}$ ,  $\Delta\lambda = 0.33$   
H<sub>2</sub>O:  $\lambda_c = 3.06 \mu\text{m}$ ,  $\Delta\lambda = 0.15$   
L':  $\lambda_c = 3.78 \mu\text{m}$ ,  $\Delta\lambda = 0.70$



# Exoplanet mission timelines.

