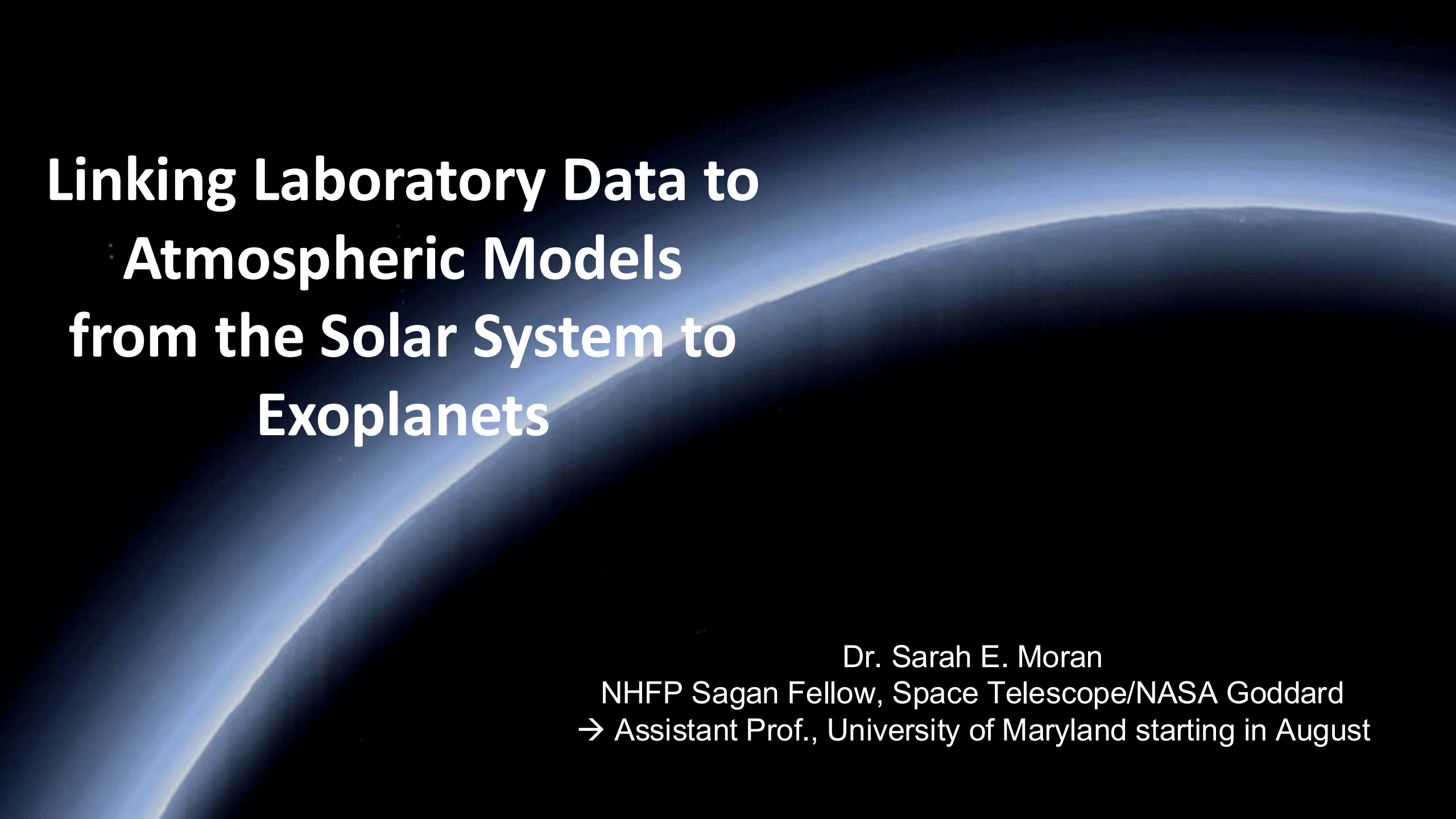
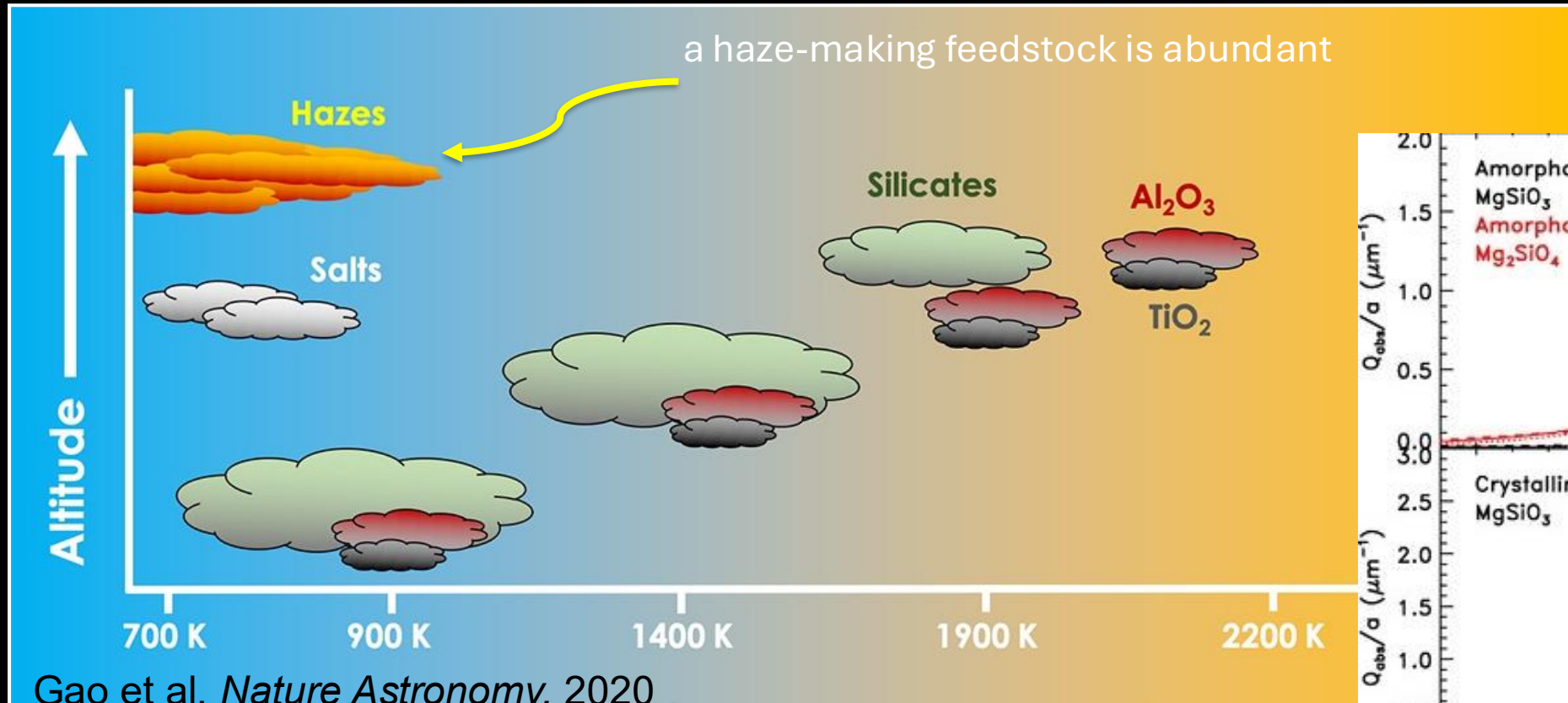




Linking Laboratory Data to Atmospheric Models from the Solar System to Exoplanets

Dr. Sarah E. Moran
NHFP Sagan Fellow, Space Telescope/NASA Goddard
→ Assistant Prof., University of Maryland starting in August

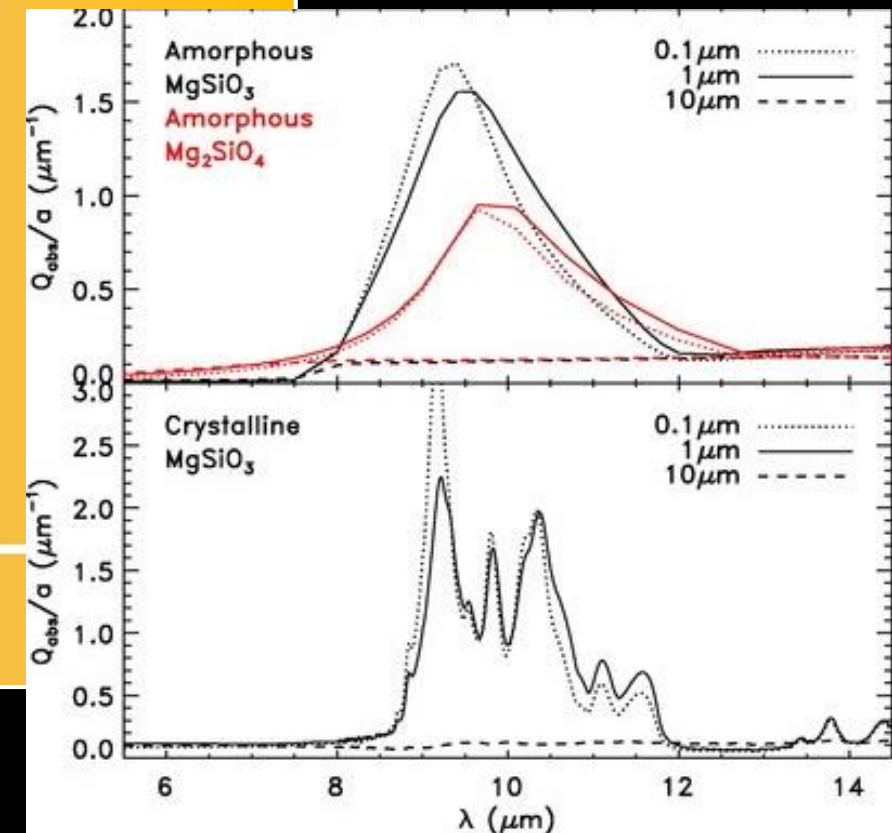
Clouds (and hazes) are a fundamental part of atmospheres whose compositions and morphologies trace **temperature** and **chemical** formation conditions



Gao et al. *Nature Astronomy*, 2020

← many hundreds of degrees this way to solar system worlds

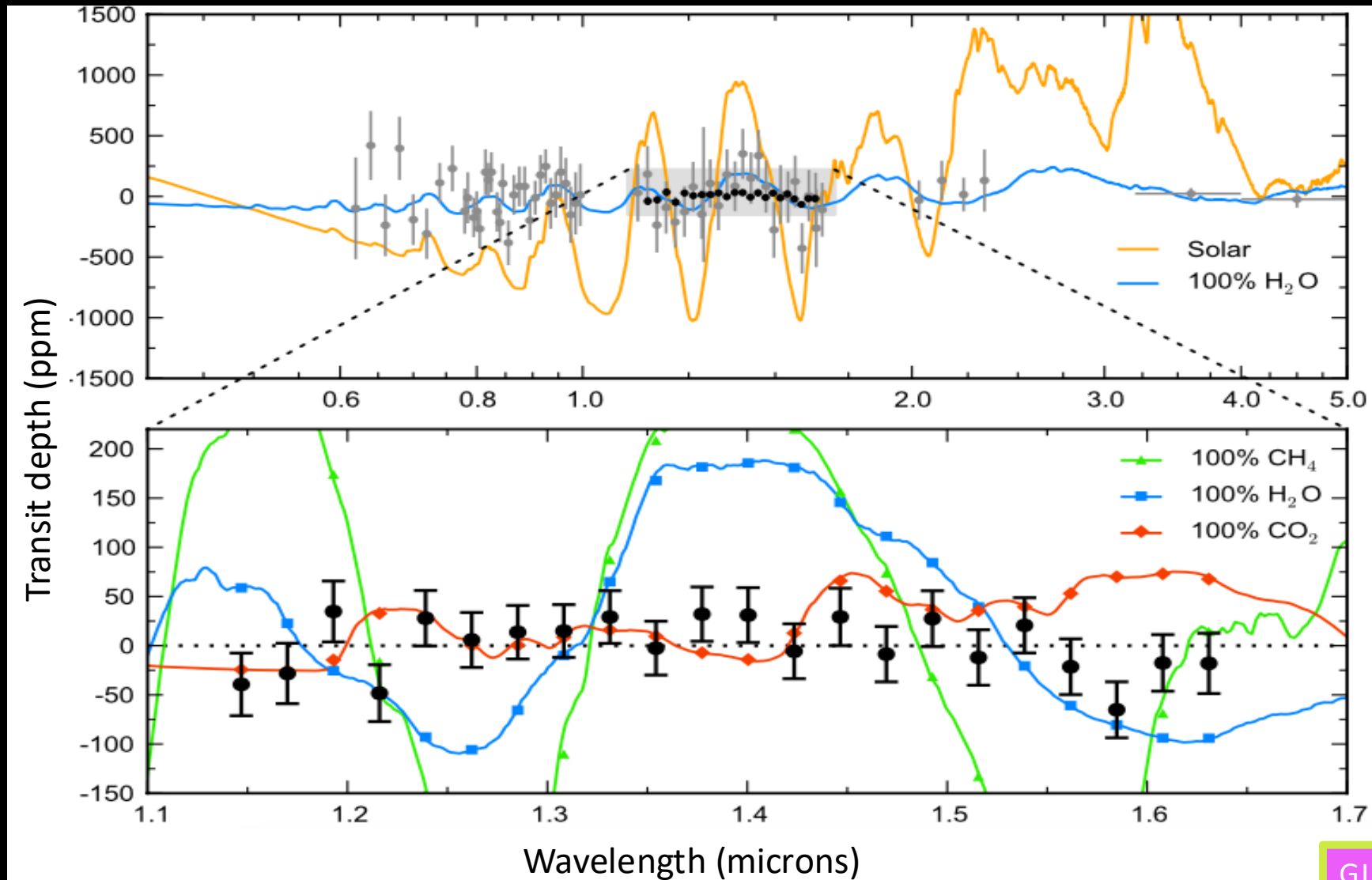
"Quenched", i.e.,
condensed and
supercooled **rapidly**



Crystallized, i.e., condensed and cooled
slowly

Cushing et al., *ApJ*, 2006

Clouds or hazes are some of the possibilities for our inability to see anything in some exoplanet atmosphere observations with telescope observations...



Kreidberg et al., *Nature*, 2014

GJ 1214b – a warm sub-Neptune (500K; 2.7 R_⊕)

Both haze and cloud **chemistry** and **morphology** can be constrained in the lab, which feeds into models, which is how we interpret observations

Haze



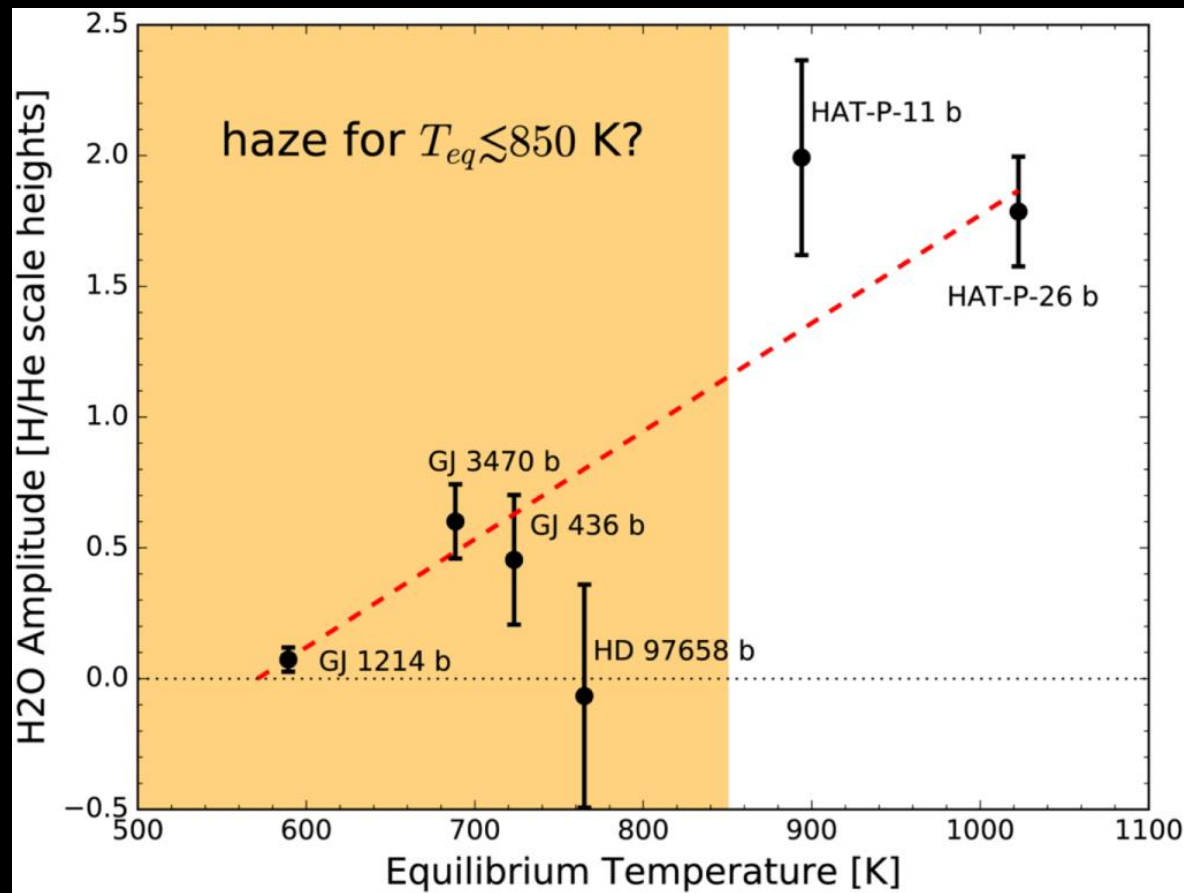
Clouds



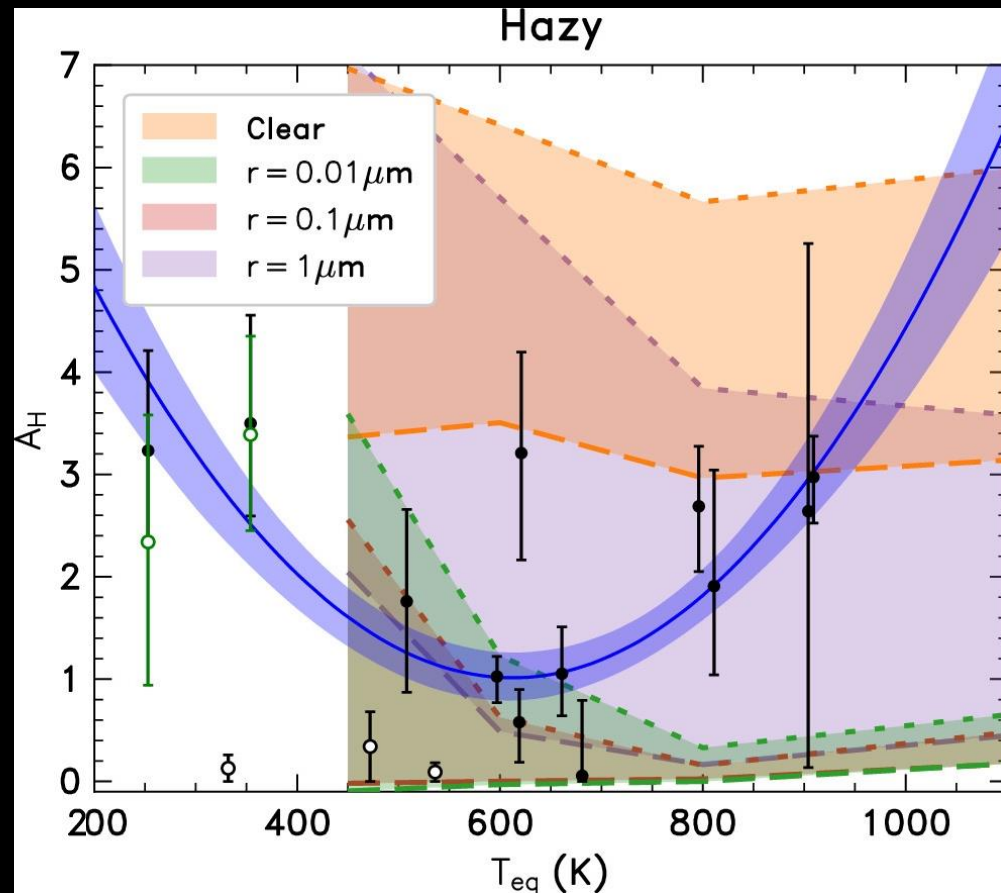


Haze: *Chemistry*

The shift to a haze-dominated regime *might* be due to methane being the major carbon reservoir at cooler temperatures



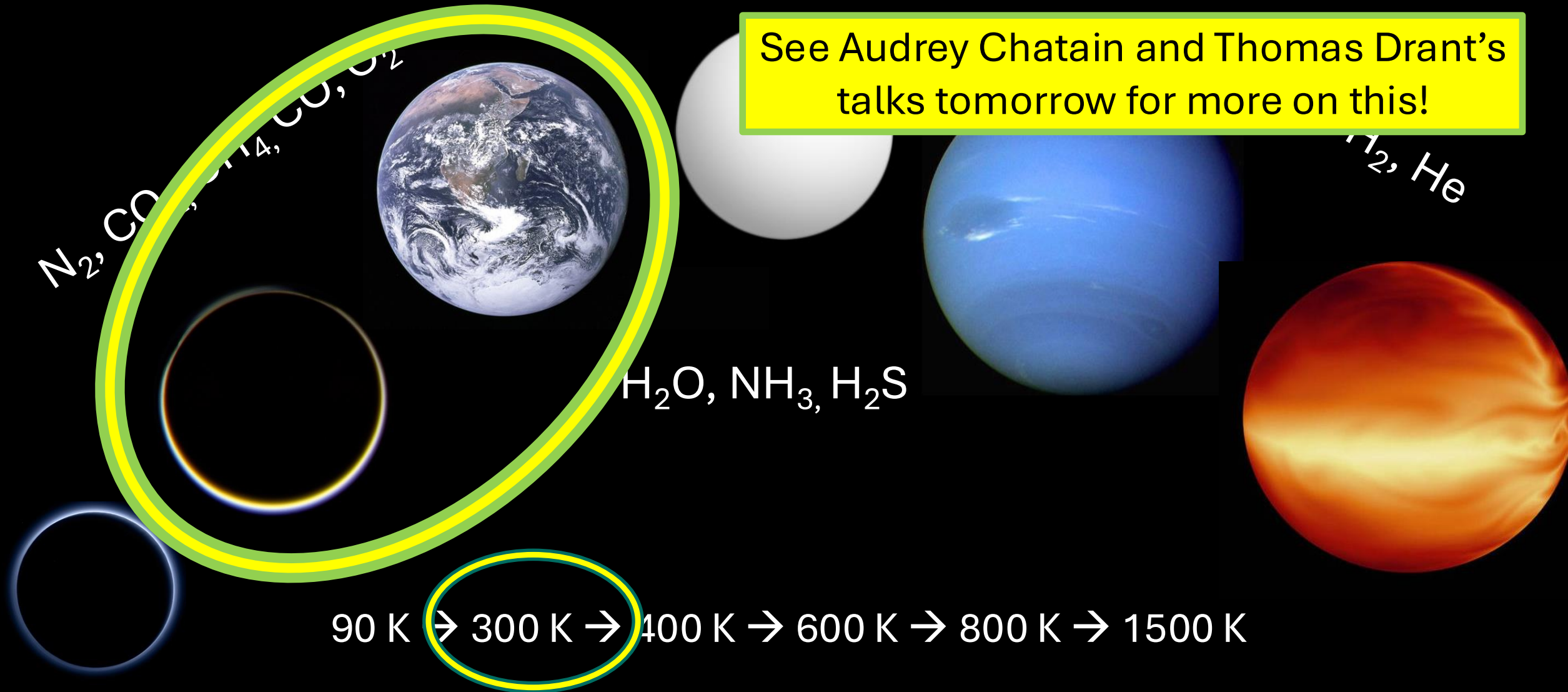
Crossfield & Kreidberg, *AJ*, 2017



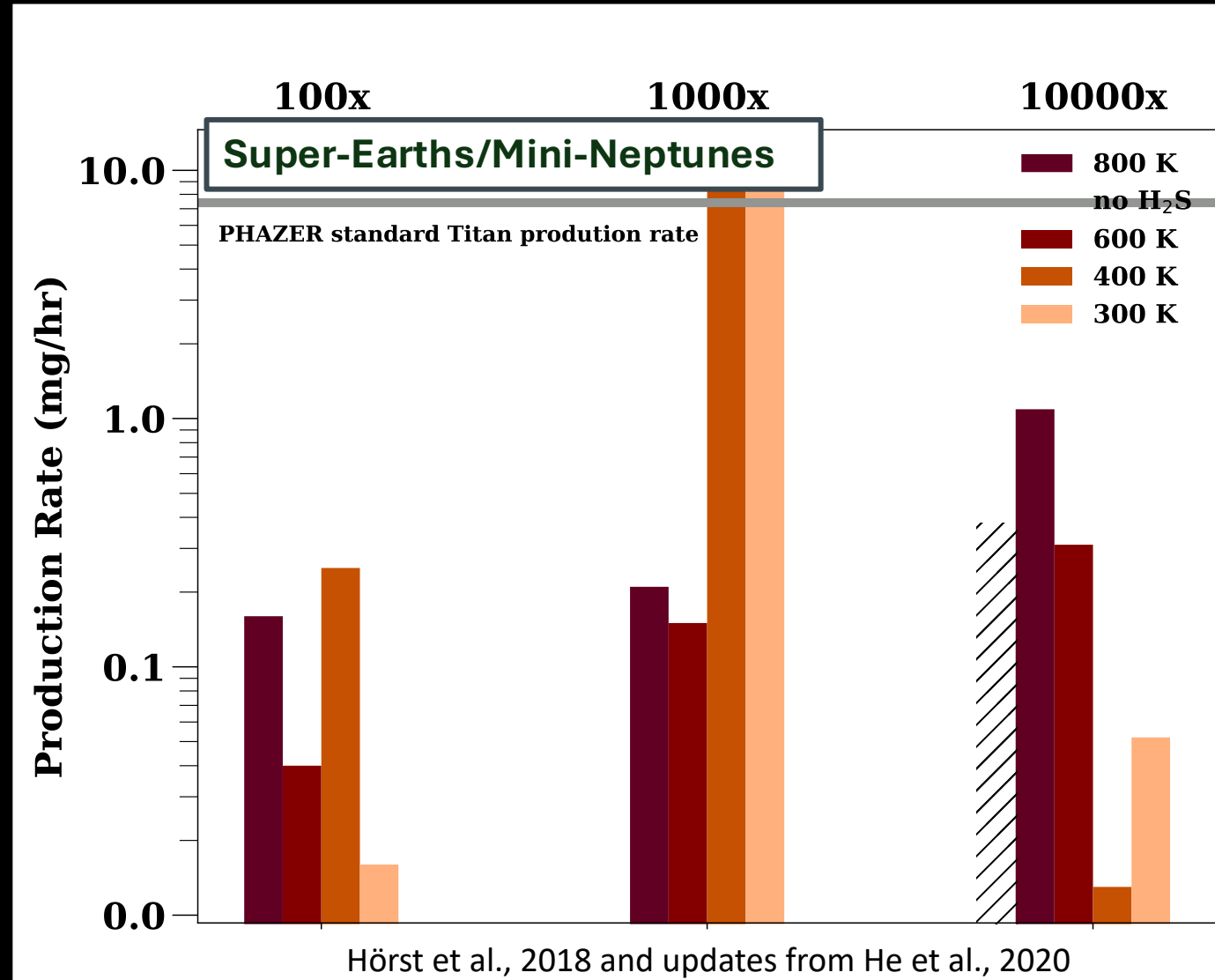
Brande et al., *ApJL*, 2024

solar system lab studies and exoplanet lab studies are complementary

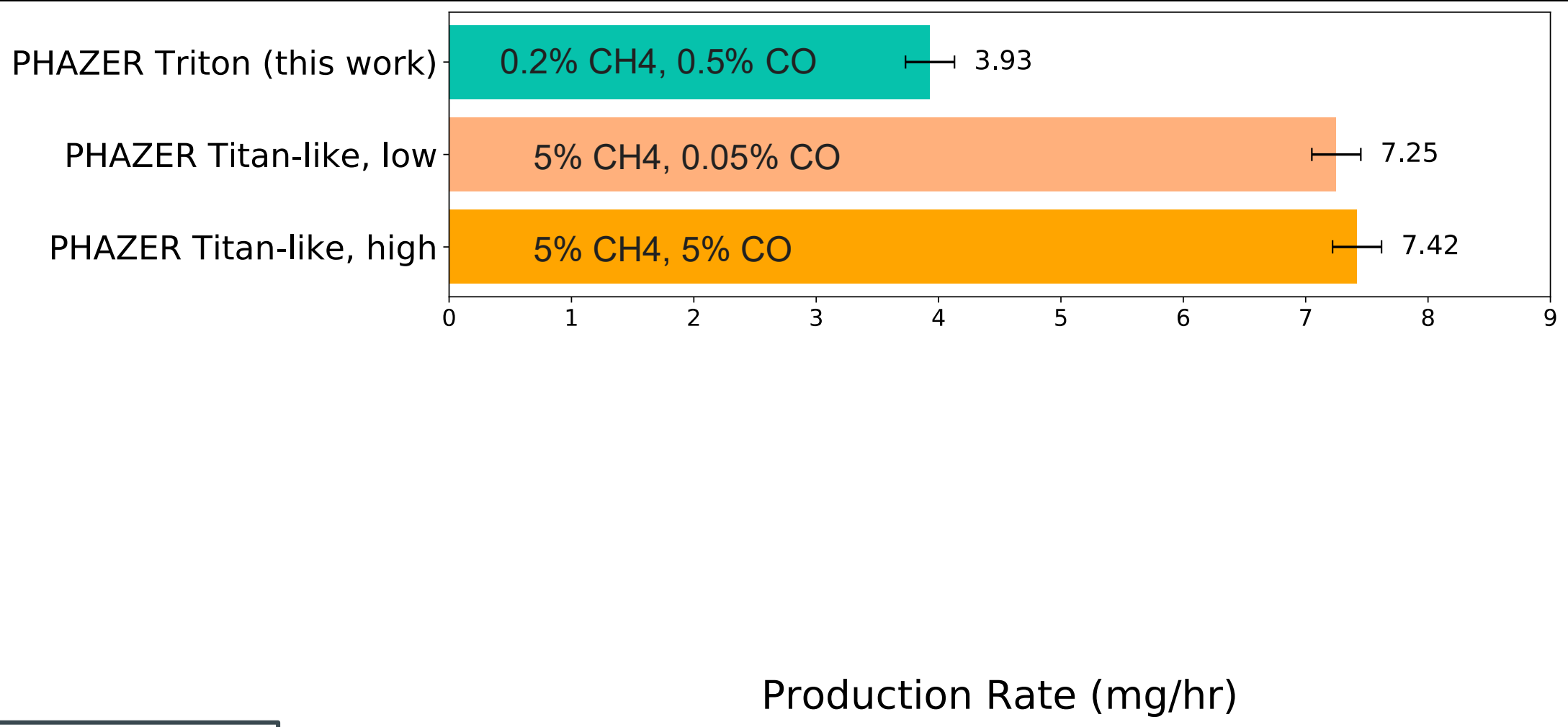
See Audrey Chatain and Thomas Drant's talks tomorrow for more on this!



The amount of haze produced varies by composition

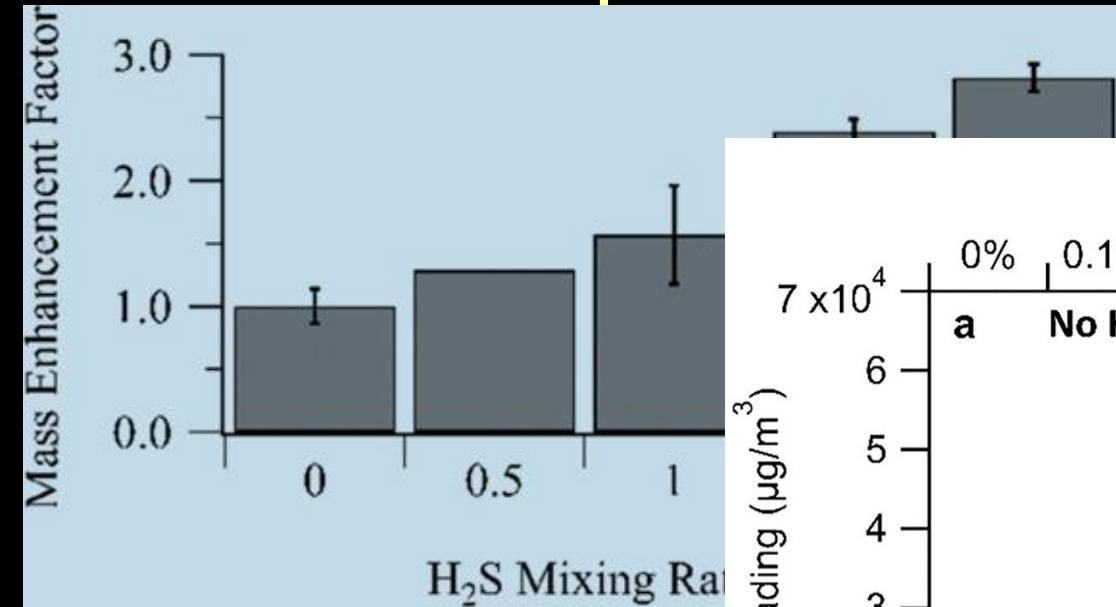


CH₄ drives haze formation, but it's *not* the only formation pathway



Hydrogen sulfide increases haze production in diverse atmospheres

N₂/CH₄/H₂S Atmospheres

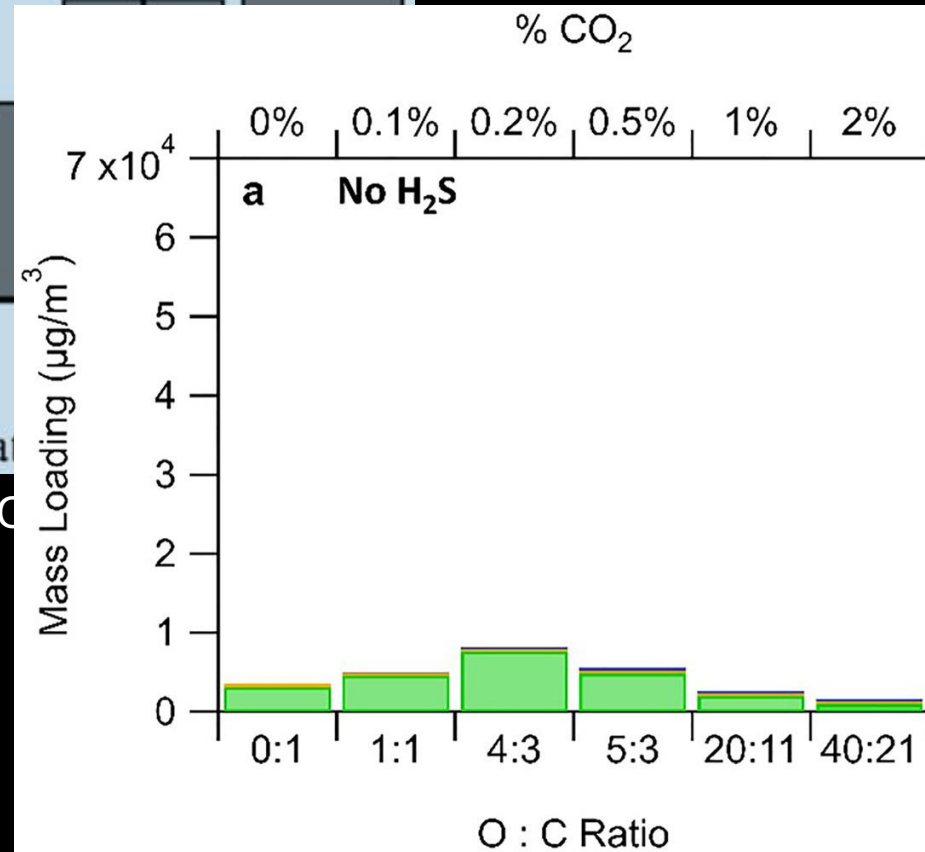


Reed et al., ACS Earth and Space Chemistry

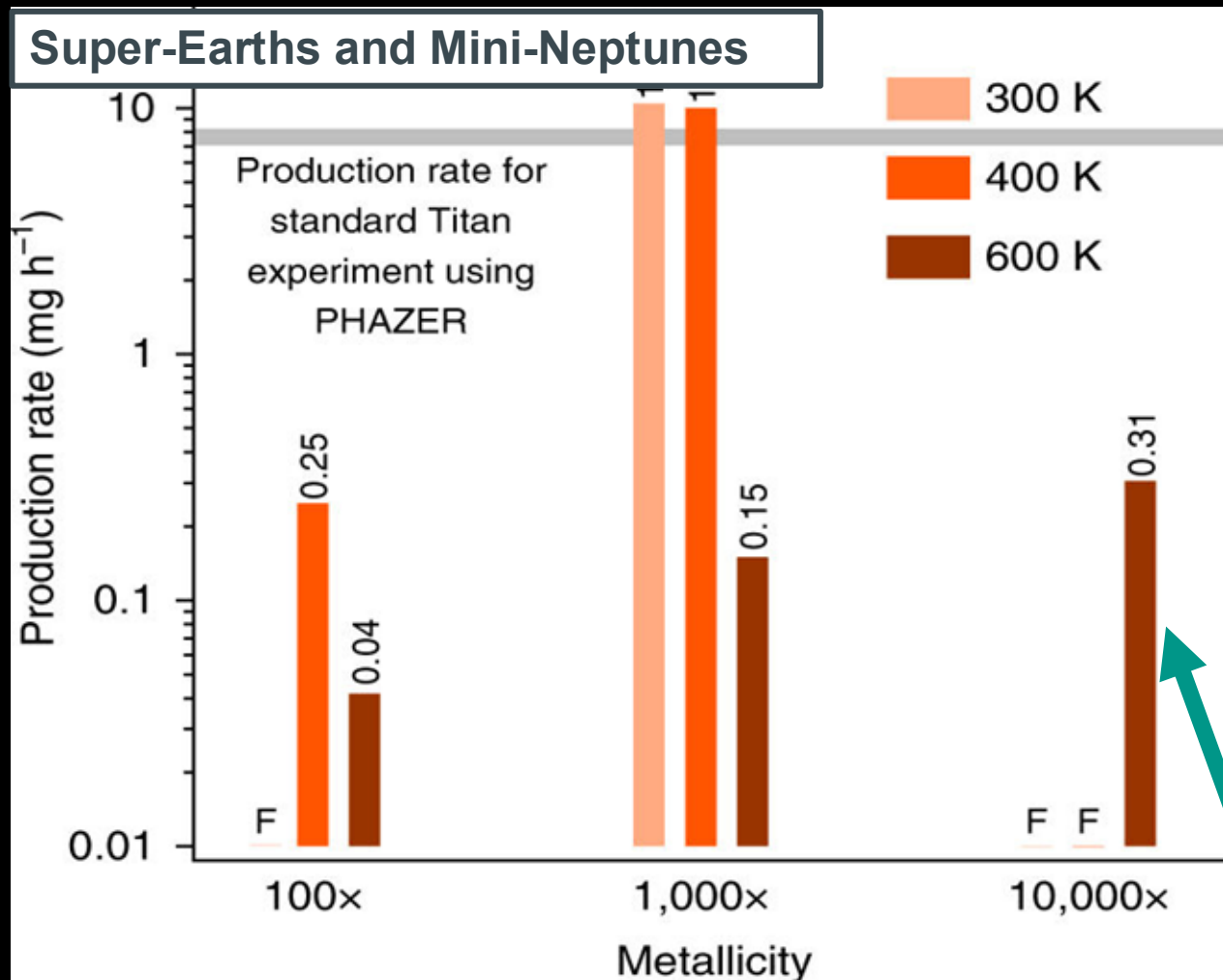
Early Earth atmospheres

(Adapted from) Reed et al., GRL, 2022

N₂/CH₄/CO₂/H₂S Atmospheres



Exoplanet lab haze studies show us that methane doesn't need to be present to drive haze formation



Hörst et al., *Nature Astronomy*, 2018

Hot Jupiter-like Atmospheres



Blank



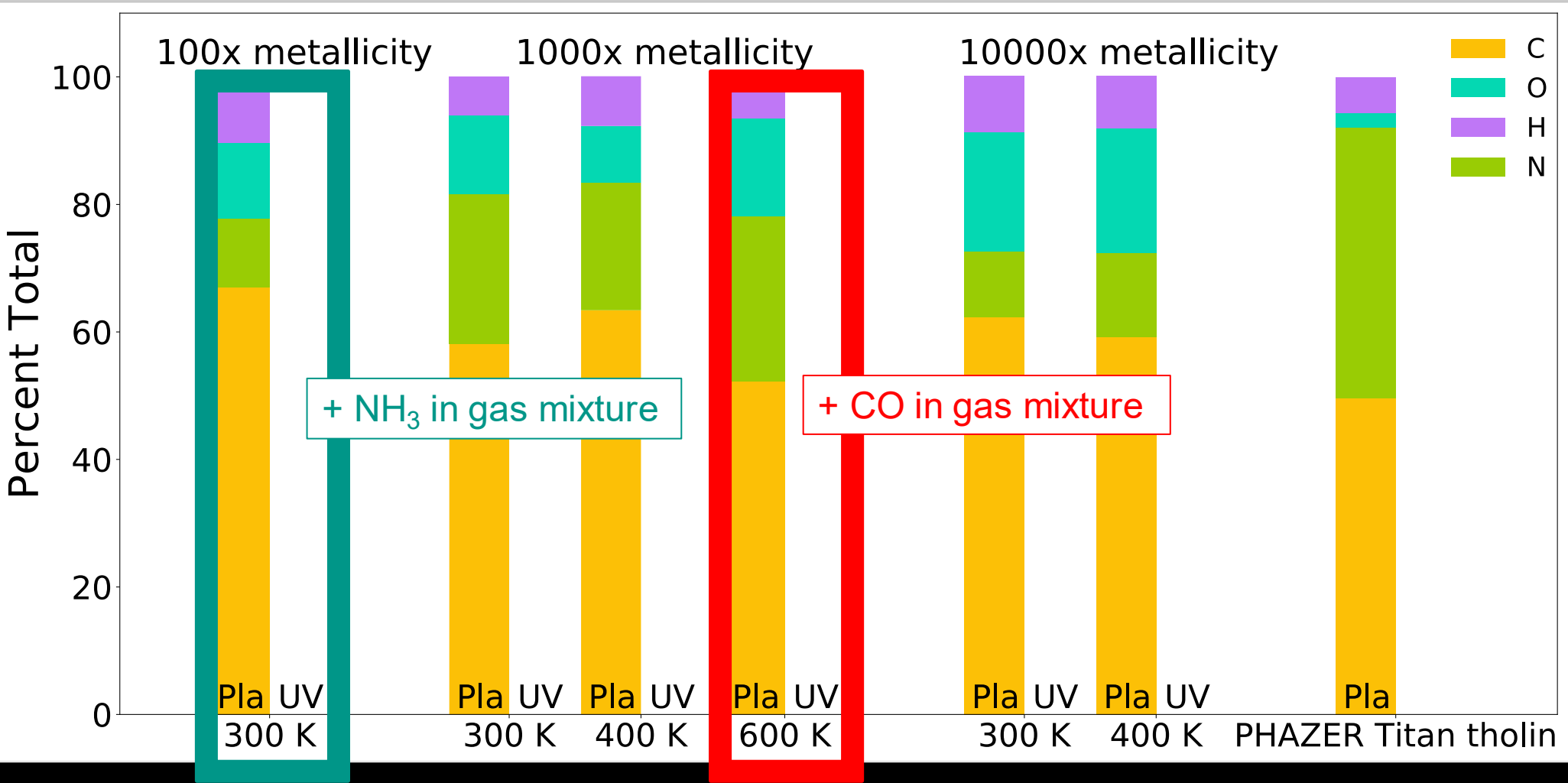
Sample 1

1473 K, H_2/CO gas mix (99.7%/0.3%) under Ly-alpha

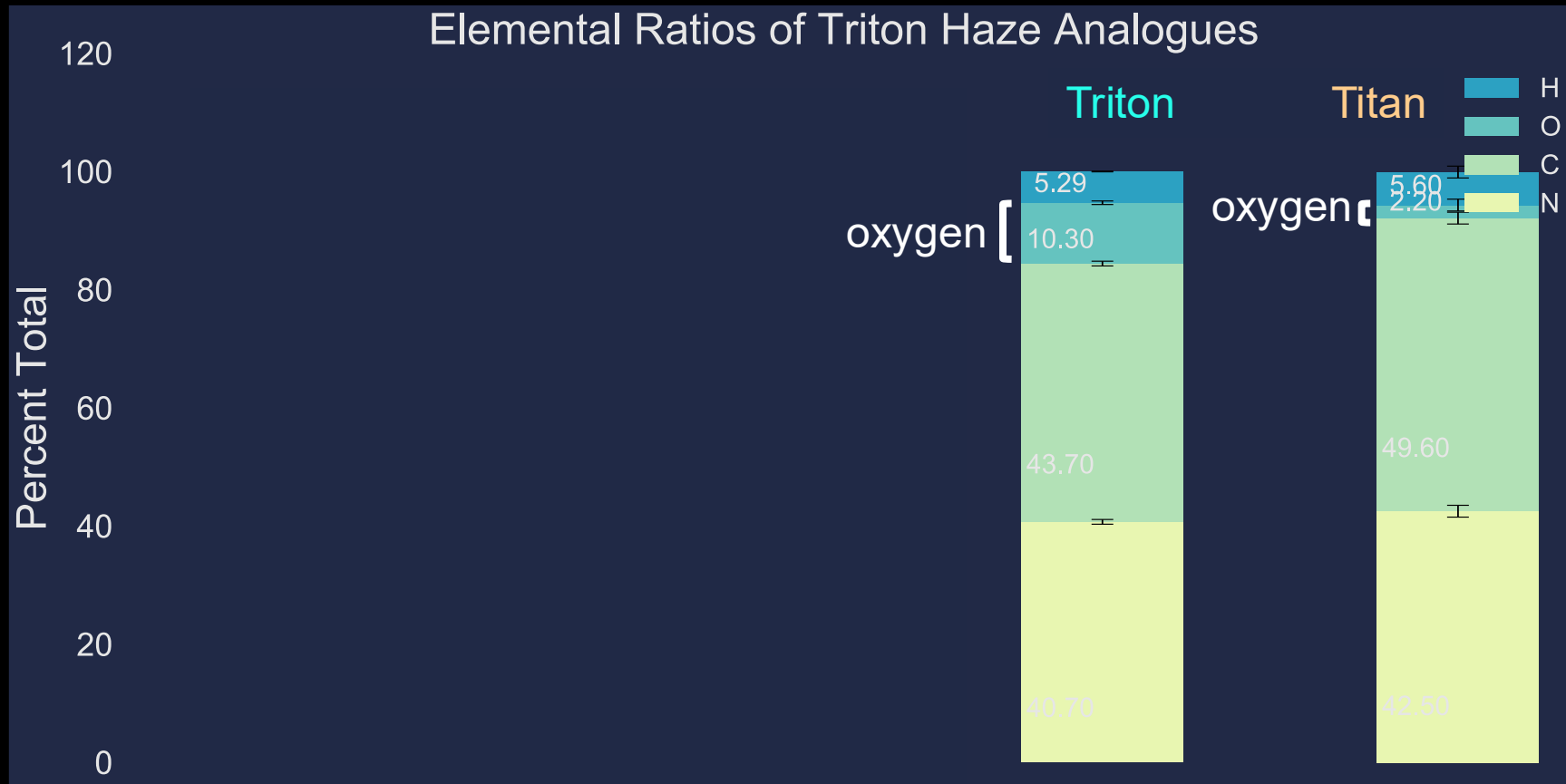
Fleury et al., *ApJ*, 2019

Only contained CO not CH_4 !

Composition of the solid is not straightforward – tiny changes in the amount and kind of molecule participating in haze formation matters



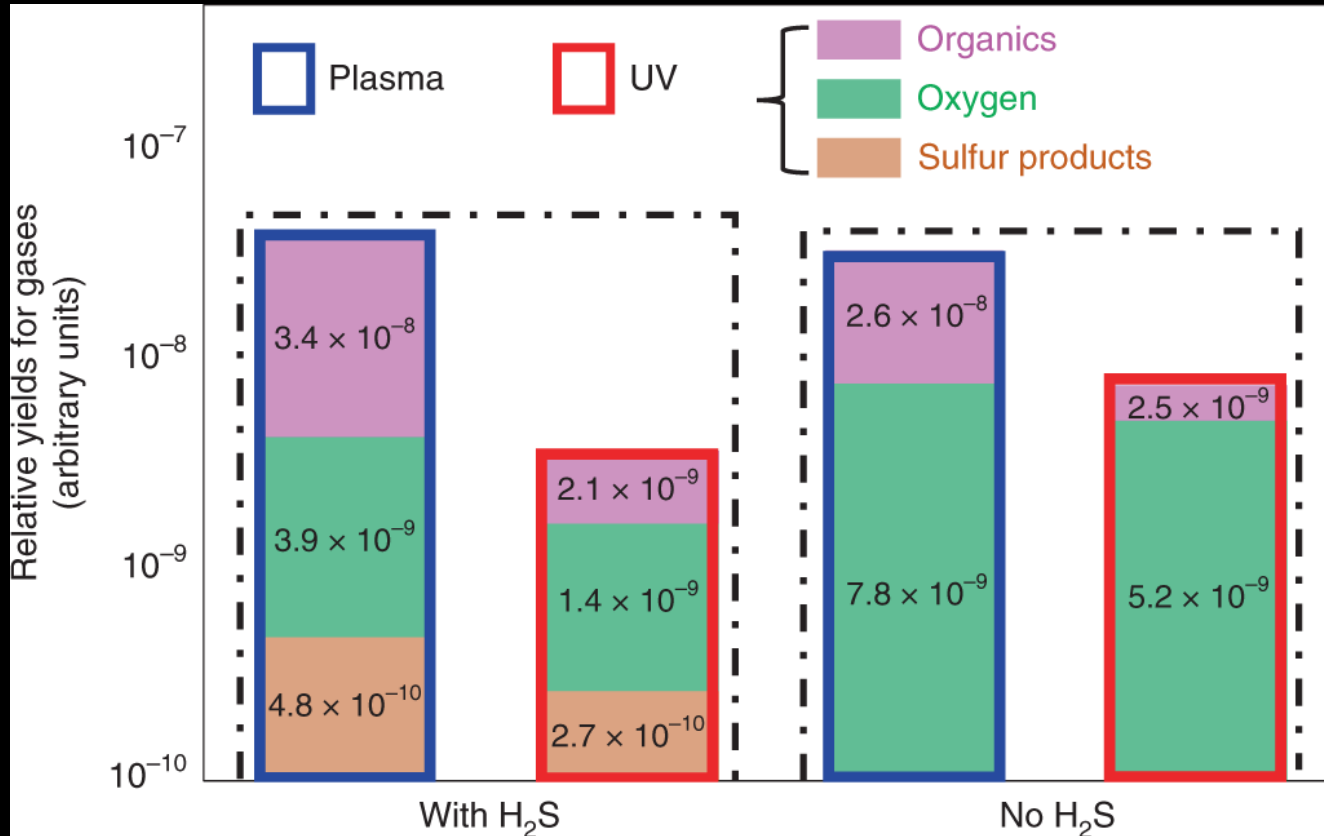
When $\text{CO} > \text{CH}_4$, oxygen is much more strongly incorporated to the solid particles



Moran et al., *JGR— Planets*, 2022

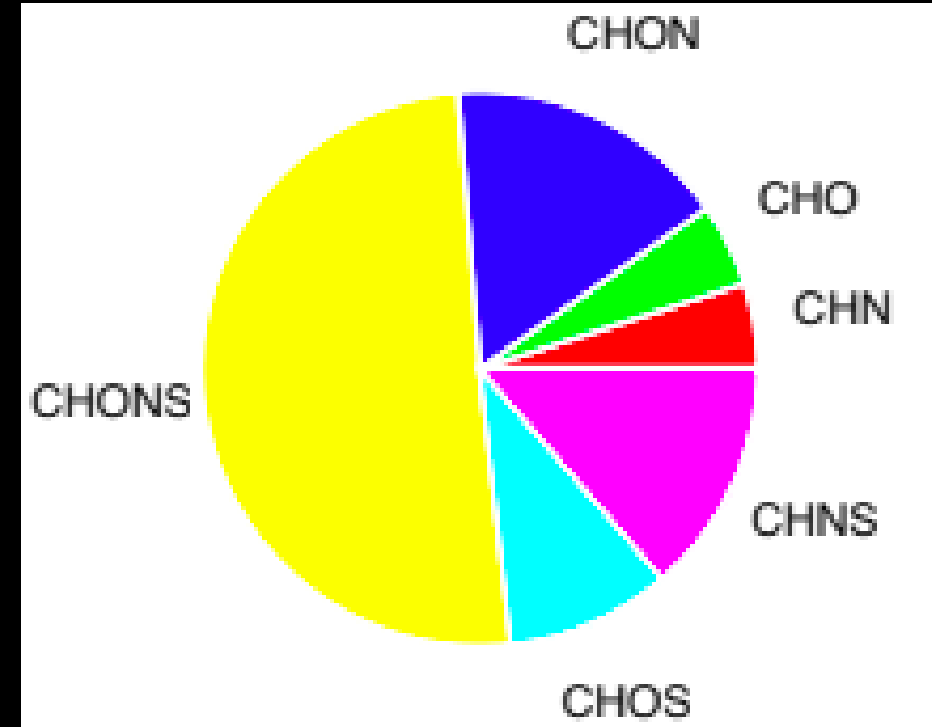
Trace species reactants in the gas phase are critical for ultimate haze composition

Gas Phase Products, measured with RGA



He et al., *Nature Astronomy*, 2020

Solid Products, measured with MS

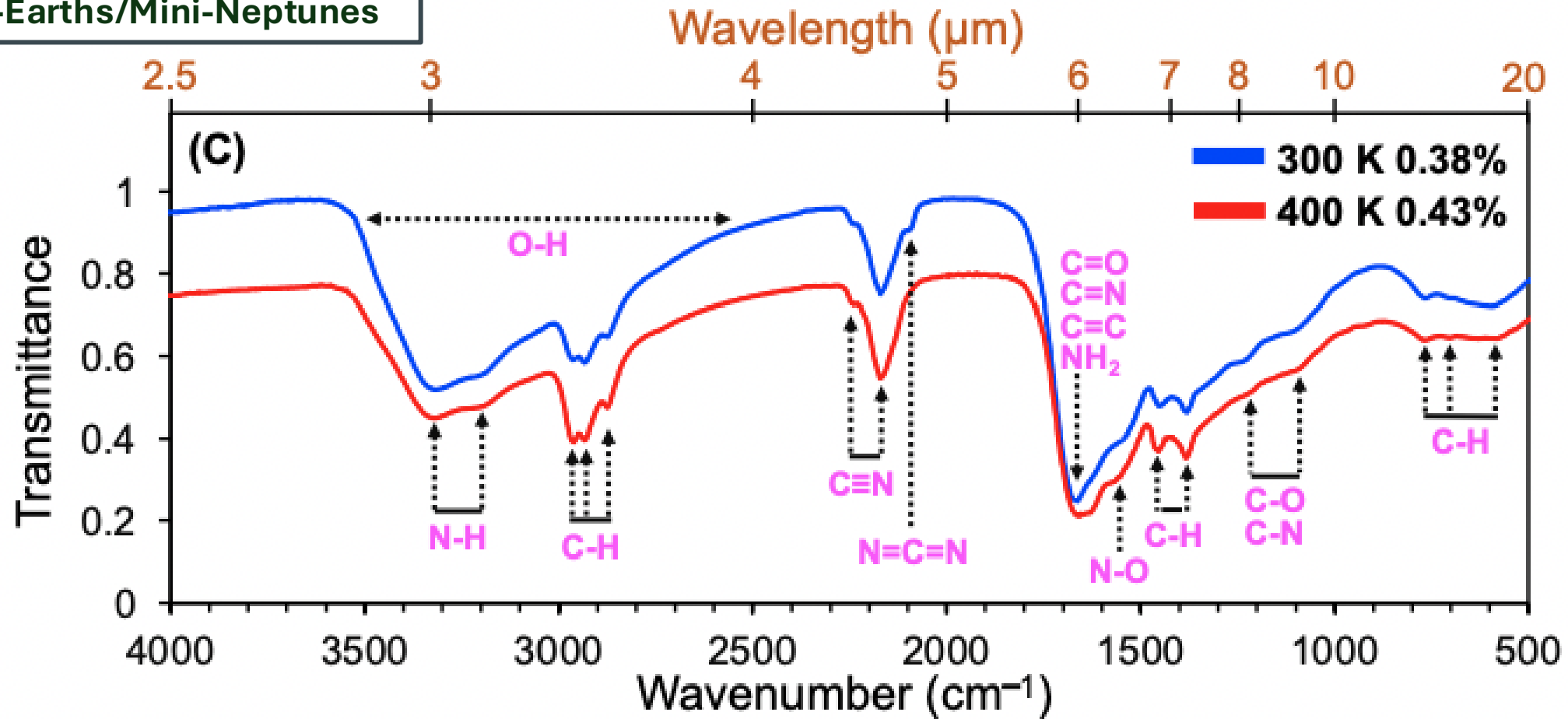


Vuitton, Moran et al., *PSJ*, 2021

Both oxygen and sulfur are readily incorporated into the haze solids!

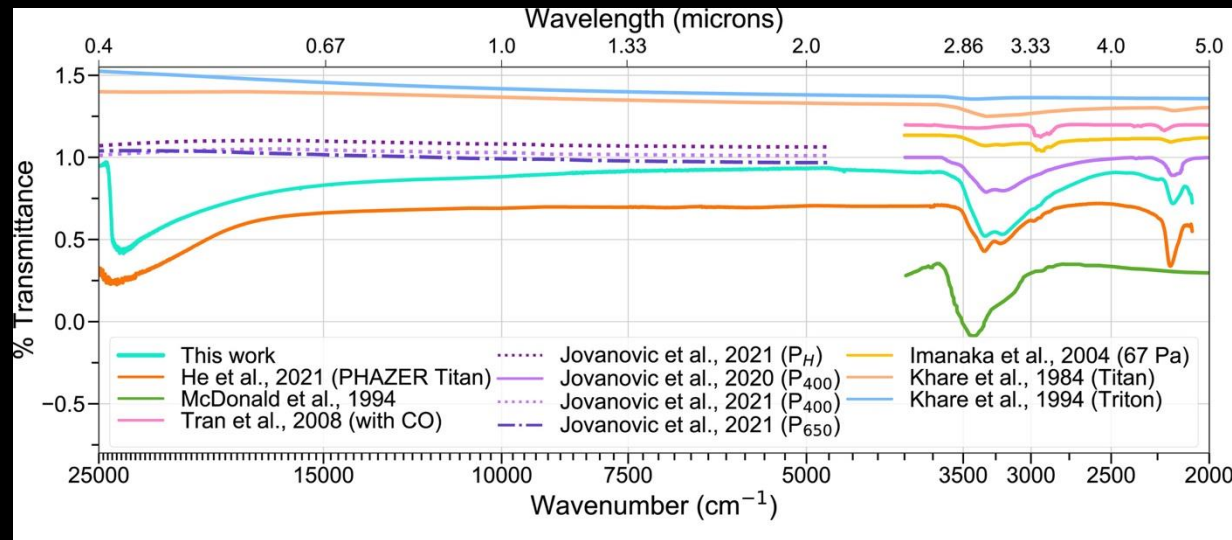
NIR-MIR spectroscopy corroborates mass spectrometry results on the functional groups that make up the haze particles

Super-Earths/Mini-Neptunes

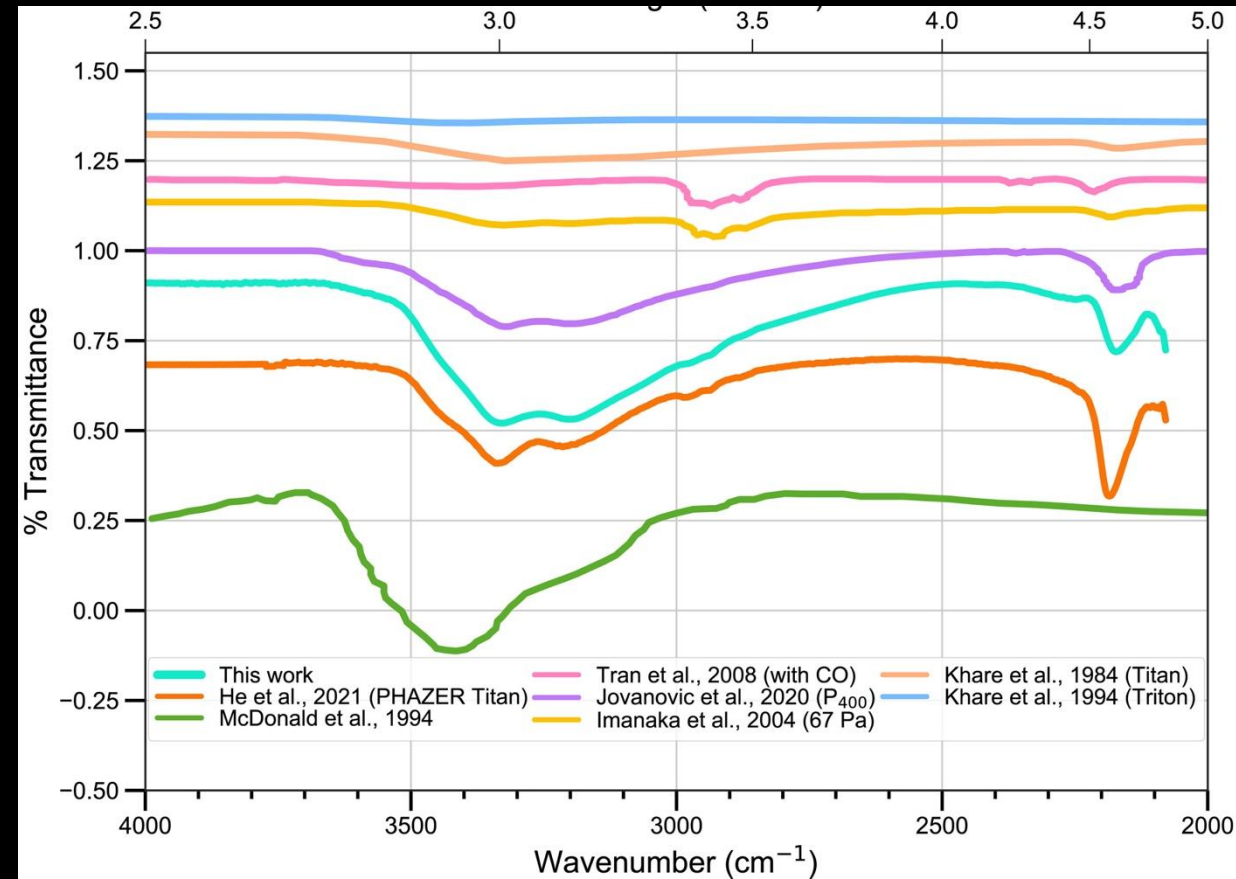


He, Radke, Moran, et al., *Nature Astronomy*, 2024

NIR-MIR spectroscopy corroborates mass spectrometry results on the functional groups that make up the haze particles



Titan, Triton, and Pluto



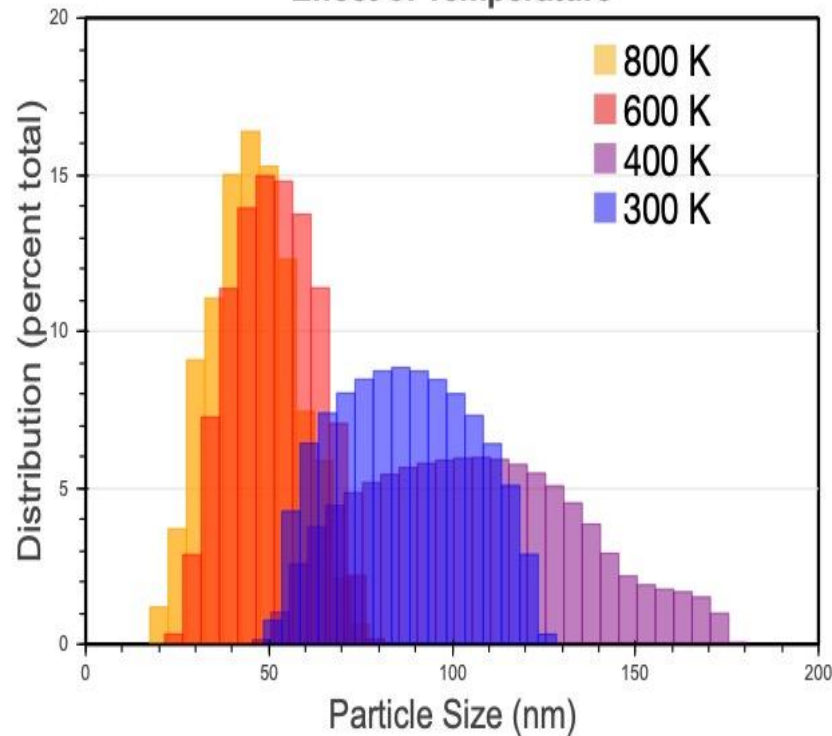


Haze: *Morphology*

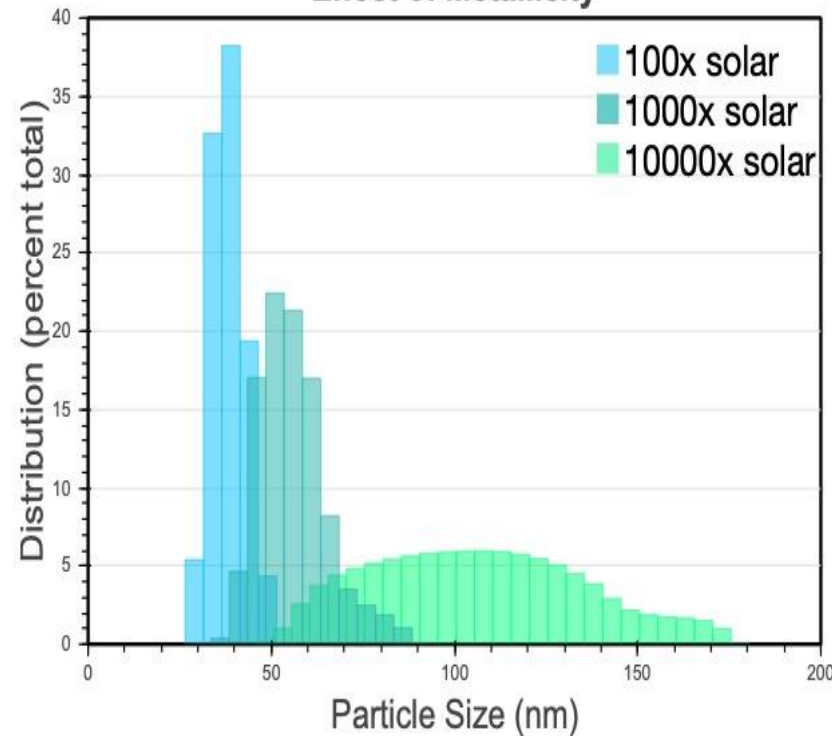
Haze particle sizes from the lab vary, but they're all small enough for Rayleigh scattering...

Super-Earths and Mini-Neptunes

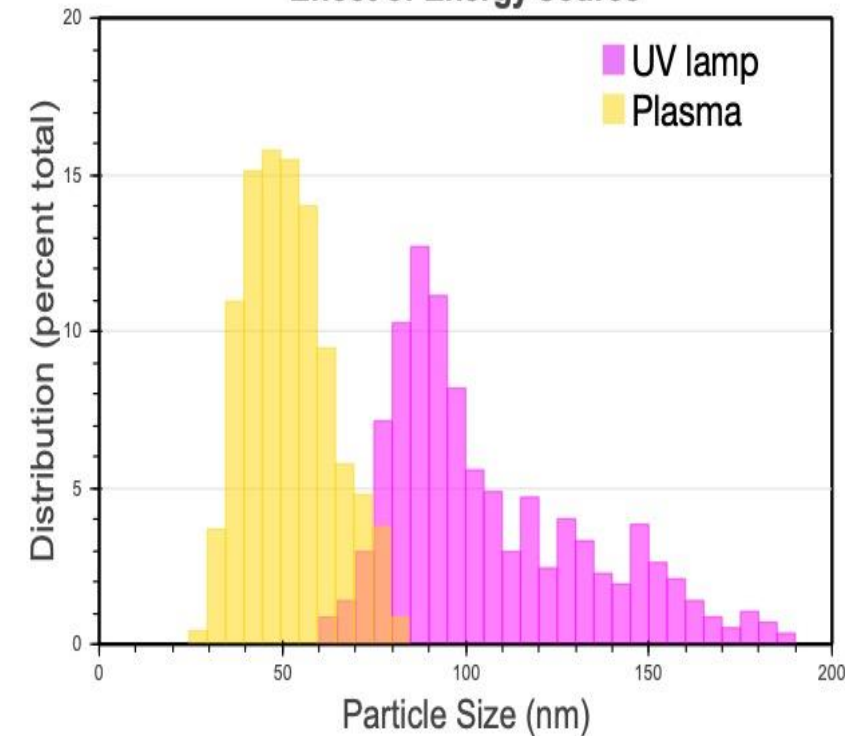
Effect of Temperature



Effect of Metallicity



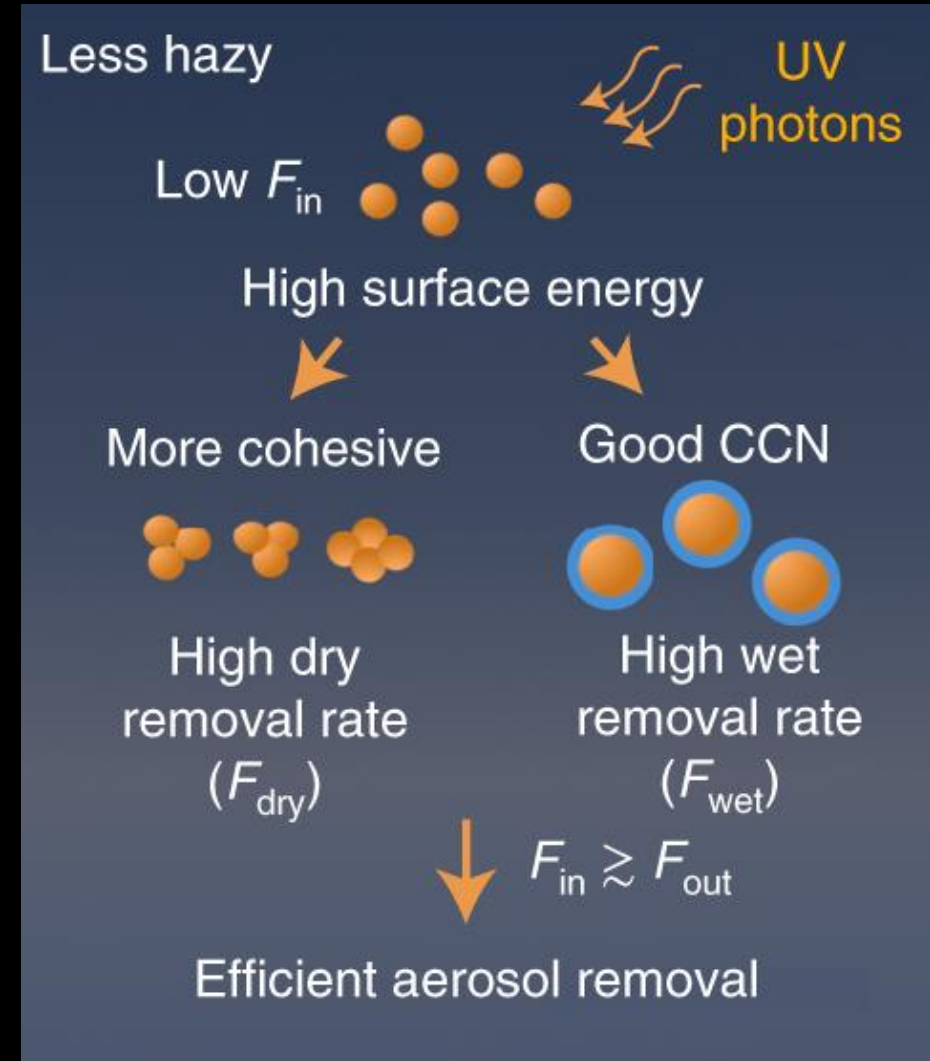
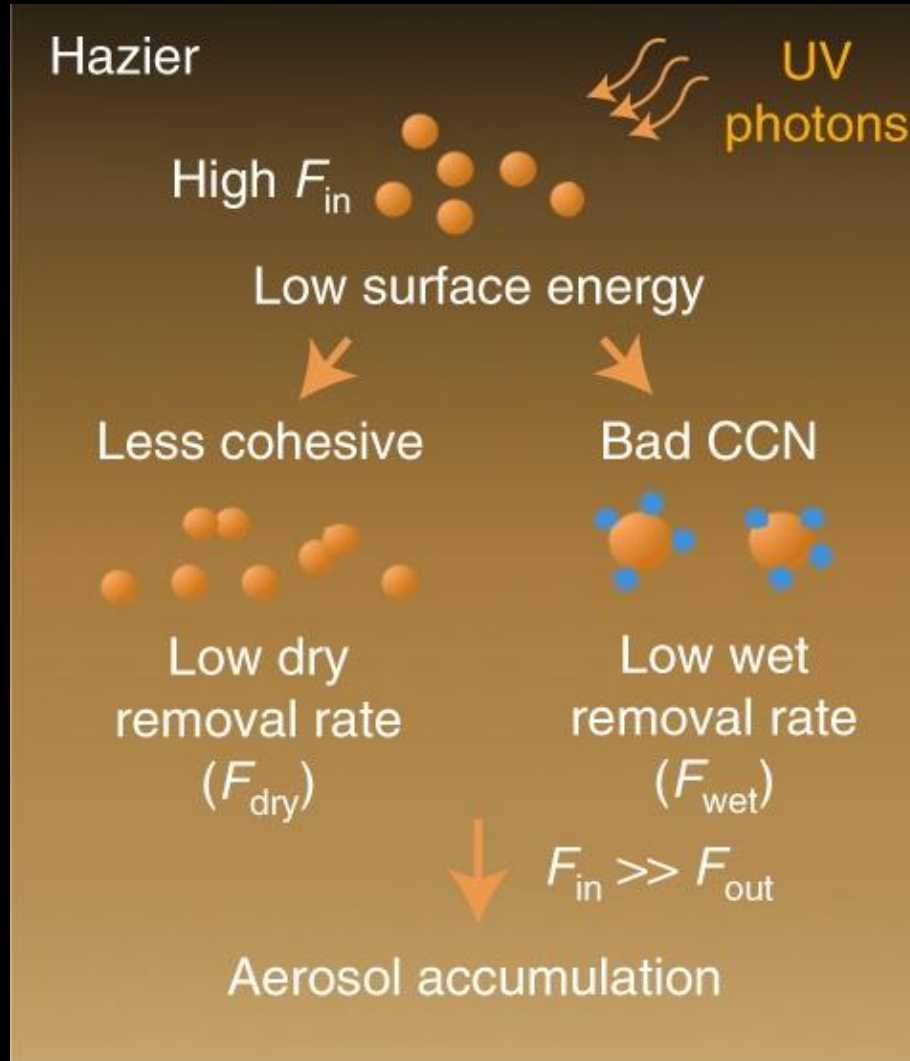
Effect of Energy source



Gao, Wakeford, Moran & Parmentier, *JGR – Planets*, 2021
(summarizing He et al., 2018a, 2018b, 2020a)

Material properties affect how aerosols evolve through the atmosphere: particles can be quite sticky and cohesive, which means they can easily get act as cloud condensation nuclei and/or conglomerate

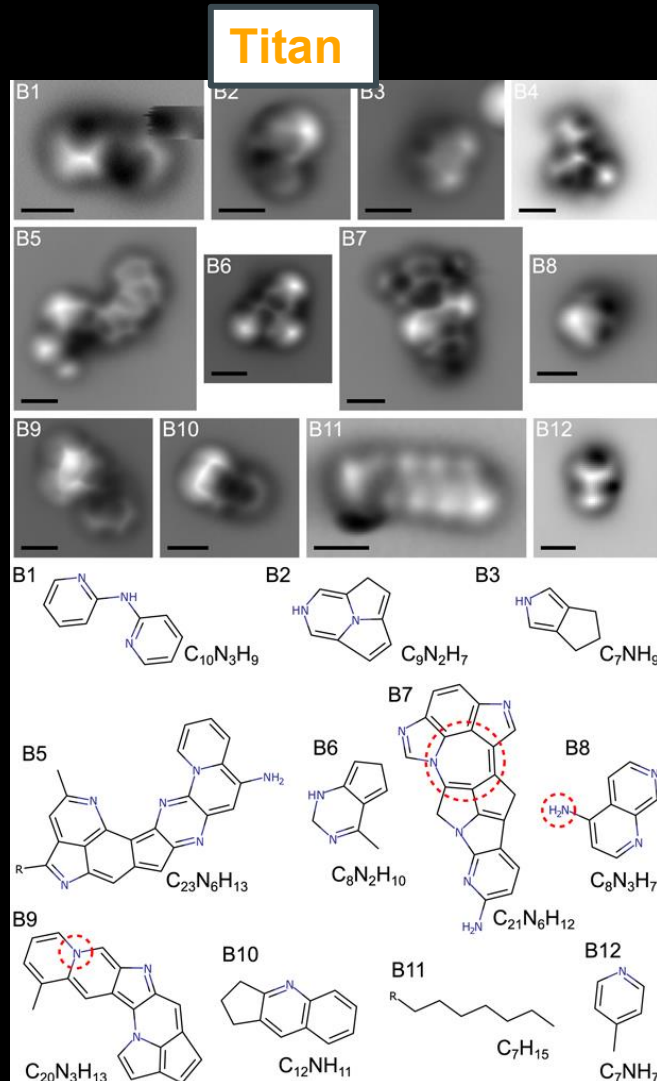
Super-Earths and Mini-Neptunes



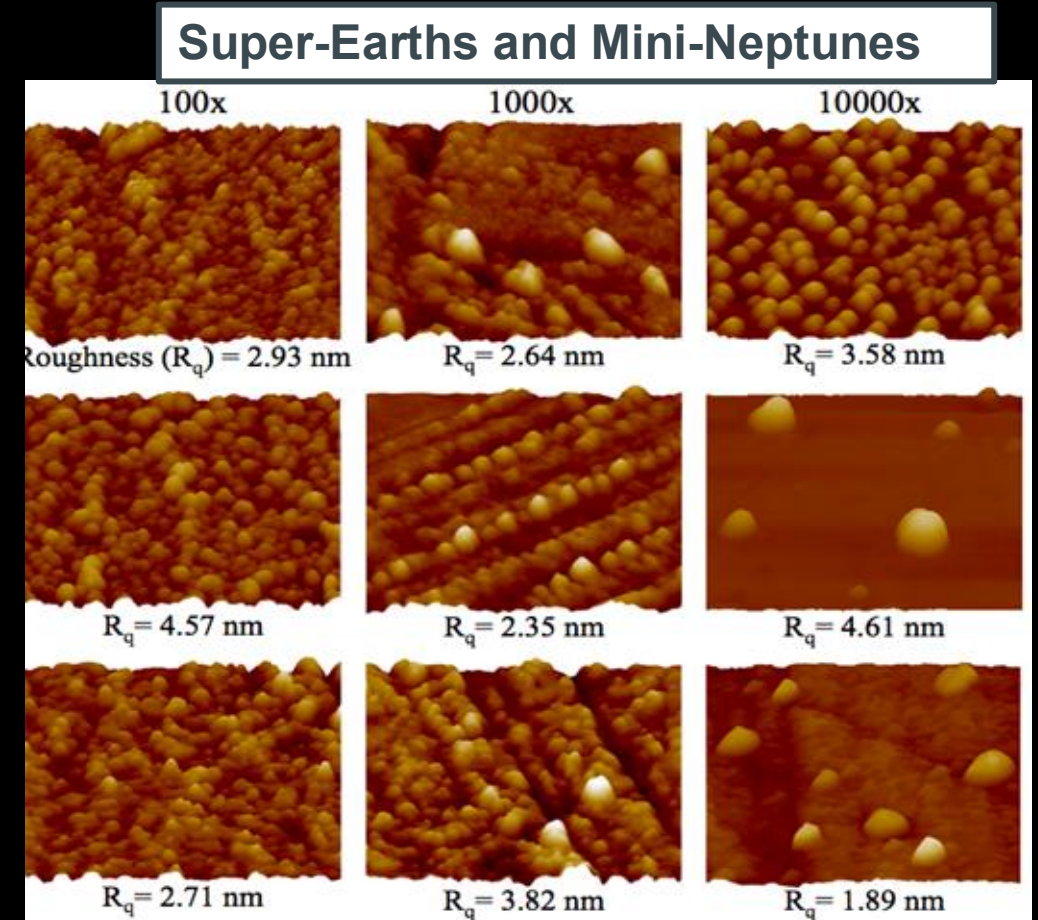
Yu et al., *Nature Astronomy*, 2021

see also
Pesciotta et
al., *ApJ*, 2026;
Huseby et al.,
PSJ, 2026

These material properties controlling particle size and shape often result in *non-spherical particles*



Schulz et al., ApJL, 2021

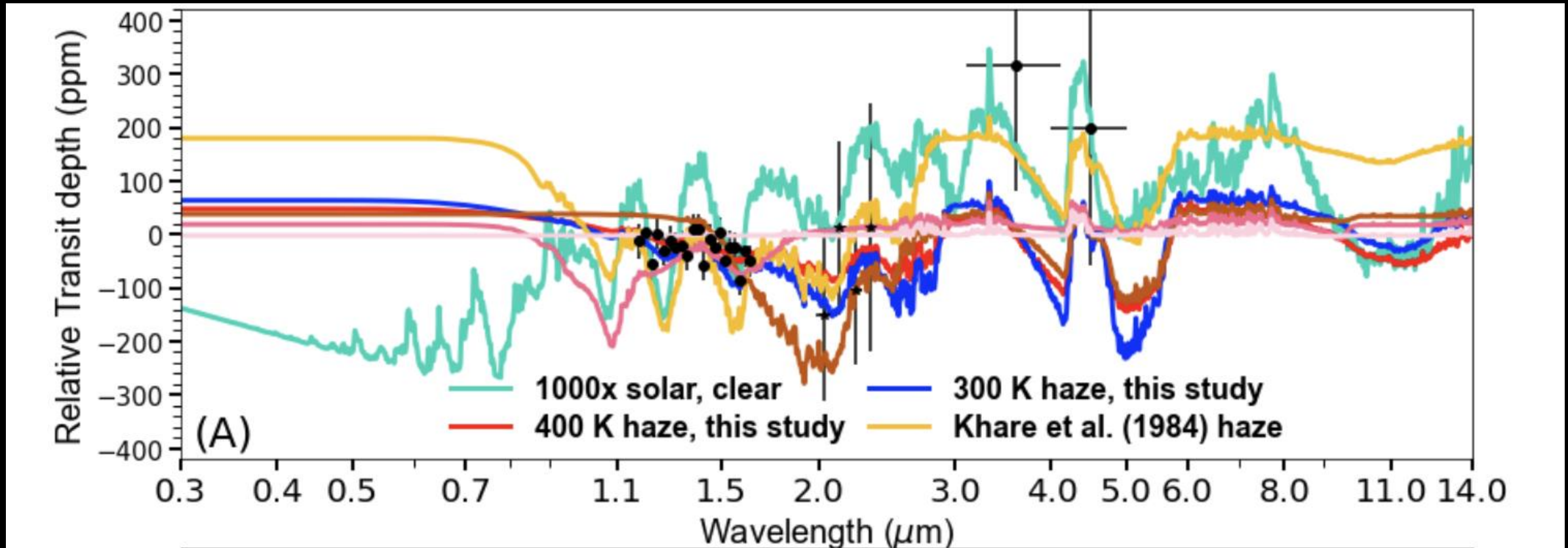


He et al., AJ, 2018



Haze:
Composition & Morphology
→ *Remote Sensing*

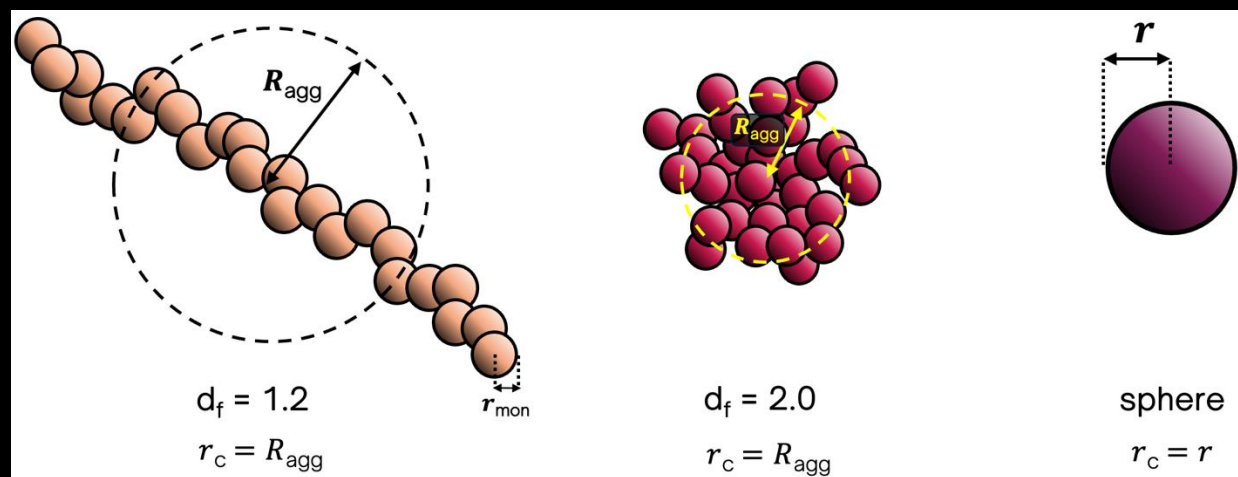
Composition via optical properties and particle sizes (via production and growth) are both needed to produce atmospheric spectral models to compare to observations



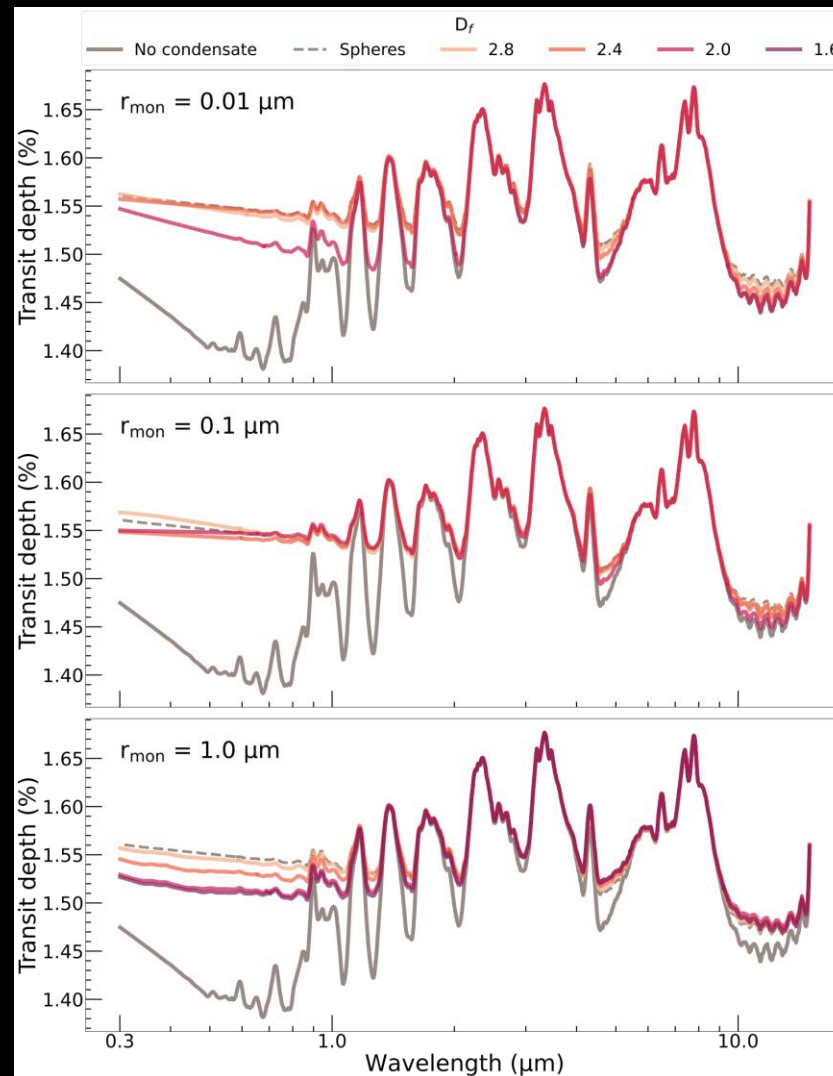
Mie theory!
only spherical
particles

He, Radke, Moran, et al., *Nature Astronomy*, 2024
(along with results of Corrales et al., *ApJL*, 2023 in pink colors)
also more now out from Thomas Drant, talking tomorrow! ☺

Hazes' size and shape can be better modeled by *fractal aggregates* in atmospheric spectral models to compare to observations

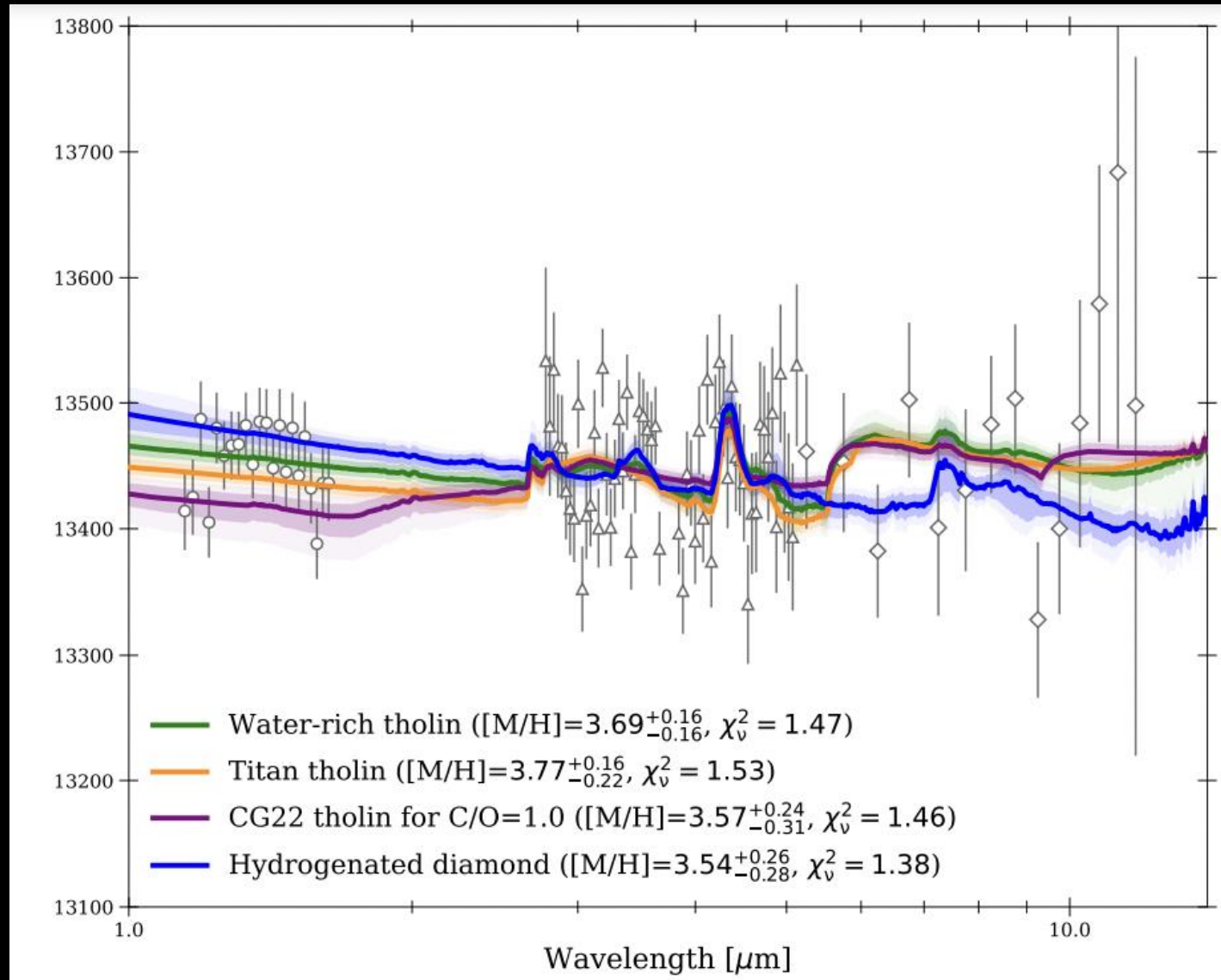


Moran & Lodge et al, *ApJ*, 2025
Lodge & Moran et al, *ApJ*, 2026



see also Ohno et al 2020; Samra et al 2022, Vahidinia et al 2024

JWST NIRSpec seems to break through the haze. Very high metallicity atmosphere –haze features are suppressed and high SNR needed

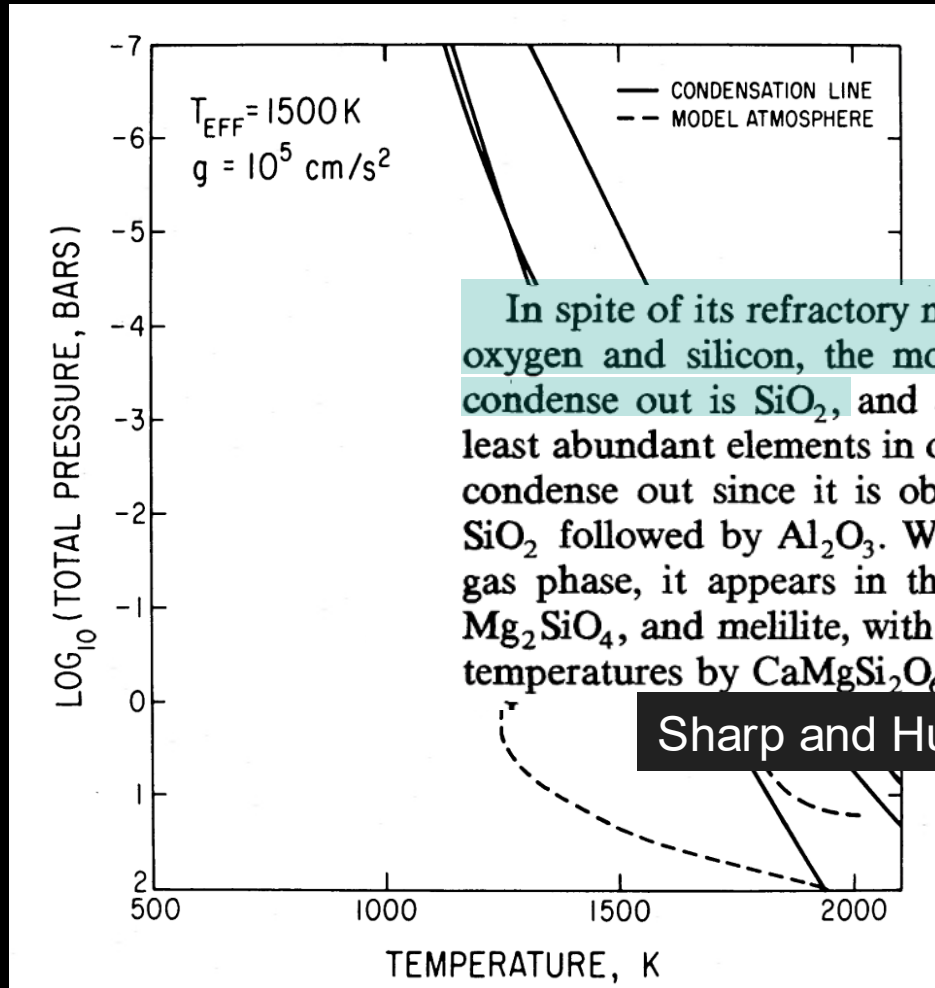


see also Ohno et al., 2024;
Schlawin et al., 2024

An aerial photograph showing a vast expanse of white, fluffy clouds over a deep blue ocean. The clouds are dense and cover most of the frame, with some darker blue patches of water visible between them. The sky above the clouds is a clear, light blue. The overall scene is bright and airy, suggesting a high-altitude or satellite perspective.

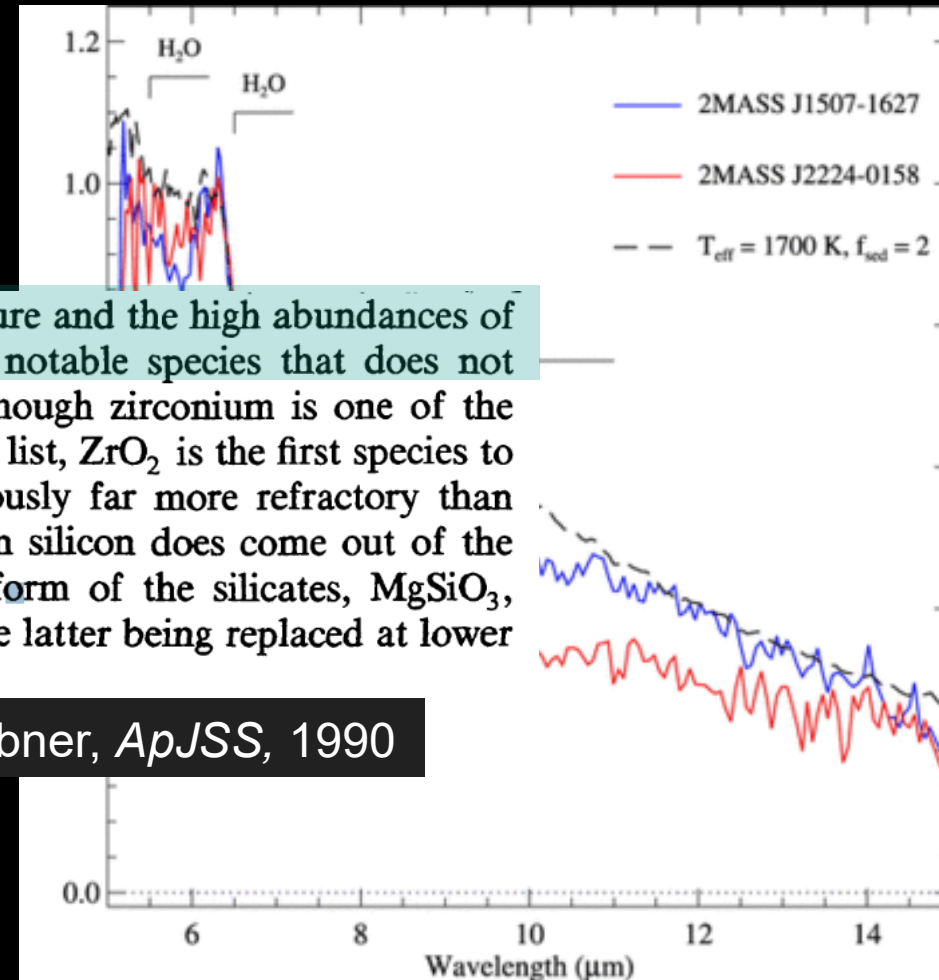
Clouds: *Chemistry*

Spitzer provided *observational* confirmation that L-dwarf clouds were likely composed of silicates, long expected by theory



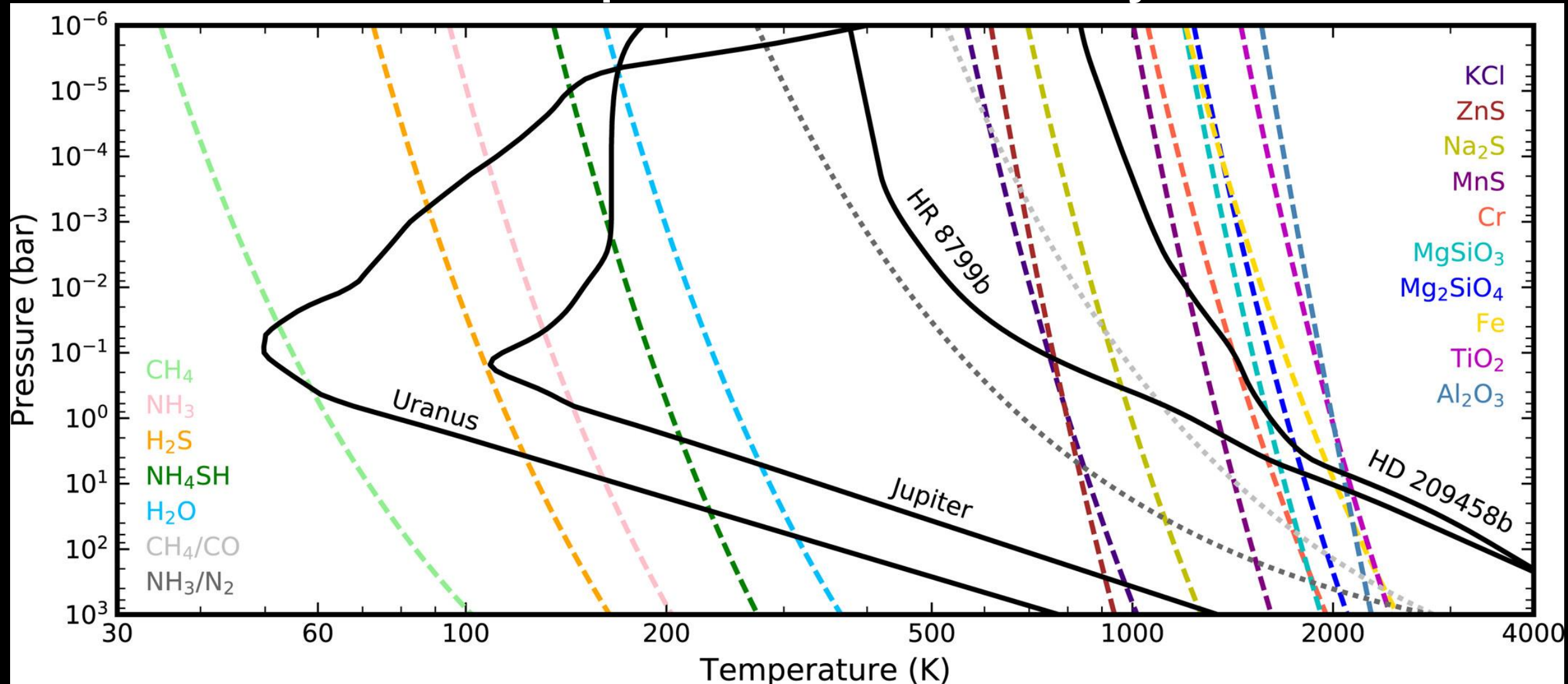
Sharp and Huebner, *ApJSS*, 1990

Lunine, Hubbard, and Marley, *ApJ*, 1986



Burgasser et al., *ApJ*, 2008

Cloud condensation chemistry is highly diverse ~~but simpler than haze chemistry~~



Cloud condensation chemistry is highly diverse: heterogenous nucleation and metallicity dependent compositions

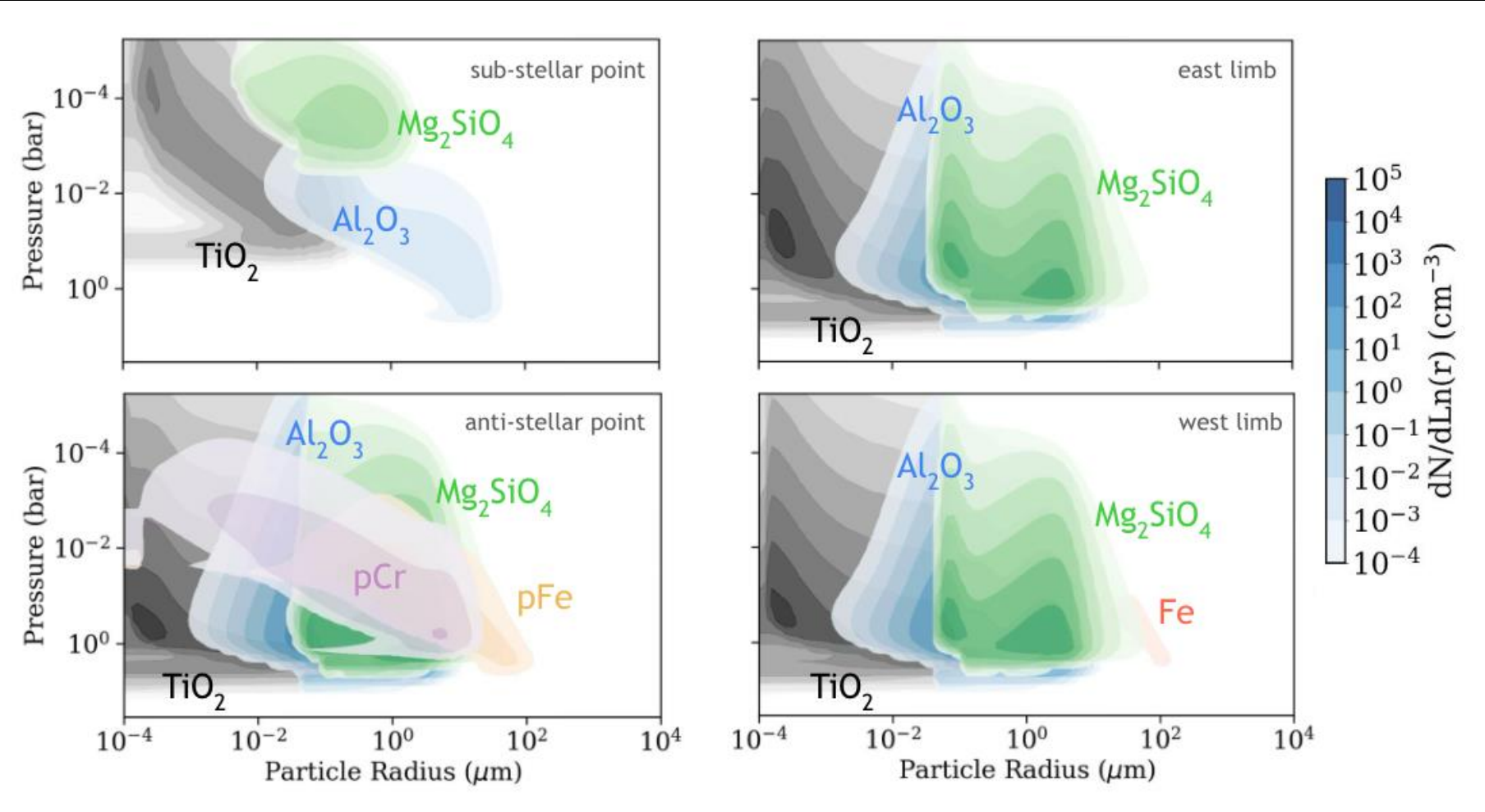


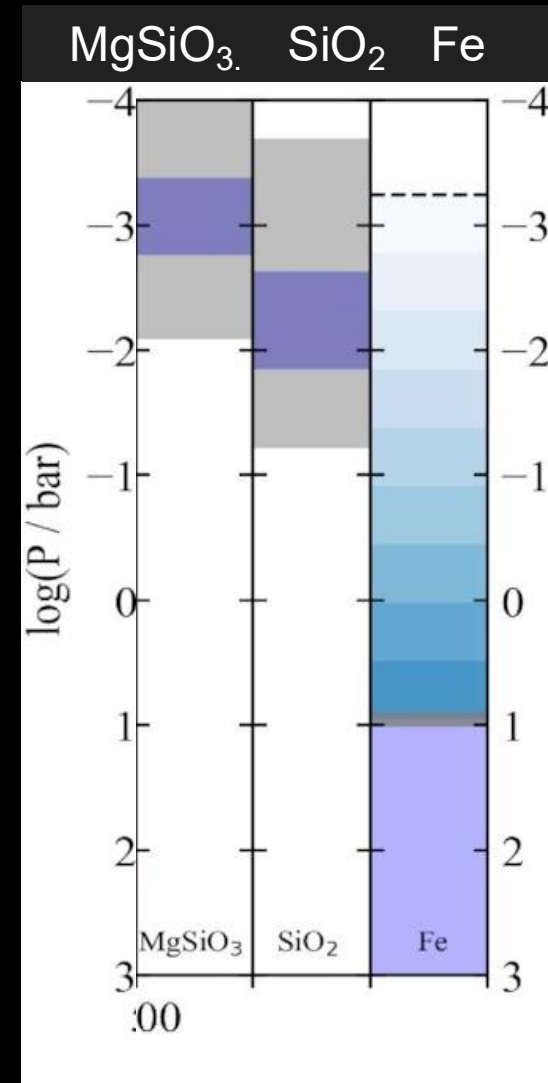
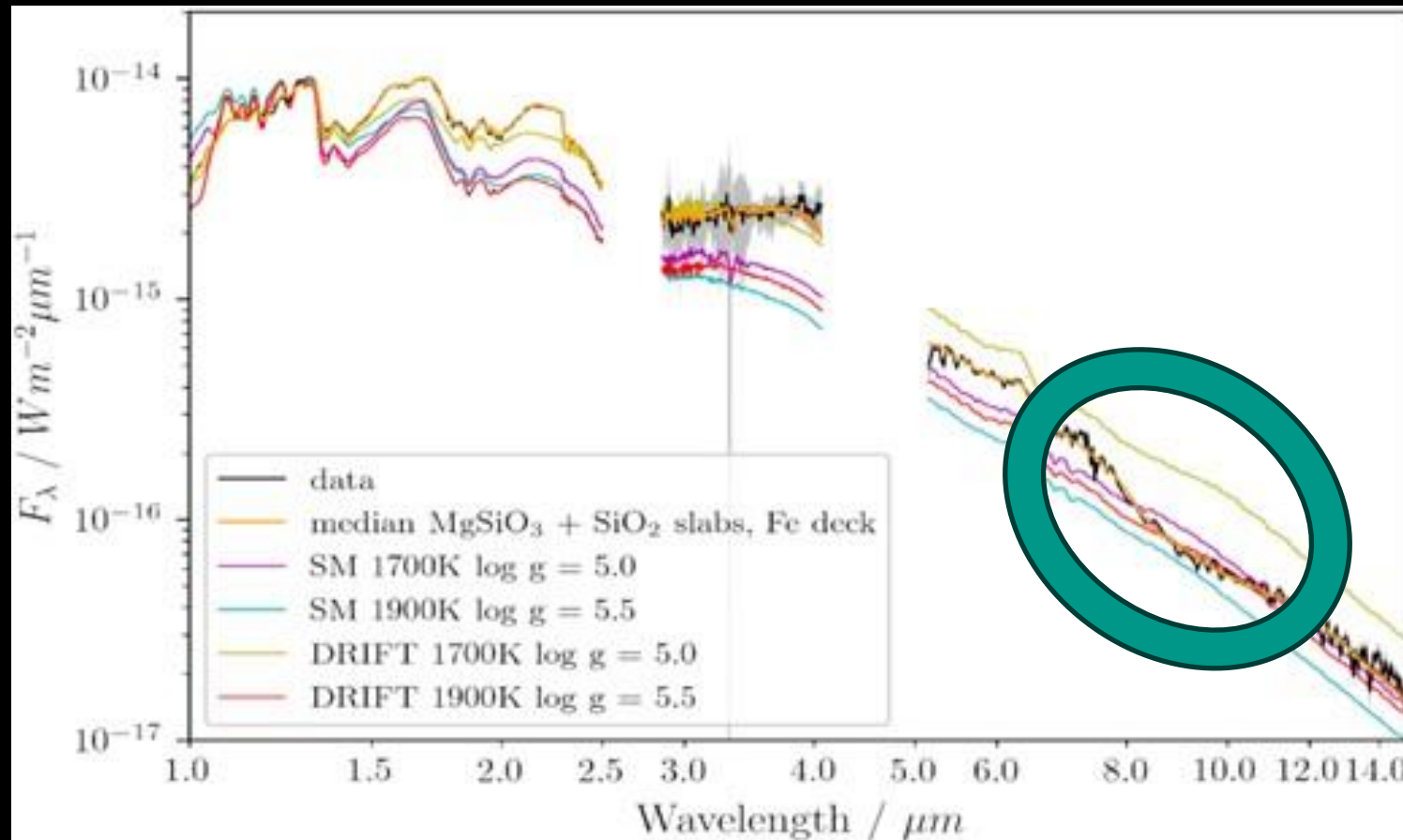
Table 1. Relative Cloud Masses and Condensation Temperatures for $P_T = 0.1$ bar and $[Fe/H] = 0.0$, after Lodders (2002).

Name	Formula	Relative Cloud Mass [†]	Condensation Temperature (K)
<i>Initial Al-bearing condensates</i>			
Hibonite	CaAl ₁₂ O ₁₉	2091	1914
Grossite	CaAl ₄ O ₇	2442	1848 [‡]
Corundum	Al ₂ O ₃	1915	...
<i>Initial Ti-bearing condensates</i>			
Ca titanate	Ca ₄ Ti ₃ O ₁₀	170	1854
Ca titanate	Ca ₃ Ti ₂ O ₇	180	1818 [‡]
Perovskite	CaTiO ₃	149	1707 [‡]
<i>Other condensates</i>			
Gehlenite	Ca ₂ Al ₂ SiO ₇	3678	1796 [‡]
Fe metal	Fe	21032	1682
Spinel	MgAl ₂ O ₄	2673	1663 [‡]
Akermanite	Ca ₂ Mg ₂ Si ₂ O ₇	3657	1626 [‡]
Ti oxide	Ti ₃ O ₅	82	1610 [‡]
Ti oxide	Ti ₂ O ₃	79	1610 [‡]
Forsterite	Mg ₂ SiO ₄	32180	1592
Diopside	CaMgSi ₂ O ₆	5809	1560 [‡]
Anorthite	CaAl ₂ Si ₂ O ₈	5227	1513 [‡]
Enstatite	MgSiO ₃	44585	1508
Cr metal	Cr	303	1416 [‡]
Ti oxide	Ti ₄ O ₇	83	1290 [‡]
Mn sulfide	MnS	360	1271
Na sulfide	Na ₂ S	≡ 1000	925

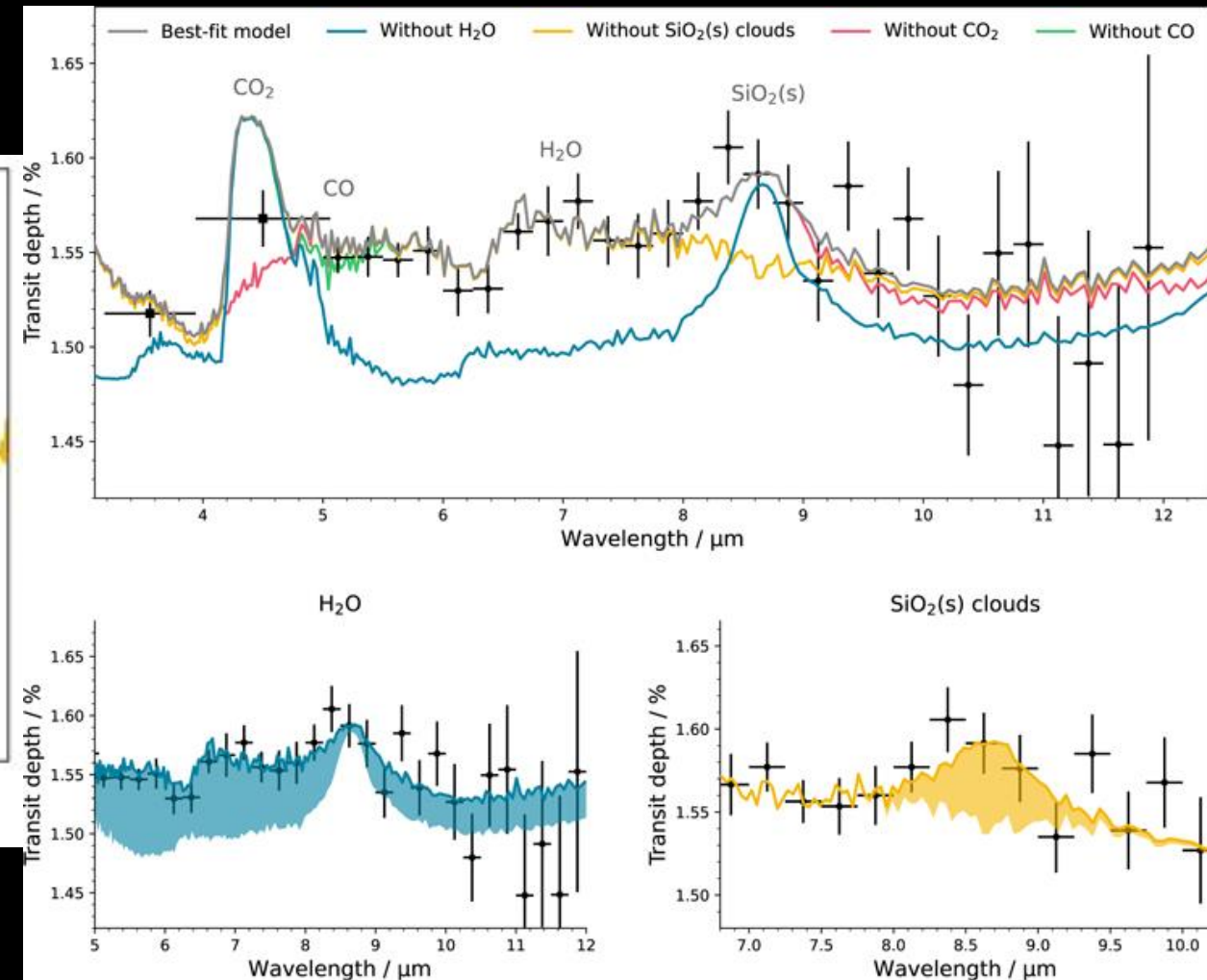
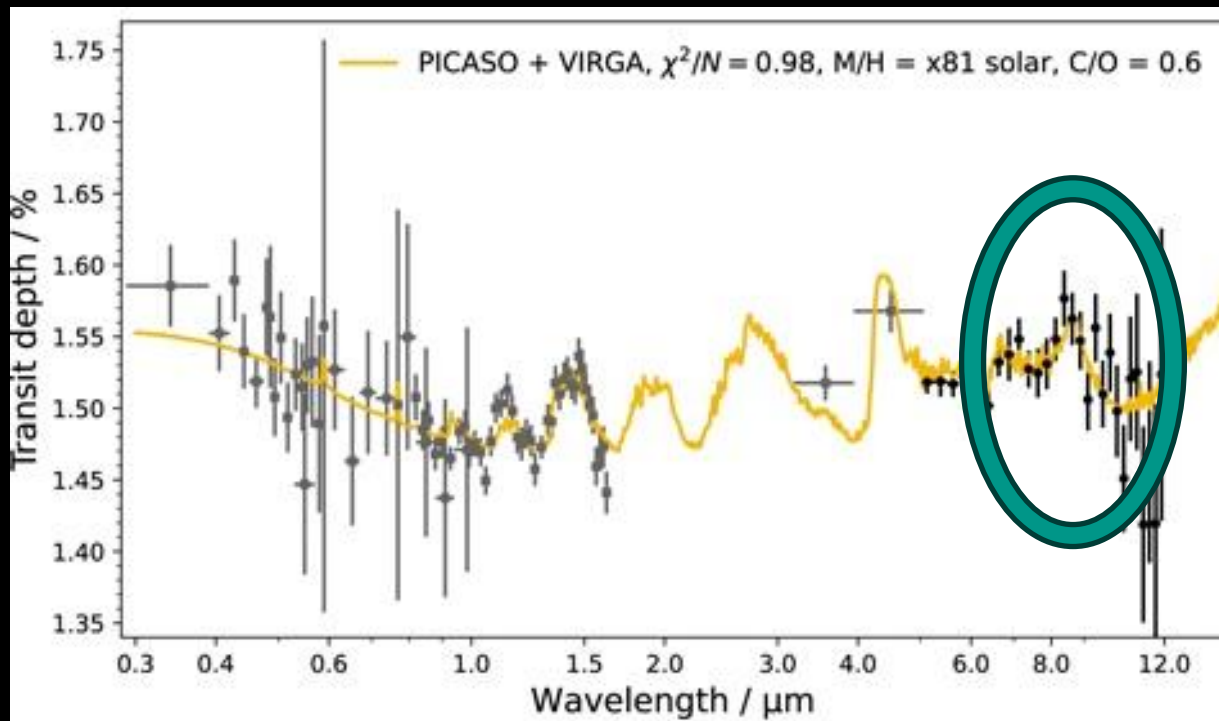
Wakeford et al., *MNRAS*, 2017

Fromont et al, AAS Journals, submitted

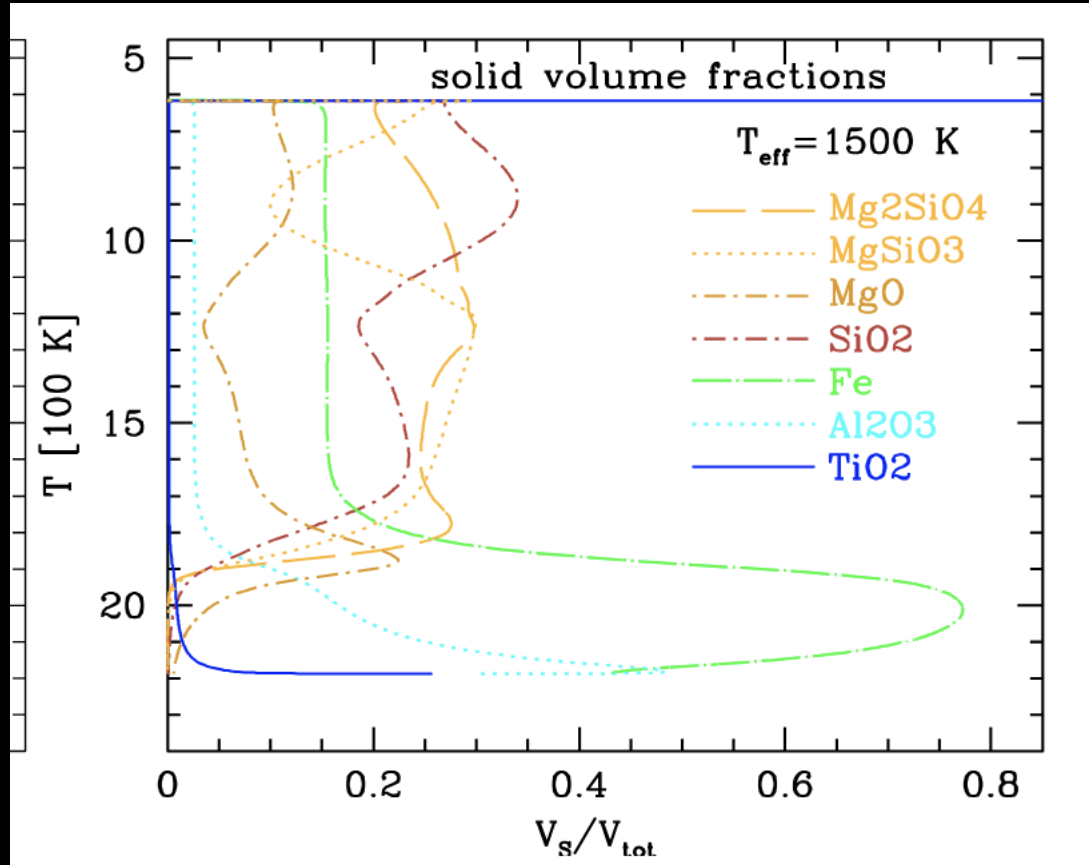
SiO_2 , not just MgSiO_3 or Mg_2SiO_4 , is discovered in an L dwarf....(and it looks amorphous not crystalline)



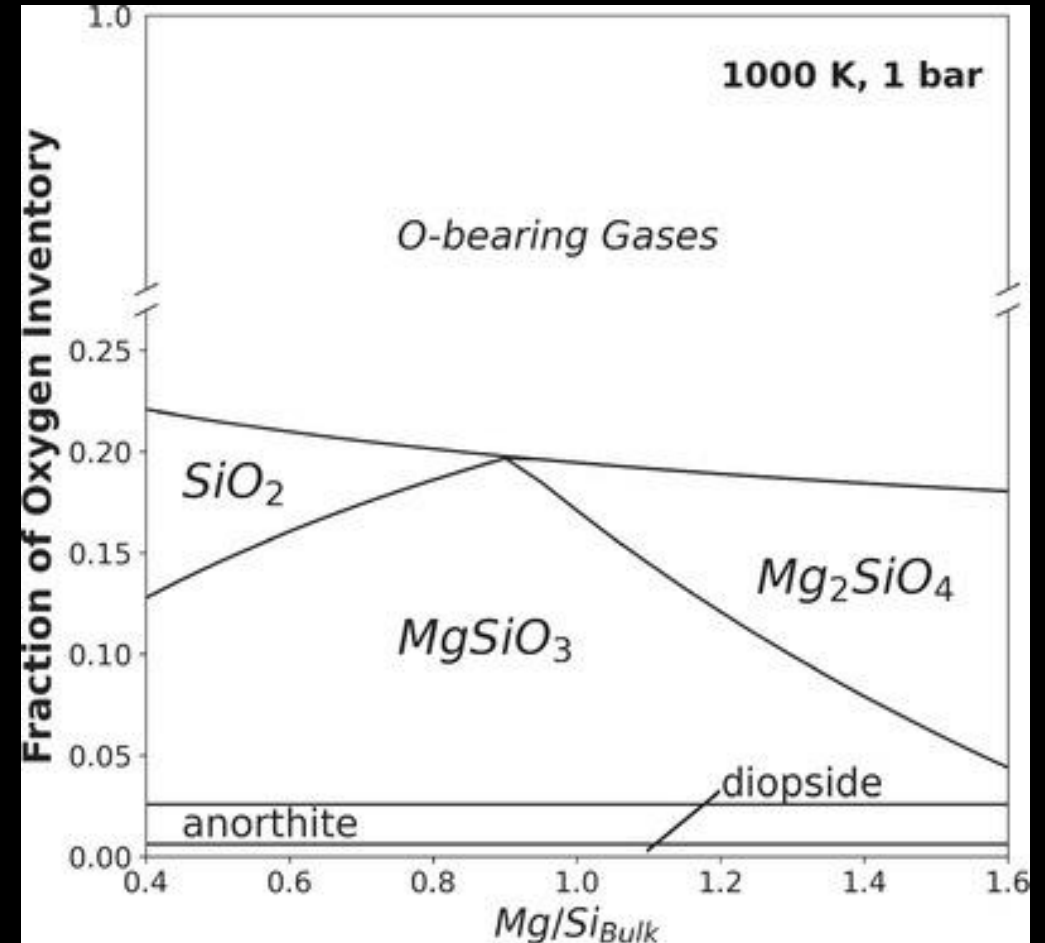
With JWST MIRI LRS, SiO_2 is discovered in the hot Jupiter WASP-17b



The cloud condensation sequence (where silicates dominate) and thus **oxygen sequestration** is highly dependent on the bulk chemistry of the atmosphere



Helling et al., A&A 2006

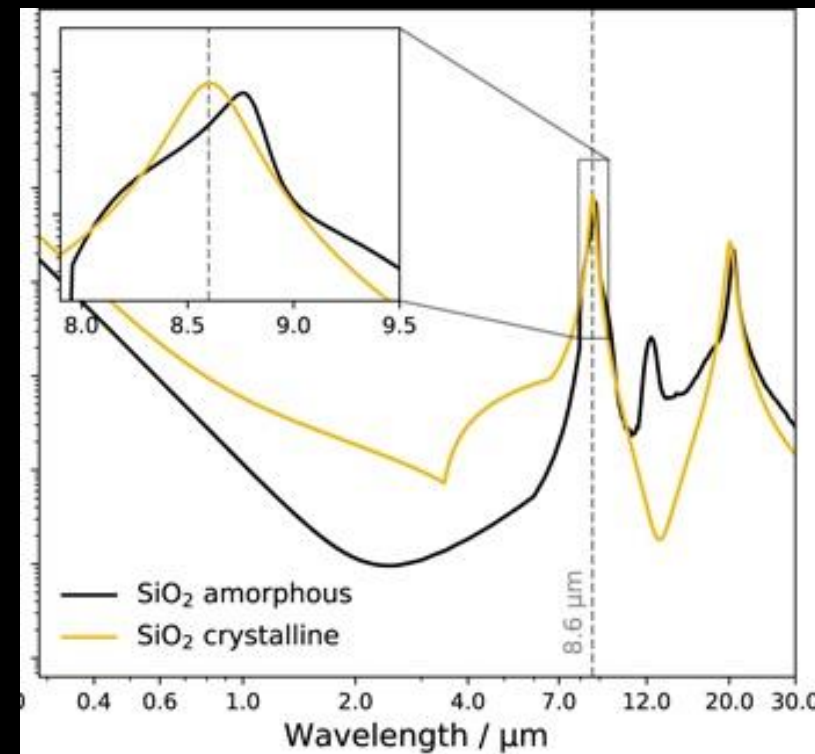
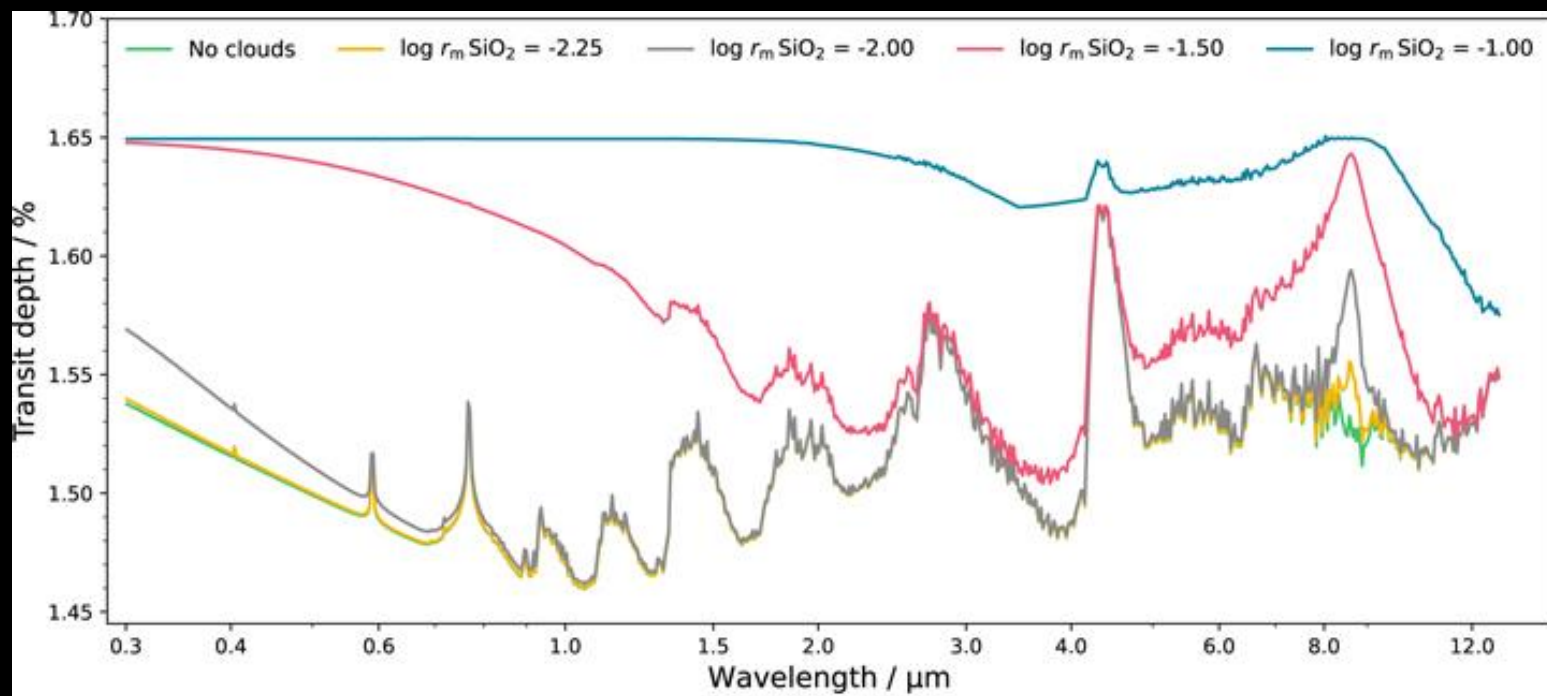


Calamari et al., *ApJ* 2024; Calamari et al., *ApJL*, 2026

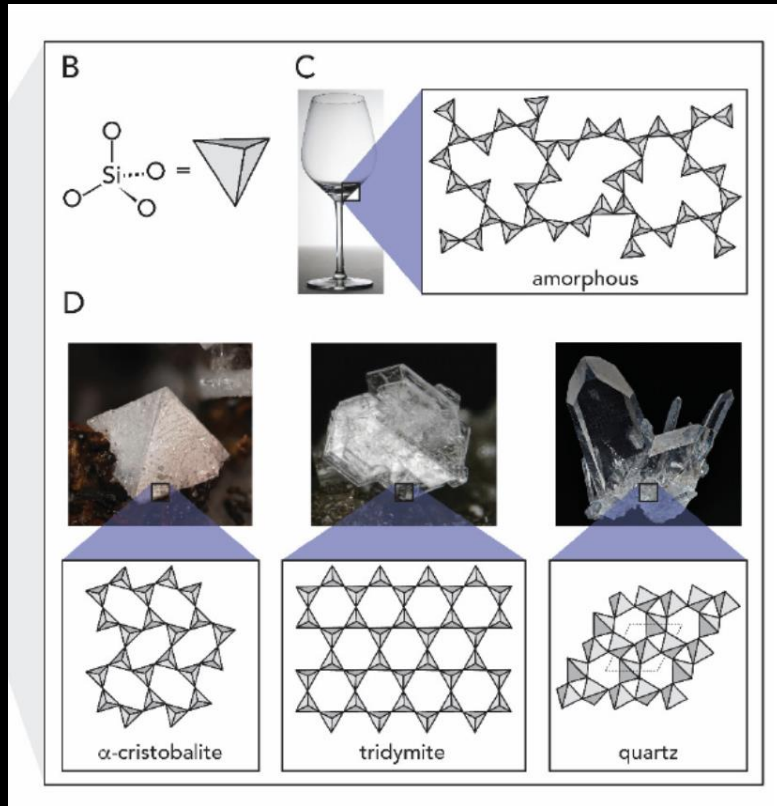
An aerial photograph showing a dense, textured layer of white and light gray clouds. The clouds are viewed from directly above, creating a pattern of soft, rounded shapes. In the upper left, a small portion of a blue sky and a white aircraft wing are visible. The overall scene is bright and expansive.

Clouds: *Morphology*

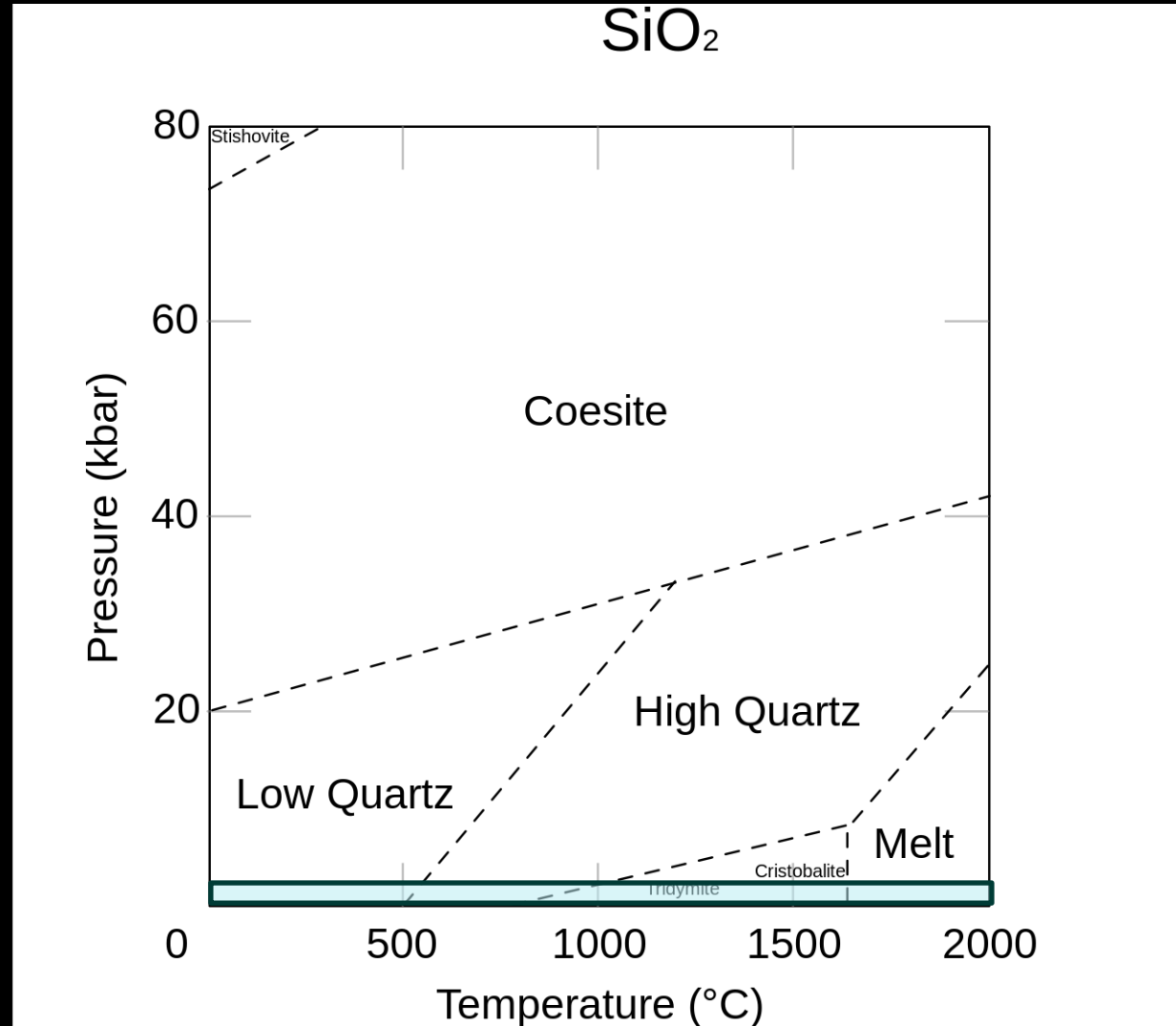
WASP-17b's SiO_2 clouds seem to be crystalline, not amorphous, with sub-micron sized particles



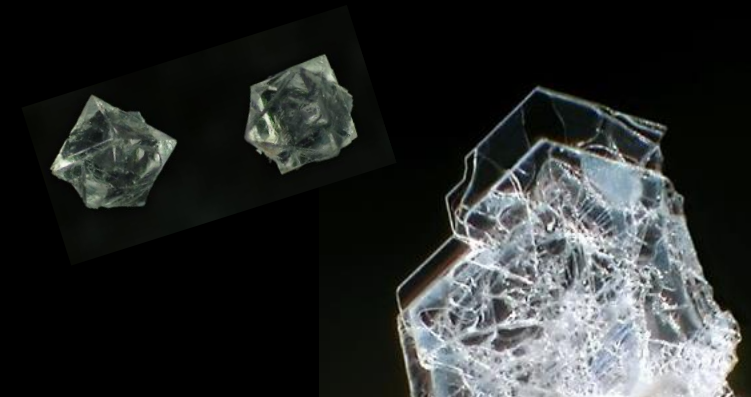
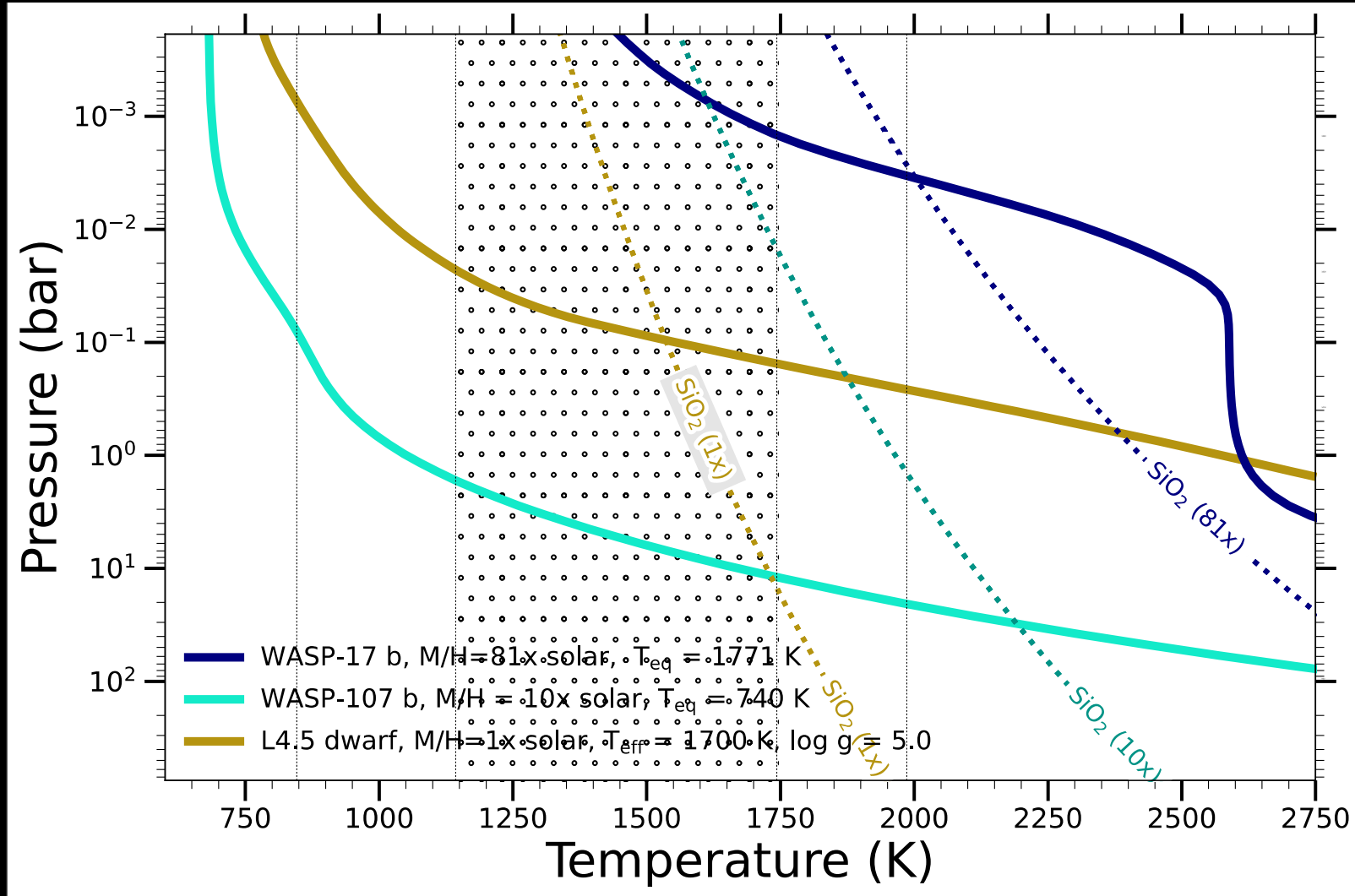
There are multiple stable polymorphs of many minerals – including SiO_2 – at high temperature/low pressure conditions



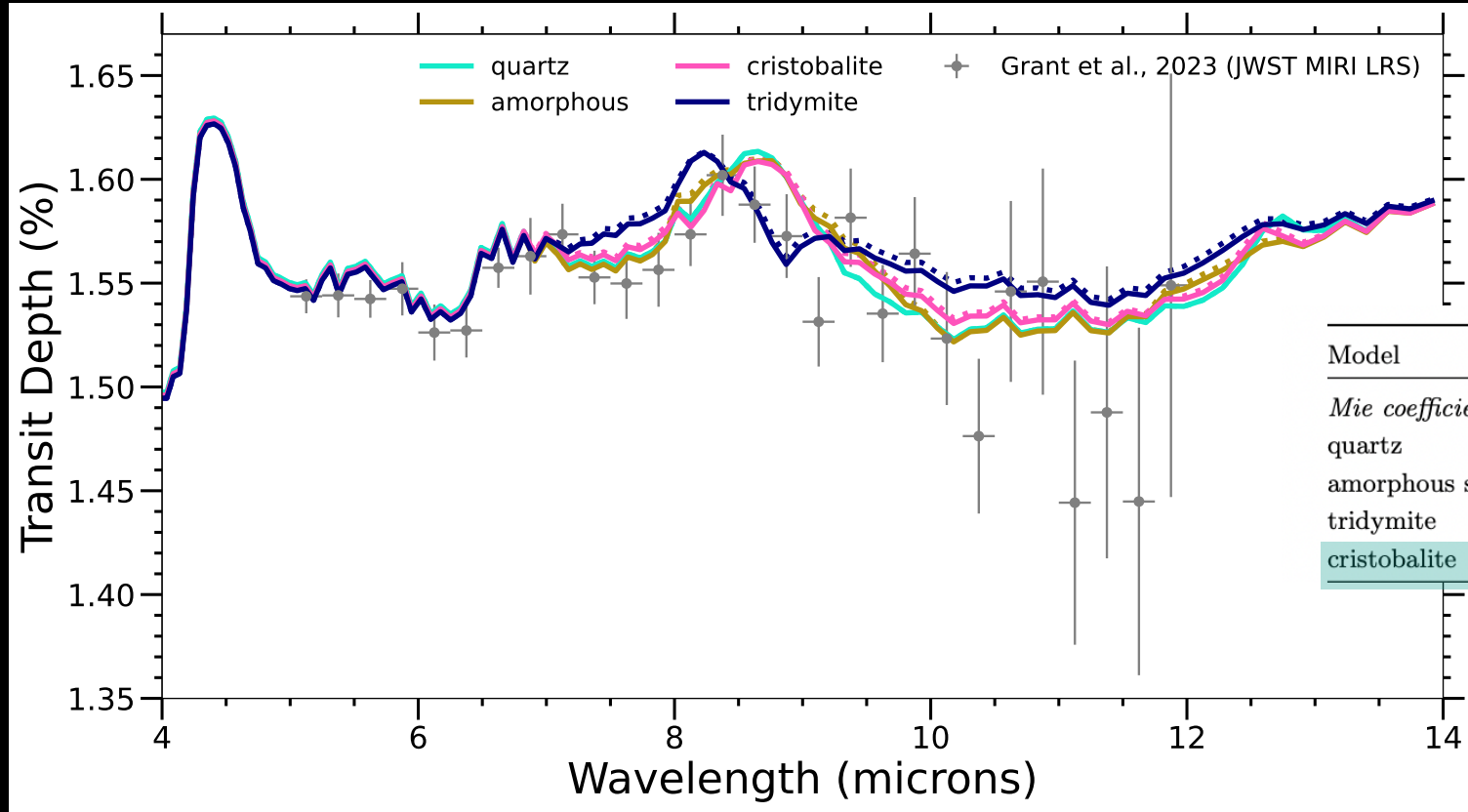
Moura et al., 2020, *Biomimetics*



There are multiple stable polymorphs of SiO_2 at the high temperature/low pressure conditions of substellar atmospheres

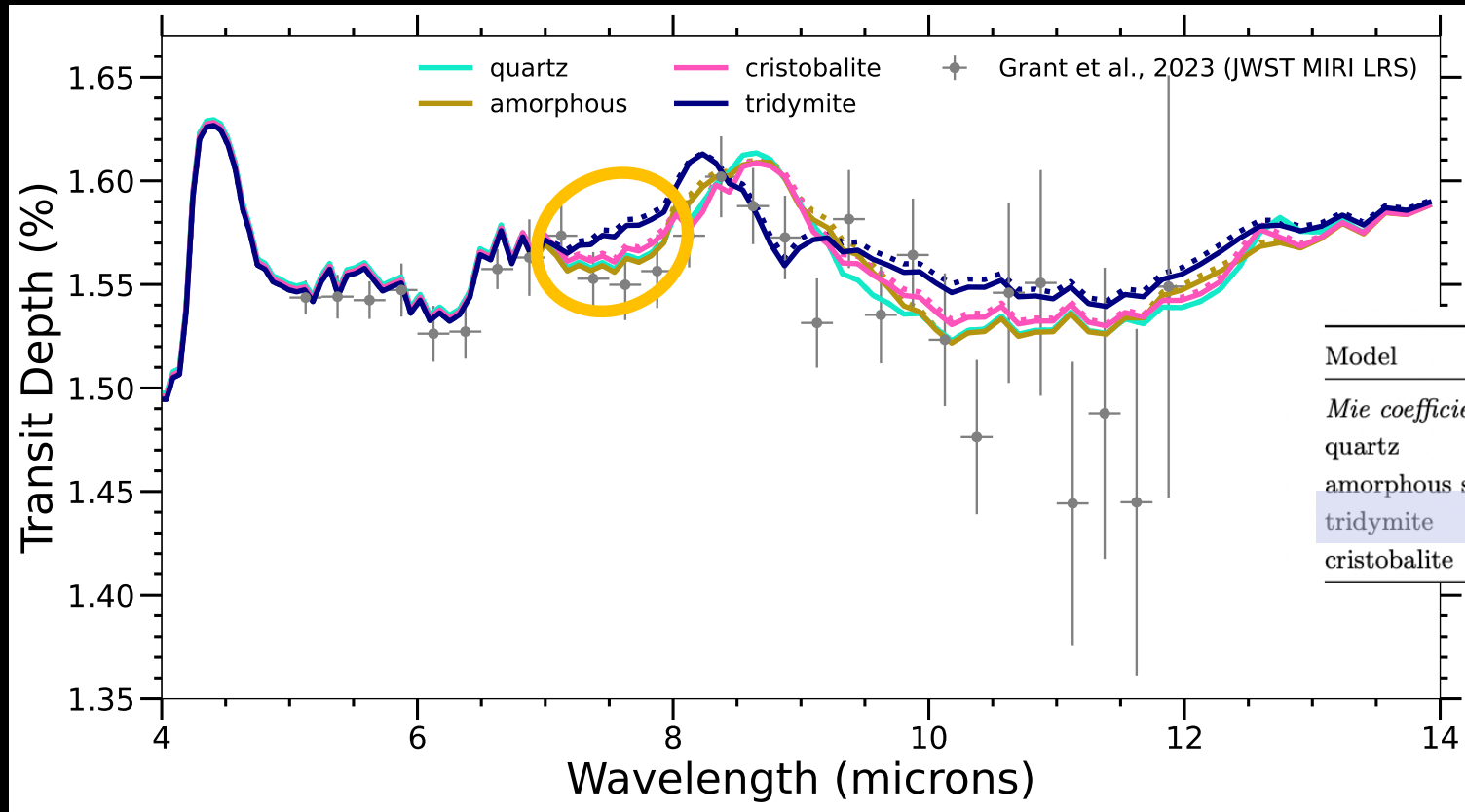


Cristobalite clouds are a better fit to the WASP-17 b JWST data compared to either quartz or amorphous silica



Model	χ^2	χ^2/n	BIC	Δ BIC
<i>Mie coefficients, BIC $k = 1$, $n = 95$, $dof = 94$</i>				
quartz	126.3	1.330	130.9	0.6
amorphous silica	126.0	1.327	130.6	0.3
tridymite	131.0	1.379**	135.6	5.3
cristobalite	125.7	1.323	130.3	–

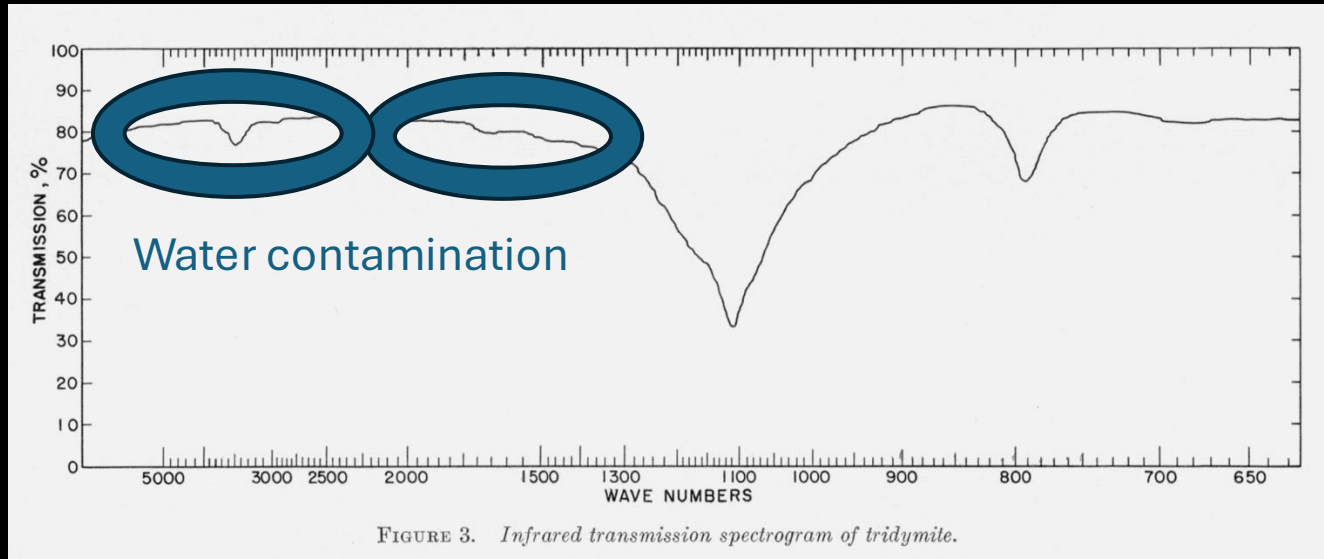
Tridymite clouds **are *not* a better fit**** to the WASP-17 b JWST data compared to either quartz or amorphous silica



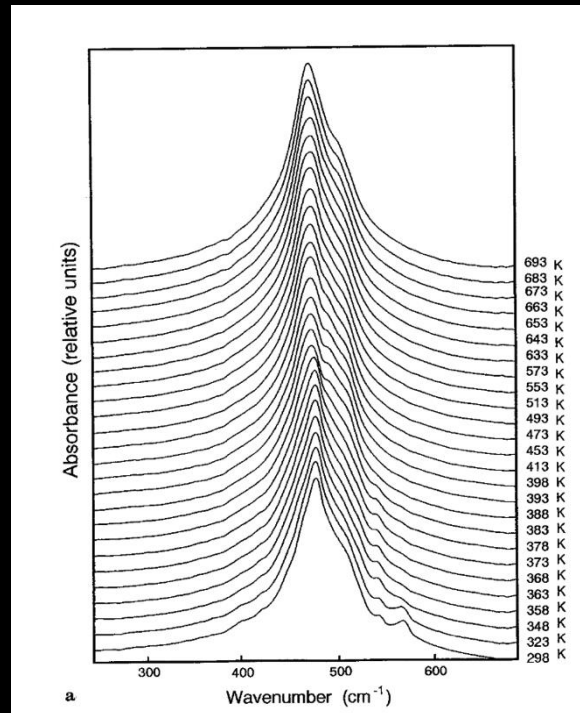
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tridymite	131.0	1.379**	135.6	5.3
cristobalite	125.7	1.323	130.3	–

**But! The region that causes the bad fit is right where we had to do the most egregious stitching and scaling of the old lab data....

Measurements of tridymite leave something to be desired

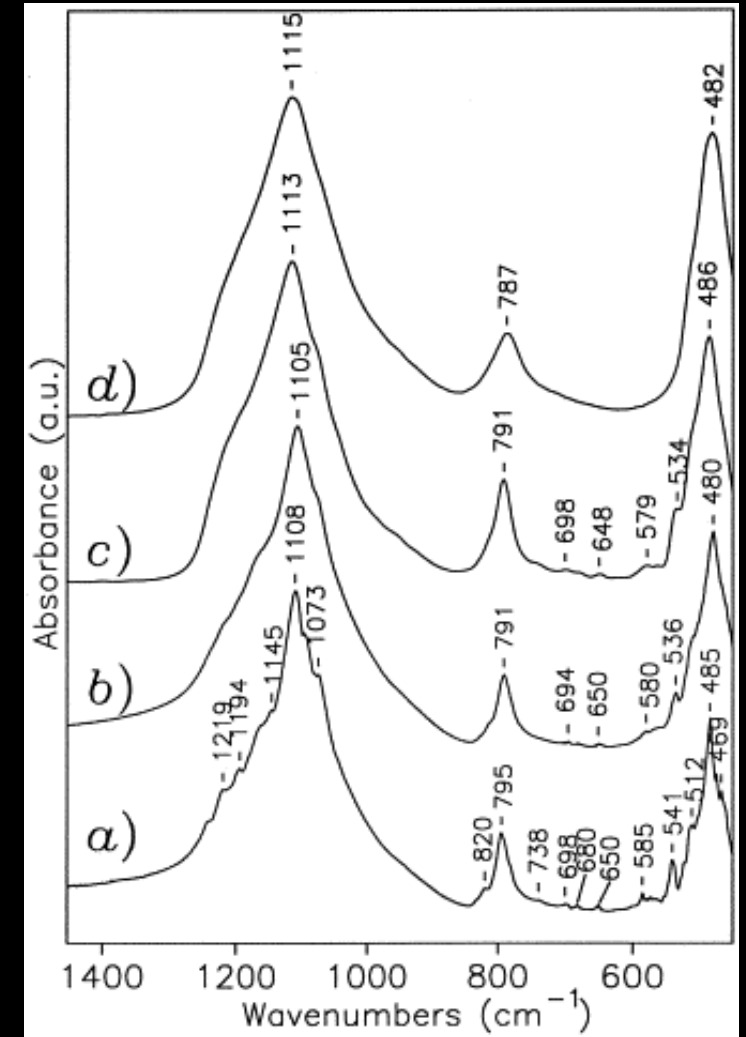


Lippincott et al., 1958



Cellai et al., 1995

“Samples were prepared by the standard KBr pellets method.”



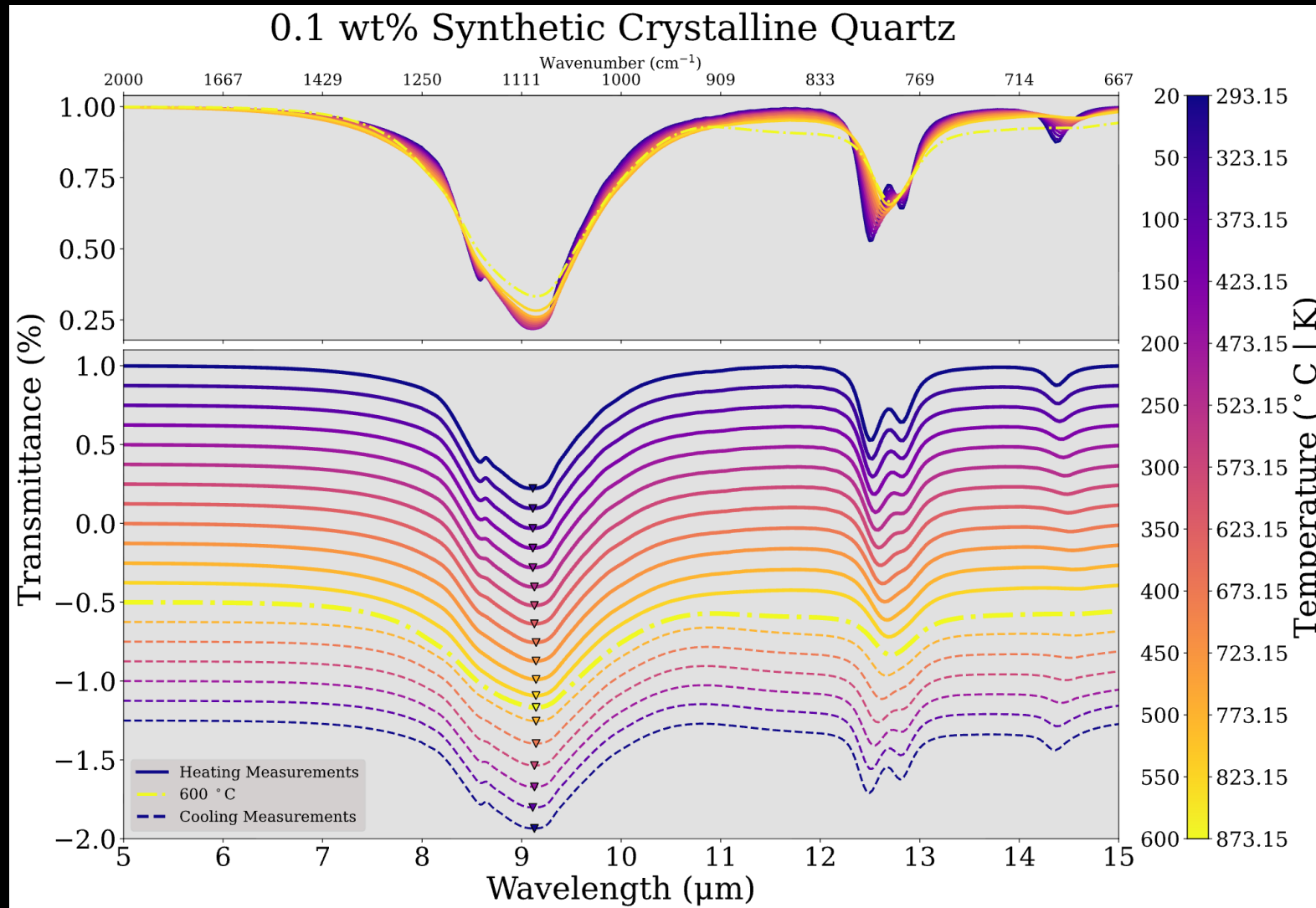
Sitarz et al., 2000

Modern labs can step in to provide new, well-vetted and applicable
silicate material laboratory measurements

From here on out, many in prep results...
so no photos* or social media please where you see this icon



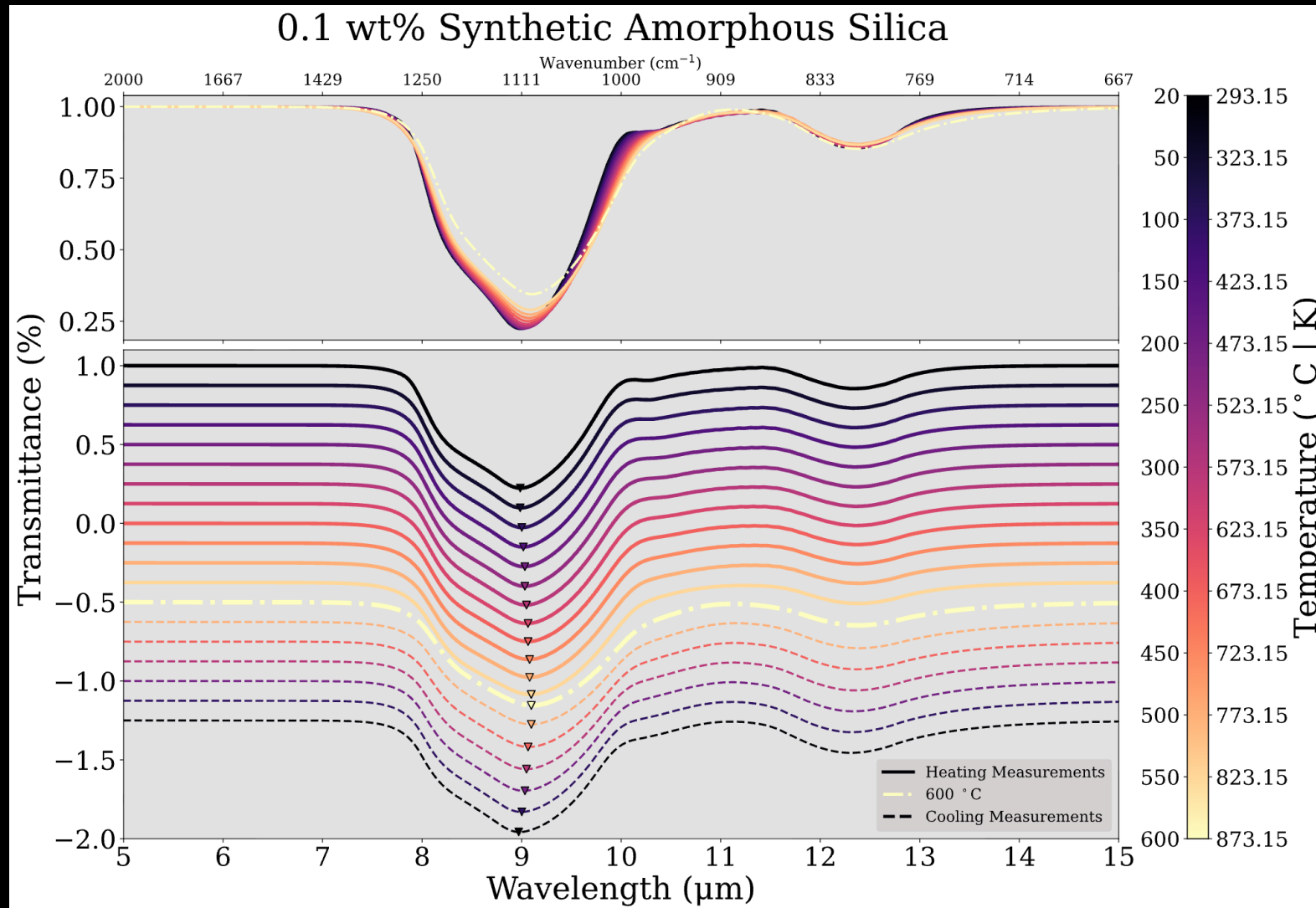
Quartz absorption shifts near instantaneously, and this transition is *reversible*



Mullens, Terragni, Moran, et al. submitted



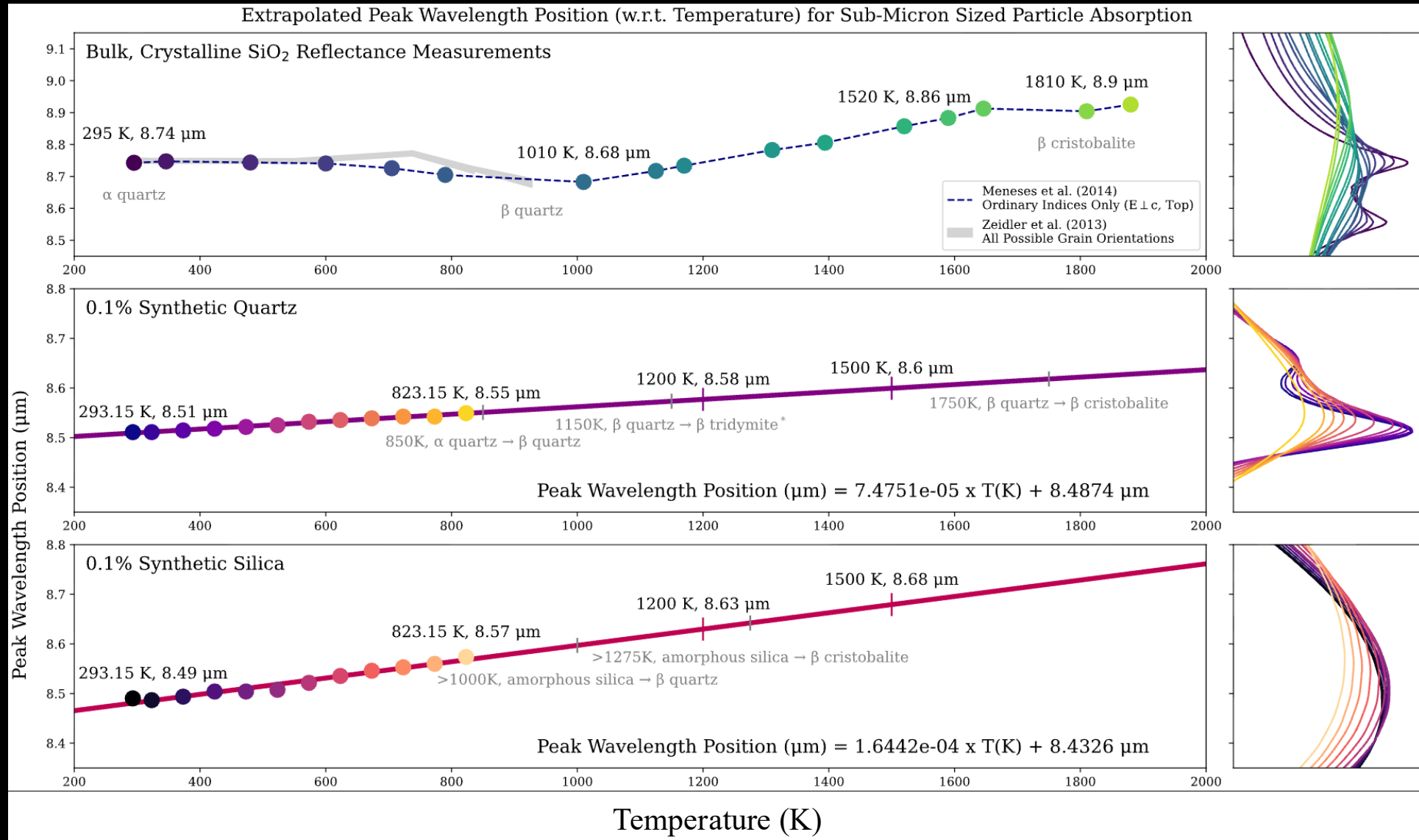
Even *amorphous* SiO₂ absorption shifts near instantaneously, making such clouds a precise probe of atmospheric temperature



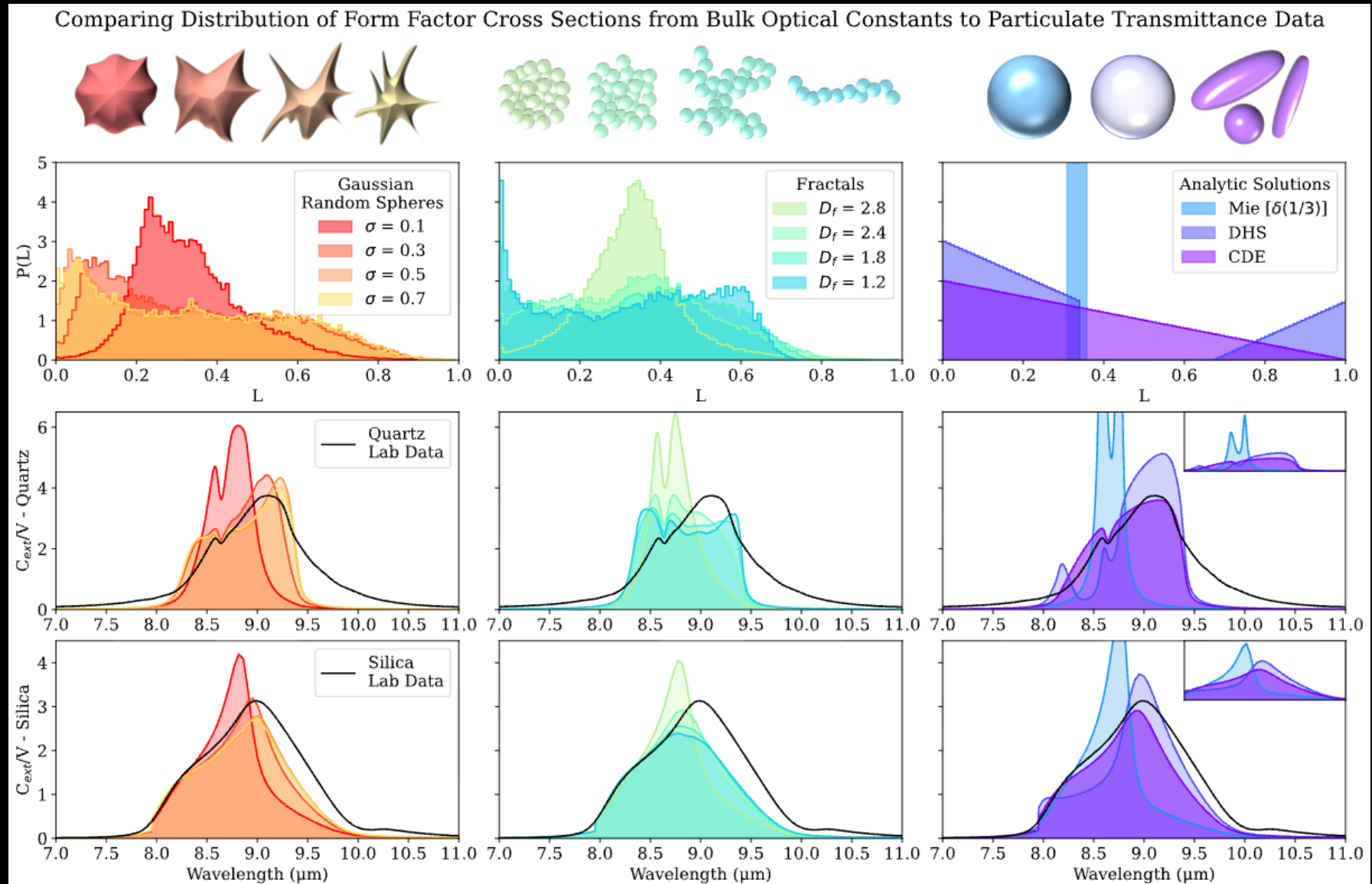
Mullens, Terragni, Moran, et al. submitted



Extrapolating from our (current) lab upper limit to our planets shifts peak wavelength up to 0.3 microns *just for* SiO_2



Most optical properties in the literature are from bulk reflectance and then most of us use Mie theory for our models...which is probably biasing our inferences



There are some incredible databases of optical properties with extensive docs and some incredible, actively developed models using the newest lab data

Mullens, Lewis & MacDonald, ApJ, 2024



Silica						
SiC	Moissanite / α Carborundum (SiC)		Kitzmann & Heng (2018) ↔ GitHub	Laor & Draine (1993) (C) Phillip & Taft (1960) in Caras (1965) Bohren & Huffman (1983) [Sec 9.1, 12.3.4]	0.2–30 μm	Crystalline (cubic, isotropic). Lab data + Damped Oscillator
SiO	Silicon Monoxide (SiO)		Kitzmann & Heng (2018) ↔ GitHub	Phillip in Palik (1985) (Vol 1, Sec 36) (C) Wetzel (2013)	0.2–30 μm	Amorphous (glass, isotropic) Palik Compilation + Thin Film KH18 filled empty Palik entries
SiO ₂	$\alpha + \beta$ Quartz (SiO ₂)		Wakeford & Sing (2015) ↔ Link	Phillip in Palik (1985) (Vol 1, Sec 34) (C) Zeidler (2013) ↔ DOCCD Link (SiO ₂ at 928K, EJC)	0.2–30 μm	Short wavelengths is α Quartz Infrared wavelengths is β Quartz 928K, Extraordinary (EJC) ray v
SiO ₂	α Quartz (SiO _{2_crystalline_2023})		Mullens et al. (2024) ↔ GitHub	Herve Herbin & Petitprez (2023)	0.25–15.37 μm	Crystalline (trigonal, uniaxial) Airborne quartz particles, random
SiO ₂	α Quartz (SiO _{2_alpha_palik})		Mullens et al. (2024) ↔ GitHub	Phillip in Palik (1985) (Vol 1, Sec 34) (C)	0.2–30 μm	Crystalline (trigonal, uniaxial) Variety of lab sources Kramers-Kronig analysis was used ↔ pyElli (Kramers-Kronig code) Indices averaged by polarization
SiO ₂	α Quartz + Silica Glass (SiO _{2_amorph})		Kitzmann & Heng (2018) ↔ GitHub	Henning & Mutschke (1997) Phillip in Palik (1985) (Vol 1, Sec 34) (C) ↔ DOCCD Link (Amorphous SiO ₂ , 300K)	0.2–30 μm	Short wavelengths is α Quartz Long wavelengths is amorphous
SiO ₂	Silica Glass (SiO _{2_glass_palik})		Mullens et al. (2024) ↔ GitHub	Phillip in Palik (1985) (Vol 1, Sec 34) (C)	0.2–30 μm	Amorphous (glass, isotropic) Kramers-Kronig analysis was used ↔ pyElli (Kramers-Kronig code)

~70 rocks, salts, and ices in base collection, out now!
In depth readme file on how lab data was taken.

 **Optical Constants db**

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Optical Constants Database

The Optical Constants database (OCdb) is a data repository developed to provide published, peer-reviewed, optical constants of materials relevant to planetary and astrophysical environments to the scientific community for the analysis and interpretation of observational data.

Ices

Ice Tholins

Gas Tholins

managed by Ella Sciamma-O'Brien at NASA Ames



e.g., Lodge & Moran et al., ApJ, 2026

Takeaways

Hazes readily incorporate **oxygen** and **sulfur** as well as **carbon**.
They are probably **fractal aggregates**.

Clouds can be both minerals and organics & therefore depend on **bulk planet chemistry**,
For minerals, **polymorphs** matter. For organics, **fractal aggregates** matter.

These differences are observable existing telescopes, and thus
clouds and hazes *are tracers* of atmospheric condition via remote sensing

**We require high accuracy, high precision laboratory data to be folded into the models
used to interpret observational data**