ASTROCHEMISTRY

FROM THE BIG BANG TO LIFE

Global Astrochemistry Lecture Series (GALS) 2024

CHEMISTRY IN (EXO)PLANET ATMOSPHERES

Laura Kreidberg. *Max Planck Institute for Astronomy, Germany*

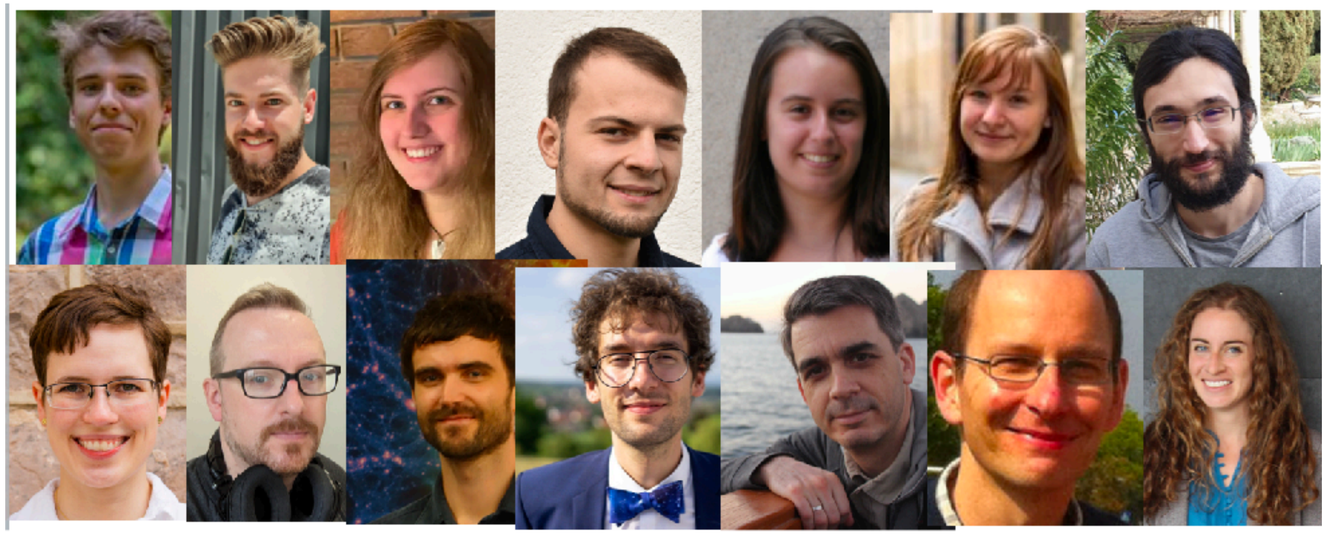
11.03.2024 | 15:00 - 17:00 CET

cost EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY
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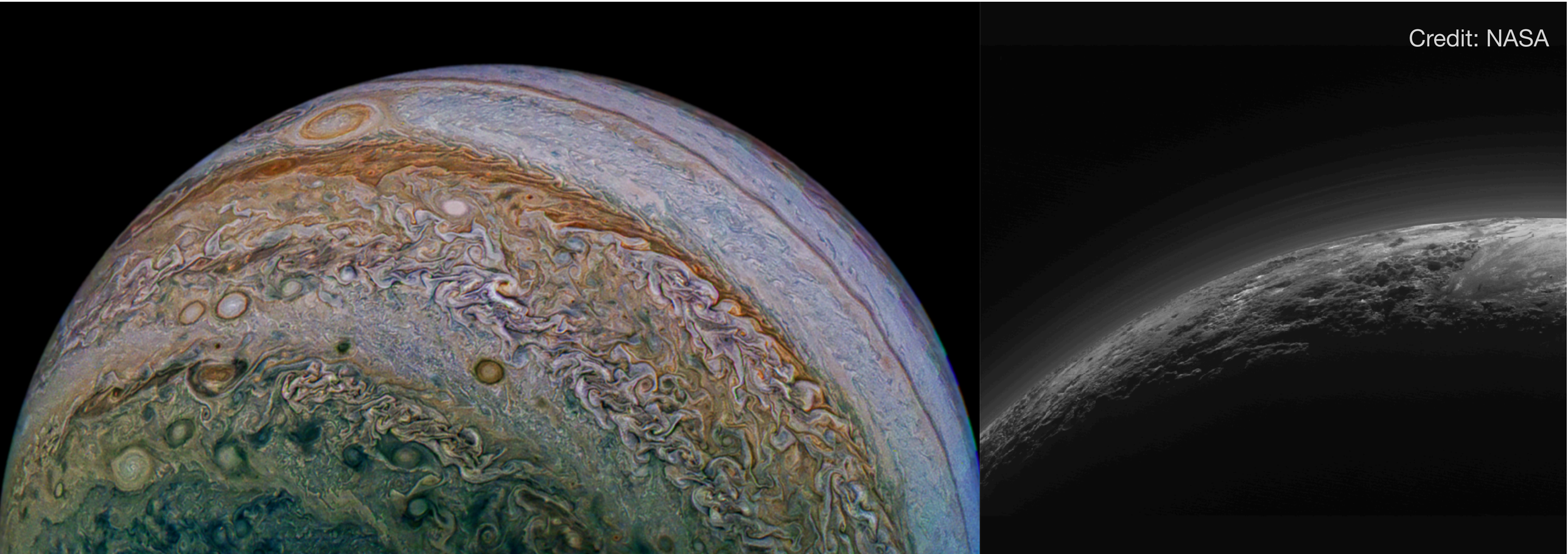
Atmospheric Physics of Exoplanets

- New department at the Max Planck Institute of Astronomy, founded in 2020
- Focus is observations, theory, and instrumentation for exoplanet atmospheres!
- Advertisement: we are hiring at all levels! Jobs are advertised in the fall on the AAS job register



Why is chemistry important in exoplanet atmospheres?

Chemistry encodes formation history, evolution, and even habitability

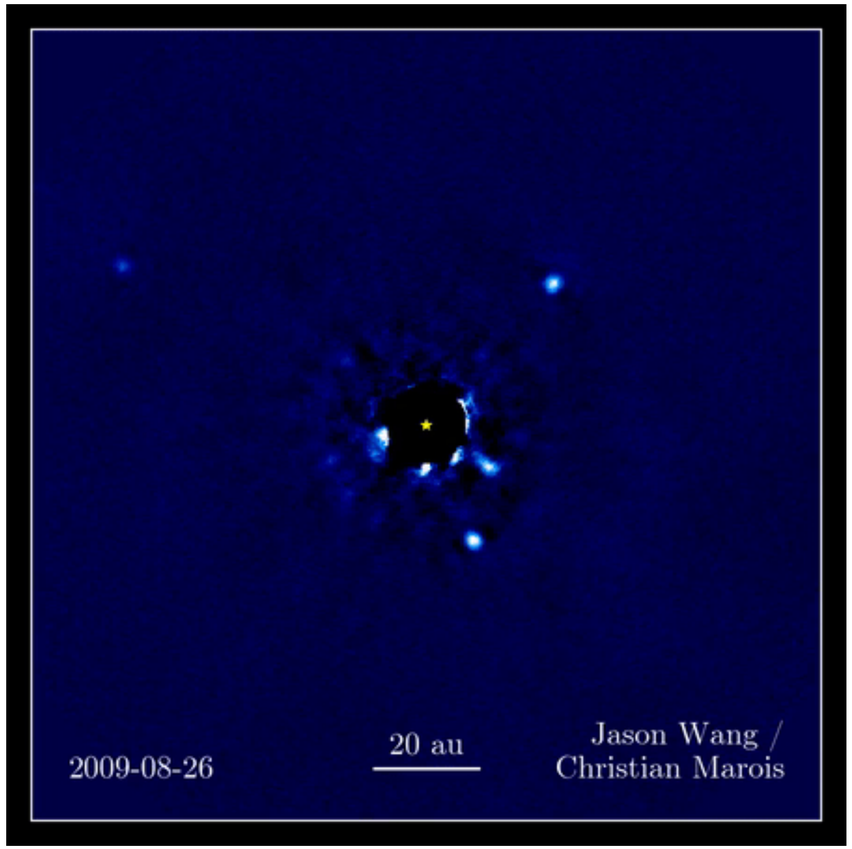


Agenda

1. How do we study the chemistry of exoplanet atmospheres?
2. Chemical composition of gaseous planets
3. What kind of clouds and hazes do exoplanets have?
4. Rocky planet atmospheres, biosignatures, and the future

Atmosphere characterization is HARD

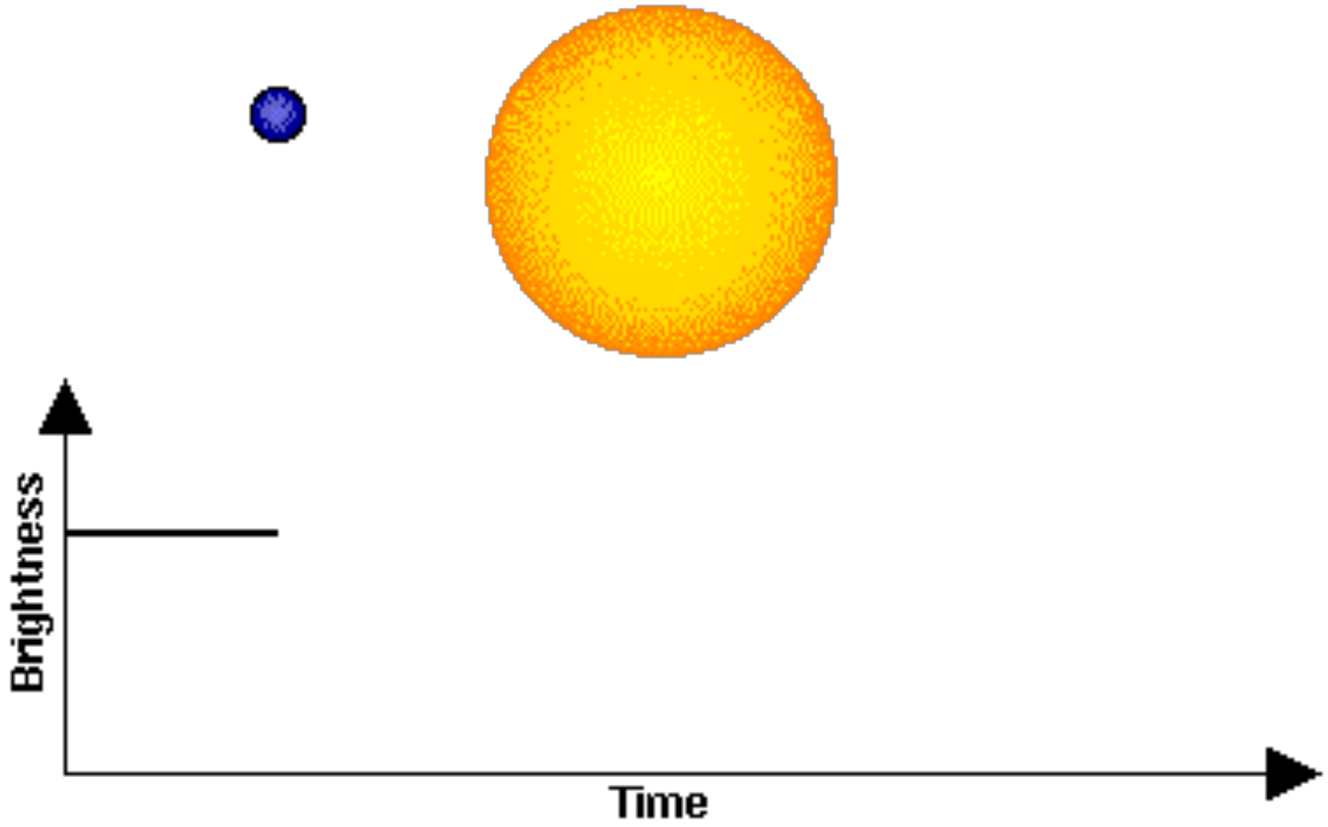
- Ideally, we would directly image planets and measure their spectra
- But planets are *at least* 10000x fainter than their stars!
- Current facilities are sensitive to massive gas giants far away (~10 AU) from their host stars



The famous HR 8799 system

Transiting planets: a fast track to atmospheres!

Even though we can't spatially separate the planet from the star, we *can* measure changes in brightness over time!

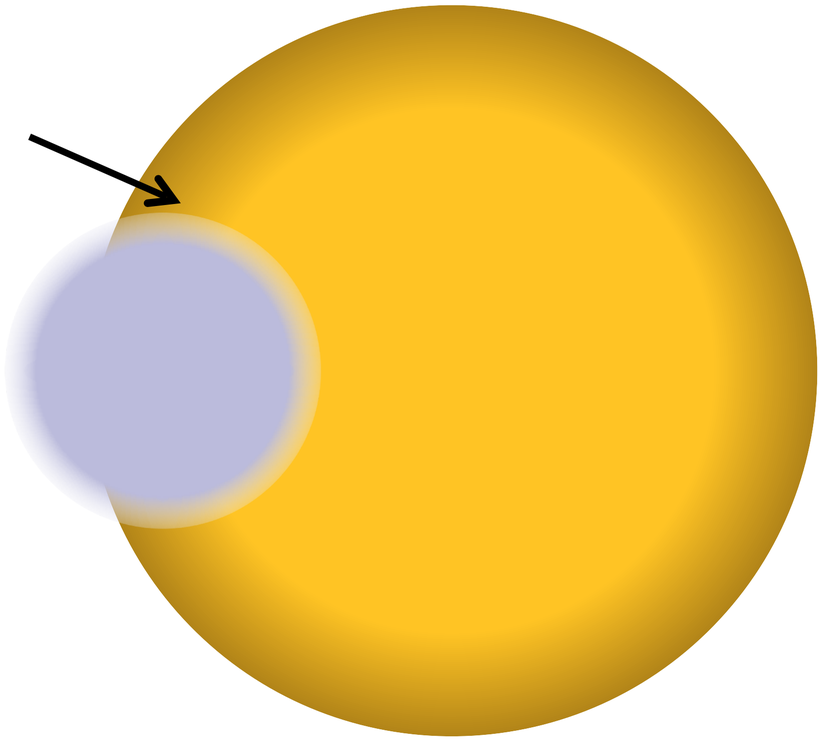


https://fluxphysics.github.io/

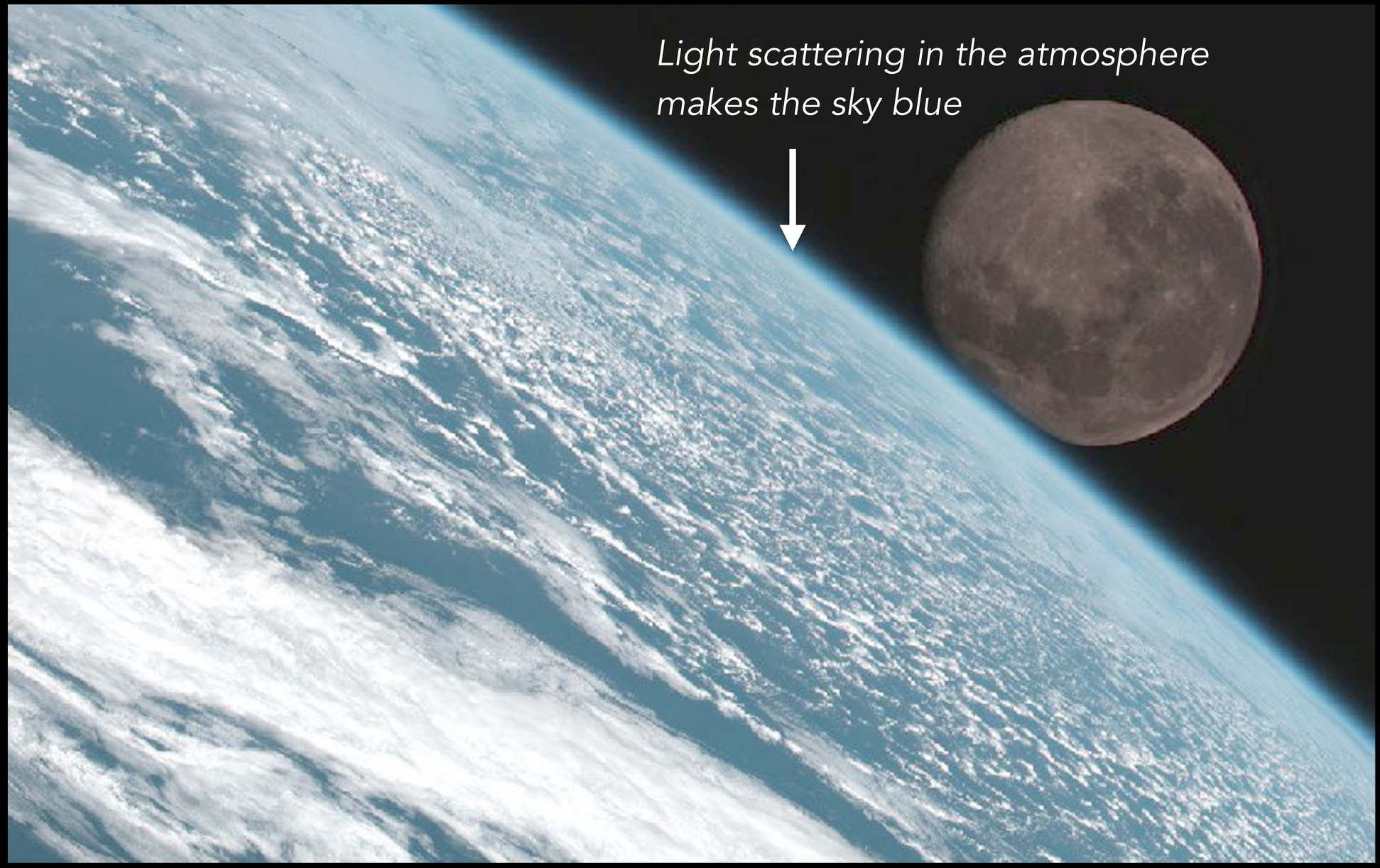
Atmosphere characterisation methods

I. Transmission spectroscopy

starlight filters through planet atmosphere during transit

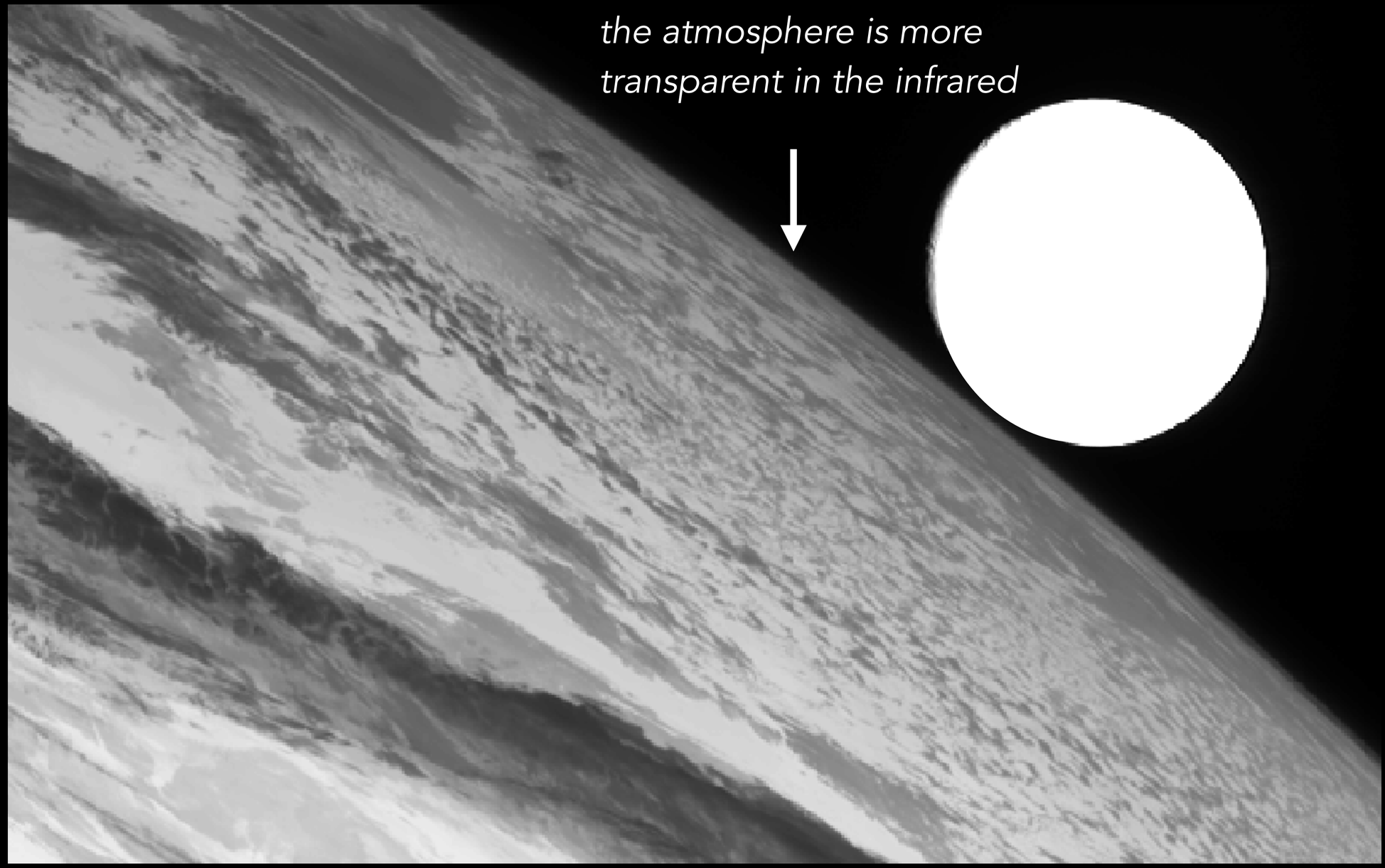


Earth in real color



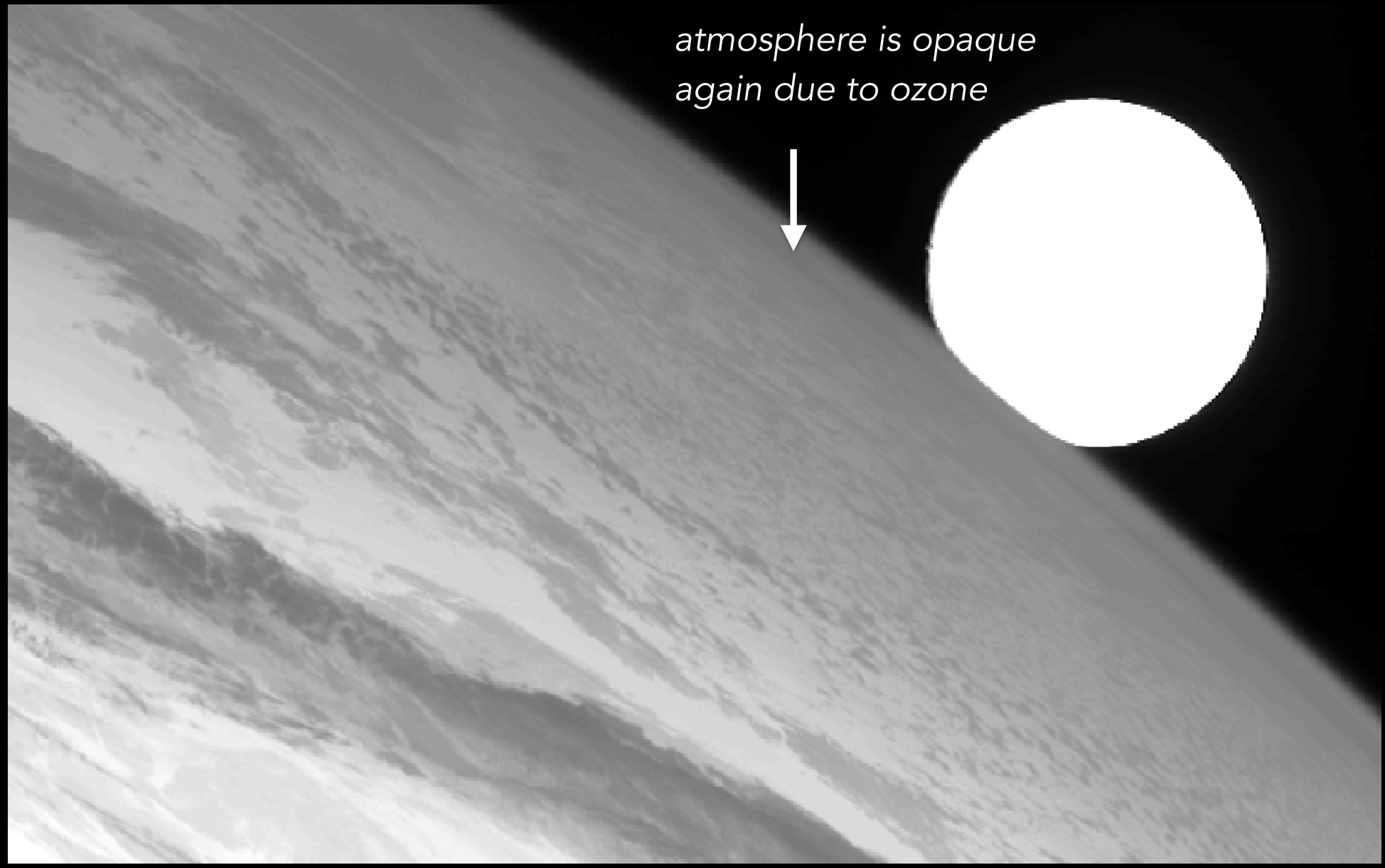
Credit: Himawari/Simon Proud/Vivien Parmentier

Earth in the infrared



Credit: Himawari/Simon Proud/Vivien Parmentier

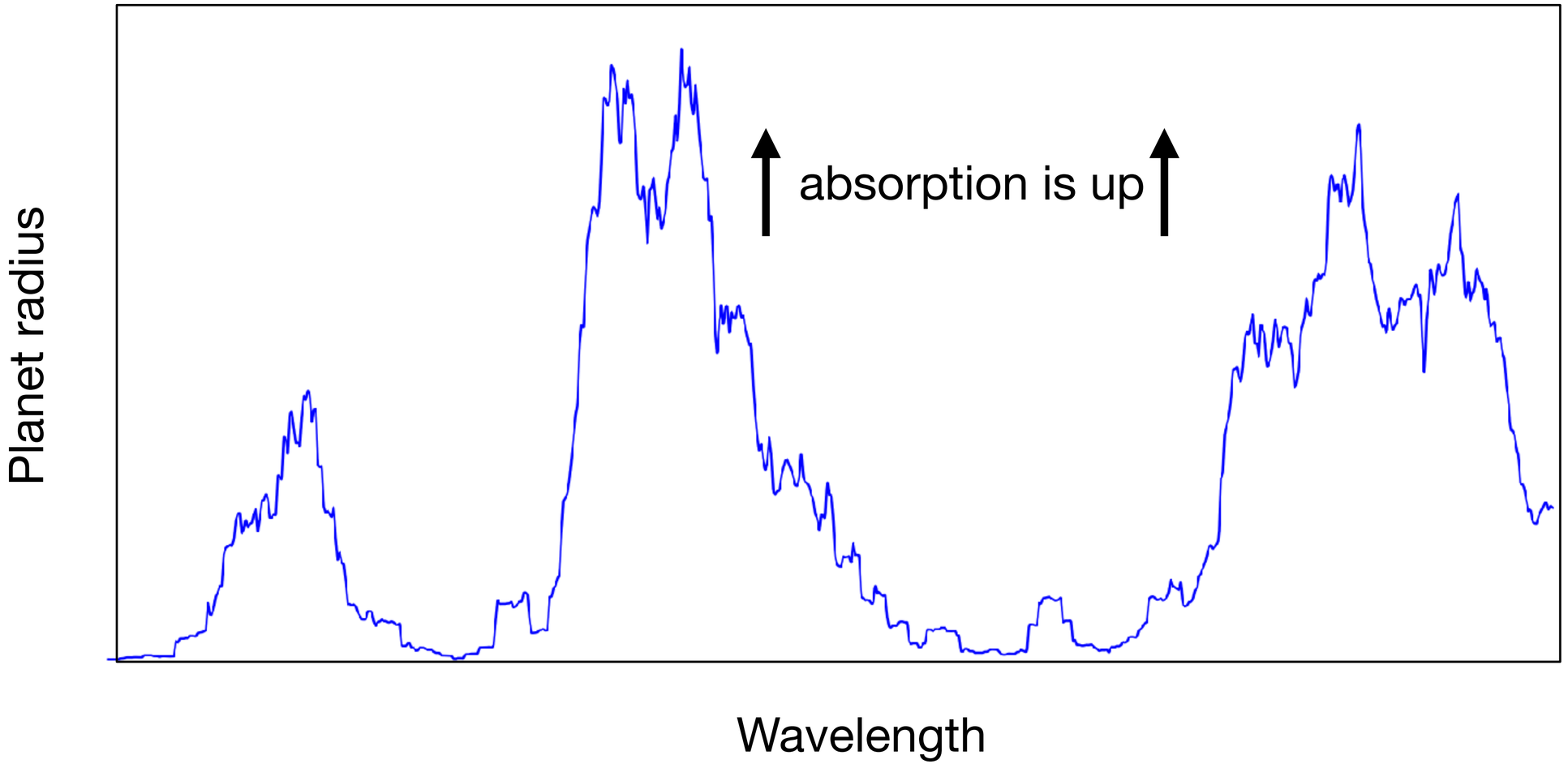
Earth in the infrared ozone band



Credit: Himawari/Simon Proud/Vivien Parmentier

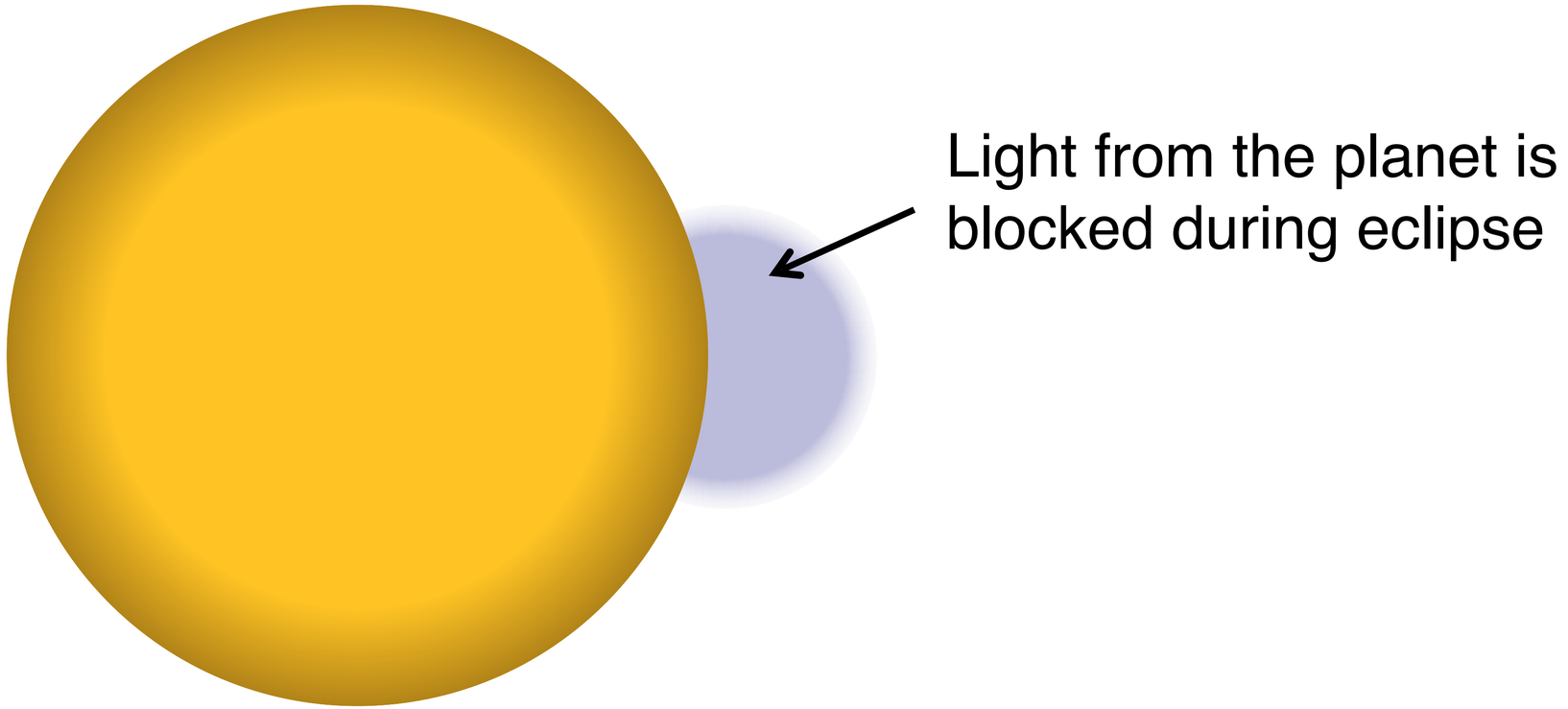
Transmission spectrum

Size of the planet versus wavelength



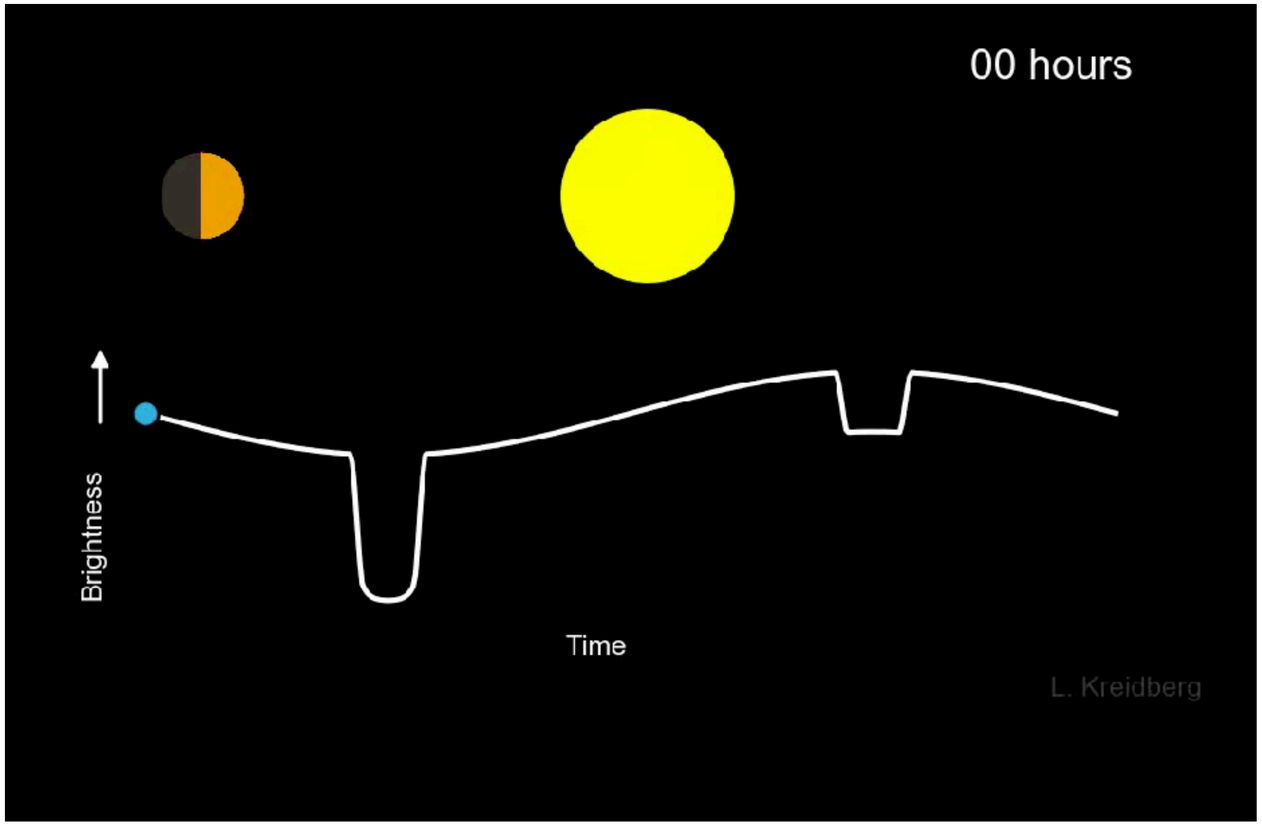
Atmosphere characterisation methods

II. Emitted and reflected light



Putting it all together

III. Phase curves

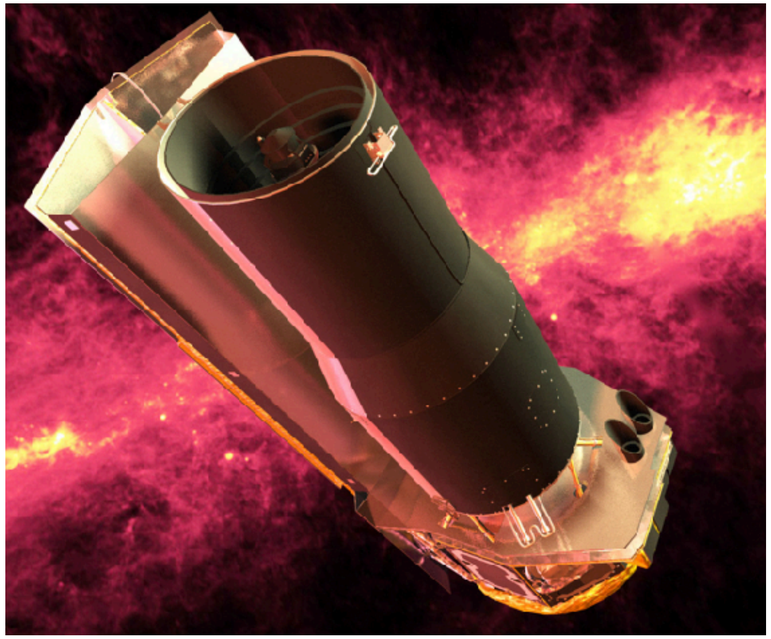


- Observe a complete orbital revolution
- Changing viewing angle reveals different regions of the atmosphere over time
- Can map the global climate and chemical composition!

Key facilities

Space

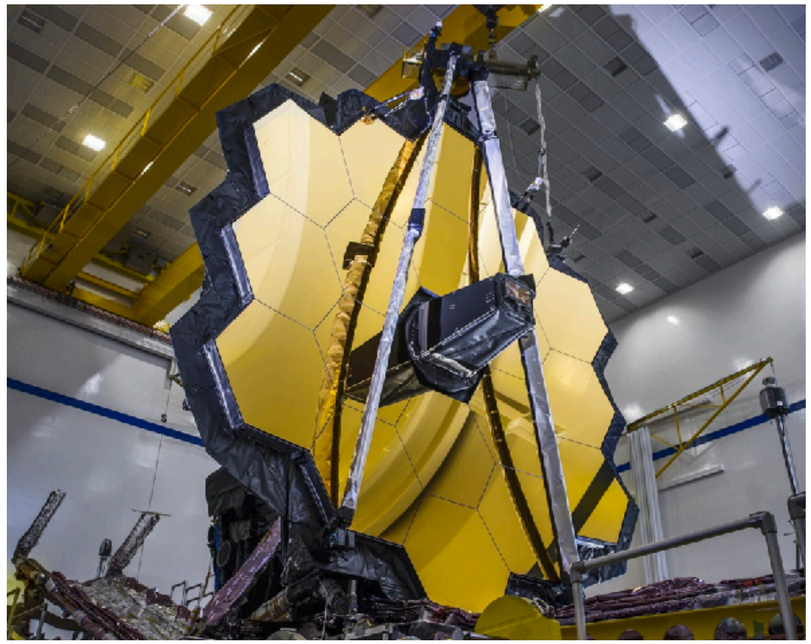
Atmosphere characterisation is easier when Earth's atmosphere is not in the way!



Spitzer Space Telescope
Launch date: 2003
85 cm mirror
Infrared; 3.6 - 160 micron



Hubble Space Telescope
Launch date: 1990
2.4 m mirror
UV-near-IR: 0.1 - 1.7 micron



JWST
Launch date: 2021
6.5 m mirror
Optical - IR: 0.6 - 30 micron

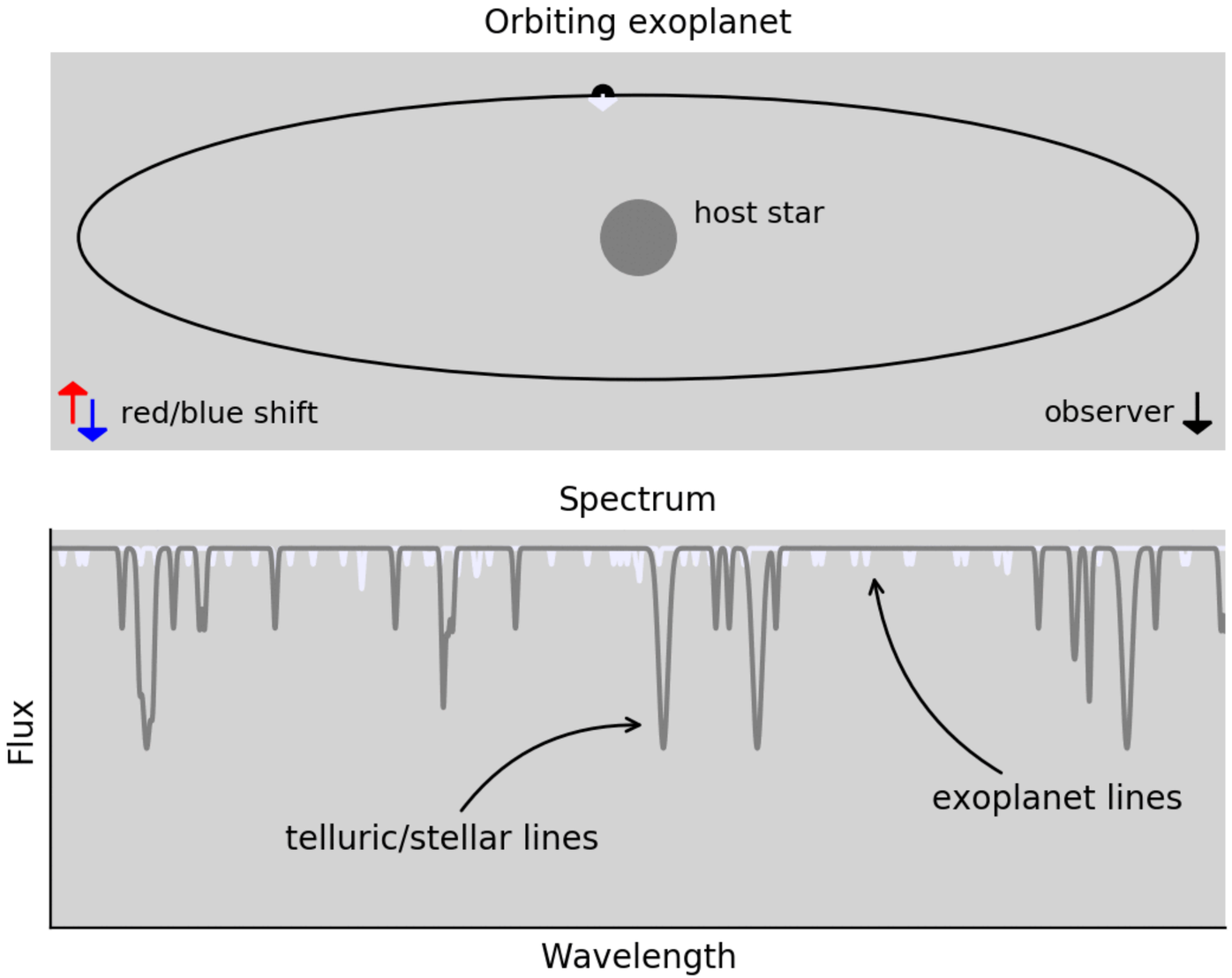
Key facilities

Ground

We can outsmart Earth's atmosphere with high-resolution spectroscopy!

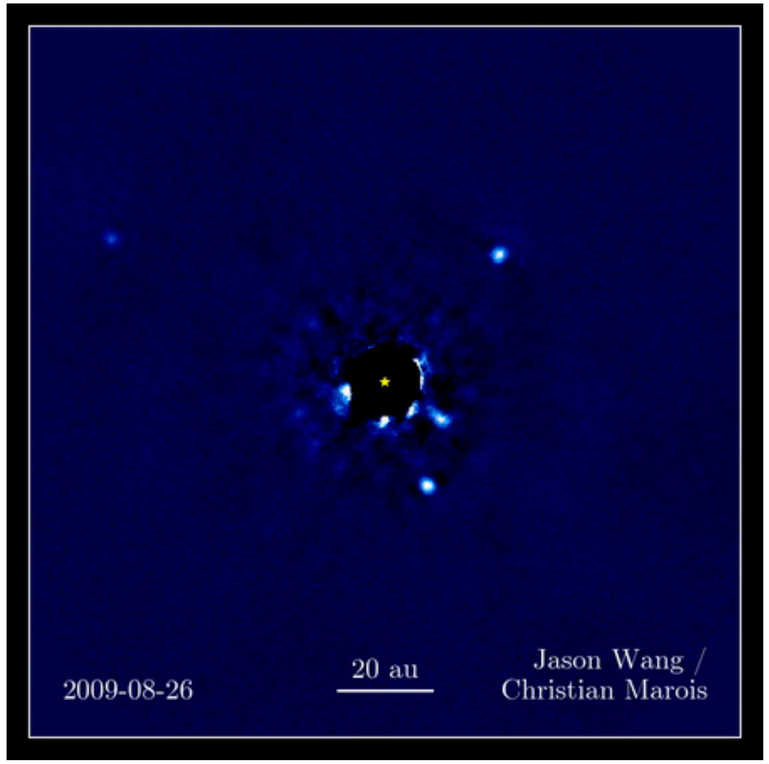
VLT/CRIRES was the first; now there are HARPS, ESPRESSO, Spirou, CARMENES, GIANO, LBT/PEPSI, Gemini/MAROON-x, IGRINS, and many more …

Credit: Lennart van Sluijs



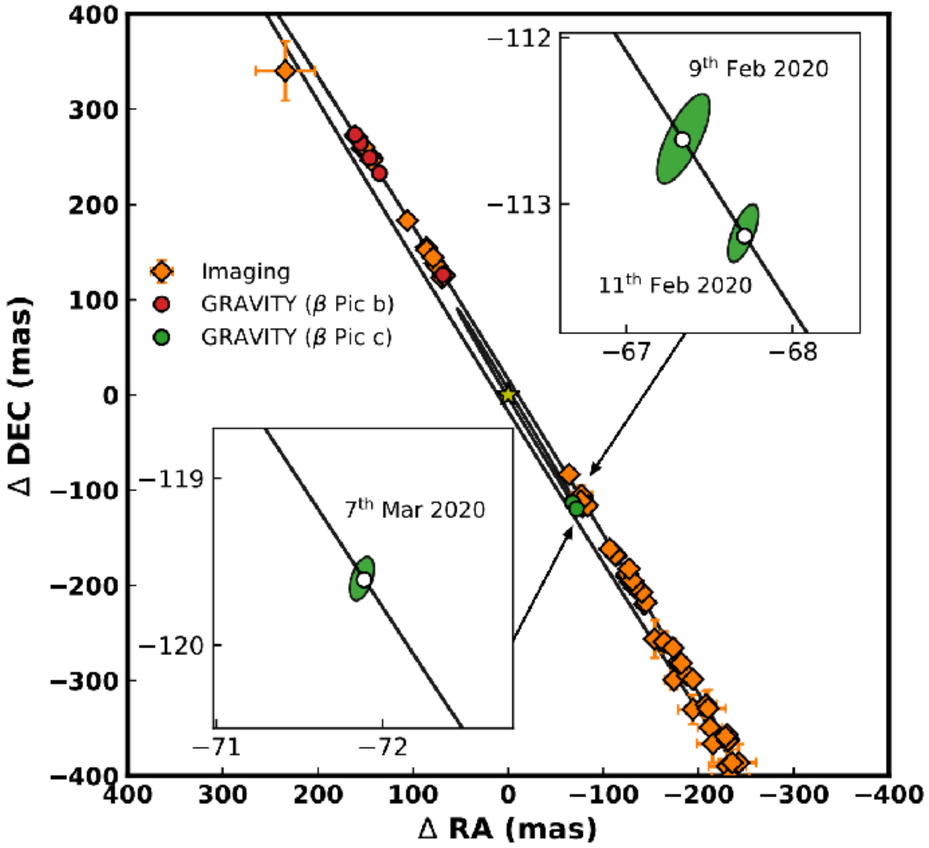
Key facilities

Ground



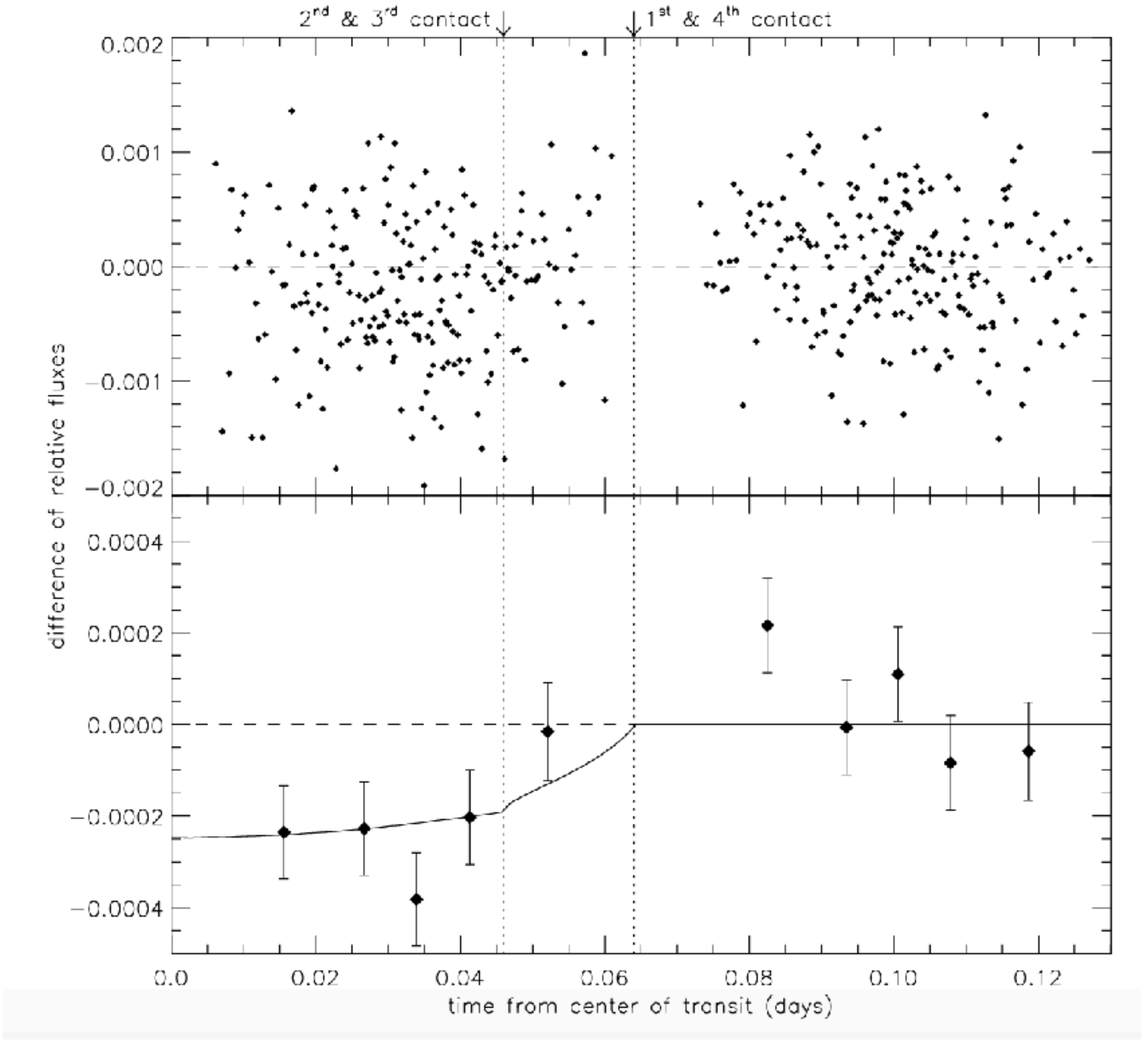
Mask out stellar light with a coronagraph (e.g. SPHERE, GPI)

Nowak et al. 2020, A&A



Spatially separate the star from the planet with interferometry (VLTI/GRAVITY)

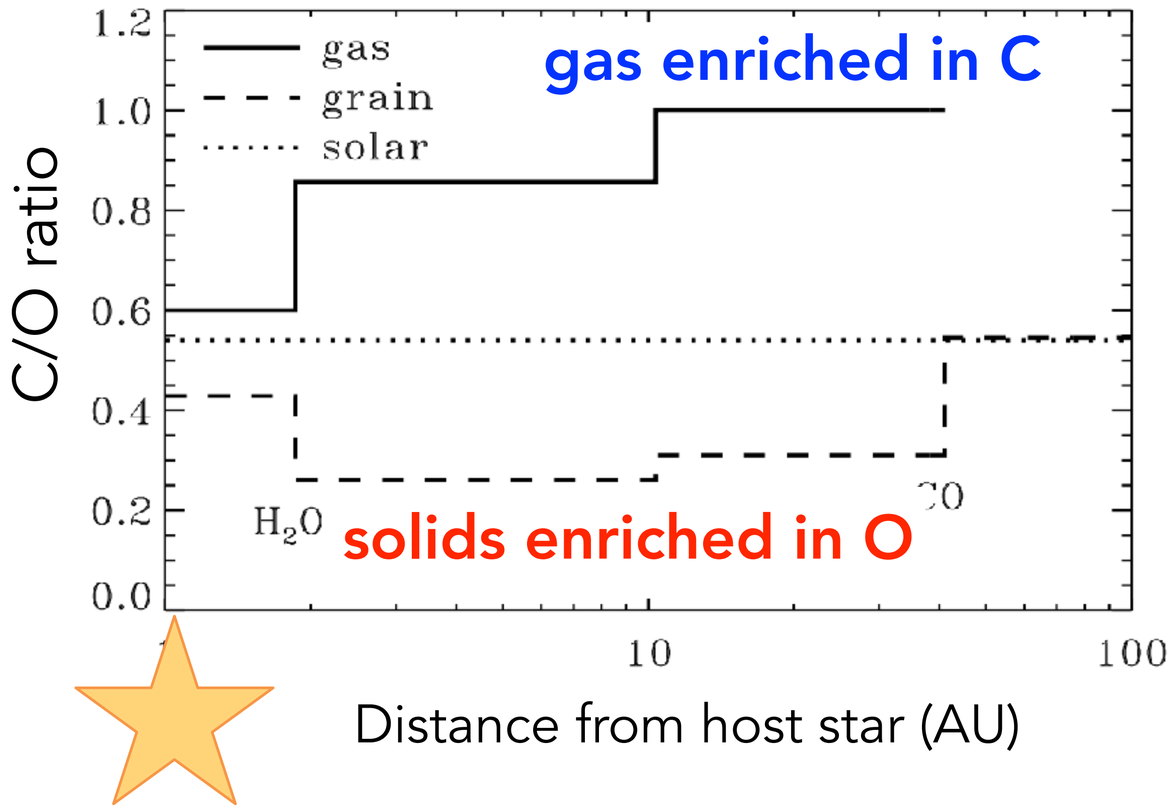
It *is* possible to reach the photon noise limit and detect small features from atmospheres



- The *FIRST* detection of an exoplanet atmosphere: sodium absorption detected in the hot Jupiter HD 209458b with four transits from the Hubble Space Telescope
- Feature amplitude :
  delta_d = 2.3e-4 +/- 0.57

— Charbonneau et al. 2002

Why do we care what atmospheres are made of? They teach us about planet formation and evolution



Gas giant atmospheres are sensitive to:

- formation location
- ratio of gas/solid accretion
- Formation time

— Öberg et al. 2011,
Eistrup et al. 2018

Terminology

How do we talk about the ingredients that planets are made of?

We classify elements based on their condensation temperature:

- **Gas** - hydrogen/helium
- **Volatile** - C, N, O (often in molecular form [e.g. H2O, CO] and called **ices**)
- **Refractory** - Fe, Si

Metallicity - [Fe/H], often referred to in units of solar metallicity (e.g. 10x solar)

Elemental abundance ratios: C/O, C/H, O/H

Expectations for gas giant atmospheres

Which molecules *should* be present at a given temperature, pressure?
Gibbs free energy minimisation

$$G(p,T) = U + pV - TS,$$

credit: wikipedia

- U is the internal energy (SI unit: joule),
- p is pressure (SI unit: pascal),
- V is volume (SI unit: m^3),
- T is the temperature (SI unit: kelvin),
- S is the entropy (SI unit: joule per kelvin),

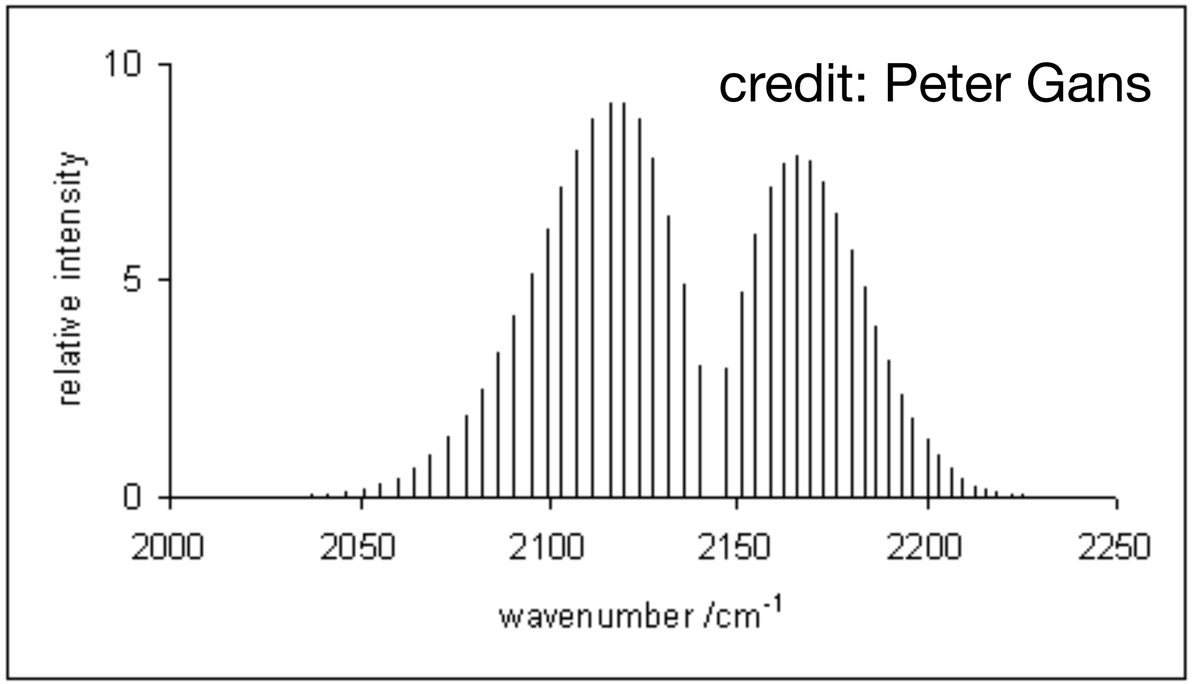
7 2018A&A...614A...1W 2018-06 cited: 122

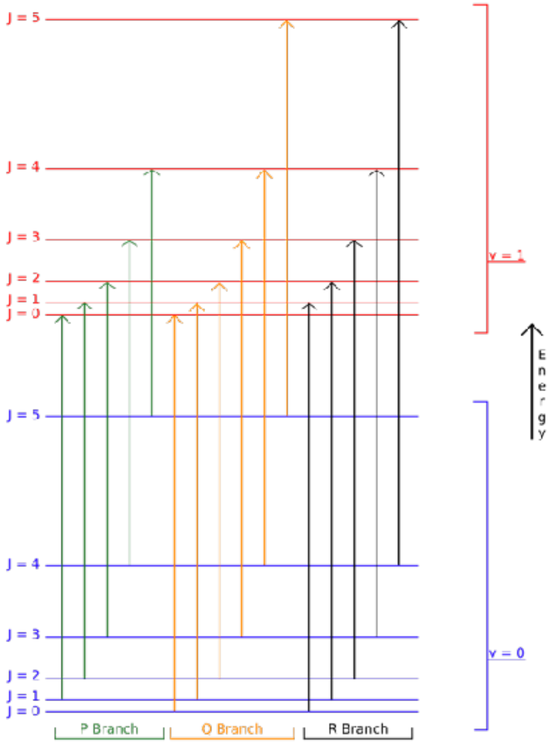
Equilibrium chemistry down to 100 K. Impact of silicates and phyllosilicates on the carbon to oxygen ratio

Woitke, P.; Helling, Ch.; Hunter, G. H.; Millard, J. D.; Turner, G. E.; Worters, M.; Blecic, J.; Stock, J. W.

Expectations for gas giant atmospheres

Which molecules are most spectrally active (= easiest to observe)?

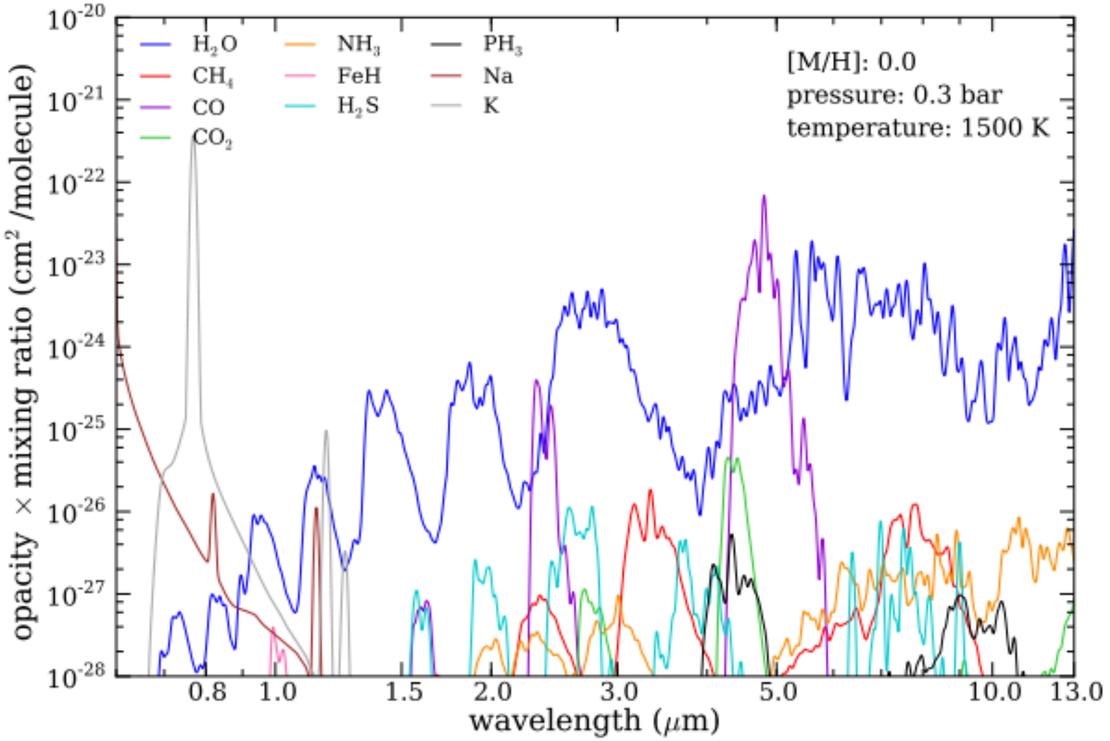


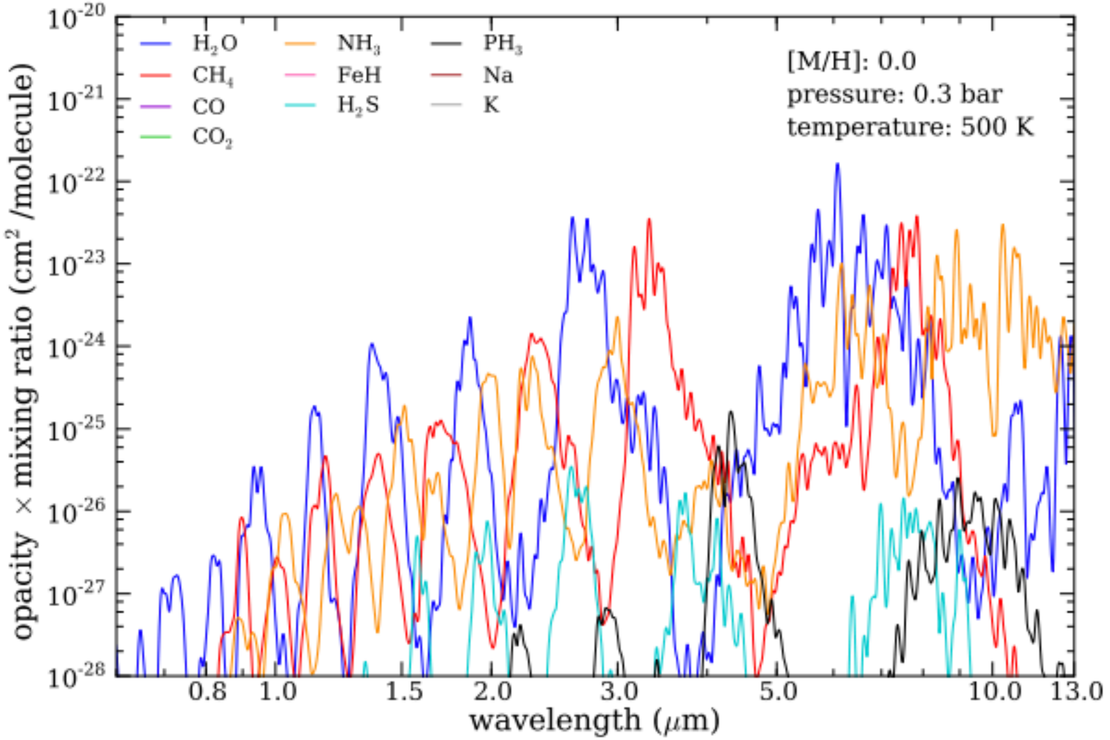


Left: Simulated vibration-rotation line spectrum of CO
Right: Schematic ro-vibrational energy level diagram for a linear molecule

Expectations for gas giant atmospheres

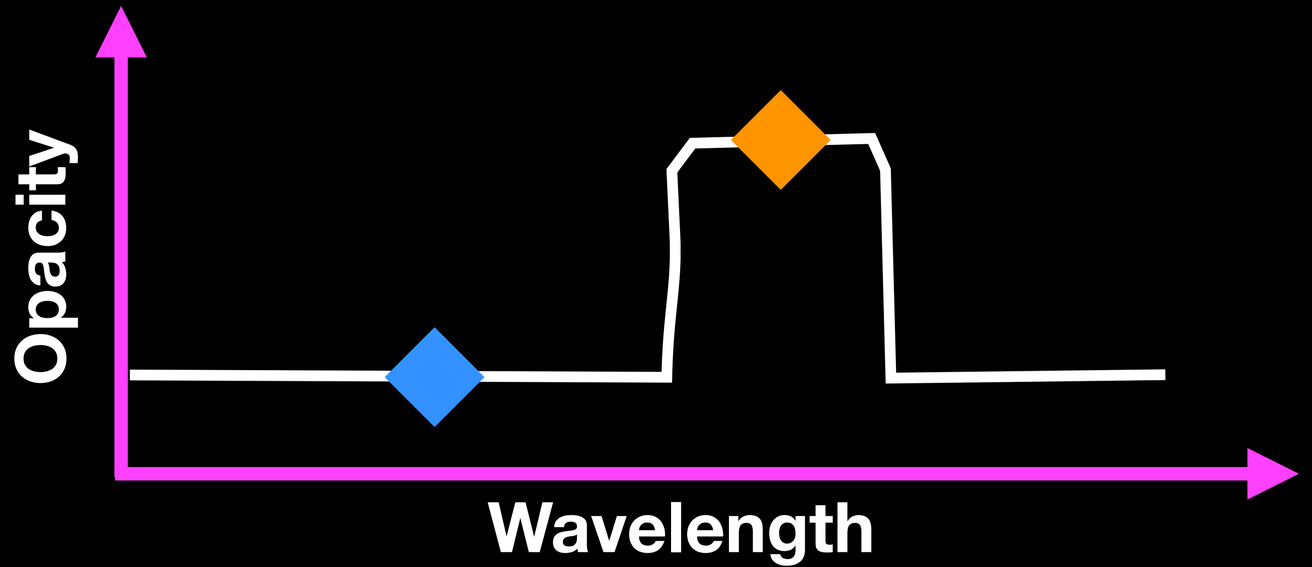
Credit: Caroline Morley

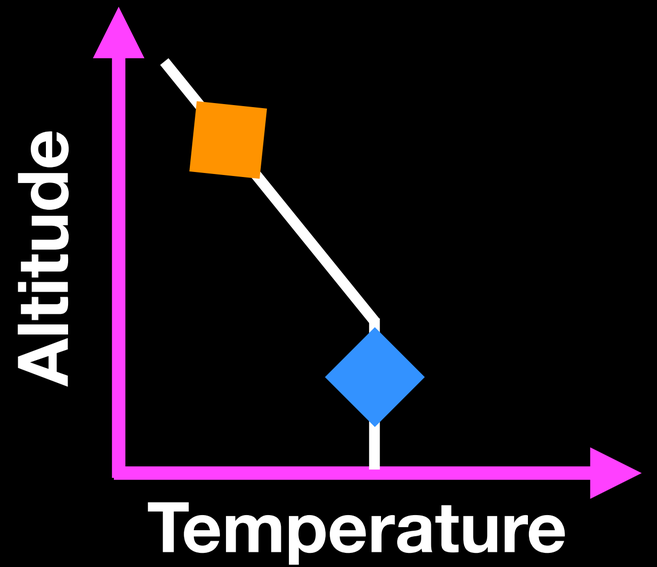


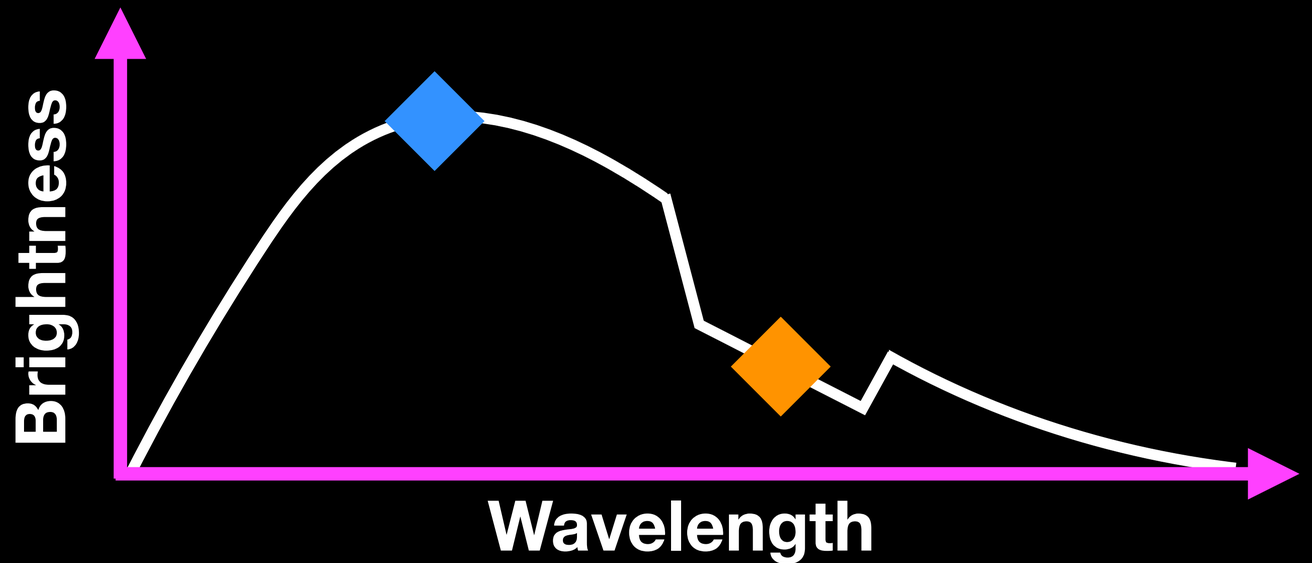


Dominant absorbers depend on temperature, metallicity, and elemental abundance ratios
H2O, CO, CO2, CH4, NH3, Na, K are all possibilities

Linking atmosphere properties to observed emission

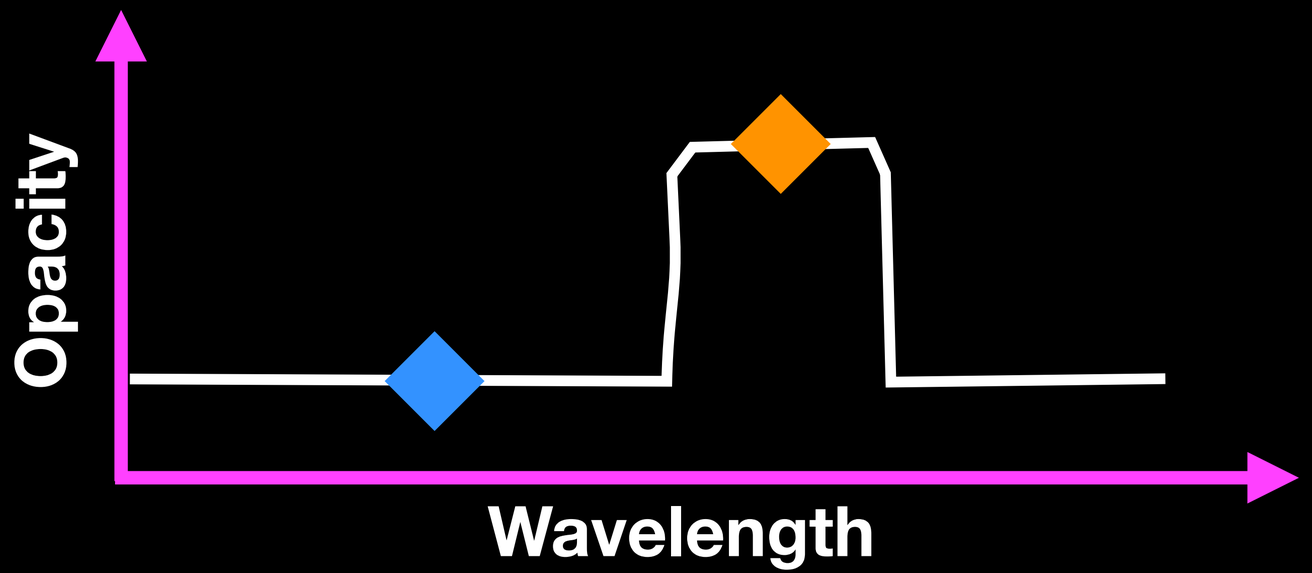


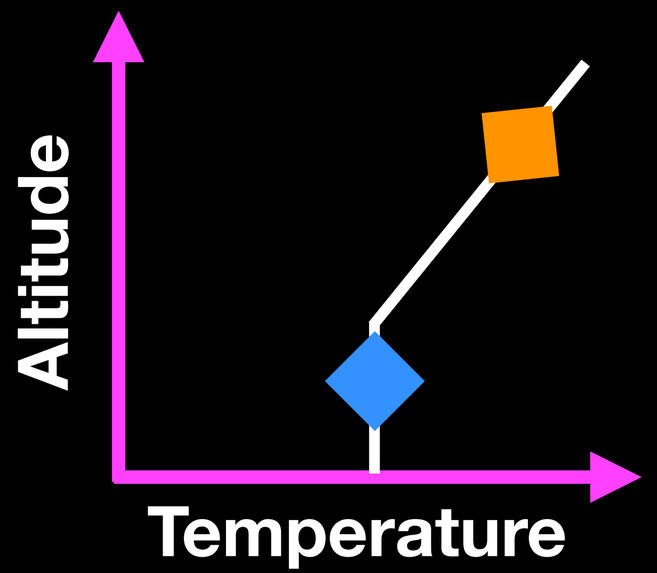


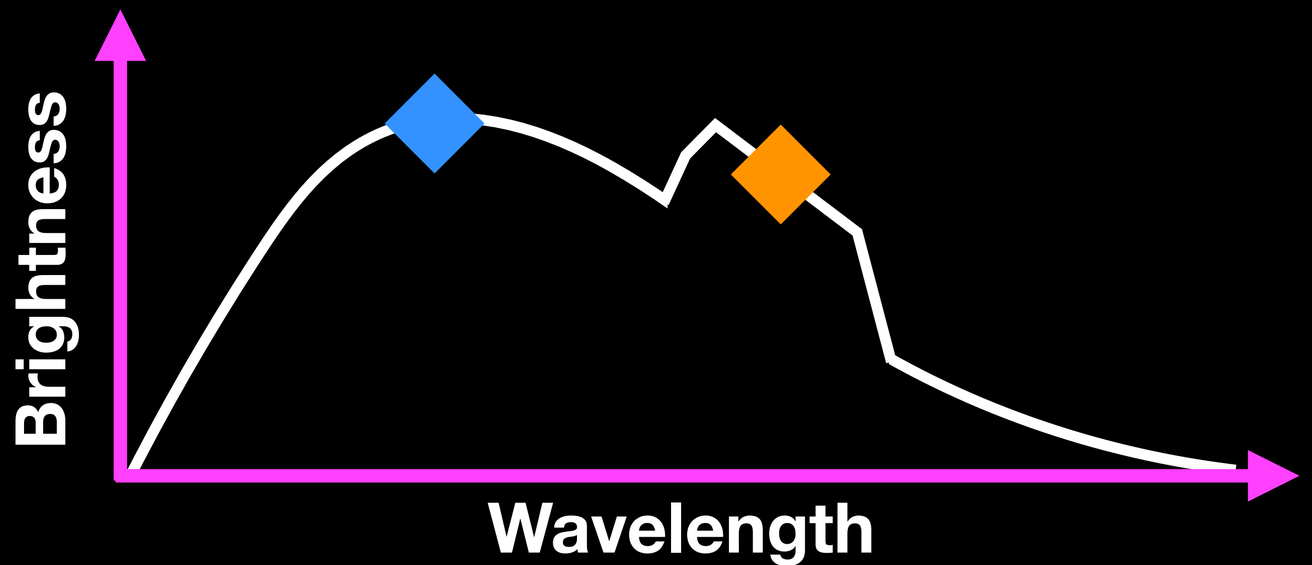


Credit: Tom Mikal-Evans

Linking atmosphere properties to observed emission

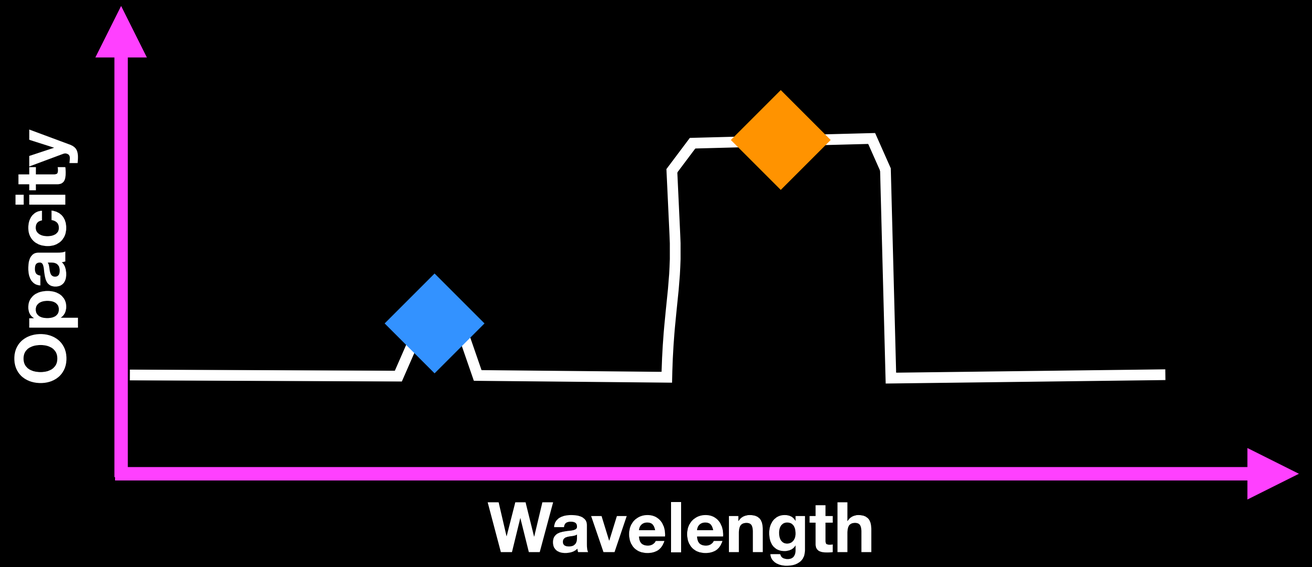


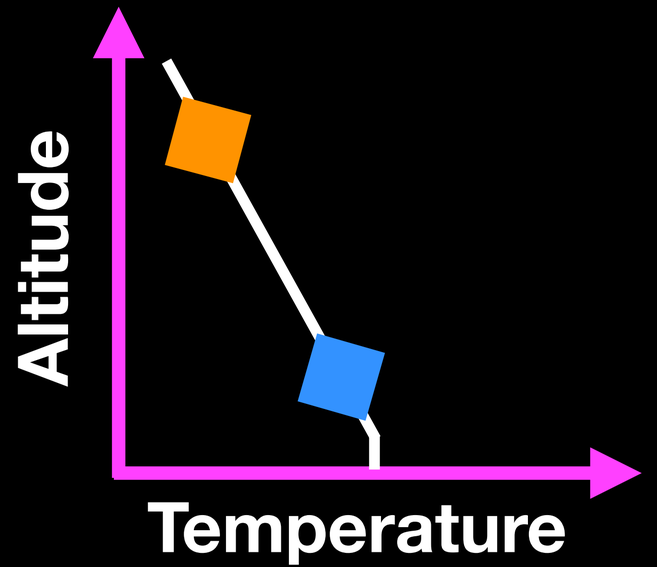


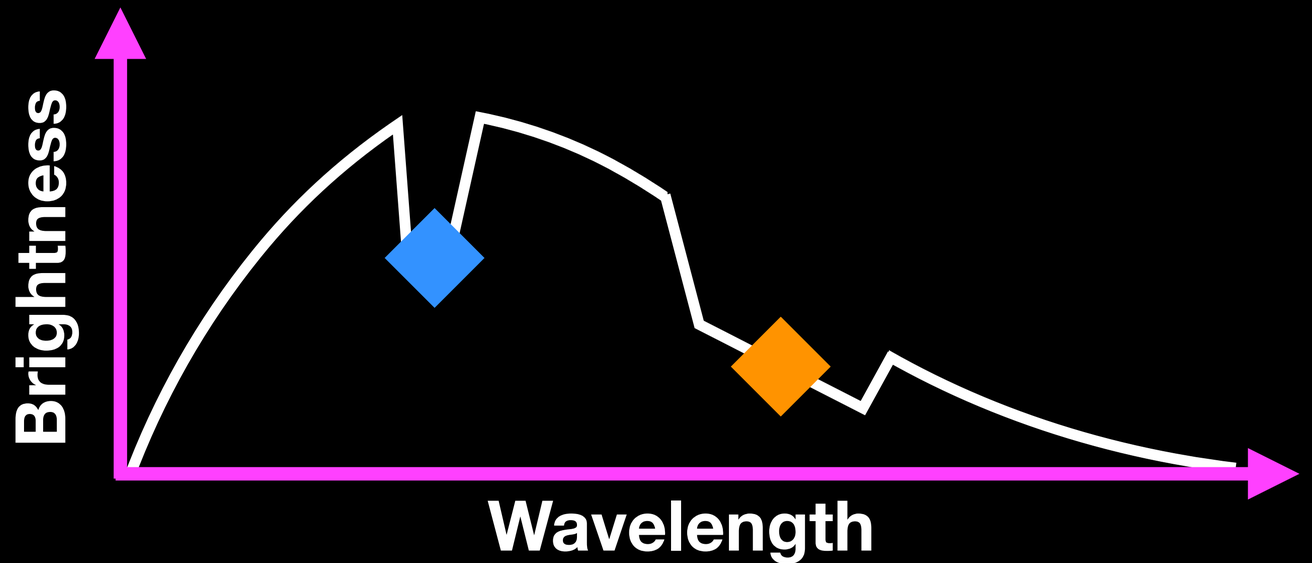


Credit: Tom Mikal-Evans

Linking atmosphere properties to observed emission

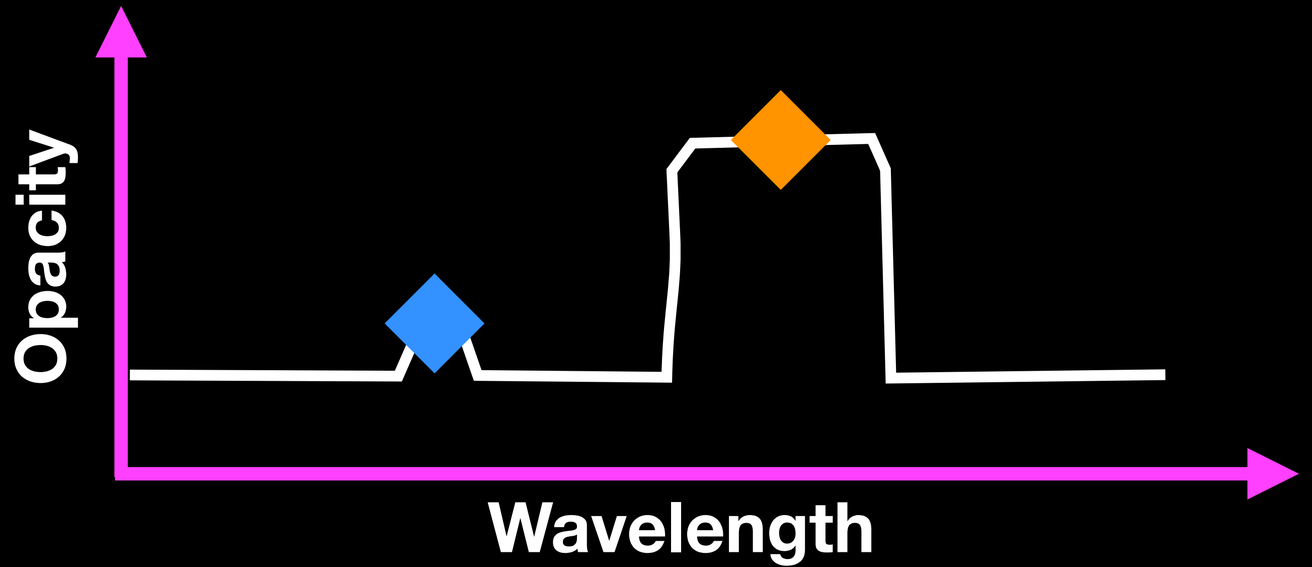


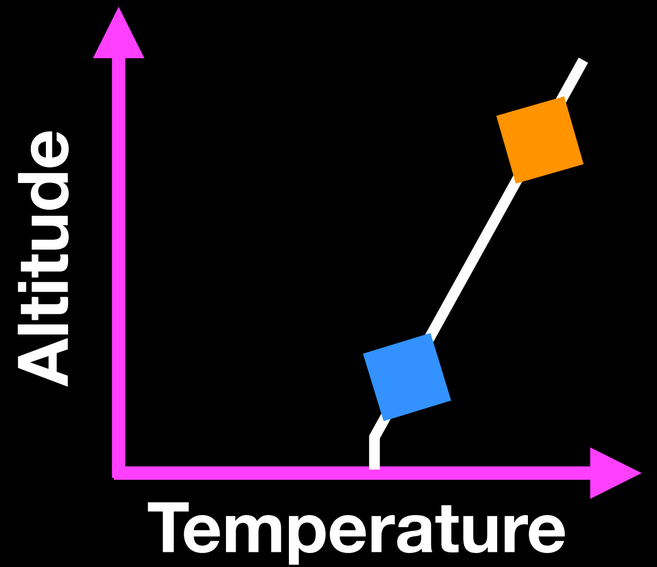


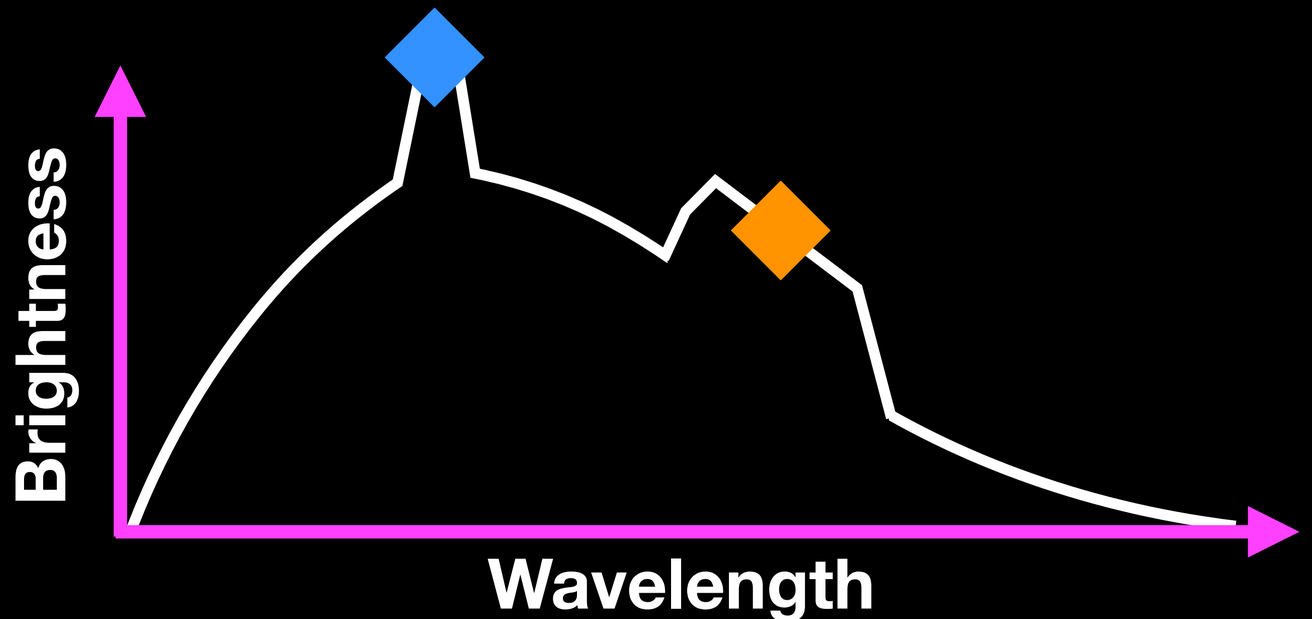


Credit: Tom Mikal-Evans

Linking atmosphere properties to observed emission

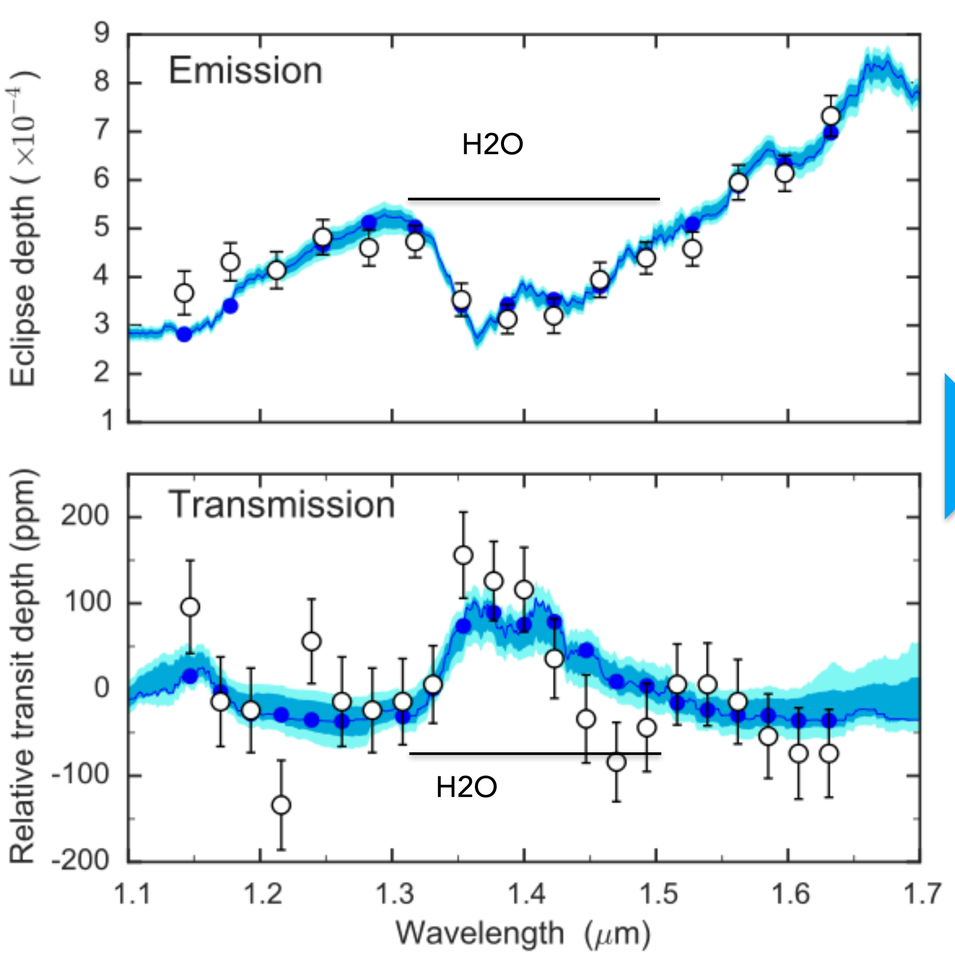


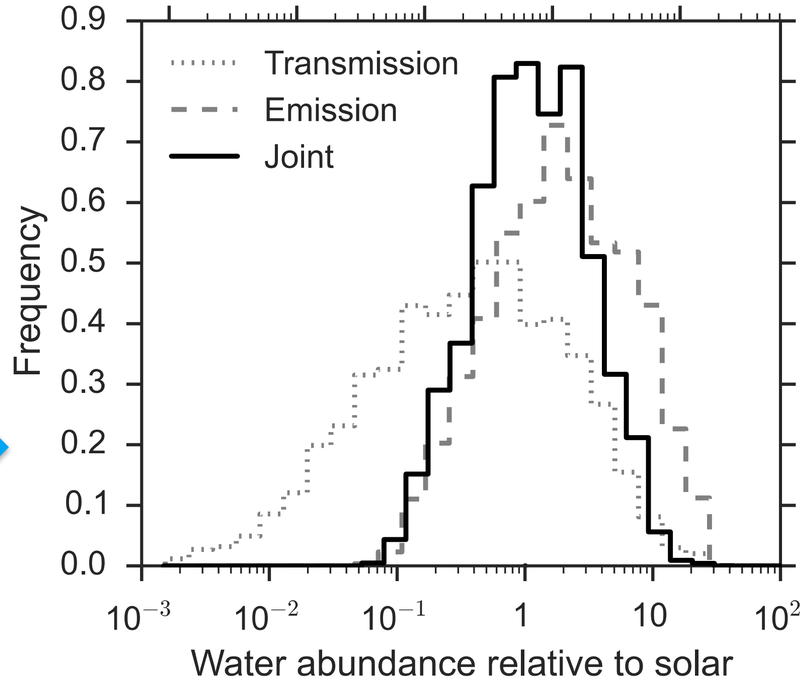




Credit: Tom Mikal-Evans

Measurements of hot Jupiter chemical composition

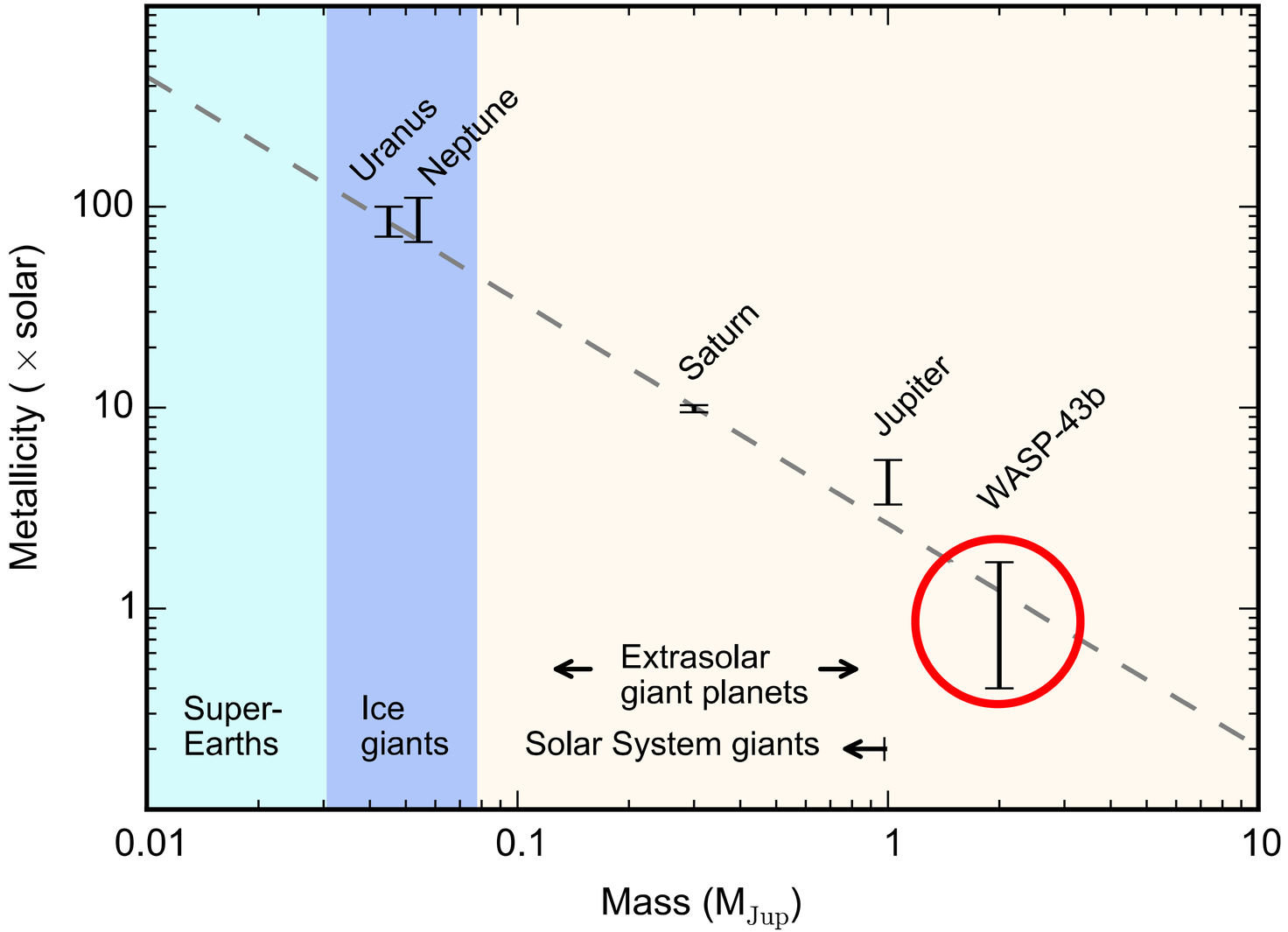




~solar abundance of water for the hot Jupiter WASP-43b from HST/WFC3 spectra

— Kreidberg et al. 2014

WASP-43b follows the Solar System metal enrichment trend

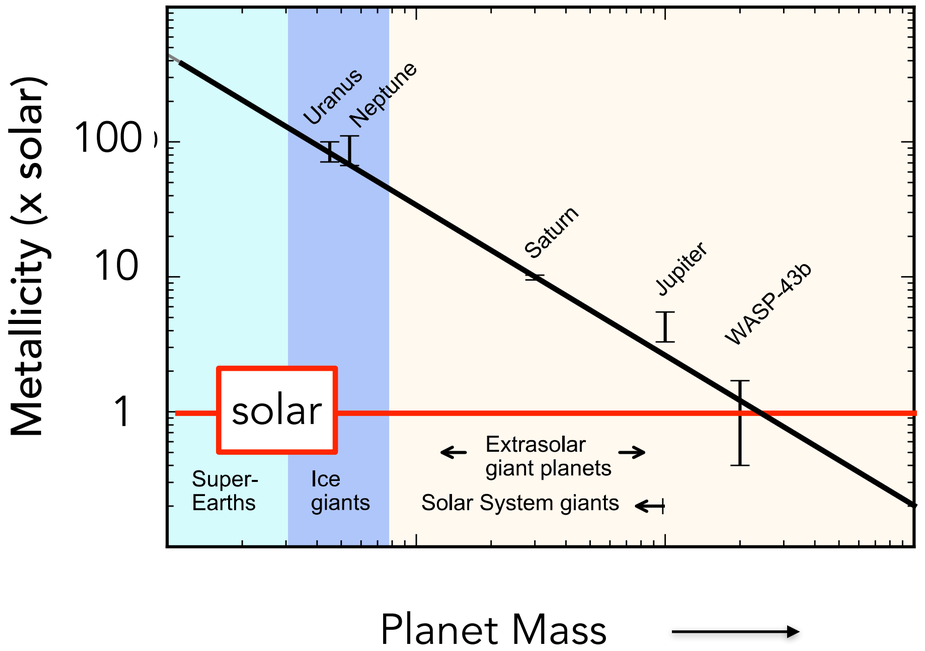


— Kreidberg et al. 2014

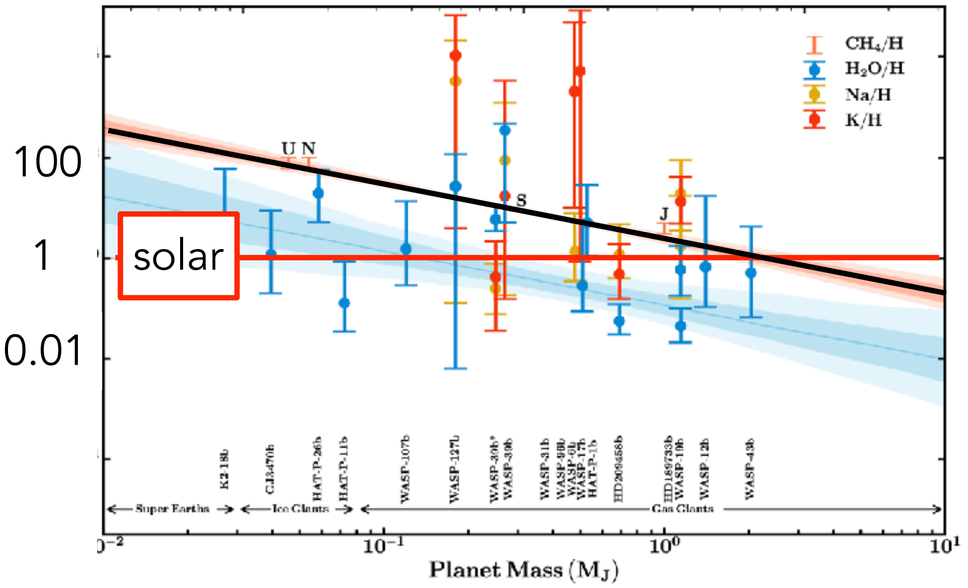
How it started

How it's going

Kreidberg et al. 2014b

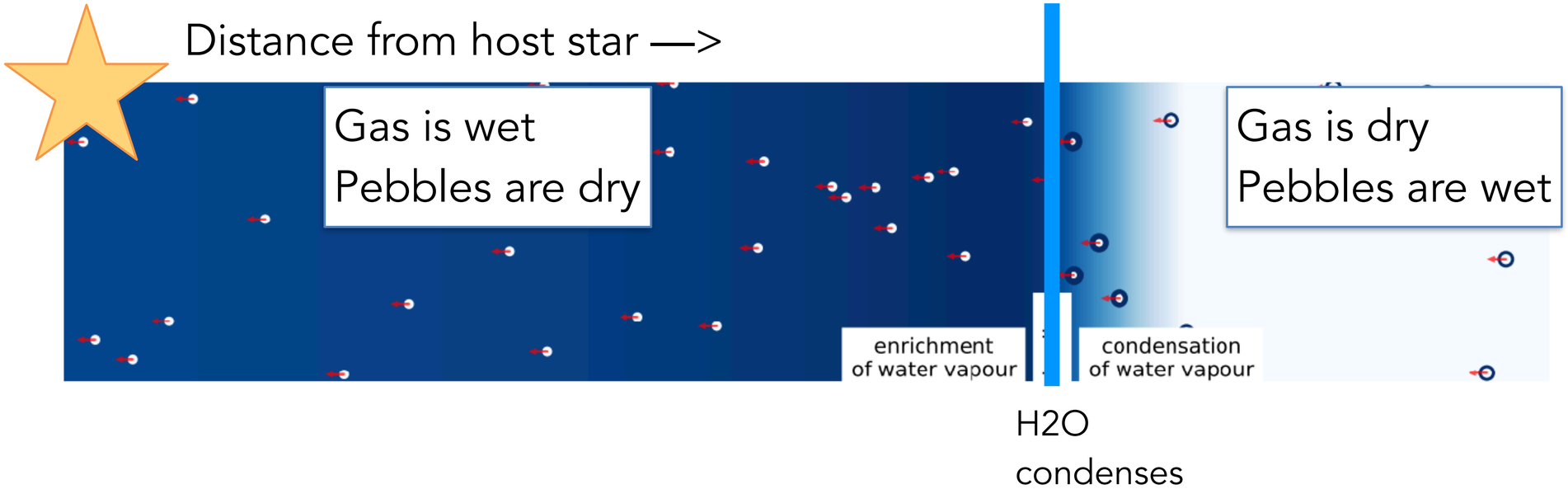


Welbanks et al. 2019



- As usual, exoplanets are much more diverse than the SS!
- Many gas giants appear to be depleted in H2O (?)

Are low atmospheric water abundances physically plausible? yes!



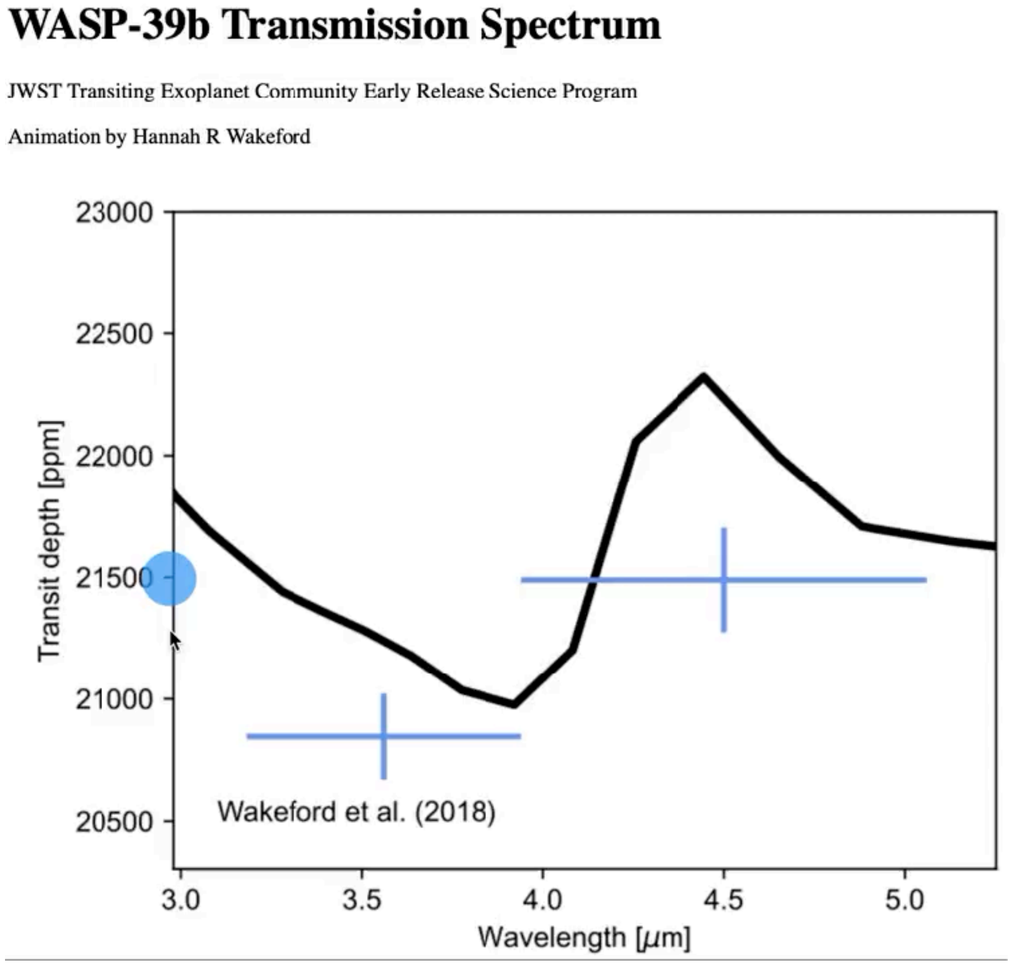
Dry atmospheres naturally arise in the pebble accretion model for planets accreting dry gas beyond the water ice line
— Schneider & Bitsch 2021

Get ready for a JWST glow up!!!!!



JWST has a big mirror (10x larger collecting area than Hubble)
JWST has broad wavelength coverage (0.6 - 12 micron spectroscopy, up to 30 micron photometry)

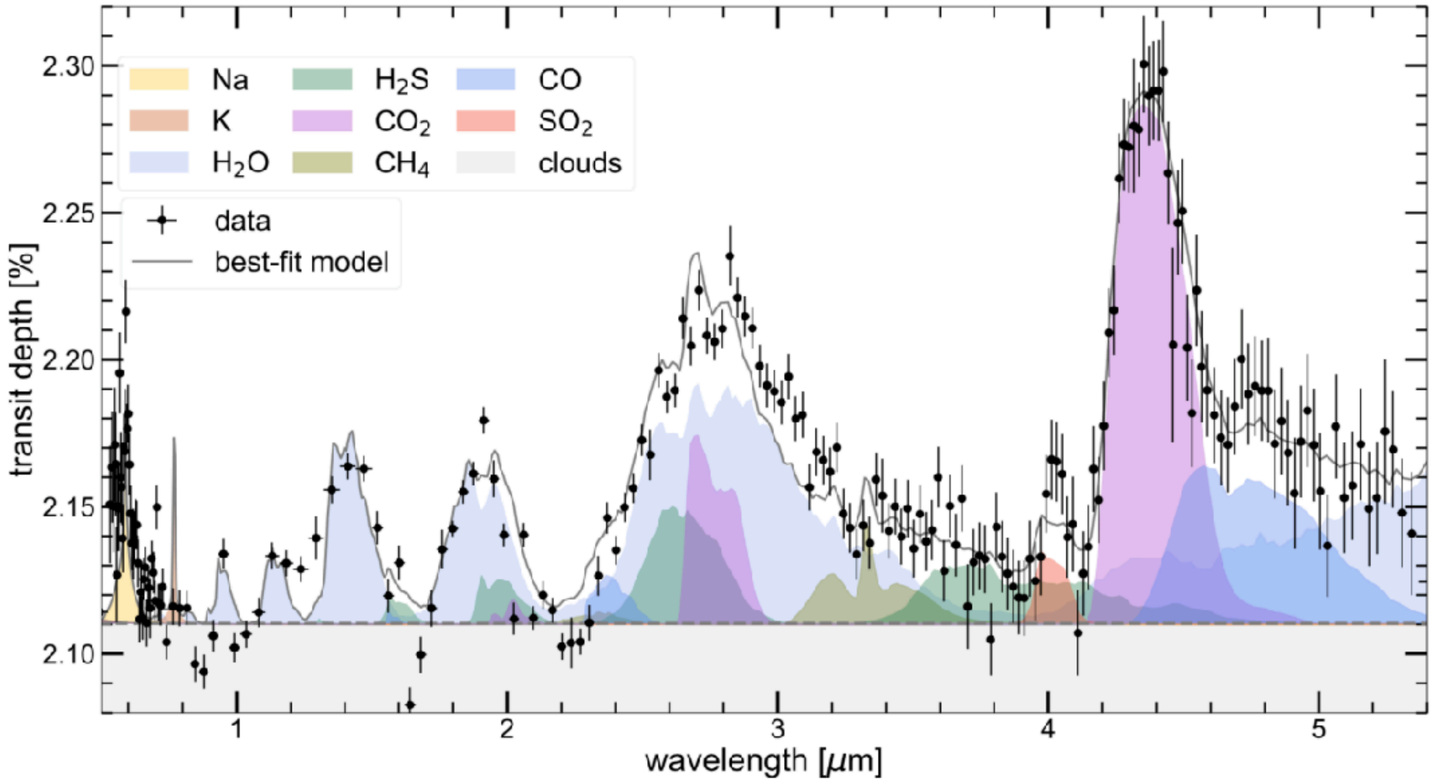
What do spectra typically look like? Post-2022



WASP-39b through the eyes of JWST

— Hannah Wakeford and the Transiting Exoplanet Community ERS team

JWST opens the door to measuring abundances of multiple species

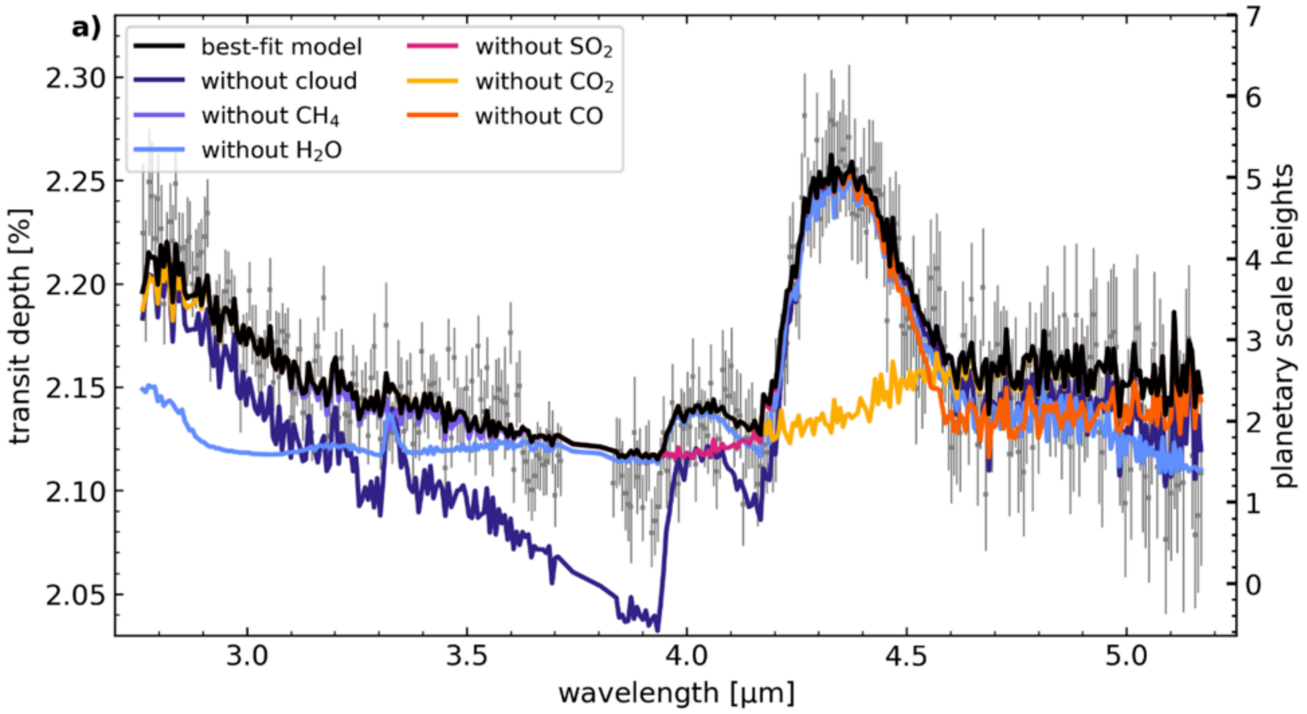


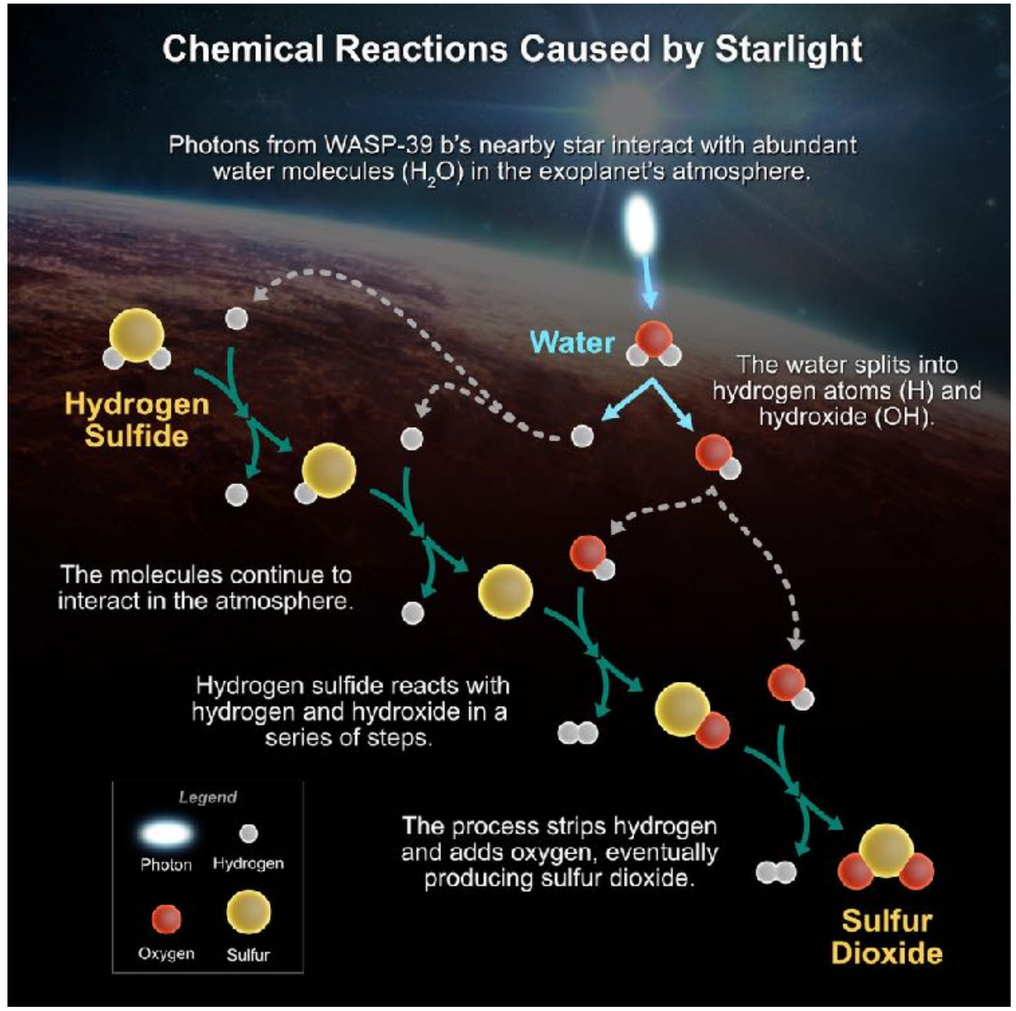
Transiting Exoplanet Community JWST Early Release Science Program results:

Feinstein et al. 2023,
Alderson et al. 2023,
Ahrer et al. 2023,
Rustamkulov et al. 2023

Presence of CO2 -> metallicity ~ 10x solar

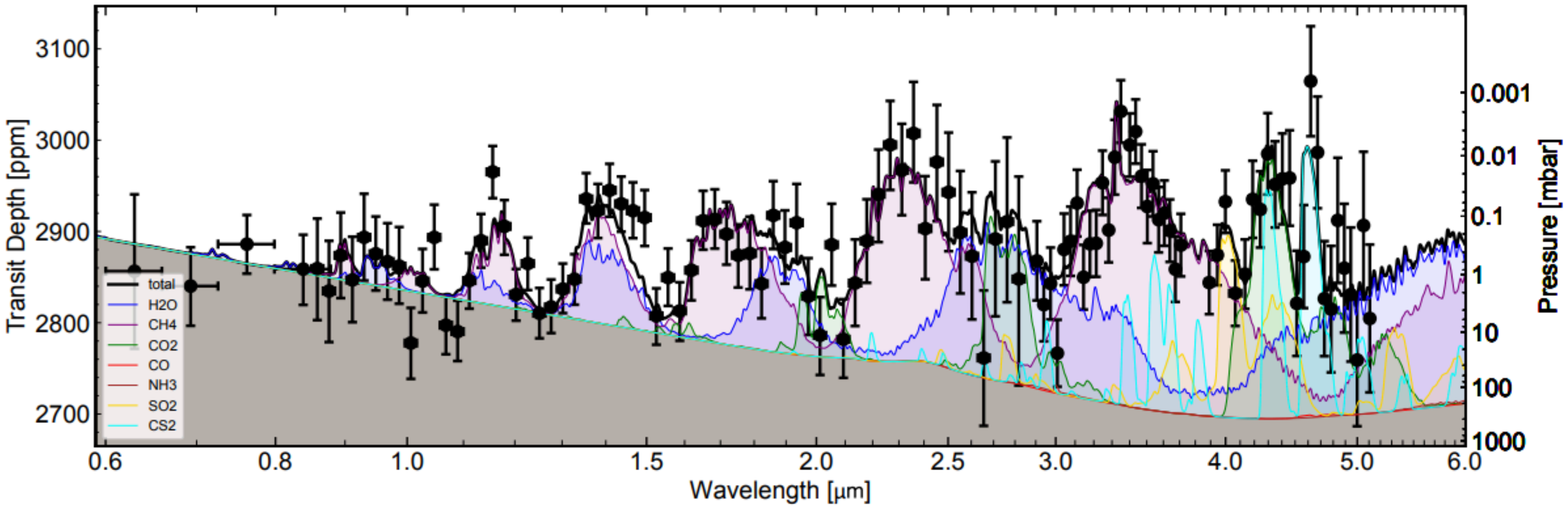
Photochemistry shapes the observed spectrum of WASP-39b





Alderson et al. 2023
Tsai et al. 2023

Panchromatic spectrum for sub-Neptune TOI 270d
Photochemistry and vertical mixing!

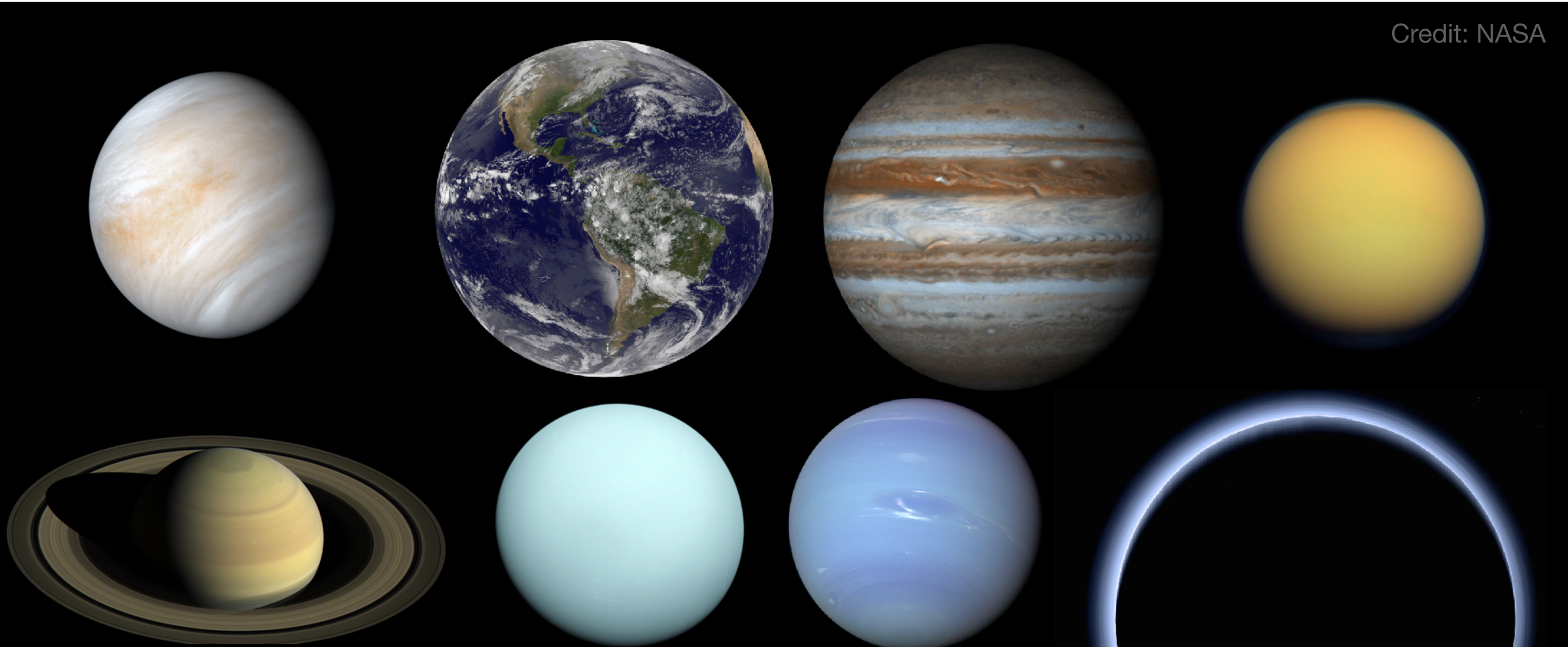


Metal-rich atmosphere (MMW = 5 +/-1 ; metal mass fraction near 50%)

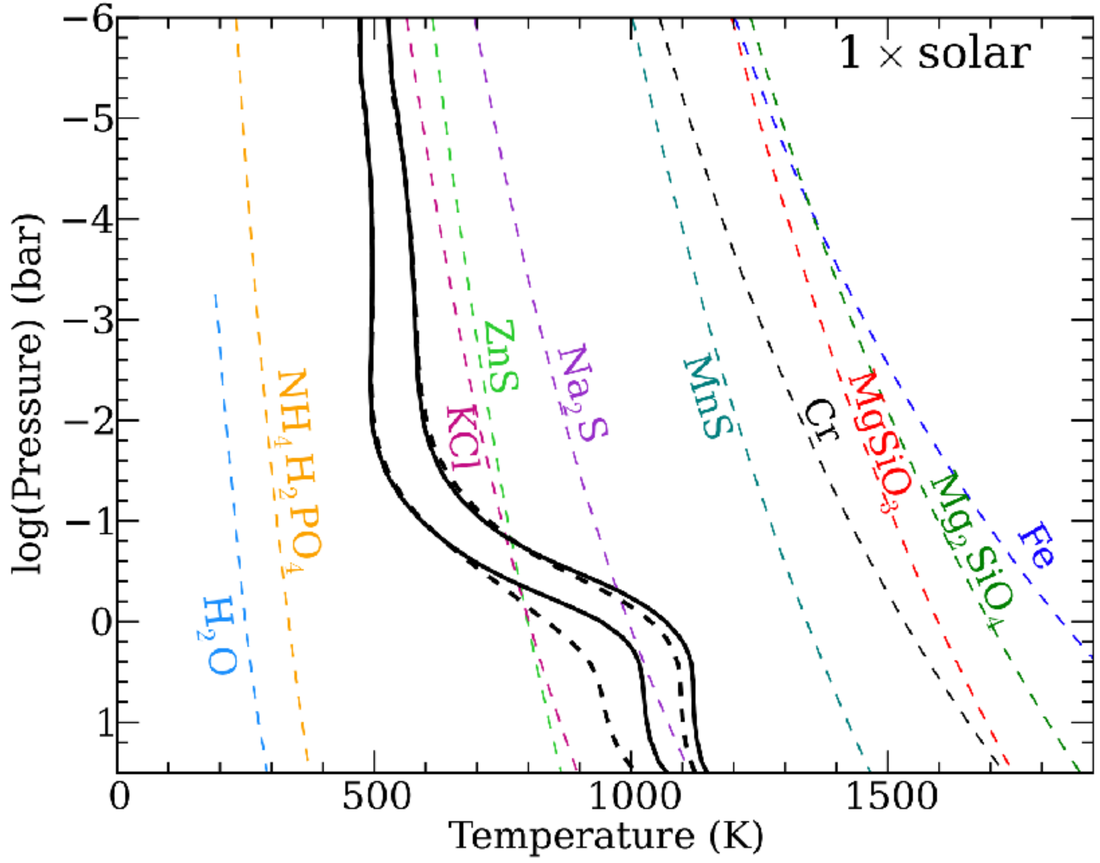
Benneke et al., submitted

Clouds in exoplanet atmospheres

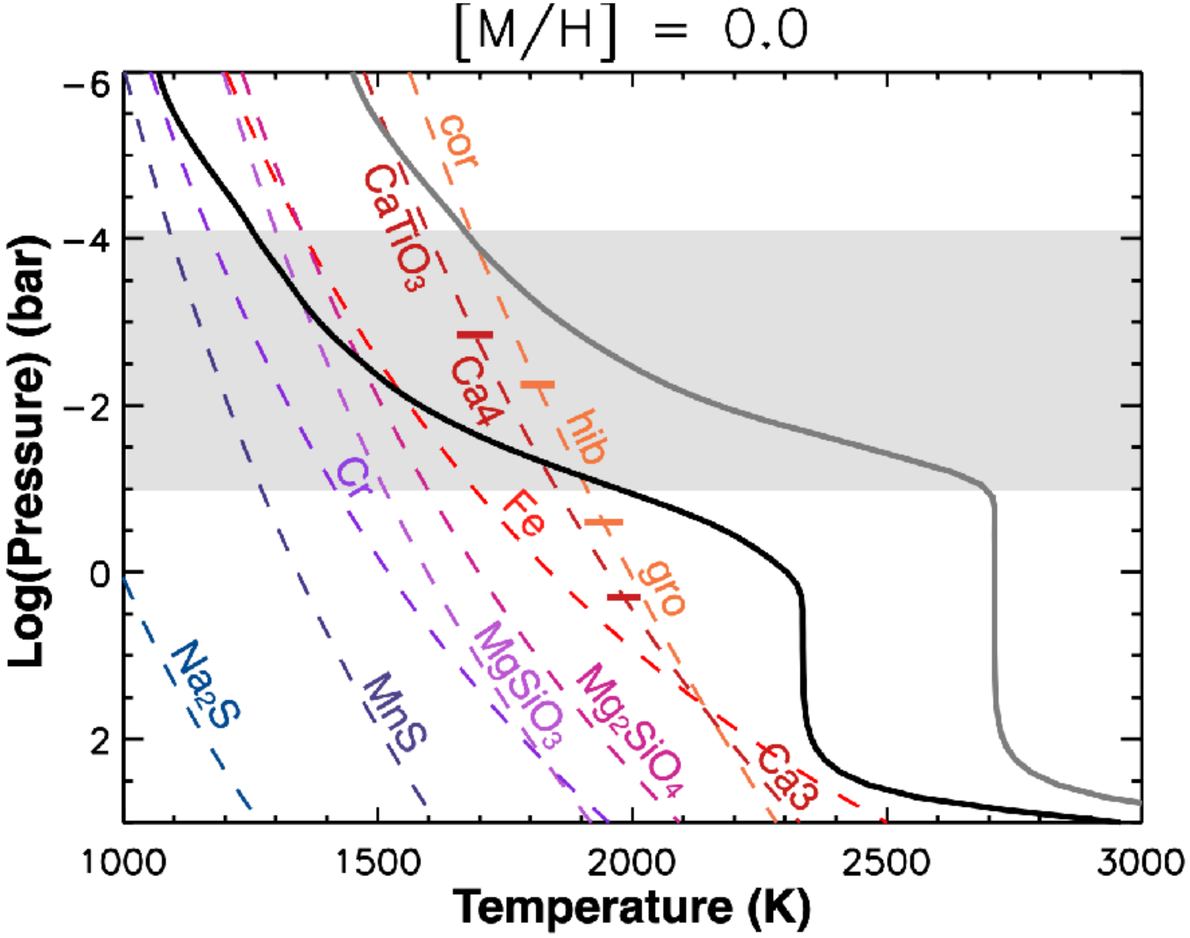
What do all these planets have in common? Clouds and hazes!



Theoretical models predict many different condensates I. Equilibrium clouds

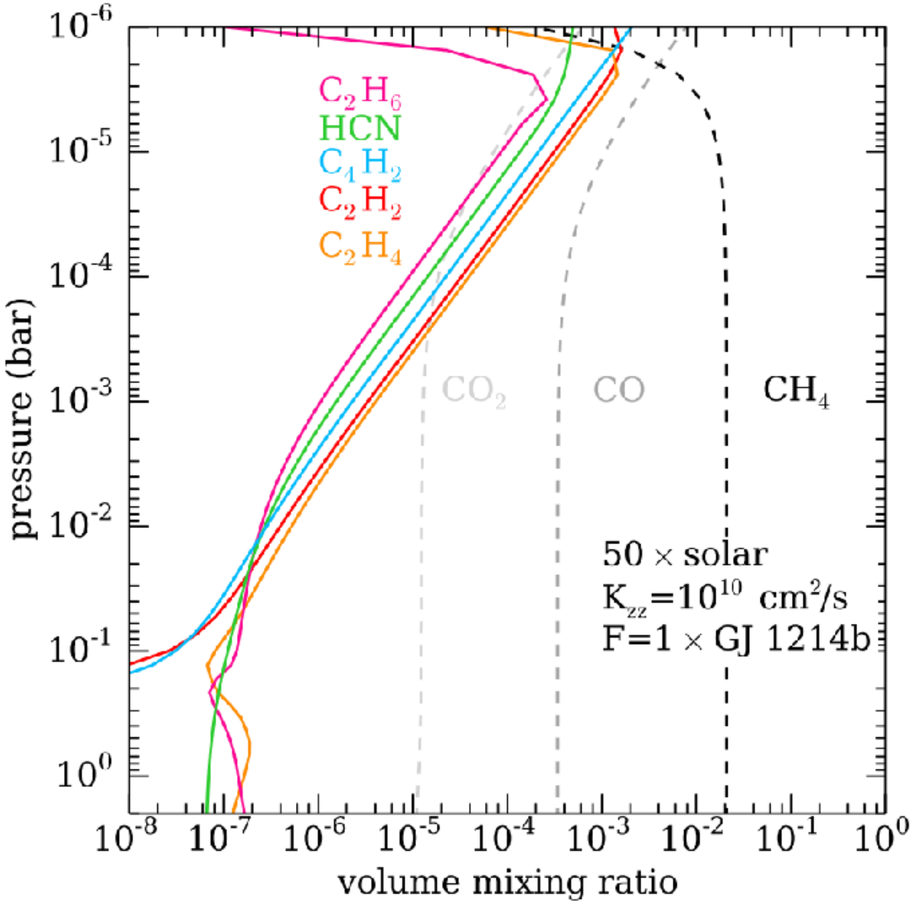


Morley et al. 2013

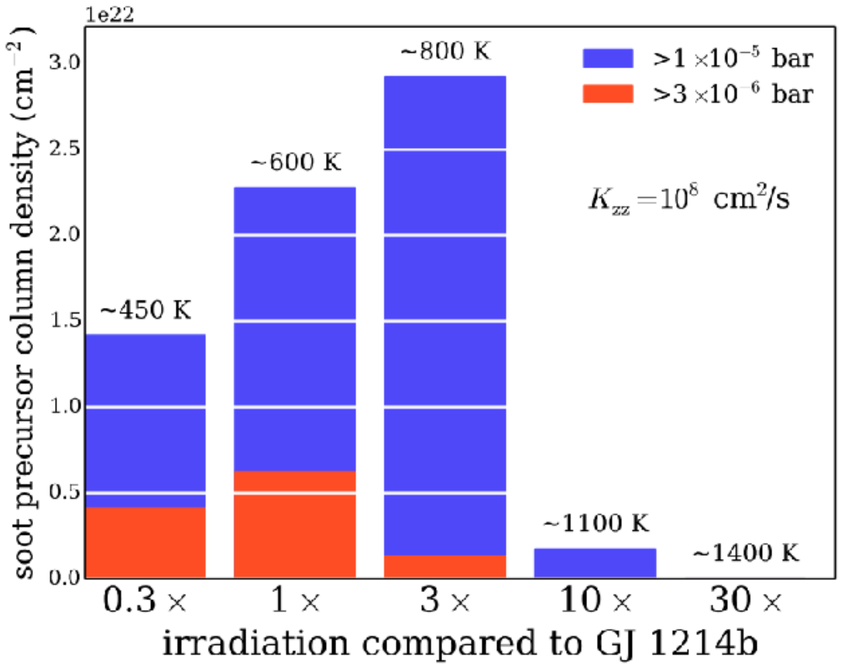


Wakeford et al. 2017

Theoretical models predict many different condensates
I. Photochemical hazes



Morley et al. 2015

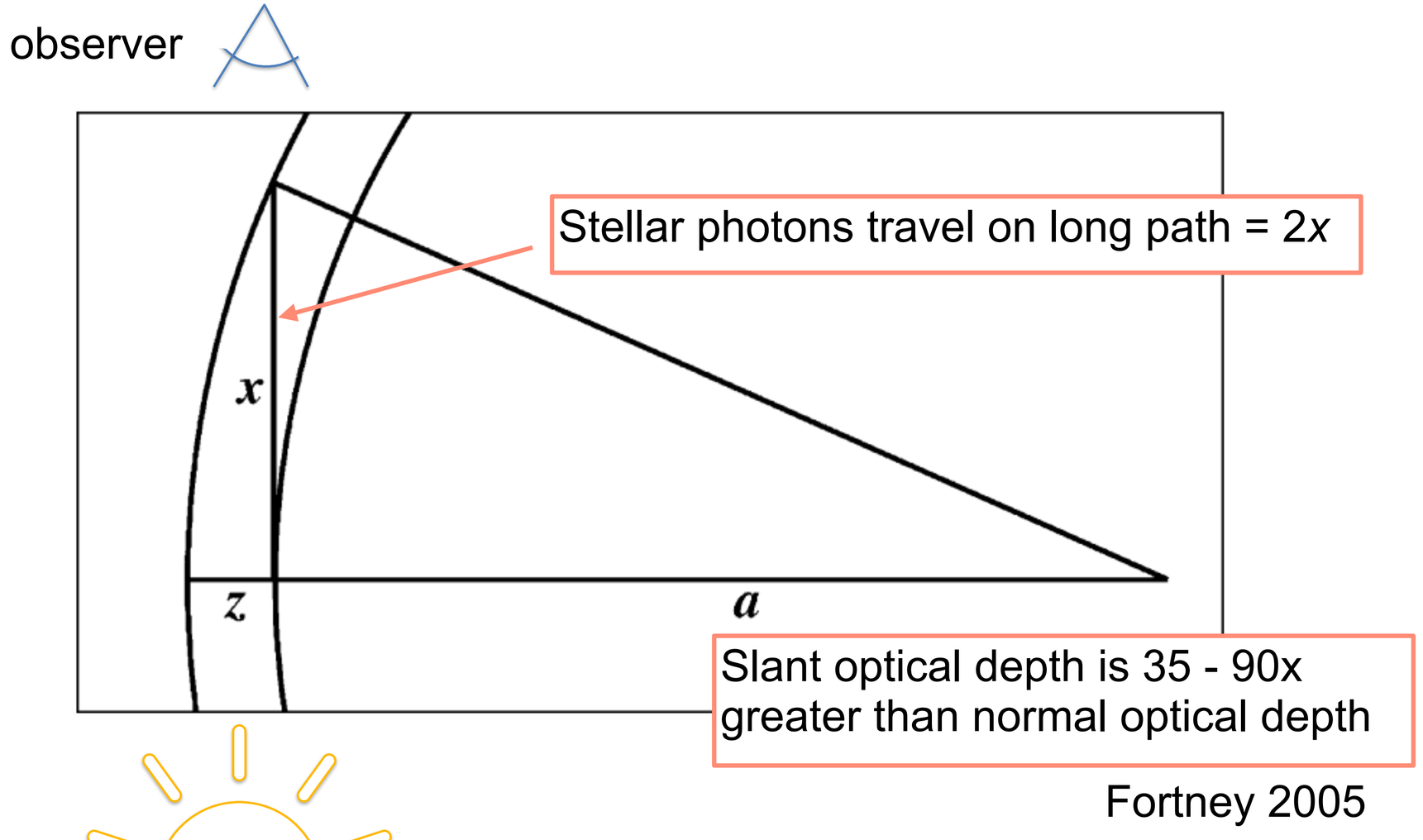


Photochemistry generates haze precursors

Carbon and sulphur hazes are common

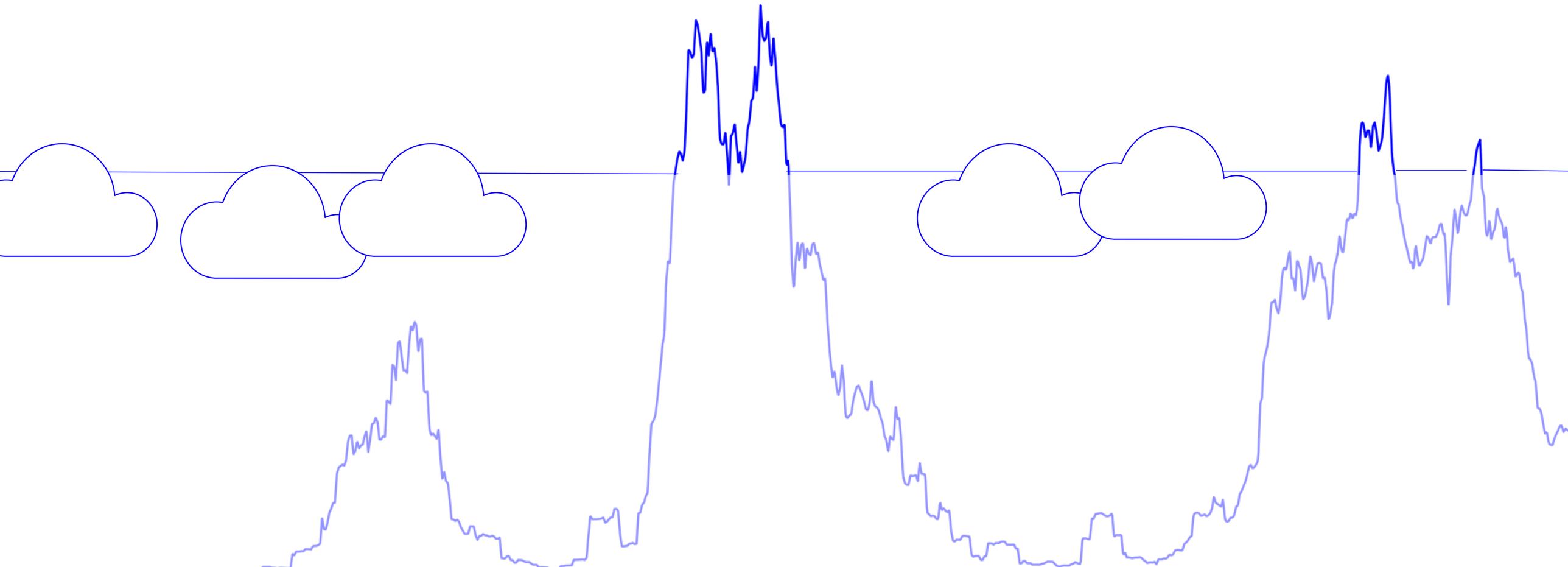
“Tholin” a synonym for hydrocarbon hazes

Transmission spectra are strongly affected by clouds

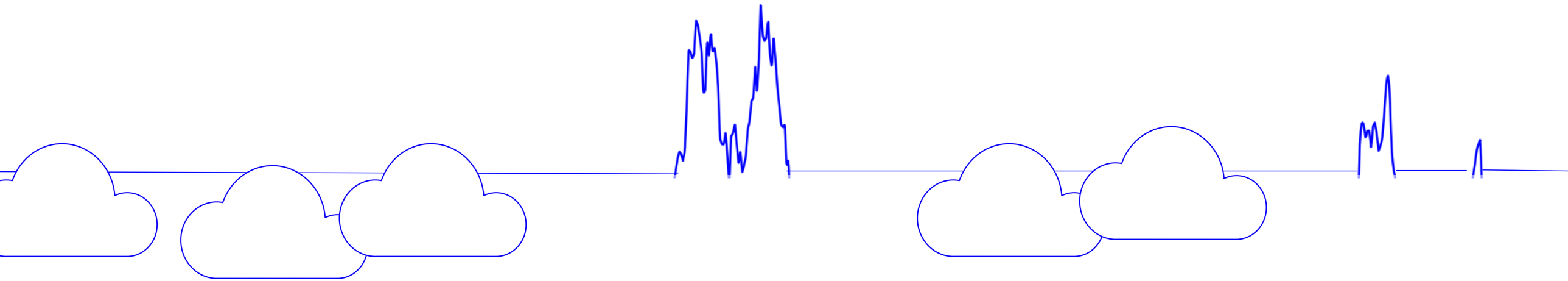


Fortney 2005

What do clouds/haze look like in transmission spectra?

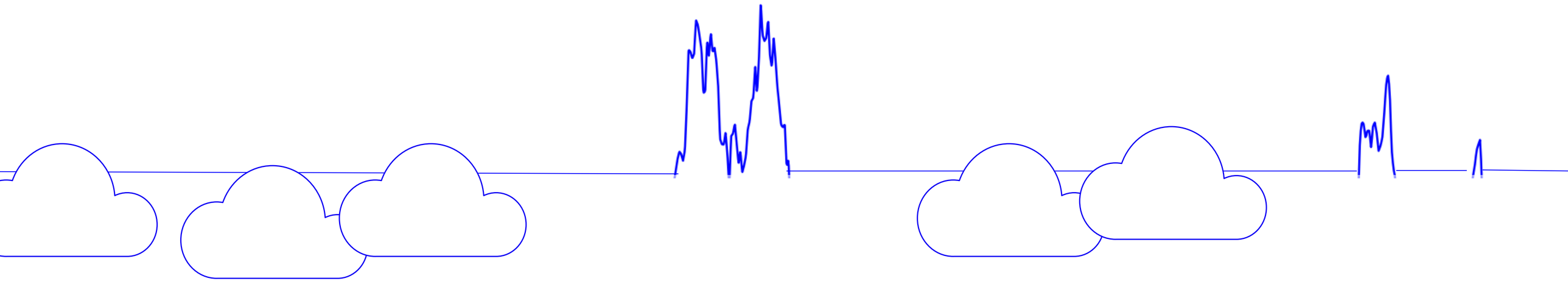


What do clouds/haze look like in transmission spectra?



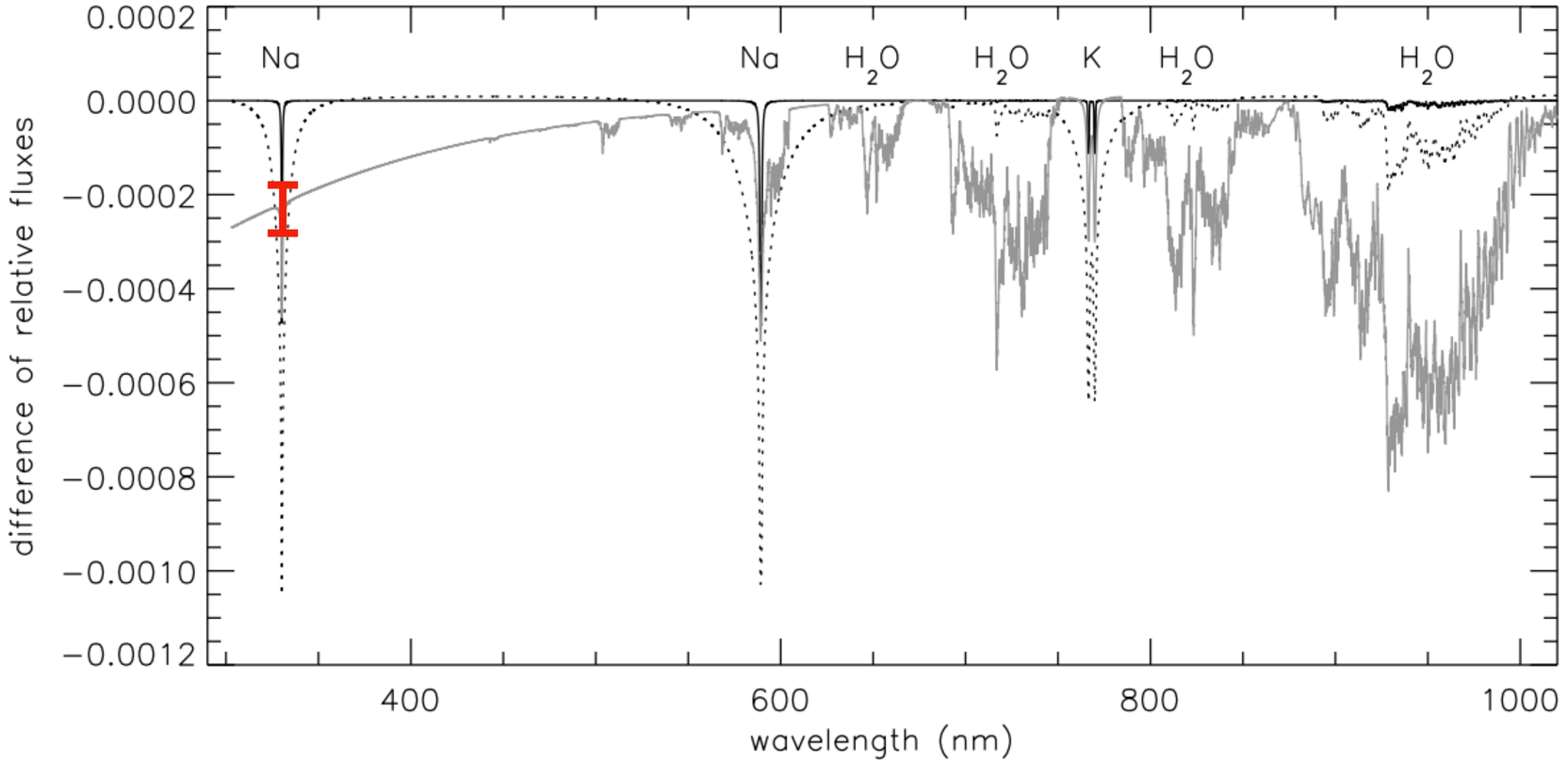
“gray cloud” approximation — condensates have constant opacity with wavelength

What do clouds/haze look like in transmission spectra?



Note: clouds properties are somewhat degenerate with mean molecular weight in atmospheric retrieval

Observational evidence for condensates
I. Truncated features in transmission spectra

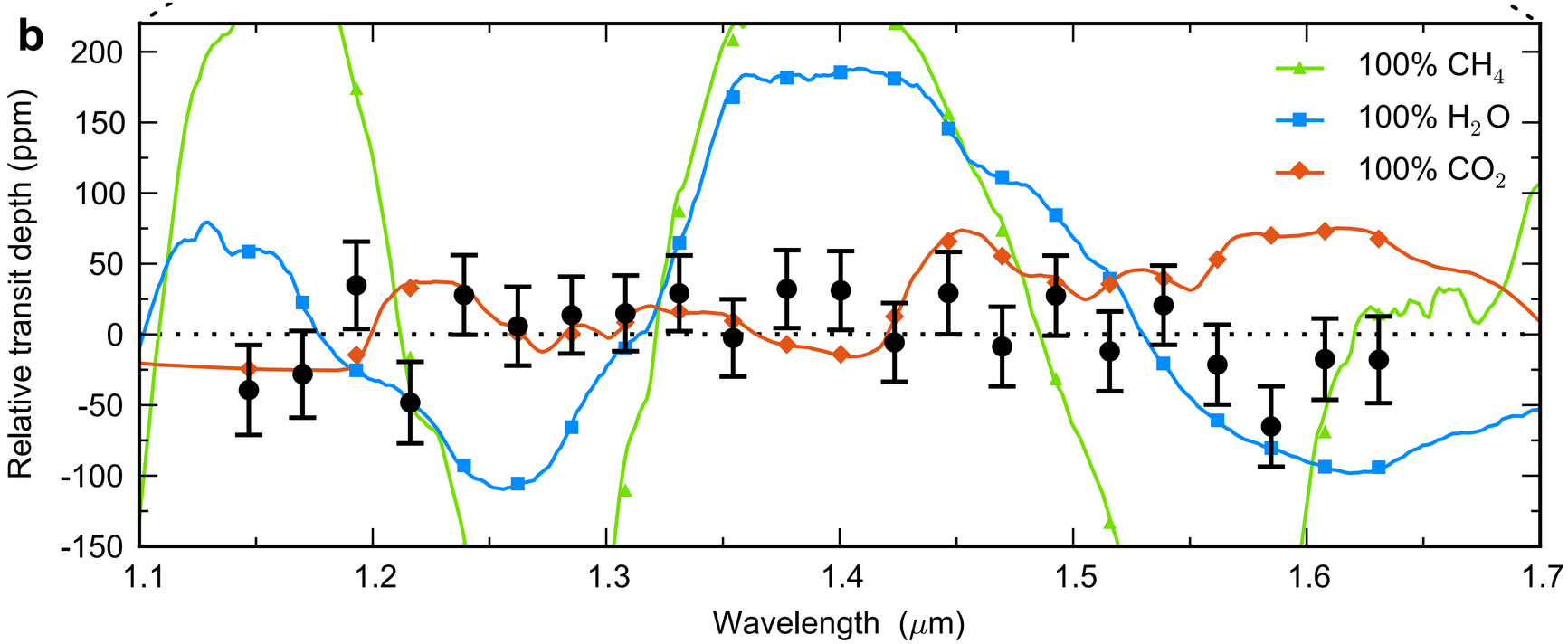


Sodium absorption signature in the hot Jupiter HD 209458b, compared to model spectra

1x solar; deep cloud
1x solar; high cloud
subsolar Na

Charbonneau et al. 2002

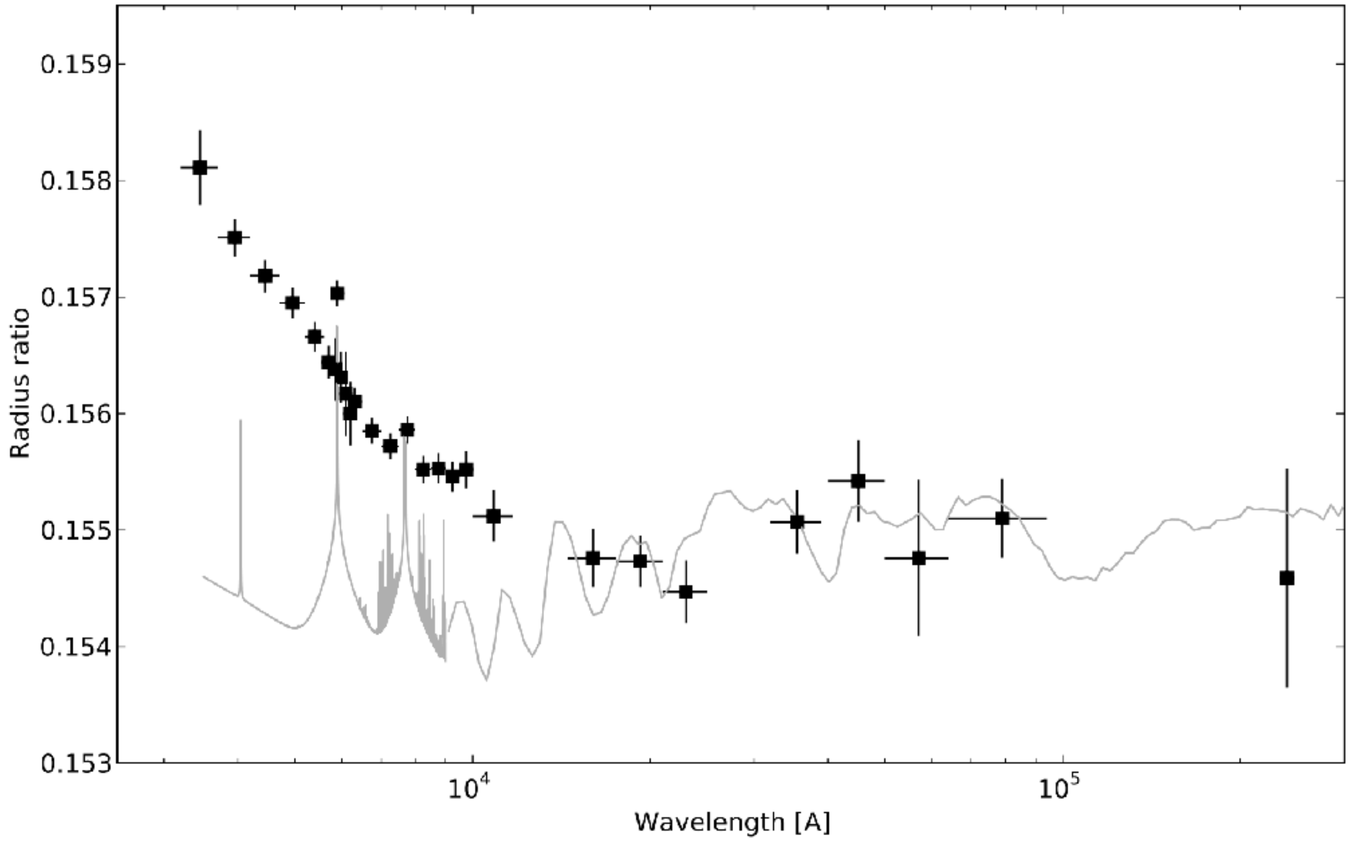
Observational evidence for condensates
I. Truncated features in transmission spectra



Cloud deck at < 0.1 mbar pressure for sub-Neptune archetype GJ 1214b

— Kreidberg et al. 2014

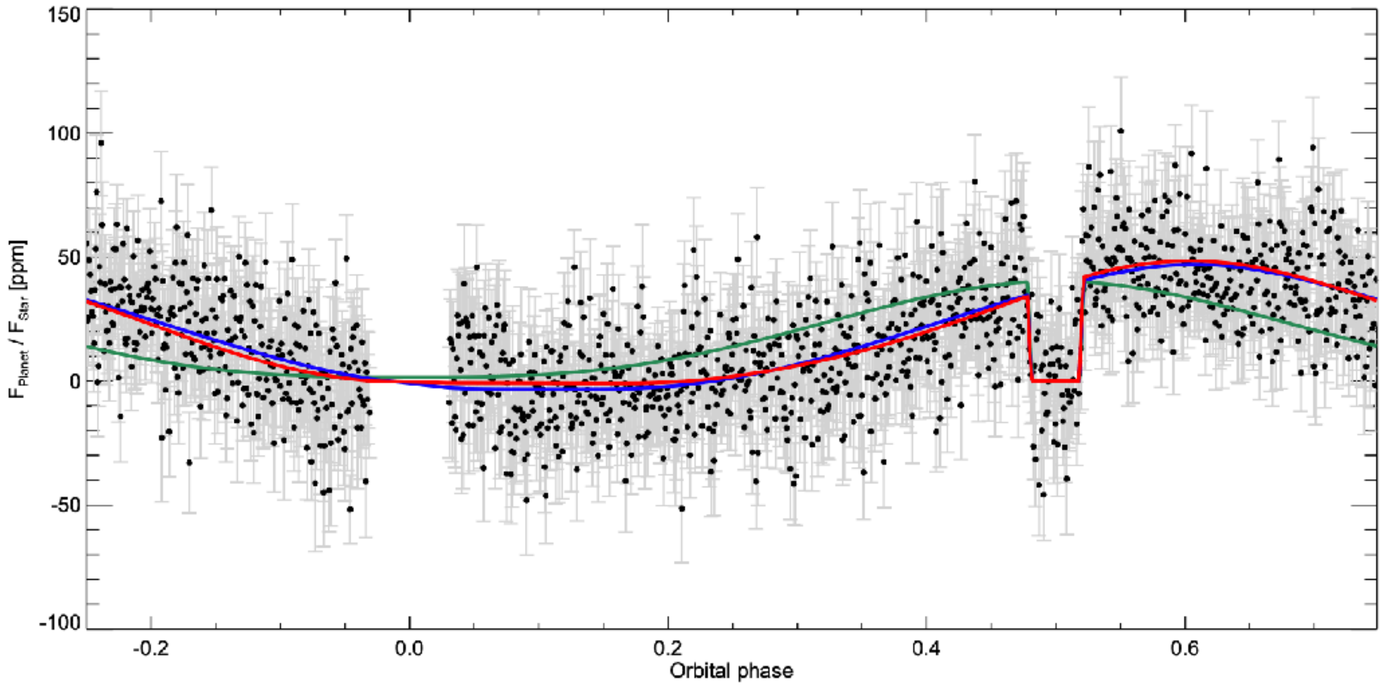
Observational evidence for condensates II. Haze scattering slope in the optical

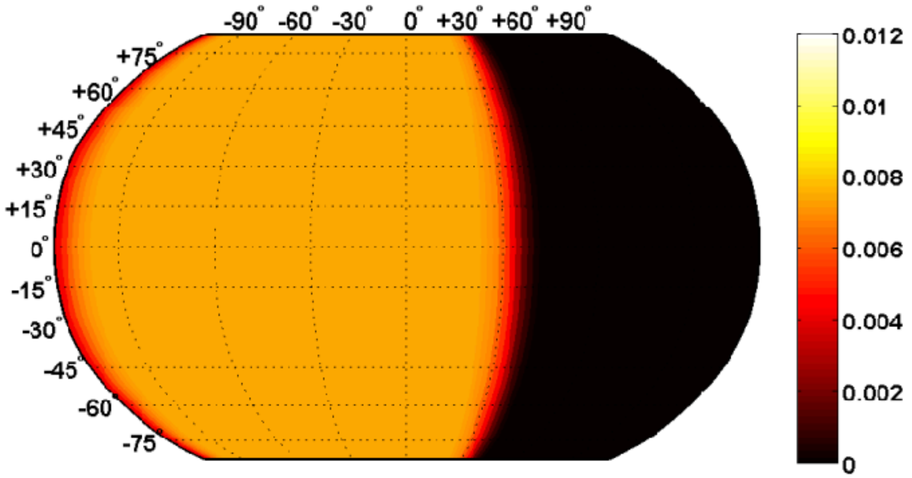


Evidence for sub-micron haze particles in the hot Jupiter HD 189733b

— Pont et al. 2013

Observational evidence for clouds
III. Phase curve amplitudes and offsets

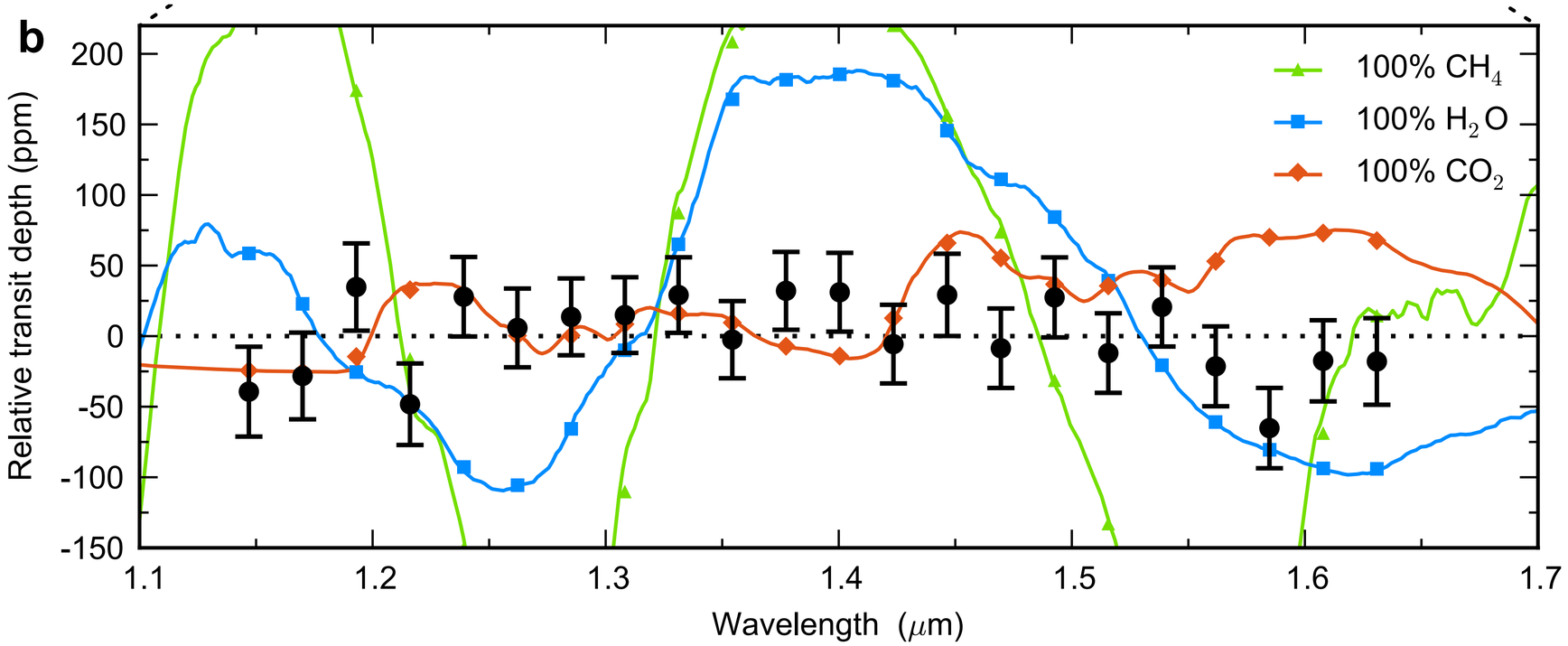




Westward offset in the optical phase curve of the hot Jupiter Kepler-7b indicates inhomogenous cloud coverage — Demory et al. 2013

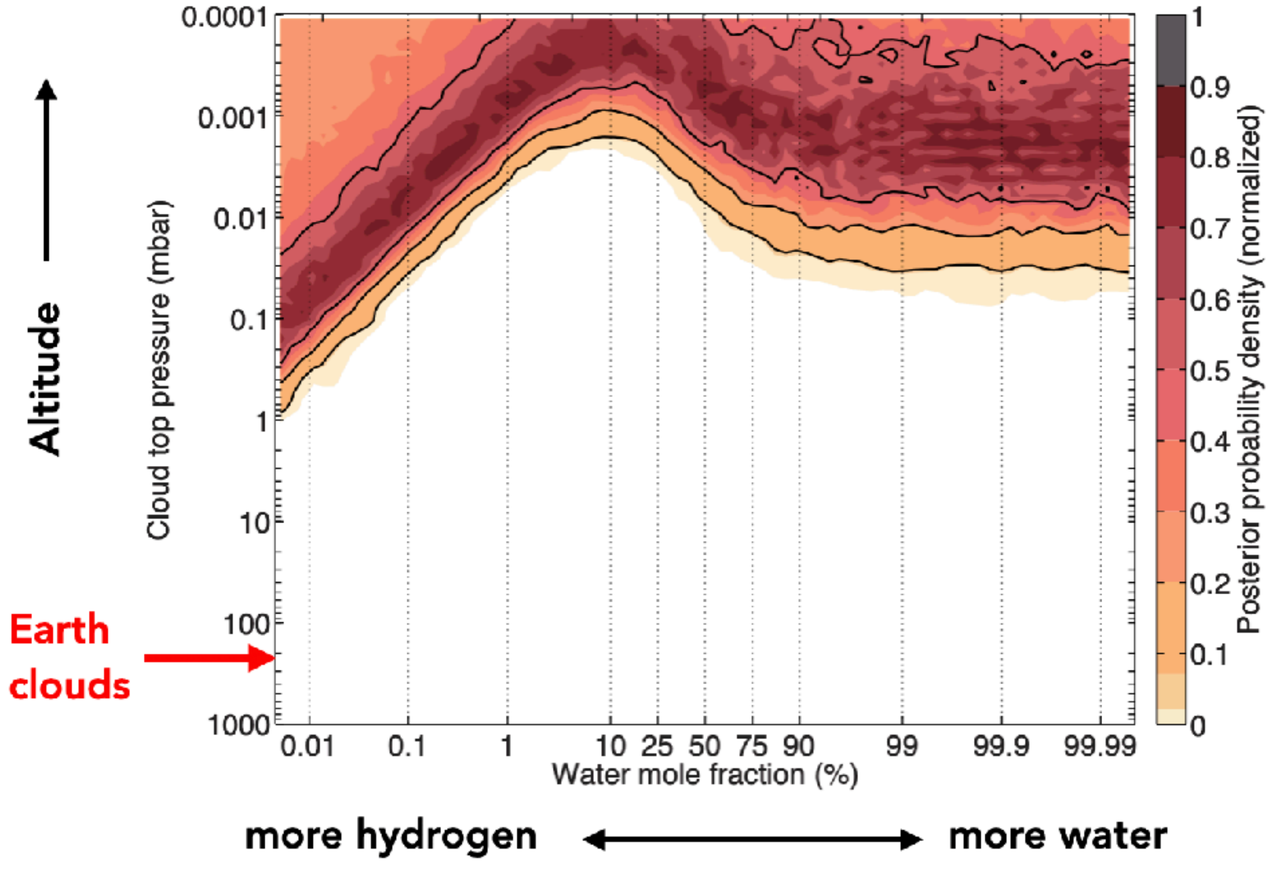
What are the clouds/haze made of? In-depth studies of individual objects

Kreidberg et al. 2014



GJ 1214b has a REALLY featureless spectrum!

What are the clouds/haze made of? In-depth studies of individual objects

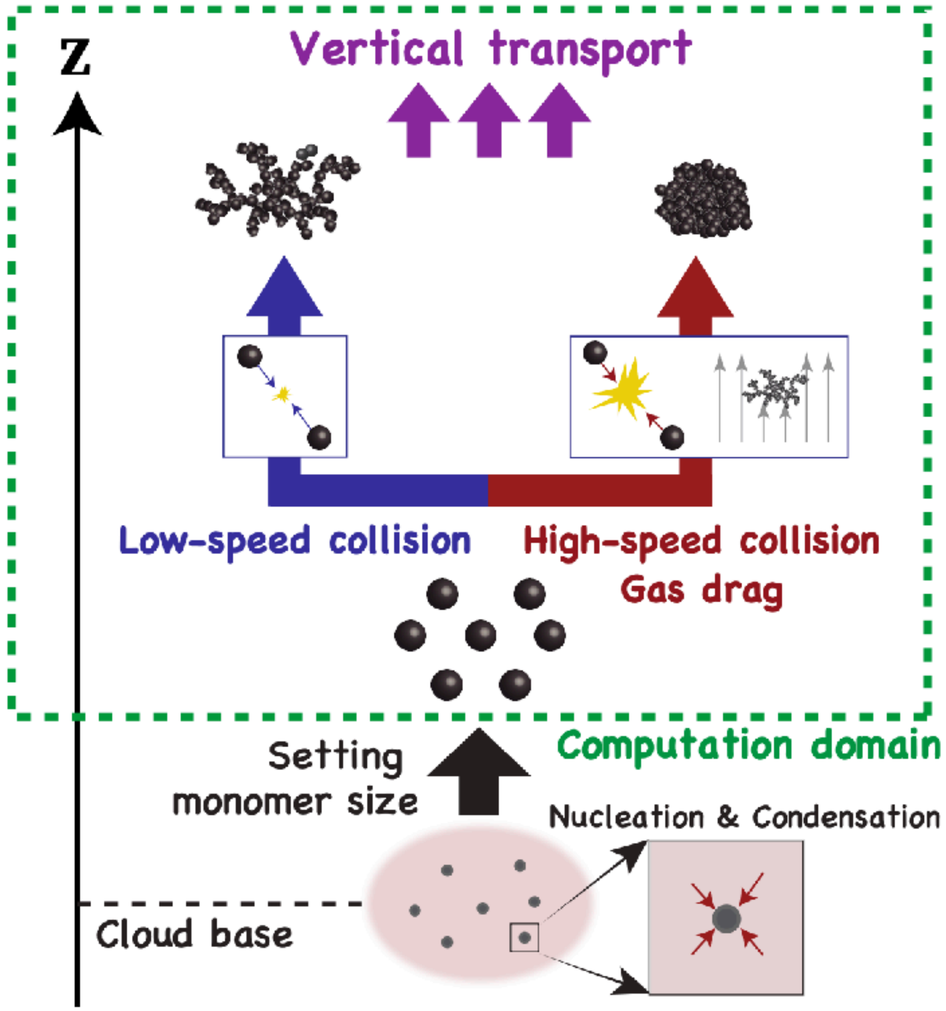


Cloud deck pressure must be 0.1 mbar or lower

Equilibrium condensation of salts/sulfides, or photochemical hazes possible

Kreidberg et al. 2014

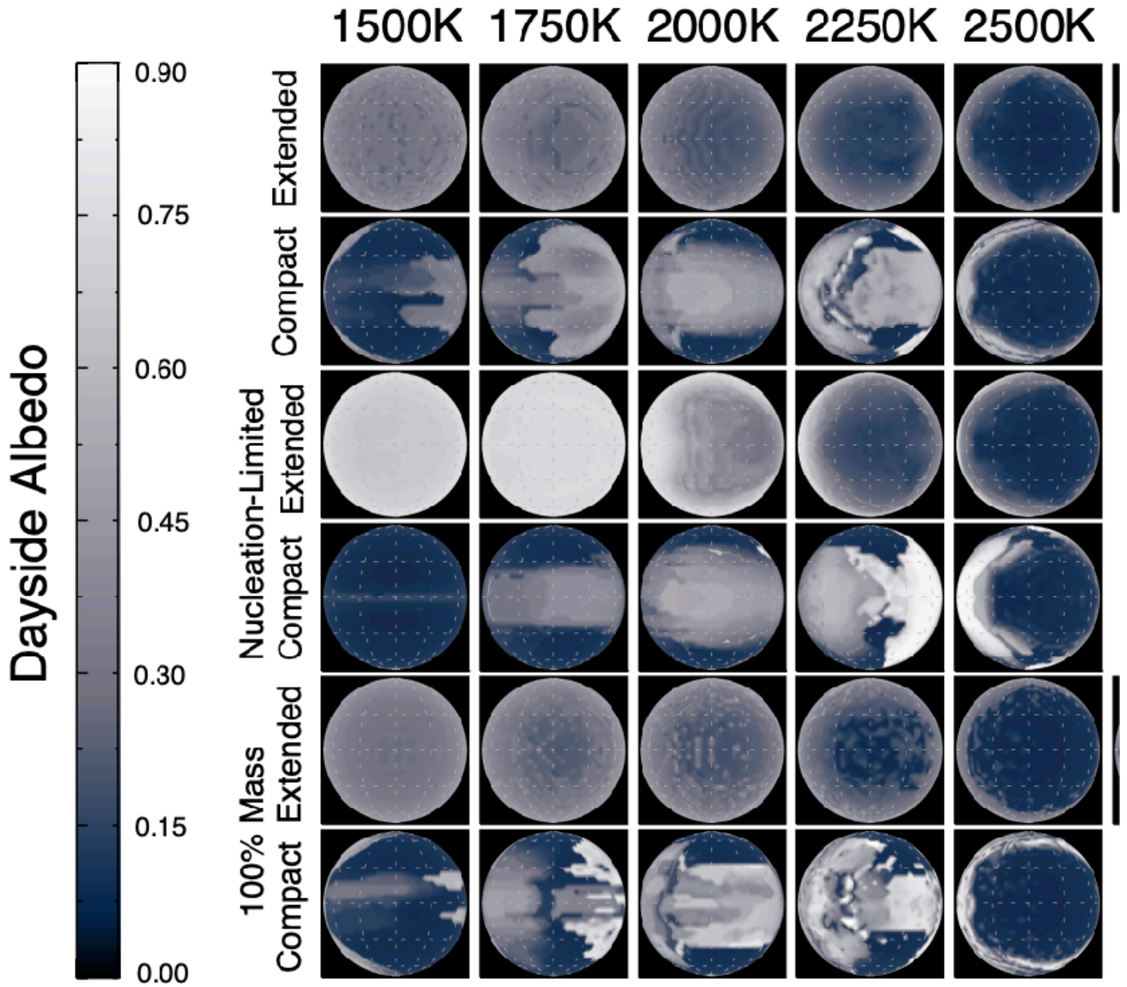
Challenge: how do the clouds and haze stick around at such high altitudes?



Porosity can decrease the density of cloud particles by 1 -3 orders of magnitude!

Ohno et al. 2020

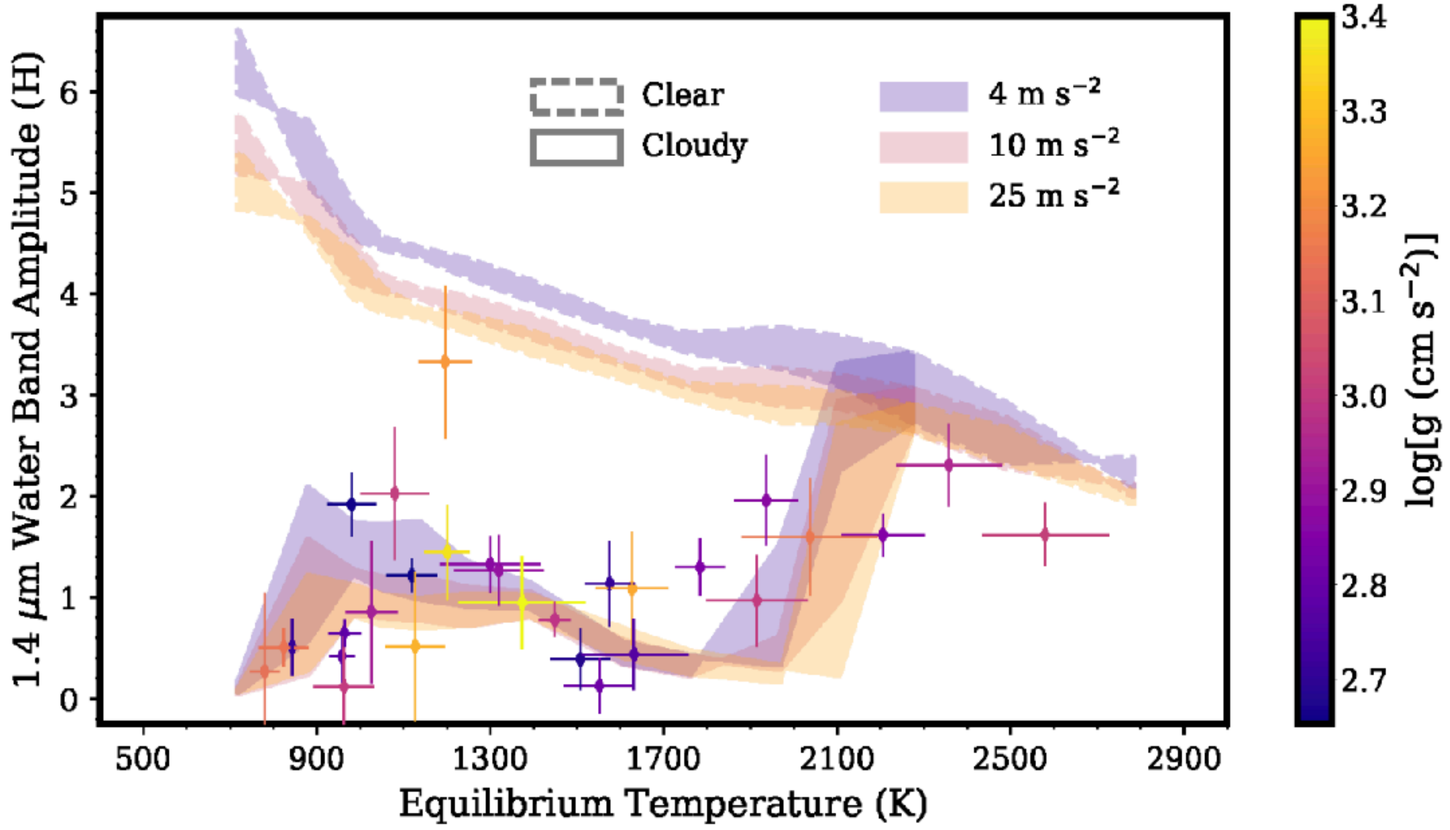
Where are the clouds and hazes?



Maybe everywhere,
maybe somewhere,
maybe nowhere

Roman et al. 2021

What are the clouds/haze made of? Evidence from population-level trends

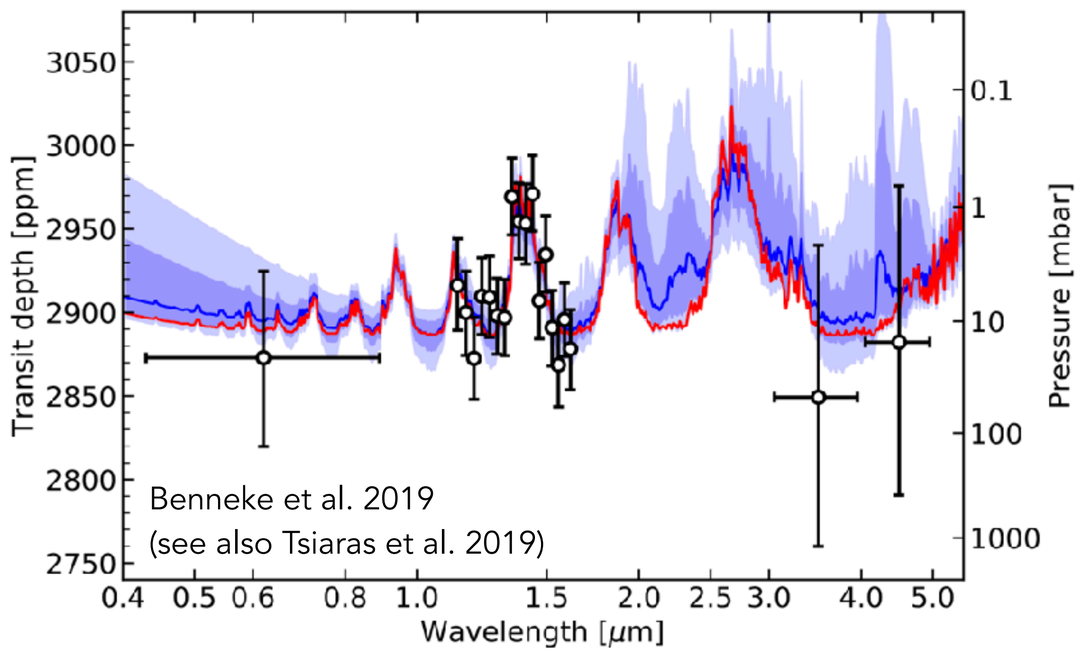


Gao et al. 2020

For gas giants:

- *Photochemical hazes dominate at low temp below 950 K*
- *Silicate cloud opacity increases from 1100 - 1800 K*

What are the clouds/haze made of? Evidence from population-level trends



K2-18b: A cloud-free atmosphere in the habitable zone?

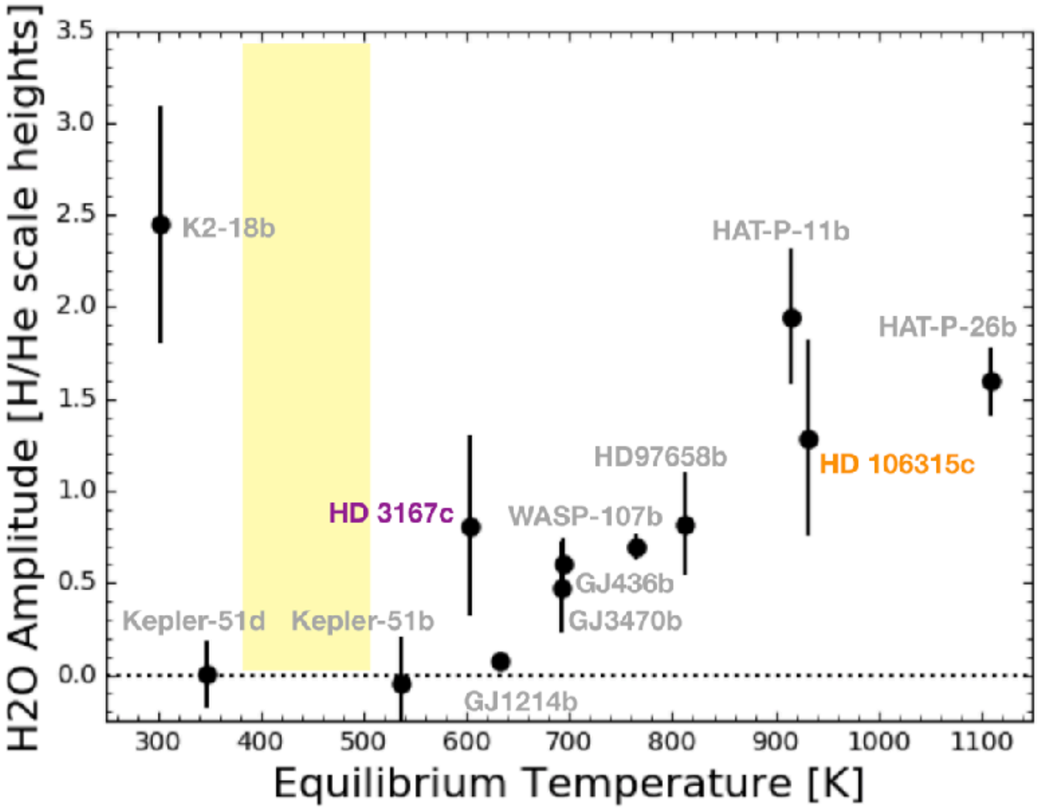
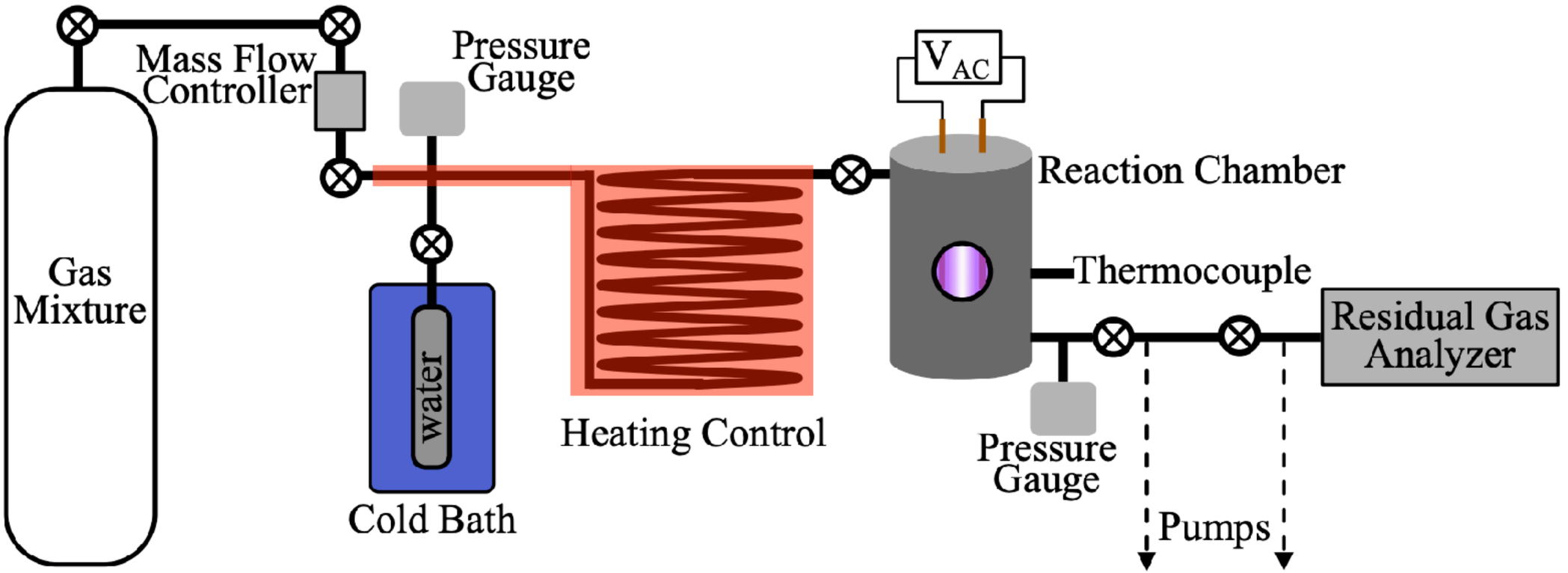


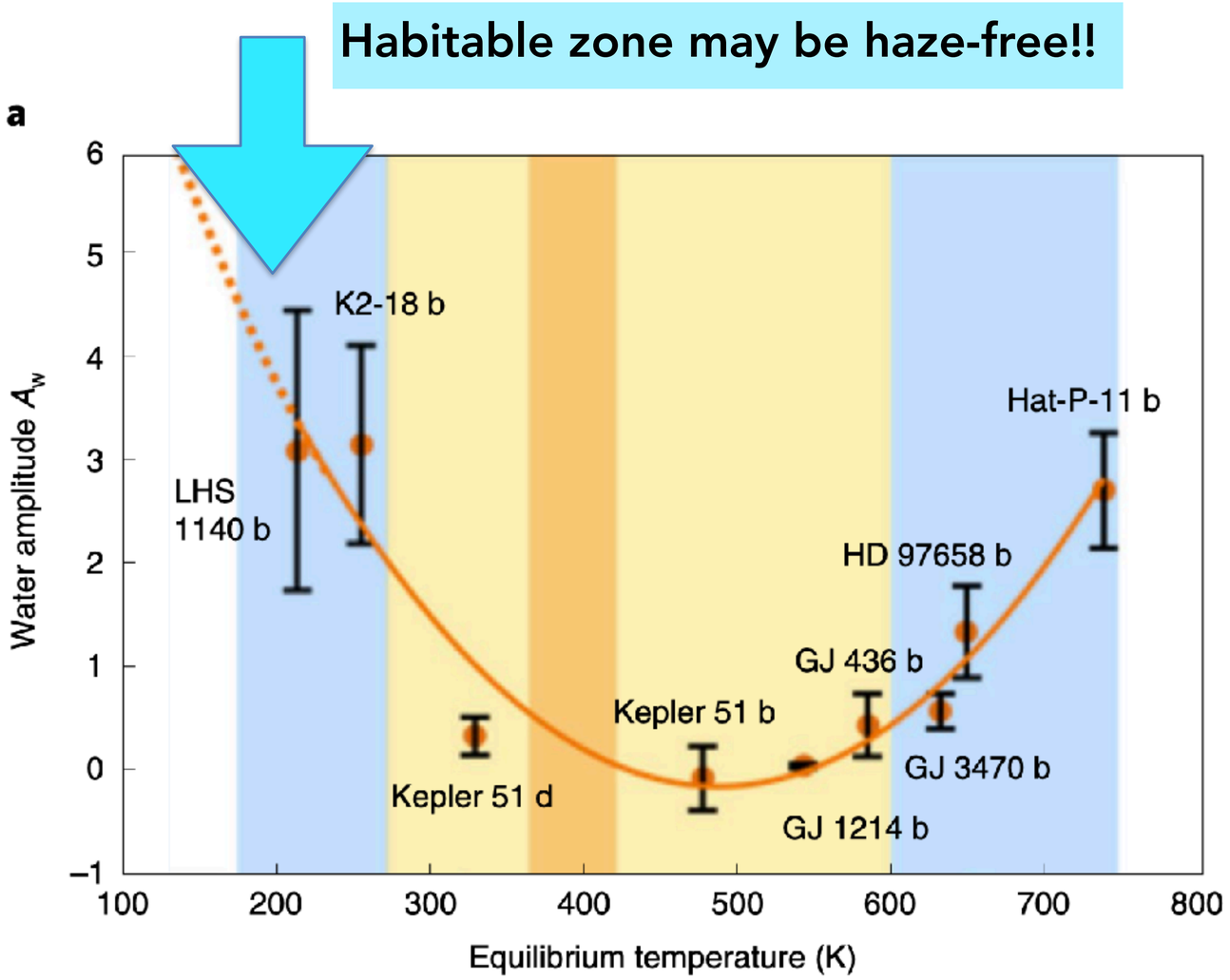
Figure c/o Ian Crossfield

Lessons learned from work in the lab



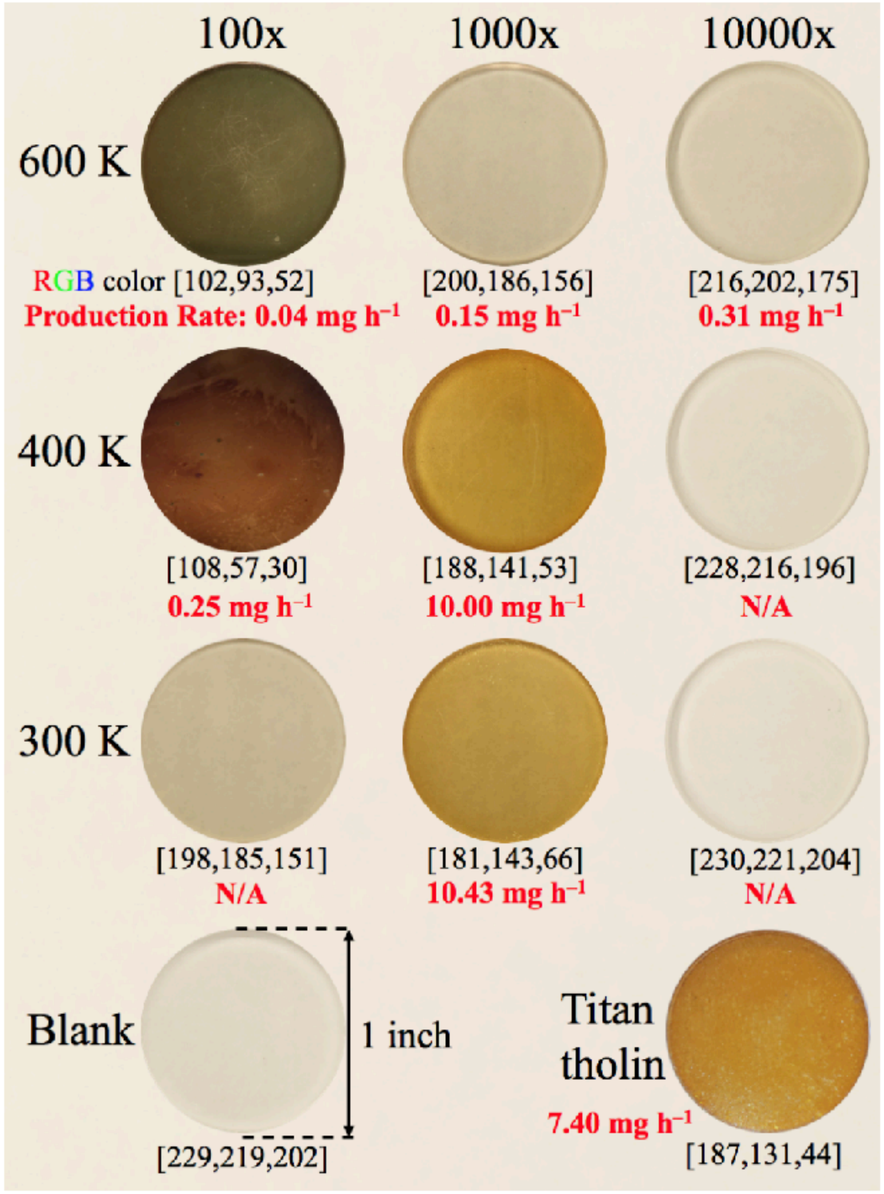
He et al. 2018

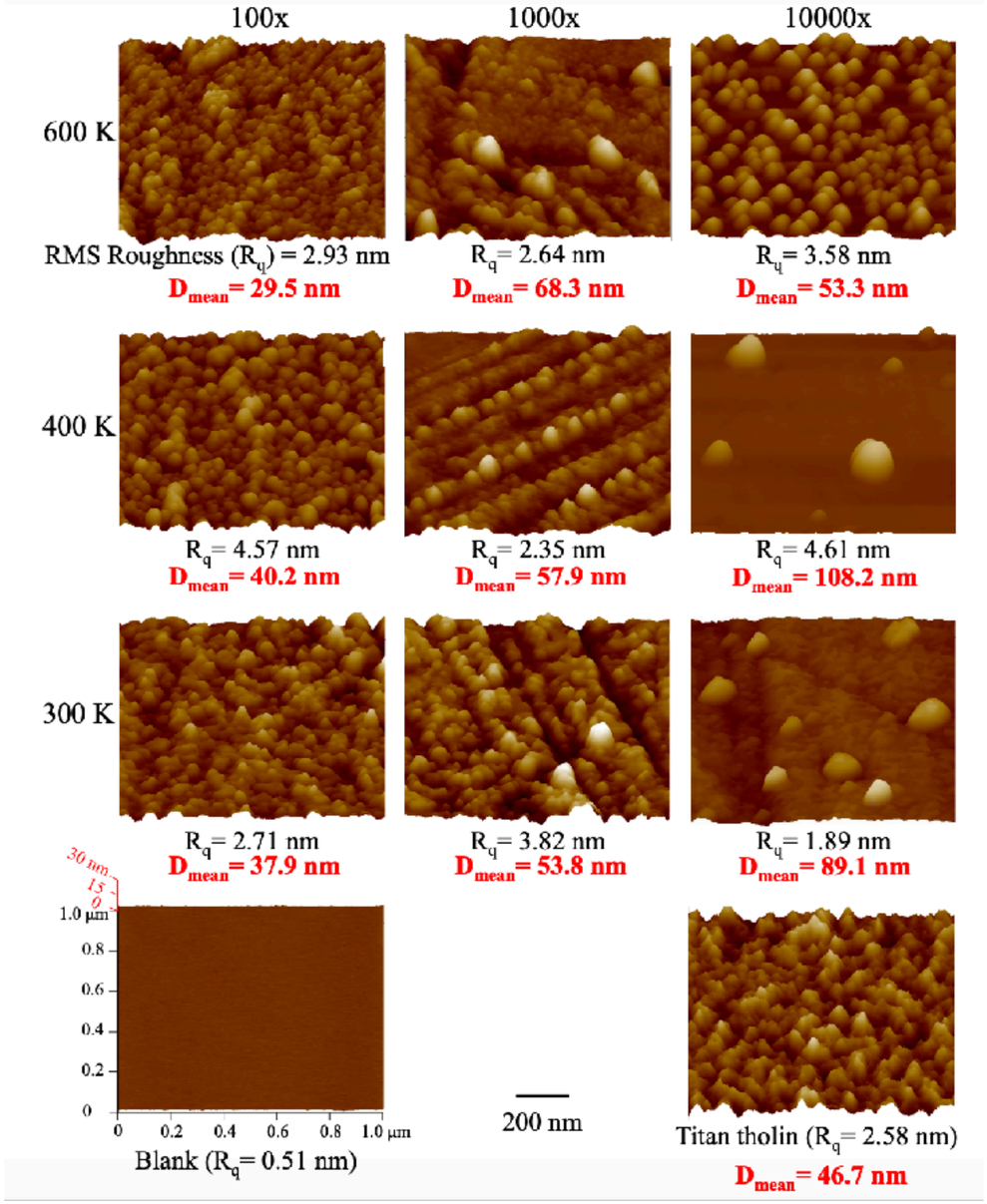
Lessons learned from work in the lab

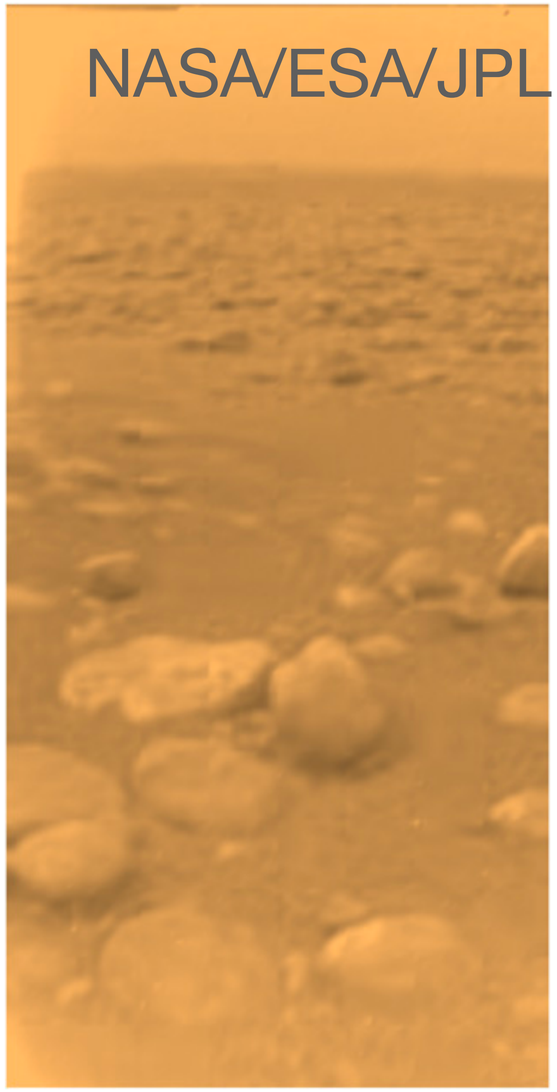


High surface energy particles grow and rain out, low surface energy particles linger in upper atmosphere

Yu et al. 2021



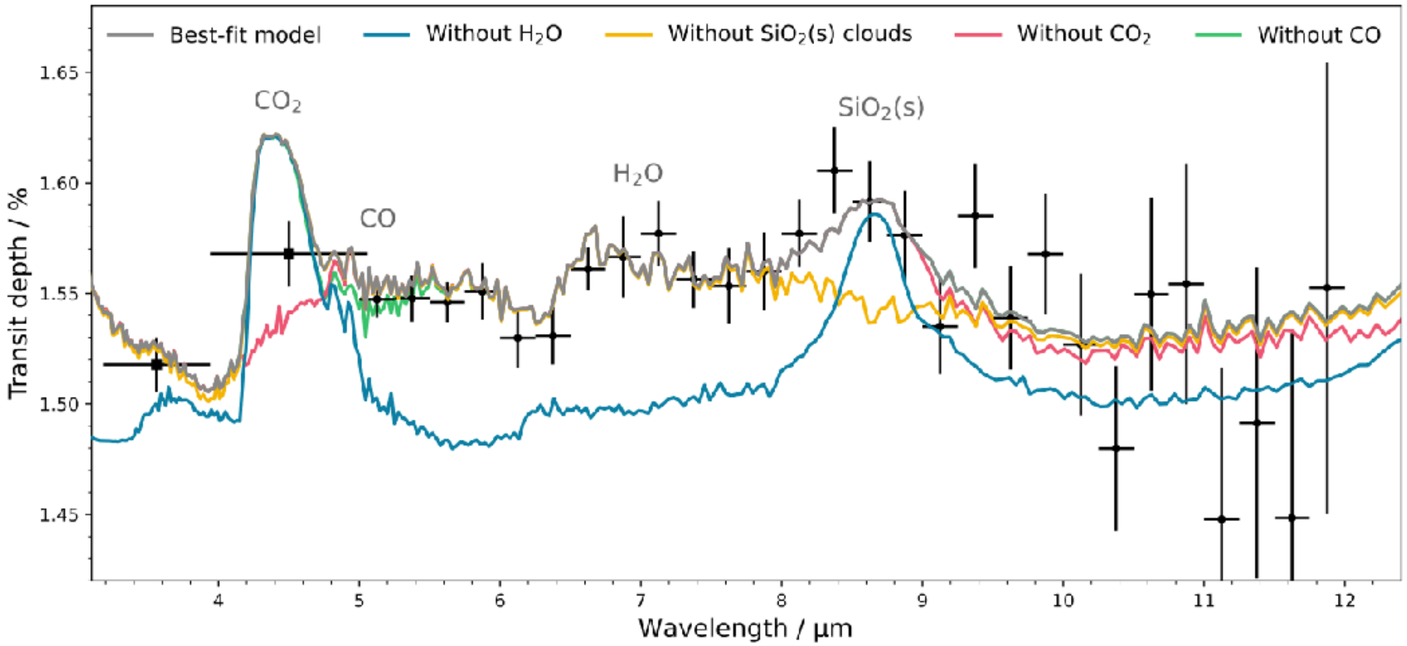


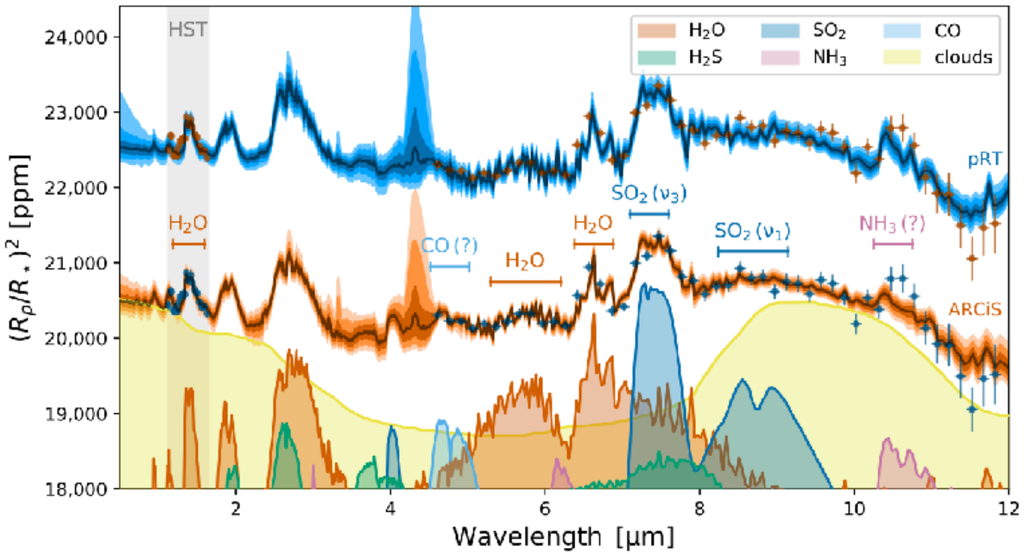


Haze colors and haze particles ! He et al. 2018

Huygens lander view from the surface of Titan

First direct measurement of cloud composition - silicates in WASP-17b and WASP-107b!





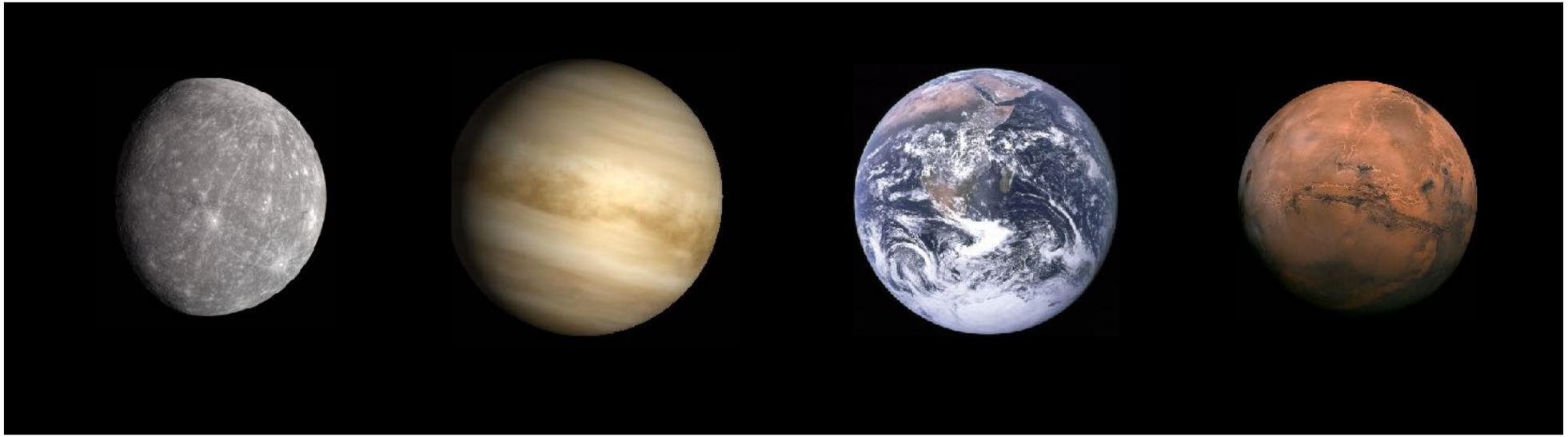
- *WASP 117b (left) : SiO2(s) clouds are small particles (~ 0.01 μm) with Pcloud ≲ 1 mbar (Grant et al. 2023)*
- *WASP 107b (right): opacity from some silicate cloud (MgSiO3, SiO2, or SiO) strongly favoured (Dyrèk et al. 2023)*

Rocky planet atmospheres, biosignatures, and the future

Laura Kreidberg
Max Planck Institute for Astronomy

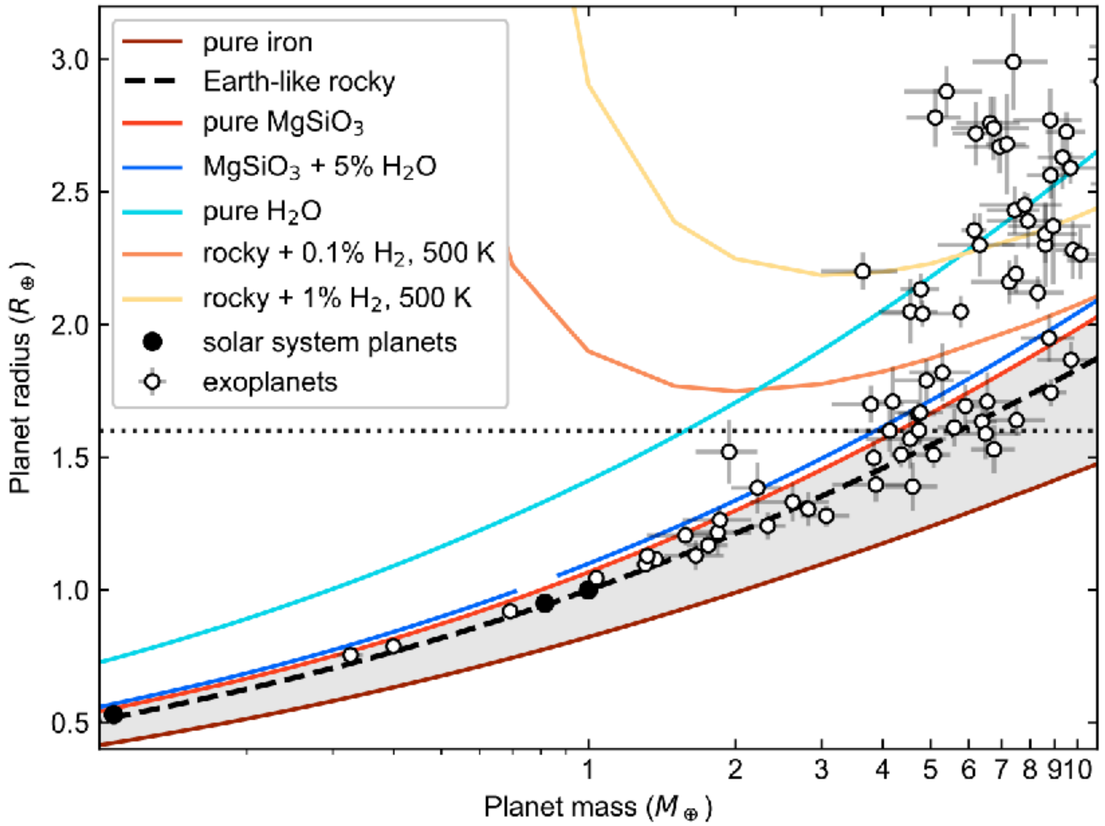
- What do we expect rocky planet atmospheres to look like?
- Which rocky planets can we observe with our current techniques? What have we learned so far?
- What is a biosignature? How will we identify inhabited planets?
- Upcoming telescopes (soon and not so soon)

What do we expect rocky planet atmospheres to look like?



Already in the Solar System we see a diversity of compositions shaped by many processes

Clues from masses and radii:
Rocky planet atmospheres are probably not hydrogen-rich



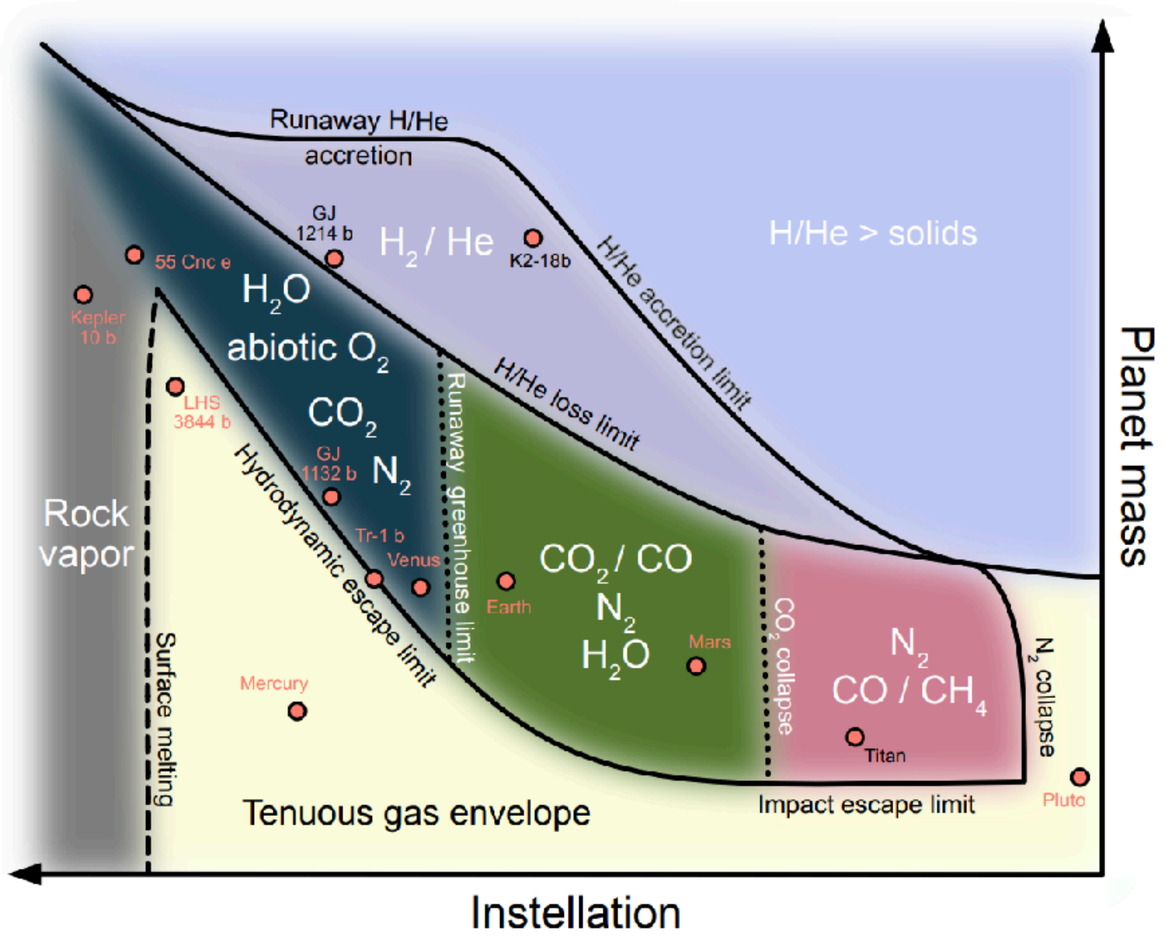
Even a small amount of hydrogen — 1% by mass — increases the planet radius to 2 Re

Less massive H2 envelopes easily evaporate

Wordsworth & Kreidberg 2022 ARA&A

But a diversity of secondary atmospheres is possible!

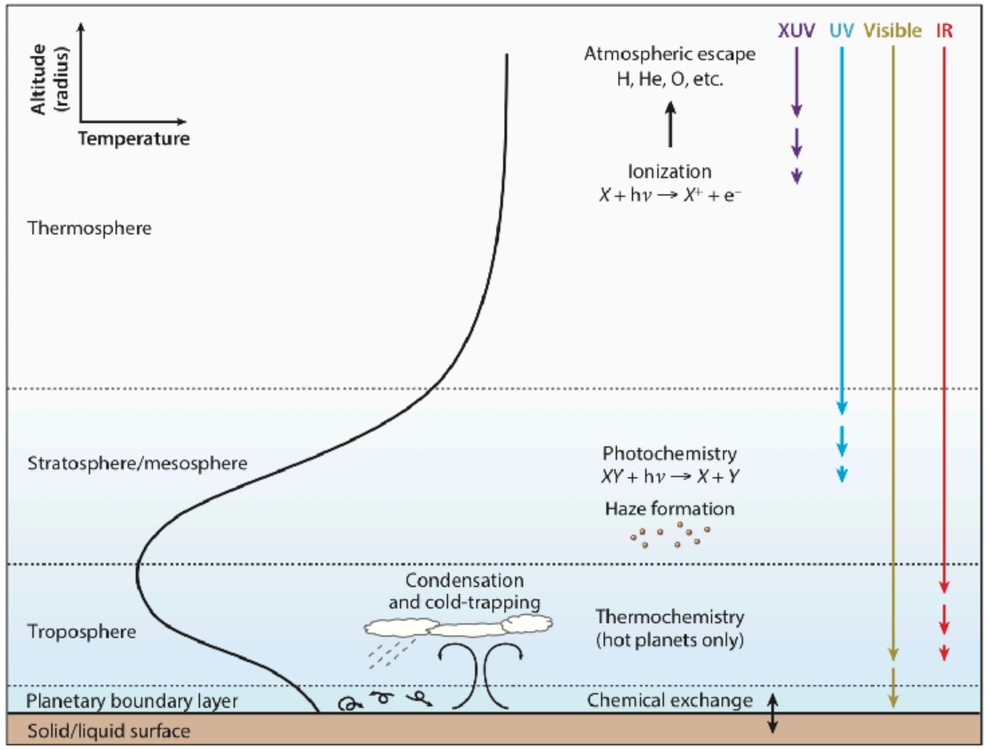
Depending on temperature, the atmosphere may be dominated by N_2, CO, CH_4, H_2O, CO_2, O_2, rock vapor…



Lichtenberg et al. 2022

A diversity of processes shape rocky planet atmospheres

Altitude ⟶



Escape

Photochemistry

Haze formation

Condensation

Interior exchange

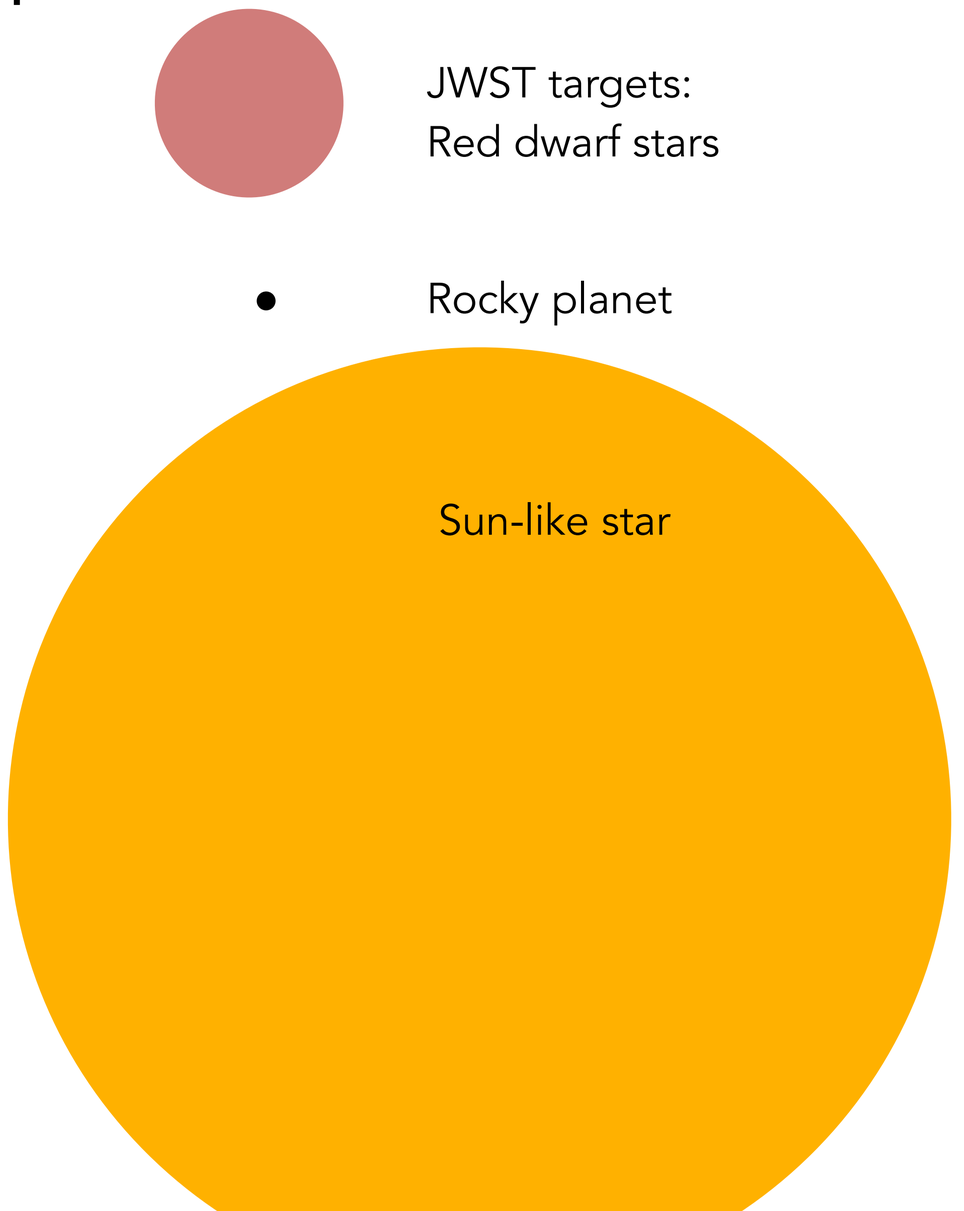
Wordsworth & Kreidberg 2023, ARA&A

+ circulation, cold-trapping, atmospheric collapse, impacts

- What do we expect rocky planet atmospheres to look like?
- Which rocky planets can we observe with our current techniques? What have we learned so far?
- What is a biosignature? How will we identify inhabited planets?

Rocky planets around M-dwarfs: searching for keys under the lamp post

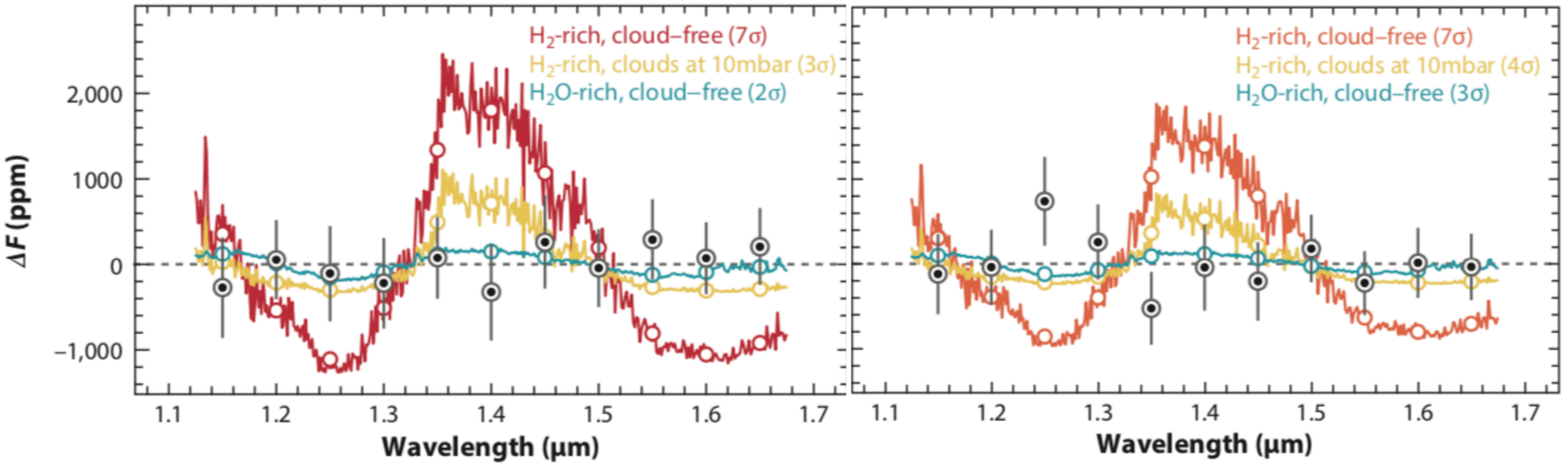
- Most of the known rocky planets in the galaxy orbit M-dwarfs
- The habitable zone is closer to cooler M-dwarf stars, leading to higher transit probability
- The smaller the star, the easier it is to characterize the planet atmosphere



The first transmission spectra for rocky planets around M-dwarfs were featureless

TRAPPIST-1b

TRAPPIST-1c



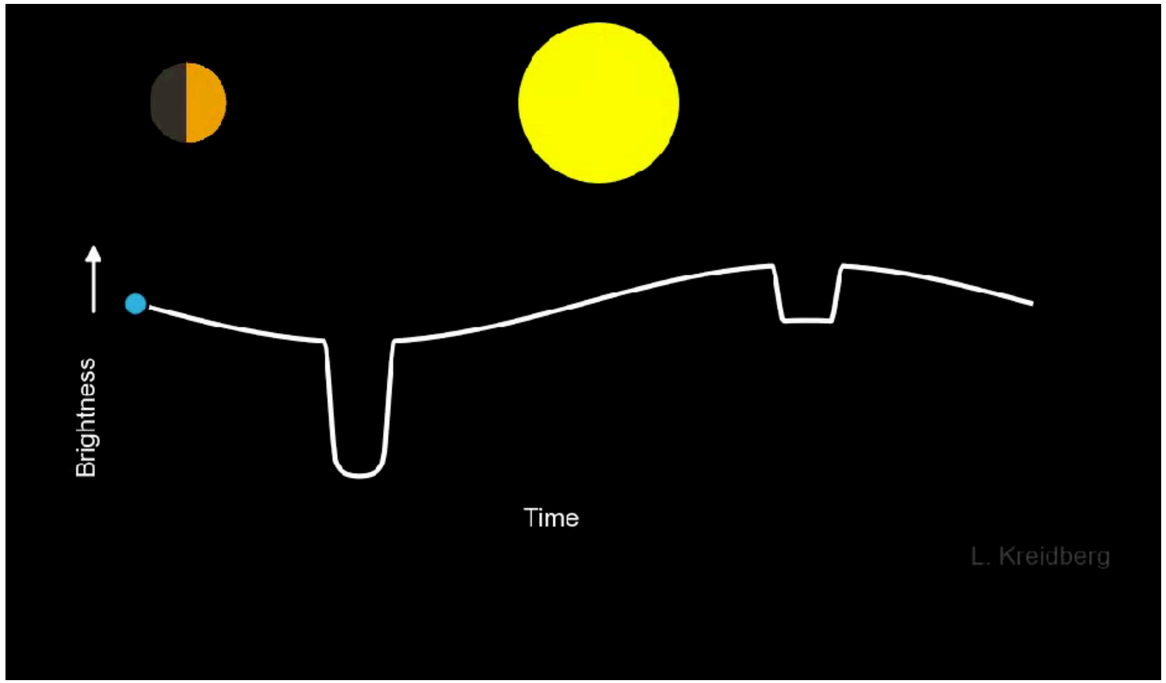
De Wit et al. 2016

Flat spectra put upper limits on hydrogen-rich atmospheres for 9 planets. High mean molecular weight, clouds, or no atmosphere — all still possible!

Planet	Result	Facility
GJ 1132 b	solar composition ruled out (16.3σ)	HST/WFC3
LHS 1140 b	marginal evidence for H_2O (2.7σ);	HST/WFC3,
	may be due to stellar contamination	Magellan/IMACS & LDSS3C
LHS 3844 b	solar composition ruled out (5.2σ)	Magellan/LDSS3C
TRAPPIST-1 b	solar composition ruled out (7σ)	HST/WFC3
TRAPPIST-1 c	solar composition ruled out (7σ)	HST/WFC3
TRAPPIST-1 d	solar composition ruled out (8σ)	HST/WFC3
TRAPPIST-1 e	solar composition ruled out (6σ)	HST/WFC3
TRAPPIST-1 f	solar composition ruled out (4σ)	HST/WFC3
TRAPPIST-1 g	solar composition disfavored (2σ)	HST/WFC3

Wordsworth & Kreidberg 2022, ARA&A

Results from transmission spectroscopy are ambiguous, so how else can we search for atmospheres? Phase curves!



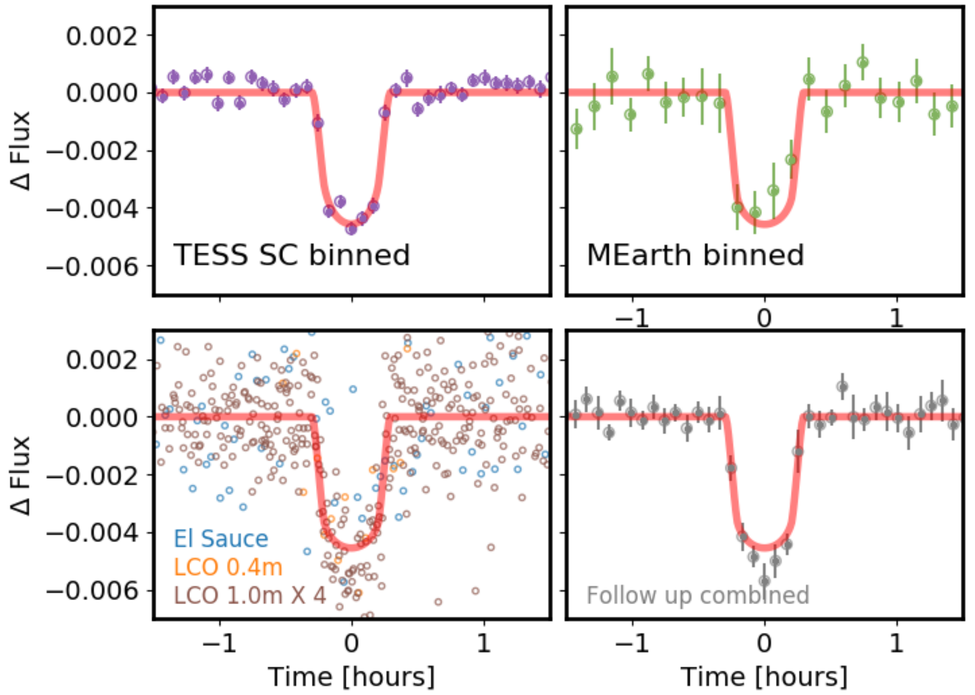
Thicker atmospheres are better are circulating heat, leading to more equal temperatures on the dayside and nightside

(Seager & Deming 2009, Selsis et al. 2011, Koll & Abott 2015, Kreidberg & Loeb 2016)

LHS 3844b — the first rocky planet accessible for thermal phase curve observations

- Rp = 1.3 Re
- P = 11 hours
- Teq = 1000 K

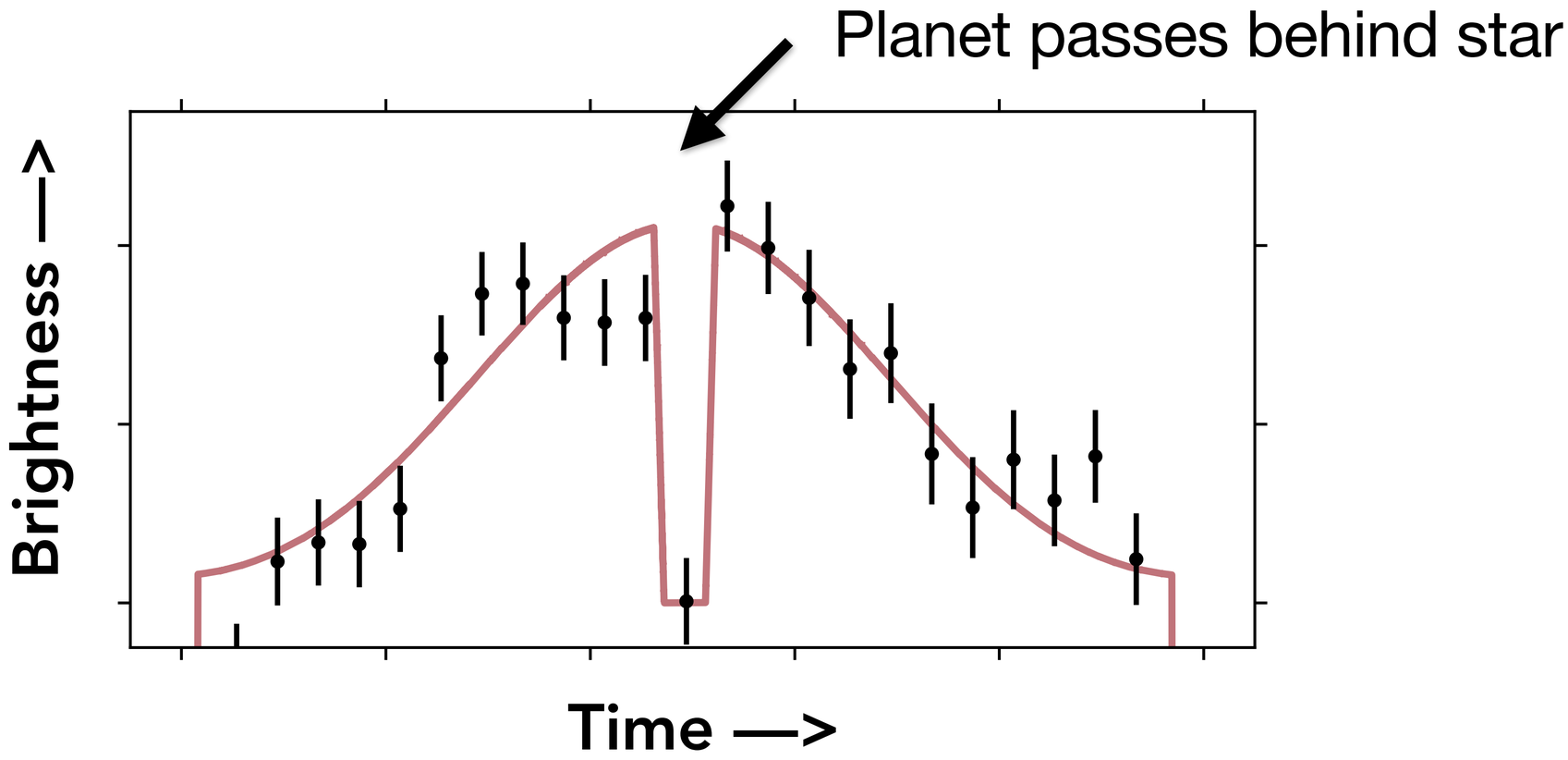
- R_* = 0.2 Rs
- D = 15 parsecs



Vanderspek et al. 2019

First rocky planet phase curve, LHS 3844b

Does it have an atmosphere?



Kreidberg et al. 2019

First rocky planet phase curve

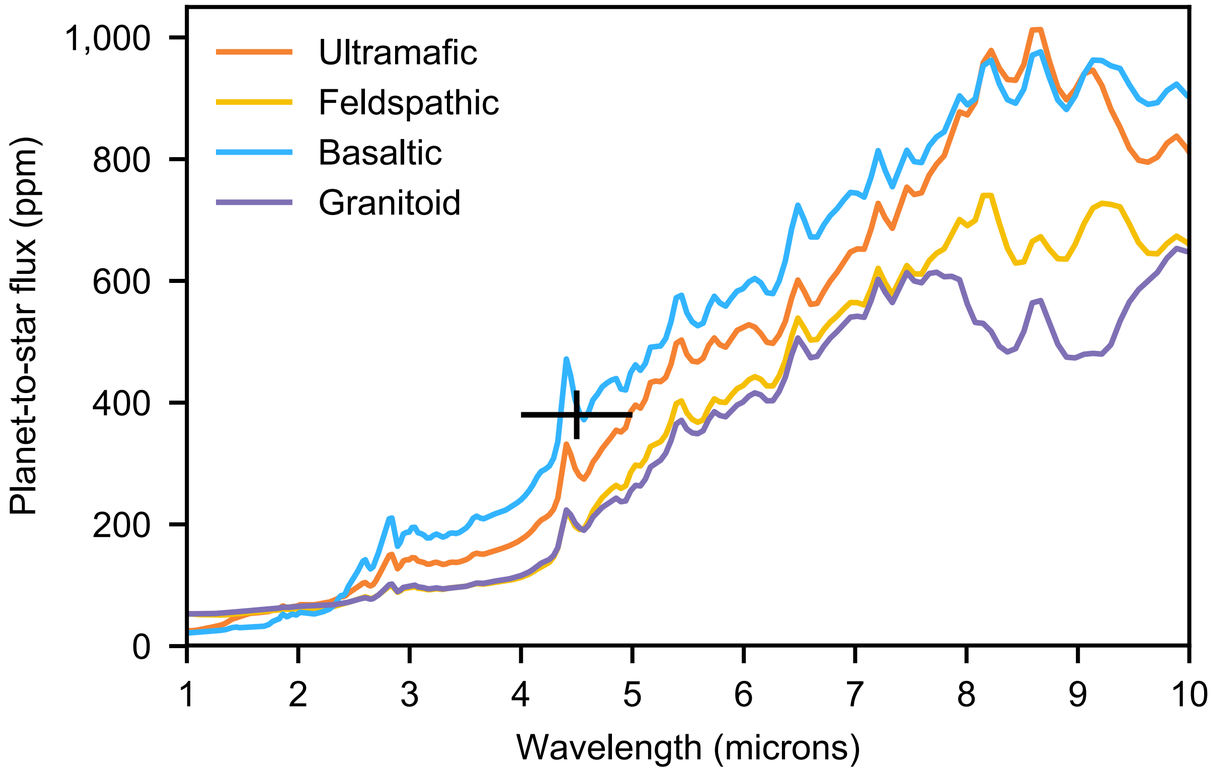
Does it have an atmosphere?

NO

We’re seeing dark rock, like the basalt on the slopes of Mt. Etna (minus the friendly life forms)



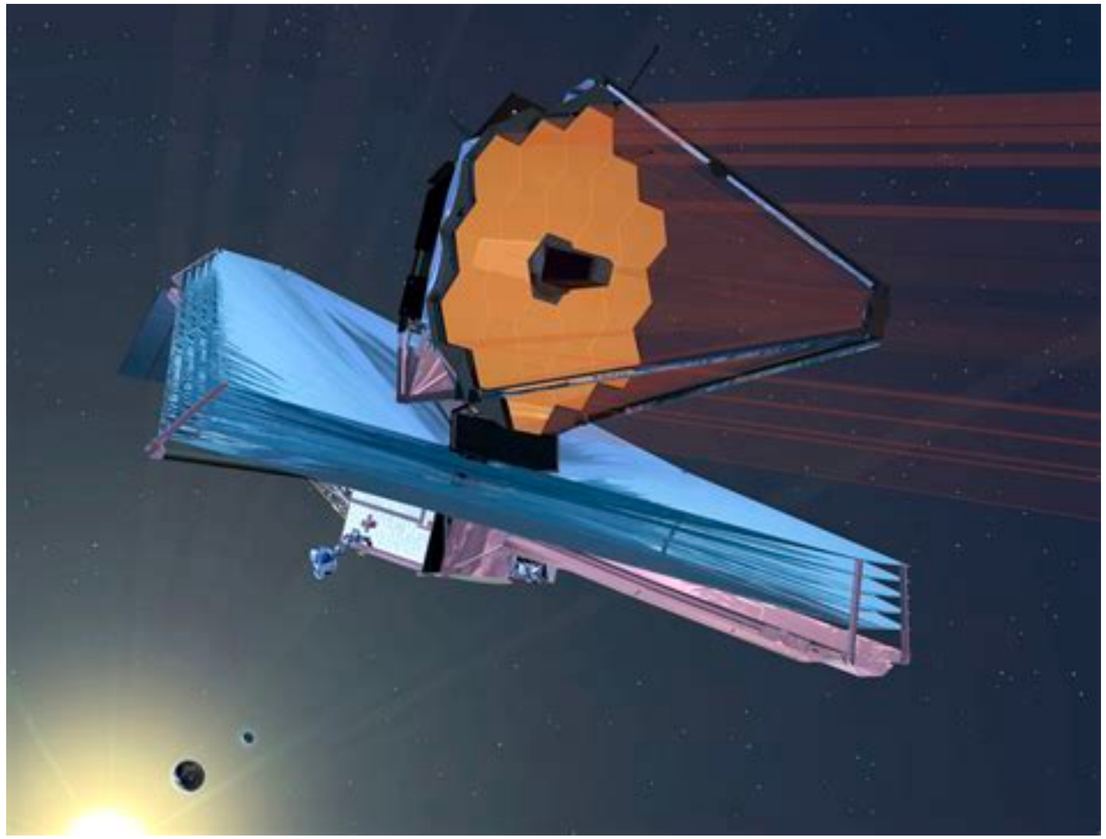
What is the rocky surface made of??



Kreidberg et al. 2019, Nature

Best fit compositions are basaltic, similar to the lunar mare and Mercury

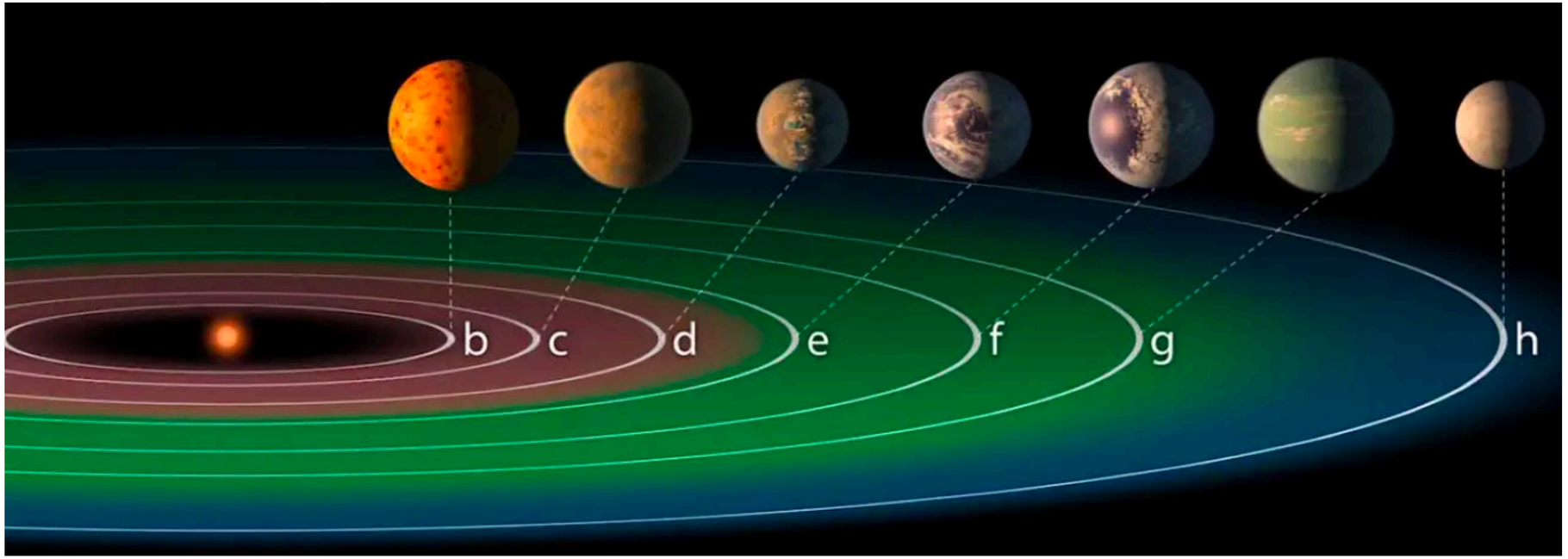
As per usual JWST is a game changer



What have we found so far?

Atmosphere ratings with Laura’s atmosphere-ometer

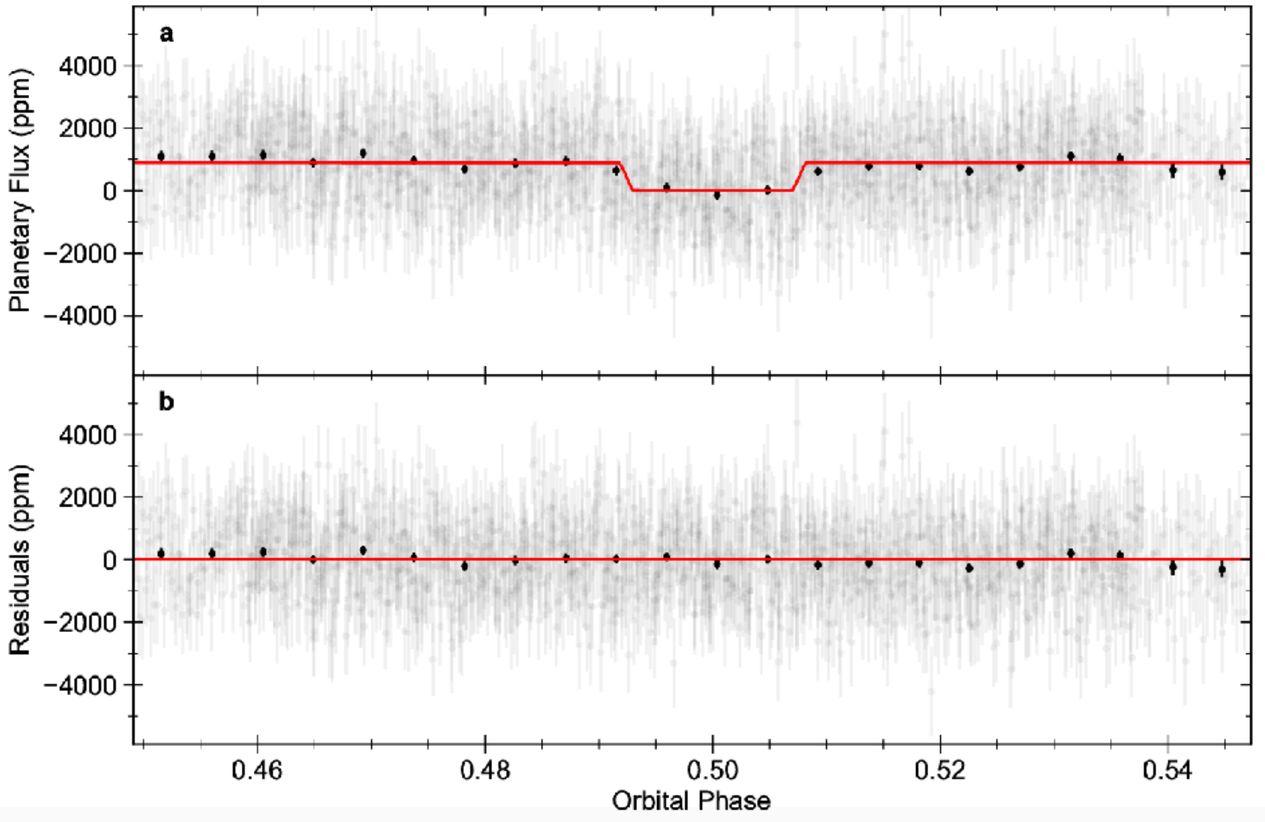
First look at the TRAPPIST-1 system



- Seven rocky planets transiting a nearby ultra cool dwarf star
- Three potentially habitable worlds (planets e, f, and g)
- One Venus analog (planet c)

First JWST observations of rocky planets

TRAPPIST-1b secondary eclipse detected with MIRI at 15 micron



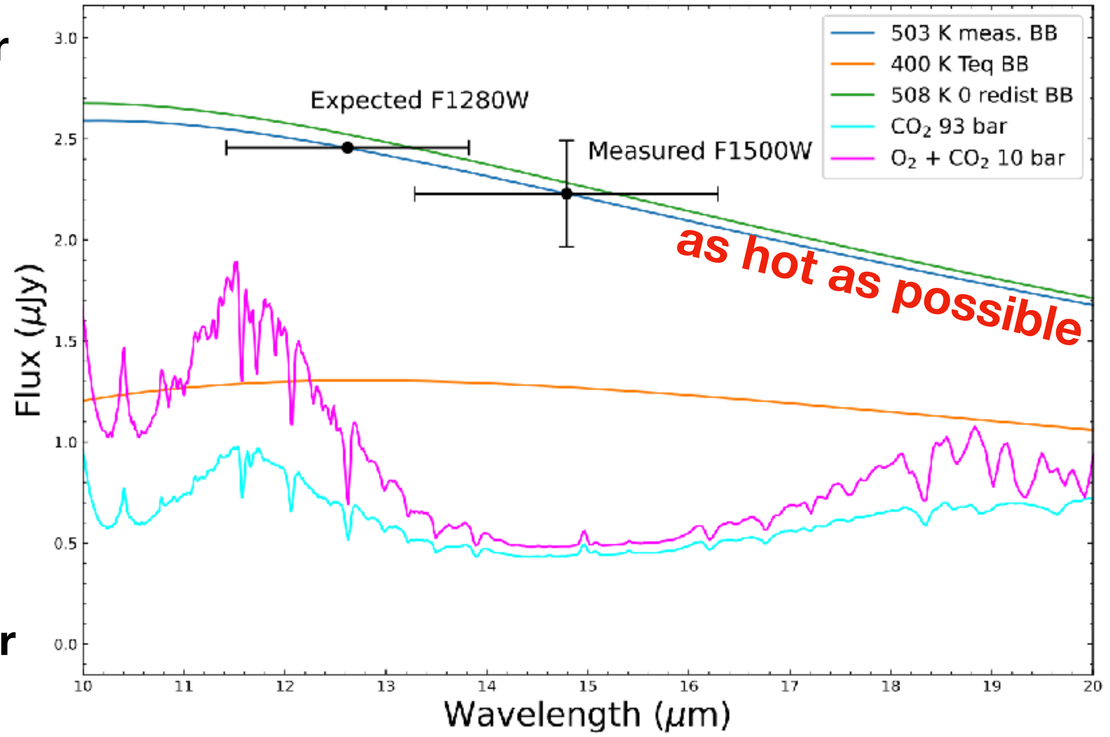
Greene et al. 2023. Nature

Revisiting the TRAPPIST-1 system

Dayside temperature of the innermost planet

Hotter

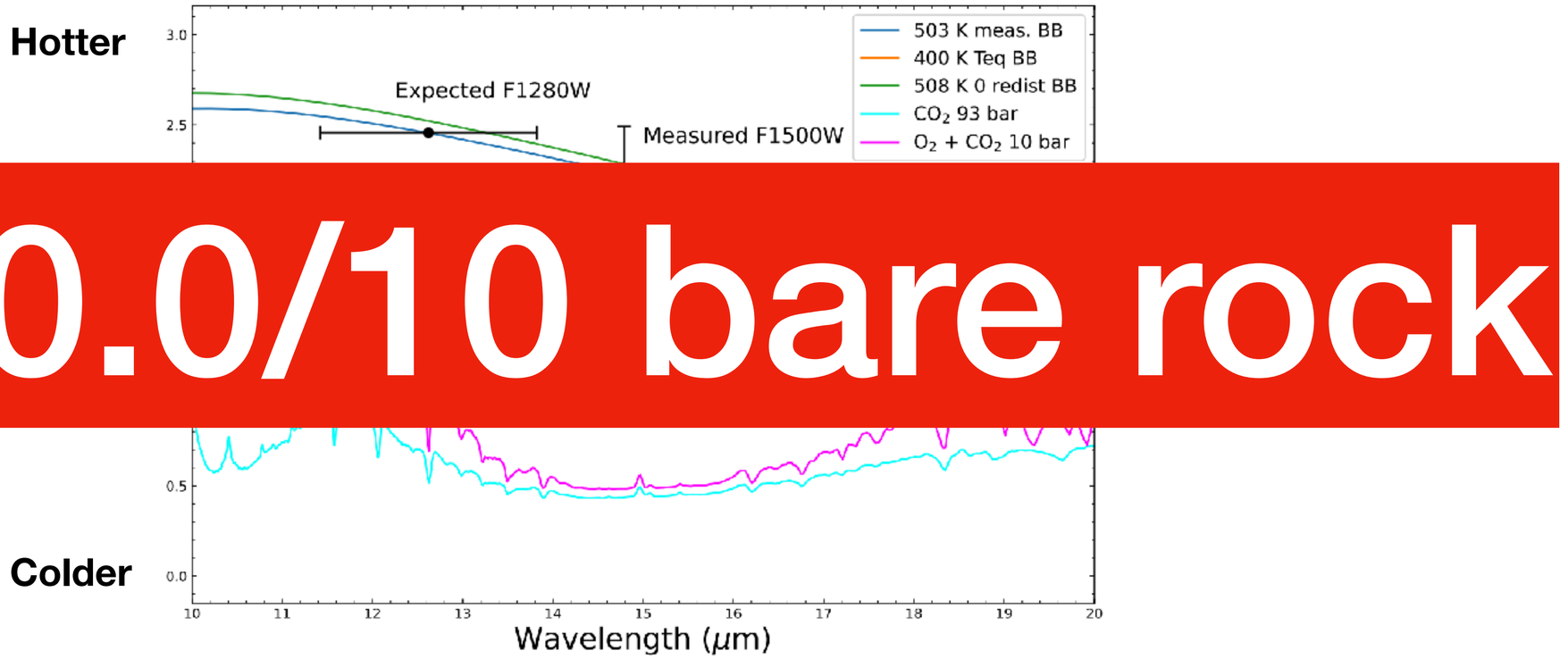
Colder



Greene et al. 2023. Nature

Revisiting the TRAPPIST-1 system

Dayside temperature of the innermost planet

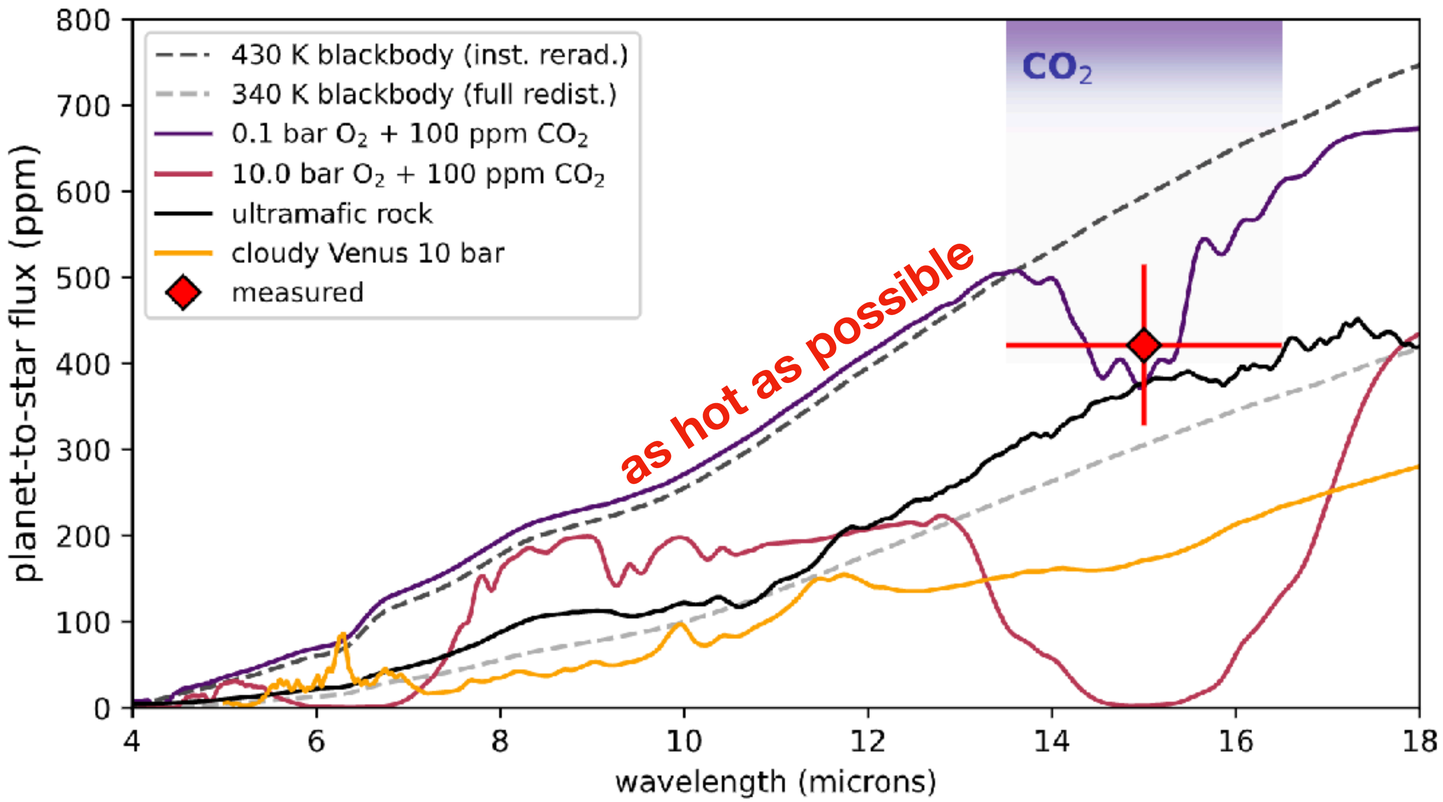


0.0/10 bare rock

Greene et al. 2023. Nature

Revisiting the TRAPPIST-1 system

Dayside temperature of planet c

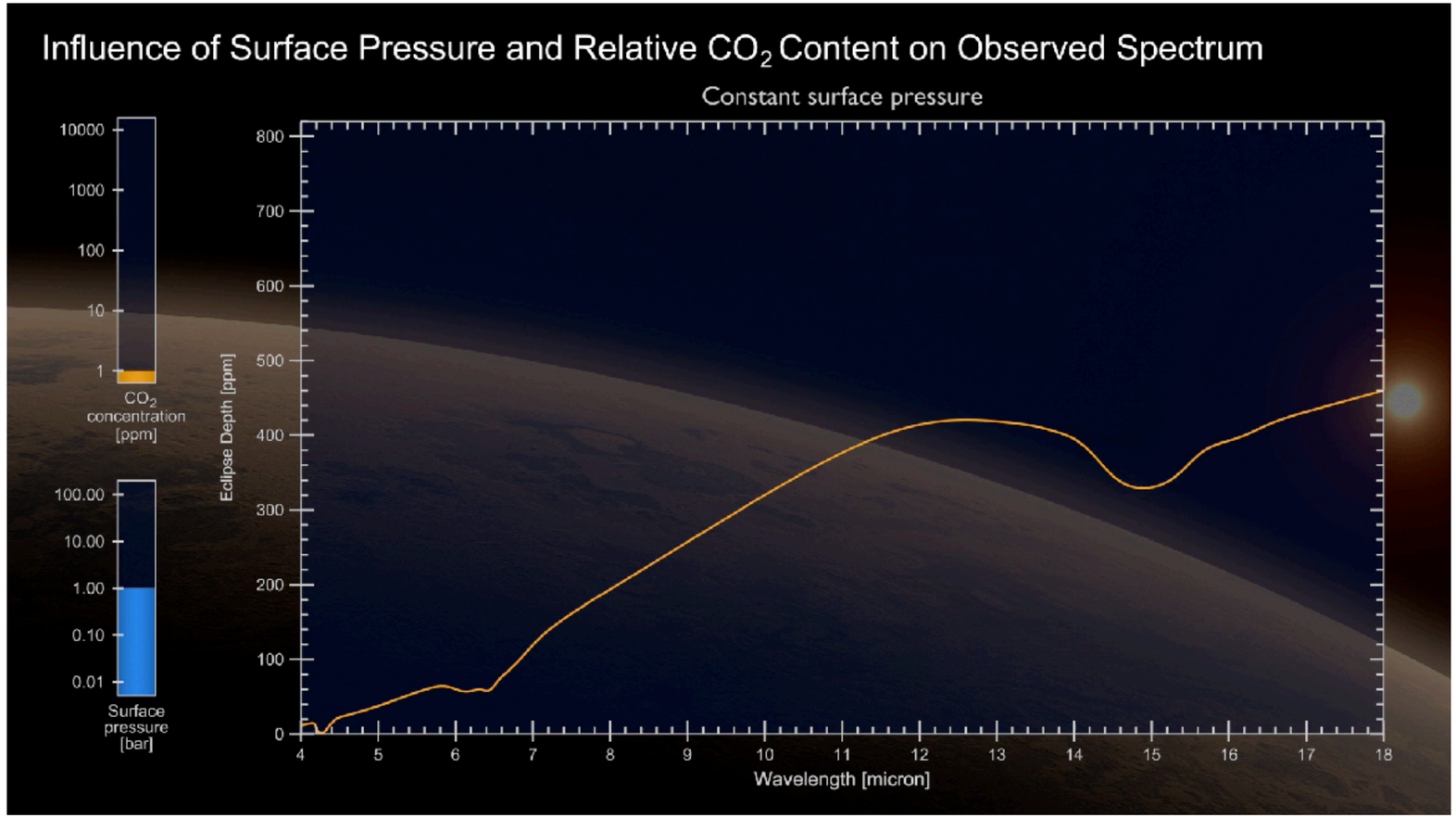


Zieba et al. 2023, Nature

Sebastian Zieba is on the job market :)



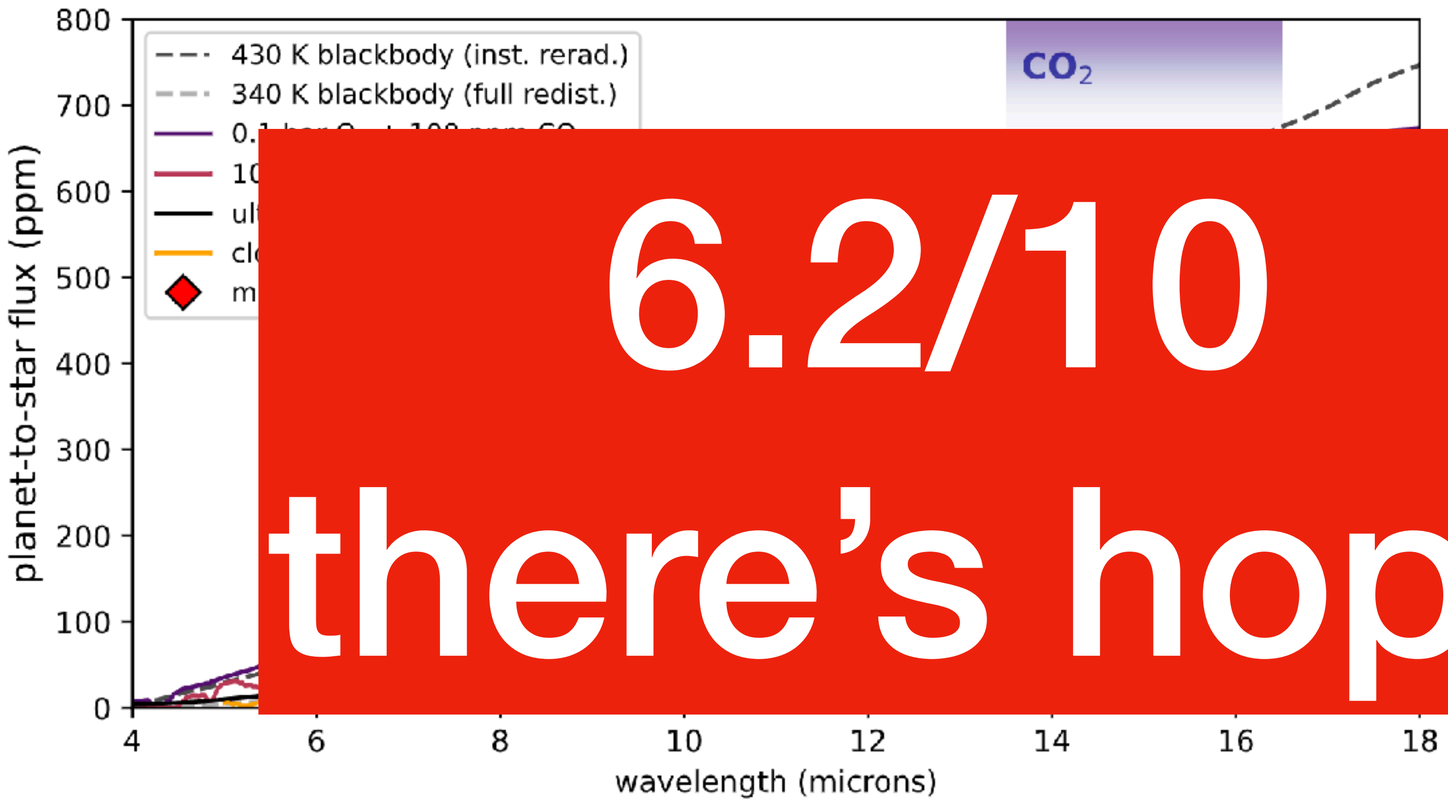
What kind of atmosphere *could* exist on TRAPPIST1-c? Constraints on surface pressure and CO2 abundance



Credit: Thomas Müller, Haus der Astronomie

Revisiting the TRAPPIST-1 system

Dayside temperature of planet c



6.2/10

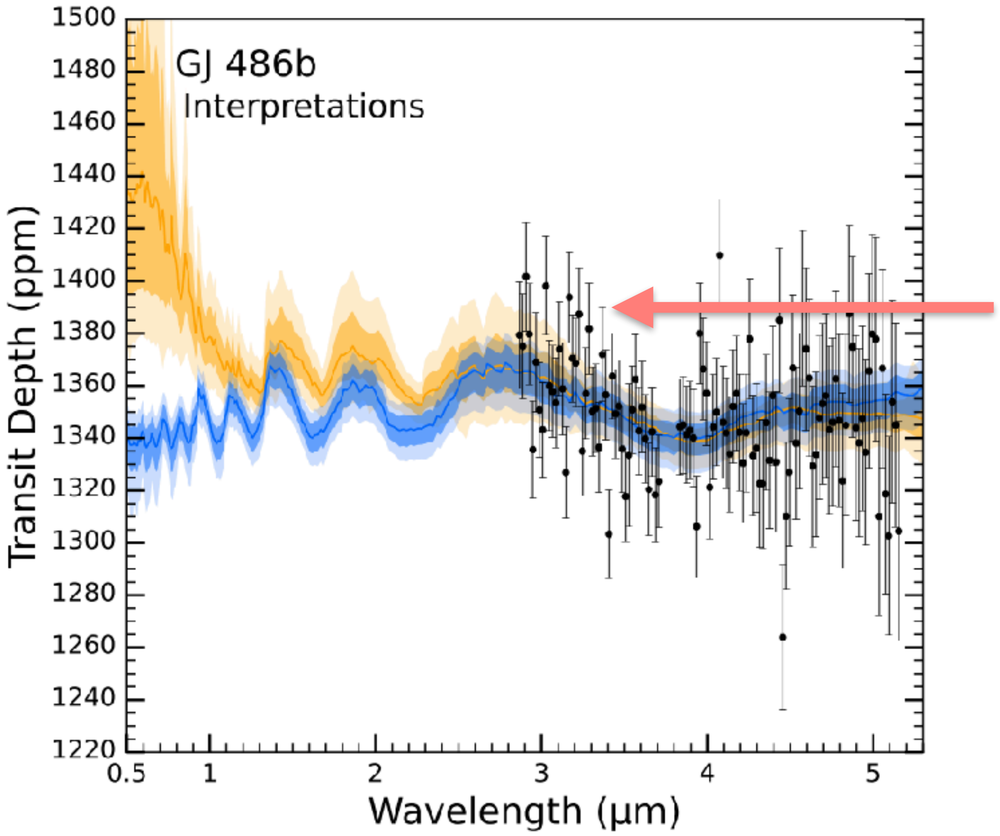
there's hope

…tian Zieba
…the job
…et :)



Zieba et al. 2023, Nature

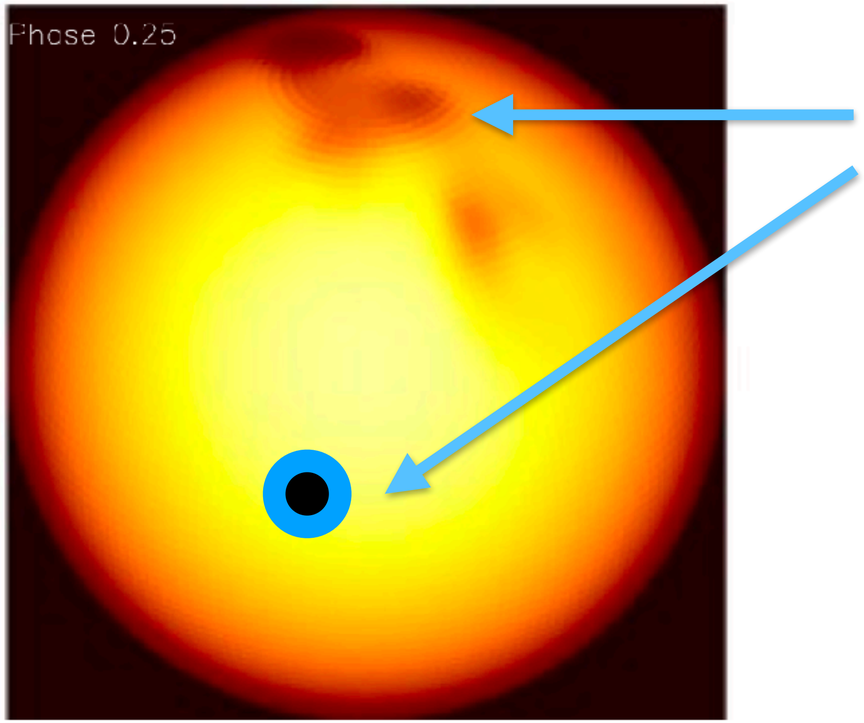
First rocky planet transmission spectrum, GJ 486b



Small feature is present!

Moran et al. 2023

Atmospheric “features” could come from the star…



There is water vapour in cool star spots that can masquerade as water in the planet’s atmosphere

Barnes et al. 2015, Rackham et al. 2018

Atmospheric “features” could come from the star…



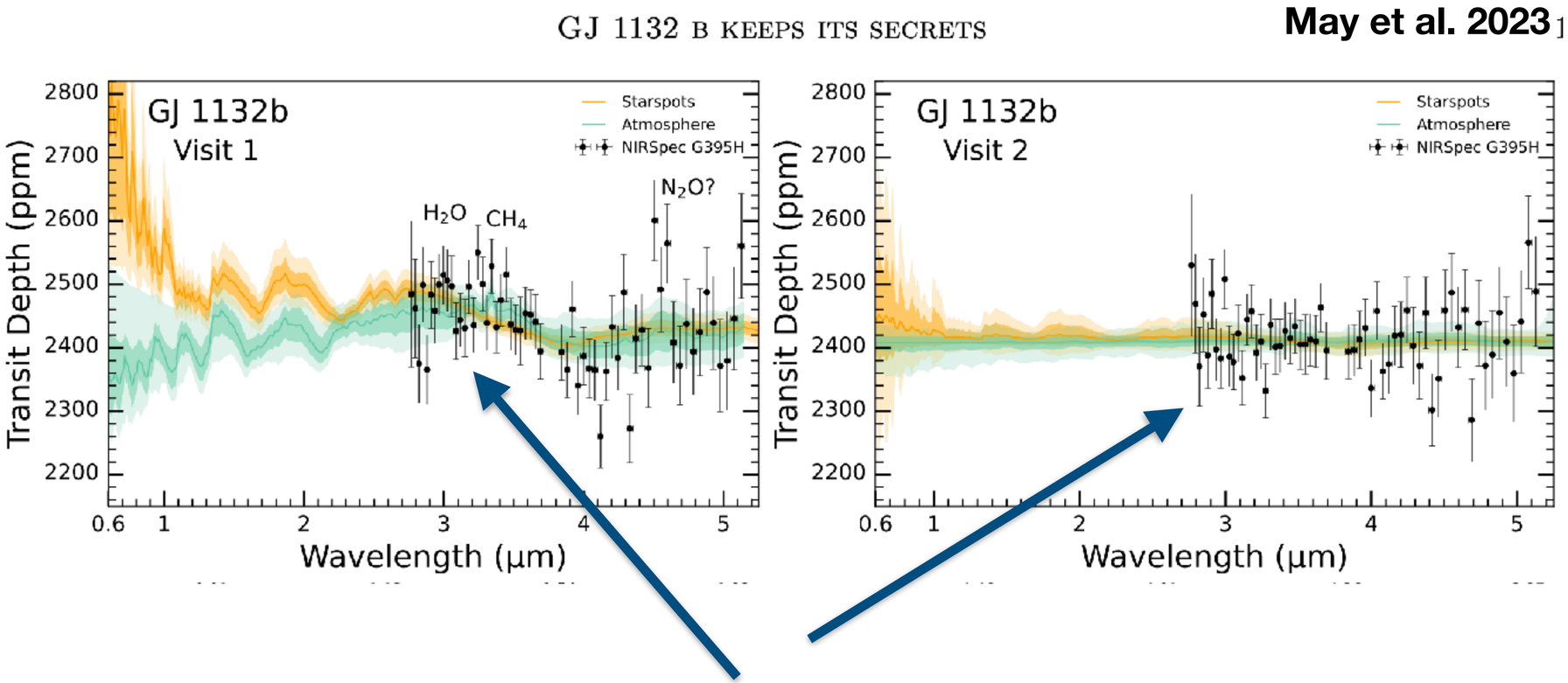
There is water vapour in cool star spots that can masquerade as water in

5.0/10 this star is on notice

Barnes et al. 2015, Rackham et al. 2018

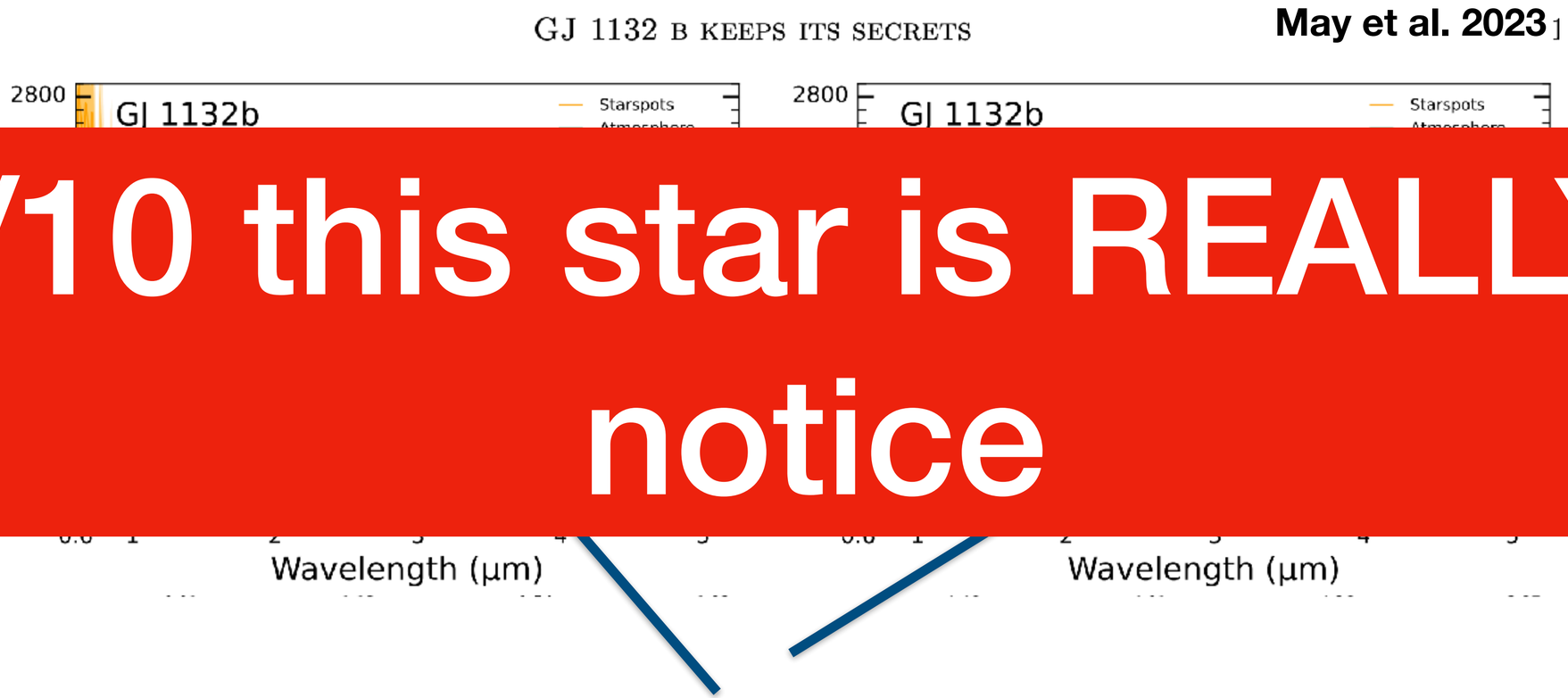
Signs of an atmosphere - now you see them, now you don't

May et al. 2023



"Feature" vanishes on second observation

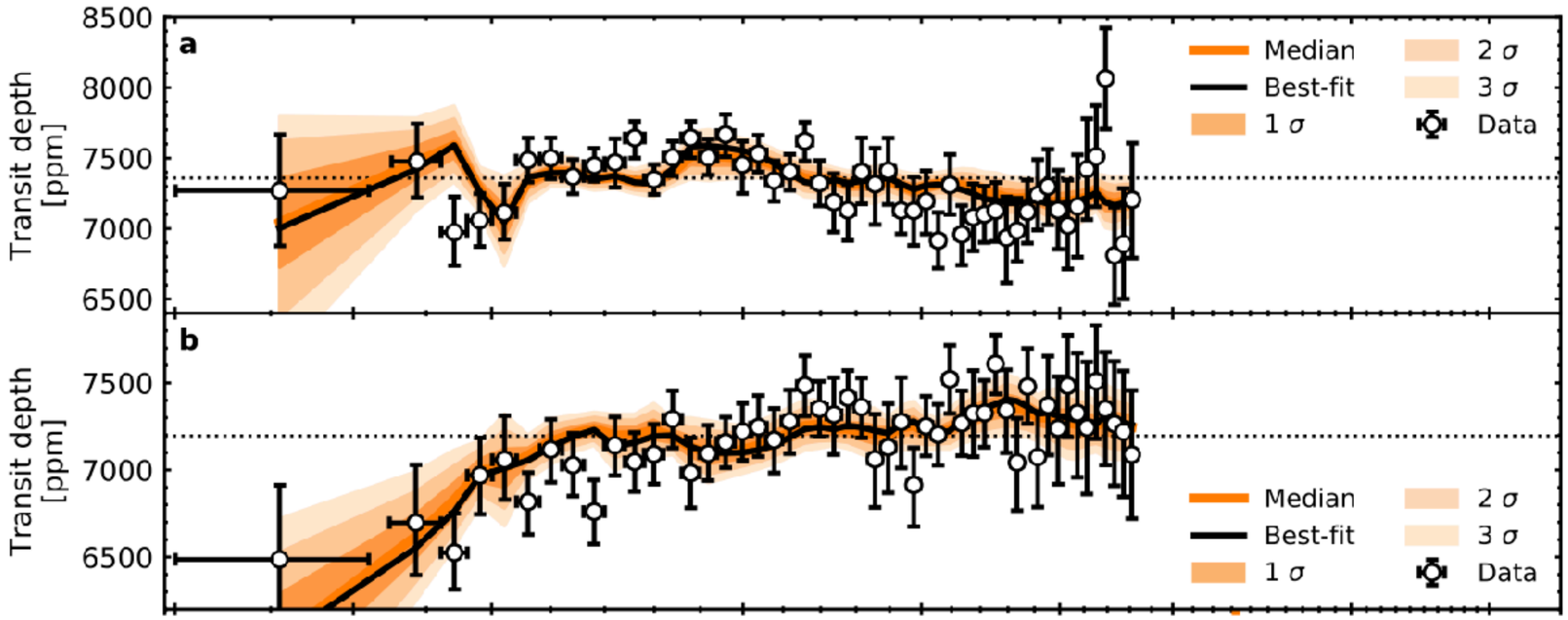
Signs of an atmosphere - now you see them, now you don't



0.2/10 this star is REALLY on notice

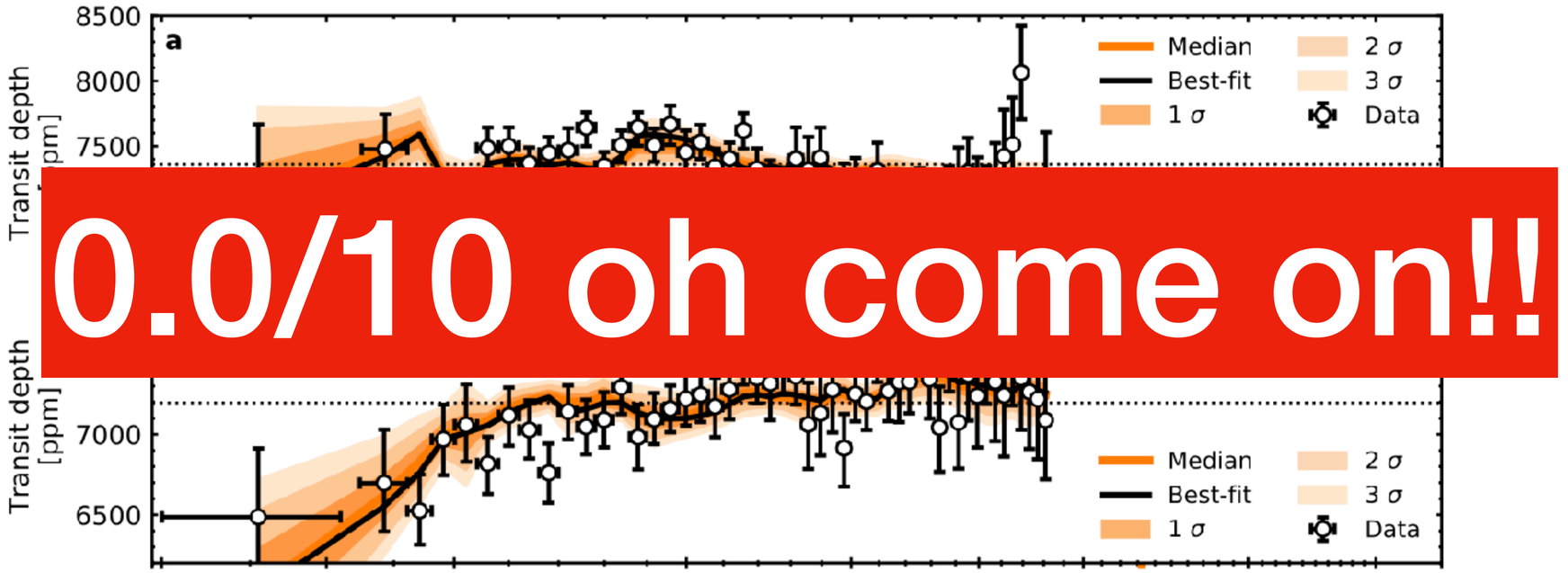
"Feature" vanishes on second observation

We even see “features” in the transmission spectrum of the bare rock TRAPPIST-1b



TRAPPIST-1b, Lim et al. 2023

We even see “features” in the transmission spectrum of the bare rock TRAPPIST-1b



0.0/10 oh come on!!

TRAPPIST-1b, Lim et al. 2023

What have we learned?

No atmosphere 2

Badly behaving star 3

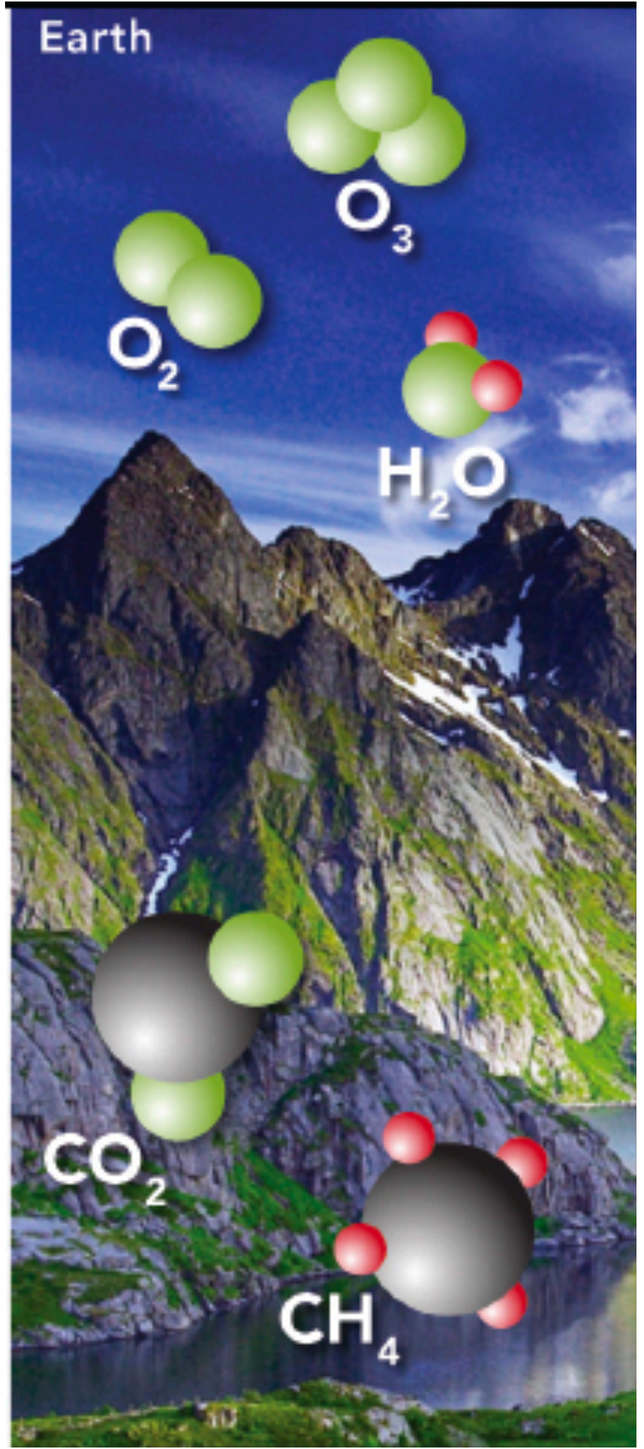
Possible atmosphere 1

JWST observations of rocky planets have just begun — how far can we push the limits?

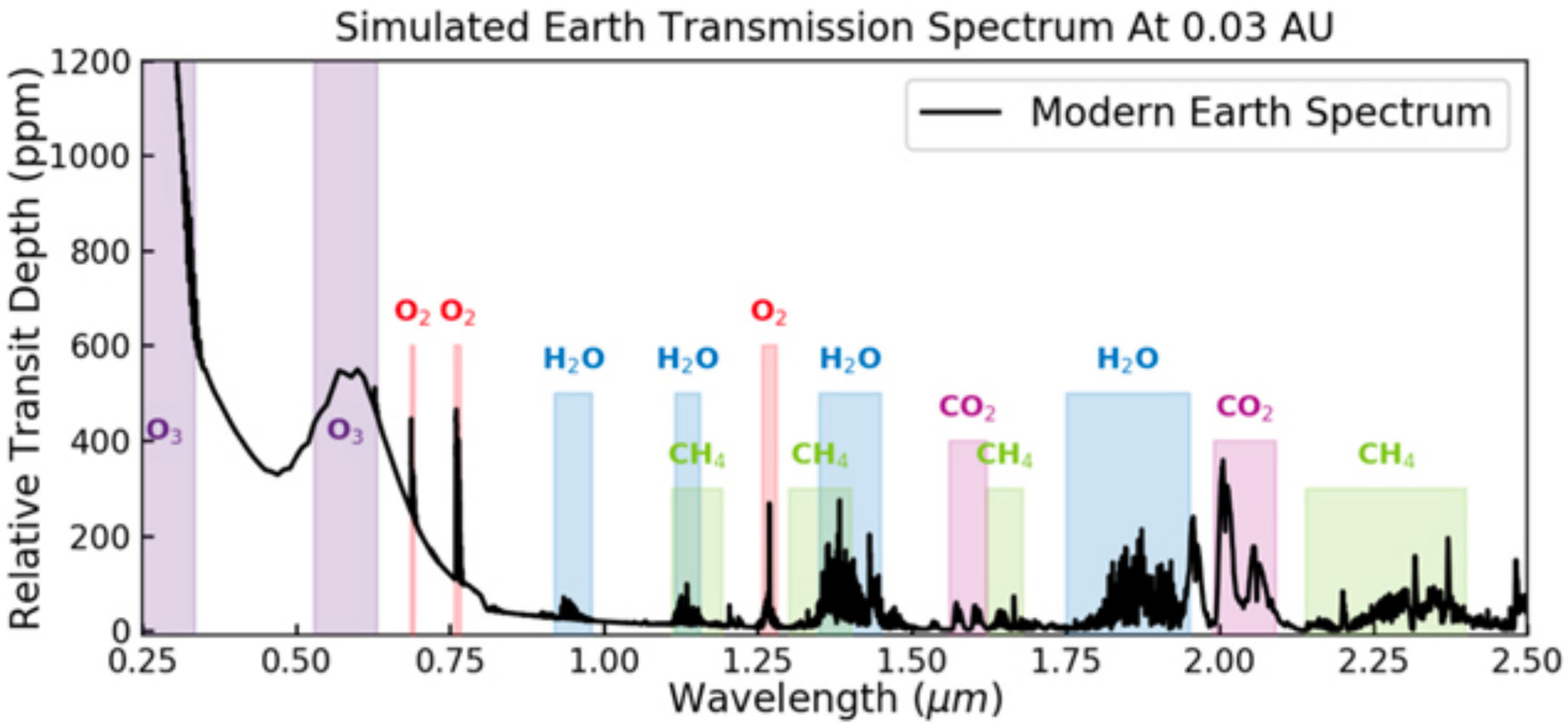
- What do we expect rocky planet atmospheres to look like?
- Which rocky planets can we observe with our current techniques? What have we learned so far?
- What is a biosignature? How will we identify inhabited planets?

What is a biosignature?

- Atmospheric chemistry *out of equilibrium*, due to biologic activity (and no other types of disequilibrium)
- The classic biosignature is the simultaneous presence of oxygen and methane on Earth
- Other possibilities: CH4+CO2, PH3, O2-X CIA, …

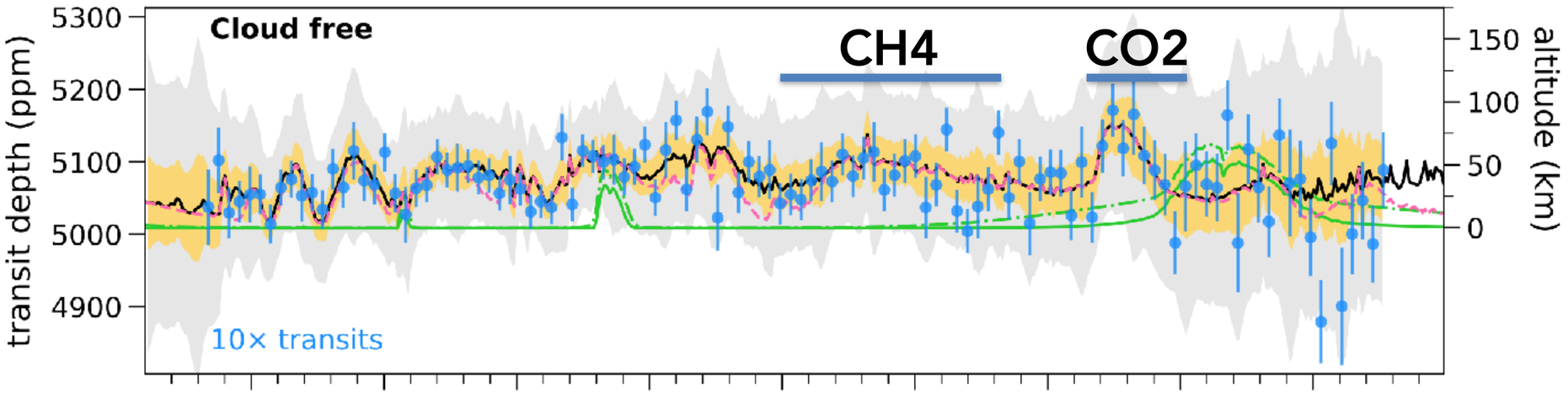


This is what Earth's transmission spectrum looks like



Mayorga et al. 2021

Detectability of CH4-CO2 biosignature on TRAPPIST-1e with JWST



For the clear atmosphere and cloud/haze layer pressures of 600-100 mbar, strong (5σ) detections of both CH4 and CO2 are found to be possible with approximately 5-10 co-added transits measured using the Near Infrared Spectrograph (NIRSpec) prism, assuming a dry stratosphere. However, approximately 30 coadded transits would be required to achieve the same result if a cloud/haze-layer is present at 10 mbar.

Mikal-Evans et al. 2022

WHAT IS NEXT?

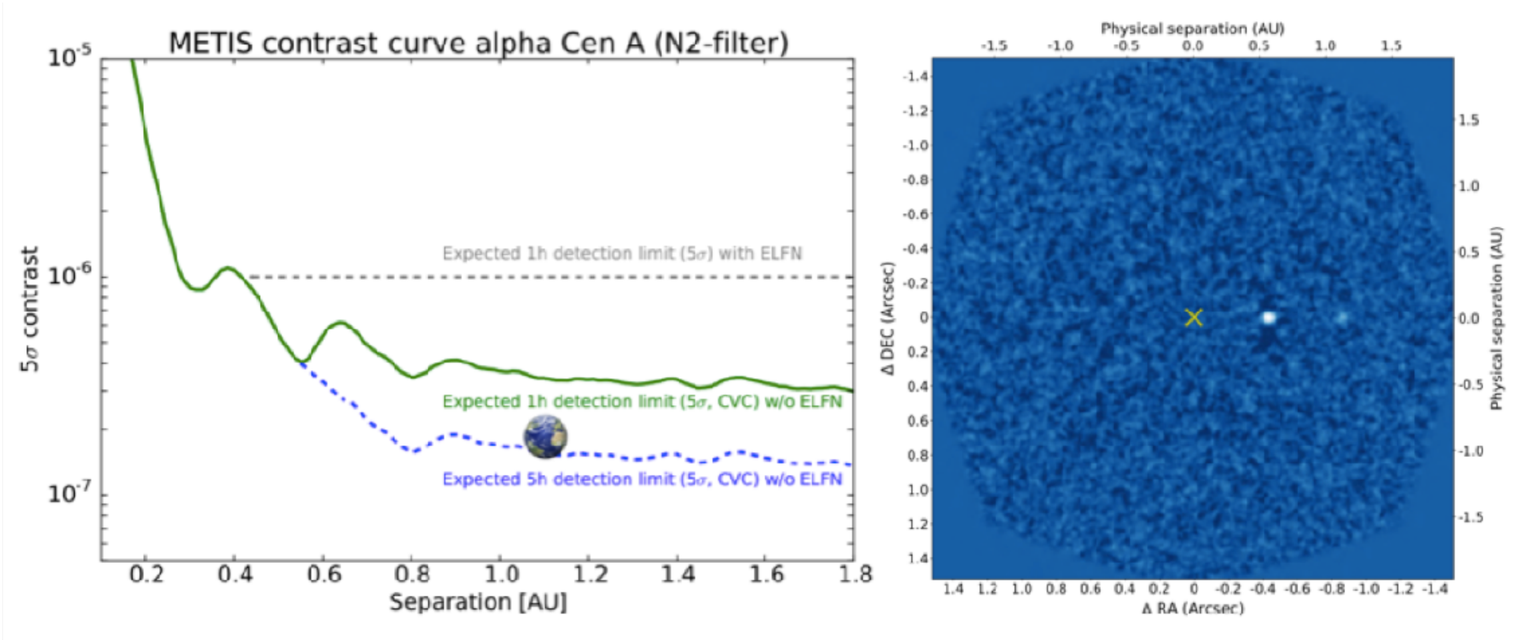
30-m class telescopes

Next-generation space telescopes

30-m class telescopes

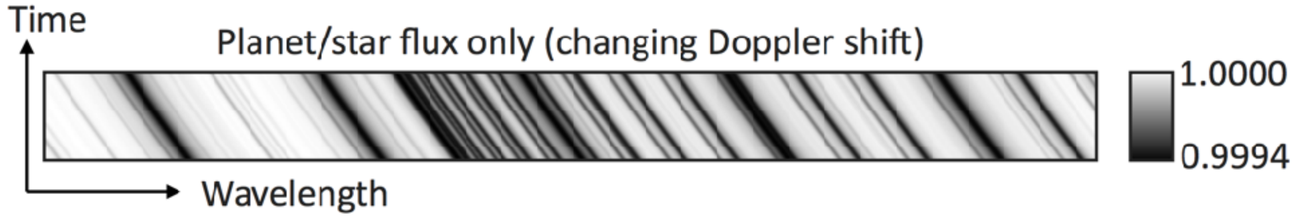
Possible first direct images of rocky planets

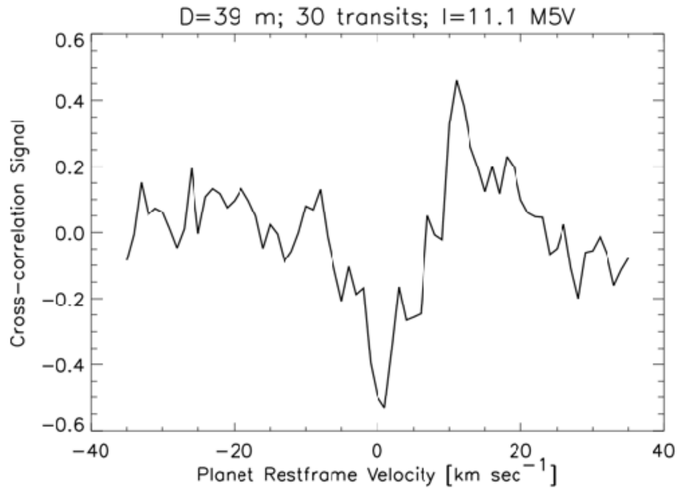
c/o Michael Meyer



30-m class telescopes

Possible detections of molecular oxygen at high spectral resolution





Oxygen detectable for a “best case scenario” planet, assuming dozens of transit observations

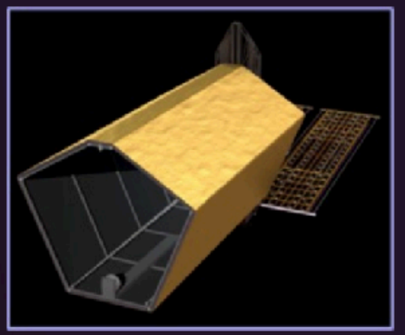
–Snellen 2013

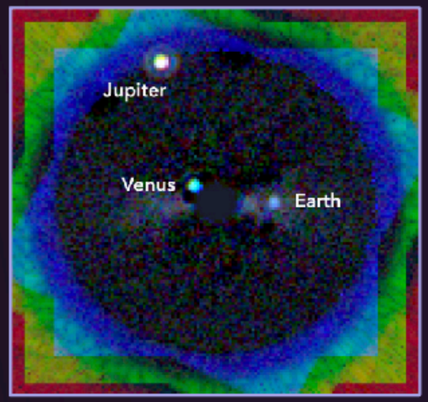
But - need to correct for Earth’s atmosphere orders of magnitude better than we currently do

Next generation telescopes

Pathways to Habitable Worlds

- Decadal Survey (ASTRO2020) priority science area
  - Are there habitable planets harboring life elsewhere in the universe?
  - Survey sun-like, nearby stars for habitable planets anmd search for evidence of life
- Primary recommendation:
  - Space telescope similar in wavelength coverage to Hubble, with an aperture of ≥6 meter and coronagraphic imaging capability
  - Observe ~100 nearby stars, and successfully detect potentially habitable planets around at least a quarter of the systems.
- Primary Technical requirements
  - 6 meter Segmented mirror telescope with active control of optics to achieve ultrastability
  - Coronagraph achieving contrast levels of 10^{-10}
- **Habitable Worlds Observatory**





Next generation telescopes



An ambitious mission employing a formation-flying nulling interferometer in space working at mid-infrared wavelengths. As such, LIFE is grounded in the heritage of ESA's Darwin and NASA's TPF-I concepts from the early/mid 2000s