Interpreting ~~Photometry~~ ~~&~~ Spectroscopy From A Modeling Perspective

And Lots about… Clouds

Eileen Gonzales
Assistant Professor
San Francisco State University

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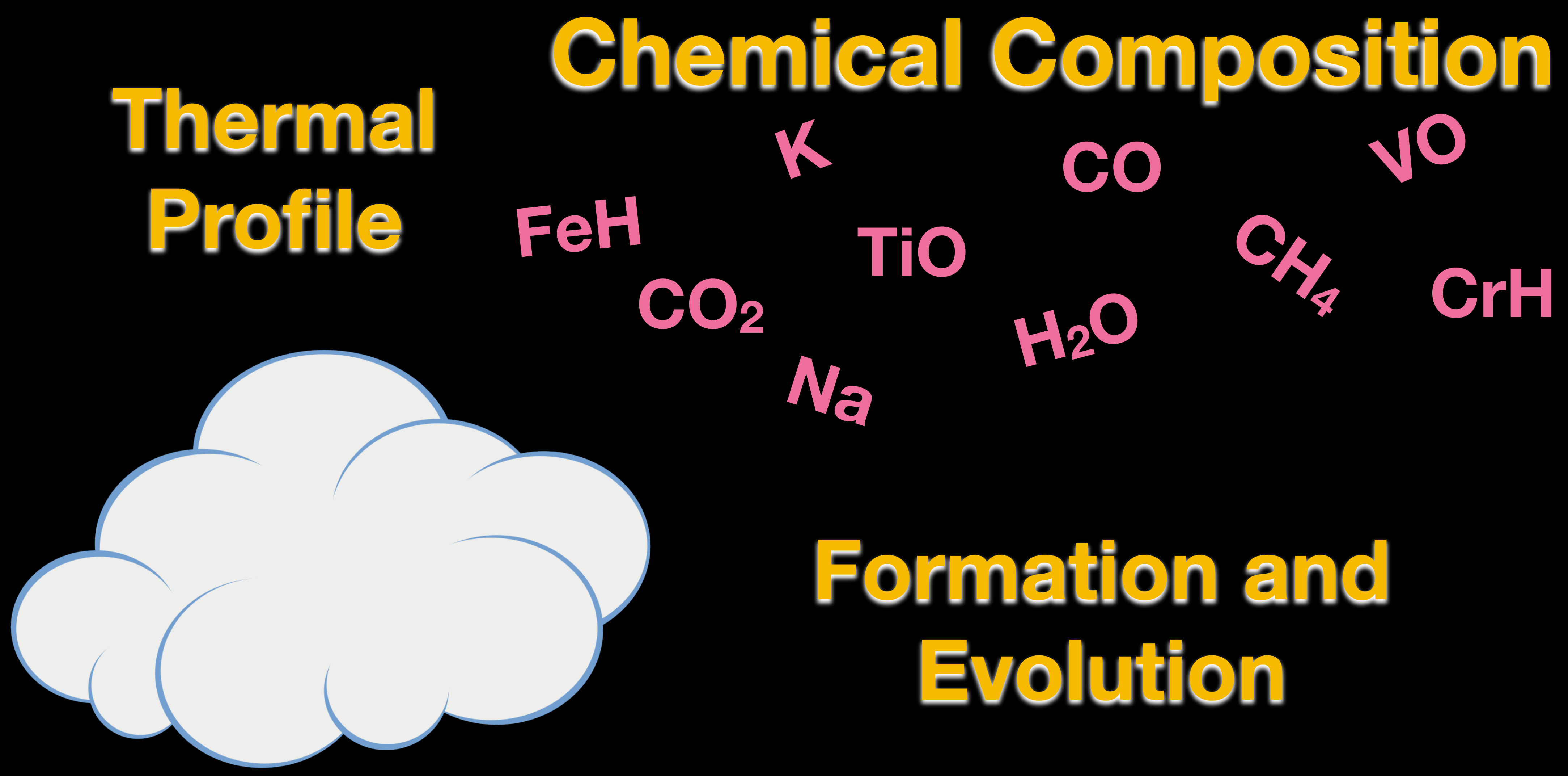
San Francisco State University

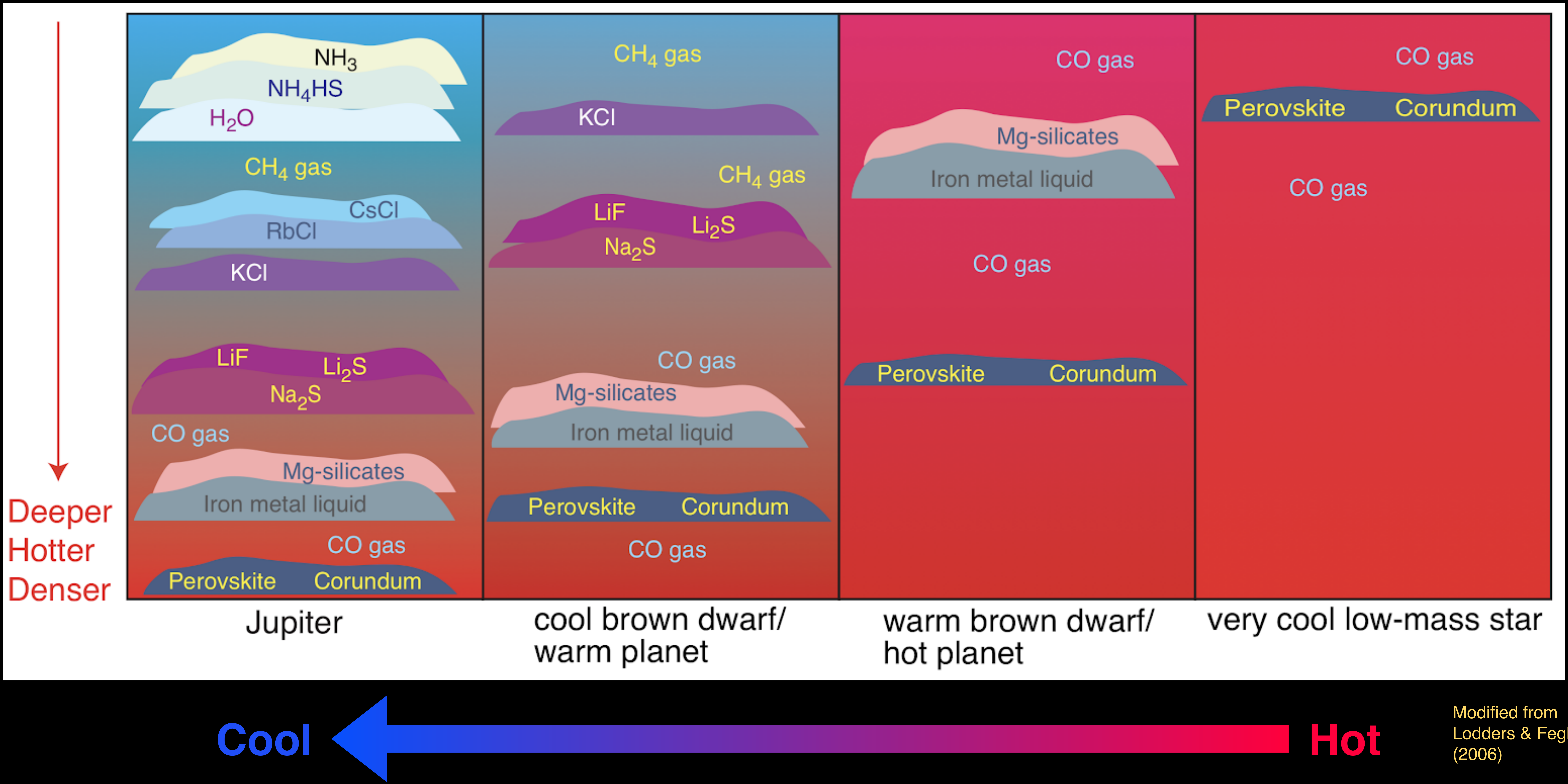
What is your science question?

What are the key bits of information you want to explore through modeling?



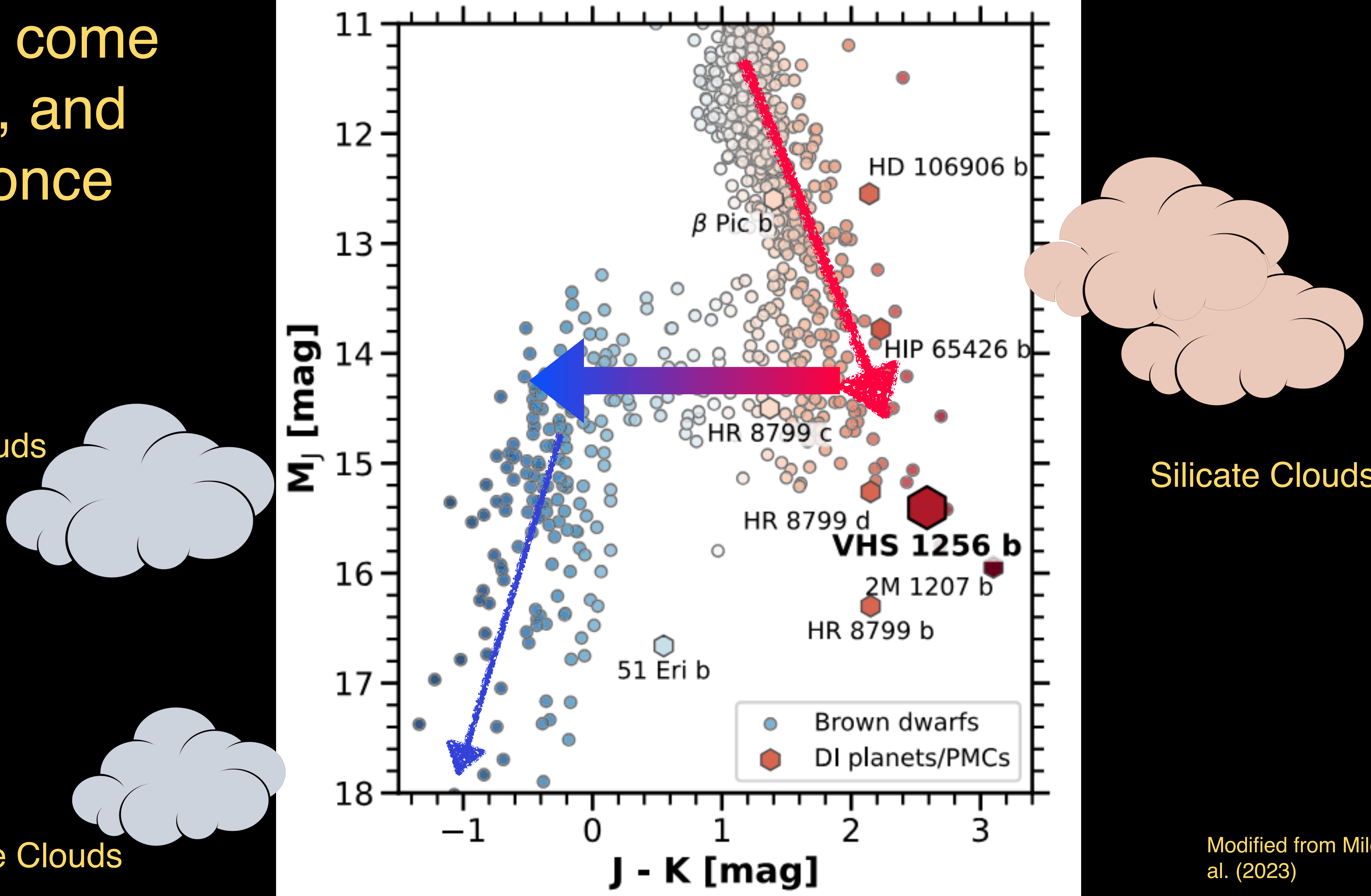
Thermal Profile
Chemical Abundances
Disequilibrium Chemistry
Vertical mixing
C/O for formation
Isotopologue abundances
Cloud particle Size
Cloud composition
Variability
Match Model to Data for fundamental properties
Predictions of missing wavelength coverage
Fit unexpected features
And more…..

Clouds in Substellar Atmospheres



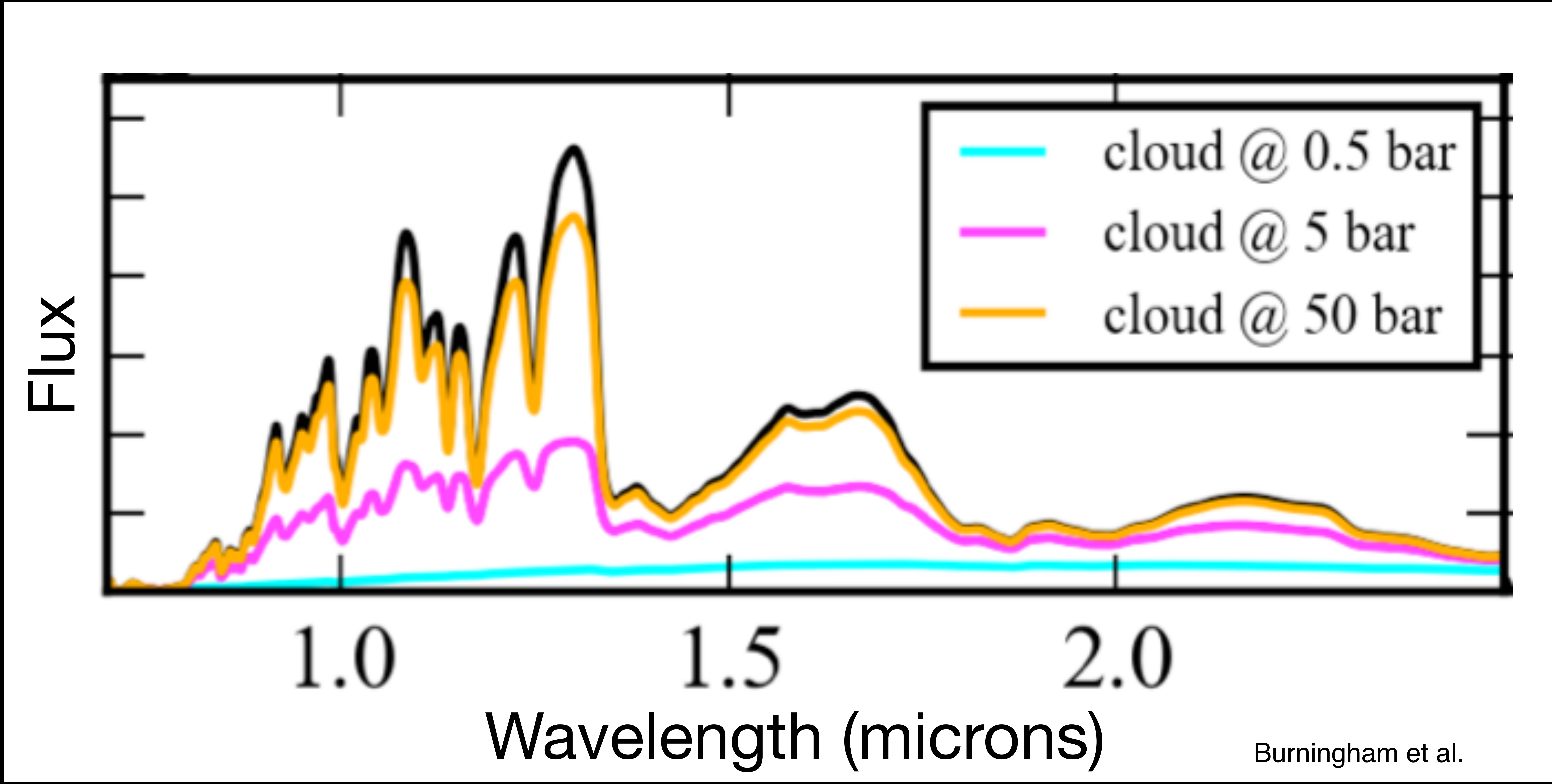
Modified from
Lodders & Fegley
(2006)

Clouds come and go, and return once more



Modified from Miles et al. (2023)

Clouds suppress spectral features



Forward Model vs Retrieval Model

Self-Consistent Grid models

Chemical Equilibrium retrievals

Free retrievals

Few knobs to turn

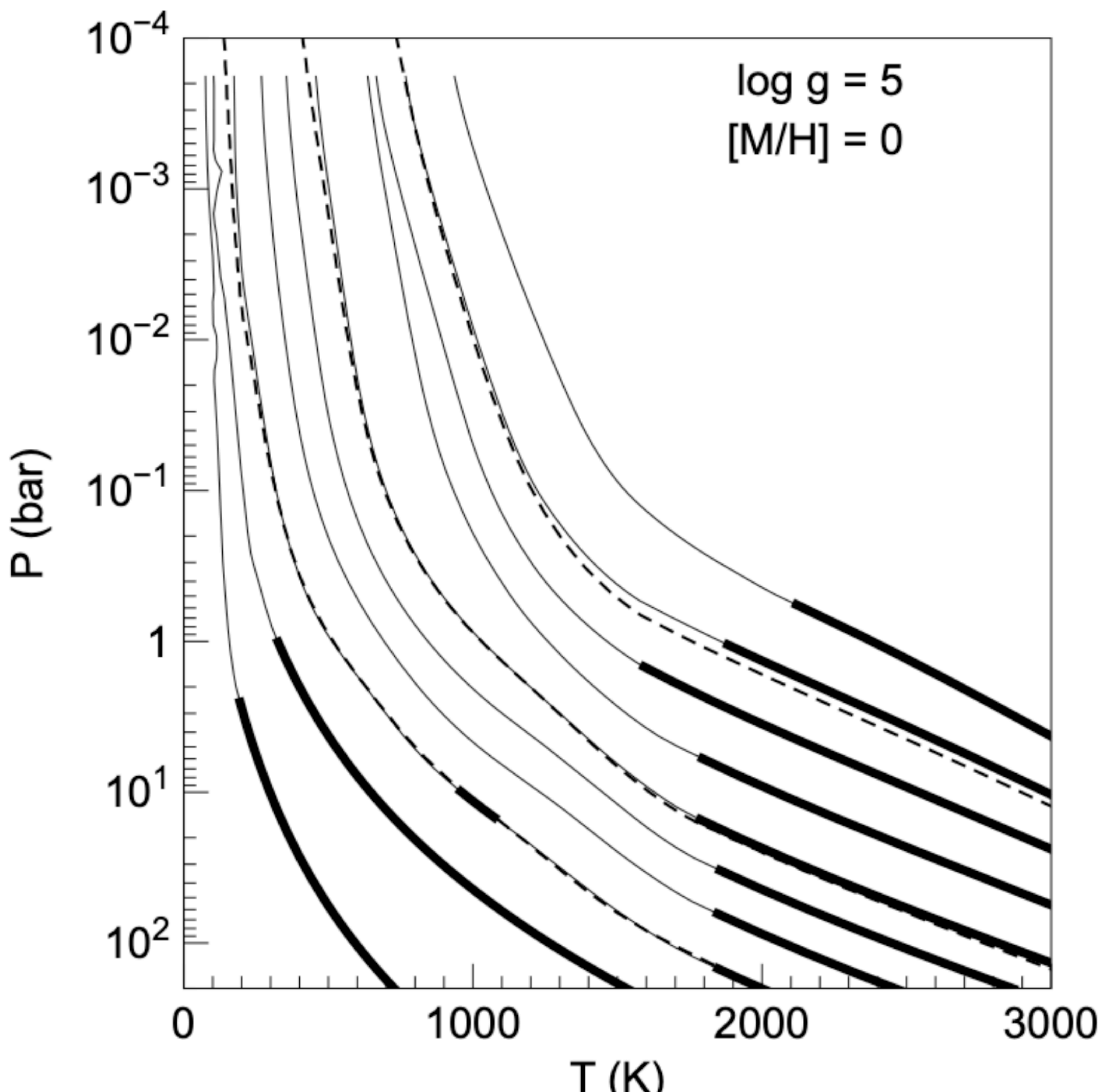
Many knobs to turn

Decreasing consistency →

What is a Forward Model

(Aka Grid Model) is self consistent model that includes all the physics and chemistry.

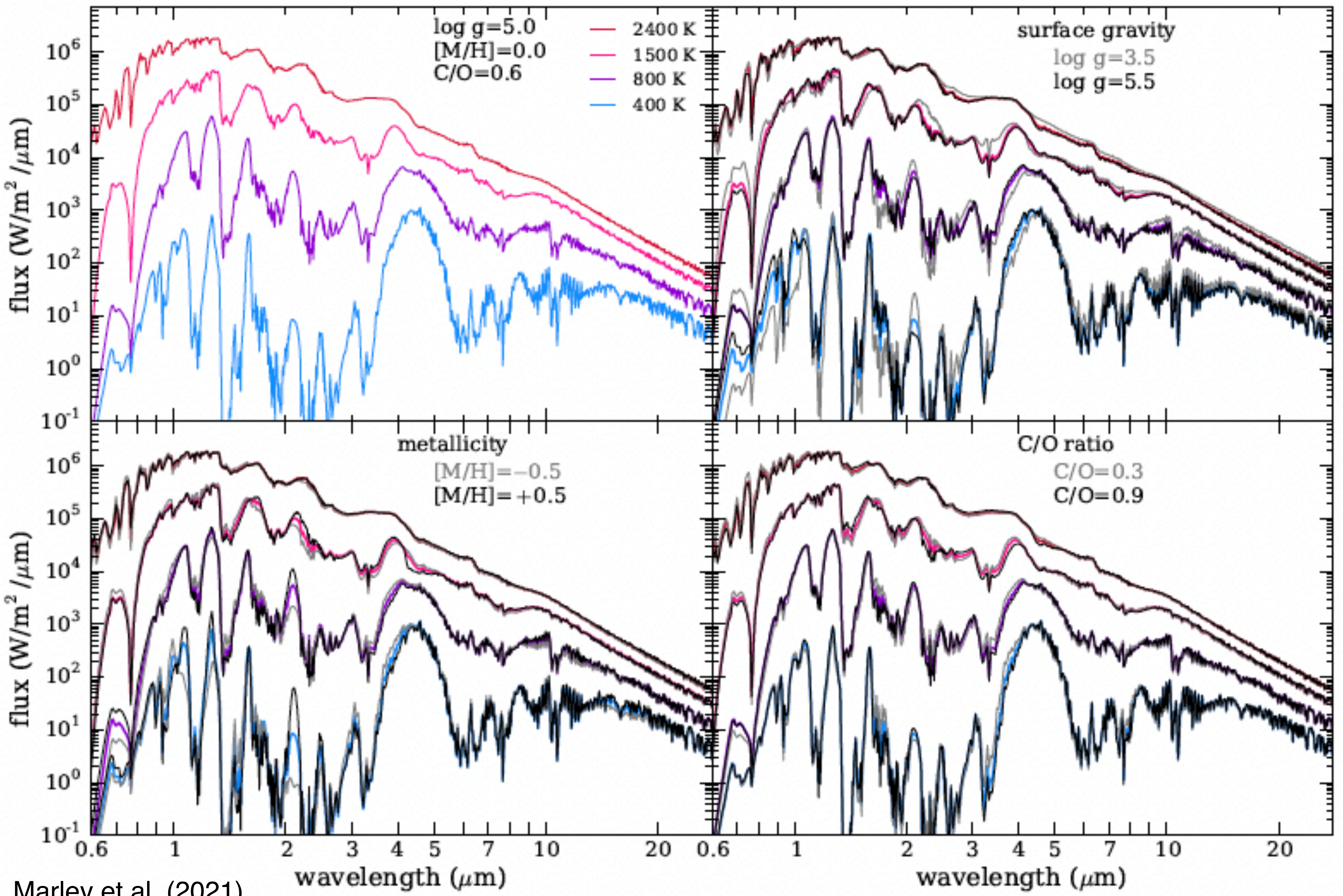
Assumes radiative-convective equilibrium, thermochemical equilibrium, and quench approximation



Marley et al. (2021)

(See Marley & Robinson 2015 and Heather Knuston 2018 SSW Talk 1D Models Slide for more detail)

Forward Models: What do they include?



Marley et al. (2021)

Effective Temperature
Surface Gravity
Metallicity
C/O
K_{zz}
F_{sed}

Forward Models: Why use them?

Easy to use to compare to observations

Great for limited data coverage

Ideal Comparisons to retrieval fits

Great as predictions for proposals

Examples of Forward Models:

- Sonora
- ATMO
- BT-SETTL
- PHOENIX
- Exo-Rem
- Lacy & Burrows
- And many more

https://emac.gsfc.nasa.gov/

What Are Atmospheric Retrievals

Theoretical inverse spectral modeling technique that makes minimal assumptions about the physics involved

Self-Consistent Grid models

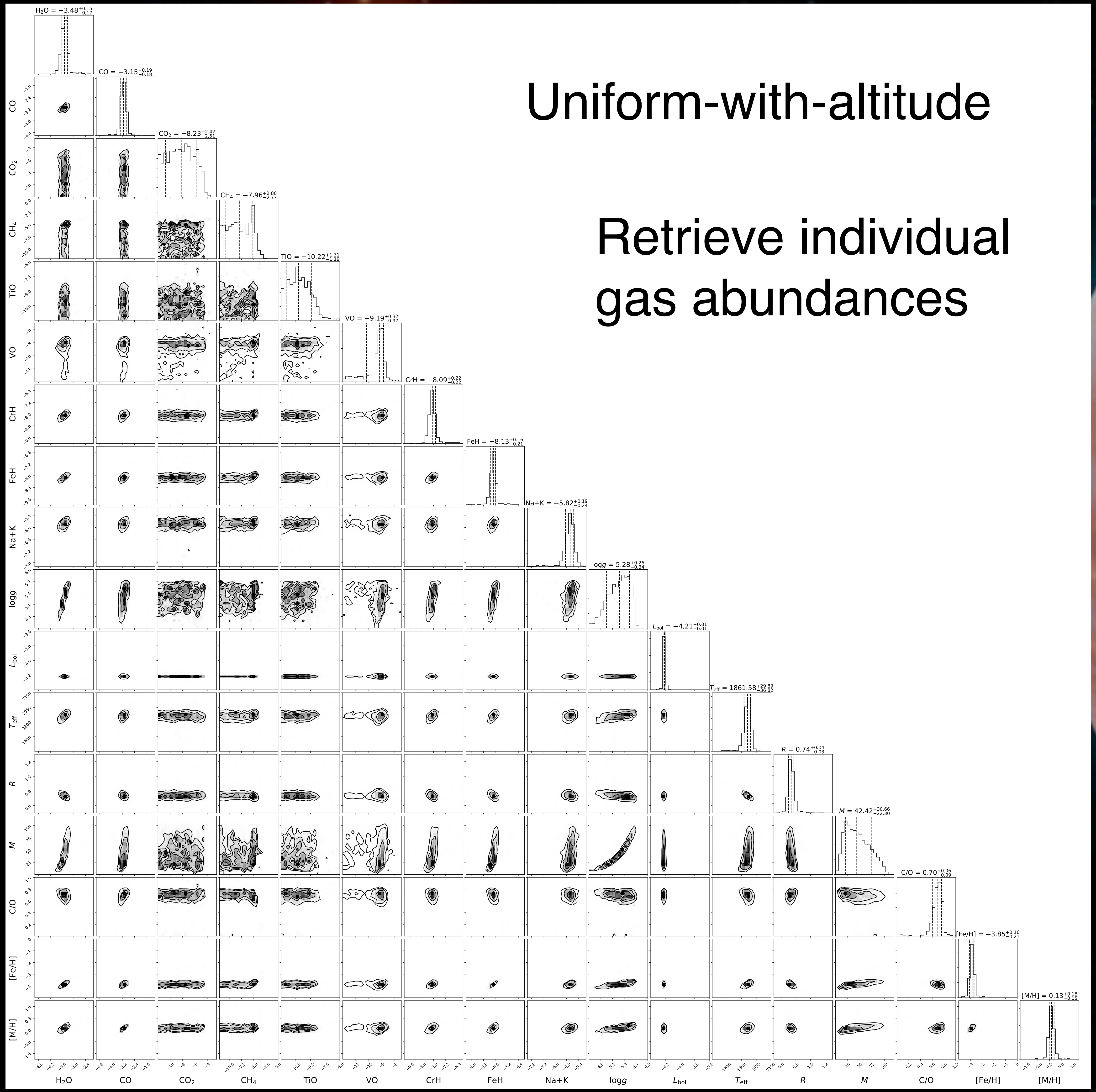
Chemical Equilibrium retrievals

Free retrievals

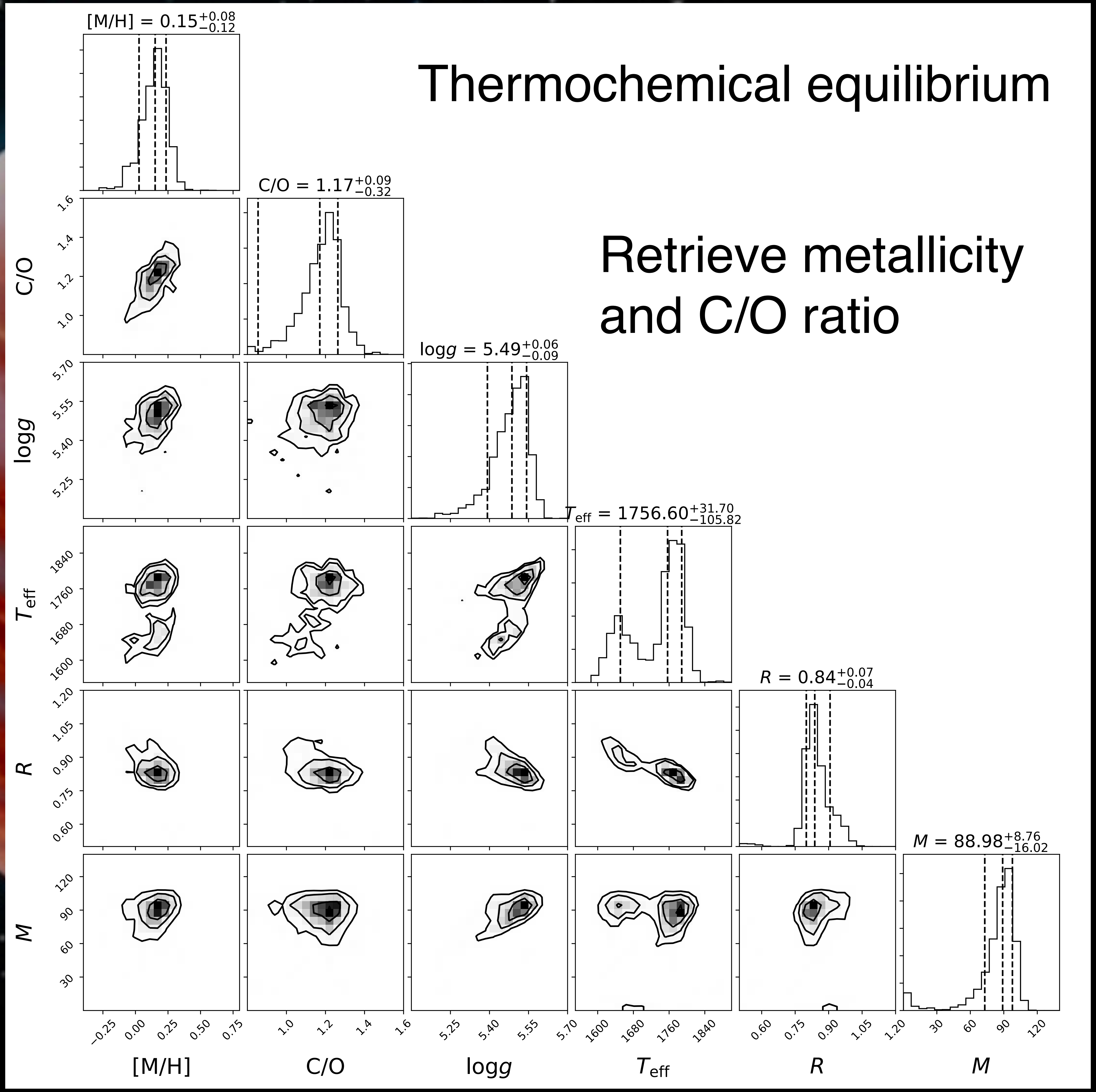
Few knobs to turn

Many knobs to turn

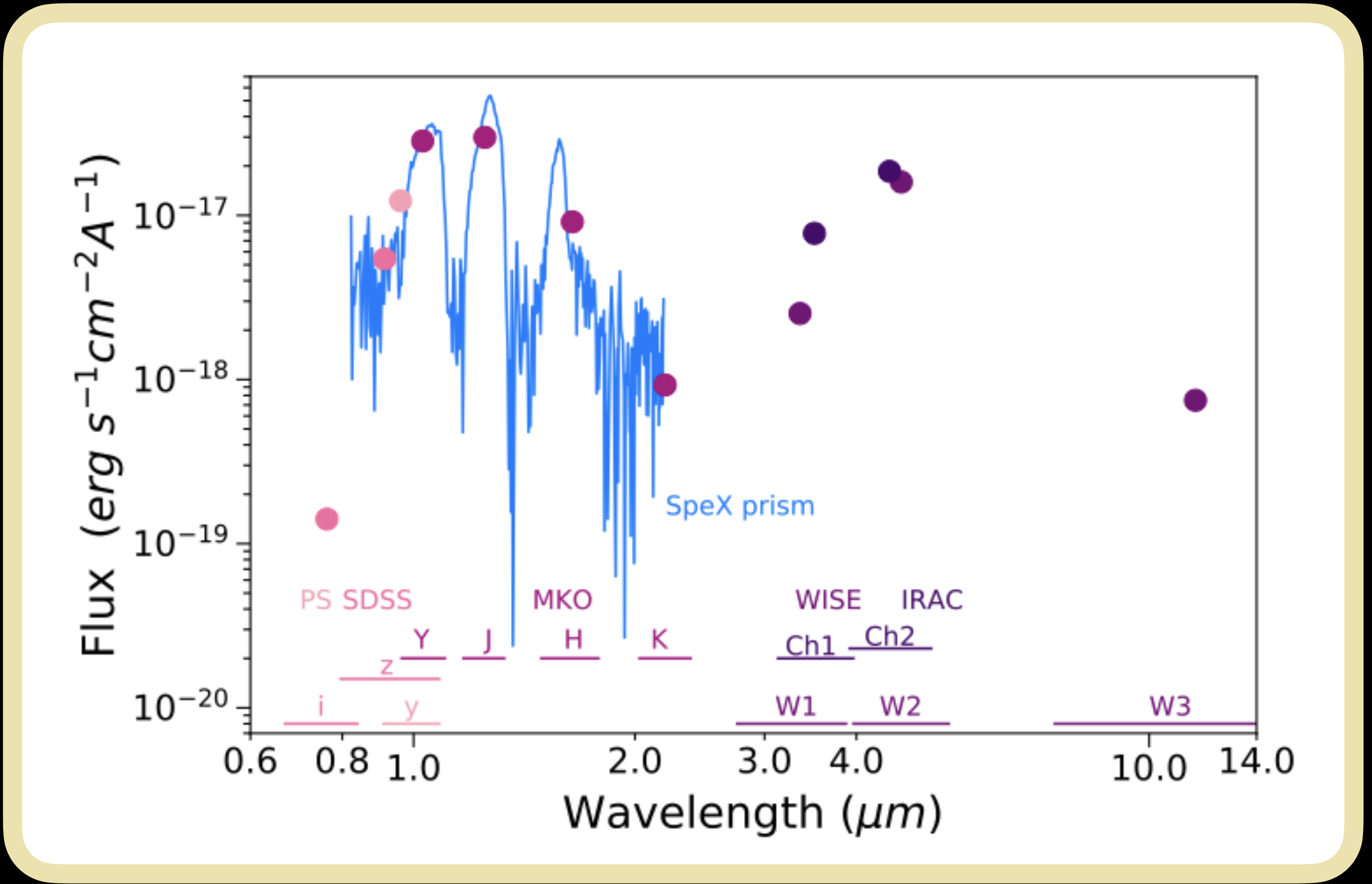
Assume gas abundance is the same no matter the altitude



Gas abundances from thermochemical grid



How do Retrievals work?



Gonzales et al. (2020)

Setup Parameters

- PT profile parameterization
- Cloud parameterization
- Chemical model

Atmospheric Retrieval

H_2O CH_4 CO

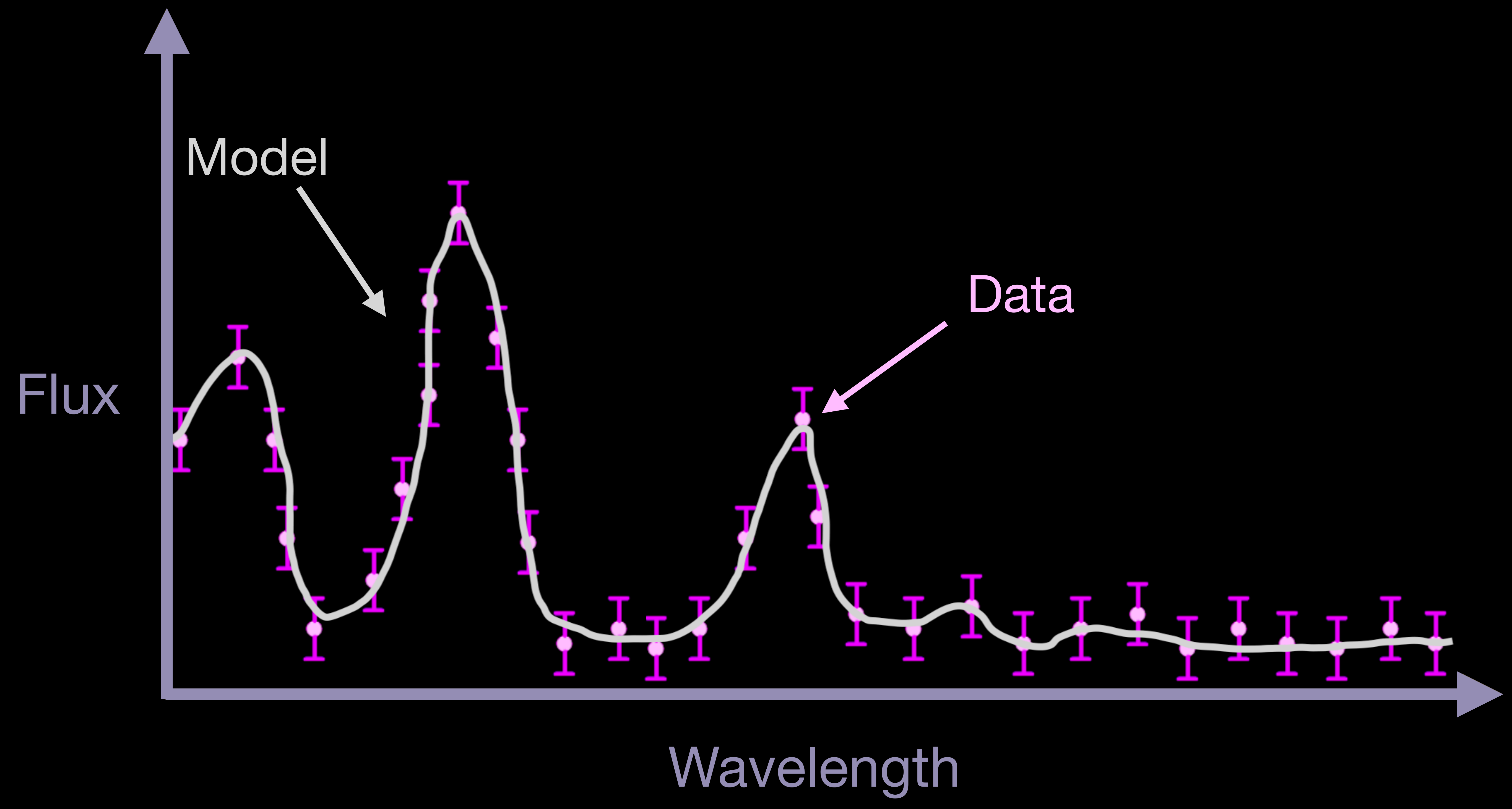
NH_3 Na K

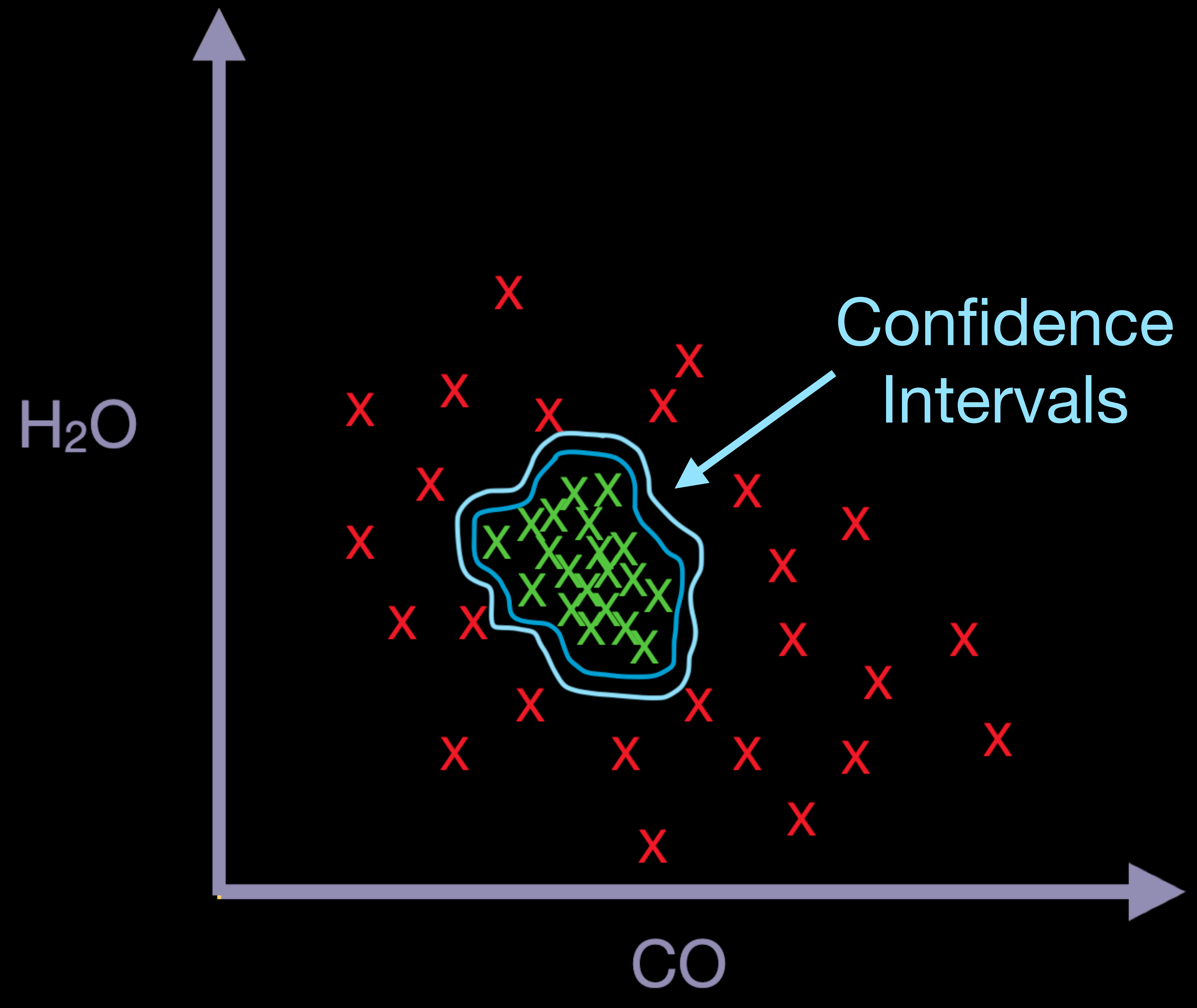
Underlying Assumptions

- Radiative transfer treatment
- Gas opacities (i.e. Line Lists)

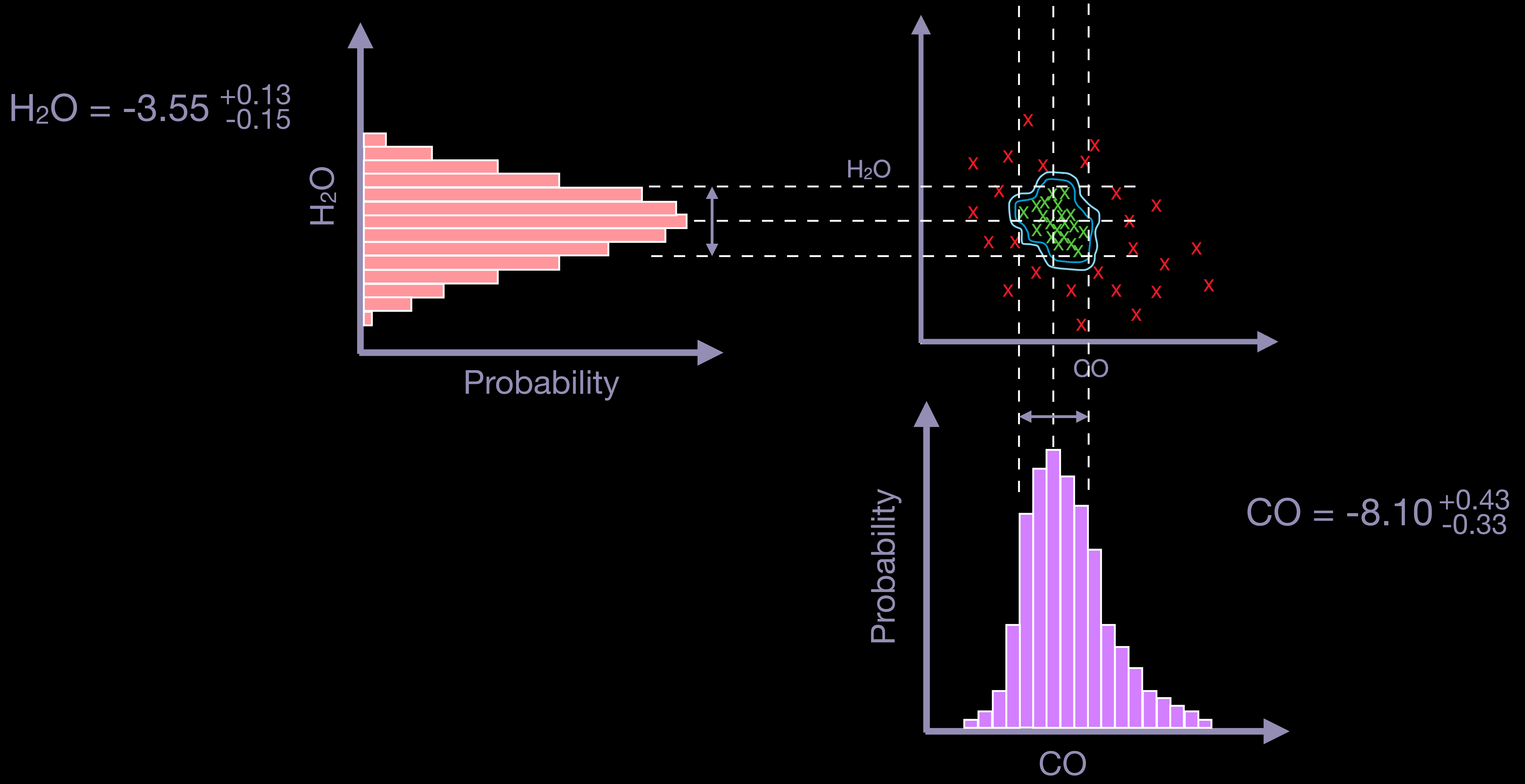
Spectrum + Assumed Gases + Setup + Underlying Assumptions =

How the Sampler Works

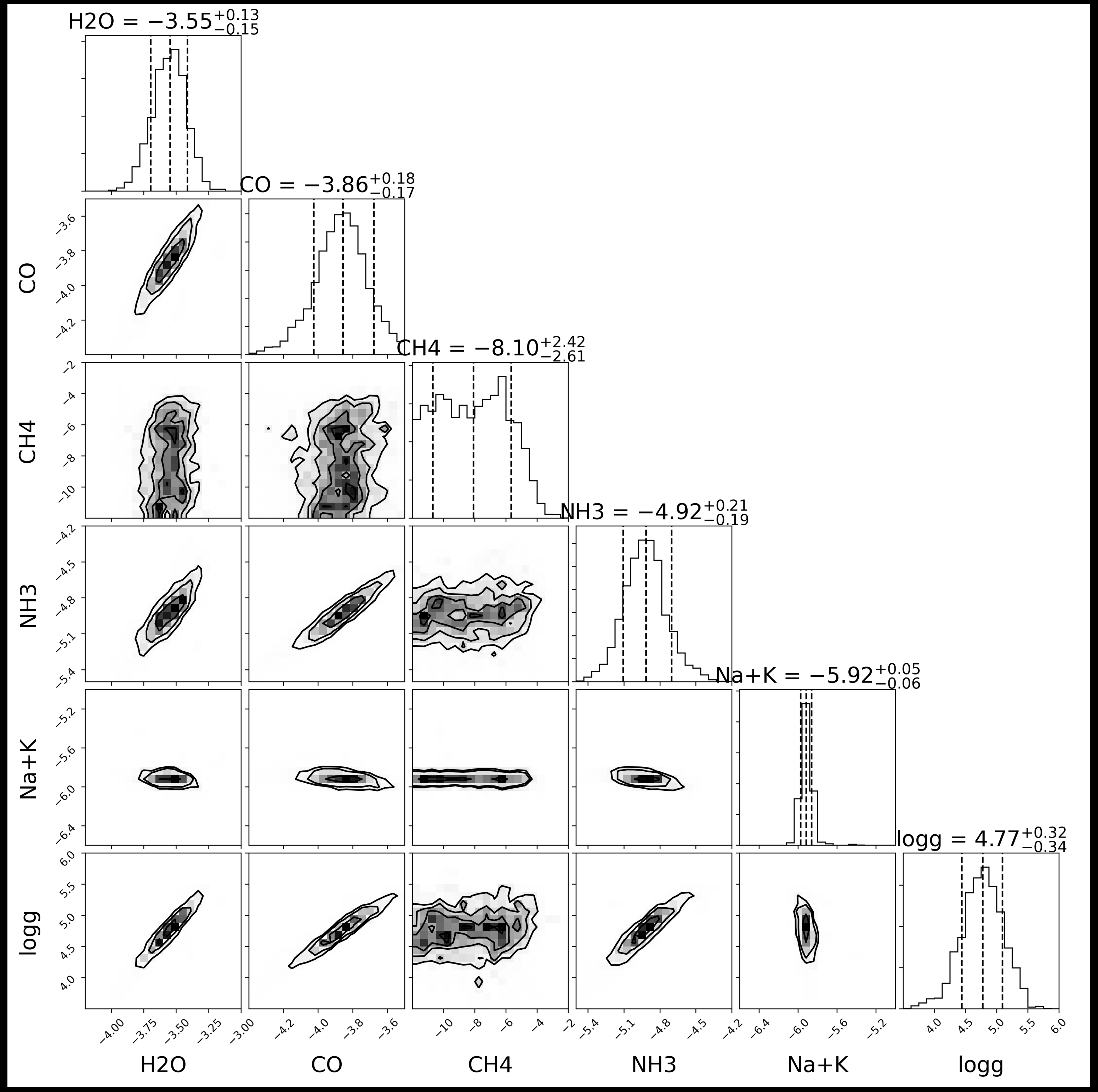


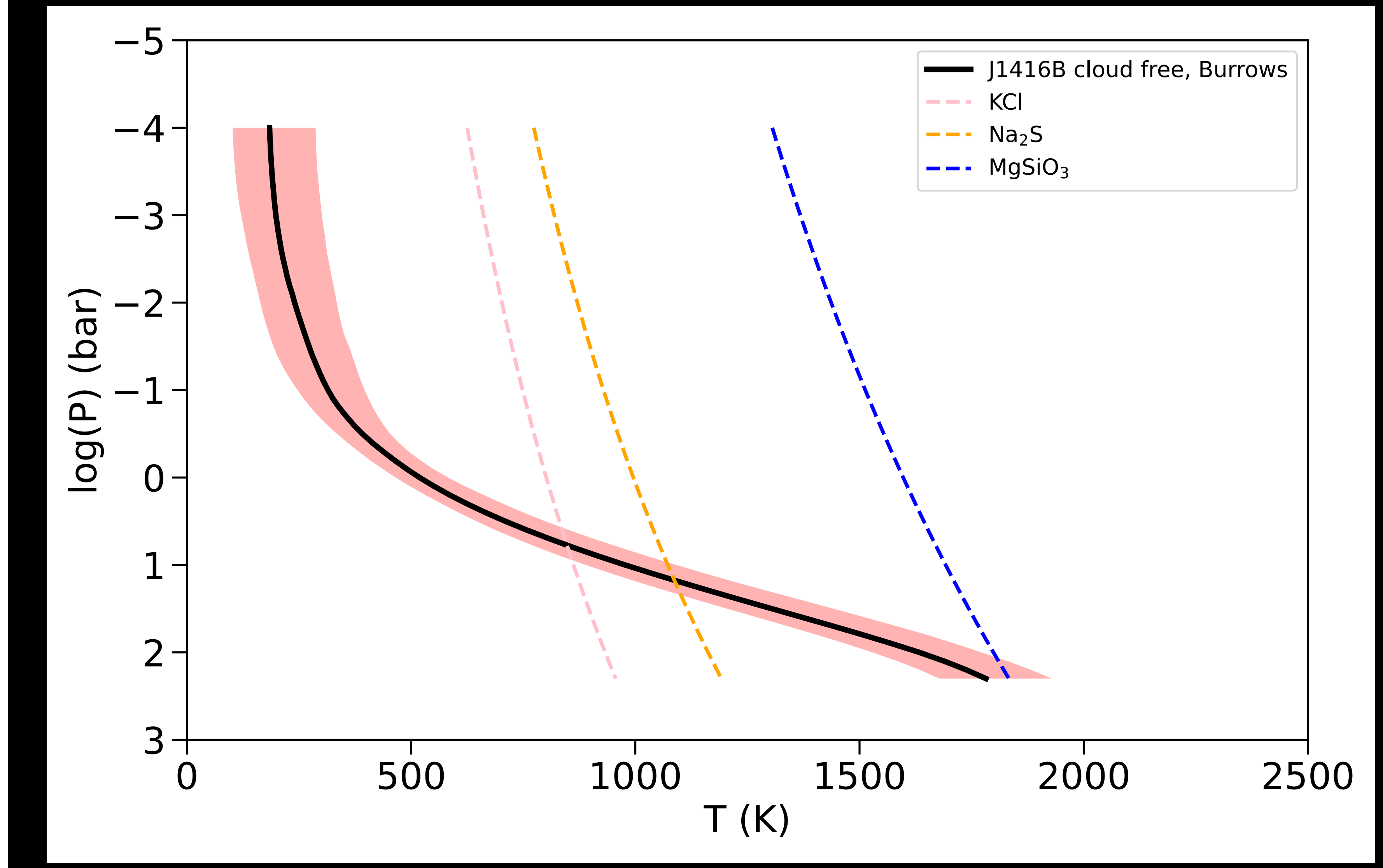


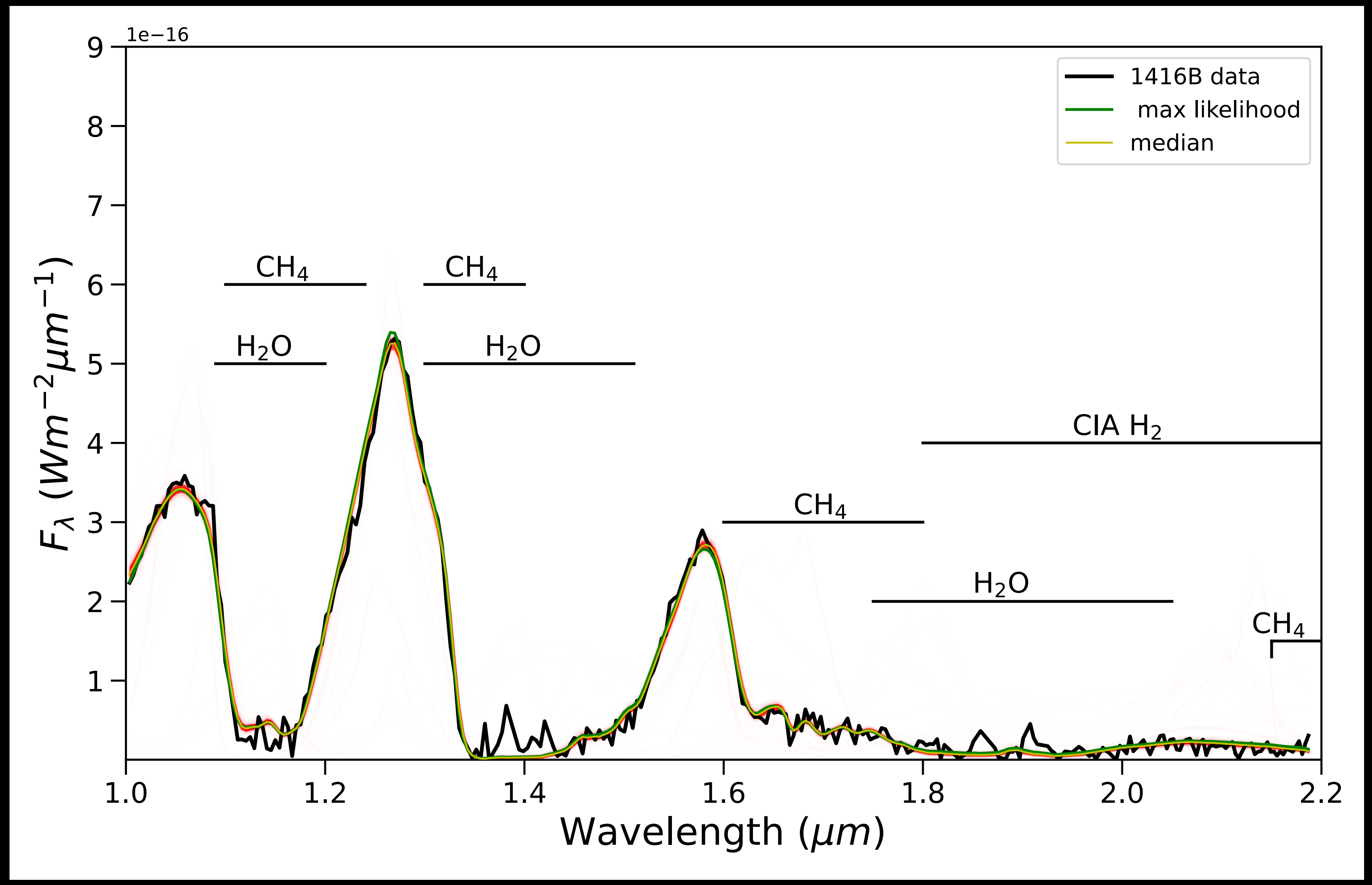
Getting Parameter Values



What Comes Out?







Gonzales et al. (2020)

= Gas Abundances + Thermal profile (cloud properties if included) + Retrieved Model Spectrum

What Retrieval Codes are there?

At least 49 published codes

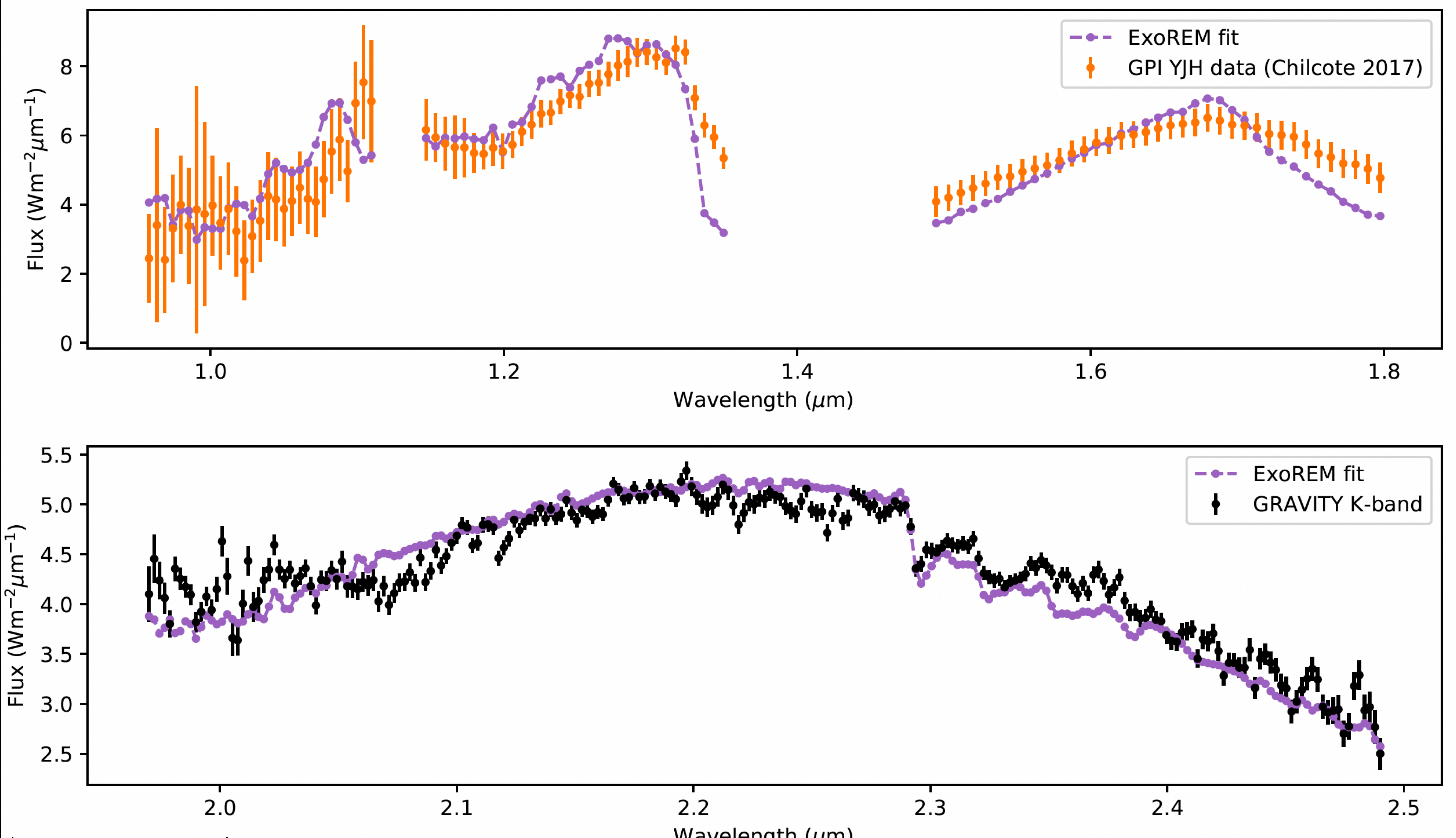
Catalogue of Exoplanet Atmospheric Retrieval Codes (https://zenodo.org/records/7675743)

Table 1. Catalogue of Exoplanet Atmospheric Retrieval Codes

Code / Authors	Spectrum Type	Parameter Exploration	Code Link	References
Sampling Based				
Madhusudhan & Seager	Transmission Emission	Grid, MCMC	—	Madhusudhan & Seager (2009)
NEMESIS	Emission Transmission Reflection	OE, NS	Link	Lee et al. (2012) Barstow et al. (2013) Barstow et al. (2014)
SCARLET	Transmission Emission Reflection	MCMC, NS	—	Benneke & Seager (2012) Benneke et al. (2019) Wong et al. (2020)
MassSpec	Transmission	MCMC	—	de Wit & Seager (2013)
CHIMERA	Emission Transmission Reflection	OE, MCMC, NS, SC-Grid	Link	Line et al. (2013) Swain et al. (2014) Piskorz et al. (2018)
TauREx	Transmission Emission	MCMC, NS	Link	Waldmann et al. (2015b) Waldmann et al. (2015a)
Lupu et al.	Reflection	MCMC, NS	—	Lupu et al. (2016)
HELIOS-R	Emission	NS	Link	Lavie et al. (2017)
APOLLO	Transmission Emission	MCMC	Link	Howe et al. (2017) Howe et al. (2022)
POSEIDON	Transmission Emission	NS	Link	MacDonald & Madhusudhan (2017) Coulombe et al. (2023)
ATMO	Transmission Emission	MCMC, NS, SC-Grid	—	Wakeford et al. (2017) Evans et al. (2017)
Brewster	Emission	MCMC, NS	—	Burningham et al. (2017)
Pyrat Bay	Transmission Emission	MCMC	Link	Kilpatrick et al. (2018) Cubillos & Blecic (2021)
HyDRA	Emission	NS	—	Gandhi & Madhusudhan (2018)
PSG	Reflection Emission Transmission	OE, NS	Link	Villanueva et al. (2018)
AURA	Transmission	NS	—	Pinhas et al. (2018)
exoretrievals	Transmission	NS	—	Espinoza et al. (2019)
Brogi & Line	Emission	NS	Link	Brogi & Line (2019)
PLATON	Transmission Emission	NS	Link	Zhang et al. (2019) Zhang et al. (2020)

When do you choose:
forward model or a retrieval model?

What kind of data do you have?



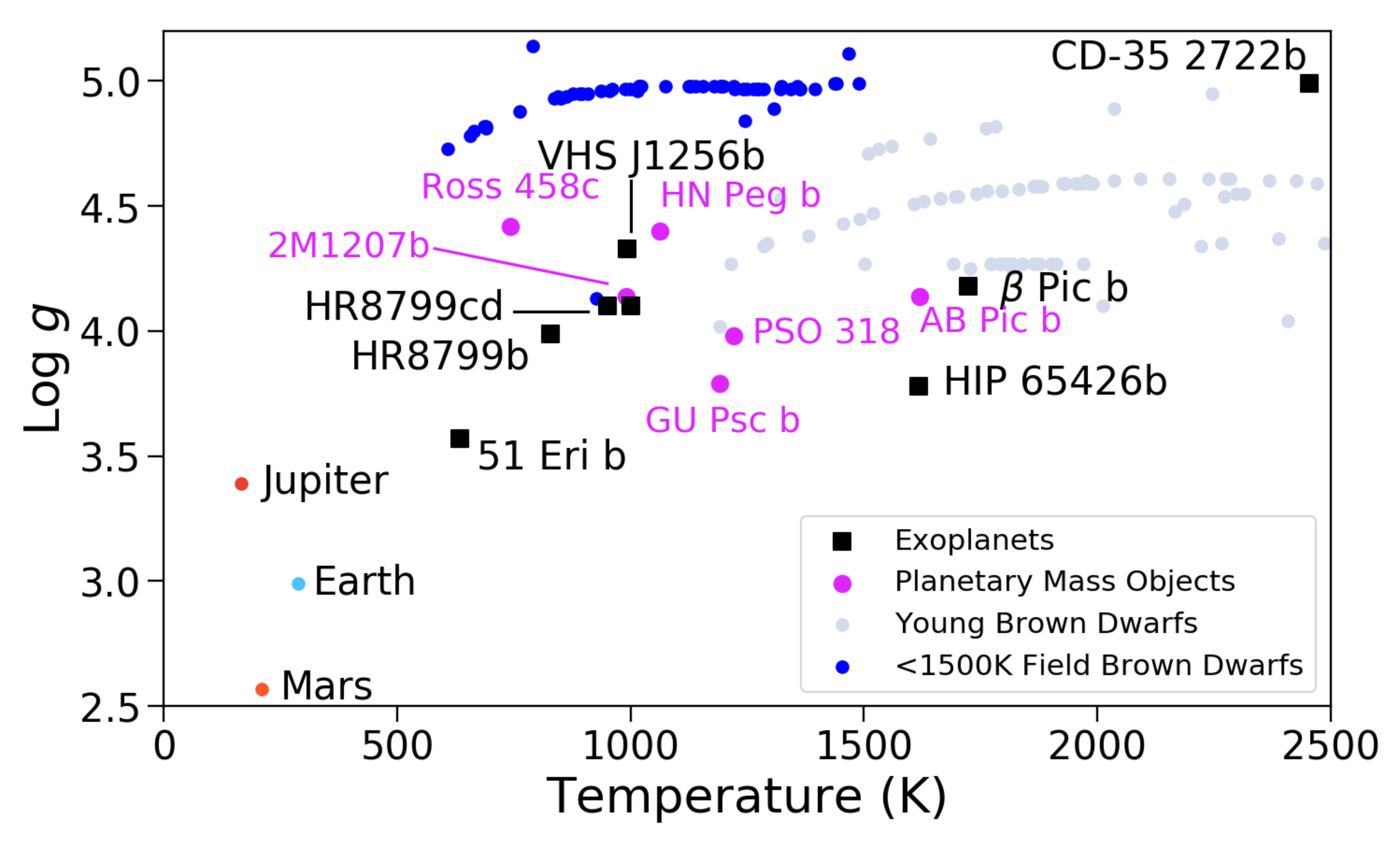
(Nowak et al. 2019)

Two Keys things to keep in mind:

1. Wavelength Coverage

2. Resolution

Brown Dwarfs Should be Your Friends

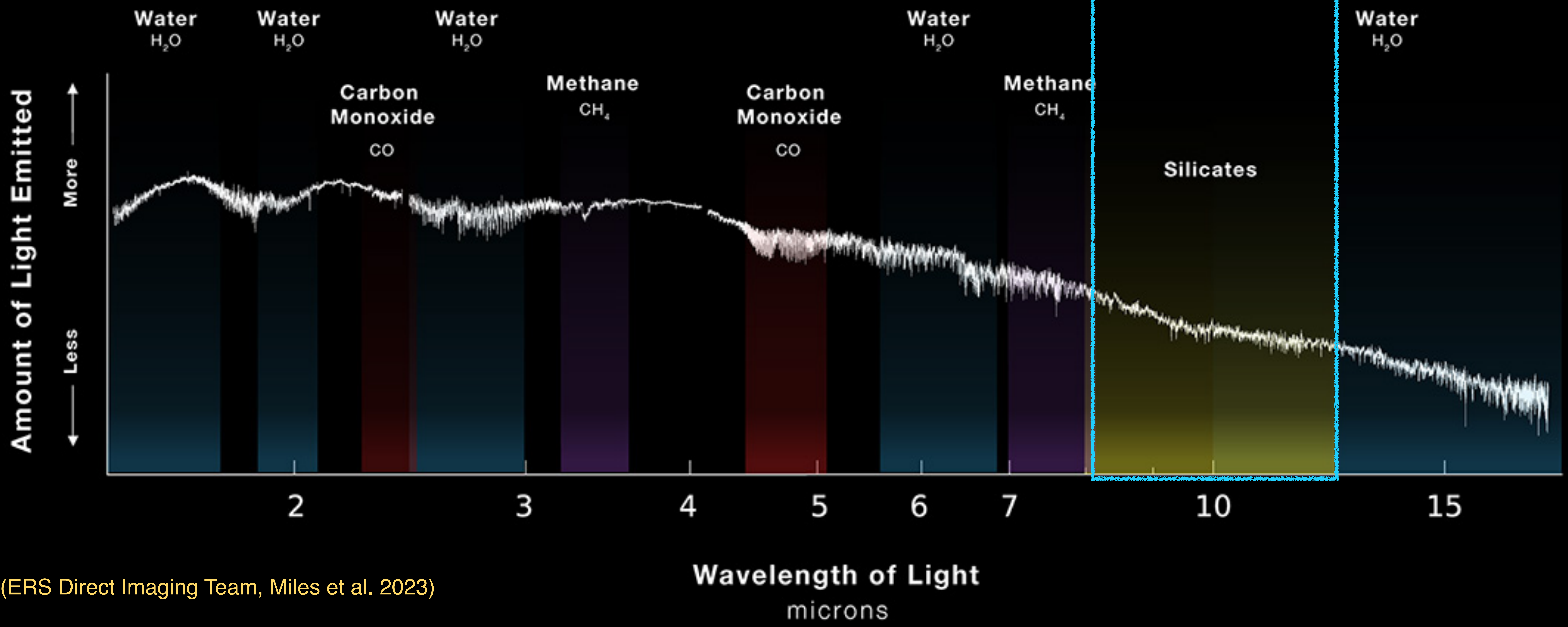


Brown Dwarfs As Exoplanet Analogs

Faherty et al. (2021)

EXOPLANET VHS 1256 b
EMISSION SPECTRUM

NIRSpec and MIRI | IFU Medium-Resolution Spectroscopy



(ERS Direct Imaging Team, Miles et al. 2023)

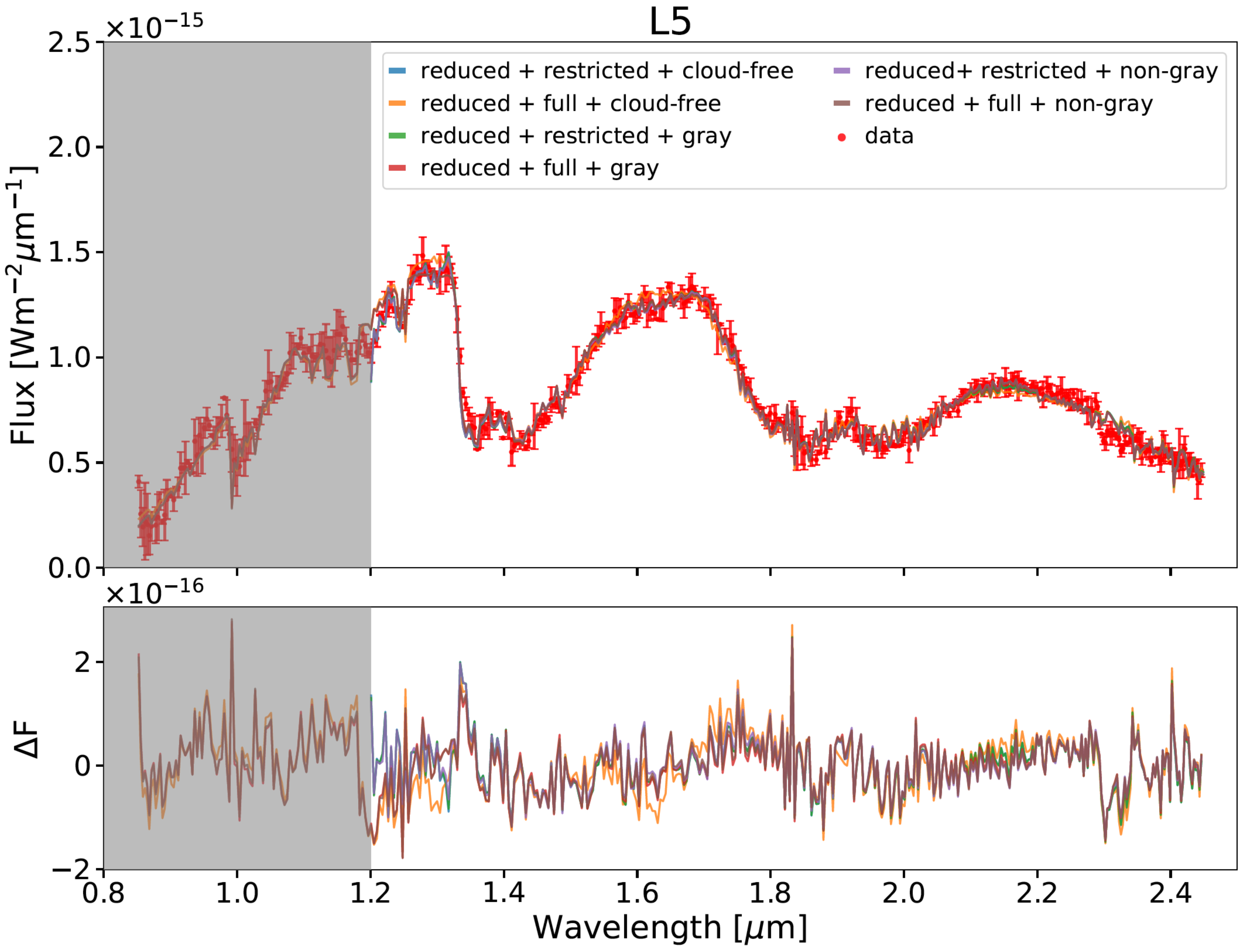
Case Studies

1. Cloud interpretations in the context of wavelength coverage and resolution

2. Chemical Abundance interpretations in the context of wavelength coverage and PT profile parameterization

3. Unphysical results that can arise

Limited Data Coverage



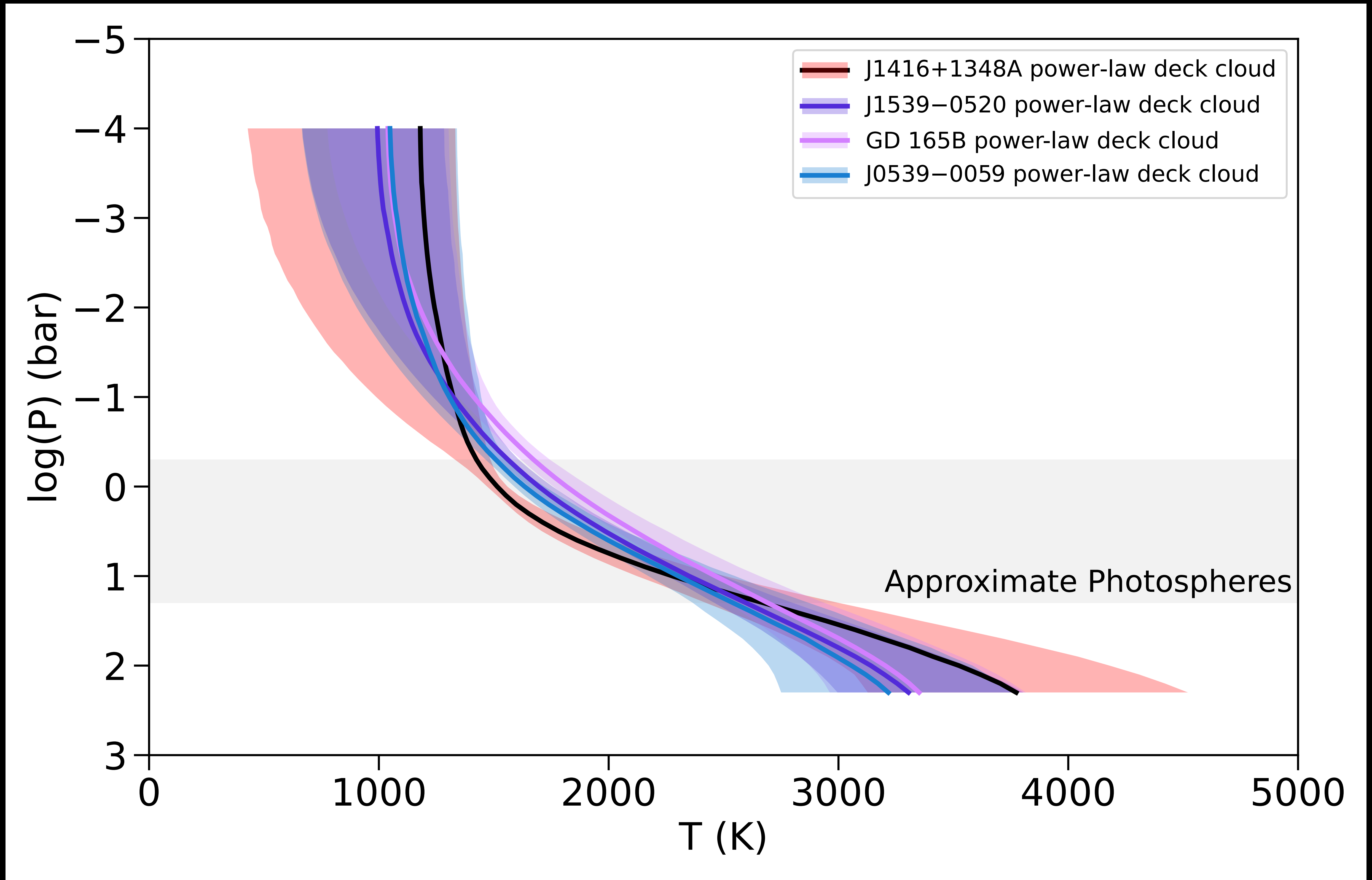
Cloud Models Indistinguishable

For early L's: gravity depends on cloud model

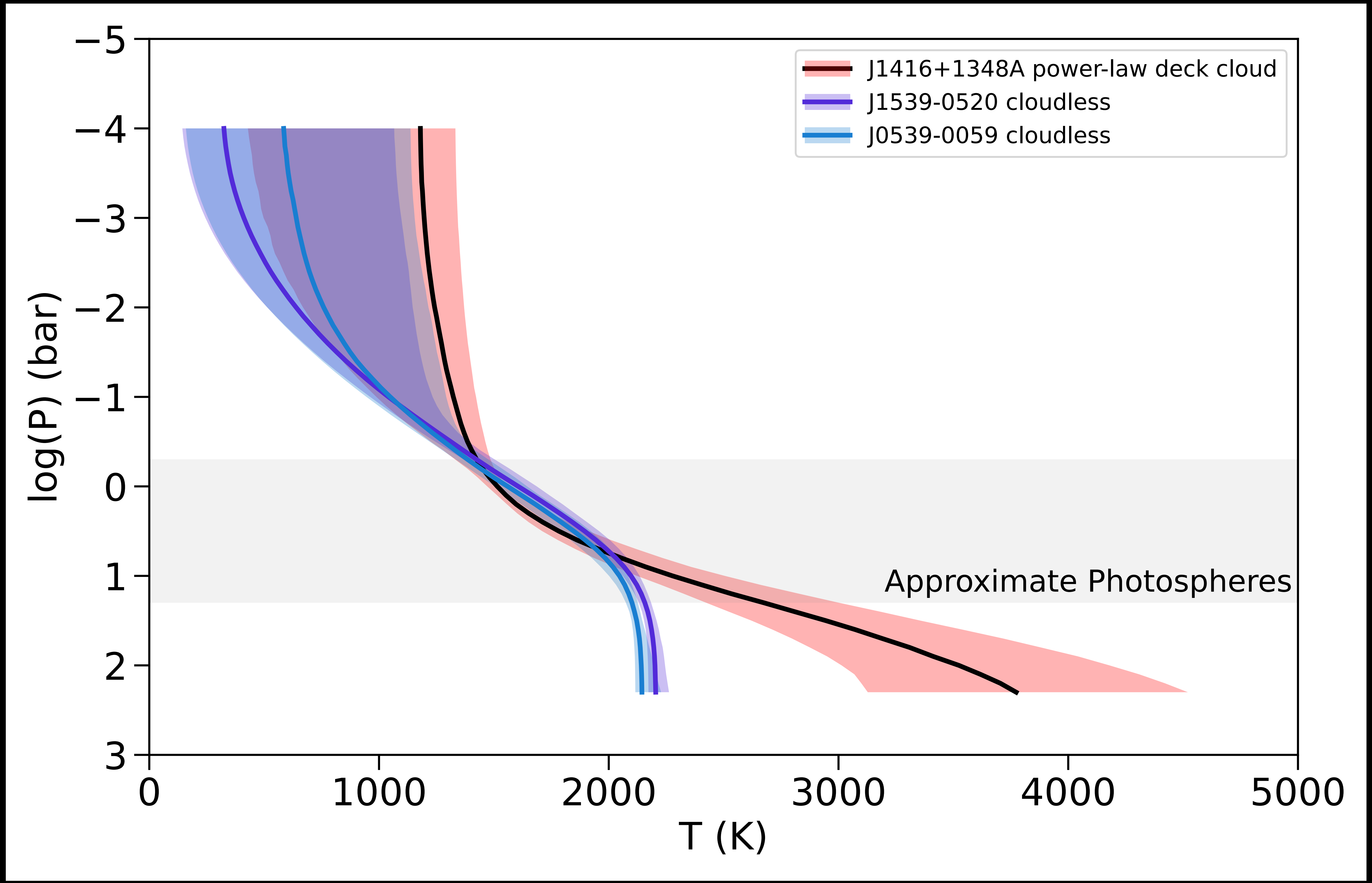
Constraining optical depth depends on priors

Lueber et al. (2022)

Indistinguishable Cloud Models



Cloudy



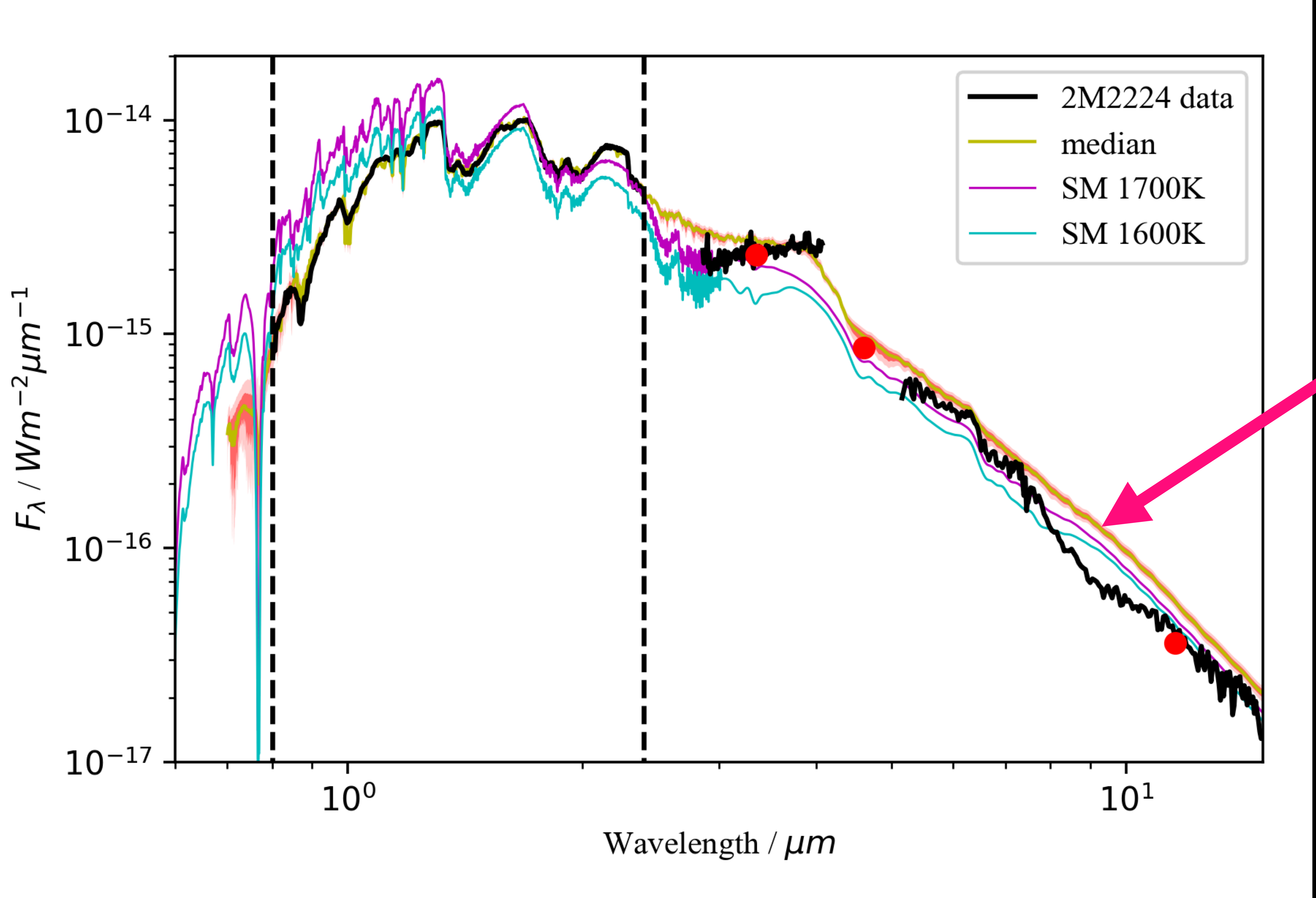
Cloud-free

C/O ratio and M/H are not affected by cloud model

Gonzales et al. (2020)

Gonzales et al. (2022)

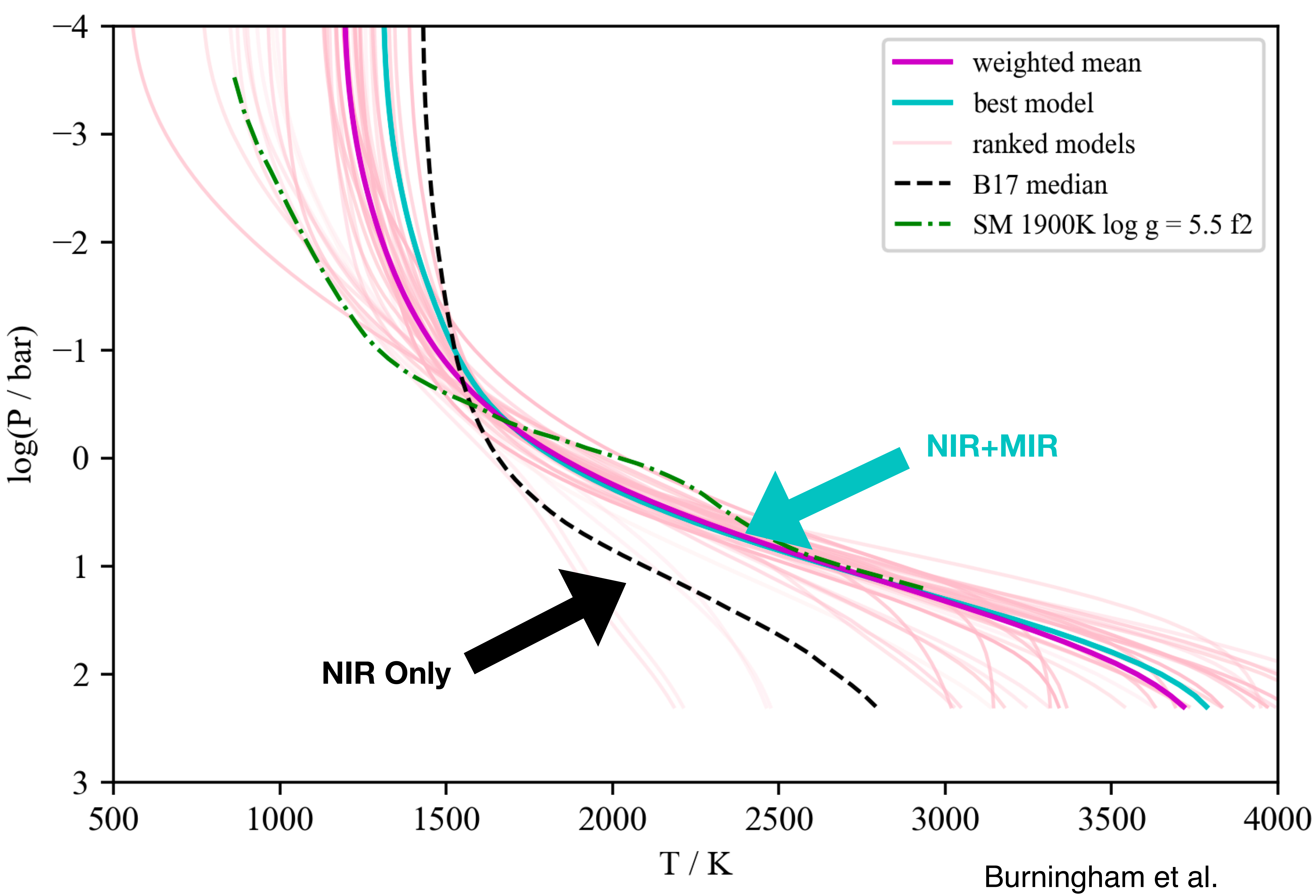
Wavelength coverage: NIR Only Spectral Fit



Silicate feature cannot be fit by retrieval using NIR data alone

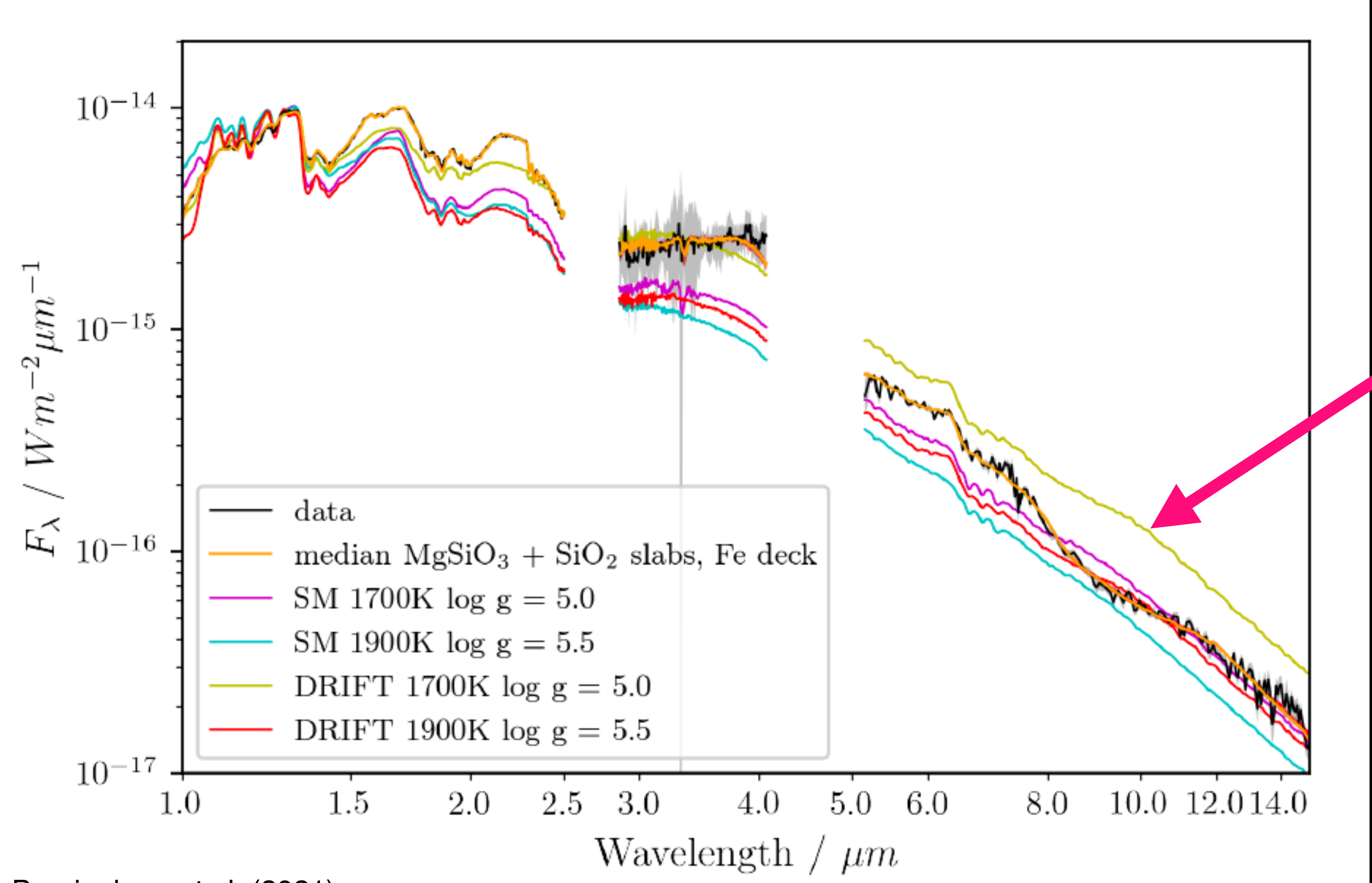
Burningham et al. (2017)

Shape of the PT profile depends on wavelength coverage



Burningham et al.

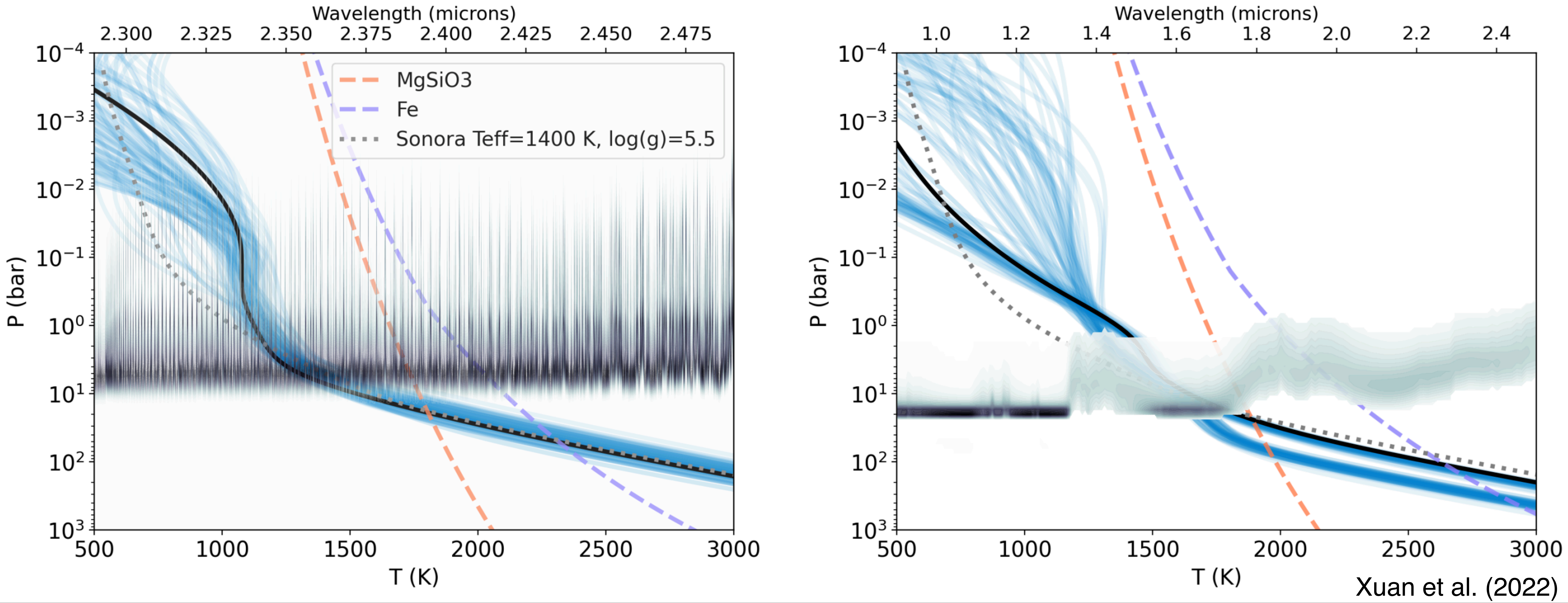
MIR Wavelength coverage can distinguish cloud species



Burningham et al. (2021)

Silicate feature fit by retrieval but *not grid models*

High Resolution Spectra and Clouds

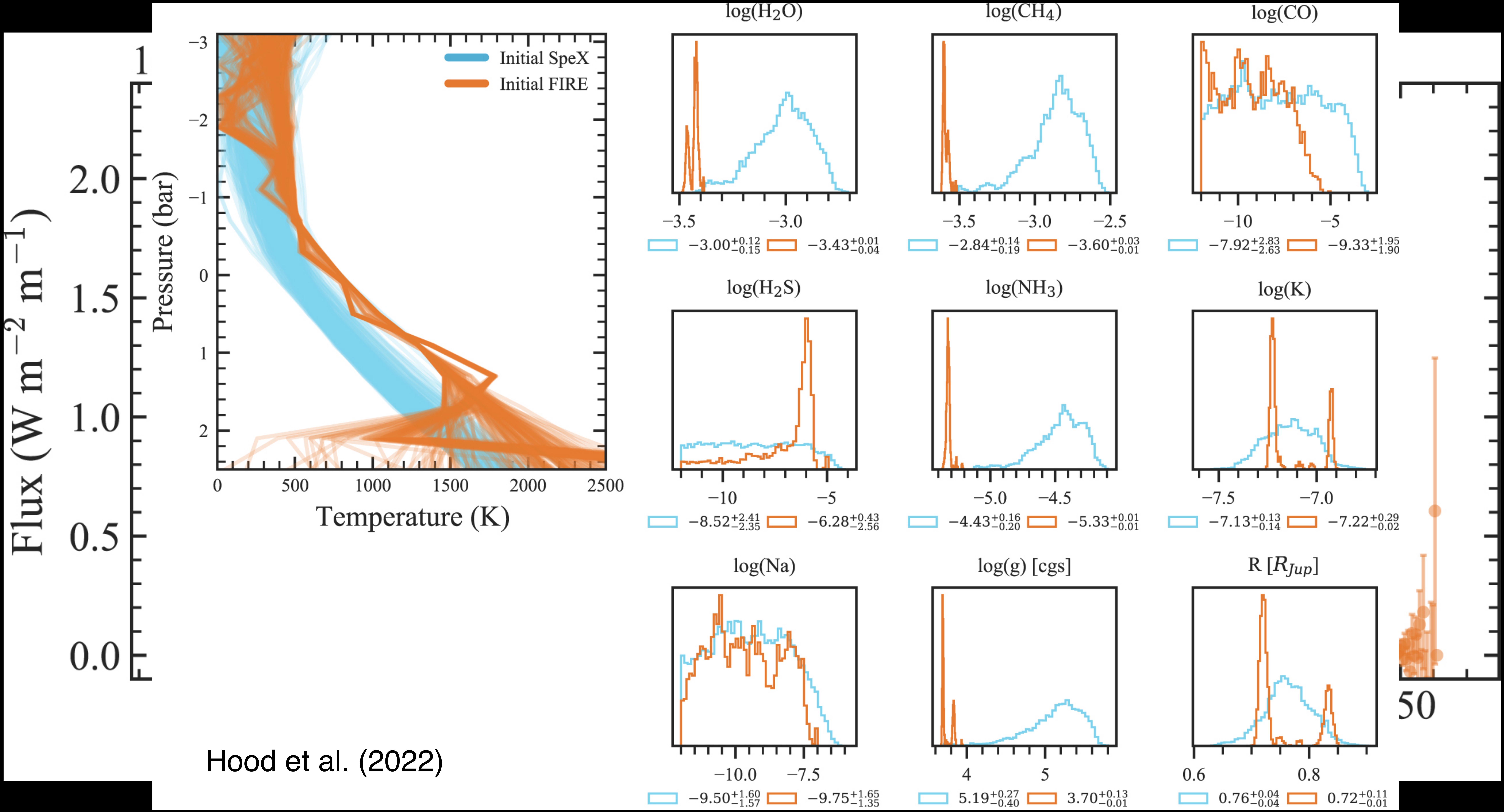


Xuan et al. (2022)

High resolution spectrum insensitive to clouds!

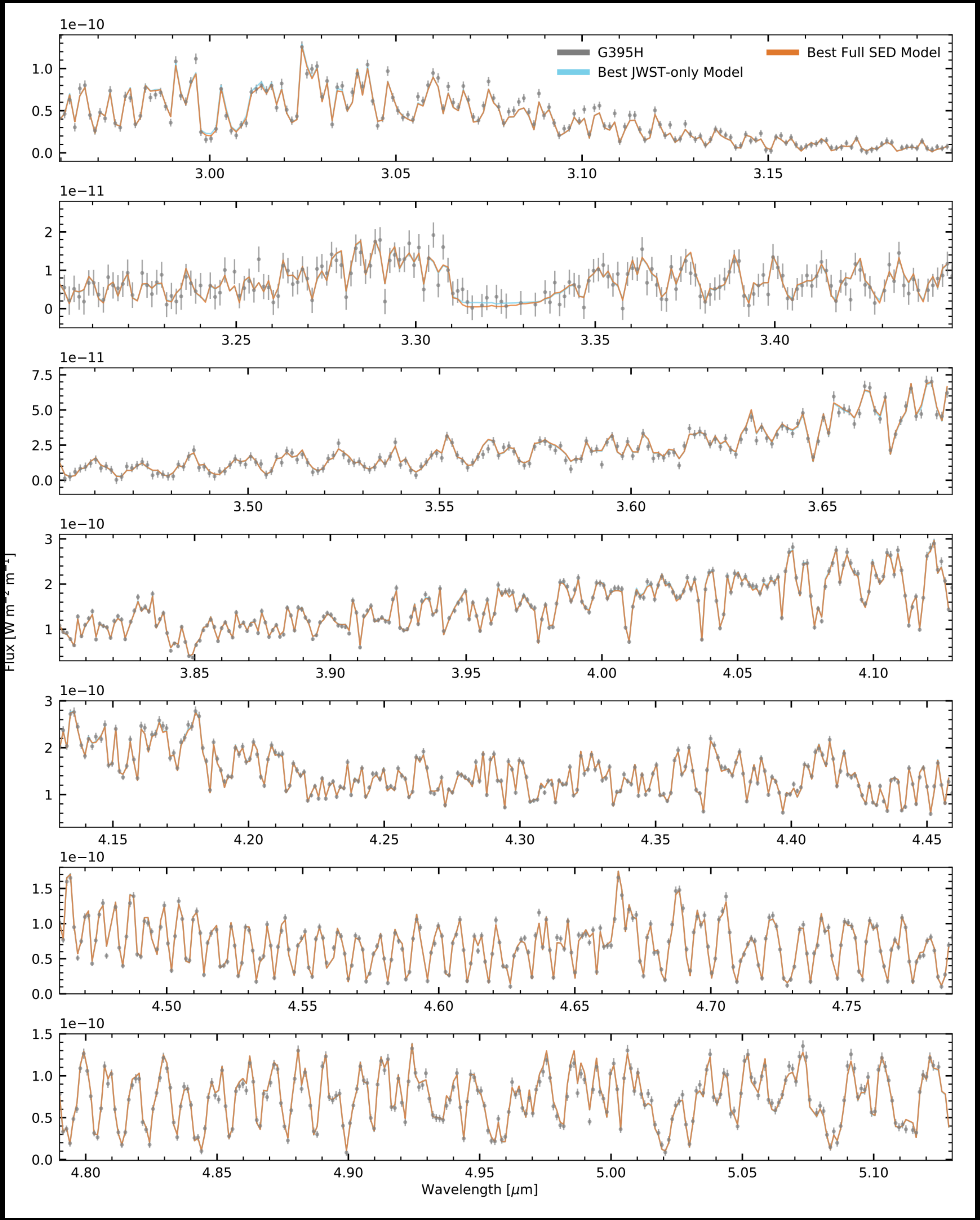
Wavelength coverage and continuum pressure level location plays a key role.

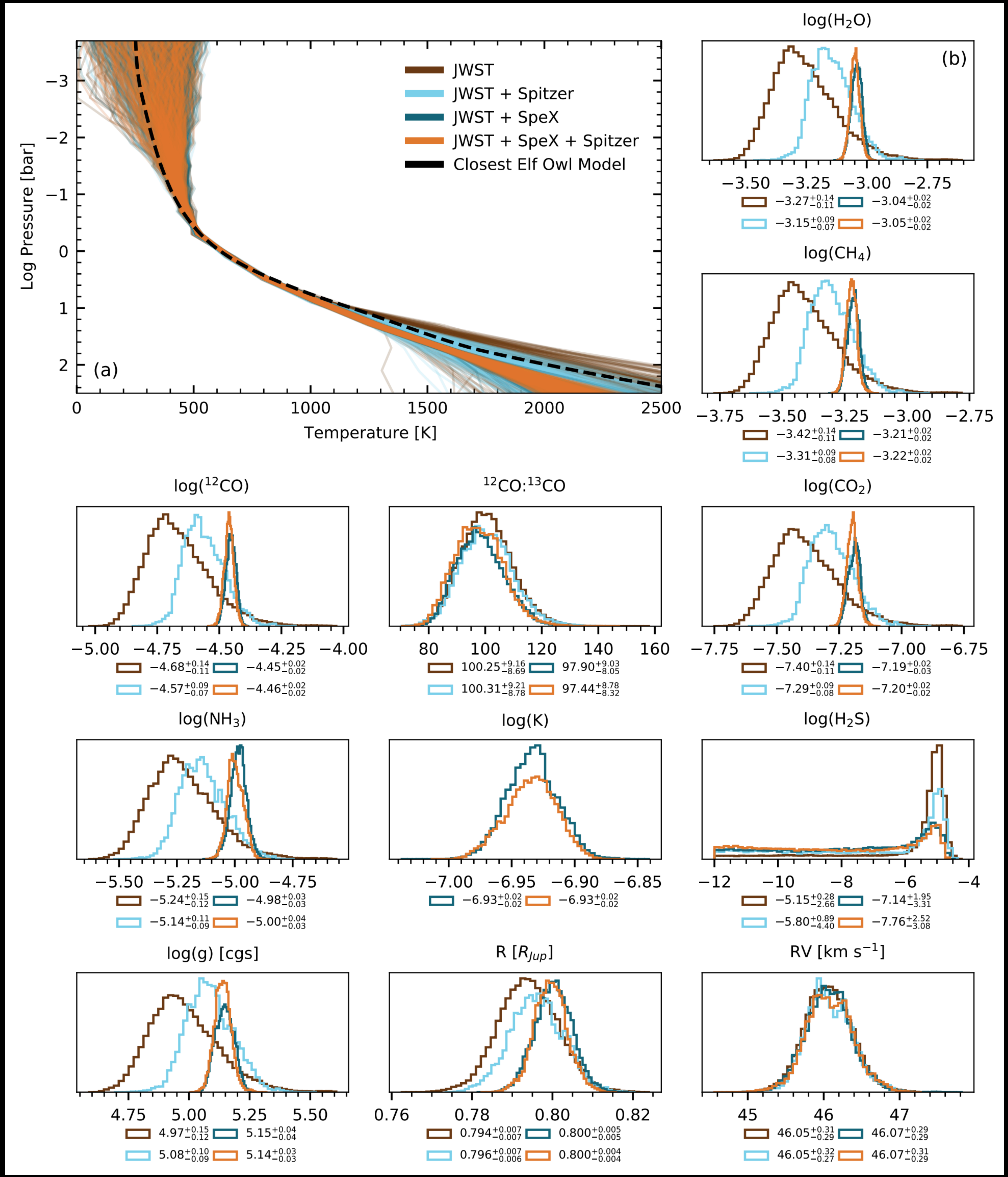
Spectral Resolution/coverage impacts abundance constraints



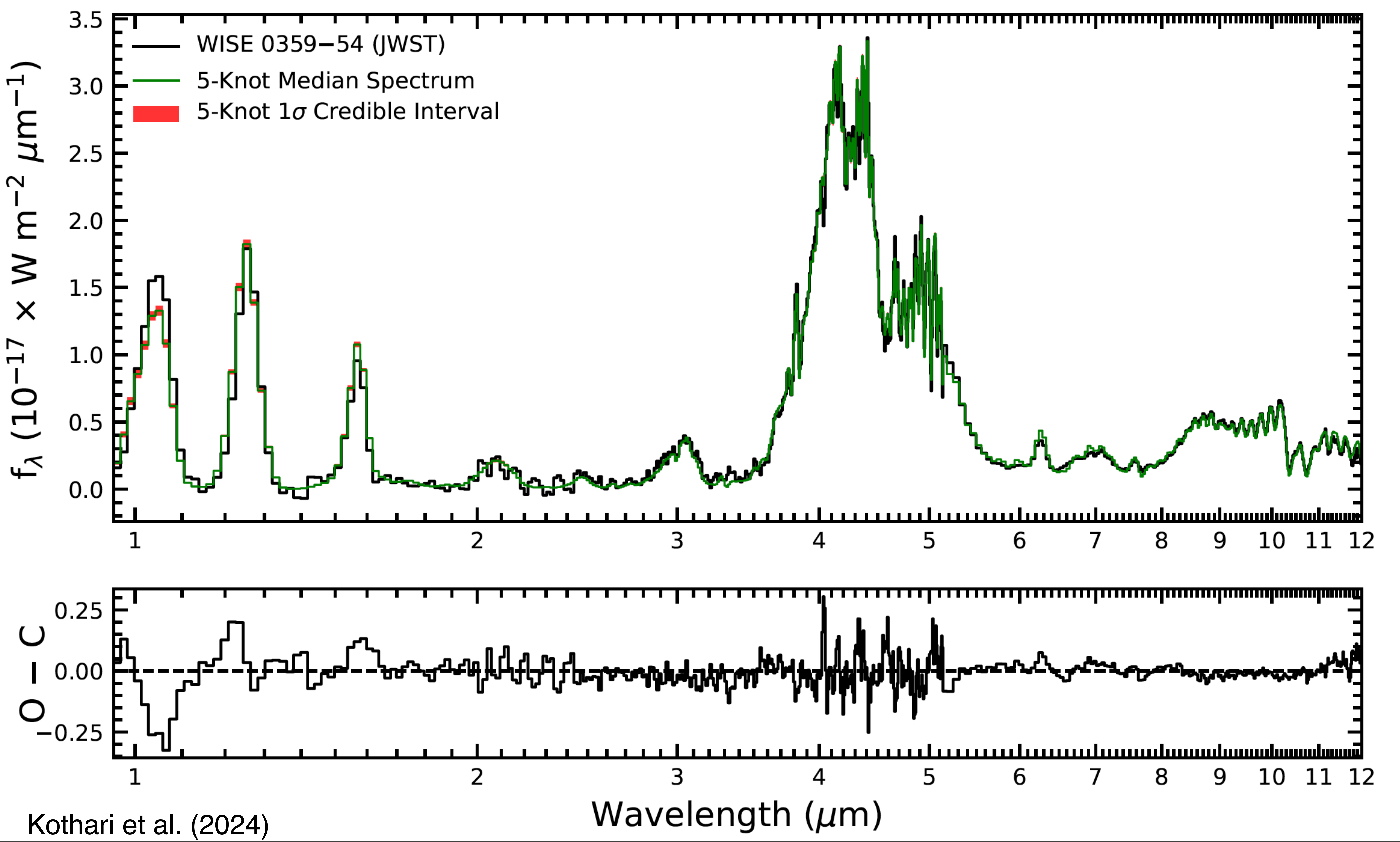
Hood et al. (2022)

Hood et al. (2024)





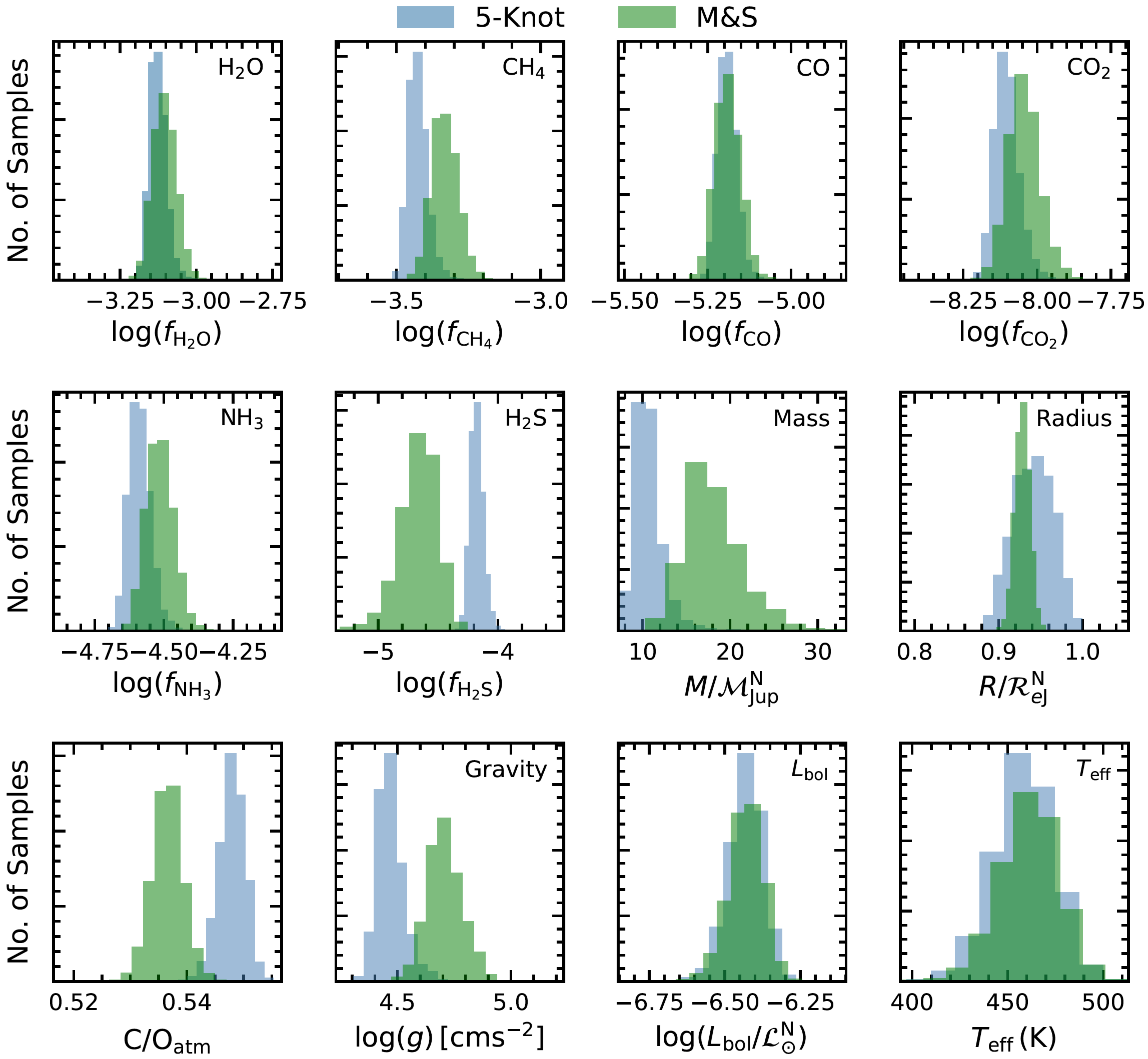
How the Profile is parameterized can impact results



Kothari et al. (2024)

How the Profile is parameterized can impact results

Two different PT profile parameterizations lead to differences in retrieved parameter values



Kothari et al. (2024)

Metallicity and Rejected Models

Table 6

Retrieved Gas Abundances and Derived Properties for SDSS J1256−0224 Indistinguishable Full Gas Set Models

Parameter	Value for Ions for Continuum Opacities			
	[M/H] = −1.5		[M/H] = −2	[M/H] = −2.5
	C/O = 1.0	C/O = 0.25		
Retrieved				
H_2O	$-4.58^{+0.16}_{-0.14}$	$-4.57^{+0.18}_{-0.16}$	$-4.71^{+0.20}_{-0.19}$	$-4.60^{+0.19}_{-0.18}$
CO	<-5.63	<-5.57	<-5.74	<-5.67
CO_2	<-4.79	<-4.91	<-5.45	<-5.49
CH_4	<-6.14	<-5.92	<-6.39	<-6.81
TiO	<-9.75	<-9.71	<-9.88	<-9.77
VO	<-9.92	<-9.98	<-9.87	<-9.87
CrH	$-8.95^{+0.14}_{-0.16}$	$-8.95^{+0.16}_{-0.19}$	$-9.08^{+0.18}_{-0.19}$	$-9.03^{+0.20}_{-0.19}$
FeH	$-9.49^{+0.59}_{-1.32}$	$-9.43^{+0.56}_{-0.97}$	$-9.41^{+0.45}_{-0.73}$	$-9.13^{+0.42}_{-0.63}$
Na+K	<-8.64	<-8.67	<-8.65	<-8.56
log g (dex)	$5.44^{+0.19}_{-0.20}$	$5.47^{+0.17}_{-0.24}$	$5.12^{+0.29}_{-0.33}$	$5.27^{+0.30}_{-0.29}$
Derived				
L_{bol}	-3.60 ± 0.01	-3.59 ± 0.01	-3.59 ± 0.01	-3.60 ± 0.01
T_{eff} (K)	$2550.46^{+194.50}_{-170.03}$	$2538.43^{+233.35}_{-152.20}$	$2648.53^{+171.58}_{-177.44}$	$2716.85^{+160.47}_{-154.07}$
Radius (R_{Jup})	$0.79^{+0.13}_{-0.12}$	$0.80^{+0.13}_{-0.15}$	$0.74^{+0.12}_{-0.09}$	$0.70^{+0.10}_{-0.09}$
Mass (M_{Jup})	$72.11^{+21.75}_{-24.24}$	$74.09^{+20.23}_{-24.40}$	$28.61^{+21.36}_{-11.56}$	$37.36^{+29.07}_{-16.60}$
C/O	…	…	…	…
[M/H][a]	$-1.53^{+0.16}_{-0.14}$	$-1.51^{+0.18}_{-0.16}$	$-1.65^{+0.20}_{-0.19}$	$-1.55^{+0.19}_{-0.18}$

Notes. Molecular abundances are fractions listed as log values. For unconstrained gases, 1σ confidence is used to determine upper limit. C/O = 1.0 is Solar abundance and C/O = 0.25 is one quarter Solar abundance.

[a] Atmospheric value.

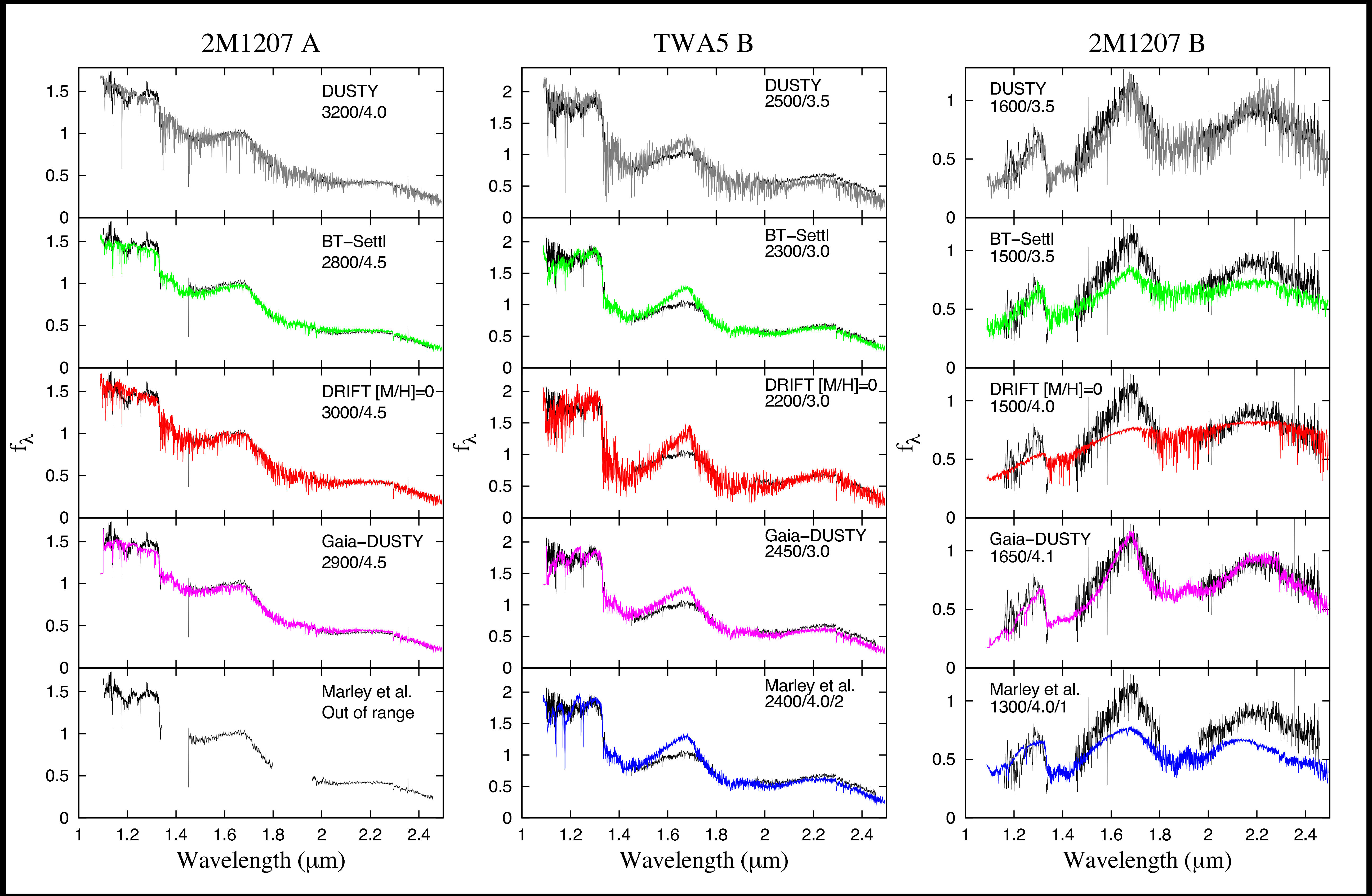
Gonzales et al. (2021)

Grid Models struggle with outliers!

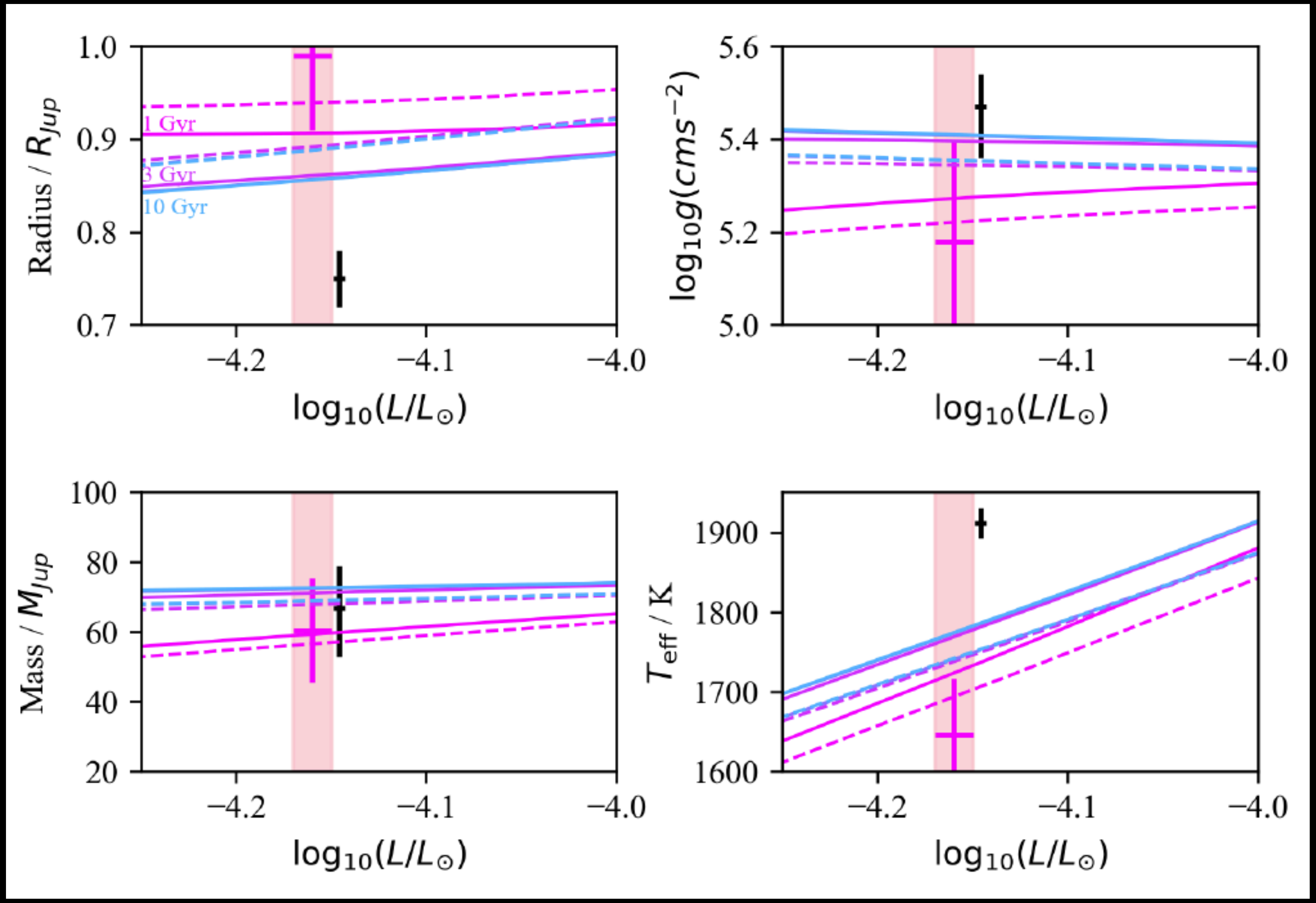
Retrievals can fit much better!

BUT one needs to examine parameters carefully

Problems with Substellar Models



Patience et al. (2012)



Burningham, Faherty, Gonzales et al. (2021)

Grid models struggle to fit spectra

Unphysical Radii
Mismatch in physical properties

Two Key Take Aways

Two Keys things to keep in mind when choosing between Forward models and retrievals:

1. Wavelength Coverage
2. Resolution

Retrieval results can't be blindly trusted. You must check if they are physical!