An Overview of Atmospheric Retrievals (aka curve fitting for planets…)

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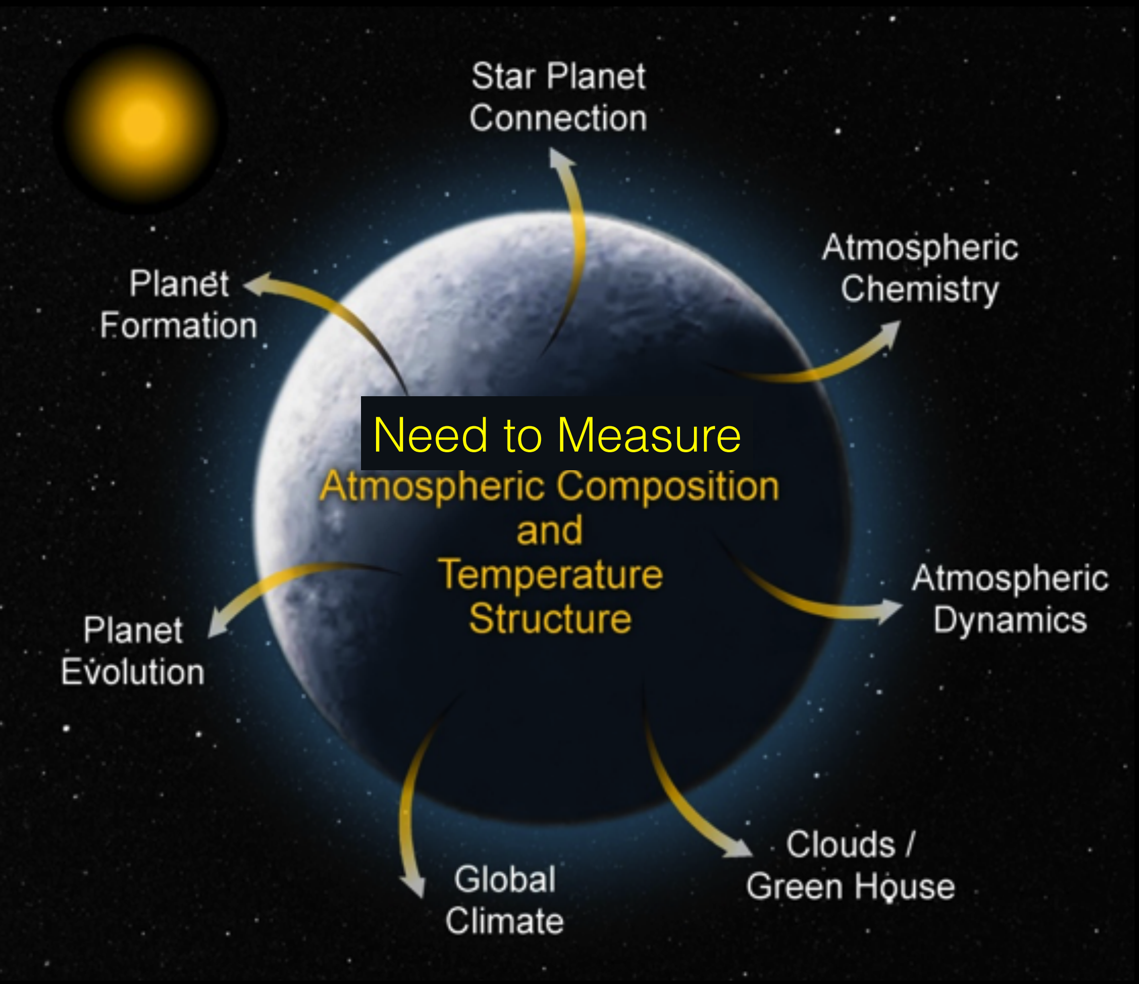
DEXTERS

Dwarf & EXoplaneT Exploration and Remote Sensing

Motivation-The Astrophysics of Exoplanets: Origins and Processes

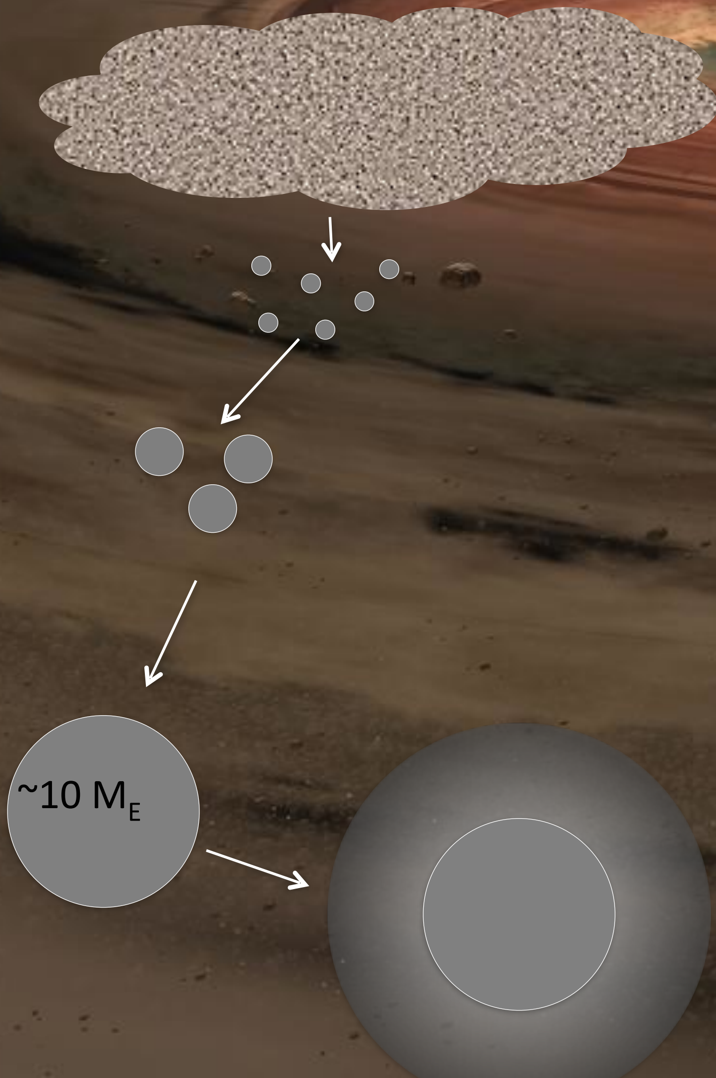


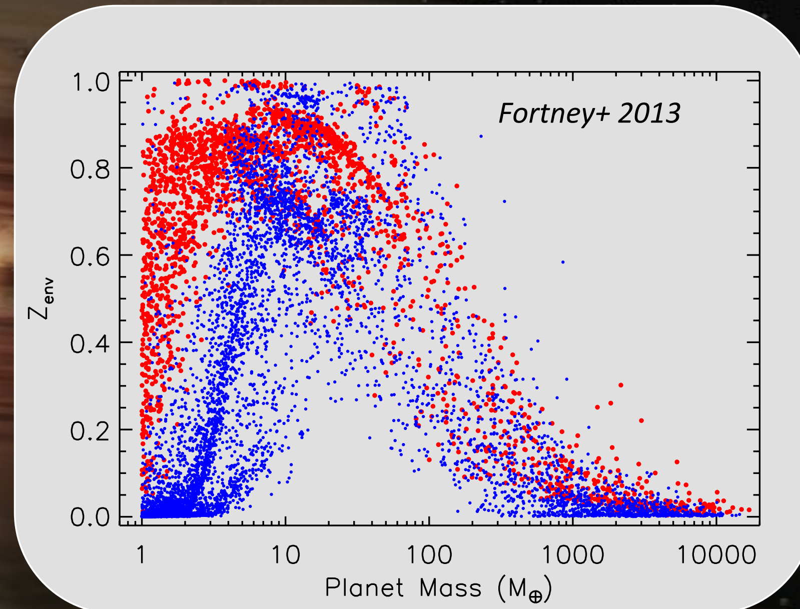
- How do atmospheres form and evolve?
- Does atmospheric composition reflect formation conditions?
- What is the range of planetary climates?
- What are the driving atmospheric chemical processes?
- What is the prevalence of biosignatures?

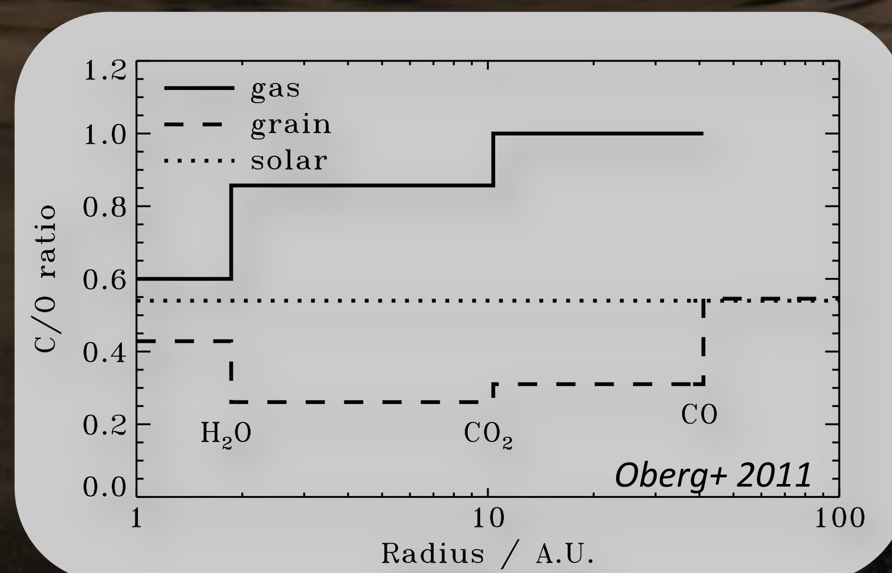
Origins: Formation Impacts Abundances

Core Accretion

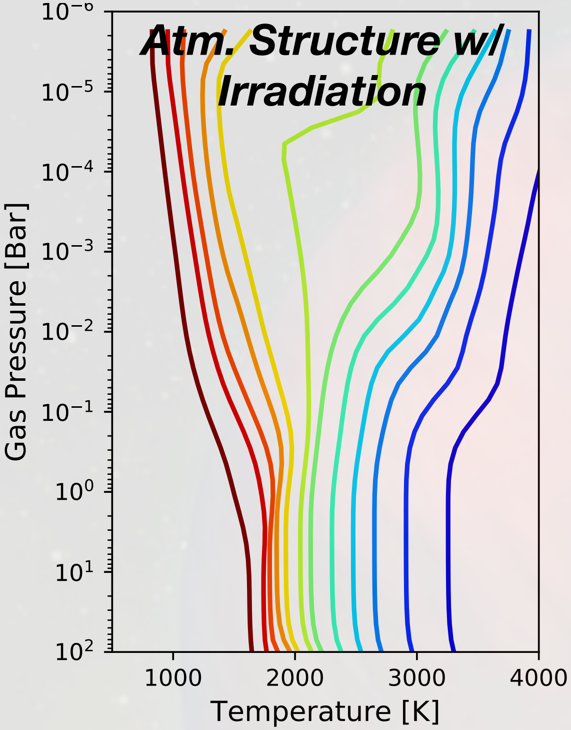
(planets only)-*Pollack 1984*



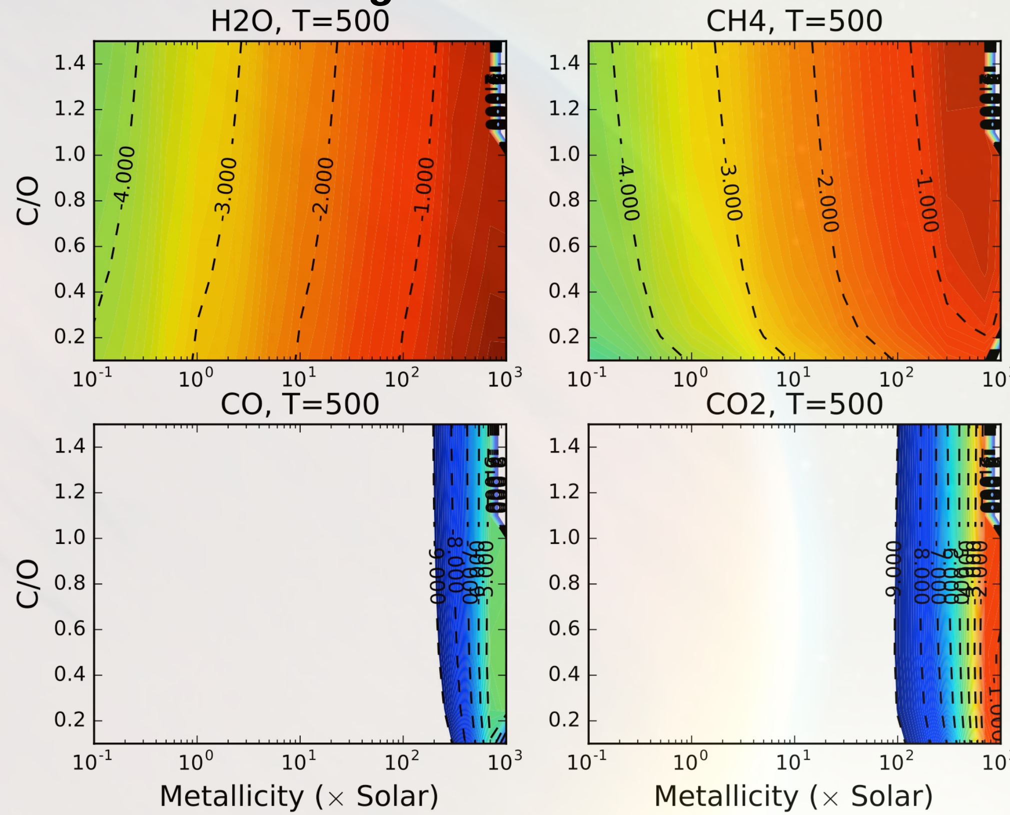




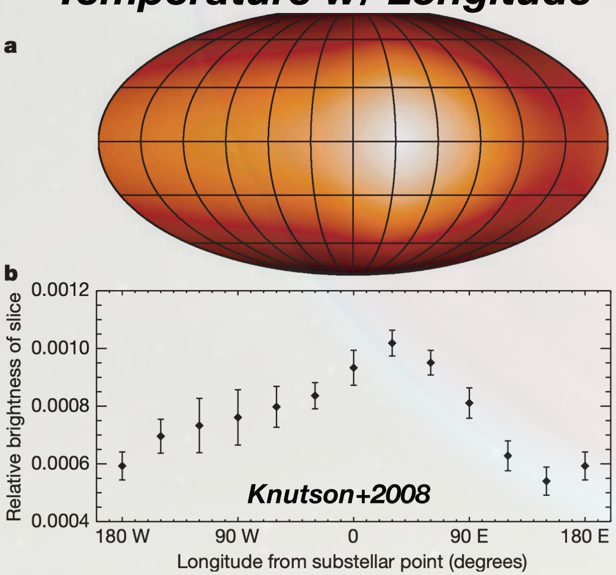
Processes: Climate & Chemistry



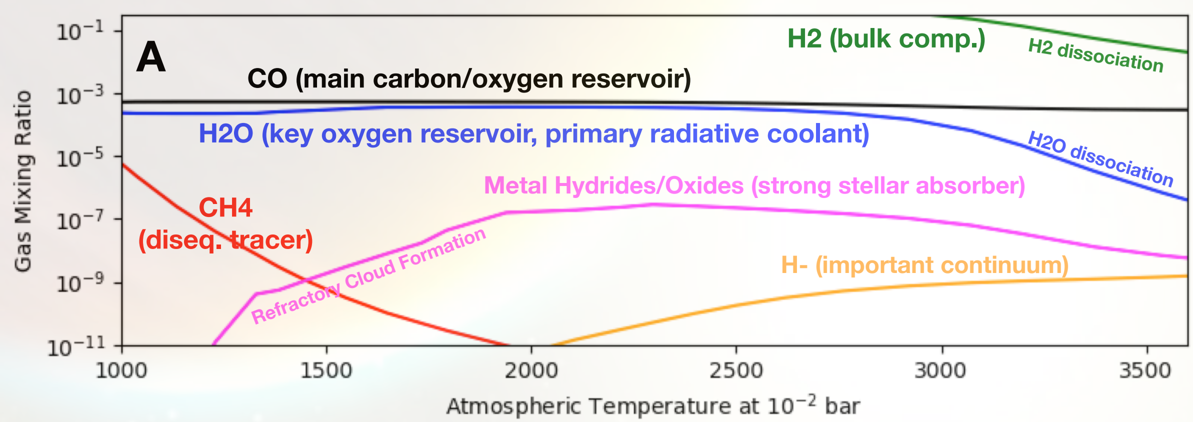
Molecules diagnostic of Elemental Abundances



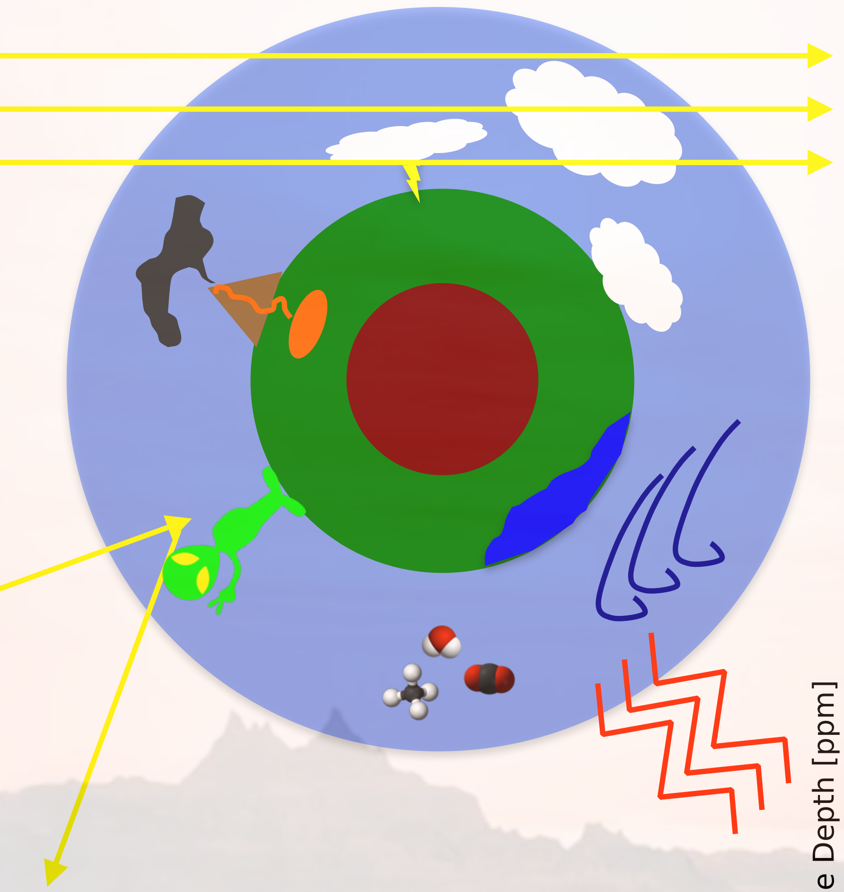
Temperature w/ Longitude

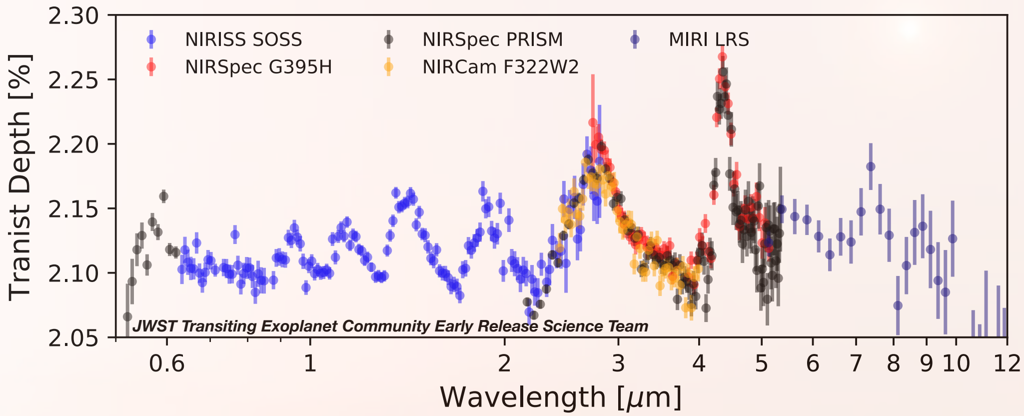


Chemical Transitions w/ Temperature

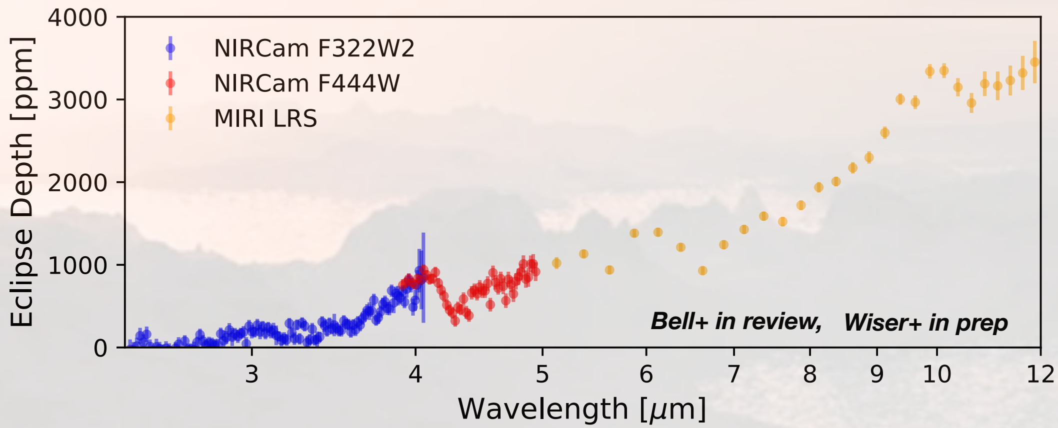


Things we want with observations we can get





$$D \propto \frac{2R_pH}{R_*^2}\ln(f_1\sigma_{1,\lambda} + \ldots + f_N\sigma_{N,\lambda})$$



$$D \propto \cdot \ln\left(\frac{\sigma_{1,\lambda_1} f_1}{\sigma_{2,\lambda_2} f_2}\right)\frac{\partial \ln T}{\partial \ln P}$$

What are we really doing?

*Things** we want with observations we can get*

Nuisance physics we don't want to deal with but have to (blah, star)

$$A = \begin{pmatrix} \frac{\partial(Obs_1)}{\partial(physics_1)} & \frac{\partial(Obs_1)}{\partial(physics_2)} & \cdots & \frac{\partial(Obs_1)}{\partial(physics_n)} \\ \frac{\partial(Obs_2)}{\partial(physics_1)} & \frac{\partial(Obs_2)}{\partial(physics_2)} & \cdots & \frac{\partial(Obs_2)}{\partial(physics_n)} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial(Obs_m)}{\partial(physics_1)} & \frac{\partial(Obs_m)}{\partial(physics_2)} & \cdots & \frac{\partial(Obs_m)}{\partial(physics_n)} \end{pmatrix}$$

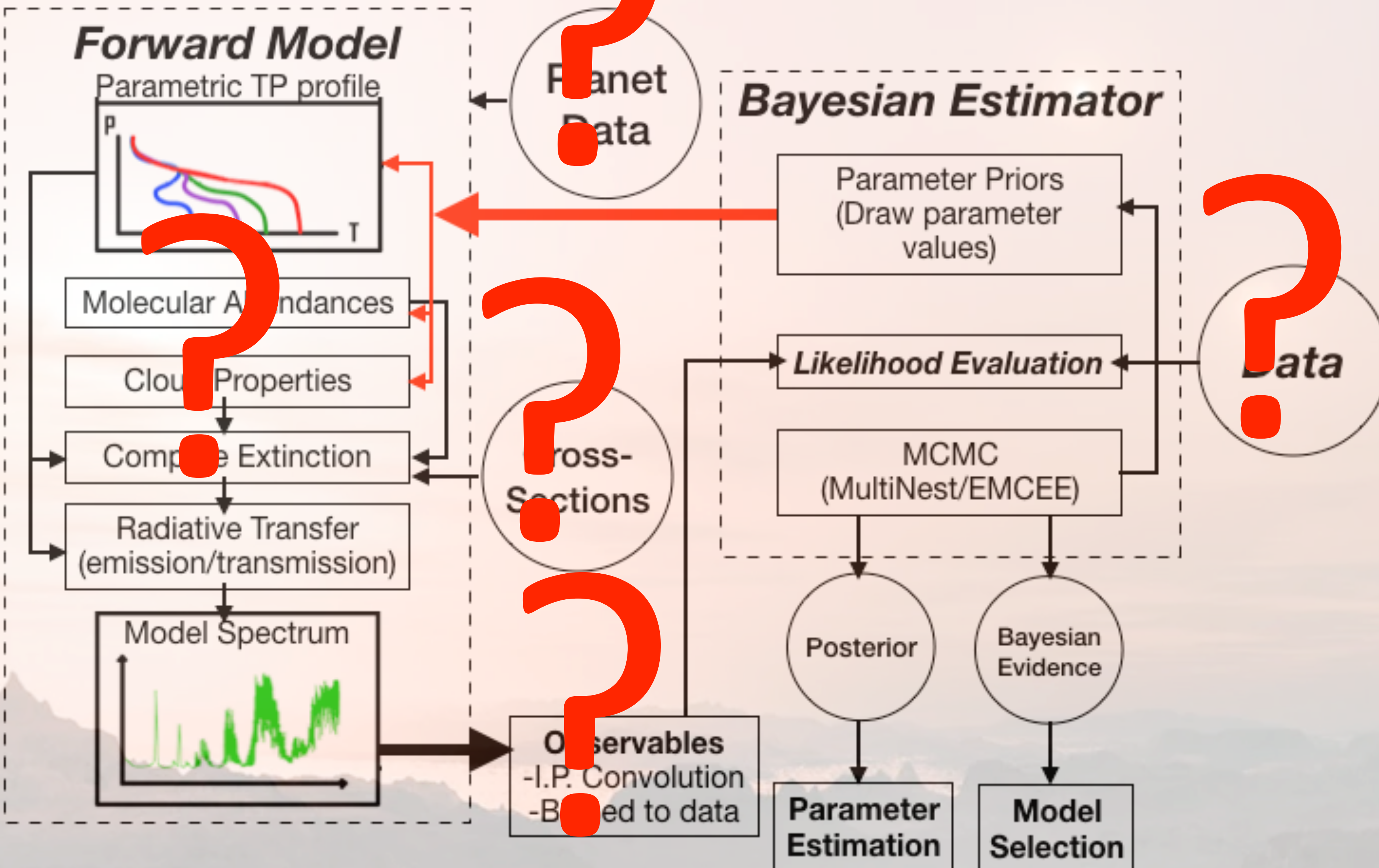
Observations we want but can't yet get (new telescope?)

Things we don't know we want with observations we don't know we need

**We often debate what "Things" we want…

$$\vec{Physics} = A^{-1}\vec{Obs}$$

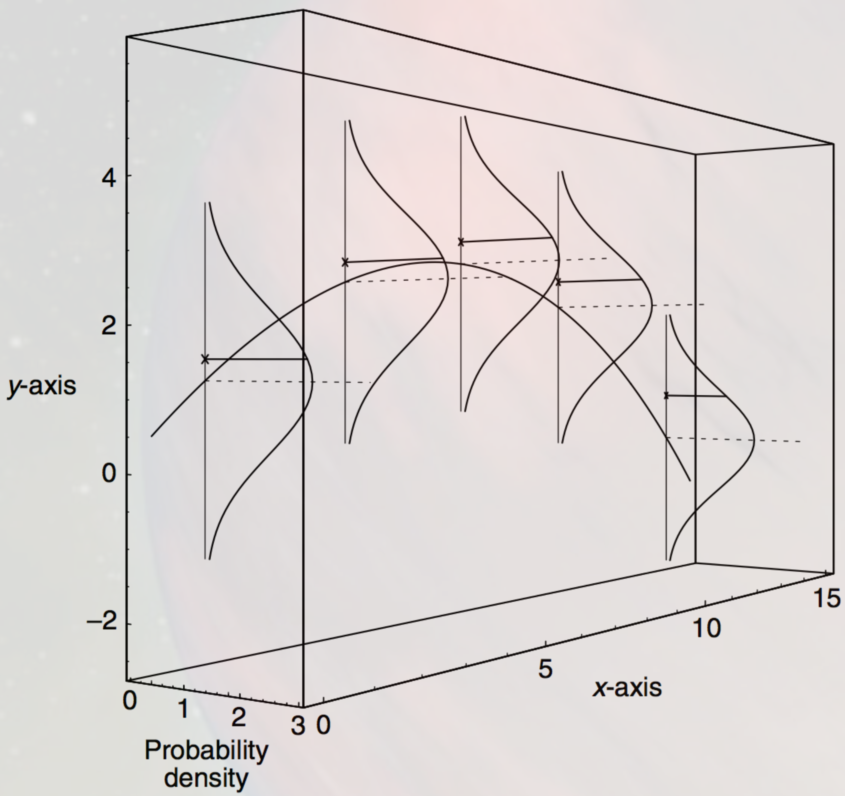
Typical Retrieval Components

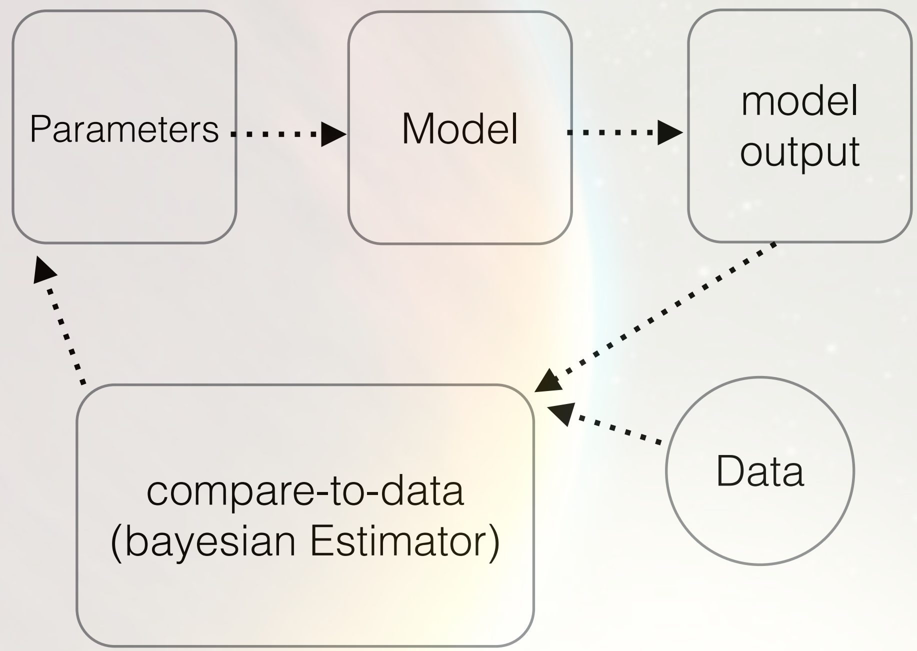


After MacDonald et al. 2017

Parameter Estimation Basics

Goal


4
2
0
−2
y-axis
0
1
2
3
Probability density
0
5
10
15
x-axis


Parameters
Model
model output
compare-to-data (bayesian Estimator)
Data

Bayes Theorem

$$p(H_i|D,I) = \frac{p(H_i|I)p(D|H_i,I)}{p(D|I)},$$

where $H_i \equiv$ proposition asserting the truth of a hypothesis of interest

$I \equiv$ proposition representing our prior information

$D \equiv$ proposition representing data

$p(D|H_i,I) =$ probability of obtaining data D, if H_i and I are true (also called the likelihood function $\mathcal{L}(H_i)$)

$p(H_i|I) =$ prior probability of hypothesis

$p(H_i|D,I) =$ posterior probability of H_i

$p(D|I) = \sum_i p(H_i|I)p(D|H_i,I)$ (normalization factor which ensures $\sum_i p(H_i|D,I) = 1$).

Two Basic Problems We care About

- Model Selection: What is the simplest model that can adequately explain my data?

- Parameter Estimation: Assuming you have the “correct” model, what are the range of parameter values that are consistent with the data?

Parameter Estimation

Hypothesis being tested are parameter (θ) "values" (e.g., a slope and an intercept for a line) given an assumed model, M

$$p(H_i|D,I) = \frac{p(H_i|I)p(D|H_i,I)}{p(D|I)} \longrightarrow p(\theta|D,M) = \frac{p(\theta|M)p(D|\theta,M)}{p(D|M)}$$

Hypotheses here are different parameter values

$p(\theta|M)d\theta$ is prior prob. that theta in $[\theta, \theta + d\theta]$

"global likelihood" $$p(D|M) = \int d\theta\; p(\theta|M)p(D|\theta,M) = \mathcal{L}(M)$$

(prob. of full model is weighted average of all parameters values weighted by prob.)

The "answer" is the posterior probability. Can summarize with "mean/median" and "confidence intervals"

Marginalization:

Only care about one parameter, but prob. depends on multiple params (e.g., only want slope, but have to also fit for intercept)

$$p(\theta|D,M) = \int d\phi\; p(\theta,\phi|D,M)$$

Built in Occam's Razor

What is the simplest model that can explain the data?

Given some set of Models,$\{M_i\}$, each with its own set of parameters,θ which model, M_i, is best?

Confusing: "Two" Uses of Bayes happening:

Within a particular model, testing hypothesis of various parameter values

$$p(\theta|D,M) = \frac{p(\theta|M)p(D|\theta,M)}{p(D|M)}$$

$$p(M_i|D,I) = \frac{p(M_i|I)p(D|M_i,I)}{p(D|I)}$$

Testing hypothesis of different models

$$p(D|M) = \int d\theta\ p(\theta|M)p(D|\theta,M) = \mathcal{L}(M)$$

I=M1 + M2 +…Mn (+="or")

Odds ratio between Model i and j

prior odds (usually cancel)

$$O_{ij} = p(M_i|D,I)/p(M_j|D,I) = \frac{p(M_i|I)}{p(M_j|I)}\frac{p(D|M_i,I)}{p(D|M_j,I)} \equiv \frac{p(M_i|I)}{p(M_j|I)}B_{ij}$$

$p(D|I)$ term drops out

Usually these cancel

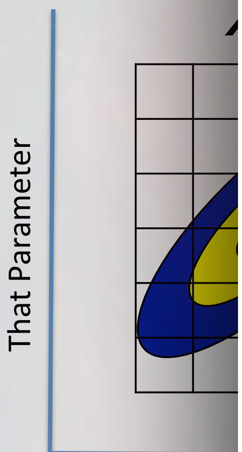
B_{ij} is called "Bayes factor". It is the ratio of the Bayesian Evidences from the "parameter estimation" version of Bayes

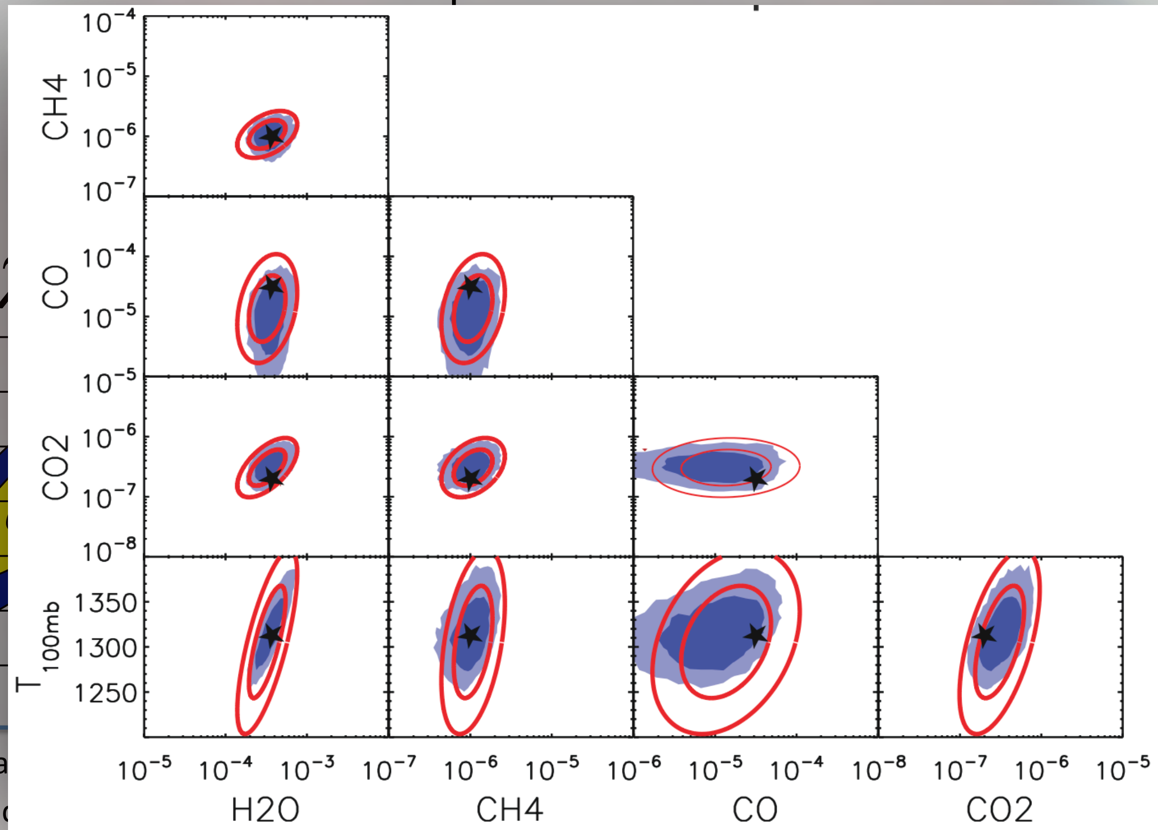
Inference Tools

Grid Search

Optimal Estimation

MCMC/NS



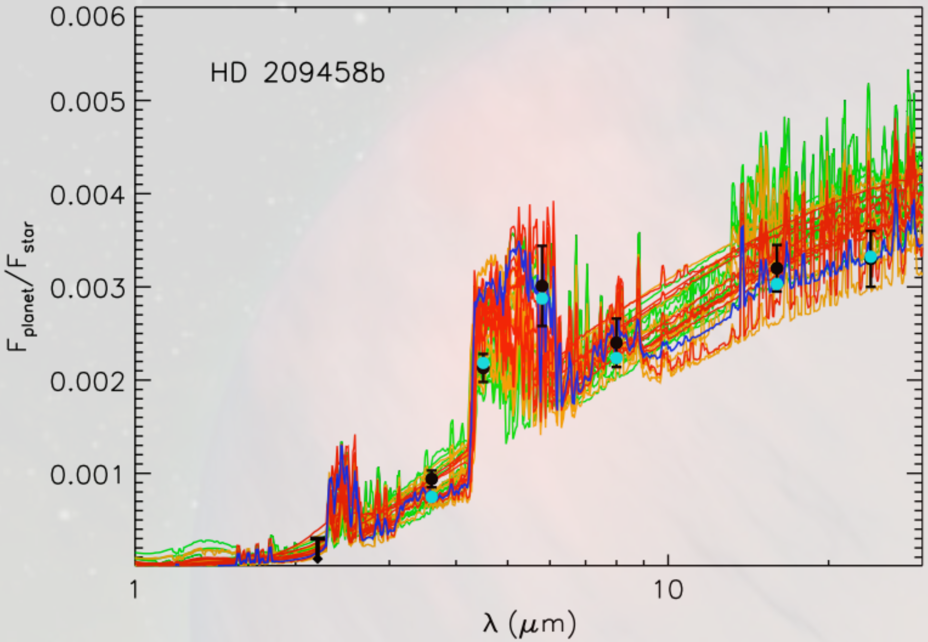


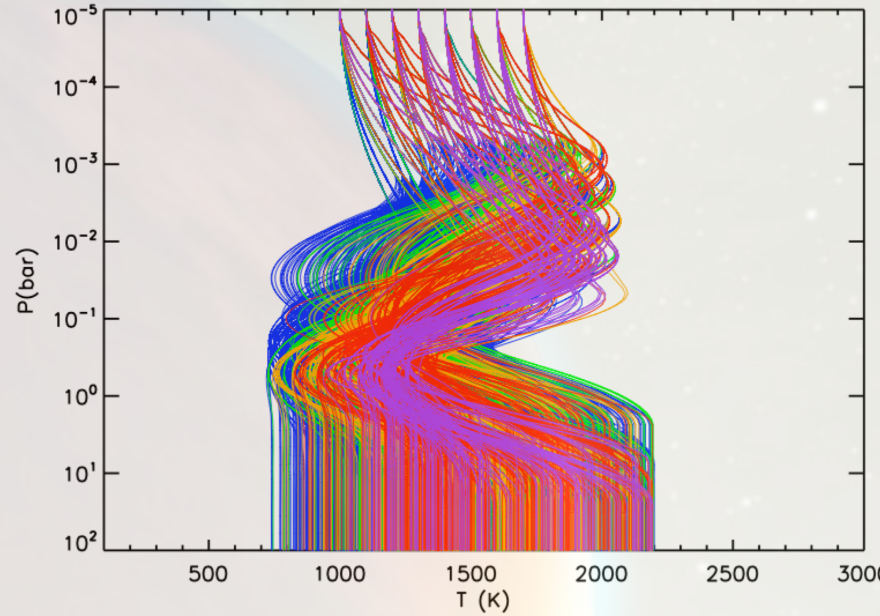
This Pa

#models=#gric

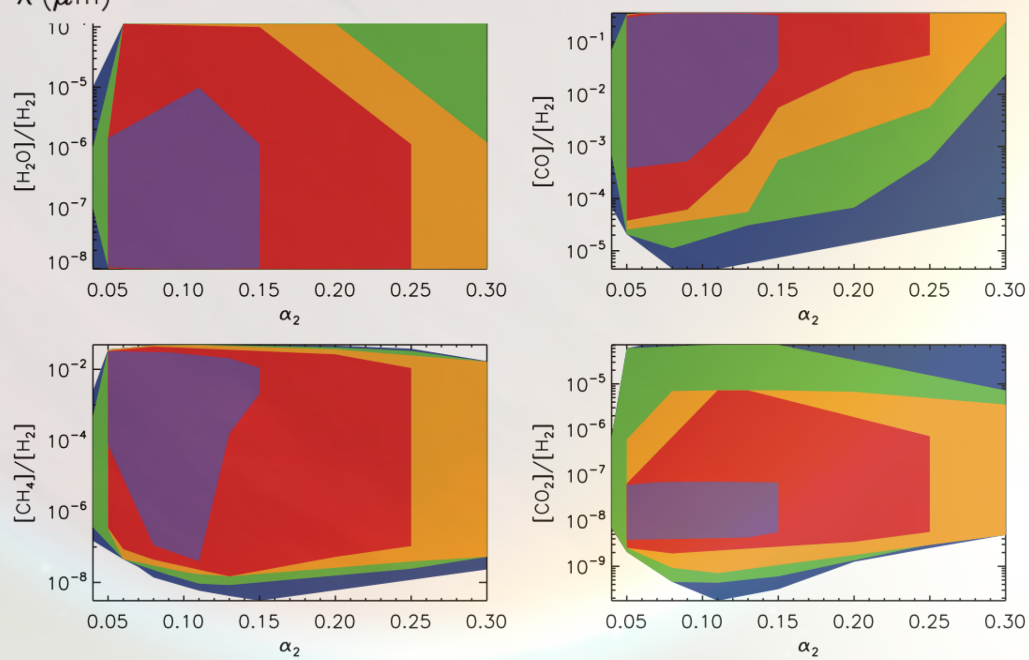
his Parameter

Grid Search: First Quantification of TP/Abundance uncertainties

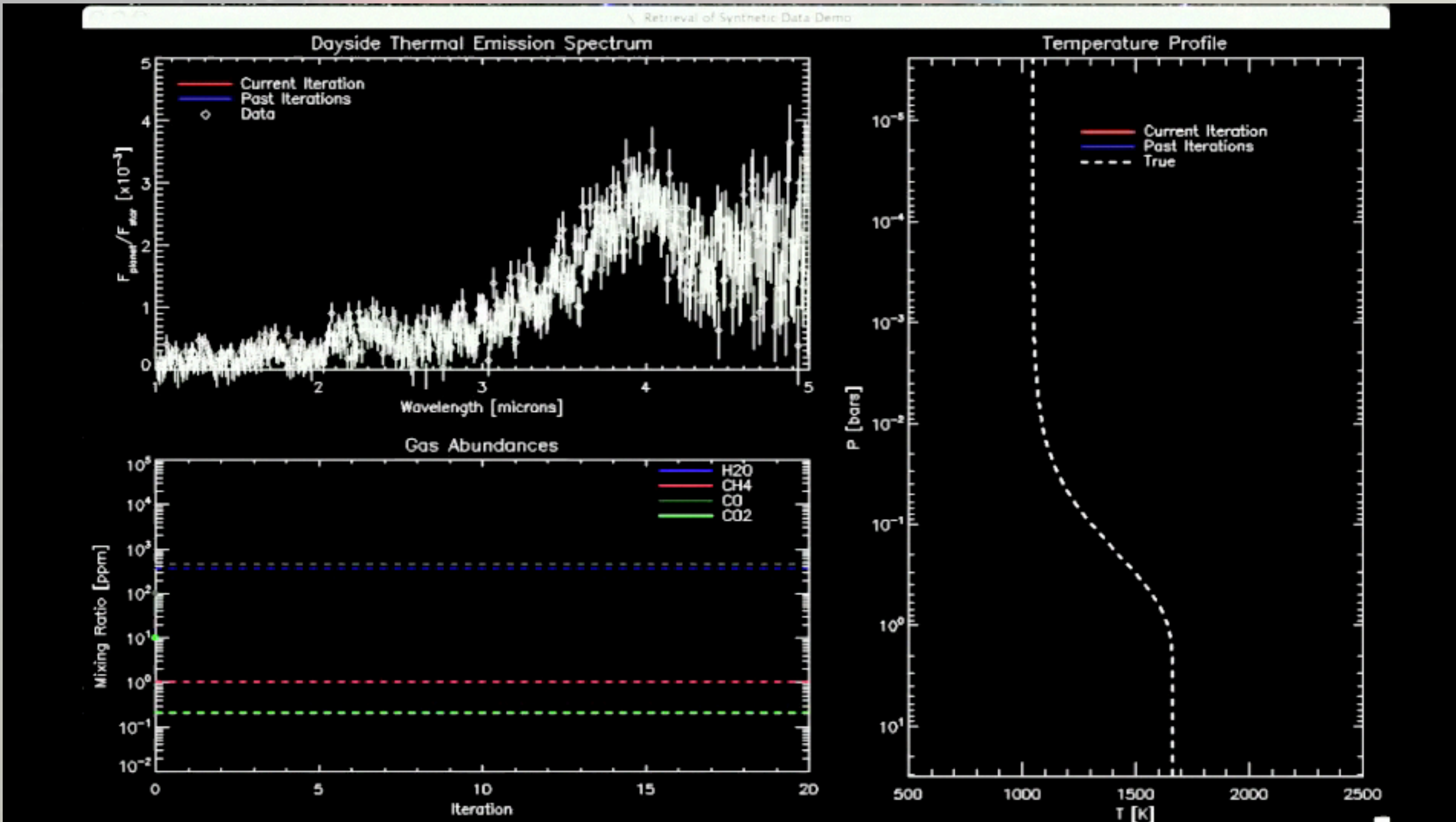




Madhusudhan
&
Seager 2009



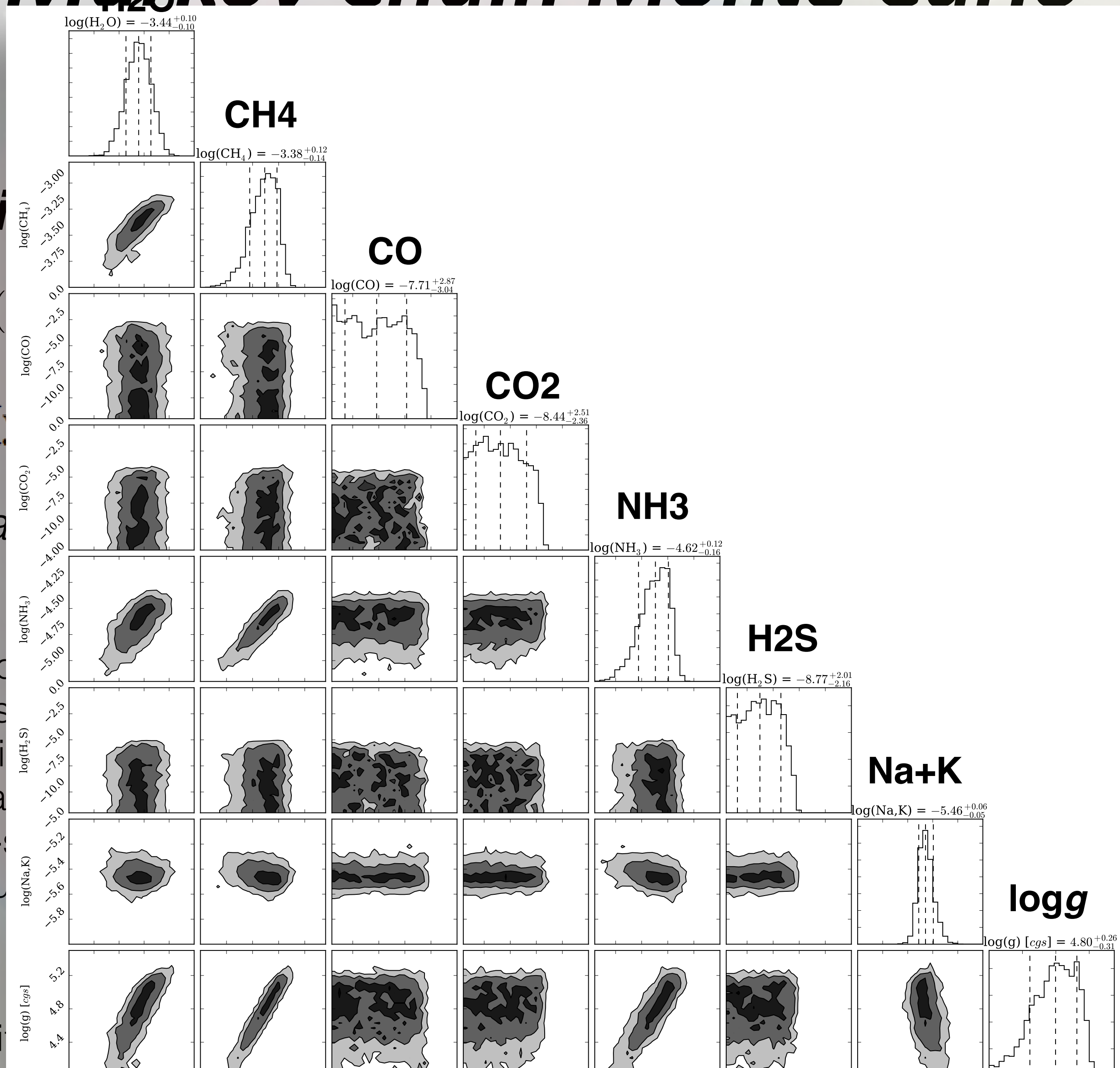
Optimal Estimation (aka, chi-square minimization…)



$H = \frac{1}{2}\ln(|\mathbf{S} \quad \mathbf{S}_a|)$

Lee+2012;13 Line+2012;13;14 Barstow+2013;14;15

Markov Chain Monte Carlo

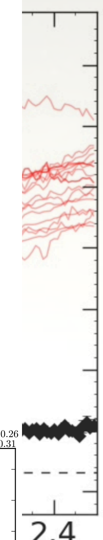


Formali

Bayes': $P($

$\ln \mathcal{L}(y|x) = ($

*lnP(**x**)=wha*



Pros:

-Full exploratio
-no posterior s
-arbitrary likeli
-can do "hiera
-many off-the-s
(emcee, pymu

Cons:

-oh so slow wi

Madhusudhan+2011, Benneke & Seager 2012;13, Line et al. 2013;14;15;16, Waldmann et al. 2015

The Forward Model: AKA, The Magic of Parameterizing an Atmosphere (Assumptions Matter!!!!!!!!!!!!!!!)

A range of model assumptions

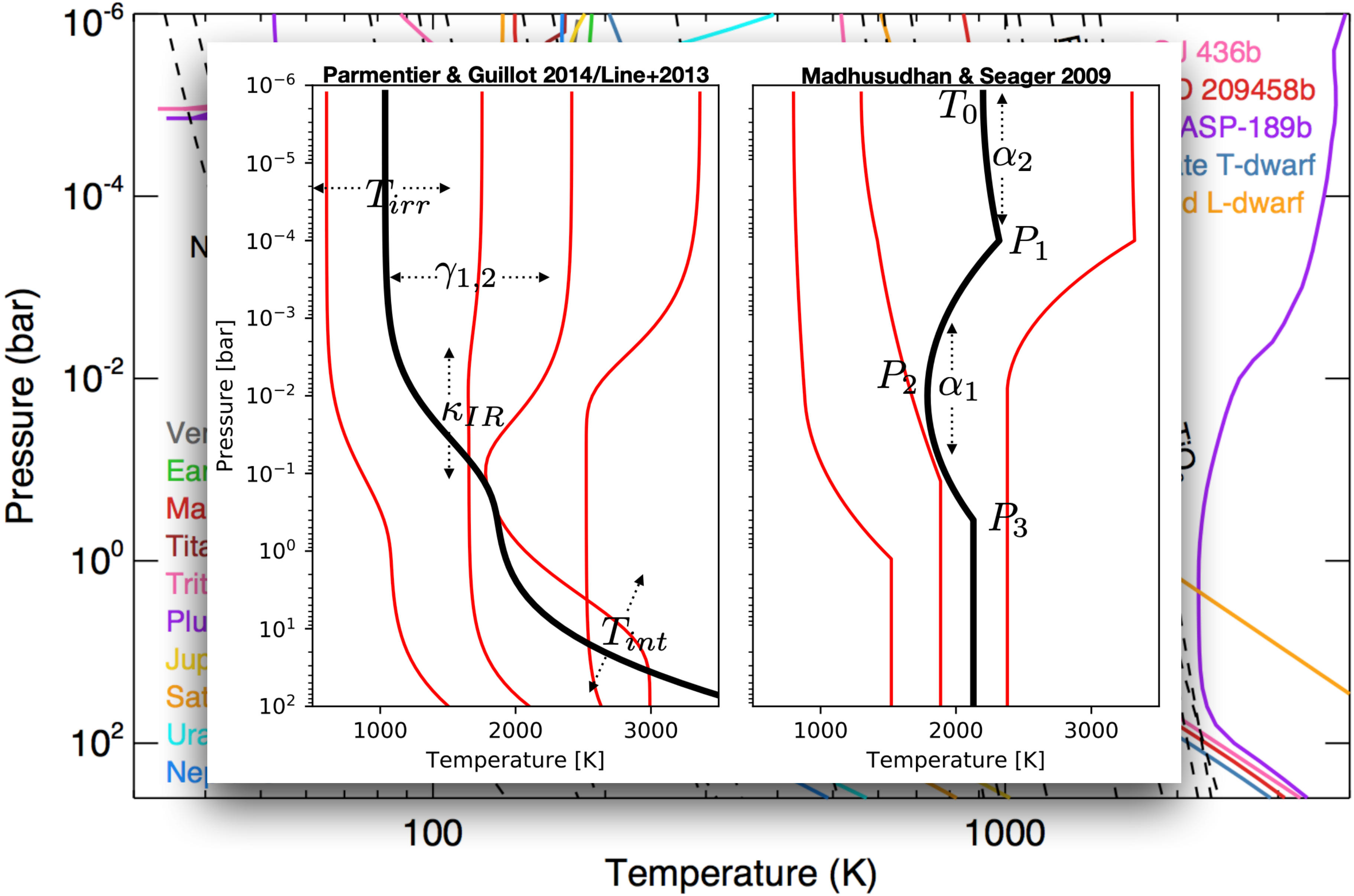
	Less assumptions More parameters		More assumptions Less parameters
Temperature profile	Free Semi-grey	1D Radiative/conv eq. Non-grey	2D/3D radiative/conv eq.
Chemistry	Free chemistry — Choice of species — Vertical profile	Equilibrium Choice of free parameters [M/H], [C/O] others ?	1/2/3D disequilibrium
Clouds	Parametrized Absorbing Grey	Simple equilibrium clouds Scattering, non-grey	Microphysics bin vs. moment ?
Geometry	1D	2D — Lat/long 2D — Limb depth	3D radiative transfer
Stars	Blackbody	1D stellar model	Inhomogeneous stellar model

"Free Retrieval"

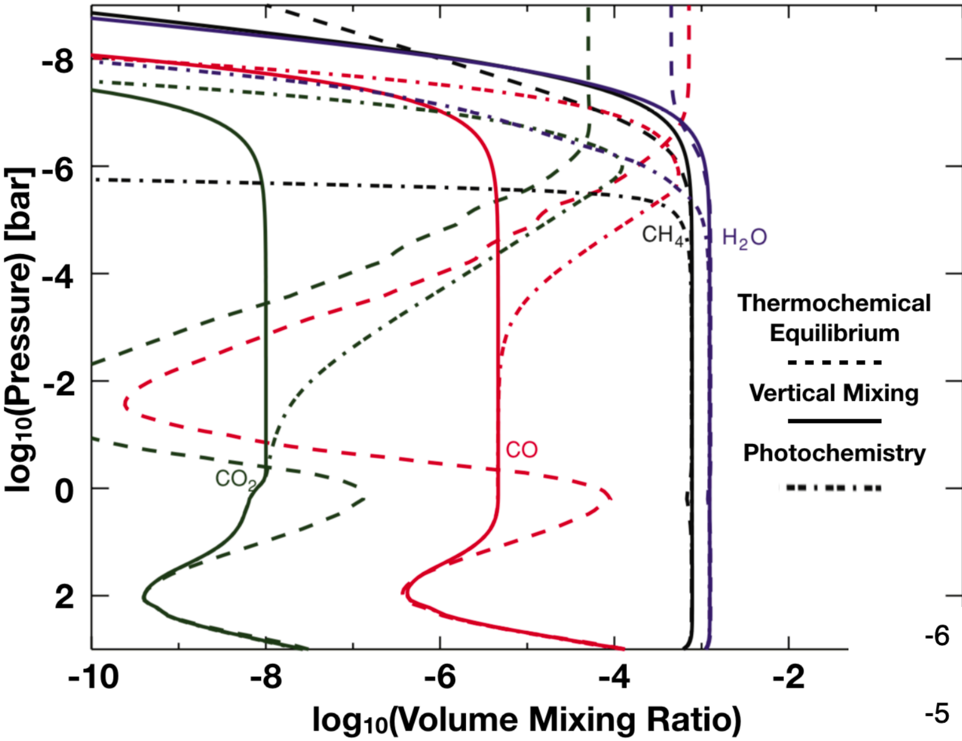
1/2/3D RCE "Gridtrievals"

"Chemically-Consistent Retrieval"

Temperature Pressure Profiles



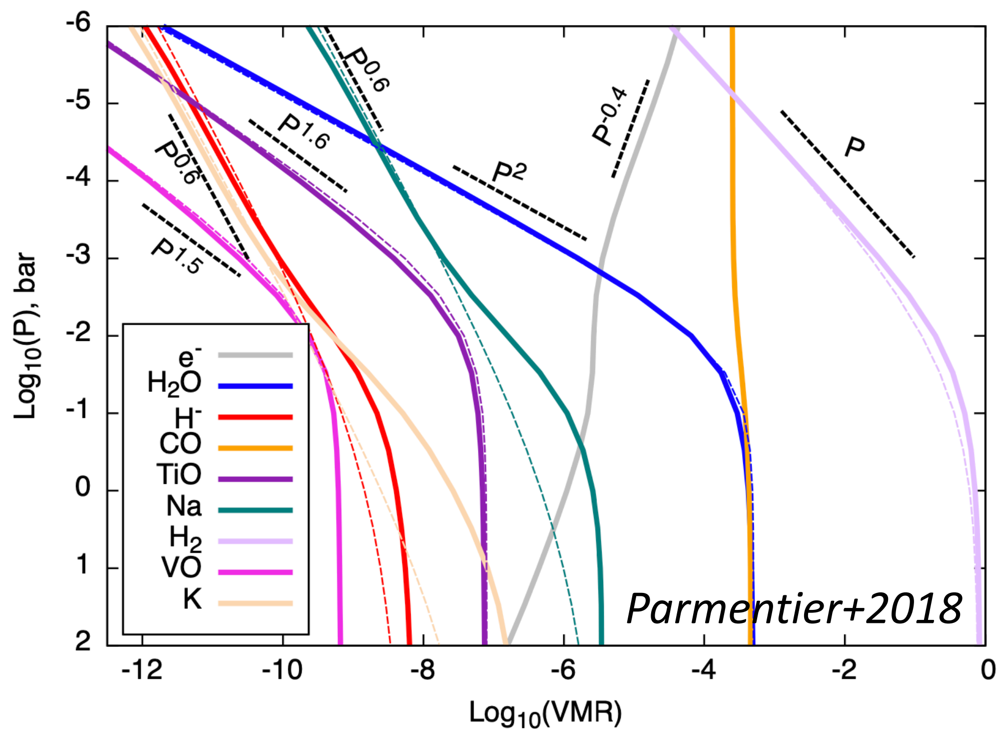
Chemistry/Abundances



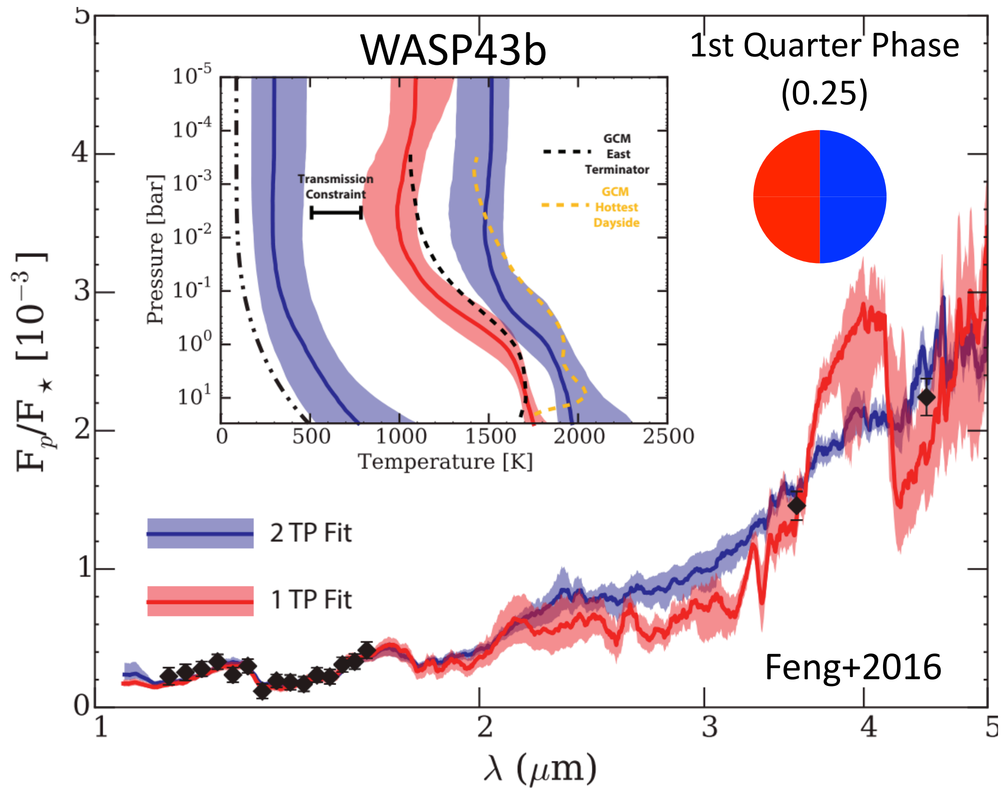
-constant with altitude?
-analytic prescription?

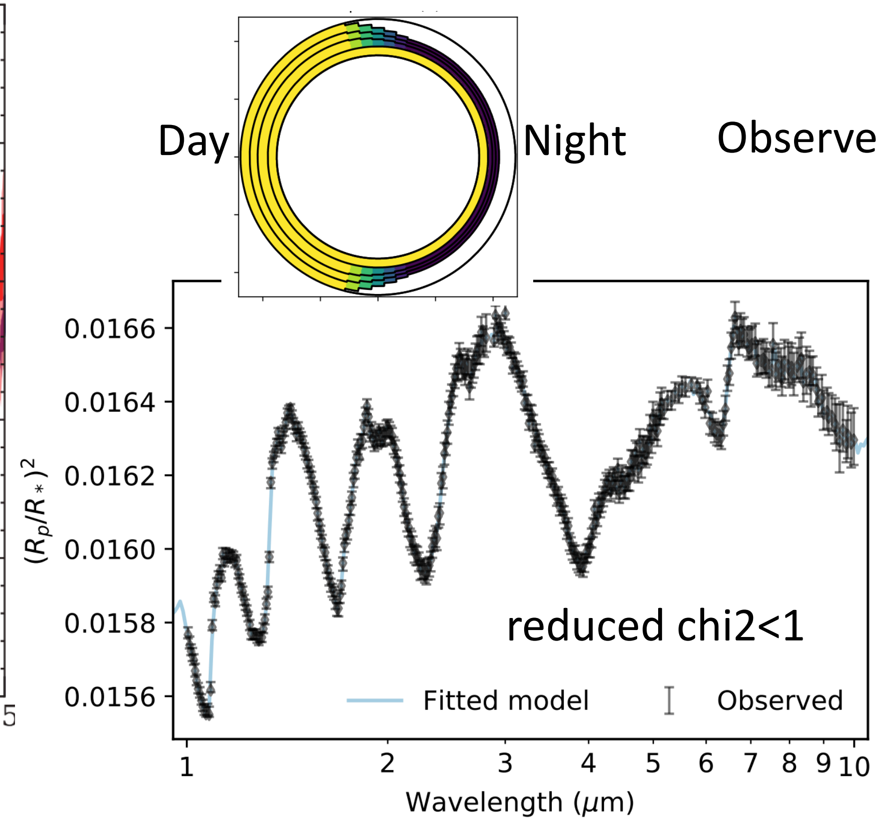
$$\frac{1}{A} = \left(\frac{1}{A_0^{0.5}} + \frac{1}{A_d^{0.5}} \right)^2,$$

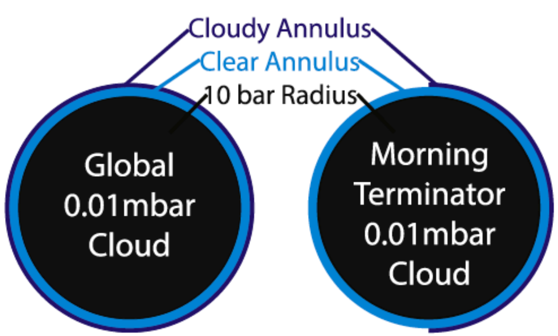
$$\log_{10} A_d \approx \alpha \log_{10} P + \frac{\beta}{T} + \gamma,$$

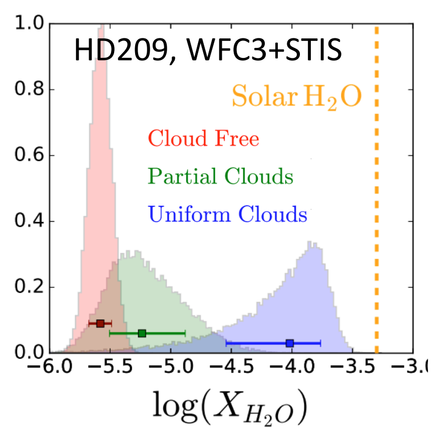


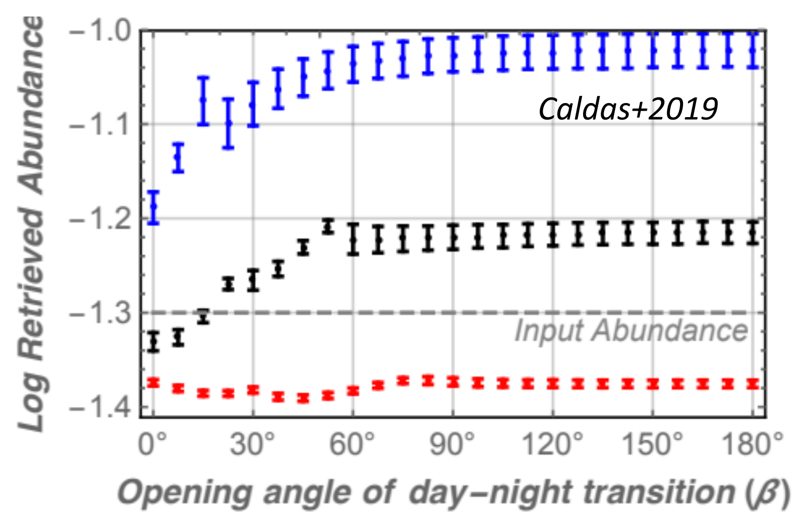
3D Effects: Non-uniform Temps, Clouds







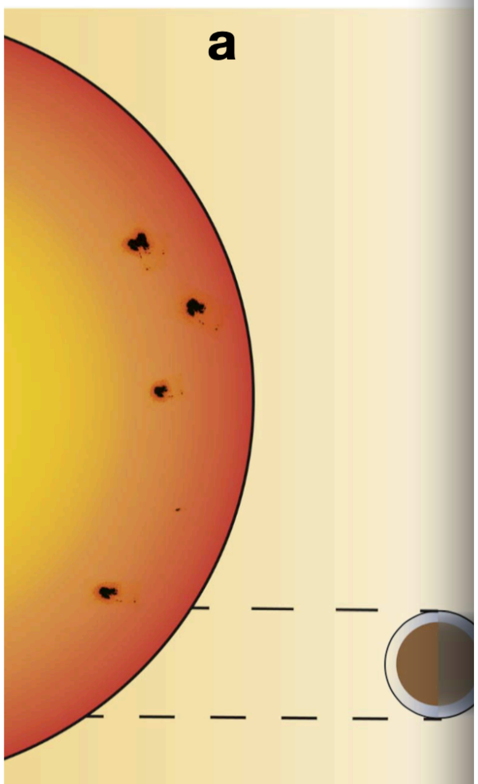


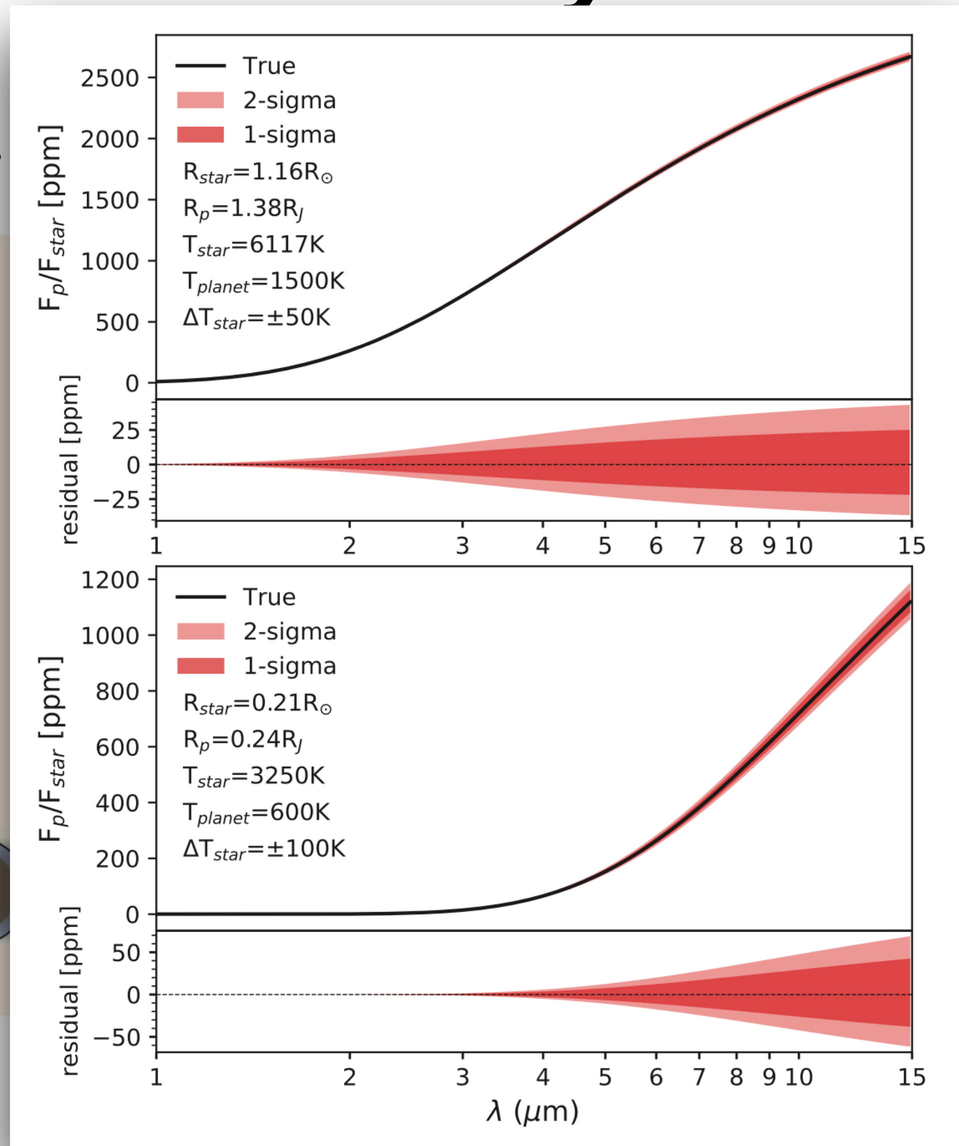


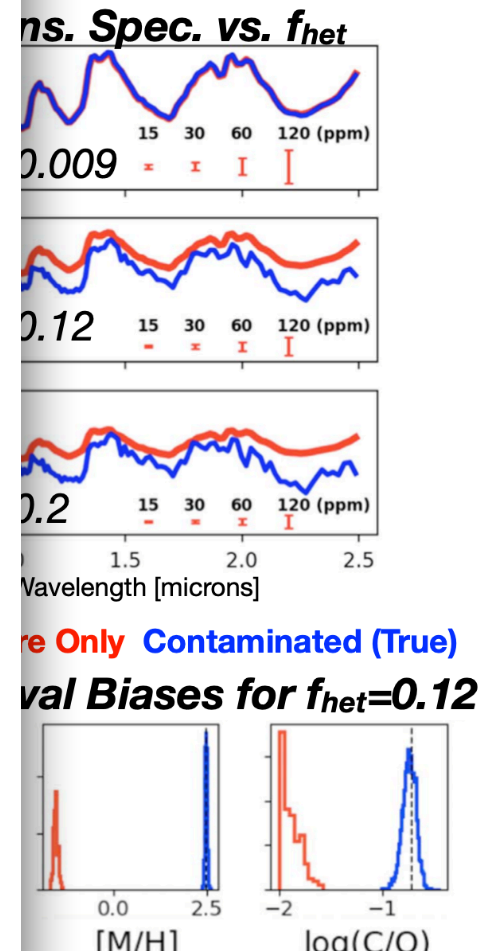
Line & Parmentier 2016; MacDonald & Madhusudhan 2017

Know thy Star

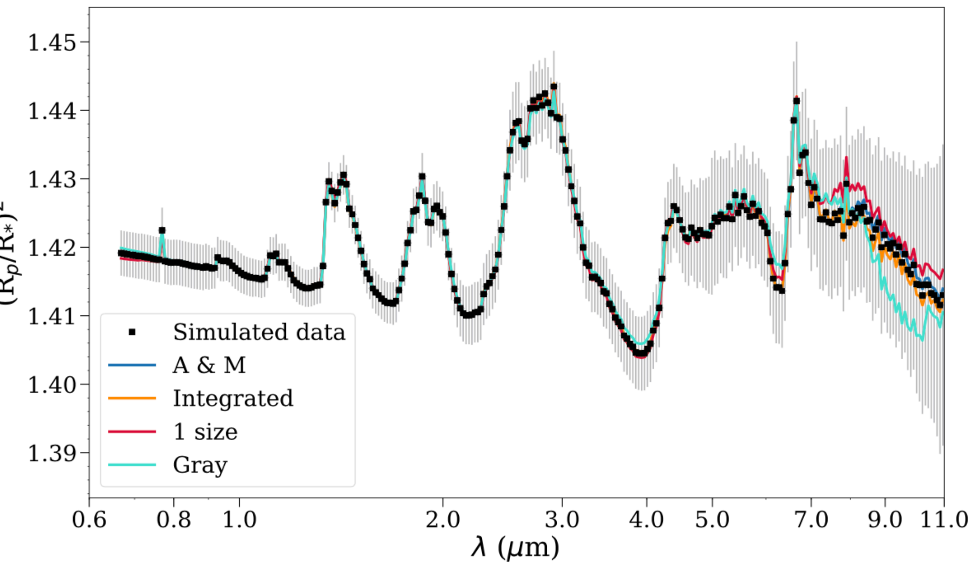
Transit Light-Source

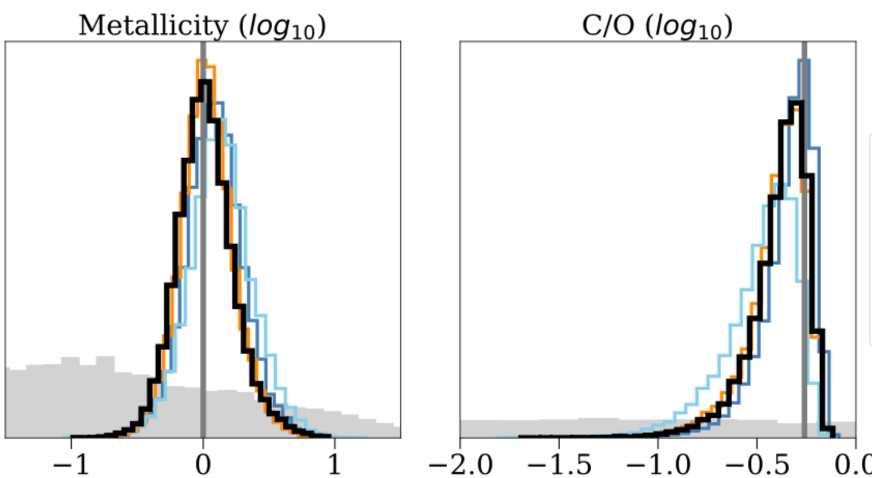


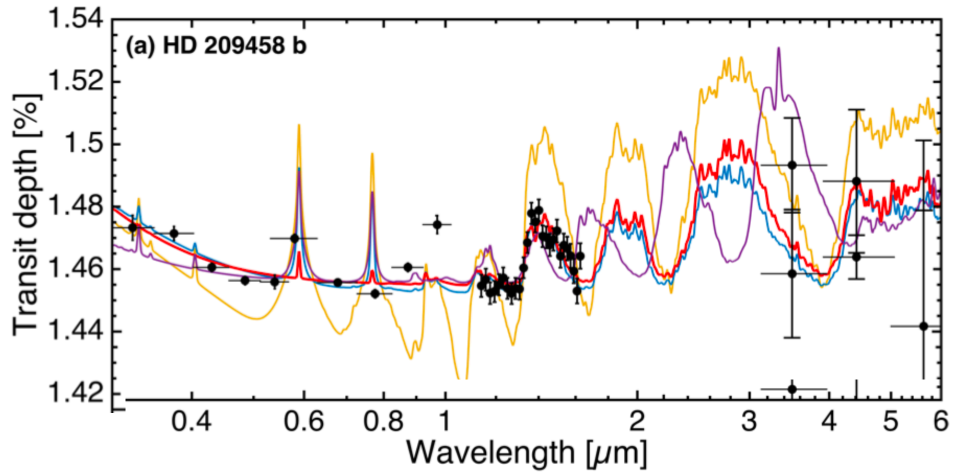


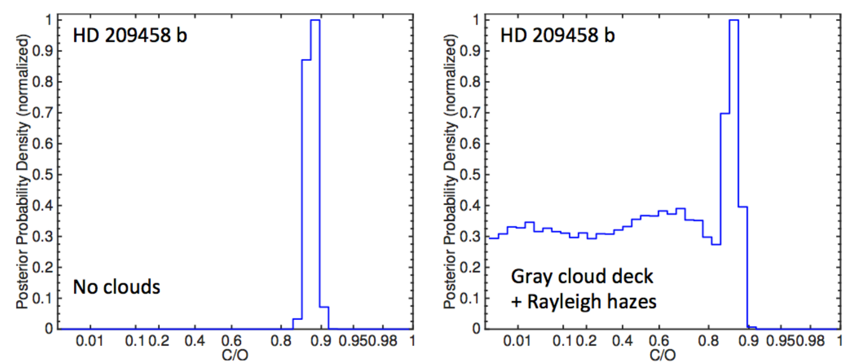


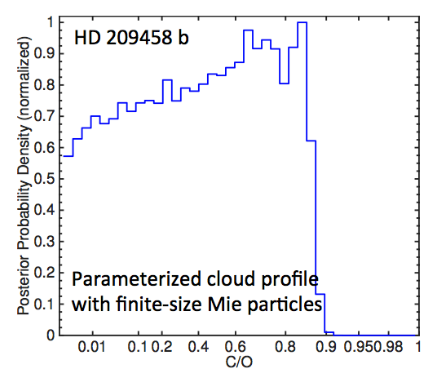
Clouds/Hazes/Aerosols/Nuisances….







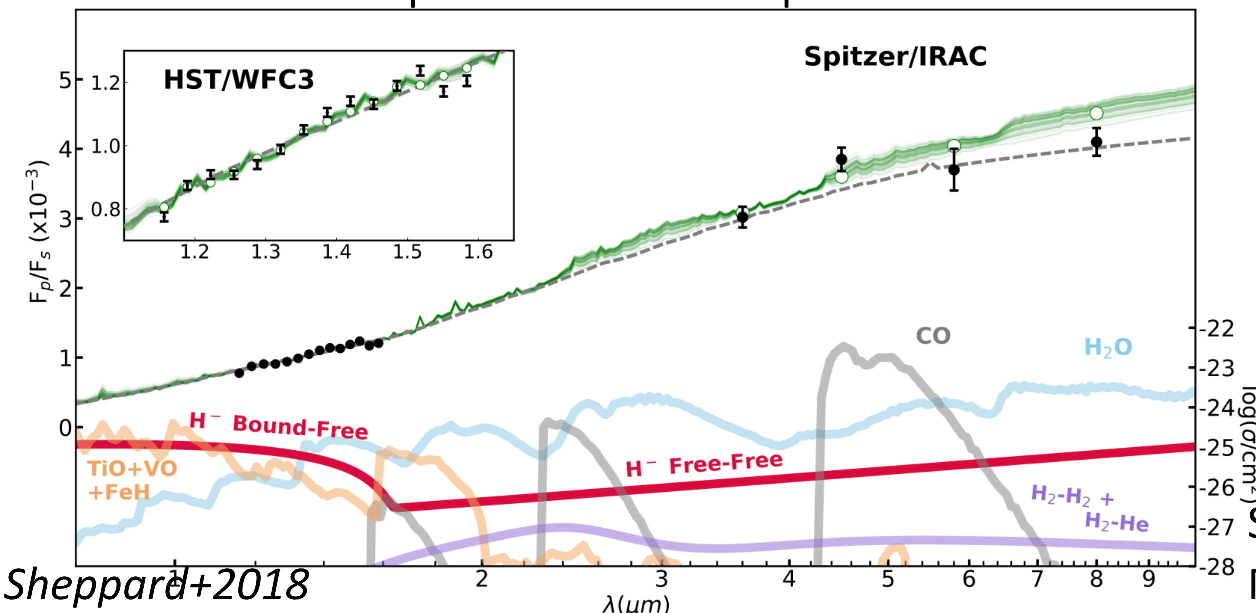




Mai & Line 2019, Benneke 2015

Degree of Self-Consistency

Hot Jupiter WASP-18b Teq~2500K

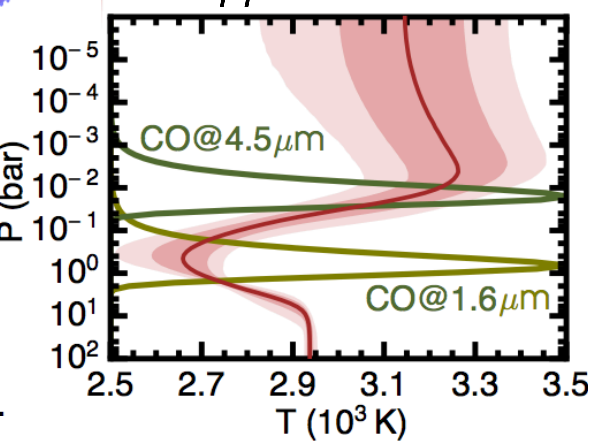


Sheppard+2018

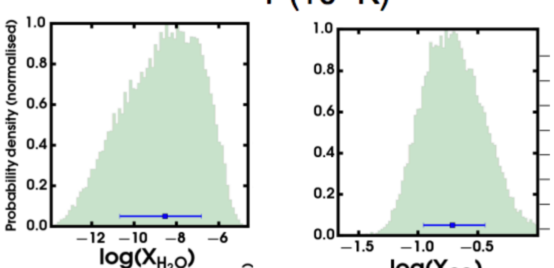
Self-Consistent 1D grid

MCMC interpolation

Arcangeli+2018



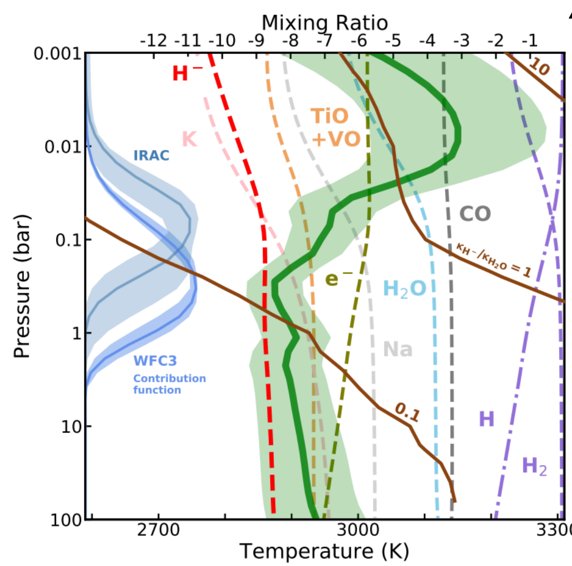
"Free Retrieval"

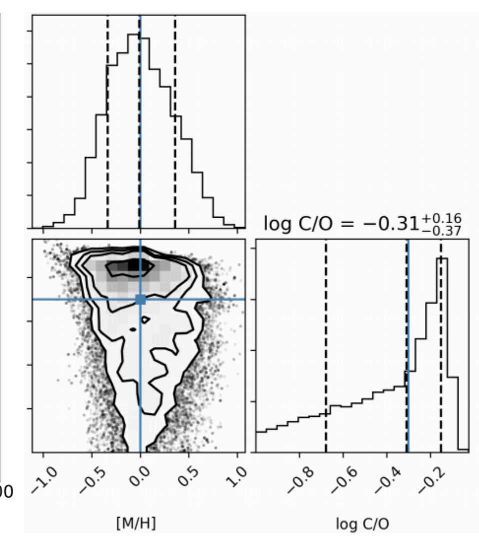


~300x Solar

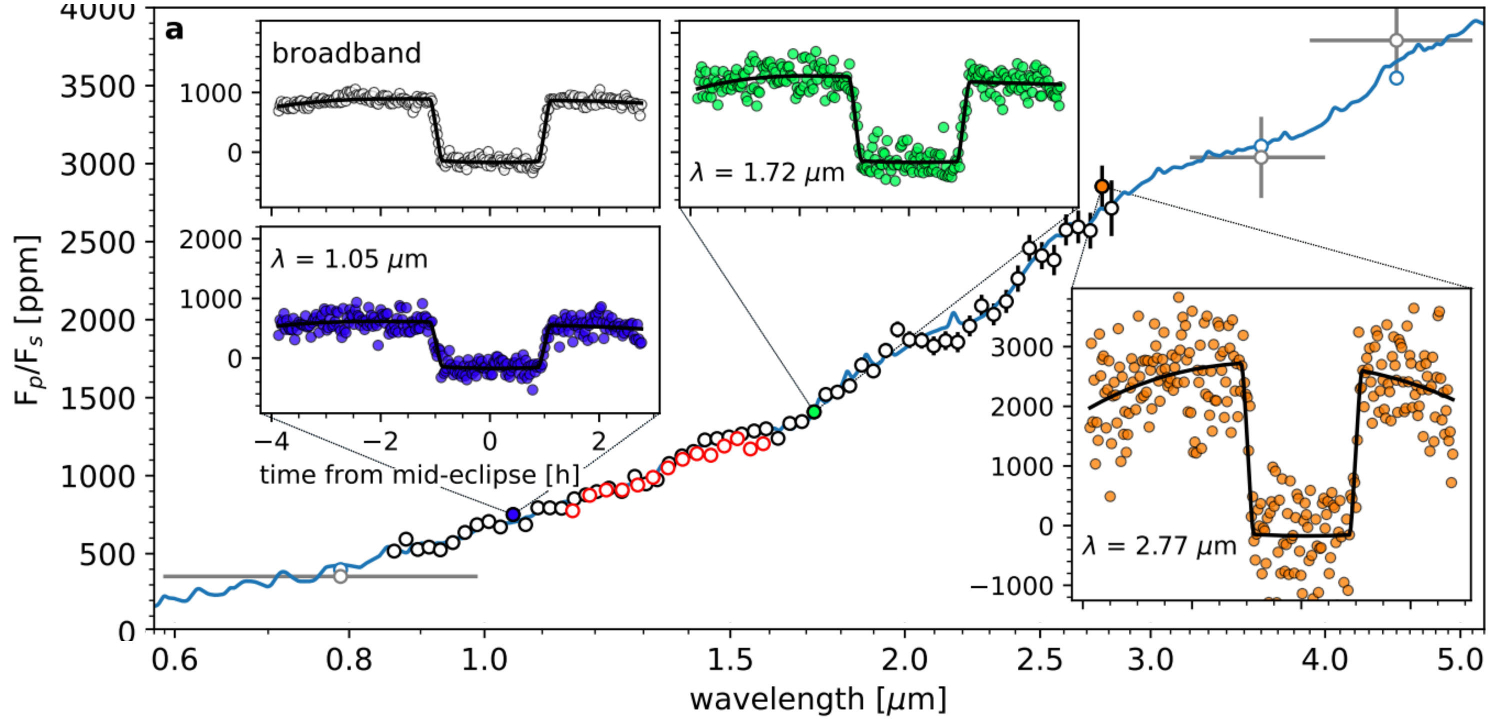
C/O~1

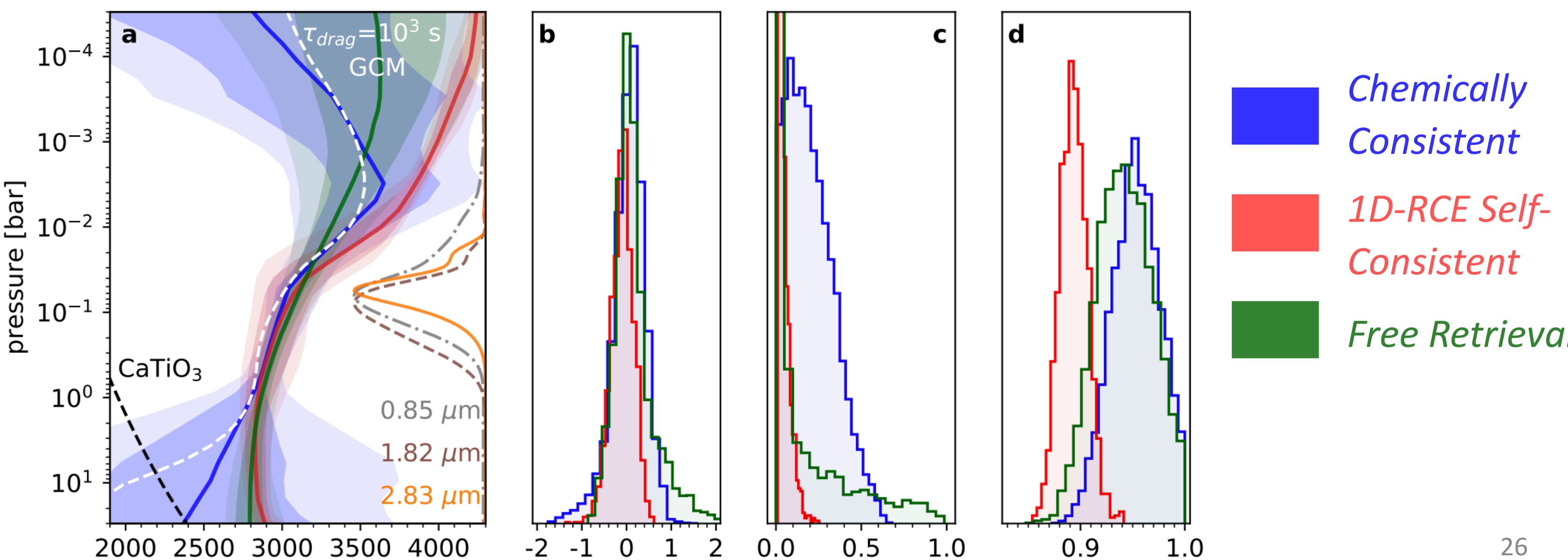
CO=20% of Atmosphere!?





Solar Comp!

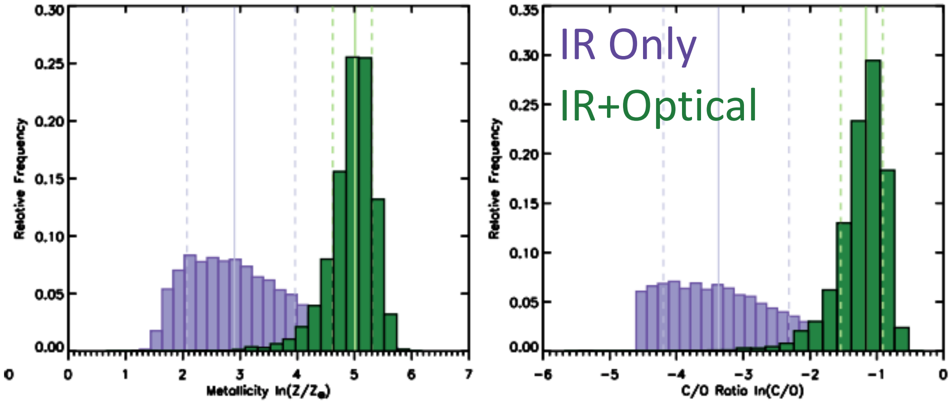




Coulombe & the ERS Team, 2023

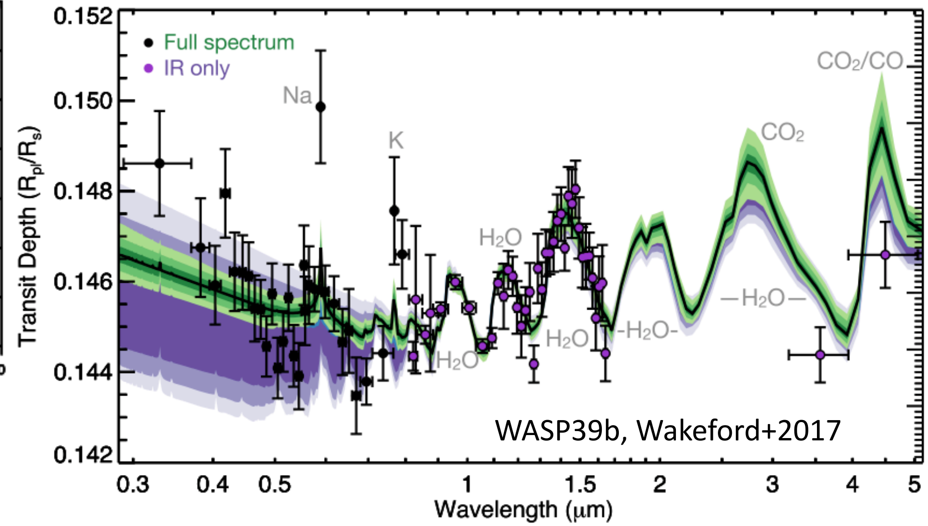
It's not me, it's you: The "Answer" also Depends on the Data!!!!

Which data sets to include?

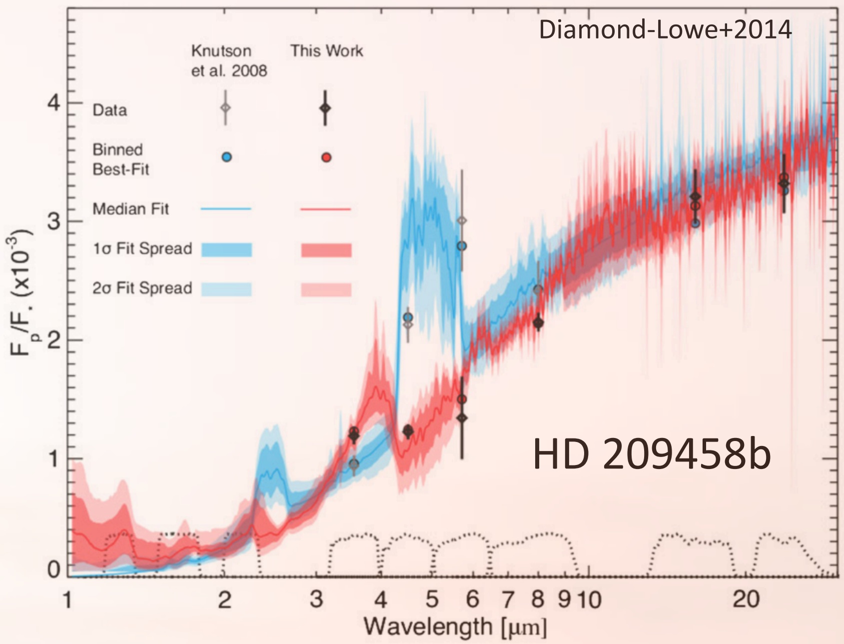


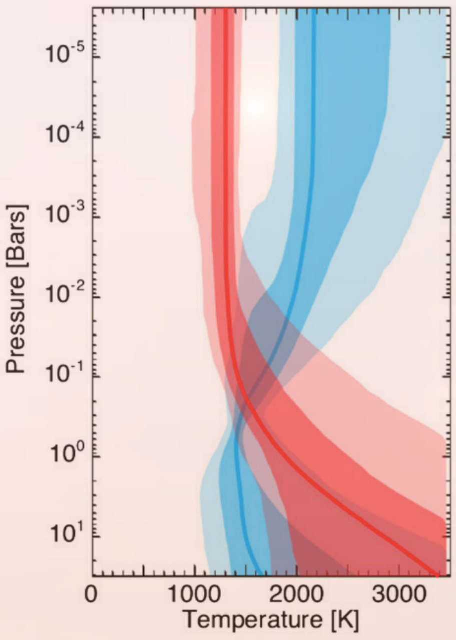
IR Only: χ^2 = 31.9, DOF=31 —> p-val=0.42)

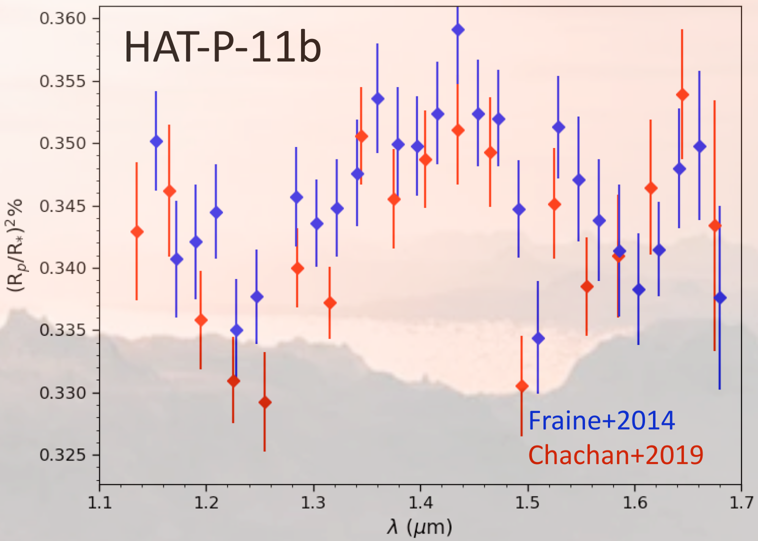
IR+Optical: χ^2 = 88.1, DOF=65 —> p-val=0.03)

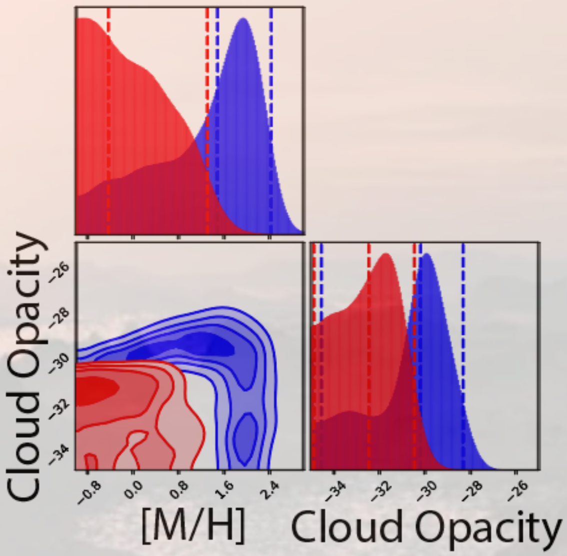


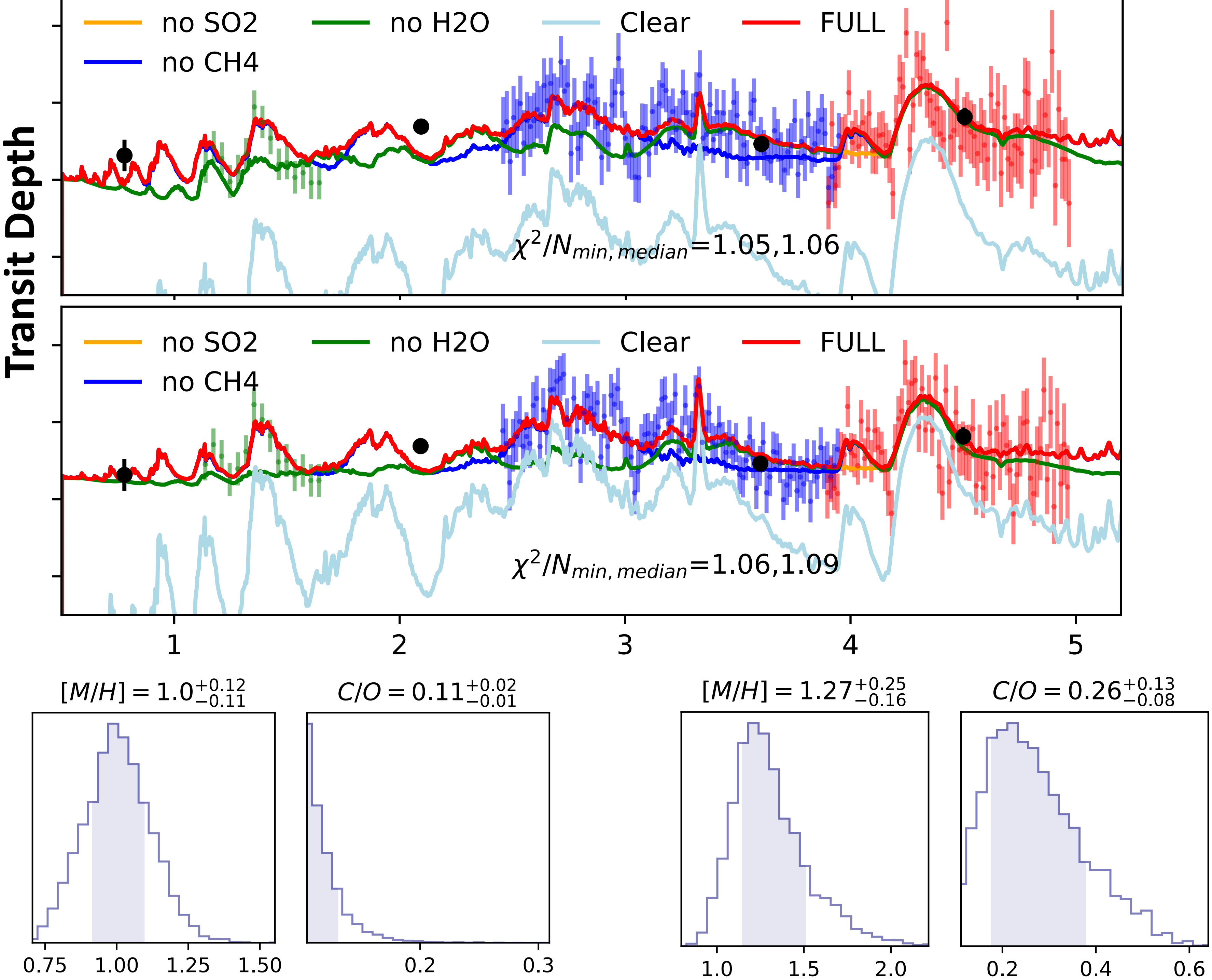
Data analysis differences





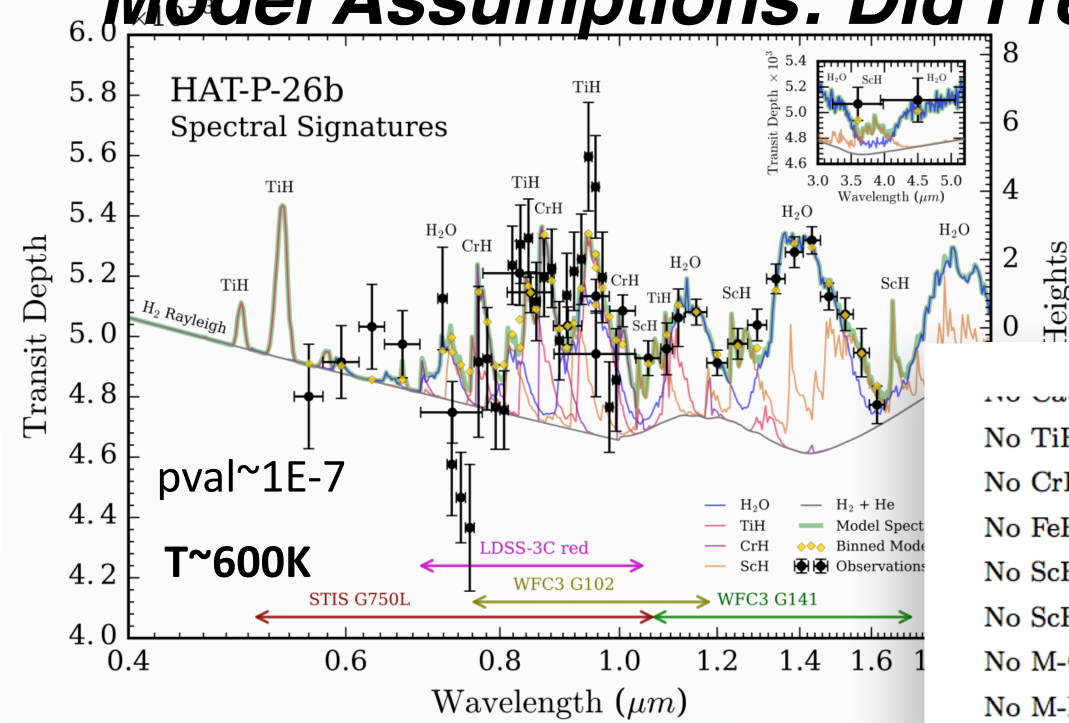






Transit Depth
no SO2
no H2O
Clear
FULL
no CH4
$\chi^2/N_{min,median}$=1.05,1.06
no SO2
no H2O
Clear
FULL
no CH4
$\chi^2/N_{min,median}$=1.06,1.09
1
2
3
4
5
$[M/H] = 1.0^{+0.12}_{-0.11}$
$C/O = 0.11^{+0.02}_{-0.01}$
$[M/H] = 1.27^{+0.25}_{-0.16}$
$C/O = 0.26^{+0.13}_{-0.08}$
0.75
1.00
1.25
1.50
0.2
0.3
1.0
1.5
2.0
0.2
0.4
0.6

Model Assumptions: Did I really detect this gas?

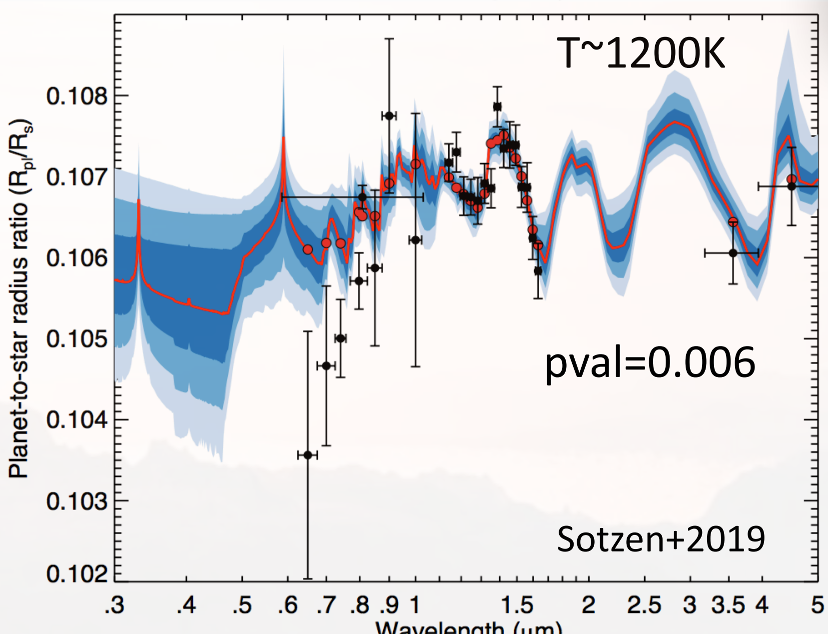


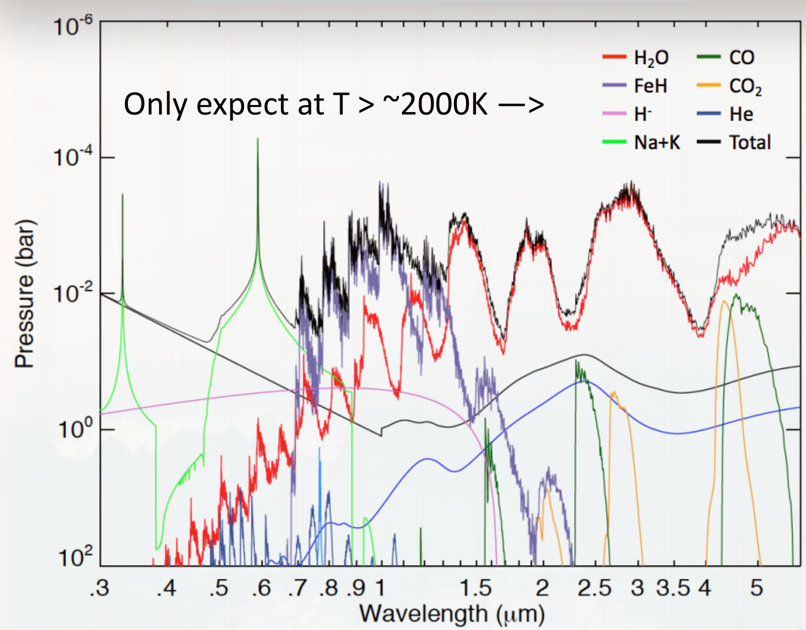
Model	Evidence $\ln(\mathcal{Z}_i)$	Best-fit $\chi^2_{r,\min}$	Bayes Factor $\mathcal{B}_{0i}$	Significance of Ref.
Full Chem	352.26	3.55	Ref.	Ref.
No H_2+He	325.59	6.32	3.82×10^{11}	7.6σ
No H_2O	328.12	6.03	3.03×10^{10}	7.2σ
No CH_4	352.41	3.39	0.86	N/A
No NH_3	352.64	3.37	0.68	N/A
No HCN	352.45	3.44	0.82	N/A
No CO	352.34	3.39	0.92	N/A

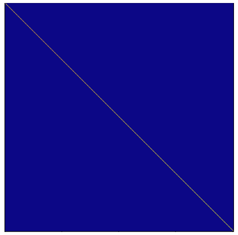
MacDonald & Madhusudhan 2019

Only expect at T > ~1800K

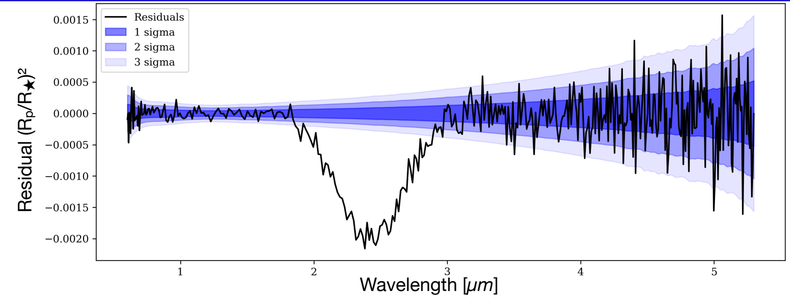
No TiH	347.45	4.08	122	3.6σ
No CrH	351.16	3.54	3.01	2.1σ
No FeH	352.43	3.46	0.84	N/A
No ScH	351.57	3.48	2.00	1.8σ
No ScH or AlO	350.25	3.72	7.44	2.5σ
No M-Oxides	354.08	3.04	0.16	N/A
No M-Hydrides	345.66	3.79	732	4.1σ





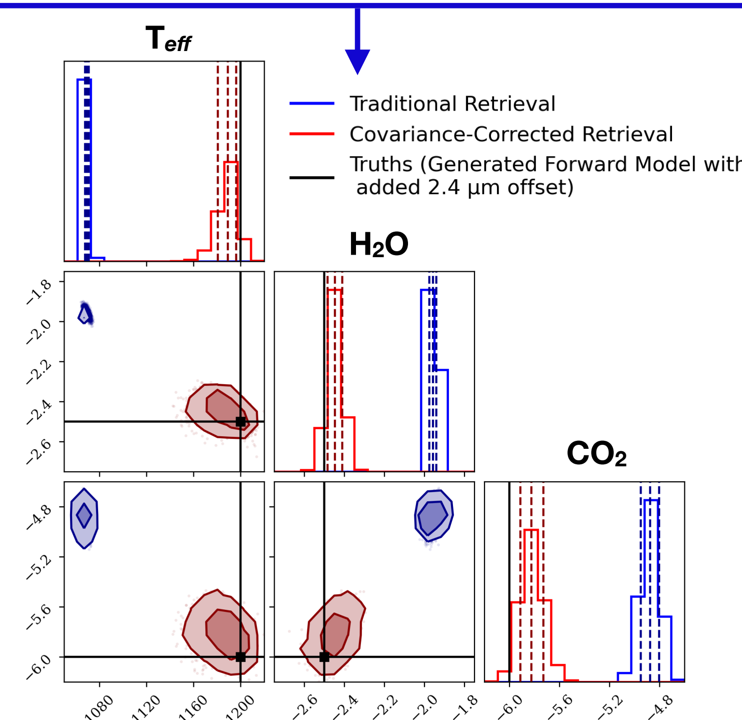


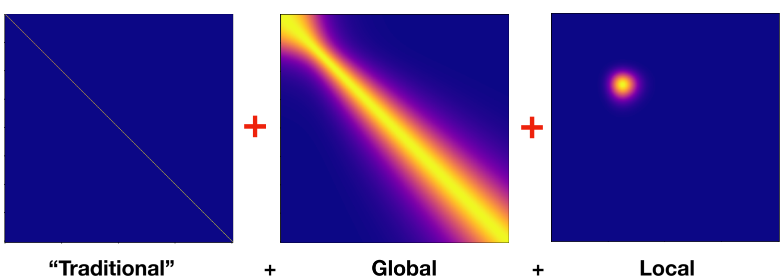
“Traditional” covariance only

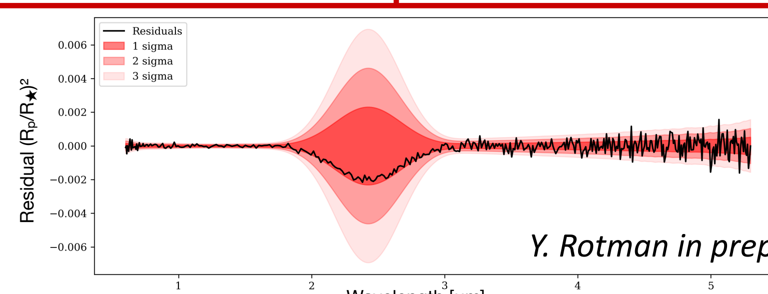


Missing features in transmission spectra from poor line lists or choice of opacity sources in retrievals **can bias posterior probability distributions** significantly

By treating uncertainties as a 2D matrix and adding in local and global covariances as free parameters in retrievals, we can account for and **downweight biasing features,** and successfully **retrieve correct parameter values to within 2 sigma**







Bayesian Leave-One-Out Cross-validation

LOO-CV gives us per-data point scores telling us how well a model explains the data.

Each data point is removed in turn and we do a retrieval on the rest of the data to see how well the left-out data point is predicted by the model.

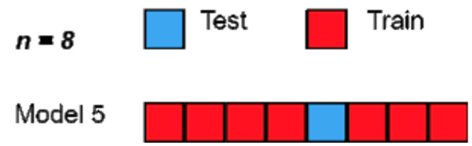
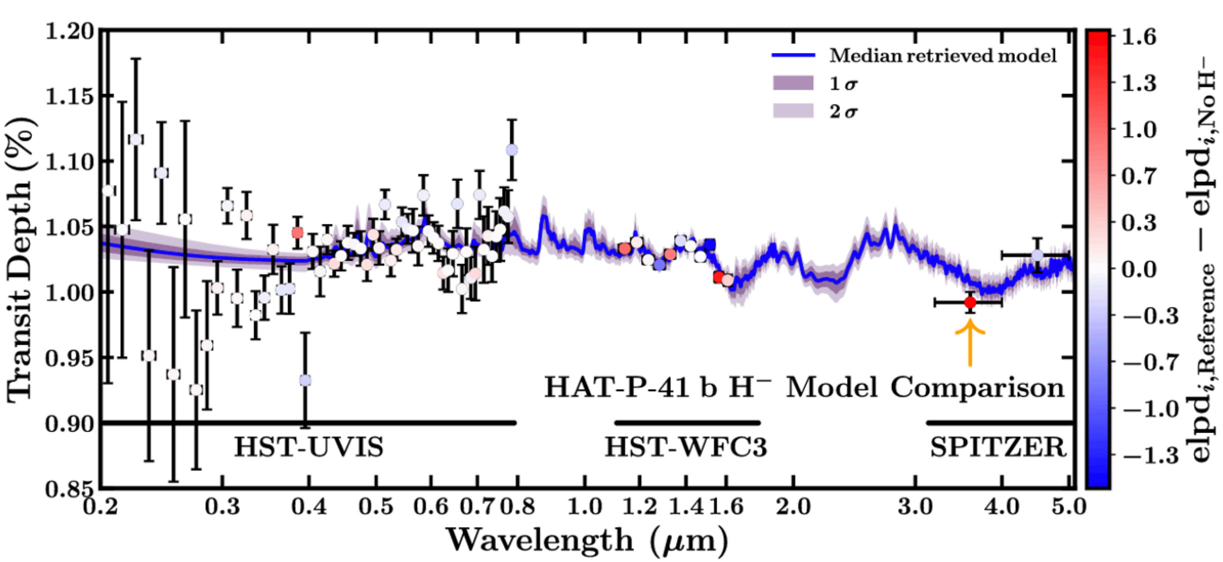


Illustration of leave-one-out cross-validation (LOO-CV) when n = 8 observations. Wikimedia Commons

LOO-CV gives us interpretable model criticism and a model selection metric
see Welbanks et al. 2023a – now possible with a single retrieval!



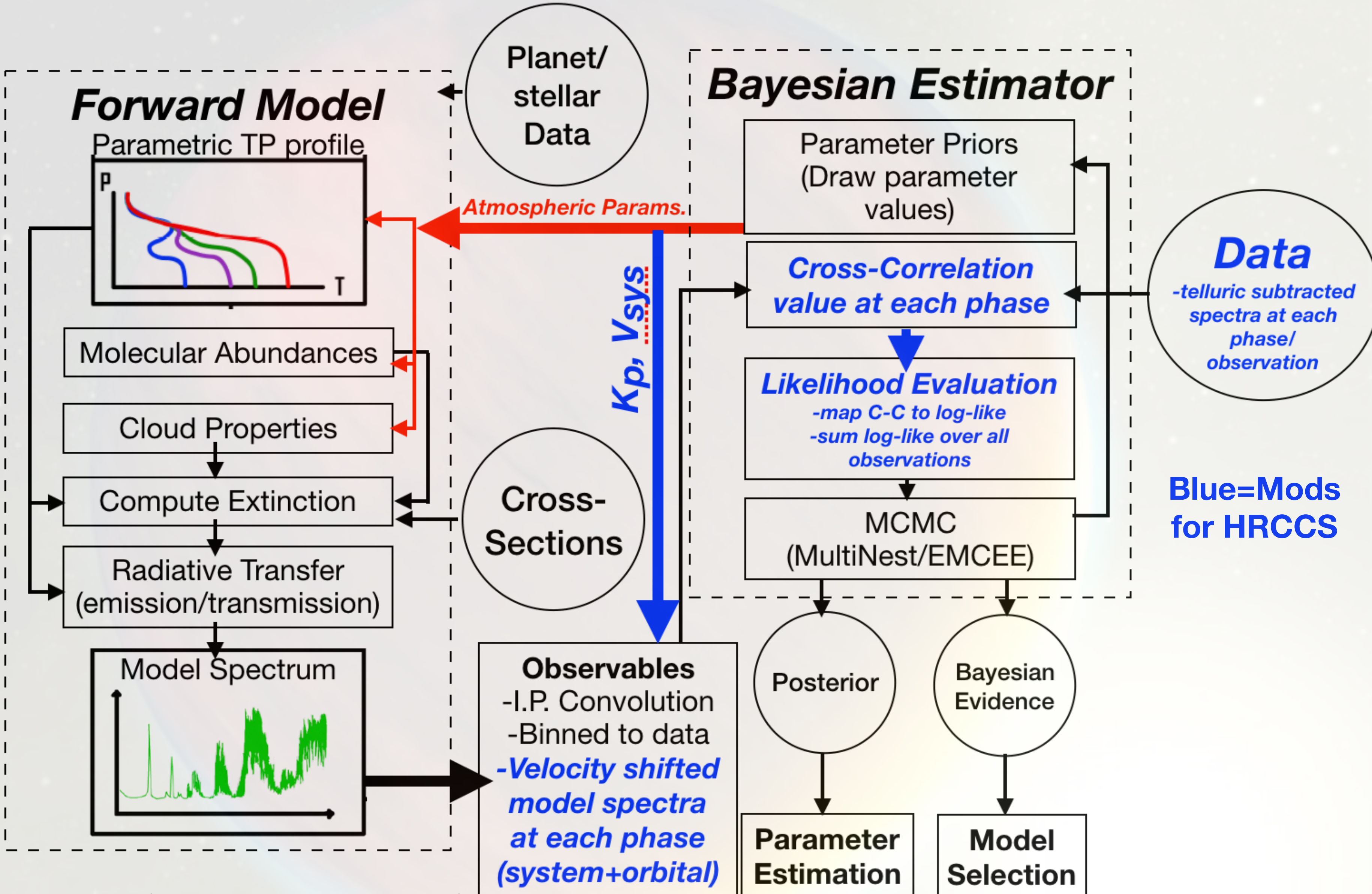
Redder points are preferably explained by the model with H^-

LOO-CV shows that the detection of H- in HAT-P-41b depends on a single Spitzer data point

Luis Welbanks

Additional Applications

HRCCS Retrievals: Crash Course



$$\ln\mathcal{L} \propto \ln\left(\sigma_d^2 + \sigma_m^2 - 2\rho\sqrt{\sigma_m^2\sigma_d^2}\right)$$

(Brogi & Line 2019)

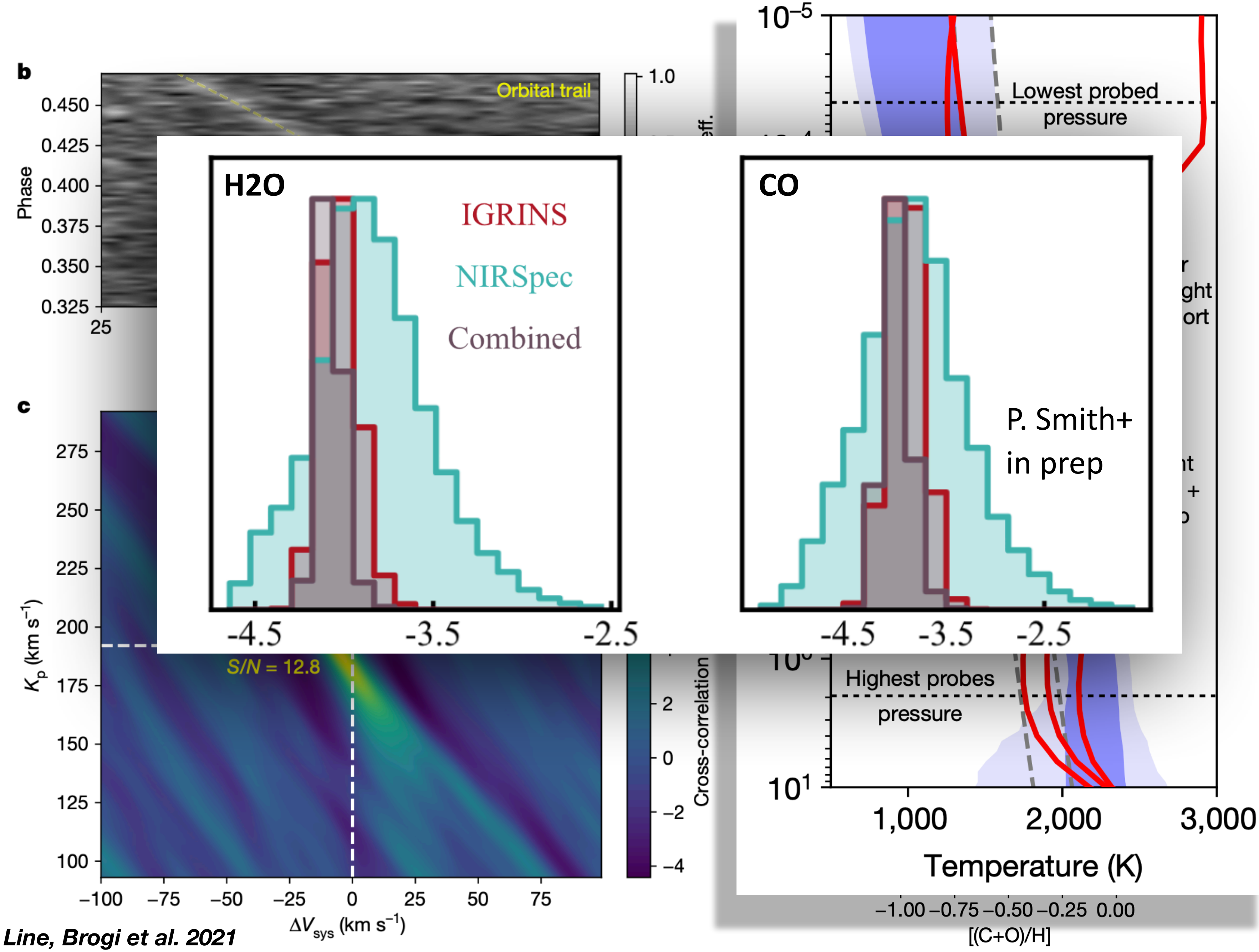
$$\ln\mathcal{L} \propto \ln(1-\rho^2)$$

(Zucker 2003)

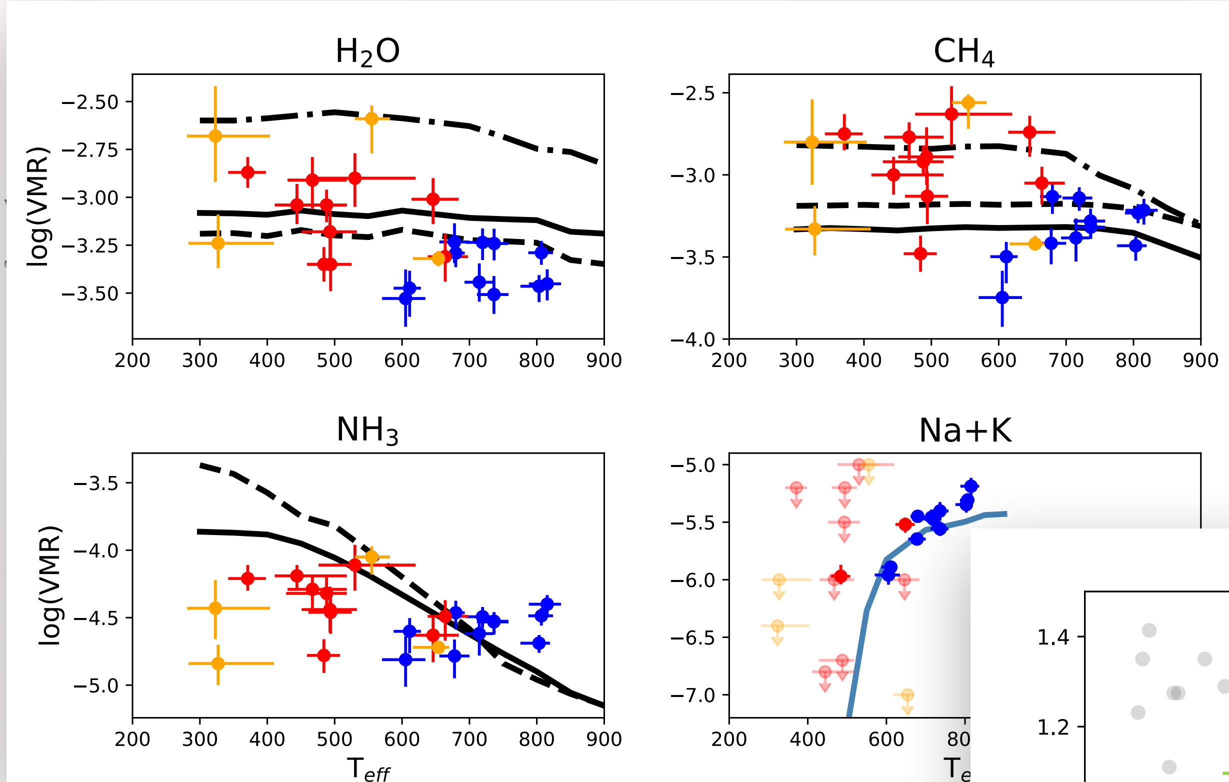
$$\ln\mathcal{L} \propto \rho$$

(Lockwood+2012)

Strong Signal Detection and “ultra-precise” Abundance/TP Constraints!



Benchmark T - Dwarfs As "Validation" Laboratories

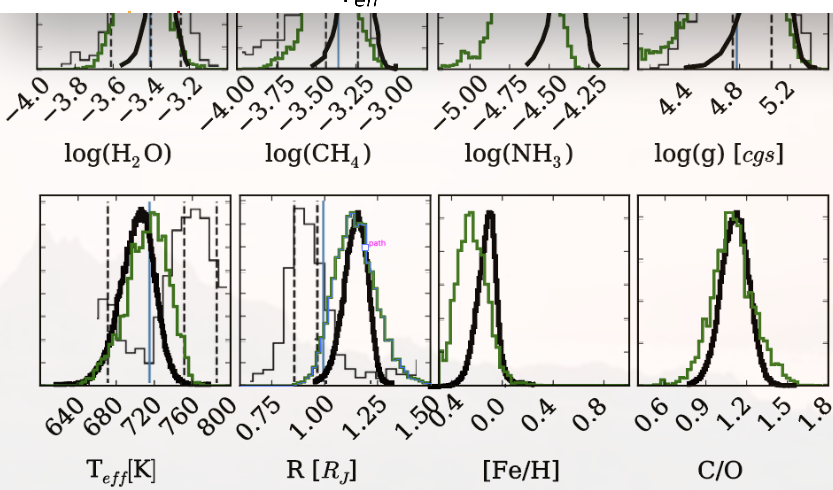


−0.22–0.12[c]

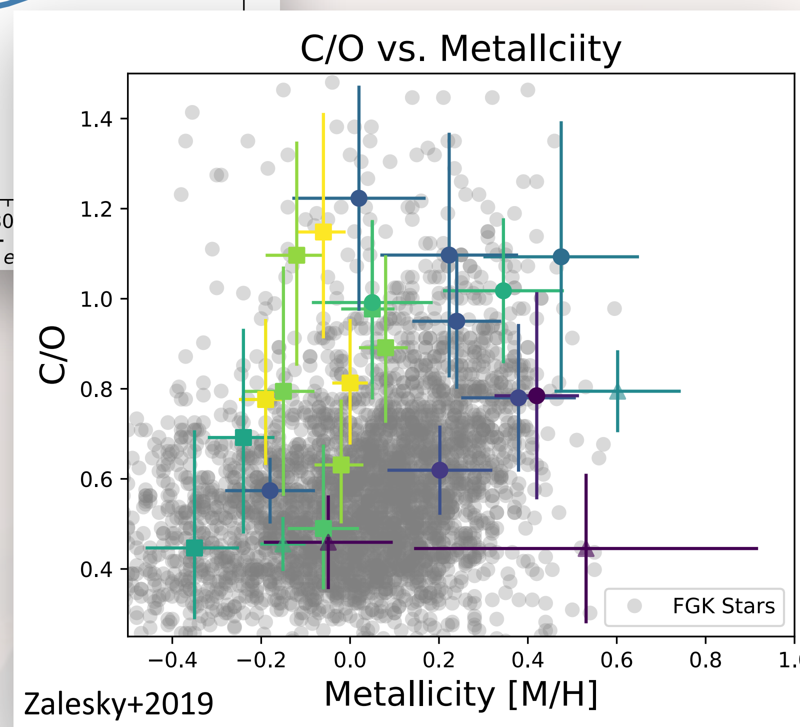
[Fe/H][e] −0.29 to −0.04

0.65–0.97

C/O[g] 0.70–0.93



(pre-rainout correction)



Lots of Tools!

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)
petitRADTRANS	Transmission Emission Reflection	MCMC, NS	Link	Mollière et al. (2019) Mollière et al. (2019) Alei et al. (2022)
MERC	Transmission	NS	—	Seidel et al. (2020)
species	Emission	MCMC, NS, SC-Grid	Link	Stolker et al. (2020)
Gibson et al.	Transmission	MCMC	—	Gibson et al. (2020)
ExoReL$^{\mathcal{R}}$	Reflection	NS	—	Damiano & Hu (2020)
Alfnoor	Transmission	NS	—	Changeat et al. (2020)
PETRA	Transmission	MCMC, SC-Grid	—	Lothringer & Barman (2020)

Table 1 *(continued)*

Code / Authors	Spectrum Type	Parameter Exploration	Code Link	References
METIS	Transmission	MCMC	—	Lacy & Burrows (2020)
Carrión-González et al.	Reflection	MCMC	—	Carrión-González et al. (2020)
ARCiS	Transmission Emission	NS	—	Min et al. (2020) Chubb & Min (2022)
PICASO	Reflection Emission Transmission	NS, SC-Grid	Link	Mukherjee et al. (2021) Miles et al. (2022) Batalha et al. (2023)
Cerberus	Transmission	MCMC	—	Swain et al. (2021)
Aurora	Transmission	NS	—	Welbanks & Madhusudhan (2021)
BART	Transmission Emission	MCMC	Link	Harrington et al. (2022)
ExoJAX	Emission	MCMC	Link	Kawahara et al. (2022)
ThERESA	Eclipse Mapping	MCMC	Link	Challener & Rauscher (2022)
p-winds	Transmission	MCMC	Link	Dos Santos et al. (2022)
smarter	Transmission	NS	—	Lustig-Yaeger et al. (2022)
tierra	Transmission	MCMC	Link	Niraula et al. (2022)
rfast	Reflection Emission Transmission	MCMC	Link	Robinson & Salvador (2023)
Machine Learning				
HELA	Transmission	RF	Link	Márquez-Neila et al. (2018)
ExoGAN	Transmission	NN	Link	Zingales & Waldmann (2018)
INARA	Reflection Emission	NN	Link	Soboczenski et al. (2018)
plan-net	Transmission	NN	Link	Cobb et al. (2019)
Fisher et al.	Transmission	RF	—	Fisher et al. (2020)
Johnsen & Marley	Reflection	MLP	Link	Johnsen et al. (2020)
Nixon & Madhusudhan	Transmission	RF	—	Nixon & Madhusudhan (2020)
MARGE+HOMER	Emission	NN+MCMC	Link	Himes et al. (2022)
exoCNN	Transmission	NN	Link	Ardevol Martinez et al. (2022)
VI-retrieval	Transmission	NN+VI	—	Yip et al. (2022)
Vasist et al.	Emission	NN+VI	—	Vasist et al. (2023)

A Catalogue of Exoplanet Atmospheric Retrieval Codes

Ryan J. MacDonald[1,*] and Natasha E. Batalha[2]

https://arxiv.org/pdf/2303.12925.pdf

Work to be done!

- What to include in more complex forward models (more physics, chemistry, and geometry—what is actually needed??)
- HRCCS Retrievals have only just begun! So much more to learn from this (and synergies with low-res)!
- Data-Model "mis-fitting" remedies (e.g., covariance/GP, Leave-One-Out)
- Speed** improvements in more complex forward models—>GPUs?
- ((What role does Machine Learning play??))

**Don't spend your PhD optimizing code! Prioritize the science (plus, the writing process is the slowest part regardless!)

Questions?