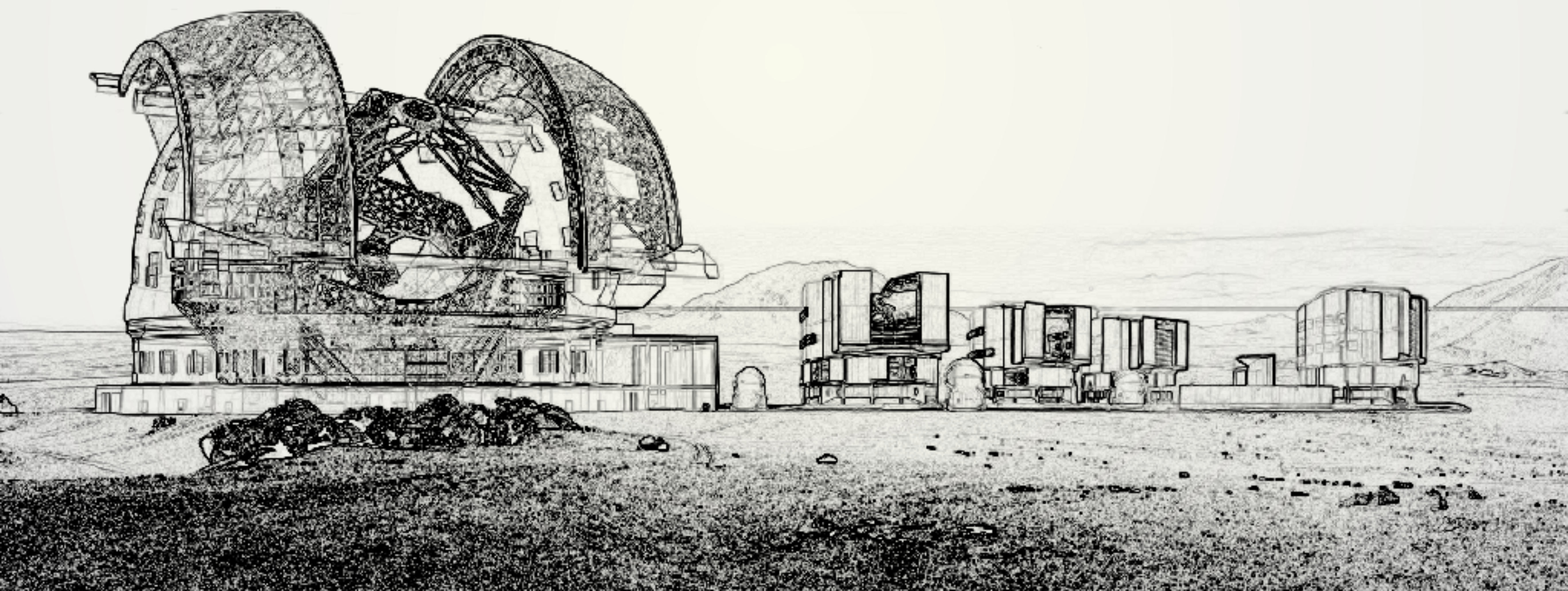
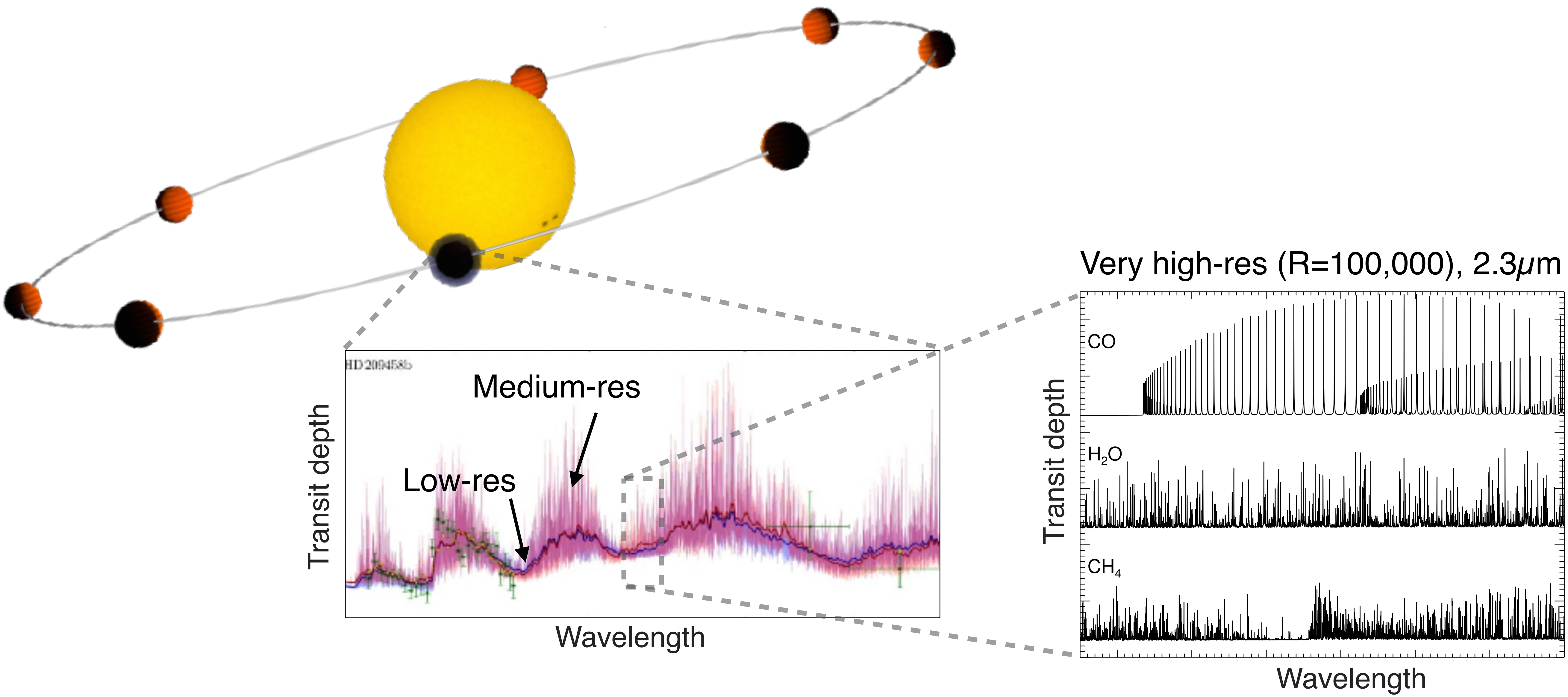
Measuring abundances
from high-resolution cross-correlation spectroscopy

See also Neale Gibson's talk tomorrow 27/08

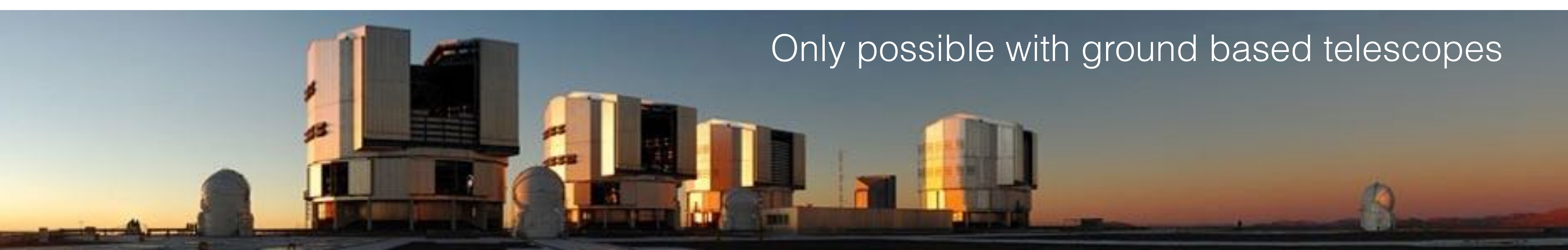
Matteo Brogi
Assistant Professor, University of Warwick



Exoplanets at high spectral resolution



Each species has a unique pattern of spectral lines
Species can be “matched” line by line to templates, e.g. via *cross correlation*

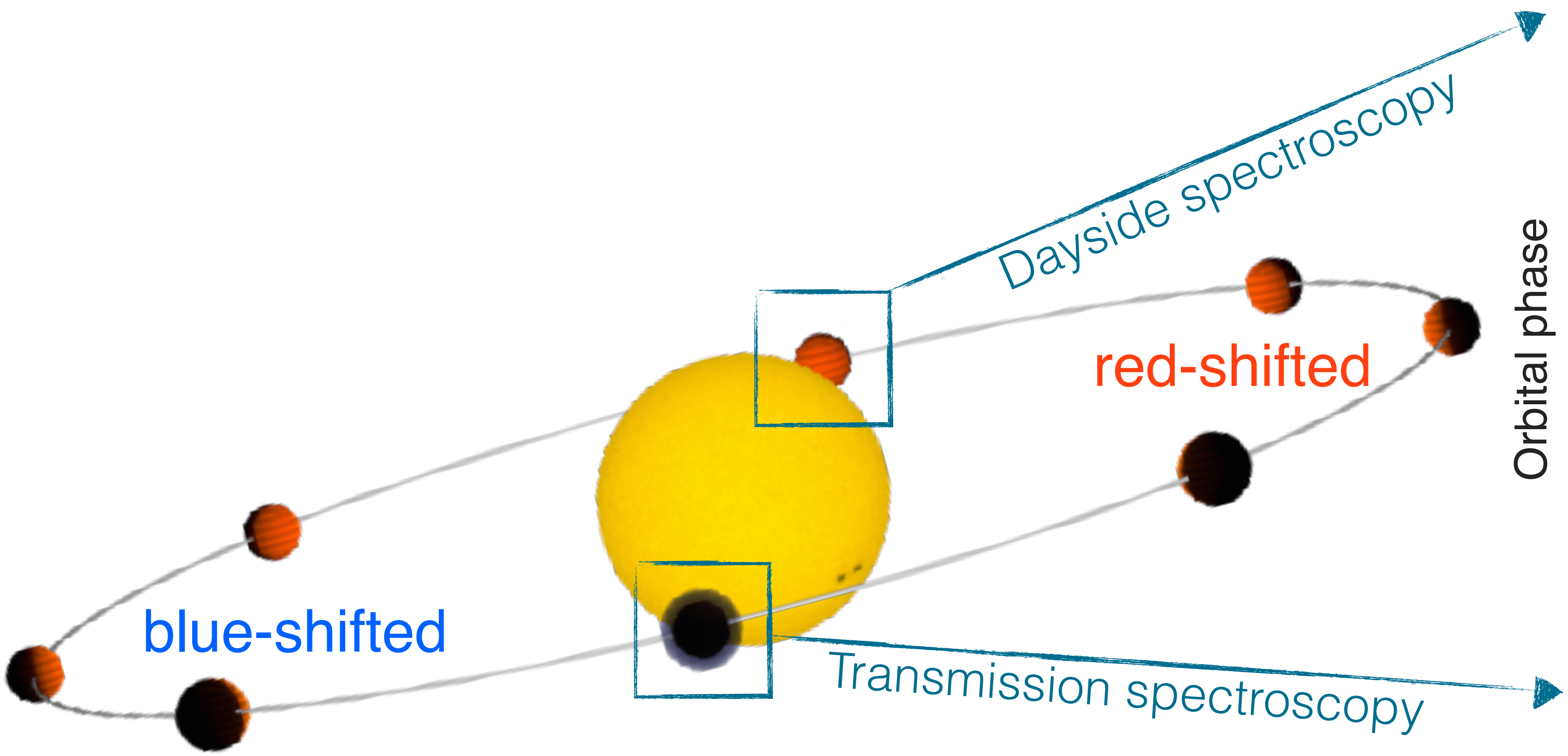


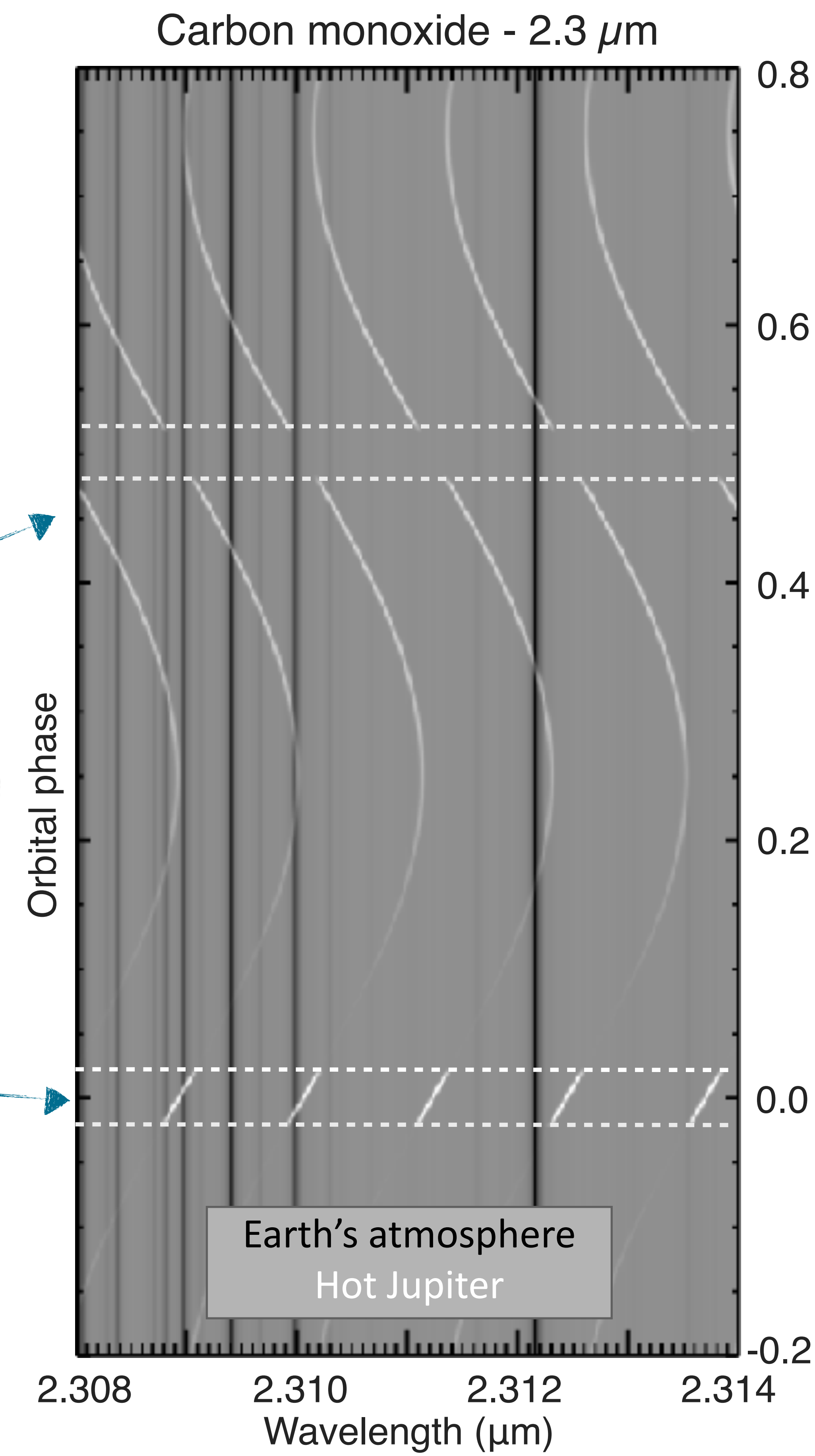
Detecting the orbital motion of close-in planets

Detecting change in planet radial velocity
during a few hours of observations
(Planet RV: 10-100 km/s; Stellar RV: 10-100 m/s)

⇒ Telluric and planet signal disentangled

⇒ Planet radial velocity directly measured

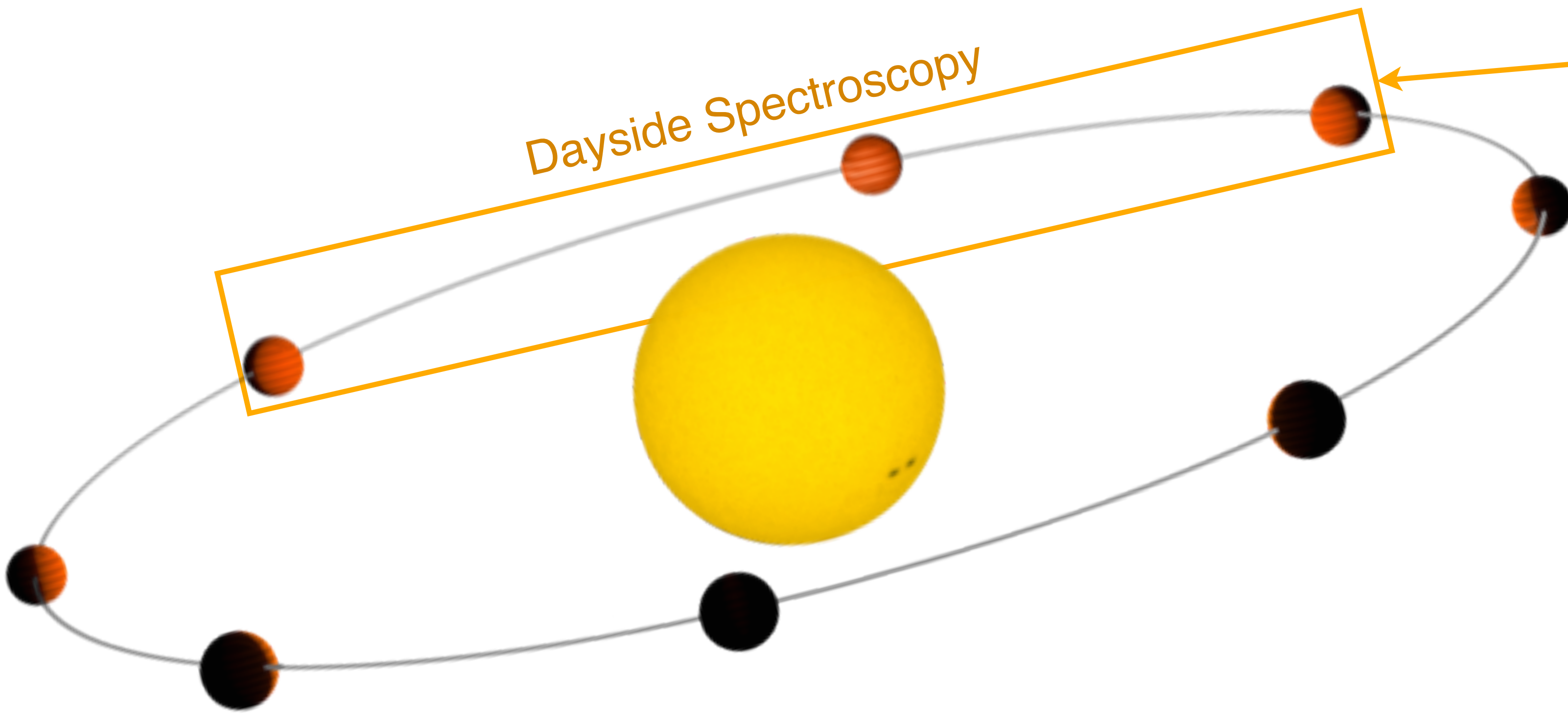


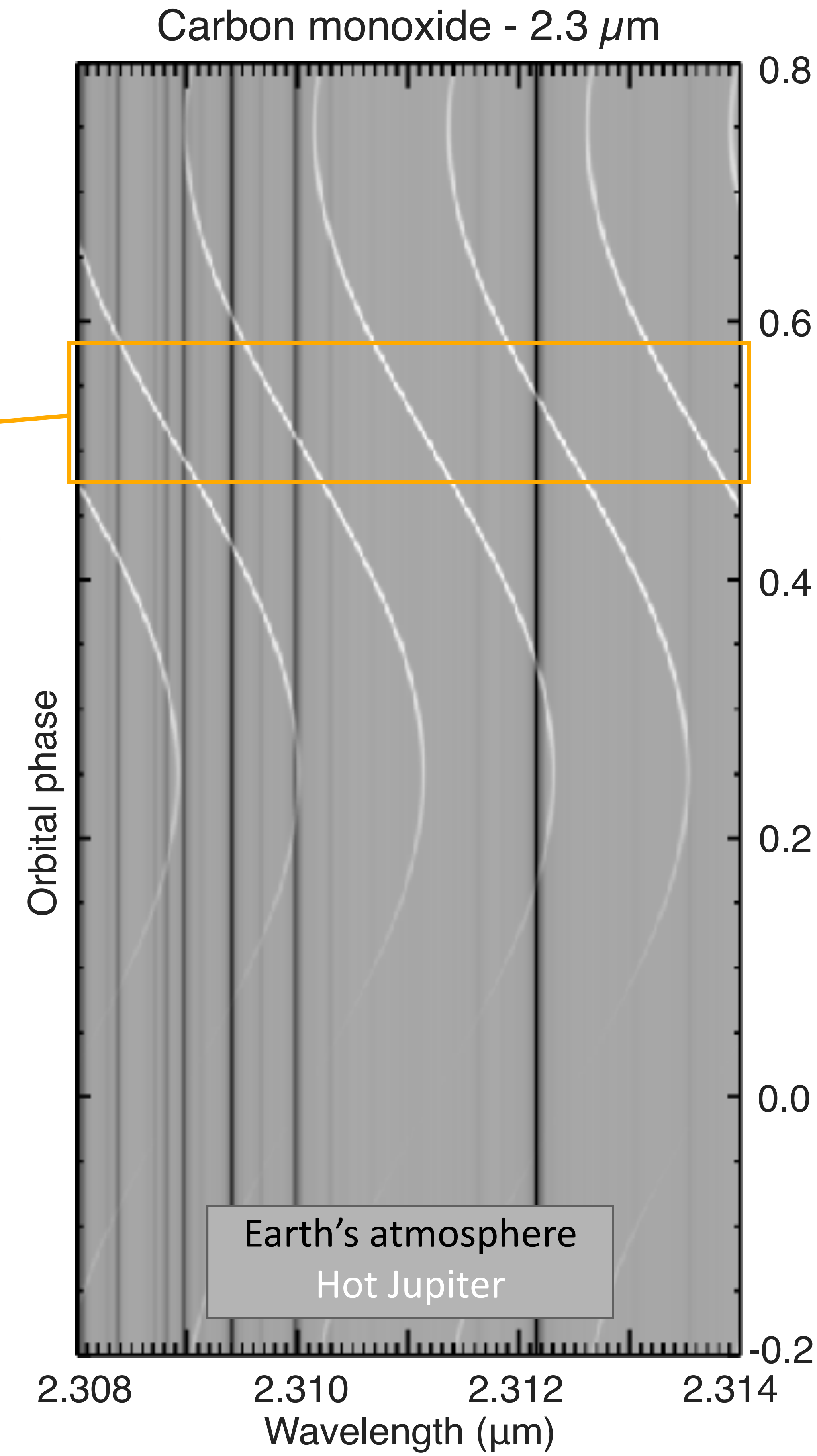


High spectral resolution of non-transiting planets

The thermal spectrum
of the planet is targeted directly

Dayside spectroscopy
applicable to non-transiting planets!



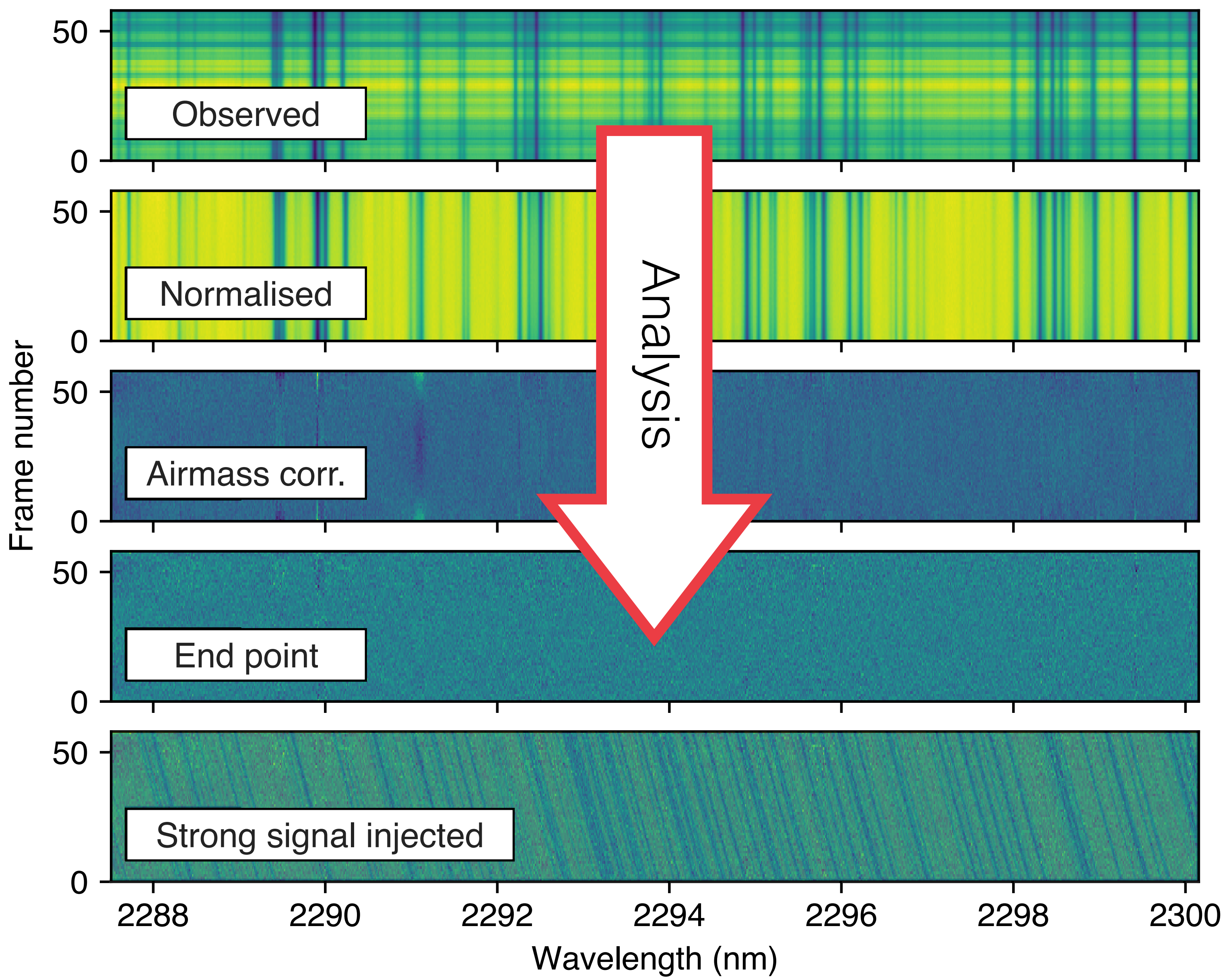


The first and only method to study
atmospheres of most non-transiting planets
(evolved, on close-in orbits)

Can solve for planet mass and orbital inclination

Processing ground-based high-res spectroscopy

Every spectral line stationary in wavelength is removed
(check my lecture on Monday)



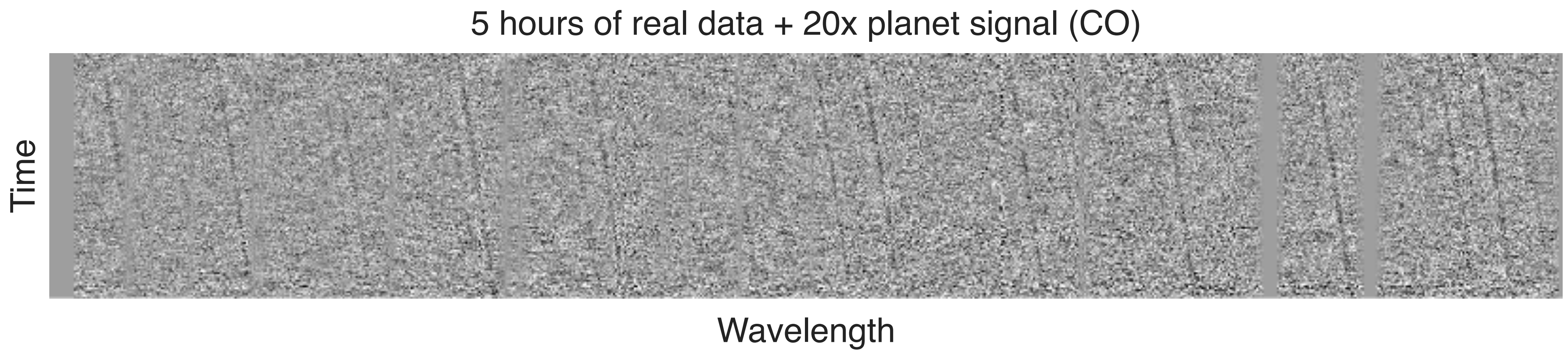
Time-correlated effects (transparency, throughput, etc.) will be "in common-mode" between spectral channels

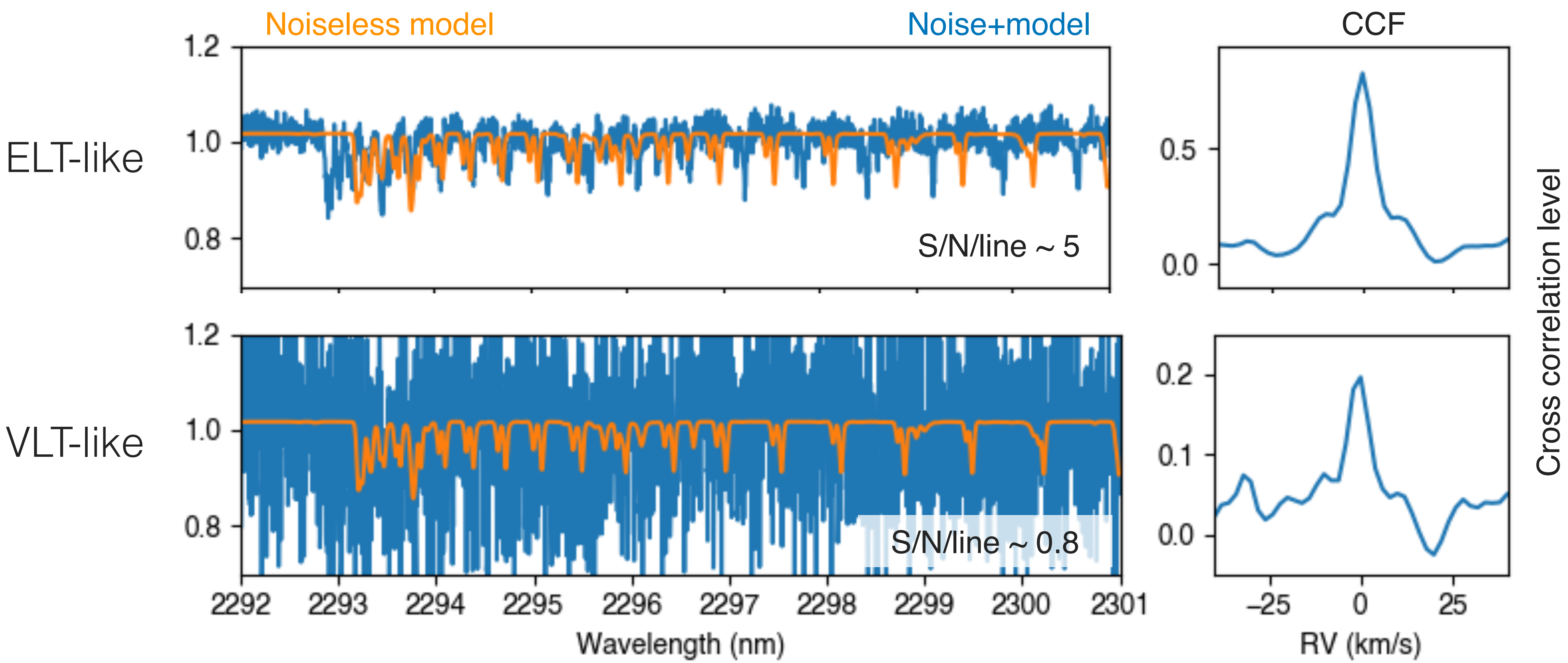
The analysis progressively "normalises" these effects

These steps can be"automated" by algorithms decomposing data into a linear combination of eigenvectors (e.g. PCA)

The process "auto-calibrates" the data: no reference star needed
However, broad-band variations are removed

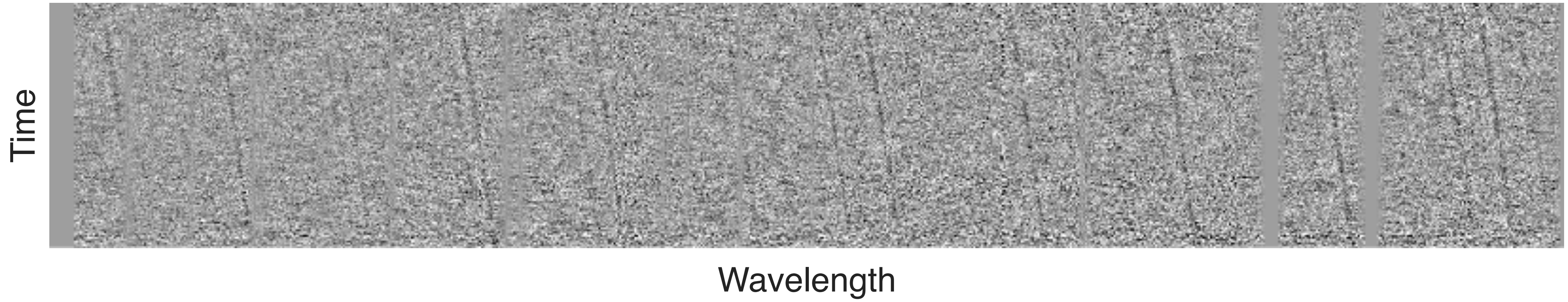
Extracting the (faint) planet signal: cross correlation





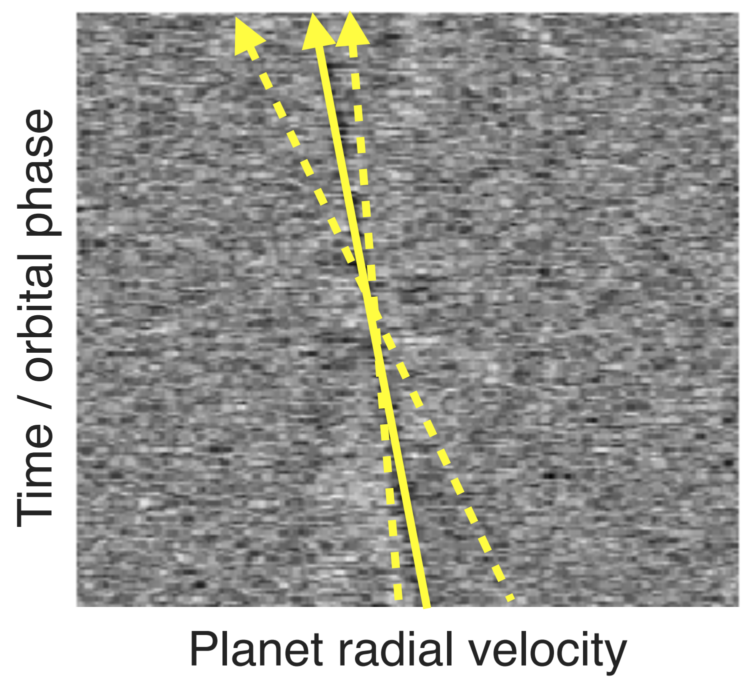
Extracting the (faint) planet signal: cross correlation

5 hours of real data + 20x planet signal (CO)



Cross-correlation with model spectra

Cross-correlation matrix
CC(RV, t)



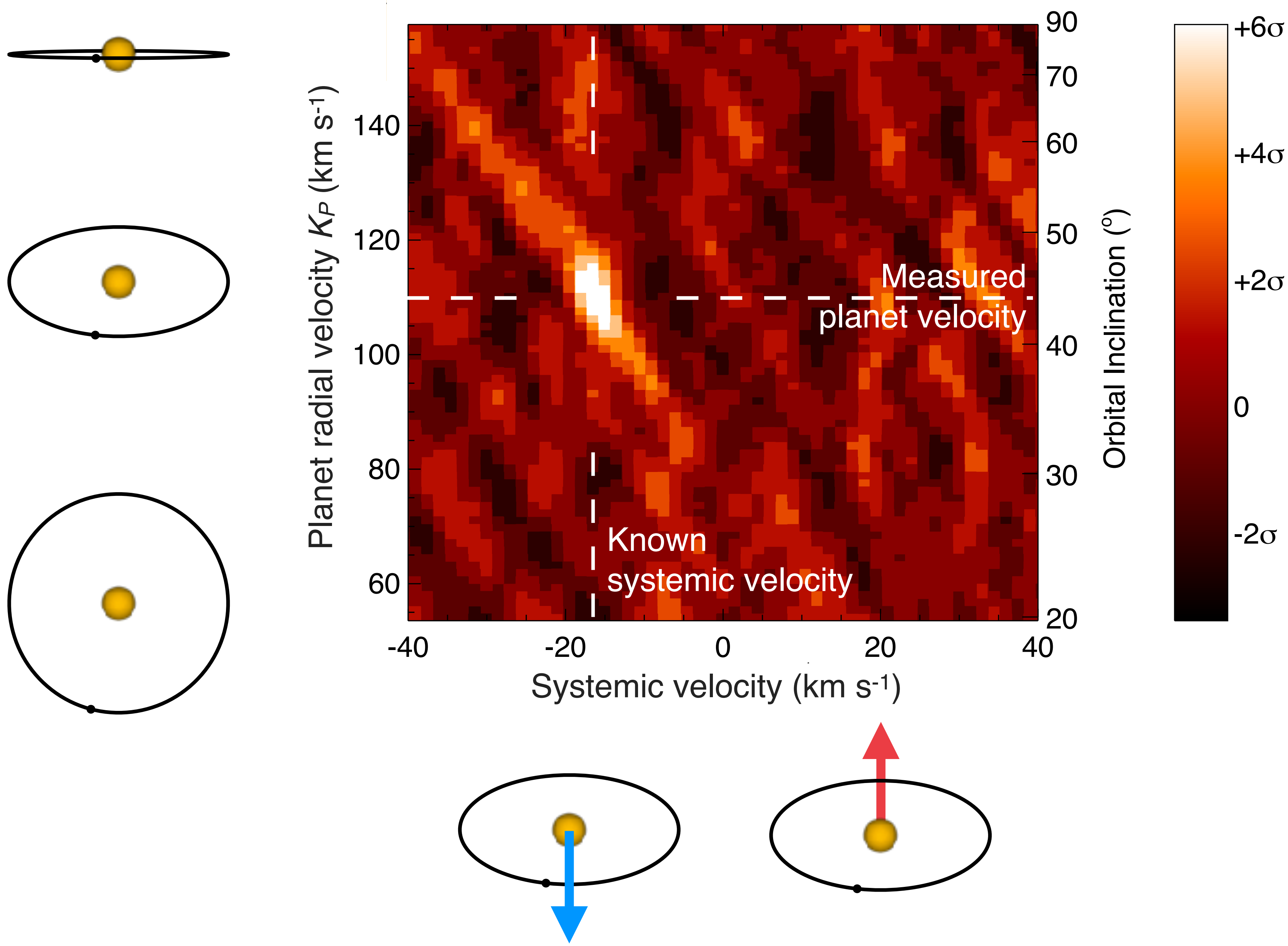
The peak CC tracks the planet radial velocity in time

Shifting and co-adding to planet rest-frame requires knowledge of planet orbital velocity (two parameters: ***slope*** and ***shift***)

Detections and velocity maps

Maximising the cross correlation value as a function of orbital parameters

2 velocities to describe a **circular orbit** ⇒ a 2-dimensional map



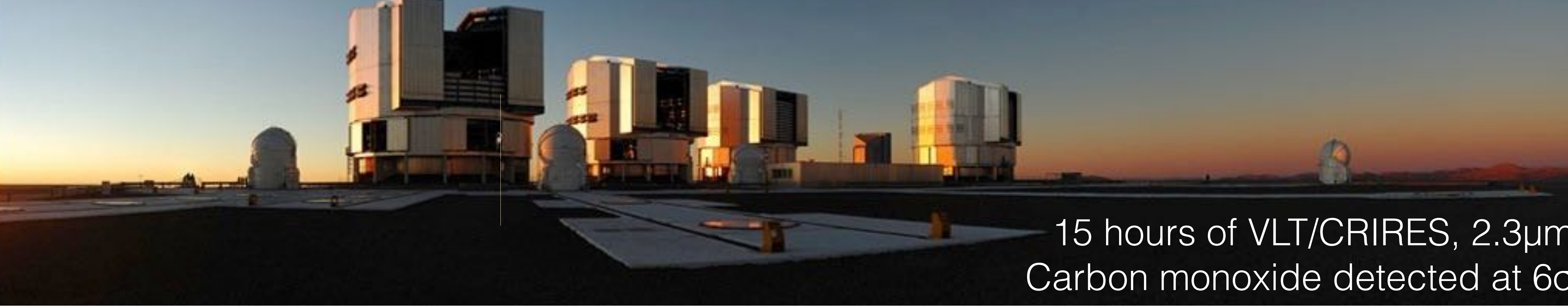
Maximum planet's orbital RV (at quadrature)

$$K_\mathrm{P} = v_\mathrm{orb}\sin(i)$$

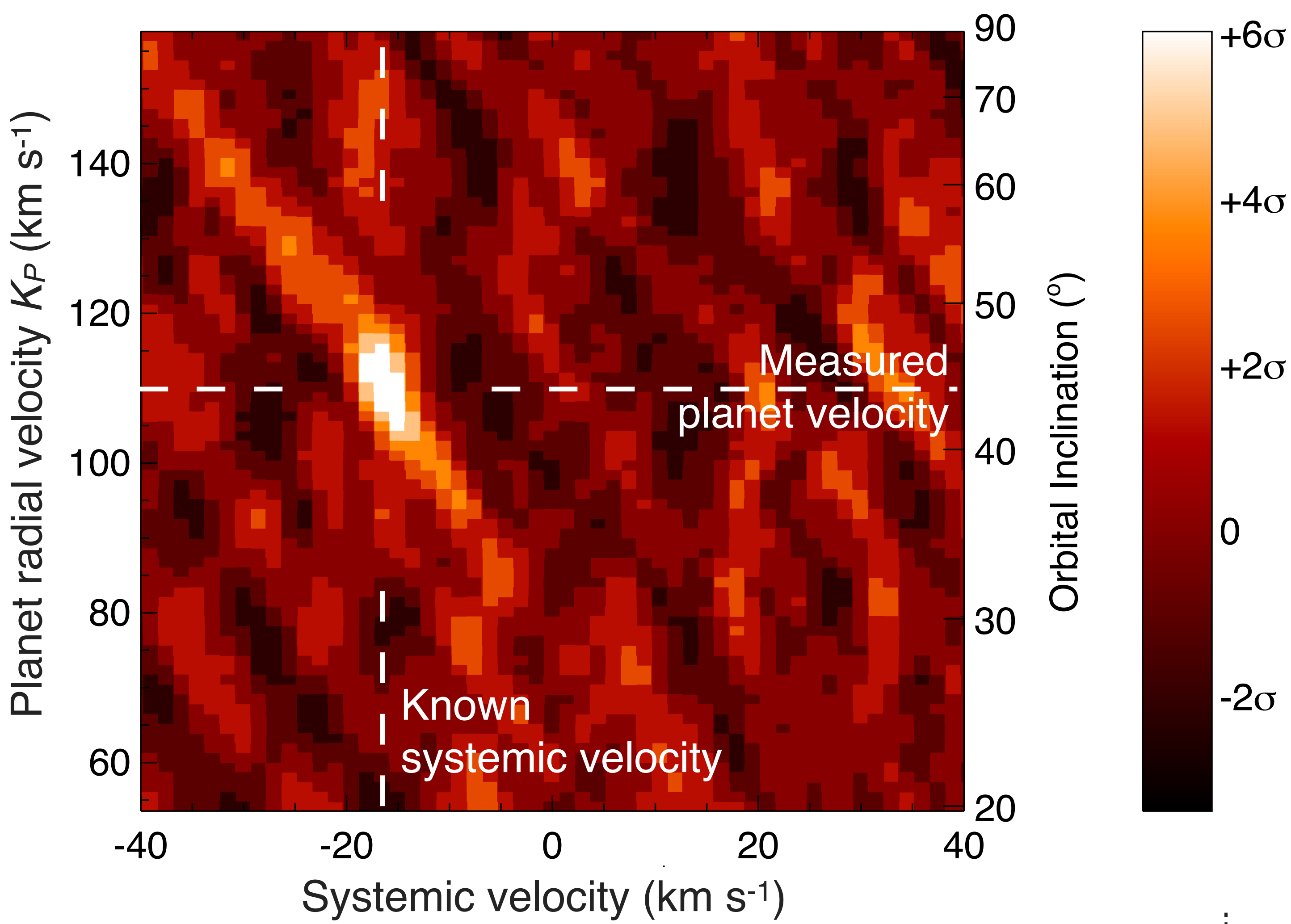
Bulk RV of the star+planet system (systemic velocity)

Star and planet as spectroscopic binaries

Pilot study: τ Boo b (Brogi+ 2012)



15 hours of VLT/CRIRES, 2.3μm
Carbon monoxide detected at 6σ



Measured:

RV semi-amplitude ratio: K_P/K_S

⇒ Mass ratio: M_P/M_S

Inferred:

Orbital inclination i

Planet mass $M_P = f(M_S)$

Uncertainties in planet mass dominated by uncertainties in stellar mass.

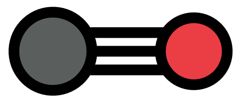
For τ Boo b:

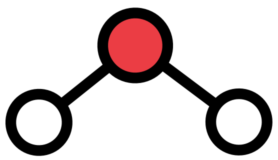
i = (45.5 ± 1.5) deg, M_P = (5.95 ± 0.28) M_{Jup}

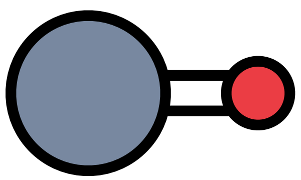
The chemical inventory at high spectral resolution

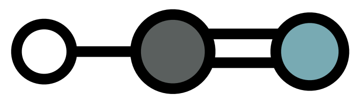
Observed sample: 30 planets
10 non-transiting, 18 transiting, 2 directly imaged

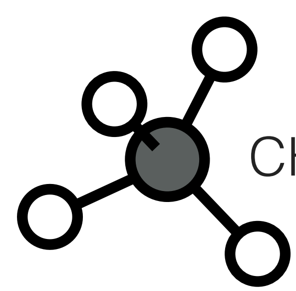
Potential sample: > 50 (currently)
15 non-transiting (K < 6.5 mag) + 40 transiting (K < 10 mag)

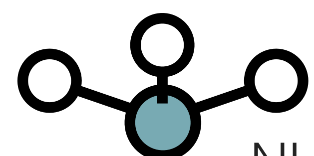
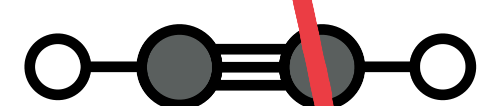
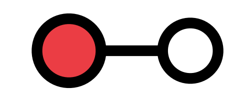
2010  CO

2013  H_2O

2017  TiO

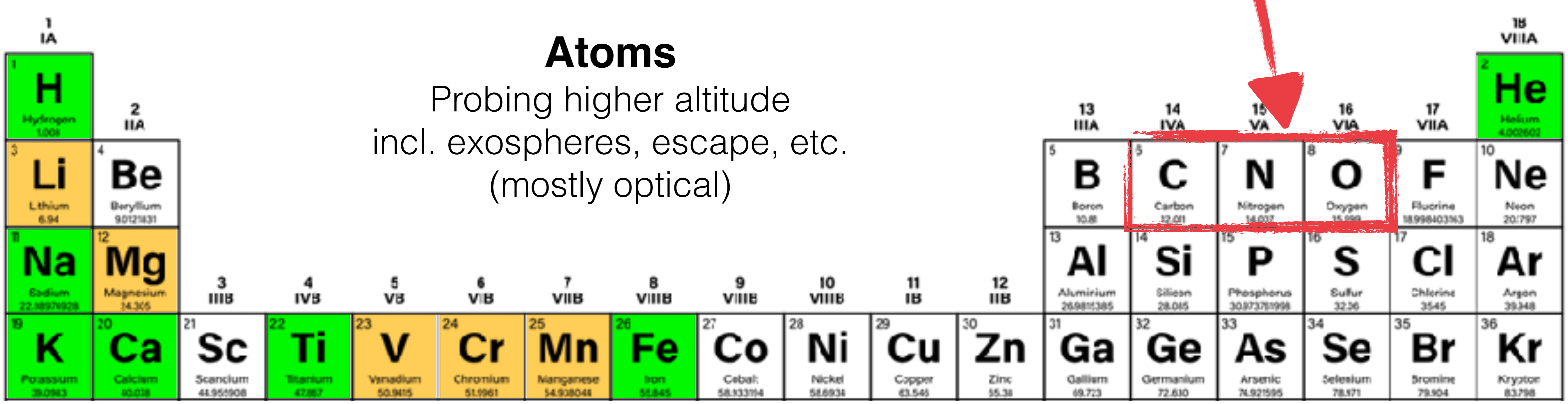
2018  HCN

2019  CH_4

2021  NH_3  C_2H_2  OH

Molecules
Constraints on T, abundances
(mostly nIR)

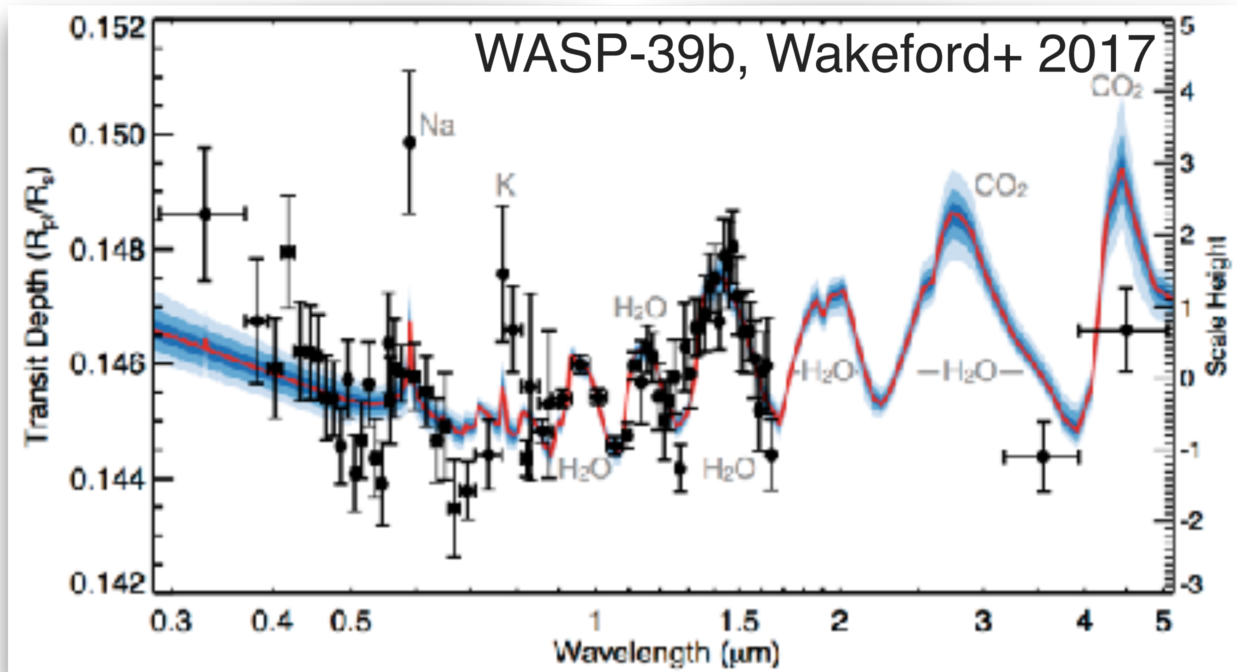
Atoms
Probing higher altitude
incl. exospheres, escape, etc.
(mostly optical)



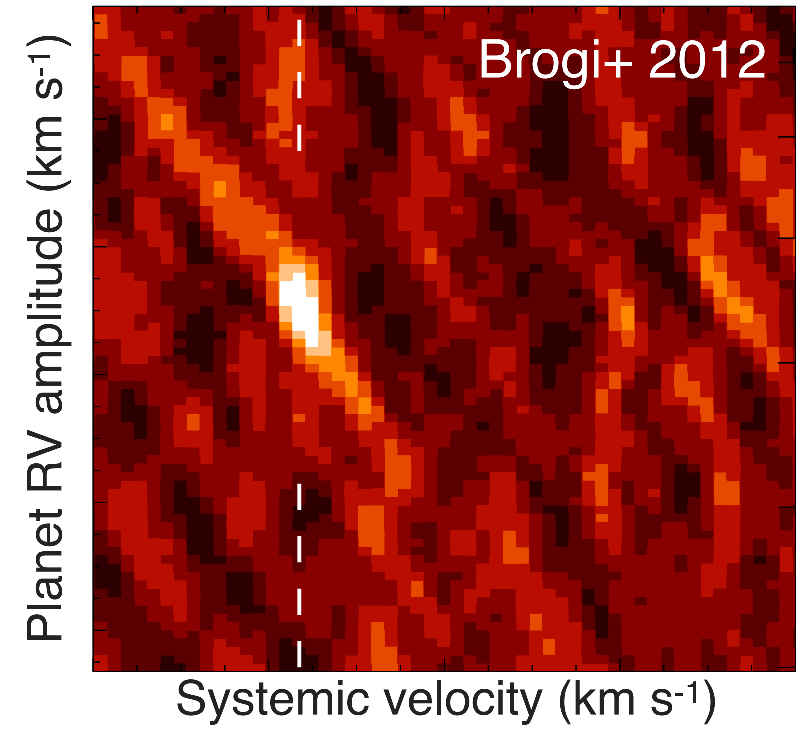
From detecting to measuring: detection significance

Quantifying the "goodness of fit" of a model is not (yet) possible at high-res

Low-res spectroscopy



High-res spectroscopy



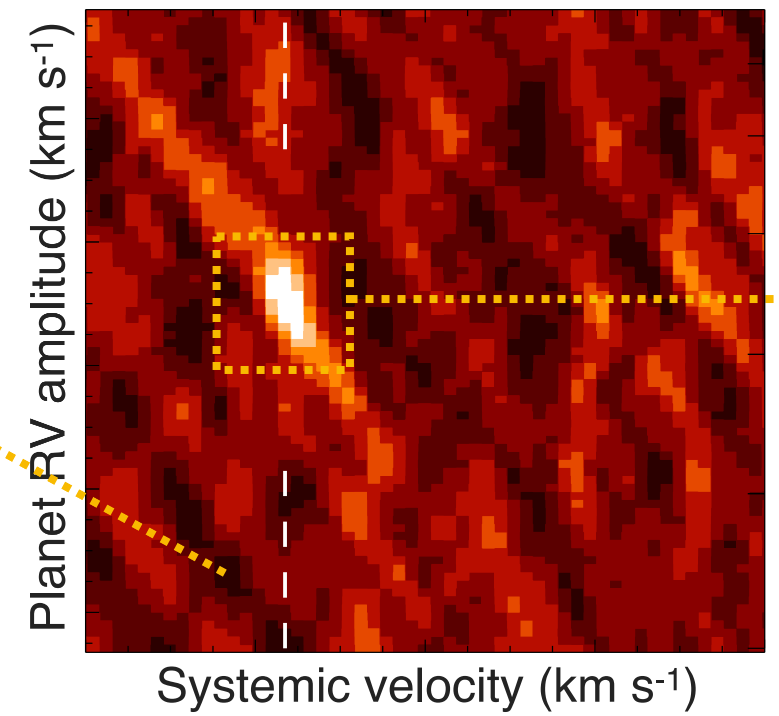
Low-res spectroscopy recovers an actual spectrum
Models can be matched to observations via chi-square fitting (also in a Bayesian way)

High-resolution spectroscopy measures a level of correlation

How do we even quantify significance?
How do we "select" models?

S/N as a proxy for detection significance

Noise: the standard deviation of all the other cross correlation values



Signal: the peak value of the total cross correlation

S/N = Peak CC / stdev(CC)

Immediate and intuitive quantity to compute

Some of the "noise" is actually auto-correlation / aliasing signal

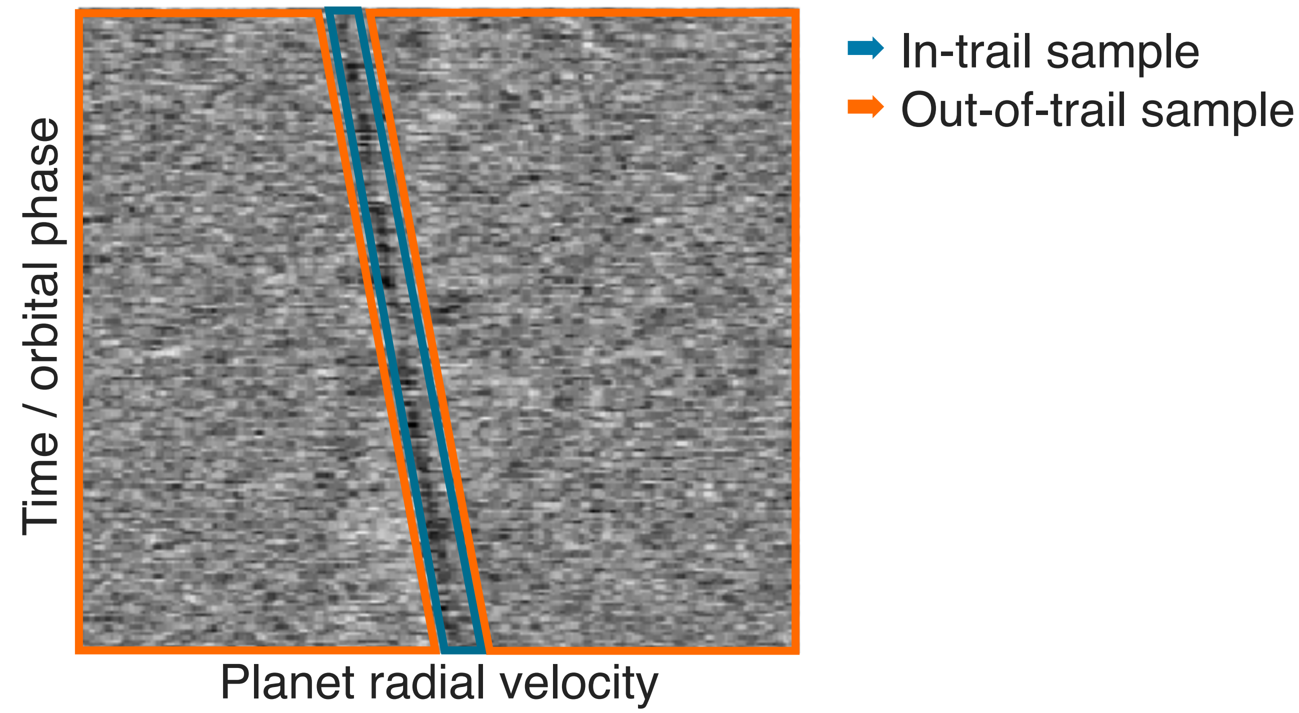
Some (V_{sys}, K_P) values will have increased noise due e.g. to residual telluric or stellar lines

At low SNR peaks can arise by just noise fluctuations

Error bars are usually defined by (V_{sys}, K_P) values corresponding to $(S/N)_{max} - 1$

Detection significance from statistical tests on the CCFs

Testing the means of the in-trail and out of trail cross-correlation values



Null hypothesis H_0: in-trail and out-of-trail sample have the same mean

Welch t-test (data samples can have ≠ size and variance) used to reject H_0
p-value ⇒ detection significance σ

Hp #1: the cross correlation values follow a Gaussian distribution (usually true)

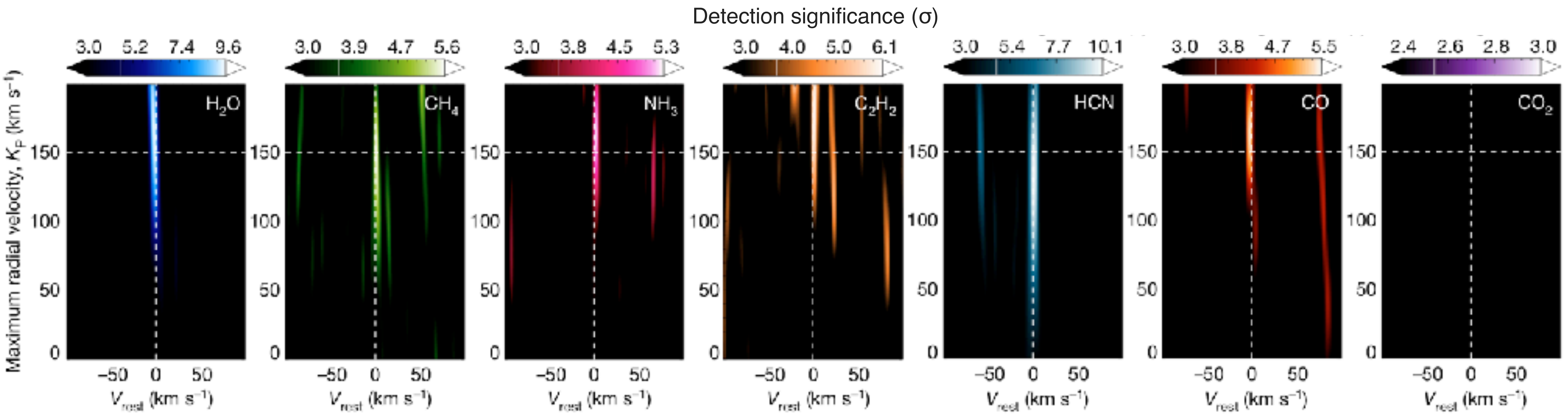
Hp #2: the cross correlation values are independent (depends on RV sampling)

Dependence on the “width” of the in-trail sample (at least 1 FWHM)

n-σ error bars can correctly be determined as $\sigma_{max} - n$

Five carbon- and nitrogen-bearing species in a hot giant planet's atmosphere

P. Giacobbe, M. Brogi, S. Gandhi et al., *Nature* **592**, 205-208 (2021)

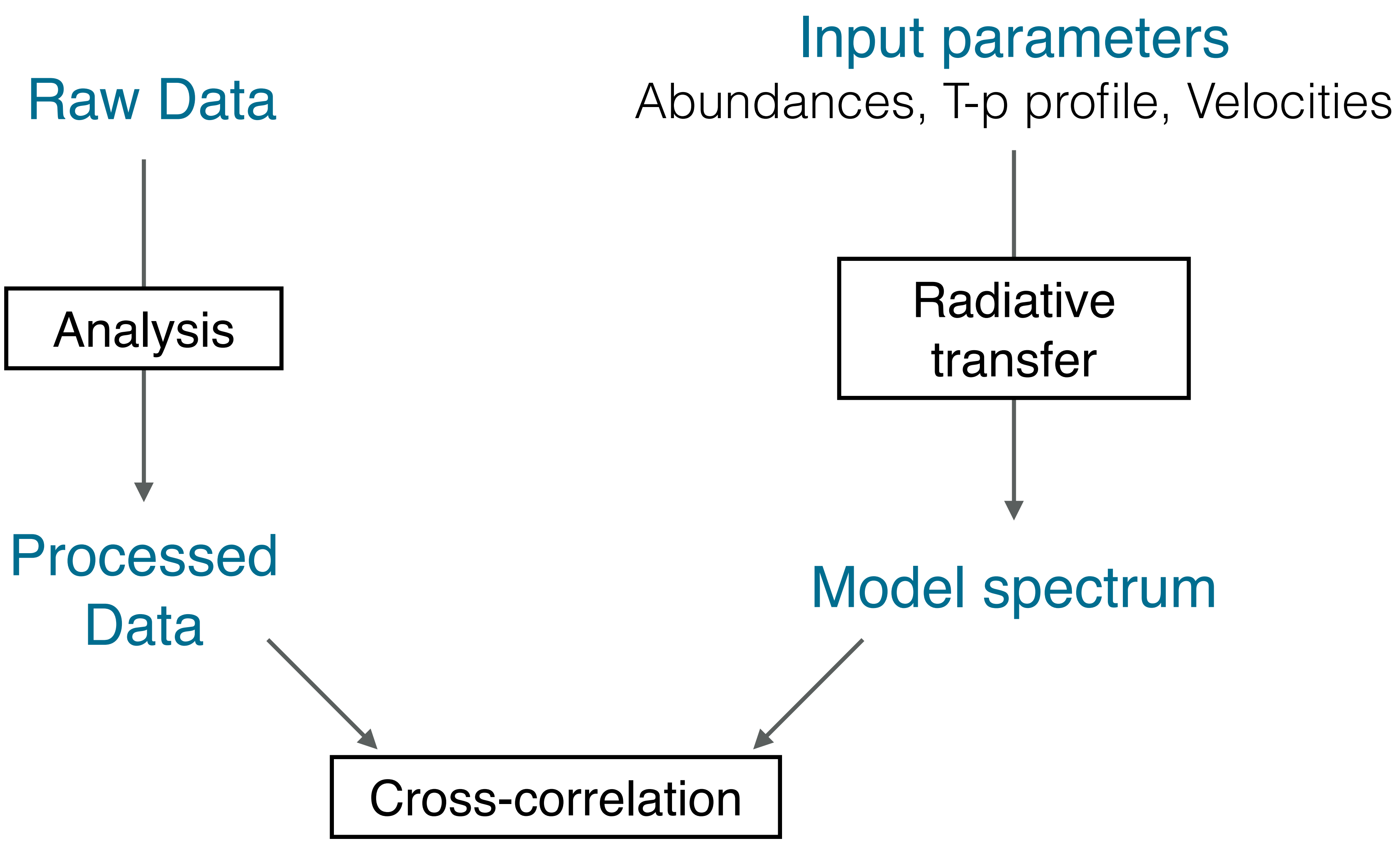


4 transits of hot Jupiter HD 209458b (1,500K) ⇒ H_2O + 5 species simultaneously detected

What does it mean for the atmosphere of HD 209548 b?

Need to move *beyond detecting* and towards *measuring*
(Just hold on for a few more slides)

From detecting to measuring: our checklist



Need to: account for any biases of the analysis

understand what's the information content at high-res

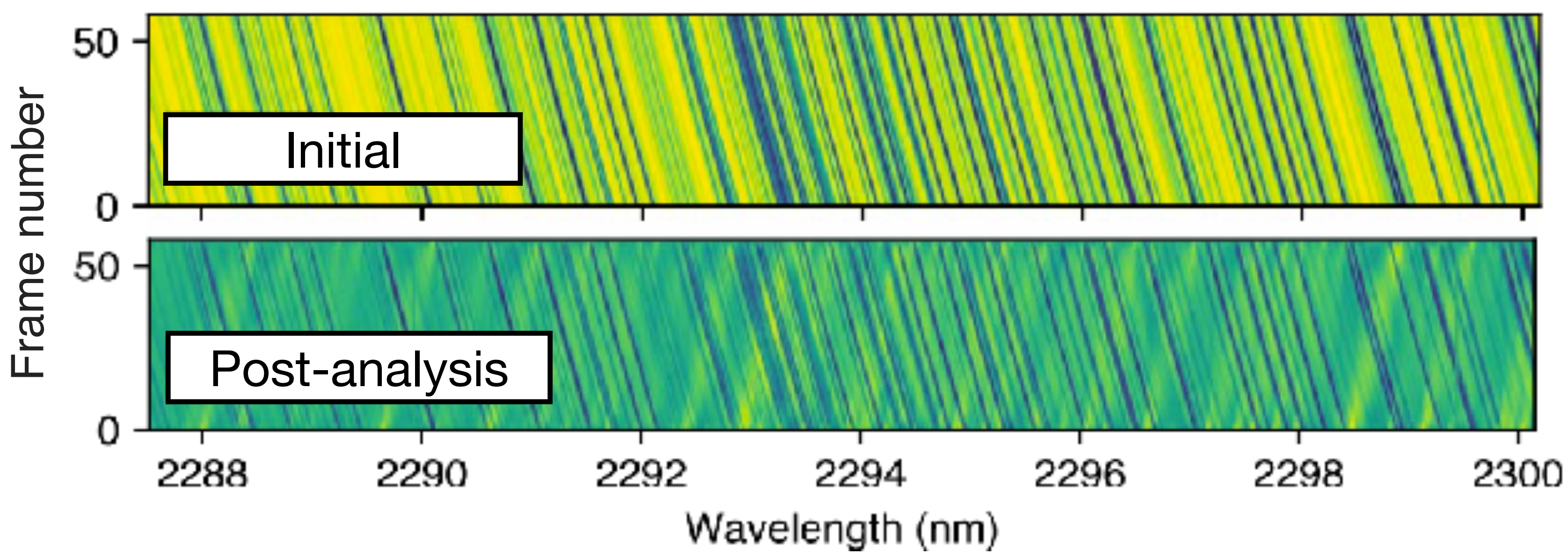
design a method to select the best model within a grid

explore the whole parameter space to understand degeneracies

The data analysis is not completely harmless

The removal of telluric and stellar lines affects exoplanet lines

Shown by Brogi & Line (2019) on simulated data - easy to see in the noiseless case



Different telluric removal techniques show different biases

see Gibson's talk

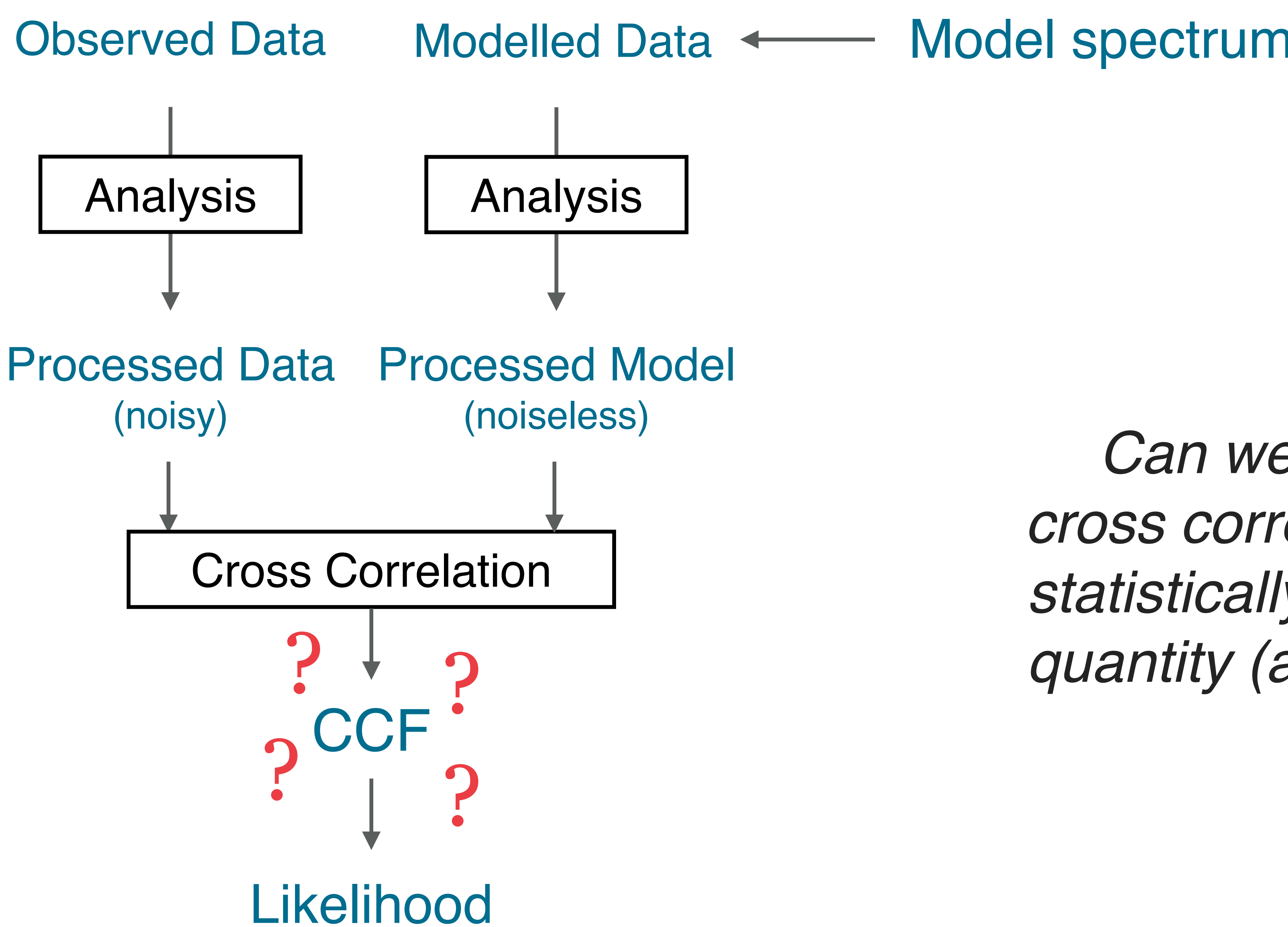
(e.g. airmass de-trending, PCA, Sysrem)

Altered shape & depth of spectral lines ⇒ biased abundances and T

Model reprocessing is **unavoidable** to obtain **unbiased measurements** from HRCCS

Model reprocessing: an unavoidable step

The model planet spectrum is injected in the data or a synthetic sequence is created



Can we translate cross correlation into a statistically meaningful quantity (a likelihood)?

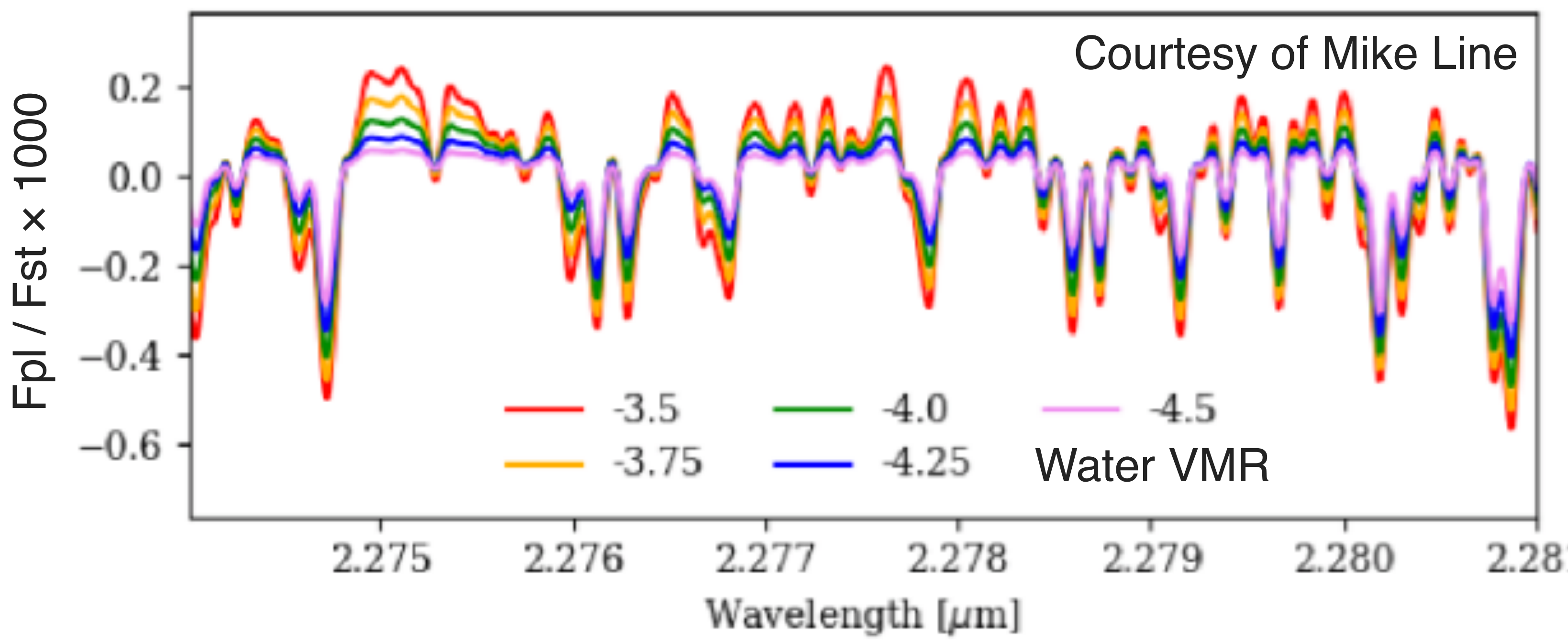
What is the information content in high-res data?

High-res data is normalised to remove stellar & telluric spectrum
(loss of absolute level of continuum in both emission and transmission)

No actual “spectrum” is visible
(no ground truth - consequences for goodness of fit)

Data is still expressed in units of stellar spectrum
(absolute line-to-line and line-to-continuum depths can still be recovered)

Line ratios and line shape change with absolute abundances and temperatures



HRCCS can measure absolute and relative abundances with the right framework

Building a likelihood function for high-res data

Brogi & Line (2019), but also Zucker (2003) and Gibson et al. (2020)

We would like to:

- use the match in line position
- distinguish between +ve and -ve correlation
- use information about line shape and amplitude

Length of array

$$\log(L) = -\frac{N}{2}\log[s_f^2 - 2R(s) + s_g^2].$$

Data Variance — Cross-covariance — Model Variance

Cross correlation

$$C(s) = \frac{R(s)}{\sqrt{s_f^2 s_g^2}}.$$

logL contains the **model** and **data variances** s^2

(it accounts for the amplitude of lines)

logL contains the **cross covariance** R

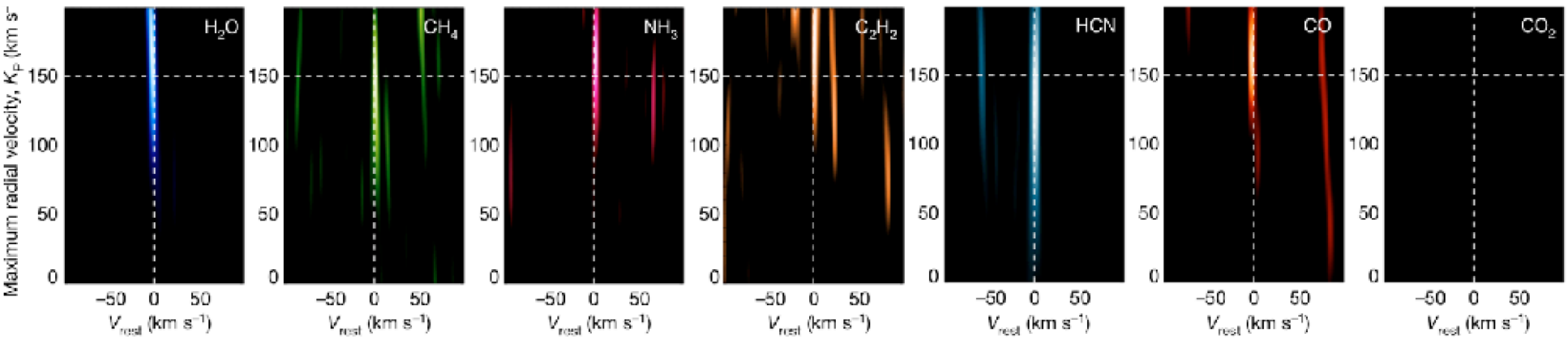
(not normalised - accounts for amplitude of lines)

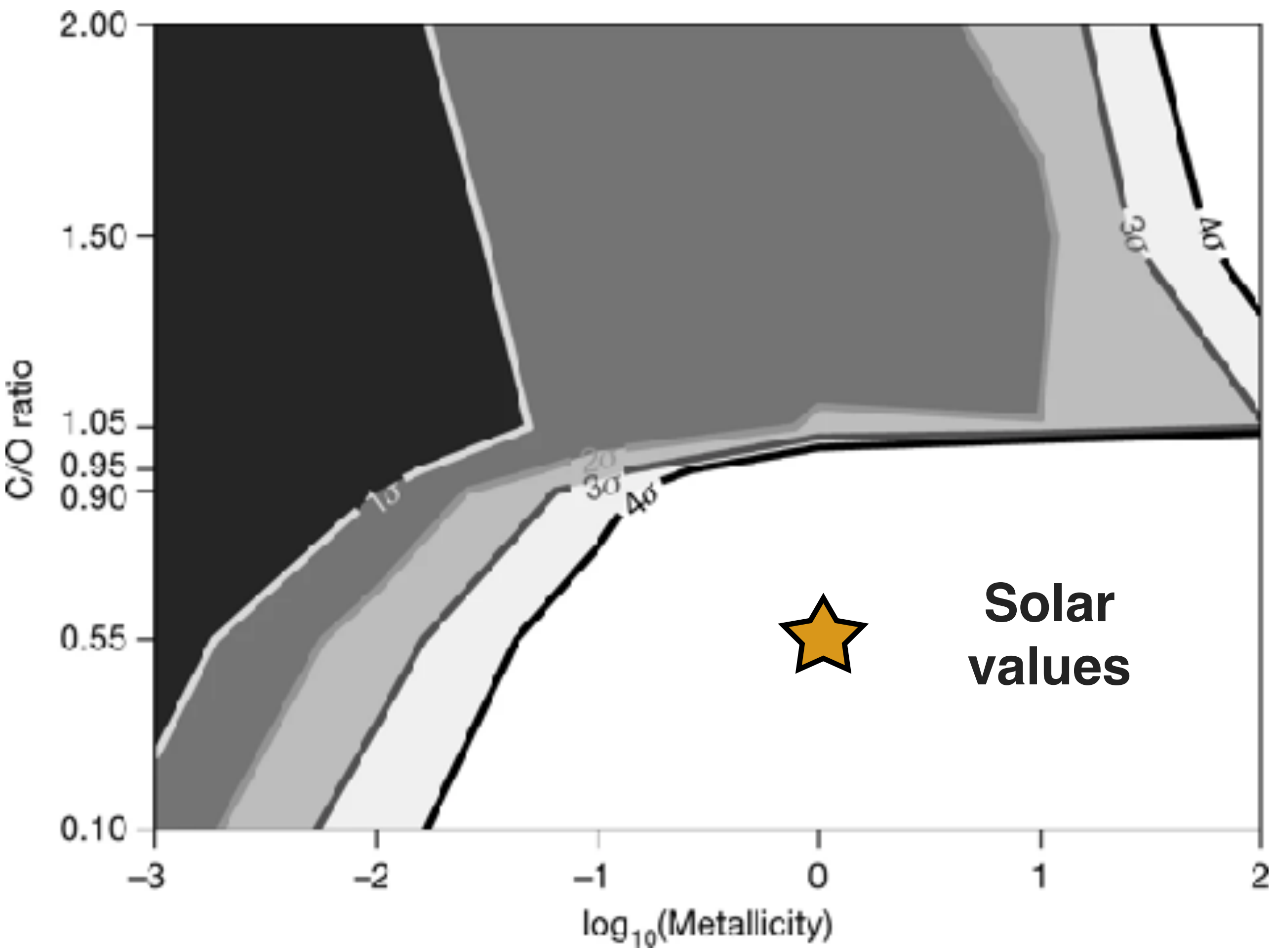
(penalises anti-correlation - accounts for emission/absorption)

Model selection through likelihood-ratio tests

Exploring a grid of equilibrium models by varying metallicity and C/O

Giacobbe, Brogi, Gandhi et al., *Nature* (2021)





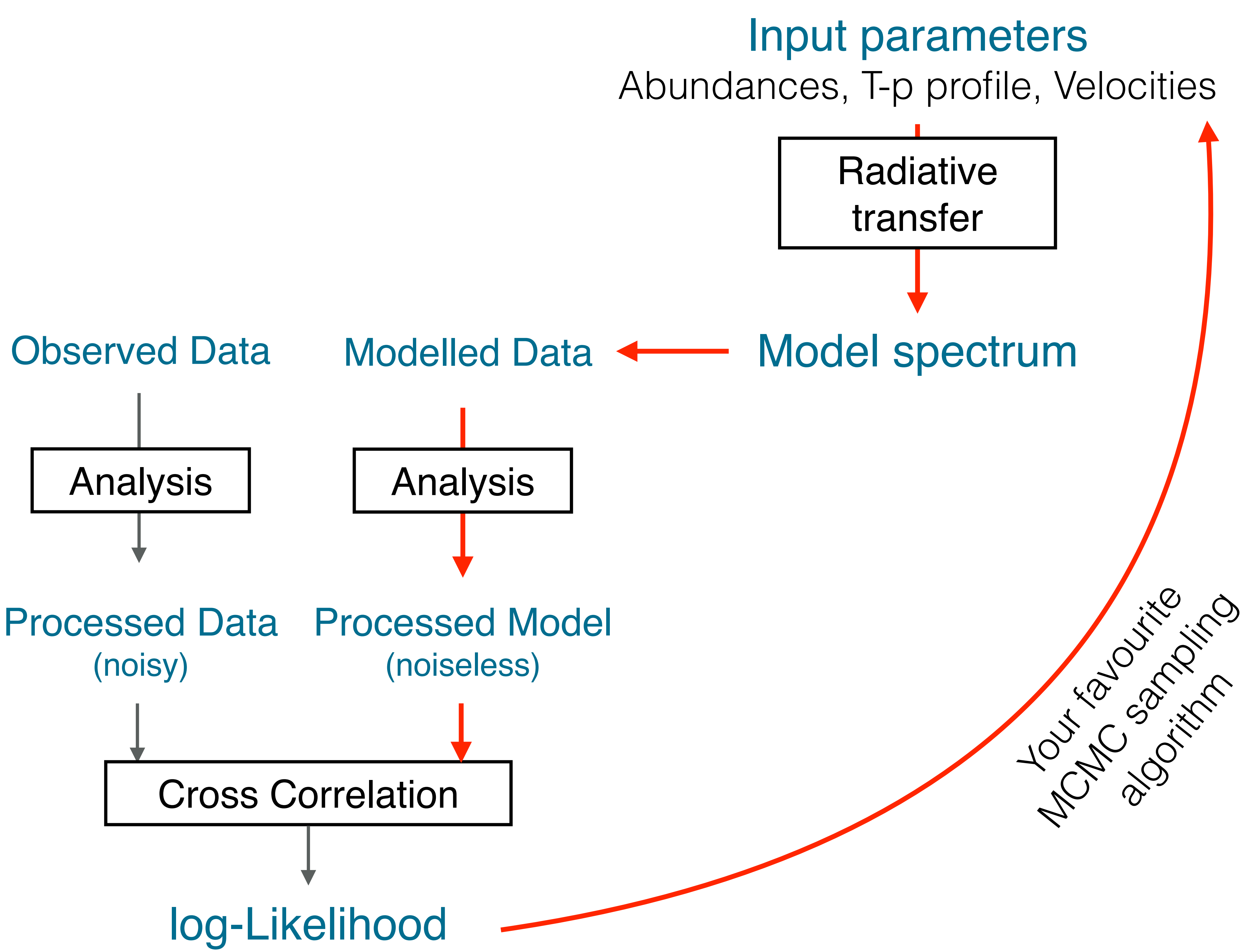
Addition of clouds (with LR parameters) highly favoured (17 sigma)

Disequilibrium chemistry disfavoured

HD 209458b formed beyond the snow line and subsequently migrated w/o accreting ice planetesimals

Running a Bayesian retrieval on HR data

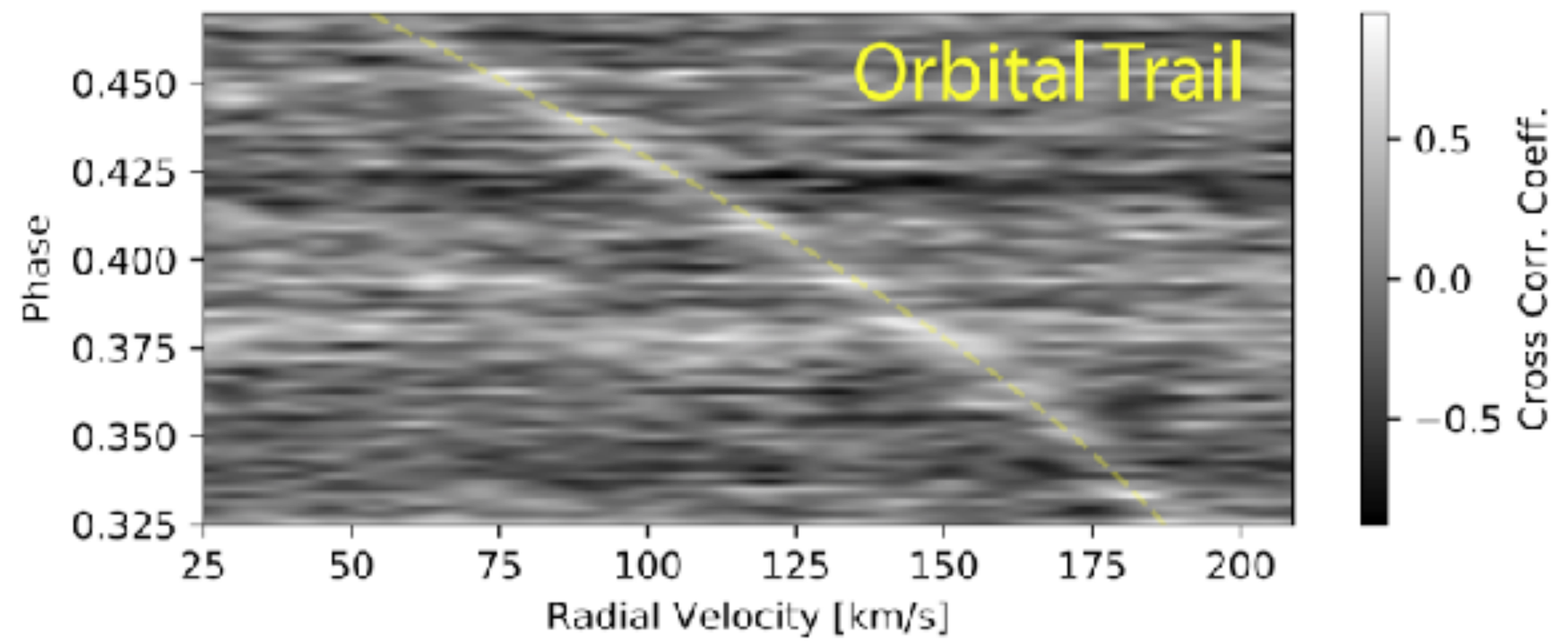
Letting the data “inform” model selection to explore full parameter space

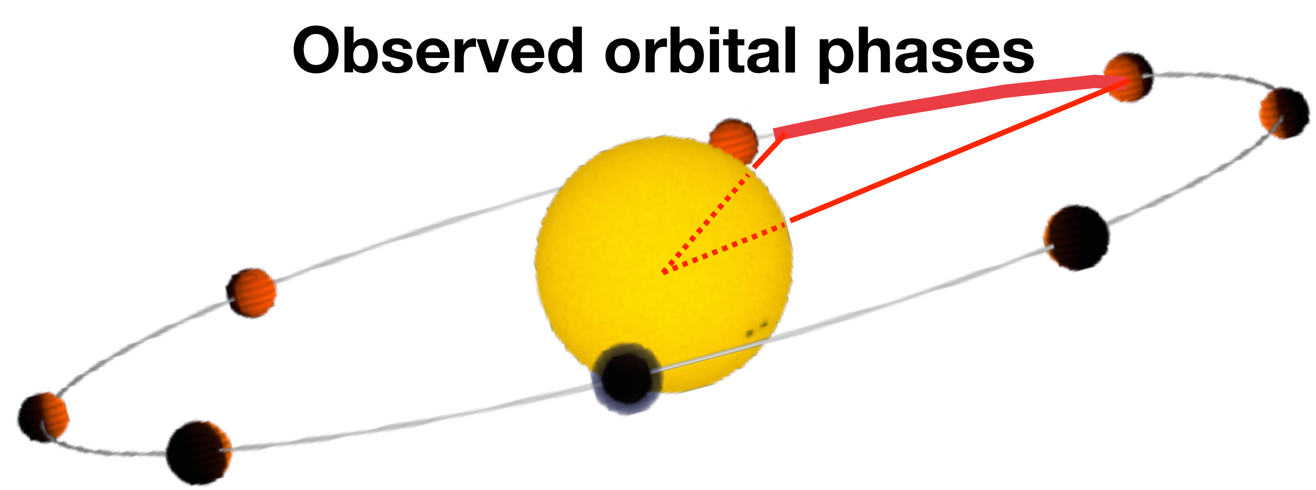


The emission spectrum of WASP-77 A b

Line, Brogi, Gandhi et al., *Nature*, accepted (coming soon!)

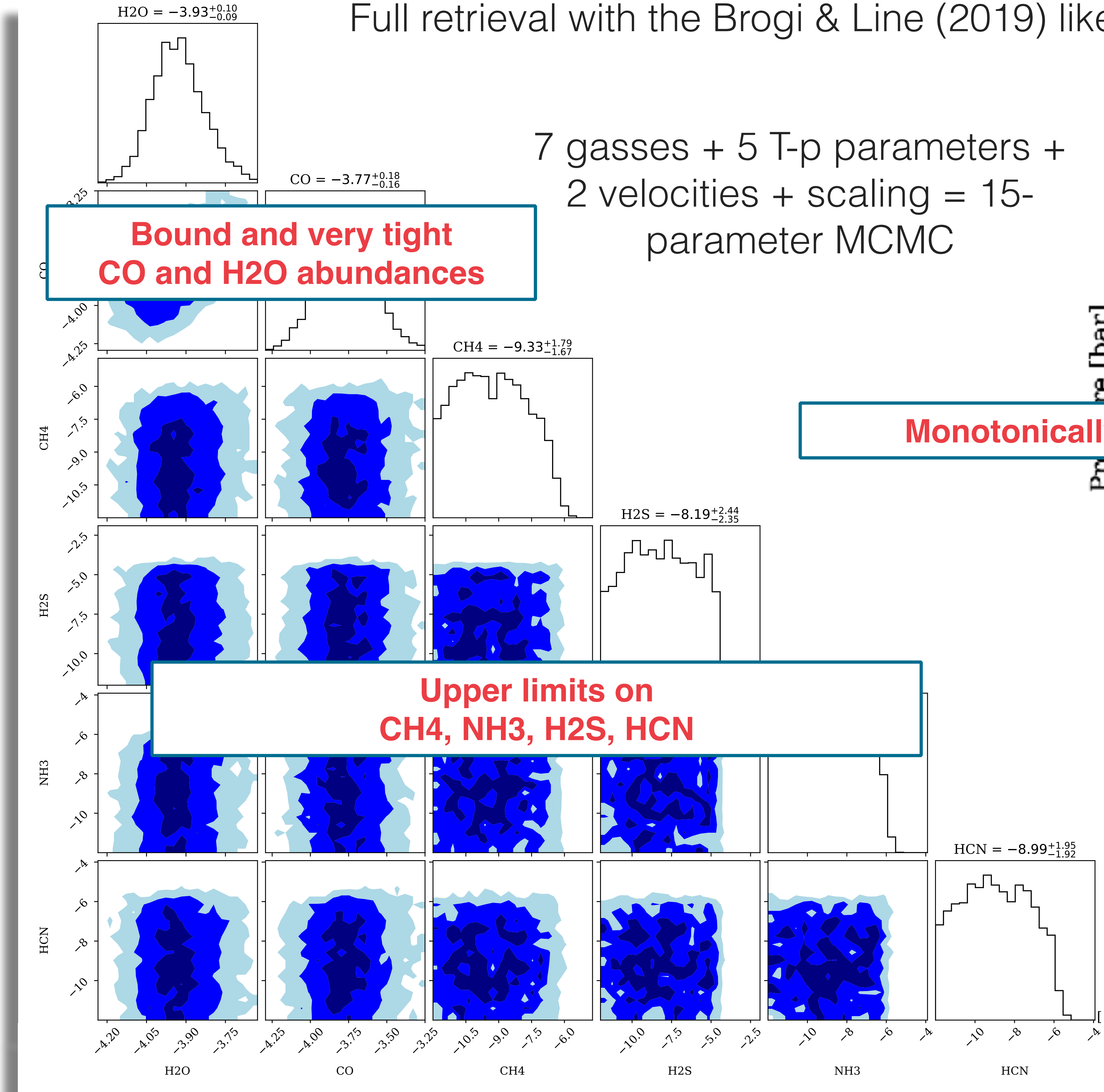
R~45,000
1.45 - 2.45 μm simultaneously
Silicon immersion grating
(keeping the instrument compact)





Achieving “solar system” precisions in the chemistry

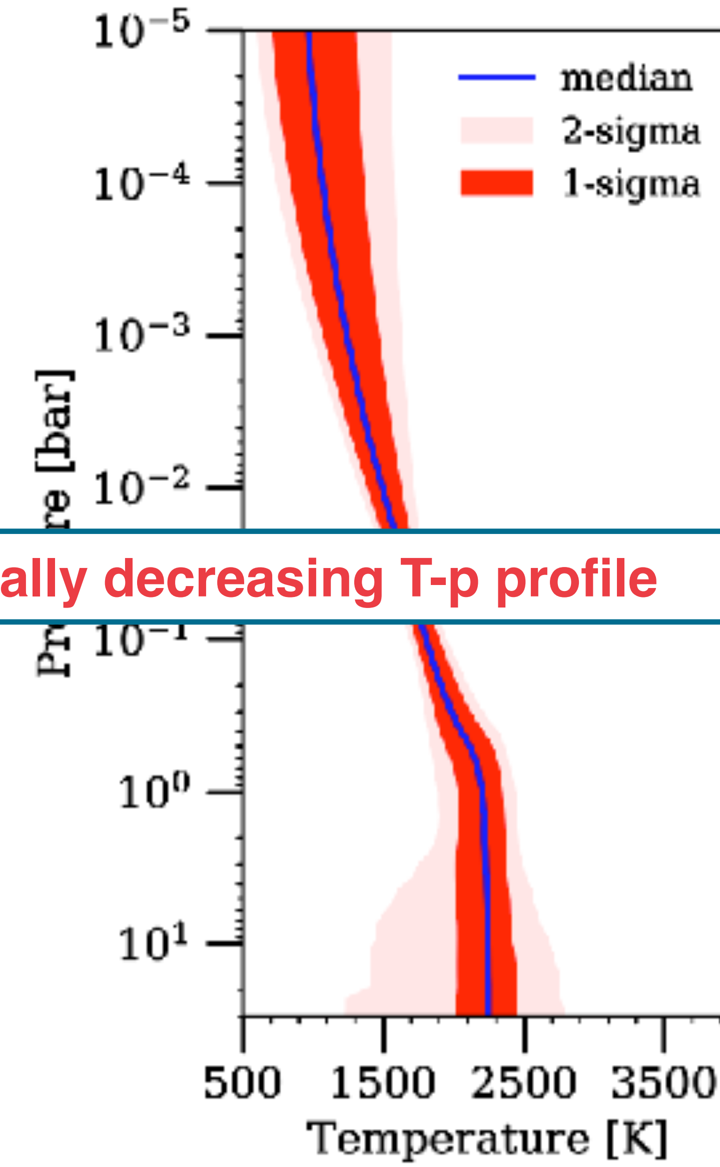
Full retrieval with the Brogi & Line (2019) likelihood



7 gasses + 5 T-p parameters + 2 velocities + scaling = 15-parameter MCMC

Bound and very tight CO and H2O abundances

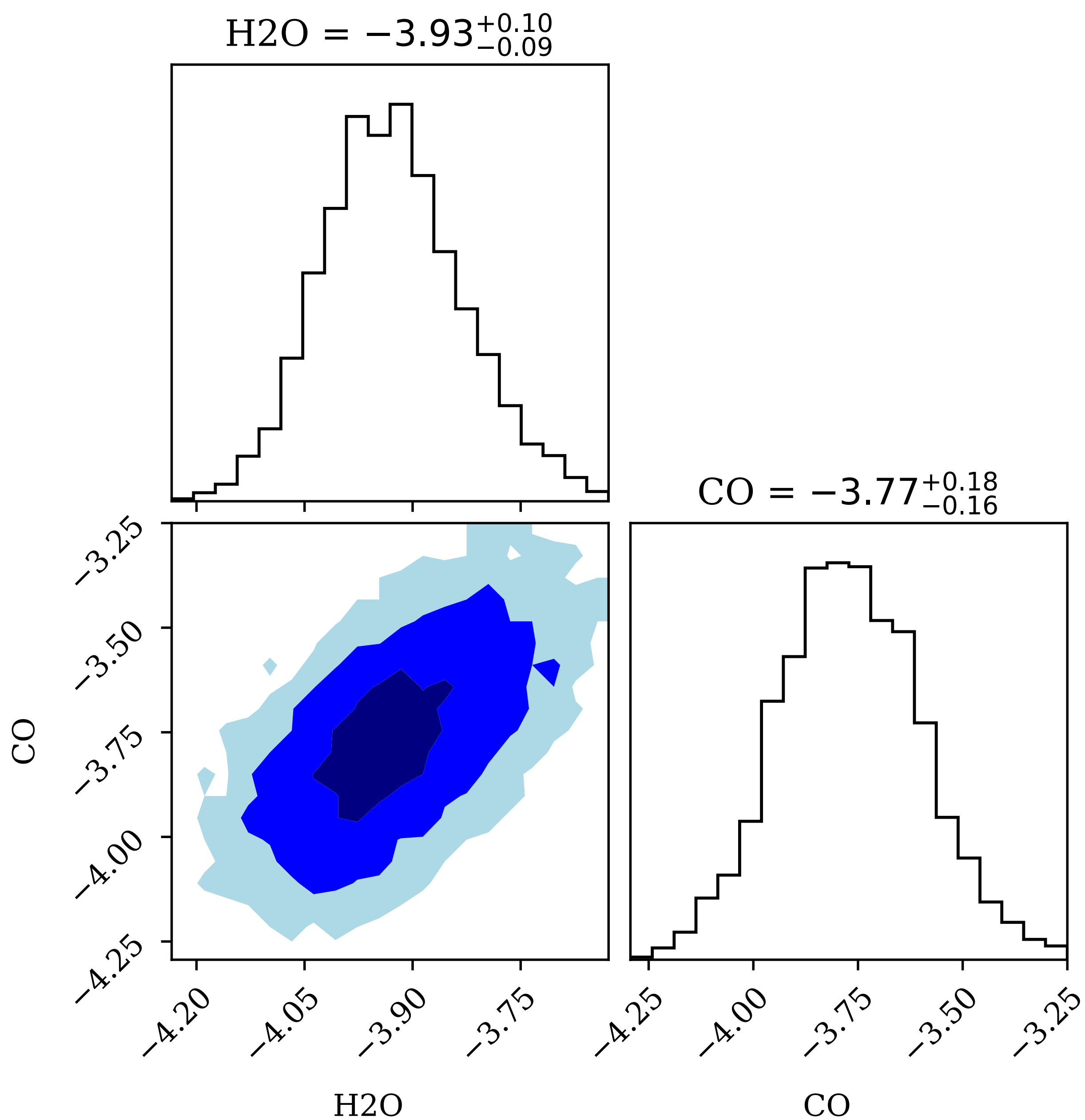
Upper limits on CH4, NH3, H2S, HCN



Monotonically decreasing T-p profile

Achieving JWST precisions in the chemistry

0.1-0.2 dex precision in **absolute abundance** for H2O and CO



Validated independently with
2 retrieval frameworks
CHIMERA (Line)
GENESIS/HyDRA-H (Gandhi)

Accuracy tested by changing:
Data processing
T-p parametrisation
Choice of line lists

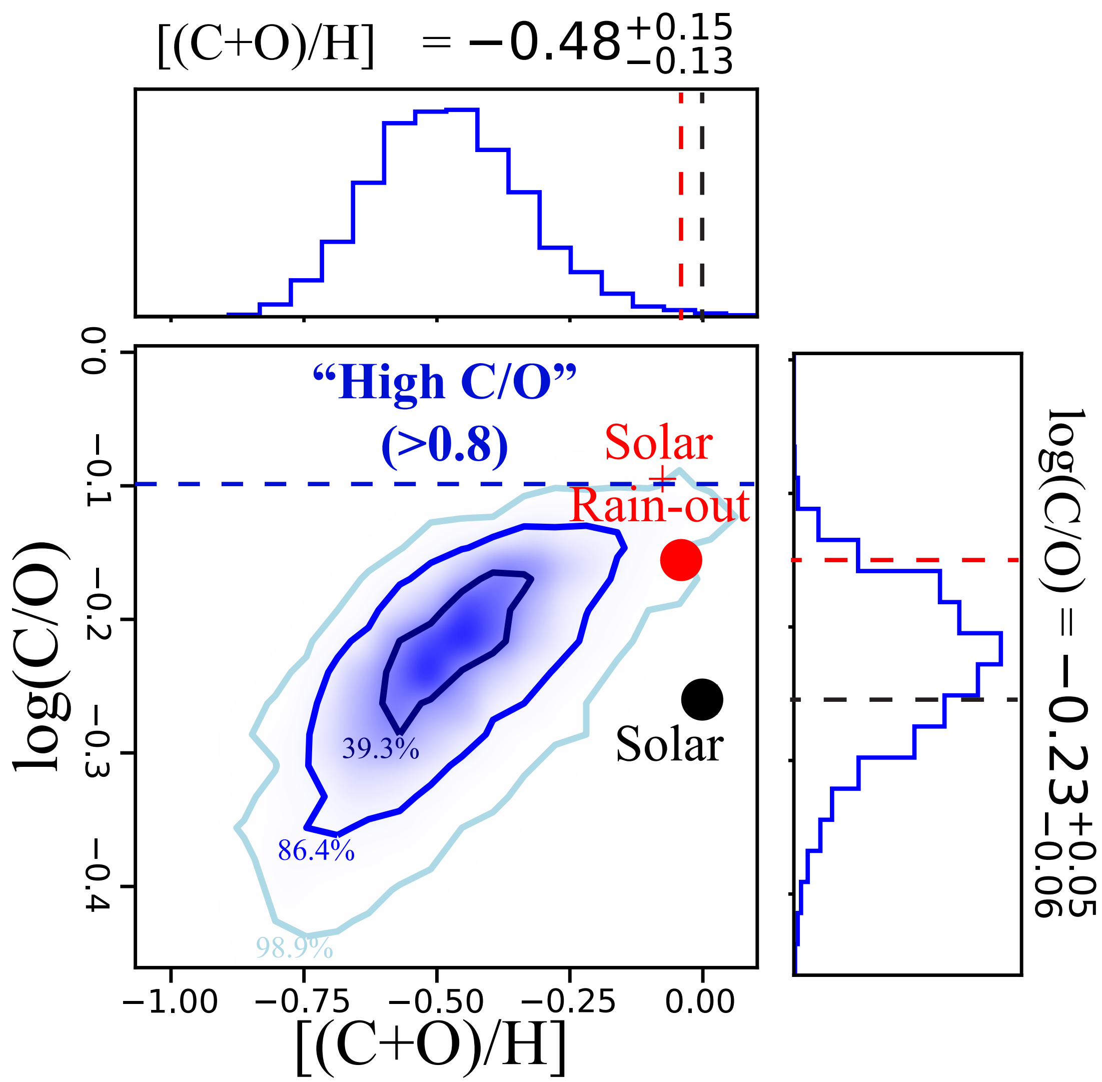
Computationally intensive
1 model evaluation =
5-10s on a single CPU core
(GPU+parallel computing)

What can we do with such precision?

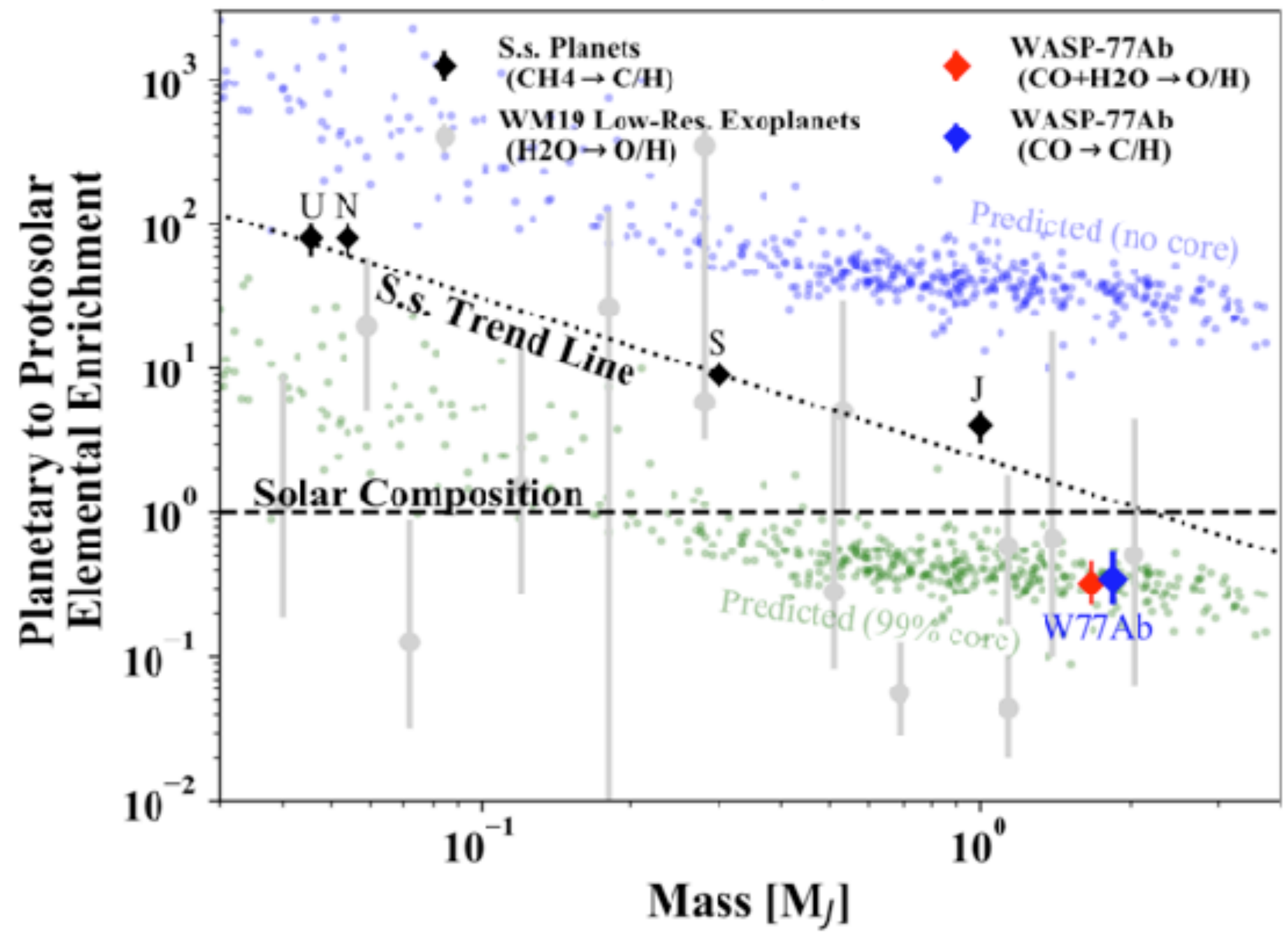
Constraints in the chemistry

WASP-77 A b has sub-solar metallicity but solar C/O

CO+H2O ⇒ Metallicity, C/O



Mass-metallicity relation



C/O & metallicity of hot Jupiters can be connected to formation and early evolution scenarios

2021 has seen three measurements of C/O & metallicity (Giacobbe+21; Line+21; Pelletier+21 - see talk!)

A joint analysis of low- and high-resolution spectra

Low res information

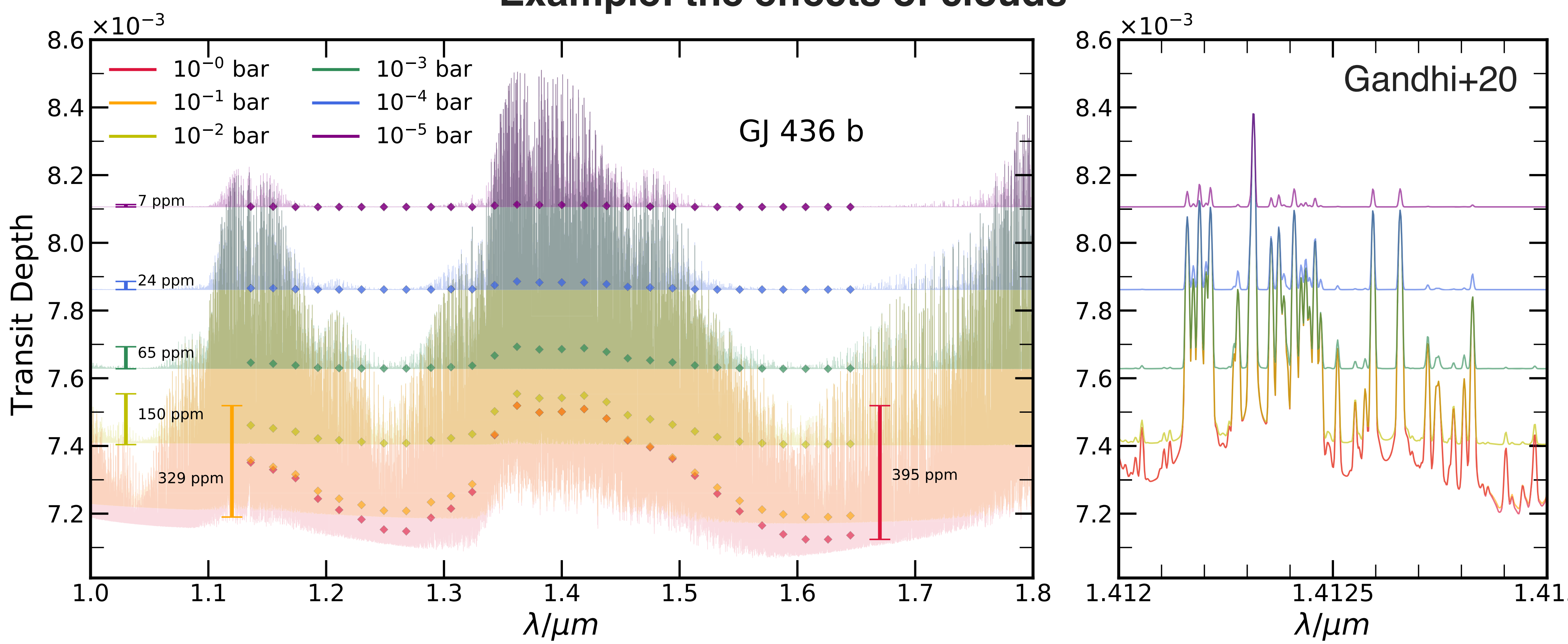
Broad-band variations (the “wiggles” in the spectrum)
Overall transit depth of planet flux (the “level of continuum”)
see Natasha’s and Ryan’s lecture on Tuesday

High-res information

Line-to-line variations, line-to-continuum variations, line shape
see Sid’s lecture on Tuesday

Independently encoding opacity sources, temperature vs pressure, gravity, etc.

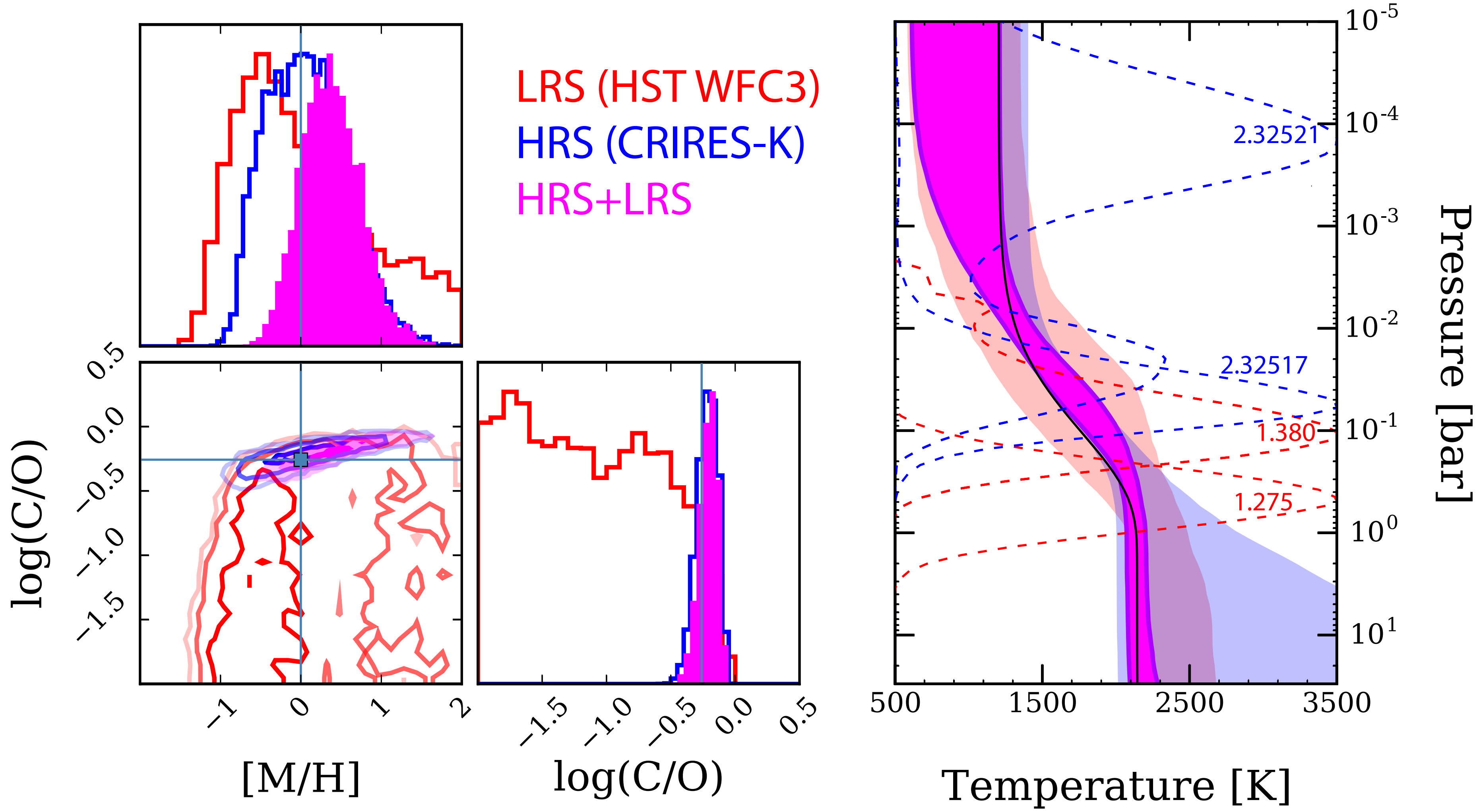
Example: the effects of clouds



Combining LR and HR within the likelihood framework

Brogi & Line (2019): simulated HST + VLT/CRIRES observations
Noise level of current observatories (1 eclipse / 5 hours)

total logL = logL (low-res) + logL (high-res)



Published LR+HR on real data are still rare
(Piskorz+18, Gandhi+ 2019, Gandhi+ in prep.)

Why should we even care with JWST incoming and such high-quality ground-based observations?

4 good reasons to combine low- and high-resolution

Robustness

Independent method, information, and instruments
Test for validity of model assumptions

Errors

Confidence intervals shrink across the whole parameter space

Reducing biases and degeneracy

Aerosols and 3-dimensional effects have different impact on HR and LR

Optimisation

Use the predictive capability of a HR dataset
to inform JWST observations

Ground and space observations are in synergy, not in competition