Spectral Retrieval
(or, I have a spectrum-- now what?)

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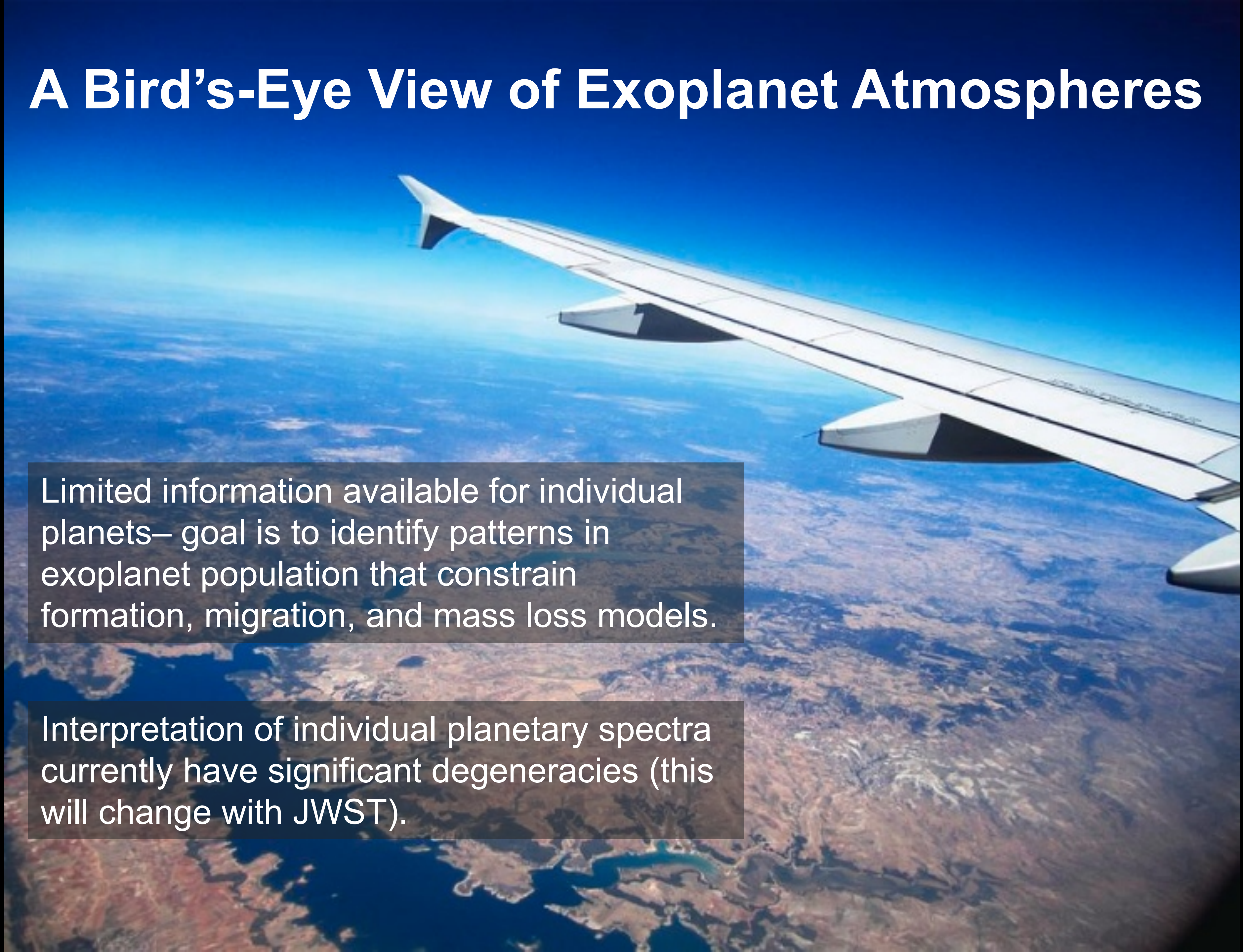
A Bird’s-Eye View of Exoplanet Atmospheres



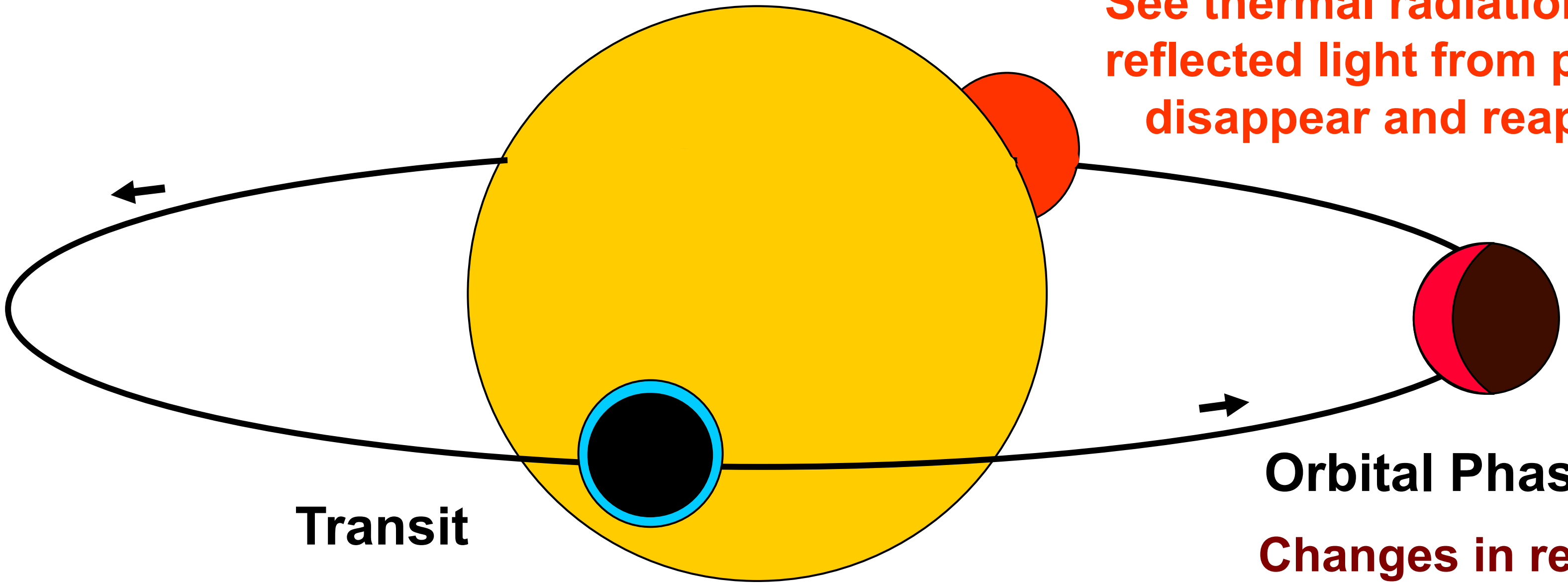
Limited information available for individual planets– goal is to identify patterns in exoplanet population that constrain formation, migration, and mass loss models.

Interpretation of individual planetary spectra currently have significant degeneracies (this will change with JWST).

Observations of Eclipsing Systems Allow Us to Characterize Exoplanet Atmospheres

Secondary Eclipse

See thermal radiation and reflected light from planet disappear and reappear



Orbital Phase Variations

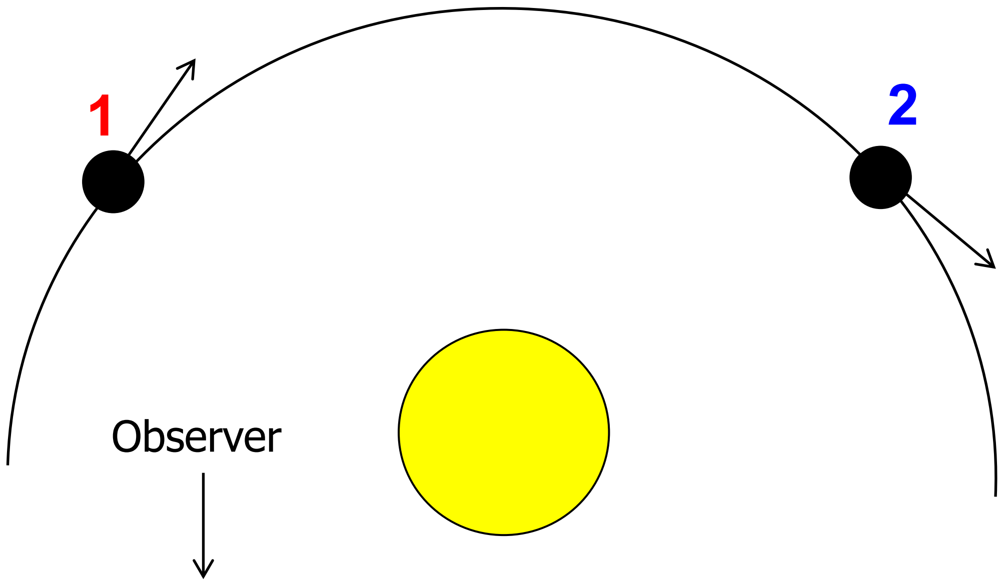
Changes in reflected/emitted light spectrum as function of orbital phase.

Transit

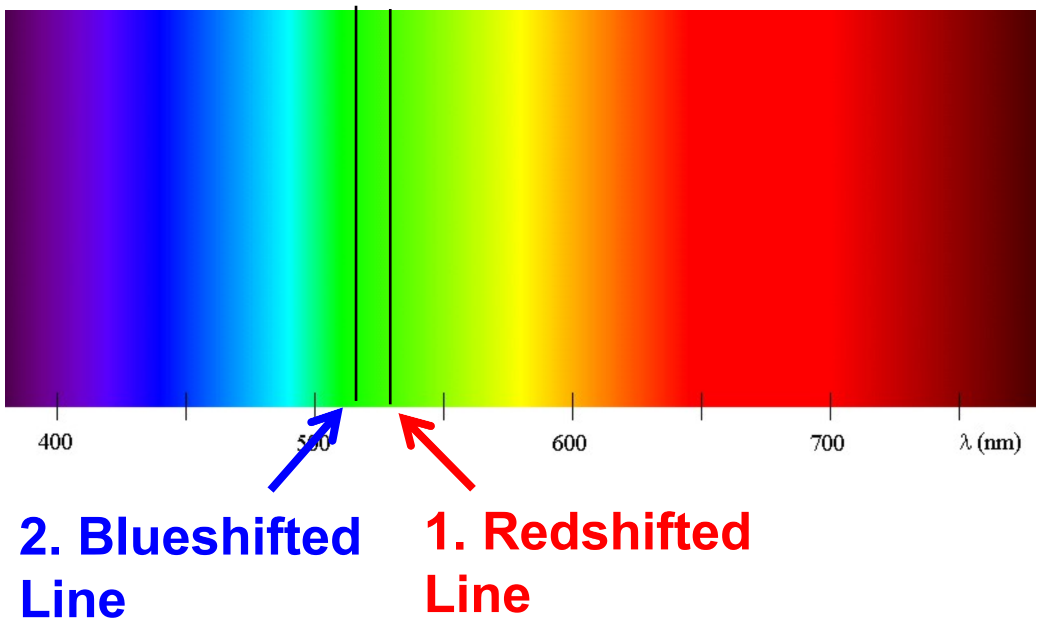
See radiation from star transmitted through the planet's atmosphere

Reviews of observational literature for transiting planets: Madhusudhan et al. (2014), Deming & Seager (2017)

Can Also Use Doppler Shift to Separate Light from Planet vs Star



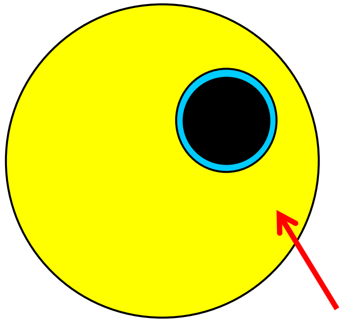
Stellar spectrum also contains a **component of planetary emission** with absorption lines that undergo large radial velocity shifts.



Examples (including both transmission and emission spectroscopy): Birkby et al. (2013), de Kok et al. (2013), Brogi et al. (2012, 2013), Lockwood et al. (2014)

Can combine with low resolution secondary eclipse data (e.g., Brogi & Line 2017).

Scaling Laws for Transiting Planets

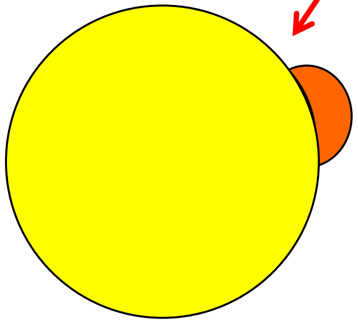


Absorption During Transit (%):

$$\frac{2R_P}{R_*^{\,2}}\left(\frac{kT_p}{\mu g}\right)$$

mean molecular weight

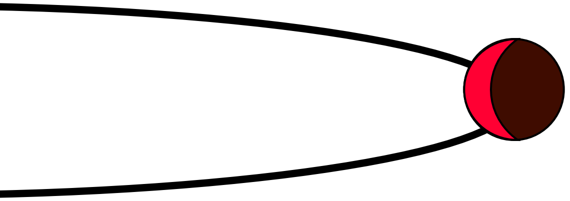
M stars preferred!



Secondary Eclipse Depth (IR):

$$\left(\frac{R_p}{R_*}\right)^2\left(\frac{T_p}{T_*}\right)$$

Three ways to decrease signal: smaller planet, lower temperature, heavier atmosphere.



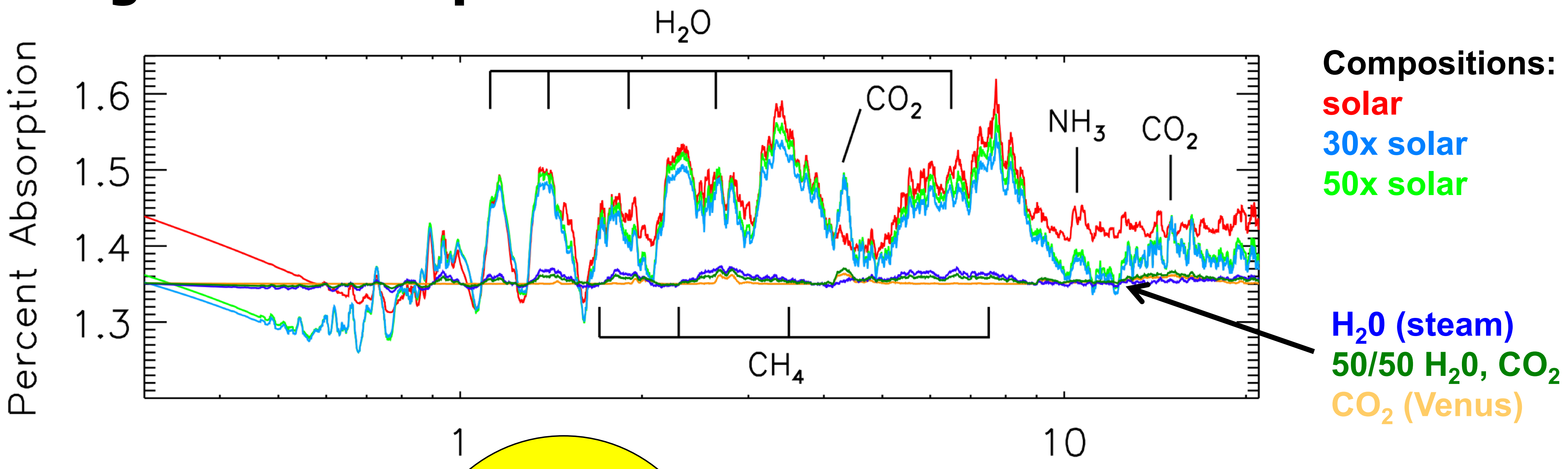
Orbital Phase Variations:

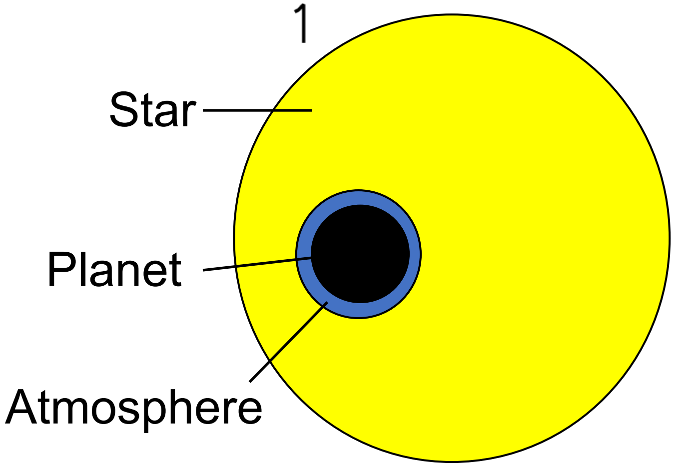
Always less than secondary eclipse depth for planets on circular orbits.

Doppler Shift:

Depends on strength of absorption/emission lines (pressure-temperature profile, clouds both important)

Transmission Spectroscopy Measures Mean Molecular Weight of Atmosphere

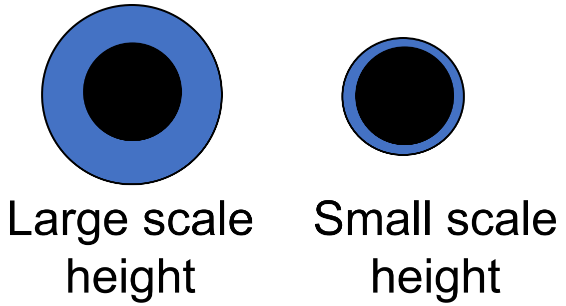




Scale Height

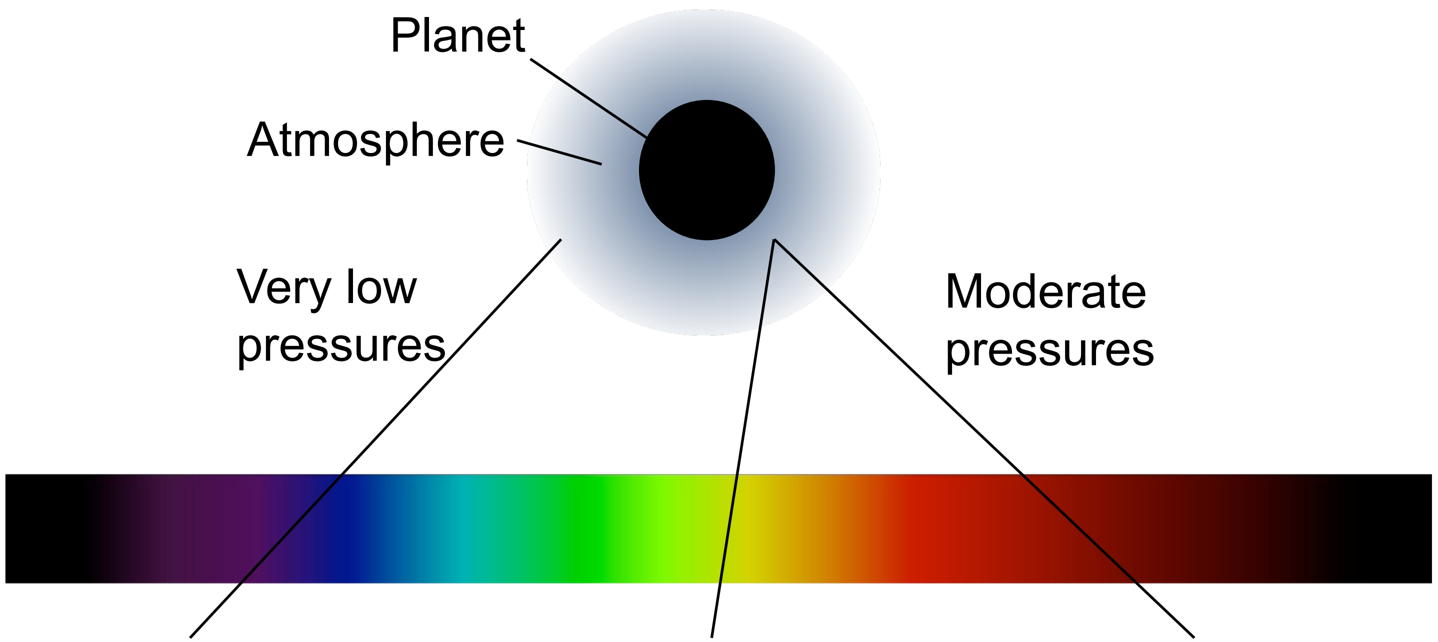
$$H = \frac{kT}{\mu g}$$

mean molecular weight



Miller-Ricci & Fortney (2010)

A Transmission Spectroscopy View of Hot Jupiters

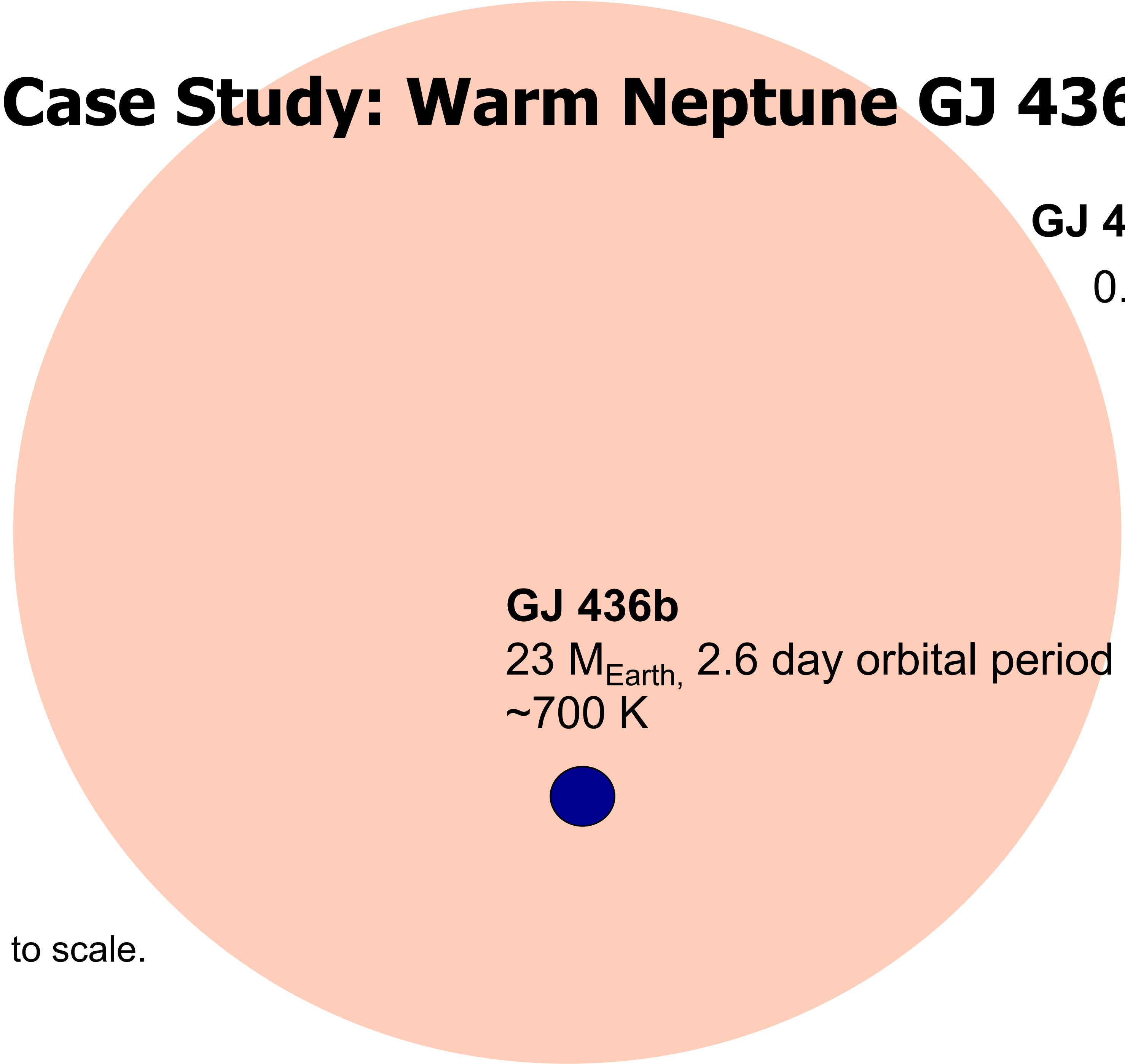


Secondary eclipse, phase variations

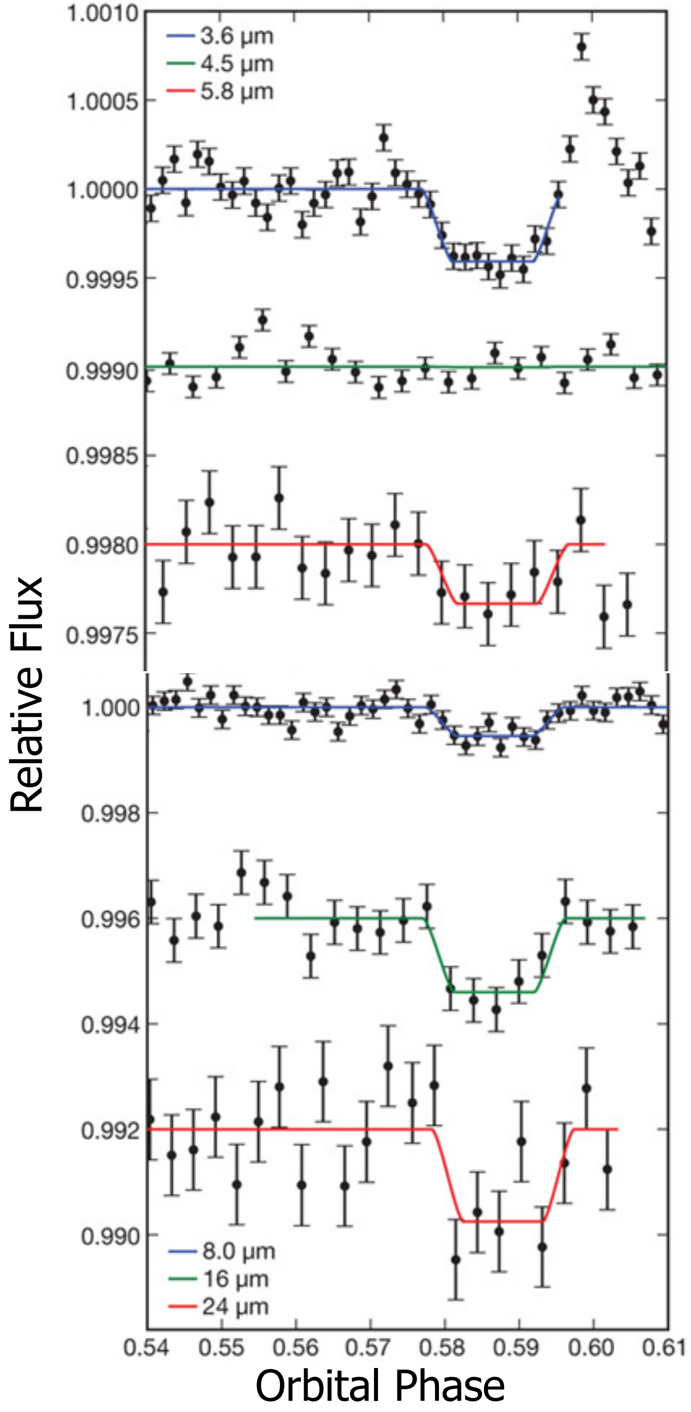
Wavelength	**UV**	**Visible**	**Infrared**
What do we measure?	Lyman alpha, ionized metals	Rayleigh scattering, Na, K, TiO	Water, methane, CO, CO_2
What do we learn?	Atmospheric mass loss	Cloud particle size distribution Cloud albedo	Is the chemistry in equilibrium? Mean molecular weight of atmosphere? Temperature vs pressure in different regions of planet

See, e.g., Madhusudhan et al. (2014)

A Case Study: Warm Neptune GJ 436b

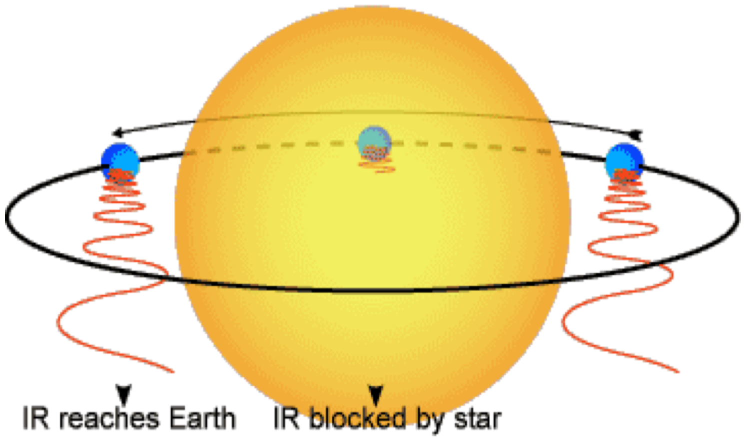


GJ 436 system to scale.



A Dayside Emission Spectrum for GJ 436b

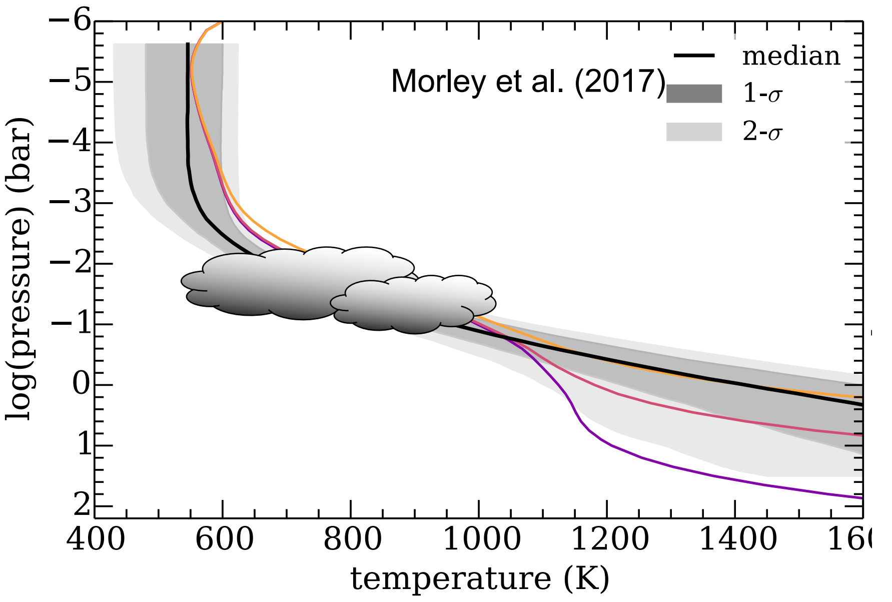
Stevenson et al. (2010, 2012), Lanotte et al. (2014), Morley, Knutson et al. (2017)



Observe the decrease in light as the planet disappears behind the star and then reappears.

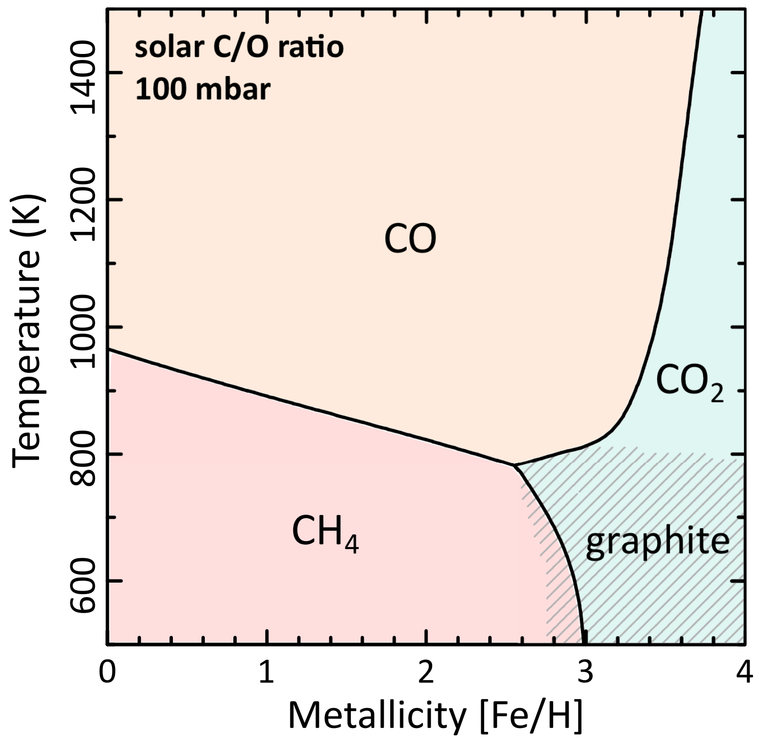
Ingredients for 1D Models

1. **Pressure temperature profile.** Can be **calculated** using a simplified solution of radiative transfer equation (energy into each atmospheric layer must equal energy out) **or fit** using a smoothly varying parameterization.



2. **List of atoms and molecules.** What elements (and molecules) are included in the model? How do elemental abundances translate into molecular abundances? Can enforce **chemical equilibrium** (given elemental abundances, can calculate molecular abundances at each pressure, temperature), use chemical reaction networks to calculate **disequilbrium abundances**, or allow **molecular abundances to be free parameters**.

Moses et al. (2013)



3. **Clouds.** Usually parameterized as an opaque cloud deck and/or an optically thin scattering haze of small particles.

For each model component, must decide: fit or predict from first principles?

Atmospheres are Complicated, Models Must Simplify for the Sake of Computational Efficiency

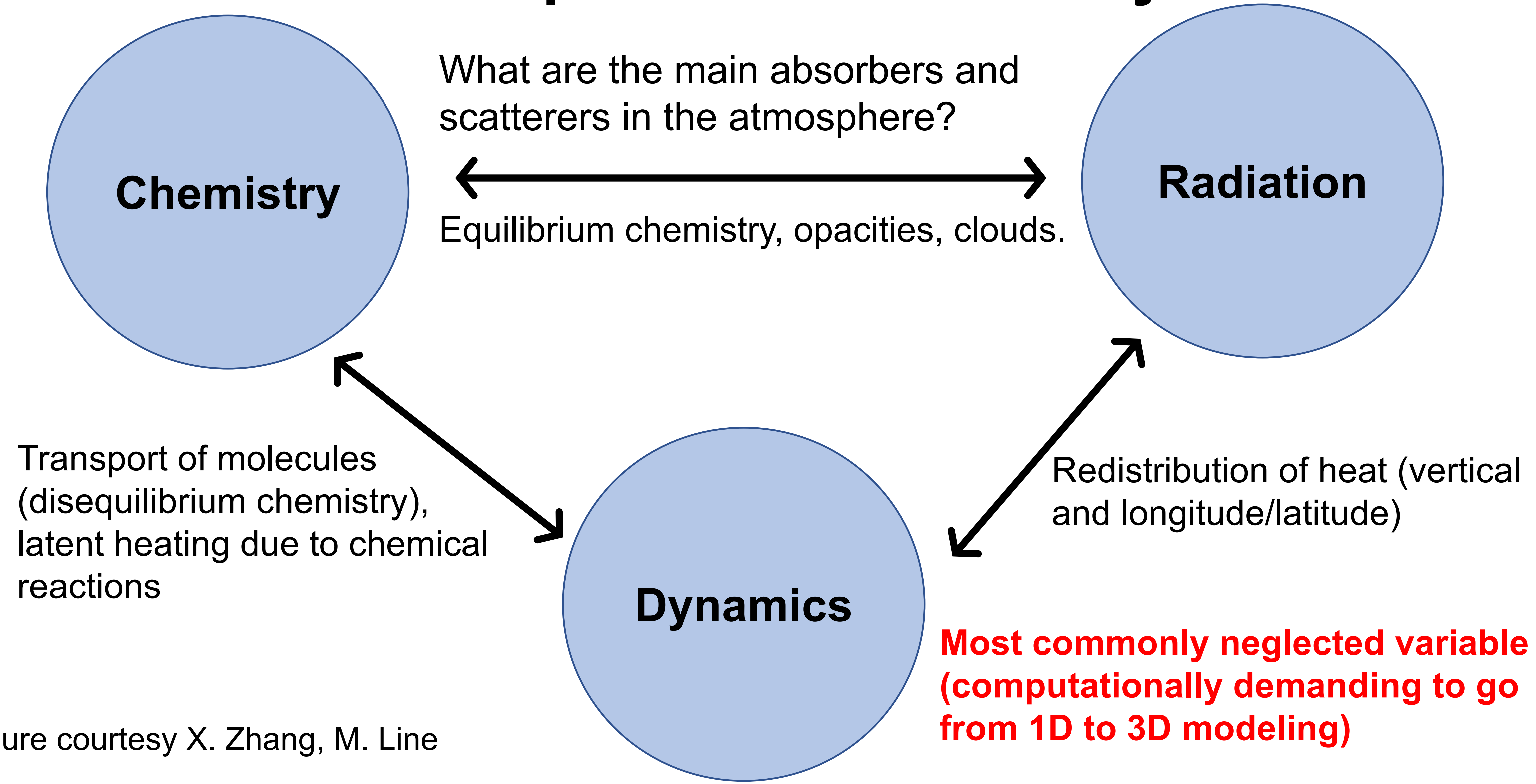
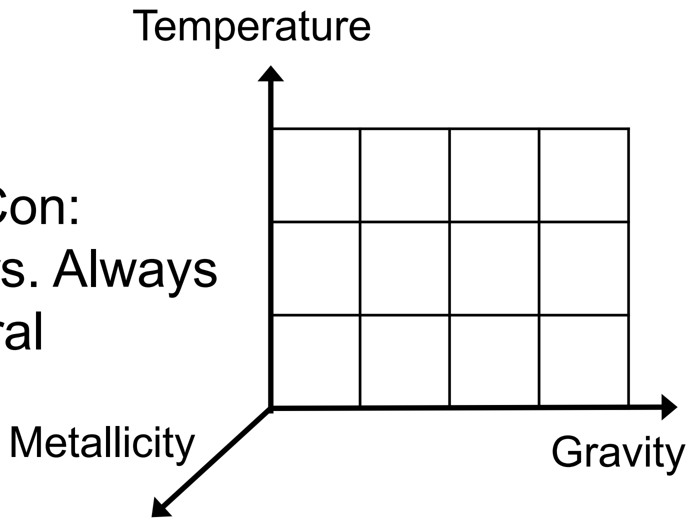


Figure courtesy X. Zhang, M. Line

Spectral Retrieval Options

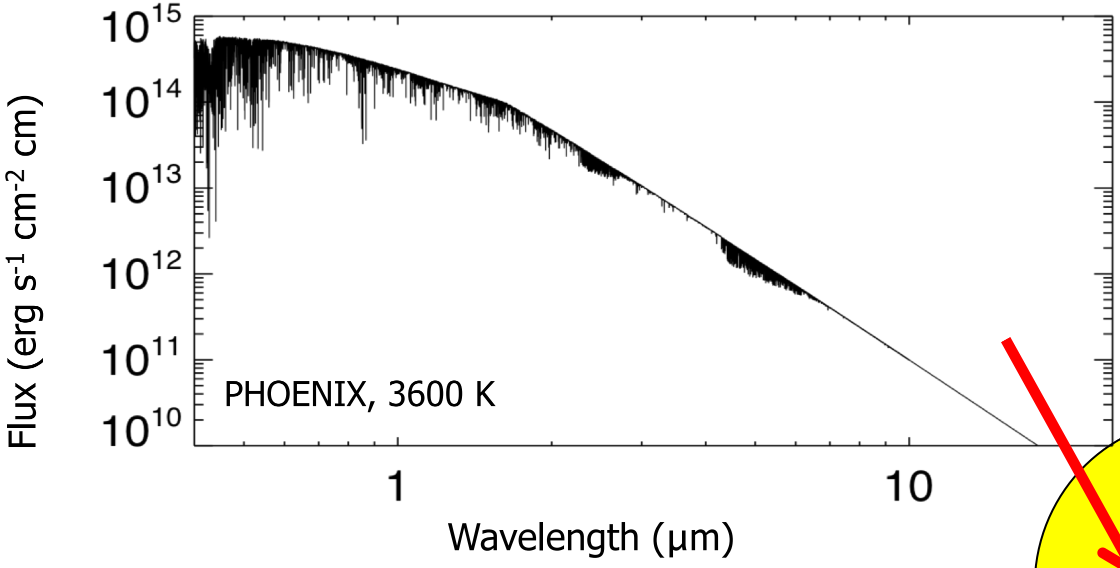


1. **Grid modeling.** Pro: forward (i.e., physically self-consistent) models. Con: limited parameter space, hard to estimate uncertainties in model parameters. Always a good place to start, best approach for marginal data (low SNR, low spectral resolution, limited wavelength coverage).

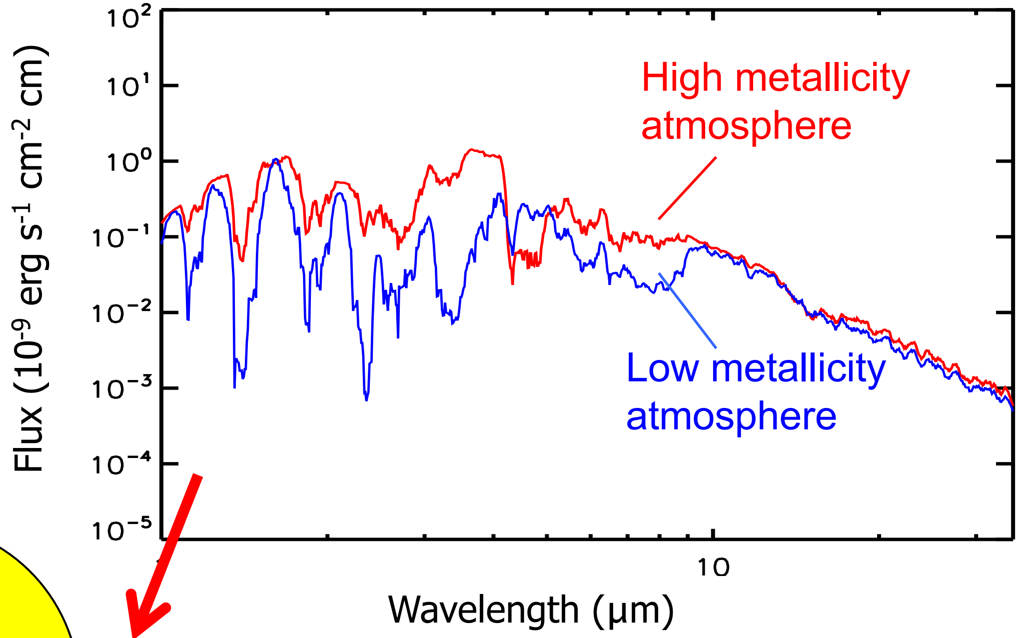
See Marley & Robinson (2015), Heng & Marley (2018).

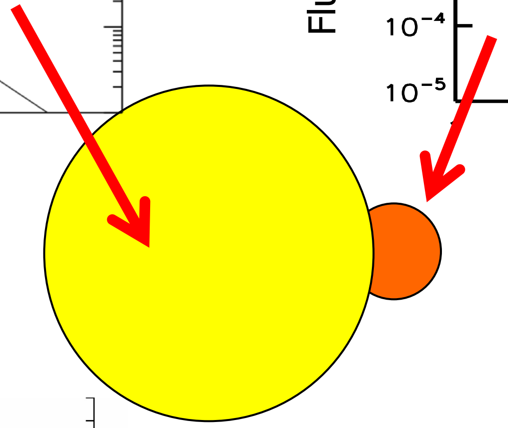
Comparison to Models

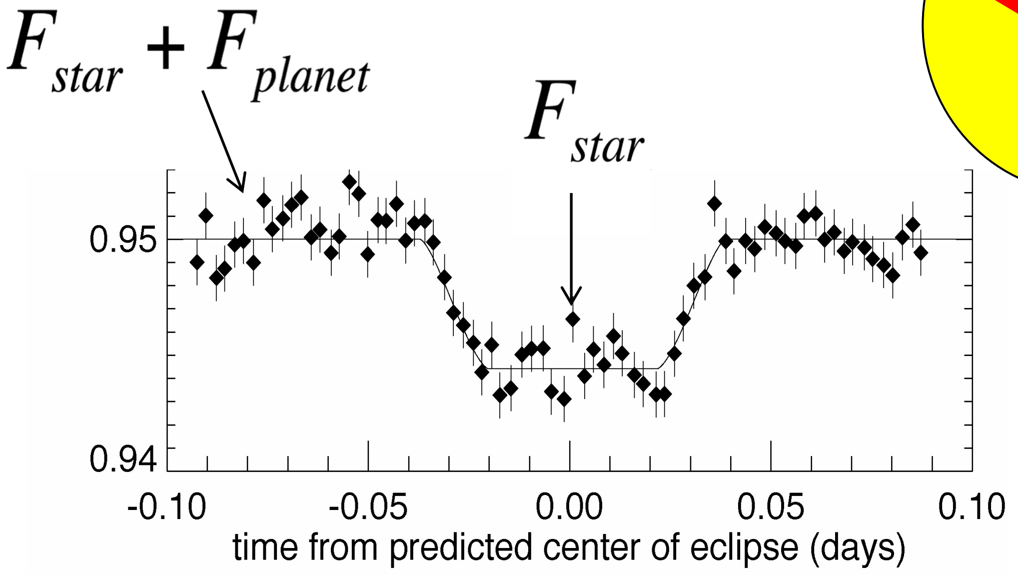
Stellar Atmosphere Model



Planet Atmosphere Models

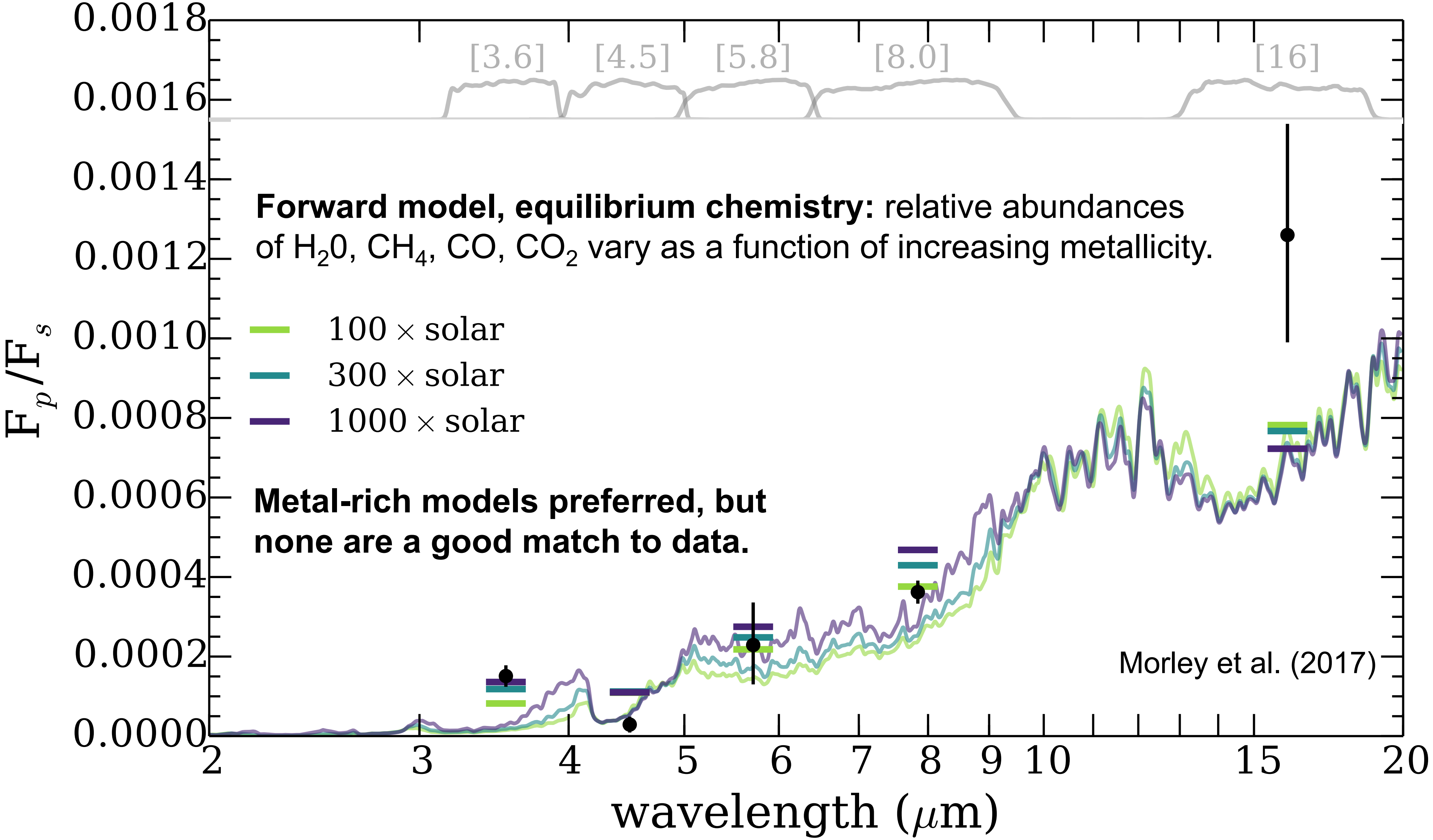






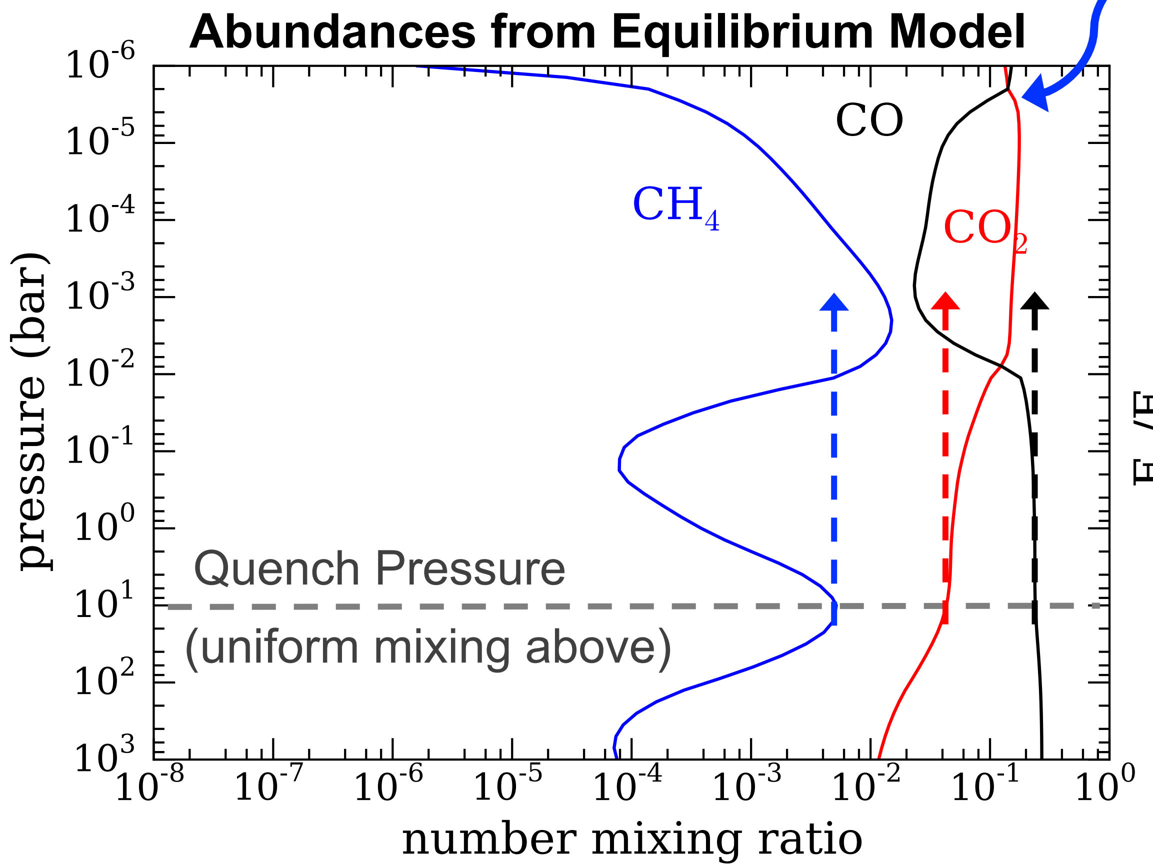
$$depth(\%) = \frac{F_{planet}}{F_{star} + F_{planet}} \approx \frac{F_{planet}}{F_{star}}$$

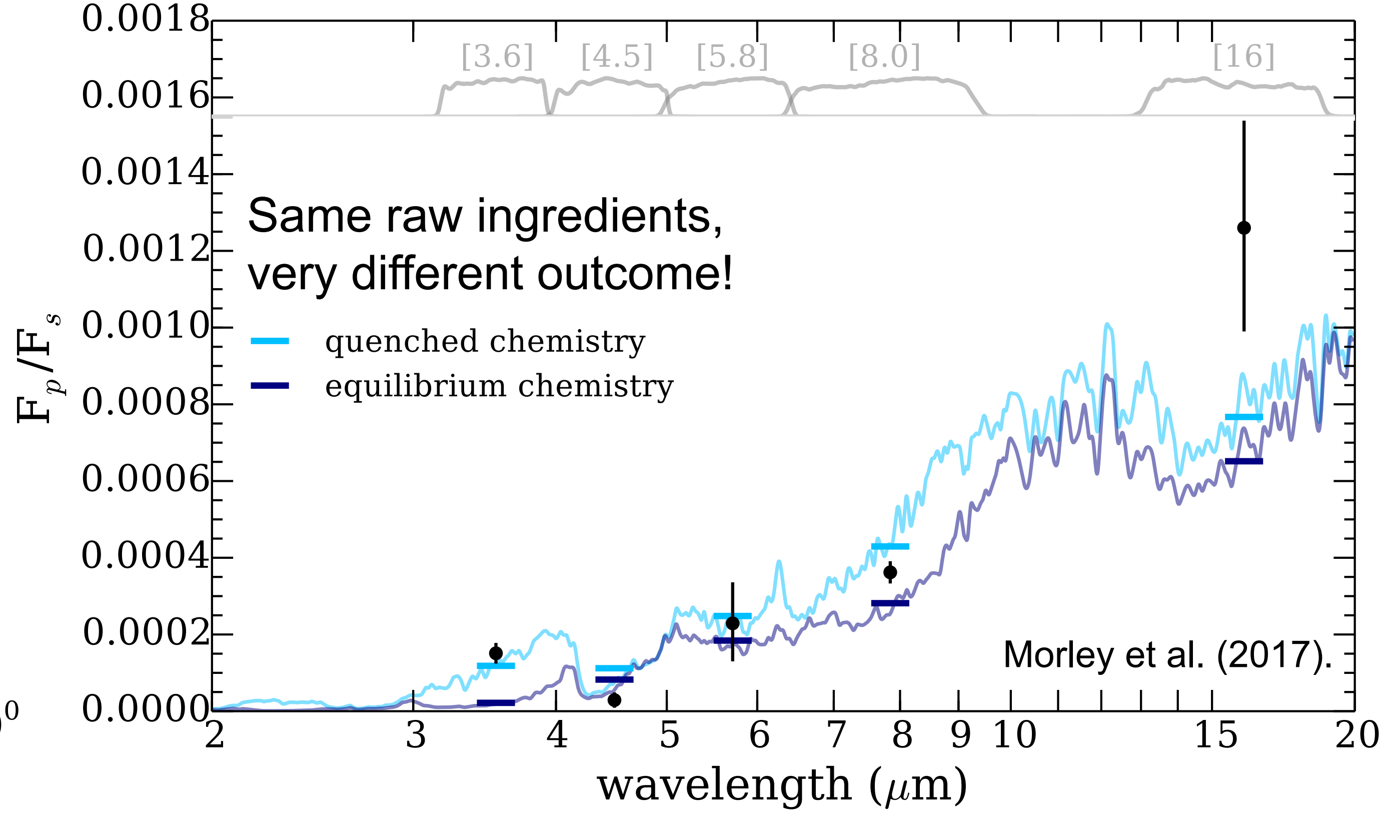
Grid Comparison to Constrain Atmospheric Metallicity



What's Missing? Vertical Mixing, UV Irradiation Can Also Affect Atmospheric Chemistry

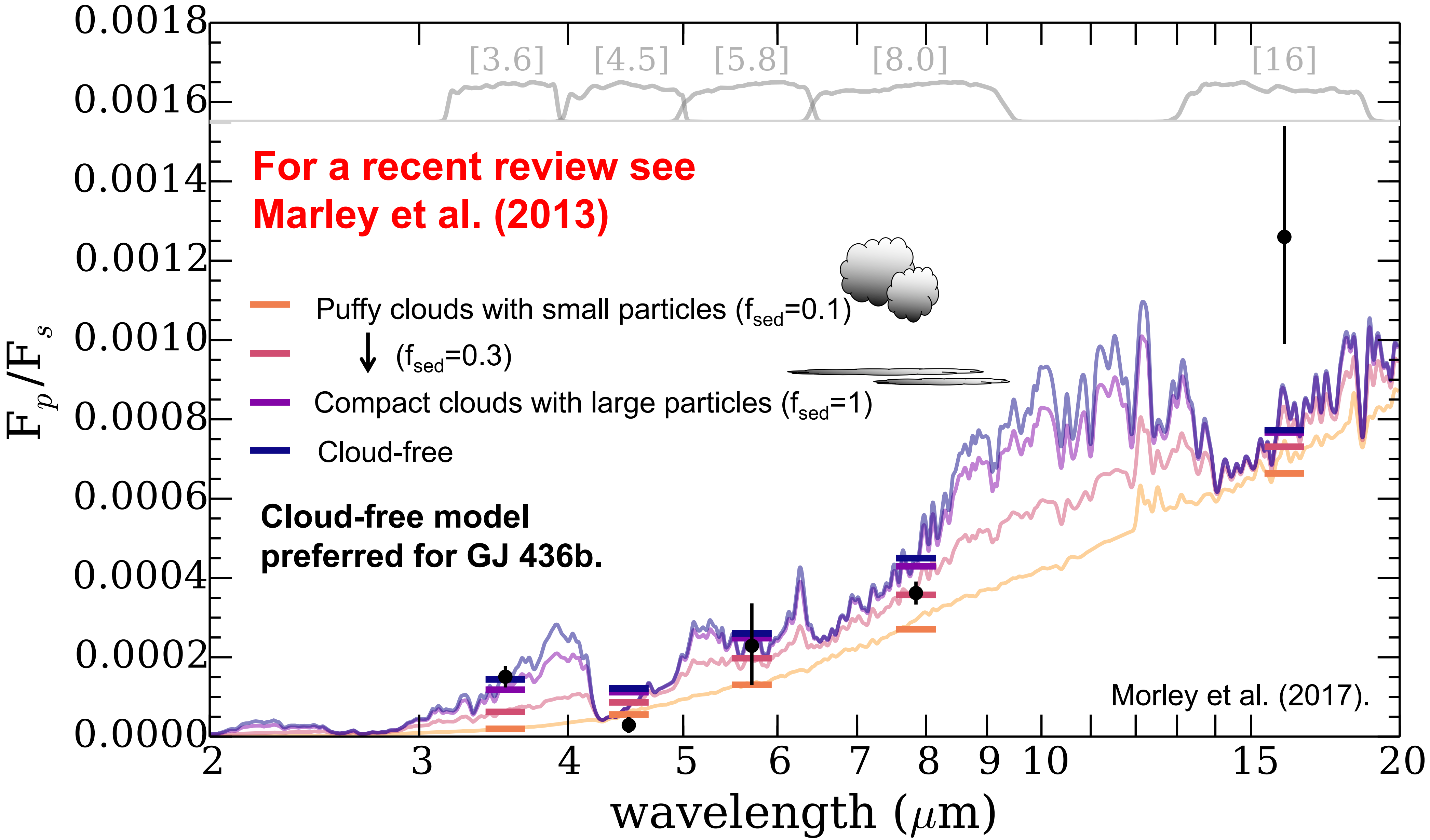
UV light from star breaks apart molecules at top of atmosphere.



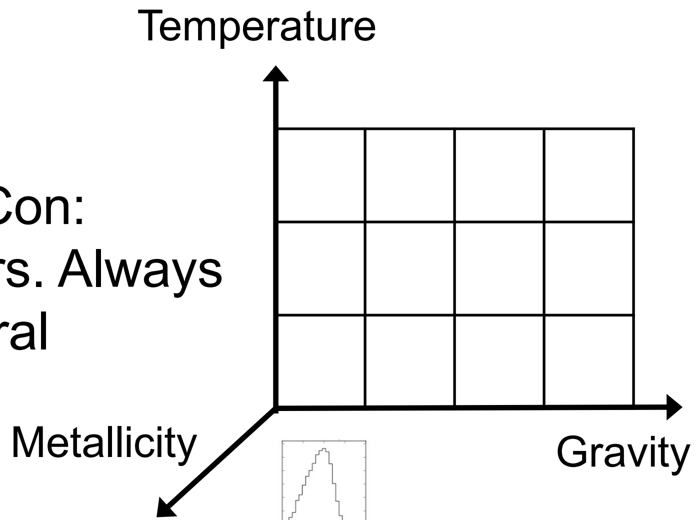


For a recent review see Moses et al. (2013)

What Effect Do Clouds Have on Emission Spectra?



Spectral Retrieval Options



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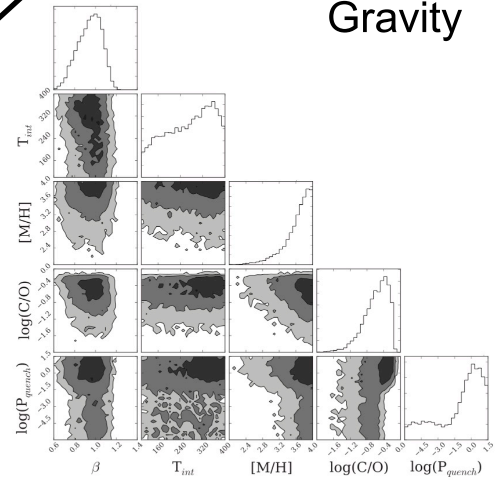


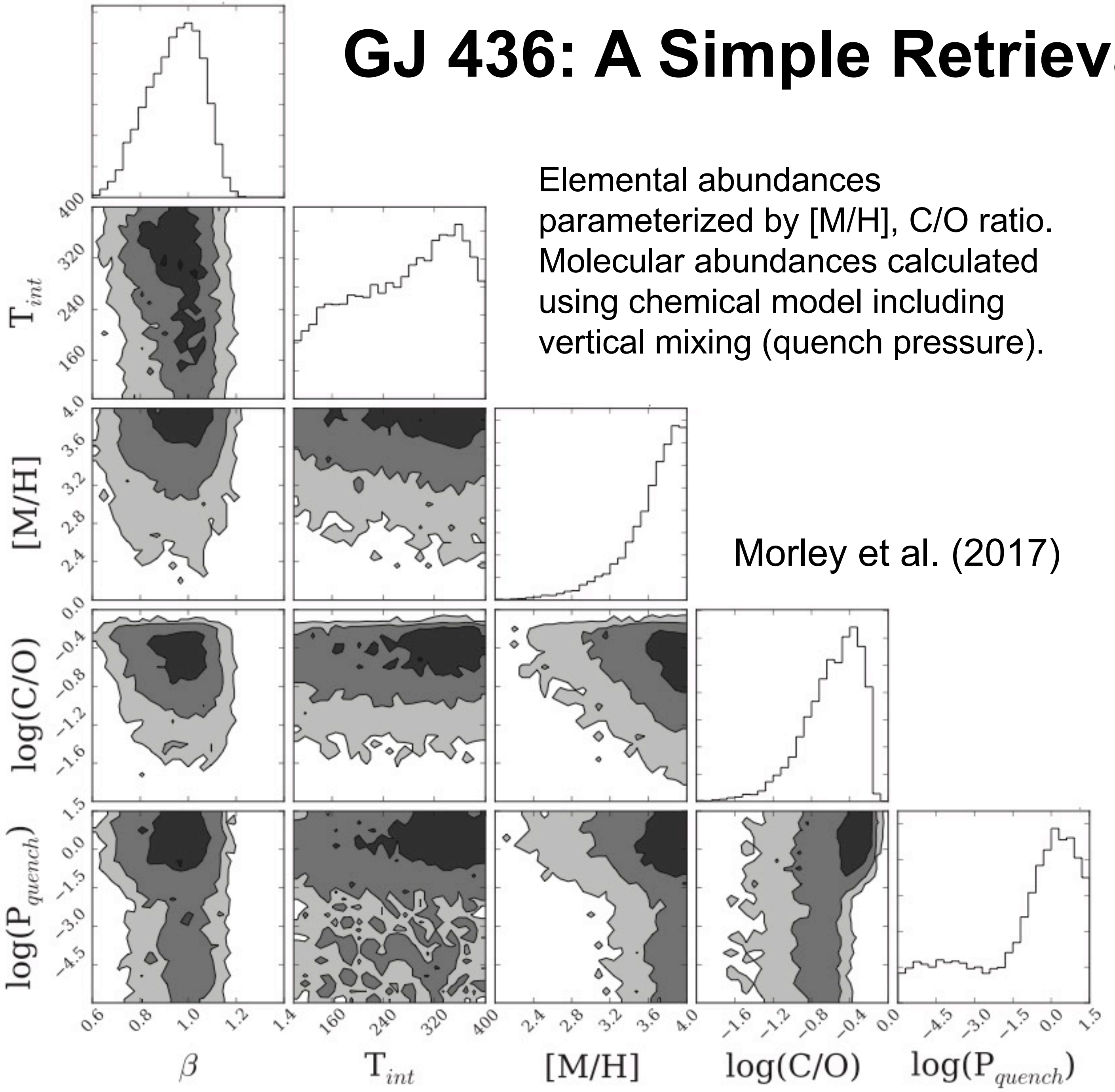
2. **Retrieval with self-consistent forward models.** Pro: allows more thorough explanation of (limited) parameter space, can marginalize over nuisance parameters. Con: models may not capture all relevant processes (vertical/horizontal transport, photochemistry, effects of clouds).

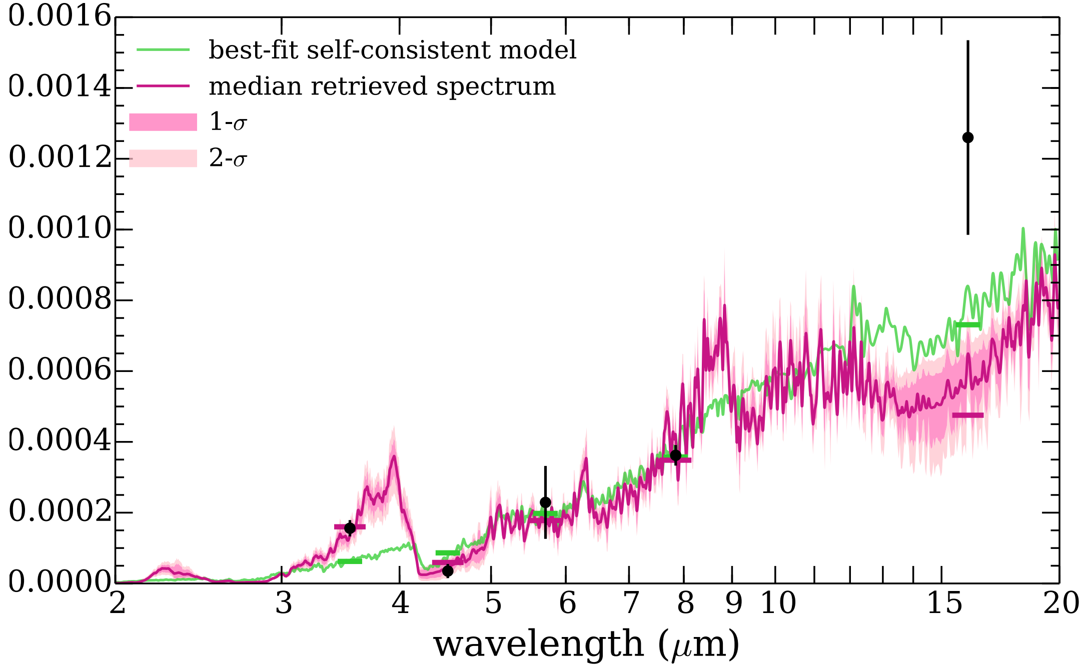
See Marley & Robinson (2015), Heng & Marley (2018).

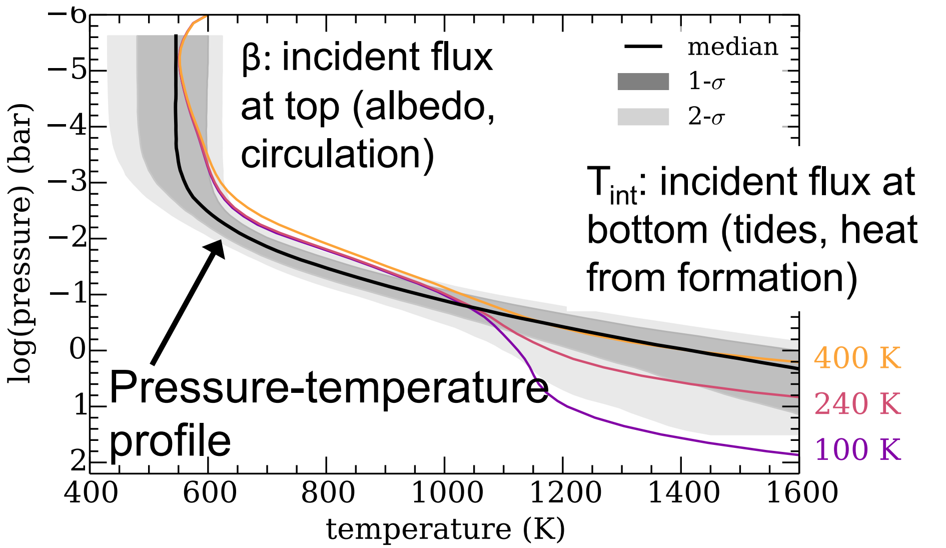
GJ 436: A Simple Retrieval With Forward Models

Elemental abundances parameterized by [M/H], C/O ratio. Molecular abundances calculated using chemical model including vertical mixing (quench pressure).

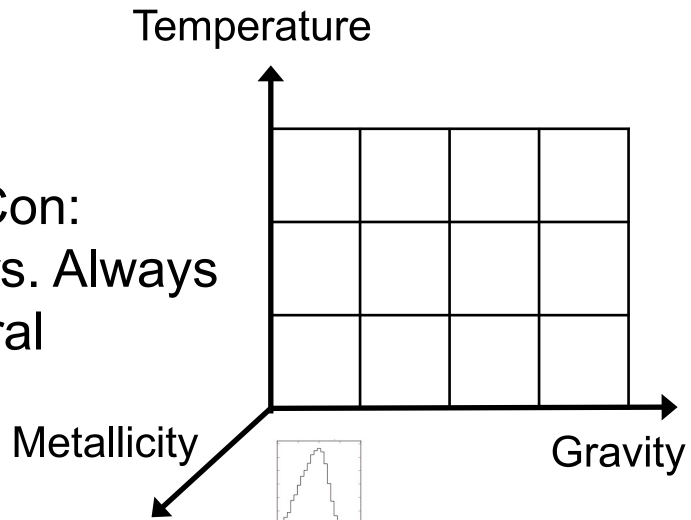
Morley et al. (2017)







Spectral Retrieval Options



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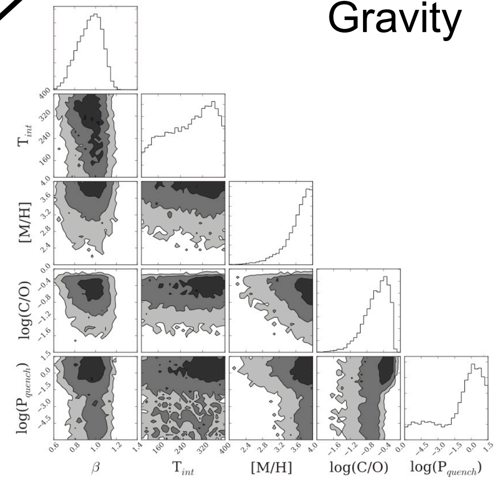


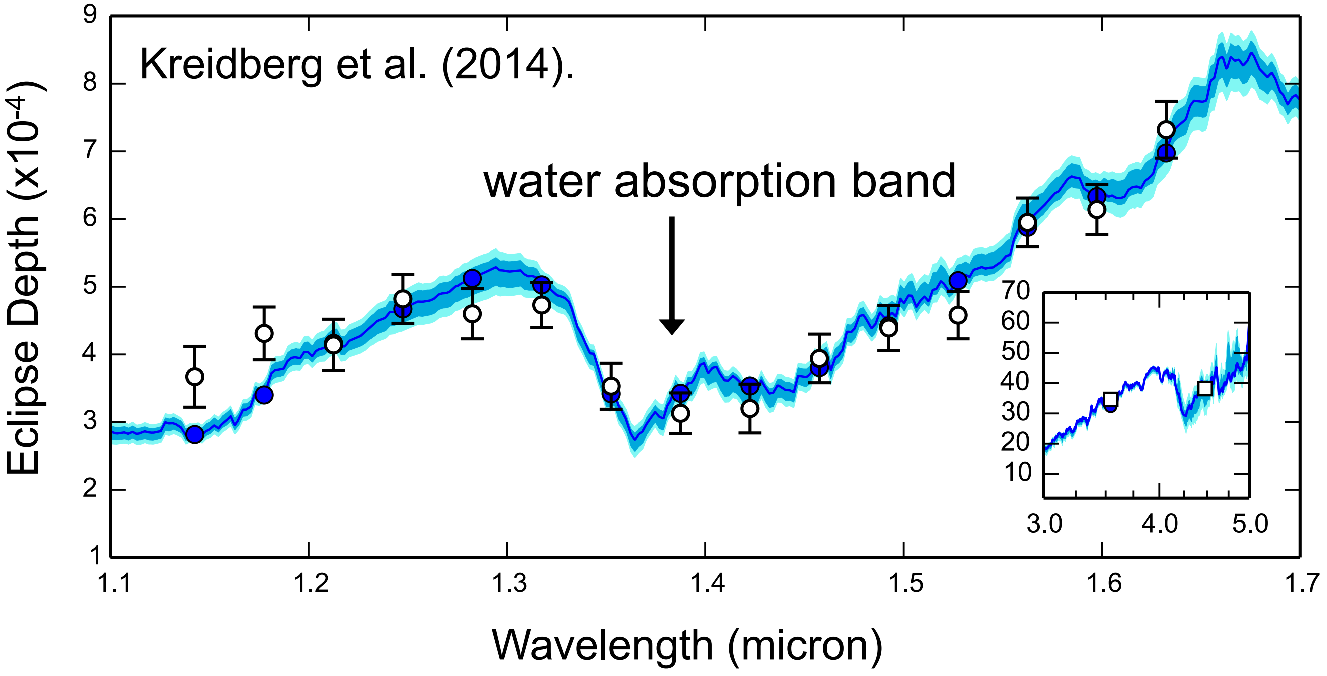
2. **Retrieval with self-consistent forward models.** Pro: allows more thorough explanation of (limited) parameter space, can marginalize over nuisance parameters. Con: models may not capture all relevant processes (vertical/horizontal transport, photochemistry, effects of clouds).

3. **Retrieval with molecular abundances as free parameters, parameterized pressure-temperature profile, clouds.** Pro: makes minimal assumptions about atmospheric processes. Con: allows for unphysical results (e.g., unstable mixes of gases, very steep pressure-temperature profiles). Need very good data to avoid unphysical solutions.

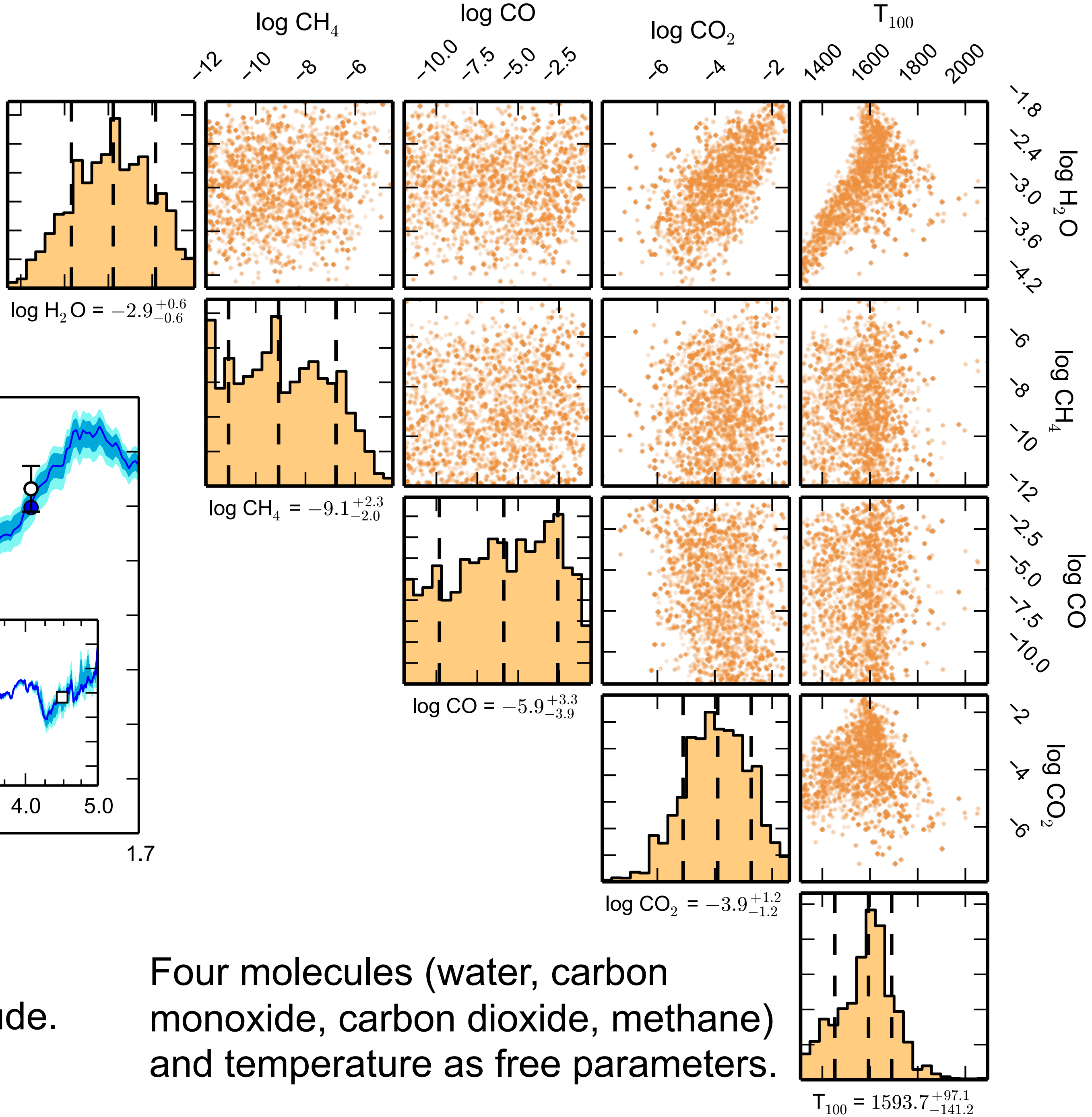
See Marley & Robinson (2015), Heng & Marley (2018).

WASP-43b: A Free Retrieval For Individual Molecules

HST/WFC3 emission spectrum (secondary eclipse): spectrally resolved molecular band!



Water abundance well-constrained, all other molecules uncertain by multiple orders of magnitude.



Four molecules (water, carbon monoxide, carbon dioxide, methane) and temperature as free parameters.

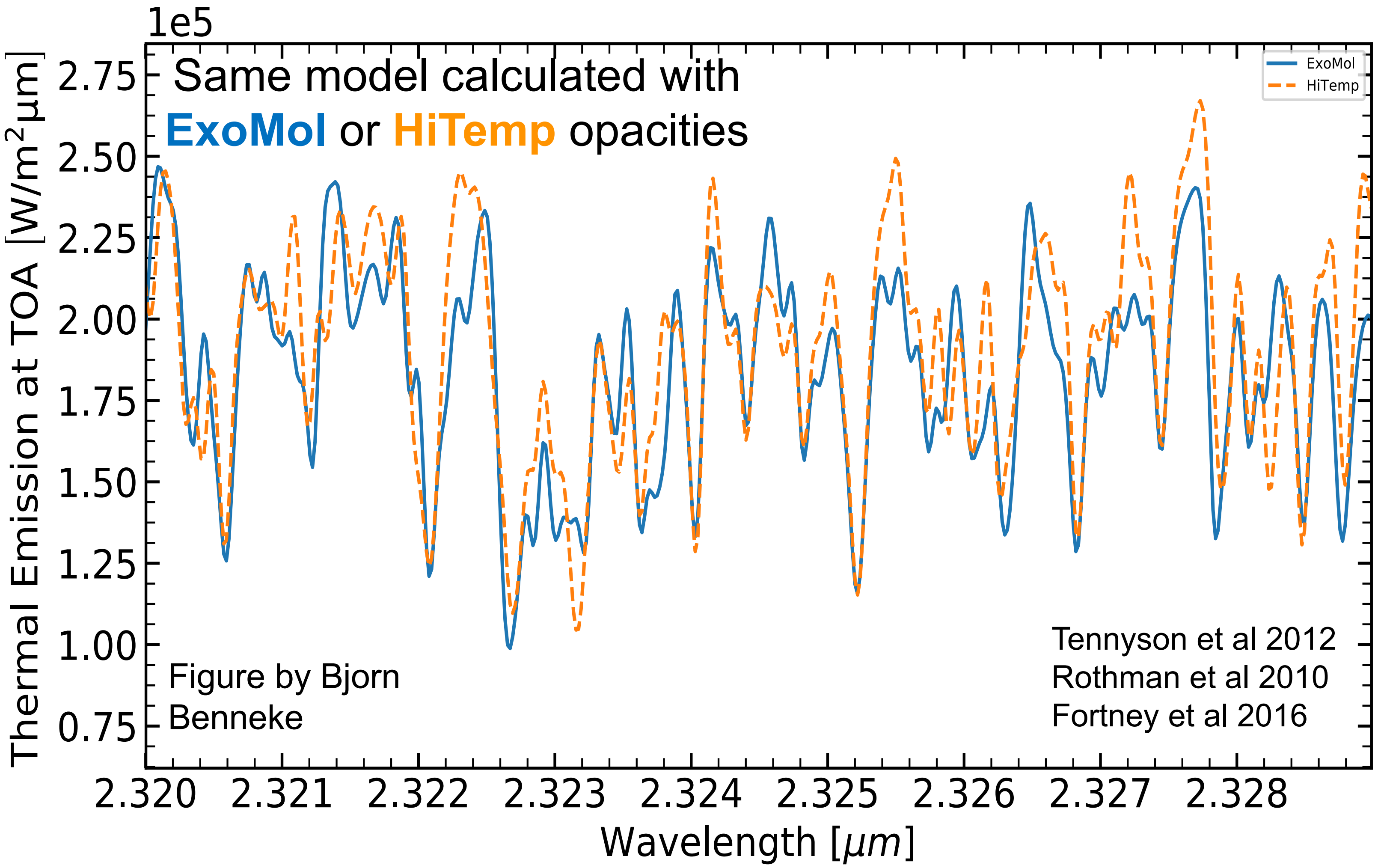
Caveat: Not Everything is Chemically (or Physically) Possible

Some mixes of gases aren't stable, will react to form other compounds.

Cloud particles may precipitate out, energy in has to equal energy out.

(h/t Kevin Heng)

Opacities: The Devil is in the Details



Can get different results using different line lists; **all line lists are wrong** in one way or another. Problems are worse for some molecules than others (e.g., methane).

Have to **compute line shapes for millions or even billions of lines** to make model, then bin that down to resolution of data. Computationally intensive, imperfect shortcuts (e.g., correlated-k) available. Pressure-broadening in wings is a fundamental unsolved problem.

(h/t Kevin Heng)

See Fortney et al. (2016)

Don't Be Misled By Your Priors or Choice of Model Parameterization

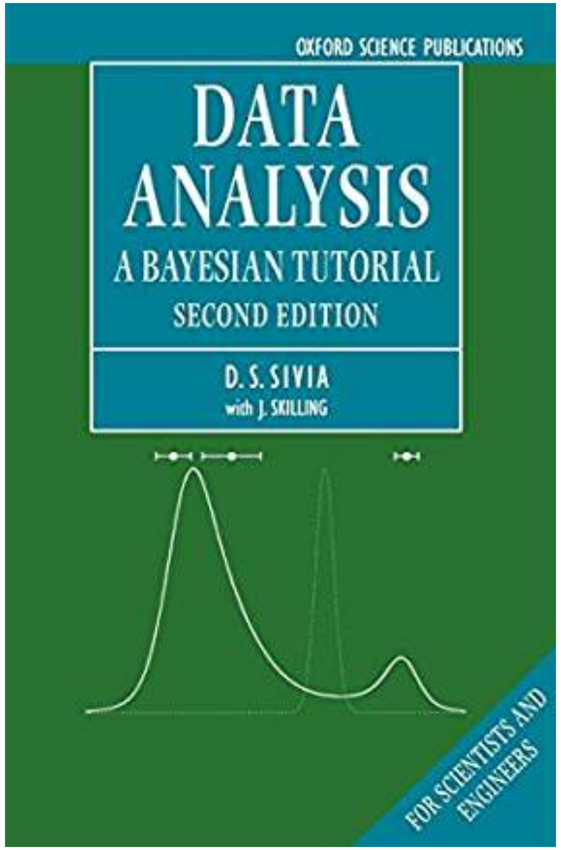
Concise, easy-to-read introduction to Bayesian statistics

$$C/O \approx \frac{\tilde{n}_{CO} + \tilde{n}_{CH_4} + \tilde{n}_{CO_2}}{\tilde{n}_{CO} + \tilde{n}_{H_2O} + 2\tilde{n}_{CO_2}},$$

If you assume a uniform prior in the mixing ratio *n* (abundance relative to H_2) of each individual molecular species you will get **artificial peaks** in the posterior probability distribution for C/O whose location depends on the dominant molecular species.

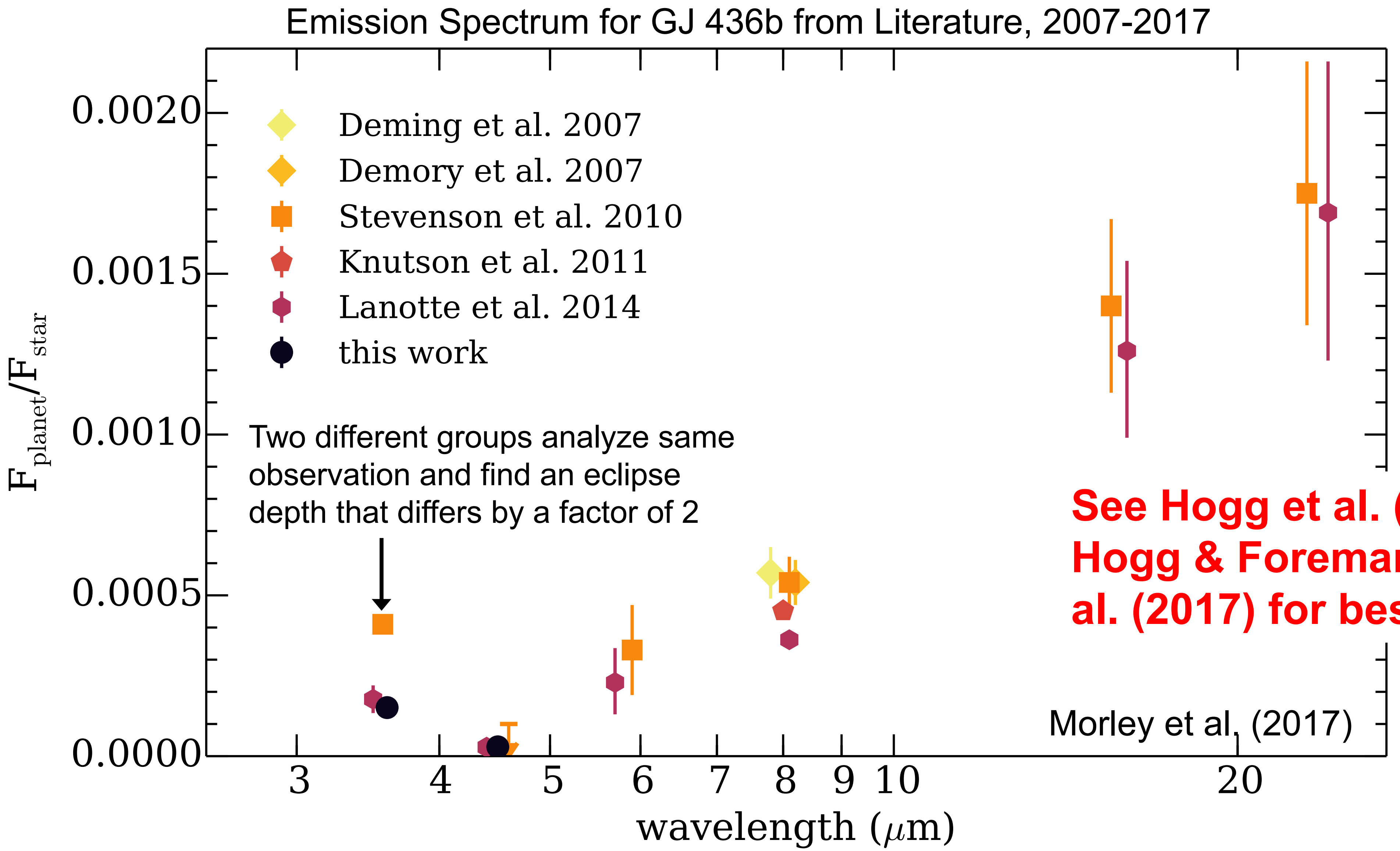
Matters most when model parameters are **poorly constrained** by data. **Important corollary:** try multiple model parameterizations to see if you get the same answer.

For more information, see Line et al. (2013)



(h/t Kevin Heng)

You Need to Understand the Data, Too!



See Hogg et al. (2010), Hogg & Foreman-Mackey et al. (2017) for best practices.

Always remember: use common sense.

Your retrieval is only as good as your understanding of the measurements and your choice of model.

(garbage in, garbage out)