

# Theoretical Models of Exoplanet Atmospheres



CARL SAGAN  
INSTITUTE



Cornell University

Ryan MacDonald  
Natasha Batalha

Atmospheres, Atmospheres!

Do I look like I care about atmospheres?

24 August 2021

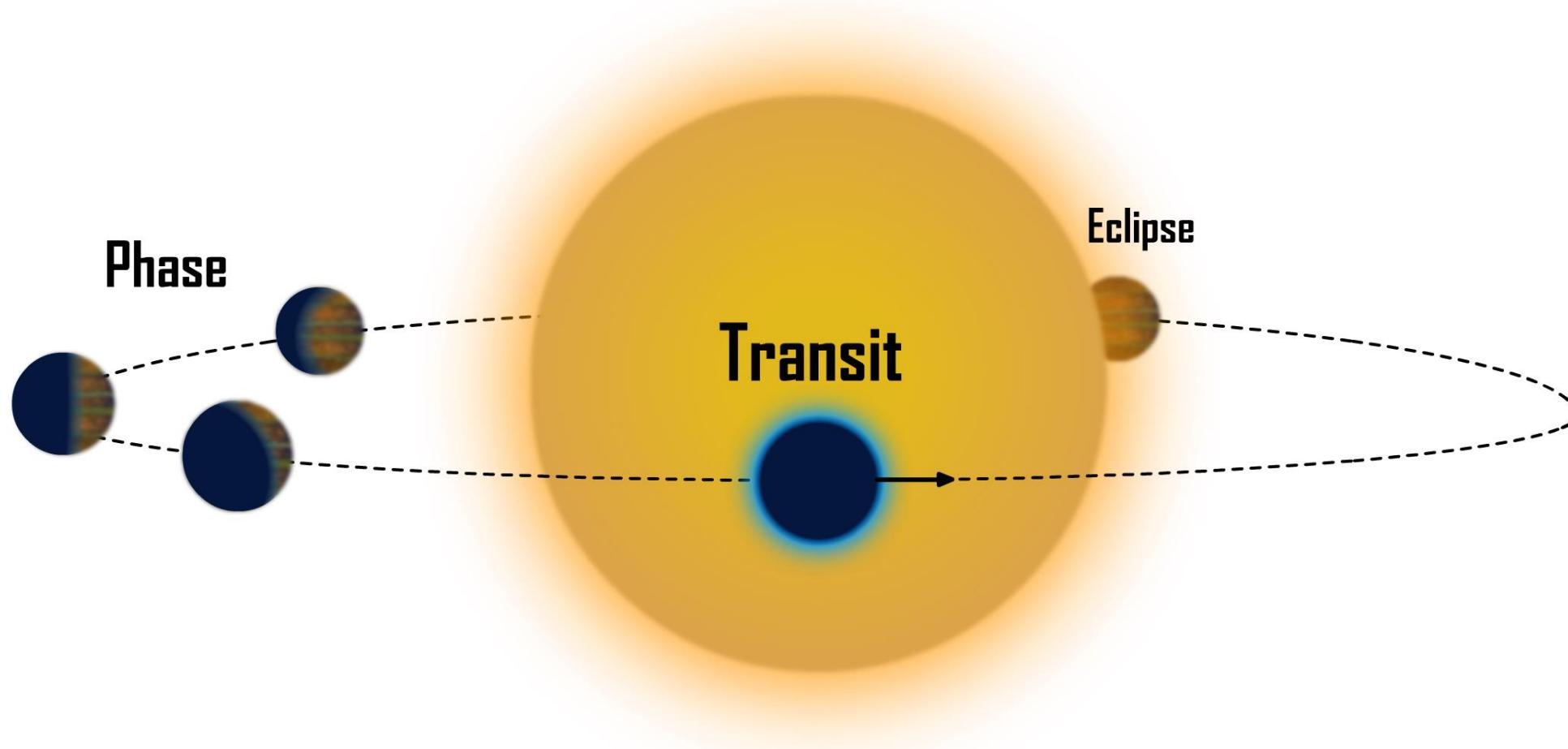


Image credit  
ESO/M. Kornmesser

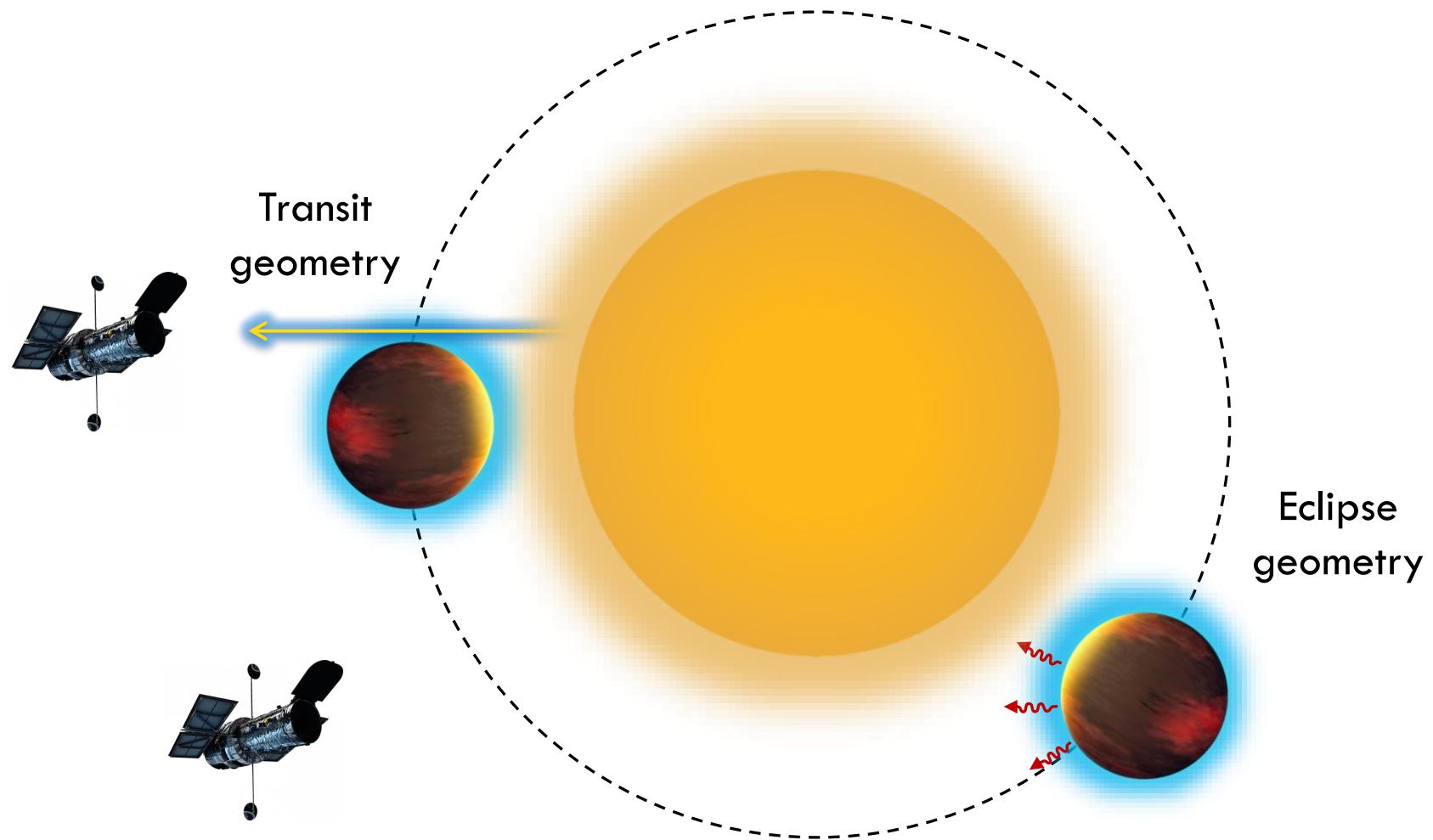
PART 1:

# SPECTRA OF EXOPLANET ATMOSPHERES

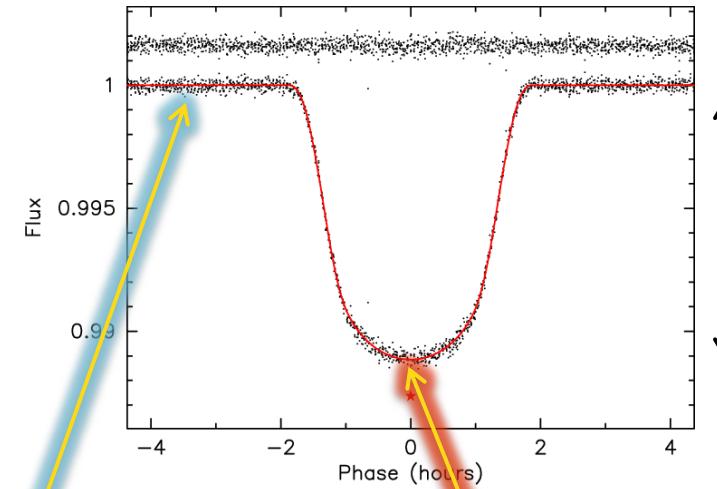
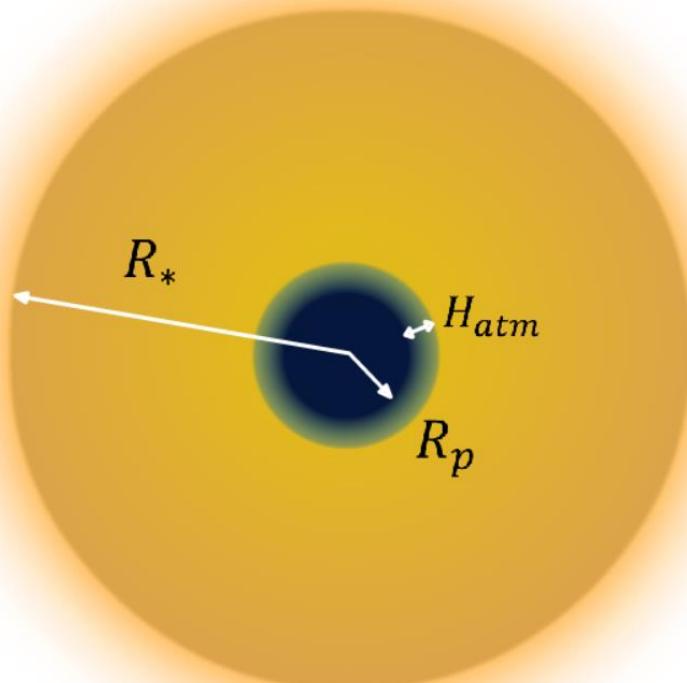
# TECHNIQUES TO PROBE EXOPLANET ATMOSPHERES



# DIFFERENT SPECTRA PROBE DIFFERENT ATMOSPHERIC REGIONS



# A TOY MODEL FOR TRANSMISSION SPECTRA



$$\delta_{trans} = \frac{F_{out} - F_{in}}{F_{out}}$$

$$F_{out} = \frac{I_* A_*}{d^2} \quad F_{in} = \frac{I_* A_* - I_* A_p}{d^2} \quad \rightarrow \quad \delta_{trans} = \frac{A_p}{A_*}$$

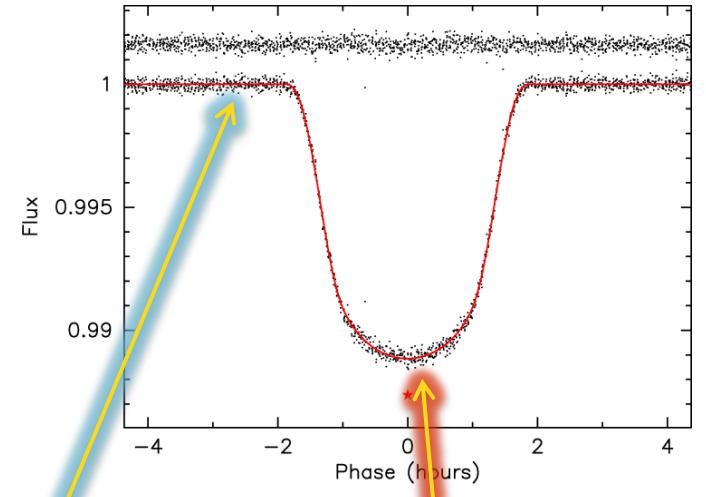
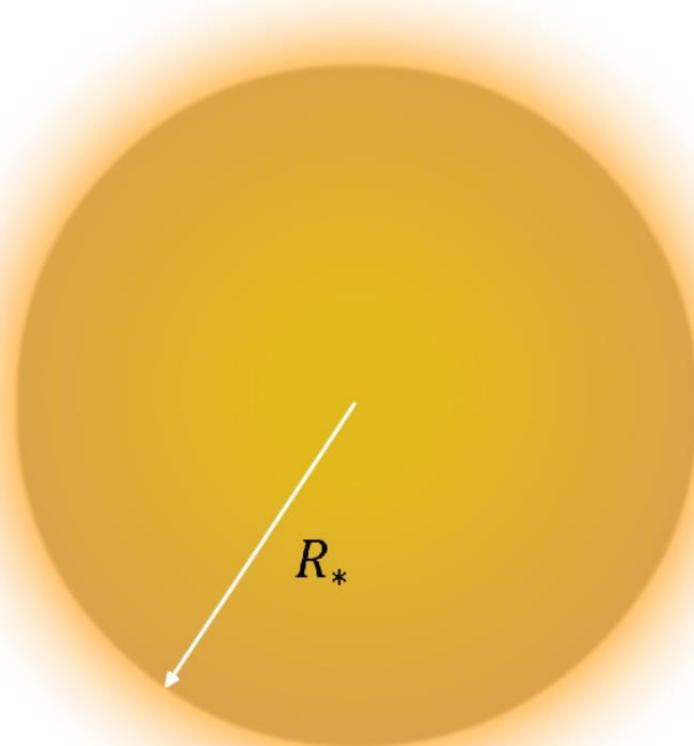
For a transparent atmosphere:

$$\delta_{trans} = \frac{R_p^2}{R_*^2}$$

For an opaque atmosphere:

$$\delta_{trans} = \frac{R_p^2}{R_*^2} + \left( \frac{2R_p H_{atm}}{R_*^2} + \frac{H_{atm}^2}{R_*^2} \right) \approx \frac{R_p^2}{R_*^2} + \frac{2R_p H_{atm}}{R_*^2}$$

# A TOY MODEL FOR EMISSION SPECTRA



$$\delta_{eclipse} = \frac{F_{out} - F_{in}}{F_{out}}$$

$$F_{out} = F_p + F_*$$

$$F_{in} = F_*$$

$$\rightarrow \delta_{eclipse} = \frac{F_p}{F_p + F_*} \approx \frac{F_p}{F_*}$$

Assume both planet and star emit as black bodies:

$$B_\lambda(T) = \frac{2hc^2}{\lambda^5} \left( \frac{1}{e^{\frac{hc}{\lambda k_B T}} - 1} \right)$$

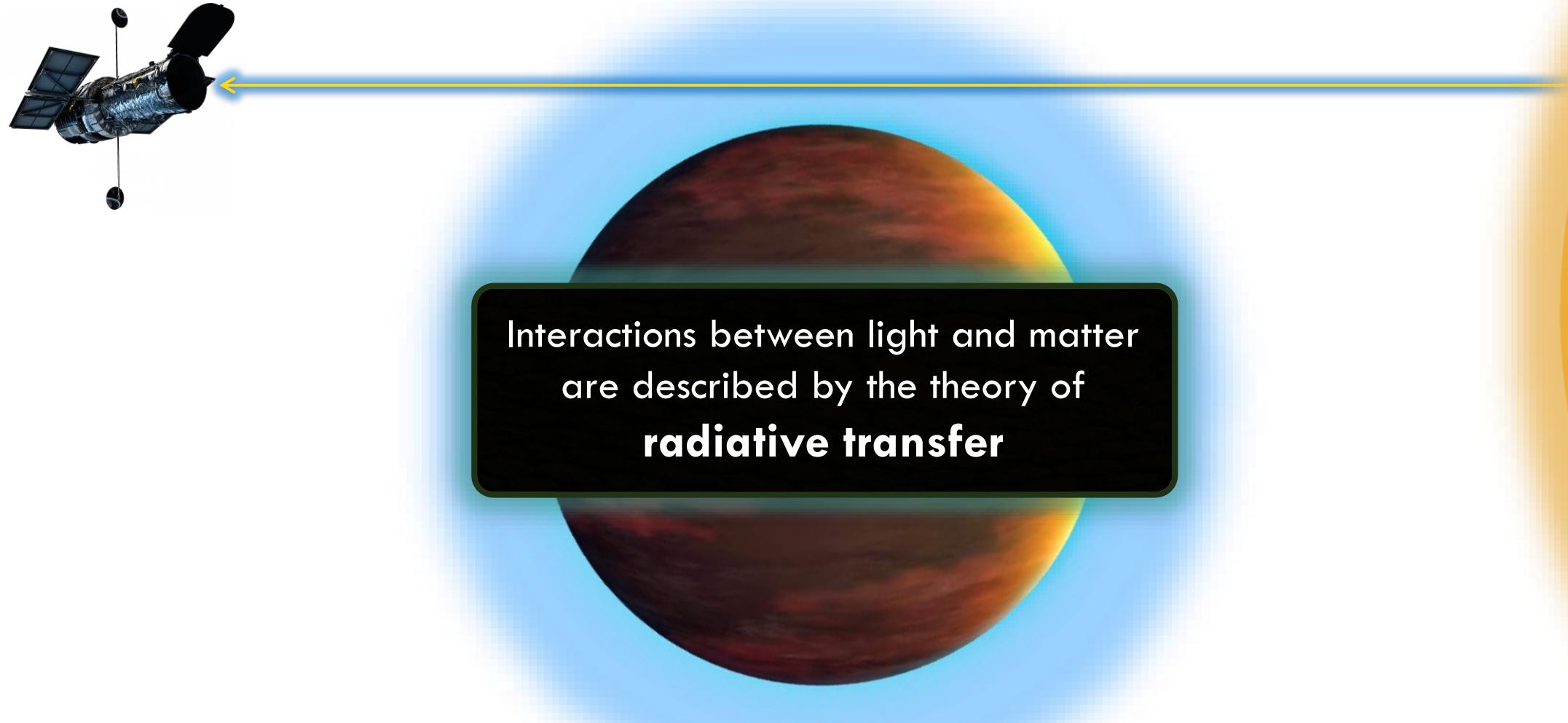
$$F_p = \frac{\pi B_\lambda(T_p) R_p^2}{d^2}$$

$$F_* = \frac{\pi B_\lambda(T_*) R_*^2}{d^2}$$

$$\therefore \delta_{eclipse} = \left[ \frac{e^{\frac{hc}{\lambda k_B T_*}} - 1}{e^{\frac{hc}{\lambda k_B T_p}} - 1} \right] \left( \frac{R_p^2}{R_*^2} \right) \approx \frac{T_p}{T_*} \left( \frac{R_p^2}{R_*^2} \right)$$

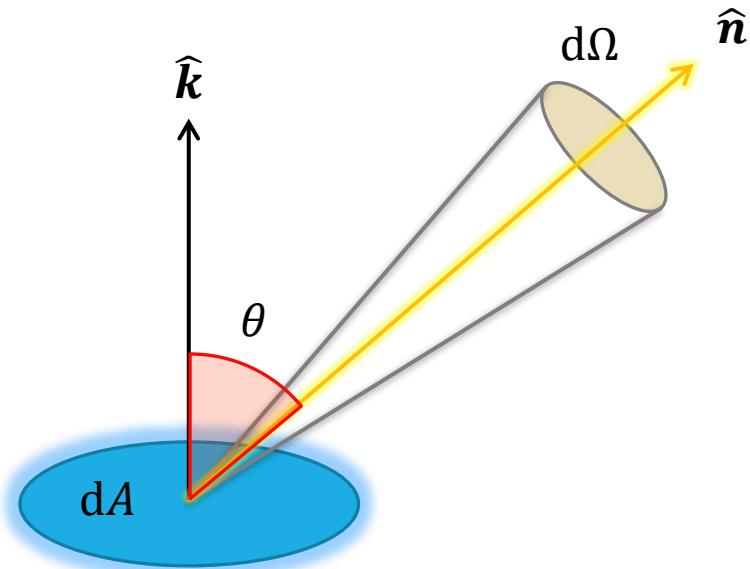
$$\frac{hc}{\lambda k_B T_p} \ll 1$$

# BUILDING A BETTER MODEL OF EXOPLANET SPECTRA



Interactions between light and matter  
are described by the theory of  
**radiative transfer**

# BASIC QUANTITIES OF RADIATIVE TRANSFER



A beam of light, travelling in direction  $\hat{n}$ , represented as a cone with solid angle  $d\Omega$ , passes through a surface of area  $dA$

The **intensity** encodes how much energy flows through the surface per time per wavelength:

$$dE_\lambda = I_\lambda (\hat{n} \cdot \hat{k}) d\Omega dA d\lambda dt$$

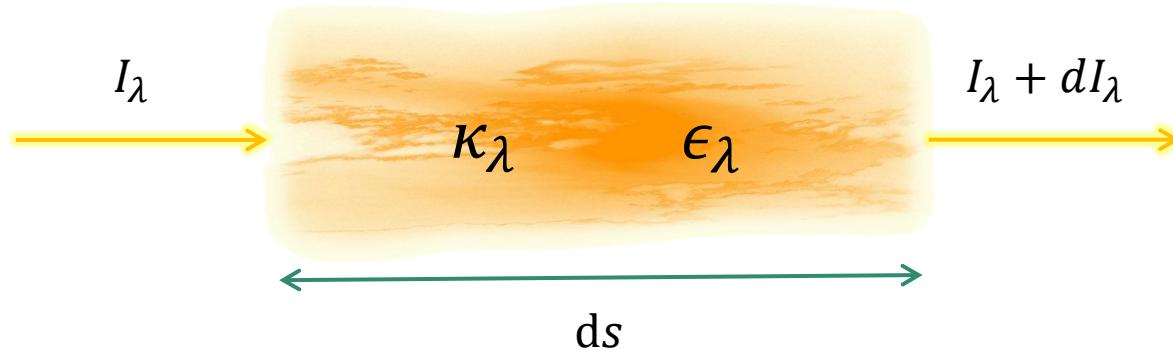
**Intensity** is a fundamental quantity of radiative transfer

We observe **flux**, which is the integrated intensity over all solid angles:

$$F_\lambda = \int I_\lambda \hat{n} \cdot \hat{k} d\Omega$$

In a vacuum, the intensity of a beam remains constant

# INTERACTIONS BETWEEN LIGHT AND MATTER



The **extinction coefficient** ( $\kappa_\lambda$ ) encodes processes that remove photons from the beam:

$$dI_{\lambda, loss} = -\kappa_\lambda I_\lambda ds$$

The **emission coefficient** ( $\epsilon_\lambda$ ) encodes processes that add photons to the beam:

$$dI_{\lambda, gain} = \epsilon_\lambda ds$$

A beam travelling through a medium can have its intensity changed

Combined effect:

$$\frac{dI_\lambda}{ds} = -\kappa_\lambda I_\lambda + \epsilon_\lambda$$

**The equation of radiative transfer**

# THE RADIATIVE TRANSFER EQUATION

Now we can introduce two important quantities

**The optical depth:**

$$\tau_\lambda = \int \kappa_\lambda ds$$

**The source function:**

$$S_\lambda = \frac{\epsilon_\lambda}{\kappa_\lambda}$$

This yields the most common form of the radiative transfer equation

$$\frac{dI_\lambda}{ds} = -\kappa_\lambda I_\lambda + \epsilon_\lambda \quad \rightarrow \quad \frac{dI_\lambda}{d\tau_\lambda} = -I_\lambda + S_\lambda$$

In local thermodynamic equilibrium (LTE)  
[and when scattering is negligible],  
Kirchoff's law gives us

$$S_\lambda = B_\lambda$$

$$\frac{dI_\lambda}{d\tau_\lambda} = -I_\lambda + B_\lambda$$

# RADIATIVE TRANSFER: TRANSMISSION SPECTRA

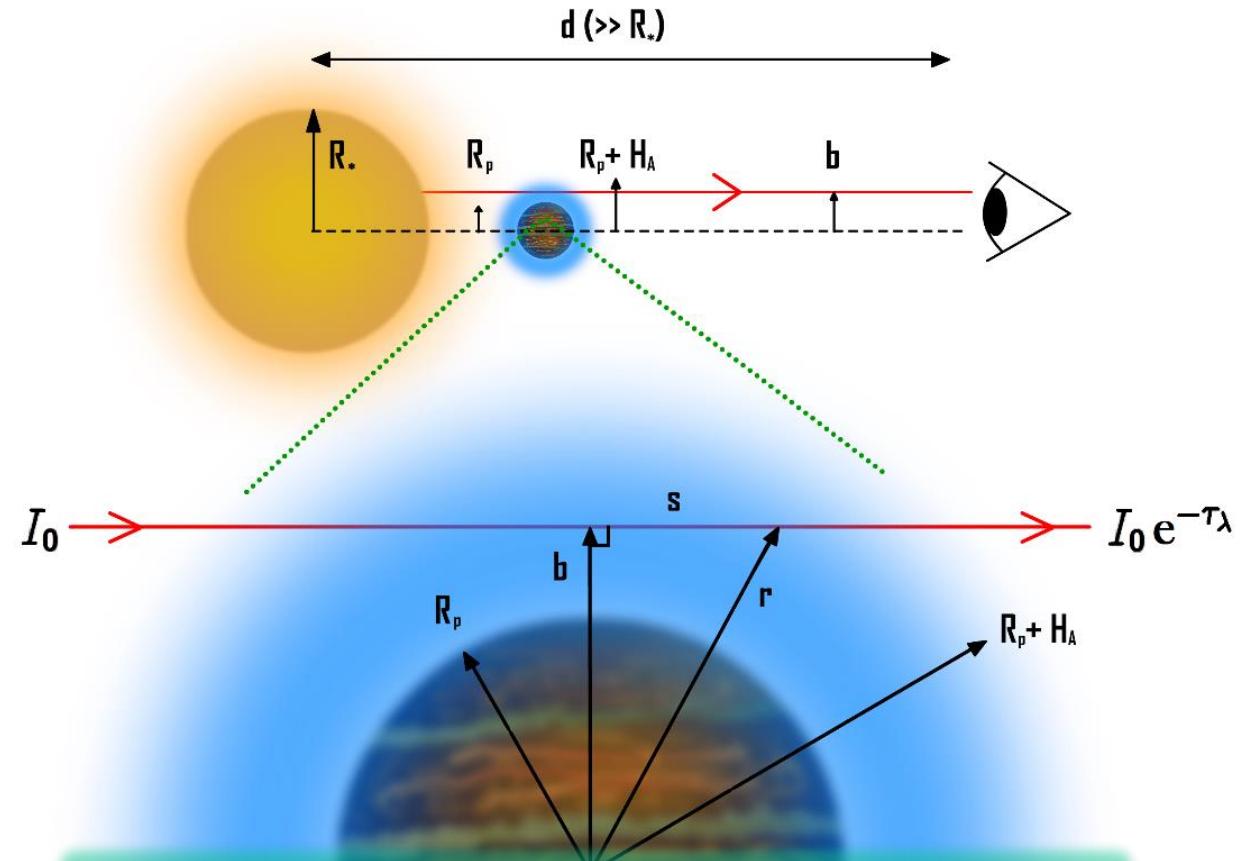
In transmission geometry, there is no emission into the beam:

$$\frac{dI_\lambda}{d\tau_\lambda} = -I_\lambda$$

$$I_\lambda(\tau_\lambda) = I_\lambda(0) e^{-\tau_\lambda}$$

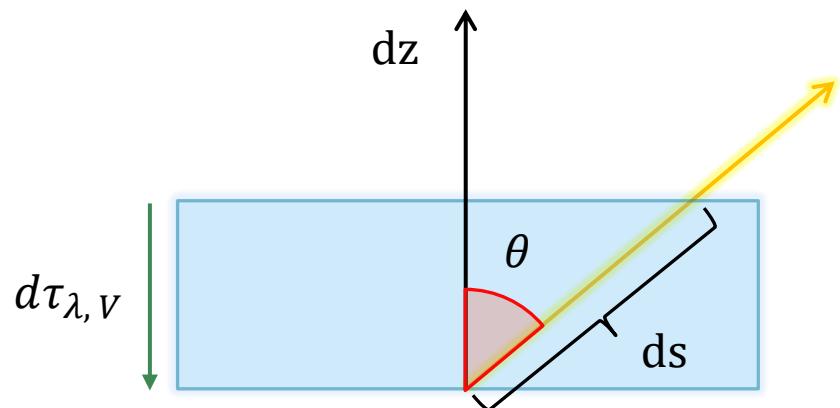
## The Beer-Lambert law

A transmission spectrum is a sum over the areas of atmospheric annuli, weighted by how strongly they absorb light ( $1 - e^{-\tau_\lambda}$ ):



$$\delta_\lambda = \frac{R_p^2 + 2 \int_{R_p}^{R_p+H_A} b \left(1 - e^{-\tau_\lambda(b)}\right) db - 2 \int_0^{R_p} b e^{-\tau_\lambda(b)} db}{R_*^2}$$

# RADIATIVE TRANSFER: EMISSION SPECTRA



Emission spectra usually consider the *vertical* optical depth instead of the path optical depth:

$$d\tau_{\lambda, V} = -\kappa_\lambda dz = -\kappa_\lambda \cos \theta ds$$

The radiative transfer equation for emission spectra then becomes:

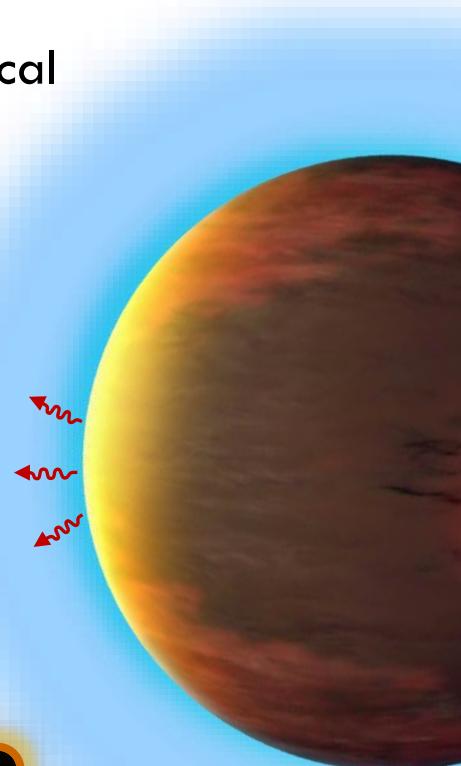
$$\mu \frac{dI_\lambda}{d\tau_{\lambda, V}} = I_\lambda - B_\lambda$$

Solution for top-of-atmosphere intensity:

$$I_{\lambda, \text{top}}(\mu) = \frac{1}{\mu} \int_0^\infty B_\lambda(\tau_{\lambda, V}) e^{-\frac{\tau_{\lambda, V}}{\mu}} d\tau_{\lambda, V}$$

Integrating over all emission angles gives us the planet flux:

$$F_{p, \lambda} = 2\pi \frac{R_p^2}{d^2} \int_0^1 \int_0^\infty B_\lambda(\tau_{\lambda, V}) e^{-\frac{\tau_{\lambda, V}}{\mu}} d\tau_{\lambda, V} d\mu$$



# DETERMINING THE OPTICAL DEPTH

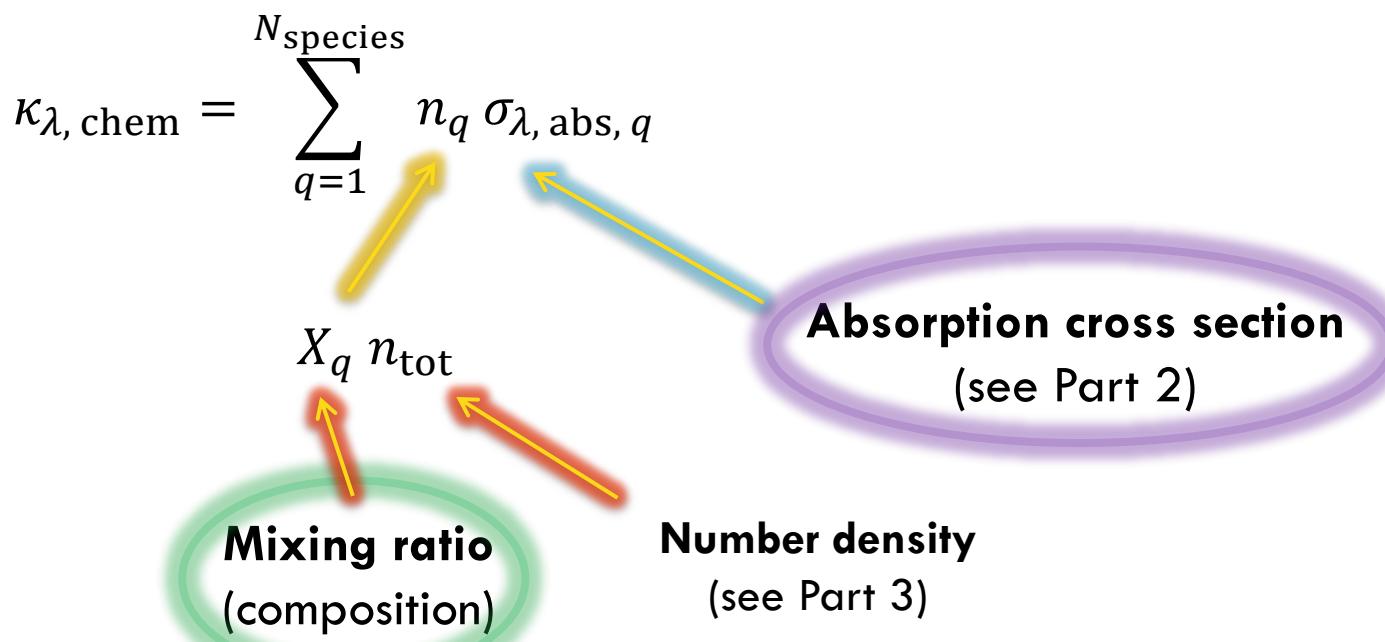
The optical depth is required to compute exoplanet spectra:

$$\tau_\lambda = \int \kappa_\lambda \, ds$$

Many different physical processes can contribute opacity to the extinction coefficient:

$$\kappa_\lambda = \kappa_{\lambda, \text{chem}} + \kappa_{\lambda, \text{Rayleigh}} + \kappa_{\lambda, \text{pair}} + \kappa_{\lambda, \text{aerosol}}$$

Let us focus on the first term ('regular absorption' by atoms, molecules, or ions):

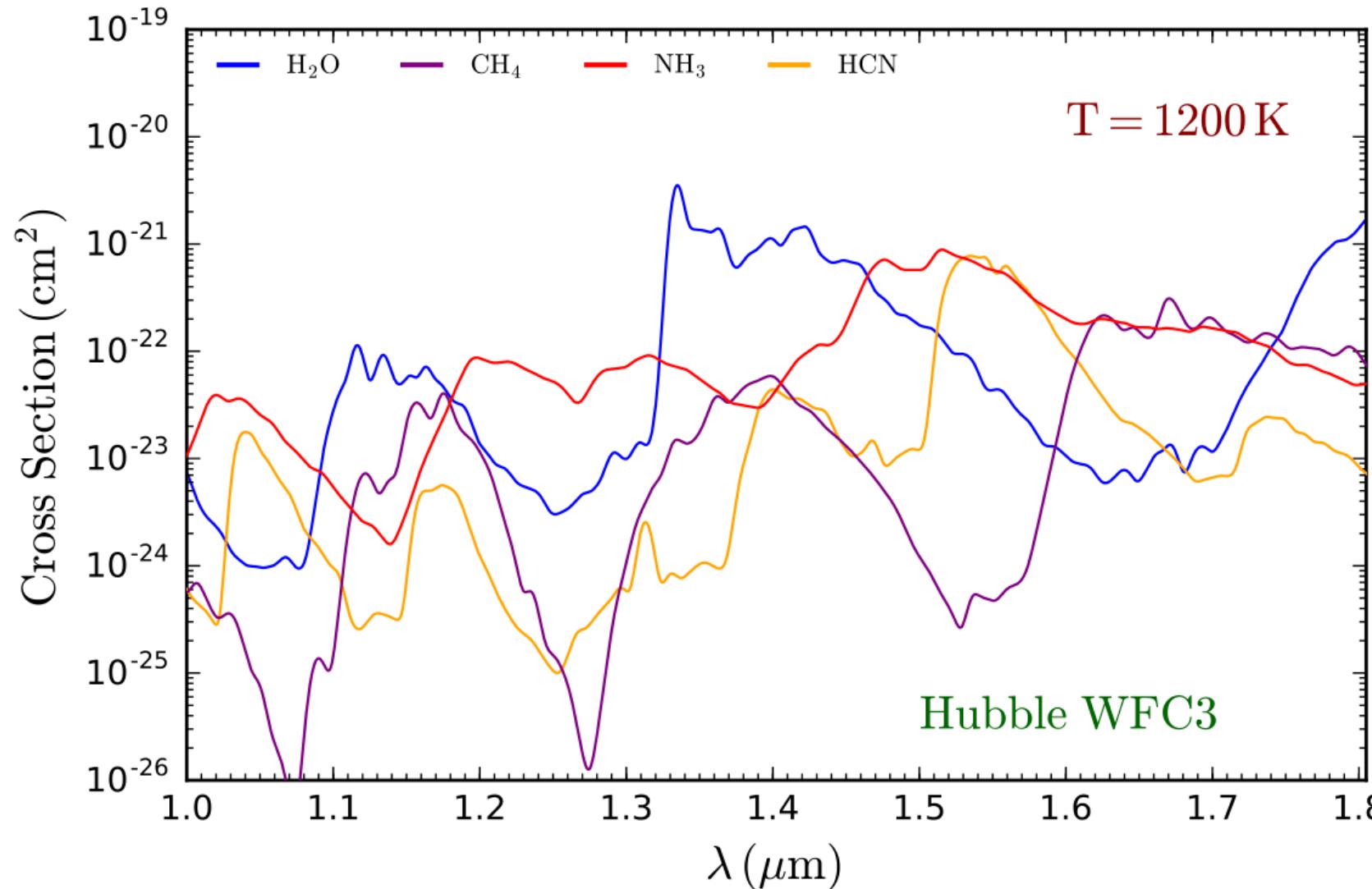


**Tutorial 1: Sequences of spectra and atmospheric compositions**

PART 2:

# OPACITY IN EXOPLANET ATMOSPHERES

# INTRODUCTION TO CROSS SECTIONS



Cross sections,  $\sigma_\lambda$ , determine how strongly a given chemical species absorbs (or scatters) light

They can be thought of as the ‘effective area’ of a chemical species

# COMPUTATION OF CROSS SECTIONS

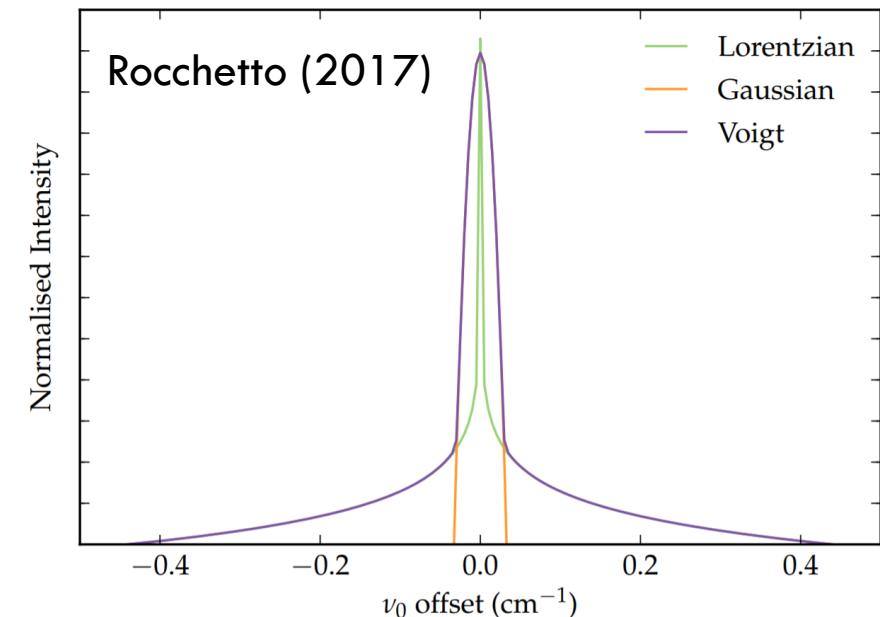
$$\sigma_\lambda(P, T) = \sum_j S_j(T) f(\lambda, \lambda_{0,j}, P, T)$$

Sum over many billions of quantum transitions

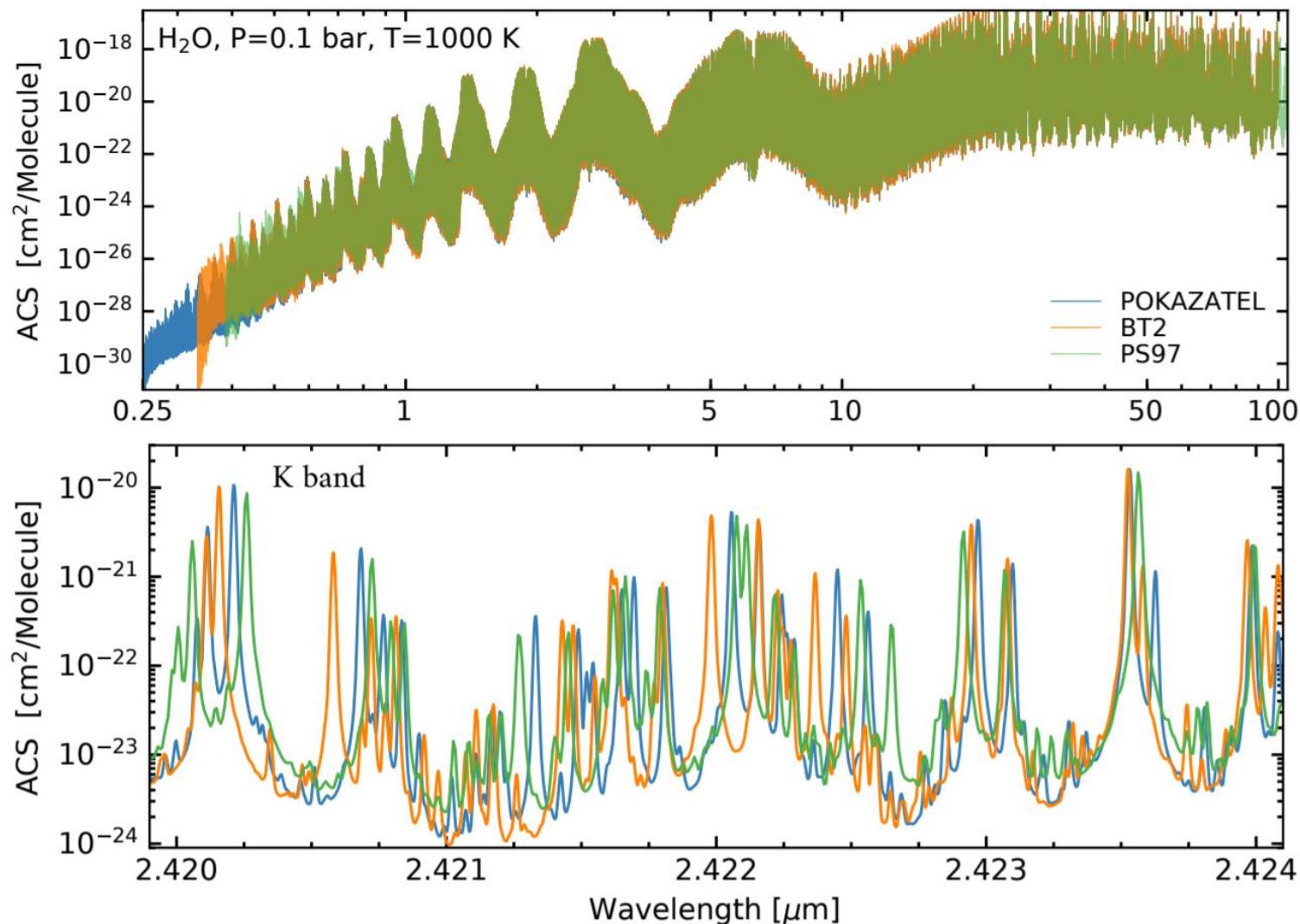
Tabulated for each transition in a **line list**

(ExoMol, HITEMP, HITRAN etc.)

**Line profiles** are normally assumed to be Voigt profiles

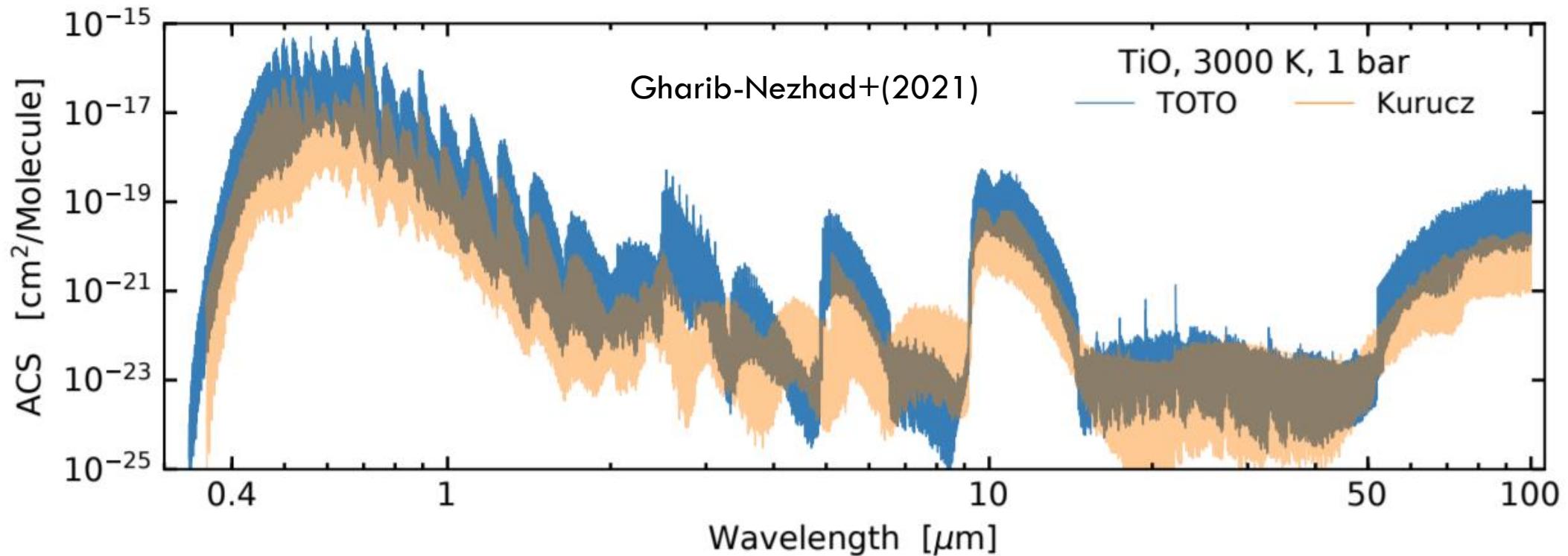


# CROSS SECTION UNCERTAINTIES



Gharib-Nezhad+(2021)

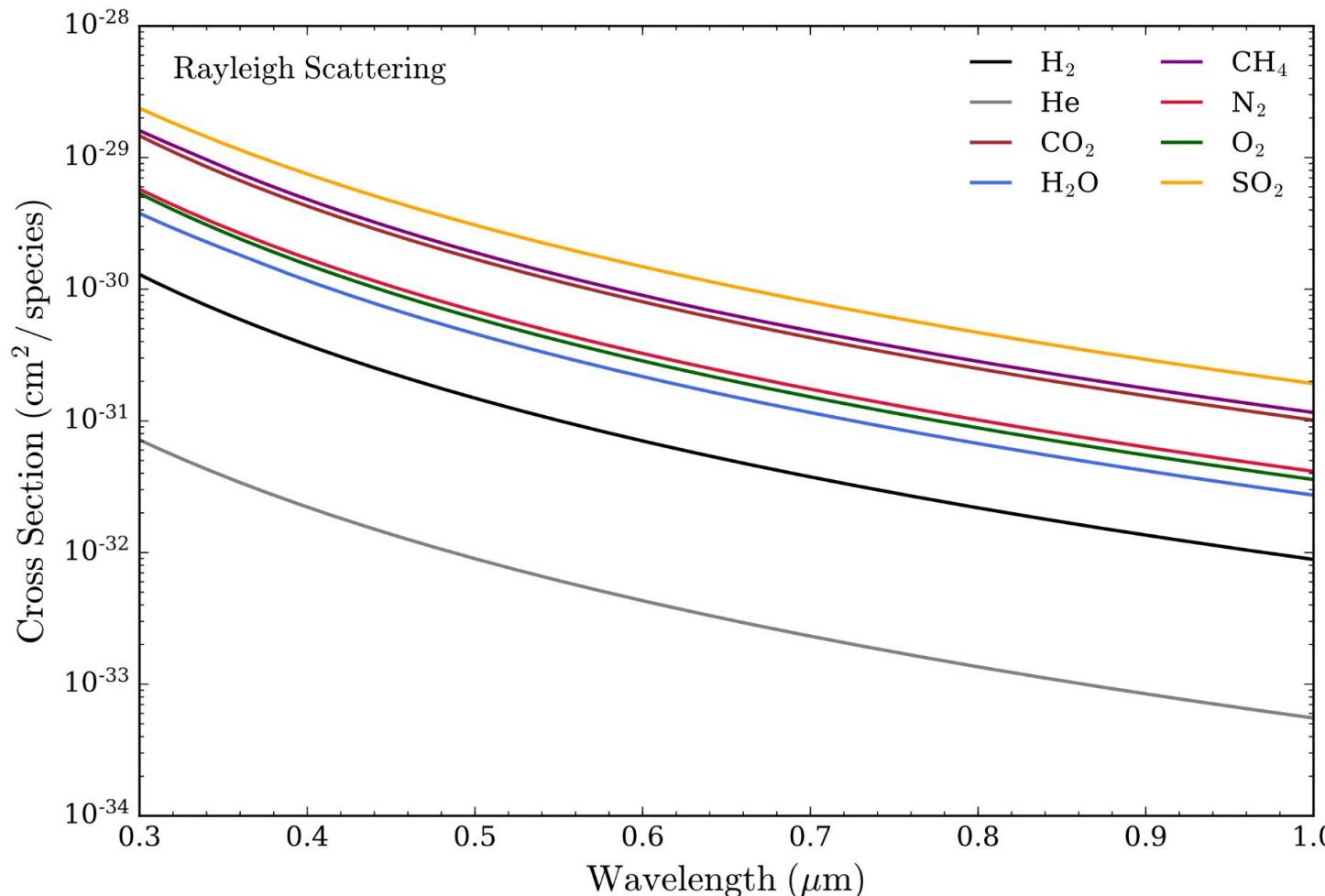
# CROSS SECTION UNCERTAINTIES



The **choice of line list** is an important consideration  
that can **significantly alter cross sections**

Cross sections are fixed inputs to atmospheric  
models, so any **uncertainties in cross sections**  
**can propagate to model inferences**

# RAYLEIGH SCATTERING

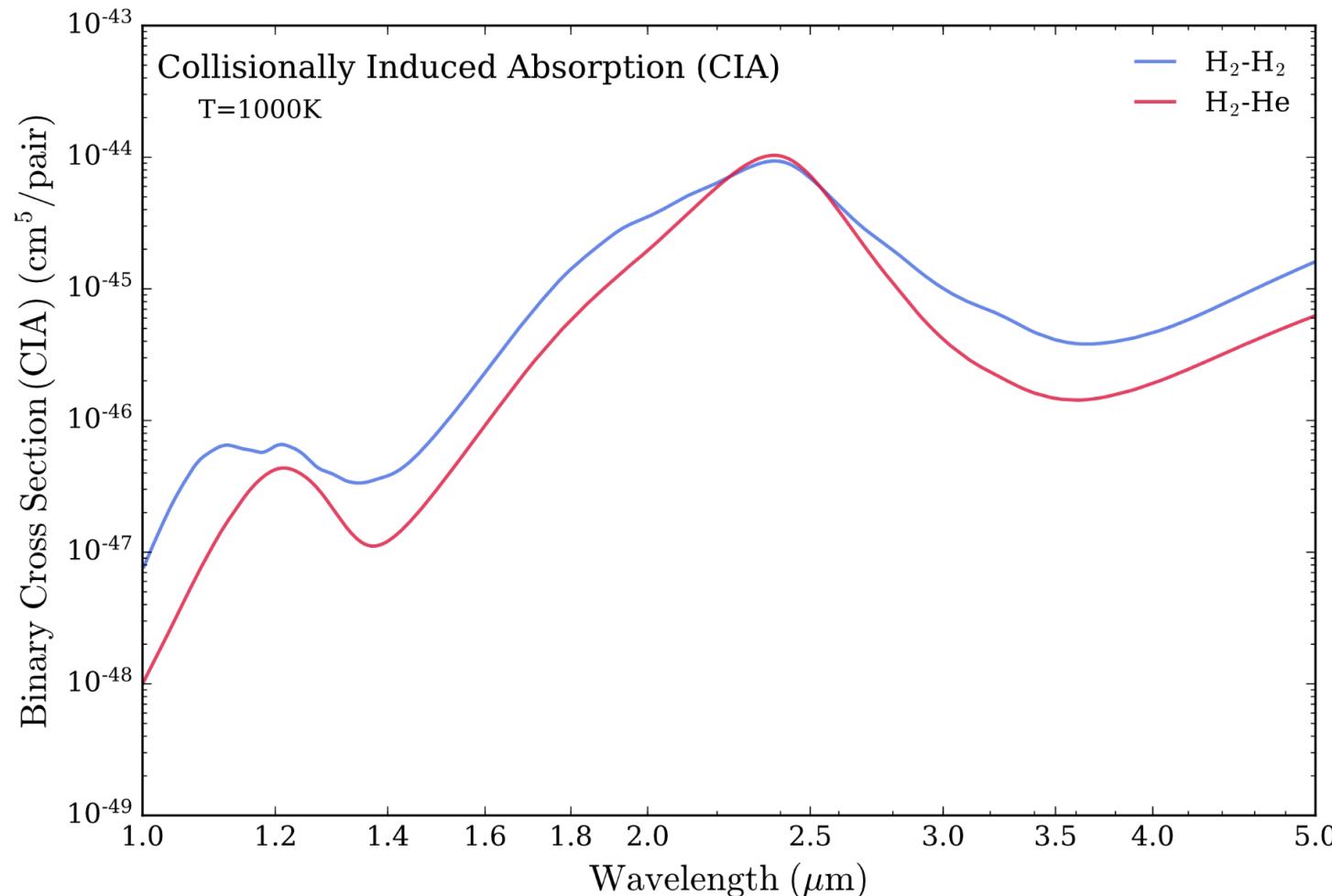


$$\kappa_{\lambda, \text{Rayleigh}} = \sum_{q=1}^{N_{\text{species}}} n_q \sigma_{\lambda, \text{Rayleigh}, q}$$

$$\sigma_{\lambda, \text{Rayleigh}, q} = \frac{128}{3} \pi^5 \alpha_q^2(\lambda) \lambda^{-4} F_{\text{King}, q}(\lambda)$$

**Rayleigh scattering provides a continuum opacity that can dominate at short wavelengths**

# CONTINUUM (PAIR PROCESS) ABSORPTION

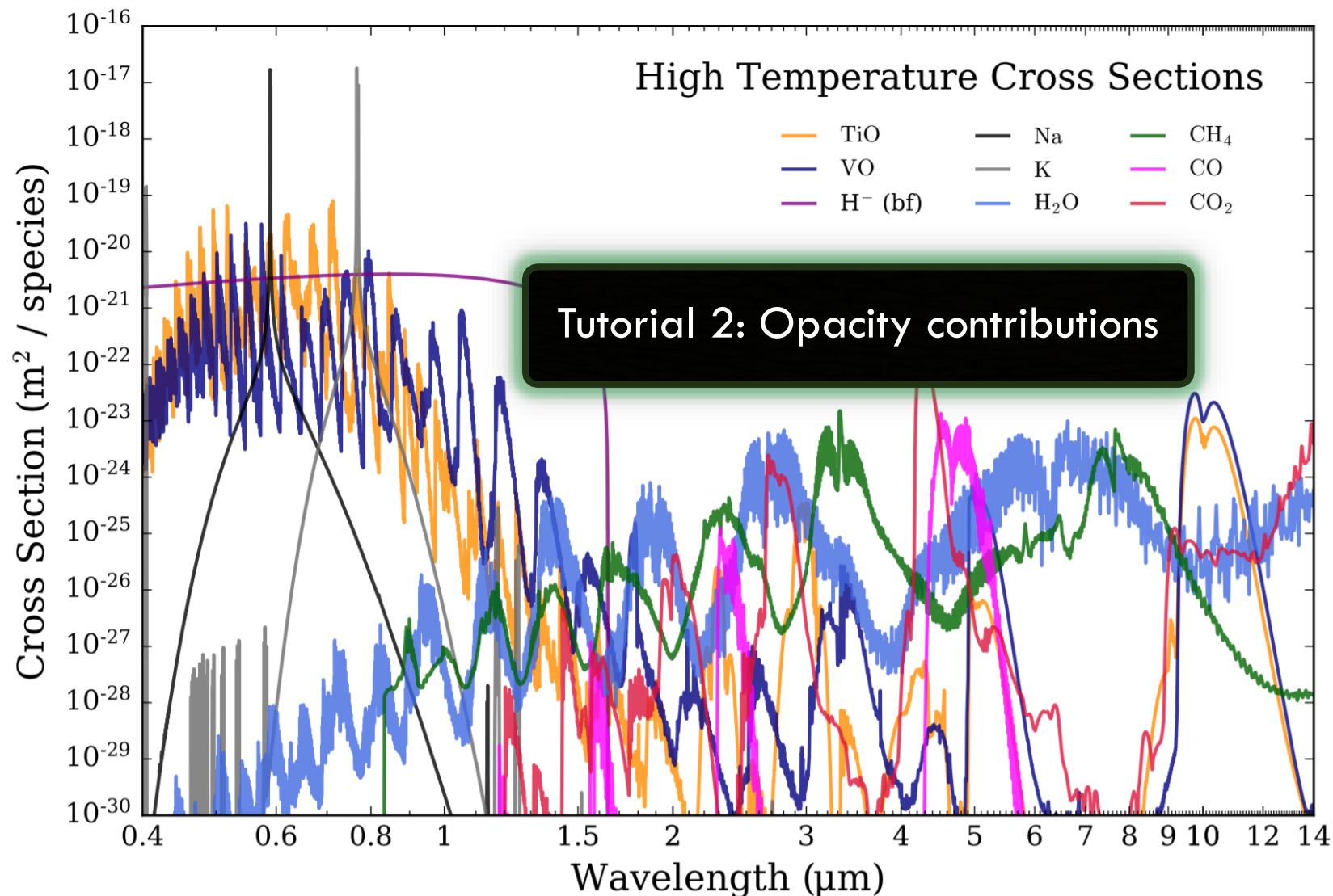


$$\kappa_{\lambda, \text{pair}} = \sum_{\text{pairs}} n_{q_1} n_{q_2} \sigma_{\lambda, \text{pair}, q}$$

**Collision-induced absorption**  
increases with  $n_{\text{tot}}^2$ , so this absorption  
dominates at high pressures

→ sets the floor of a spectrum

# CROSS SECTION DATABASES



PART 3:

# BUILDING A MODEL ATMOSPHERE

# ATMOSPHERE MODELLING

To compute optical depths, we need to know the number densities in each atmospheric layer ( $n_q$ ) and the physical spacing of each layer ( $dr$ )

$$\tau_\lambda = \int \kappa_\lambda \, ds \quad \kappa_{\lambda, \text{chem}} = \sum_{q=1}^{N_{\text{species}}} n_q \sigma_{\lambda, \text{abs}, q}$$

The number densities are given by the **ideal gas law**:

$$n_q = X_q \frac{P}{k_B T(P)}$$

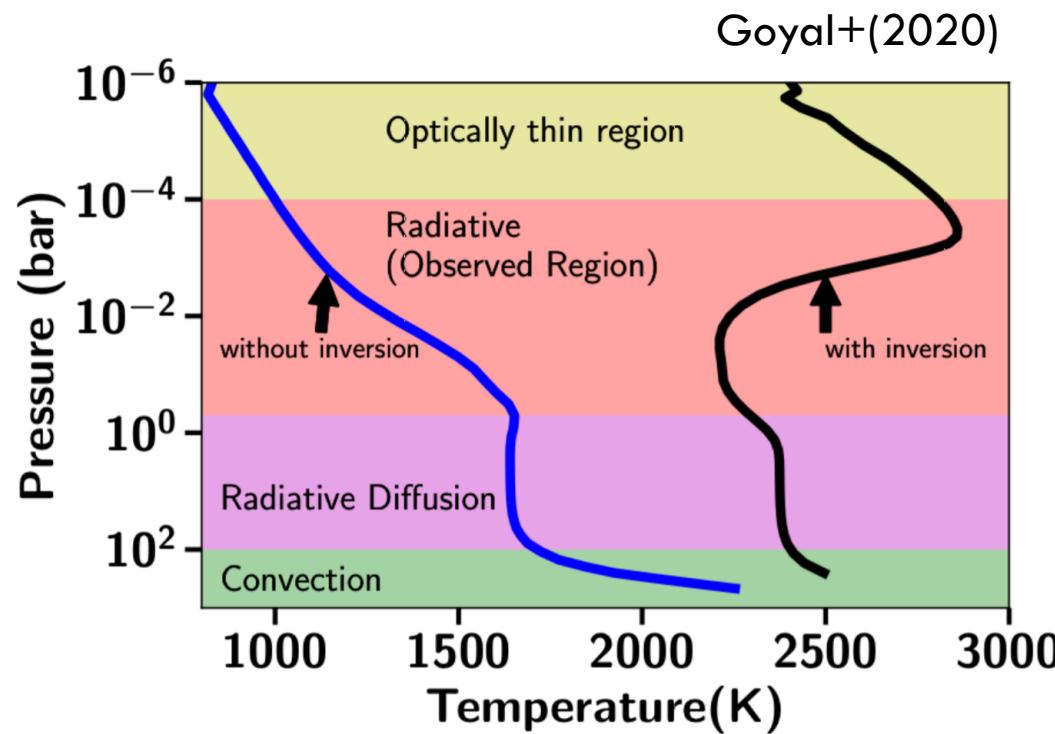
We need a prescription for  $T(P)$

The radial grid is determined by solving the equation of **hydrostatic equilibrium**:

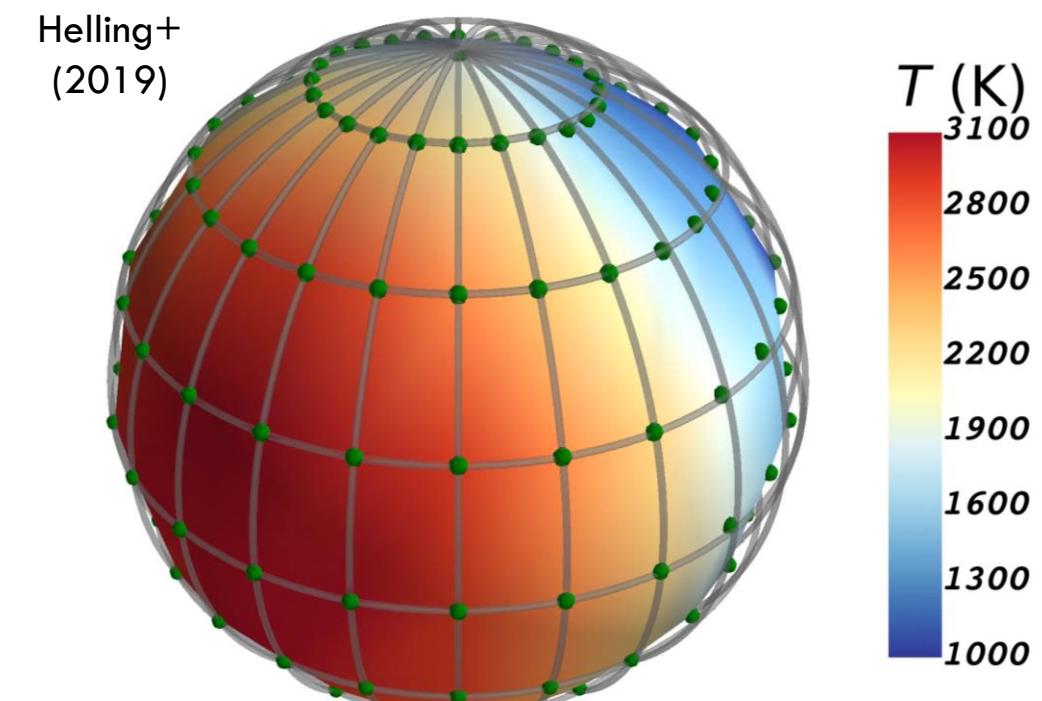
$$\frac{dP}{dr} = -\frac{GM_p \rho(r)}{r^2}$$

$$\rightarrow r(P) = \left( \frac{1}{R_{p, \text{deep}}} + \int_{P_{\text{deep}}}^P \frac{k_B T(P)}{GM_p \mu_{mmw}} \frac{dP}{P} \right)^{-1}$$

# ATMOSPHERE MODELLING: TEMPERATURE STRUCTURE

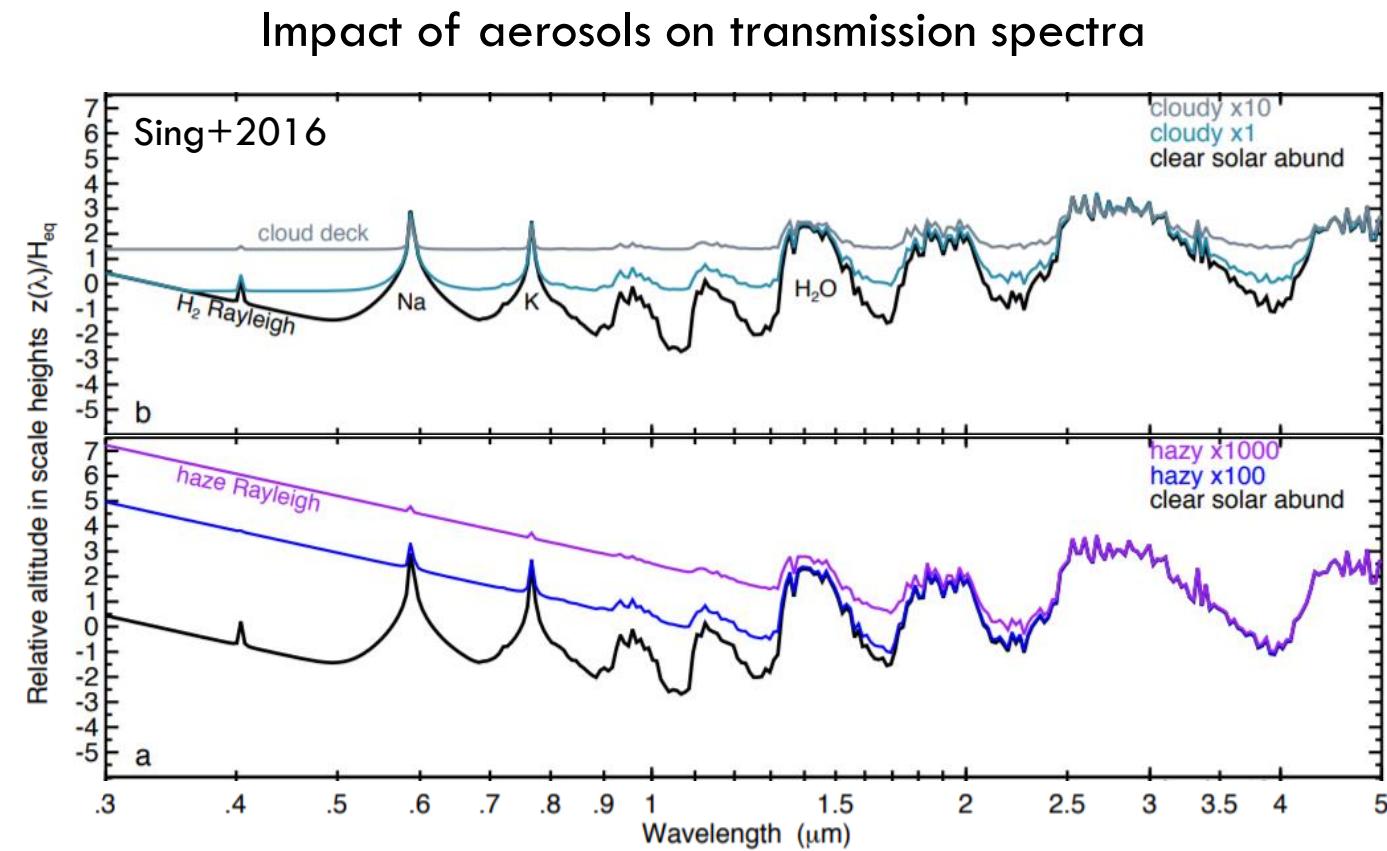
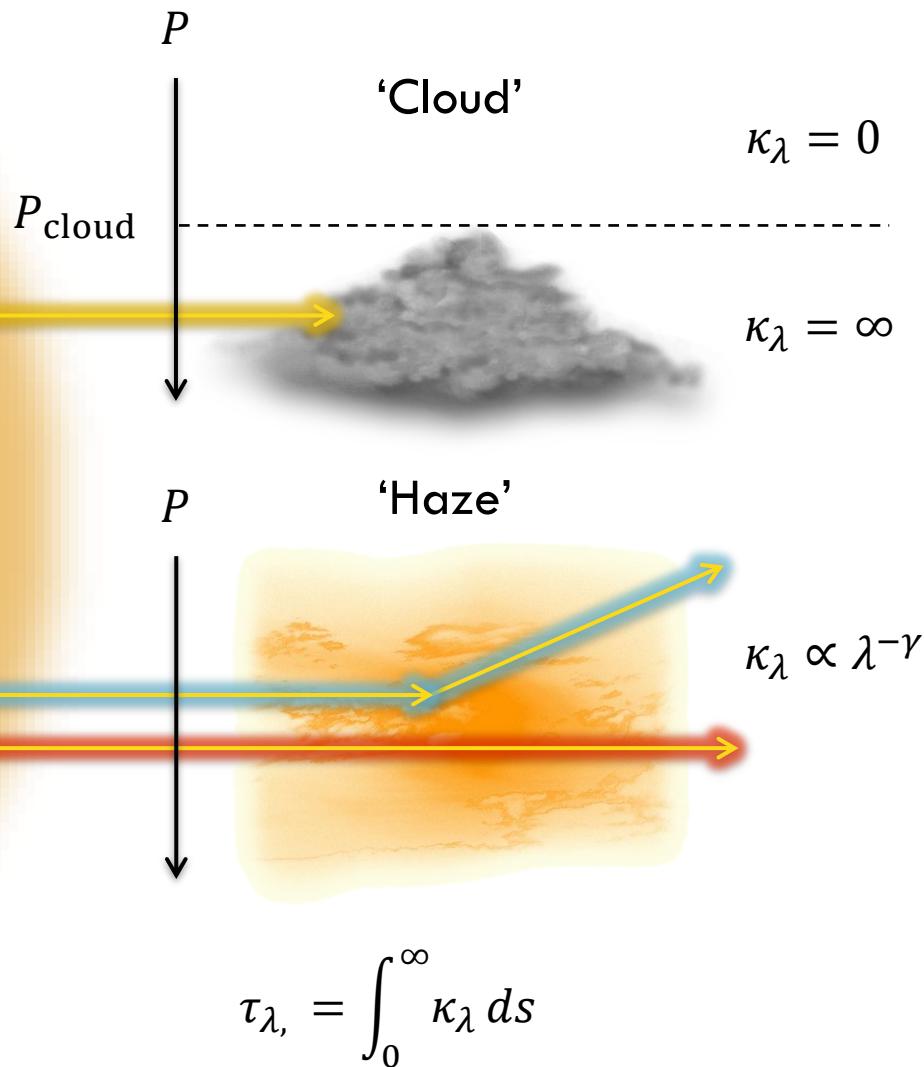


A **self-consistent P-T profile** can be computed by iteratively enforcing the condition of **radiative-convective equilibrium**



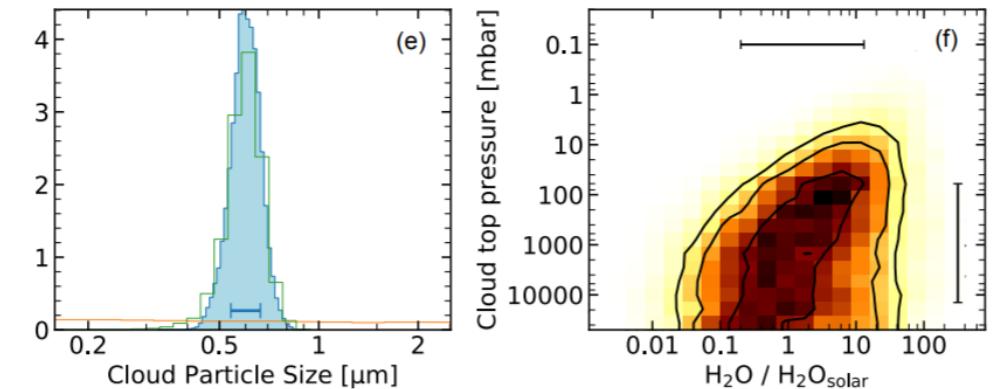
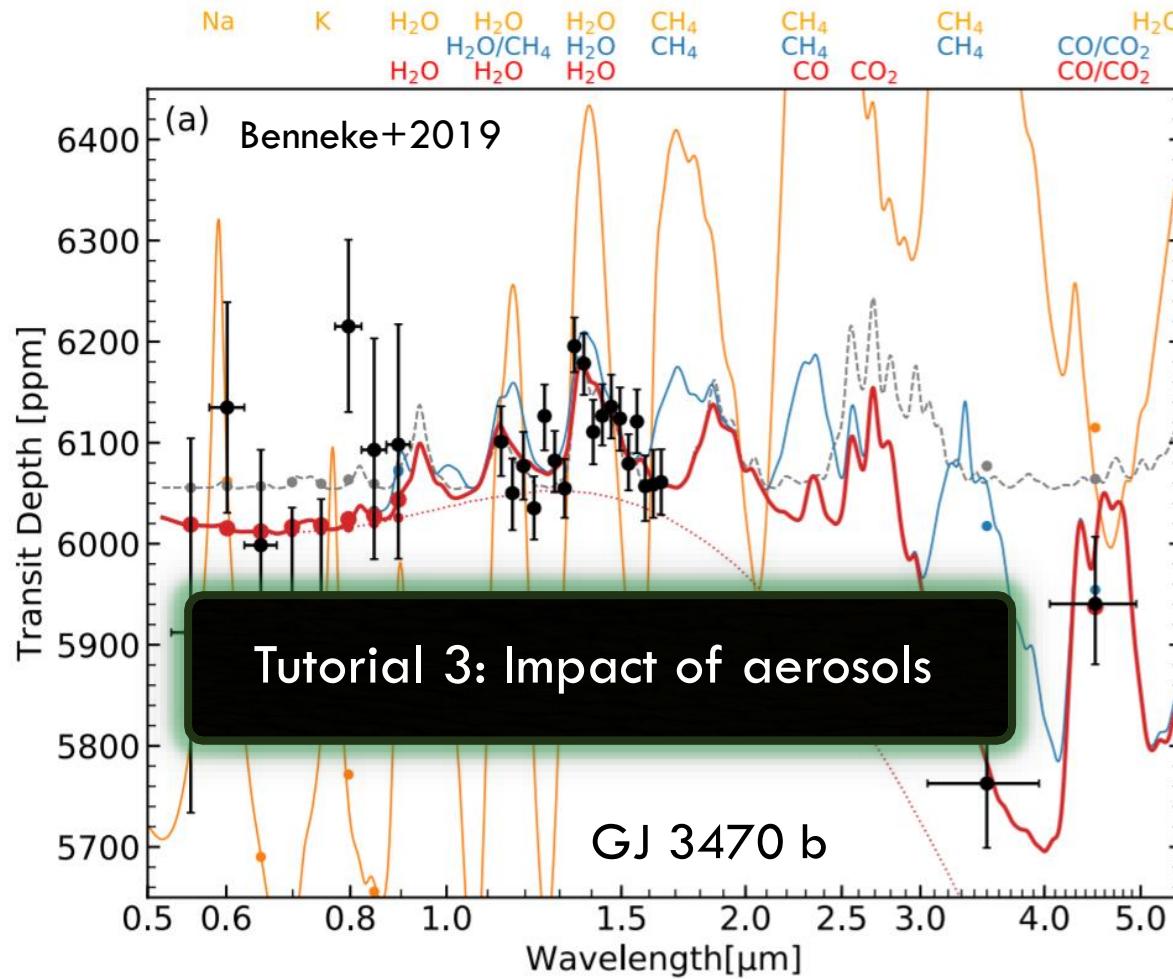
**3D models** can have temperatures and compositions that strongly vary with longitude, latitude, and altitude

# ATMOSPHERE MODELLING: AEROSOLS



Clouds → flat spectrum + muted features  
Haze → strong scattering + non-Rayleigh slope

# MIE SCATTERING AEROSOLS



**Mie scattering predicts a rapid drop off in aerosol extinction for  $\lambda \gtrsim 2\pi r$**

$$\kappa_\lambda = n_0 e^{-\frac{z}{fH_{\text{gas}}}} \int_0^\infty \pi r^2 Q_{\text{ext}} \left( m, \frac{2\pi r}{\lambda} \right) P(r) dr$$

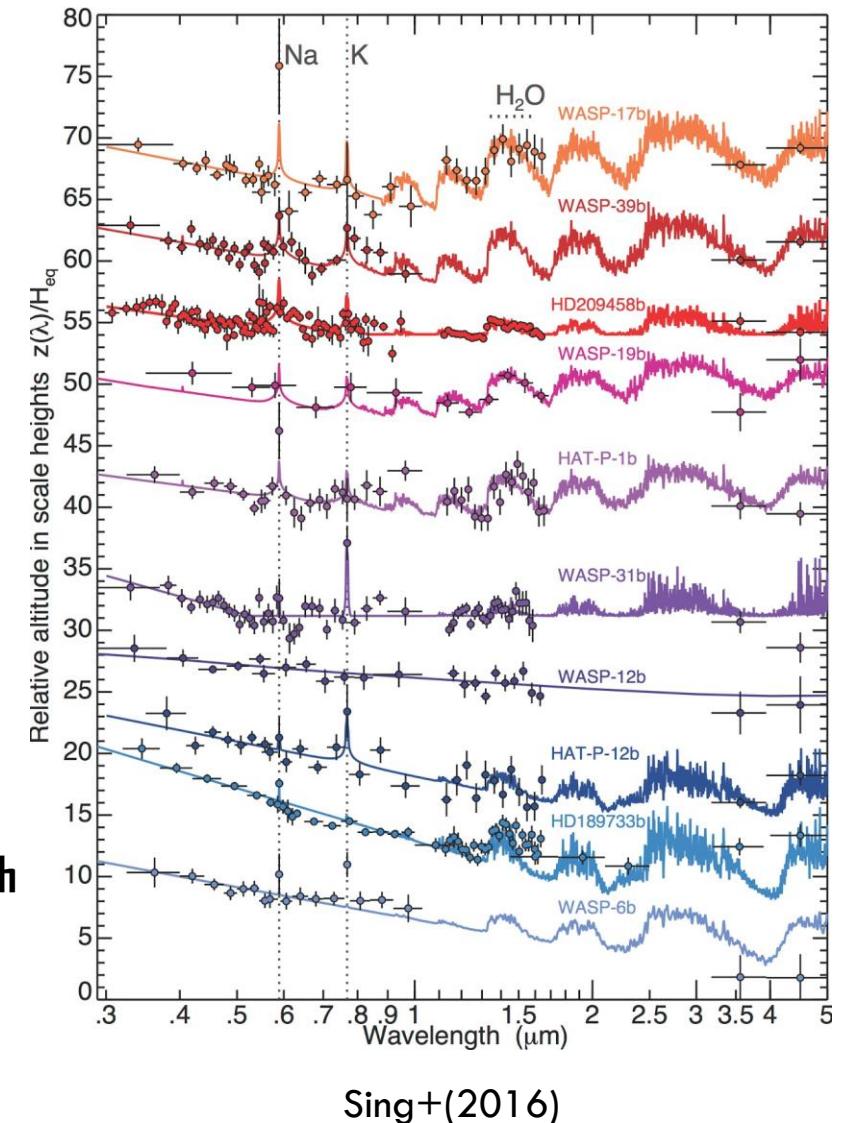
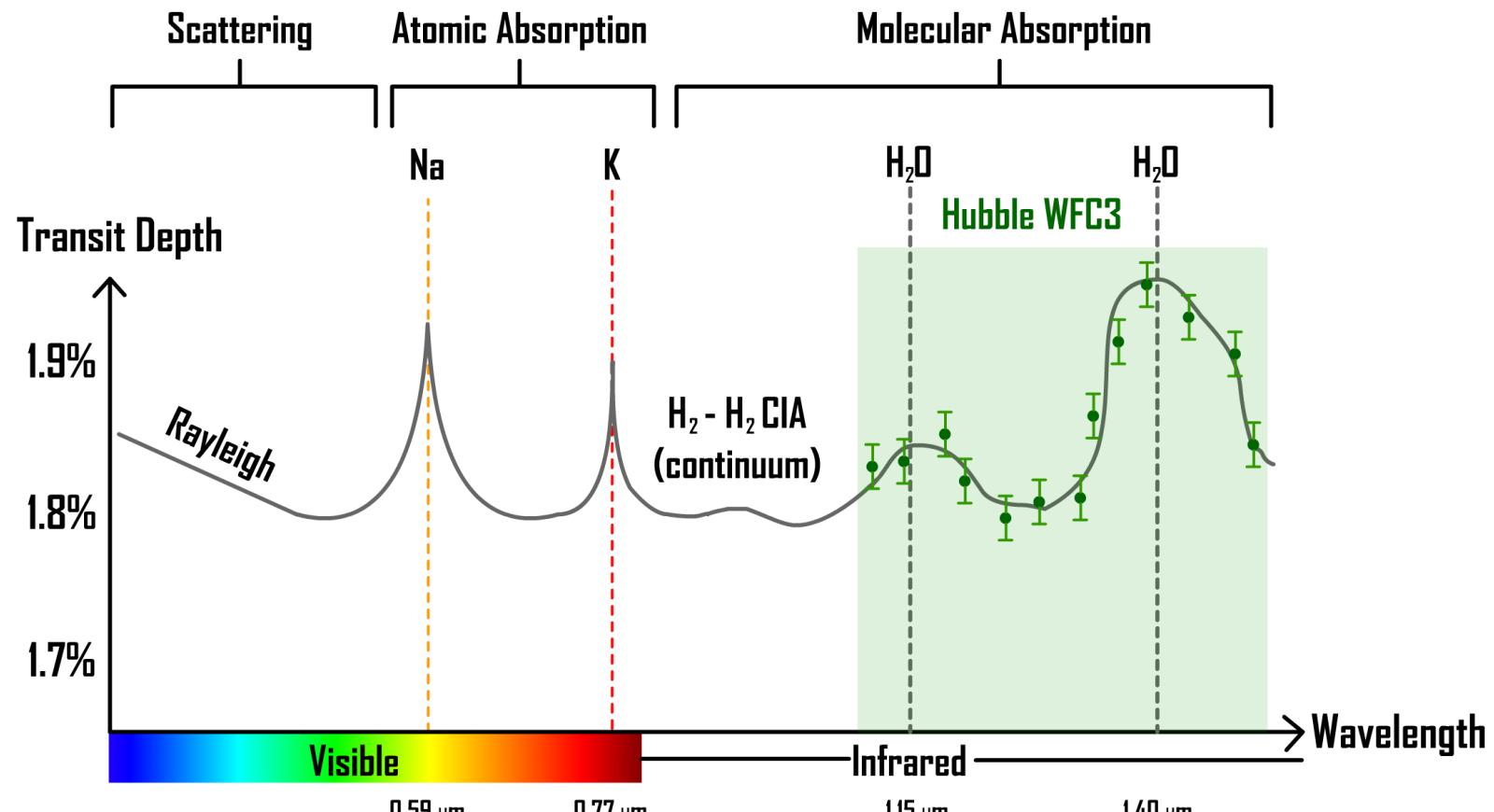
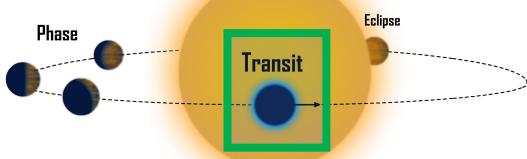
$$P(r) = \frac{1}{\sigma_g r \sqrt{2\pi}} e^{-\left(\frac{\ln r - \ln r_m}{\sqrt{2}\sigma_g}\right)^2}$$

[Equations from Zhang+2019]

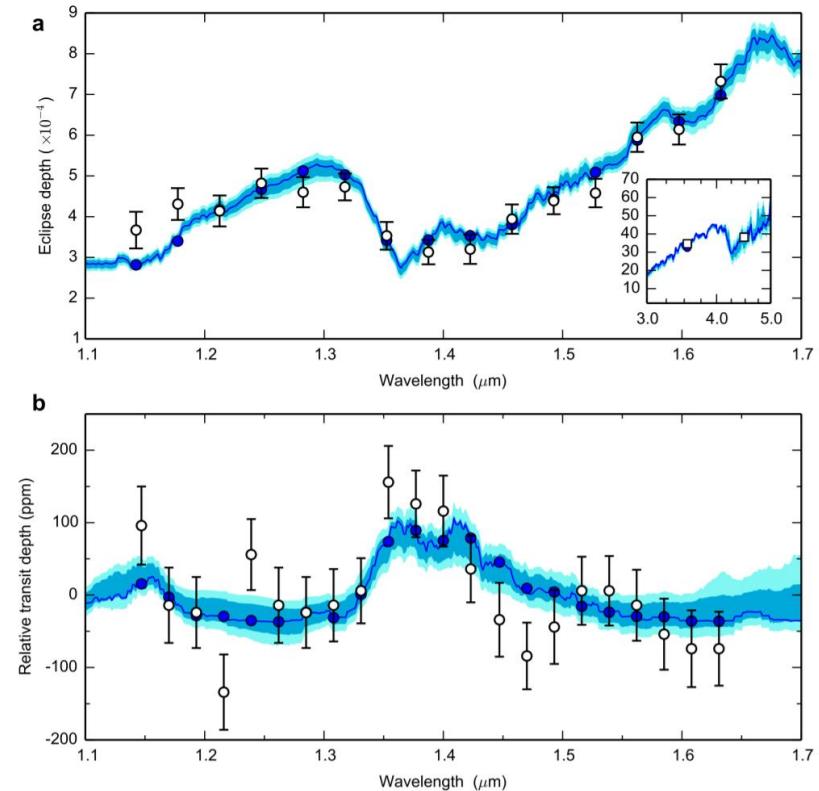
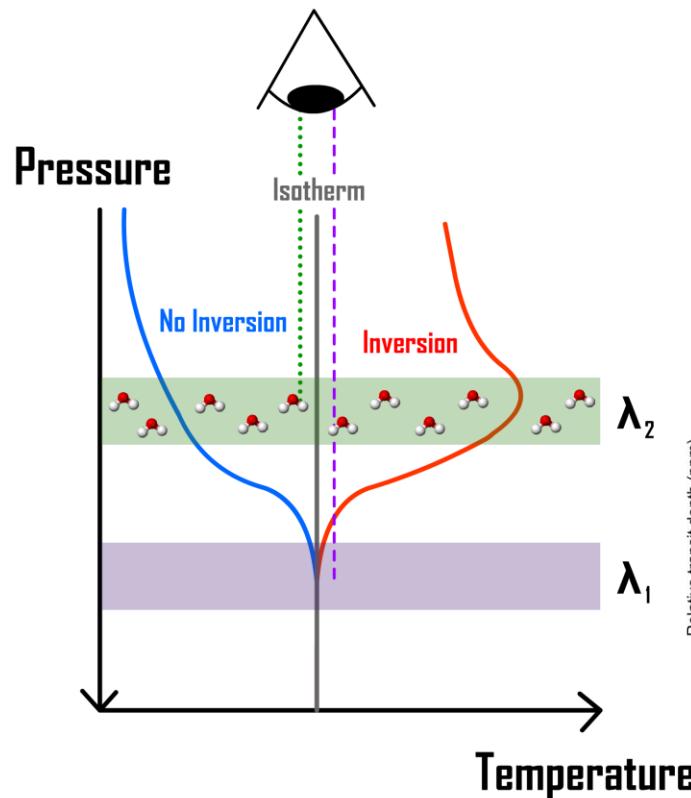
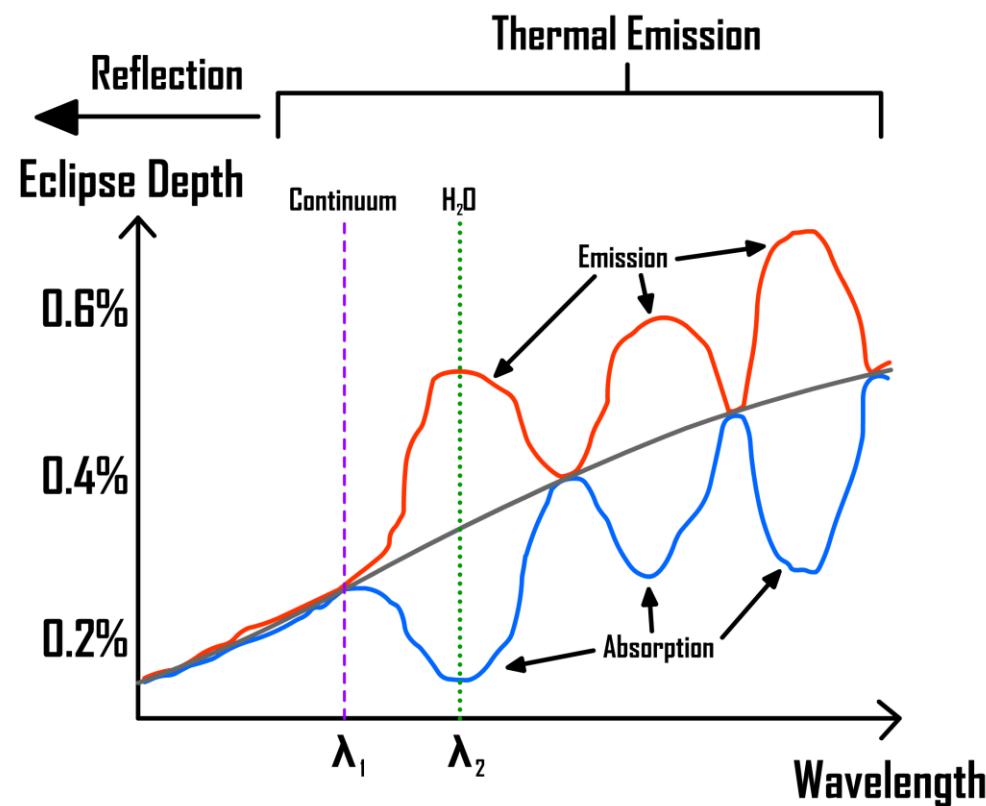
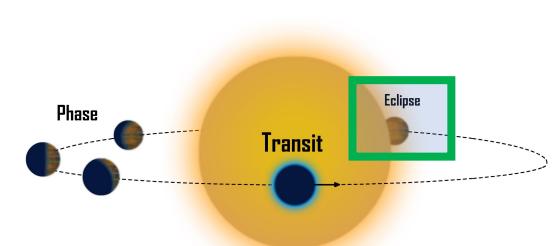
TAKEAWAYS:

# TRANSMISSION AND EMISSION SPECTROSCOPY

# TRANSMISSION SPECTROSCOPY

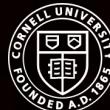


# EMISSION SPECTROSCOPY



Kreidberg+(2014)

# QUESTIONS?



Cornell University

Ryan MacDonald  
August 2021