

ESP Open-source Opacity Database

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Why an Opacity Database?

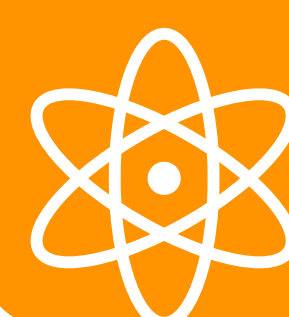
We need **opacities** (cross-sections per unit mass) of **atoms** and **molecules** in all sort of (exo)planetary atmospheric calculations!

But computing opacities is a **very difficult task** that starts with **line lists** that have **very large number of transitions**. It takes an incredible amount of **computing time** to do so! We do not want to “*reinvent the wheel*” for this tedious step of transforming line list data into opacities for **multiple points** in **T** and **P** every time, therefore we are creating a **publicly available opacity database** for the exoplanet community.

New Open Opacity Database for Exoplanetary atmospheres! Coming Soon!



Take a picture to download the papers



How do we calculate them?

Molecular and atomic opacities are calculated using **HELIOS-K** (Grimm & Heng 2015). We use line lists from different databases like **HITRAN**, **HITEMP**, **ExoMol**, **Kurucz** and **NIST**. It calculates the

molecular absorption of each line's strength and resamples the line-by-line data into a manageable **k-distribution** format. ***We use GPU's to accelerate the calculations.**

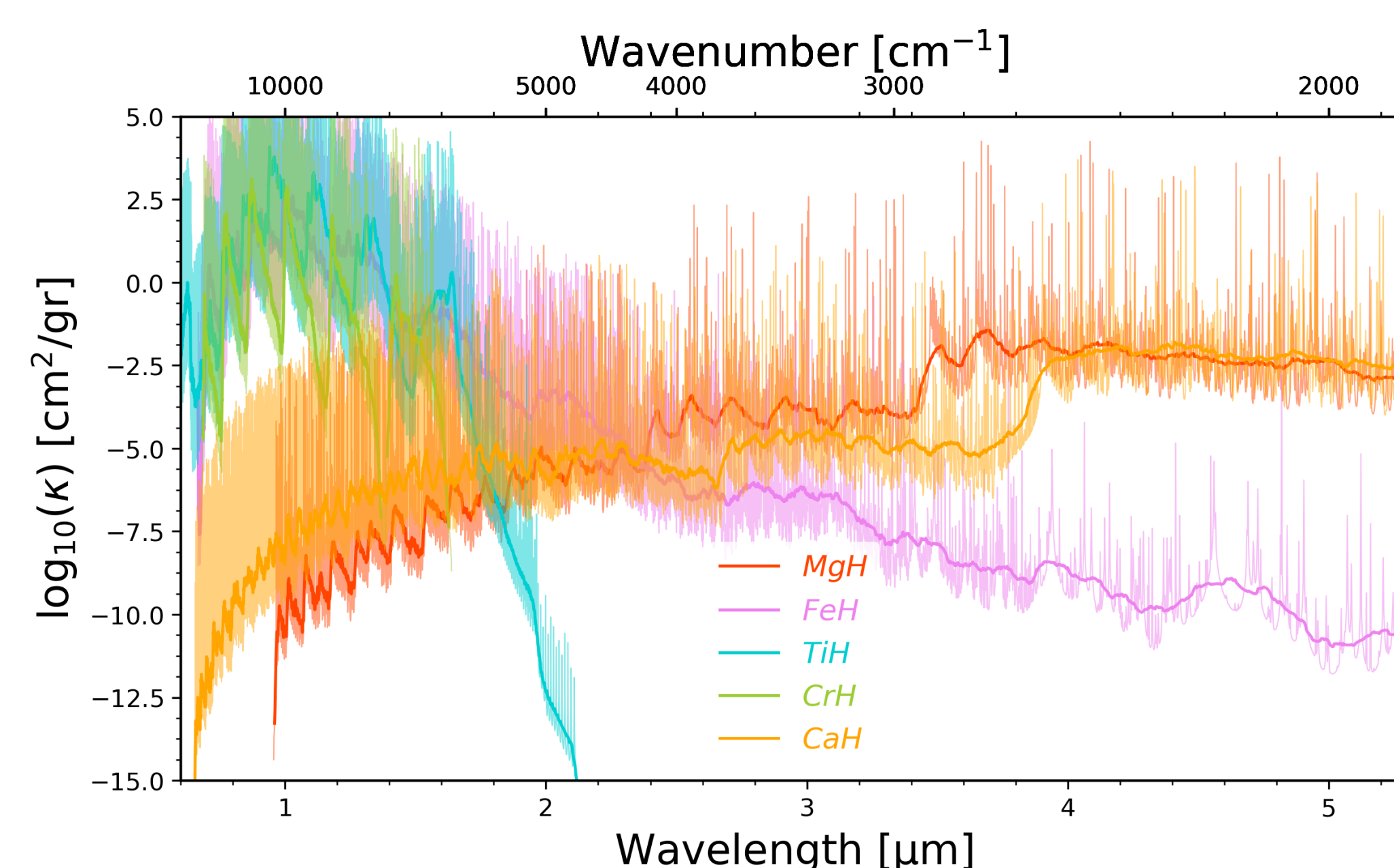
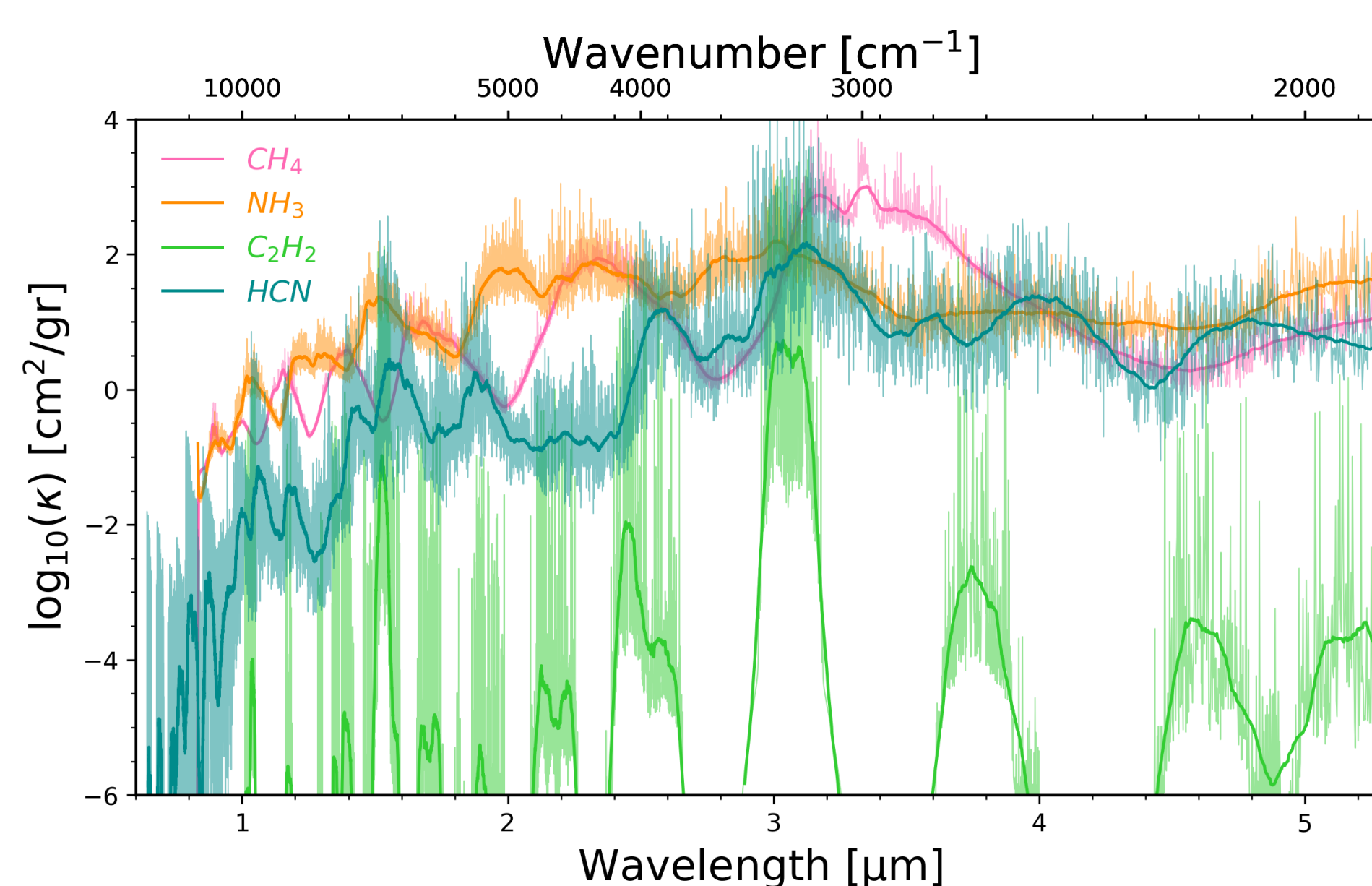
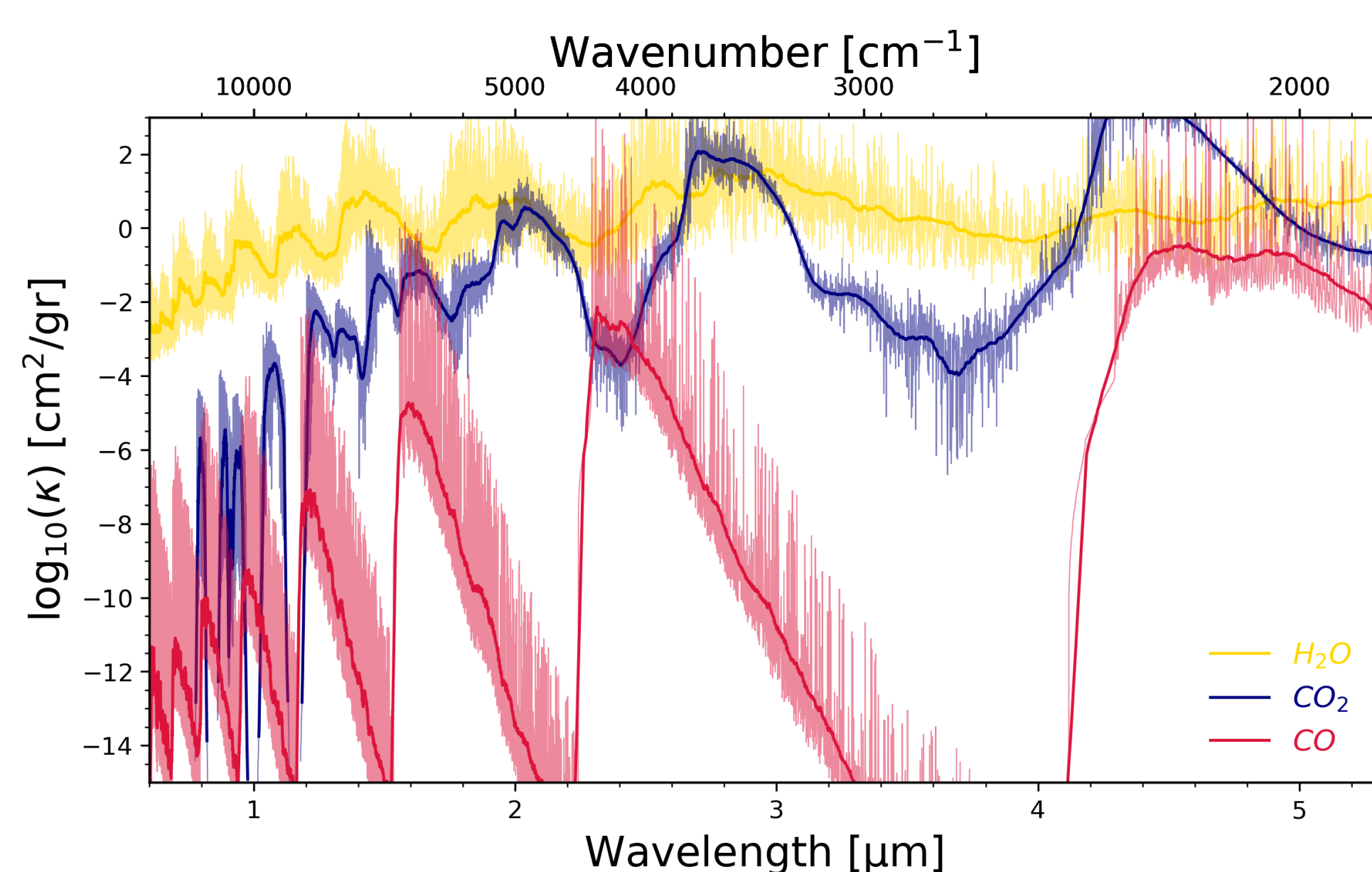


Figure 1. Examples of opacities. They were calculated using **T** = 1500 K and **P** = 10⁻³ bars

$\kappa = S \cdot \Phi$ **Opacity Function = Intensity * Line Shape**

$$\Phi = \left(\frac{\ln 2}{\pi} \right)^{\frac{1}{2}} \cdot \frac{H_v}{\Gamma_D}$$

Line Shape = The Voigt-Profile

$$H_v = \frac{a}{\pi} \cdot \int_{-\infty}^{\infty} \frac{\exp(u^2)}{(u - u')^2 + a^2} du'$$

Must be solved numerically! Computationally Expensive*

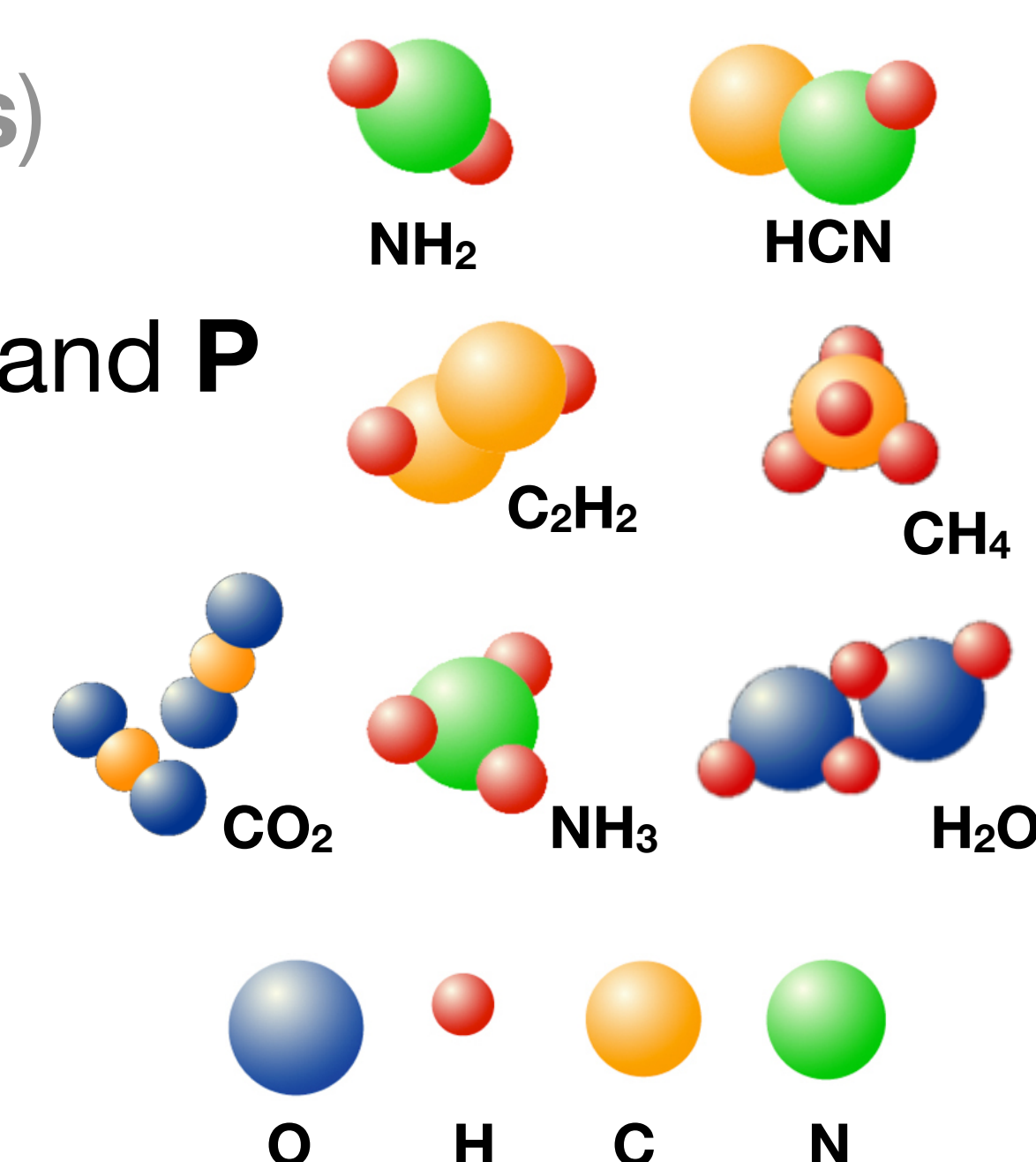
H_v : Voigt H-function Γ_D : Doppler profile a : Damping parameter

What does it have?

~ **150** molecules (isotopologues)

~ **60** Atoms and Ions

• **Grid** of opacity functions in **T** and **P**



Challenges

- **Long time** to calculate
- **Large amounts** of data
- Wavenumber **resolution** (10⁻² cm⁻¹)
- **No theory** for *cutting length* and *pressure broadening* for large amount of lines.

References

- Grimm, S.L., & Heng, K., 2015, *Astrophysical Journal*, 808,182
- Grimm, S.L., **Guzmán Mesa, A.**, et al 2019, *In prep*
- <https://github.com/exoclimes/HELIOS-K>