

# **Community Needs for Molecular & Atomic Opacities**

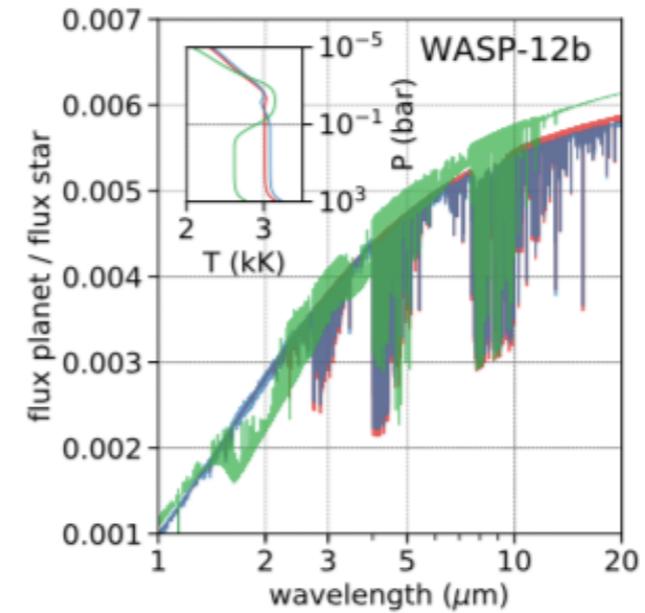
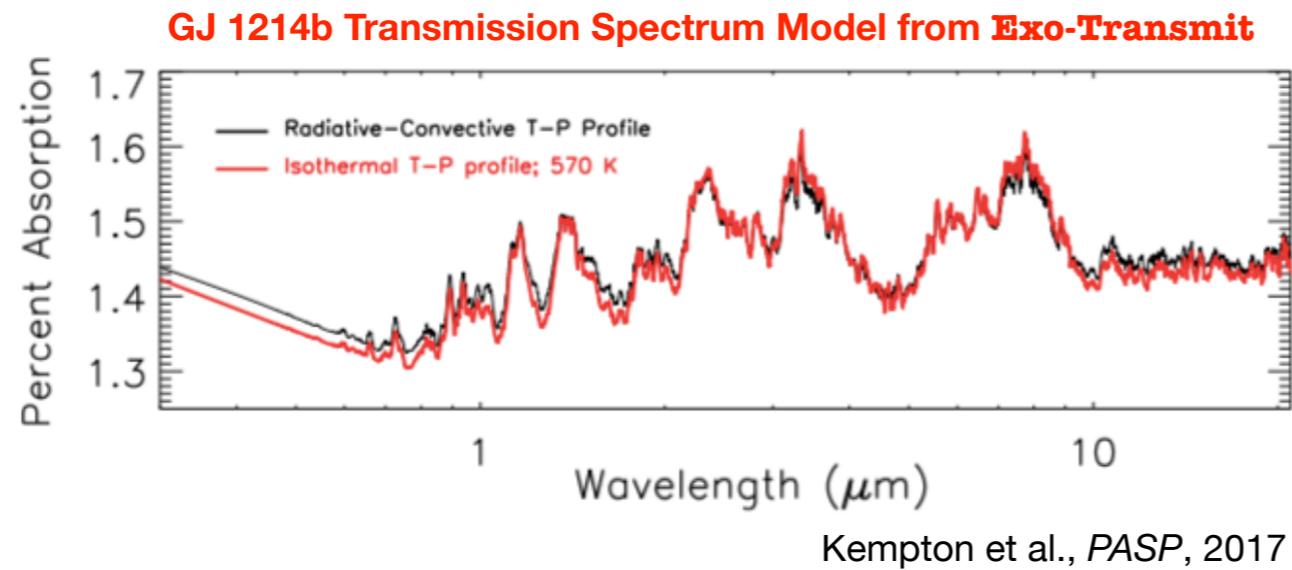
***Eliza Kempton & Natasha Batalha***

*Nikole Lewis, Clara Sousa-Silva, Richard Freedman, Mark Marley, Iouli Gordon, Sergey Yurchenko, Jonathan Tennyson, Jeff Valenti*

**ExoPAG**

# Opacities: Why do we care?

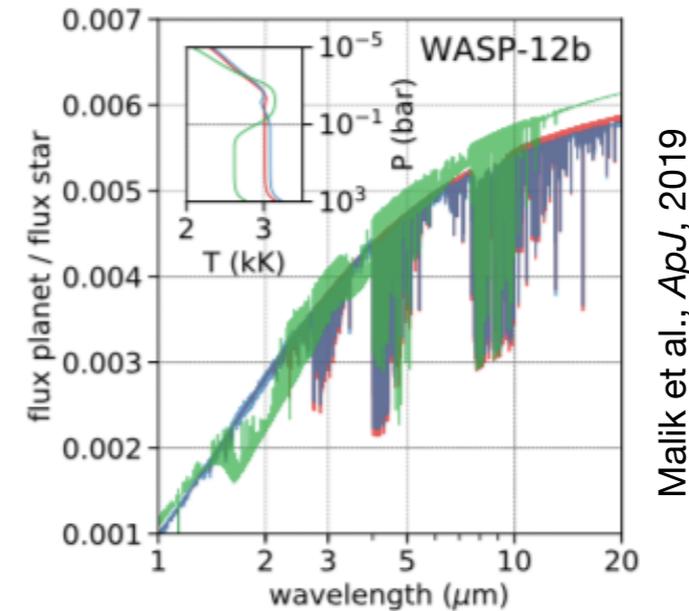
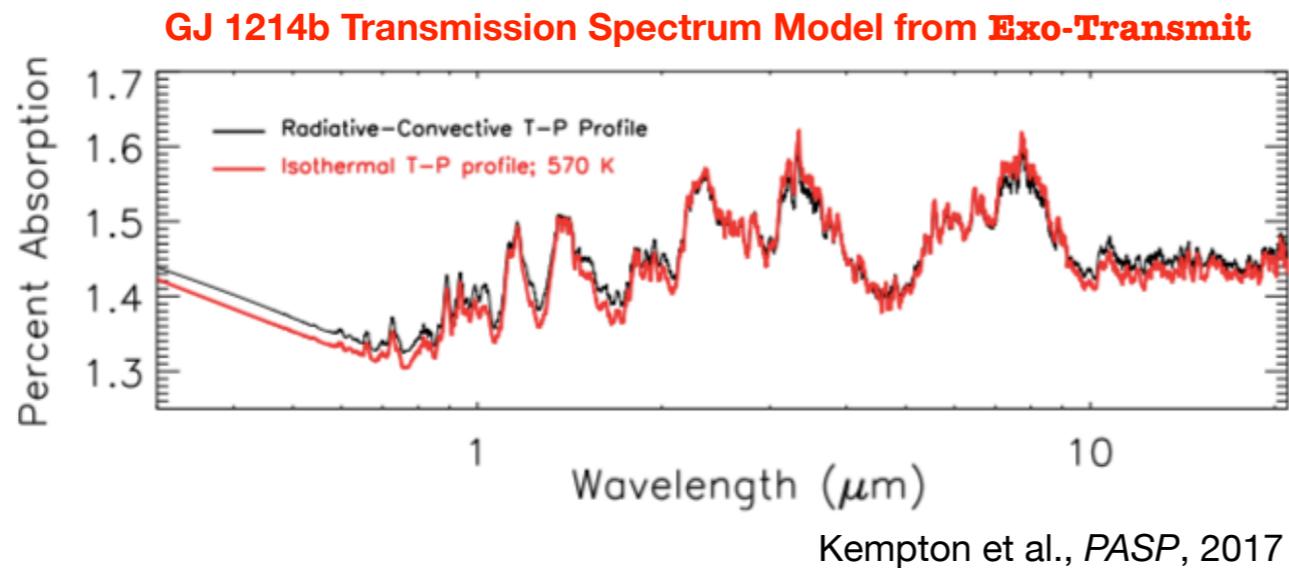
They are a critical input to exoplanet atmosphere models (like these)



**WASP-12b  
Secondary Eclipse  
Spectrum Model  
from HELIOS**

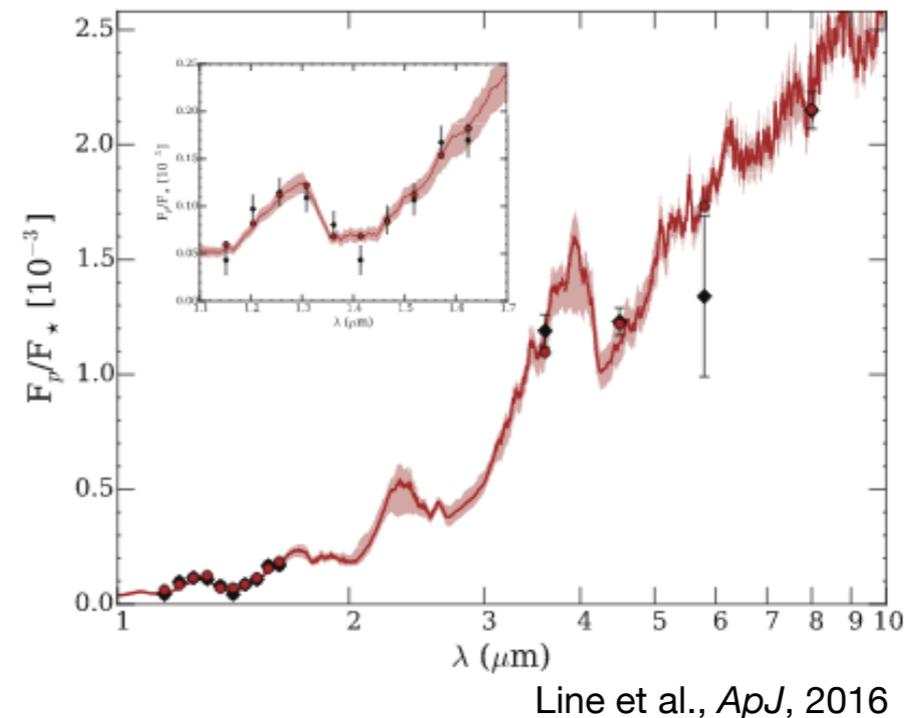
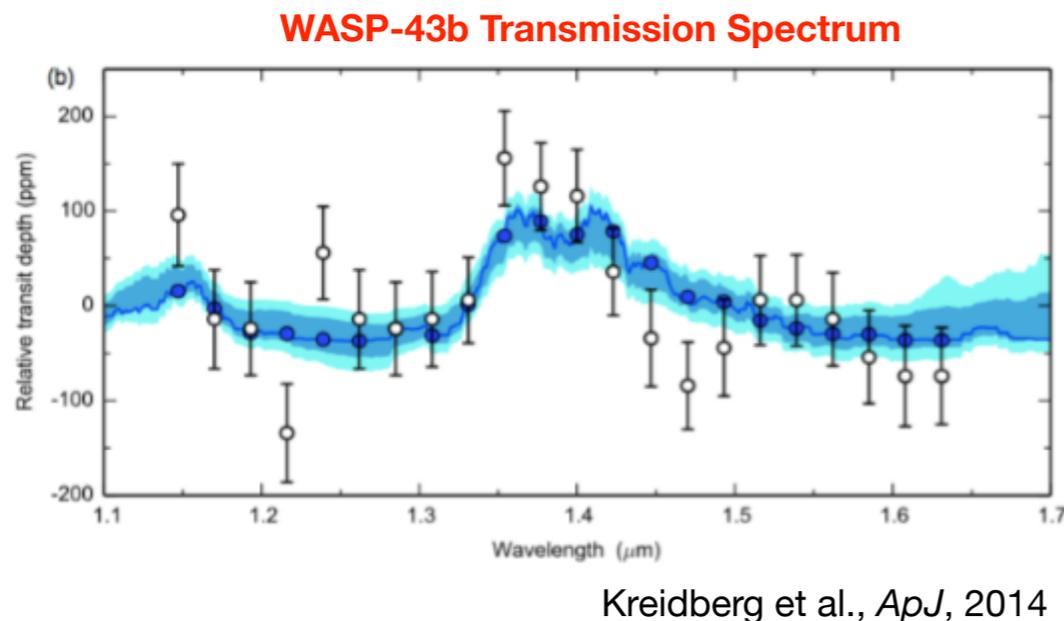
# Opacities: Why do we care?

They are a critical input to exoplanet atmosphere models (like these)



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...allowing us to predict, motivate, and interpret observations with HST, Spitzer, and ground-based telescopes (like these); and in the coming years JWST and the ELTs



**HD 209458b  
Secondary Eclipse  
Spectrum**

# Types of Opacities

- Line opacities (i.e. bound-bound)
- Bound-free and free-free opacities (e.g. H<sup>-</sup>)
- Collision-induced absorption (CIA)
- Scattering opacities

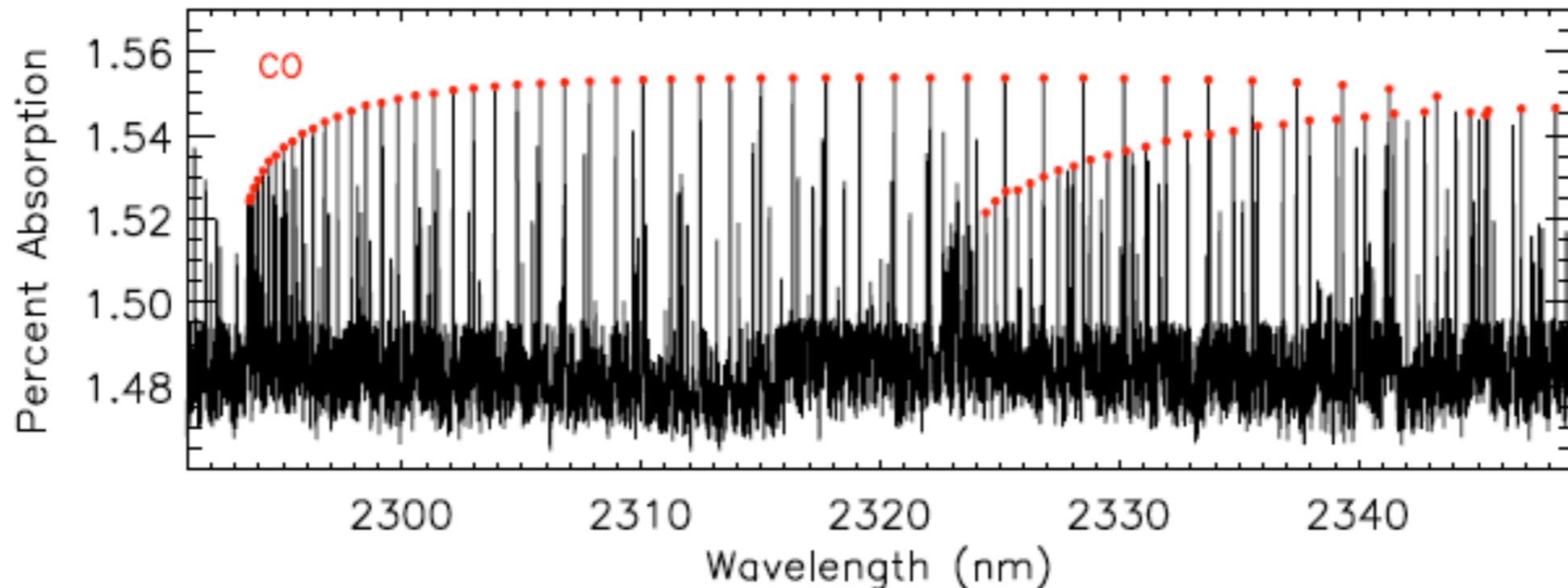
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# Line Opacities

Especially important for high-resolution spectroscopy, in which the planetary signal is recovered by cross correlating the data against a **model template spectrum**. If the model has incorrectly placed spectral lines, the signal will **fail** to be recovered.

**Model high-res. hot Jupiter transmission spectrum:**



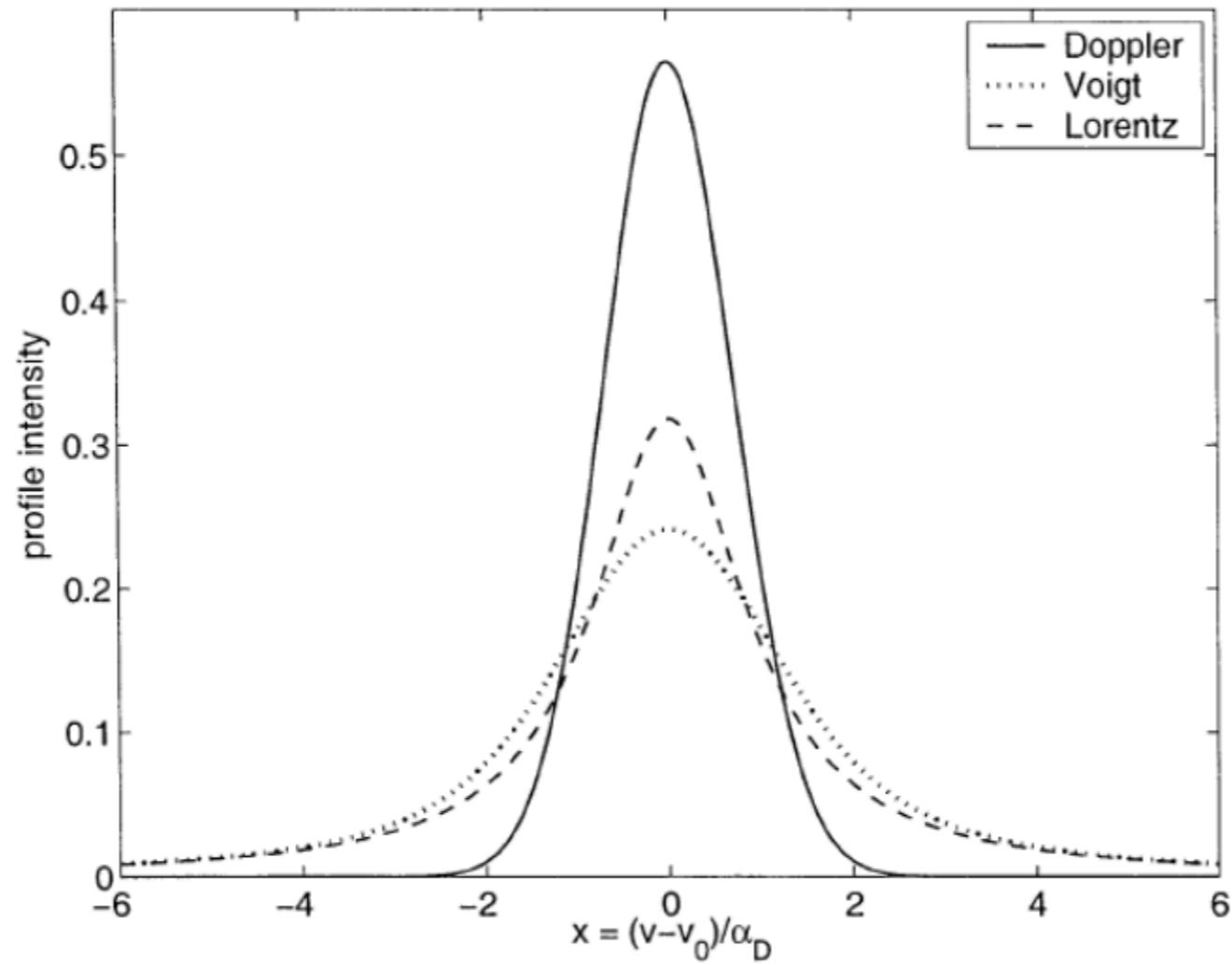
# Line Opacities

- Databases such as HITRAN and ExoMol provide line lists
- Line lists typically contain hundreds to billions of individual transitions

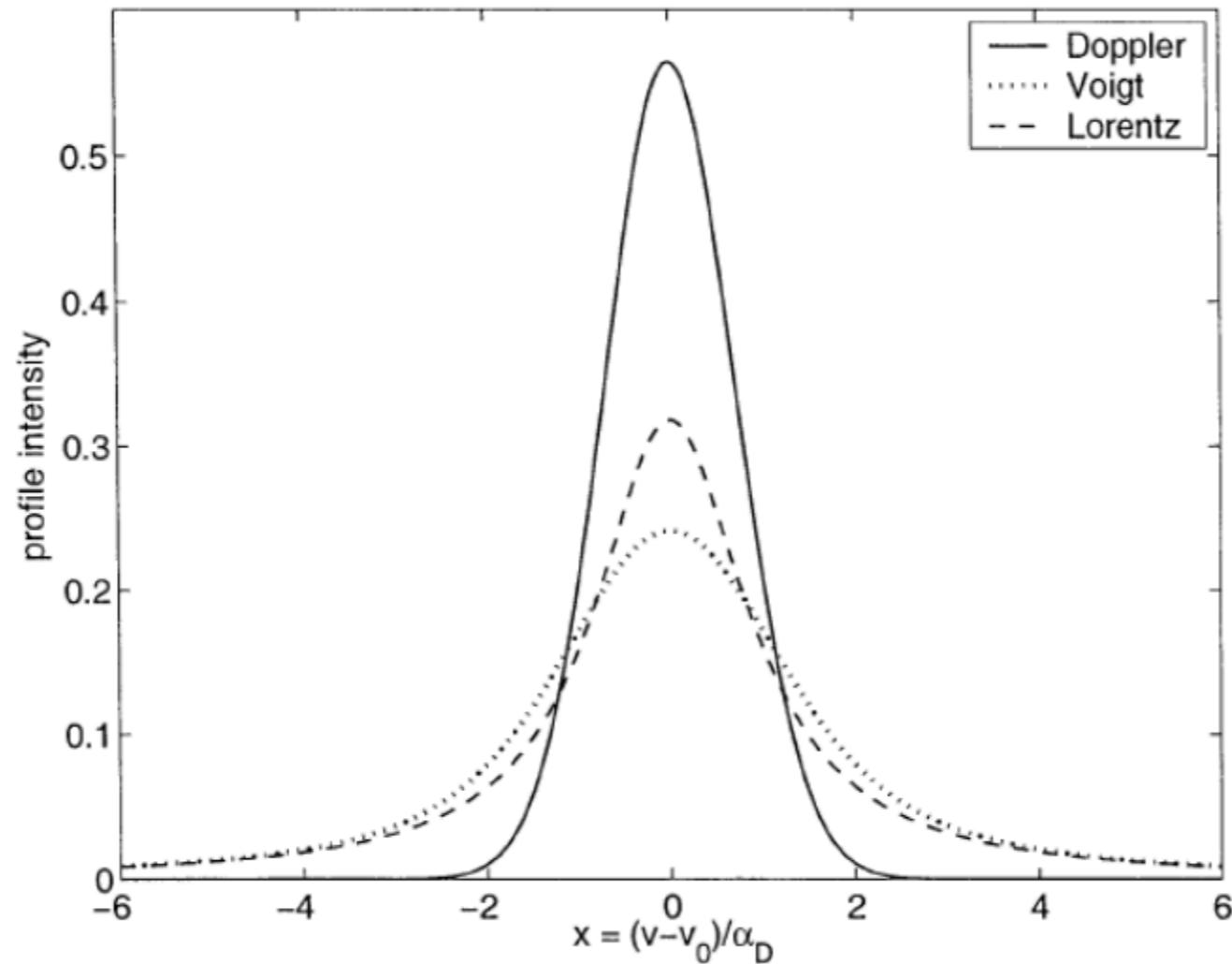
**Line Strength:** 
$$S = \frac{\pi e^2 g_i f_{ij}}{m_e c} \frac{e^{-E_i/k_B T}}{Q(T)} \left(1 - e^{-\Delta E/k_B T}\right)$$

- Line lists are generated from experiments and/or *ab initio* calculations and **may be incomplete or contain errors**
- Lines need to be broadened with a **line profile function** to produce realistic opacities

# Line Broadening – the Voigt Profile



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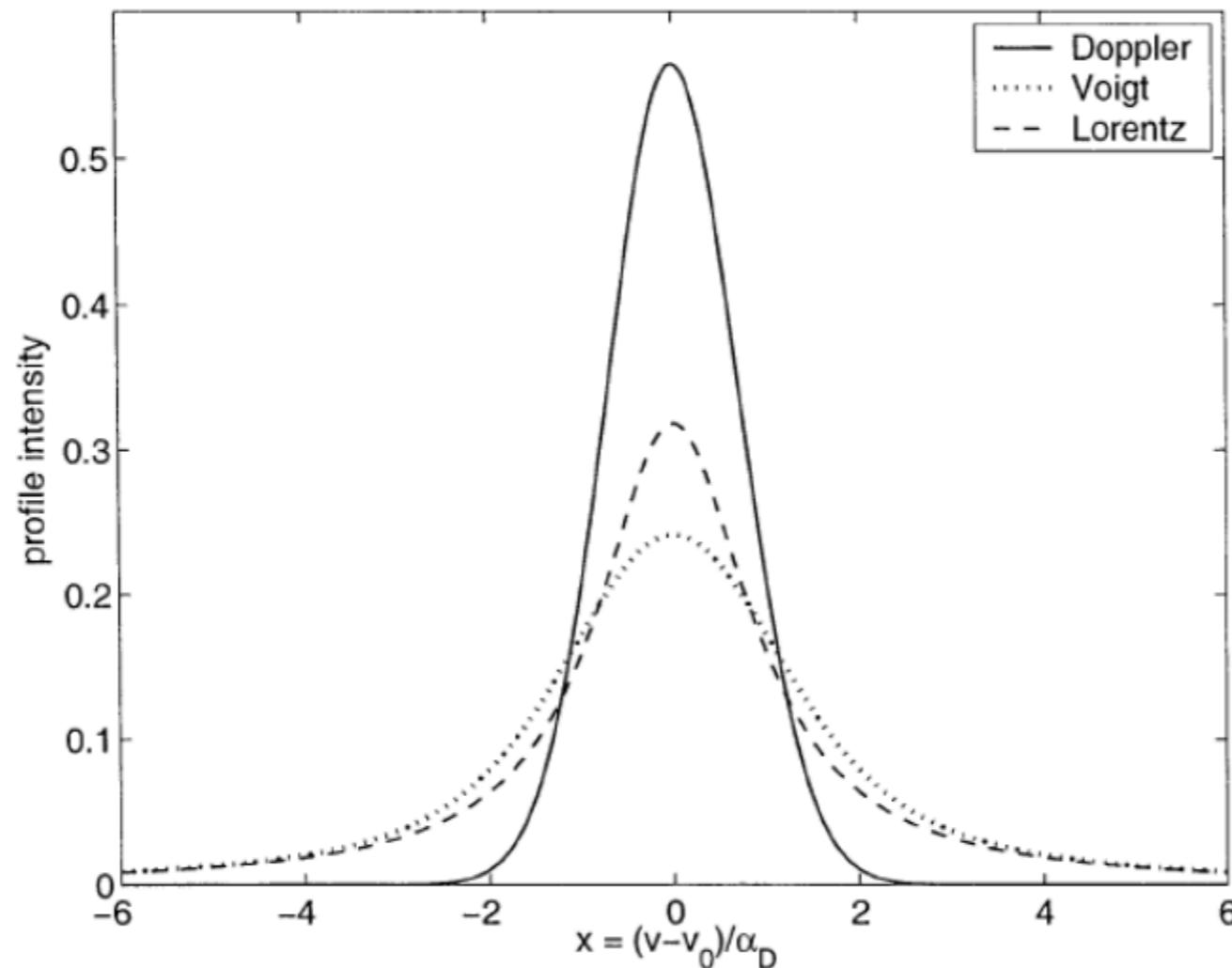
**Doppler Profile:**

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-((\nu - \nu_0)^2 / (\Delta\nu_D)^2)}$$

**Lorentz Profile:**

$$\phi(\nu) = \frac{\Gamma / 4\pi^2}{(\nu - \nu_0)^2 + (\Gamma / 4\pi)^2}$$

# Line Broadening – the Voigt Profile



Depends on temperature only

**Doppler Profile:**

$$\phi(\nu) = \frac{1}{\Delta\nu_D \sqrt{\pi}} e^{-((\nu - \nu_0)^2 / (\Delta\nu_D)^2)}$$

**Lorentz Profile:**

$$\phi(\nu) = \frac{\Gamma / 4\pi^2}{(\nu - \nu_0)^2 + (\Gamma / 4\pi)^2}$$

Depends on properties of **collisional partners (!)**

(see e.g. Gharib-Nezhad & Line, 2019)



***Line Lists***

***Specify inputs***

***Compute opacities***

## Line Lists

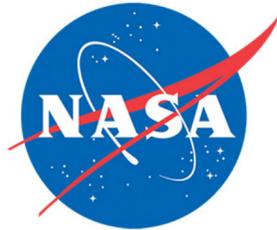
## Specify inputs

## Compute opacities

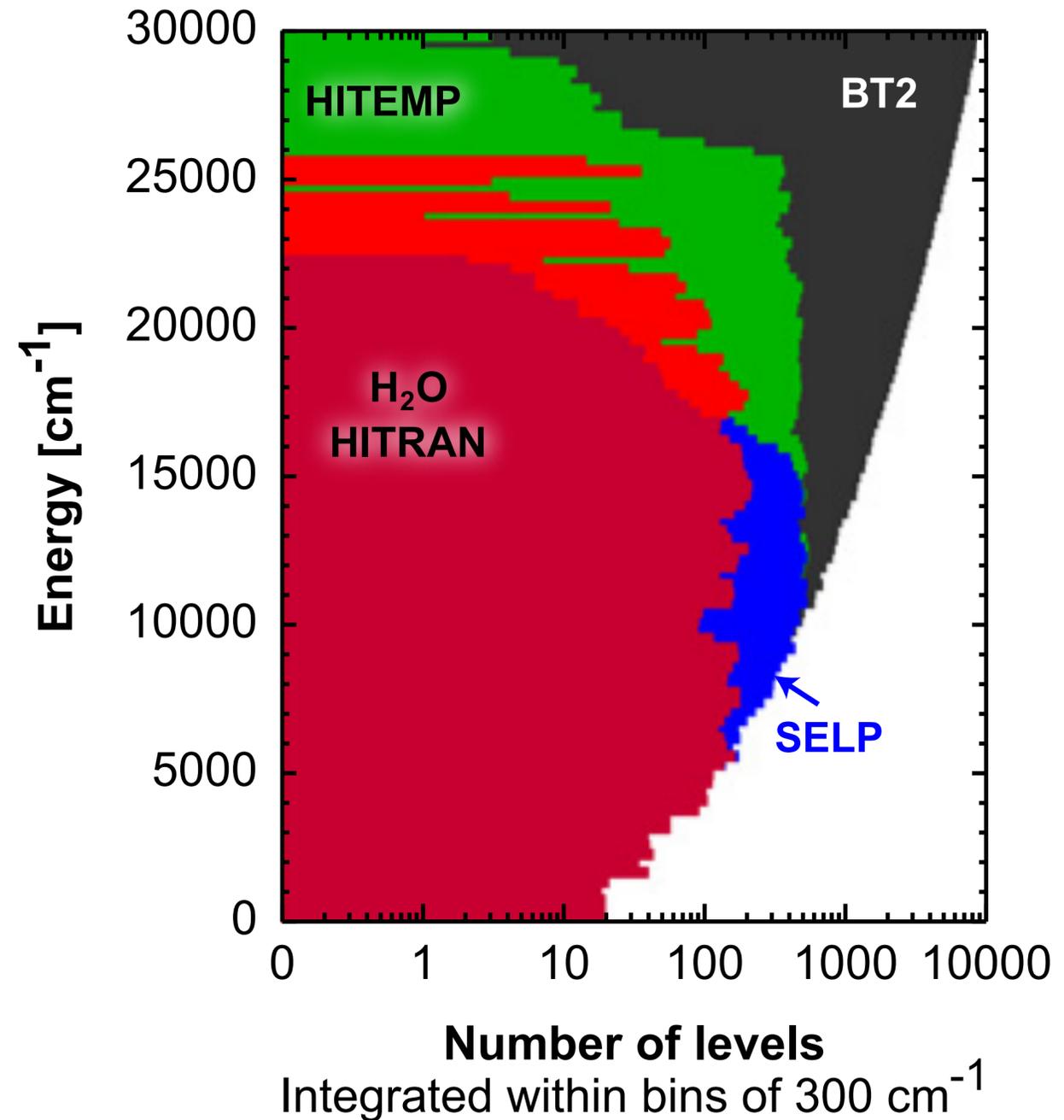
### Several databases to choose from



**ExoMol**



- *Databases differ in completeness*
- *Sometimes data does not exist for the problem at hand*
- *Data must be pre-processed*



**Villanueva+2012**

## Line Lists

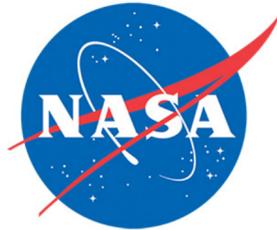
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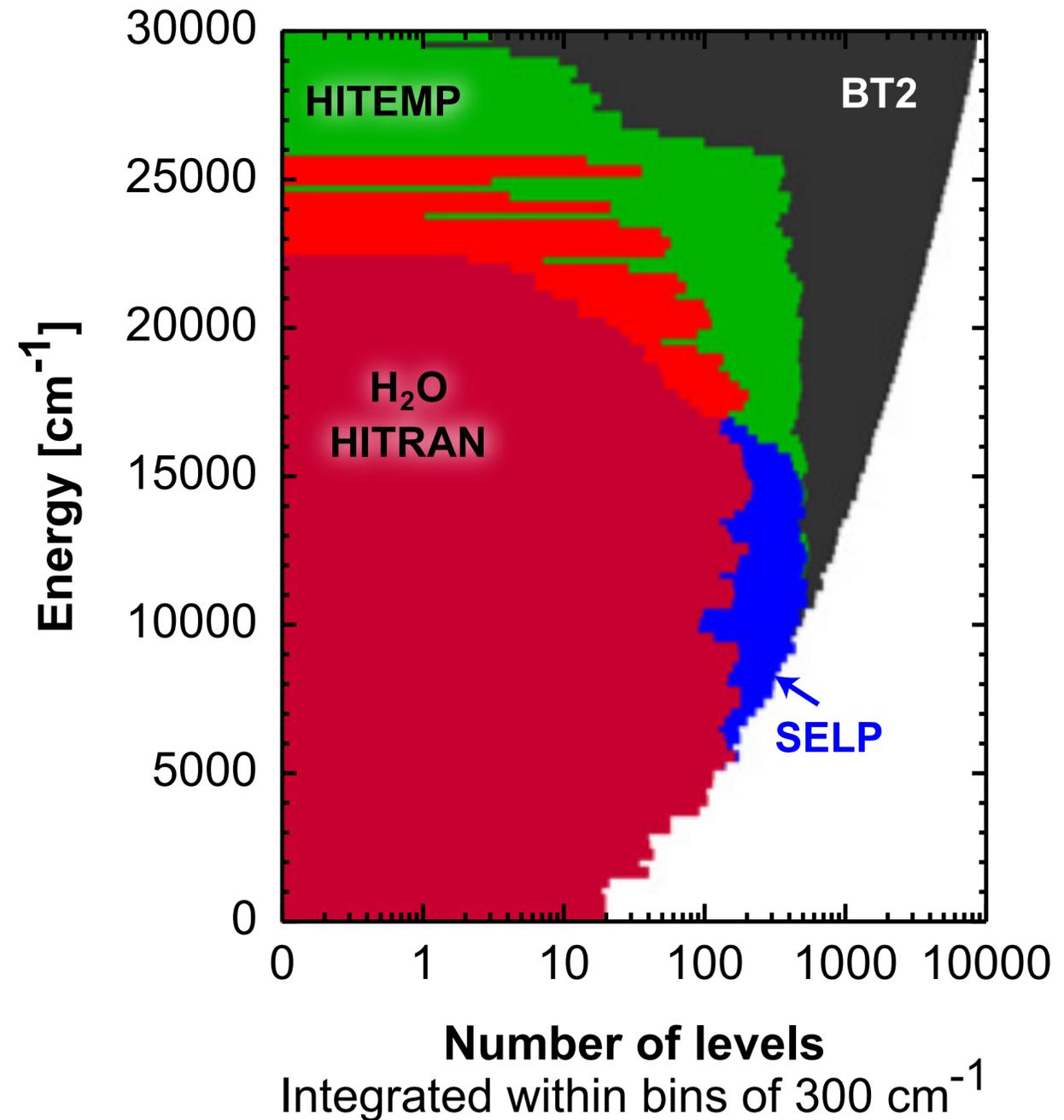


ExoMol



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Bar to entry is relatively high

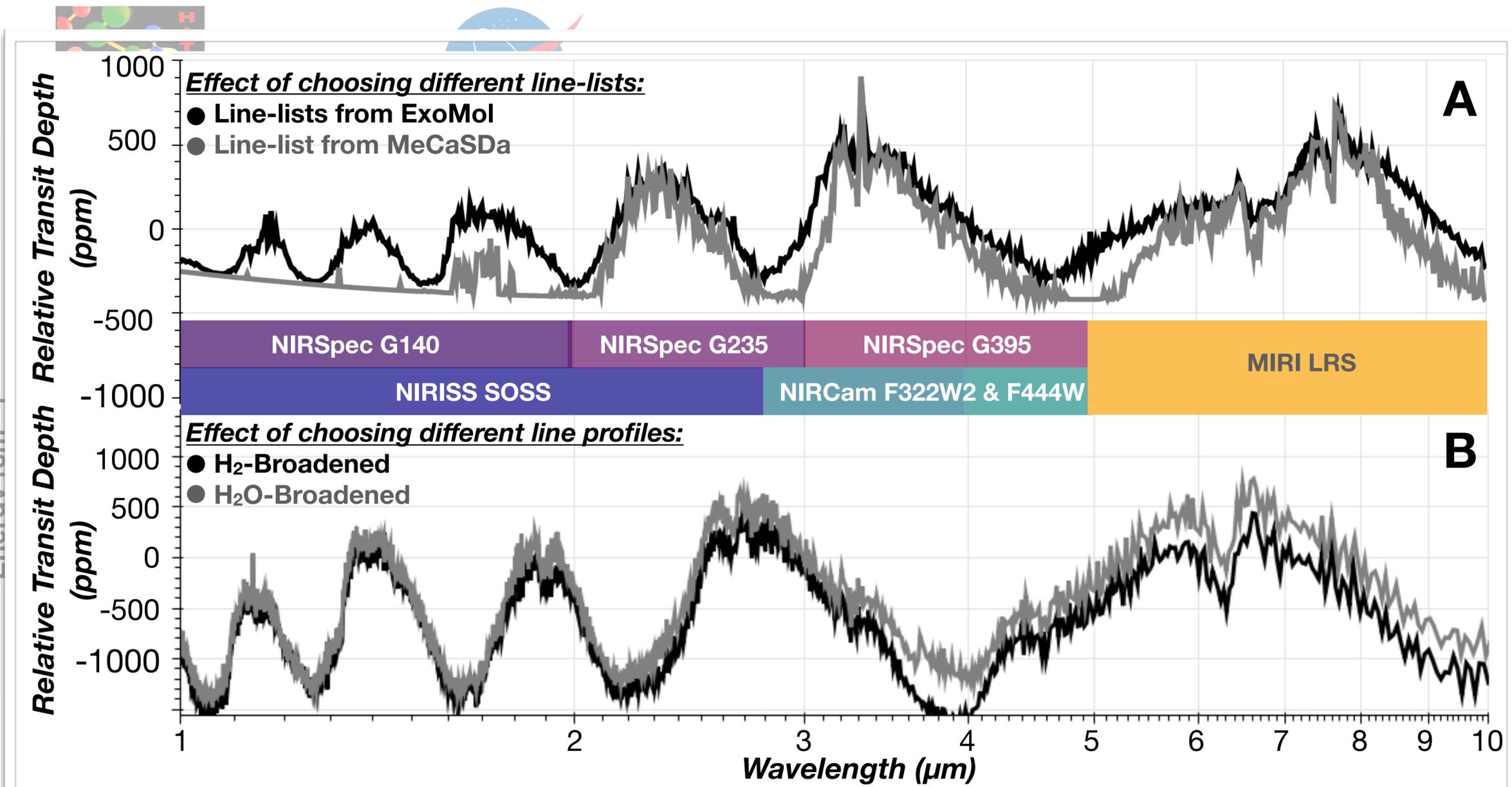


Villanueva+2012

Line Lists

Specify inputs

Compute opacities



**Choose:**

- **Line list**
- **Choose broadening profile**
- **Choose P, T, R grid**
- **Choose line width cutoff**

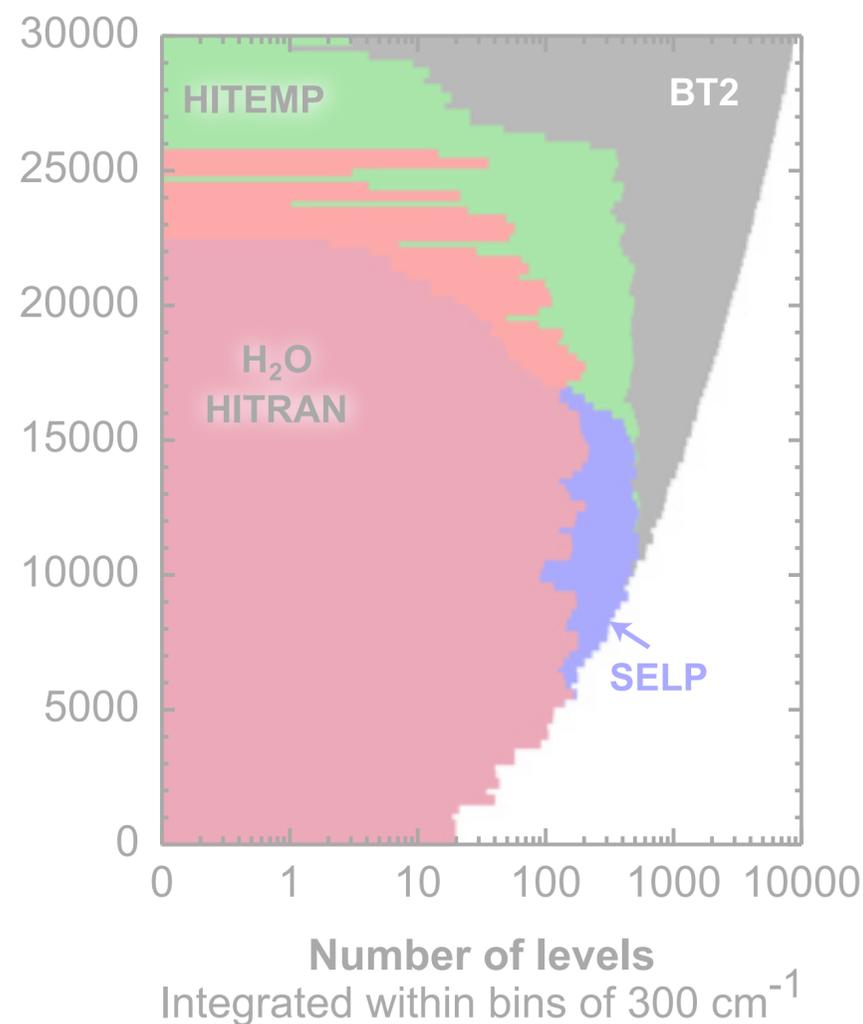
**No community standards, profiles to benchmark against**

**Bar to entry is relatively high**

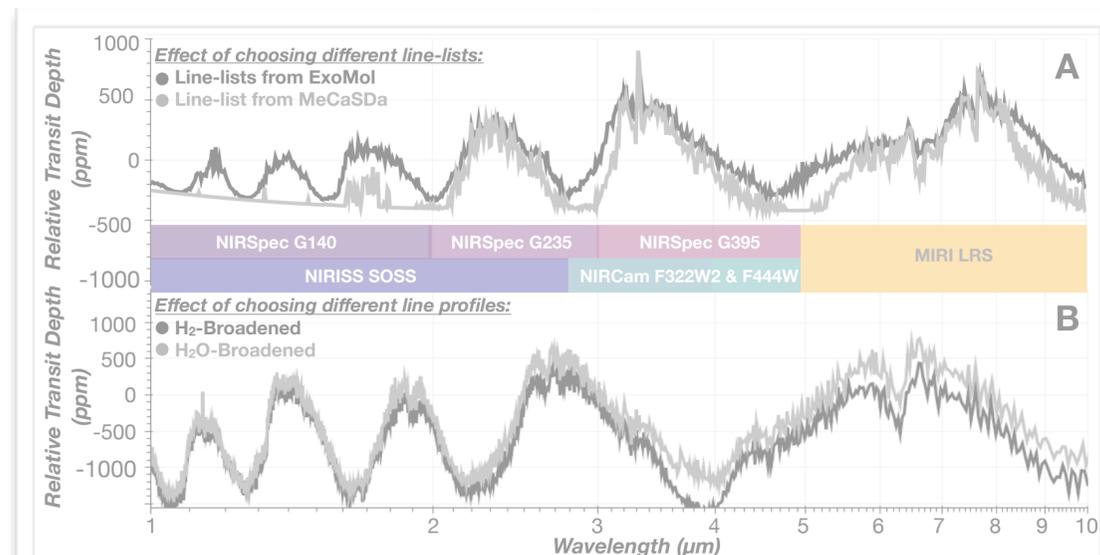
## Line Lists



ExoMol



## Specify inputs



## Compute opacities

### HELIOS-K

- *Grimm+Heng*
- *Very fast (GPU required)*
- *Handles several different kinds of data*

### ExoCross

- *Fortran*
- *Handles both ExoMol+HITRAN*

### HAPI

- *Python-Numba*
- *Query functions*
- *Visualization Tools*

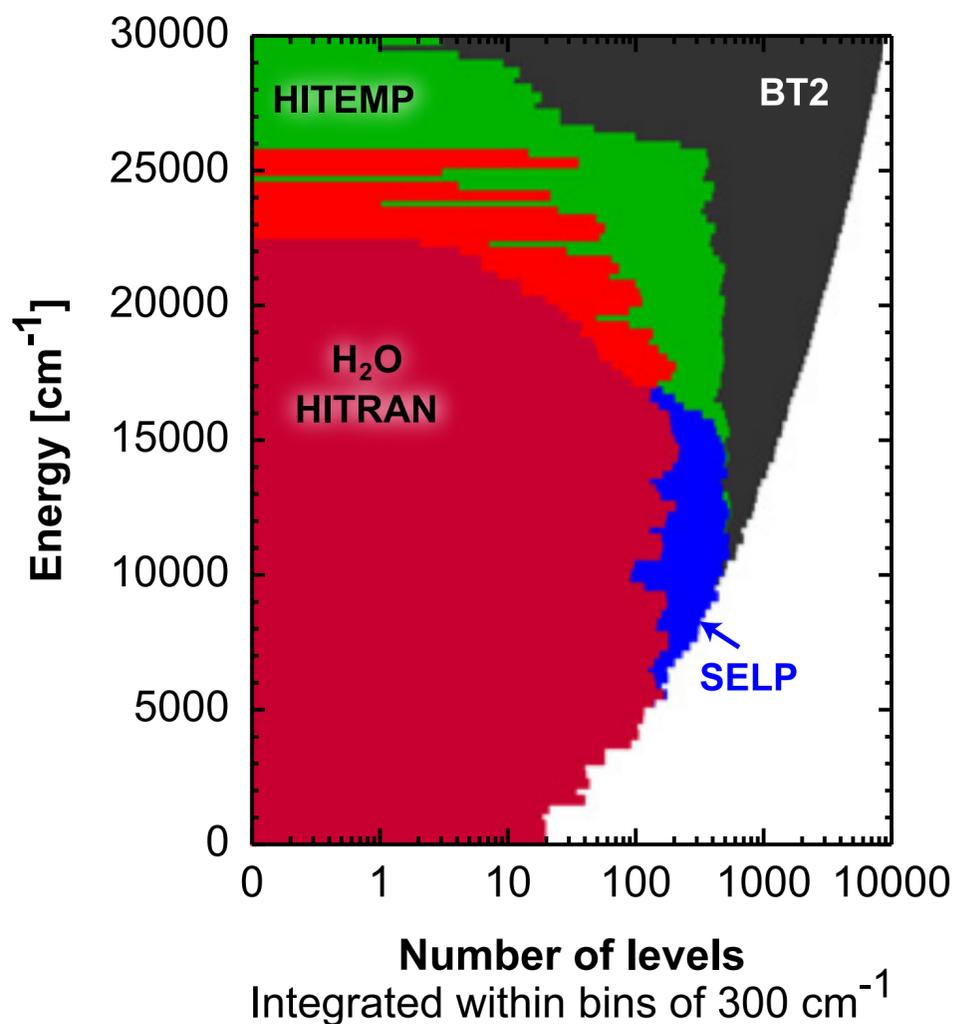
### R. Freedman

- *Fortran, not open-source*
- *Databases widely used (Marly, Fortney, Kempton, Morley, Lupu, and many more)*

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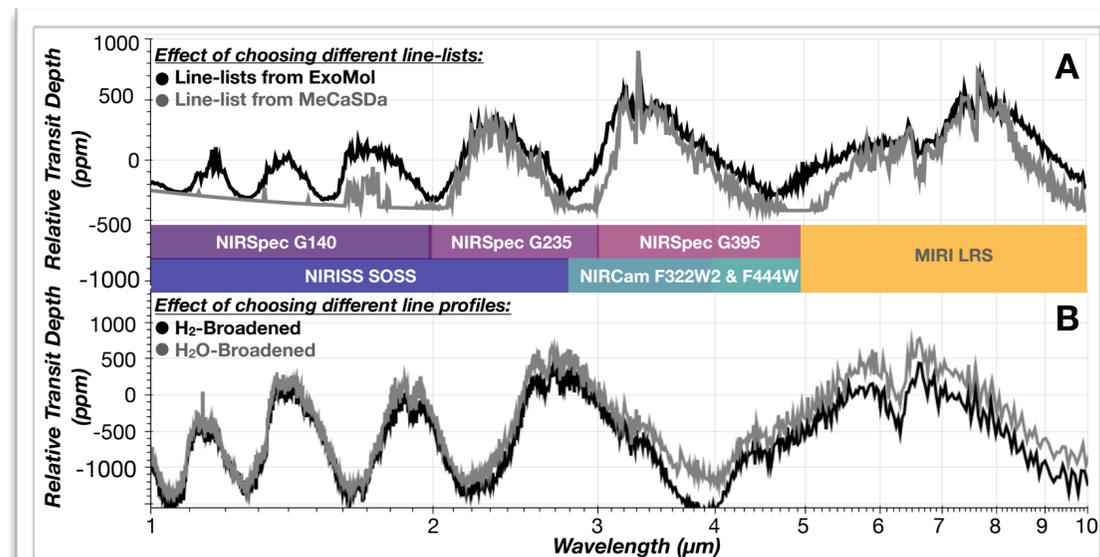


ExoMol



No uniform database

## Specify inputs



No community standards

## Compute opacities

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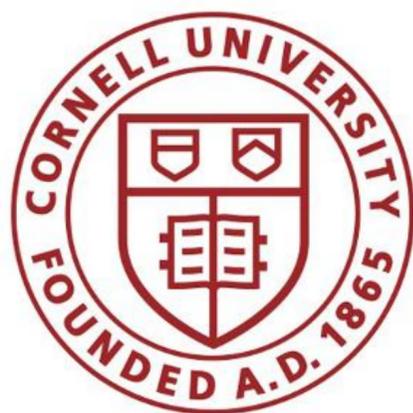
“A COMMUNITY TOOL FOR COMPUTING, VISUALIZING, AND MANIPULATING MOLECULAR & ATOMIC OPACITIES”

NASA UNSOLICITED PROGRAM: MAY 2019- 2021



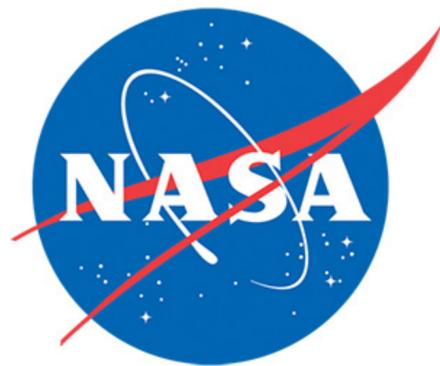
*Natasha Batalha*

*Science PI*



*Nikole Lewis*

*PI*



*Mark Marley*

*Richard Freedman*



*Iouli Gordon*

**ExoMol**

*Jonathan Tennyson*

*Sergey Yurchenko*



*Clara Sousa-Silva*



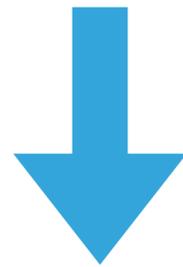
**STScI** | SPACE TELESCOPE  
SCIENCE INSTITUTE

*Jeff Valenti*

GOAL: INCREASE ACCESSIBILITY OF OPACITIES

## PROGRAM GOALS: STEPPING STONE TO INCREASING ACCESSIBILITY OF OPACITIES

Curate line lists	Compute Opacities	Easily access database	Visualize Opacities	Manipulate Opacities
Uniform meta data	Opacities for all relevant molecules	<b>Cloud hosted SQL database</b>	Web interface for opacity viz	Sum opacity weighted by abundance
Aggregate of all needed data (inc. partition functions)	Opacities for all relevant P-T combos	Informative/ searchable meta data	Interactive plotting & querying	Code to compute correlated-K tables
	Opacities for different flavors of line profiles	Automatic bibtex generation for users		
		API for fast queries		



**Novice**

*"Where does water absorb?"*

**Theorist**

*"I need opacities for my model"*

**Retrievals**

*"Do changes in opacity sources change retrieved abundances?"*

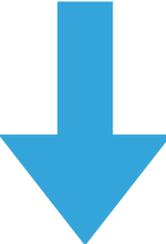
**Observer**

*"What JWST mode do I use for detecting C<sub>2</sub>H<sub>2</sub>?"*

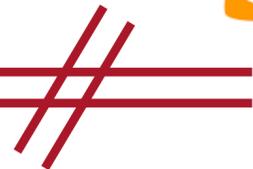
**Expert in Opacities**

*"I want to create my own line profile and contribute a pipeline module"*

USER STARTS HERE



**Constant maintenance and updates**



*seconds-minutes*



**Initial request for T,P,R power, and wave range**

*Better, if possible*  
**Go to temporary memory**

**Store permanently**

*But, if needed*

**Science with always up-to-date opacities**

Other ideas for increased productivity?

## PROGRAM PHILOSOPHY: OPEN TO COMMUNITY

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**Public Slack account with space for Q&A, discussion, and code announcements**

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**Public Trello boards where users can see upcoming tasks, releases**

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**Dedicated testing phases with monthly team hack sessions**

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**Hosting tutorials at the 1st ERS Program 1366 data challenge**

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**Development is open process. Website coming soon to get involved, submit feature requests**

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## DISCUSSION

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- What data products do you need the most? Aggregated line lists? Opacities? Correlated-K Tables
- What features do you need? E.g. Query small subsets of data? Is there code that is missing
- Are there missing molecules?
- What is most time sensitive?
- Anything else!