The Impact of Spectral Line Wing Cut-Off:

Recommended Standard Method With Application to MAESTRO Opacity Database

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

MAESTRO

Cornell University	NASA	HITRAN	ExoMol	UMass Lowell
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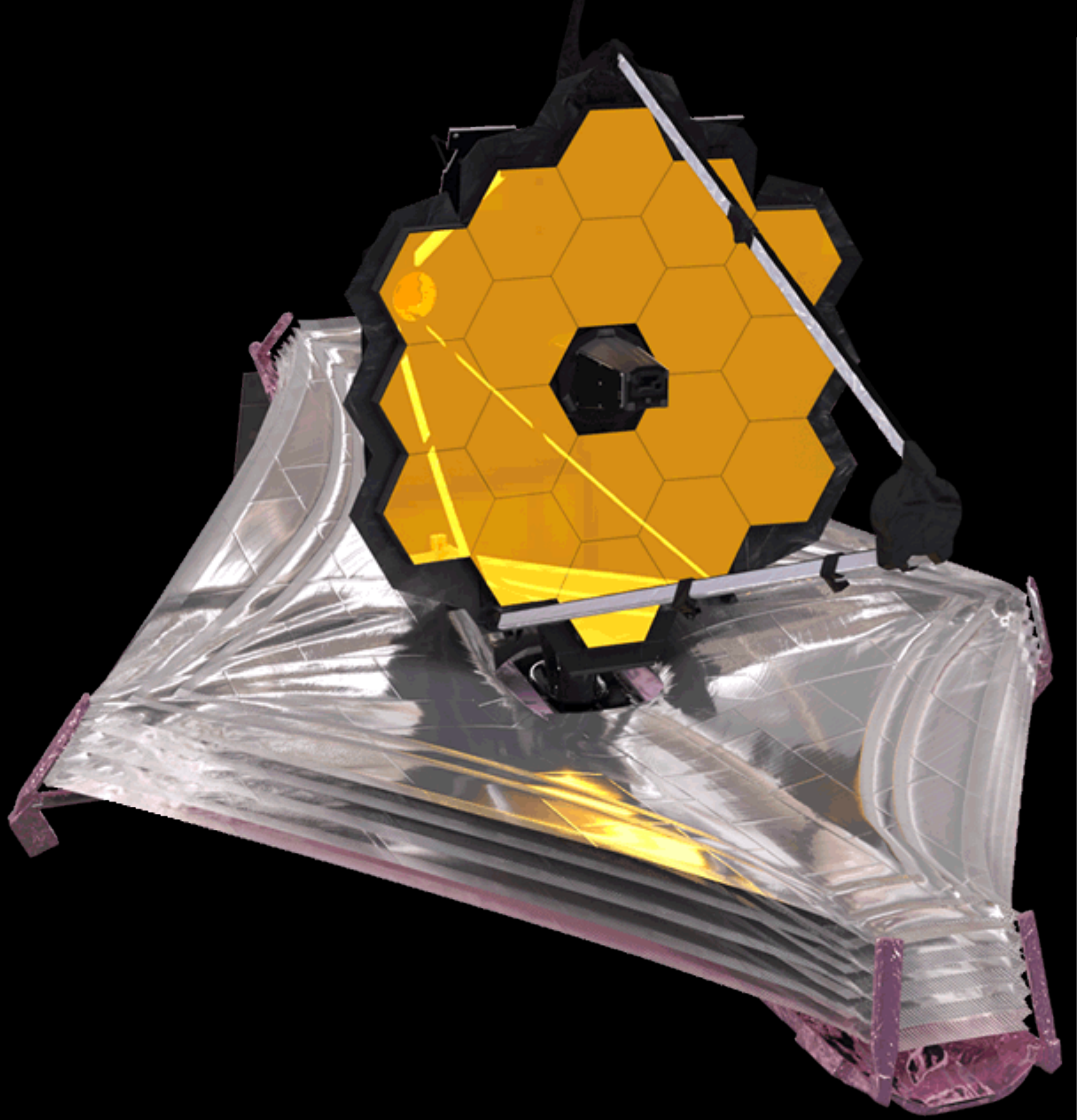
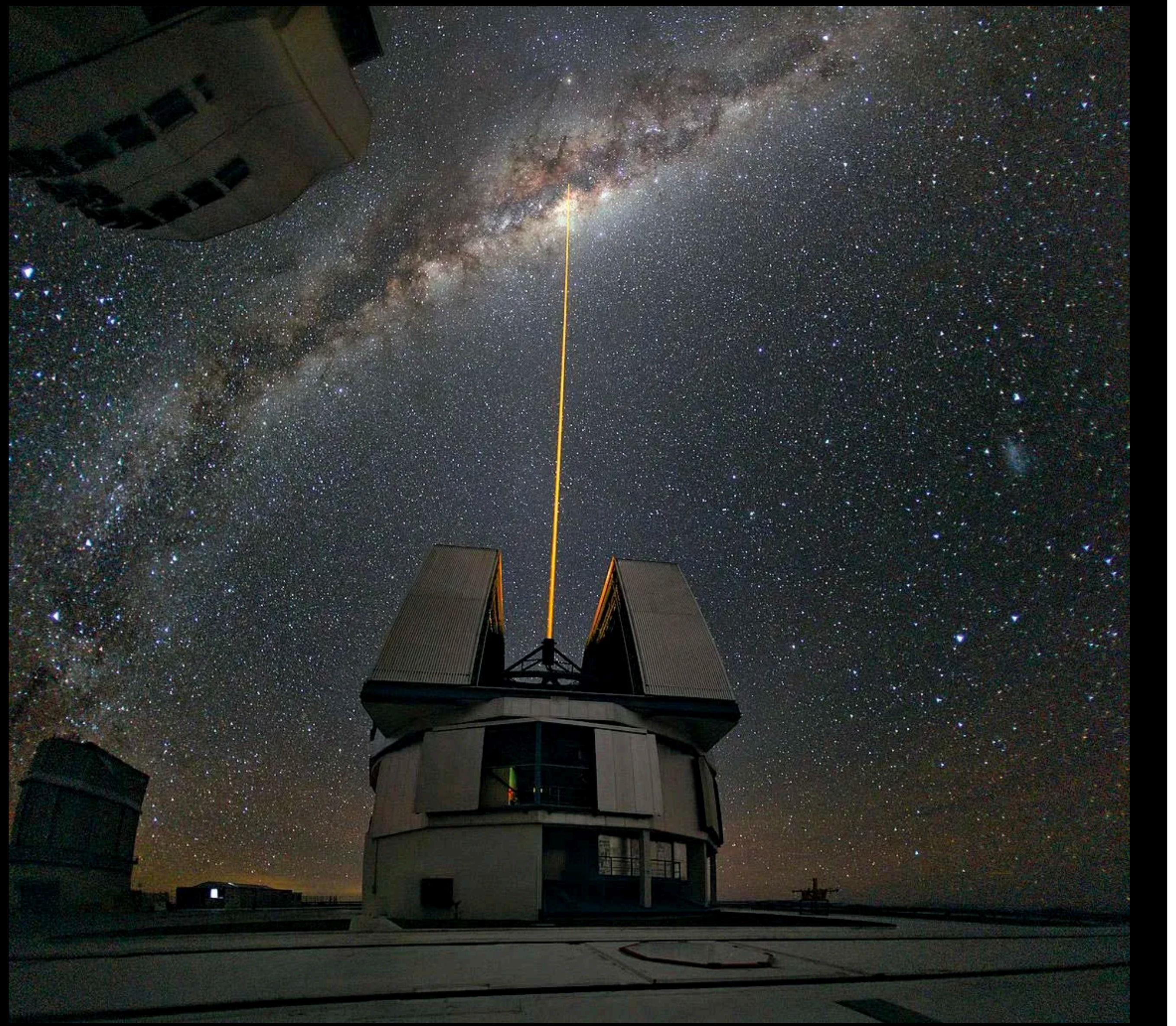
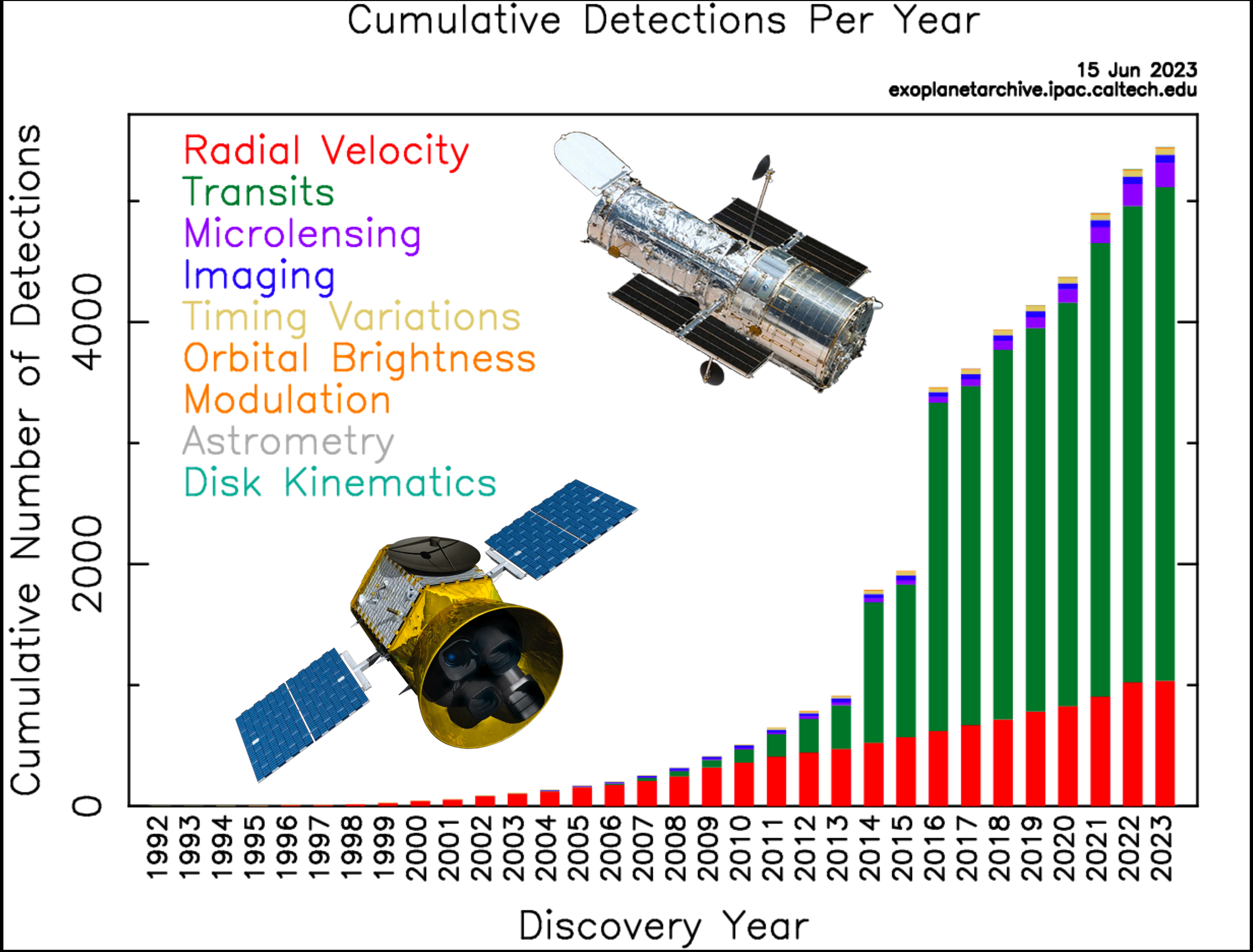
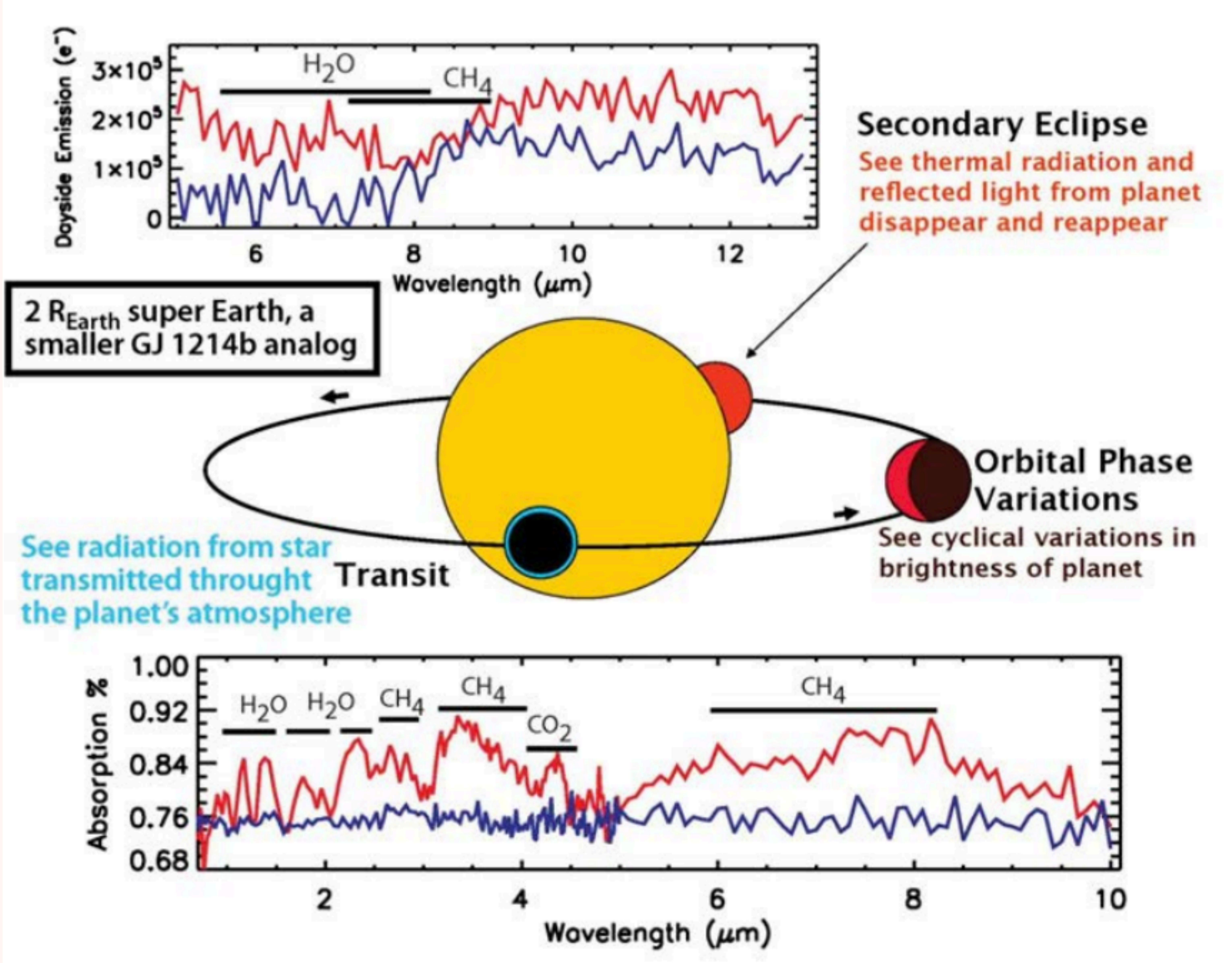
	Richard Freedman	*Rob Hargreaves*	*Sergey Yurchenko*	
	Ehsan Gharib-Nezhad		*Katy Chubb*	



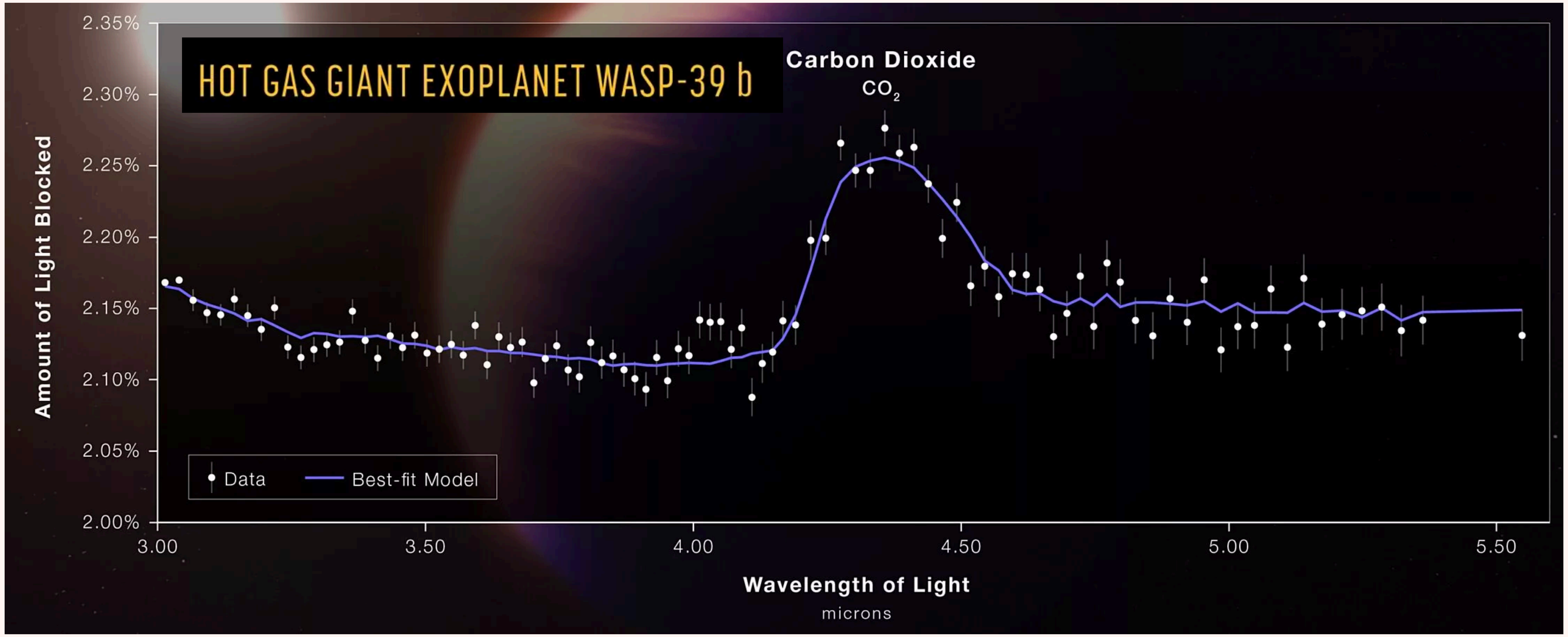



Cumulative Detections Per Year
15 Jun 2023
exoplanetarchive.ipac.caltech.edu
Radial Velocity
Transits
Microlensing
Imaging
Timing Variations
Orbital Brightness
Modulation
Astrometry
Disk Kinematics
Cumulative Number of Detections
0
2000
4000
1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021 2022 2023
Discovery Year

Transit Method



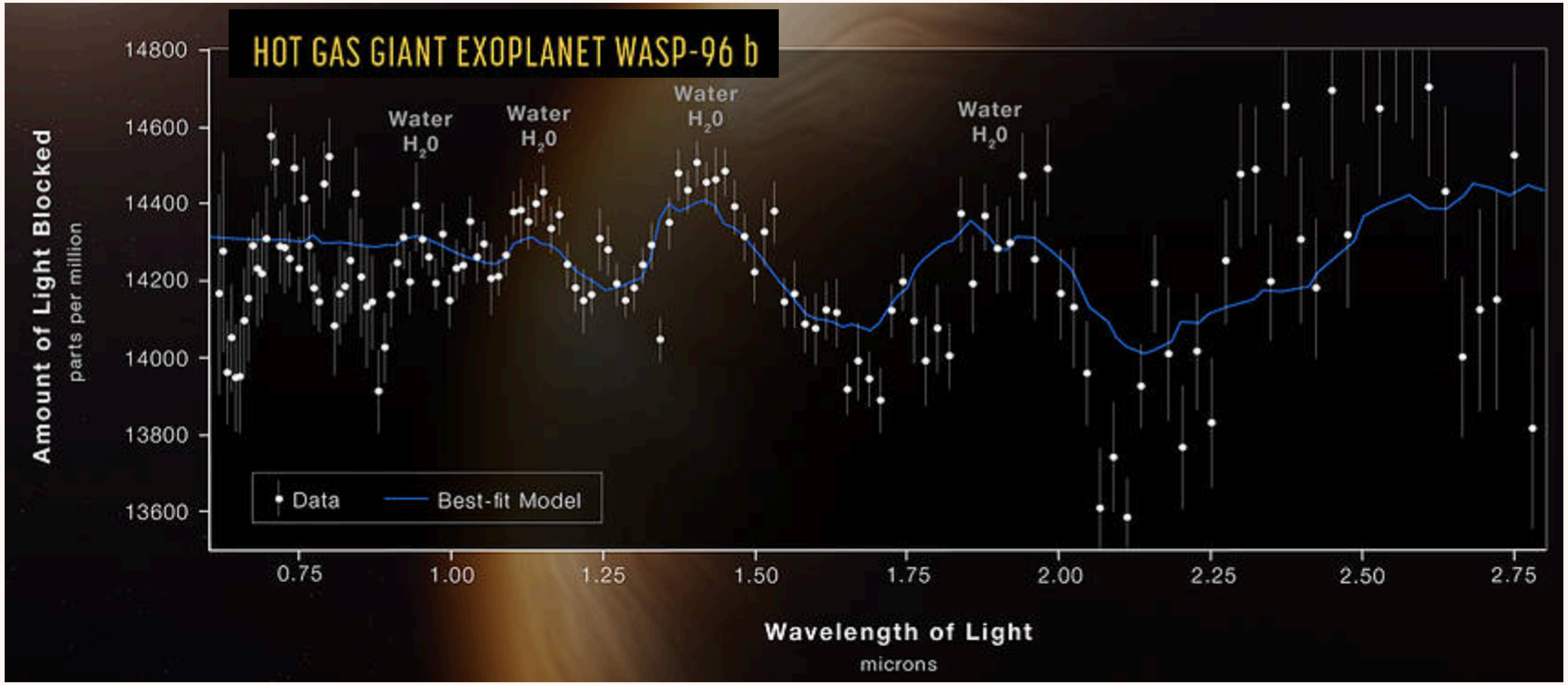
Credit: Charles Beichman *et al* 2014 *PASP* **126** 1134



WASP-39B

Transmission spectrum of a hot Jupiter known as WASP-39b, captured by JWST's Near-Infrared Spectrograph (NIRSpec) in July 2022. JWST detected carbon dioxide in WASP-39b's atmosphere, marking the first time CO2 has been detected in an exoplanet's atmosphere.

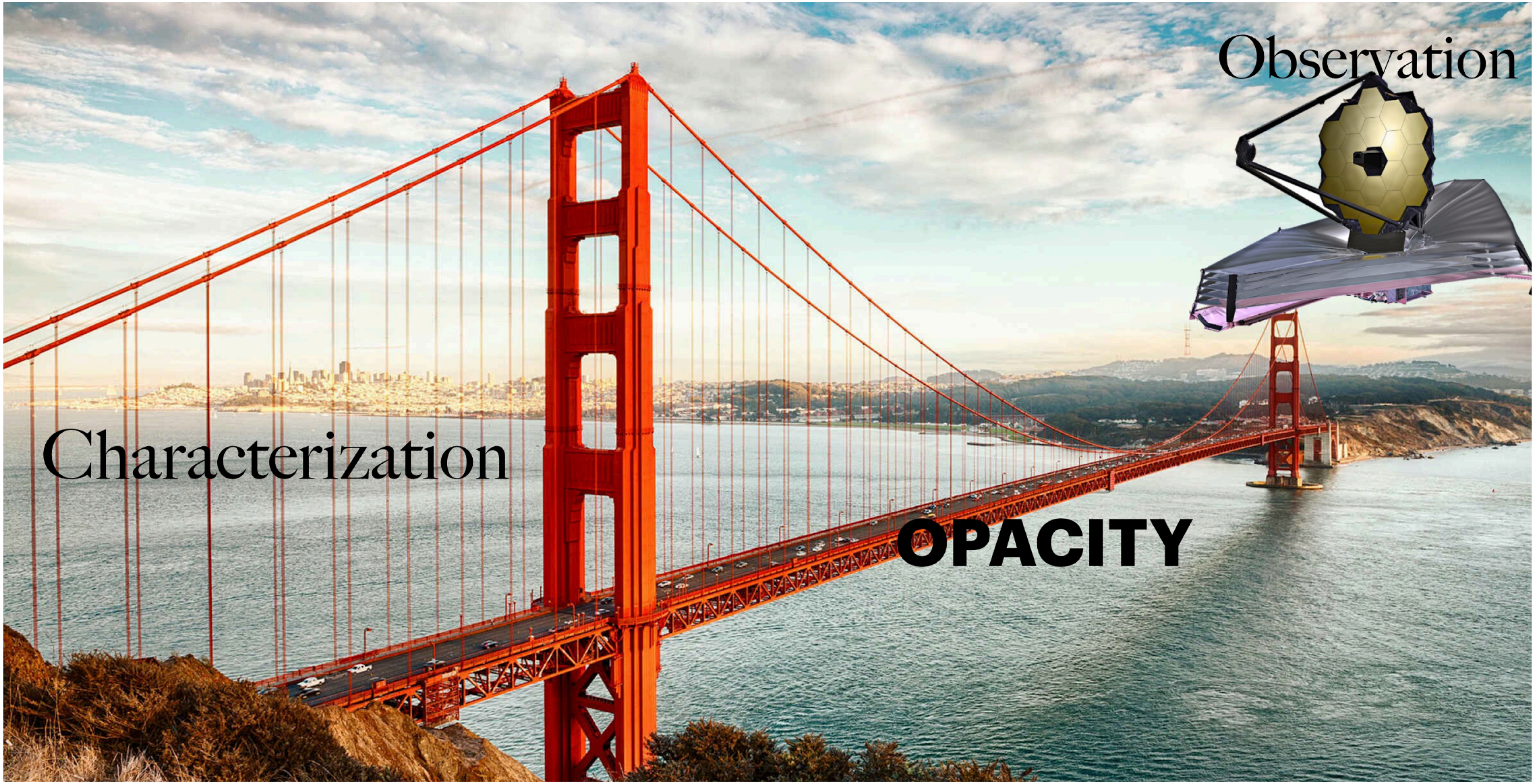
Image: NASA, ESA, CSA, and L. Hustak (STScI); Science: The JWST Transiting Exoplanet Community Early Release Science Team



WASP-96B

On June 21, Webb’s Near-Infrared Imager and Slitless Spectrograph (NIRISS) measured light from the WASP-96 system for 6.4 hours as the planet moved across the star. The result is a light curve showing the overall dimming of starlight during the transit, and a transmission spectrum revealing the brightness change of individual wavelengths of infrared light between 0.6 and 2.8 microns.

Image credit: NASA, ESA, CSA, and STScI


Observation
Characterization
OPACITY

MAESTRO

Science.data.nasa.gov/opacities/

Search a molecule to data report:

TiO

TiO

Overall Stats

Temperature Range	75.0 - 4000.0 K
Pressure Range	1e-06 - 30.0 bars
Resolution	0.003 - 0.5 cm^{-1}

Select Opacity Bundle

T (K) Kelvin — Temperature

P (bar) bars — Pressure

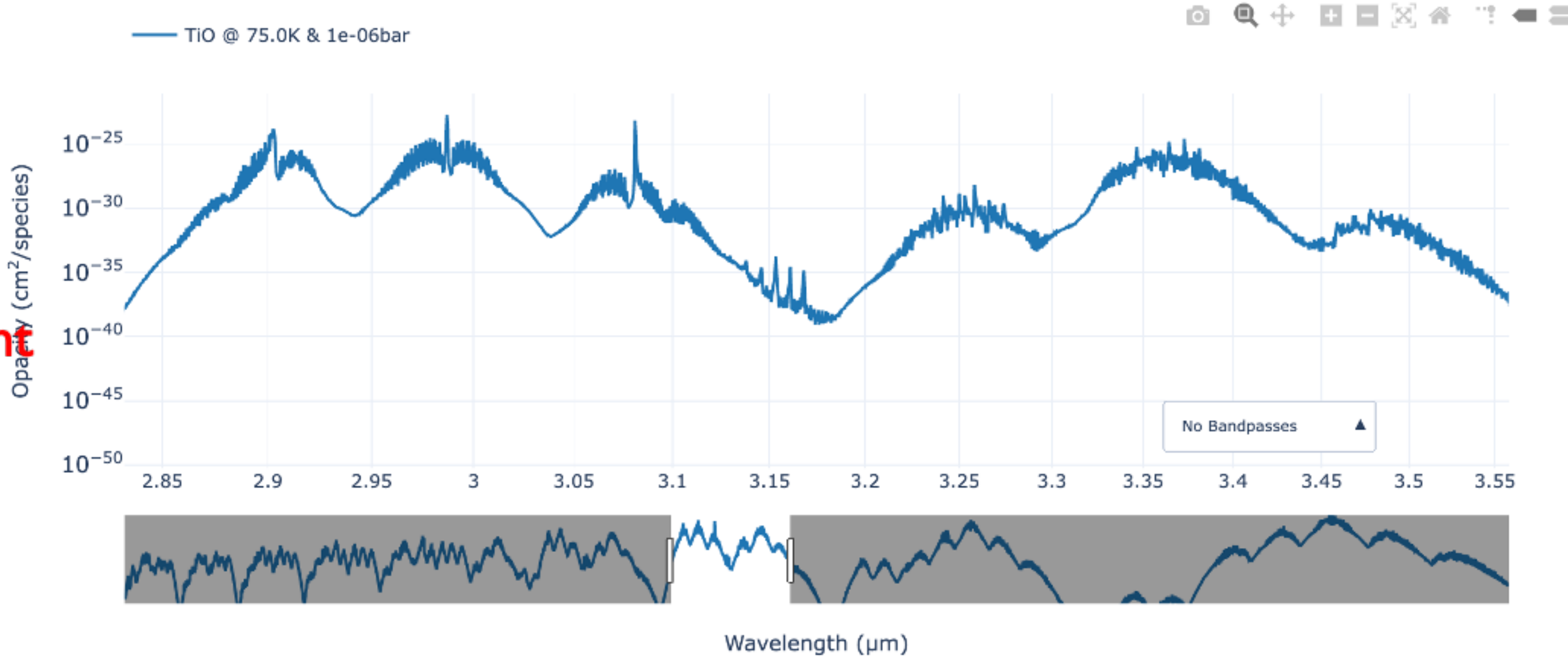
Broadened By — Broadening agent

0.26 to 333.3 µm — Wavelength

Smooth:

Submit Query

Opacities | **Calculation Cautions** 1 | **Known To Do's/Submit a Task** | **More Info**

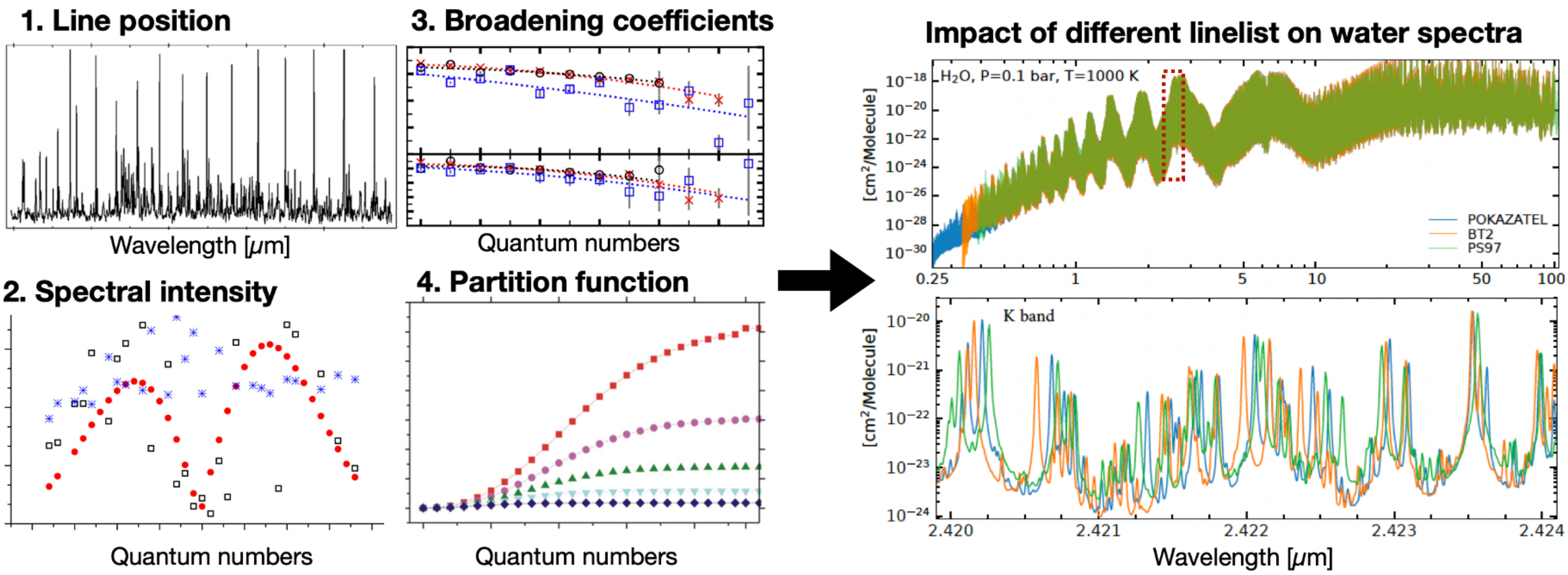


Get Meta Data | Opacities

Use the table below to explore the relevant data & citations associated with the plot above

	Product	Molecule	Temperature(K)	Pressure(bar)	Reference	Name	Wavenumber	Warning
⌄	Opacity	TiO	75.0	1e-06	Gharib-Nezhad et al. 2021	EXOPLINES: Molecular Absorption...	30.0-38300.0	1

Main components of a line list control the generated Opacity data



Credit: Ehsan Gharib-Nezhad *et al* 2021 *ApJS* **254** 34

Key Point

"

The inclusion of the non-Lorentz behavior in the ACS data is challenging due to the lack of complete spectroscopic parameters. The main technique used in astrophysics to mitigate the issue is to introduce a wing cut-off.

In addition to the inconsistency problem, inaccurate choice of wing cut-off results in many types of errors in the opacity continuum: Over-estimation and Under-estimating.

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The inclusion of the **non-Lorentz behavior** in the ACS data is challenging due to the **lack of complete spectroscopic** parameters. The main technique used in astrophysics to **mitigate** the issue is to introduce a **wing cut-off.**

In addition to the **inconsistency** problem, **inaccurate choice** of wing cut-off results in many types of **errors** in the opacity continuum: **Over-estimation** and **Under-estimating.**

“

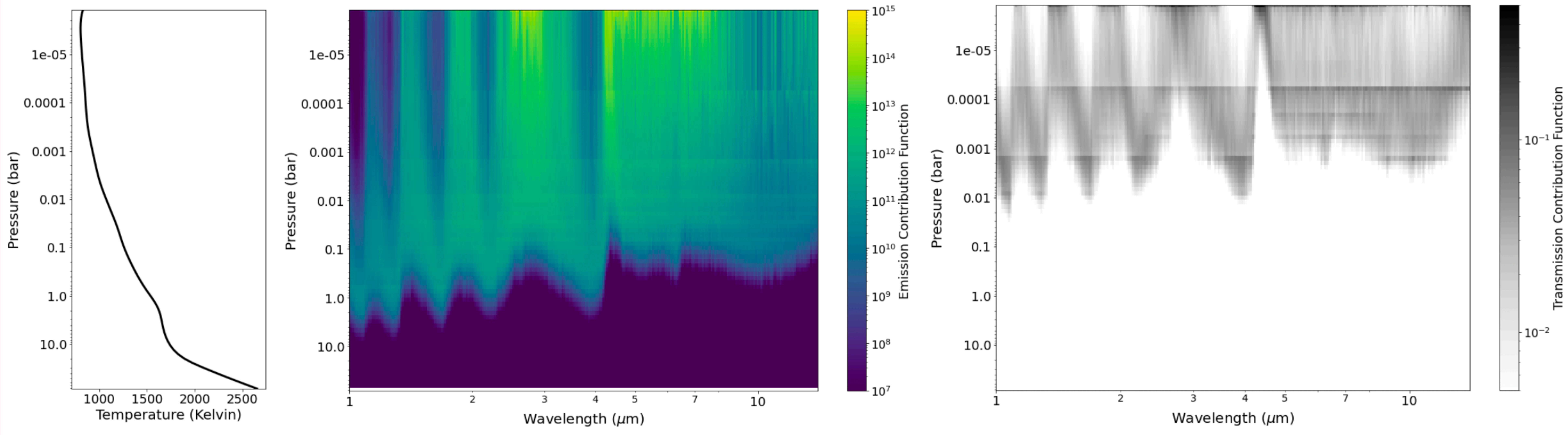
Insights on the Pre-Computed Absorption Cross-Section (ACS)

But first, we want to ask about ...

- T - P - lambda ranges relevant to modeling exo-atmospheres
- Challenges with accurate line profiles for high-P
- Not enough spectroscopic measurements for high-Ts
- Voigt profile

- Challenges, lake of necessary spectroscopic informations

Why Do We Need Opacity Data for Such a Wide T-P Range?



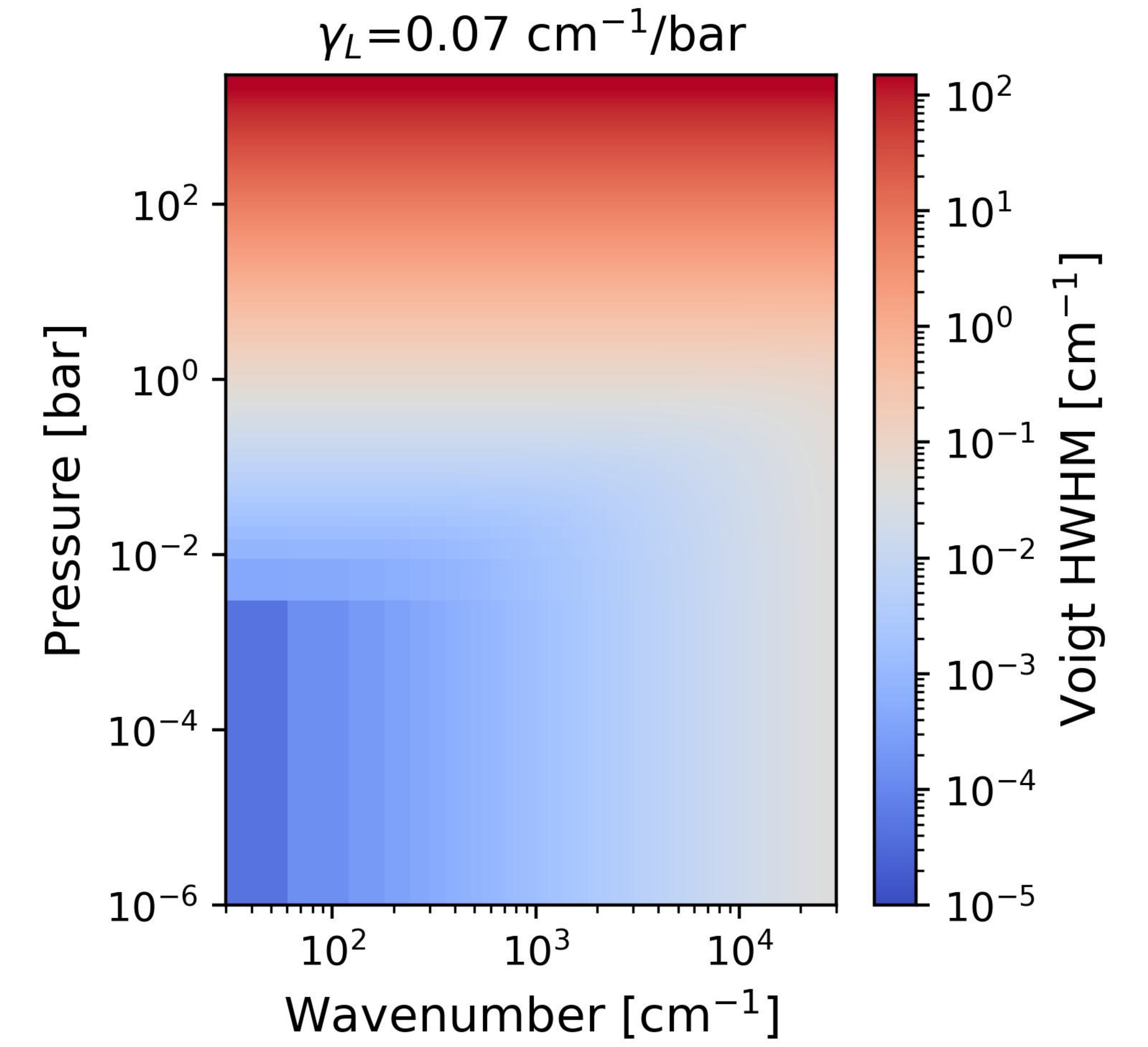
Typical hot Jupiter pressure-temperature profile (left) and associated contribution functions over relevant JWST wavelengths. Contribution functions dictate the pressure regions that the observable spectrum is sensitive to. The emission contribution function (middle) is defined in {Lothringer2018ApJ}. The transmission contribution (right) is defined in {molliere2019}.

POC: Natasha Batalha / NASA

Voigt Width Range Across P and WN

Estimated Voigt HWHM across a wide range of spectral range and pressure for CH4-in-air system with a constant Lorentz coefficient of 0.07 cm^{-1} / bar and for room temperature.

$$\Gamma_V = 0.5346\ \Gamma_L + \sqrt{0.2166\ \Gamma_L^2 + \Gamma_G^2}$$

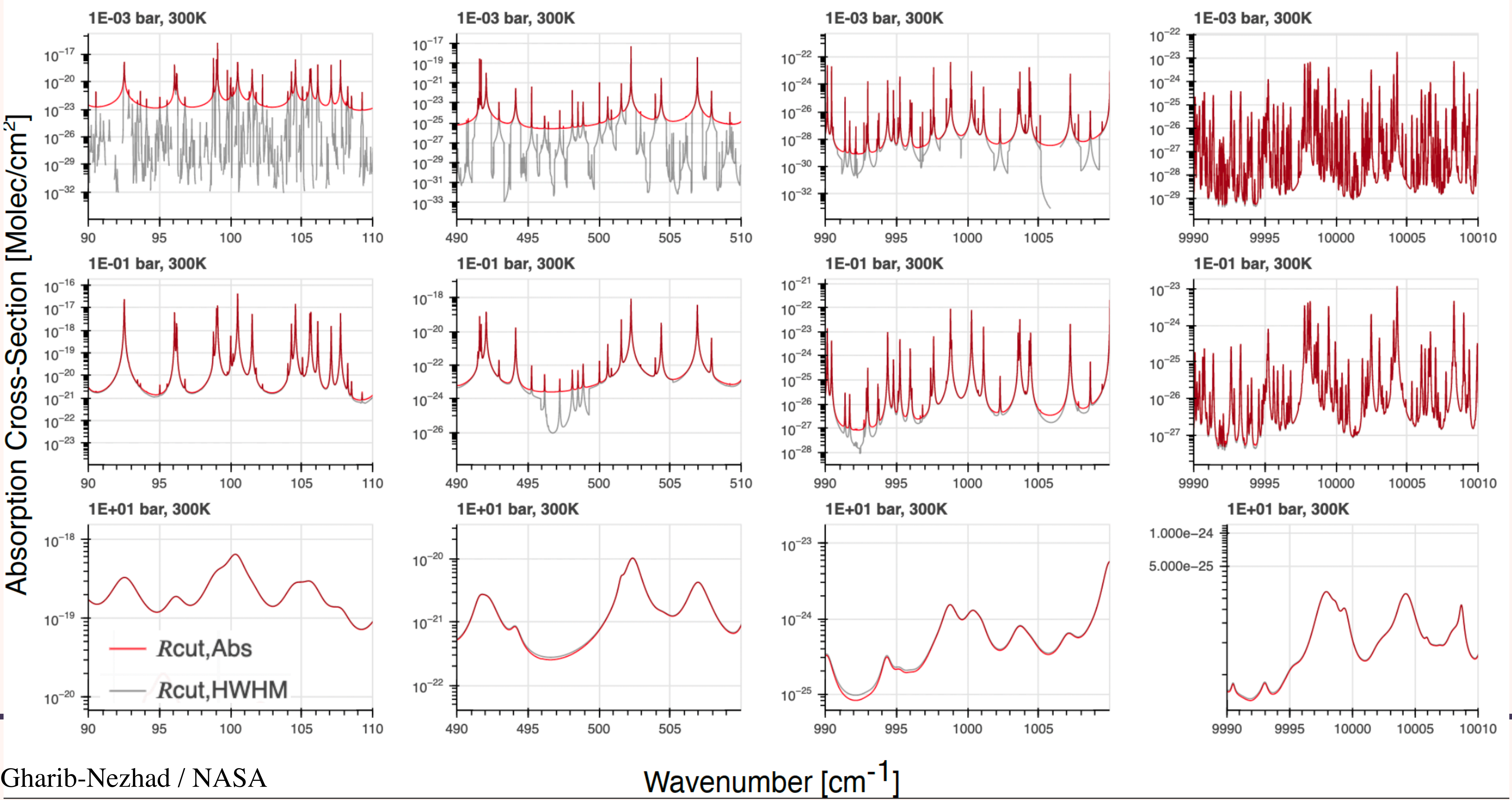


POC: Ehsan Gharib-Nezhad / NASA

CH4-in-Air: Benchmark the Effect of Different Wing Cut-Off Methods - Part 1

$$R_{\text{cut,Abs}} = \begin{cases} 30\ \text{cm}^{-1} & \text{for P} \leqslant 200\ \text{bar} \\ 150\ \text{cm}^{-1} & \text{for P} > 200\ \text{bar} \end{cases}$$

$$R_{\text{cut,HWHM}} = 500 \times \gamma_{\text{Voigt}}$$



POC: Ehsan Gharib-Nezhad / NASA

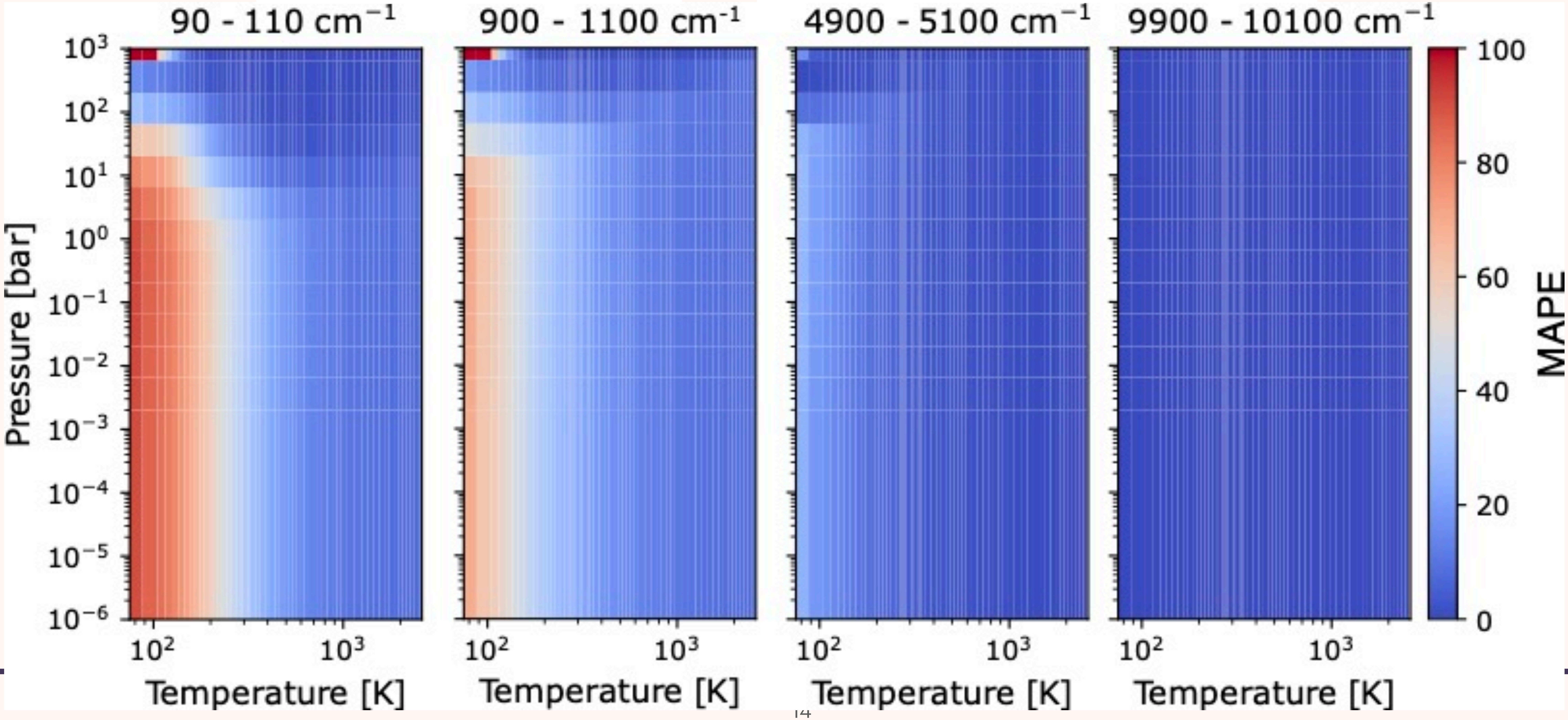
CH4-in-Air: Benchmark the Effect of Different Wing Cut-Off Methods - Part 2

$$R_{\text{cut,Abs}} = \begin{cases} 30\ \text{cm}^{-1} & \text{for P} \leqslant 200\ \text{bar} \\ 150\ \text{cm}^{-1} & \text{for P} > 200\ \text{bar} \end{cases}$$

$$R_{\text{cut,HWHM}} = 500 \times \gamma_{\text{Voigt}}$$

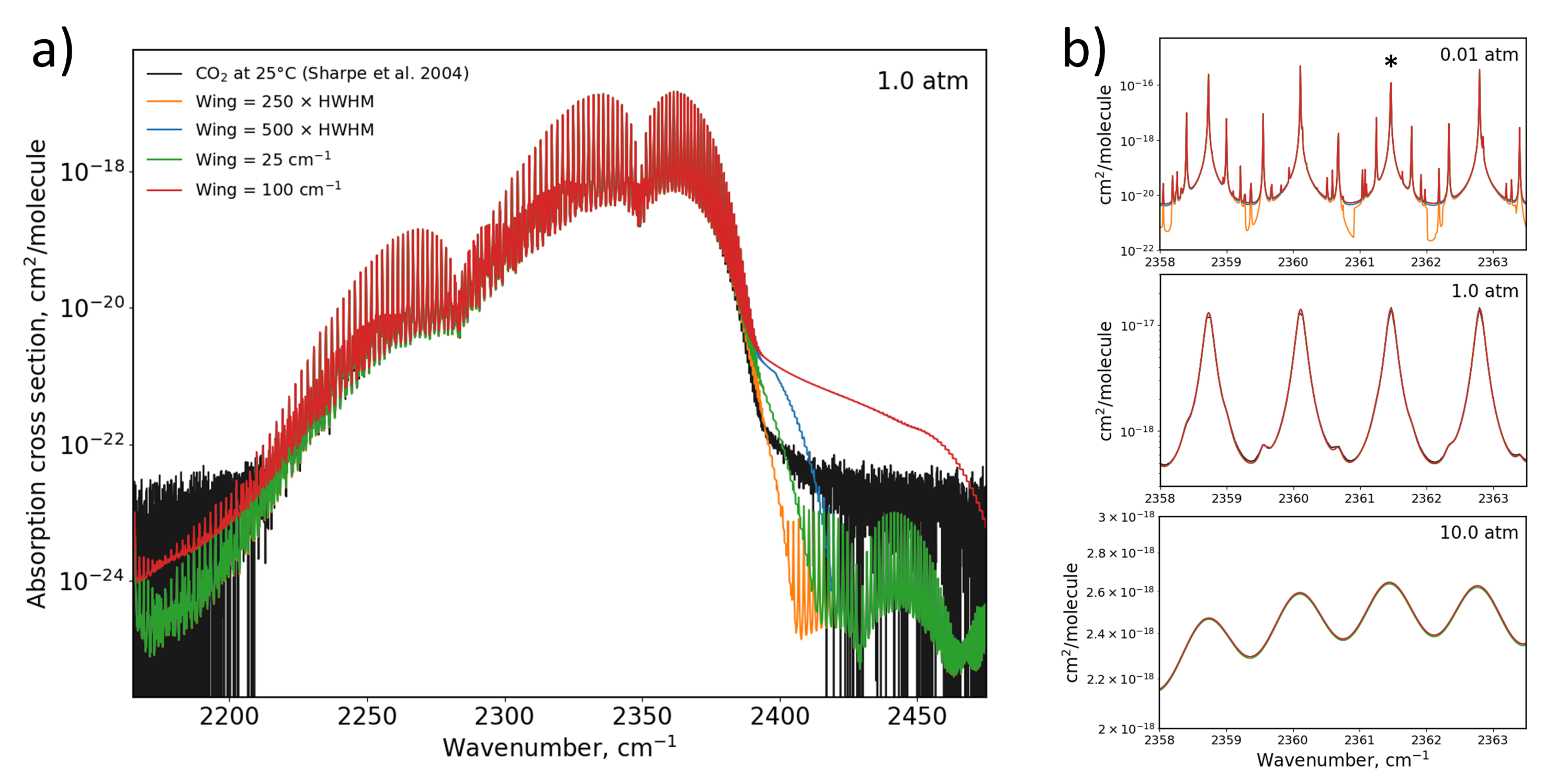
If we take the $R_{\text{cut,Abs}}$ as the actual value, then MAPE formula is expressed as follows:

$$\text{MAPE} = \left(\frac{100}{n_{\text{gp}}}\right) \sum_{i=1}^{\nu_{\text{gp}}} \left| \frac{\sigma_{R_{\text{cut,Abs}}}(\nu,T,P) - \sigma_{R_{\text{cut,HWHM}}}(\nu,T,P)}{\sigma_{R_{\text{cut,Abs}}}(\nu,T,P)} \right| \tag{3}$$



POC: Ehsan Gharib-Nezhad / NASA

CO2-in-N2: Benchmark the Effect of Different Wing Cut-Off Methods



POC: Robert Hargreaves / HITRAN team

Our Recommendation for Choosing the Wing Cut-Off

$$R_{\mathrm{cut,Abs}} = \begin{cases} 25\ \mathrm{cm}^{-1} & \text{for P} \leqslant 200\ \text{bar} \\ 100\ \mathrm{cm}^{-1} & \text{for P} > 200\ \text{bar} \end{cases}$$

This method is chosen for the following reasons:

1. For intermediate pressures and high wavenumber (>5000 cm^{-1}): Very good agreement
   For very low pressures: Significant difference

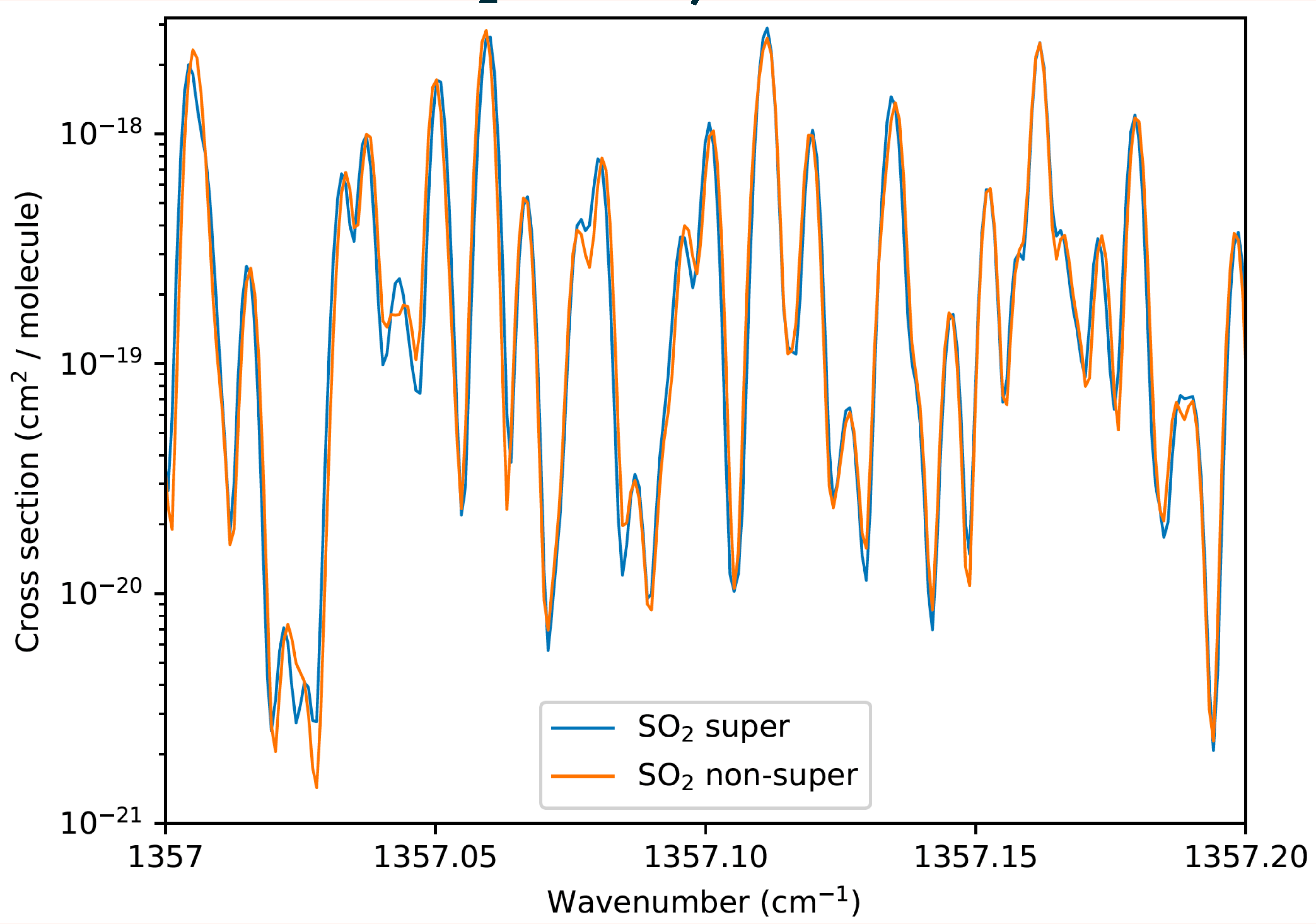
2. For very high pressures (> 200 bars), the Voigt HWHM is more than 20 cm^{-1} and so to model the core of the line profile and a part of the wing, an absolute value of 100 cm^{-1} is proposed.

3. A line wing of 25 cm^{-1} is typically used for calculations of terrestrial radiative transfer. Hence, our proposed method is very well aligned with the planetary community and could be utilized for their modeling studies as well.

SO2-in-H2/He: Assess the Impact of the Super-Lines Method on Wing Cut-Off

Temperature (K)	Pressure (bar)	MAPE (%)
1500	1	7.8×10^{-4}
1500	1×10^{-2}	0.09
1500	1×10^{-5}	0.18
1000	1	5.90×10^{-3}
1000	1×10^{-2}	0.21
1000	1×10^{-5}	0.83
500	1	0.03
500	1×10^{-2}	0.03
500	1×10^{-5}	6.34

SO_2 - 500 K, 10^{-5} bar



POC: Katy Chubb & Sergei N. Yurchenko / ExoMol team

Challenges and Lessons Learned…

- The simulation of a spectrum has a number of several complications, most are associated with the line shape:

line-coupling effects (or line-mixing effects)

- The **choice of a line-shape model** beyond Lorentzian
- The **lack of pressure broadening data** for pressure and temperature ranges relevant to exo-atmospheres
- More sophisticated line shapes are required to account for **non-binary collisions**
- Very sensitive to the choice of **wing cut-off**, particularly in certain pressure and temperature ranges across the wavelength space
- **Consistency** in atmospheric modeling results

Stay Tuned! In Revision at RAS Techniques and Instruments Journal.

The impact of spectral line wing cut-off: Recommended standard method with application to MAESTRO opacity database

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