SAG 26: Exoplanet Reflectance Spectroscopy for HWO

Jan 2025 Update

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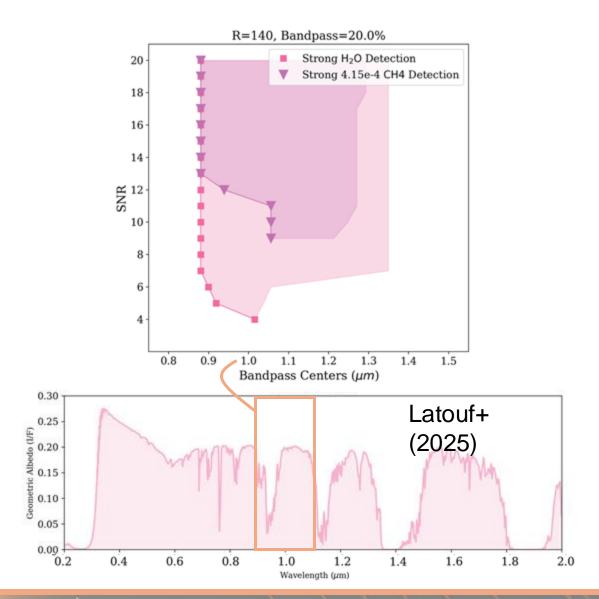
Lightning Summary

- **Motivation**: Prepare and validate the suite of tools that will help define the measurables and requirements for HWO.
- Goals: Execute a community-driven intercomparison of spectrum generating tools and determine a set of best practices for spectral simulation/retrieval.
- Timeline: Spring 2024 Fall 2025
- **Participants**: 23, with active participation from 6+ US and international research groups.
- Status: Roughly 50% of intercomparison cases completed. Report in-prep.



Motivation

- HWO responds to Astro2020's challenge to pursue a "robust sample of ~25 atmospheric spectra of potentially habitable exoplanets[.]"
- Understanding of how direct imaging instrument performance connects to spectrum quality (and subsequent environmental inferences) is strongly modelbased.



Risk

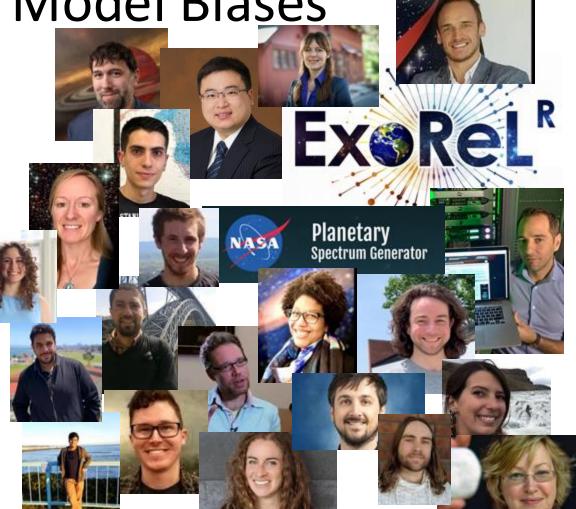
- Model-derived errors and/or biases could translate to overly stringent (or overly loose) instrument requirements for HWO.
- E.g., Model X says that SNR of 10 at 1.1 μ m yields a strong H₂O detection while Model Y says that SNR of 20 is required.





SAG 26: Addressing Spectral Model Biases

- Develop common understanding across all engaged research groups.
- Compare and validate opacities, spectral forward models, retrieval;
- Understand required model complexities.
- Identify best practices.
- Find any important areas of disagreement that could impact HWO science and design.



Organization

- Participants assembled after wide advertising.
- Kick-off April 2024.
- Bi-weekly telecons.
 - Recorded.
 - Notes and homework circulated.
- Maintaining:
 - Shared Google Drive where all participants upload results.
 - Living SAG 26 report.



Approach

- Intercomparisons start with fundamental inputs, increase in complexity.
- Compare:
 - 1. Opacities
 - 2. Spectral Models
 - 3. Retrievals
- Each comparison case has a welldefined setup document.

Experimental Setup

CH4 Line Absorption

Inputs

Case: CH4 line absorption Purpose: Comparison of high-resolution ro-vibrational opacities for CH4 Pressure(s) (Pa); {1e3,1e5} Temperature(s) (K); {300} Broadening: {foreign (native to model), self [optional]} Isotopologues: (whatever is native to given model) Wavelength Range (um): 0.2–5.0 Resolving Power; >10,000 (cross sections); >1,000 (transmission)

Outputs

- 1. Cross section file
 - a. ASCII-formatted
 - b. Columns of wavelength (um), absorption cross section (cm²/molecule)
- 2. Transmission file
 - a. ASCII-formatted
 - b. Columns of wavelength (um), transmission through a column: $N_c = p/g/m$

where N_c is the number of molecules per unit area, p is the pressure for this case (e.g., 1e3 Pa or 1e5 Pa), $g = 10 \text{ m s}^2$, and m is the molecular weight for the line absorbing gas.

3. Supplementary file

- a. Model details (e.g., citation, line cutoff)
- b. Example Python script to read cross section file

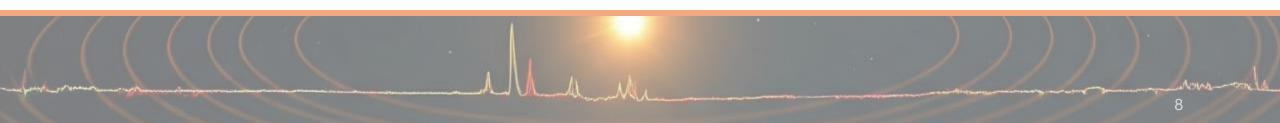
Naming Conventions

- 1. Cross section file
 - a. ch4_[model]_[linelist]_[pressure]_[temperature]_[broadener]_[submitter].dat
 - b. e.g., ch4_abstool_hitran2020_1e3Pa_300K_N2_sagan.dat
- 2. Transmission file
 - a. ch4_[model]_[linelist]_[pressure]_[temperature]_[broadener]_[submitter].trn
- 3. Supplementary file
 - a. ch4_[model]_[linelist]_[submitter].txt

Approach

- Participants upload results to Google Drive.
- Digest plots created and circulated prior to telecons.
 - Thanks Armen!
- Discrepancies analyzed during telecons.
 - Iterate as needed.

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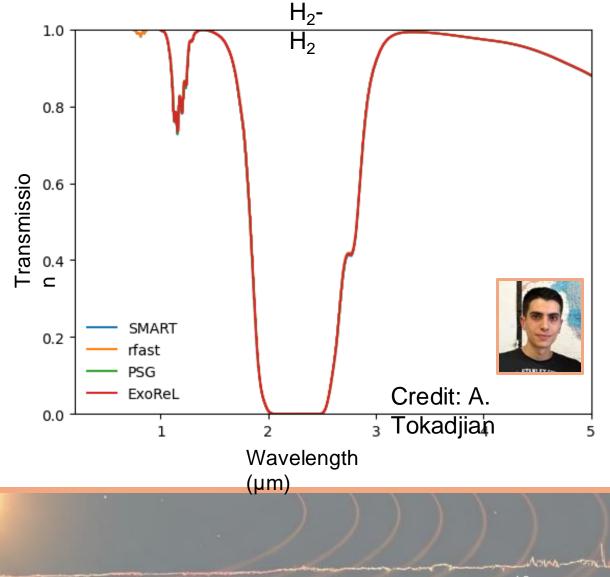


Results: Overview of Progress To-Date

- Completed intercomparison of:
 - Line absorption (сн₄, со₂, со, н₂о, о₂, о₃)
 - Rayleigh scattering (CH₄, CO₂, CO, H₂, H₂O, O₂, N₂, O₃)
 - Collision-Induced Absorption (H₂-H₂, O₂-O₂, N₂-N₂)
- For all opacity cases, differences attributable to known model assumptions.
- Ongoing intercomparison of spectral models.
 - Single-component, scattering cases.

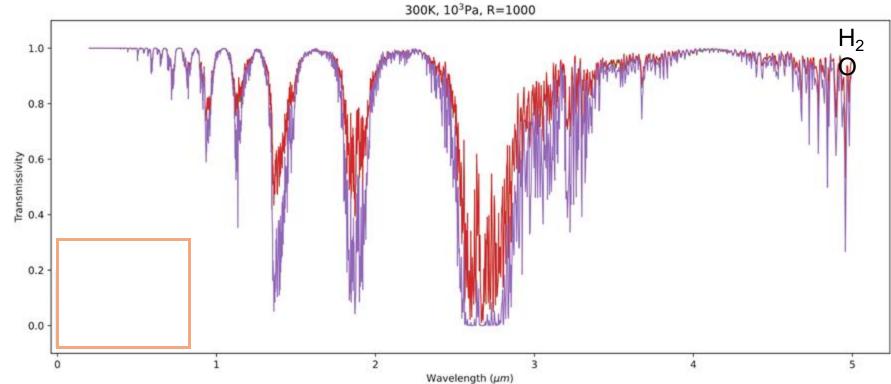
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Earliest comparisons revealed:

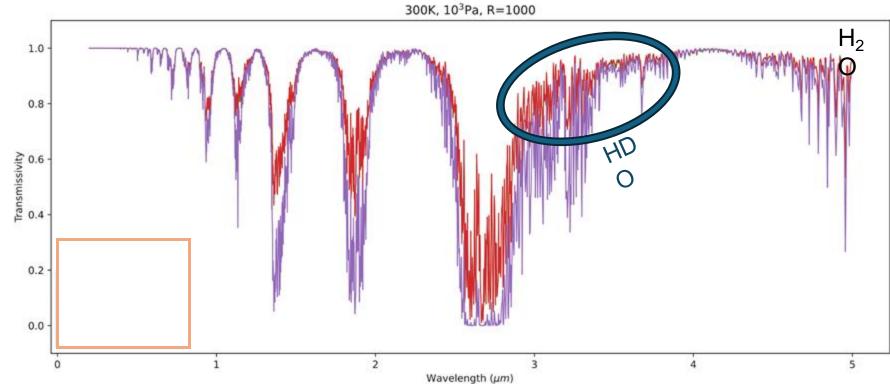
- major model differences, and
- flaws in experiment design.



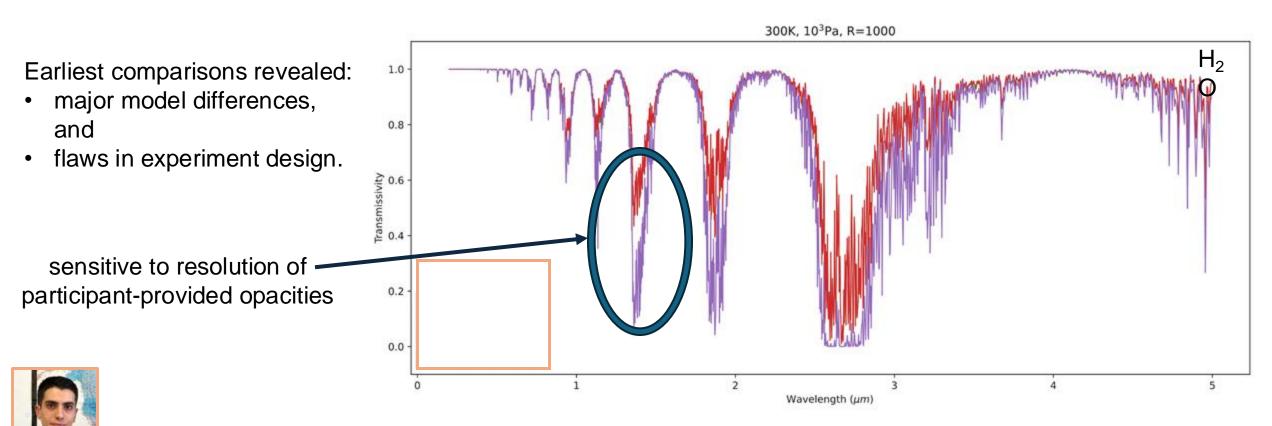


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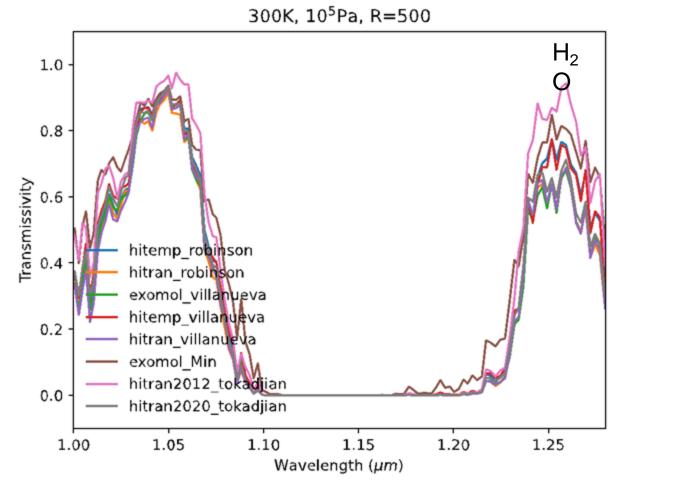
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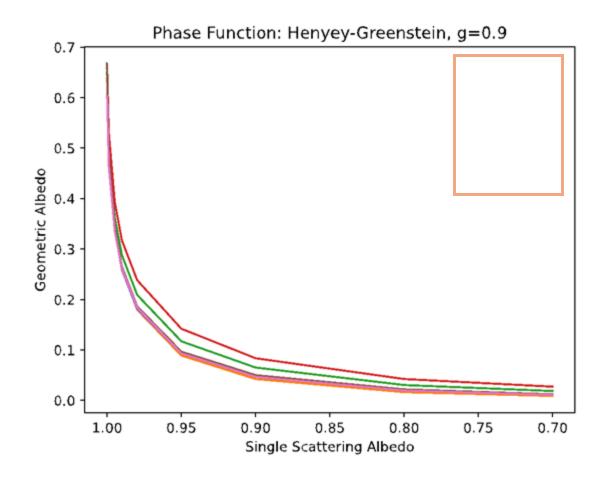
Credit: A.





Credit: A.

Results: Spectral Models





Credit: A.

Lessons Learned

- Empower teamwork. Seek complementarity.
 - CUISINES MALBEC/RISOTTO and Turnbull Precursor Science
- Opacity comparisons (esp. line absorption) benefits from a nested approach.
- Results likely sensitive to adopted linelist.
 - E.g., HITRAN 2012 vs. 2024.
- Spectral models have first-order sensitivity to adopted radiative transfer approach(es).



Next Steps

- Complete ongoing comparisons of forward (spectral) models. (Sp25)
 - Propagate opacity spread through RT models.
 - Consider cases w/cloud scattering.
- Design, execute retrieval intercomparison. (Su25)
 - Work with ongoing RISOTTO intercomparison (Young/Aiei).
- Update and complete SAG 26 report. (Sp25-Fa25)
- Package results for long-term preservation and long-lived utility.

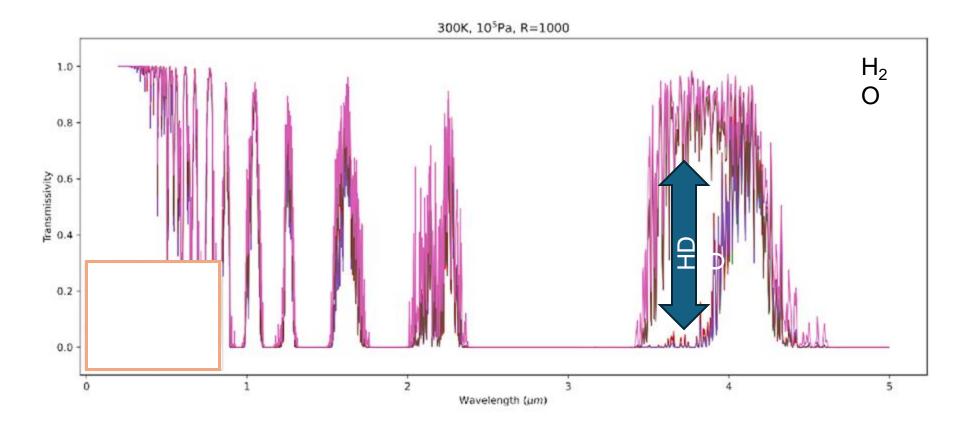
Summary Redux

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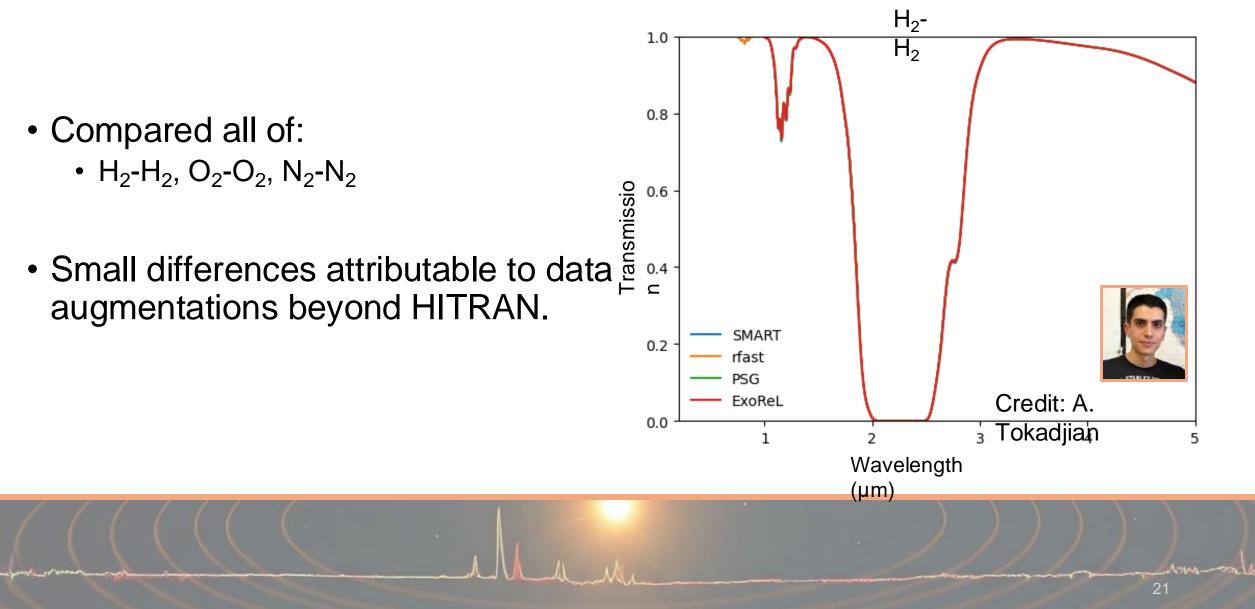
Begin Backup Slides



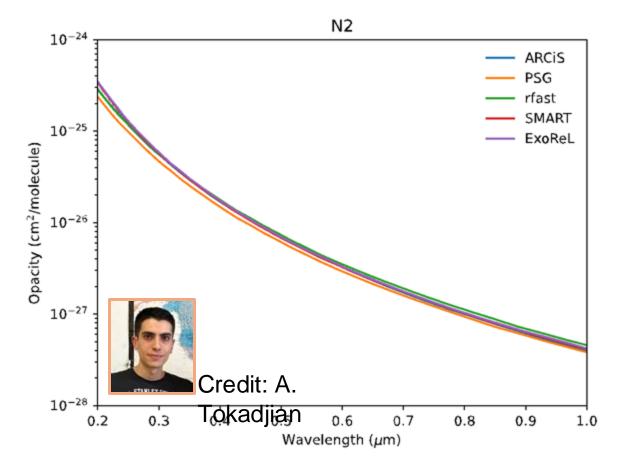


Credit: A.

Results: Collision-Induced Absorption

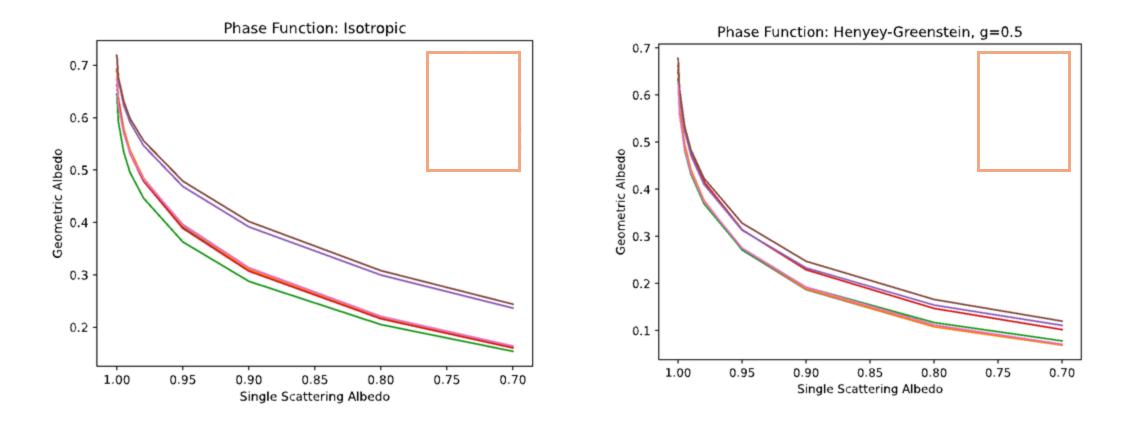


Results: Rayleigh Scattering Cross Sections



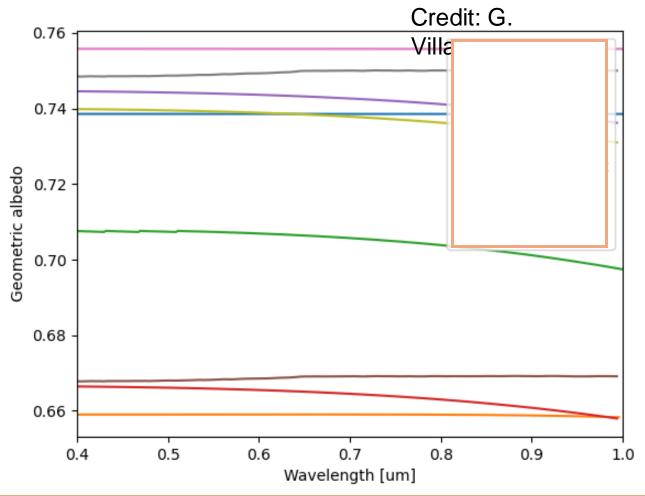
- Strong agreement for all of:
 - CH₄, CO₂, CO, H₂, H₂O, O₂, N₂, O₃
- Small differences attributable to model assumptions.

Results: Spectral Models



Credit: A. Tokadjian

Results: Spectral Models



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