Atmospheric retrieval for the ARIEL spectral database

Michiel Min (SRON)
Ingo Waldmann (UCL)
Joanna Barstow (UCL)

Netherlands Institute for Space Research

Netherlands Organisation for Scientific Research (NWO)

Aim of retrieval

- Derive the atmospheric composition from the ARIEL spectra
  - 1) molecular abundances
  - 2) elemental abundances
  - 3) thermal structure of the atmosphere

- The retrieval is always right (your question might be irrelevant though...)
  - Retrieval answers the question:

What is the best set of parameters - and the accompanying uncertainty - representing the data given all the assumptions in the forward model?

What are the exact physical parameters of the system observed?

Sometimes it feels like....

This is the retrieval giving us the answer 42

This is us thinking about what the real question actually was. Using:

- Complex disequilibrium chemistry
- GCM modelling
- Cloud formation models

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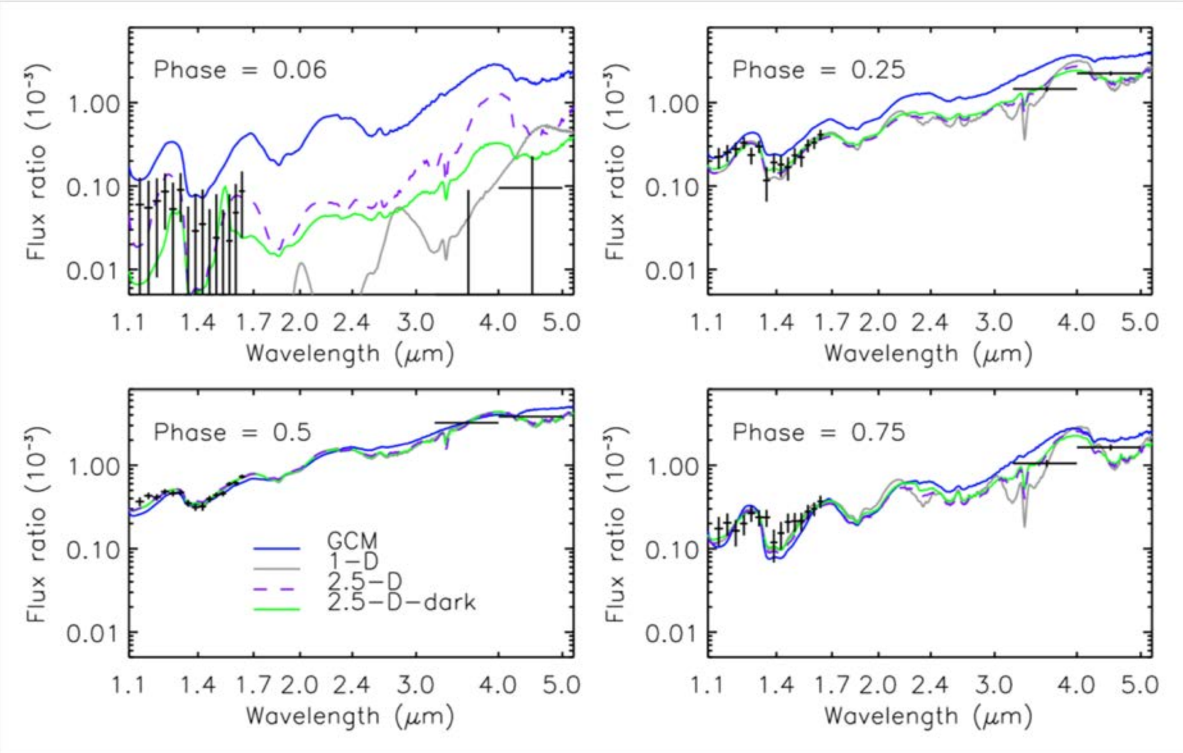
TauREx, NEMESIS, ARCiS

RETRIEVAL CODES USED

NEMESIS

NEMESIS

- Correlated-k approximation for opacities
- Either nested sampling or optimal estimation
- Not linked to thermal or chemical equilibrium models so free retrieval
- Includes multiple scattering and reflected light
- Suitable for Solar System objects -> brown dwarfs
- 2.5D retrieval mode for simultaneous retrieval of phase curve observations NEW!



Irwin et al. (2019)

UCL

TauREx 3

UK SPACE AGENCY

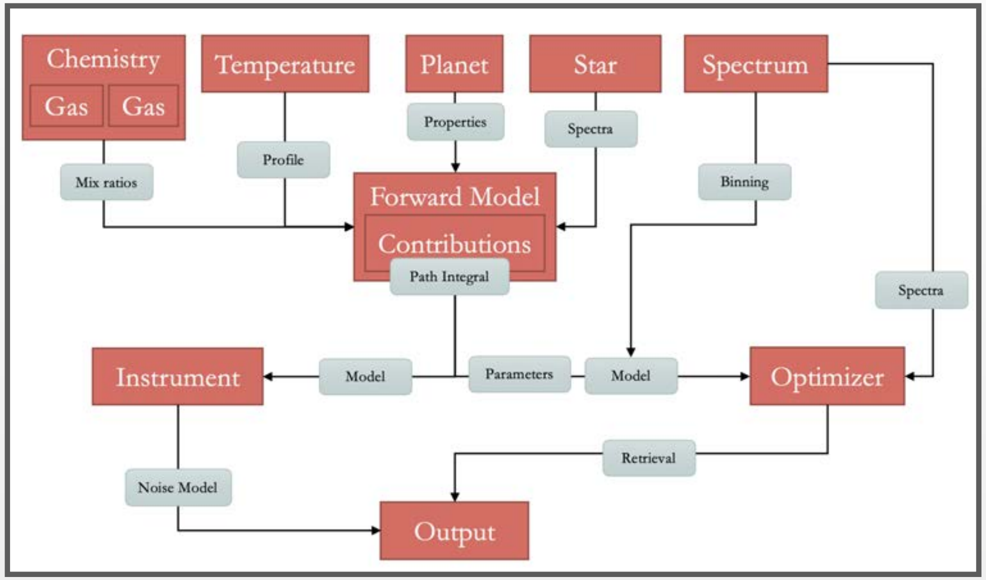
Horizon 2020

erc European Research Council
Established by the European Commission

Science & Technology Facilities Council

TauREx 3

- Built from the ground up as full python stack
- 10 - 200 times faster than TauREx 2
- Fully tested against TauREx 2 which has been benchmarked against NEMESIS, CHIMERA, ARCiS
- For full installation type: “pip install taurex”
- Plugin features and TauREx extensions
- New and fast cross sections
- Fully open under BSD license



Al-Rafaie et al. arXiv: 1912:07759

Ultra-Fast retrievals

- TauREx 3 was built for speed. 10 to >100 times faster than TauREx 2.
- Fully Python 3.x but achieves speeds of compiled languages like C
- Uses JIT compilation of forward models with Numba
- Full use of numpy vectorisation and numexpr for faster numpy operations
- TauREx 3.1 includes full GPU support -> No more performance loss for JWST wavelengths and large line-by-line retrievals

R	TauREx 2 xsec (s)	TauREx 3 xsec (s)
7000	0.57	0.039
10000	0.85	0.062
15000	1.02	0.092

Molecules	TauREx 2 xsec (s)	TauREx 2 k-tables (s)	TauREx 3 xsec (s)
1	7.23	0.45	0.61
2	8.90	0.78	0.74
4	12.42	1.49	0.92
7	19.02	2.63	1.23
15	263.56	8.21	2.34

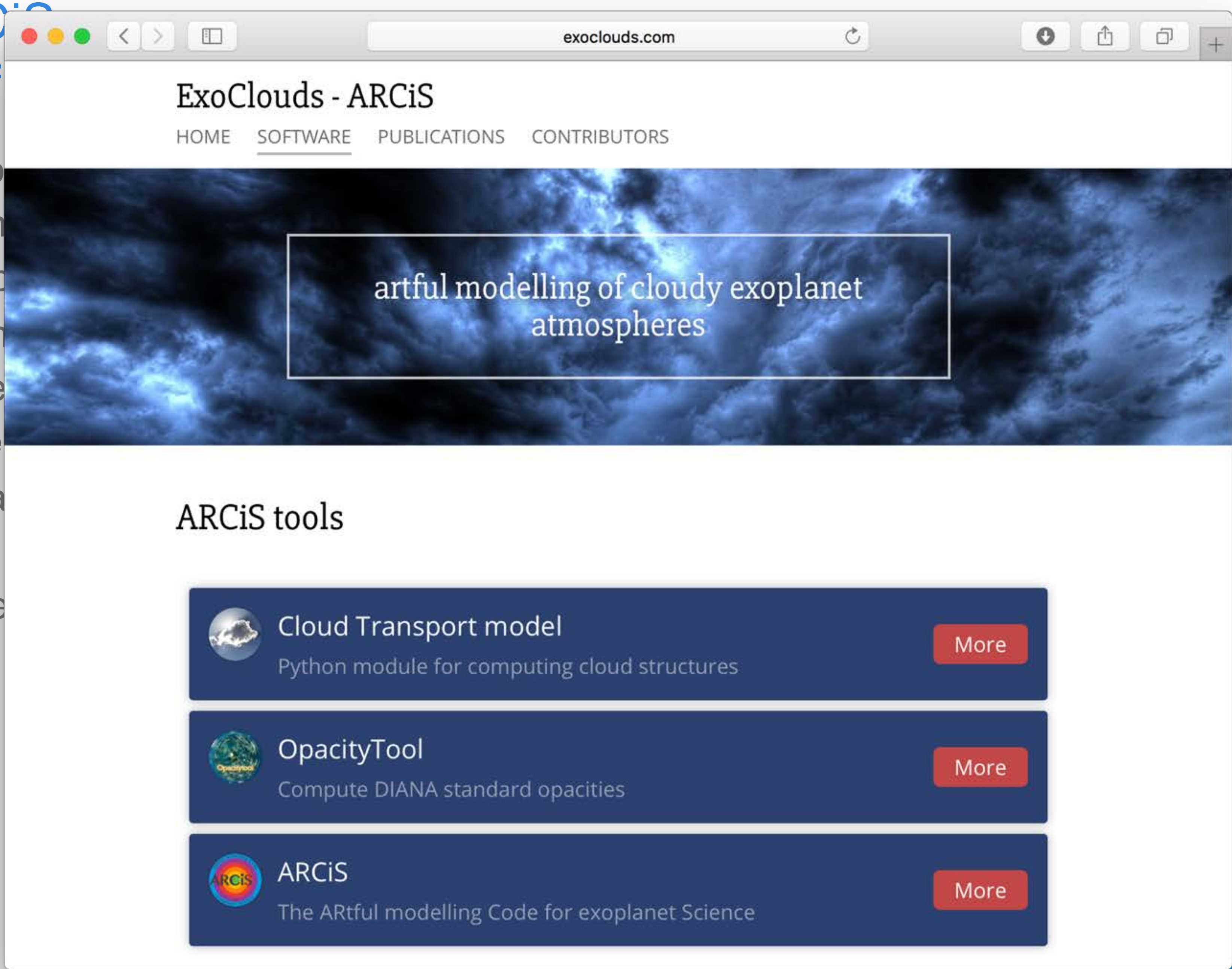
Layers	TauREx 2 xsec (s)	TauREx 2 k-tables (s)	TauREx 3 xsec (s)
50	2.24	0.20	0.24
100	8.60	0.79	0.62
150	19.29	1.81	1.53
200	35.53	3.04	2.29
600	876.24	28.90	15.35

Al-Rafaie et al. arXiv: 1912:07759

ARC

ARtf

- Fo
- An
- Op
- Ch
- Se
- Ite
- Pa
- Re



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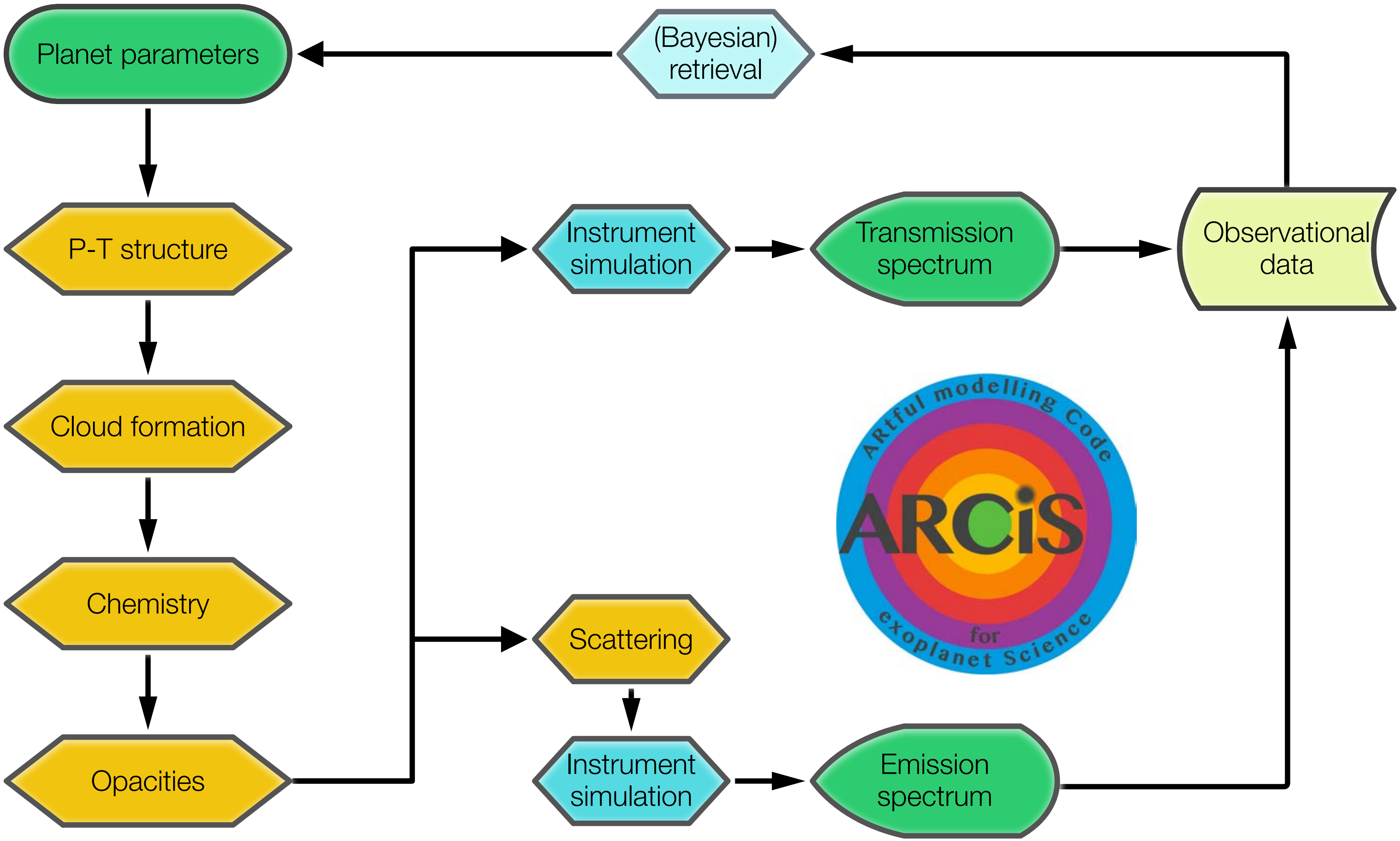
ARCiS scheme



Opacities for exoplanet atmospheres

Cross-sections (R=15,000)
and k-tables (R=1000)

All molecules in ExoMol database
+ HITEMP + MOLLIST (80+ molecules)

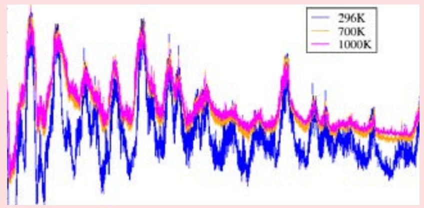
Retrieval codes:
ARCiS (k-tables), TauREx (xsecs),
NEMESIS (k-tables,
petitRADTRANS (k-tables)

Available soon on www.exomol.com

27 temperatures

22 pressures

594 T/P points / molecule



Chubb, Rocchetto, Yurchenko, Min, Waldmann, Barstow, Molliére, Al-Refaie, Tennyson (In prep)

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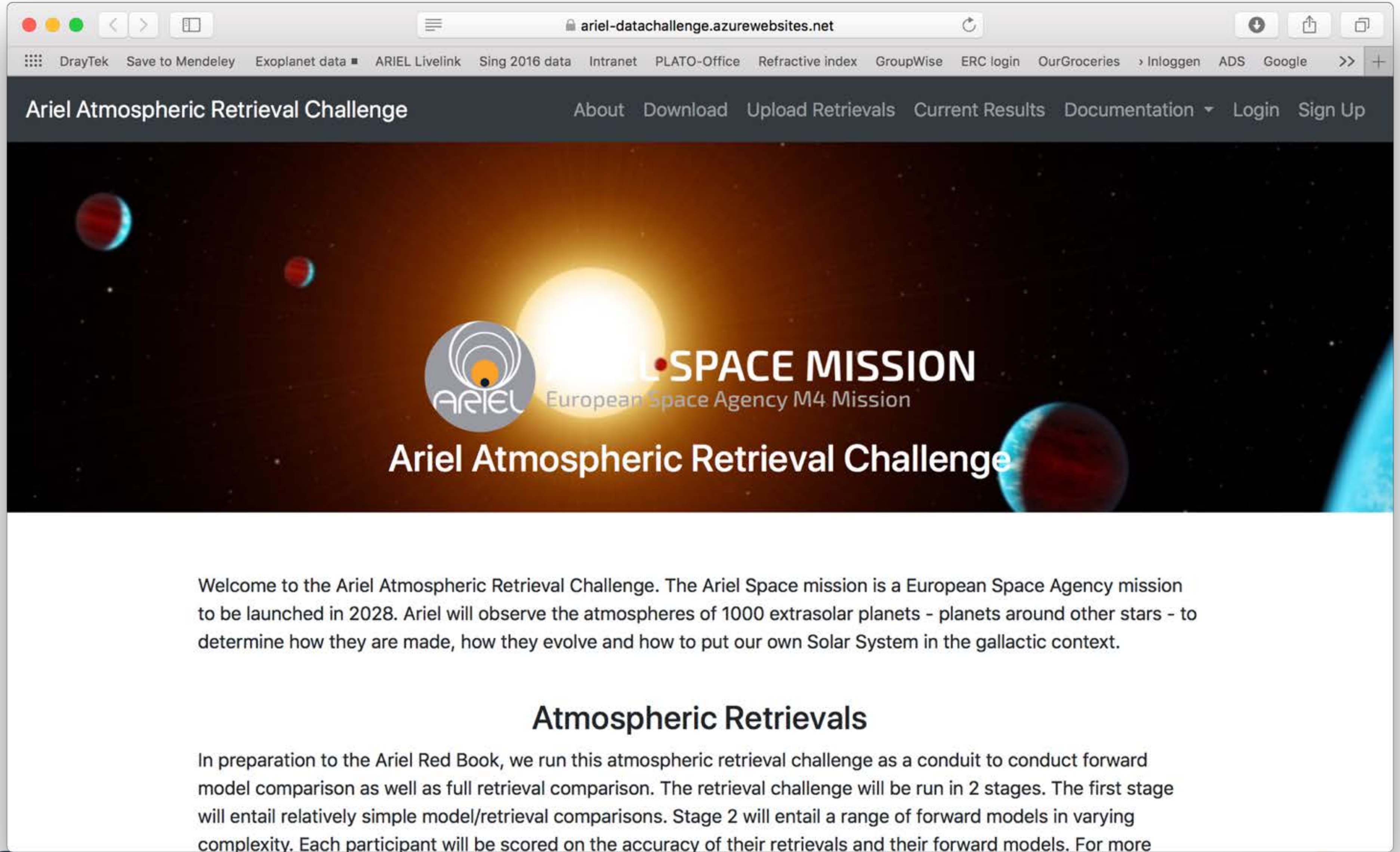
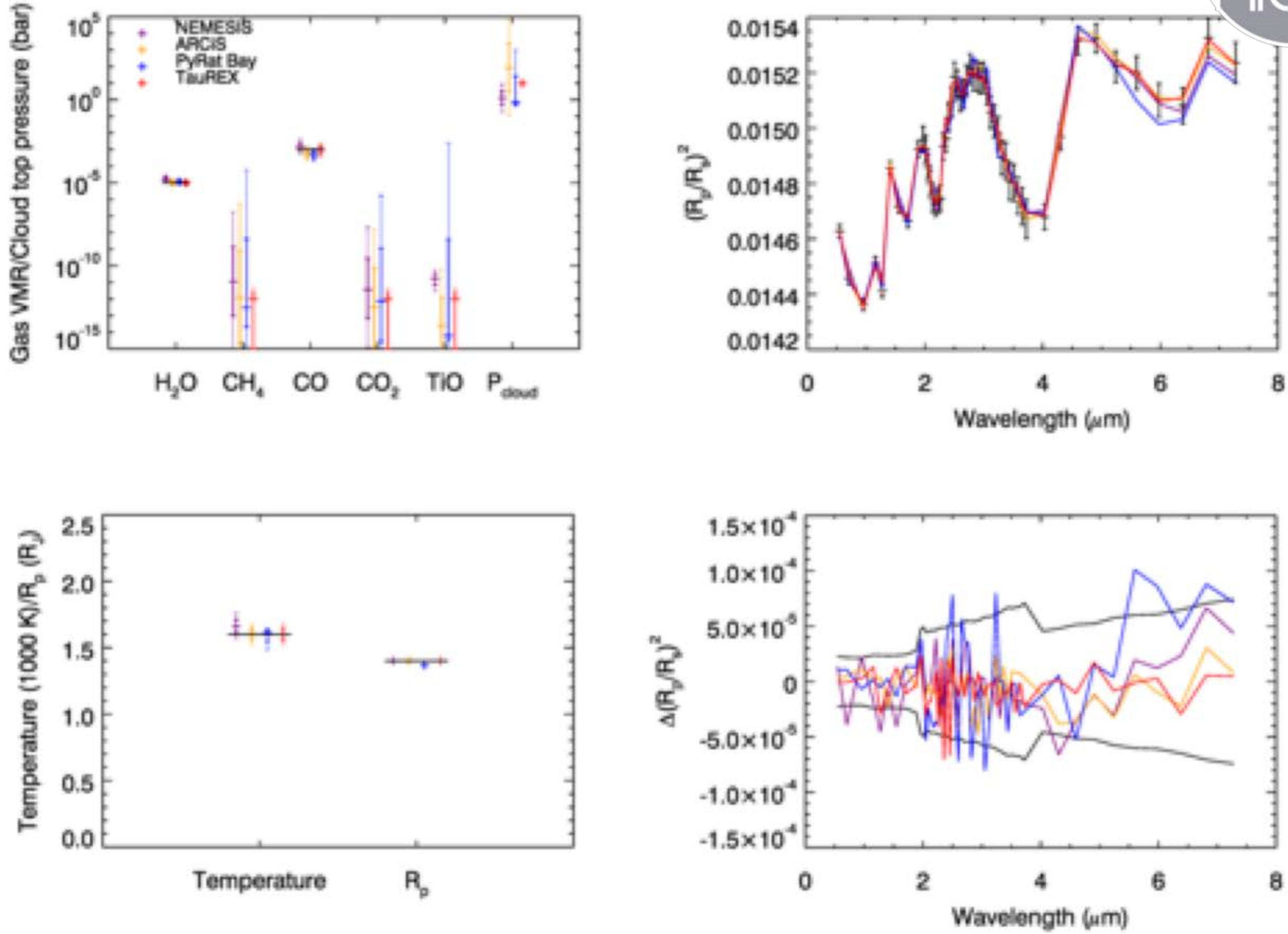
ARIEL retrieval challenge



ARIEL retrieval challenge



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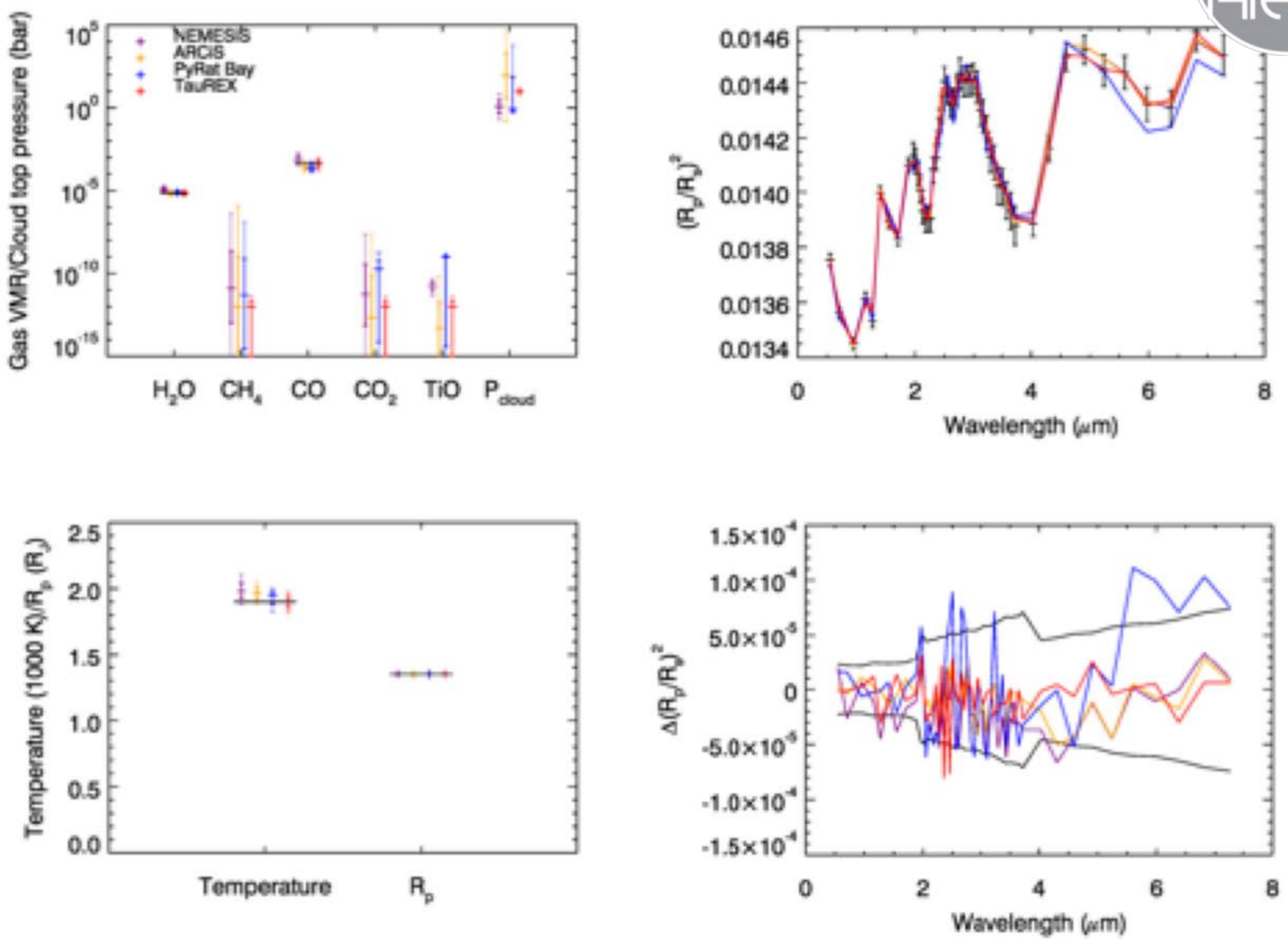
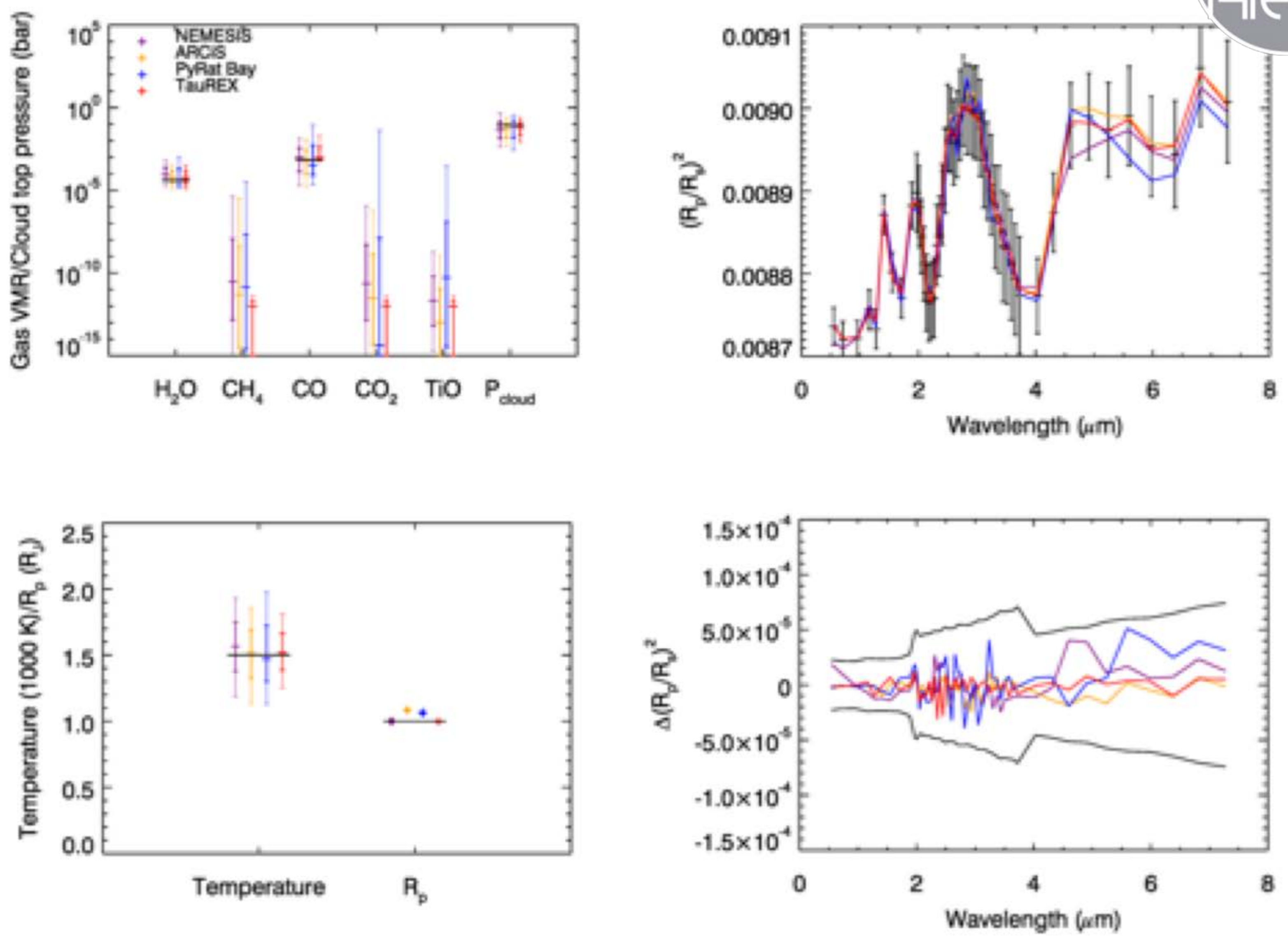


Prepared by Jo Barstow

ARIEL retrieval challenge



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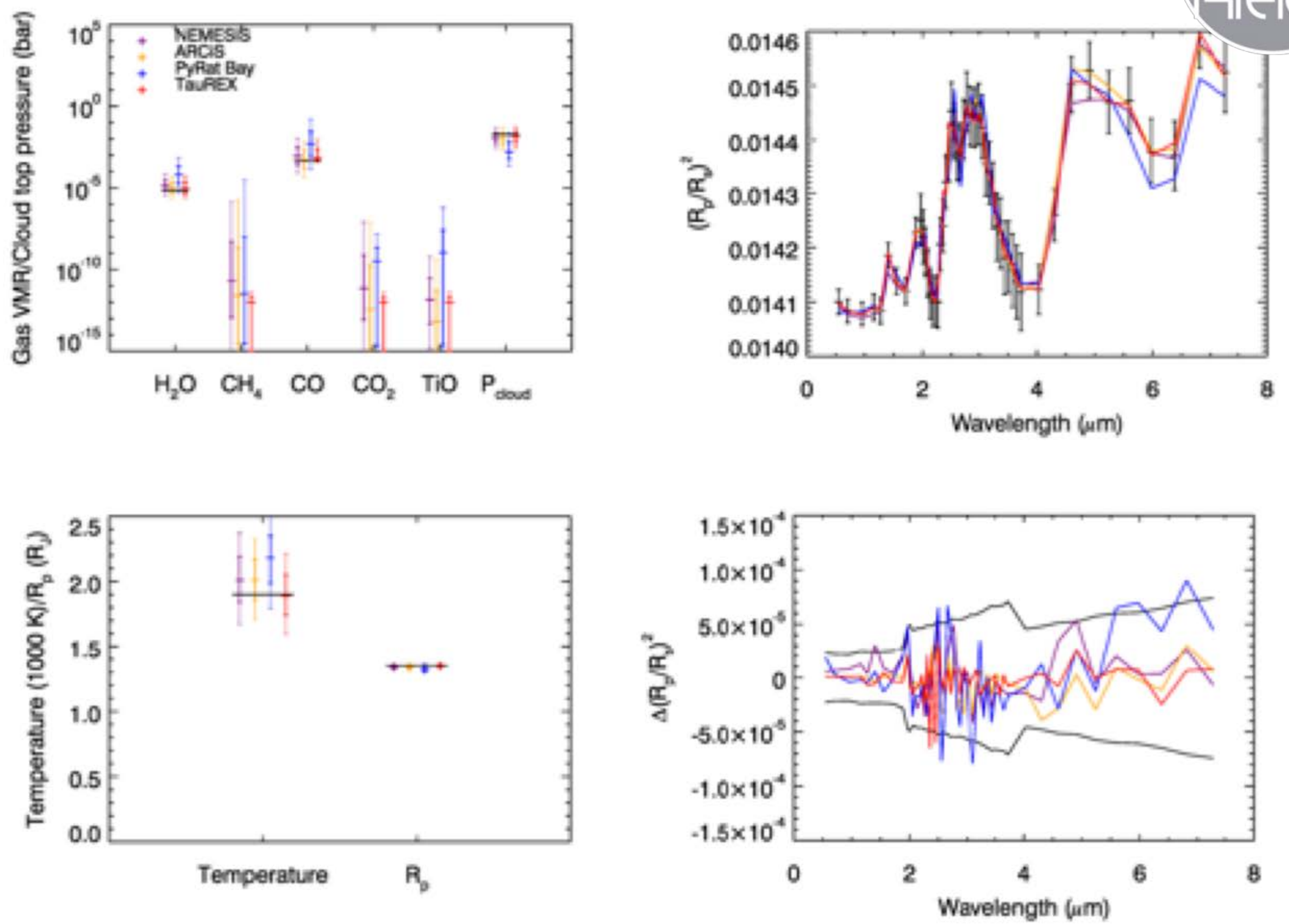

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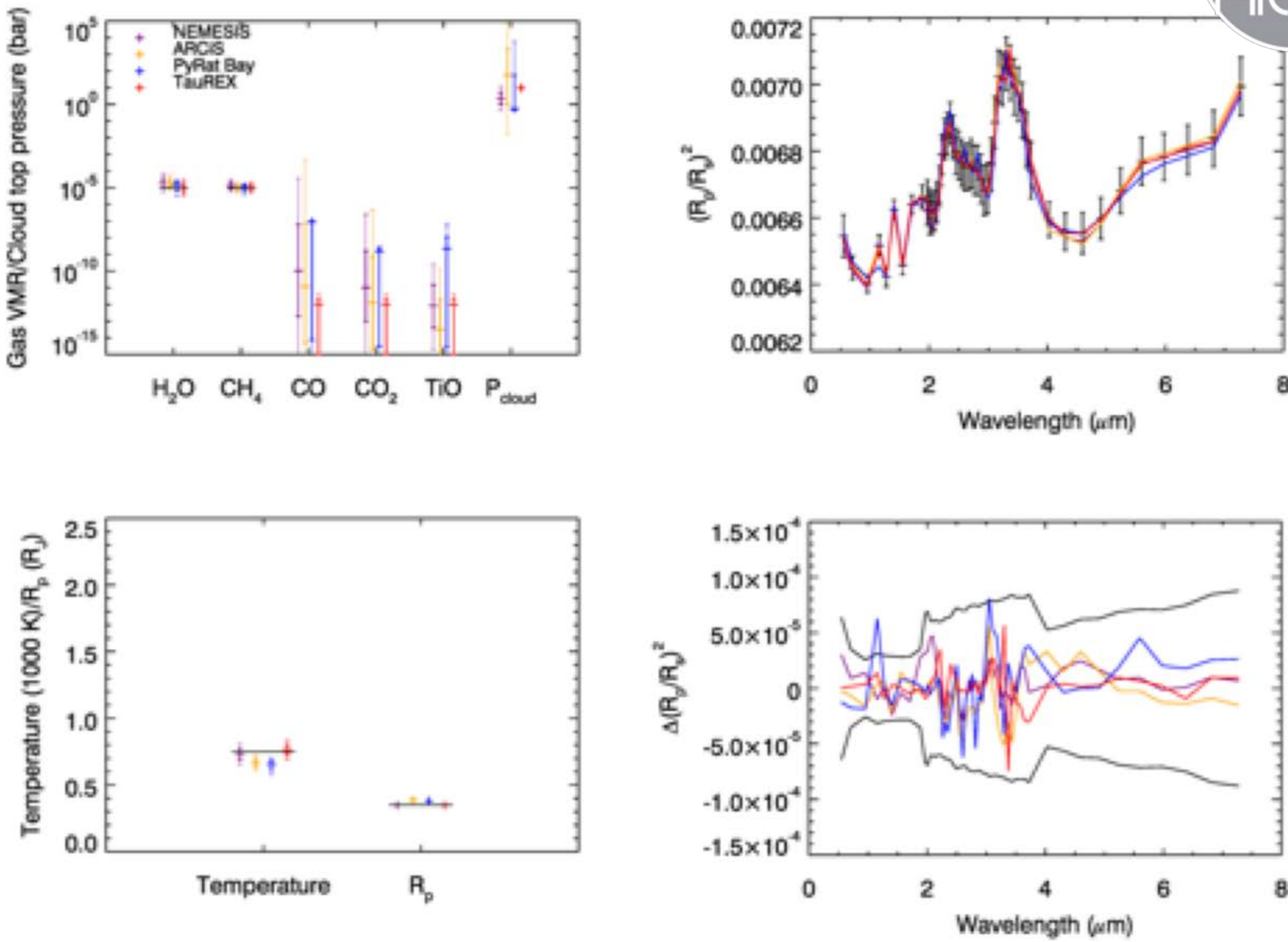

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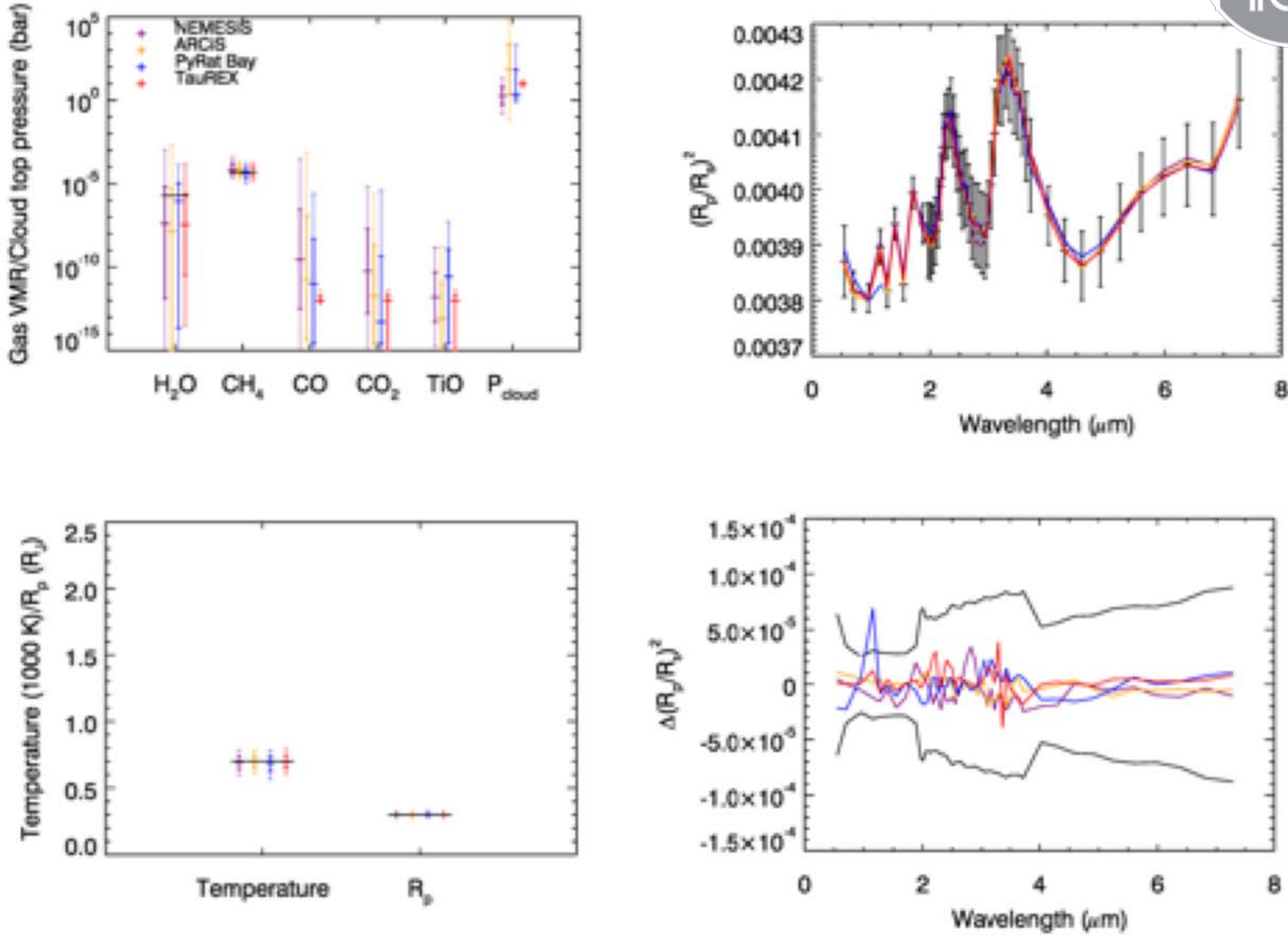

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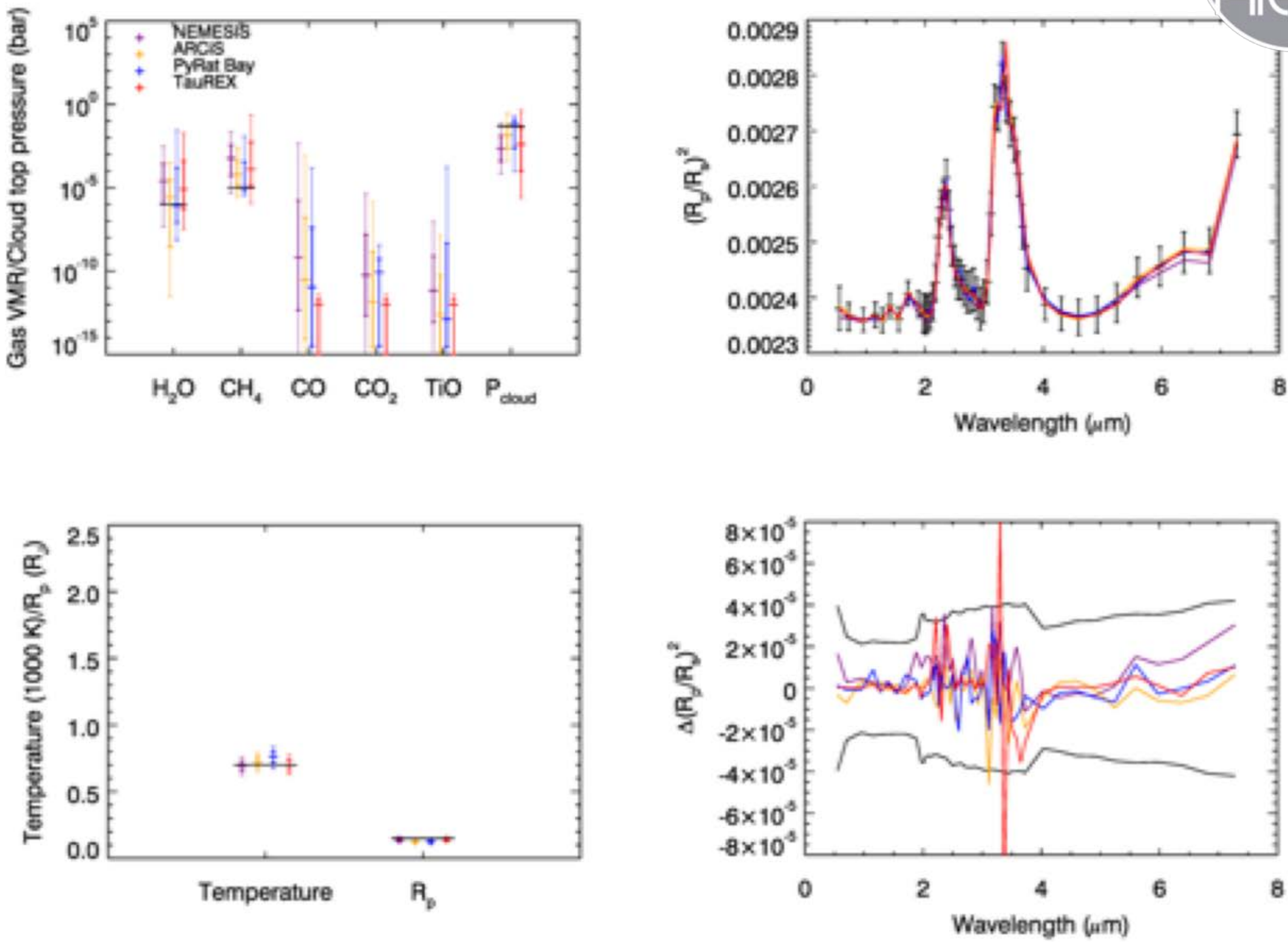

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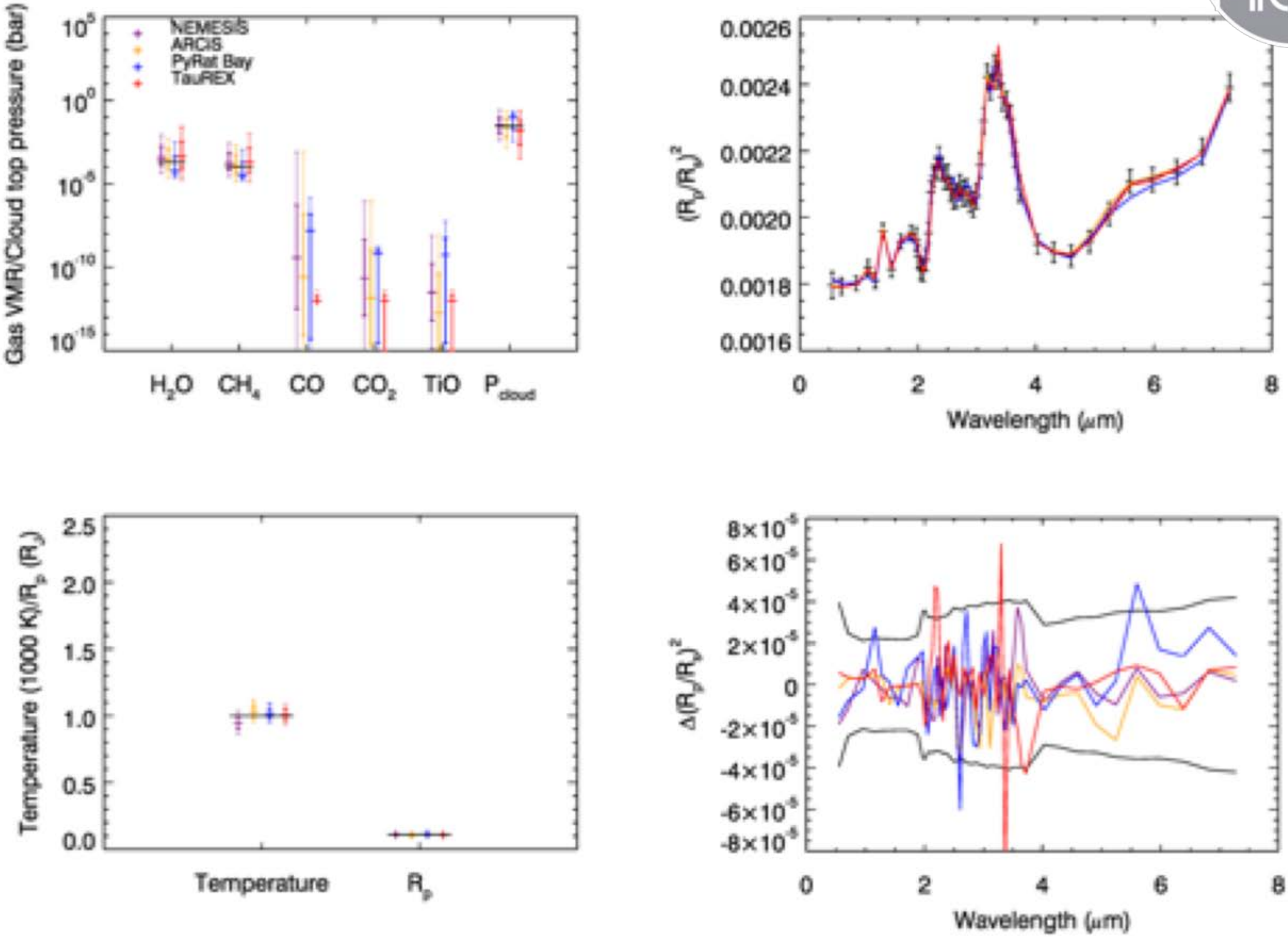


Sensitivity study - molecules

Targets to include for this:

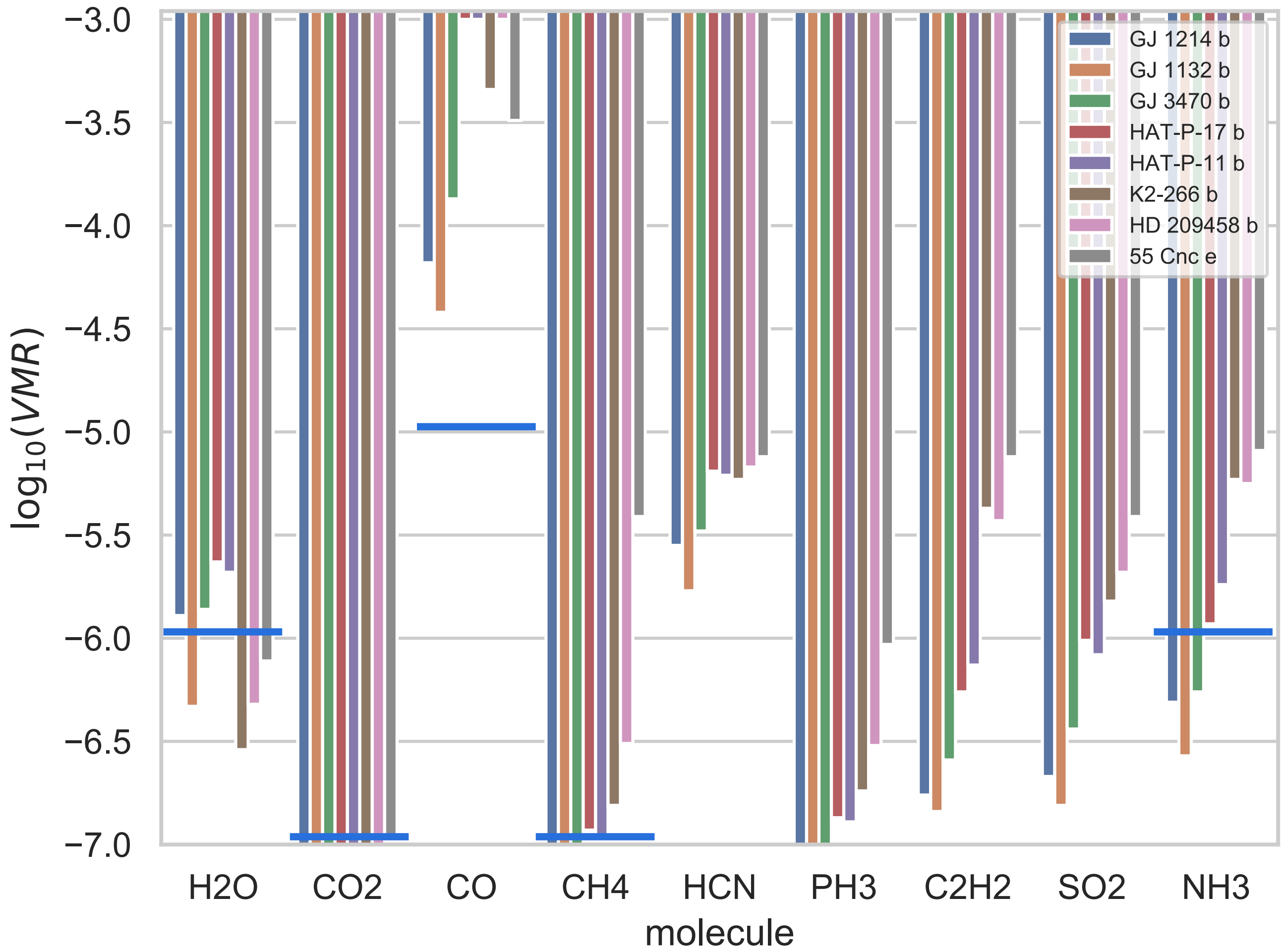
- 55 Cnc e
- GJ 1132 b
- GJ 1214 b
- K2-266 b
- GJ 3470 b
- HD 209458 b
- HAT-P-11 b
- HAT-P-17 b

Standard model contains:

- H_2O (1e-4 level)
- CH_4 (1e-5 level)
- CO (1e-5 level)
- CO_2 (1e-4 level)

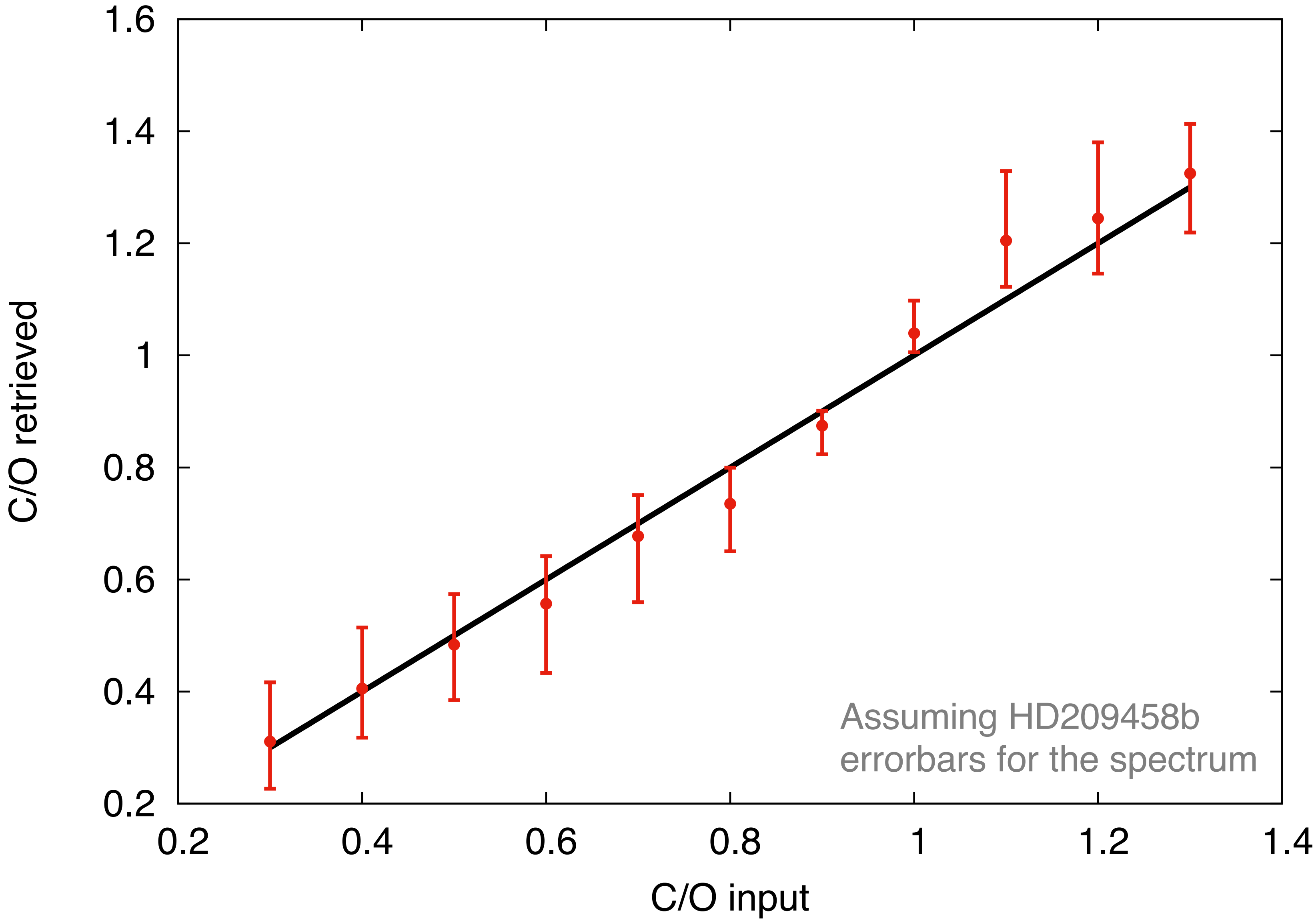
Doing these tests came down to doing ~700 full retrievals

Sensitivity study - molecules



Alfnoor results
(talk by Lorenzo Mugnai)

Sensitivity study - chemistry



Cloud formation model

- **Condensation of MgSiO3 (pyroxene) using vapour pressure equations**
- **Particle settling (rain)**
- **Particle coagulation**
- **Diffusion parameterized using diffusion strength**
- **Nucleation rate is a free parameter**

$$\frac{\partial \mathcal{M}_c}{\partial z} = \mathcal{S}_c$$

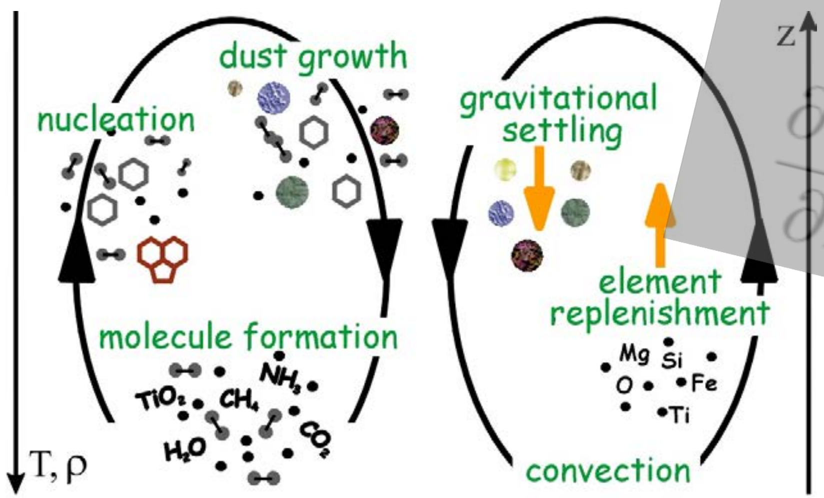
$$\frac{\partial \mathcal{M}_n}{\partial z} = \mathcal{S}_n$$

$$\frac{\partial x_c}{\partial z} = x_c v_{\mathrm{sed,p}}/K_p - \mathcal{M}_c/K_p \rho_{\mathrm{gas}}$$

$$\frac{\partial x_n}{\partial z} = x_n v_{\mathrm{sed,p}}/K_p - \mathcal{M}_n/K_p \rho_{\mathrm{gas}}$$

$$\frac{\partial x_v}{\partial z} = -\mathcal{M}_v/K_v \rho_{\mathrm{gas}}$$

Fundamental physics is captured while unknowns are parameterized



Ormel & Min (2019)

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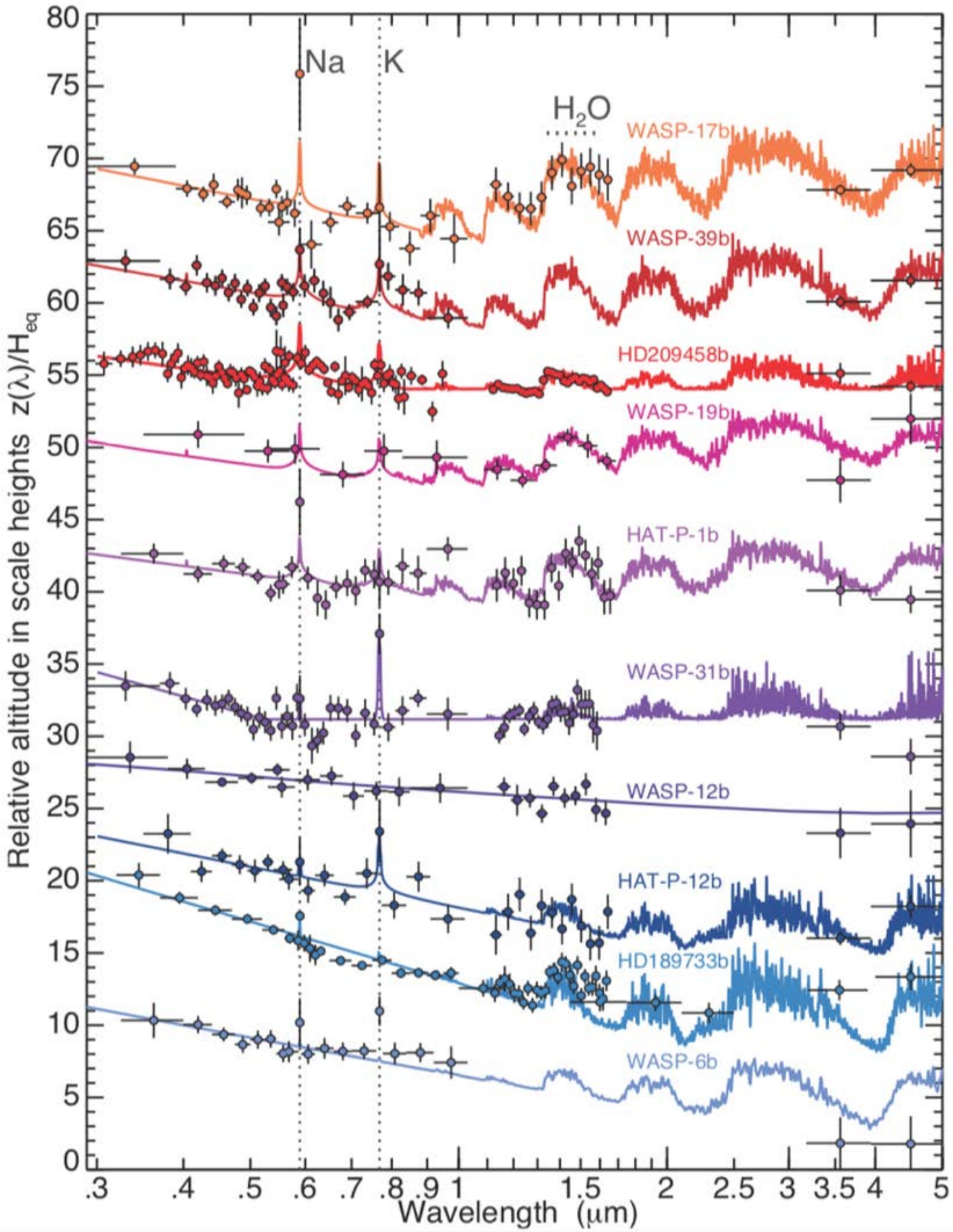
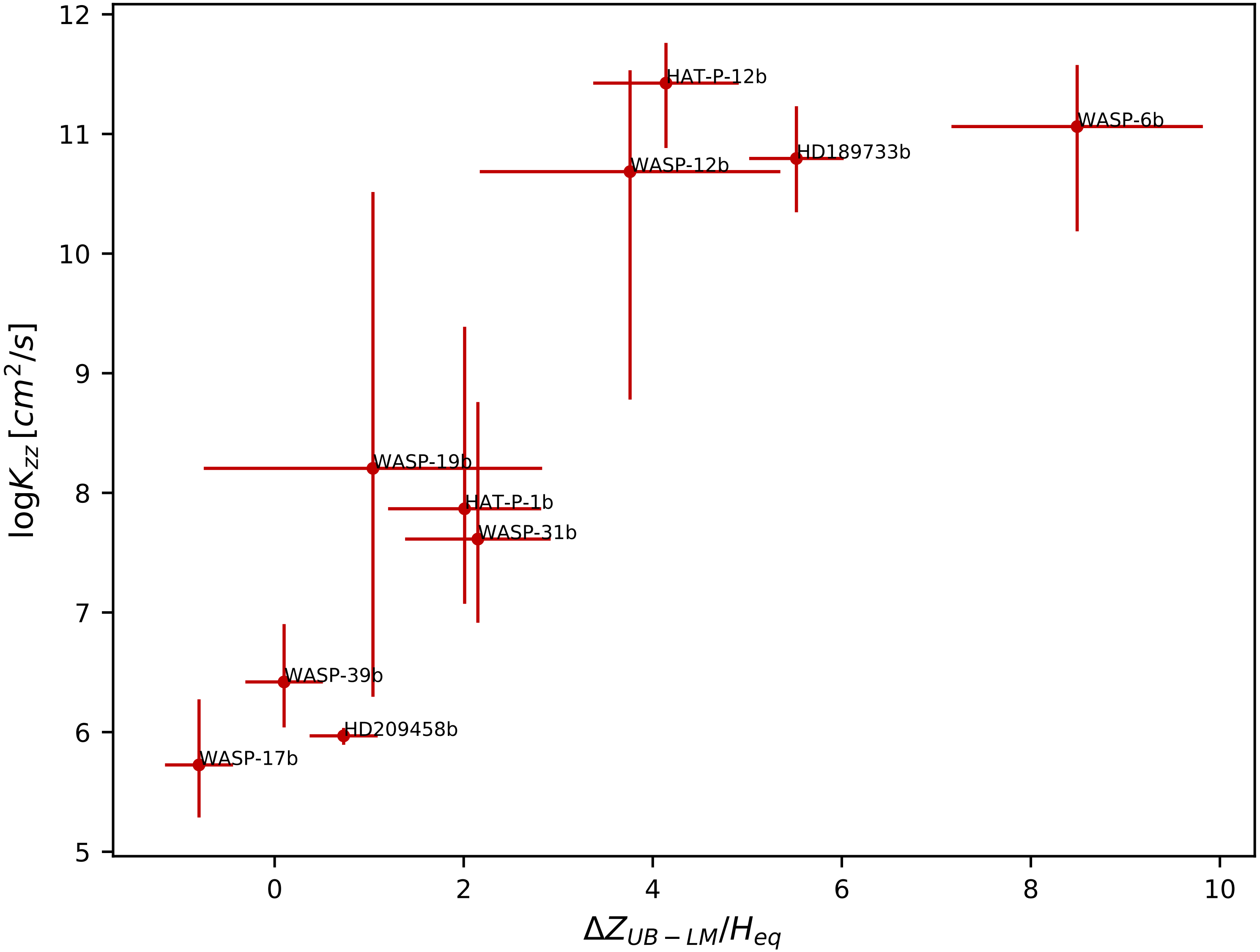
Clouds and hazes



Sing et al. 2016, Nature



Min et al. (submitted)

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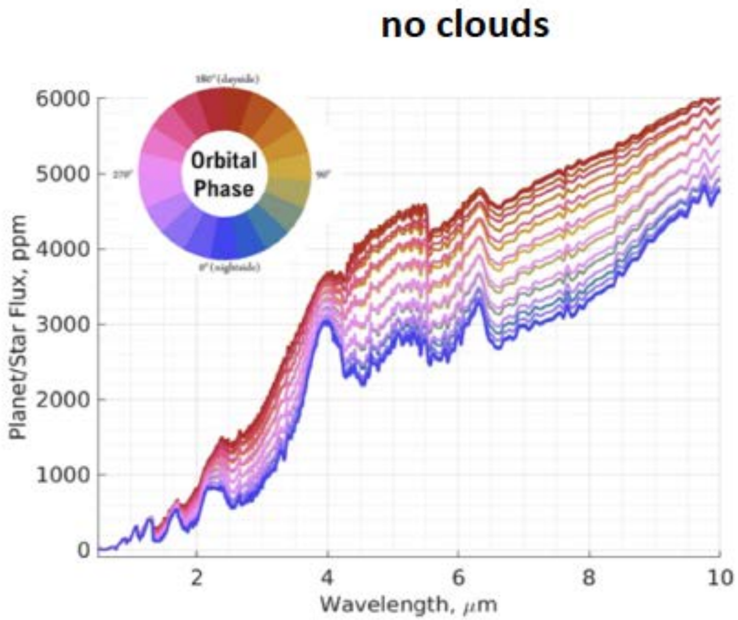
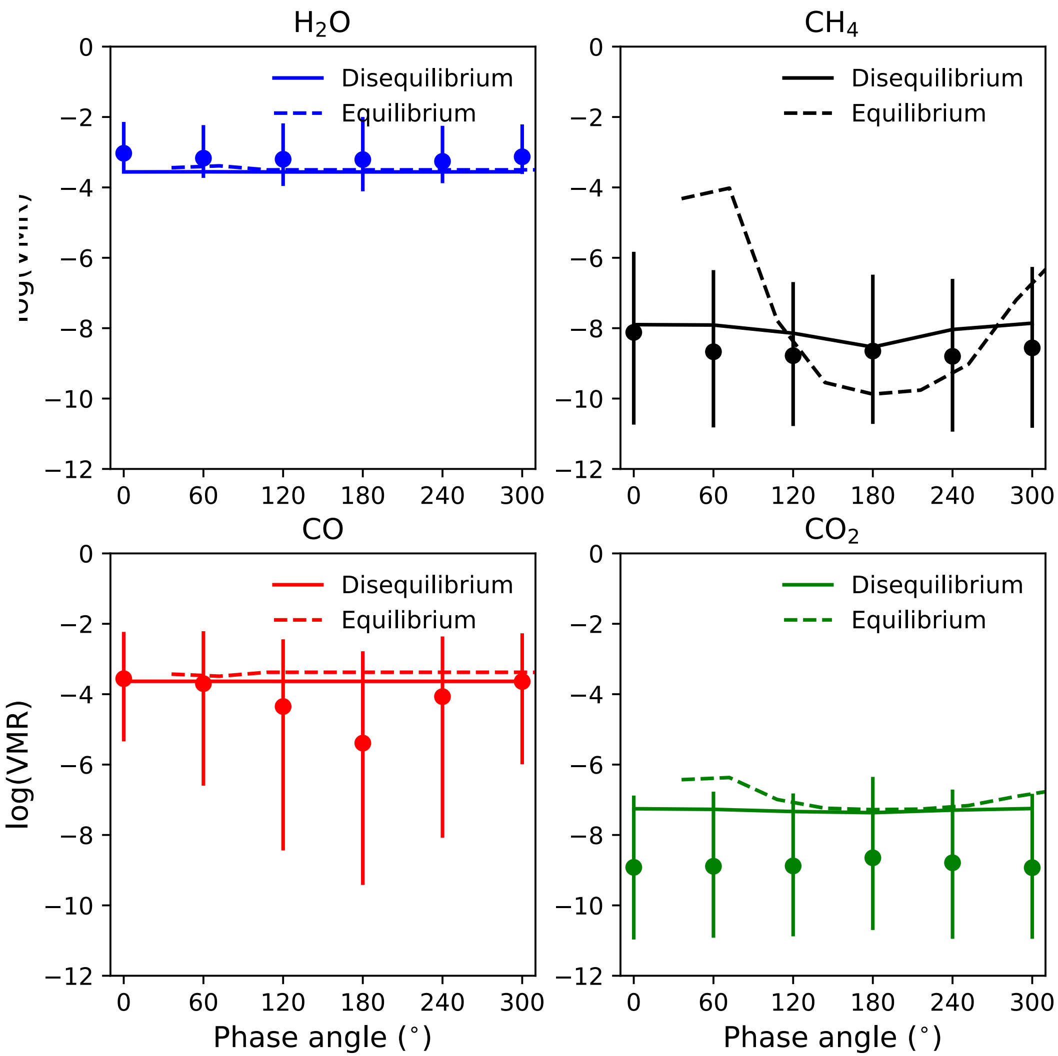
Phase curve retrieval

NEMESIS



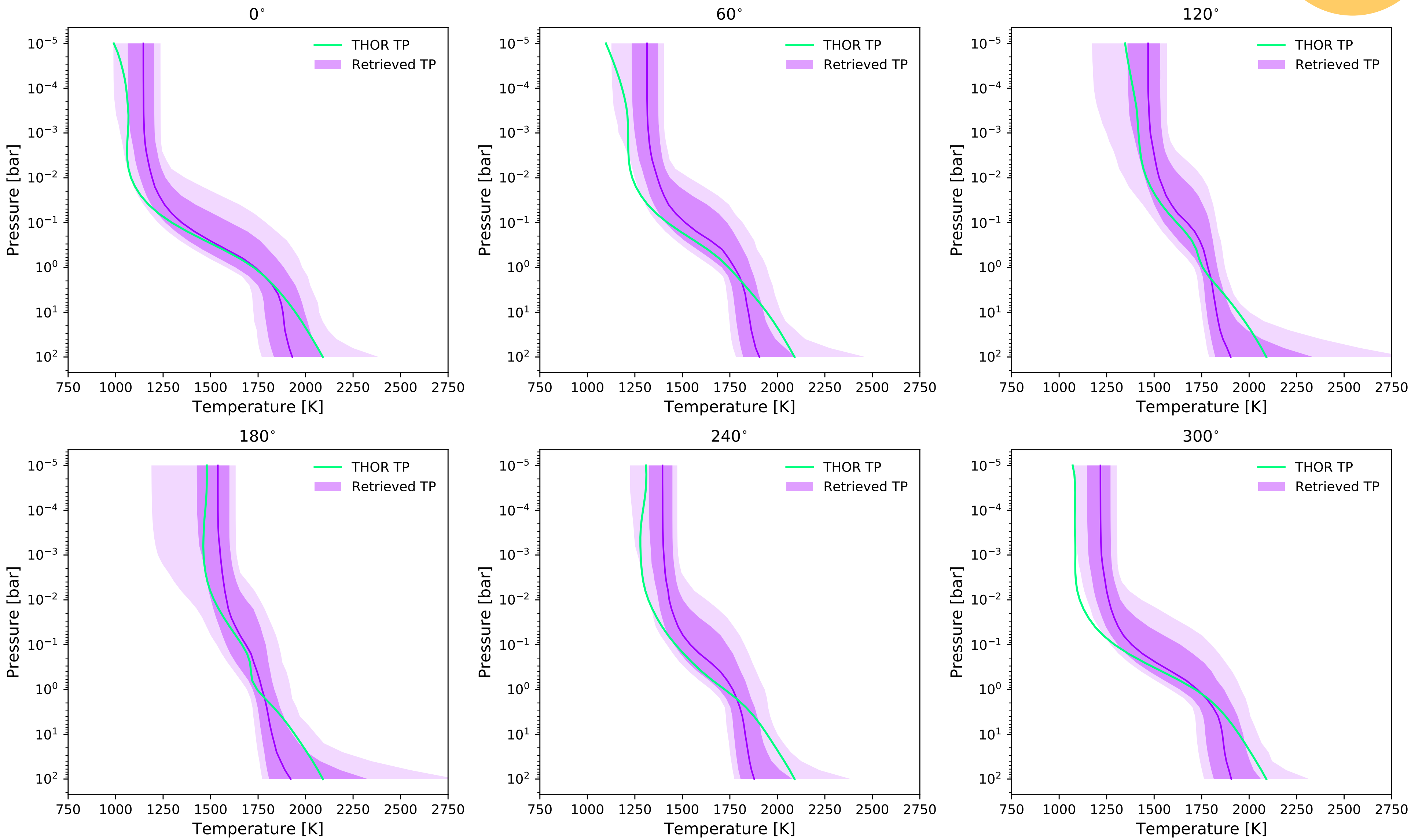


Work from Jake Taylor for the phase curve WG report

GCM model for WASP43b using THOR (Mendonca et al (2018)

Phase curve retrieval

NEMESIS



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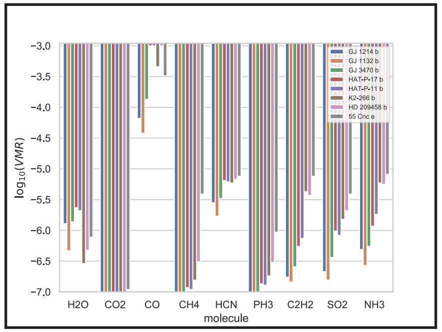
Summary/takeaway message

- Your retrieval is only as good as the underlying forward model. Always remember the question you asked.
- We have many tools available

NEMESIS

ARCiS

- ARIEL will be able to measure accurate molecular abundances for many molecules



- Adding complexity is possible, can be advantageous and sometimes even needed
  - (diseq.) Chemistry
  - Clouds
  - 3D structures