Thermochemical Calculations and Modeling of Exoplanetary Atmospheres

Jasmina Blecic

Exoplanetary Atmospheres and Habitability
Nice, October 15th, 2015

UCF

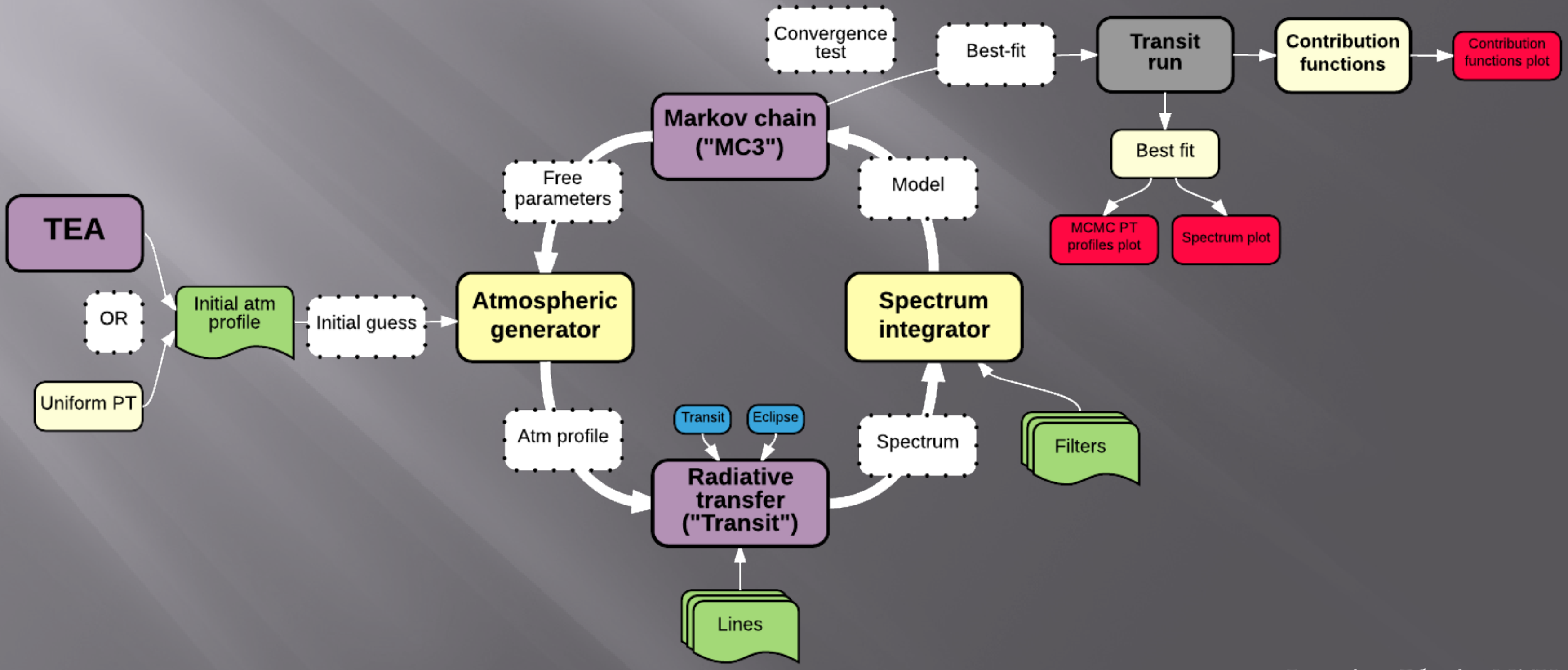
NEW YORK UNIVERSITY ABU DHABI

- Open-source Bayesian Atmospheric Radiative Transfer (*BART*) code and application to WASP-43b

  Blecic et al. 2015b, Cubillos et al. 2015, Harrington et al. 2015

- Open-source Thermochemical Equilibrium Abundances (*TEA*) code and application to several hot Jupiters

  Blecic et al. 2015a



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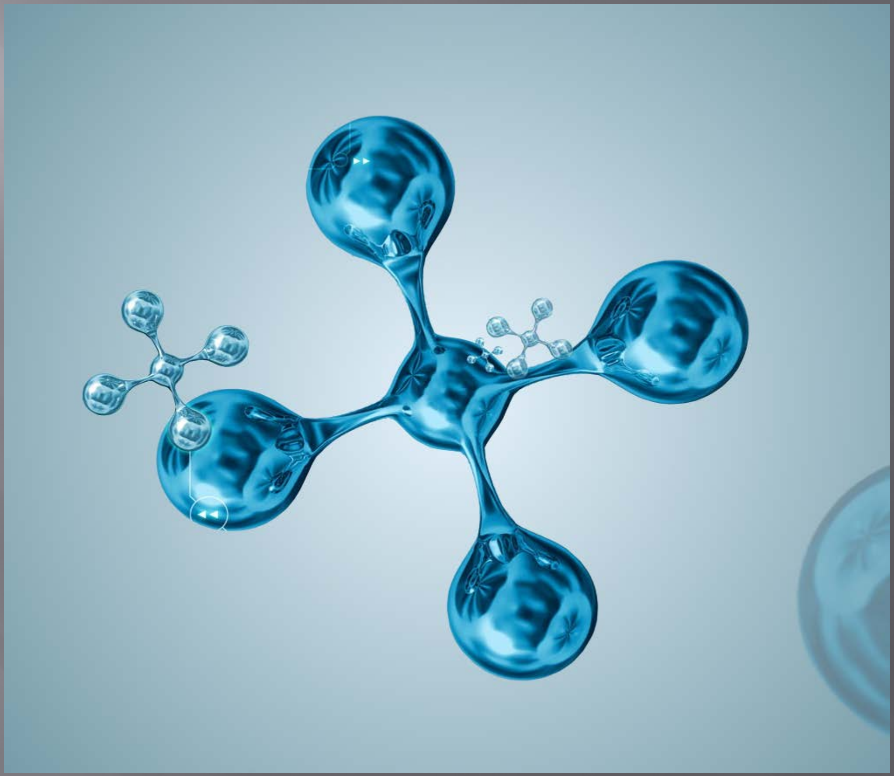
TEA

Thermochemical Equilibrium Abundances



Credit - wallconvert.com

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Submitted to APJ Supplemental Series, ArXiv

- Chemical equilibrium methods:
  - Equilibrium constants and reaction rates
  - Minimizing the free energy of the system
- Comprehensive 1D models (Moses et al. 2011, Line et al. 2011, Visscher et al. 2010)
  - Need to know reaction rates of forward and reversed reactions
- Gibbs free energy minimization
  - Each species treated independently
- Thermochemical calculations needed:
  - Initializing any atmosphere
  - First order approximation for a variety of atmospheres

TEA

- Open-source, written in Python
- Calculates equilibrium abundances of gaseous species
- Based on White et al. (1958) and Eriksson et al. (1971)
- Implements Gibbs free energy minimization within iterative Lagrangian optimization scheme
- Free energies - JANAF tables
- Elemental abundances Asplund et al. (2009)

TEA

- Modular
- Well documented
- Handles single (T, P) point and multiple (T, P) pairs
- Available at:

https://github.com/dzesmin/TEA

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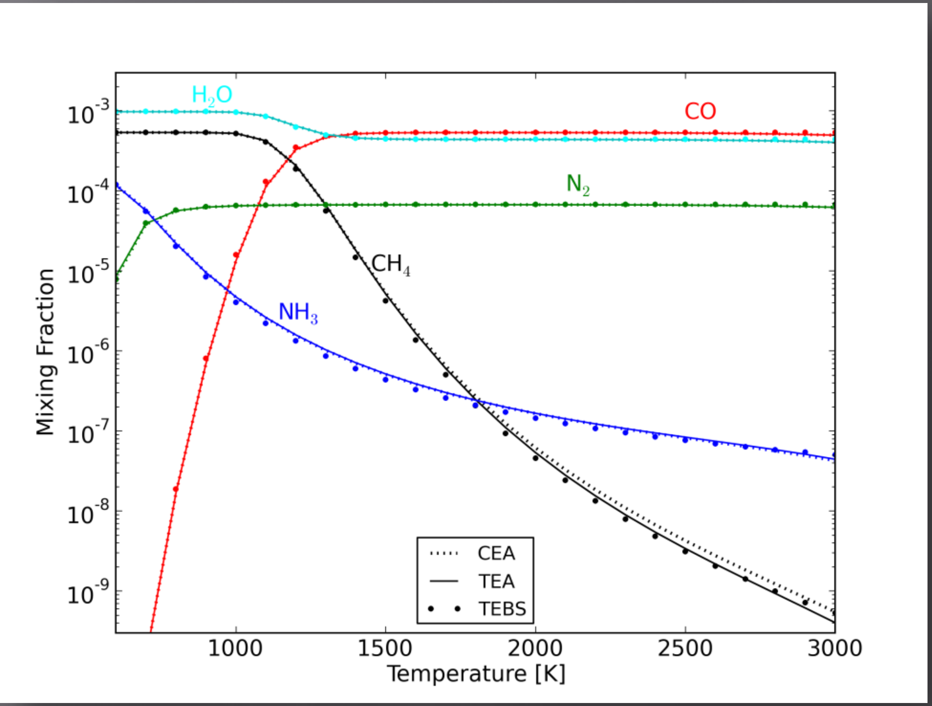
Comparison

Species	$\frac{g_i^0(T)}{RT}$	White et al. final abundances	TEA final abundances	Differences
H	-10.021	0.040668	0.04065477	-0.00001323
H_2	-21.096	0.147730	0.14771009	-0.00001991
H_2O	-37.986	0.783153	0.78318741	0.00003441
N	-9.846	0.001414	0.00141385	-0.00000015
N_2	-28.653	0.485247	0.48524791	0.00000091
NH	-18.918	0.000693	0.00069312	0.00000012
NO	-28.032	0.027399	0.02739720	-0.00000180
O	-14.640	0.017947	0.01794123	-0.00000577
O_2	-30.594	0.037314	0.03730853	-0.00000547
OH	-26.111	0.096872	0.09685710	0.00001490

- **White et al. (1958) Example (1) *vs.* TEA**



- **CEA – Chemical Equilibrium with Application**
- **TEA – Thermochemical Equilibrium Abundances**
- **TEBS – Burrows and Sharp (1999) analytic method**

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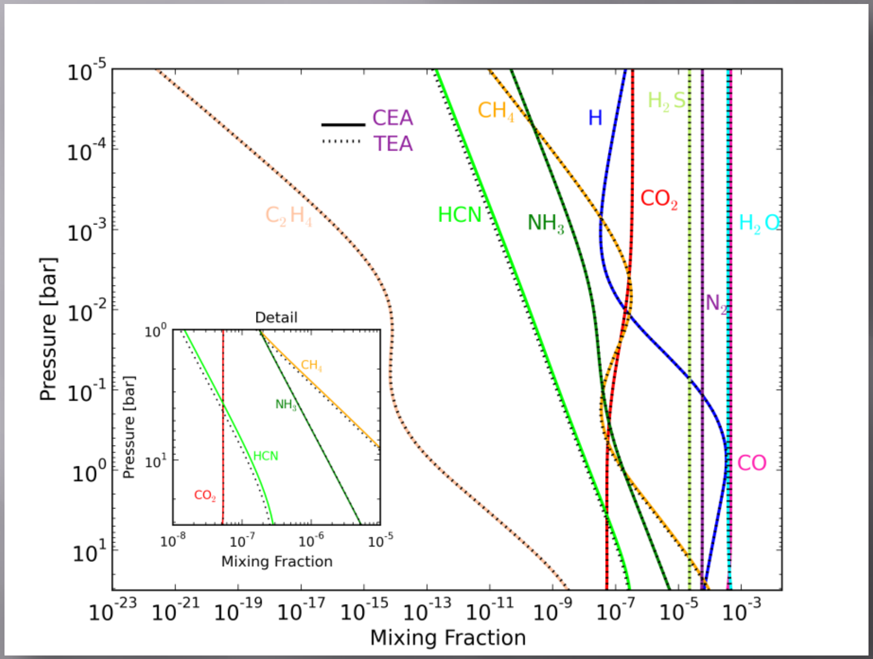
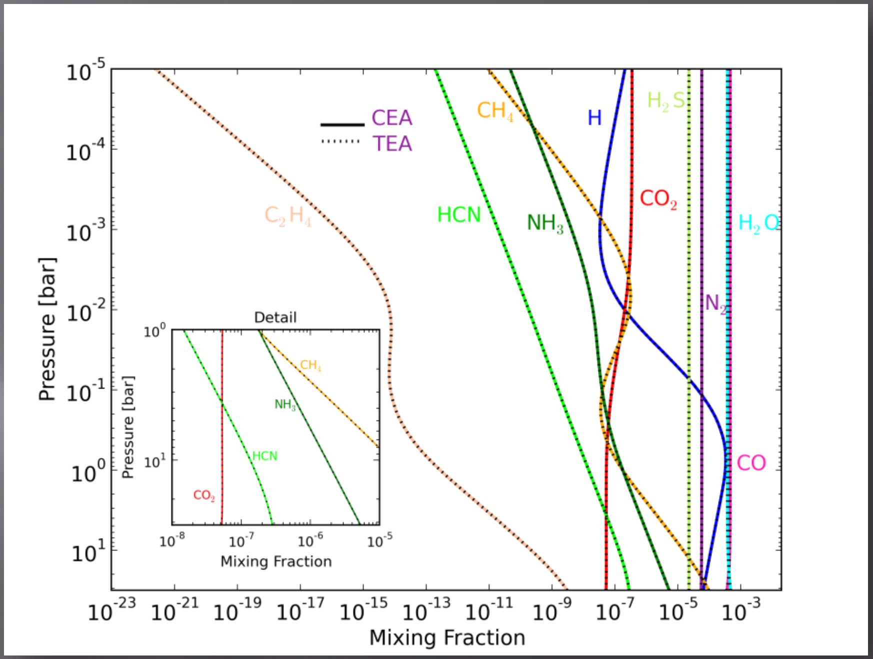
Comparison





TEA *vs.* CEA

- Output species: CO, CO_2, CH_4, H_2O, HCN, C_2H_2, C_2H_4, N_2, NH_3, HS, and H_2S

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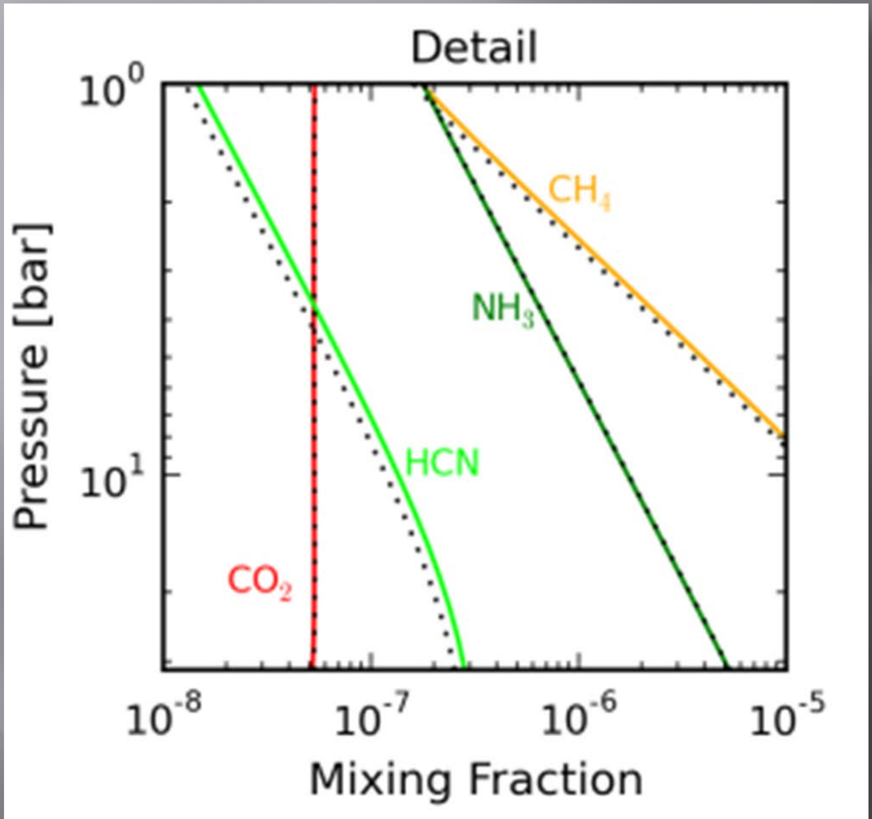
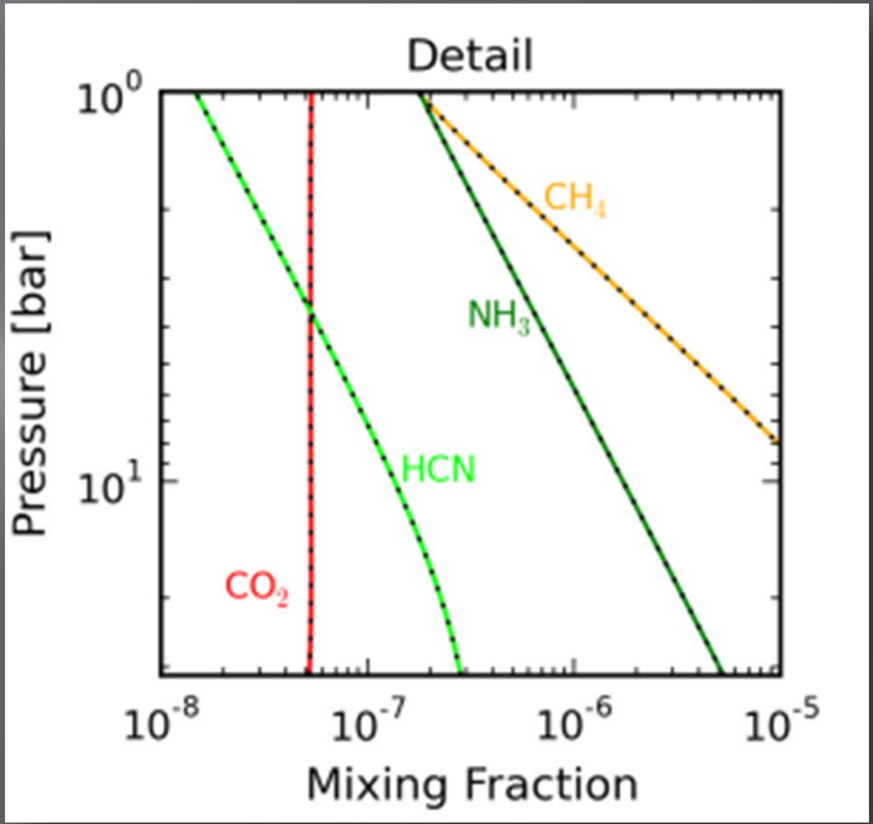
CEA *vs.* TEA





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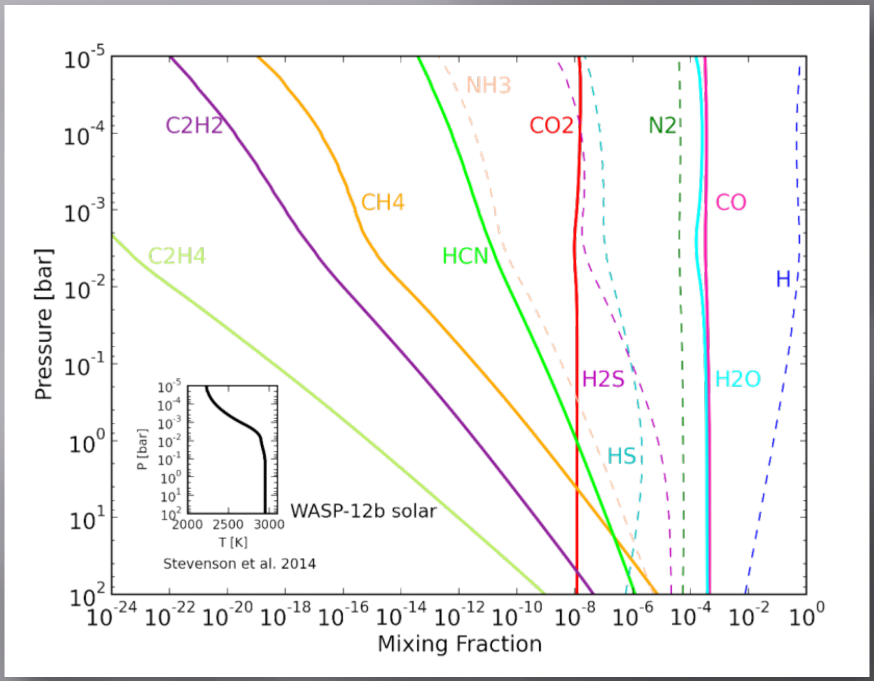
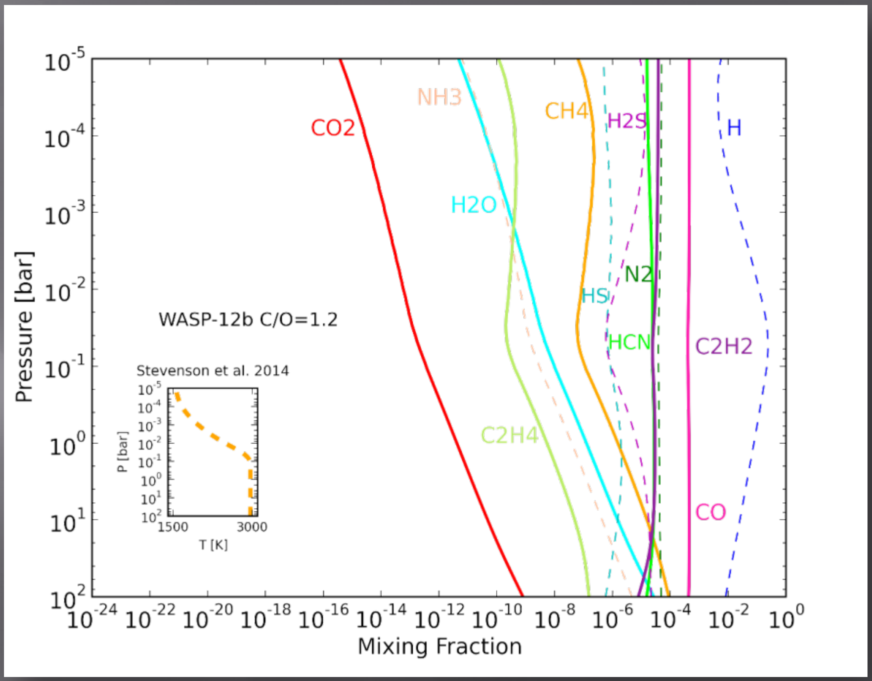
Influence of C/O Ratio





- WASP-12b O-rich, C-rich
- Output species: CO, CO_2, CH_4, H_2O, HCN, C_2H_2, C_2H_4, N_2, NH_3, HS, and H_2S

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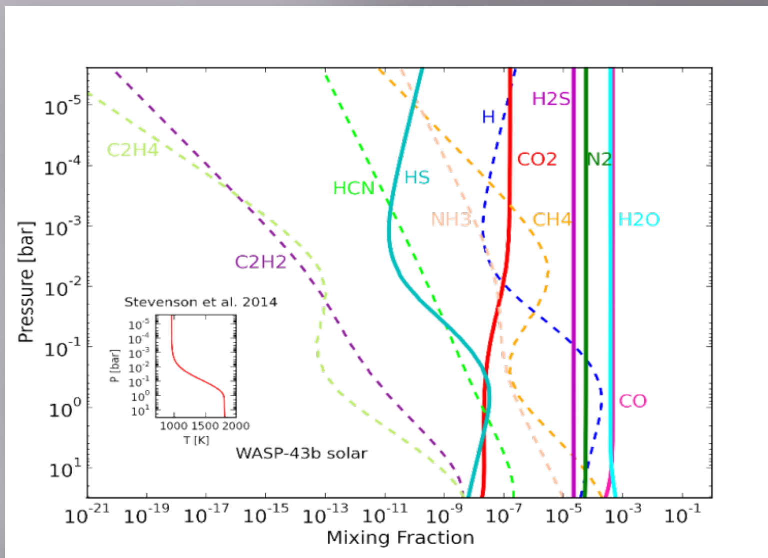
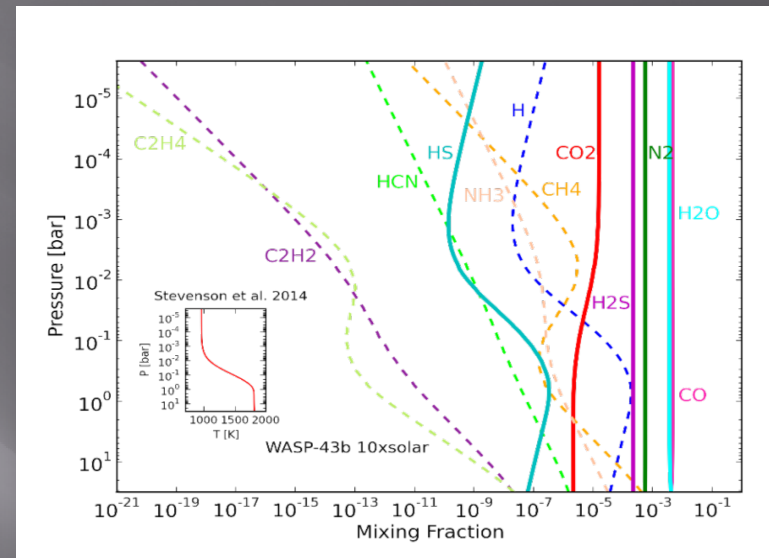
Influence of Metallicity



ζ = 0



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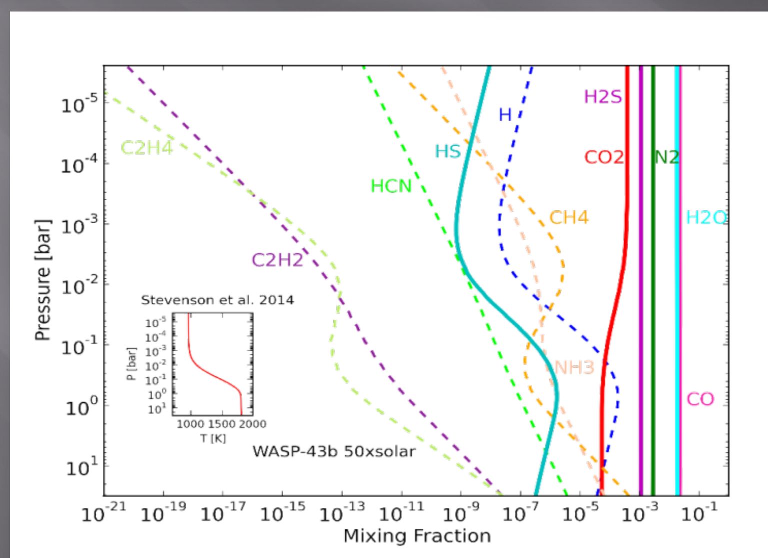

ζ = 50

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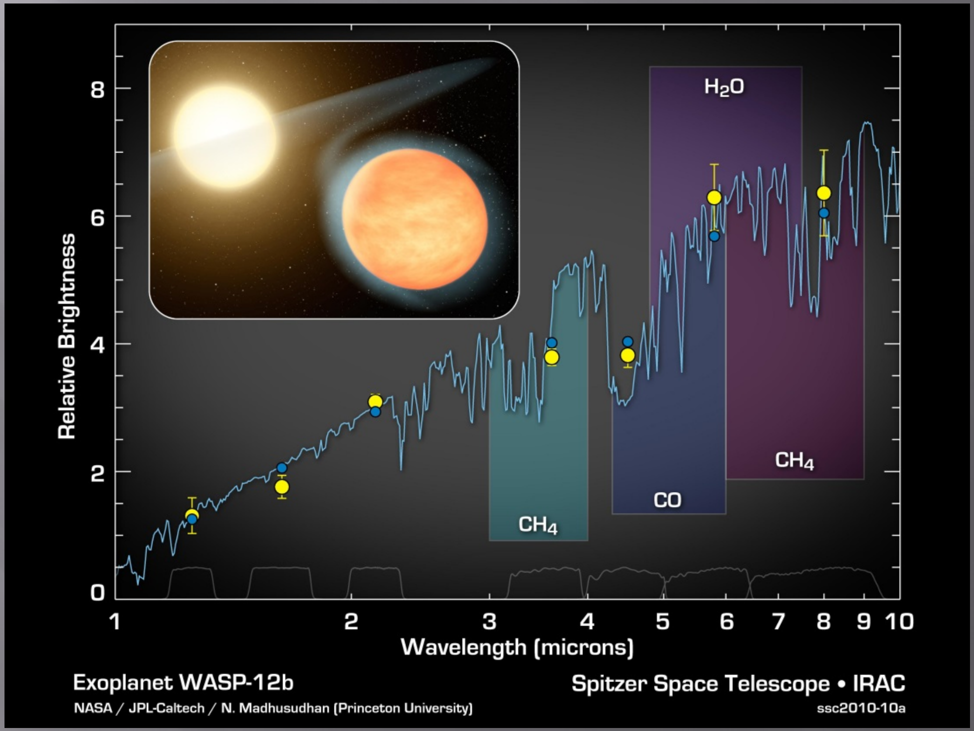
TEA

- Can be used to initiate models of any planetary atmosphere
- TEA User's Guide, Programmer's Guide, and the theory paper are provided with the code
- Tested and released version of TEA is available to the community via:

https://github.com/dzesmin/TEA/releases/tag/1.0-alpha
https://github.com/dzesmin/TEA-Examples

BART

Bayesian Atmospheric Radiative Transfer



Credit - NASA/JPL-Caltech

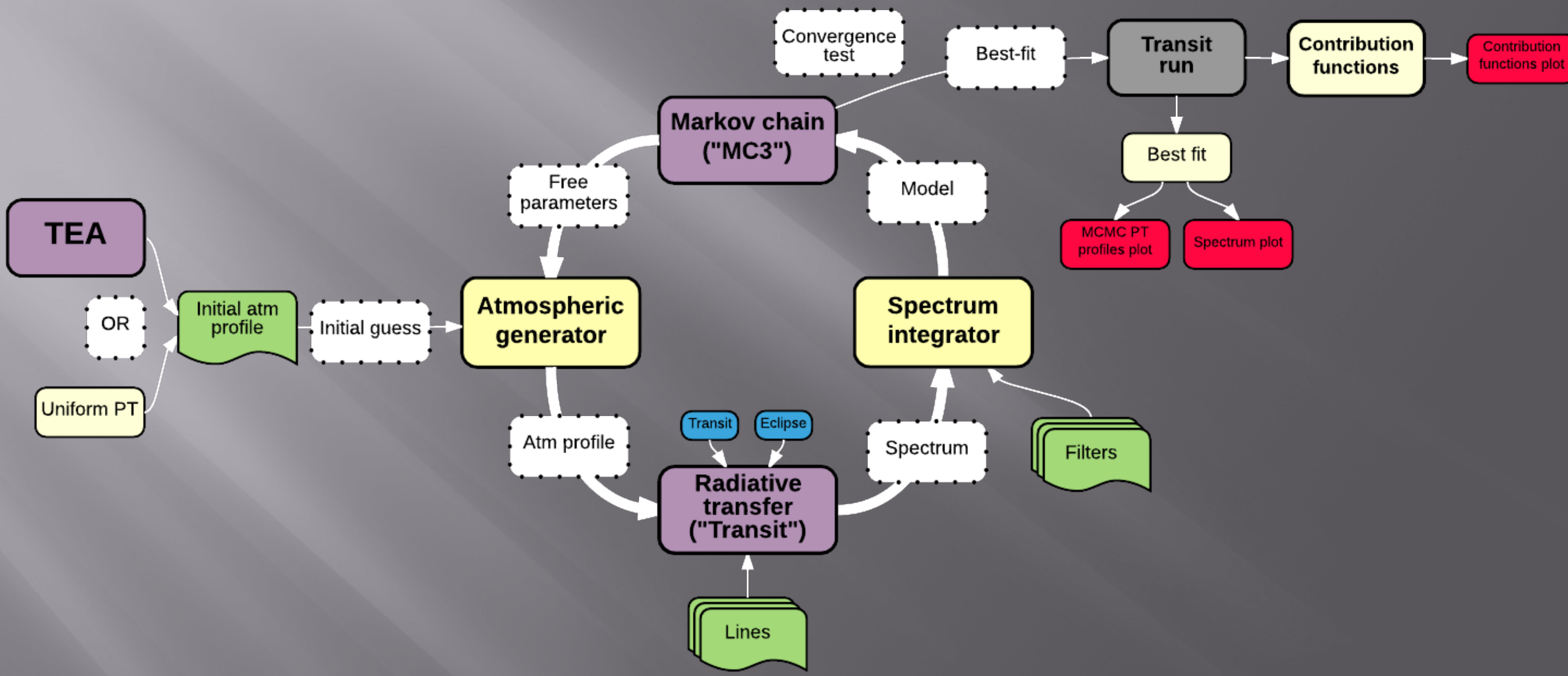
Jasmina Blecic, Joseph, Harrington, P. Cubillos et al. 2015
in preparation

- Two approaches in atmospheric modeling:
  - DIRECT
  - INVERSE
- BART – Bayesian Atmospheric Radiative Transfer code (Blecic et al. 2015b, Cubillos et al. 2015b, Harrington et al. 2015)

  https://github.com/exosports/BART

- Three self-sufficient modules, can be used for other scientific purposes:
  - TEA – Thermochemical Equilibrium Abundances module (Blecic et al. 2015a)
    https://github.com/dzesmin/TEA
  - MC^3 – Multi-core Markov-chain Monte Carlo module (Cubillos et al. 2015a)
    https:// github.com/pcubillos/MCcubed
  - Transit – Radiative-transfer module
    https://.github.com/exosports/transit

BART Flow



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WASP-43b Atmospheric Analysis

Source	Wavelength (μm)
Gillon et al. (2012) VLT/HAWK I	0.90, 1.19, 2.09
Wang et al. (2013) WIRCam	1.65, 2.19
Chen et al. (2014) GROND	0.806, 2.19
Blecic et al. (2014) Spitzer	3.6, 4.5
Zhou et al. (2014) IRIS2/AAT	2.15
Stevenson et al. (2014) HST	1.1425 - 1.6325 (15)
Stevenson et al. (2015) Spitzer	3.6, 4.5

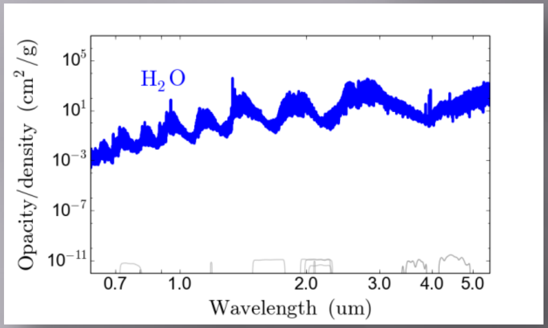
- All available secondary eclipse data from the ground- and space-based observations

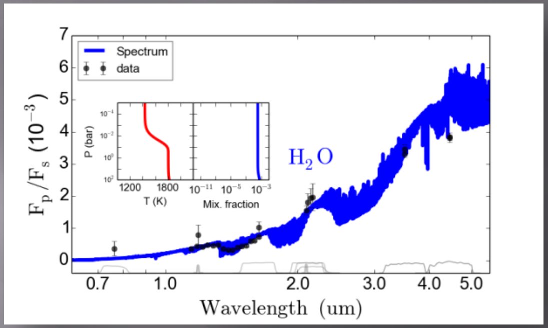
- HITRAN/HITEMP opacity sources + Swenke 1998 (TiO), Plez 1999 (VO) + Borysow et al. 2001, 2002 (CIA H_2-H_2), Richard et al. 2012 (CIA H_2-He)
- Atmospheric cases:
  - 4 major molecules (H_2O, CO_2, CO, CH_4)
  - 7 major molecules (+HCN, C_2H_2 , C_2H_4)
  - 11 major molecules (+NH_3, H_2S, TiO, VO)
  - C/O ratio
- Best-fit assessment:

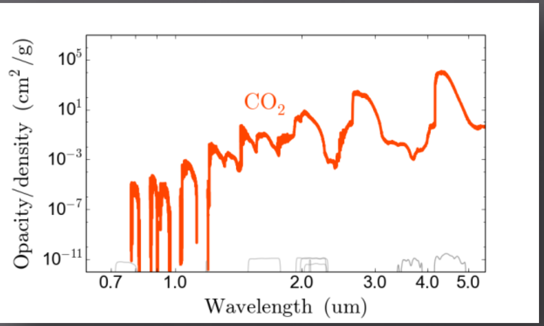
$\chi^2_{red} = \chi^2 / (N - k)$, BIC = $\chi^2 + k \ln(N)$, SDR

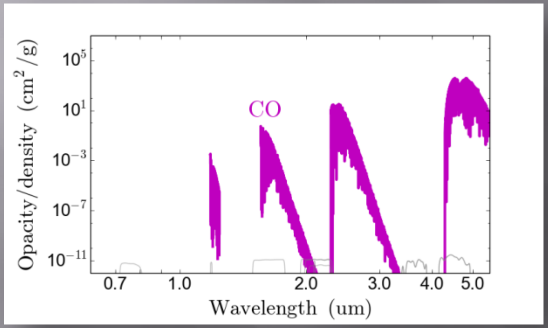
BART

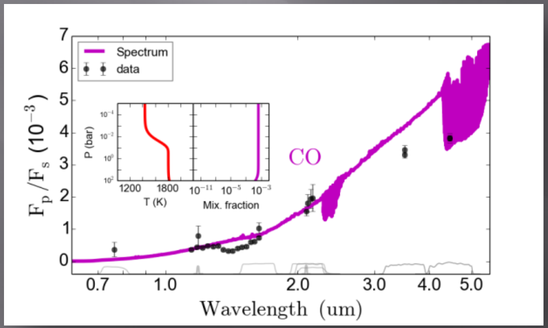
Opacities - Major

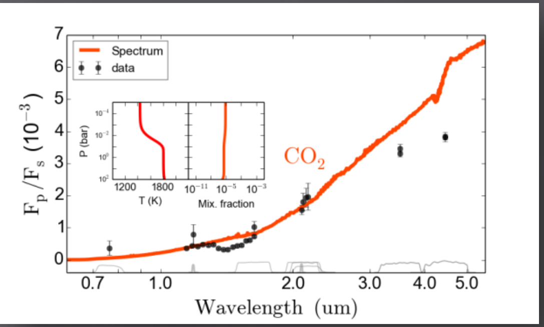


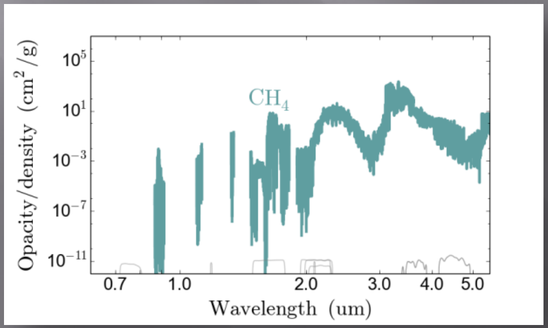


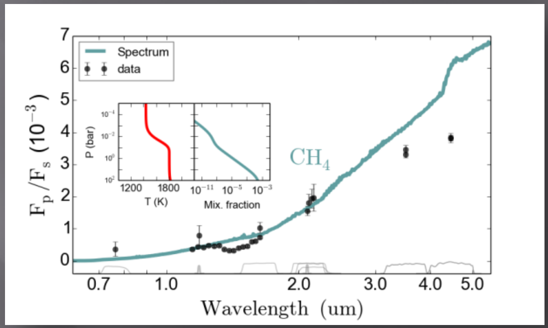












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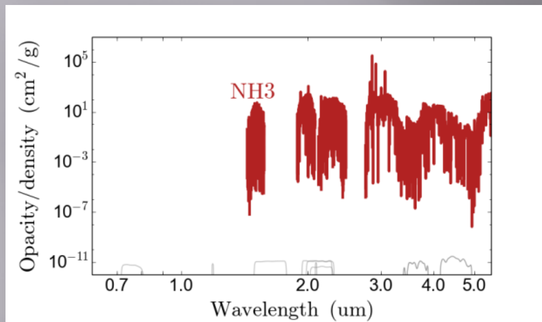
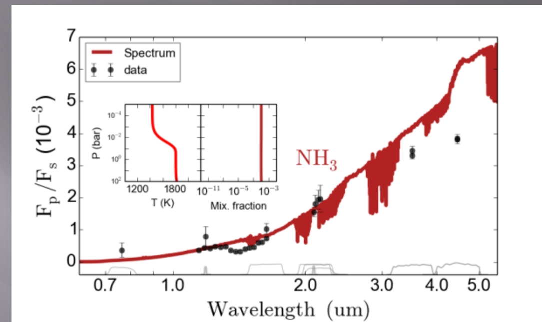
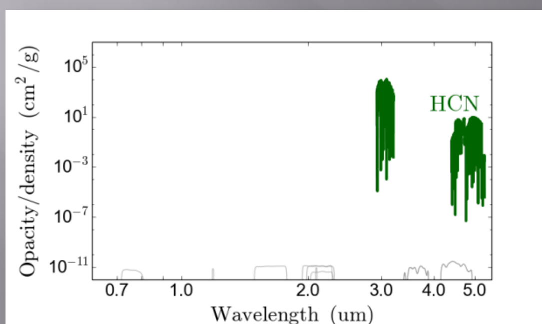
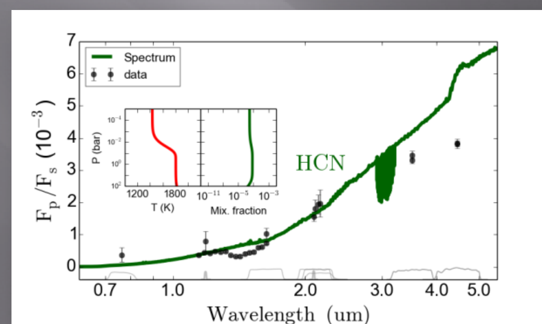
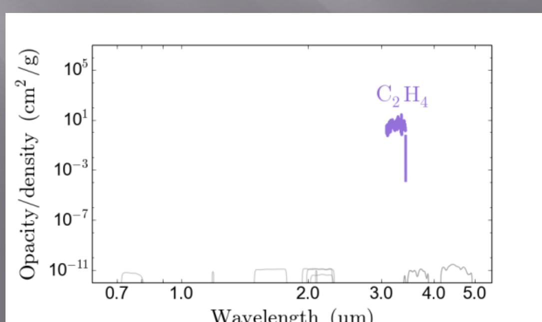
Opacities - C/O

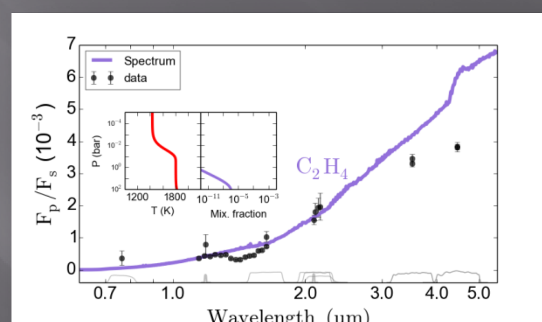


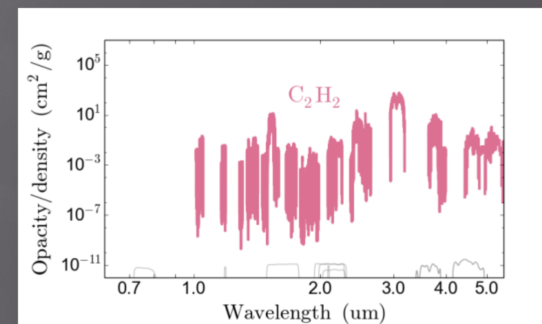


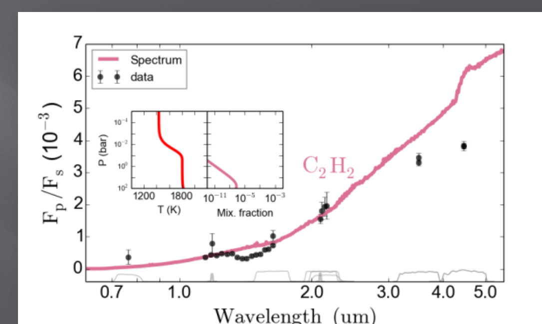












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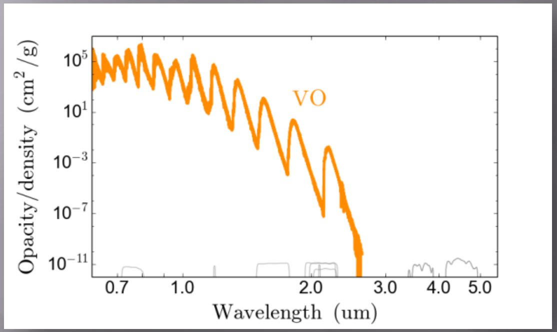
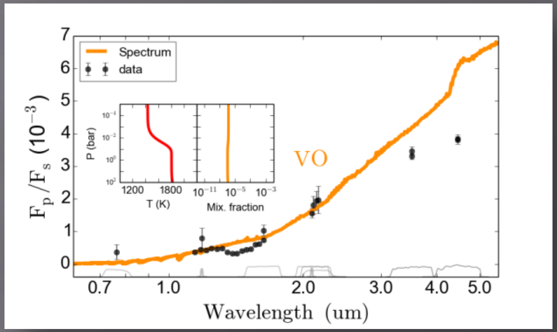
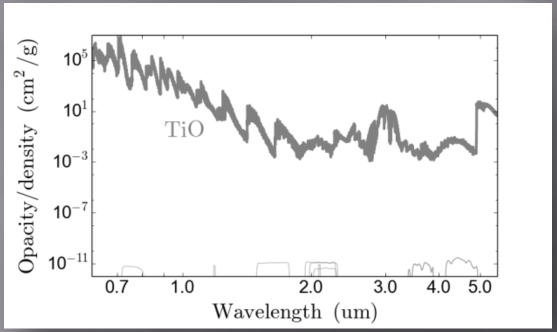
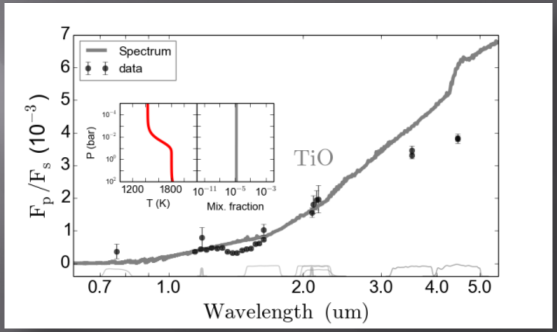
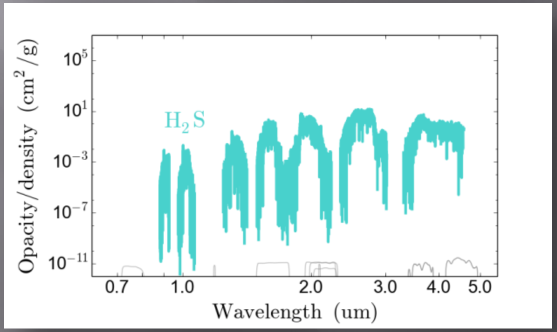
Opacities - Inversion

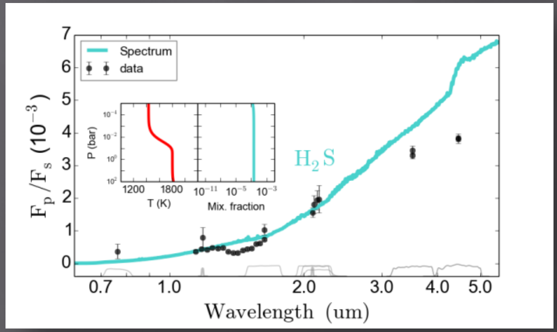








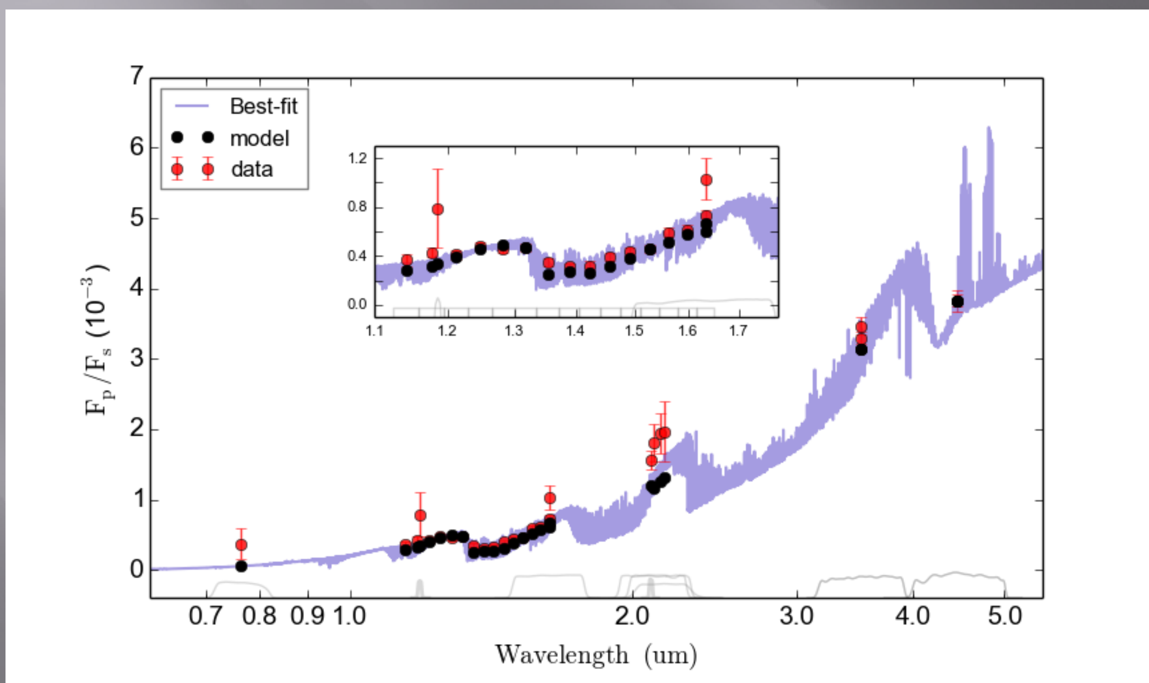


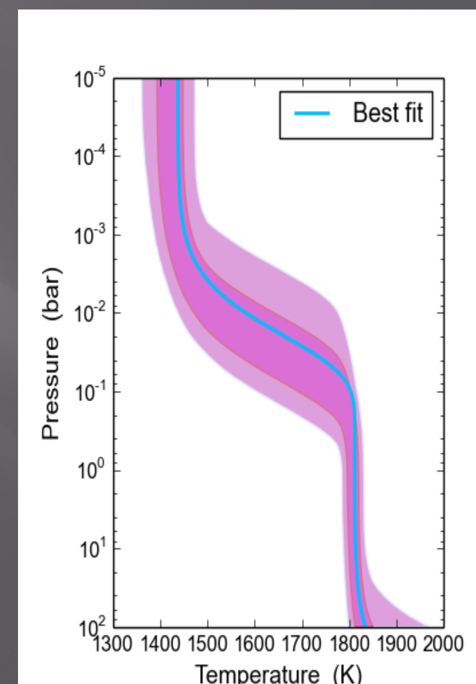


BART

4 Species - 4 Opacities

	χ^2_{red}	BIC	SDR
4 opacities	1.9709	60.2547	0.000202287
7 opacities	1.9849	60.5198	0.000209638
11 opacities	2.0542	61.8365	0.000208284





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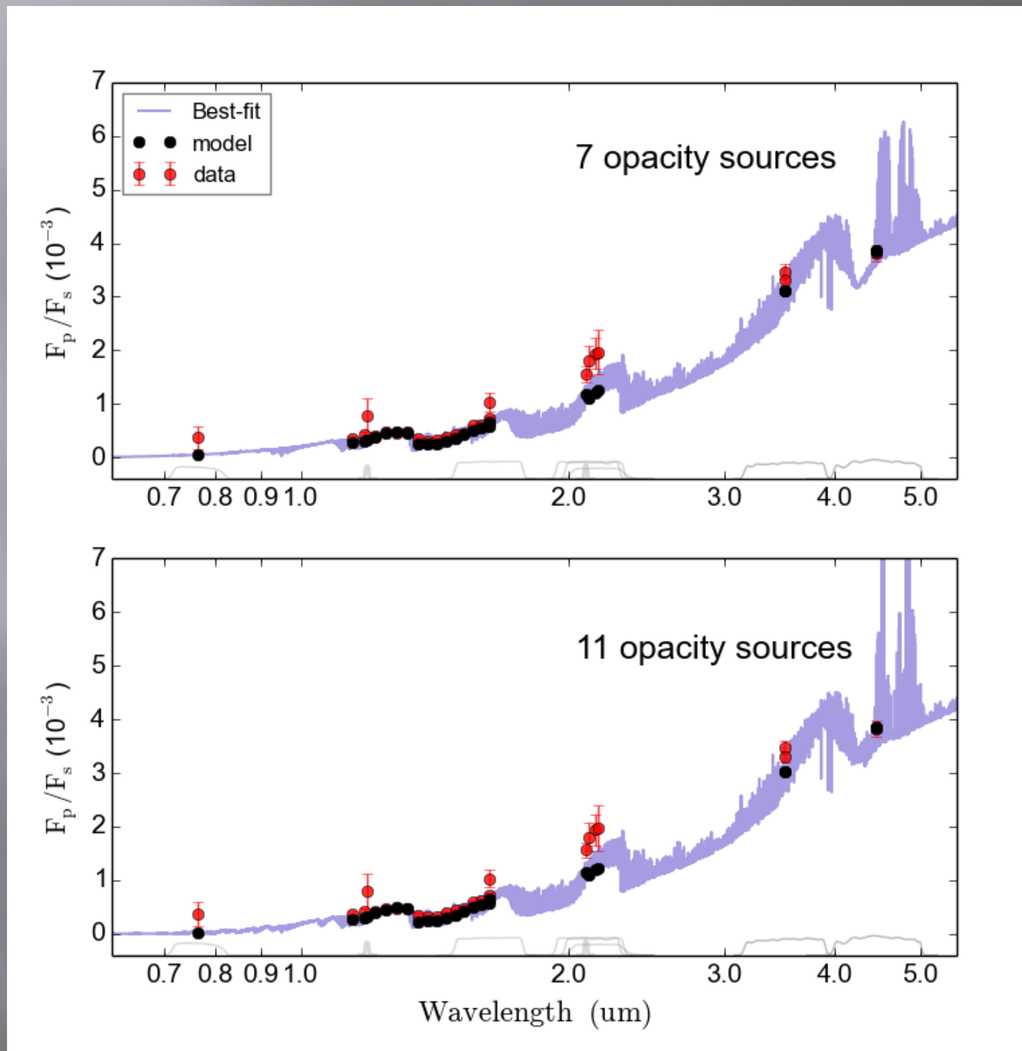
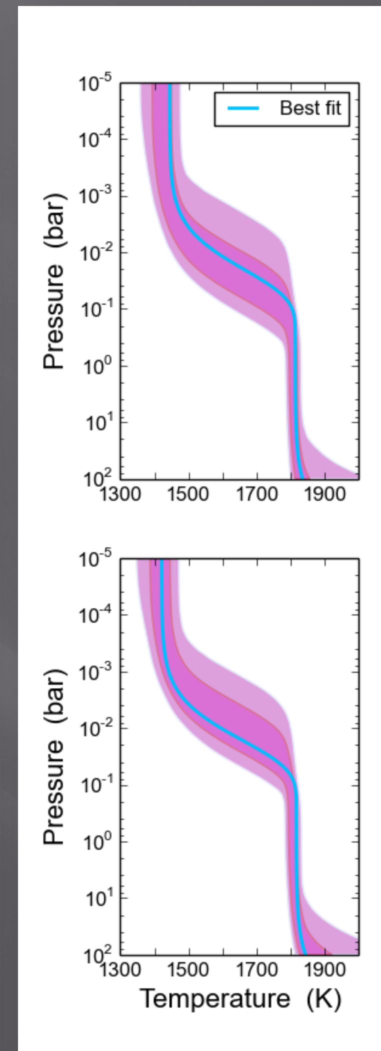
4 Species - 7 and 11 Opacities





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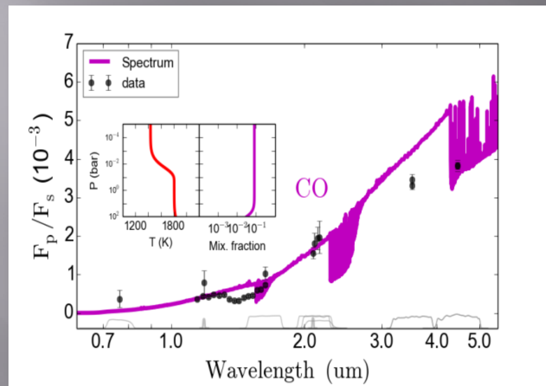
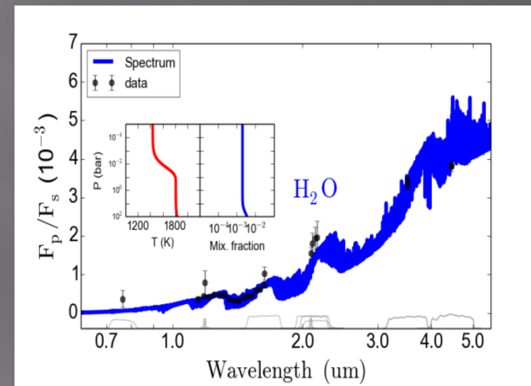
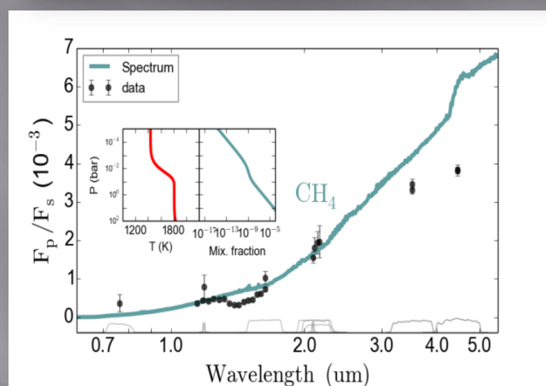
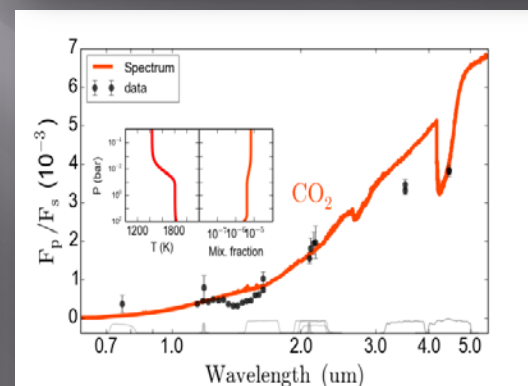
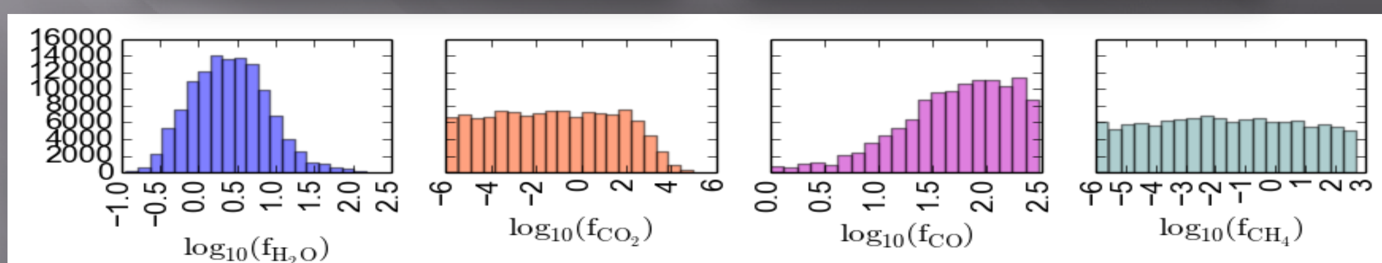
4 Species - 4 Opacities











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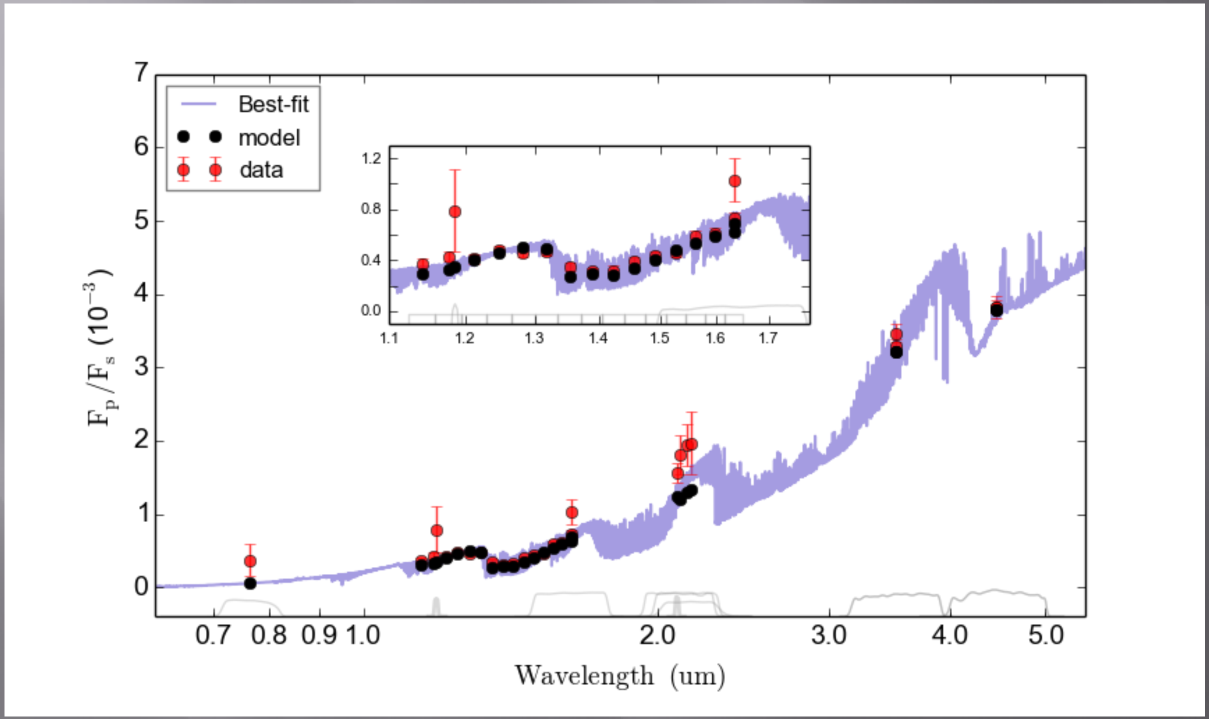
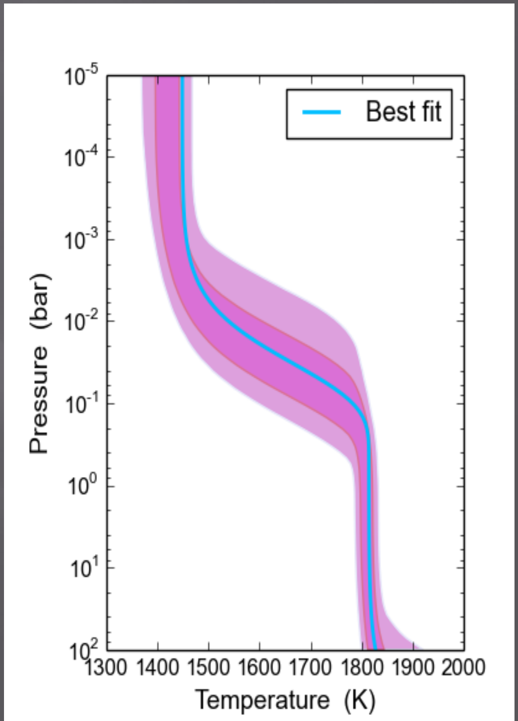
7 Species - 7 Opacities

	χ^2_{red}	BIC	SDR
Equilibrium	2.3385	69.9968	0.000203473
11 opacities	2.4337	71.5197	0.000203565





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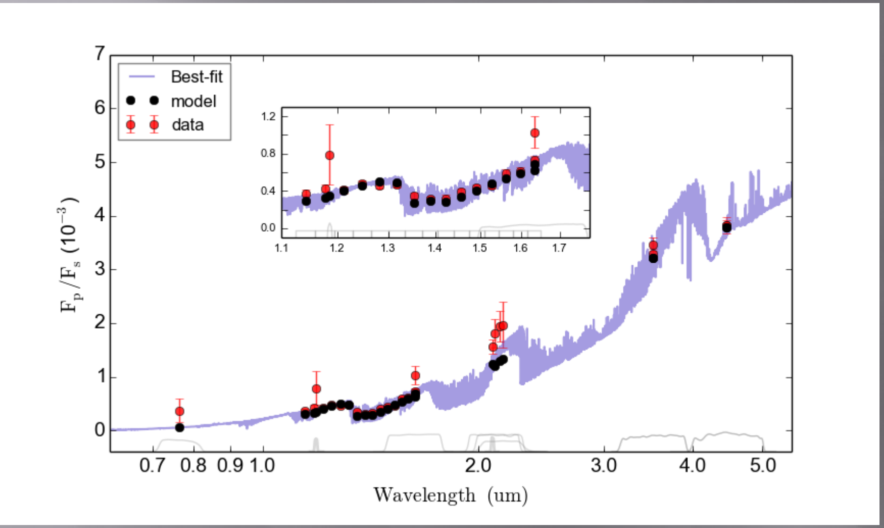
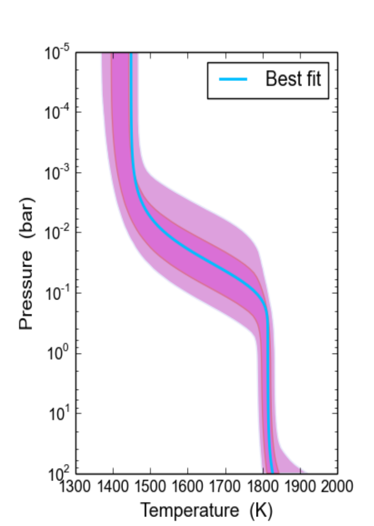
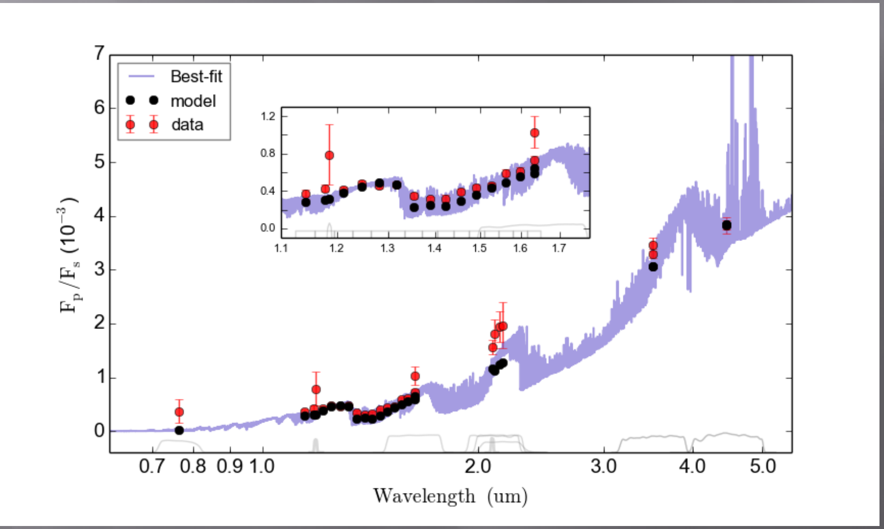
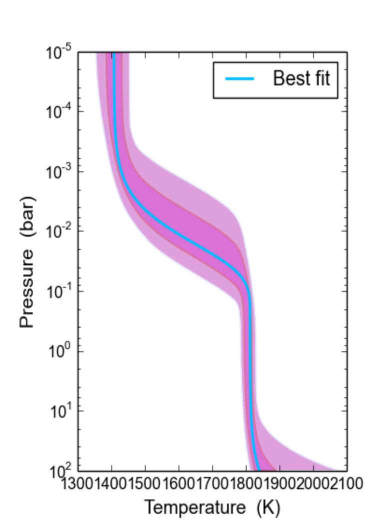
7 Opacities *vs.* 11 Opacities









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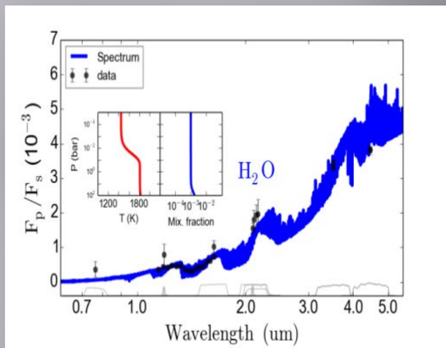
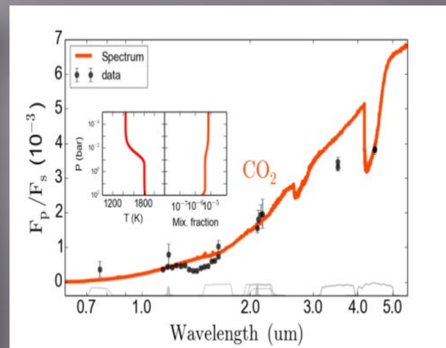
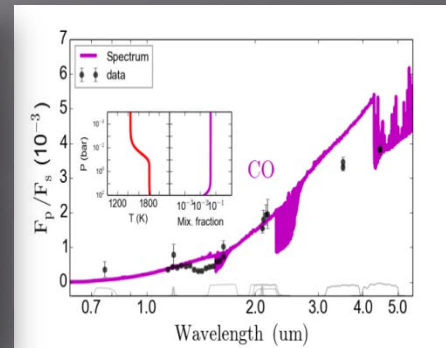
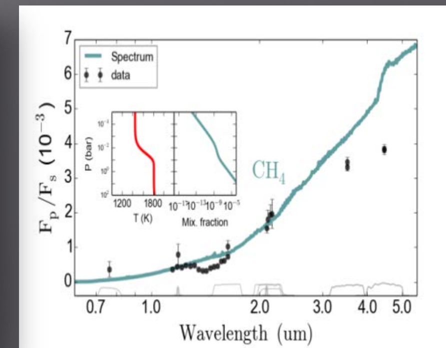
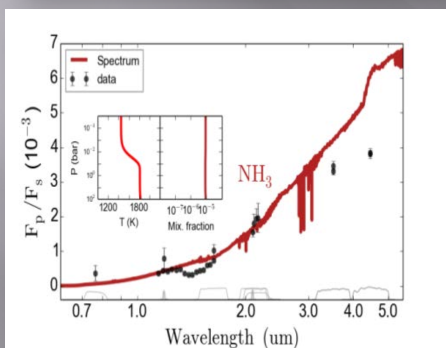
7 Species - 7 Opacities

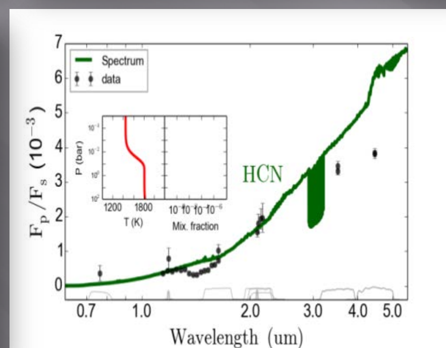


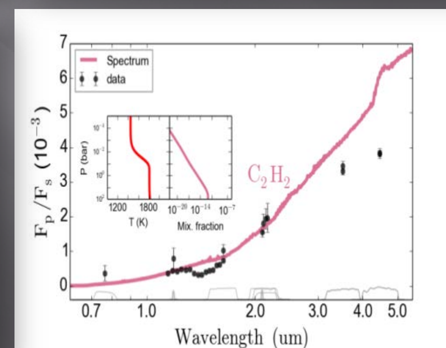


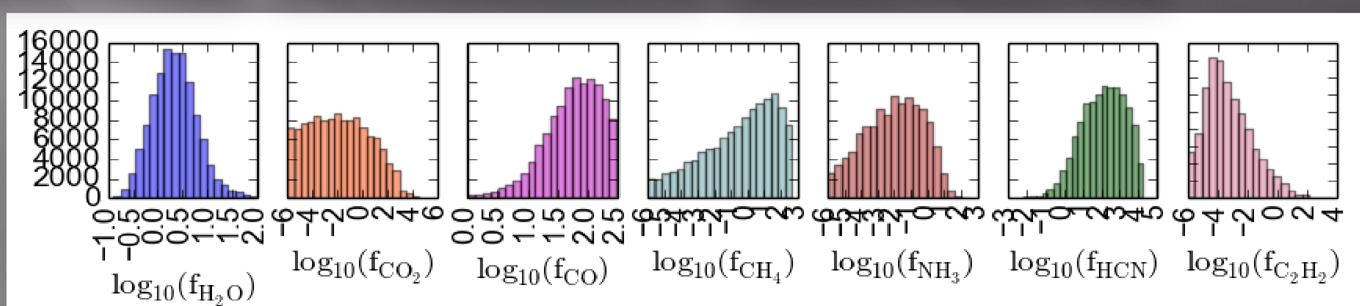












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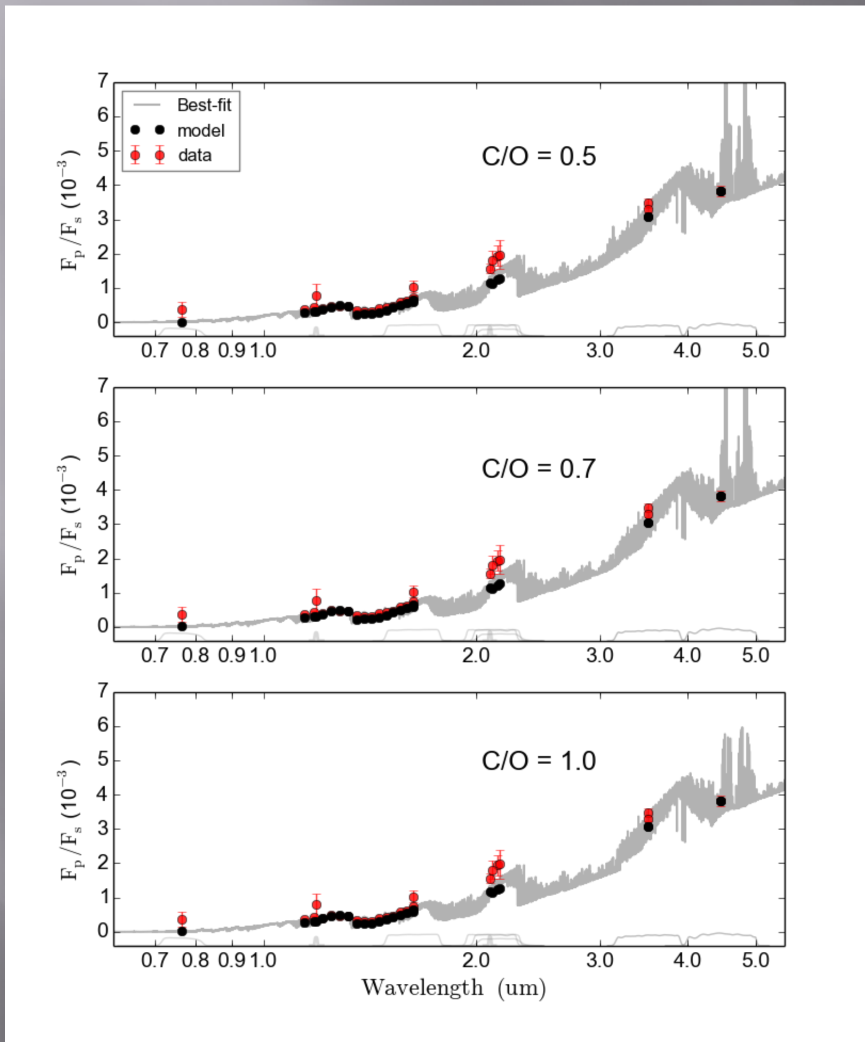
WASP-43b C/O Ratio



	χ^2_{red}	BIC	SDR
C/O=0.5	2.4377	71.5197	0.000203565
C/O=0.7	2.4236	71.3587	0.000202348
C/O=1.0	2.4018	71.0097	0.000202891

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WASP-43b Atm. Results

- T(p) profile consistent with previous work
- No thermal inversion
- Inclusion of additional sources does not improve the fit
- Spectrum dominated by H_2O
- H_2O abundance calculated to 1-10x solar, consistent with previous work
- High abundance of CO compared to the results of other groups:
  - Number of data points included
  - Difference in the molecular line-list data and/or missing/including different opacity sources

Summary

- TEA – user manual, programmer's guide, documented code, theory paper - Blecic et al. 2015a, available via open-source reproducible-research license via:

  https://github.com/dzesmin/TEA

- BART – Blecic et al 2015b, Cubillos et al. 2015b, Harrington et al. 2015 in preparation

  https://github.com/exosports/BART


THANK YOU!