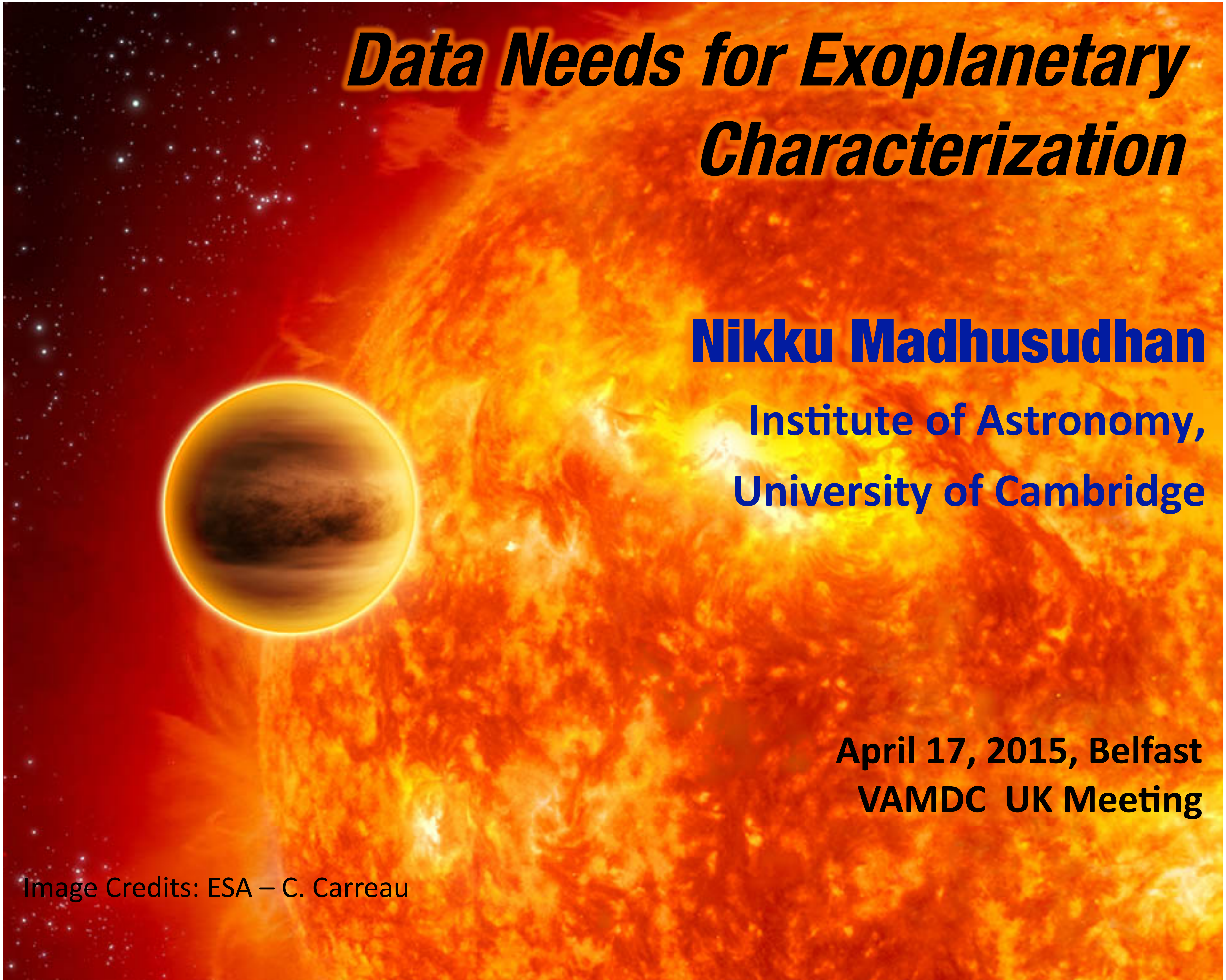


Data Needs for Exoplanetary Characterization

Nikku Madhusudhan

Institute of Astronomy,

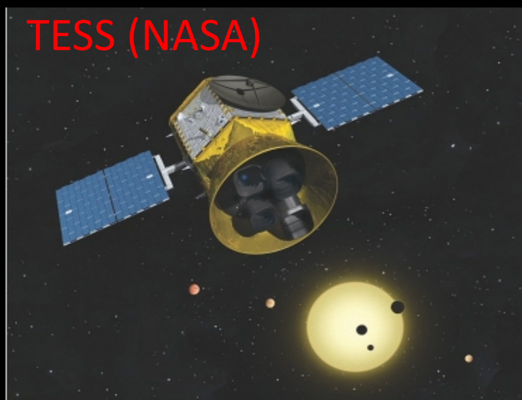
University of Cambridge

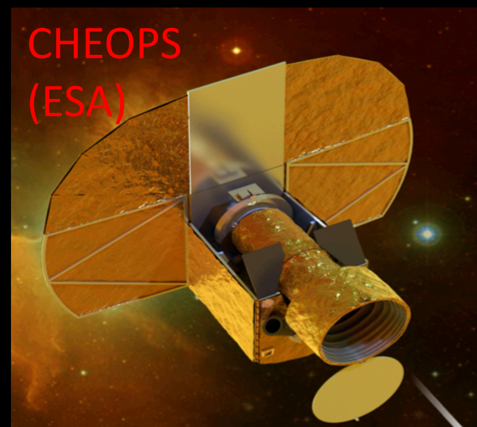
April 17, 2015, Belfast
VAMDC UK Meeting

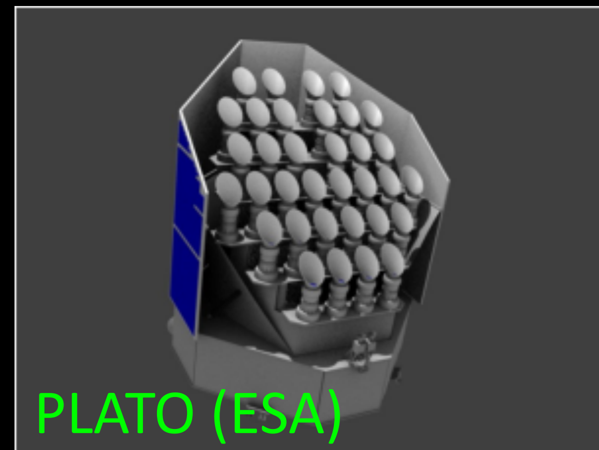
Image Credits: ESA – C. Carreau

The Future of Exoplanet Science

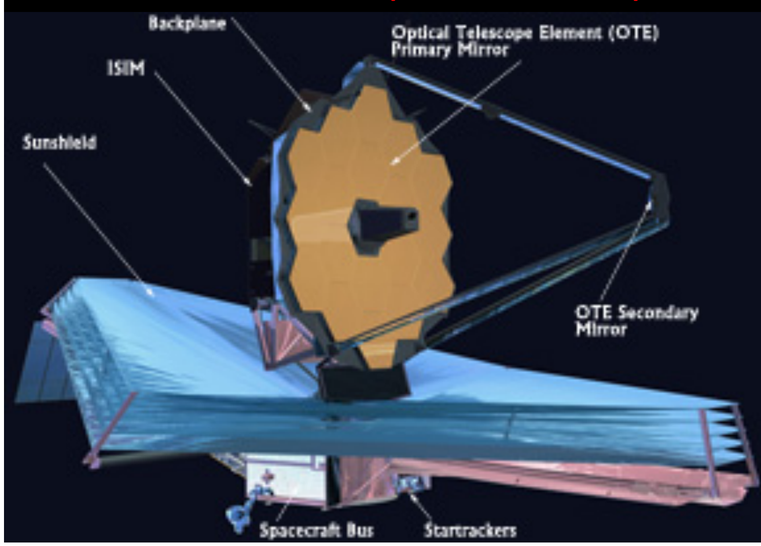
NGTS
NEXT-GENERATION TRANSIT SURVEY





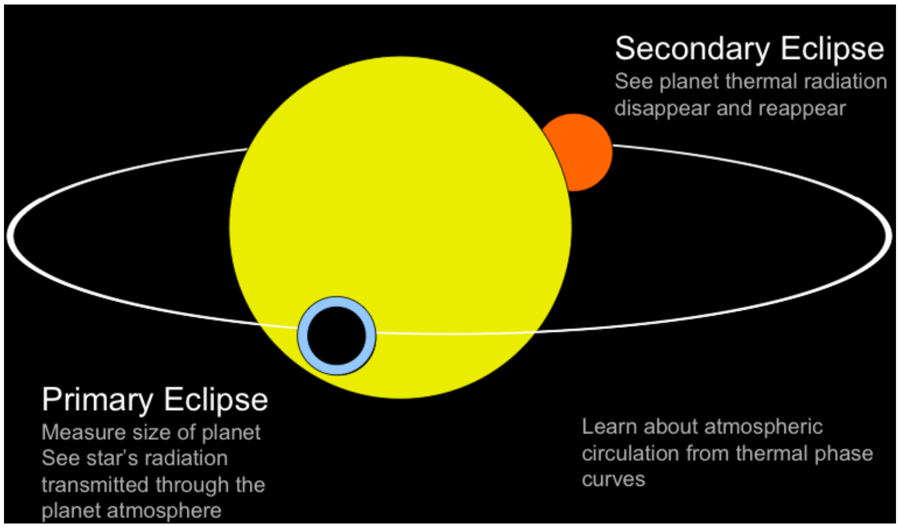


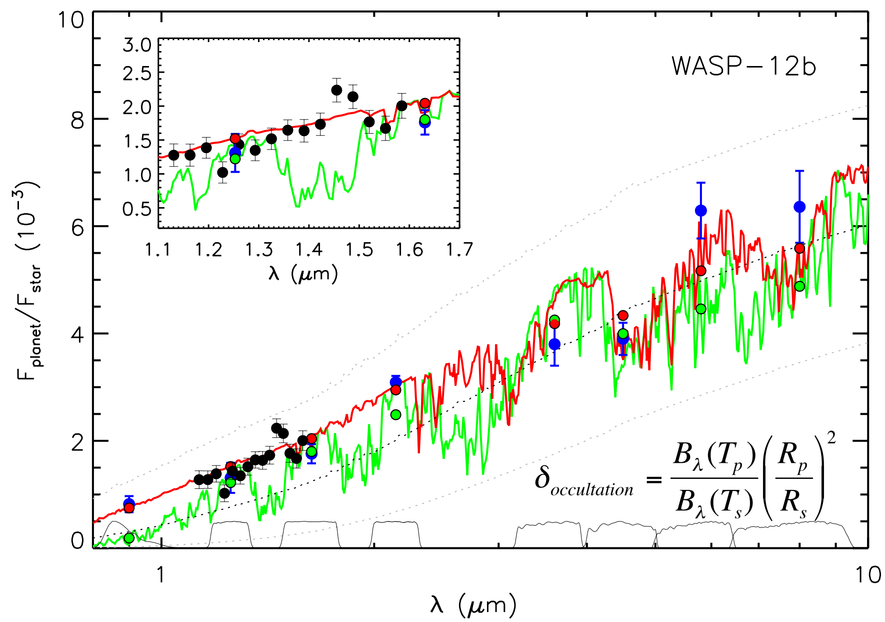
The James Webb Space Telescope

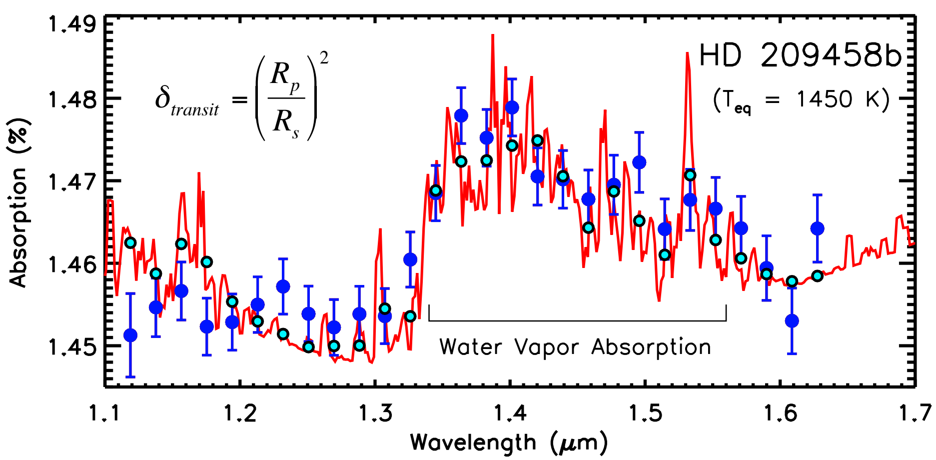


The future from ground
E-ELT, GMT, TMT

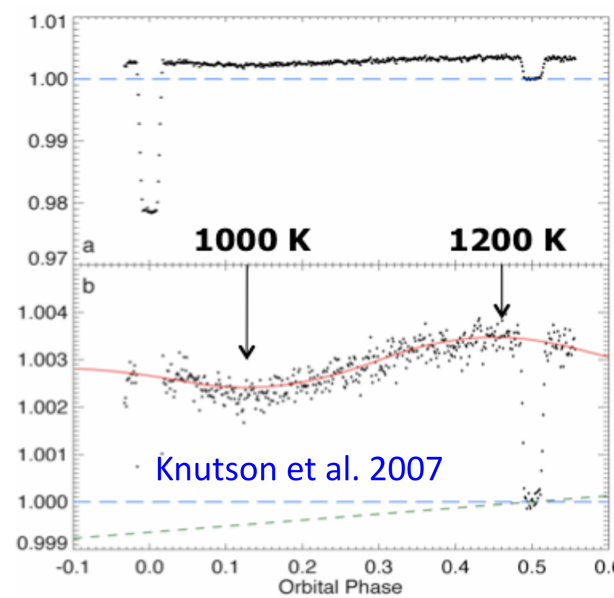
Spectroscopy of Transiting Exoplanets







Deming et al. 2013, Madhusudhan et al. 2014



Knutson et al. 2007

Exoplanetary Atmosphere Models

1-D models of irradiated atmospheres with line-by-line radiative transfer

$$\frac{dP}{dr} = -\rho g$$

$$\frac{dI_\lambda}{d\tau_\lambda} = -(1 + \frac{\sigma_\lambda}{\kappa_\lambda})I_\lambda + \frac{j_\lambda}{\kappa_\lambda}$$

$$\int_0^\infty \kappa_\lambda [J_\lambda - B_\lambda] \, d\lambda = 0$$

$$\frac{dT}{dr} = -\frac{\gamma - 1}{\gamma} \frac{\mu g}{k_B}$$

$$P = \frac{\rho k_B T}{\mu}$$

Boundary Conditions

- Stellar Irradiation (Kurucz Model)
- Intrinsic Energy source

Chemical Equilibrium

$$[X] = f_z \times [X]_{solar}$$

$$\frac{G(T)}{RT} = \sum_{i=1}^{m} \left\{ n_{\phi i} \left[\frac{\Delta G_{\phi i}(T)}{RT} + \ln P + \ln\left(\frac{n_{\phi i}}{N}\right) \right] \right\}_{\phi=1} + \frac{1}{RT} \sum_{\phi=2}^{s+1} [n_{\phi i} \Delta G_{\phi i}(T)]_{i=1}$$

$$\sum_{i=1}^{m} [\nu_{\phi ij} n_{\phi i}]_{\phi=1} + \sum_{\phi=2}^{s+1} [\nu_{\phi ij} n_{\phi i}]_{i=1} = b_j \quad \text{for } j = 1 \rightarrow k$$

$$B_{CO} = A_C + A_O + \frac{P_{H_2}^2}{2K_1(T)} - \sqrt{\left[A_C + A_O + \frac{P_{H_2}^2}{2K_1(T)}\right]^2 - 4A_C A_O}$$

Model Parameters

- Day-night redistribution: P_n, P_1, P_2
- Extra absorber: $P_{abs}, (\lambda_0, \lambda_1), \kappa_e$
- Composition (f_z) + clouds, etc.

Caveats

- Parameters
- Chemical equilibrium and compositions
- Computation time
- Artificial sources and sinks

Seager & Sasselov 1998, Sudarsky et al. 2003
Fortney et al. 2006, Burrows et al. 2007

Exoplanetary Atmosphere Models

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$$\frac{dT}{dr} = -\frac{\gamma - 1}{\gamma} \frac{\mu g}{k_B}$$

$$P = \frac{\rho k_B T}{\mu}$$

$$\kappa = \Sigma_i (n_i \times \sigma_i)$$

Boundary Conditions

z Model)

Chemical Equilibrium

$$[X] = f_z \times [X]_{solar}$$

Chemistry

Absorption Cross-section

$$\sum_{i=1}^{m} [v_{\phi ij} n_{\phi i}]_{\phi=1} + \sum_{\phi=2}^{s+1} [v_{\phi ij} n_{\phi i}]_{i=1} = b_j \quad \text{for } j = 1 \rightarrow k$$

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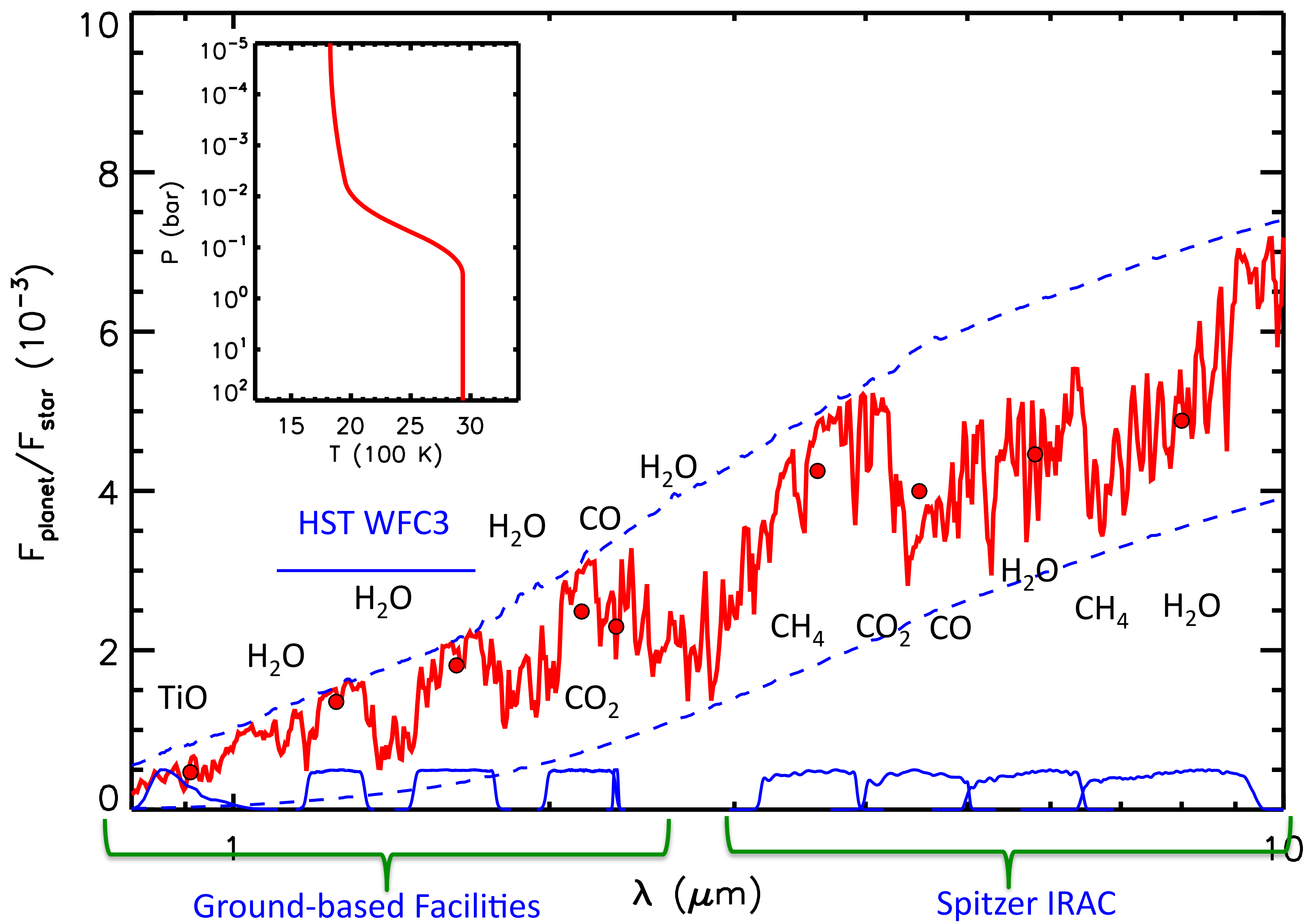
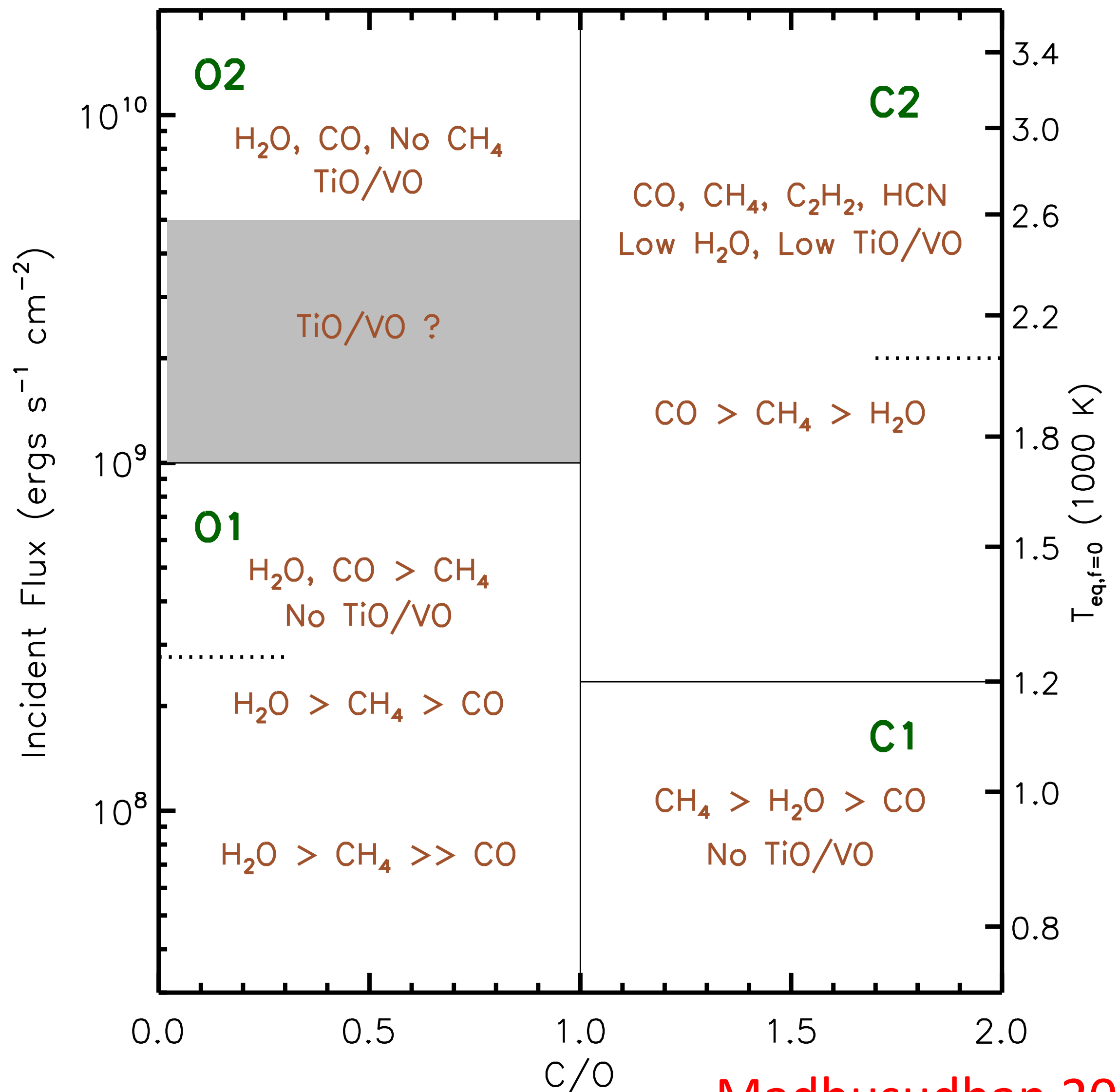
Spectral Signatures of hot Jupiter Atmospheres



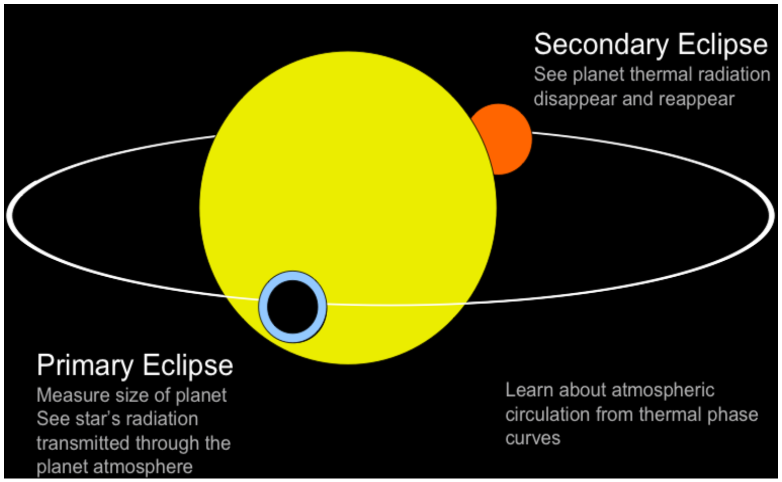
Chemistry in Hot Giant Exoplanets

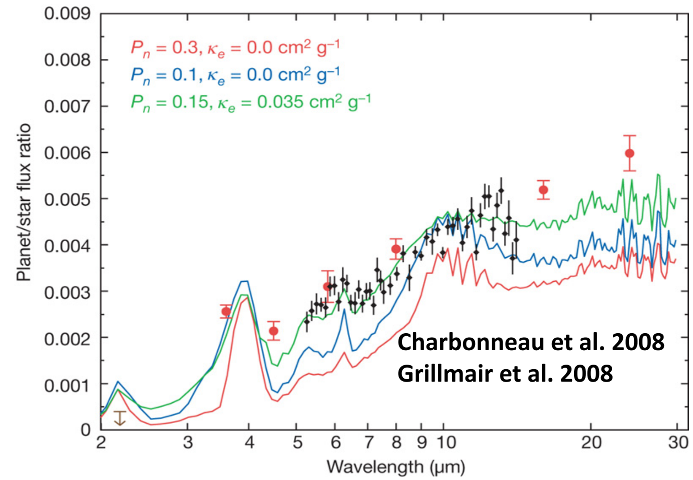


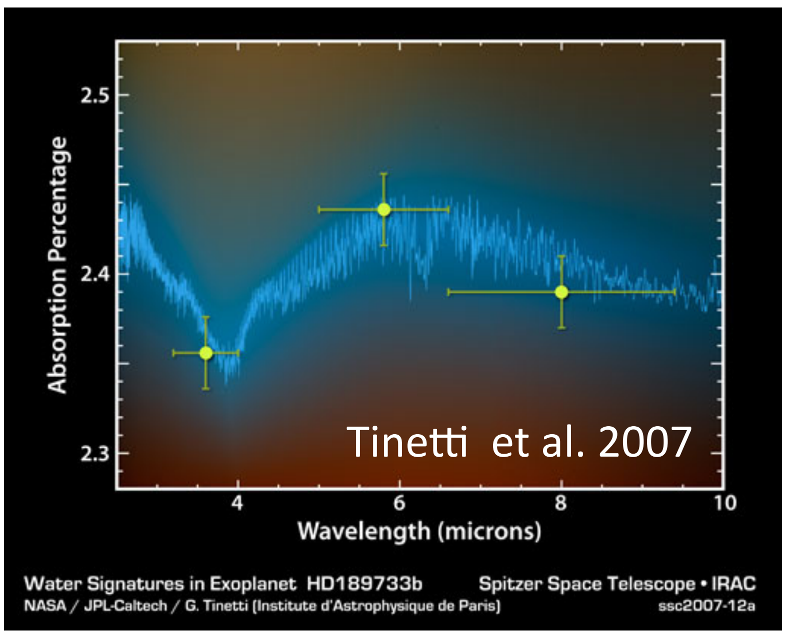
Madhusudhan 2012, ApJ, 758, 36

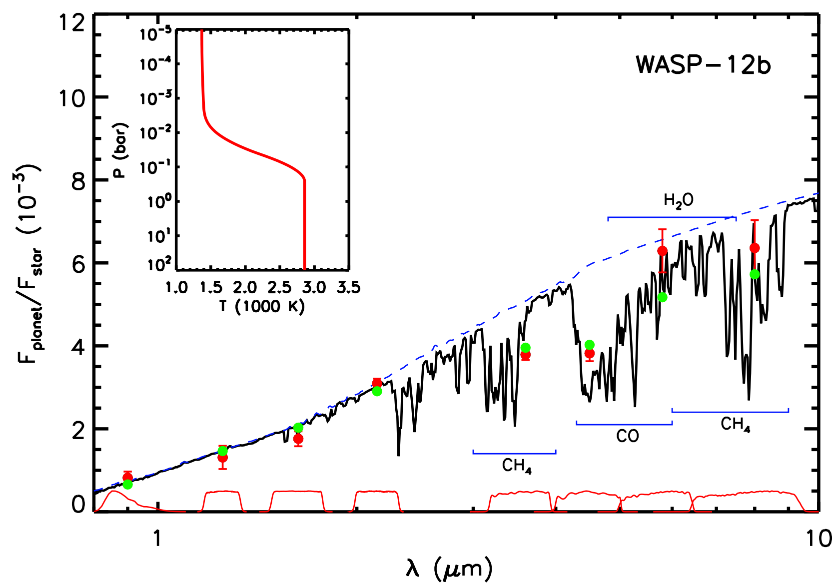
Need for Accuracy and Completeness in Molecular Line lists

1. Exoplanetary Atmospheres – Early Days



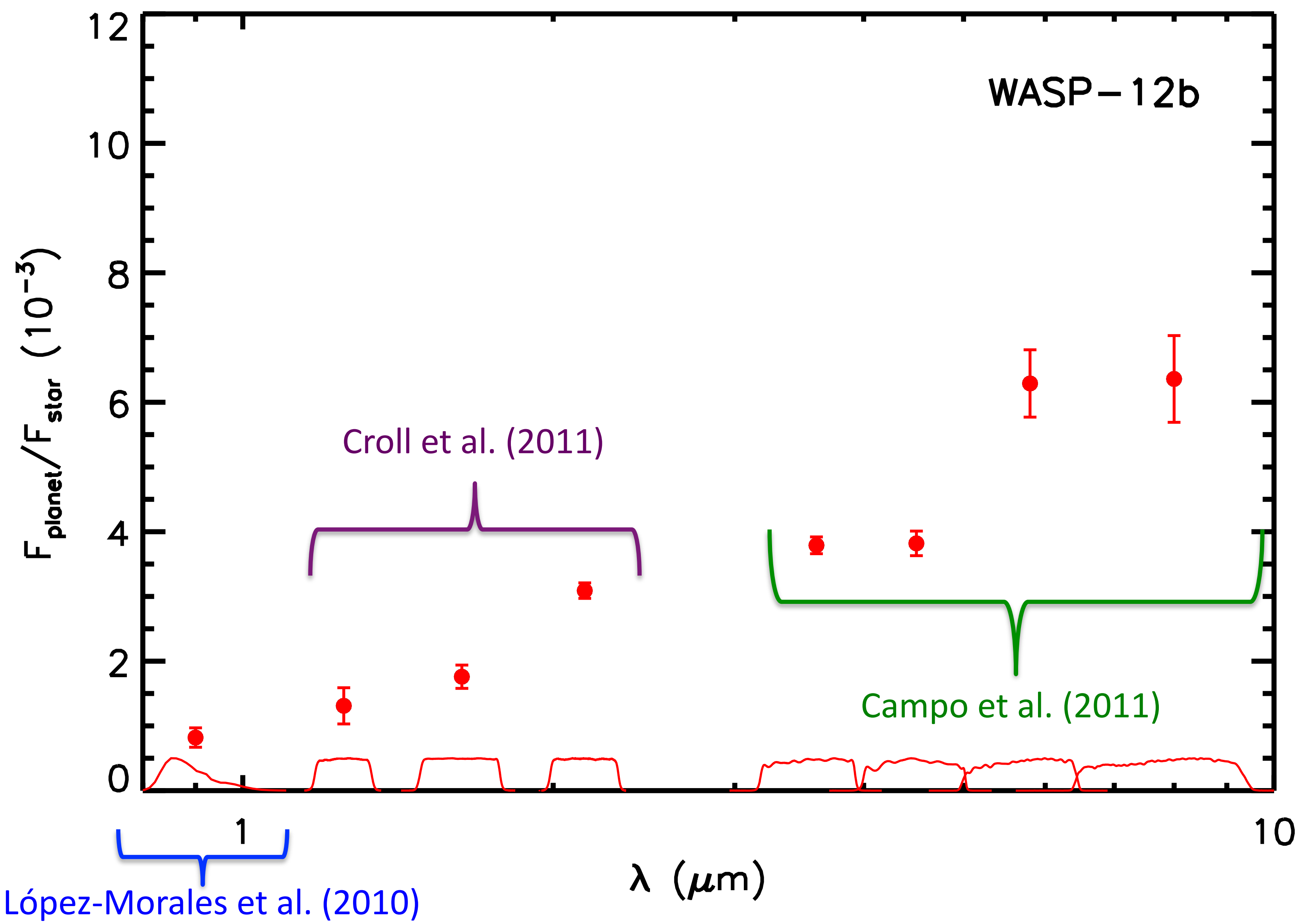




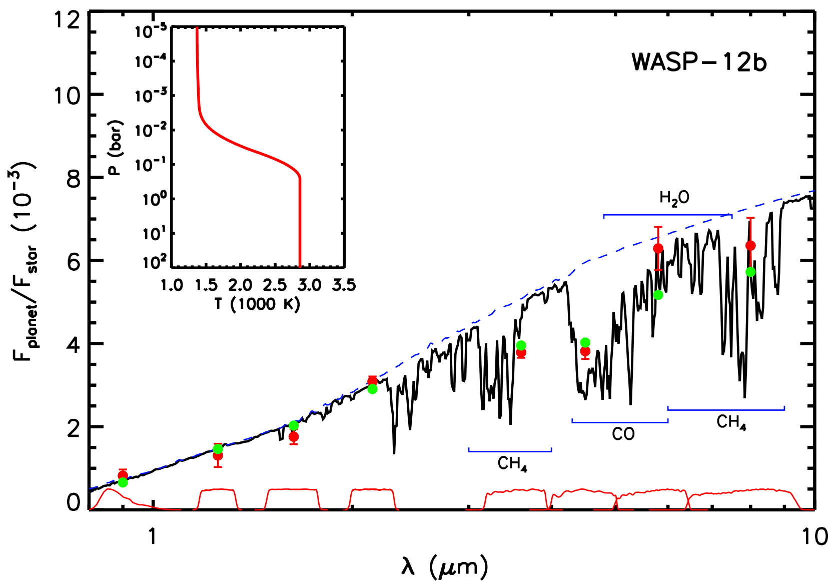


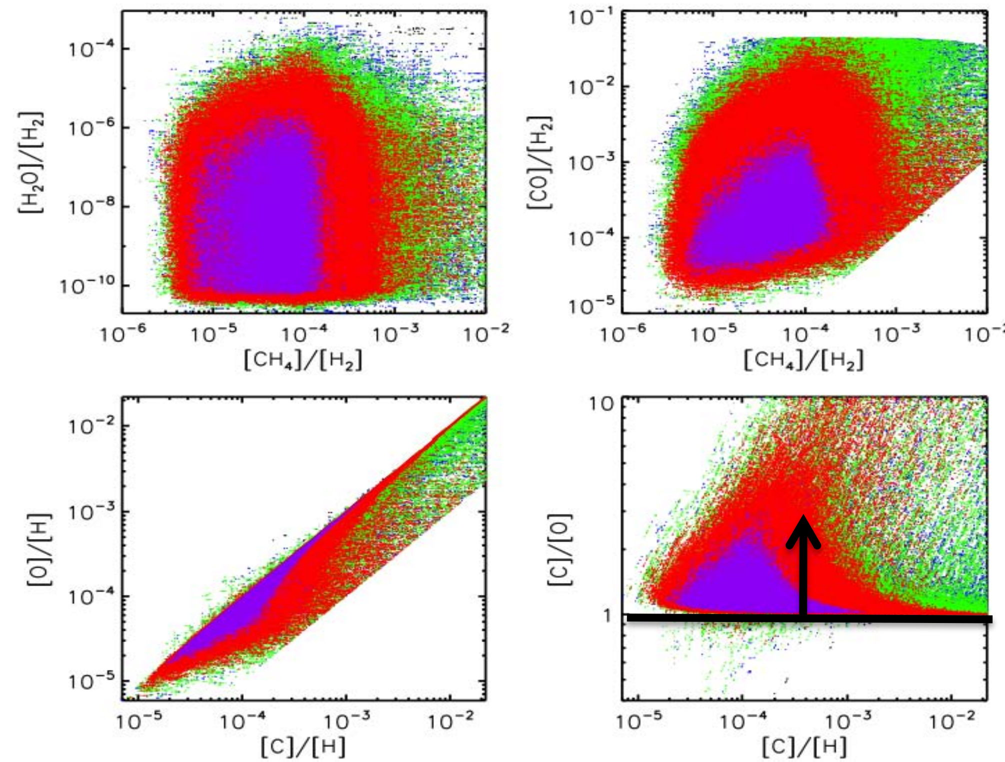
Madhusudhan et al. 2011

Ground-based Photometry and Spectroscopy



Measurement of atmospheric C/O in a giant planet





Key Molecular Constraints

- $H_2O/H_2 \leq 6 \times 10^{-6}$
- $CH_4/H_2 \geq 8 \times 10^{-6}$

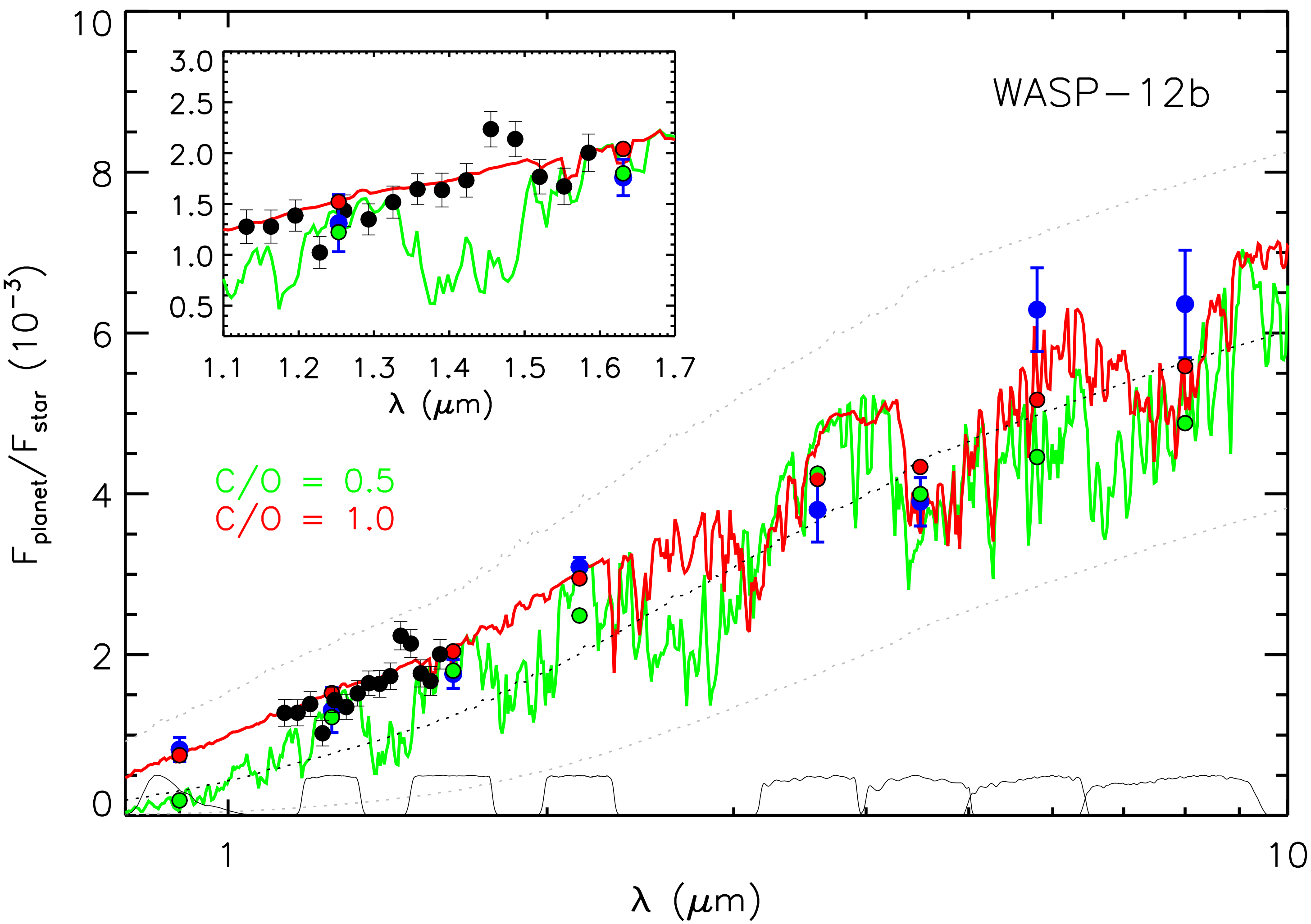
C/O ≥ 1

Adapted from Madhusudhan et al. 2011, Nature, 469, 64

Data from Lopez-Morales et al. 2010; Croll et al. 2010; Campo et al. 2011

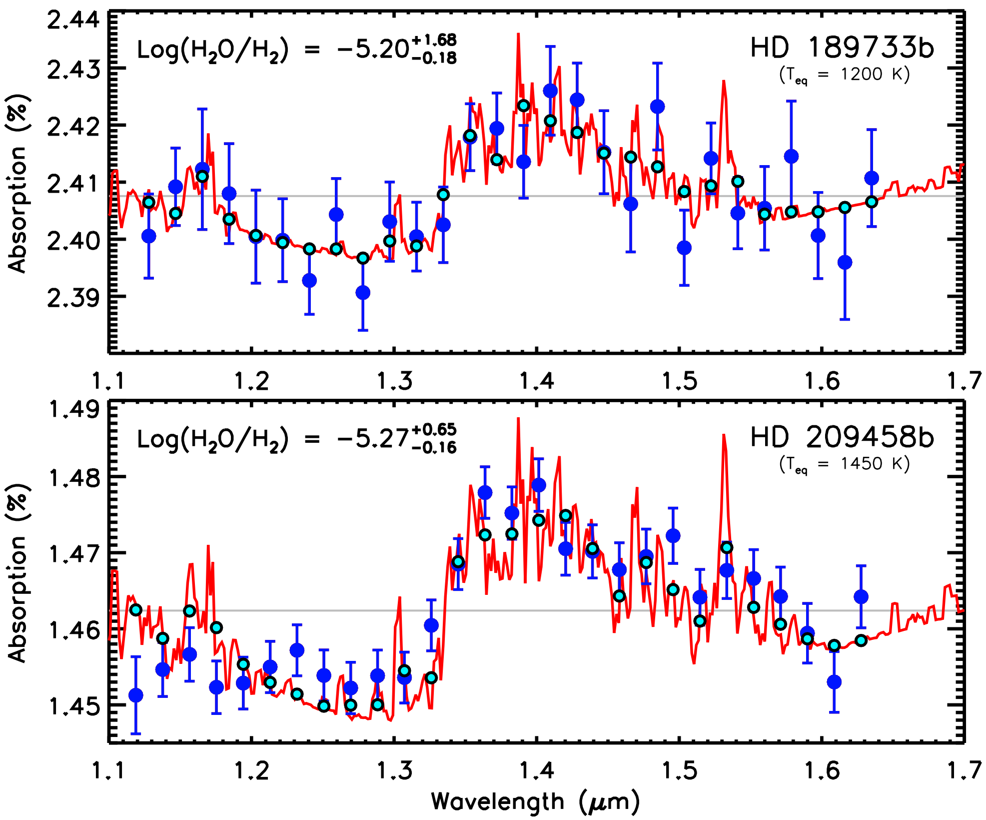
But cf Crossfield et al. 2012, Cowan et al. 2012, Swain et al. 2012, Stevenson et al. 2014

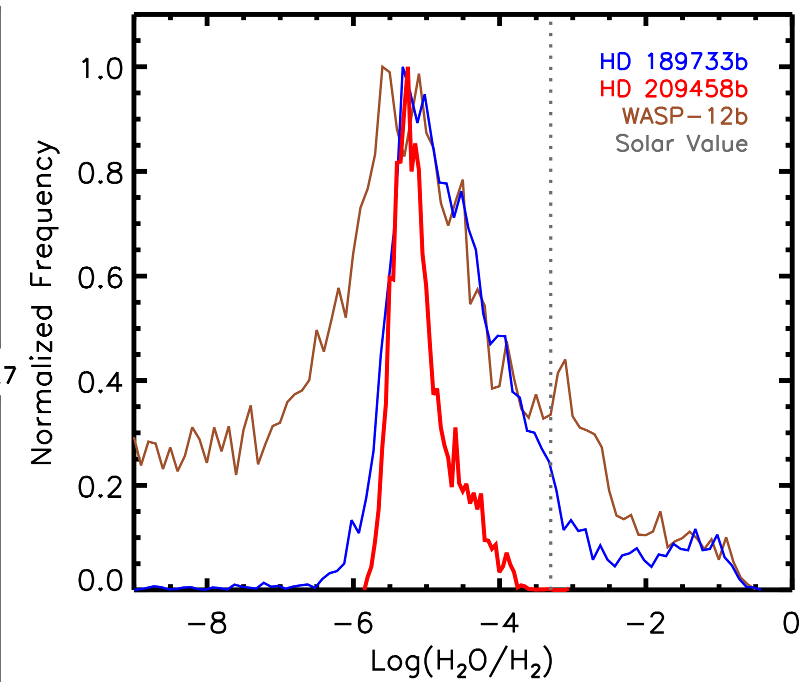
New Advances with HST WFC3



Swain et al. 2012, Madhusudhan 2012, Stevenson et al. 2014

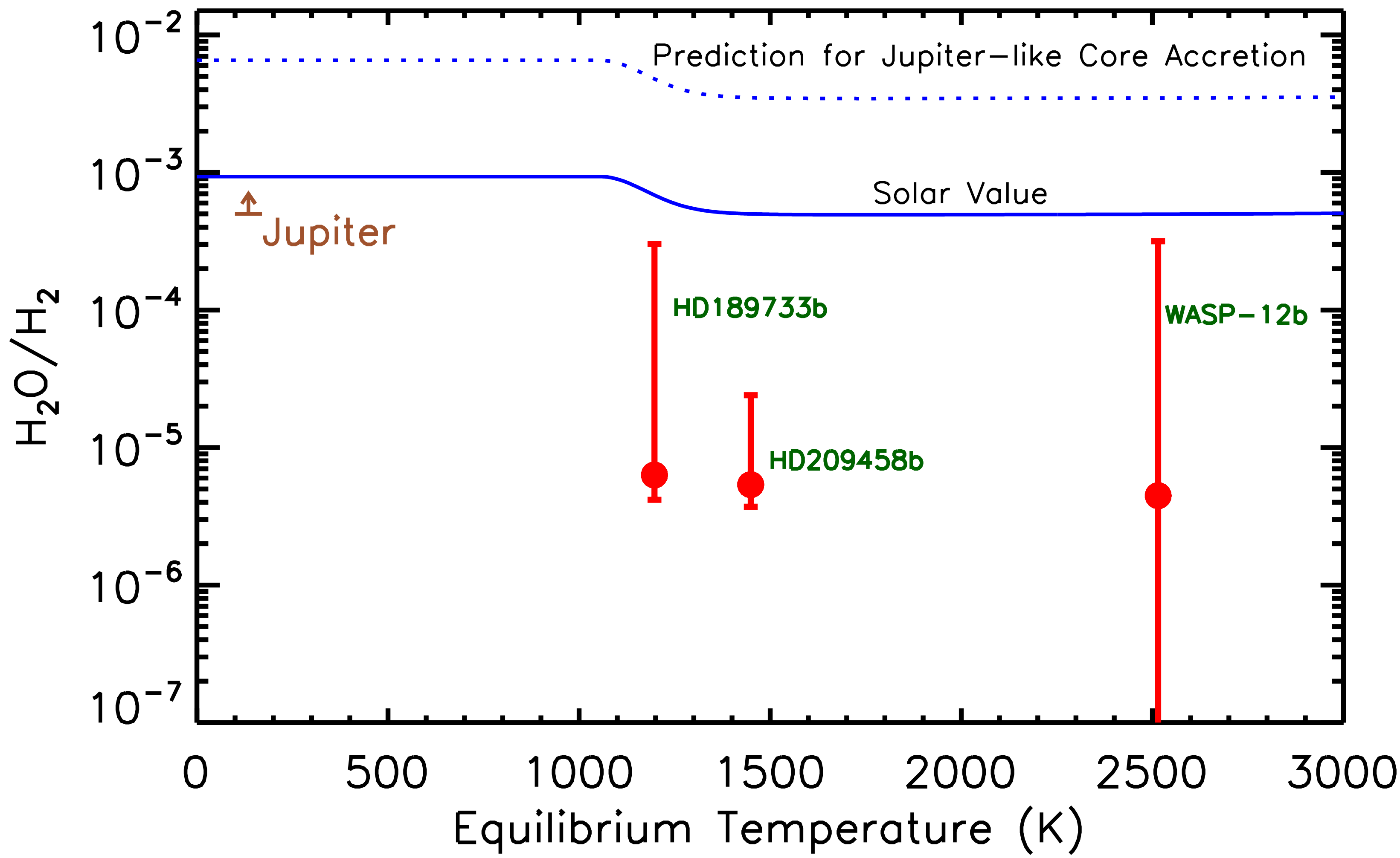
New H_2O detections with HST Transit Spectroscopy





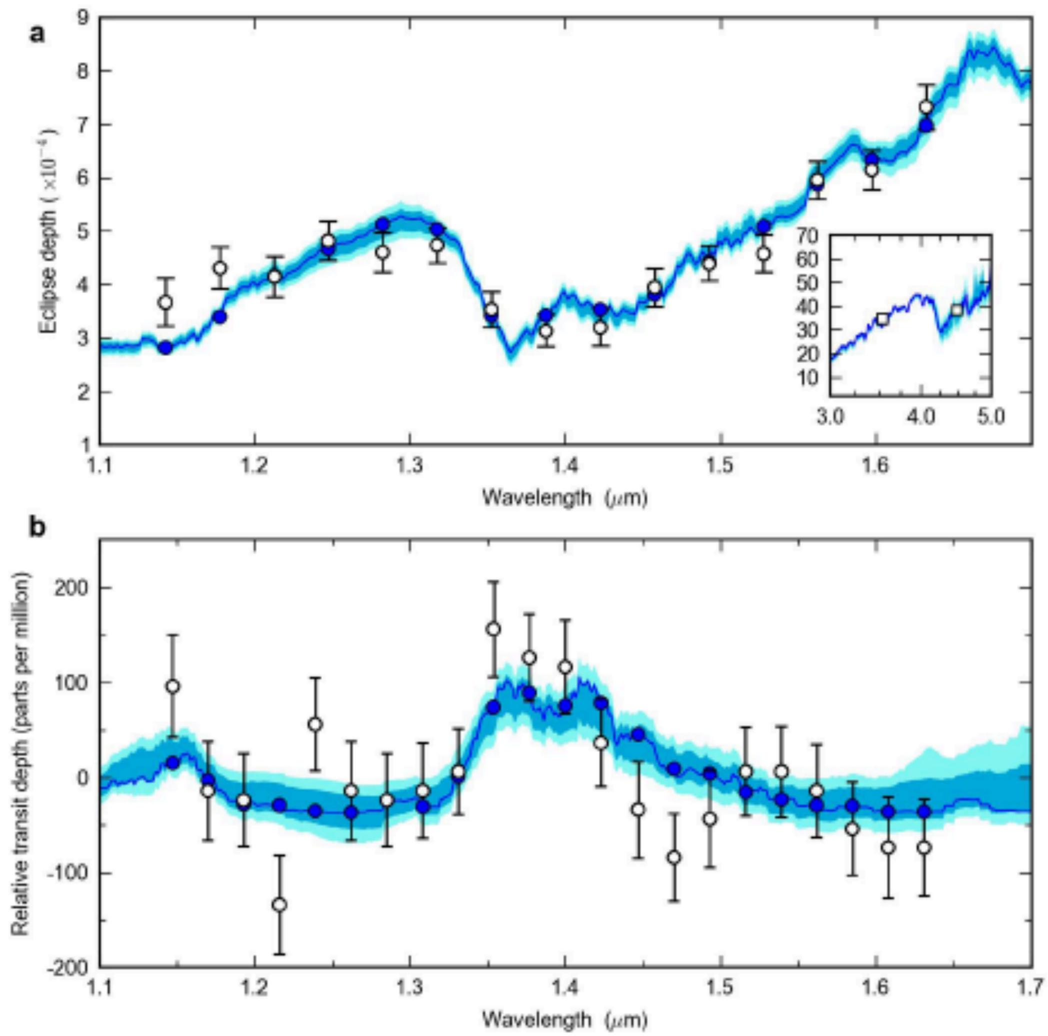
Deming et al. 2013; Madhusudhan et al. 2014a
McCullough et al. 2014

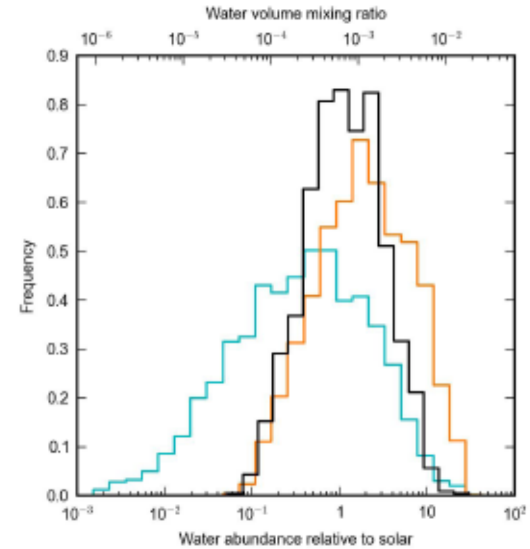
High-precision H_2O Measurements

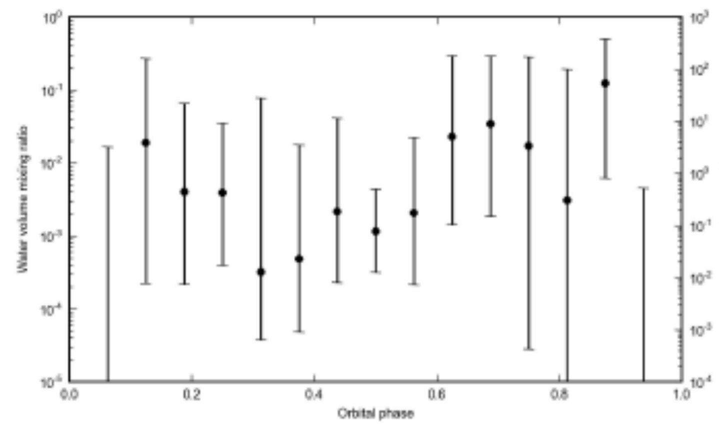


Madhusudhan et al. 2014a

H_2O in the atmosphere of WASP-43b

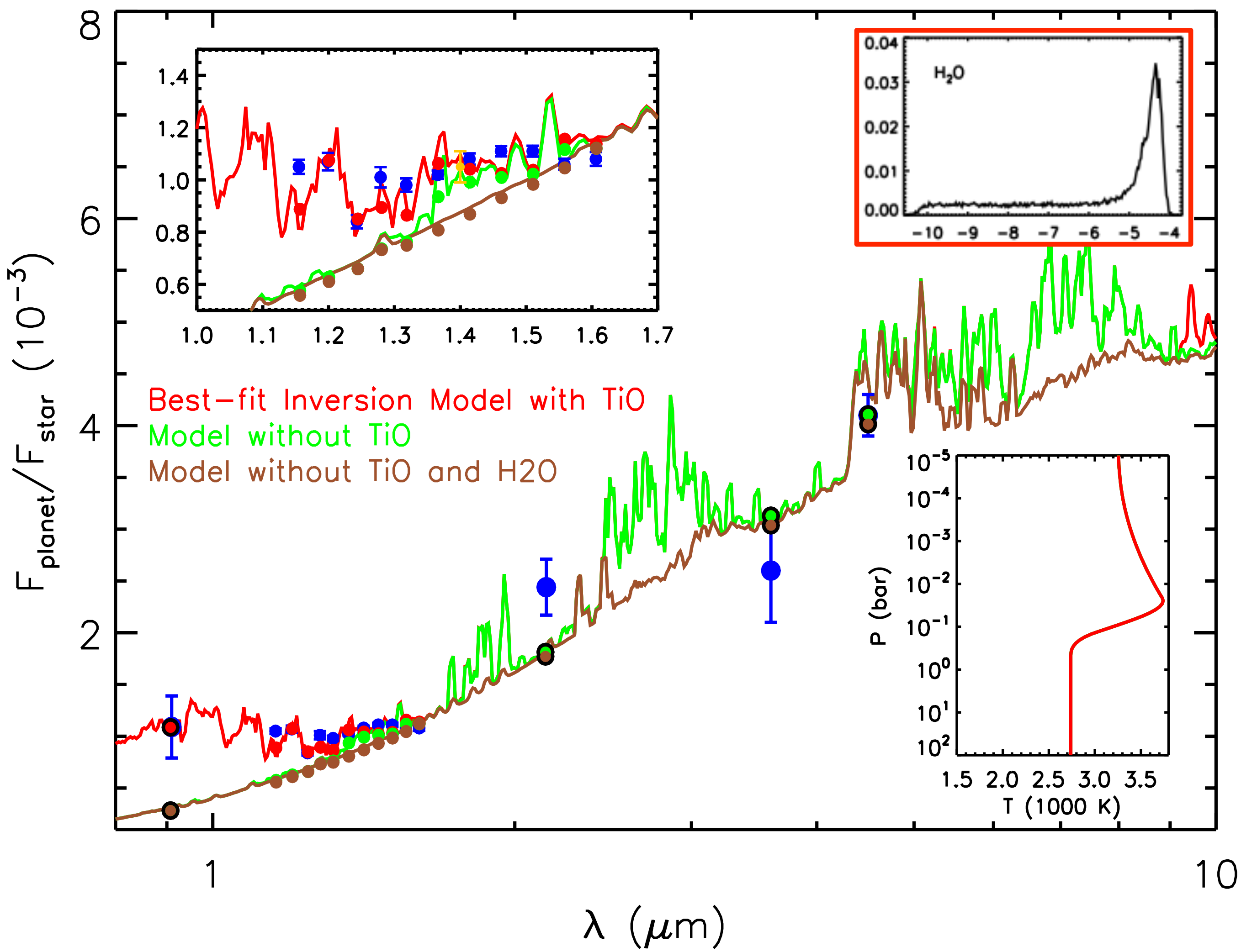






Kriedberg et al. 2014, ApJ

Precision Atmospheric Science for Exoplanets

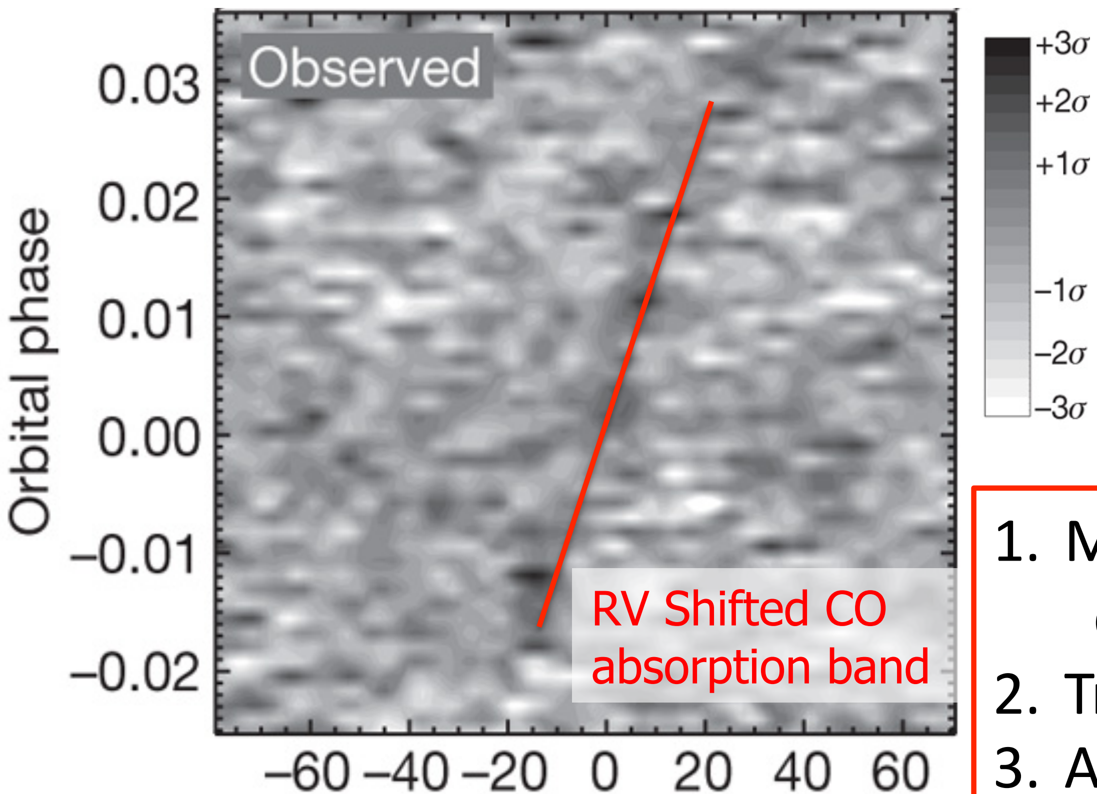


Haynes et al. (2015)

The best current observations are already at the accuracy limit of molecular line lists!

2. Very High-resolution Spectroscopy

RV-Shifted Absorption from HD 209458b During Transit

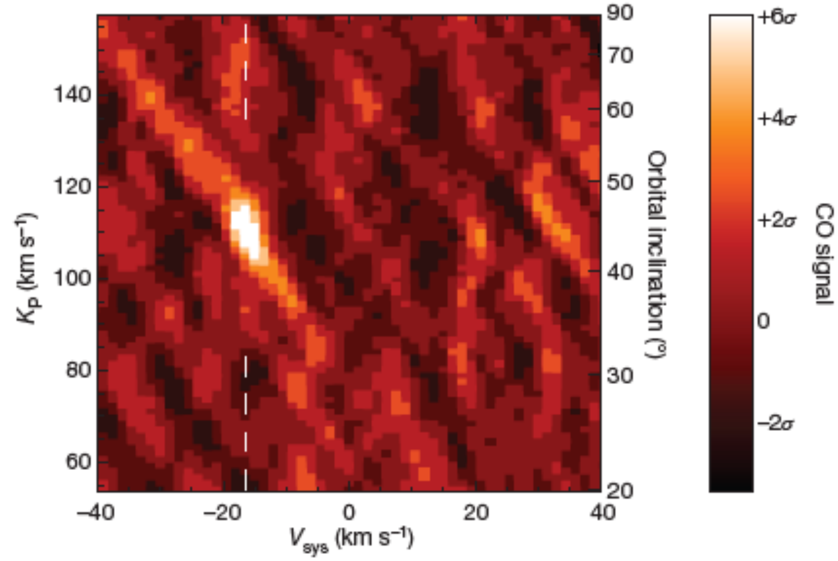


Barycentric RV + 14.8 km/s

Snellen et al. (2010)

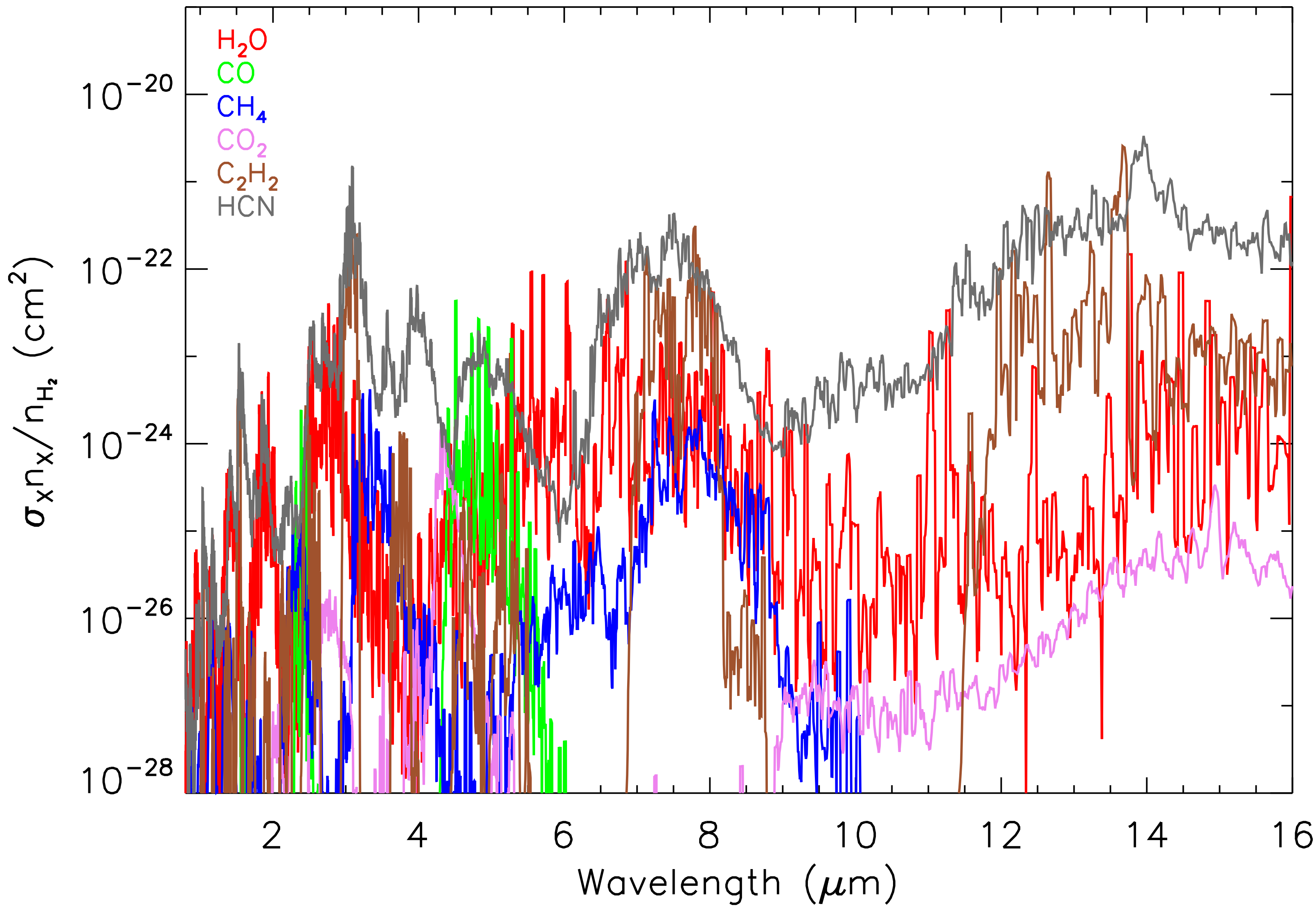
CO absorption detected at 5.6σ

CO detection in hot Jupiters

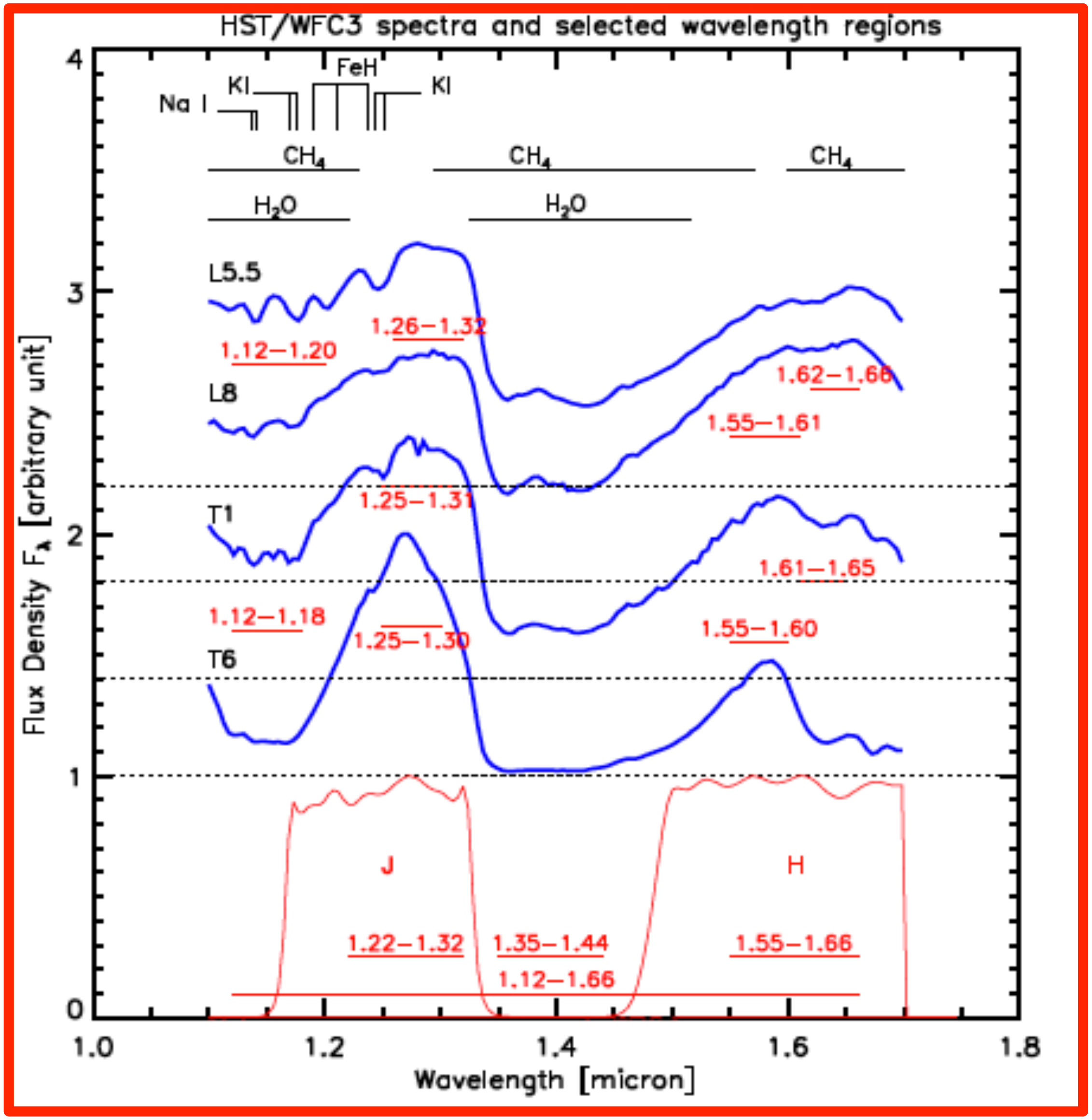


1. Molecular abundances of most dominant molecules.
2. Transiting as well as RV planets.
3. A wide range of planet types: super-Earths to Jupiters.
4. Measuring planetary rotation

Molecules in JWST/METIS Range

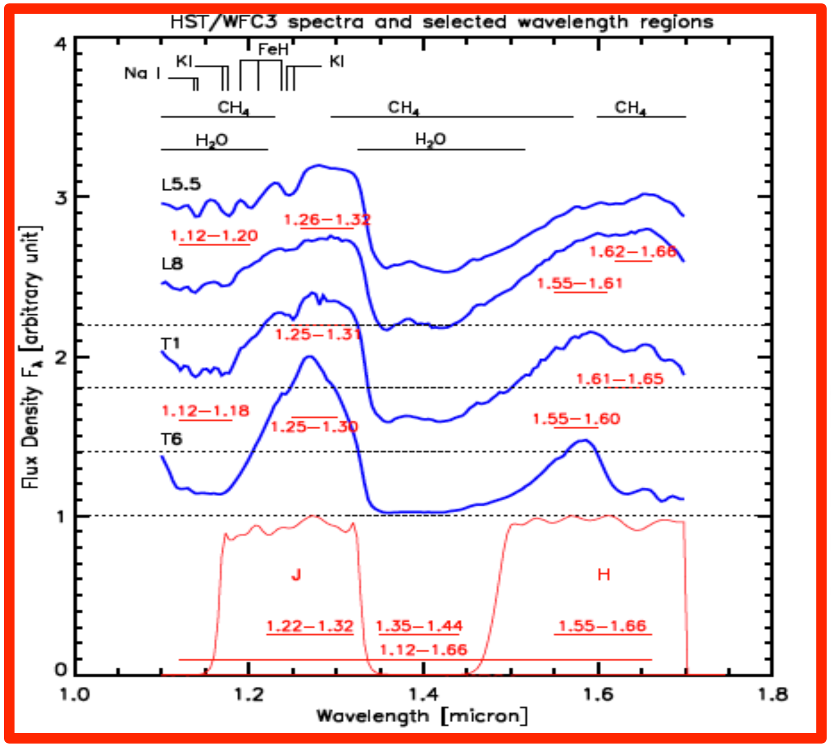


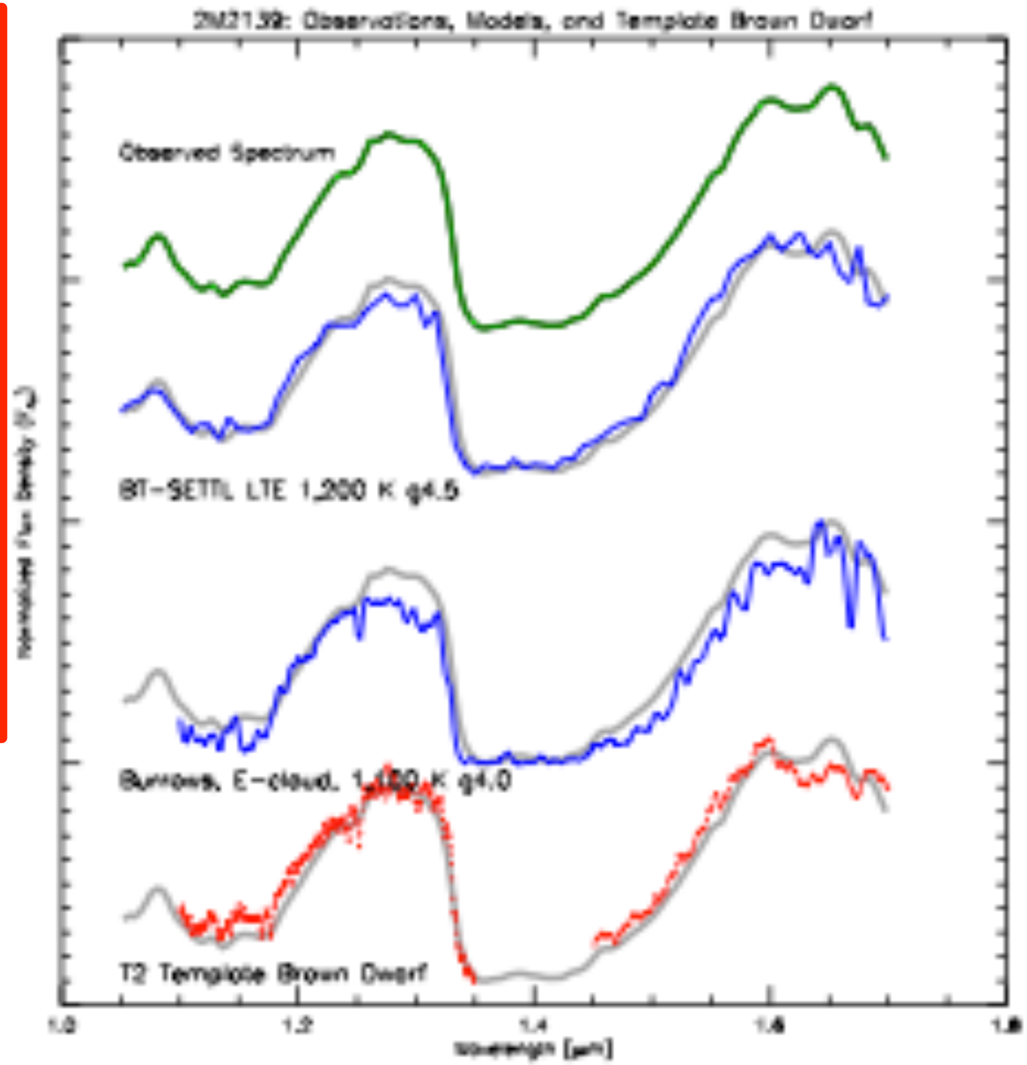
3. Brown Dwarf Atmospheres



Buenzli et al. 2014

Brown Dwarf Atmospheres

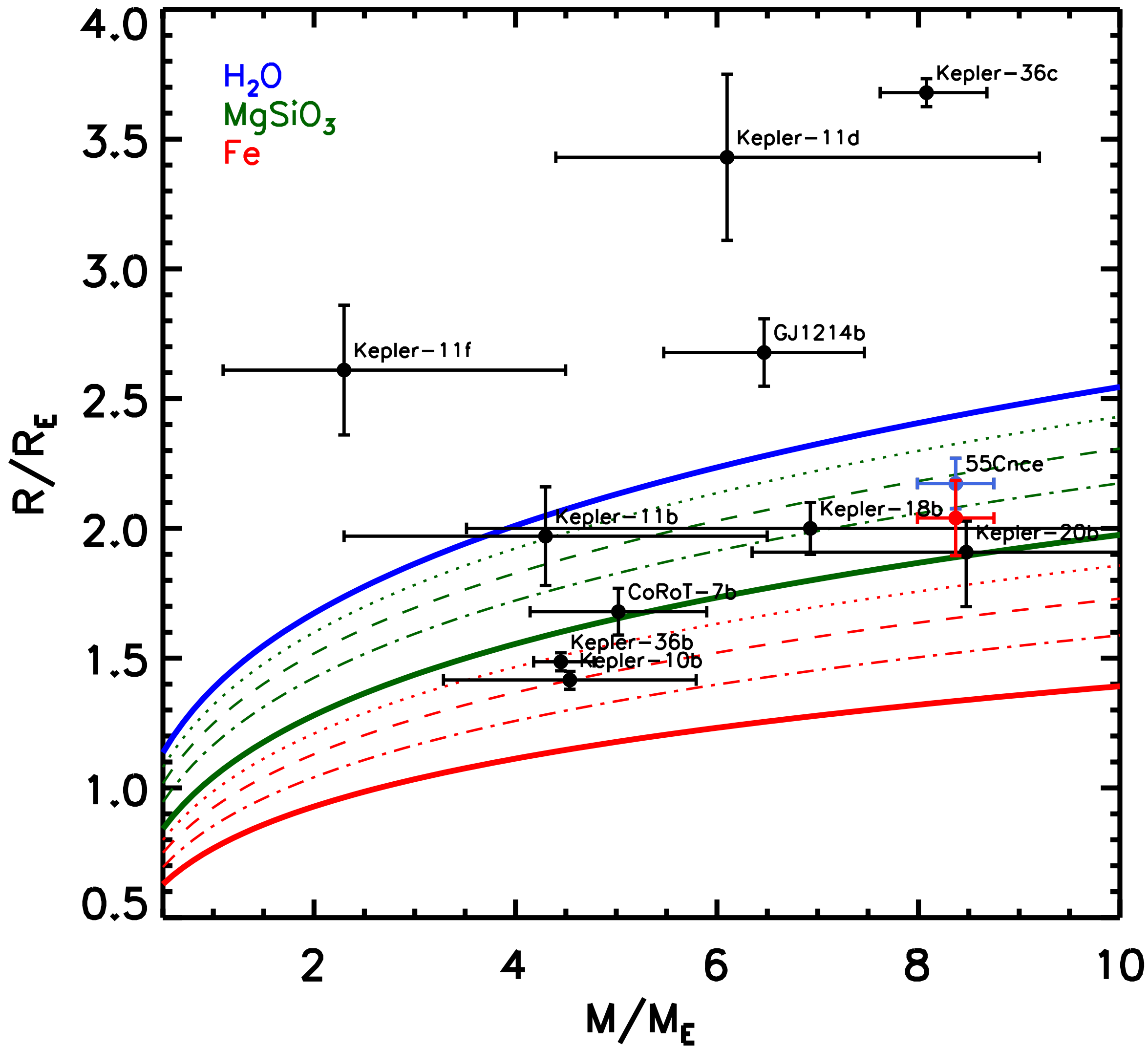




Apai et al. 2013

4. Super-Earth Interiors and Atmospheres

Need for high-T EOS



Valencia et al. 2006, Fortney et al. 2007, Seager et al. 2007, Sotin et al. 2007, Rogers & Seager 2009, 2010, Lopez et al. 2012, Madhusudhan et al. 2012

New Data require High-T Spectroscopic Line lists for

Molecules: H_2O, CO, CH_4, CO_2, NH_3, HCN, C_2H_2, TiO, VO, TiH, FeH

Requirements from Laboratory Astrophsyics

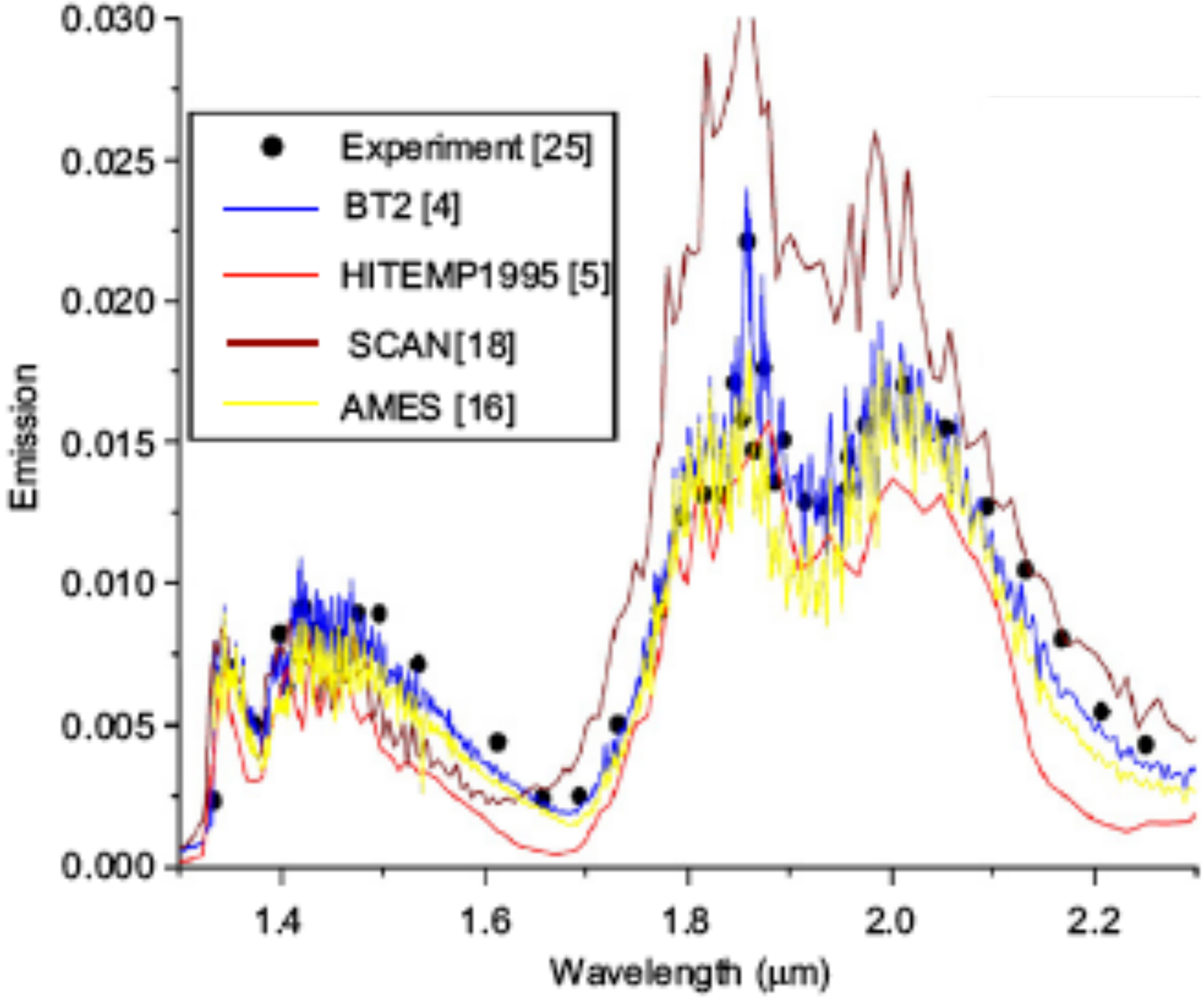
Primary Molecules: H_2O, CO, CH_4, CO_2, NH_3, HCN, C_2H_2, TiO, VO, TiH, FeH

Molecule	Ref	Method	Isotopologues	T^{max} [c]	N	Available[d]
C_2	Kurucz (2011)	semi		5200 K	3459595	Kurucz
CH	Kurucz (2011)	semi		3000 K	71591	Kurucz
CN	Kurucz (2011)	semi		5000 K	1644597	Kurucz
CO	Rothman et al. (2010)	expt		4000 K	113631	HITEMP
CaH	Weck et al. (2003d)	semi		3500 K	89970	UGAMOP
CrH	Burrows et al. (2002)	semi	$^{50}Cr, ^{53}Cr, ^{54}Cr$	1300 K	13824	Bernath
FeH	Bernath and co-workers[a]	semi	$^{54}Fe, ^{57}Fe, ^{58}Fe$	1600 K	116300	Bernath
HD^+	Coppola et al. (2011)	ai		all	10120	ExoMol
HeH^+	Engel et al. (2005)	ai	all[e]	all	8573	ExoMol
LiCl	Weck et al. (2004)	semi		4000K	3357811	UGAMOP
LiH	Coppola et al. (2011)	ai		all	18981	ExoMol
LiH^+	Coppola et al. (2011)	ai		all	329	ExoMol
MgH	Weck and co-workers[b]	semi		1300 K	23315	UGAMOP
OH	Rothman et al. (2010)	expt		4000 K	41577	HITEMP
NH	Kurucz (2011)	semi		3000 K	36163	Kurucz
NO	Rothman et al. (2010)	expt		4000 K	115610	HITEMP
SiH	Kurucz (2011)	semi		3000 K	78286	Kurucz
SiO	Langhoff & Bauschlicher (1993)	semi				
SiO	Kurucz (2011)	semi		5300 K	1827047	Kurucz
TiH	Burrows et al. (2005)	semi		1800 K	199073	Bernath
TiO	Schwenke (1998)	semi		6200 K	37744499	Kurucz

Molecule	Ref	Isotopologues	T^{max}	$10^{-6}N$	Available
H_3^+	Neale et al. (1996)	H_2D^+ (Sochi & Tennyson 2010)	3000 K	12	ExoMol
H_2O	Barber et al. (2006)	HDO (Voronin et al. 2010)	3000 K	503	ExoMol
HCN/HNC	Harris et al. (2006)	$H^{13}CN$ (Harris et al. 2008)	3000 K	240	ExoMol
C_3	Jørgensen et al. (1989)		3100 K		
CO_2	Tashkun & Perevalov (2011)	all	5000 K	626	CDSD
NH_3	Yurchenko et al. (2011a)		1500 K	1014	ExoMol

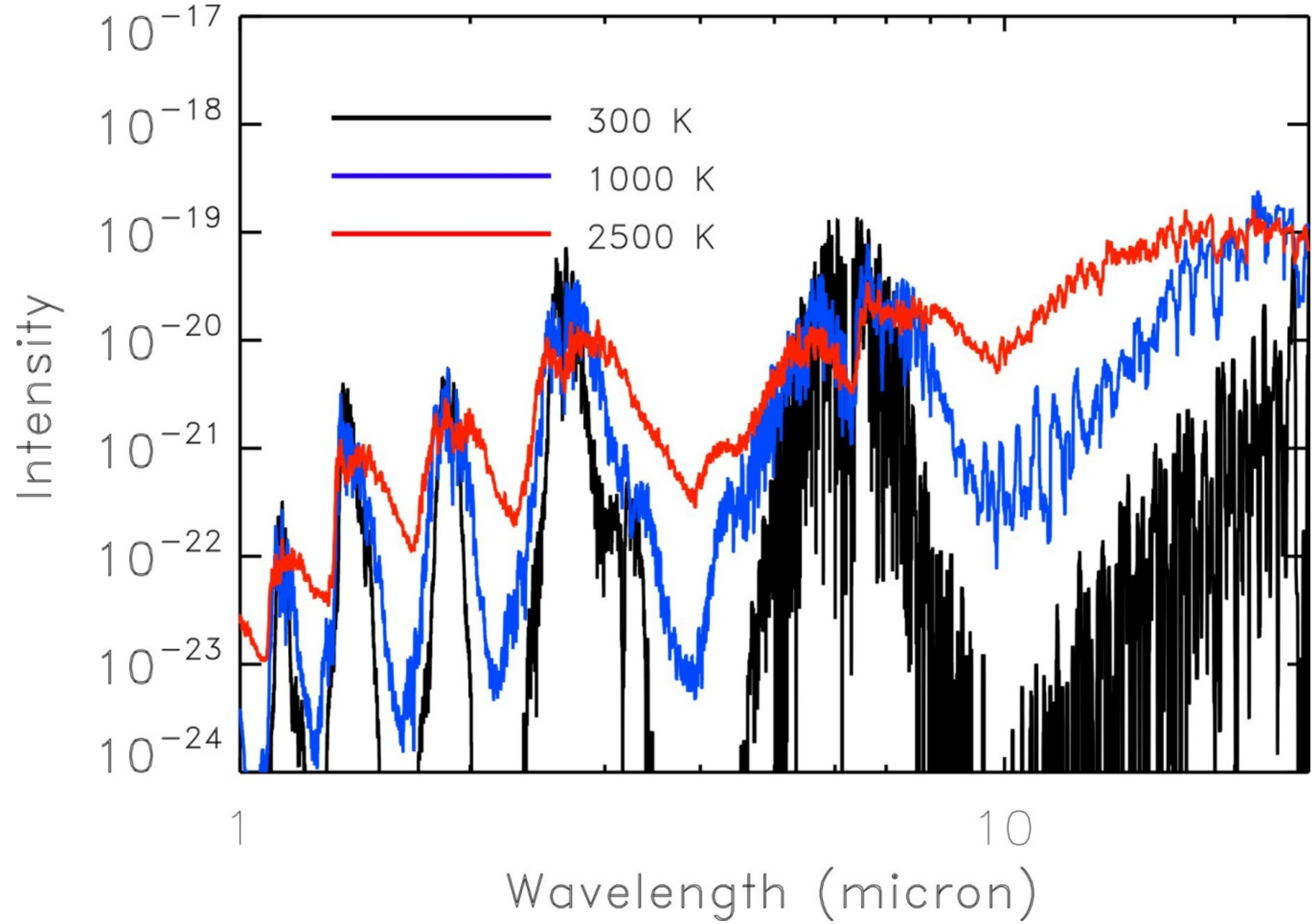
Tennyson & Yurchenko, MNRAS, 2012

High T (3000 K) Line Lists of H_2O



Rothman et al. 2010

Temperature dependence of H_2O Spectra

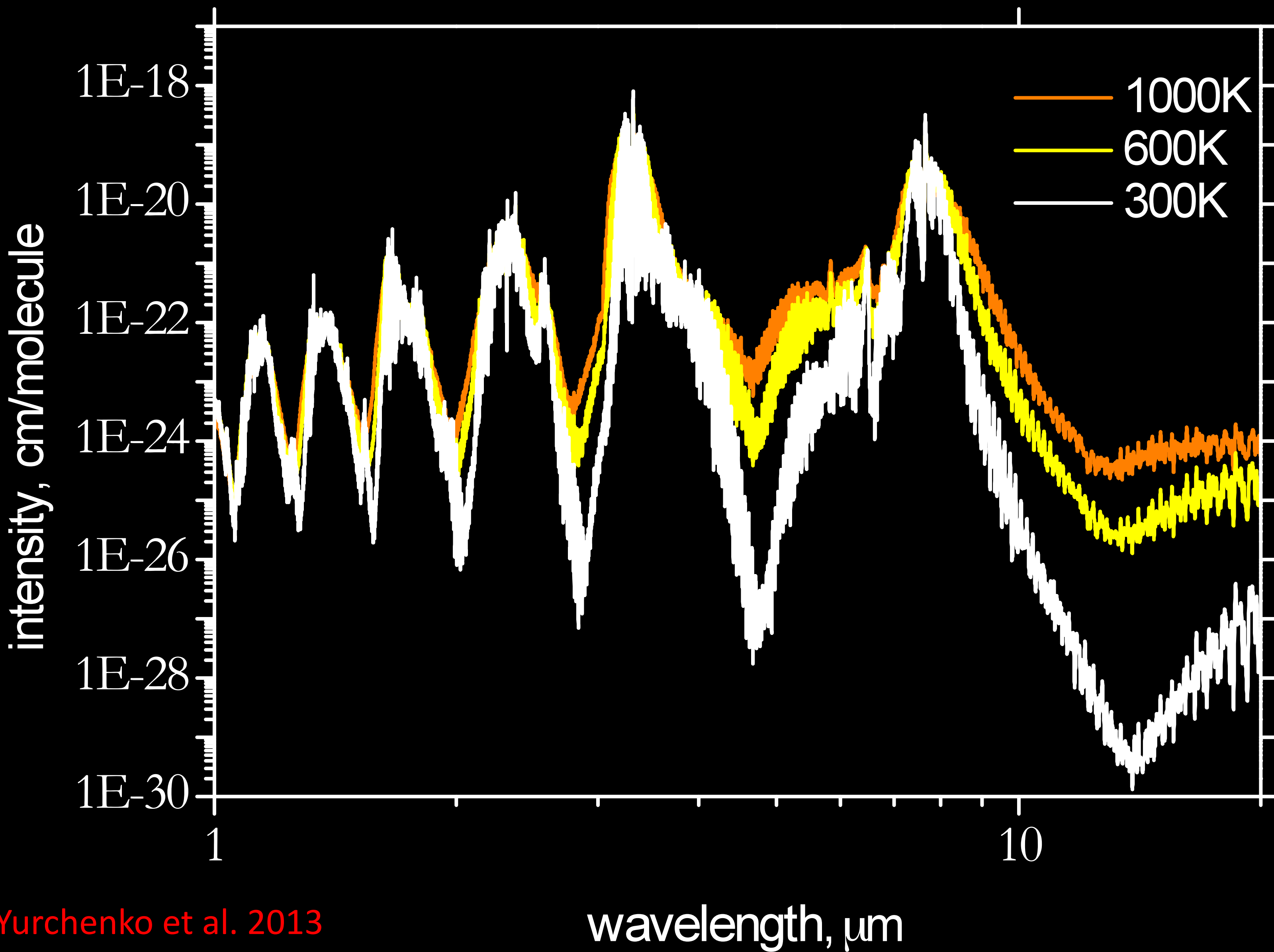


Barber et al. MNRAS 368, 1087 (2006).

- Reliable high-T Line lists have been available for H_2O, CO, and CO_2

(Rothman et al. 2005, Barber et al. 2006, Freedman et al. 2008, Rothman et al. 2010)

Absorption spectra of CH_4: Temperature Effect



Yurchenko et al. 2013

Line list Requirements

Relatively Complete line lists exist only for H_2O, CH_4, CO, CO_2, NH_3

Experimental high-temperature line lists for:

HCN, C_2H_2, TiO, VO, H_2S, SiO, SO_3, PH_3, Metal Hydrides (TiH, FeH, MgH, AlH, CrH), etc.

Theoretical ab initio line lists for:

C_2H_2, VO, Metal Hydrides (TiH, FeH, MgH, CrH), etc.

Theoretical line lists in progress (requiring validation):

H_2S, SiO, PH_3, AlH, SO_3, CrH, Al_2O_3

Both Experimental and Theoretical work on:

Higher-order hydrocarbons, self-broadened line lists for super-Earth atmospheres, aerosols, and atomic species (Na, K).

Summary

- New observations are leading to unprecedented constraints on molecular compositions and elemental abundance ratios (e.g. C/O) of exoplanetary atmospheres
  - Major implications for atmospheric processes and planet formation
- Observational constraints on chemistry are beginning to be limited by spectroscopic line list data on molecules $\kappa = \Sigma_i (n_i \times \sigma_i)$
- New advancements in experiments and theoretical calculations are critical to the future of exoplanet characterization with present and upcoming facilities (e.g. HST, JWST, E-ELT).