Equilibrium and Disequilibrium Chemistry in Hot Jupiters

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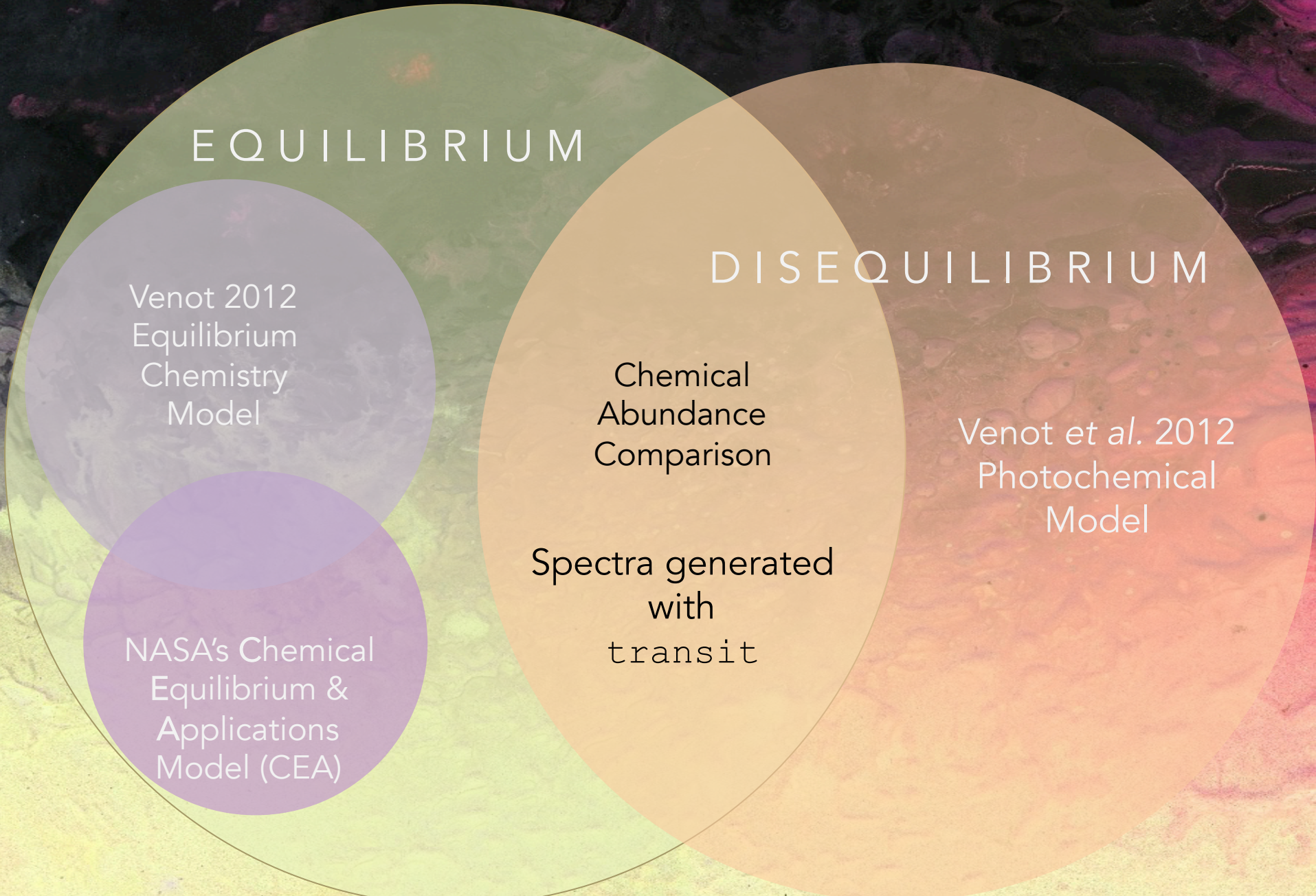
TDE

Thursday, October 15, 2015



Gordon & McBride 1994; Venot *et al,*. 2012; Cubillos *et al*., 2015 in prep.; Blecic *et al*., 2015b in prep.; Harrington *et al*., 2015 in prep.; Rojo Thesis 2007

PLANETARY LINEUP

T

HD 97658 b

T_{eq} = 757 K

M_{planet} = 0.02 R_{Jup}

R_{planet} = 0.20 R_{jup}

a = 0.08 AU

Stellar Type = K1V

HD 189733 b

T_{eq} = 1191 K

M_{planet} = 1.138 R_{jup}

R_{planet} = 1.138 R_{jup}

a = 0.03 AU

Stellar Type = K1-K2

HD 209458 b

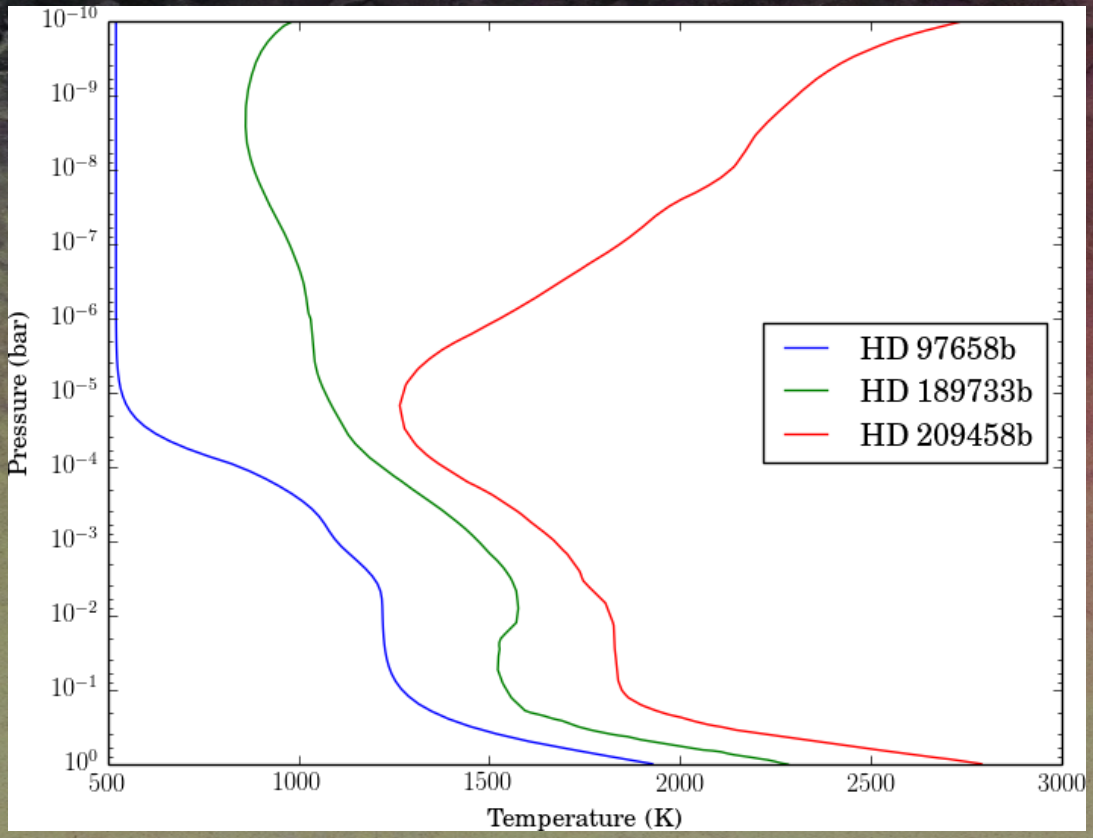
T_{eq} = 1447K

M_{planet} = 0.69 R_{Jup}

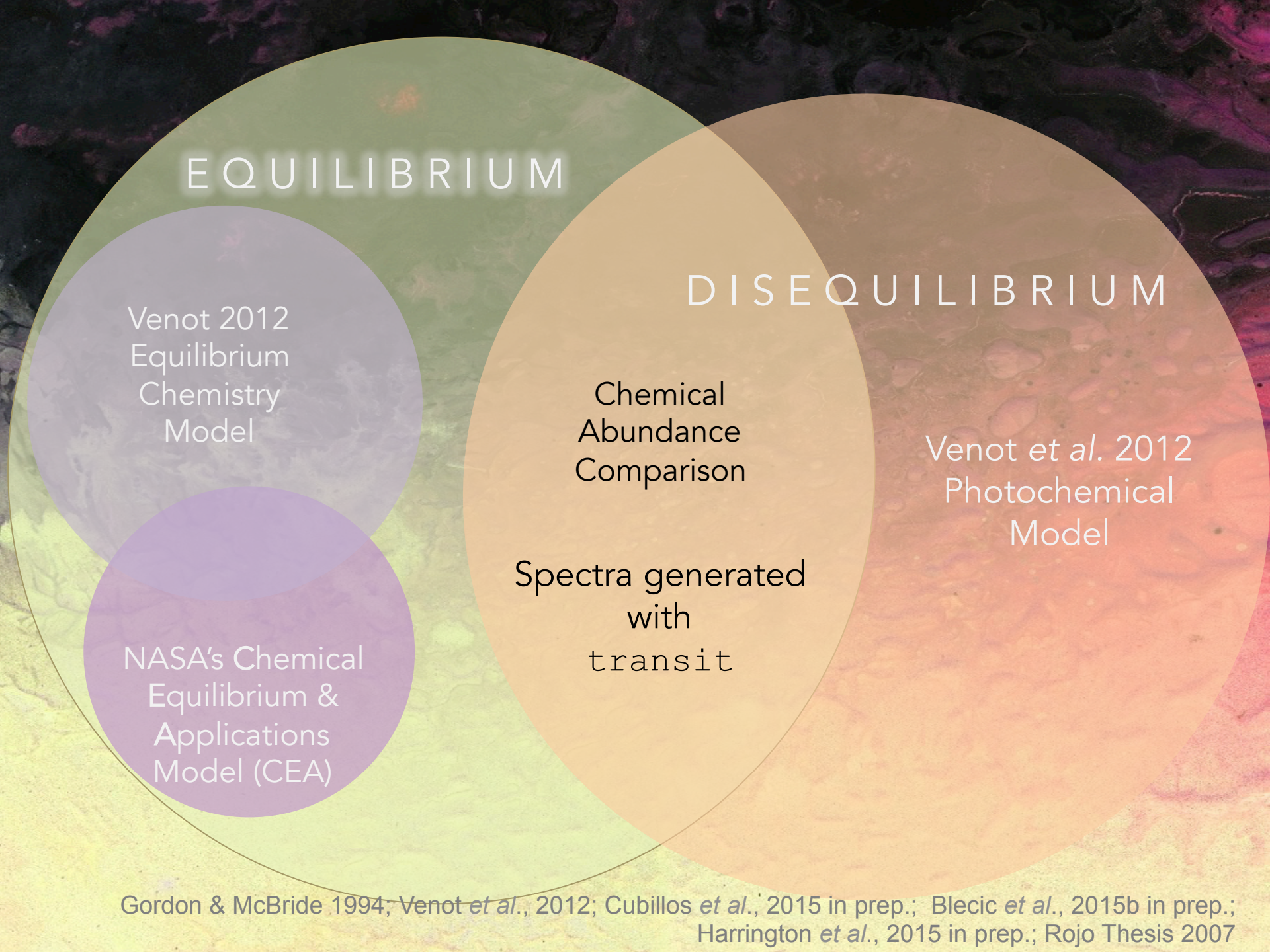
R_{planet} = 1.38 R_{Jup}

a = 0.047 AU

Stellar Type = G0V



exoplanet.eu; Venot *et al*., 2012; Miguel *et al*., 2013; Moses *et al*., 2011; Hu & Seager 2014



Gordon & McBride 1994; Venot *et al*., 2012; Cubillos *et al*., 2015 in prep.; Blecic *et al*., 2015b in prep.; Harrington *et al*., 2015 in prep.; Rojo Thesis 2007

Gordon & McBride 1994; Venot *et al*., 2012; ANL-05/20

! Differences in Thermodynamic Data!
Also seen in Tsai, Blecics, and Hébrard's talks

Venot 2012 TECA
105 species
neutral, including radical species
7 coefficients

Output by which new CEA is validated by

Burcat library
~25 species
Includes radical species (grab bag)
400 revised CEA species

CEA
~60 species included
~1401 total
Ionic and neutral species
9 coefficients

85 relevant species
~2500 species total

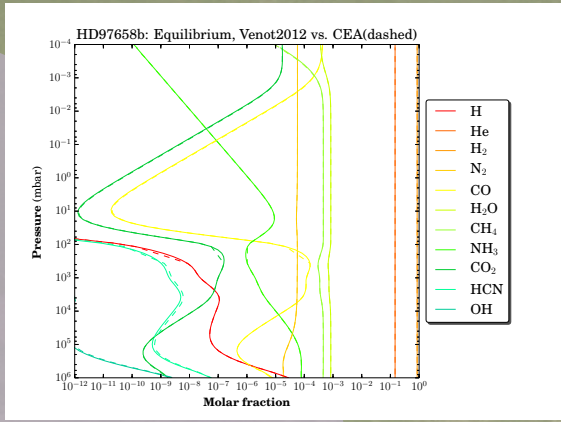
Gordon & McBride 1994; Venot *et al.*, 2012; ANL-05/20

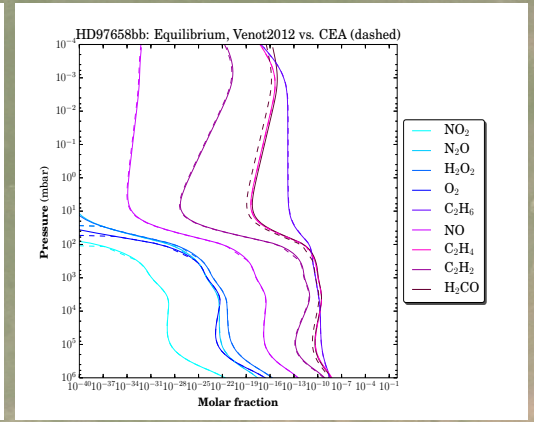
EQUILIBRIUM

Venot 2012 TECA

Burcat library

CEA





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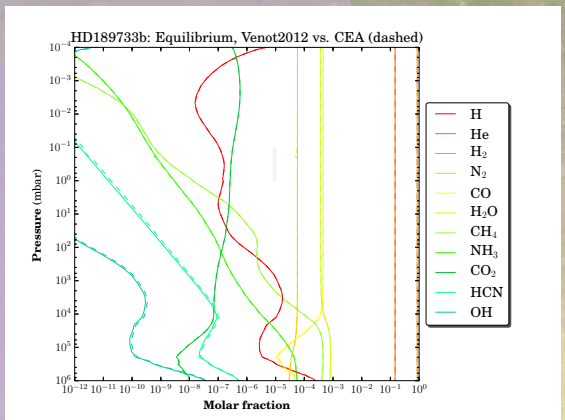

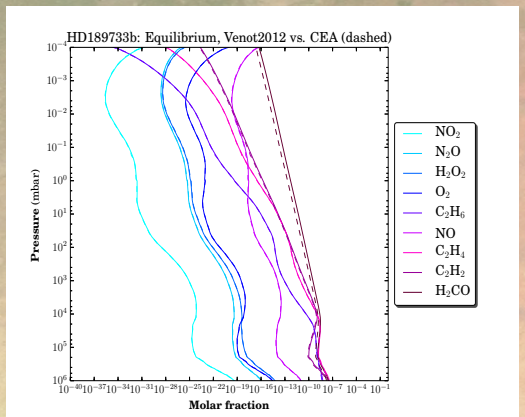

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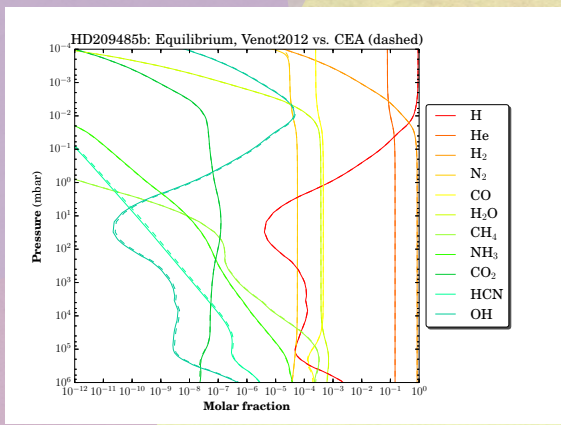
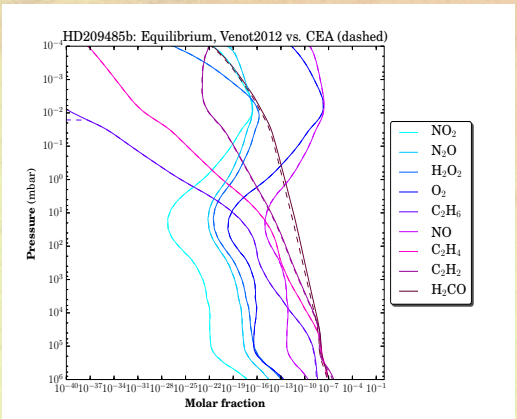
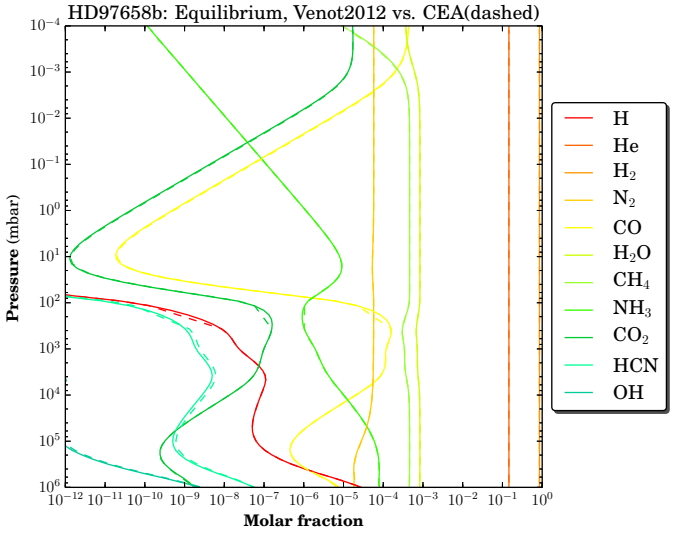
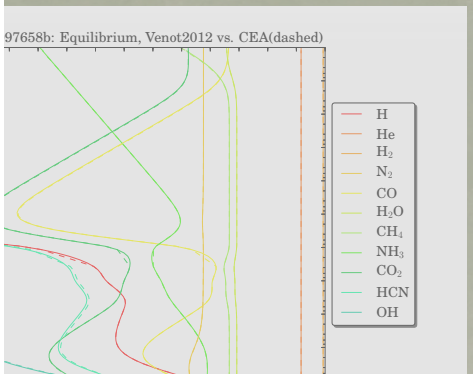


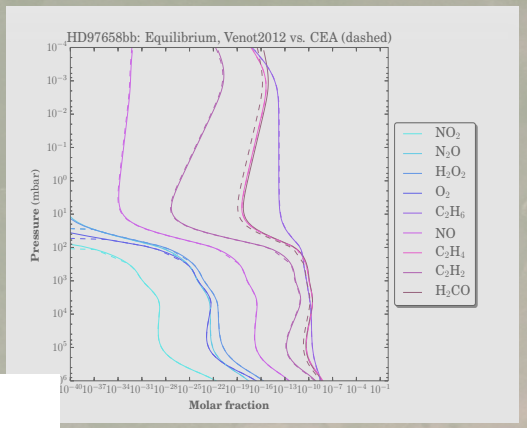


HD209458b

EQUILIBRIUM







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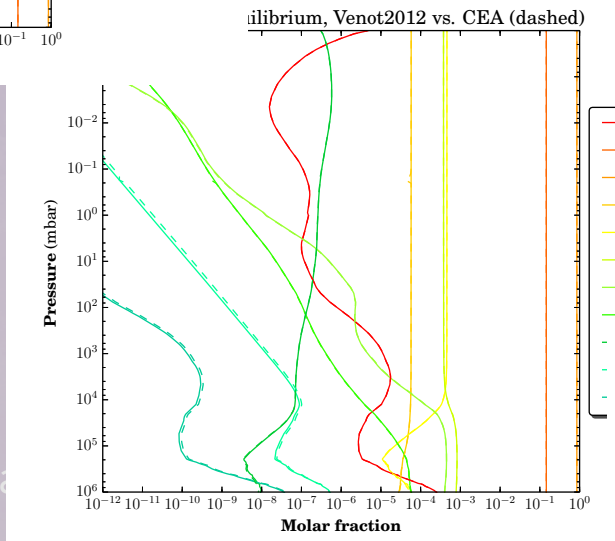
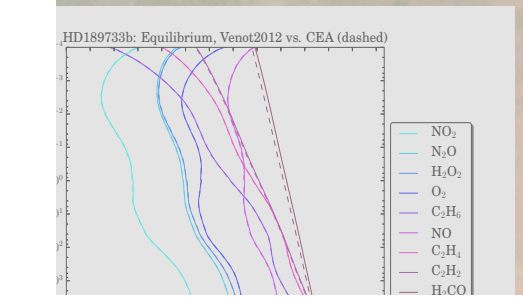
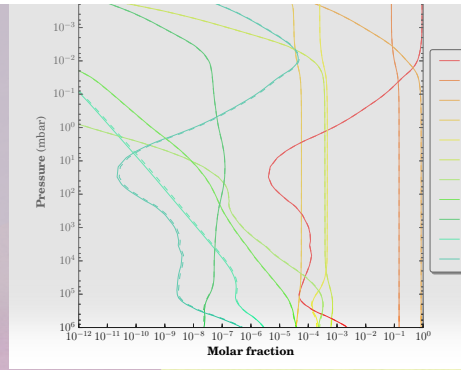
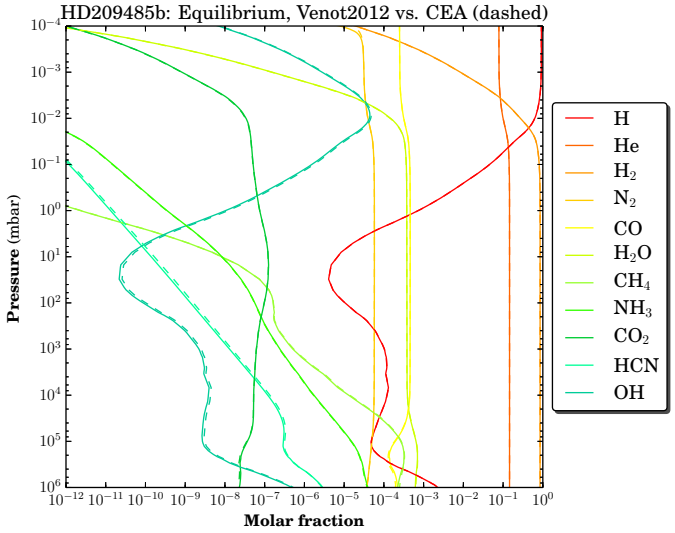




HD189





Burcat libra

CEA

Gordon & McBride 1994; Venot *et al*., 2012; Cubillos *et al*., 2015 in prep.; Blecic *et al*., 2015b in prep.; Harrington *et al*., 2015 in prep.; Rojo Thesis 2007

DISEQUILIBRIUM

Venot *et al.* 2012 Photochemical Model

C_o – C_2 verified

957 reversible and 6 irreversible reactions

300 - 2500 K

Venot *et al.*, 2012

Venot *et al.* 2012 Photochemical Model

C_o – C_2 verified

957 reversible and 6 irreversible reactions

300 - 2500 K

HD 97658 b	HD 189733 b	HD 209458 b
T_{eq} = 757 K	T_{eq} = 1191 K	T_{eq} = 1447 K
T(P=1bar) = 1927 K	T(P=1bar) = 2228 K	T(P=1bar) = 2789 K
dG = 788 J/mol	dG = 1.81 J/mol	dG = 0.05 J/mol

Venot *et al.*, 2012; Krissansen-Totton *et al.*, 2015; Miguel *et al.*, 2013; Hu & Seager 2014

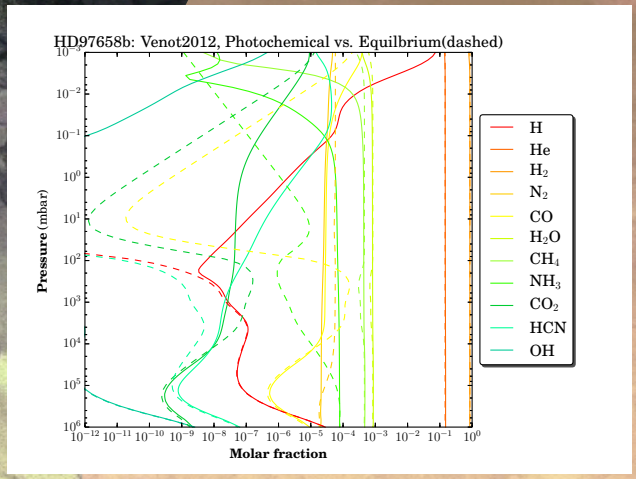
DISEQUILIBRIUM

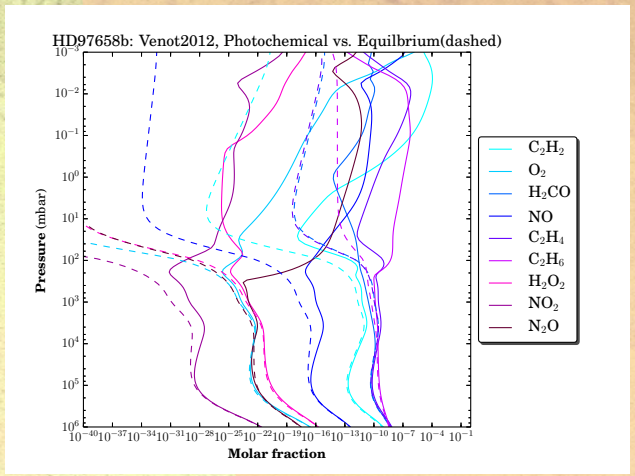
HD97658b

T_{eq} = 757 K

T(P=1bar) = 1927 K

dG = 788 J/mol



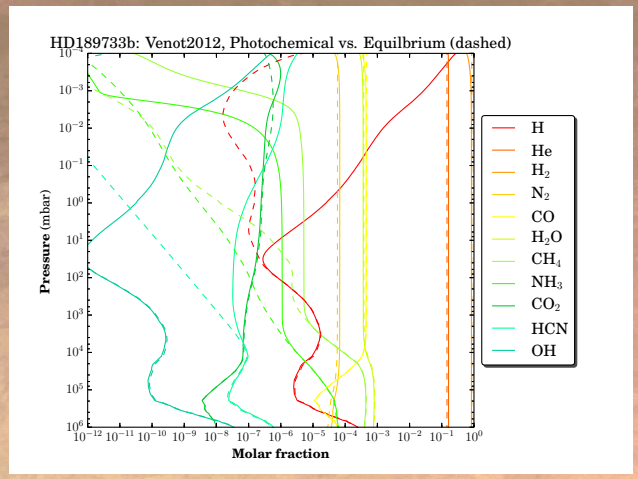


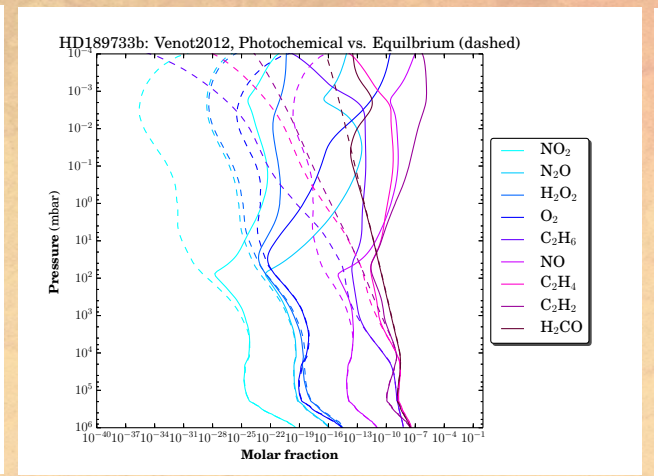
HD189733b

T_{eq} = 1191 K

T(P=1bar) = 2228 K

dG = 1.81 J/mol



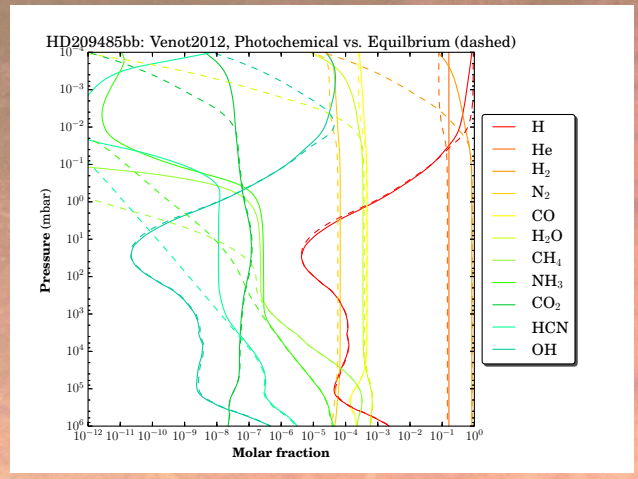


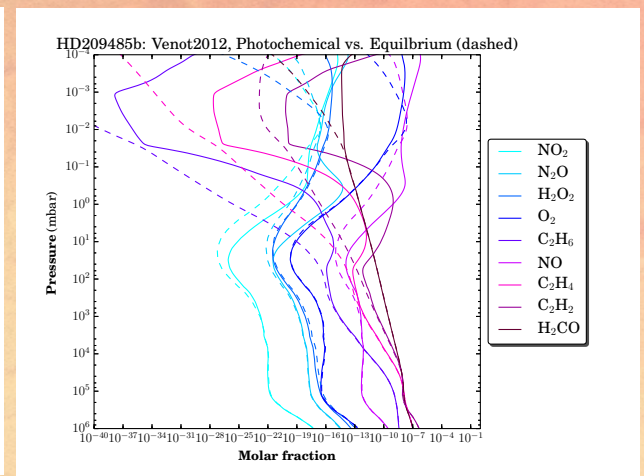
HD209458b

T_{eq} = 1447 K

T(P=1bar) = 2789 K

dG = 0.05 J/mol





DISEQUILIBRIUM

HD97658b

T_{eq} = 757 K

T(P=1bar) = 1927 K

dG = 788 J/mol

HD189733b

T_{eq} = 1191 K

T(P=1bar) = 2228 K

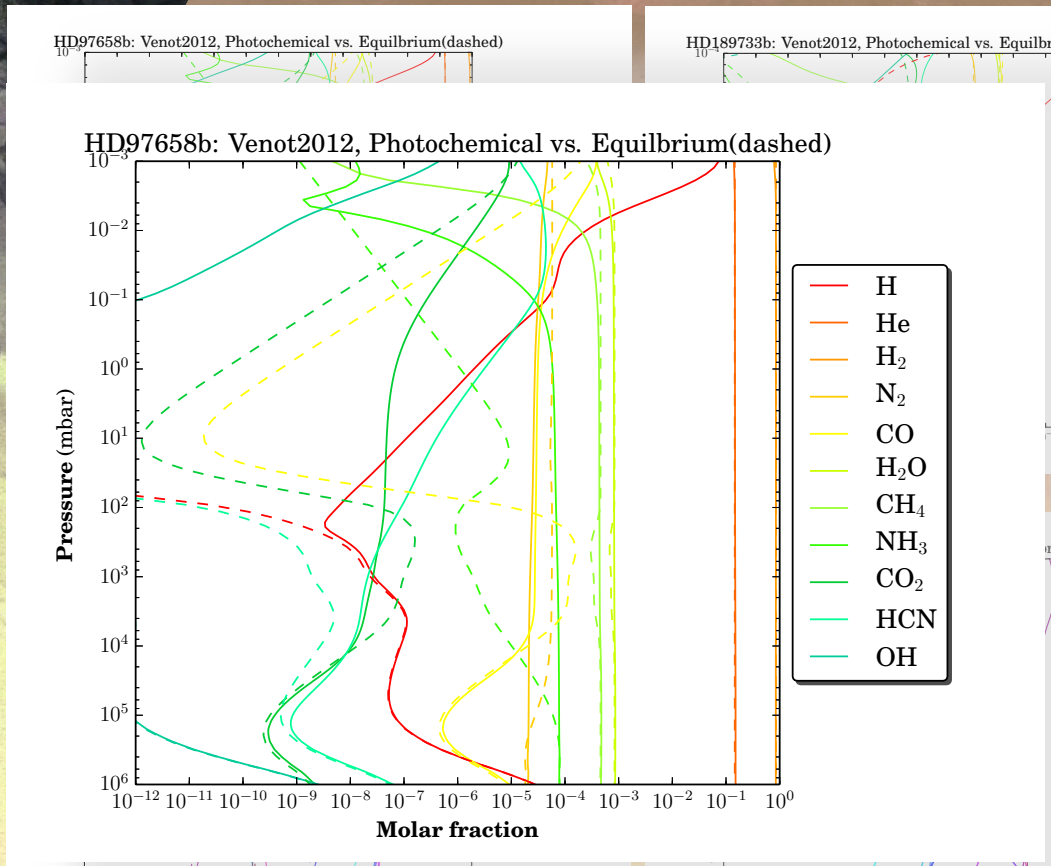
dG = 1.81 J/mol

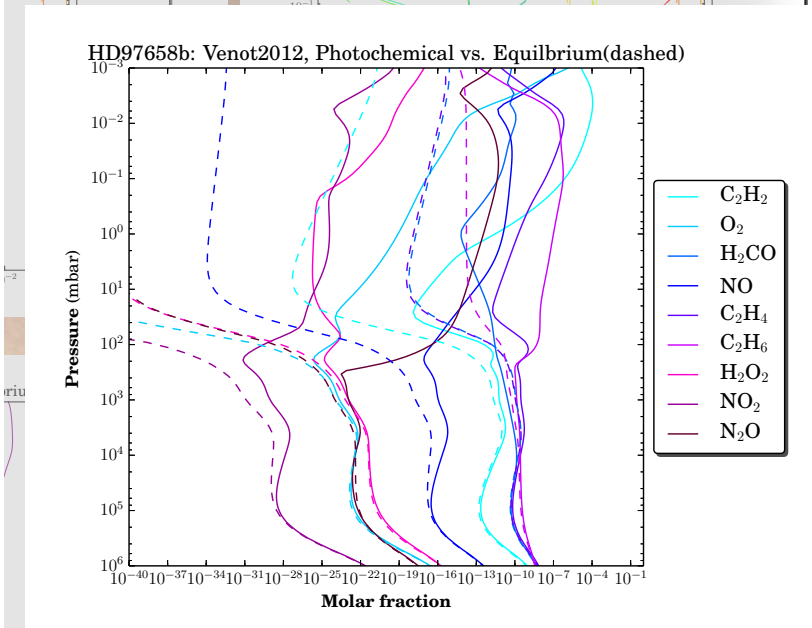
HD209458b

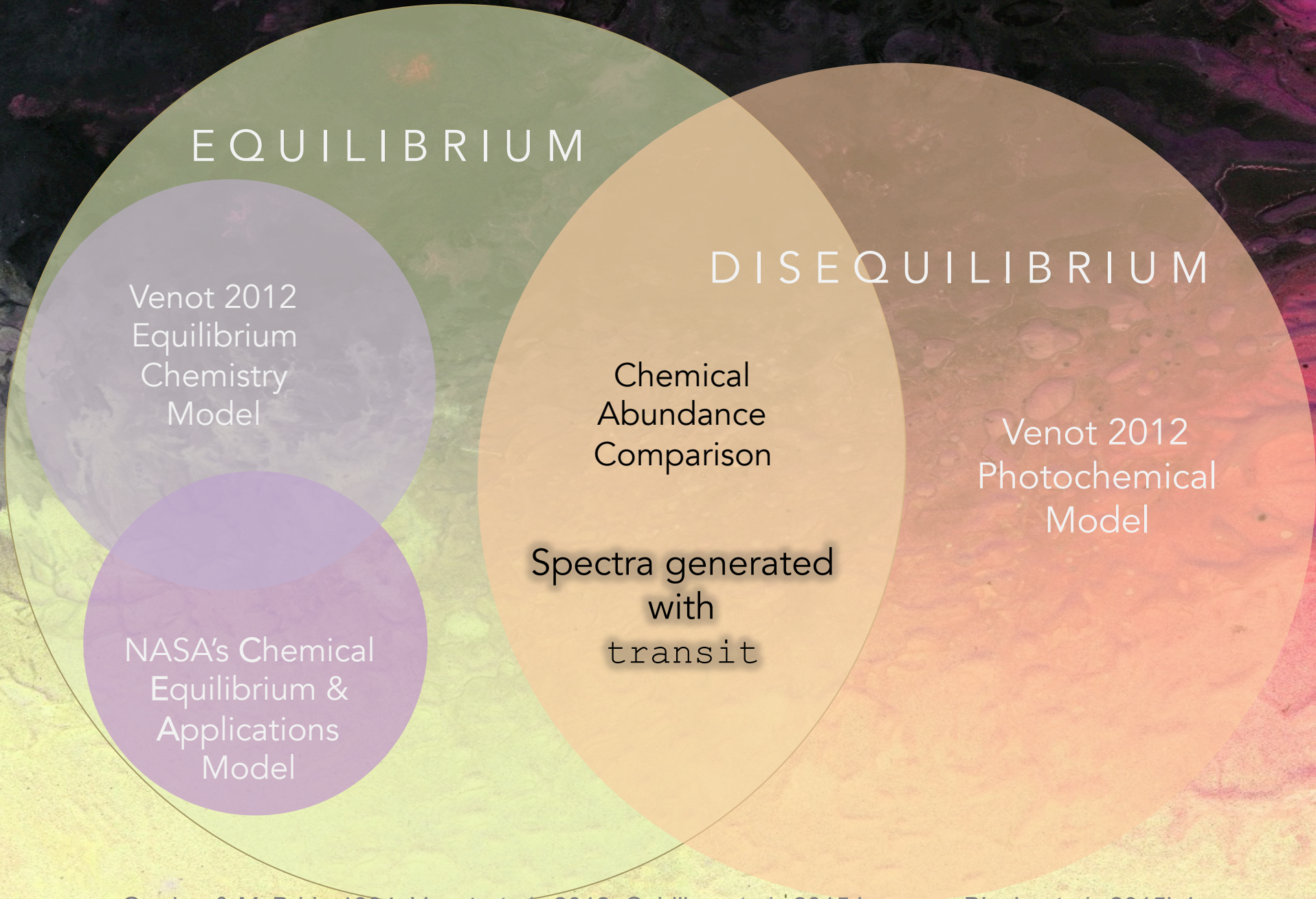
T_{eq} = 1447 K

T(P=1bar) = 2789 K

dG = 0.05 J/mol







Gordon & McBride 1994; Venot *et al*., 2012; Cubillos *et al*., 2015 in prep.; Blecic *et al*., 2015b in prep.; Harrington *et al*., 2015 in prep.; Rojo Thesis 2007

Chemical
Abundance
Comparison

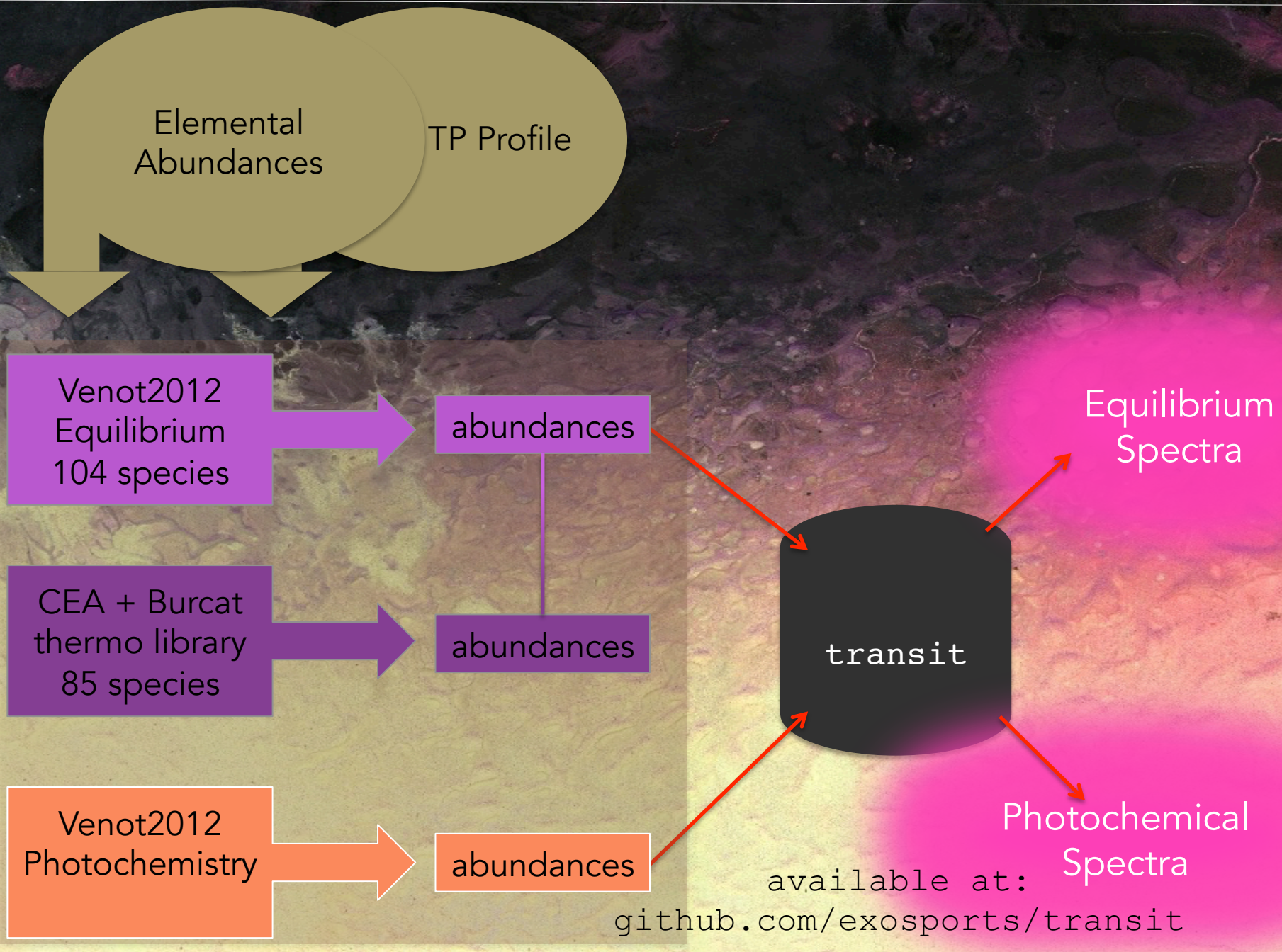
Spectra generated
with
`transit`

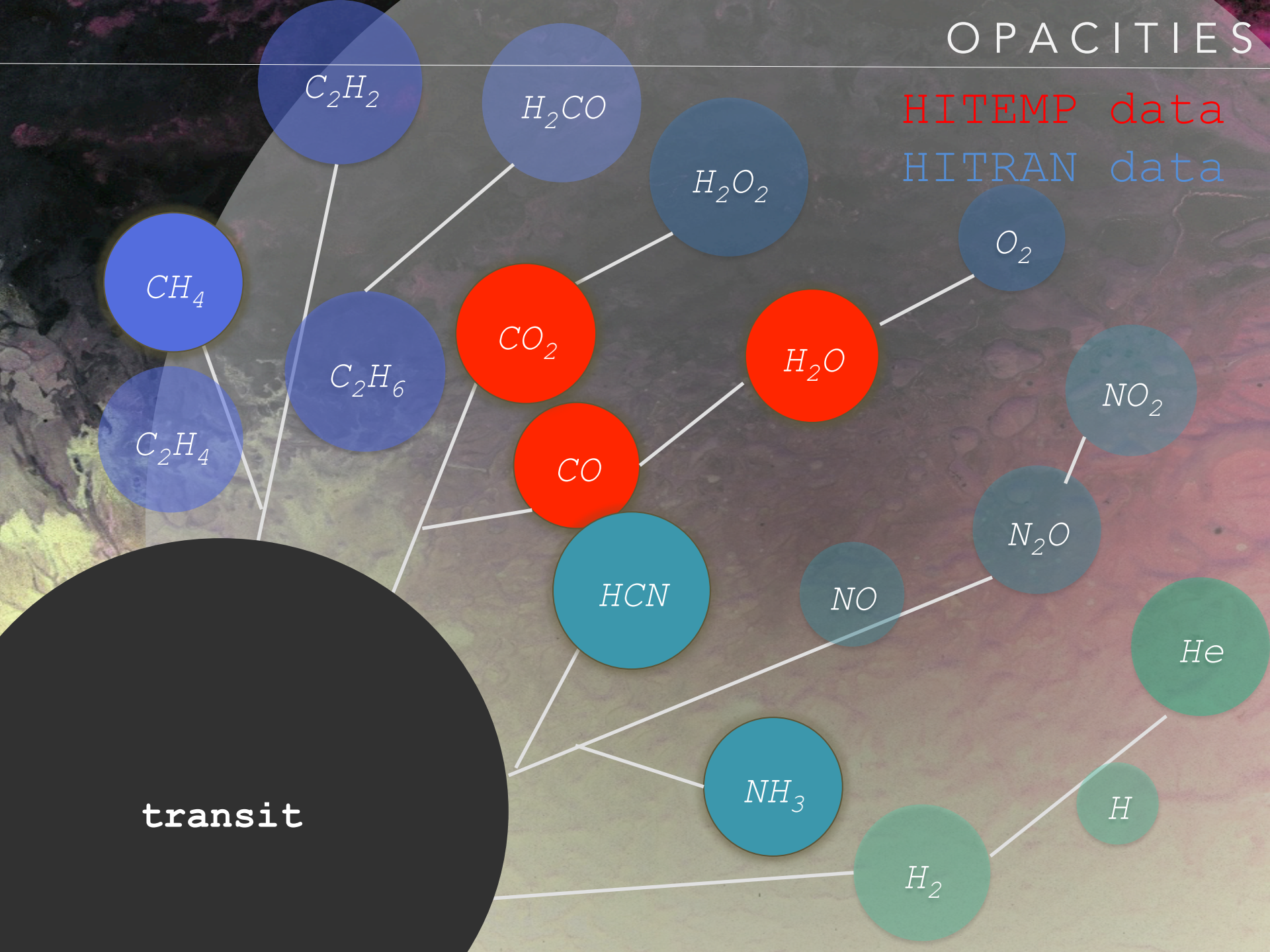
BART

available at:
github.com/exosports/transit

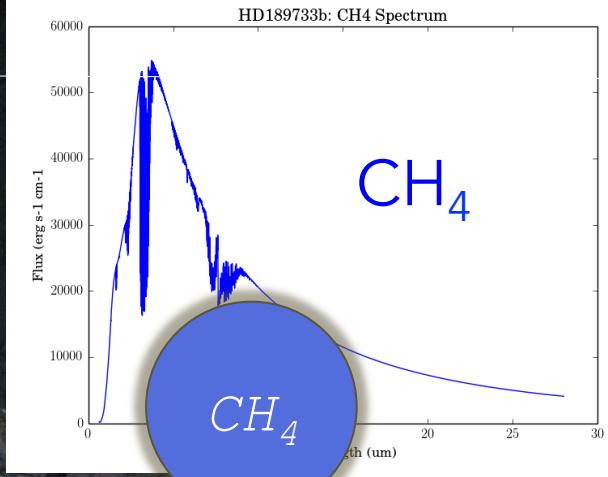
Cubillos *et al*., 2015 in prep; Blecic et al., 2015b in prep; Harrington et al., 2015 in prep.; Rojo Thesis 2007

PIPELINE

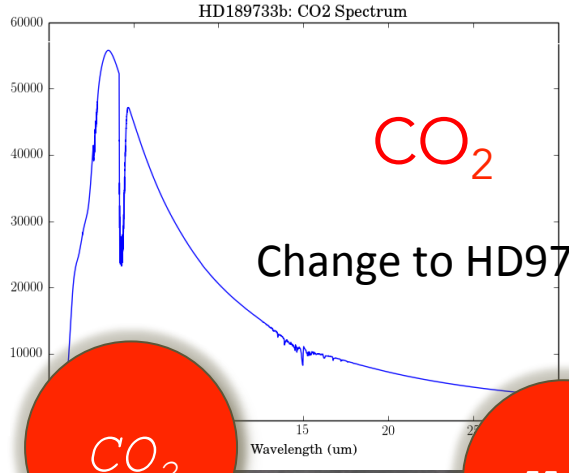

Elemental Abundances
TP Profile
Venot2012 Equilibrium 104 species
abundances
CEA + Burcat thermo library 85 species
abundances
Venot2012 Photochemistry
abundances
transit
Equilibrium Spectra
Photochemical Spectra
available at:
github.com/exosports/transit


OPACITIES
HITEMP data
HITRAN data
C_2H_2
H_2CO
H_2O_2
O_2
CH_4
CO_2
C_2H_6
H_2O
NO_2
C_2H_4
CO
N_2O
HCN
NO
He
NH_3
H
H_2
transit

HD189733b

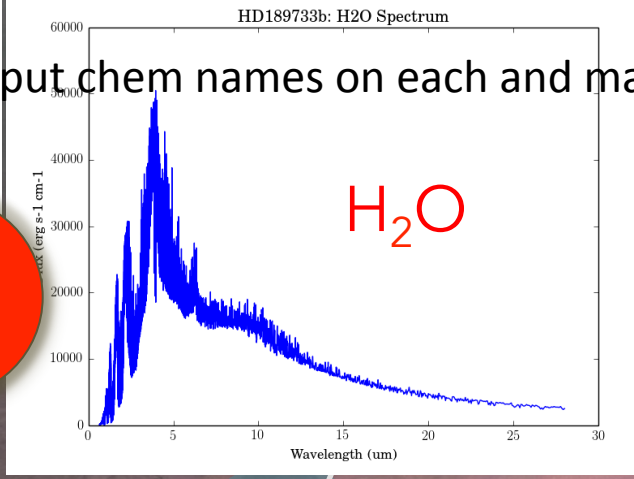


CH_4

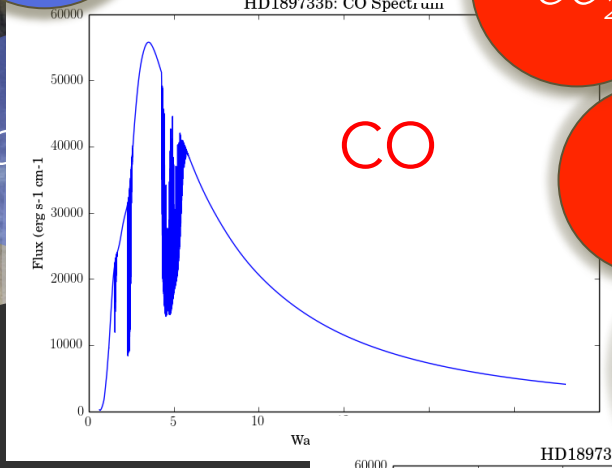


CO_2

Change to HD976; put chem names on each and ma



H_2O



CO

CO_2

H_2O

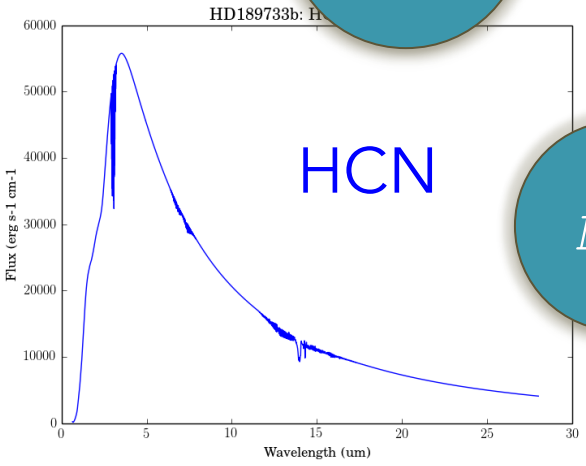
CO

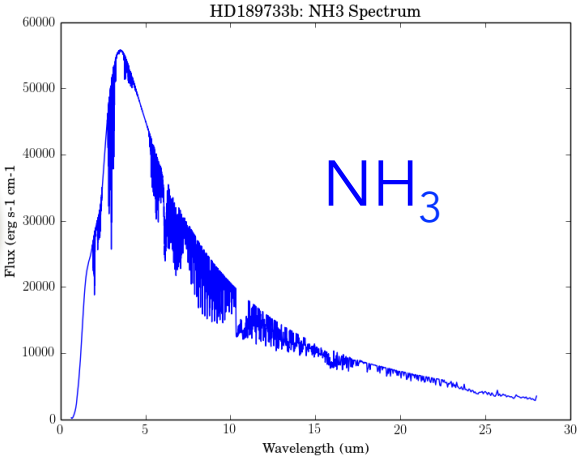
HCN

N_2O

NO

NH_3

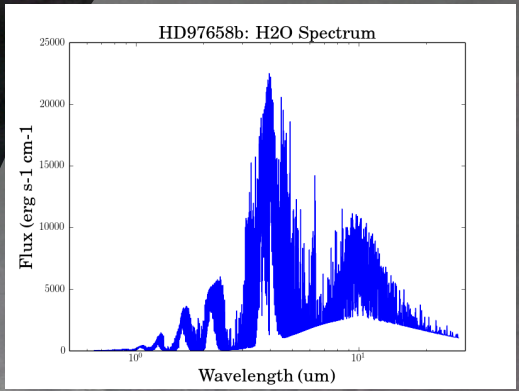


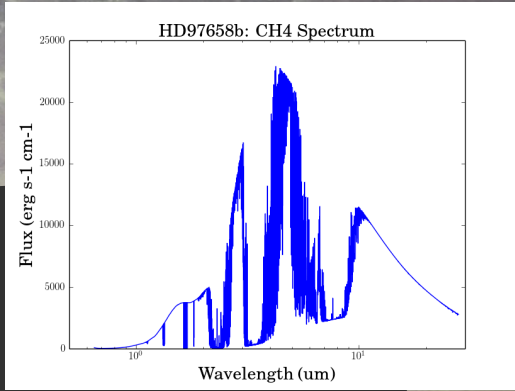


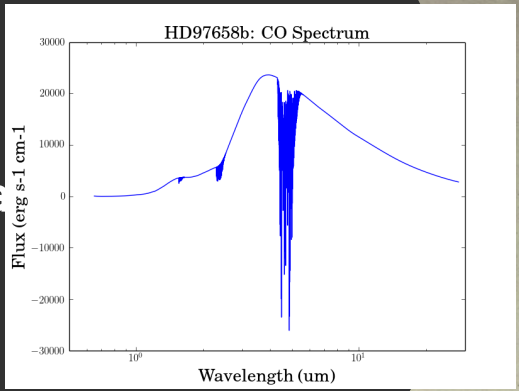
transit

HD97658b

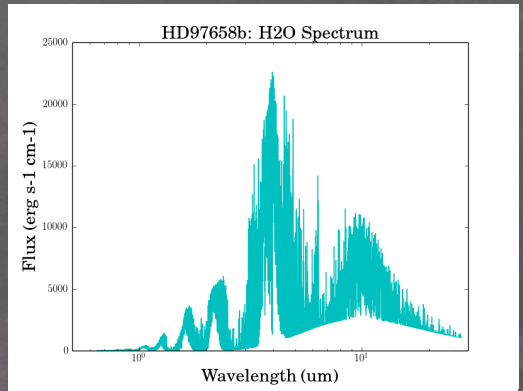
Equilibrium

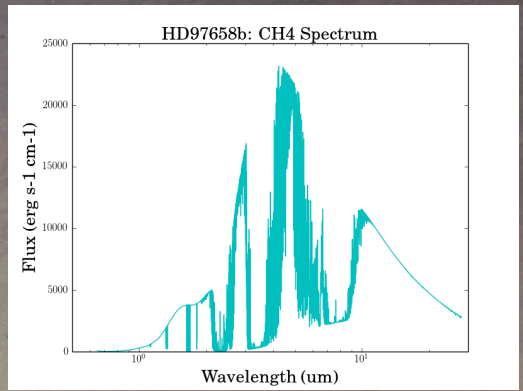


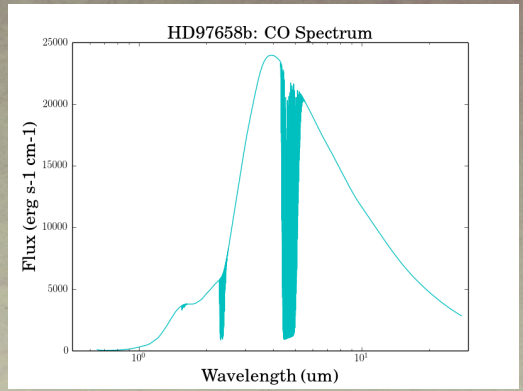


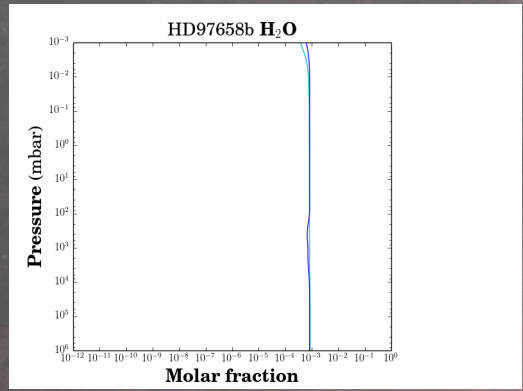


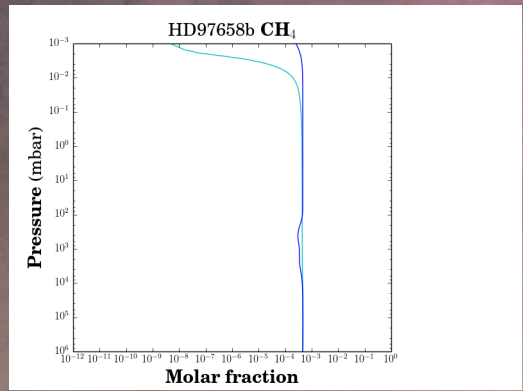
Disequilibrium

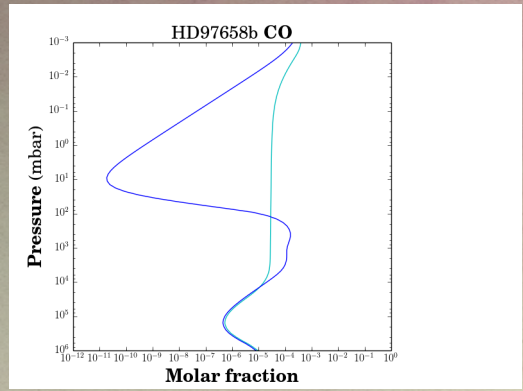








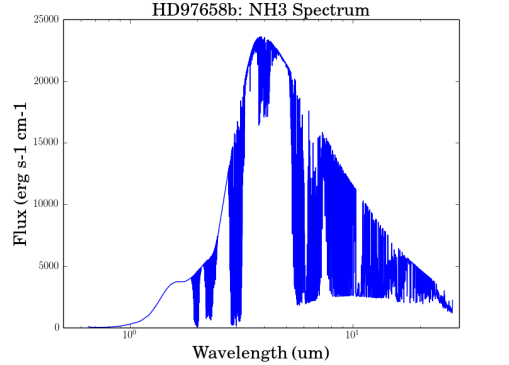




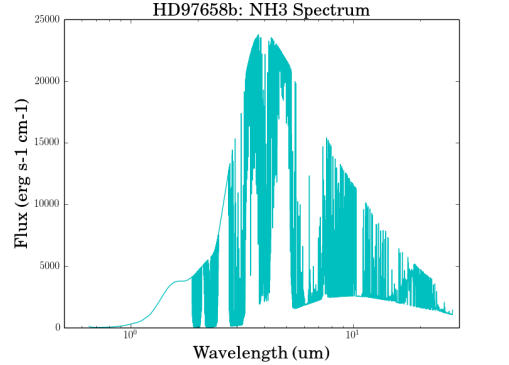
tra

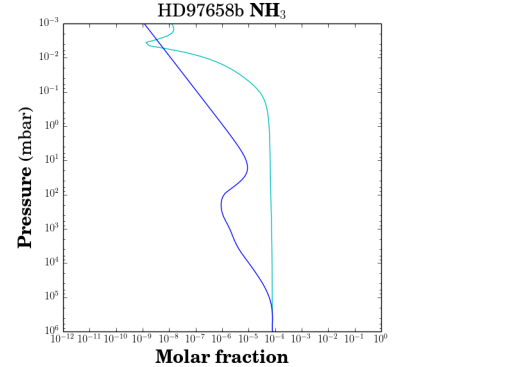
HD97658b

Equilibrium



Disequilibrium





Sulfur- and Phosphorus-containing species?

High-Temperature Experimental Data for Better Line Lists?

transit

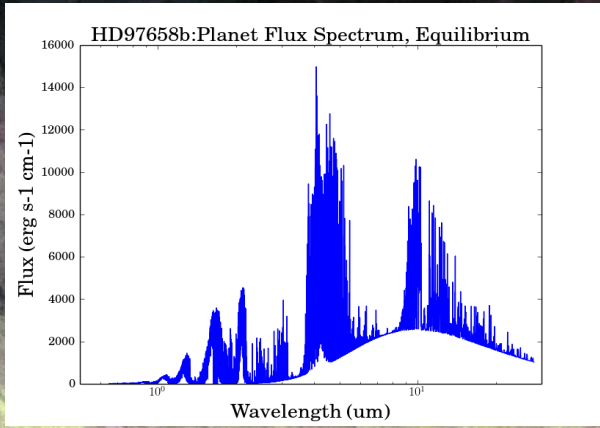
H_2O CO CO_2 CH_4

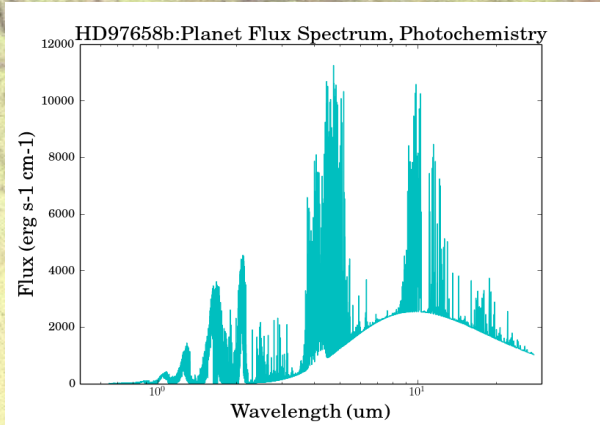
Zahnle *et al*. 2009; Rothman *et al*. 2010; Rothman *et al*. 1995; Fleckl *et al*. 2015; Hargreaves *et al*. 2015

SPECTRA : ECLIPSE, $Flux_{planet}$

HD97658b

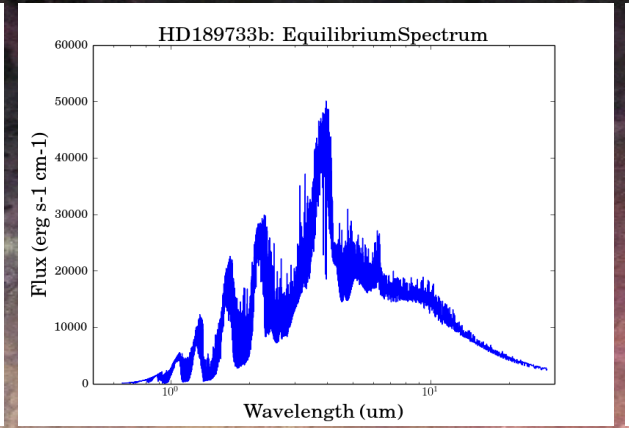
T_{eq} = 757 K

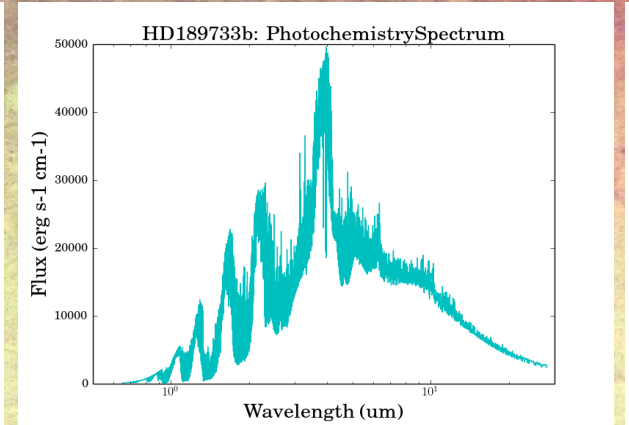




HD189733b

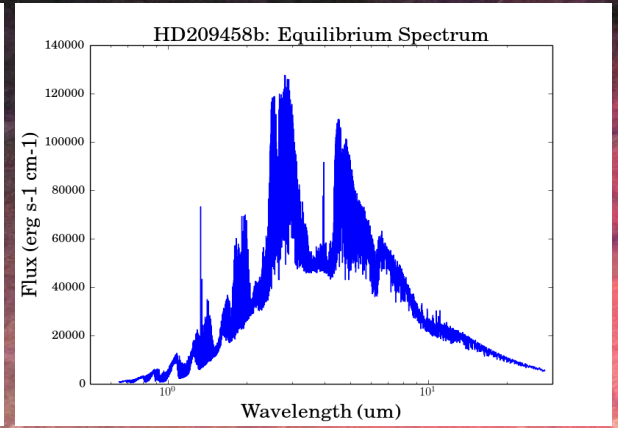
T_{eq} = 1191 K

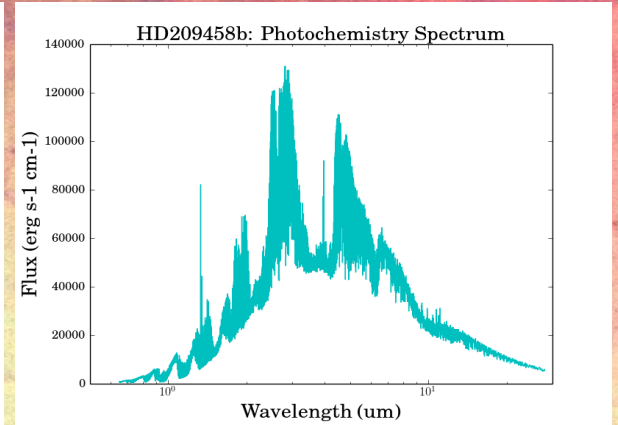




HD209458b

T_{eq} = 1447 K

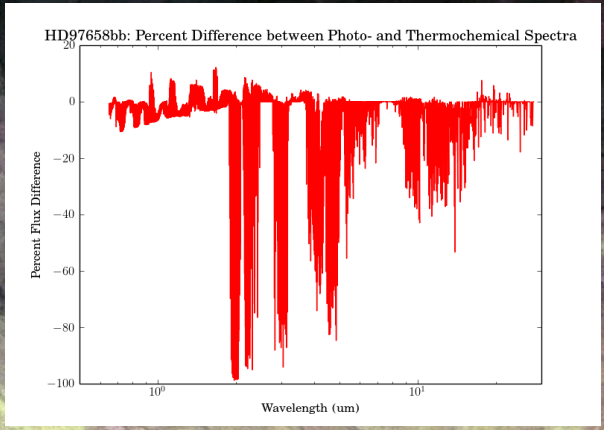


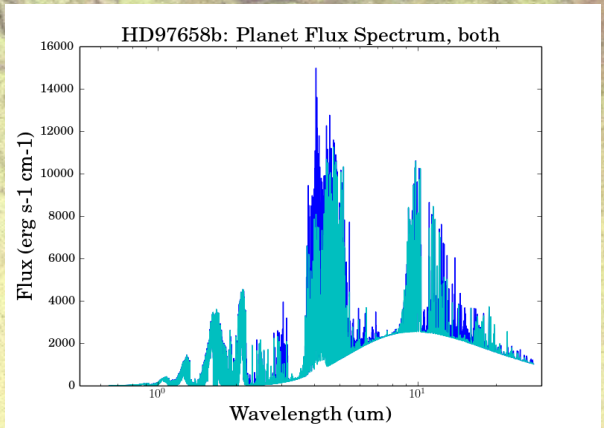


SPECTRA : ECLIPSE, $Flux_{planet}$

HD97658b

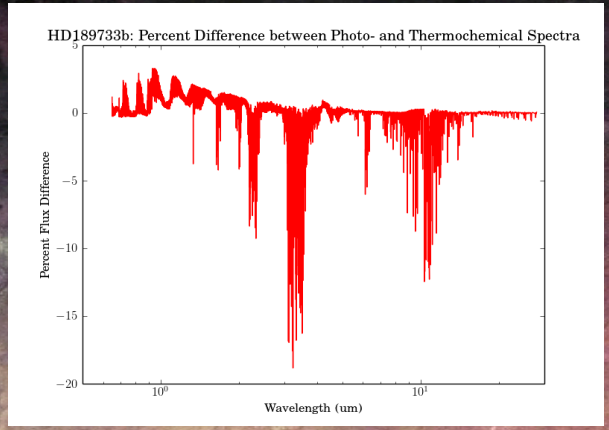
T_{eq} = 757 K

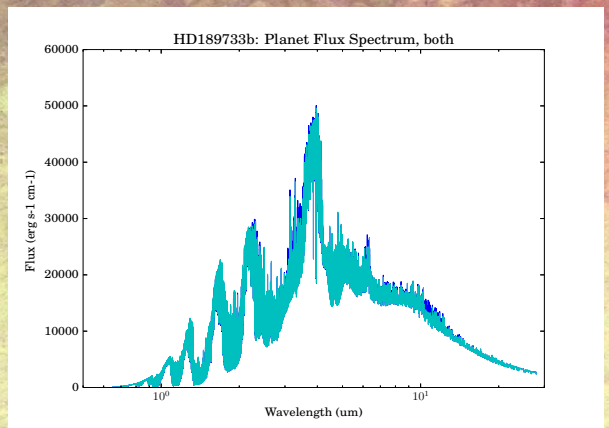




HD189733b

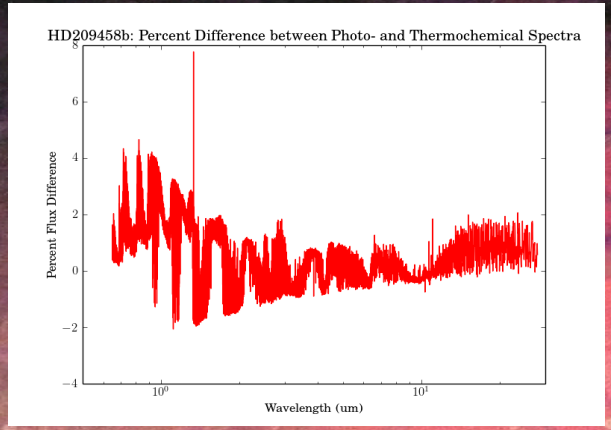
T_{eq} = 1191 K

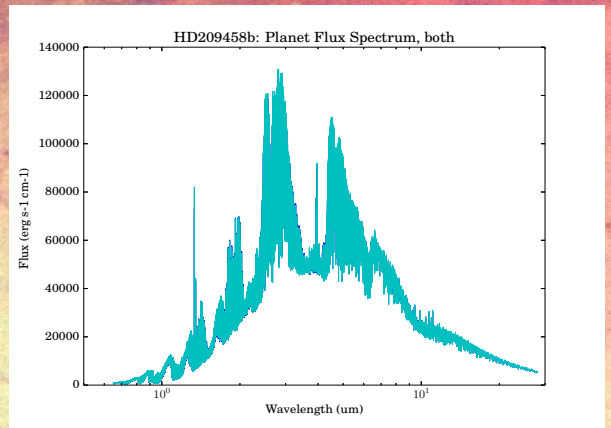




HD209458b

T_{eq} = 1447 K

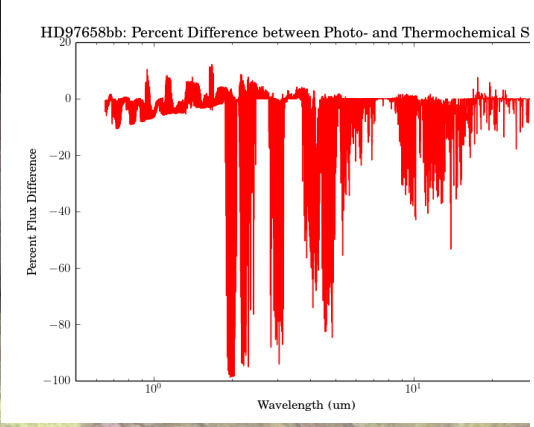


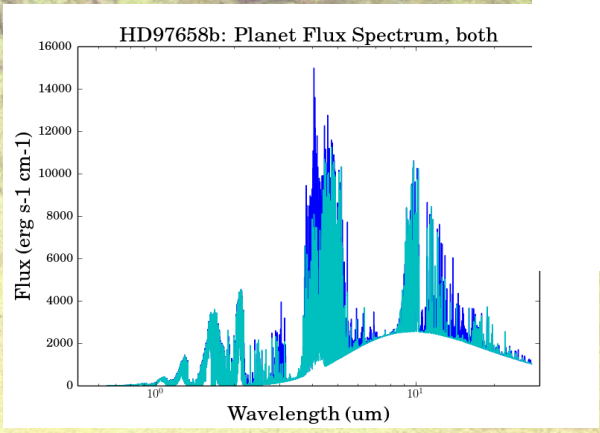


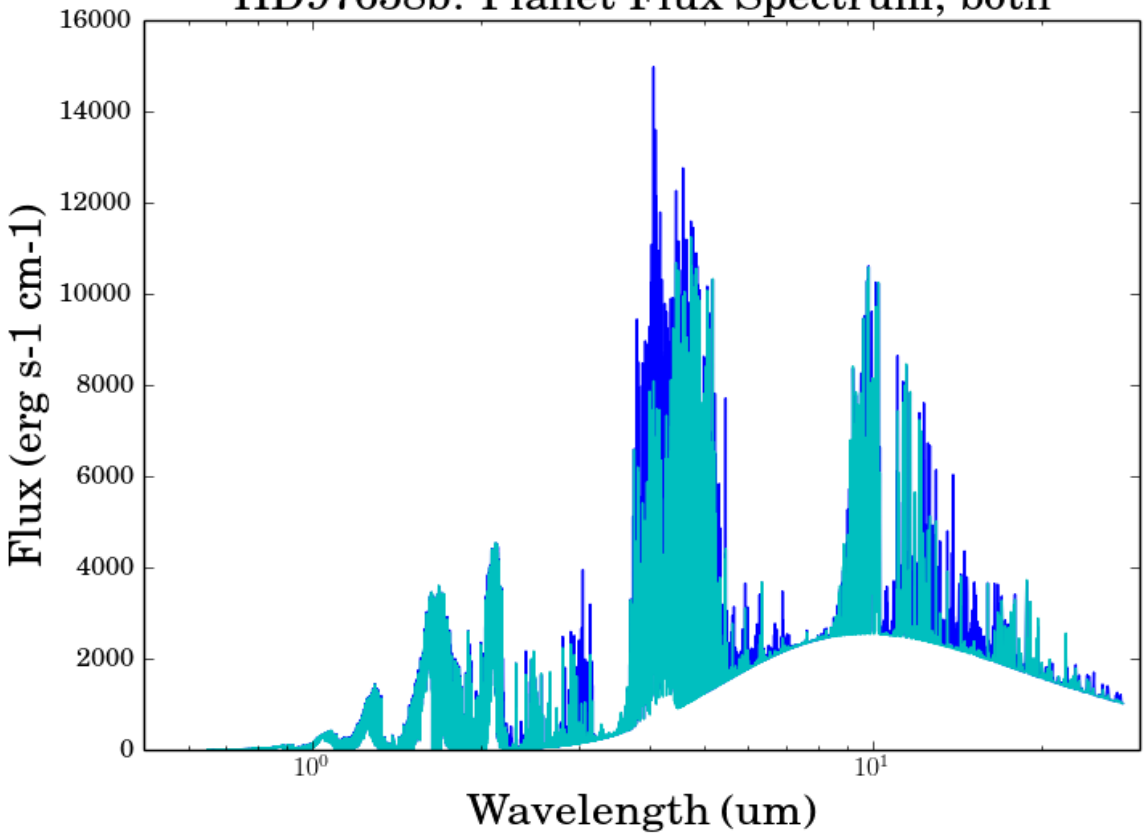
SPECTRA : ECLIPSE, $Flux_{planet}$

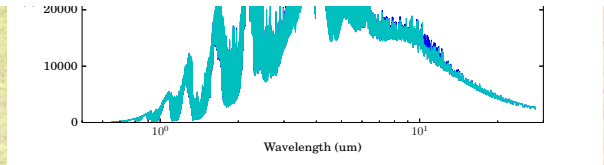
HD97658b

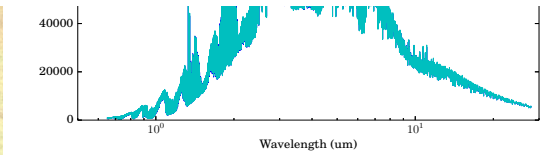
T_{eq} = 757 K







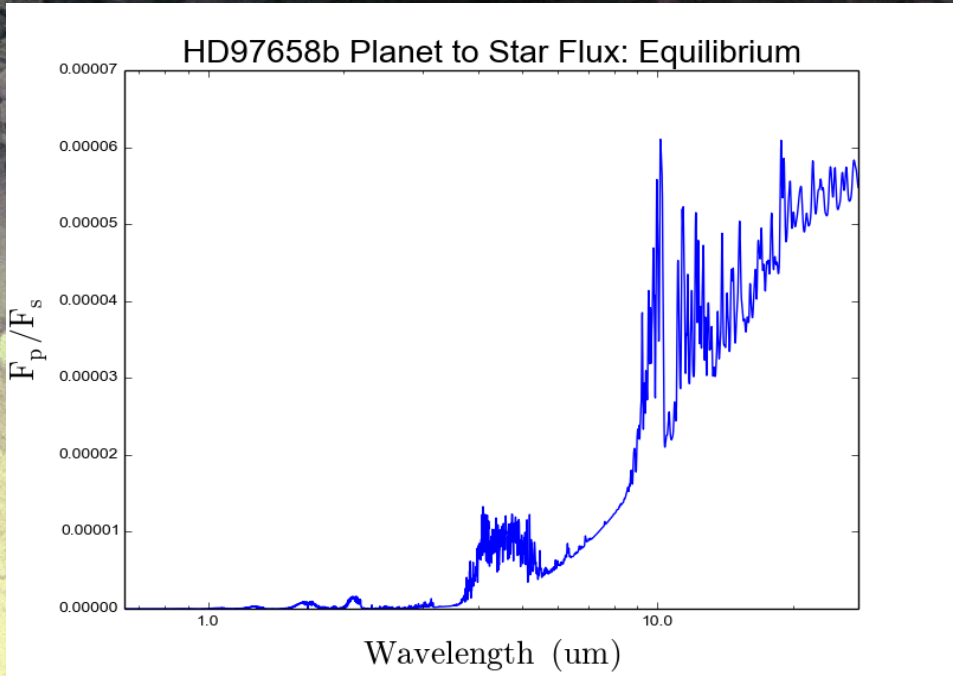


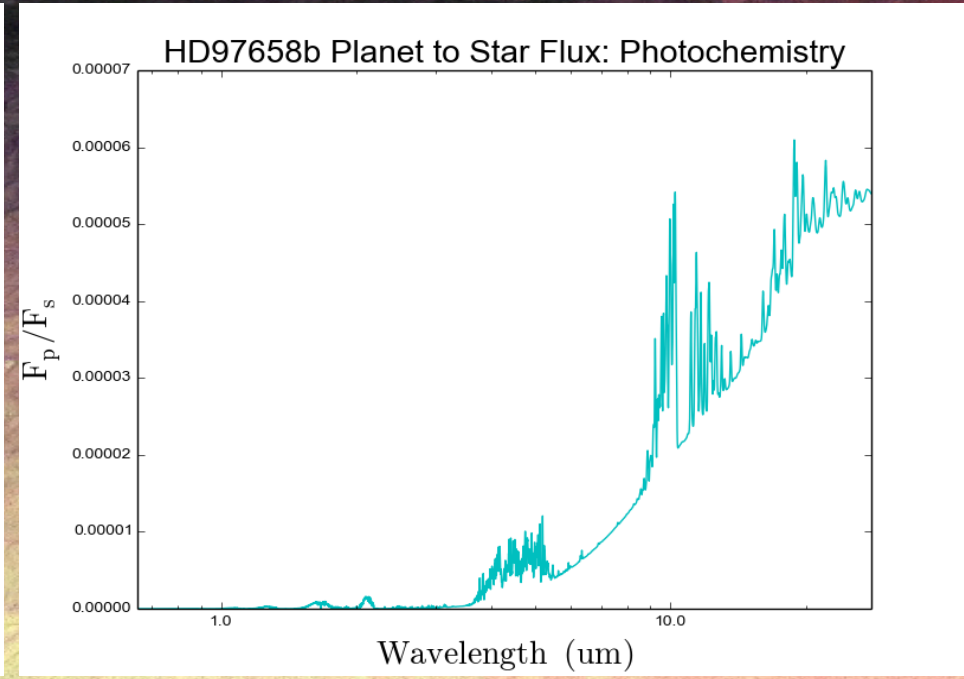


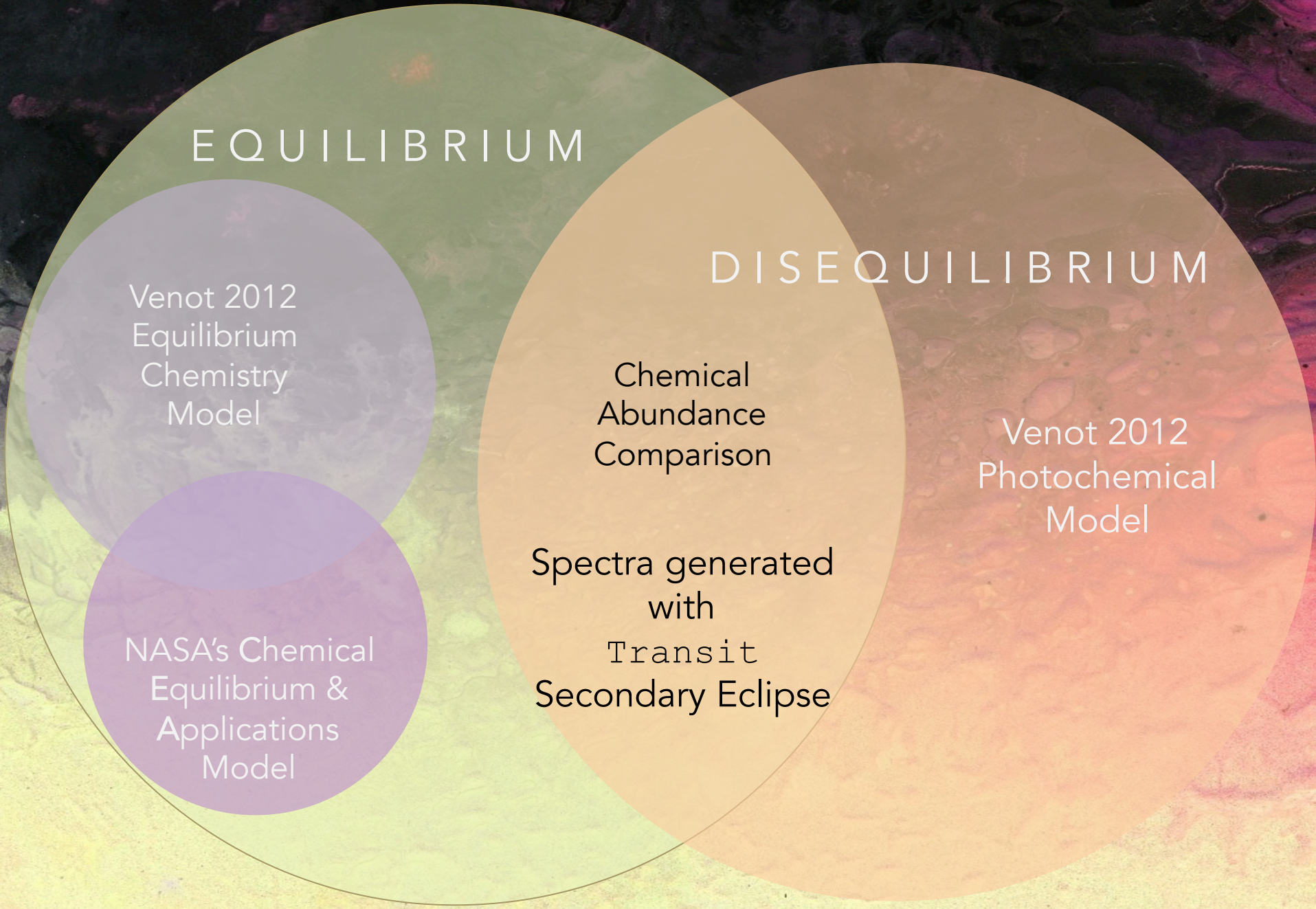
SPECTRA : ECLIPSE, $F_{planet} : F_{star}$

HD97658b

T_{eq} = 757 K






EQUILIBRIUM
Venot 2012 Equilibrium Chemistry Model
NASA's Chemical Equilibrium & Applications Model
DISEQUILIBRIUM
Venot 2012 Photochemical Model
Chemical Abundance Comparison
Spectra generated with
Transit
Secondary Eclipse

P

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EQUILIBRIUM

DISEQUILIBRIUM

Venot 2012 Equilibrium Chemistry Model

Thermochemical Equilibrium Abundances (TEA)

NASA's Chemical Equilibrium & Applications Model (CEA)

available at:
github.com/dzesmin/TEA

Chemical Abundance Comparison

more

CH_4

Spectra generated with

Transit

Secondary Eclipse

+ Transit

Venot 2012 Photochemical Model

open- source Photochemical Model?