Workshop Exoplanetary Atmospheres and Habitability
Nice - 15th October 2015

Disequilibrium chemistry and stellar flares in exoplanet atmospheres

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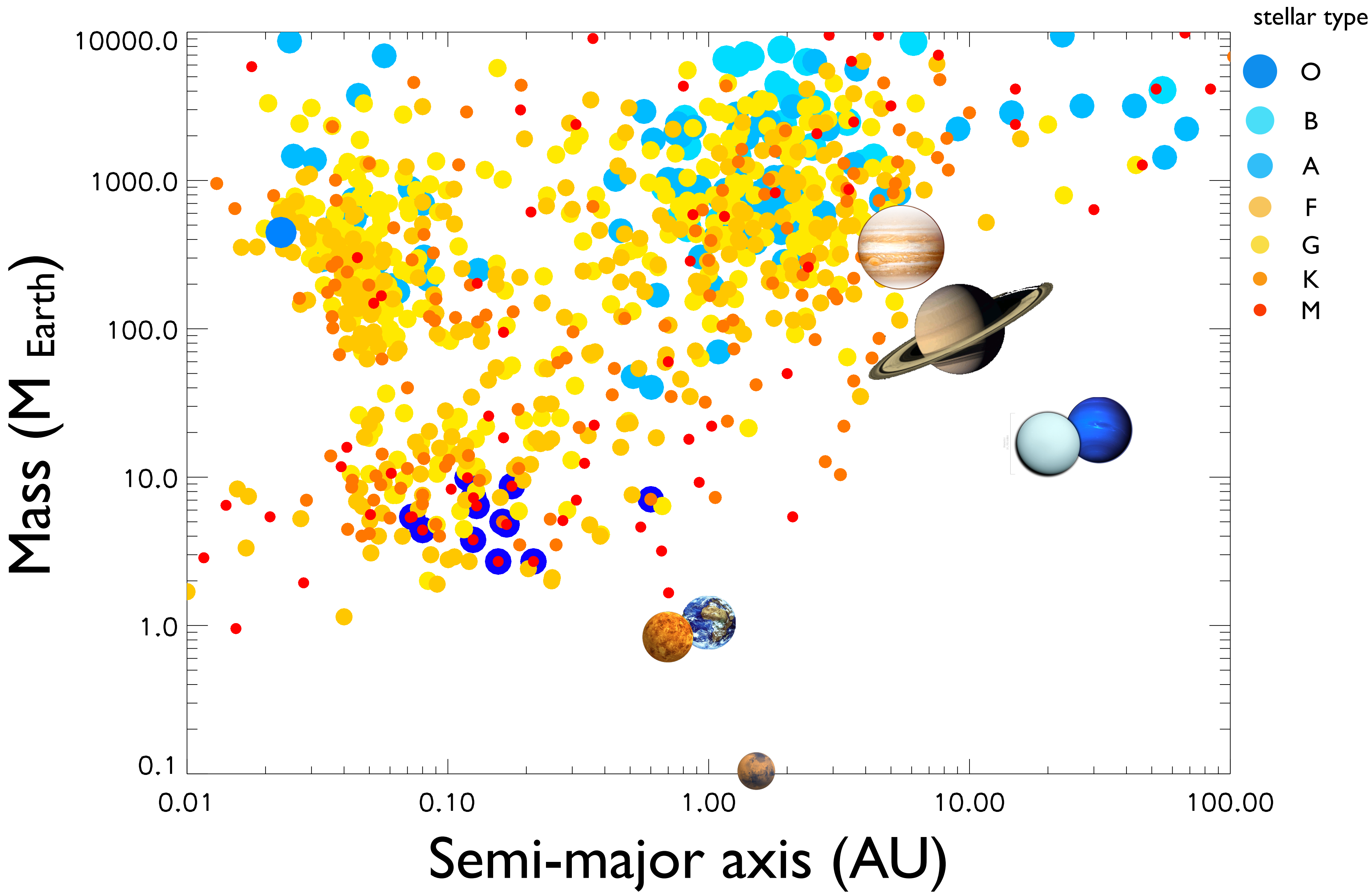
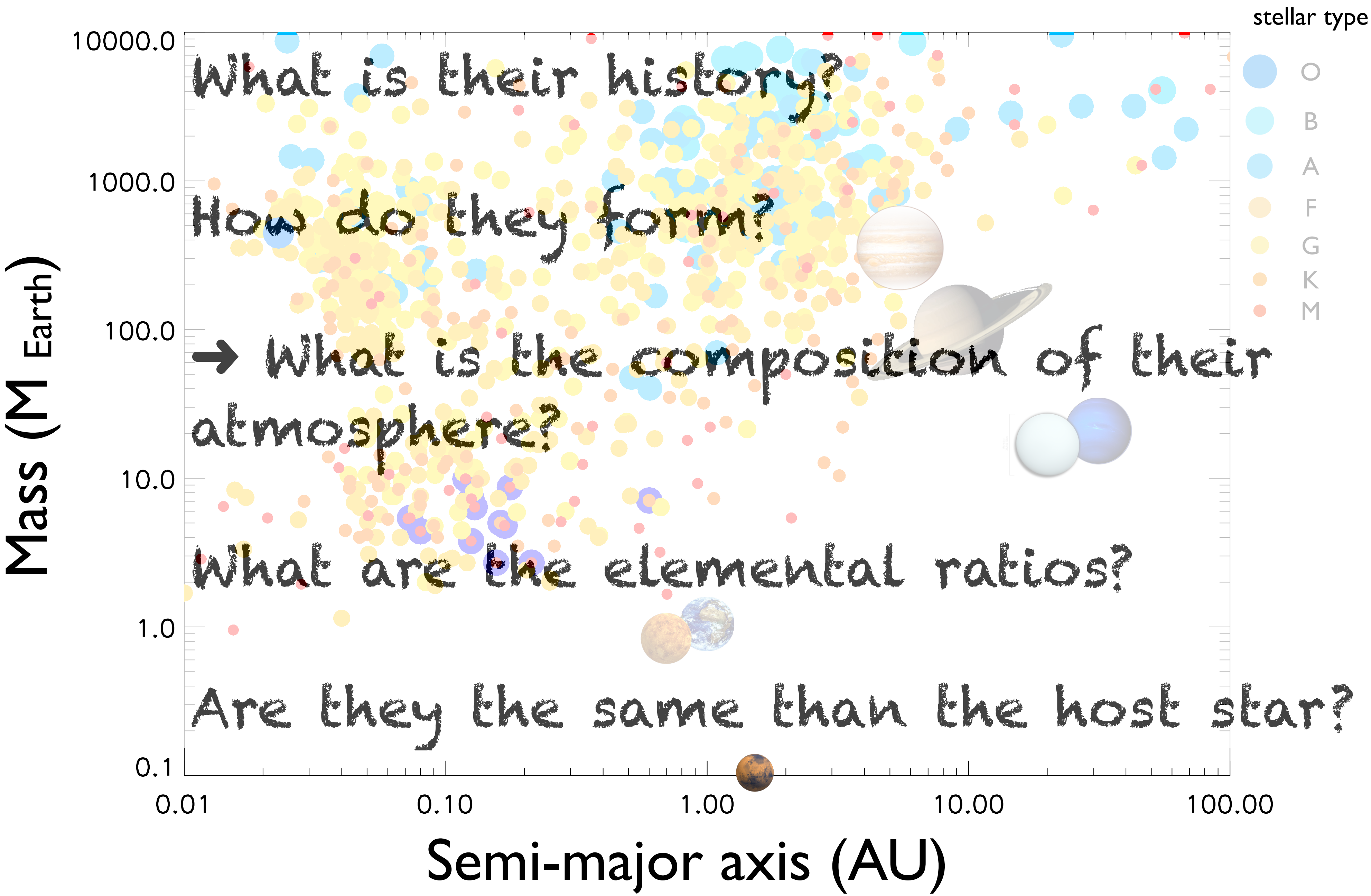
NASA, ESA, and G. Bacon (STScI)



1962 exoplanets

source : exoplanet.eu (30 September 2015)



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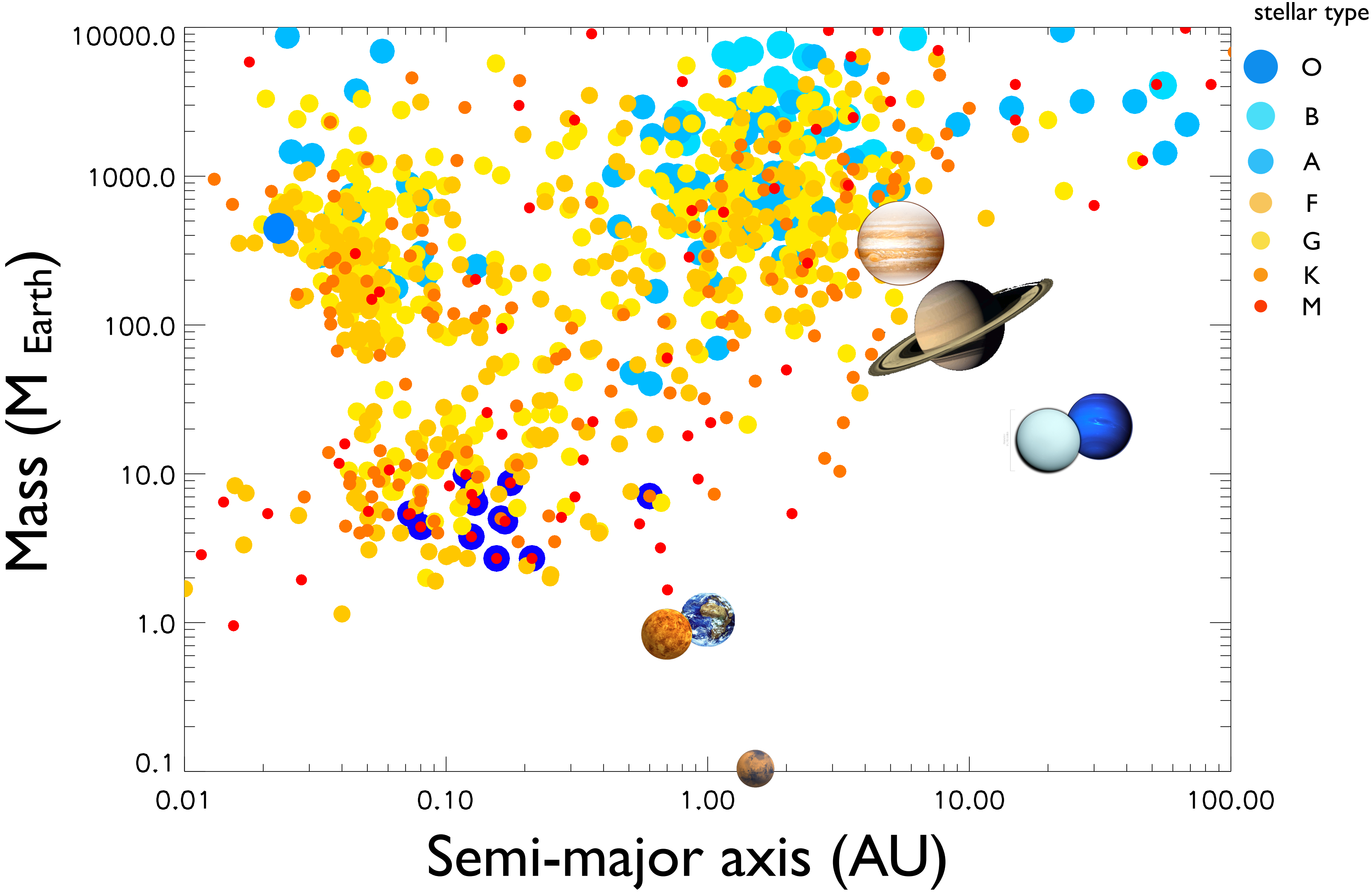

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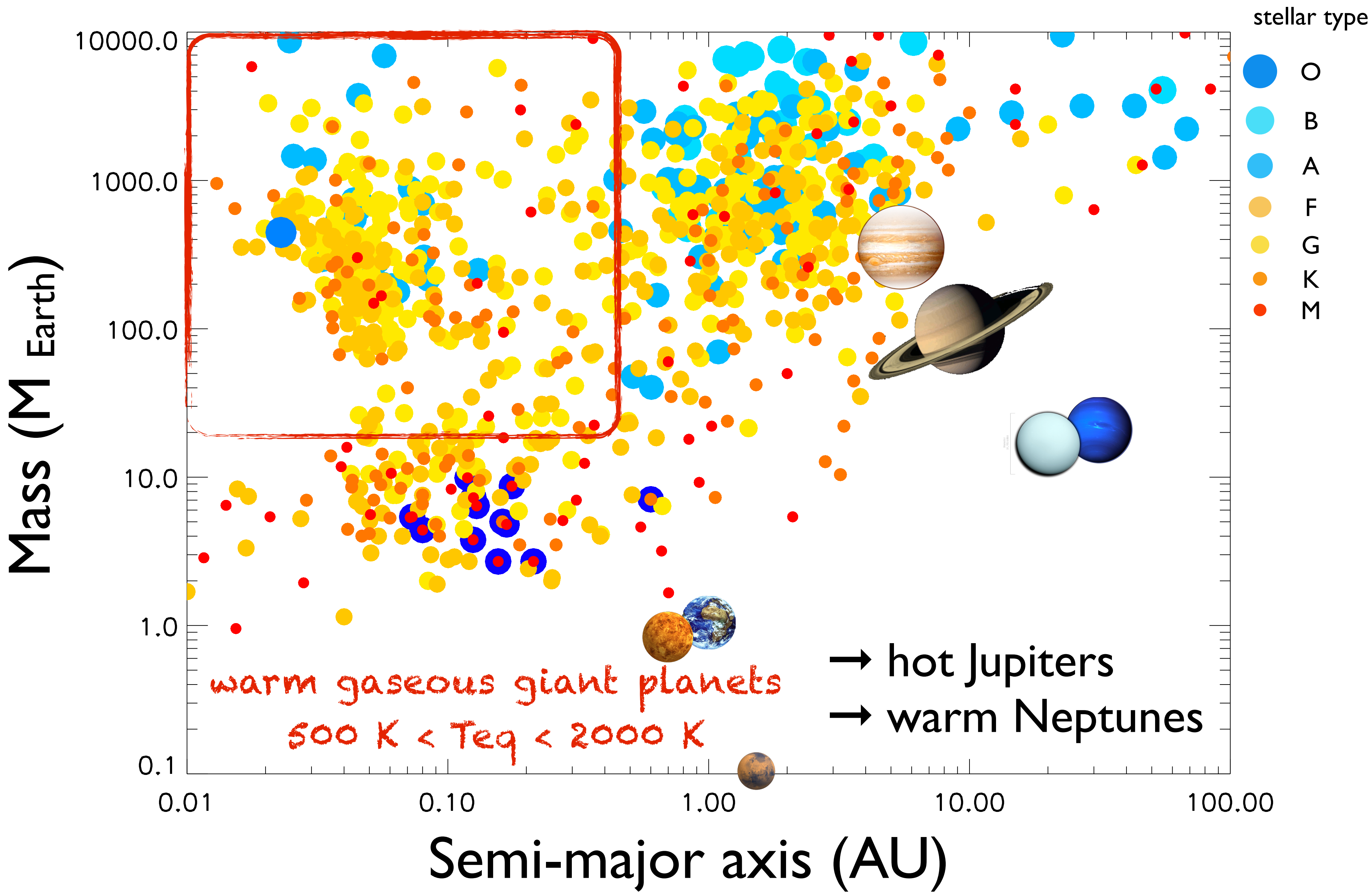

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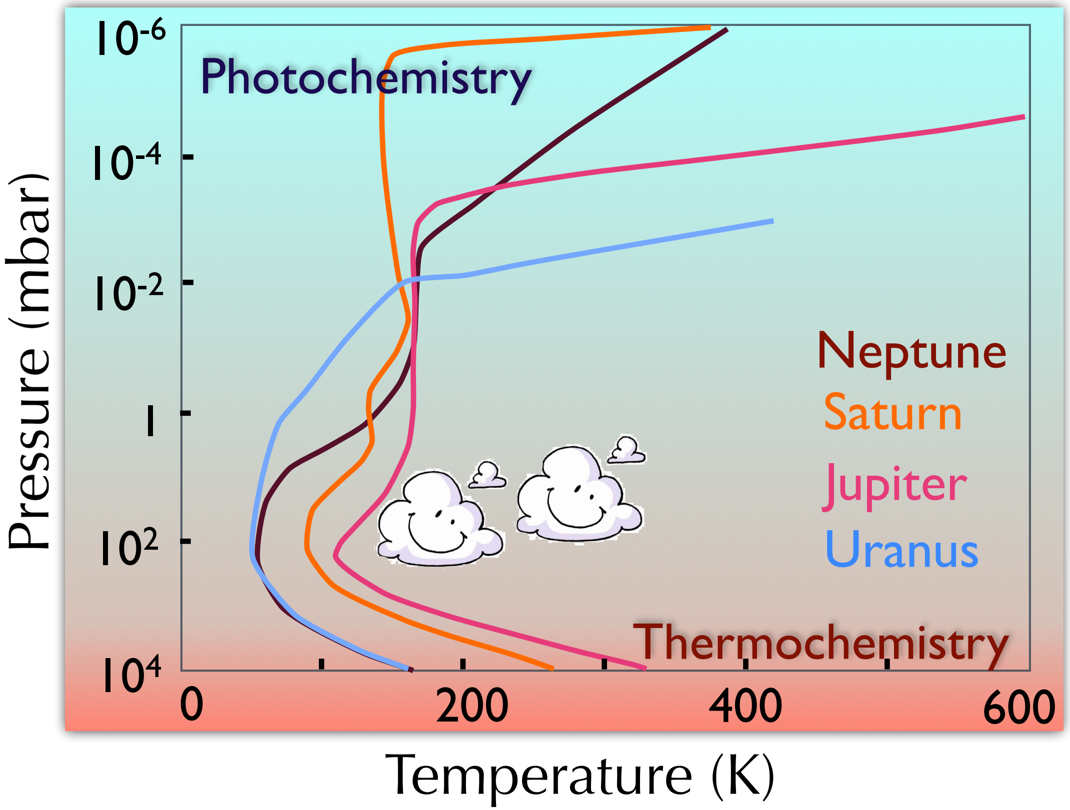
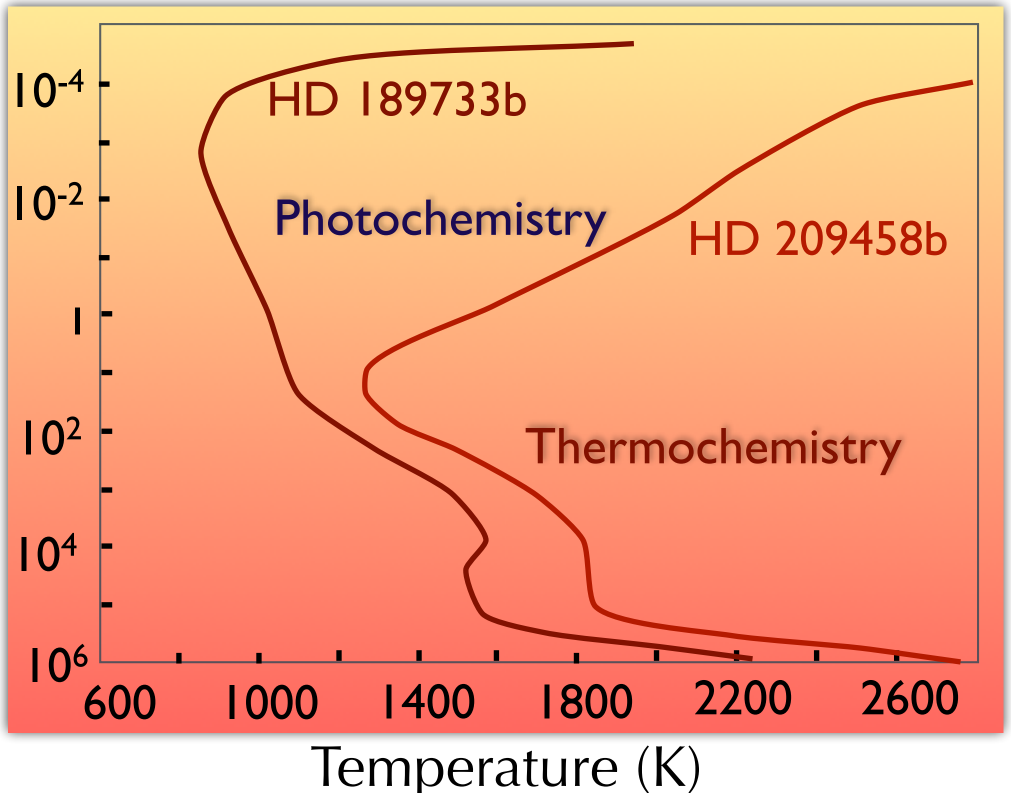
Access to elementary abundances



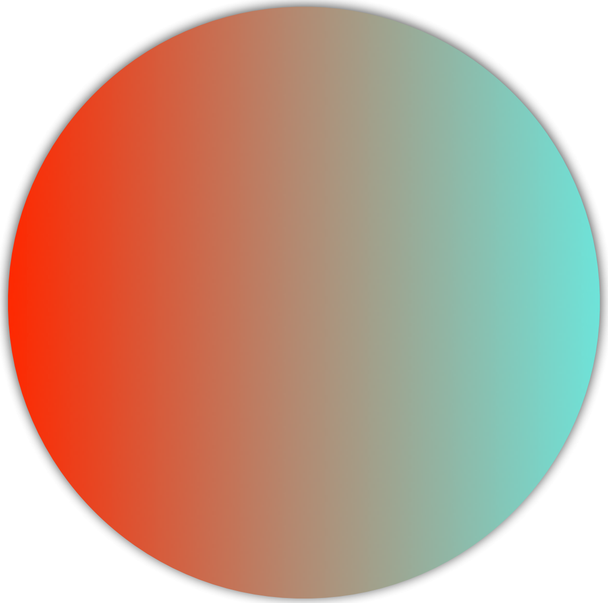


cold trap: condensation
➔ no access to the deep atmosphere

hot temperatures: no condensation
➔ access to the deep atmosphere

Out of equilibrium processes

Thermochemical equilibrium:
depends on P, T,
elementary abundances



Out of equilibrium processes

Thermochemical equilibrium:
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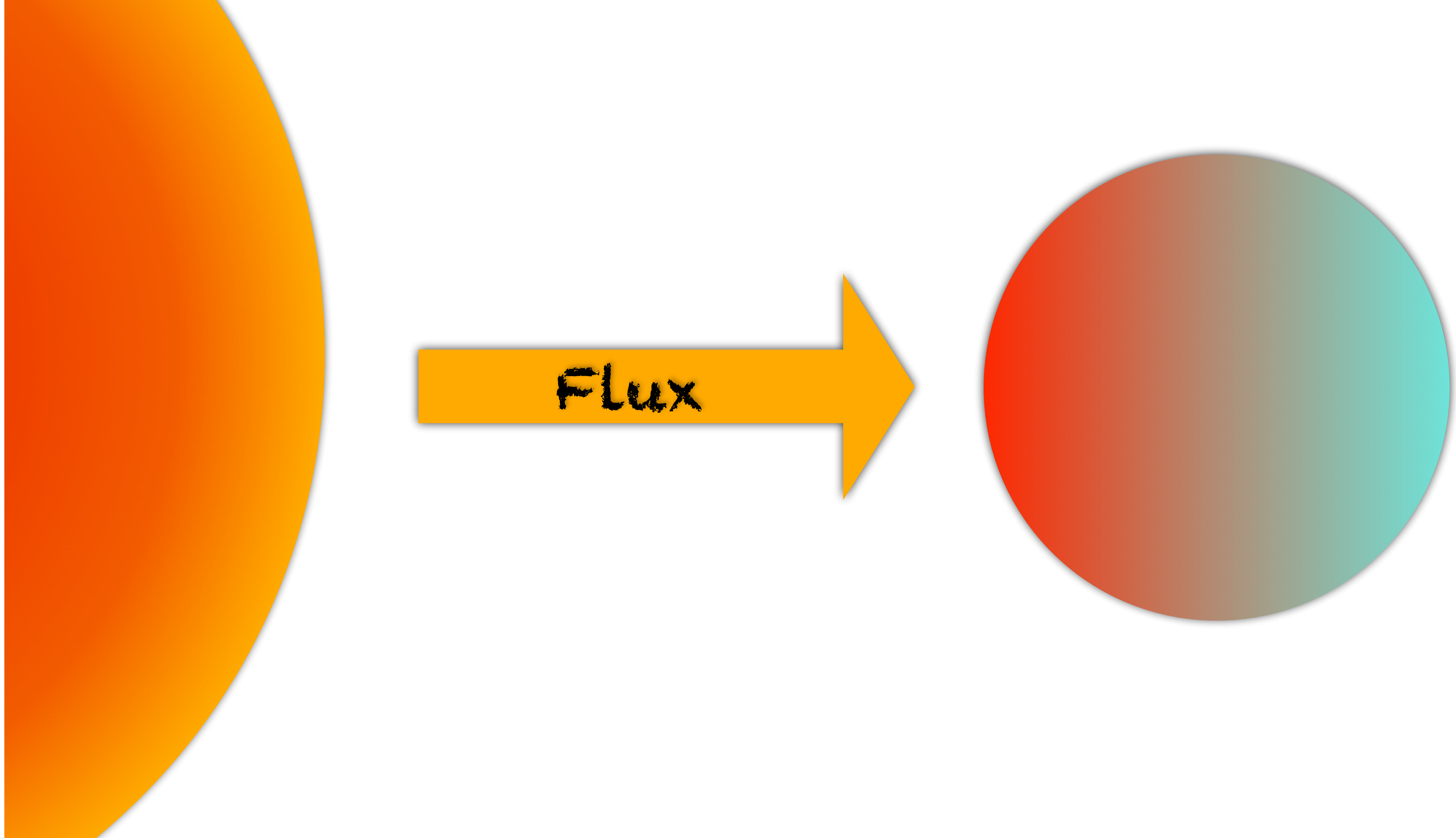
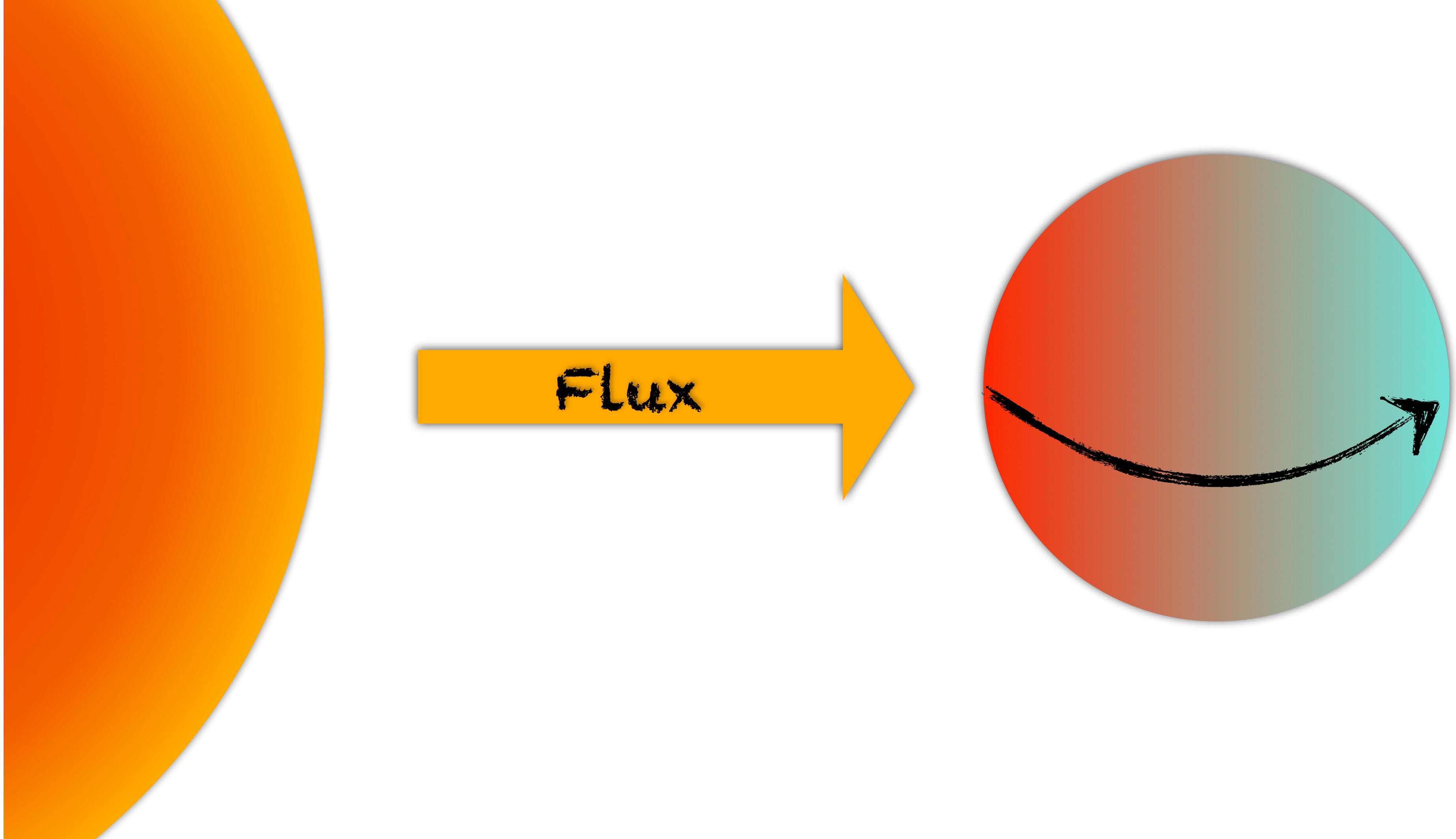


Out of equilibrium processes

Thermochemical equilibrium:
depends on P, T,
elementary abundances

1. Photodissociations
2. Horizontal circulation (winds)



Out of equilibrium processes

Thermochemical equilibrium:
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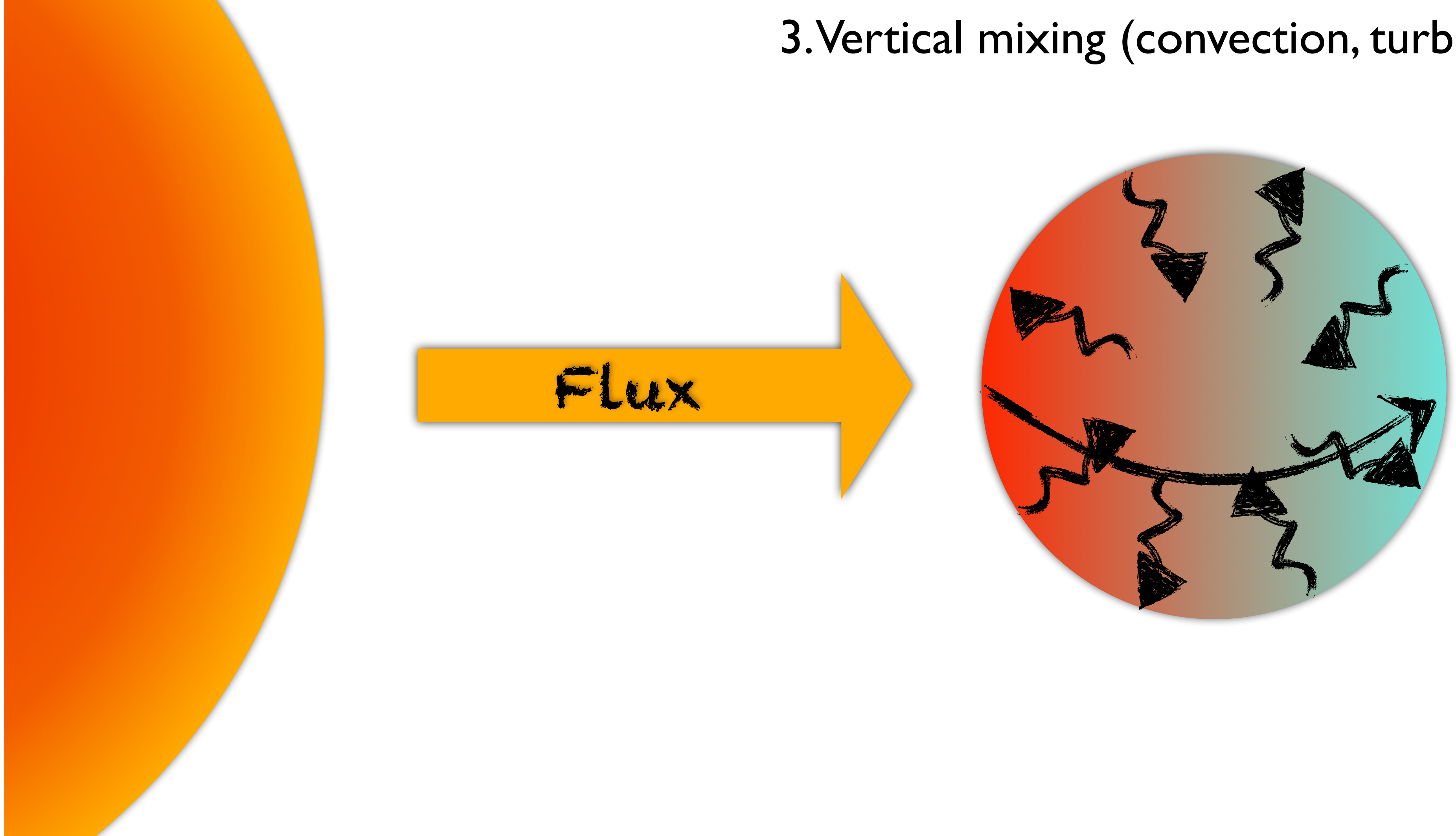
1. Photodissociations
2. Horizontal circulation (winds)
3. Vertical mixing (convection, turbulence)



Out of equilibrium processes

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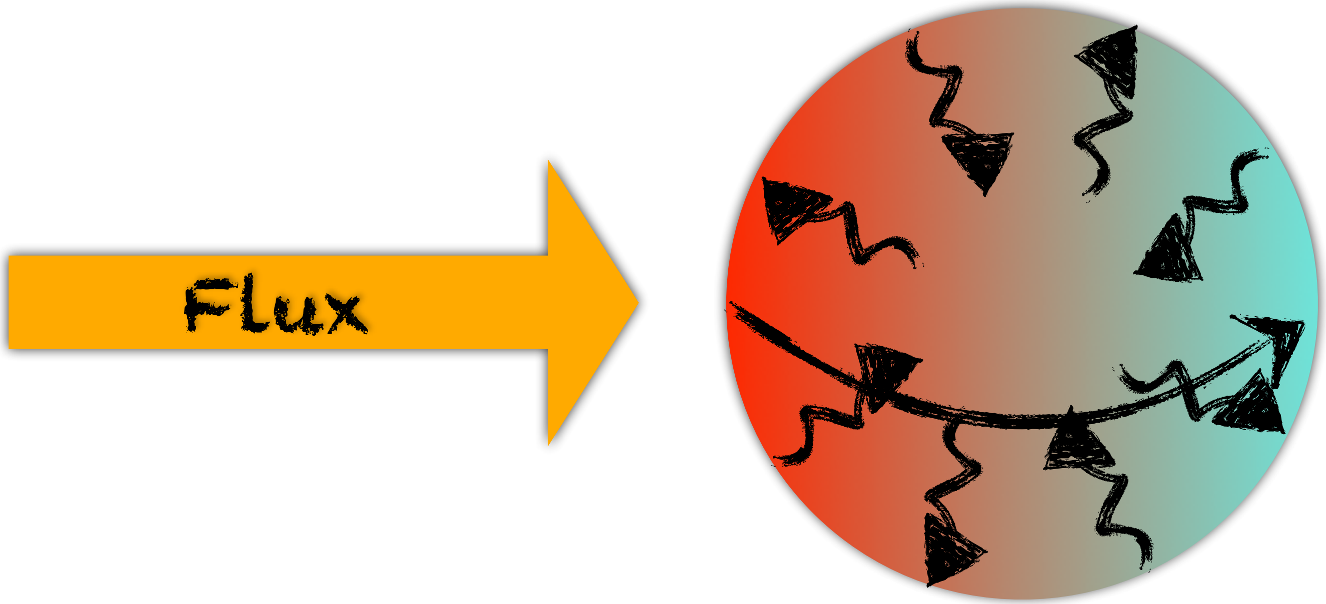
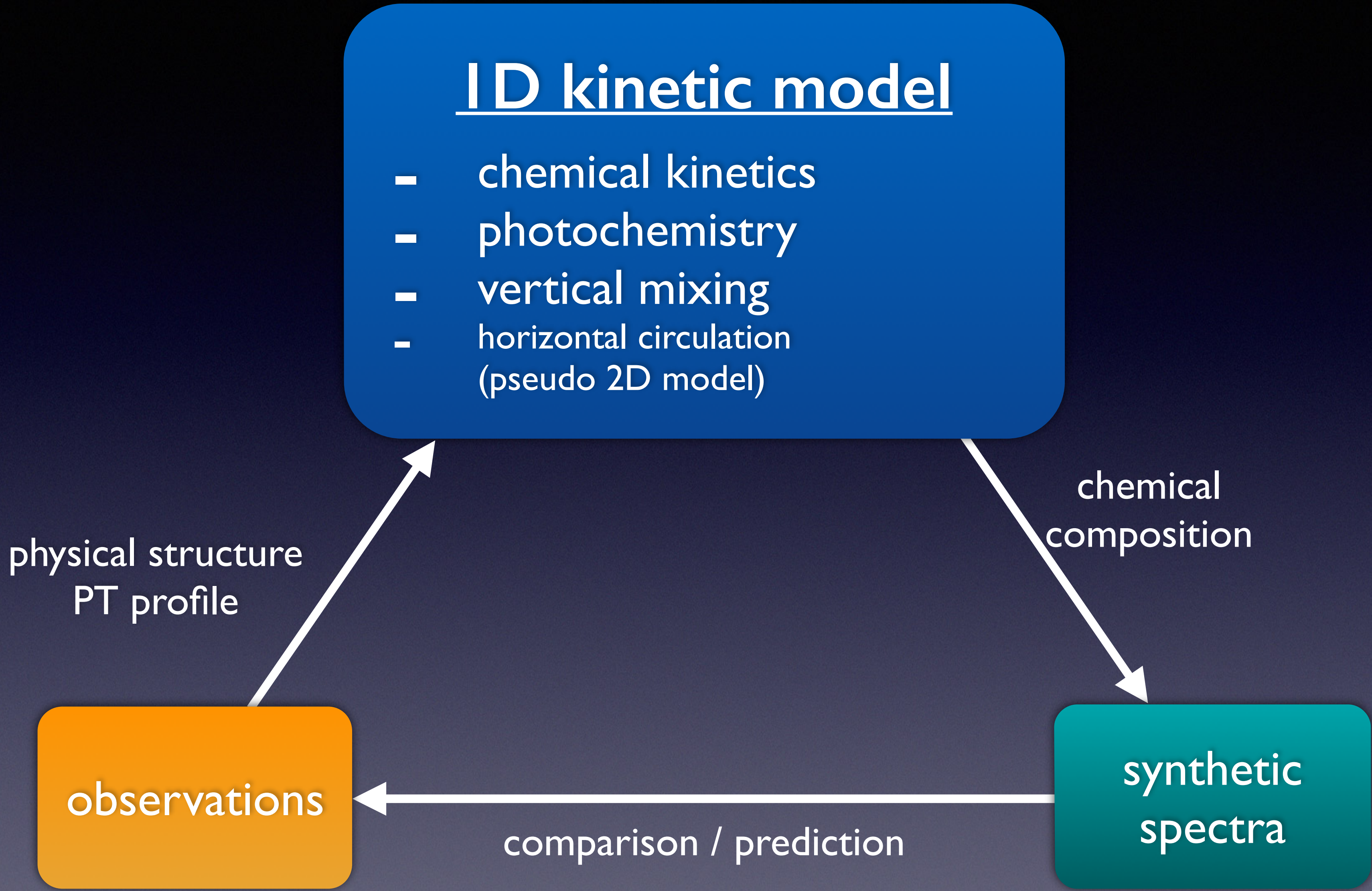


interpretation spectroscopy :

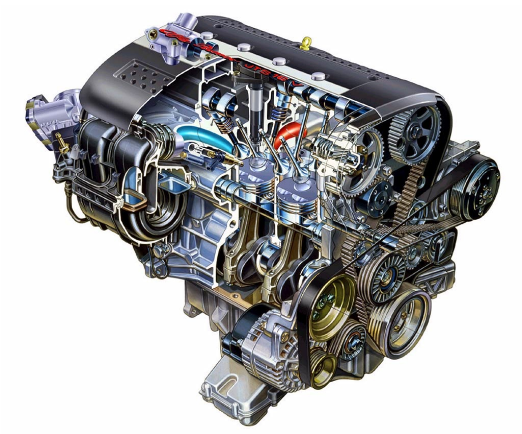
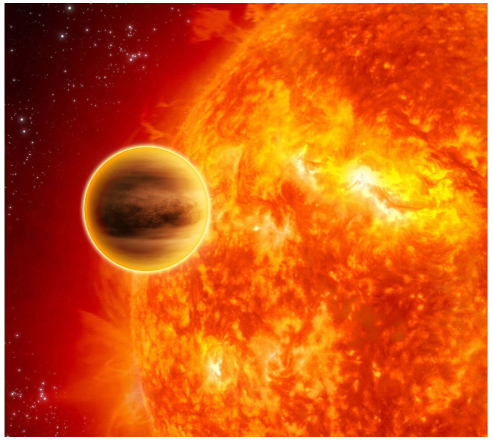
➡ need kinetic models



collaborations: forward model
M. Rocchetto (UCL) - M. Agúndez (ICMM)

Chemical networks

- Totally new in planetology:

 +  = 

- interdisciplinary collaboration - specialist of combustion (LRGP, Nancy)
- schemes validated experimentally wholes - large ranges P (10^{-3}-10^{2} bar) T (300-2500 K)
- 1920 reactions, 105 species (C,H,O,N), C_2 *Venot et al. 2012, A&A*
- 4002 reactions, 240 species (C,H,O,N), C_6 *Venot et al. 2015, A&A*
- **available for the community on KIDA (http ://kida.obs.u-bordeaux1.fr/)**

Parameters

Chemical model permits to study the influence of:

• Out of equilibrium processes:
- mixing
- photodissociations - stellar flux

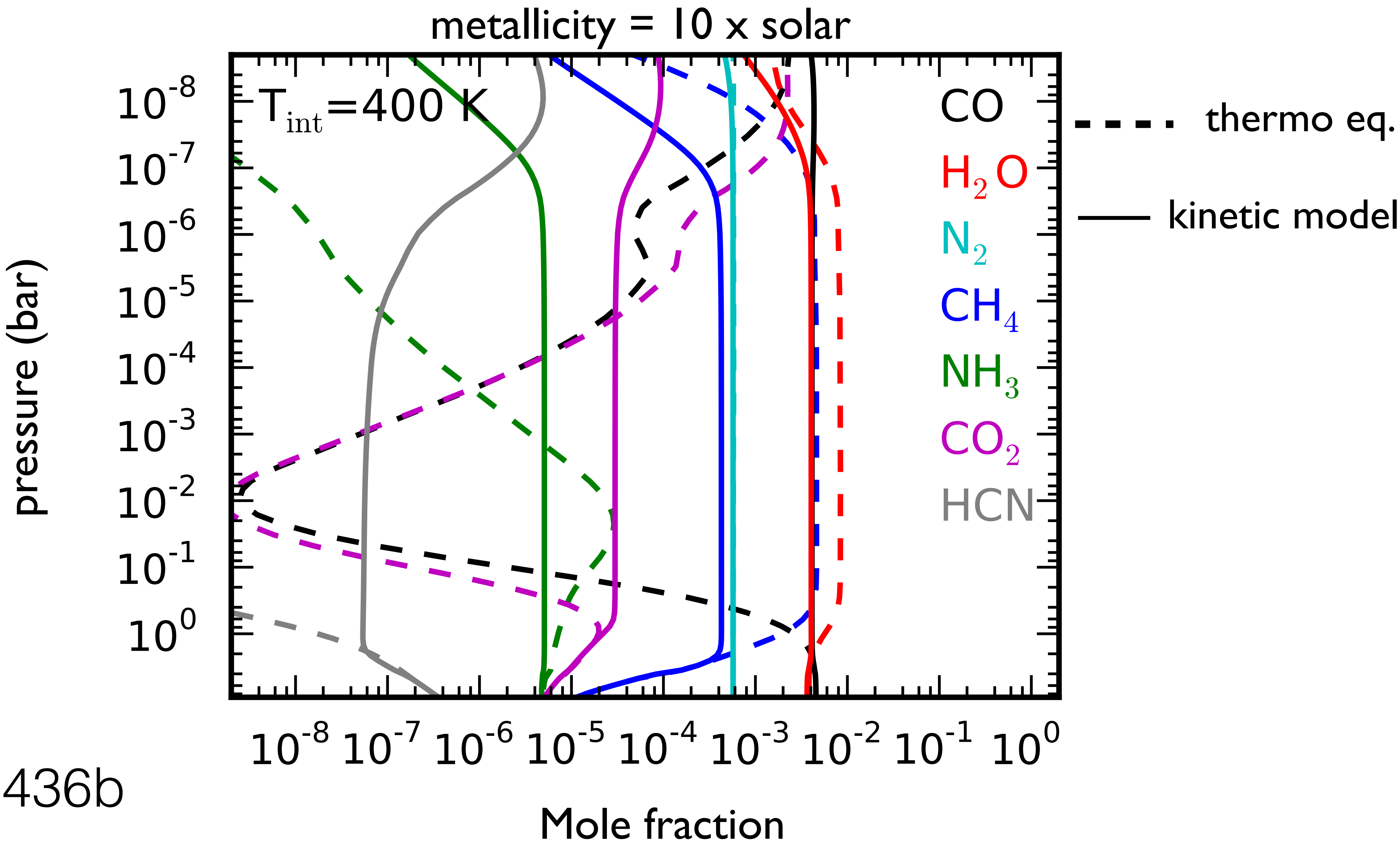
• Intrinsic properties of the planetary atmosphere:
- metallicity
- temperature
- elemental enrichment (C/O ratio)

Parameters

Chemical model permits to study the influence of:

- Out of equilibrium processes:
  - mixing
  - photodissociations - stellar flux
- Intrinsic properties of the planetary atmosphere:
  - metallicity
  - temperature
  - elemental enrichment (C/O ratio)

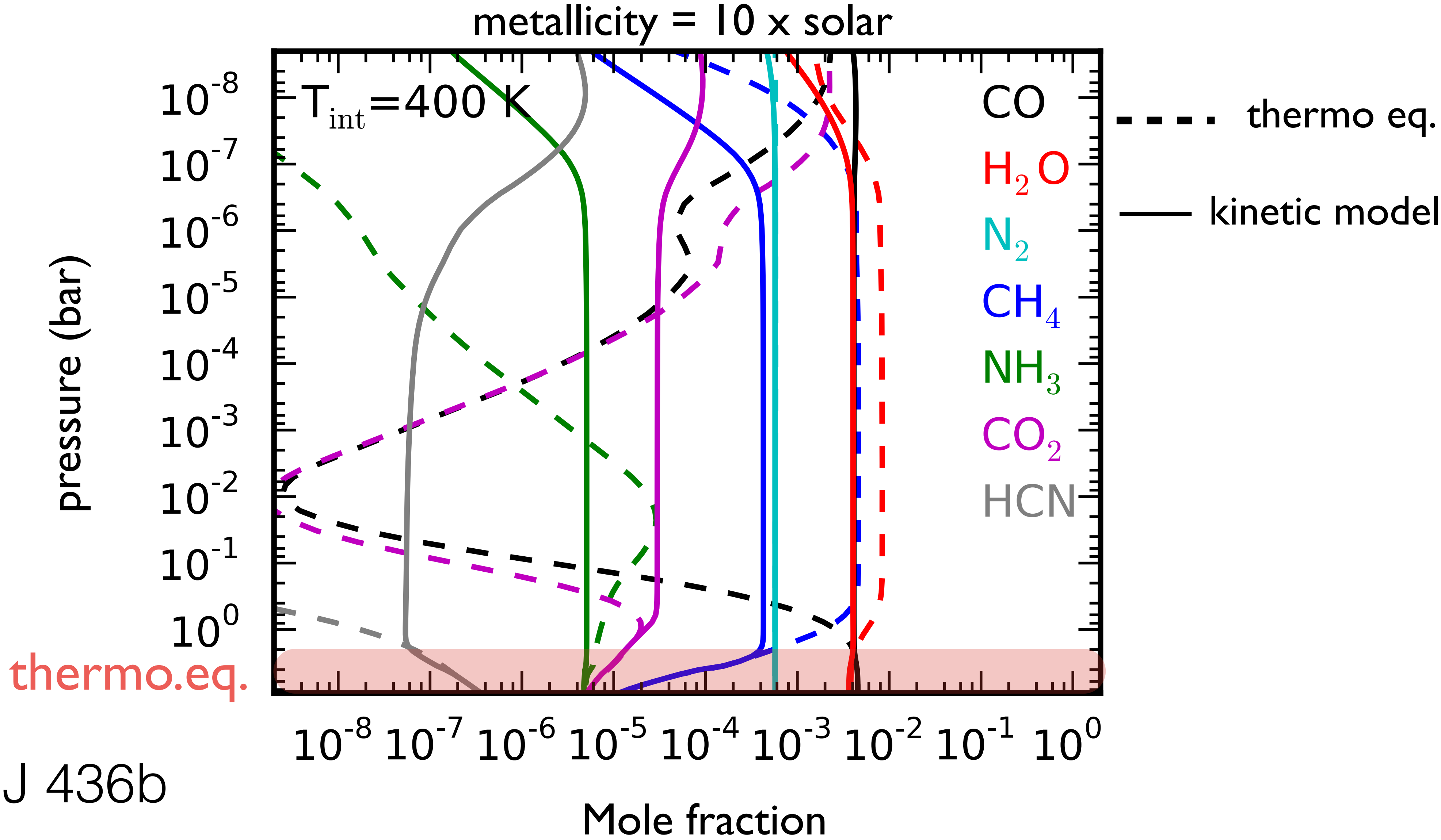
Vertical Mixing and Quenching



GJ 436b

Agúndez, Venot et al. 2014, ApJ

Vertical Mixing and Quenching



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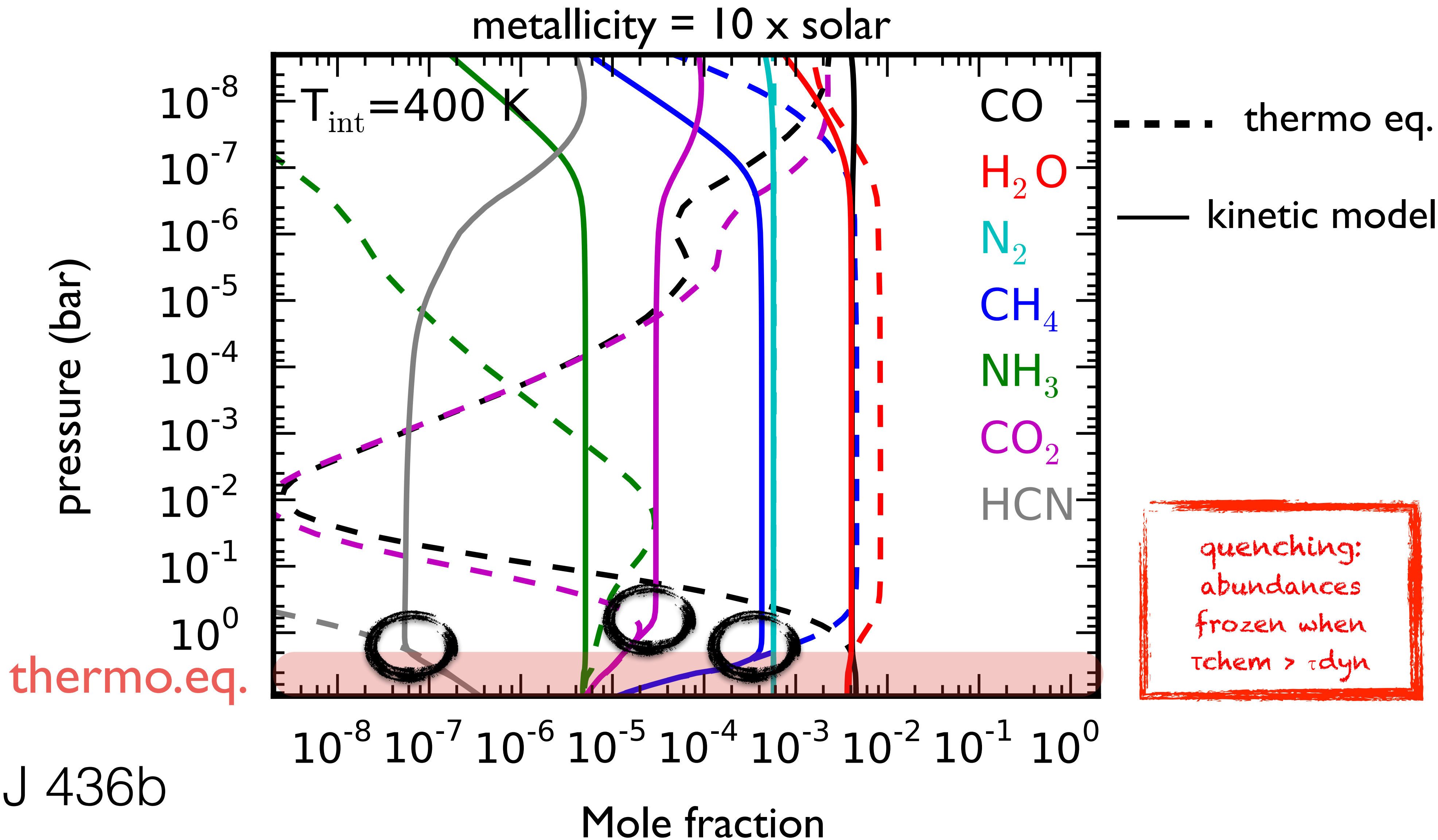
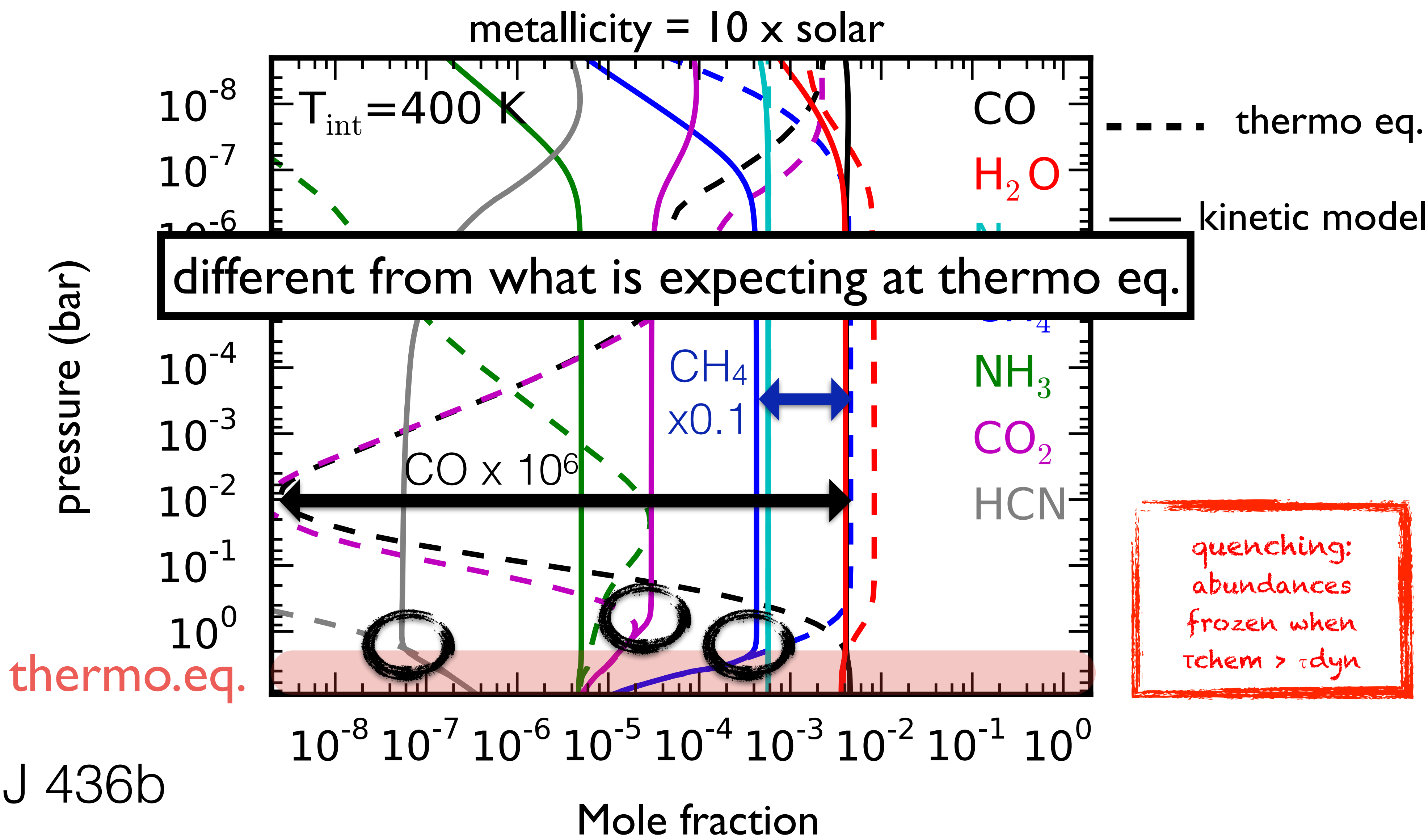


GJ 436b

Agúndez, Venot et al. 2014, ApJ

Vertical Mixing and Quenching

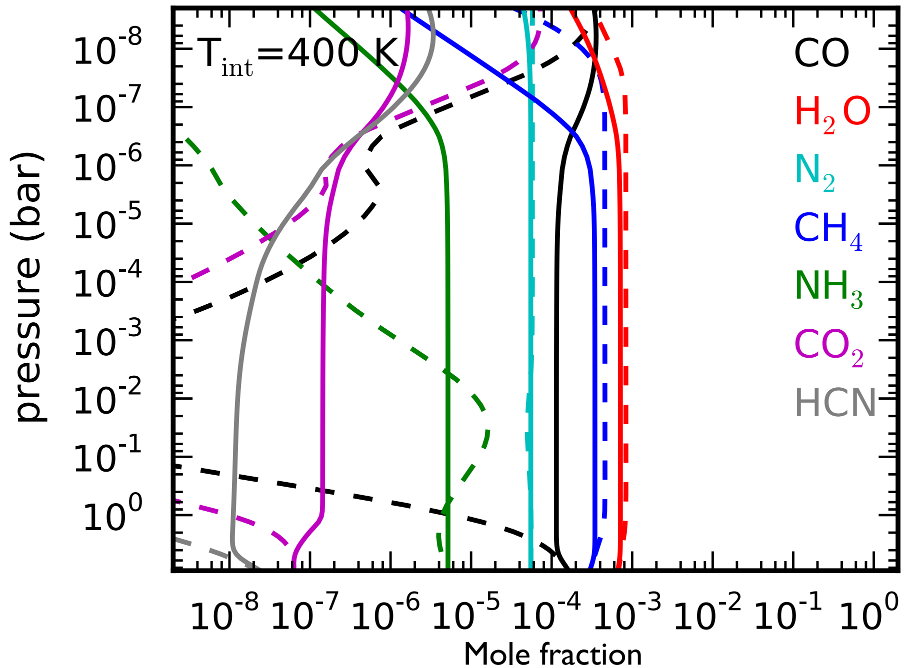


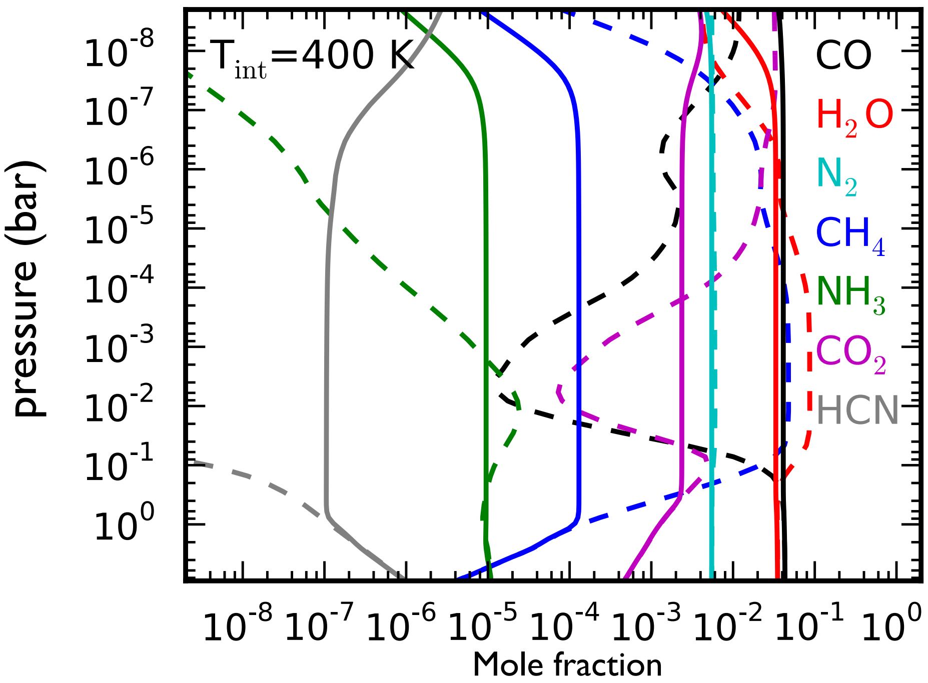
GJ 436b

Agúndez, Venot et al. 2014, ApJ

Quenching and Metallicity

1 x solar GJ 436b 100 x solar





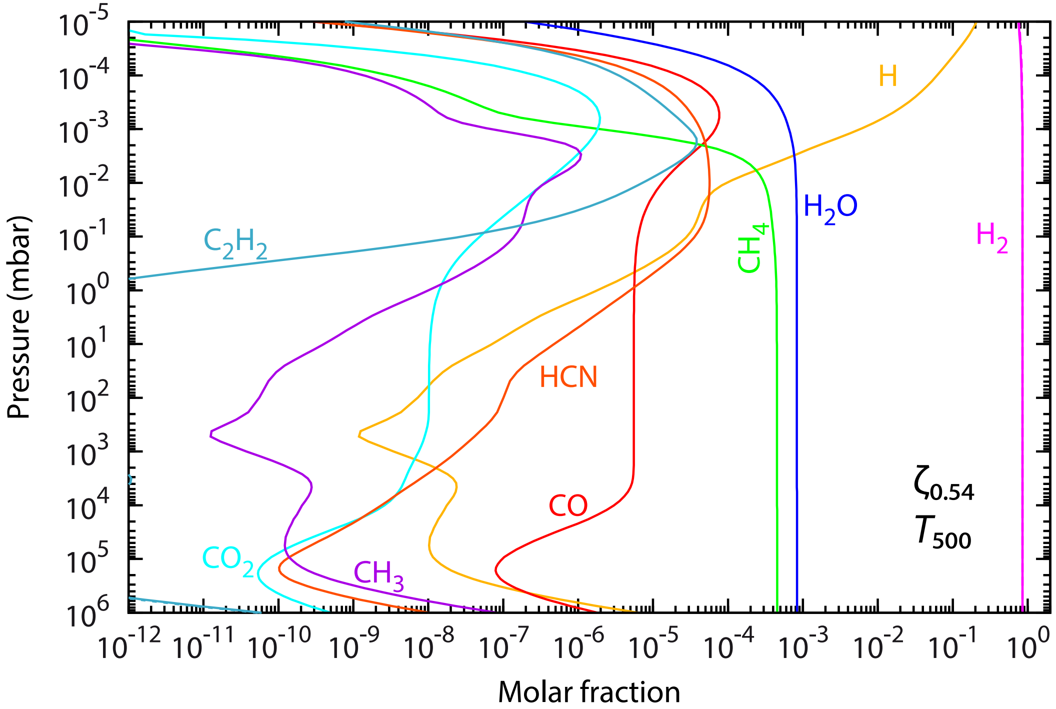
Agúndez, Venot et al. 2014, ApJ

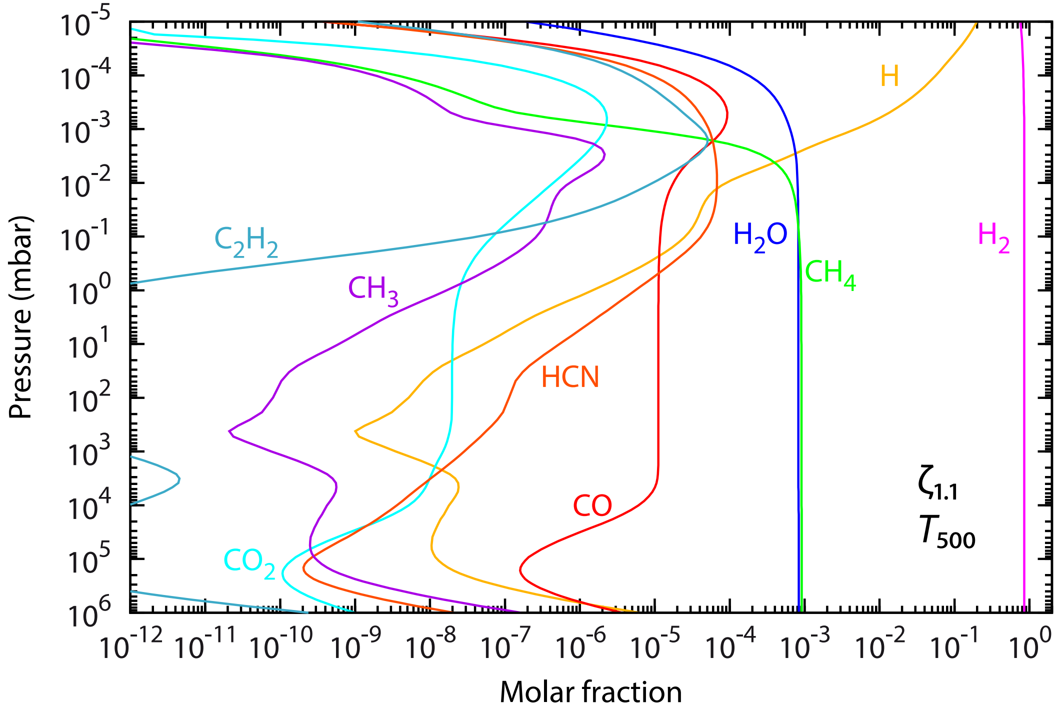
At solar metallicity: CH_4 and H_2O close to thermo eq. - more abundant than CO
With increasing metallicity: most of mole fraction increases (CO, CO_2, HCN, N_2,…)
but some decrease (CH_4) ➜ ratio CO/CH_4 increases together with metallicity

@1mbar

increase of metallicity + quenching: change in main carrier of elements (C-O)
1 x solar: H_2O and CH_4 are main O- and C-bearing species (as predicted by eq.)
100 x solar: CO is the main O- and C-bearing species (contrary to prediction of eq.)

Elemental Abundances: C/O

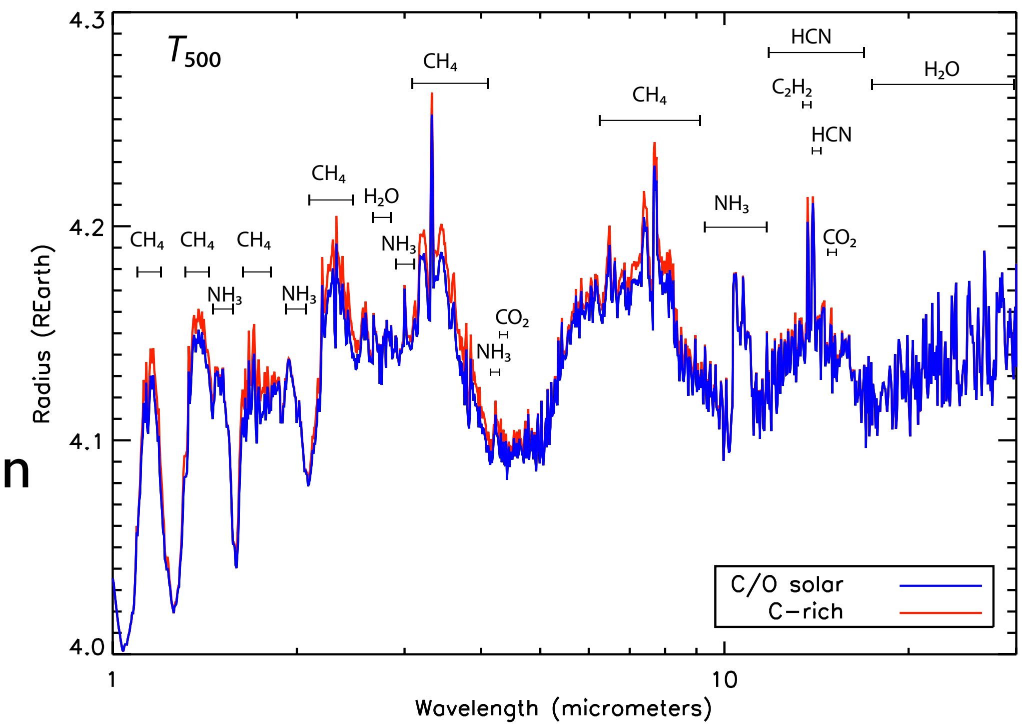




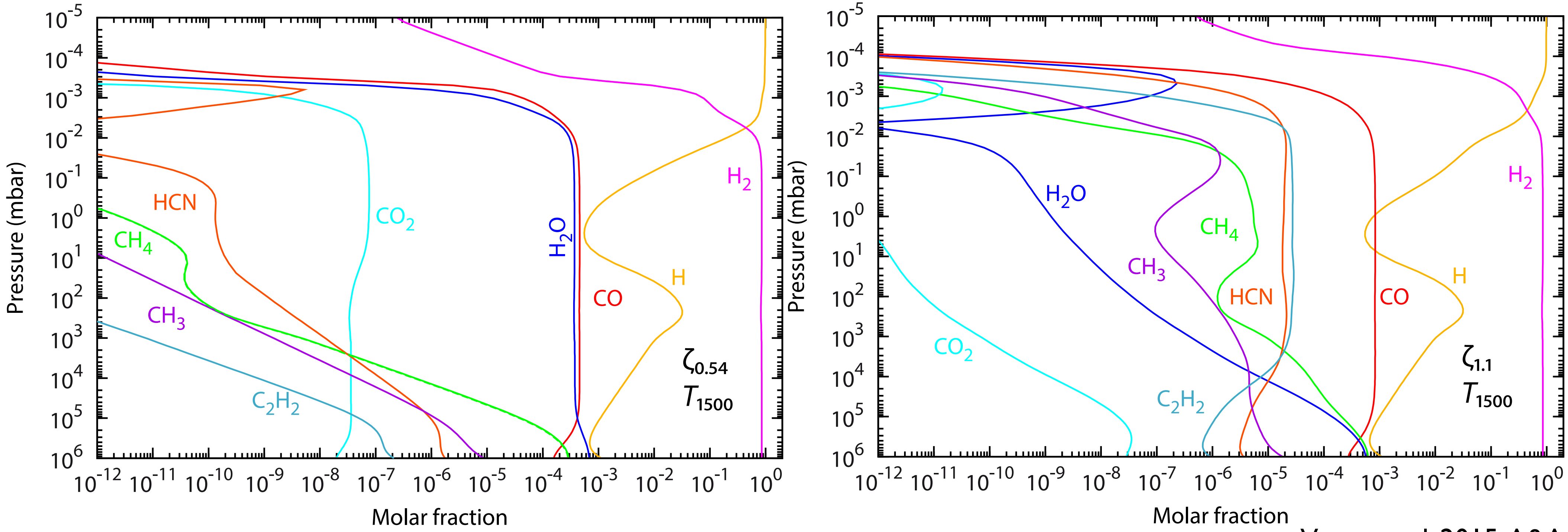
- C/O = 0.54 (solar)
- C/O = 1.1

cold atmospheres (T~500K)

C/O ratio: almost no effect on composition
small increase of C-species



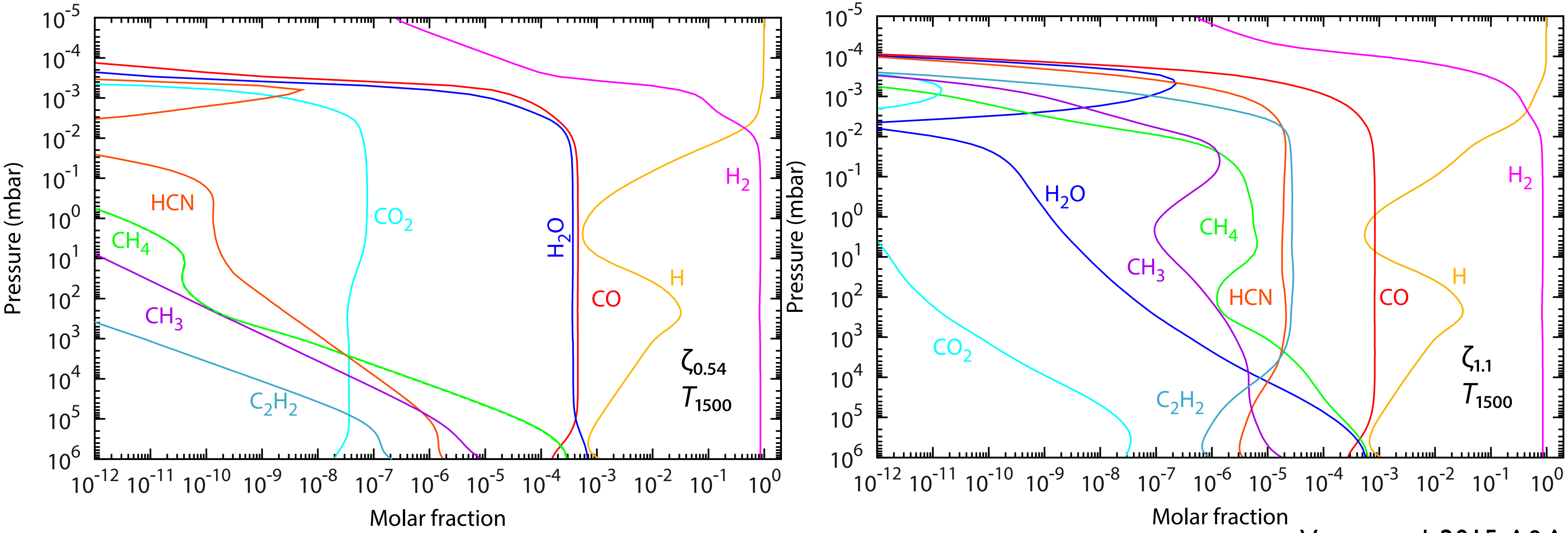
Venot et al. 2015, A&A



Venot et al. 2015, A&A

hot atmospheres (T>1000K)

C/O ratio: effect on composition
(less H_2O - more CH_4, C_2H_2, HCN...)



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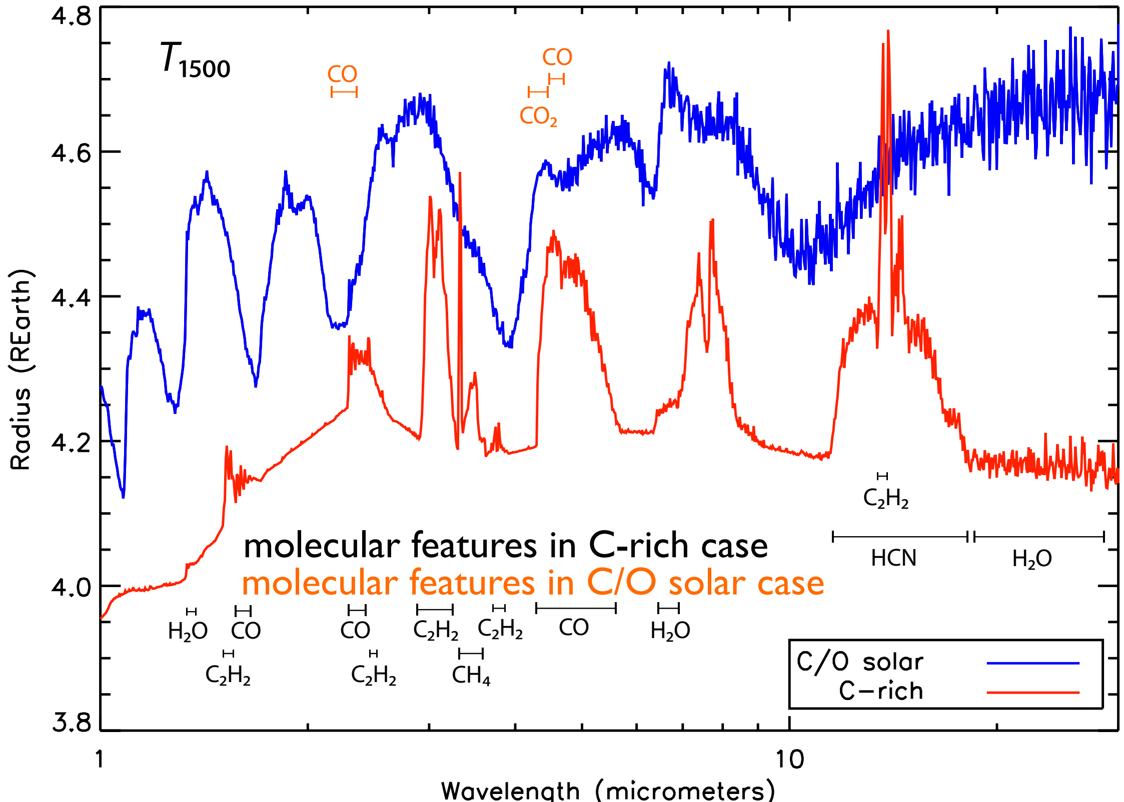
hot atmospheres (T>1000K)

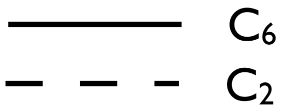
C/O ratio: effect on composition
(less H_2O - more CH_4, C_2H_2, HCN...)

C/O solar: global form due to H_2O + features of CO, CO_2

C-rich: global form due to H_2-H_2 collisions + features of CH_4, CO and C_2H_2, and HCN (15µm)
➜ tracers of C/O ratio

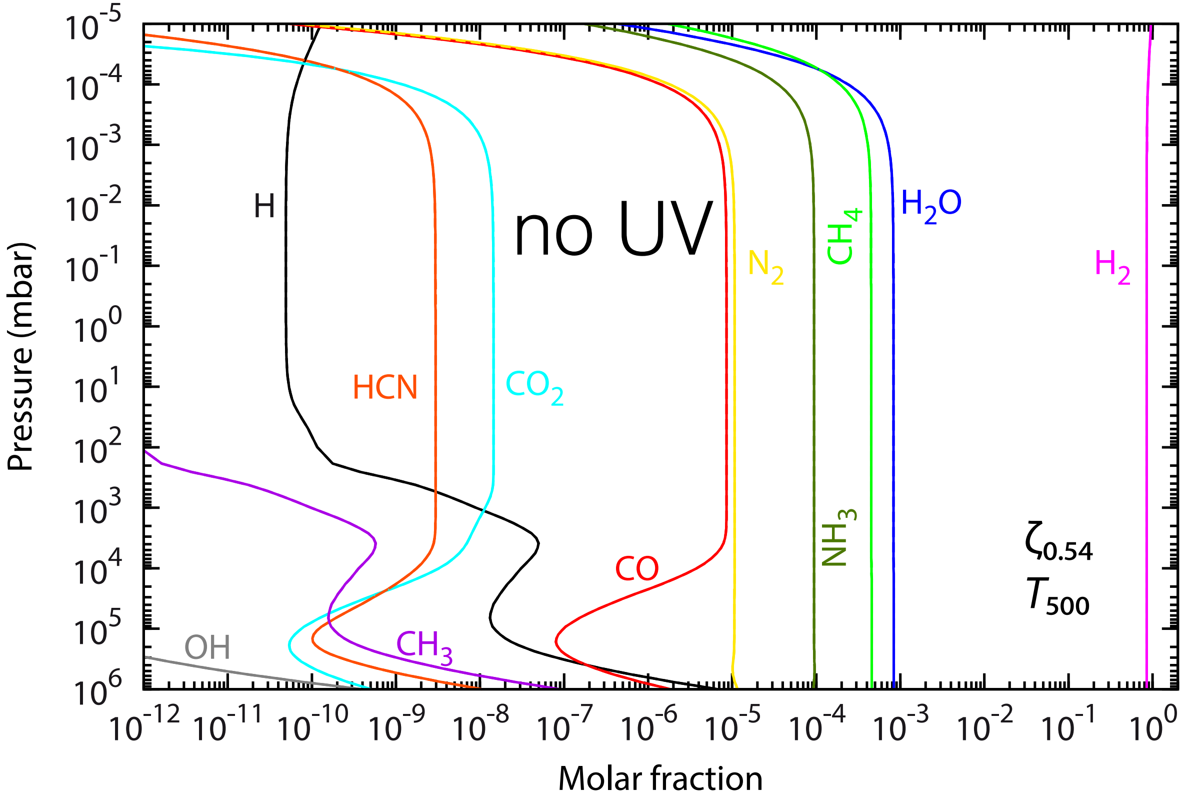


Comparison of the schemes



Venot et al., A&A, 2015

T_{500} $\zeta_{0.54}$: no UV flux, no difference



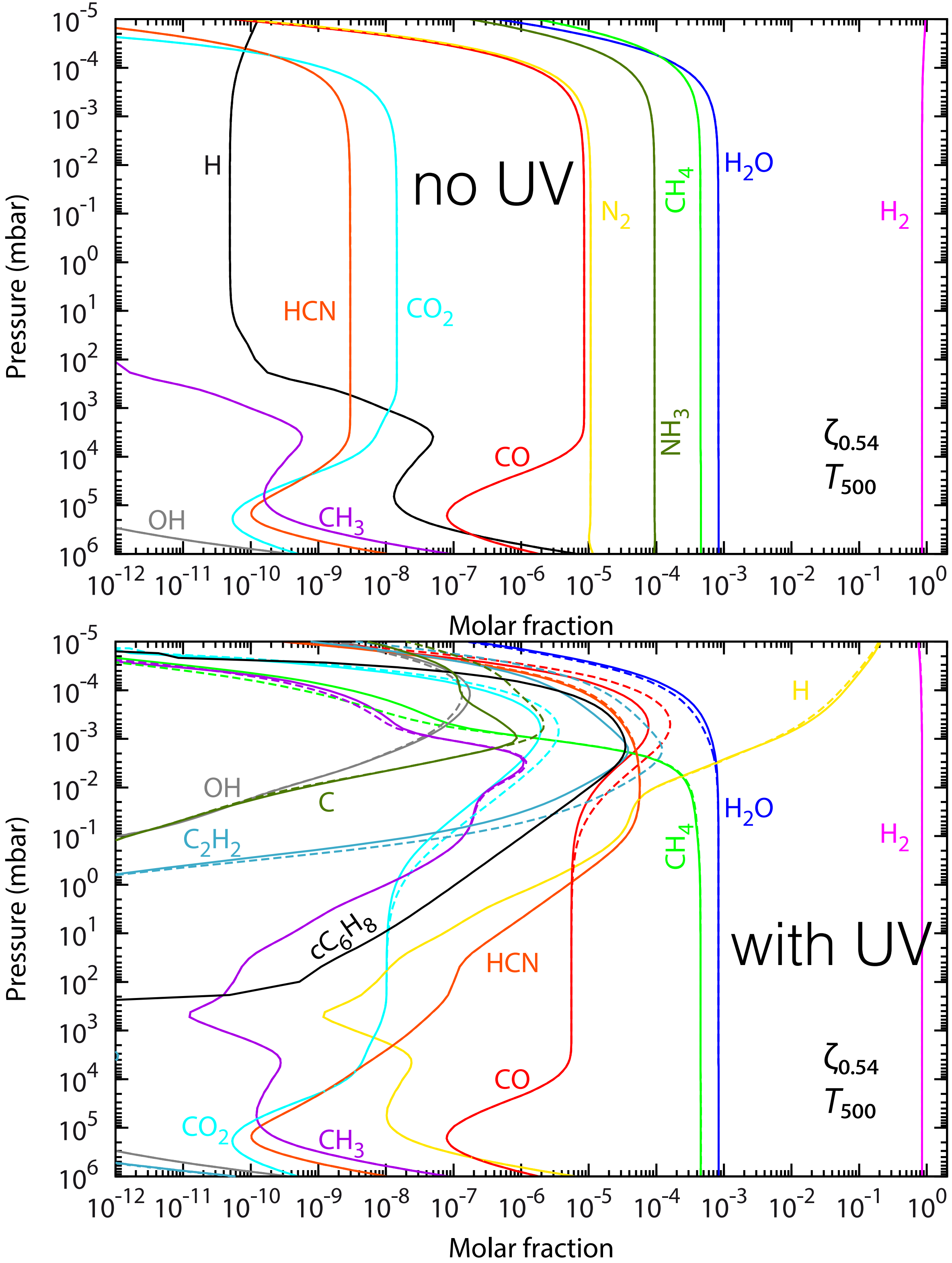
Comparison of the schemes

— C_6

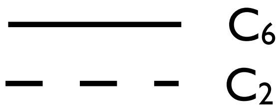
- - - C_2

Venot et al., A&A, 2015

T_{500} $\zeta_{0.54}$: with UV flux, differences at high altitude



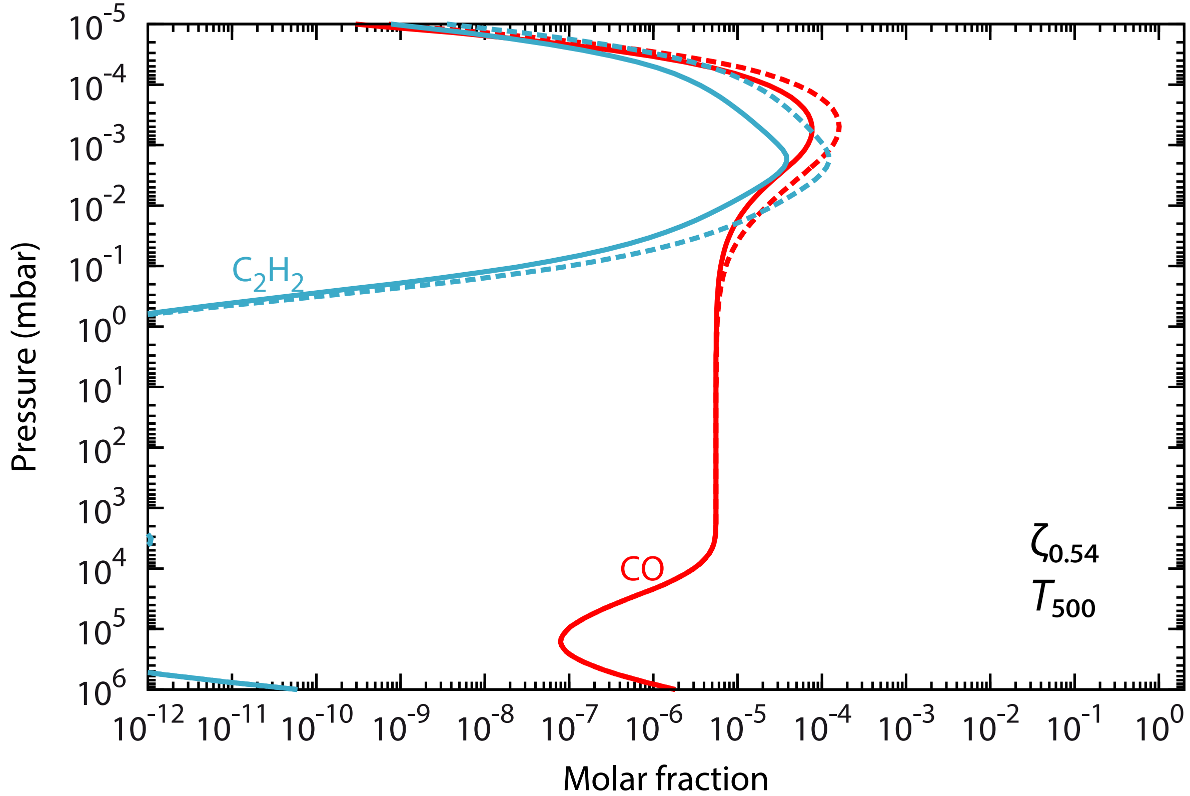
With UV flux



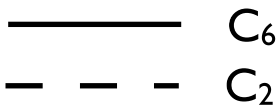
Venot et al., A&A, 2015

T_{500} $\zeta_{0.54}$: **with UV flux, differences at high altitude**

- CO et C_2H_2: more destroyed with the C_6 scheme



With UV flux



Venot et al., A&A, 2015

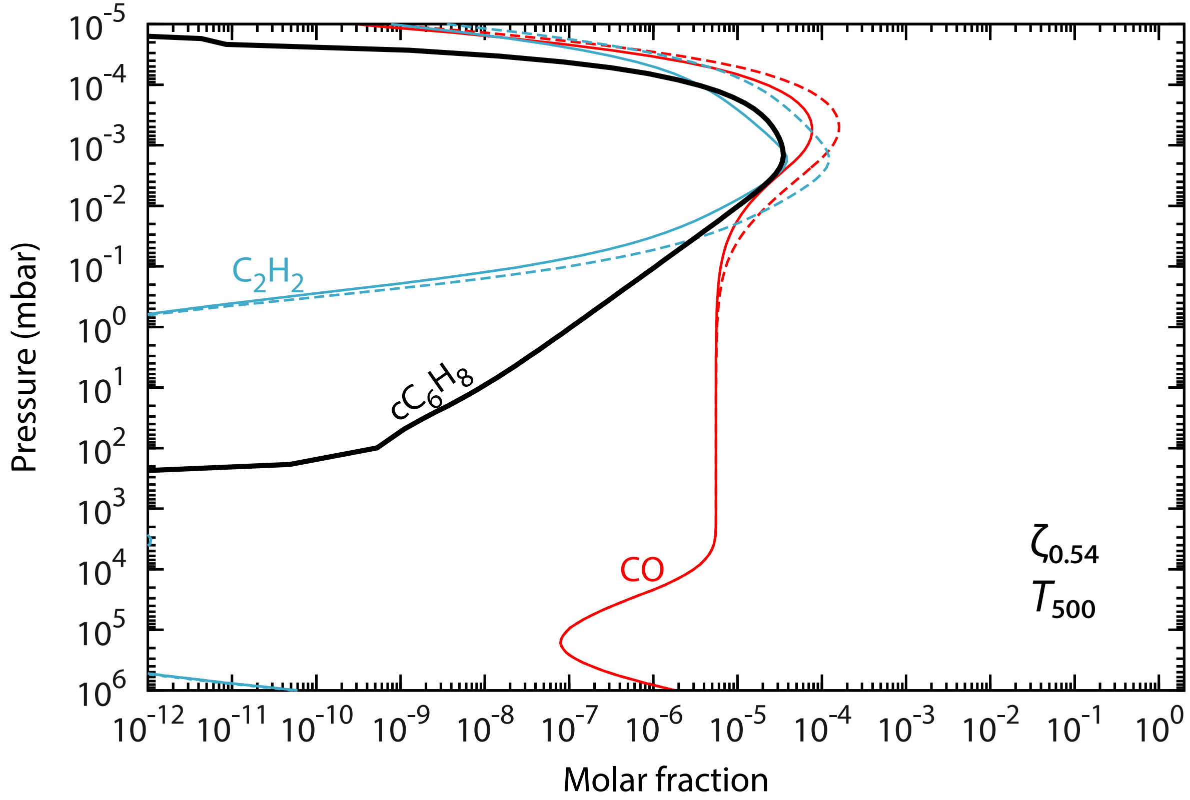
T_{500} $\zeta_{0.54}$: with UV flux, differences at high altitude

- CO et C_2H_2: more destroyed with the C_6 scheme

⇒ the carbon ends up in cC_6H_8

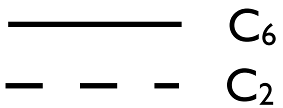
$$\mathbf{CO} + h\nu \longrightarrow C + O^{3P}$$
$$CH_4 + h\nu \longrightarrow CH + H_2 + H$$
$$CH + H2 \longrightarrow {}^3CH_2 + H$$
$${}^3CH_2 + C \longrightarrow C_2H + H$$
$$C_2H + H \longrightarrow C_2H_2$$
$$\mathbf{C_2H_2} + \mathbf{C_2H_2} + C_2H \longrightarrow lC_6H_5$$
$$lC_6H_5 \longrightarrow cC_6H_5$$
$$cC_6H_5 + H \longrightarrow cC_6H_6$$
$$cC_6H_6 + H \longrightarrow cC_6H_7$$
$$cC_6H_7 + H \longrightarrow cC_6H_8$$

$$\mathbf{CO + CH_4 + C_2H_2 + C_2H + H \longrightarrow cC_6H_8 + O^{3P}}$$



With UV flux

Photodissociations, through complex formation pathways create species with significant abundances



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$$lC_6H_5 \longrightarrow cC_6H_5$$
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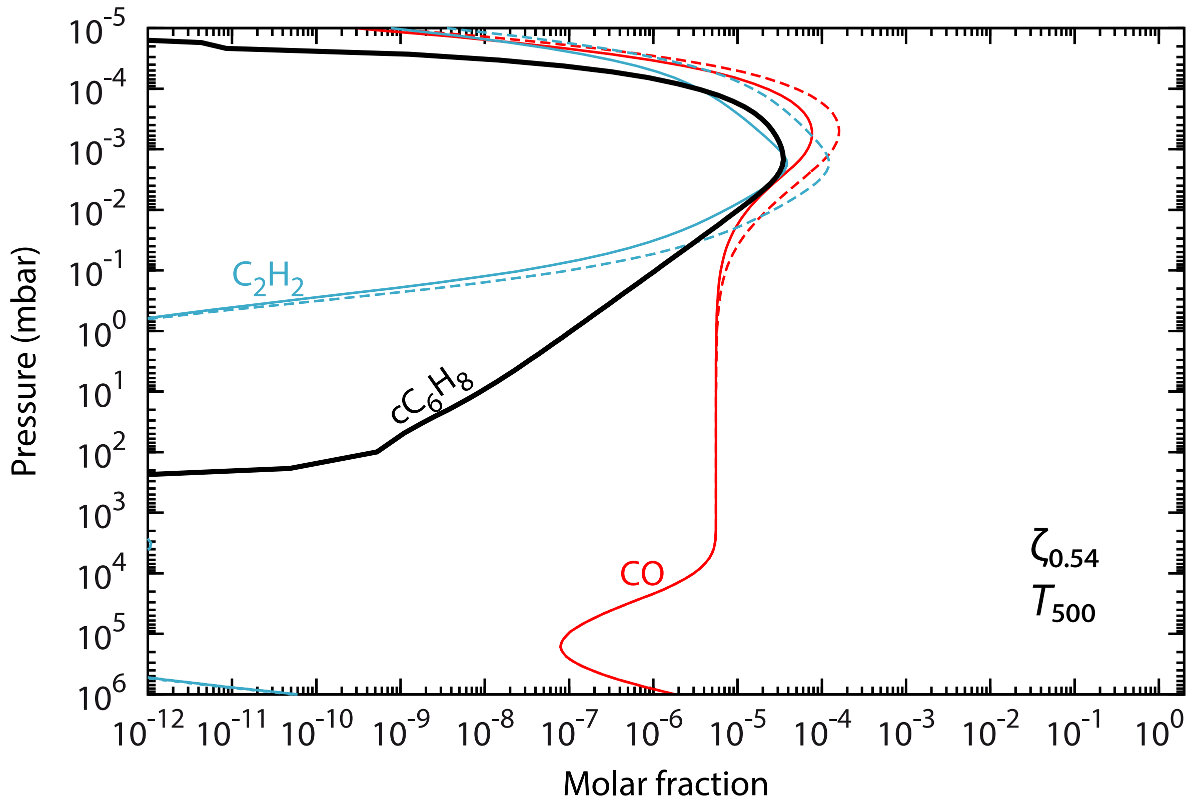


Effect of Stellar flares

M-class stars:

- very abundant in the galaxy ⇒ likely to harbour most of the planetary systems
- very active stars ⇒ subject to stellar variability (star spots, flares, …)

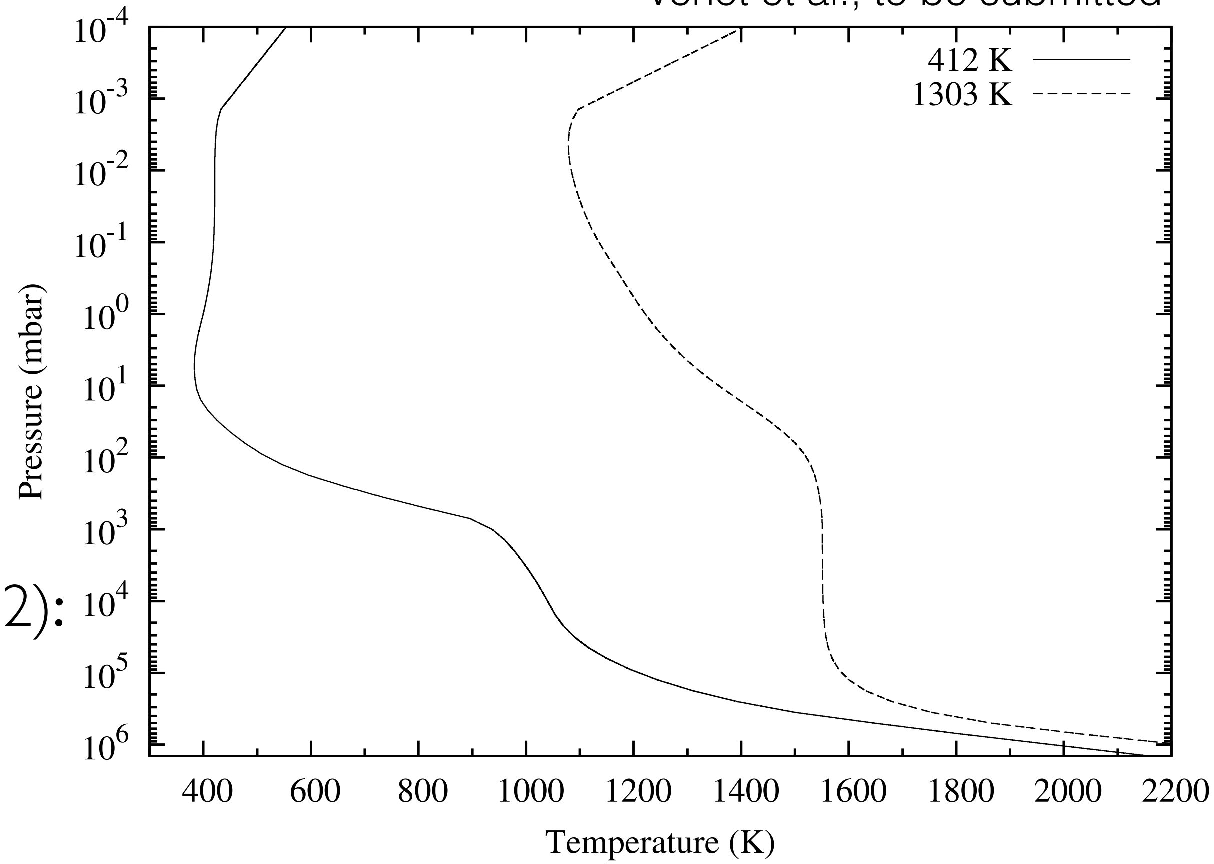
➡ In which extent can a stellar flare modify the chemical composition of an exoplanetary atmosphere and influence the resulting spectra?

2 hypothetic planets
(sub-Neptune/super-Earth)
around a very active star: AD Leo

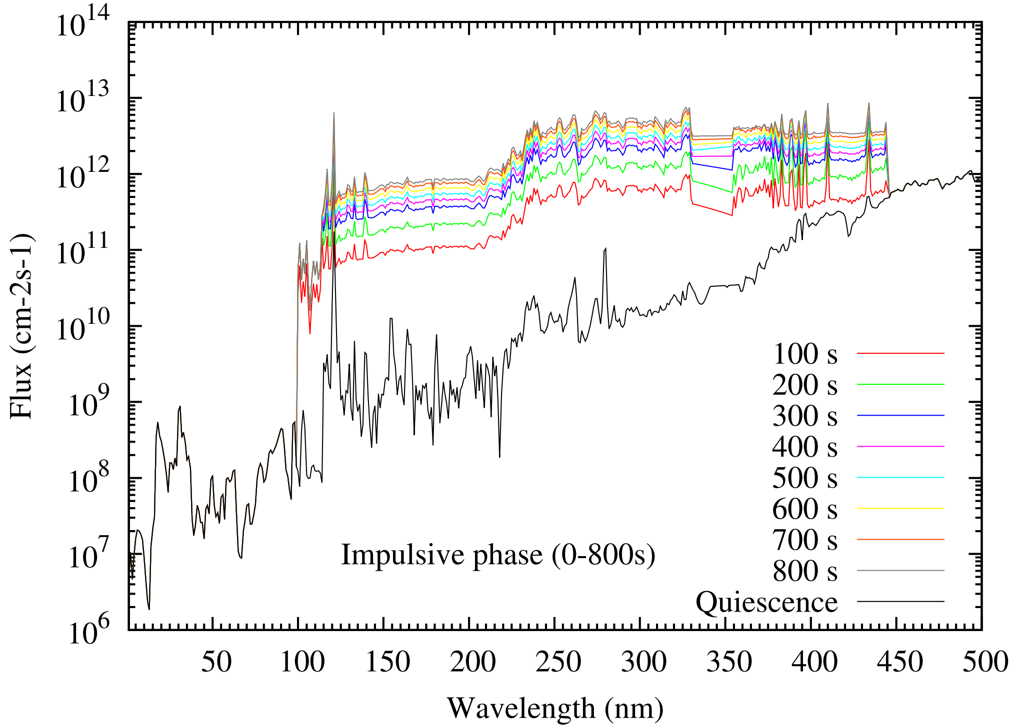
T_{eq} = 412K
T_{eq} = 1303K (from Fortney et al. 2013)

1D chemical model (Venot et al. 2012):
steady-state composition
with quiescent stellar spectra

Venot et al., to be submitted



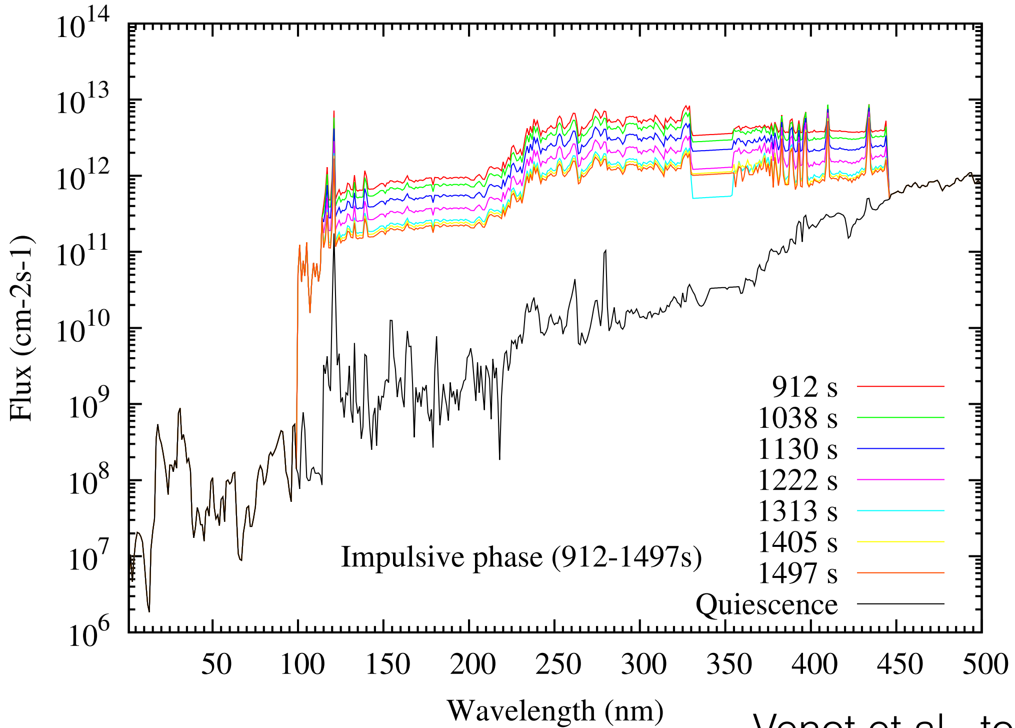
UV flux during flare

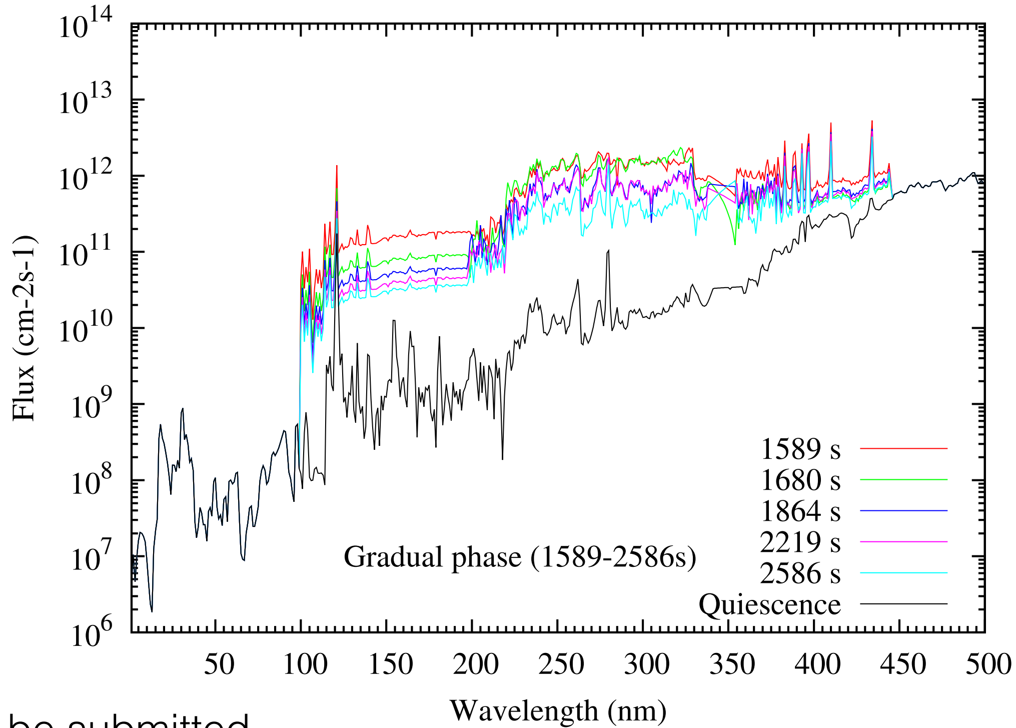


AD Leo flare of 1985

- observed by Hawley & Pettersen (1991)
- scaling and interpolation by Segura et al. 2010

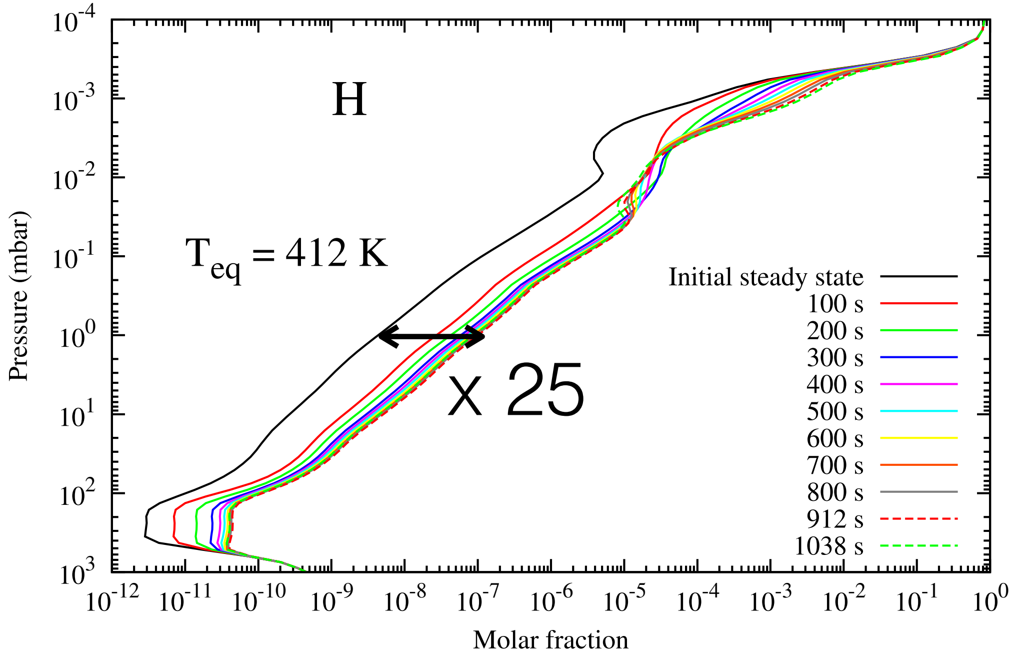
maximum irradiation at 912 s (~ x10^3)
after 2586s: return to quiescent stellar flux





Venot et al., to be submitted

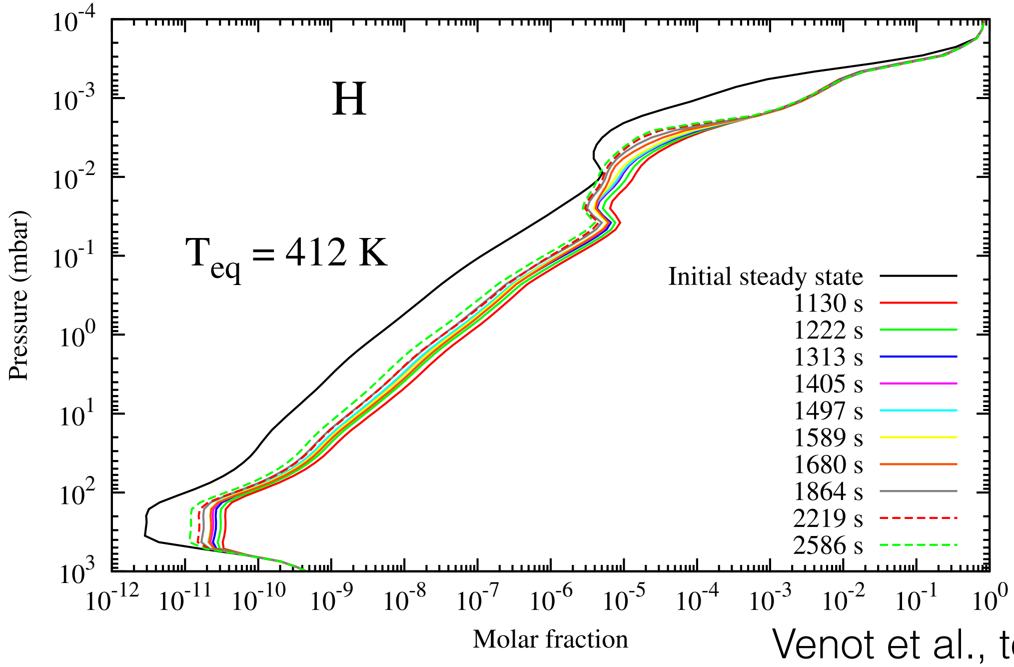
Chemical composition

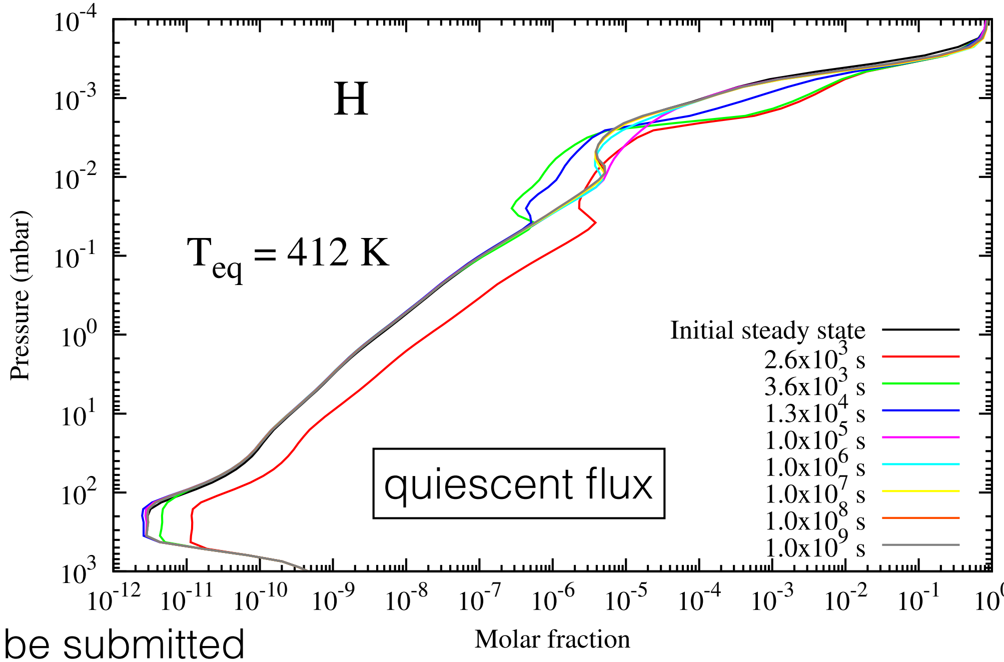


y_H globally increases for P<1 bar during the first impulsive phase (0-912s) then decreases

→ comes back to the initial steady state in 10^9s

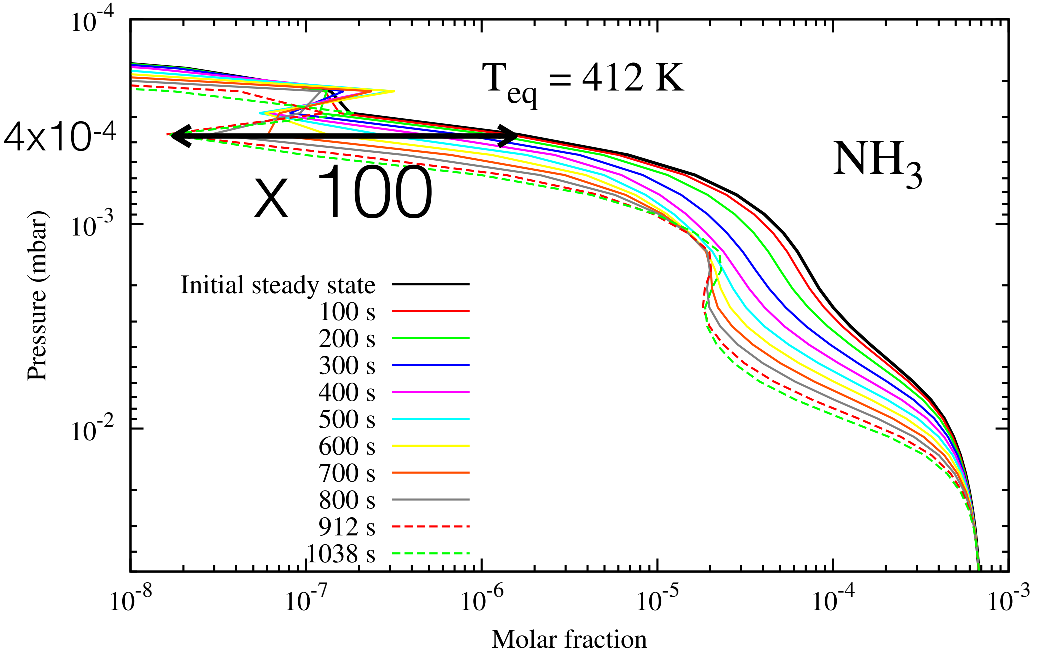
Teq = 412K





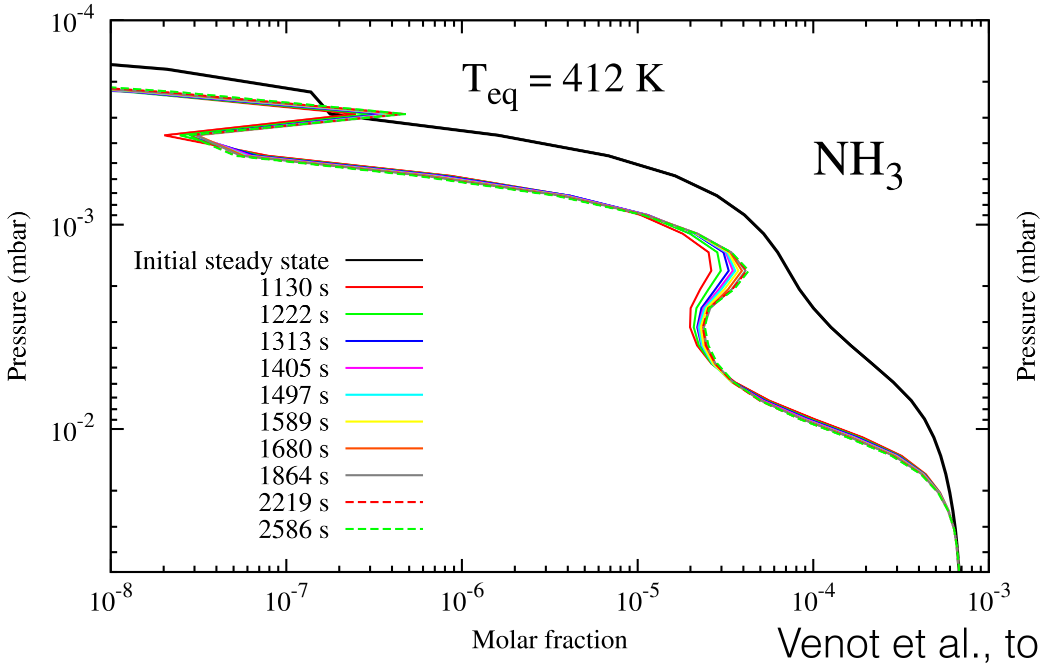
Venot et al., to be submitted

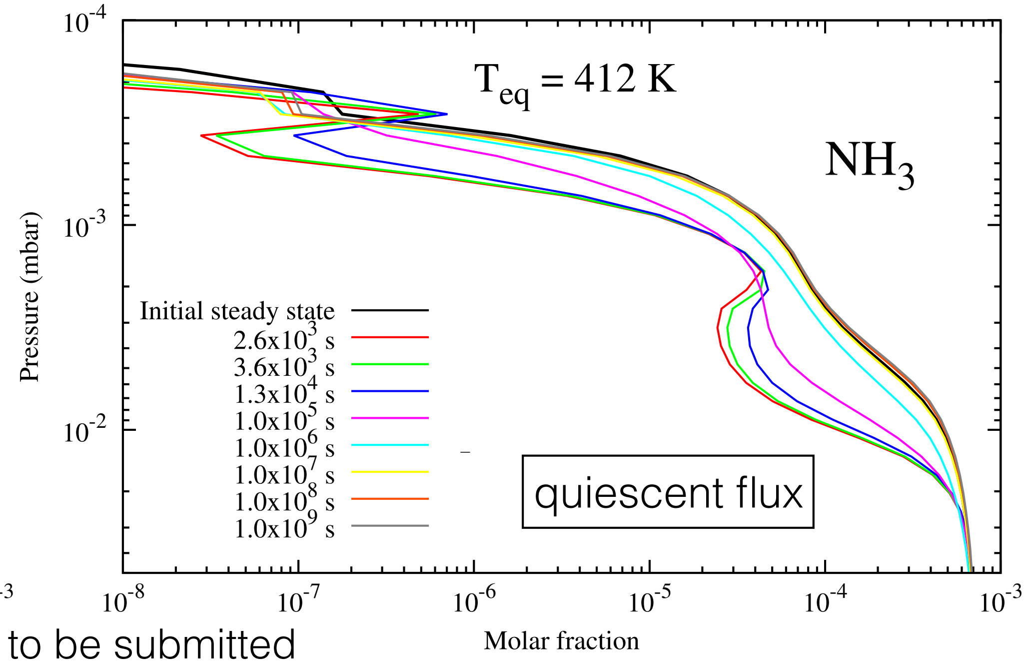
Chemical composition



on the contrary y_{NH3} globally decreases during the first phase (0-912s) then increases → comes back to the initial steady state in 10^9s

Teq = 412K





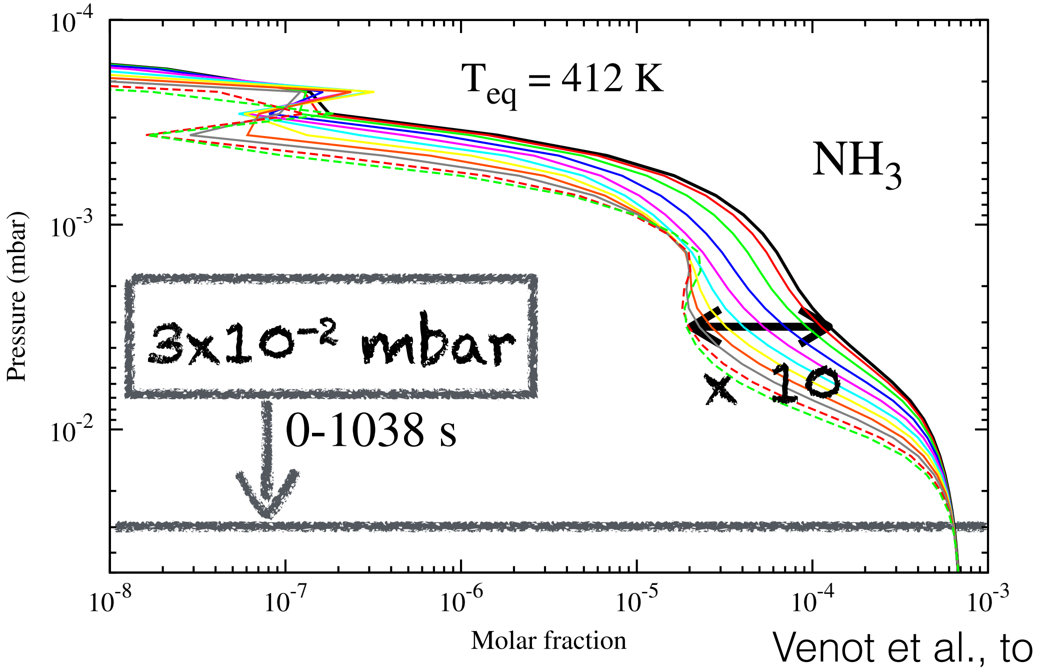
Venot et al., to be submitted

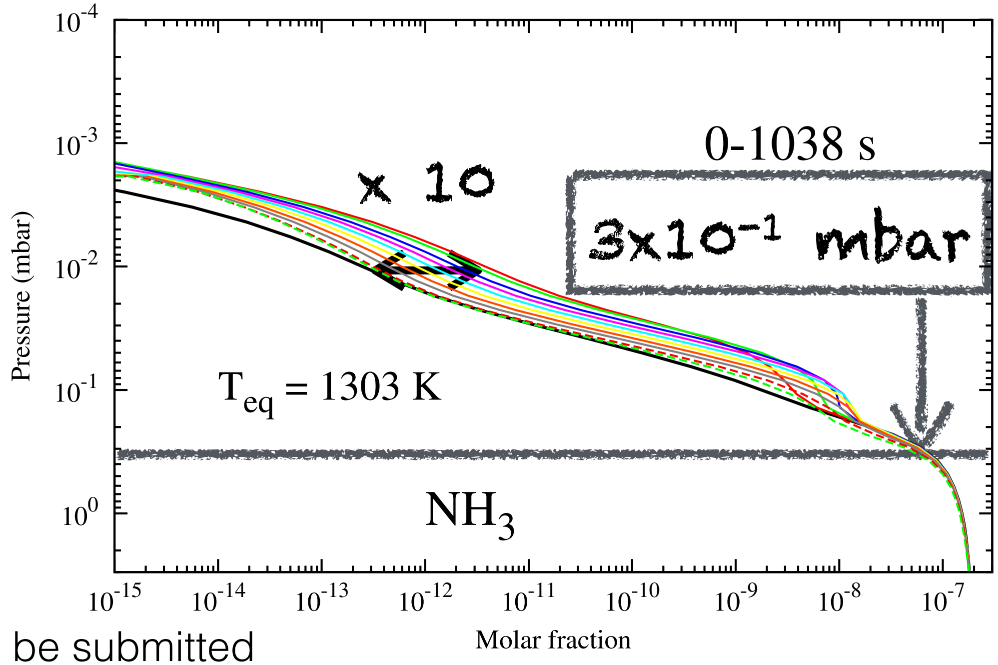
Chemical composition

For both PT profiles: same kind of evolution of abundances during flare

depth and amplitude of variation are species-dependent

for a NH3: deeper effect in the hot case

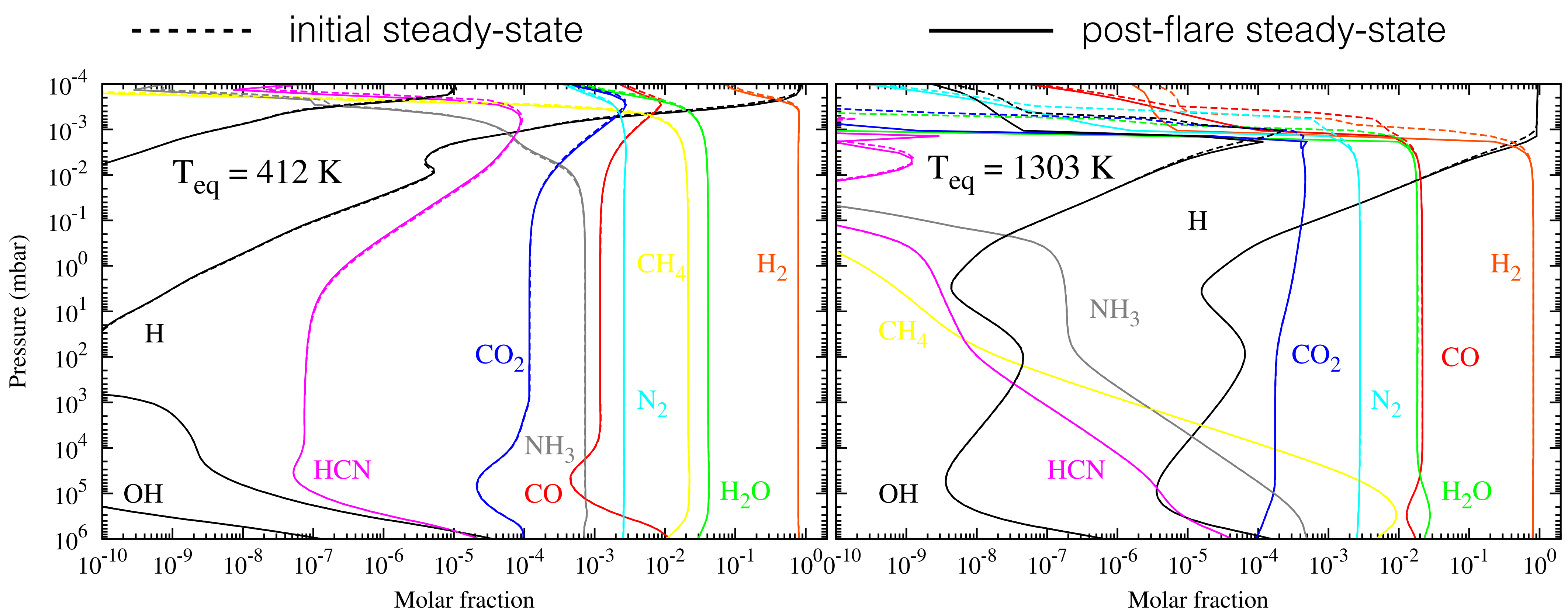




Venot et al., to be submitted

Long-term effect on the chemical composition

After the end of the flare (2586s): stellar flux comes back to quiescence
Steady-state reached after 10^9 / 10^8 s
Hot thermal profile keep trace of the flare in the upper atmosphere



$t=10^9$s Venot et al., to be submitted $t=10^8$s

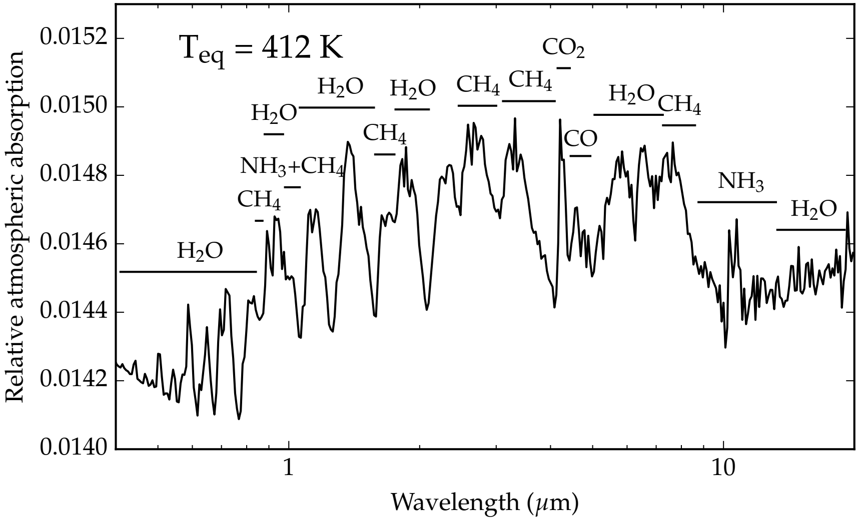
Effect on transmission spectra

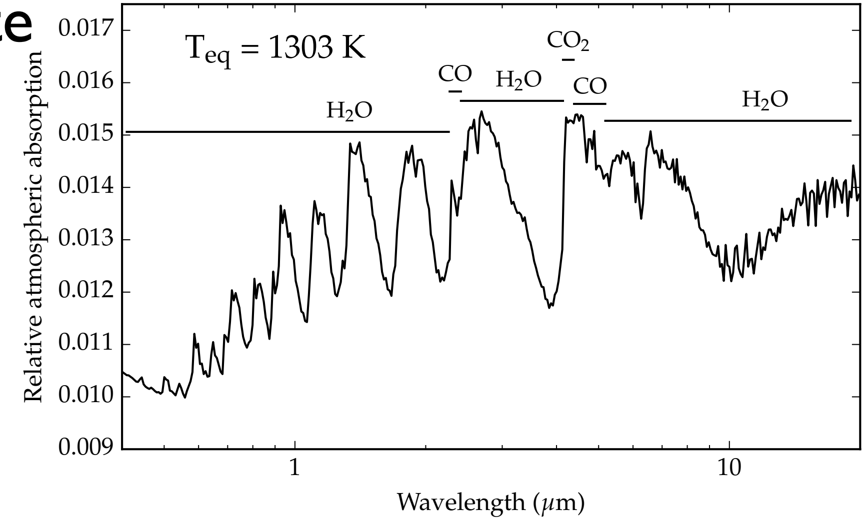
forward model (Waldmann et al. 2015)

412 K

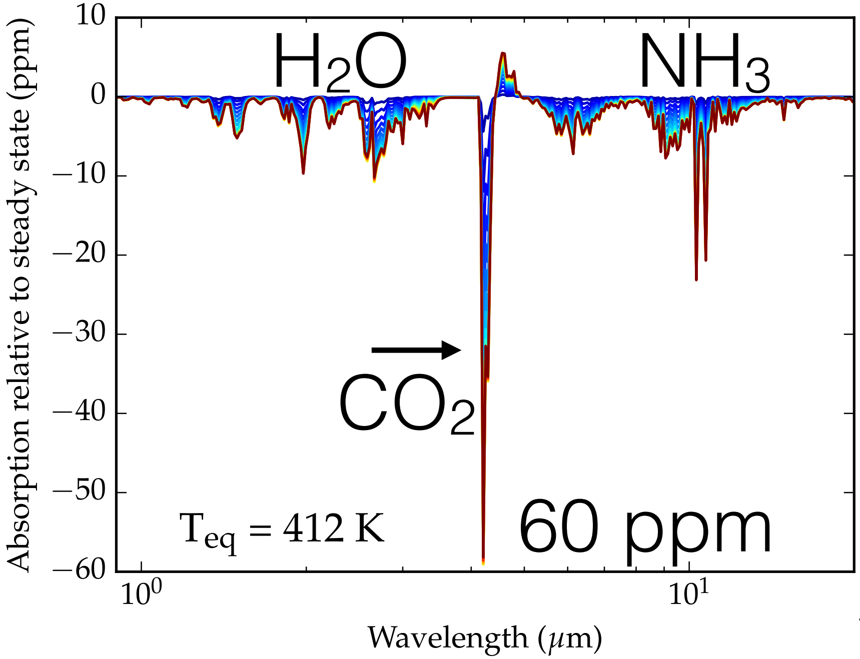
1303 K

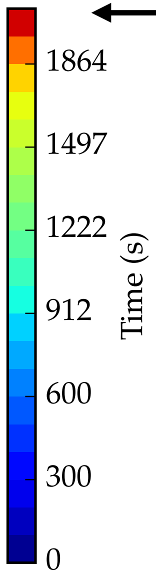
steady-state

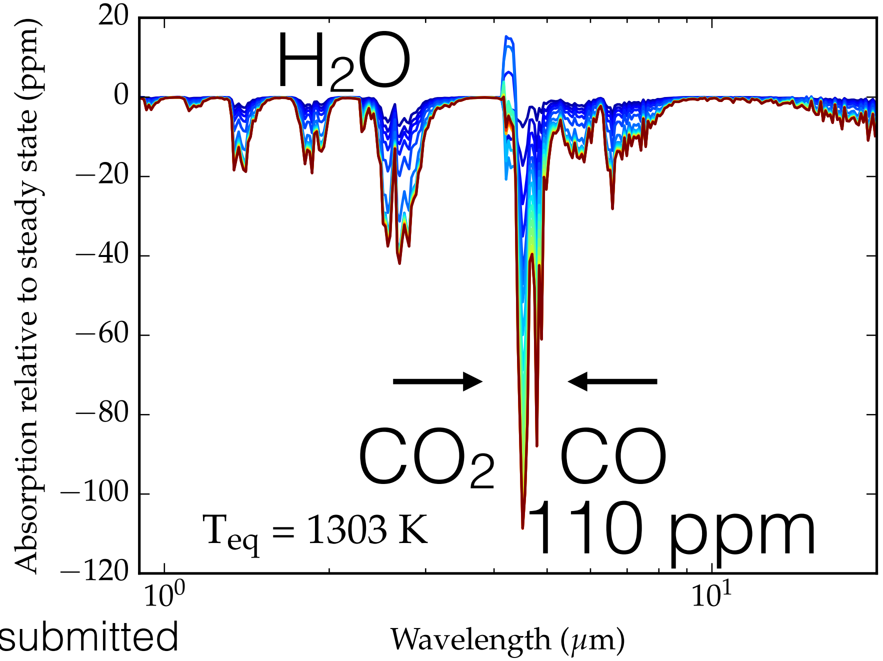




during flare



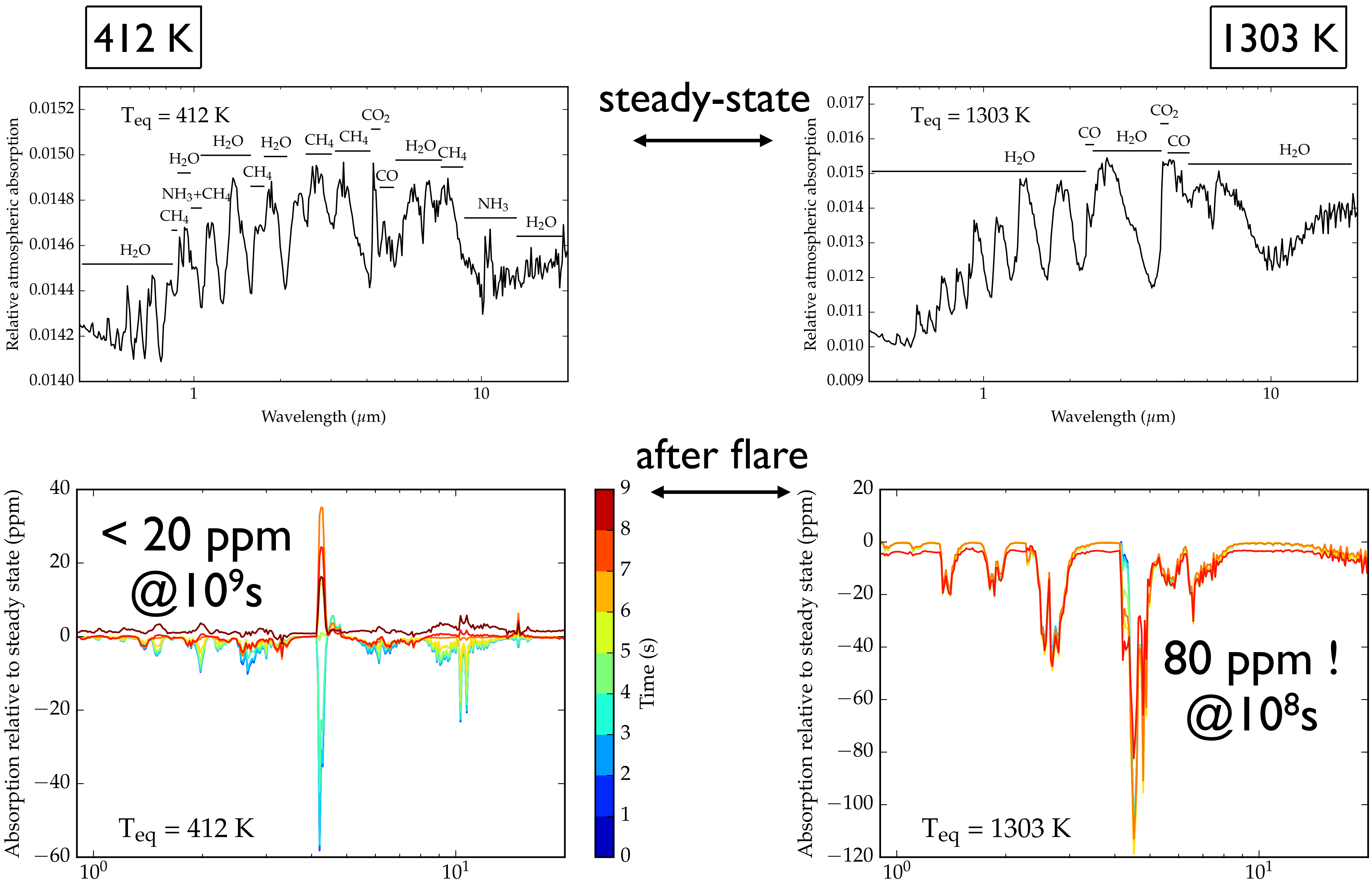




Venot et al., to be submitted

Effect on transmission spectra

forward model (Waldmann et al. 2015)



Venot et al., to be submitted

Summary

✳ High T validated chemical networks available to the community ⇒ **KIDA**

✳ Many parameters and processes influence the chemical composition of exoplanets:

- High metallicity leads to high CO/CH_4 ratio
- High metallicity + quenching leads to a change in C- & O- bearing species

- Elemental enrichment (C/O): effect at high T (> 1000K)

- C_2H_2 and HCN can be used as tracers in warm atmospheres

- Stellar flares can significantly modify the atmospheric composition of exoplanets

- Transmission spectra: variations up to 110 ppm during the flare (~sensitivity of current and future instruments)

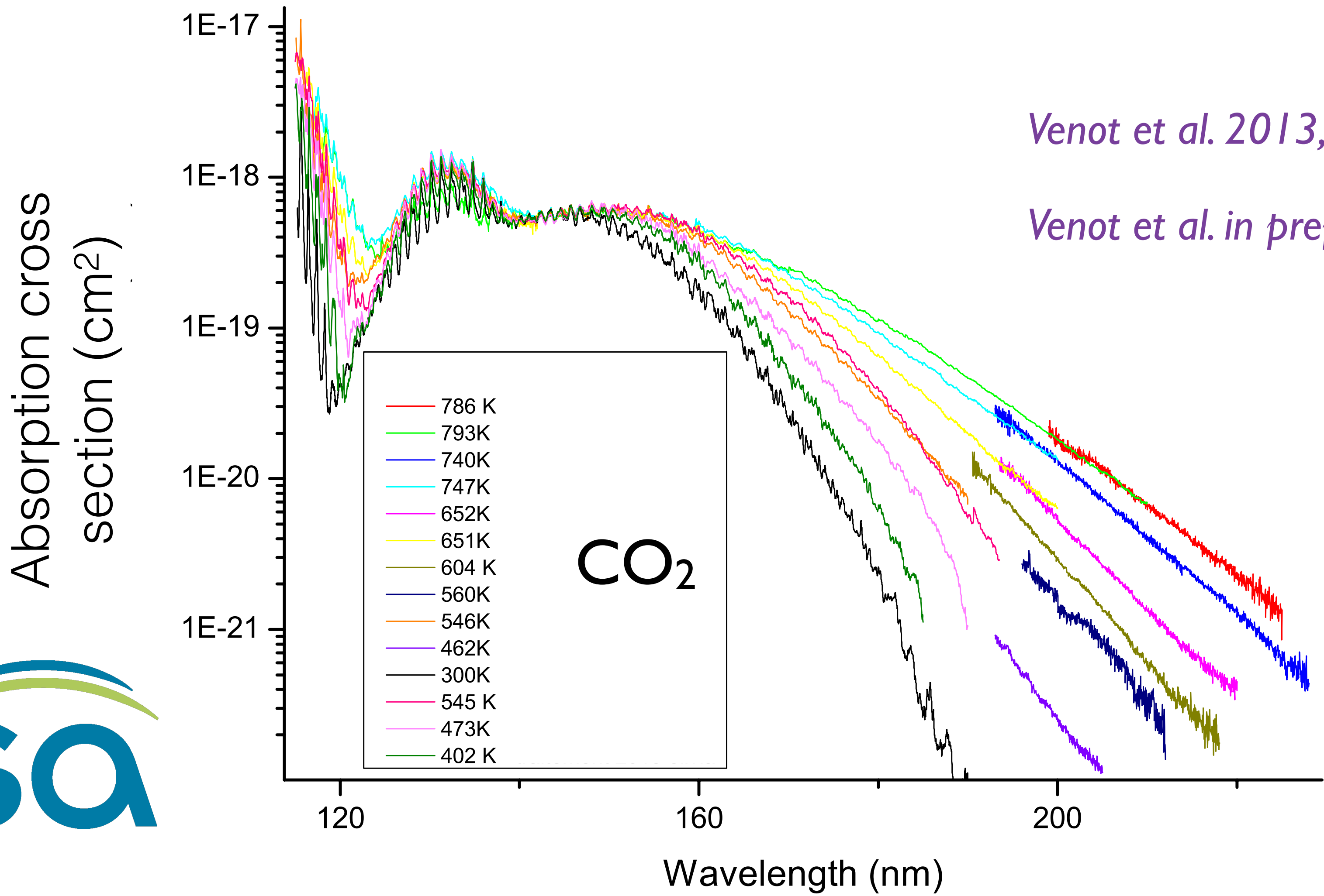
➡unlikely that flares cause significant biases in the retrieved spectrum (several transits necessary to reduced uncertainties + duration of transit ~ duration of flare (~hours))

- Upper atmosphere keeps trace of the event a long period after the end of the flare (at least 10^8s), especially in warmest exoplanets

➡possible to see variations before / after flare (spectra with high S/R)

Bonus message

- modelling performed with absorption cross sections at 300 K (except CO_2 and NH_3)
- data depend strongly on temperature
- CO_2@200 nm : 4 orders of magnitude between 300K and 800K
- higher absorption for all species could lead to different results



Venot et al. 2013, A&A

Venot et al. in prep

Bonus message

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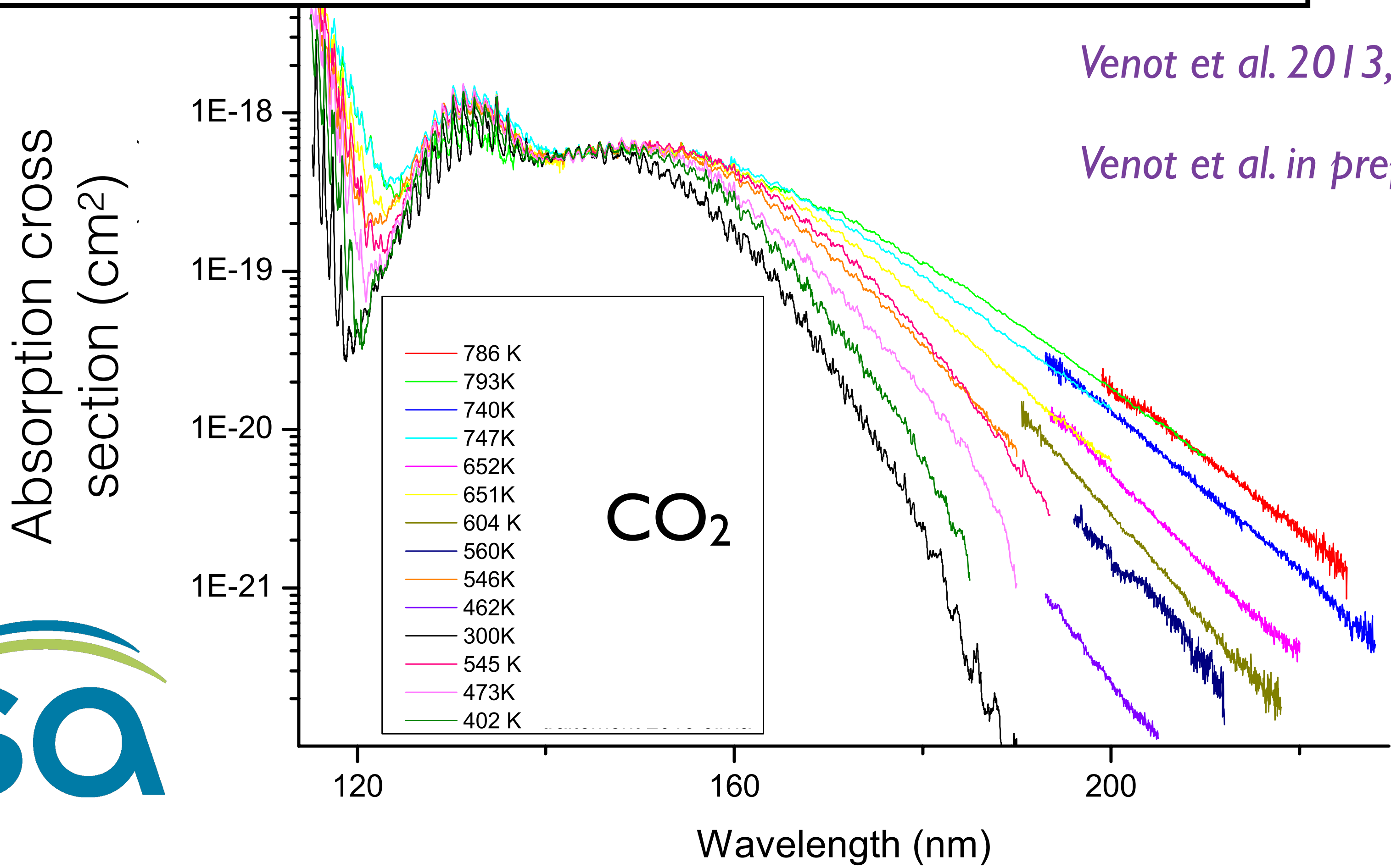
Thank you for your attention…



Venot et al. 2013, A&A

Venot et al. in prep