High-temperature chemistry and photochemistry for hot exoplanets atmospheres

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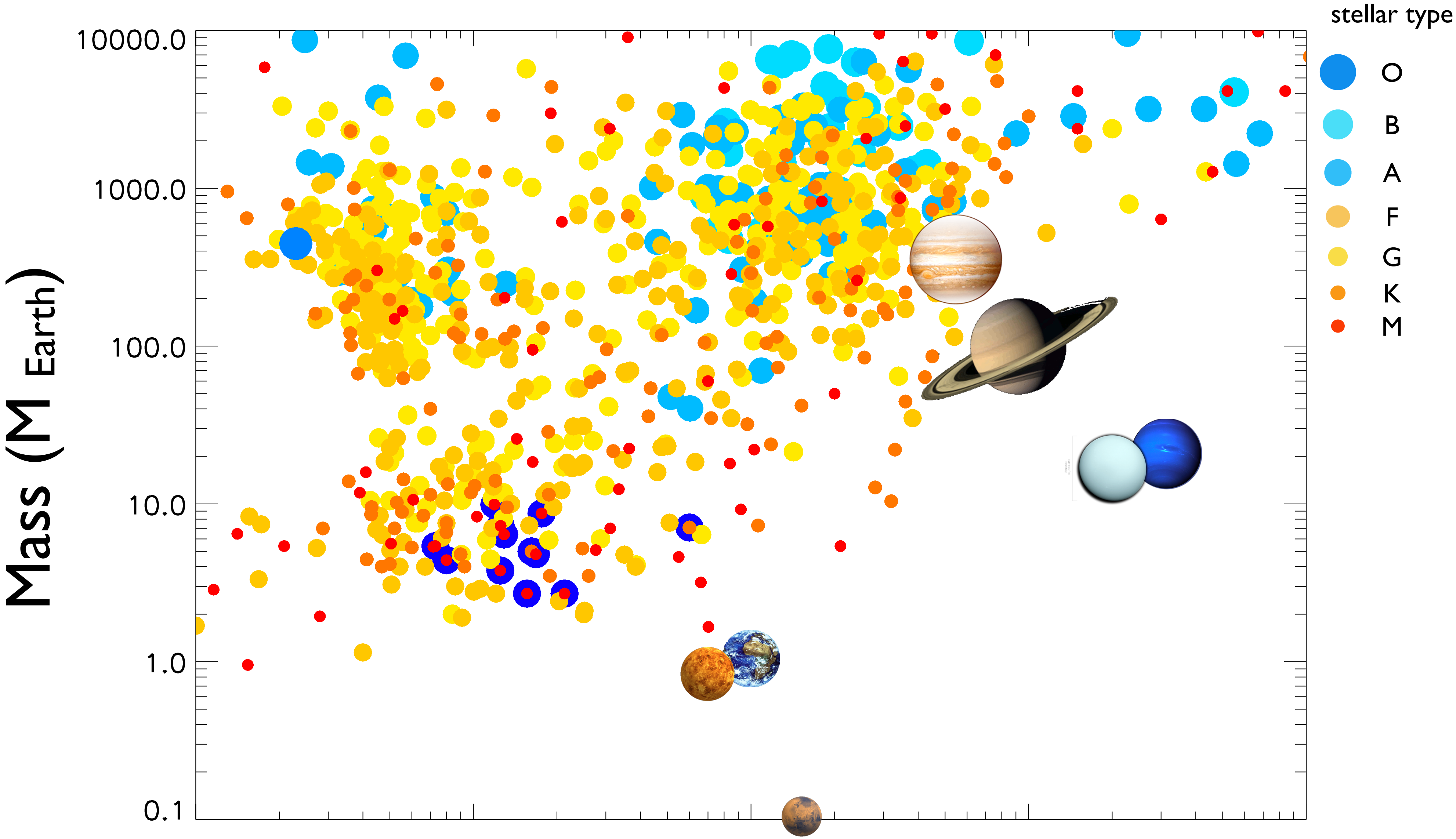


1915 exoplanets

source : exoplanet.eu (29 April 2015)

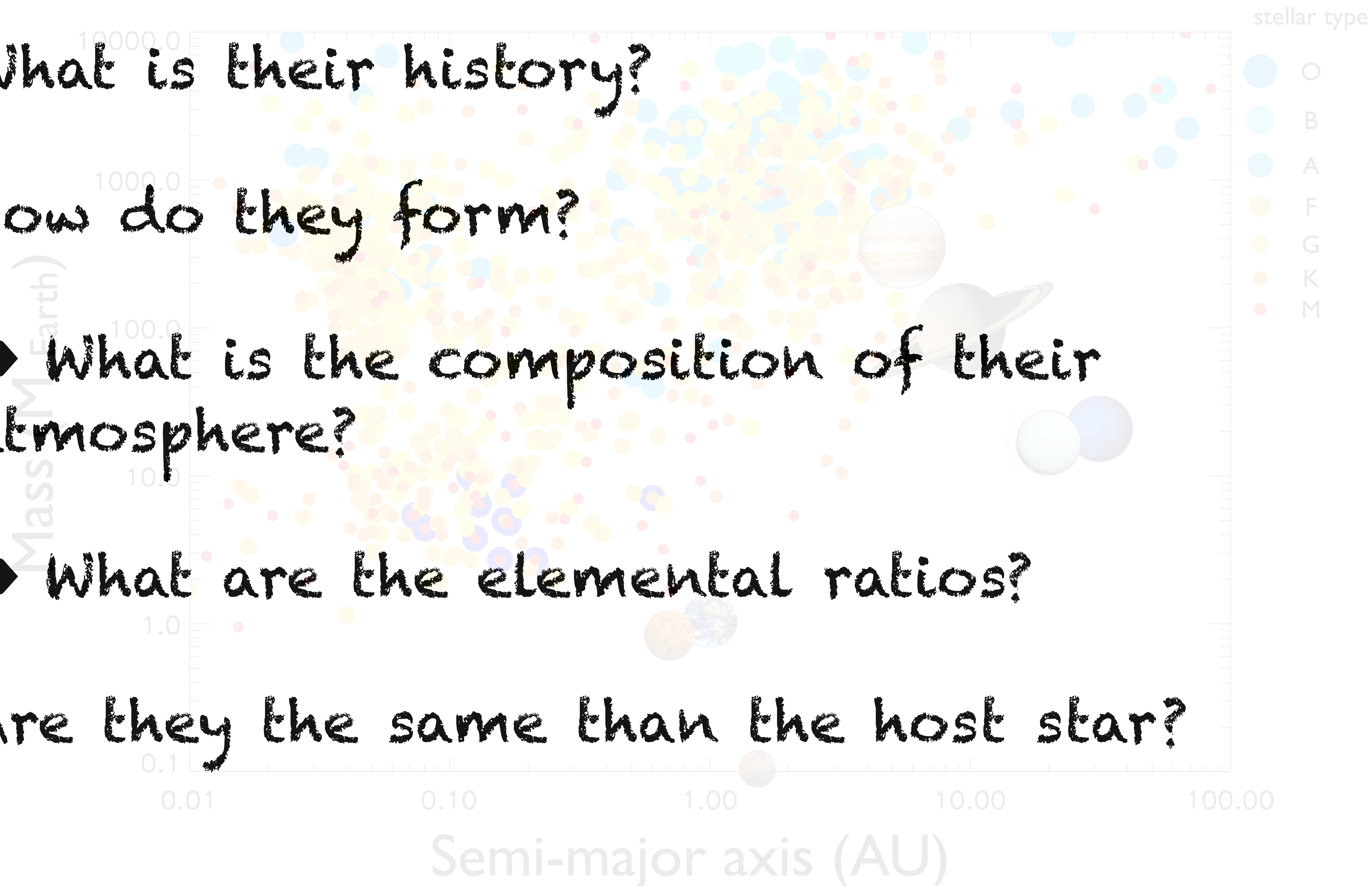
What is their history?

How do they form?

→ What is the composition of their atmosphere?

→ What are the elemental ratios?

Are they the same than the host star?



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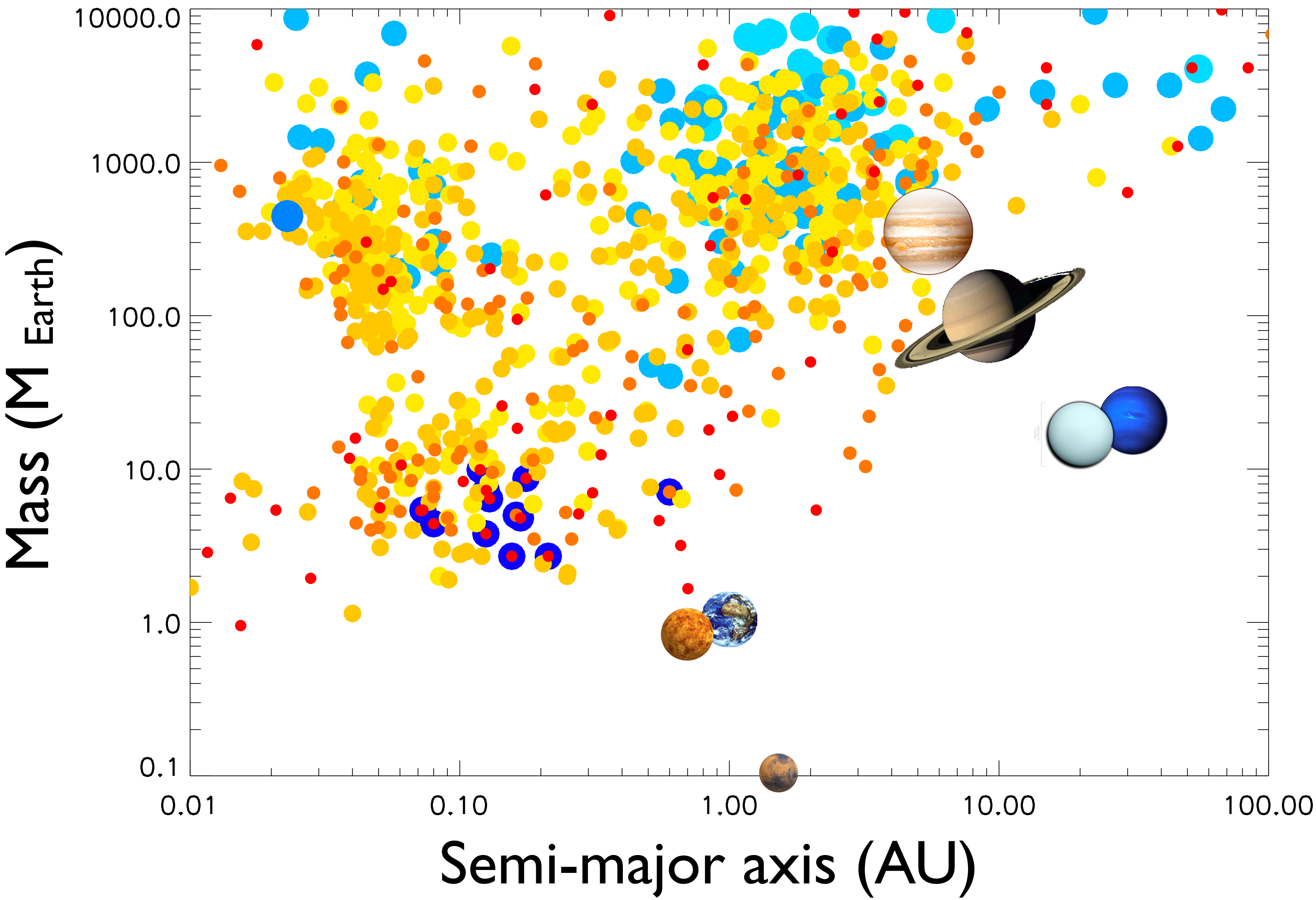

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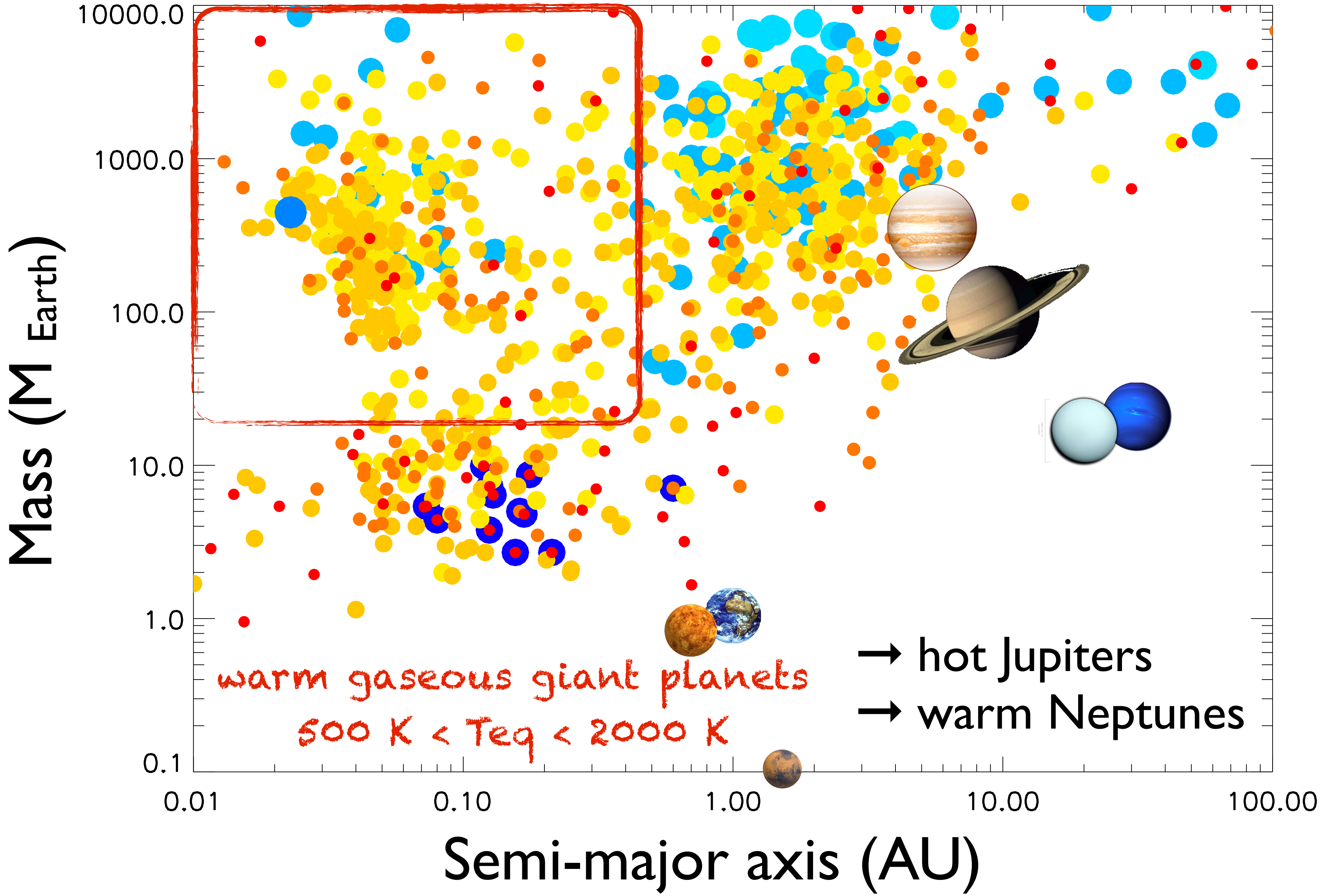

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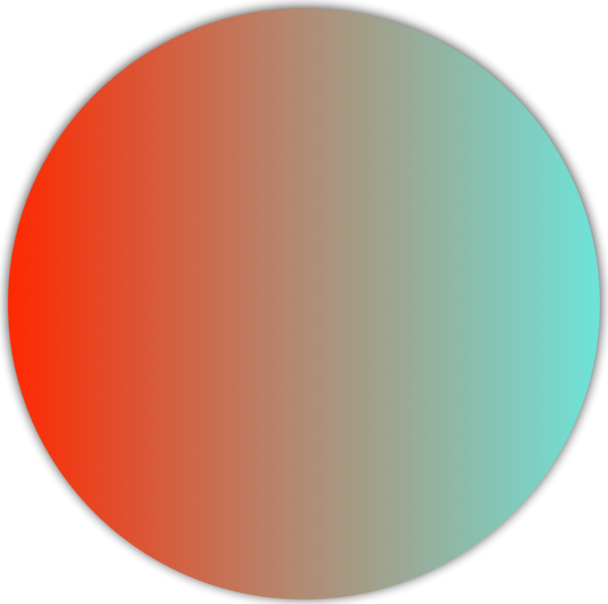
Out of equilibrium processes

Thermochemical equilibrium:
depends on P, T,
elementary abundances



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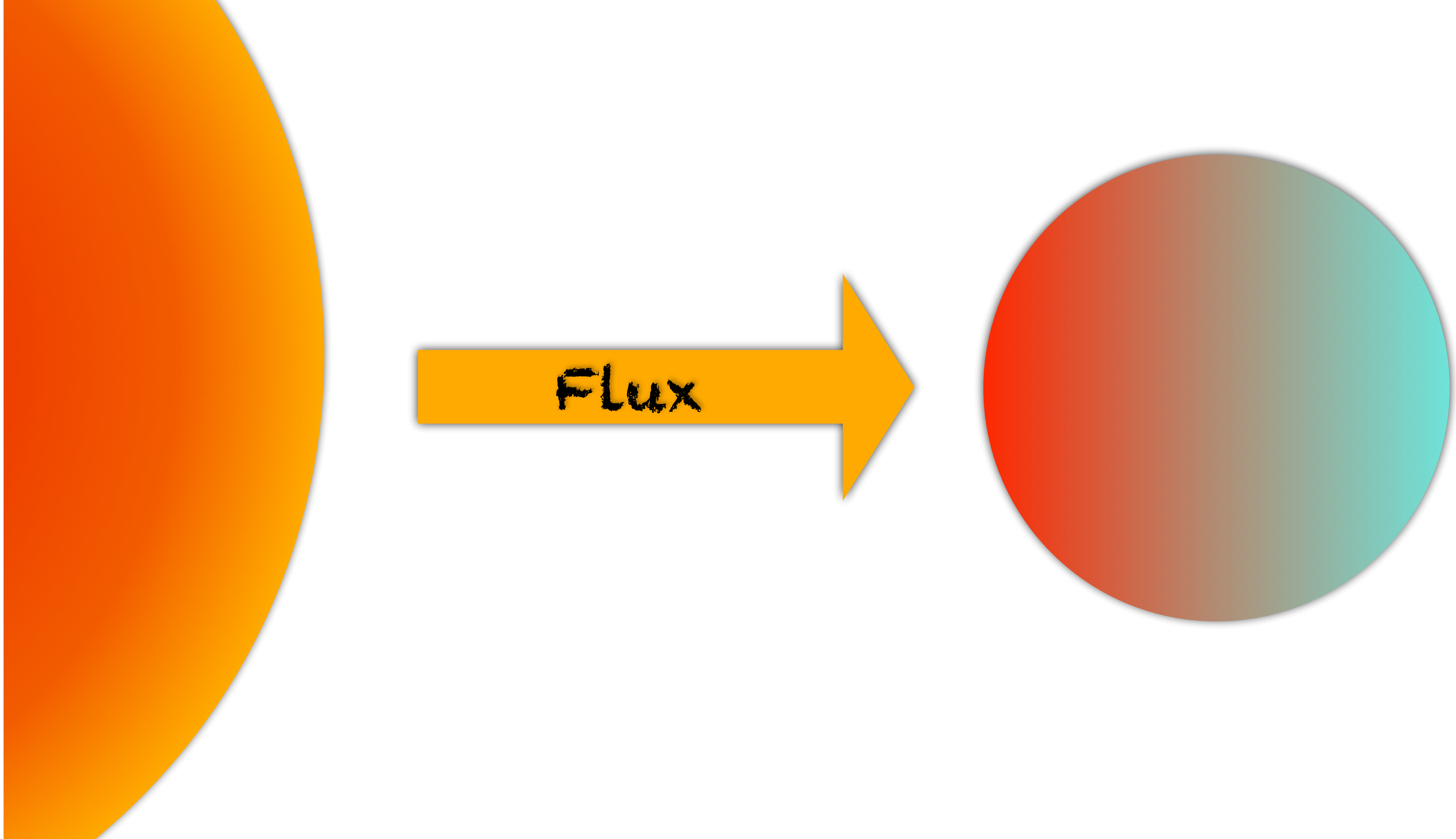

Out of equilibrium processes

Thermochemical equilibrium:
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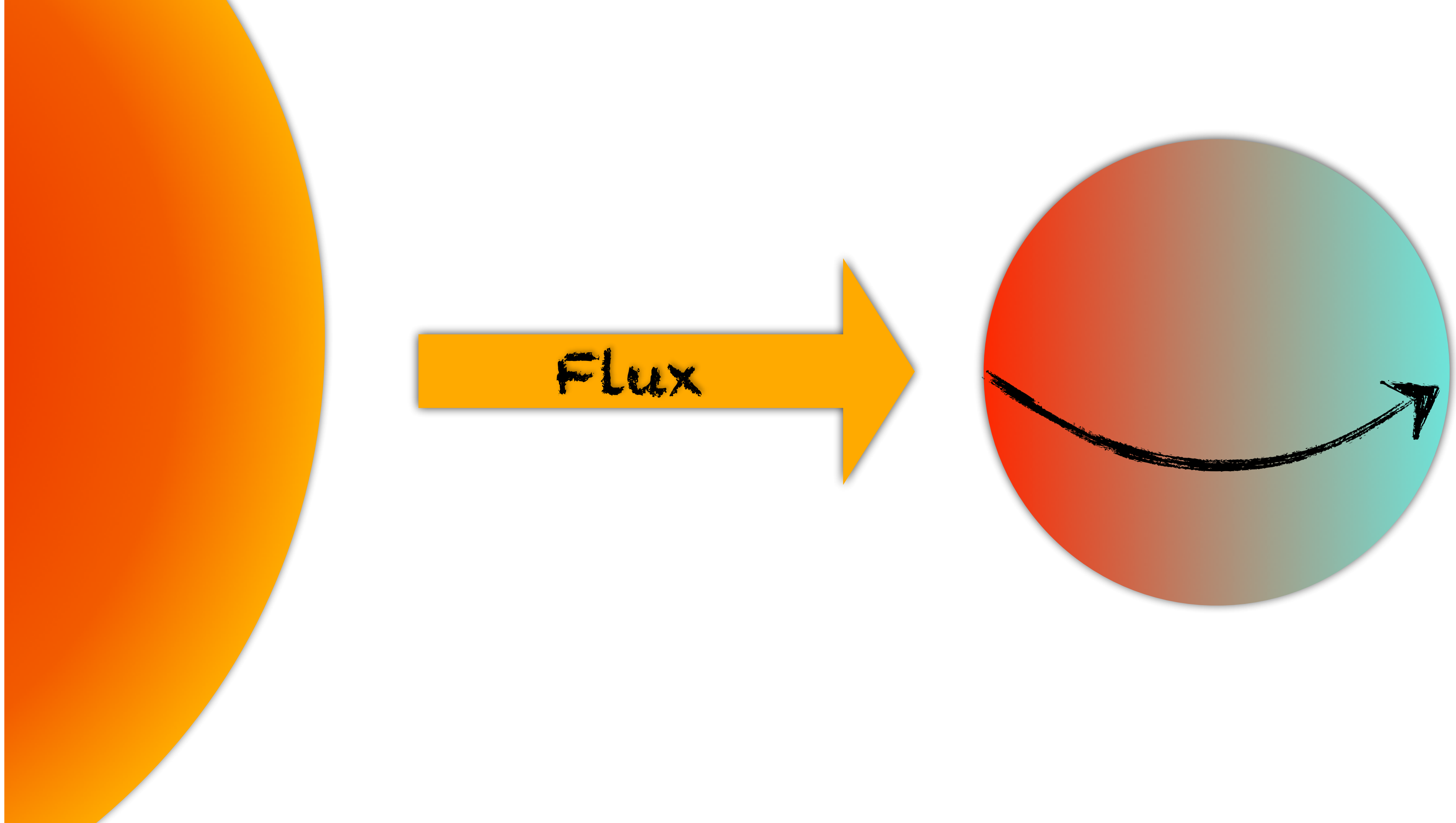
2. Horizontal circulation (winds)



Out of equilibrium processes

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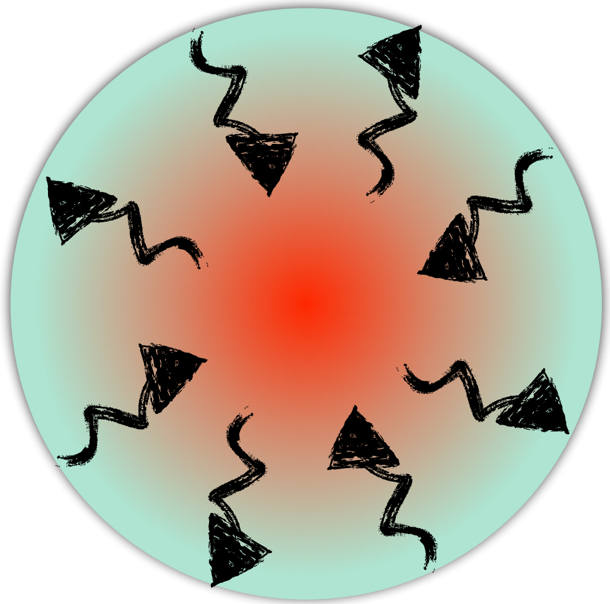
2. Horizontal circulation (winds)
3. Vertical mixing (convection, turbulence)



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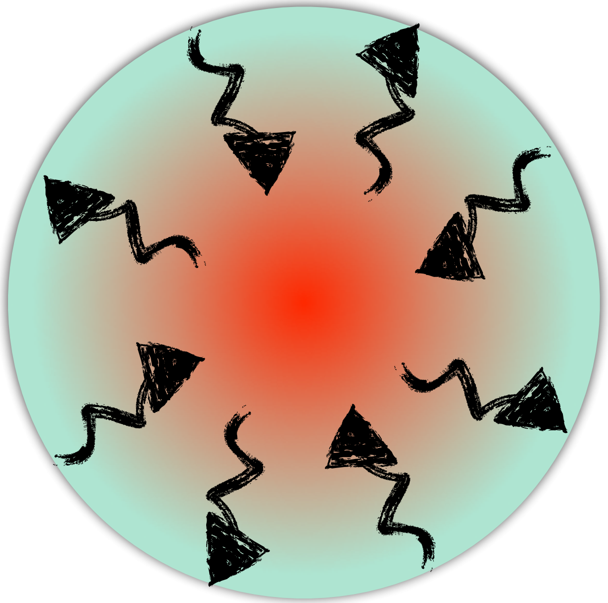
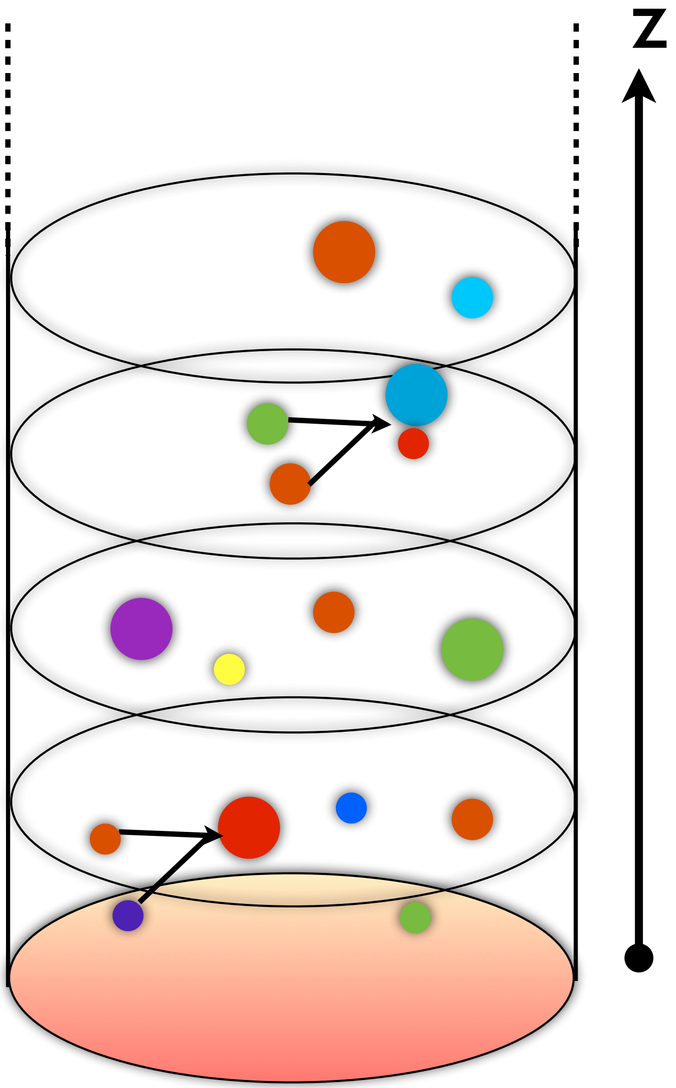


interpretation spectroscopy :

➡ need kinetic models

1D Model: kinetics, vertical mixing and photodissociations



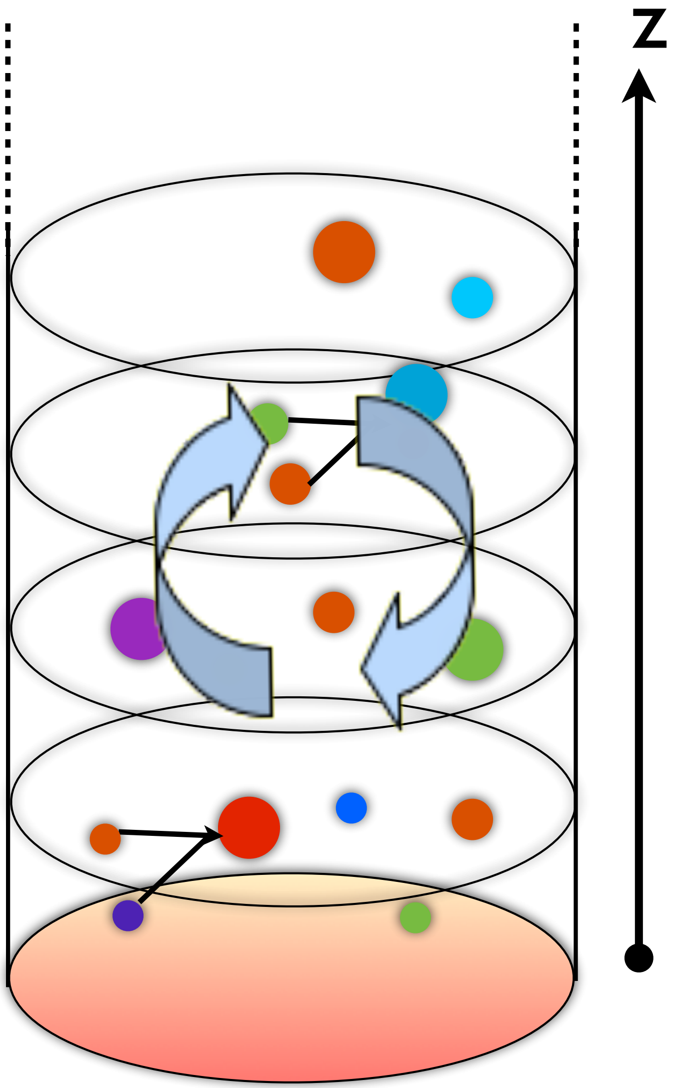
column of atmosphere with PT profile
~100 levels
chemical reactions at (P,T)

+ vertical mixing
+ UV flux ➙ photodissociations

For each compound and for each level, resolution of the continuity equation:

$$\underbrace{\frac{\partial n_i(z)}{\partial t}}_{\text{variation of the concentration } (cm^{-3}.s^{-1})} = \underbrace{P_i(z)}_{\text{production rate}} - \underbrace{n_i(z)L_i(z)}_{\text{loss rate}} - \underbrace{div(\Phi_i(z)\vec{e_z})}_{\text{vertical mixing}}$$

1D Model: kinetics, vertical mixing and photodissociations



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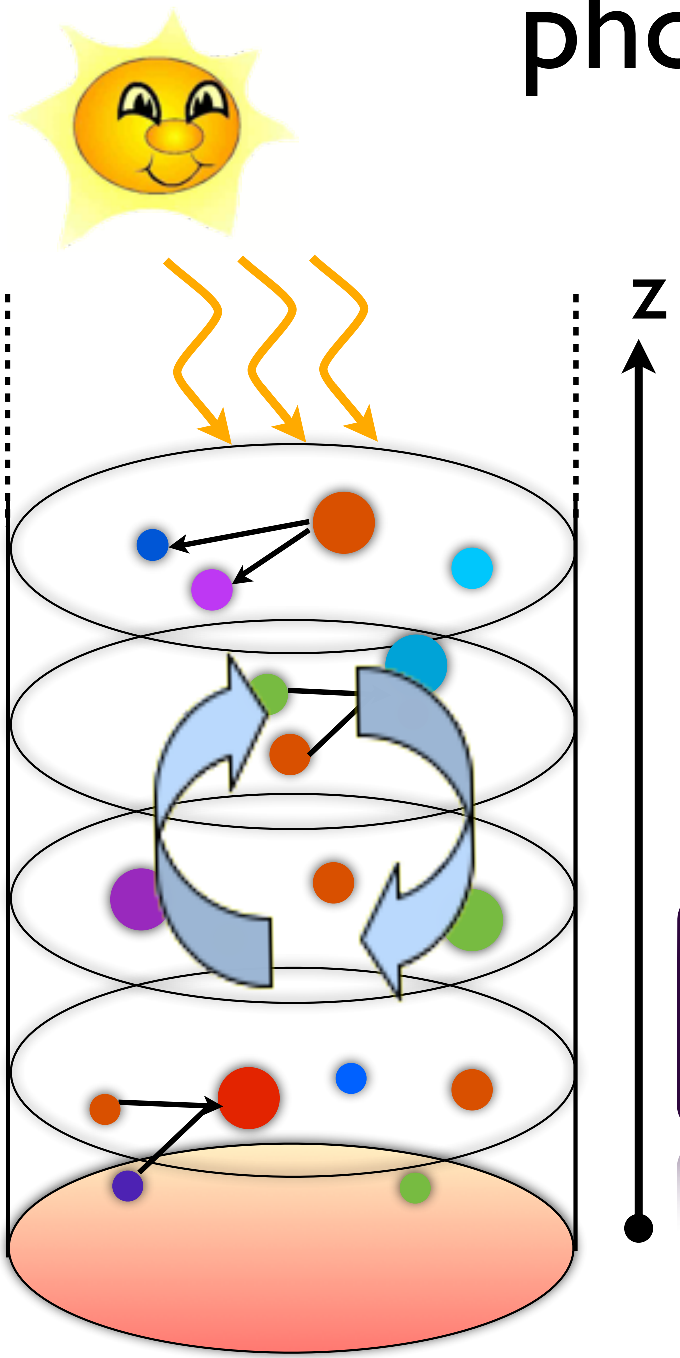
variation of the concentration ($cm^{-3}.s^{-1}$) — production rate — loss rate — vertical mixing

1D Model: kinetics, vertical mixing and photodissociations



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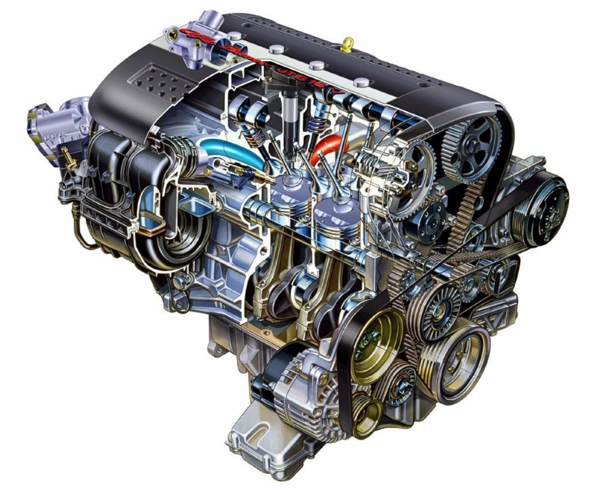
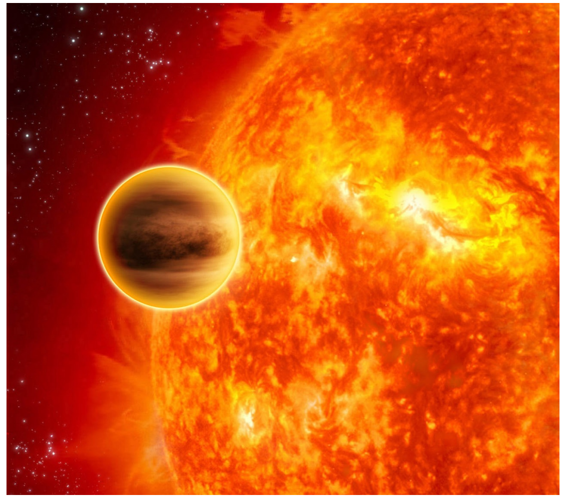
variation of the concentration ($cm^{-3}.s^{-1}$) | production rate | loss rate | vertical mixing

Development of the model:

Chemistry at high temperature

- Chemical networks **totally new** in planetology:



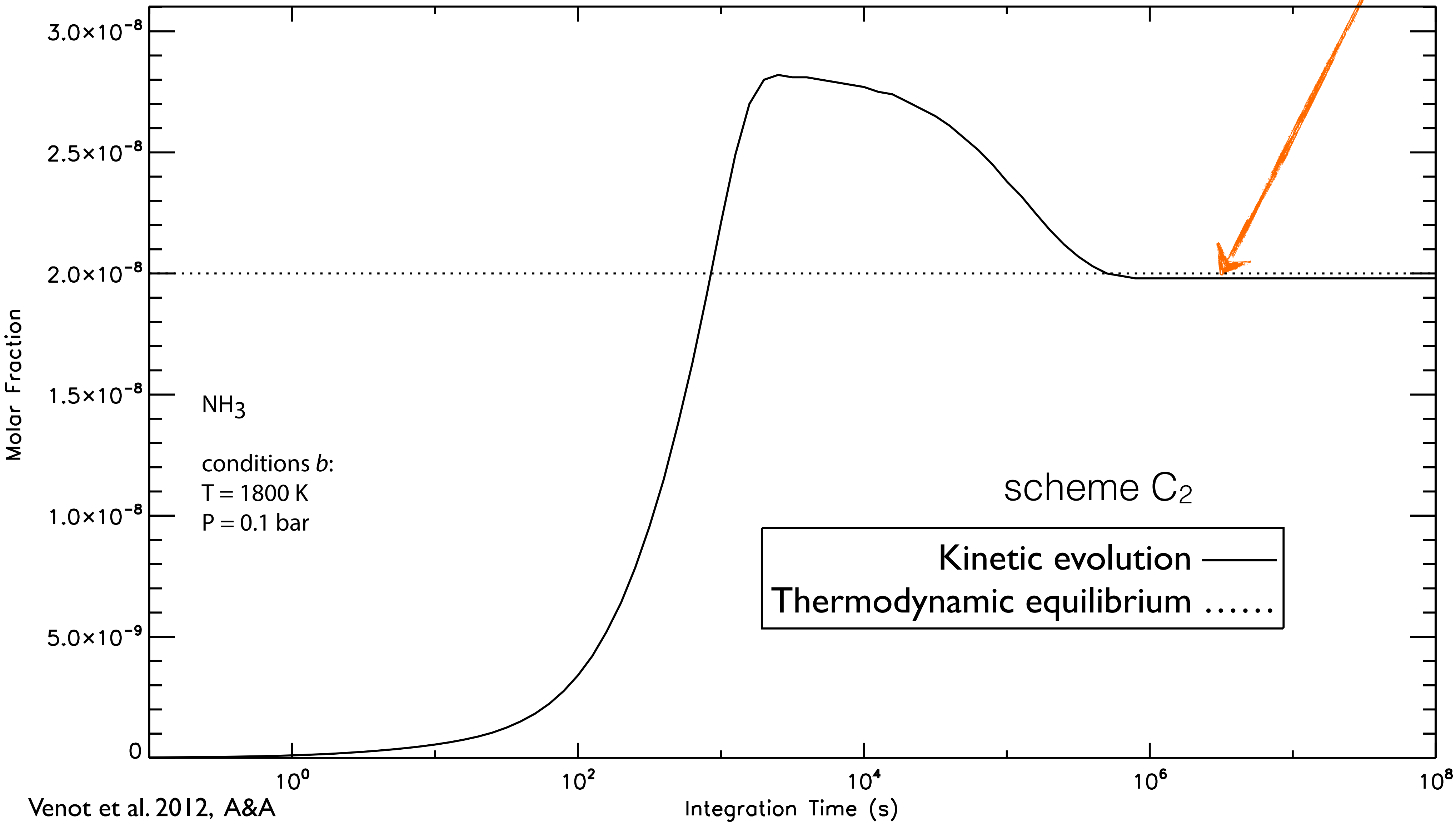


- **interdisciplinary** collaboration - specialist of combustion (LRGP, Nancy)
- schemes validated experimentally as **wholes** - large ranges P (10^{-3}-10^{2} bar) T (300-2500 K)
- 1920 reactions, 105 species (C,H,O,N), C_2 *Venot et al. 2012, A&A,*
- 4002 reactions, 240 species (C,H,O,N), C_6 *Venot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

0D Model : kinetic evolution

Initial conditions: solar elementary abundances, distributed between
H_2, CH_4, O_2, N_2, He

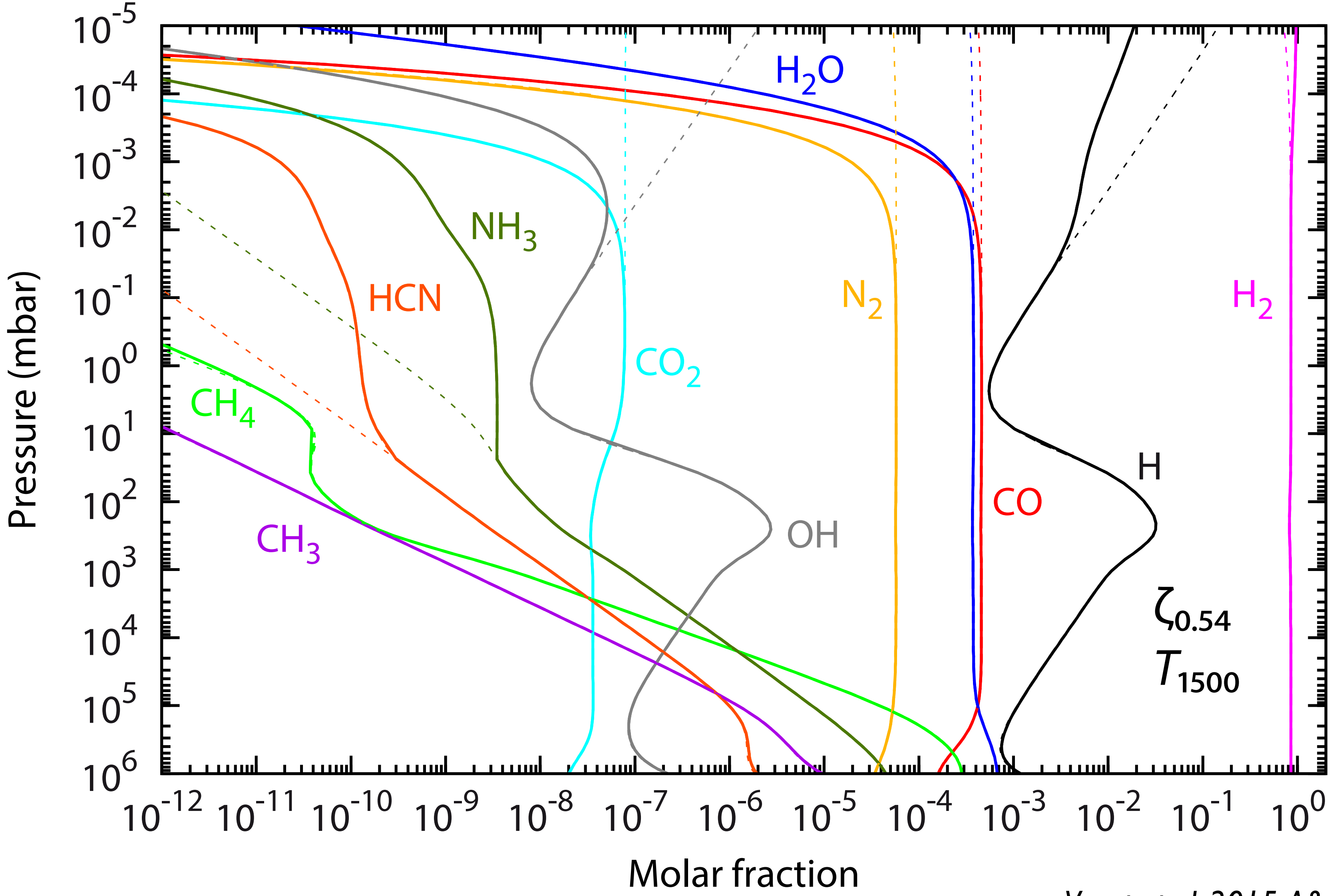
We reproduce
thermodynamic equilibrium



Venot et al. 2012, A&A

1D Model : effect of K_{zz} and $h\nu$

- - - thermo equilibrium —— kinetic model



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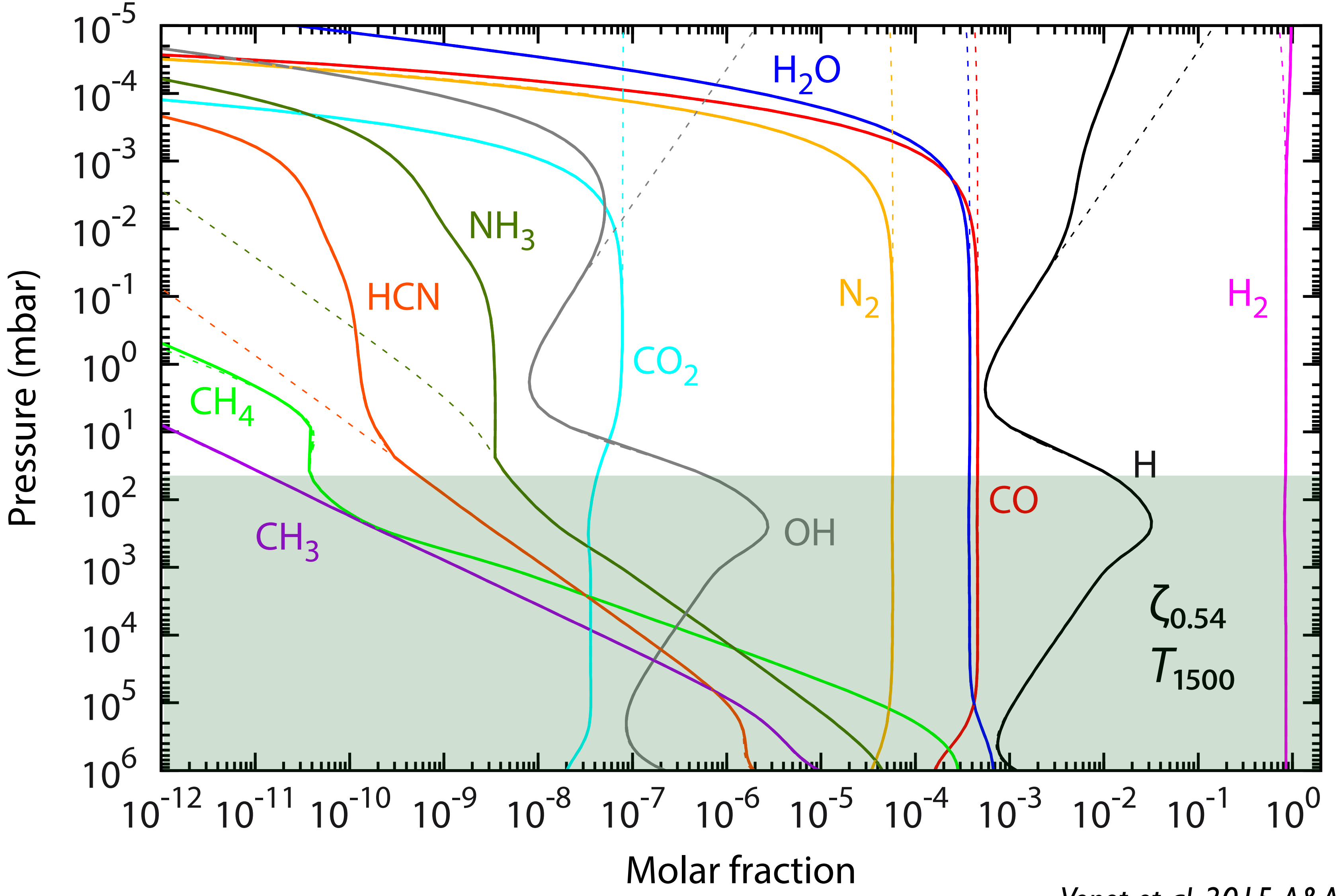


thermo eq.

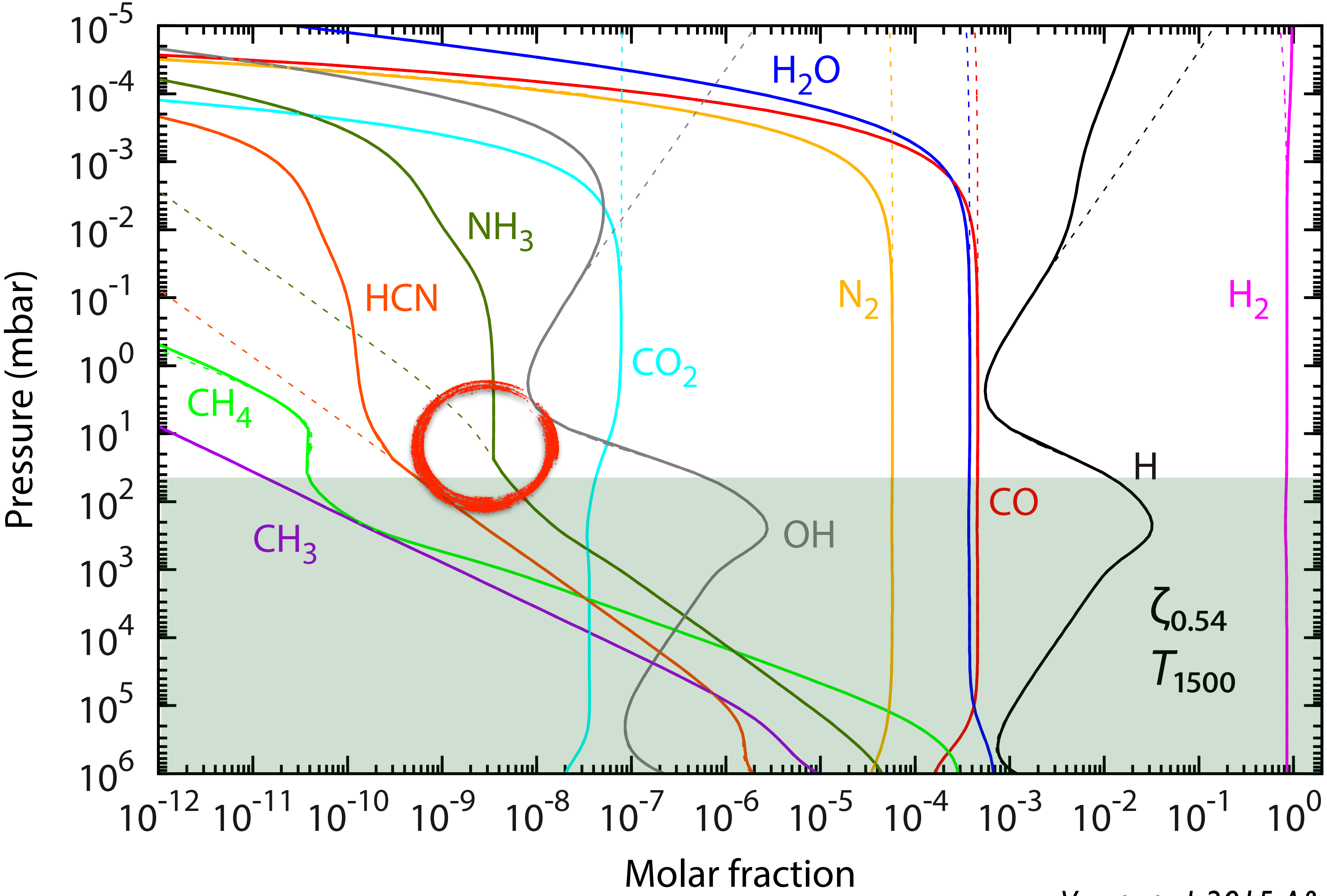
Venot et al. 2015, A&A

1D Model : effect of K_{zz} and $h\nu$

- - - thermo equilibrium —— kinetic model

quenching: abundances frozen when $\tau_{chem} > \tau_{dyn}$

thermo eq.



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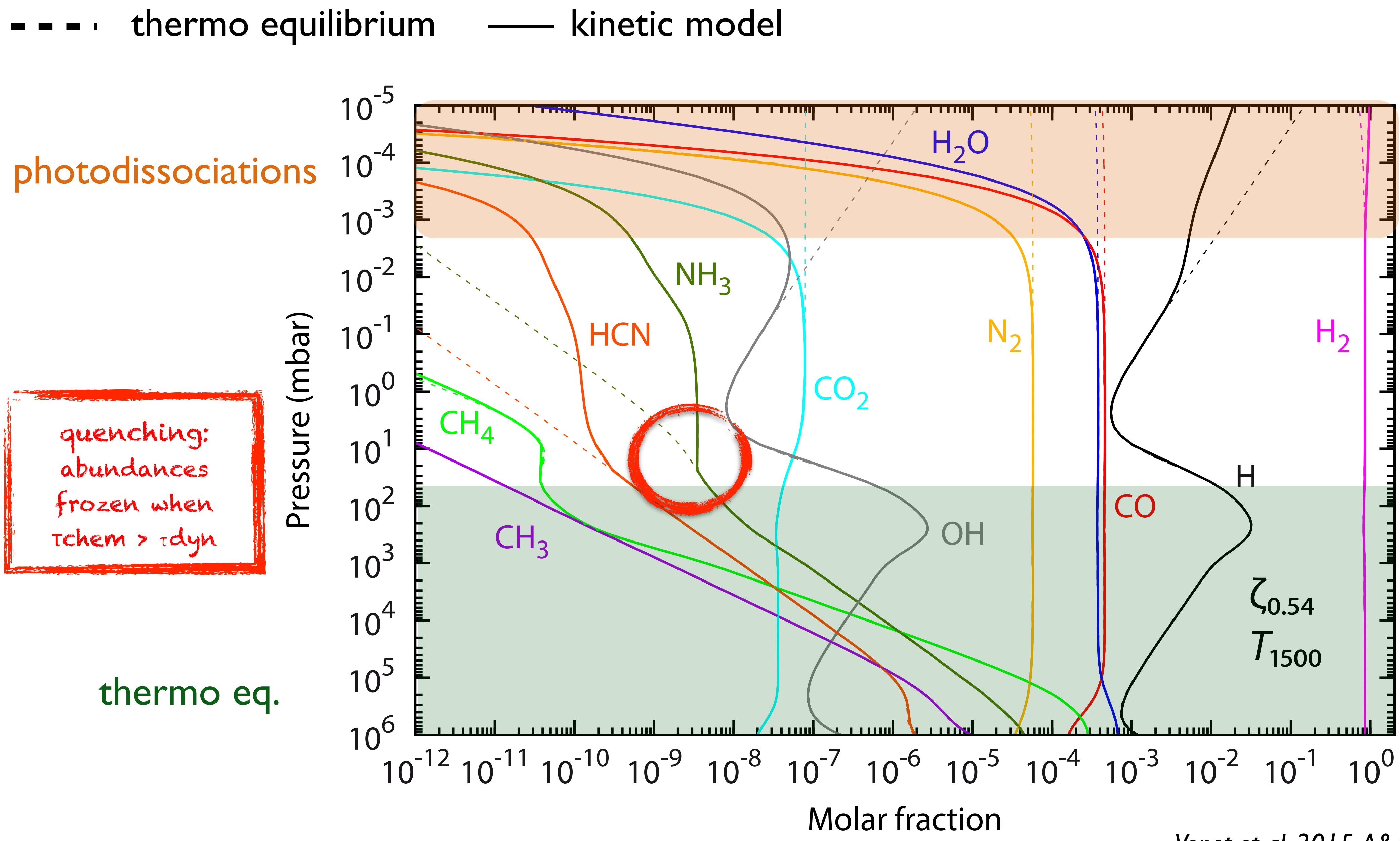


Venot et al. 2015, A&A

New chemical scheme

- strong chemical scheme indispensable
- C_2 chemical scheme might be insufficient for high C/O ratios (>1)

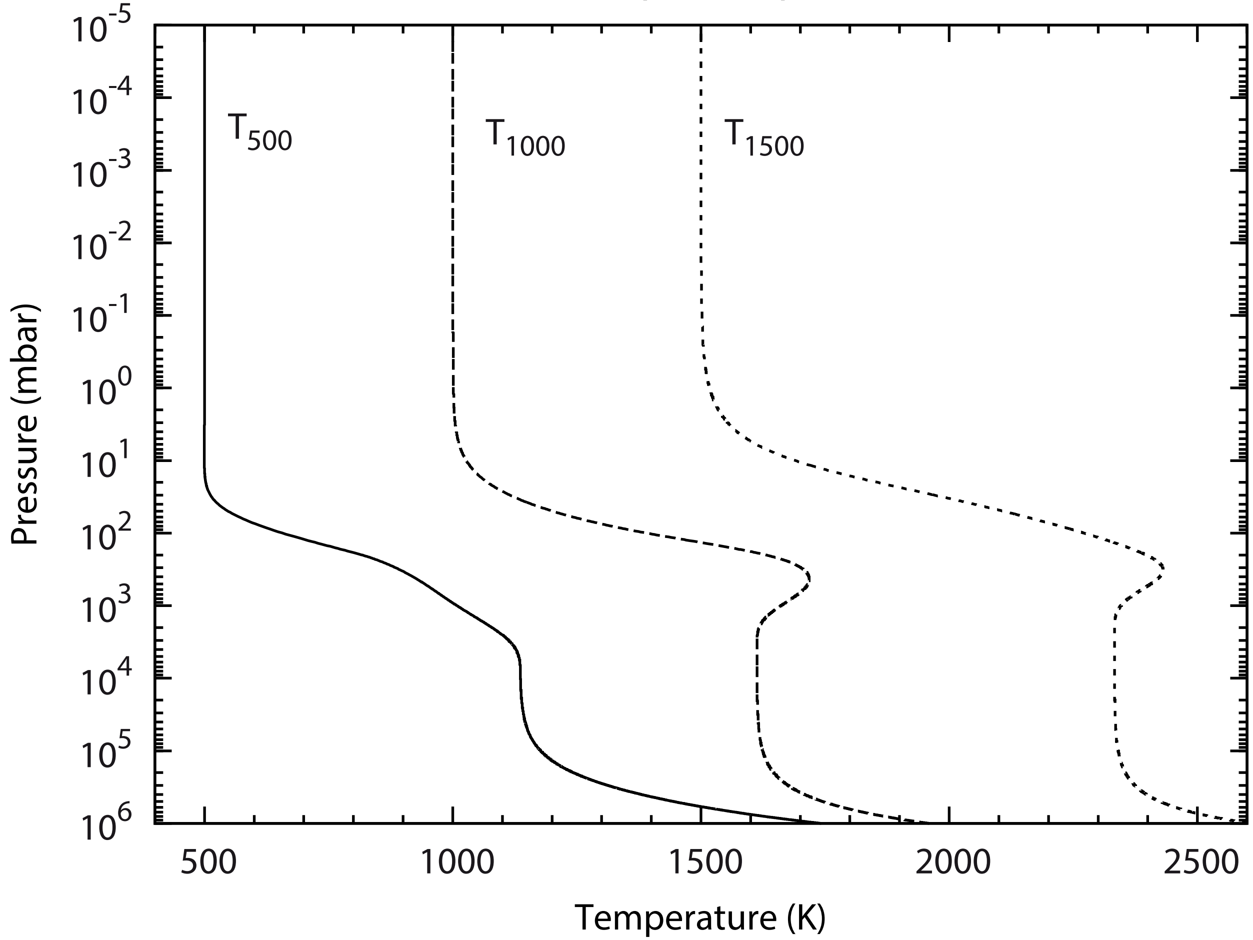
➡ C_6 chemical scheme

- 3 PT profiles with model of Parmentier & Guillot (2014)

Venot et al. 2015, A&A

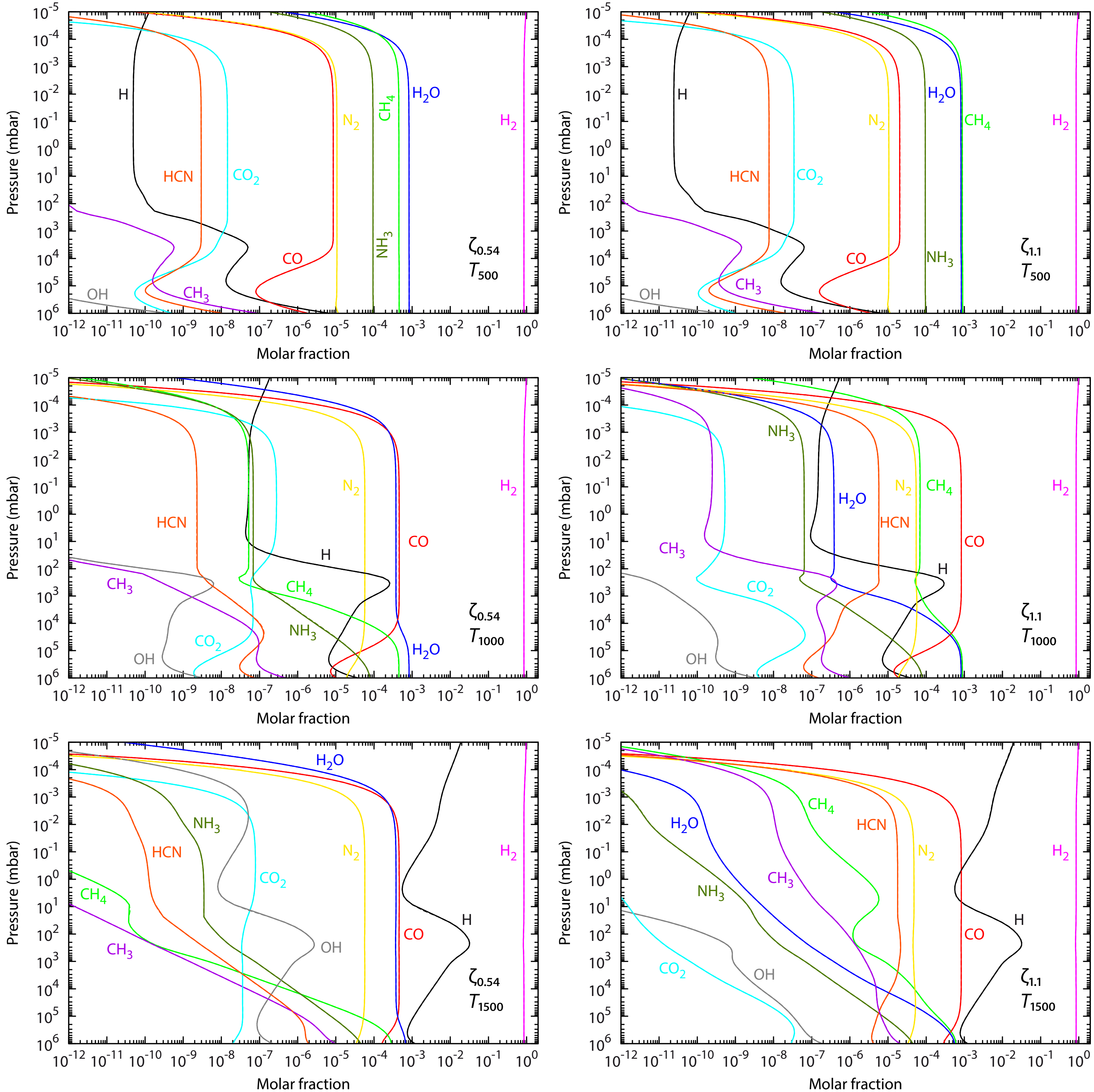
C/O ratio	0.54 - 1.1 (solar)
UV flux	with - without

⇒ 6 cases computed with both chemical schemes



No UV flux

C_6
C_2



Identical…

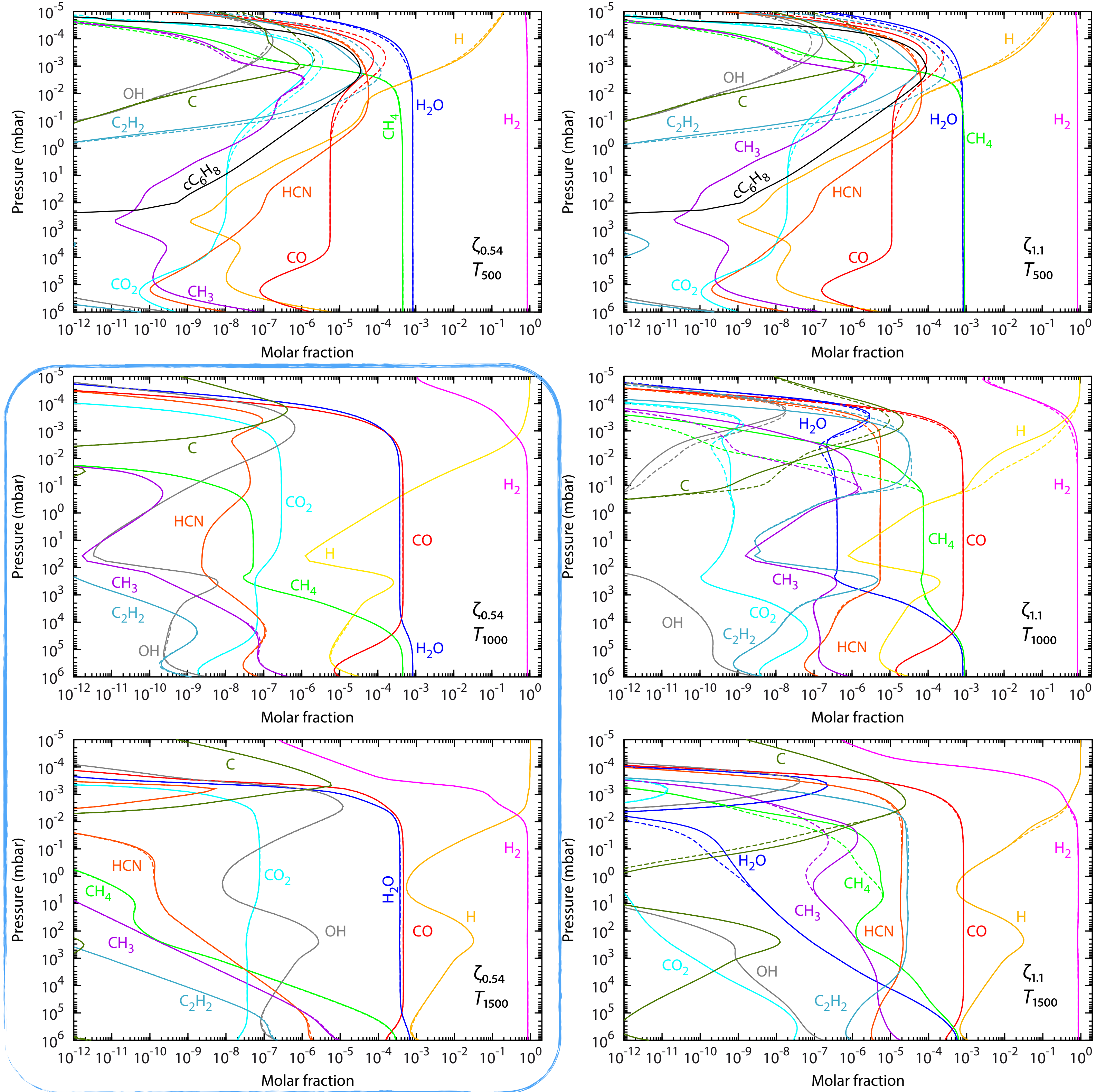
C_2 scheme very robust !

Venot et al. 2015, A&A

With UV flux

—— C_6

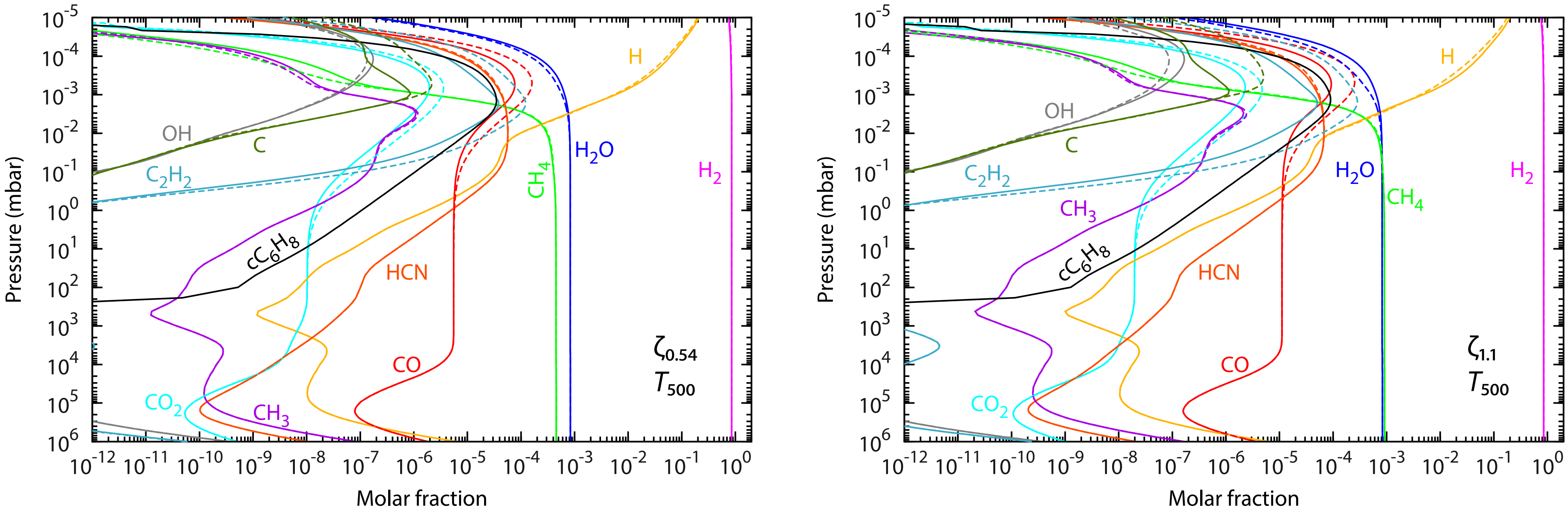
– – – C_2



Differences in the upper atmosphere

No difference for high T and C/O = solar

Venot et al. 2015, A&A



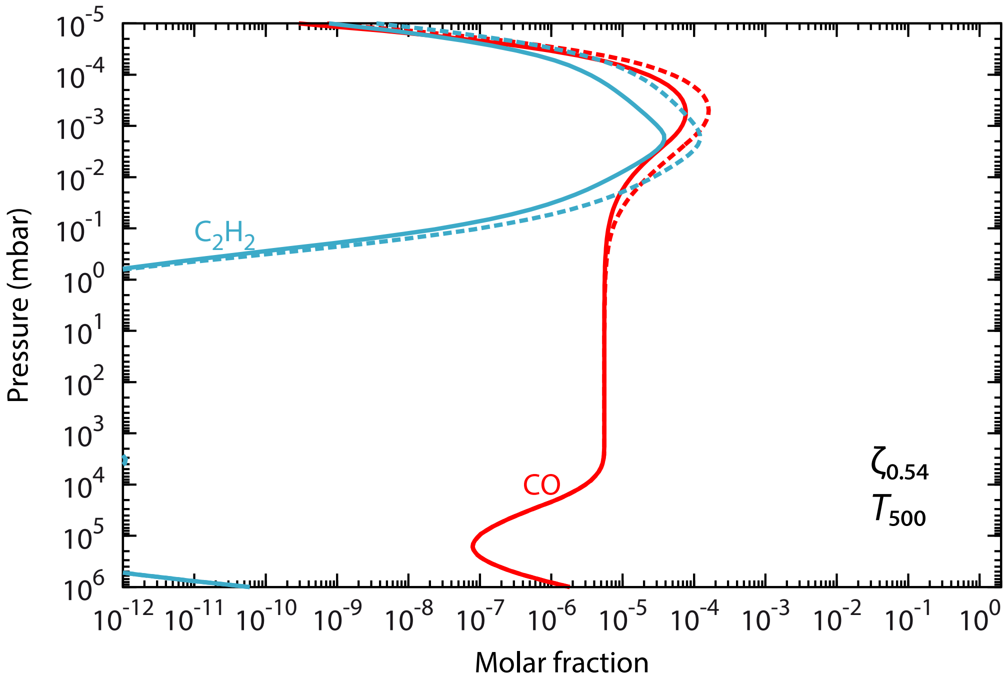
C_2

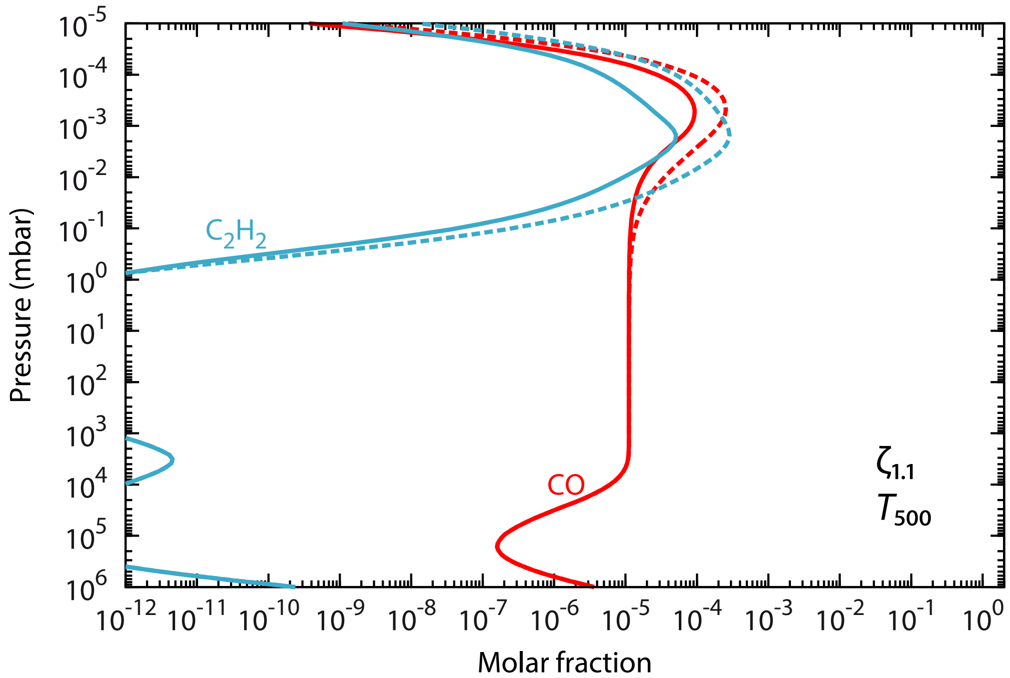
C_6

500 K

C/O (ζ) 0.54 vs 1.1 :
- slight increase of hydrocarbons amount (CH_4, CO,…)

Venot et al. 2015, A&A





.... C_2

—— C_6

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C_2 vs C_6 :
- C_2H_2, CO are less abundant with C_6 scheme

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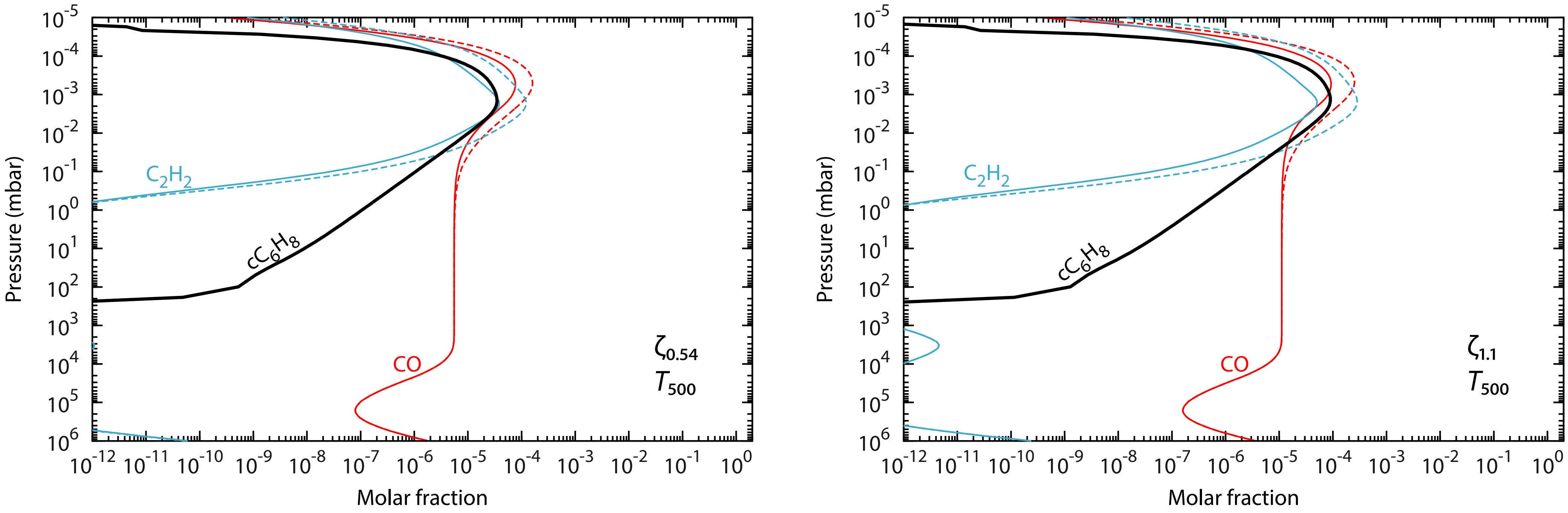

······ C_2

—— C_6

500 K

CO + hν → C + O(^{3}P)
C + H_2 → CH + H
CH + H_2 → $^3CH_2$ + H
$^3CH_2$ + C → C_2H + H
C_2H + H → **C_2H_2**
2 **C_2H_2** → nC_4H_3 + H
nC_4H_3 + **C_2H_2** → lC_6H_5
lC_6H_5 → cC_6H_5
cC_6H_5 + H → cC_6H_6
cC_6H_6 + H → cC_6H_7
cC_6H_7 + H → **cC_6H_8**

CO + 2 **C_2H_2** + 2 H_2 + C → **cC_6H_8** + O(^{3}P)

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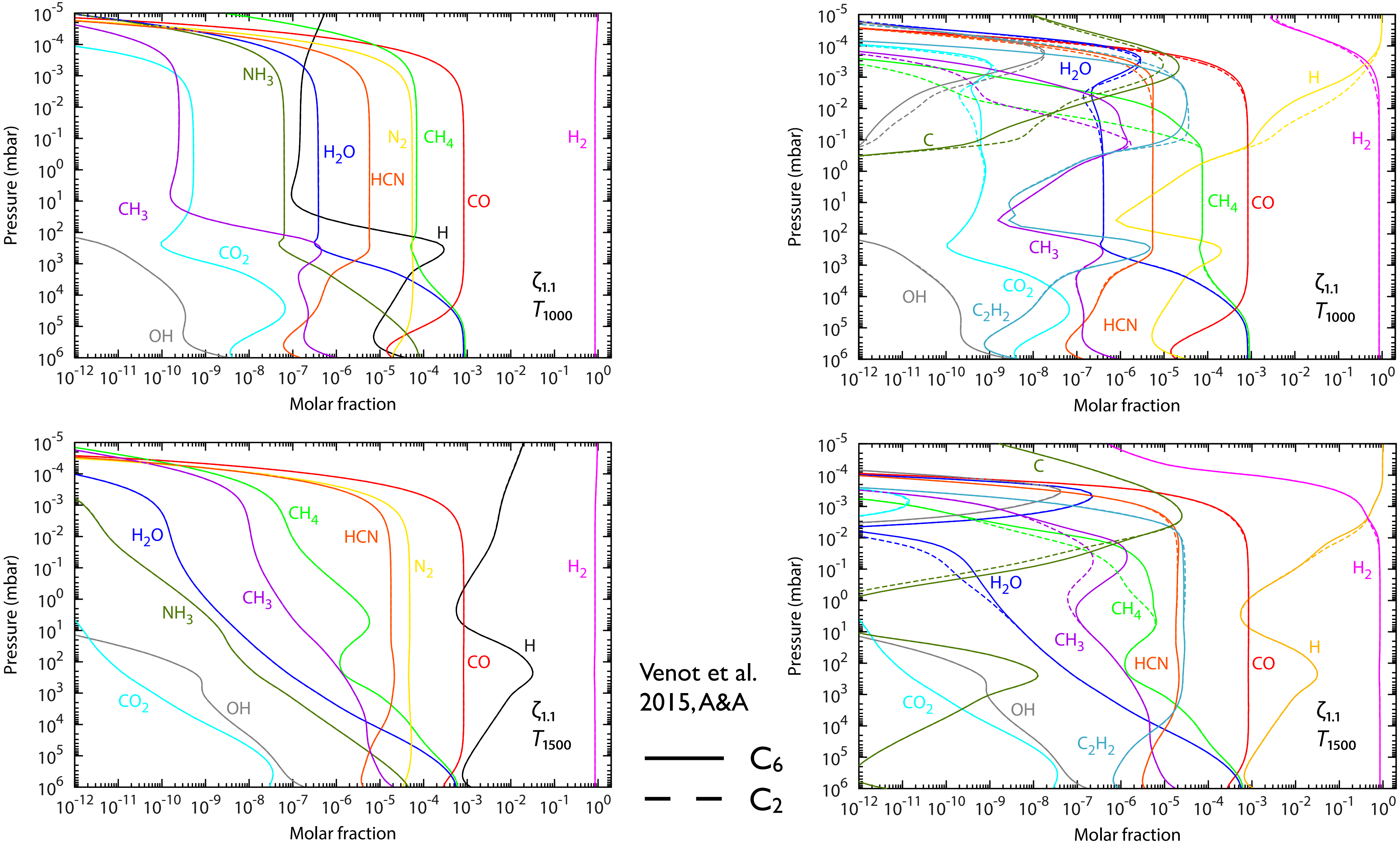
Venot et al. 2015, A&A

No UV flux

importance of photodissociations !

With UV flux

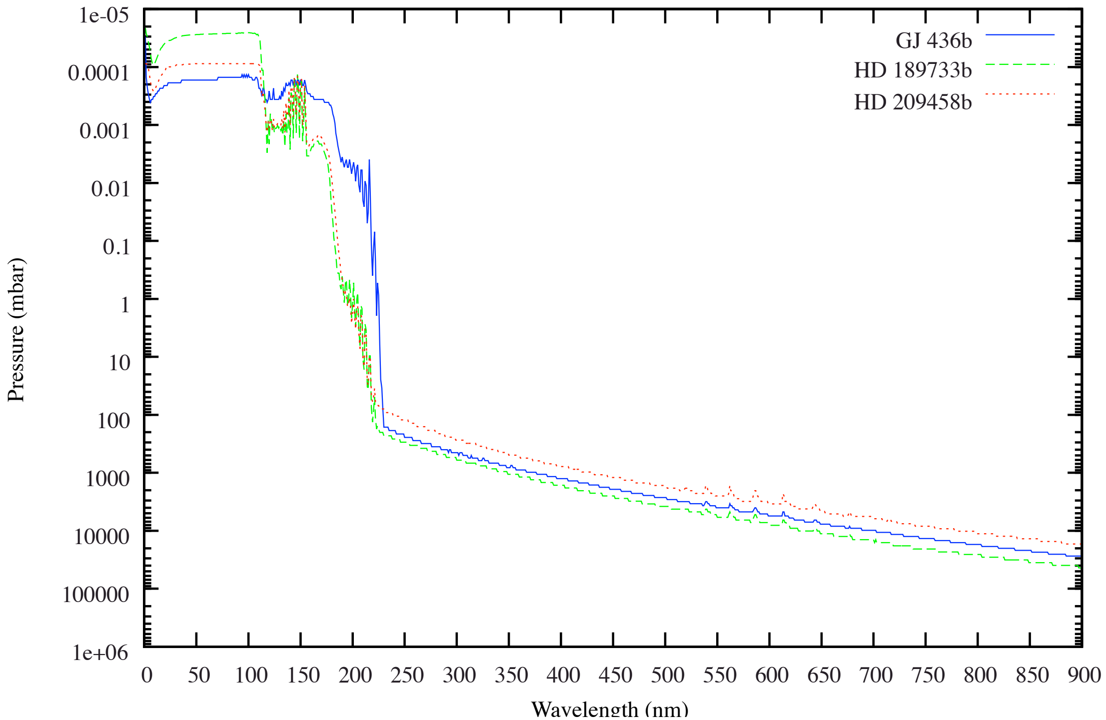


Venot et al. 2015, A&A

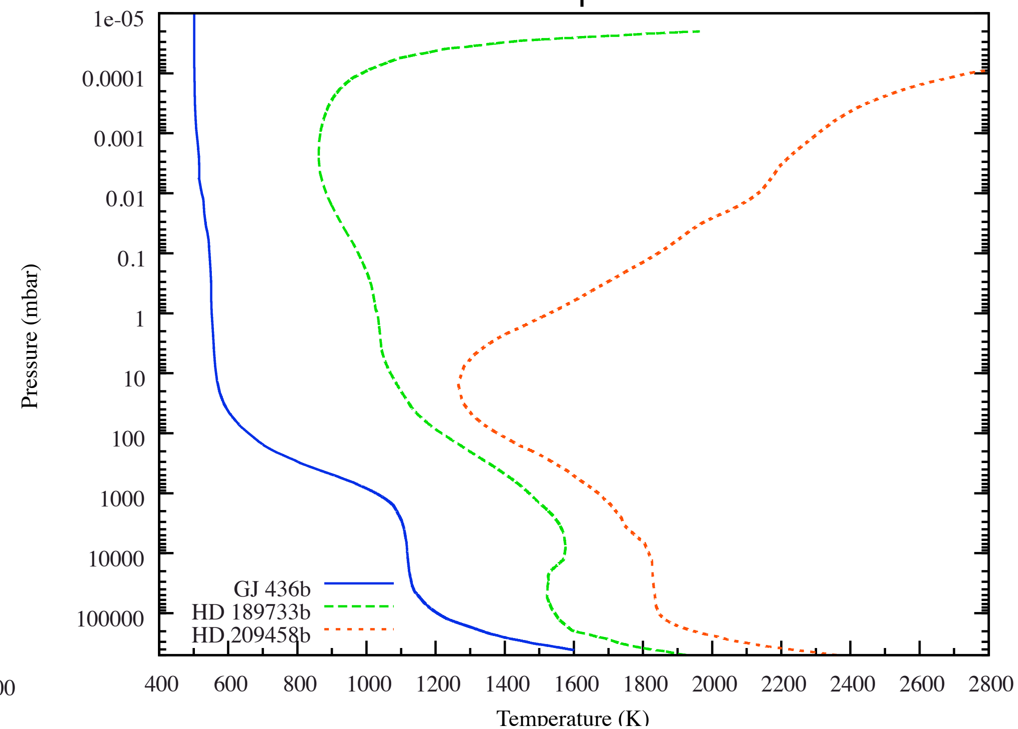
Effect of photodissociations

HD189733b, HD209458b (hot Jupiters), and GJ436b (warm Neptune)

penetration of UV flux (level where τ=1)



thermal profiles



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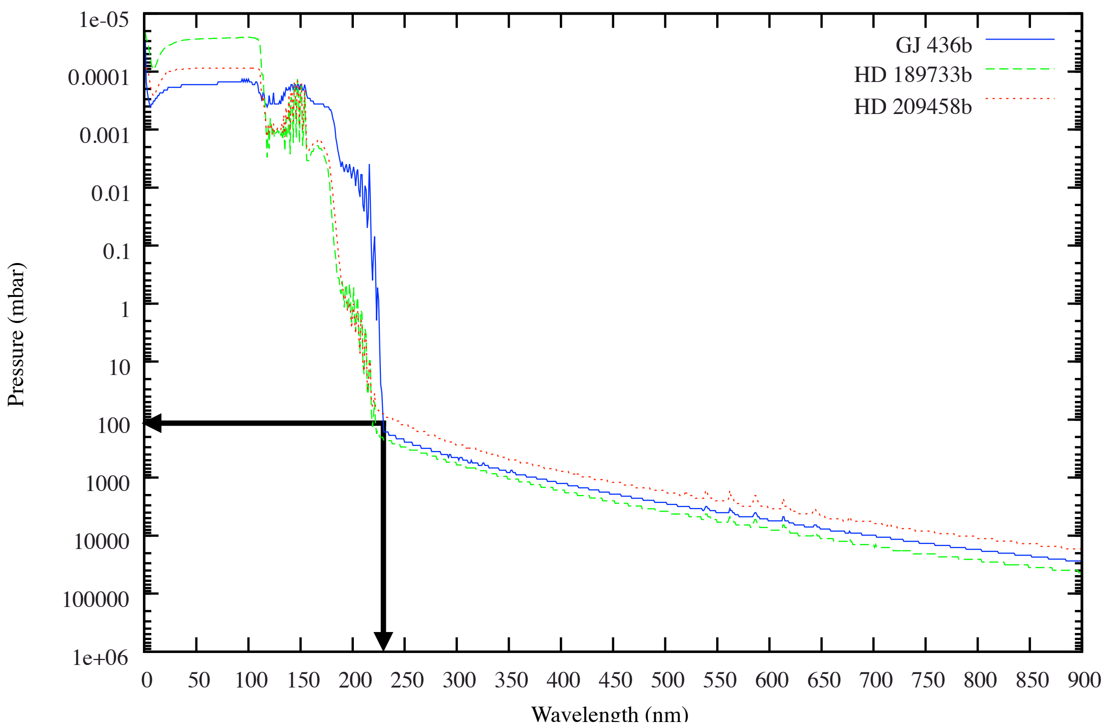

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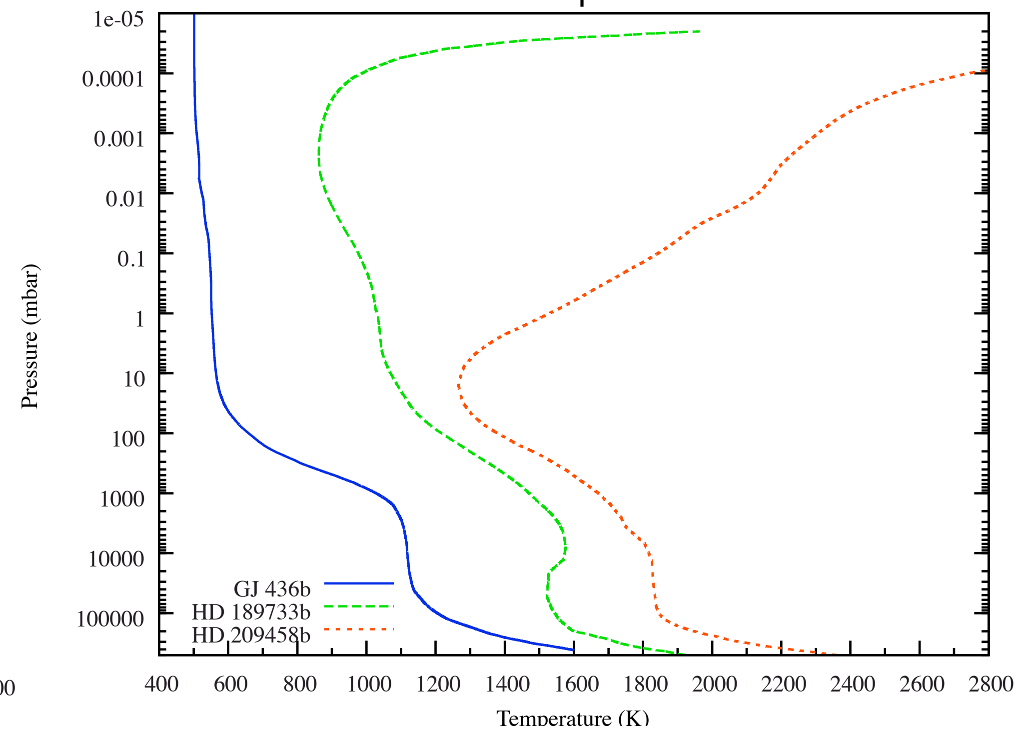

λ of interest : < 250 nm

absorbed at P < 100 mbar

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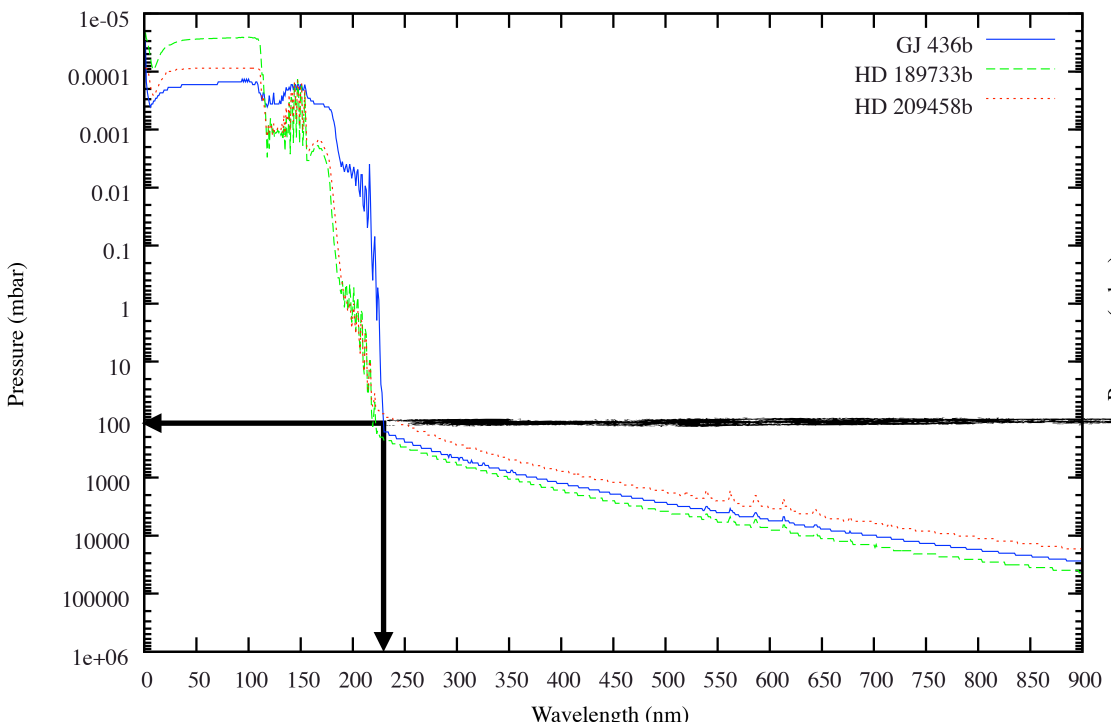

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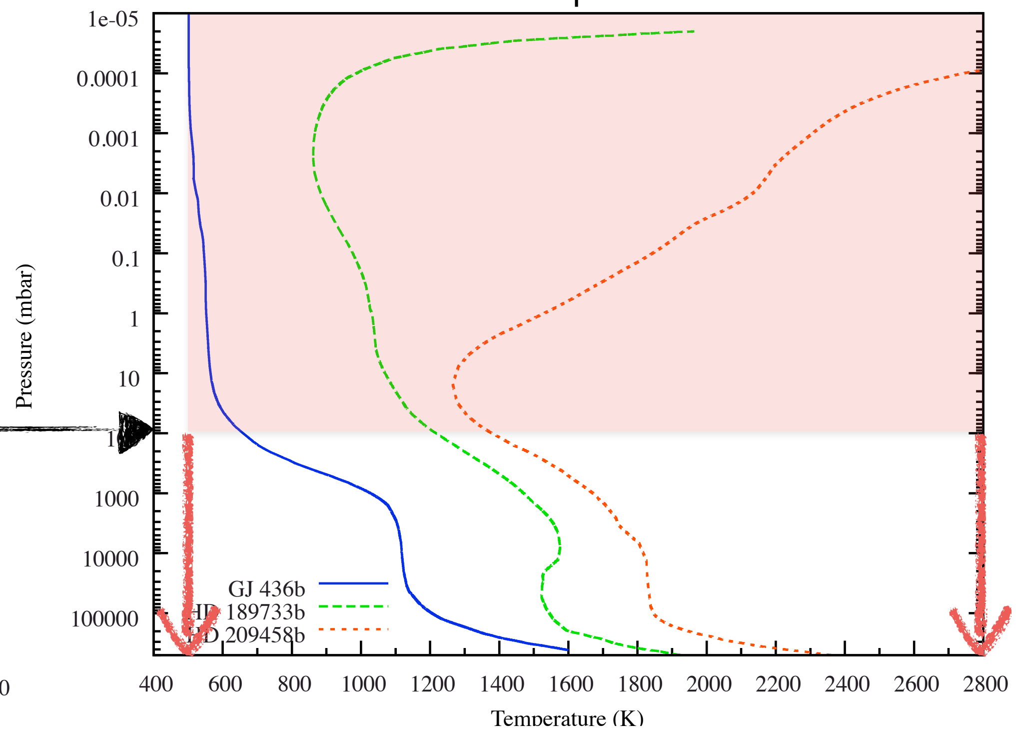


λ of interest : < 250 nm → 500 – 2800 K !

absorbed at P < 100 mbar

Absorption cross sections

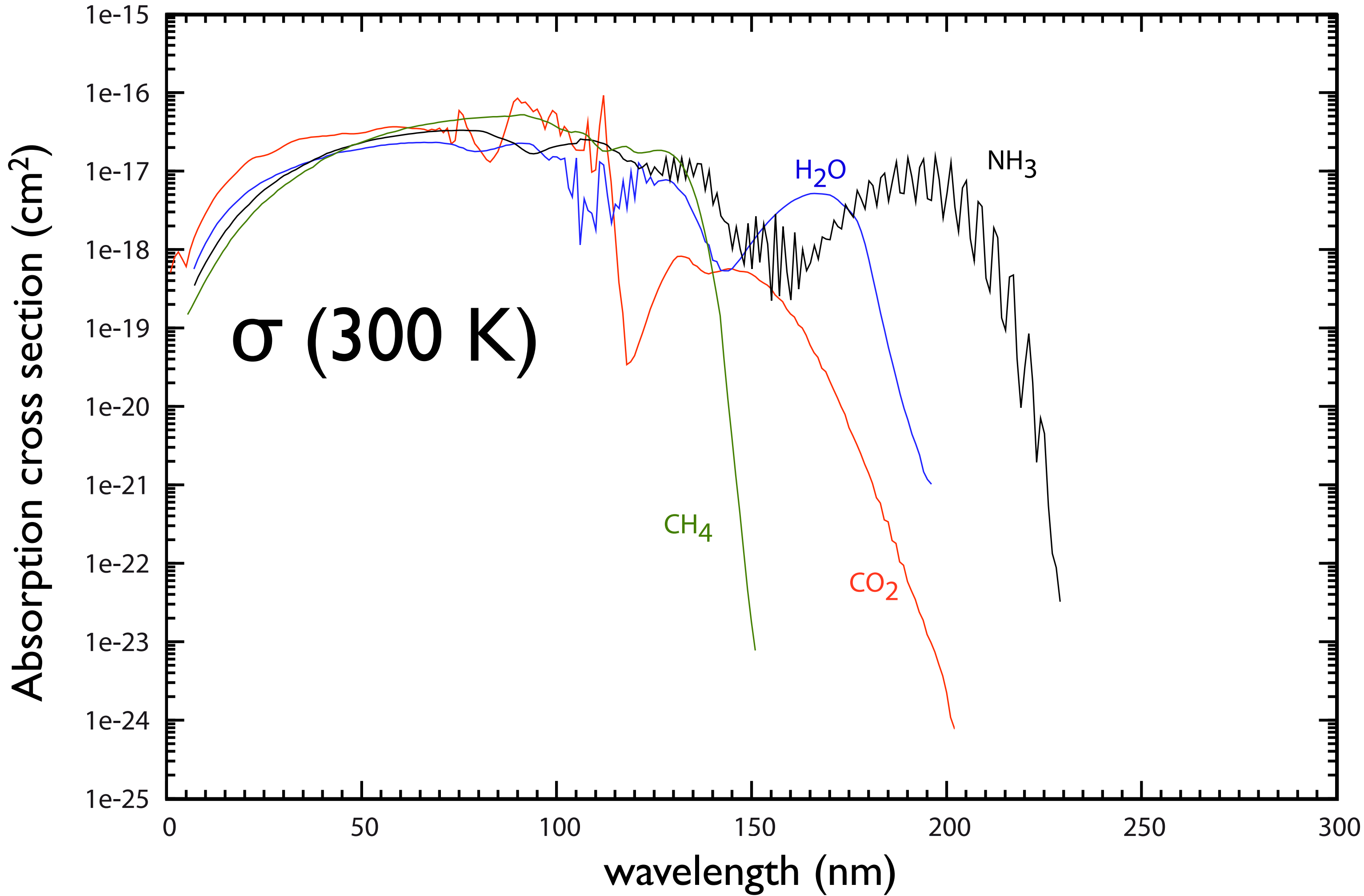
$\sigma(\lambda,T)$: capacity to absorb flux

Photodissociations rate:

$$J^k(z) = \int_{\lambda_1}^{\lambda_2} \sigma(\lambda,T) F(\lambda,z) q_k(\lambda,T) d\lambda$$

Actinic flux :

$$F(\lambda,z) = F_0(\lambda) \exp\left(-\sigma(\lambda,T)\int_z^{\infty} n(h)dh\right)$$



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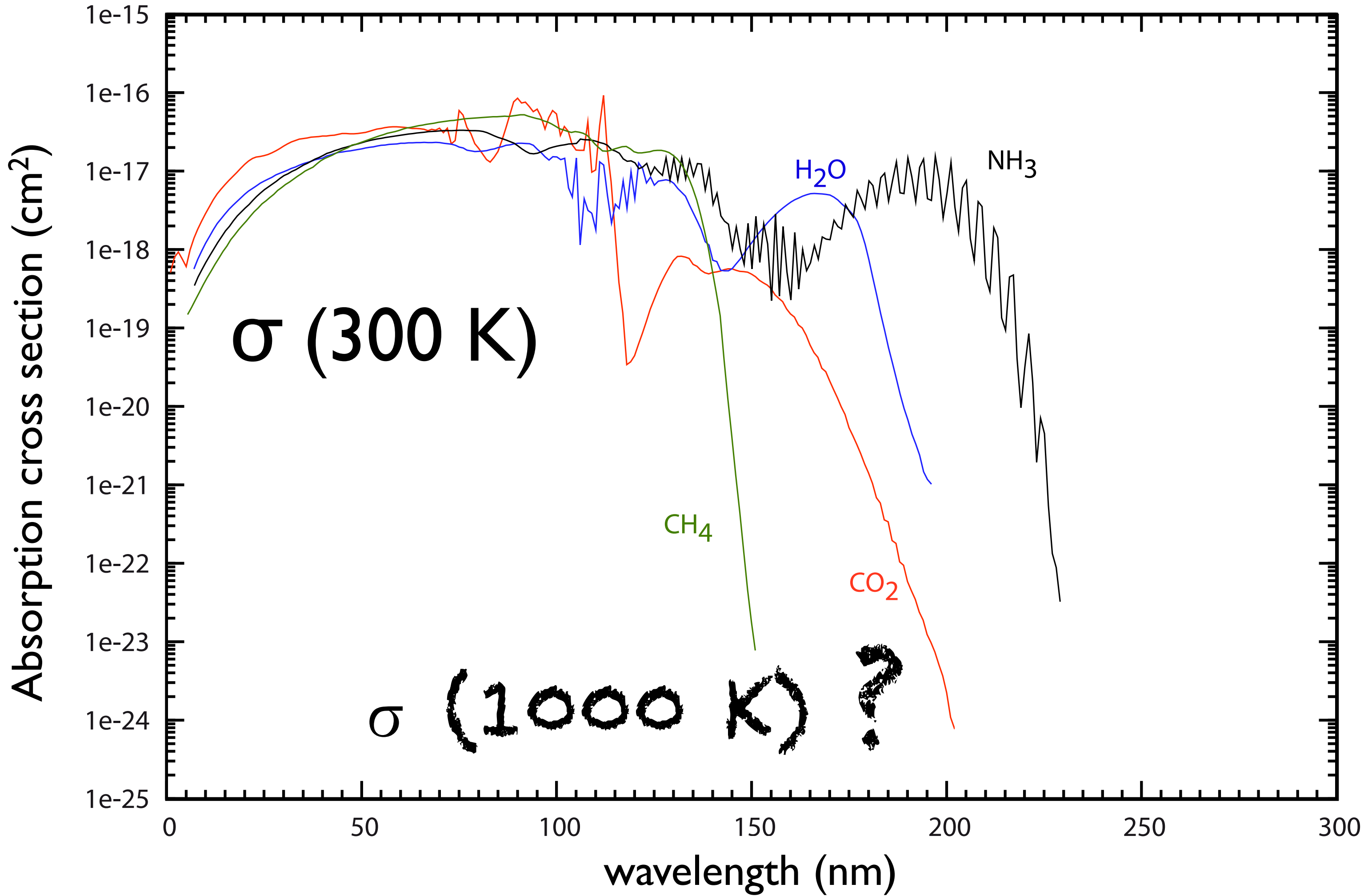


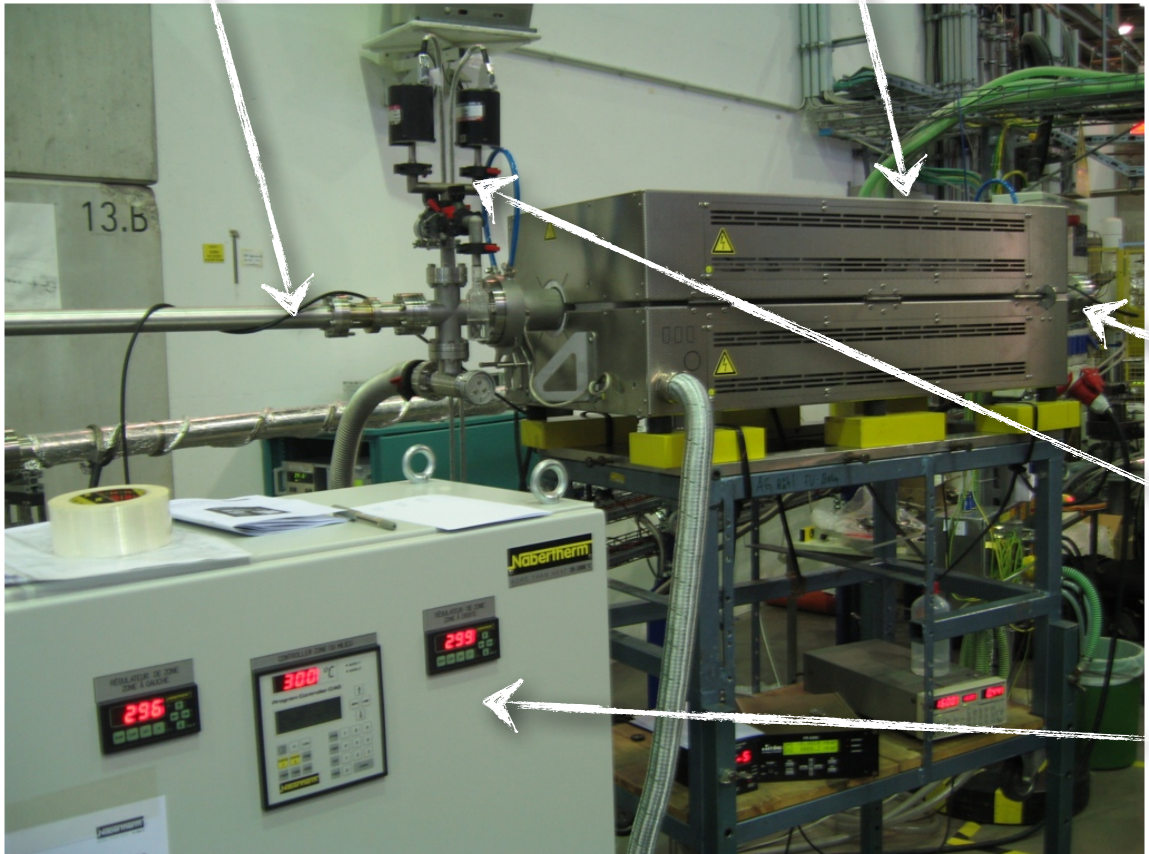
Absorption cross sections

experimental setup:

T up to 1000K

incident monochromatic flux

oven + cell



photomultiplier

injection of gas

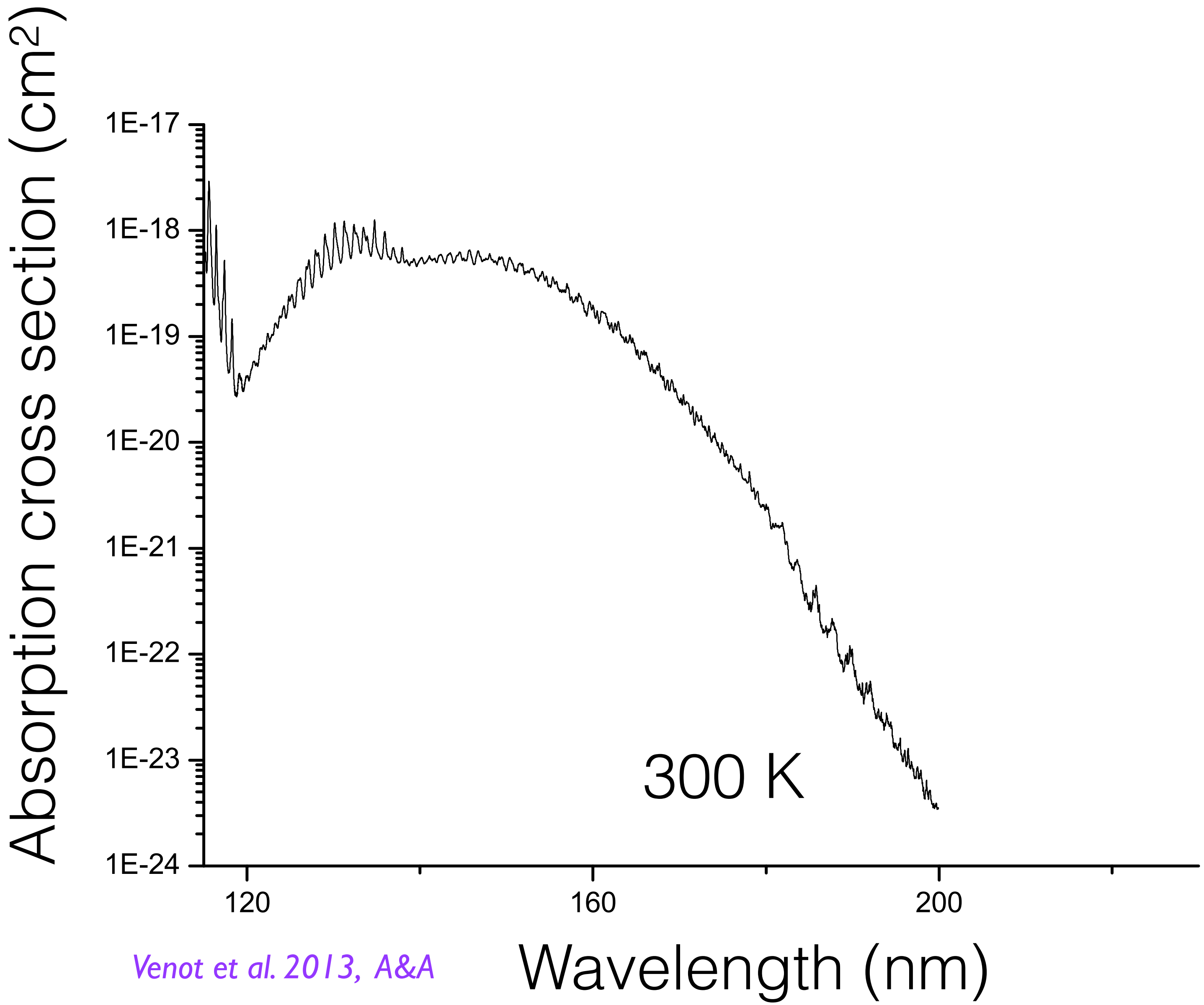
temperature control (3 zones)

115-230 nm

synchrotron facility
BESSY (Germany)
$115 < \lambda < 190$ nm

UV lamp at LISA (France)
$190 < \lambda < 230$ nm

Absorption cross sections of CO_2



Venot et al. 2013, A&A

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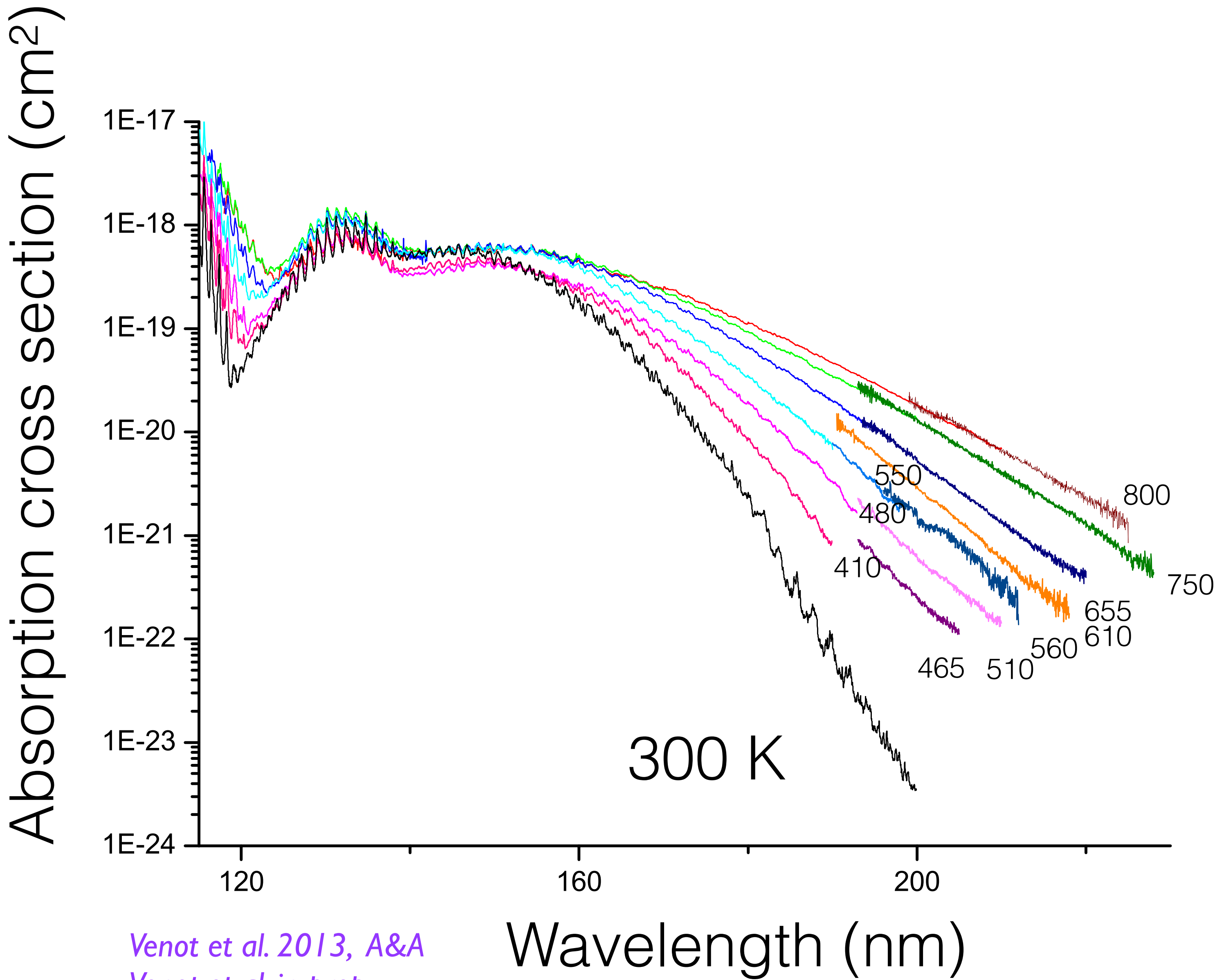

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Venot et al. in prep.

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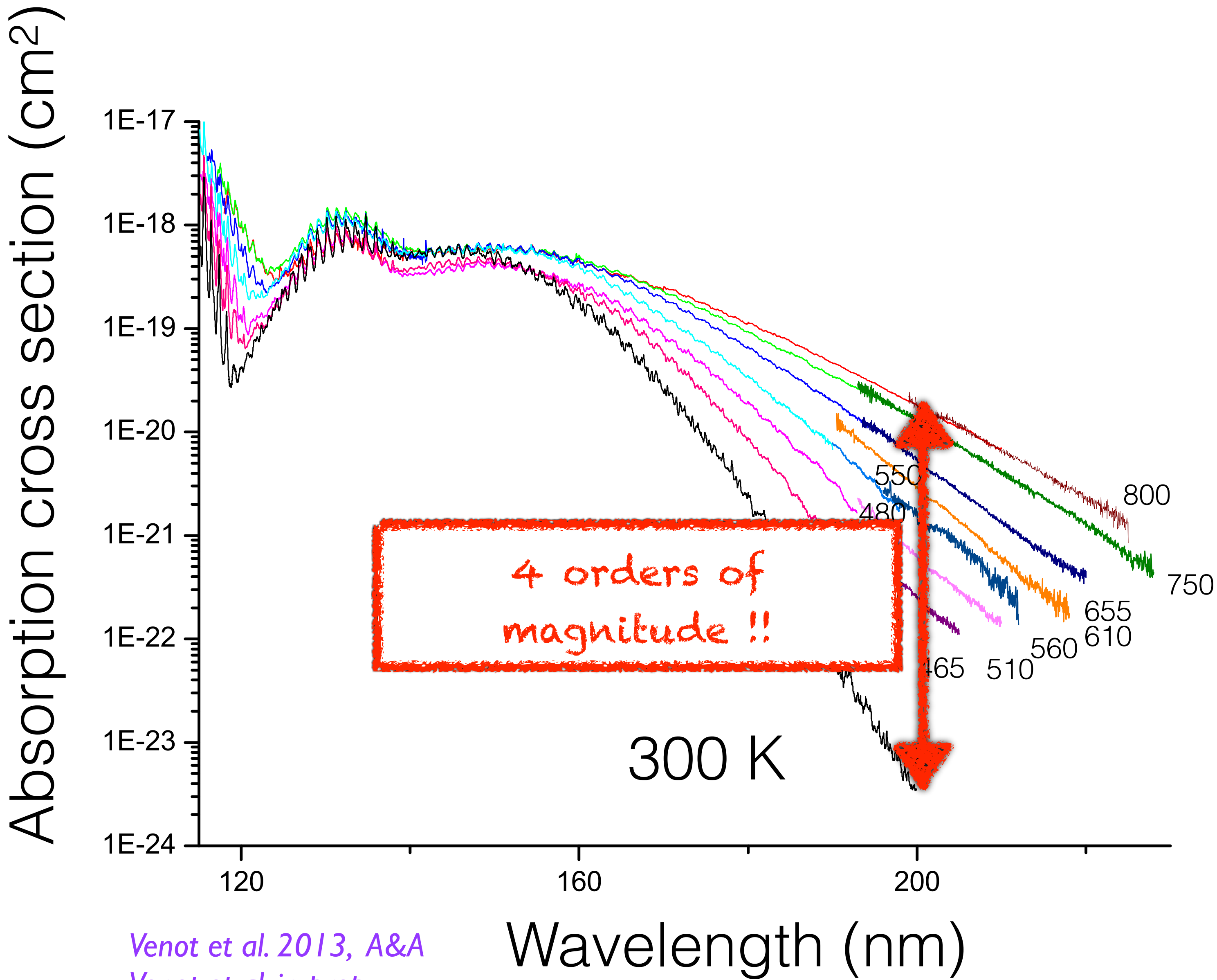

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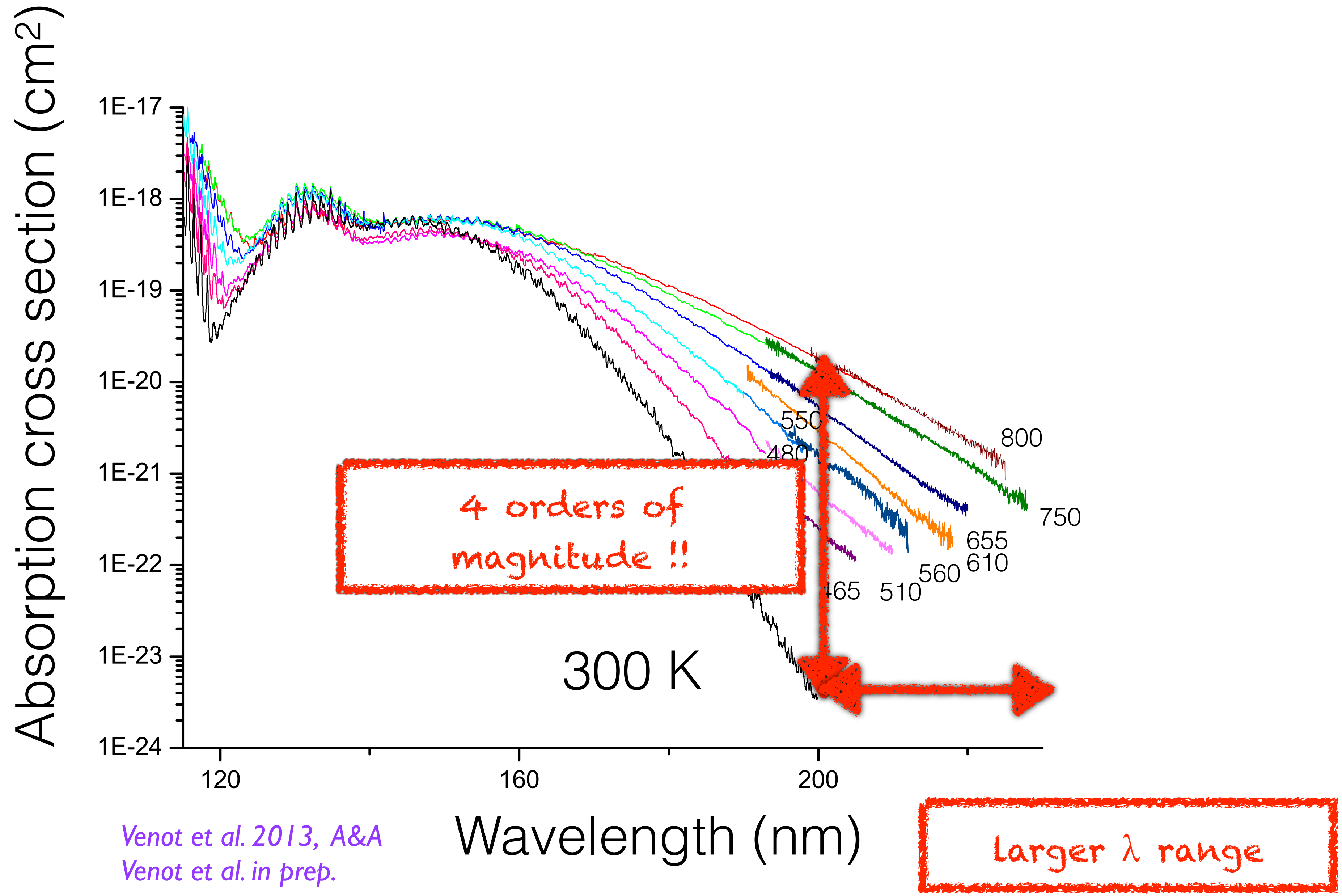

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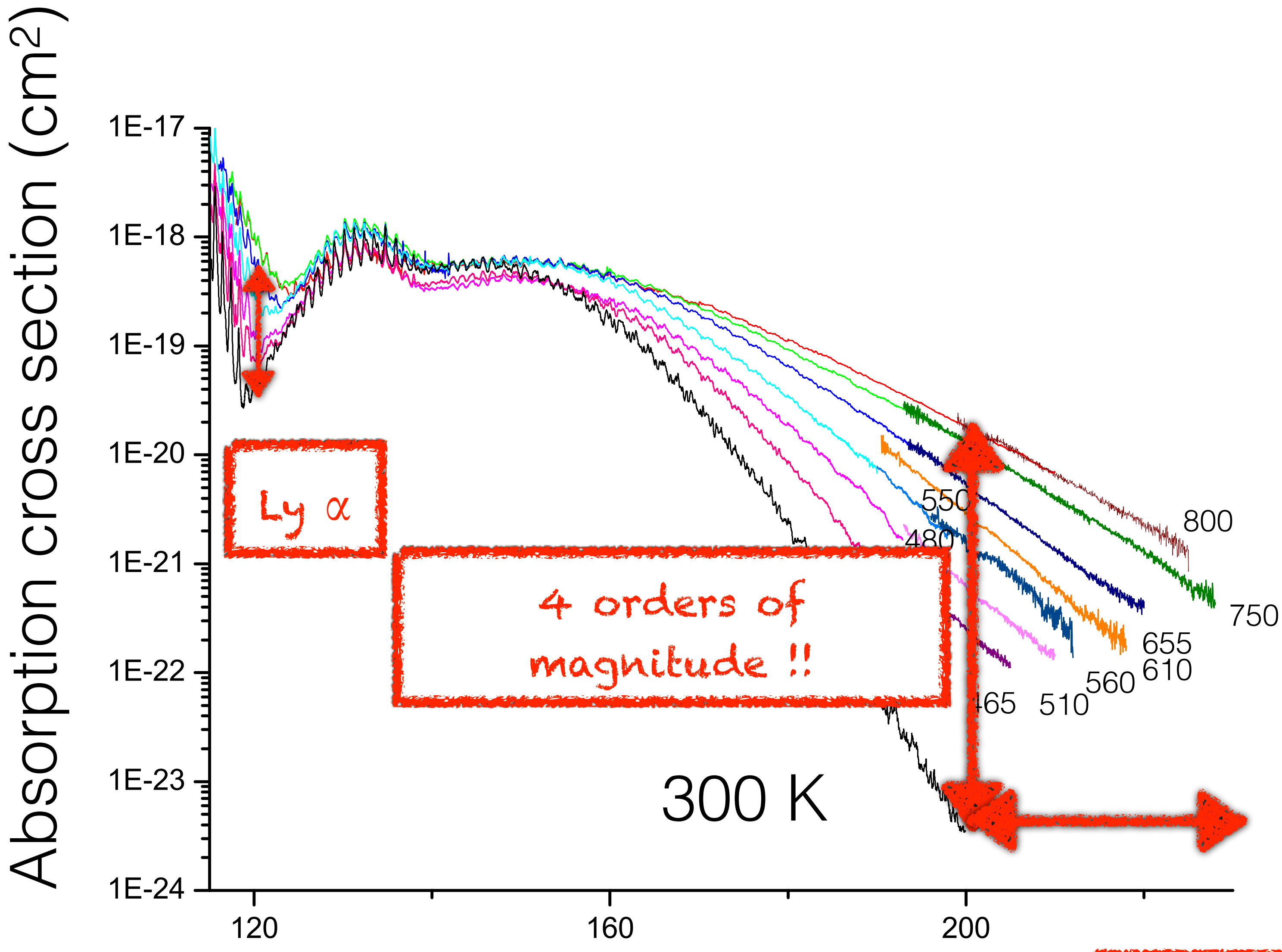

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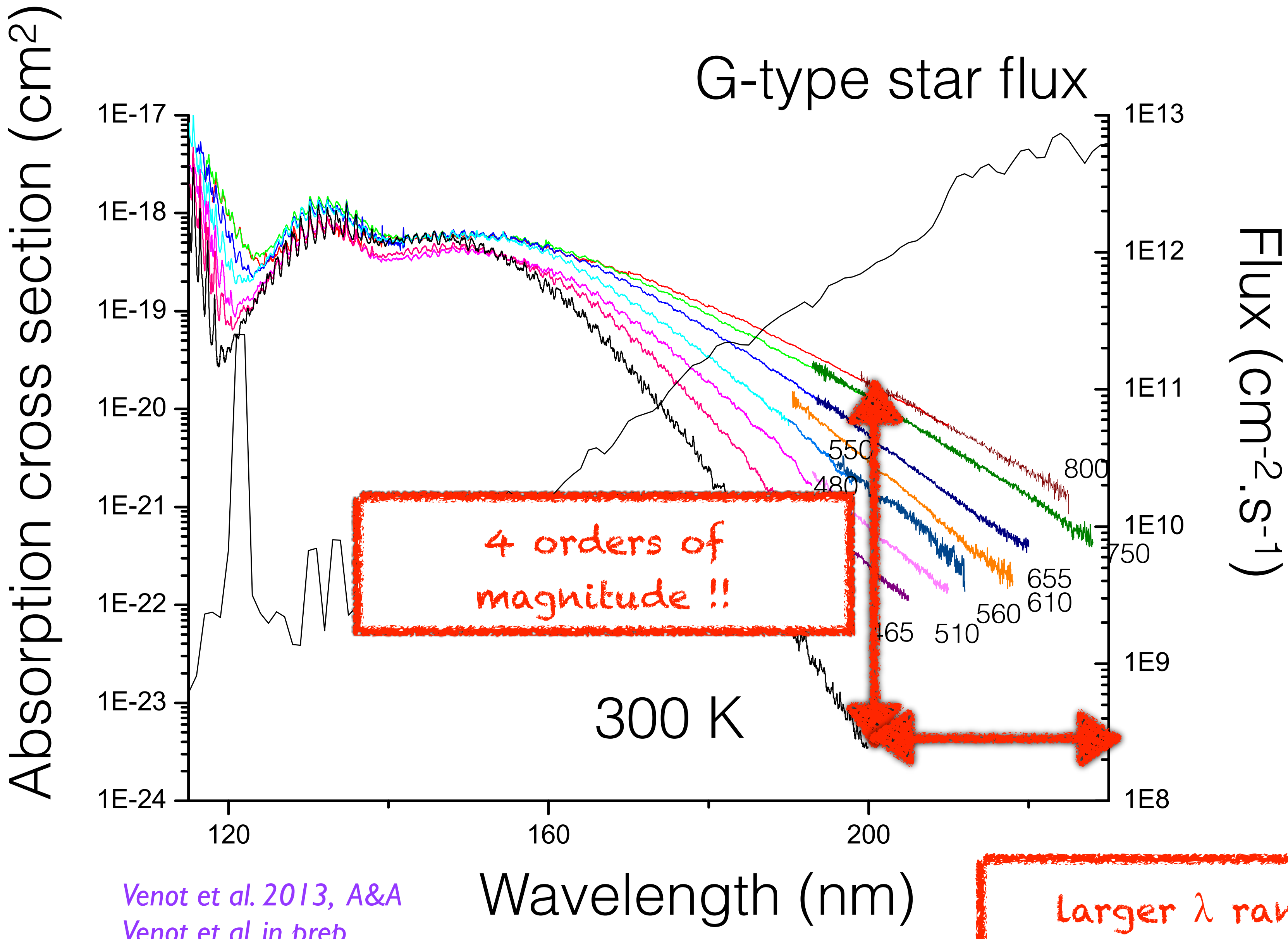
larger λ range

Absorption cross sections of CO_2



larger λ range

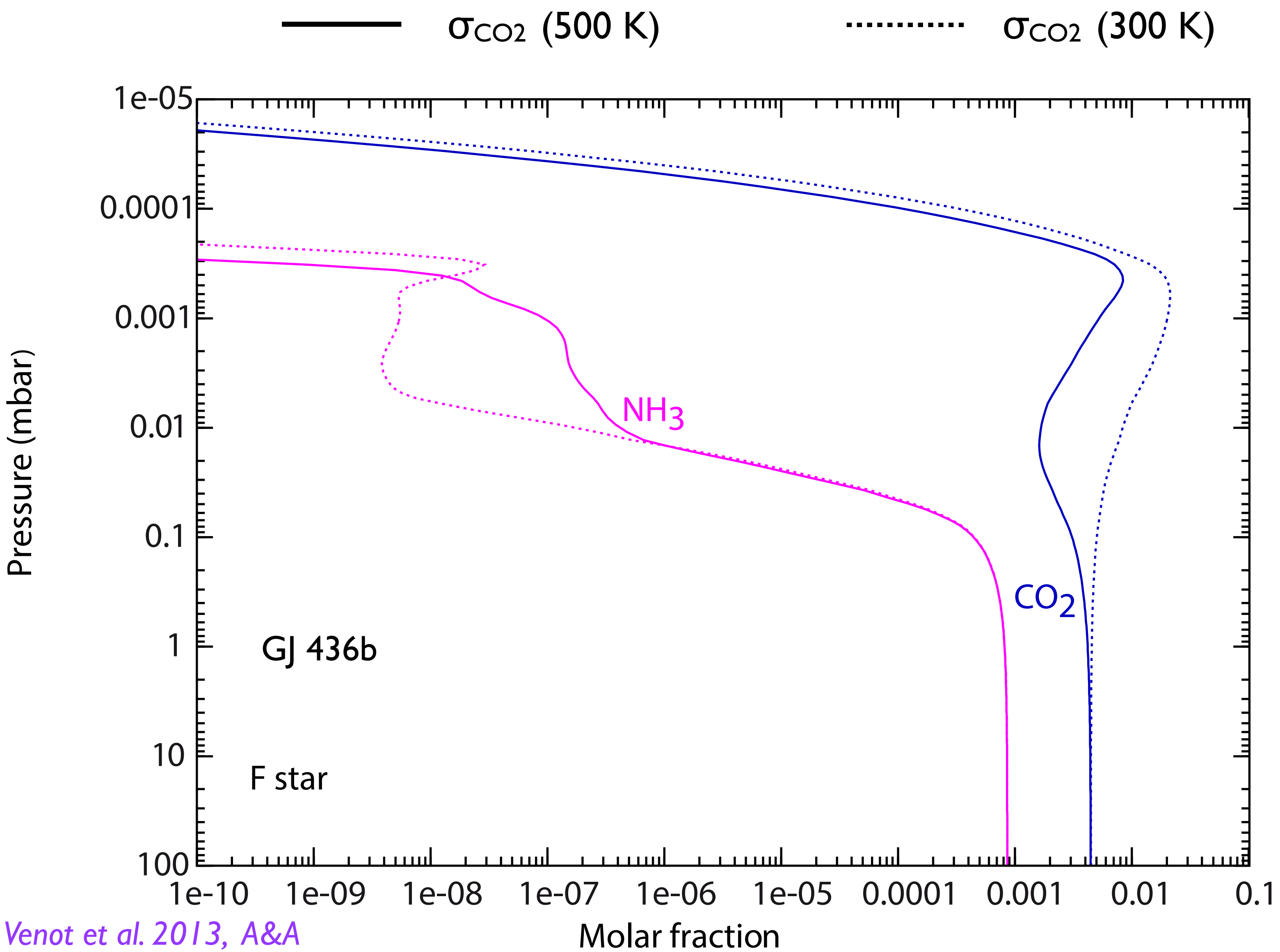
Venot et al. 2013, A&A
Venot et al. in prep.

Consequences on atmosphere

warm Neptune orbiting around a F star
$T_{atm} \approx$ 500 K (P < 100 mbar)

influence of UV flux: complex interaction between molecules

under or over-estimation of photodissociations !

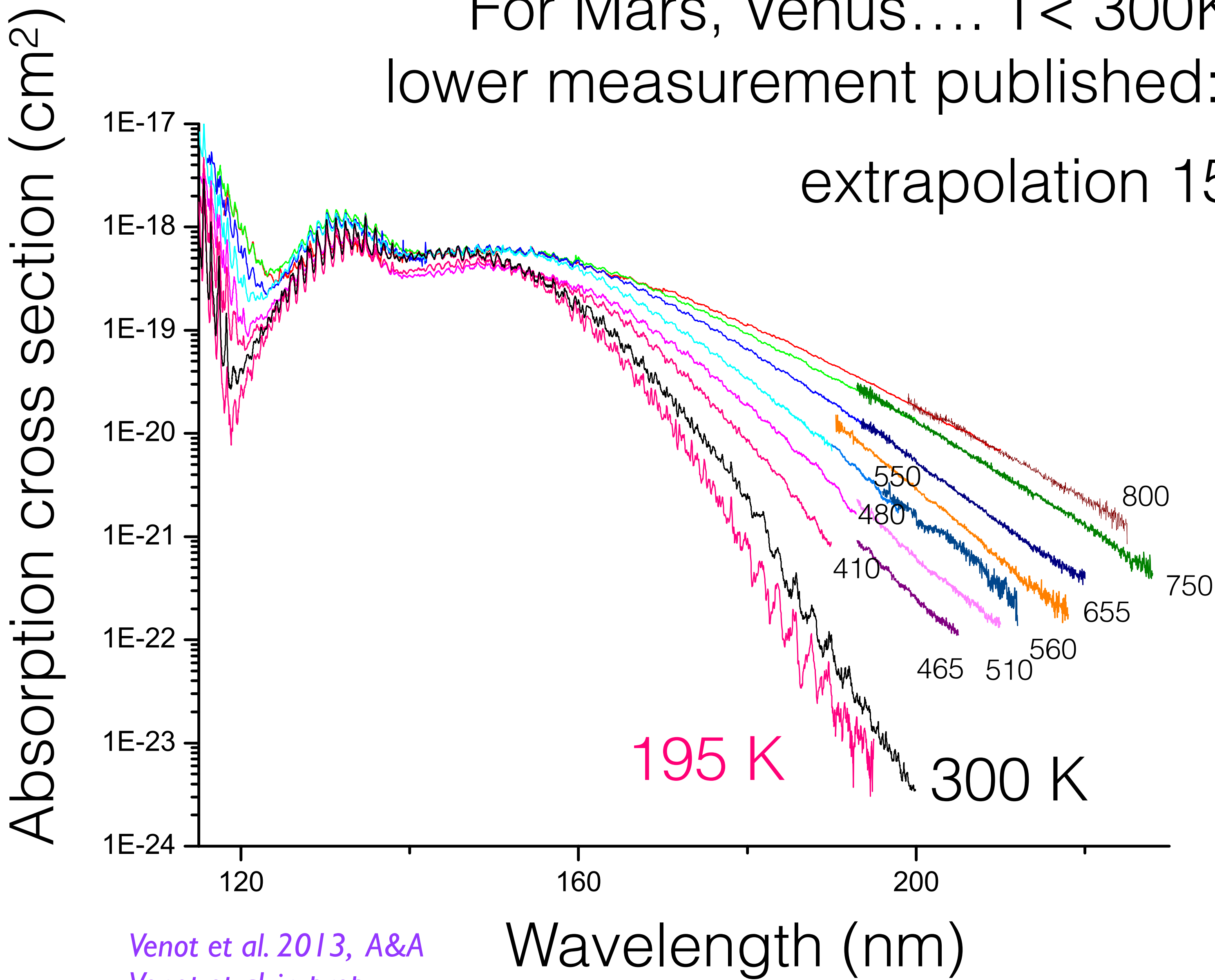


Venot et al. 2013, A&A

Absorption cross sections of CO_2

For Mars, Venus…. T< 300K…
lower measurement published: 195K

extrapolation 150 K ?



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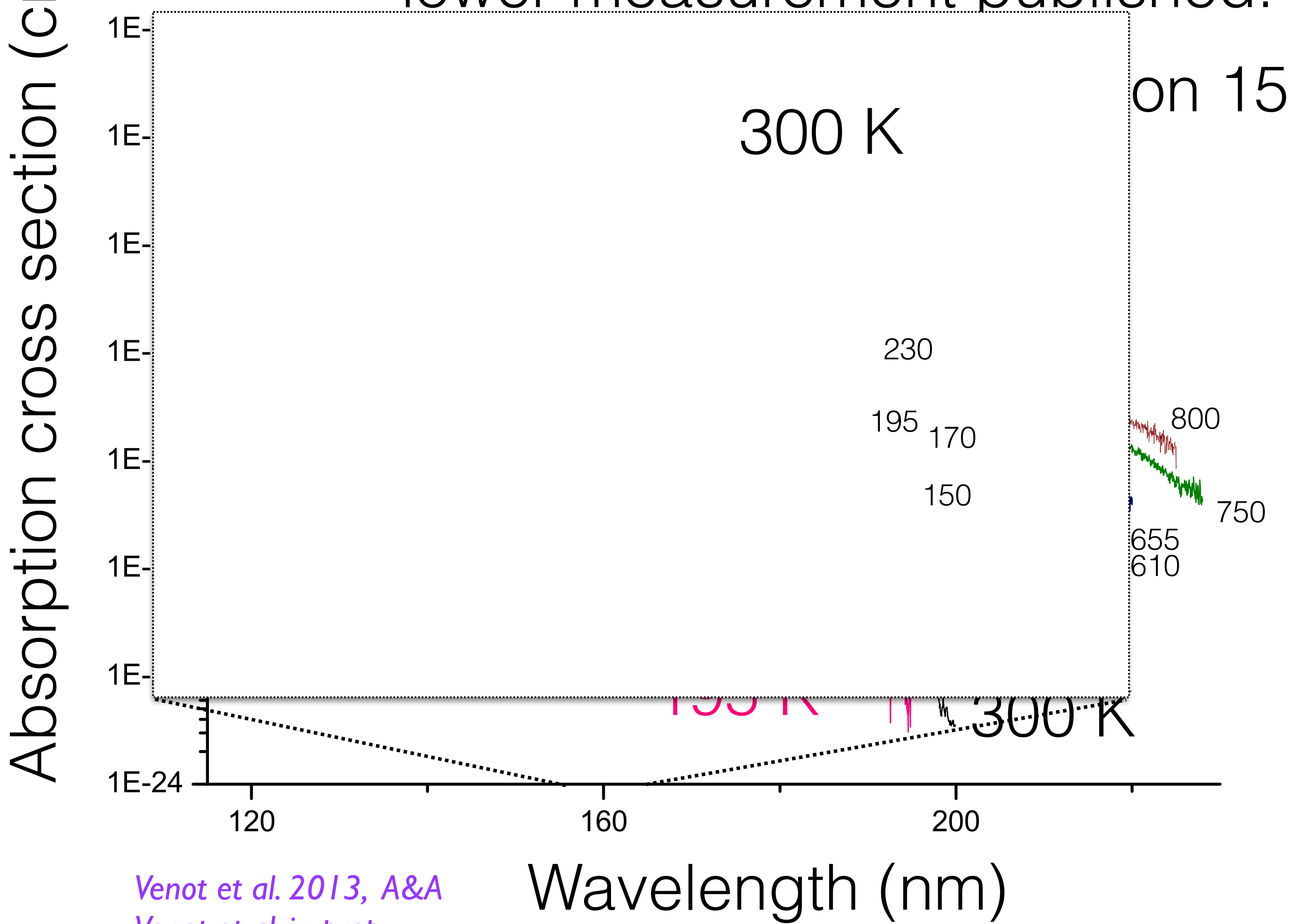

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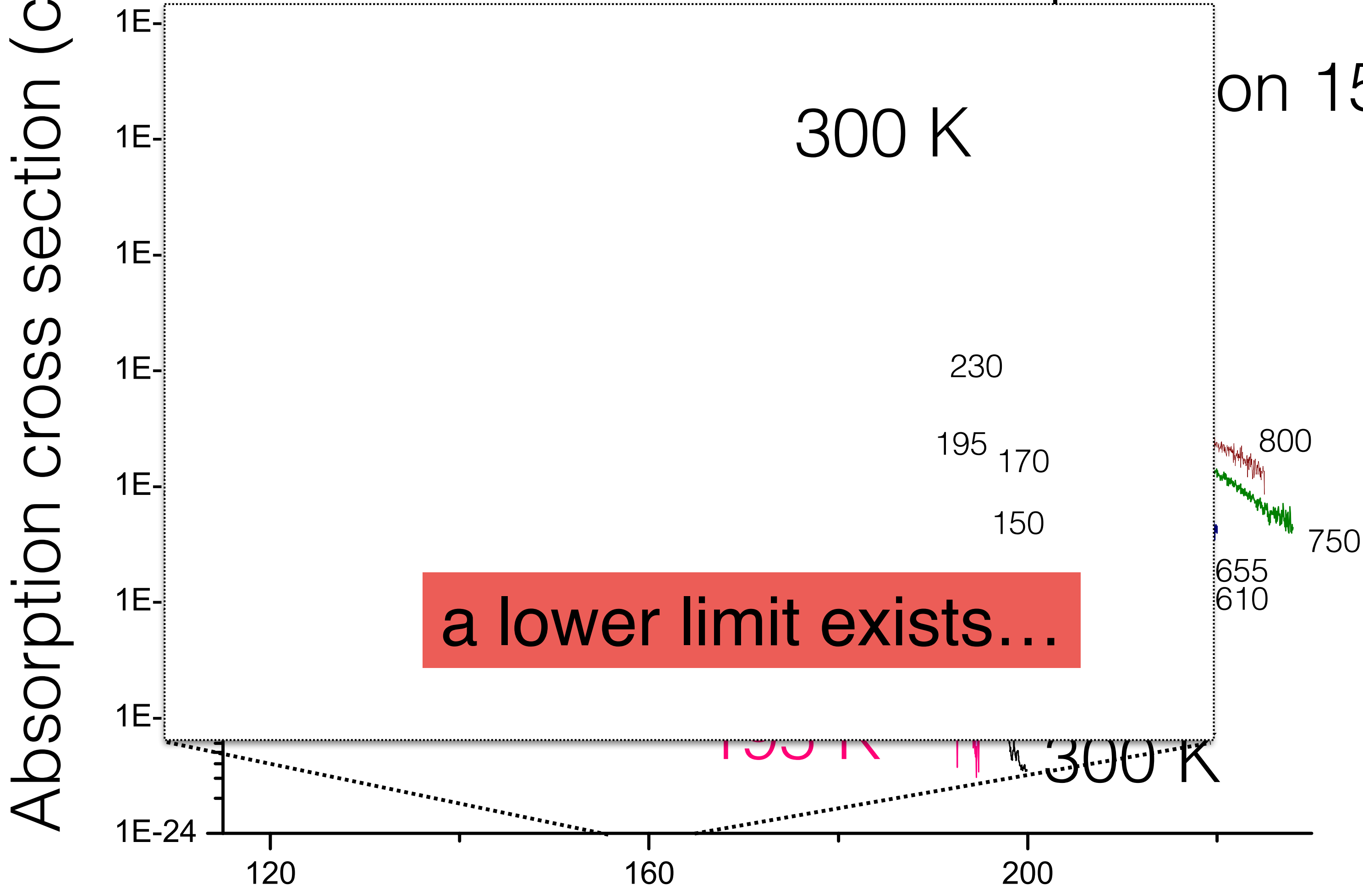
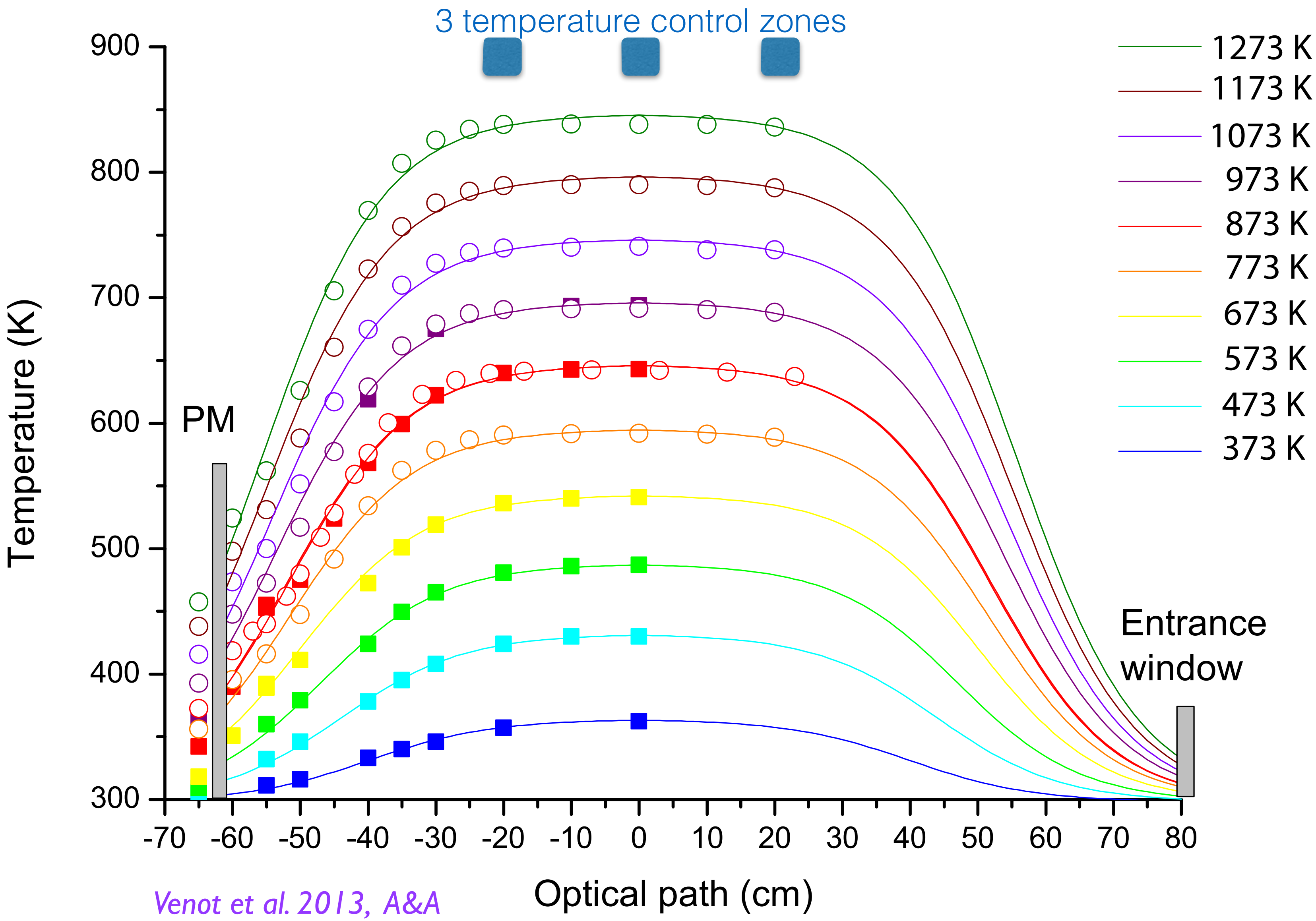


Venot et al. 2013, A&A

Venot et al. in prep.

Experimental issues

⇒ Temperature gradient

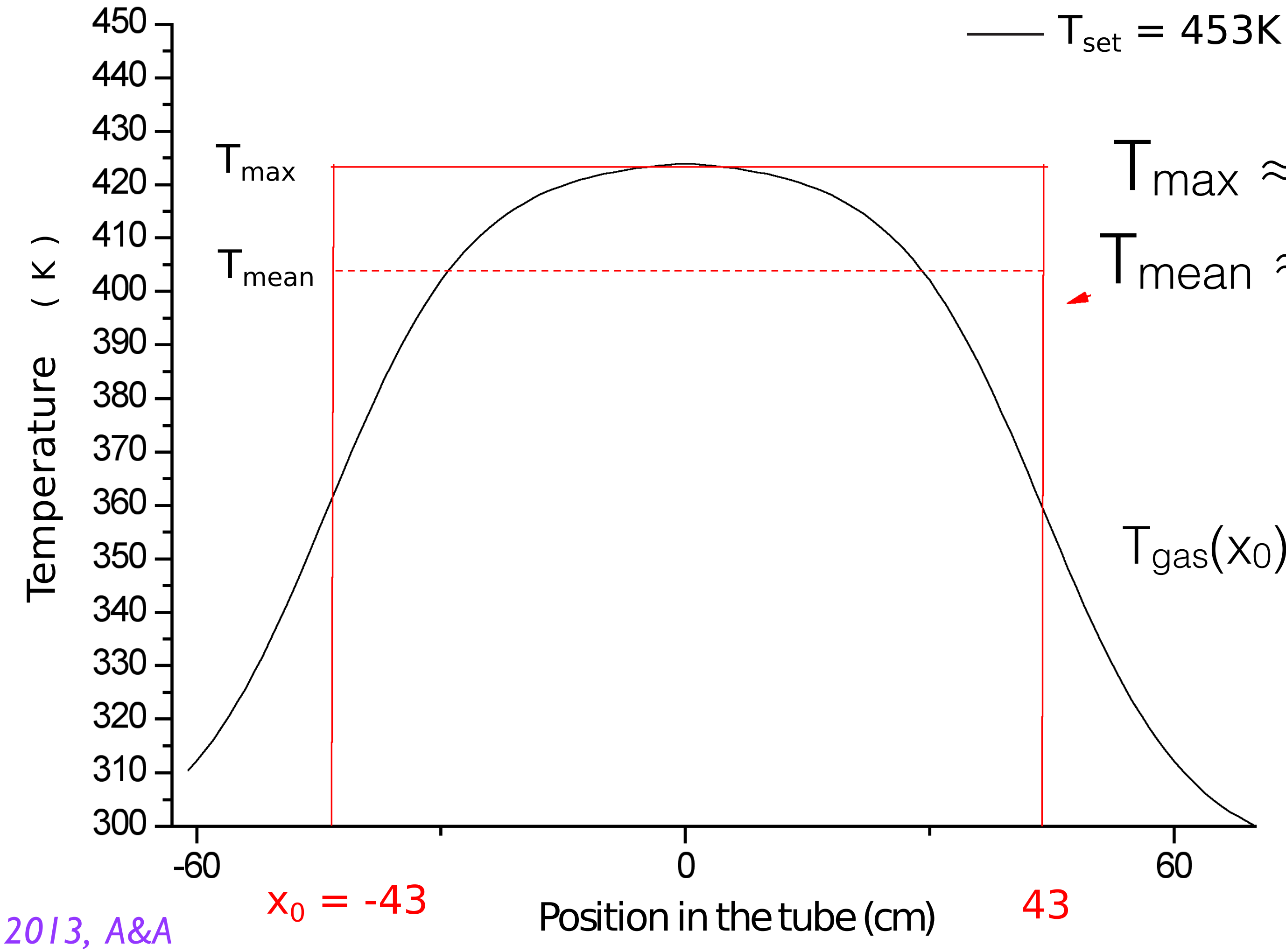


Venot et al. 2013, A&A

Experimental issues

⇒ Approximation : between x_0 and $-x_0$ → T_{mean}

elsewhere → T_{amb} (300K)



$T_{max} \approx 420$ K

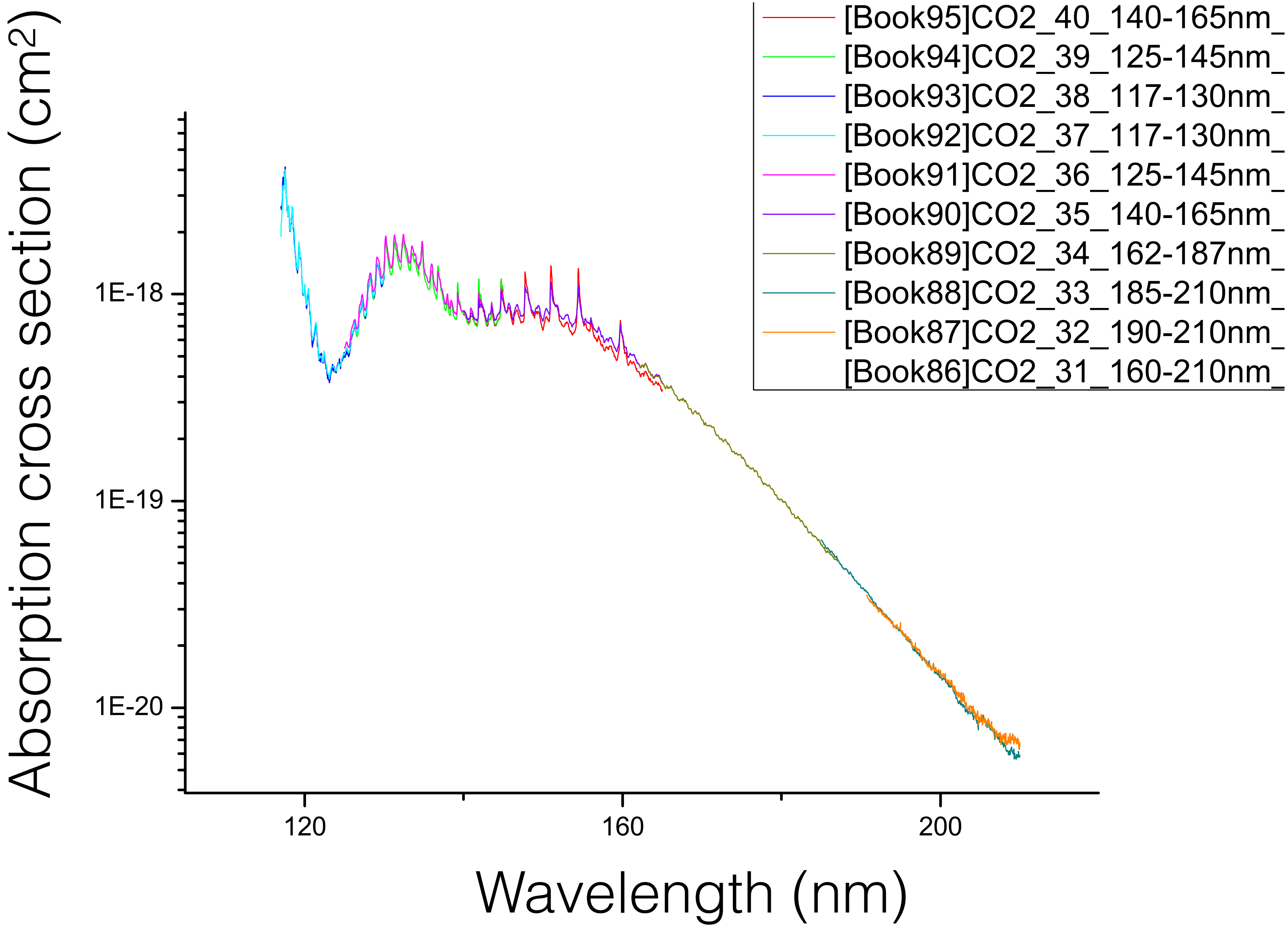
$T_{mean} \approx 405$ K

$T_{gas}(x_0) = (T_{max}+T_{amb})/2$

Venot et al. 2013, A&A

Experimental issues

⇒ Thermal decomposition



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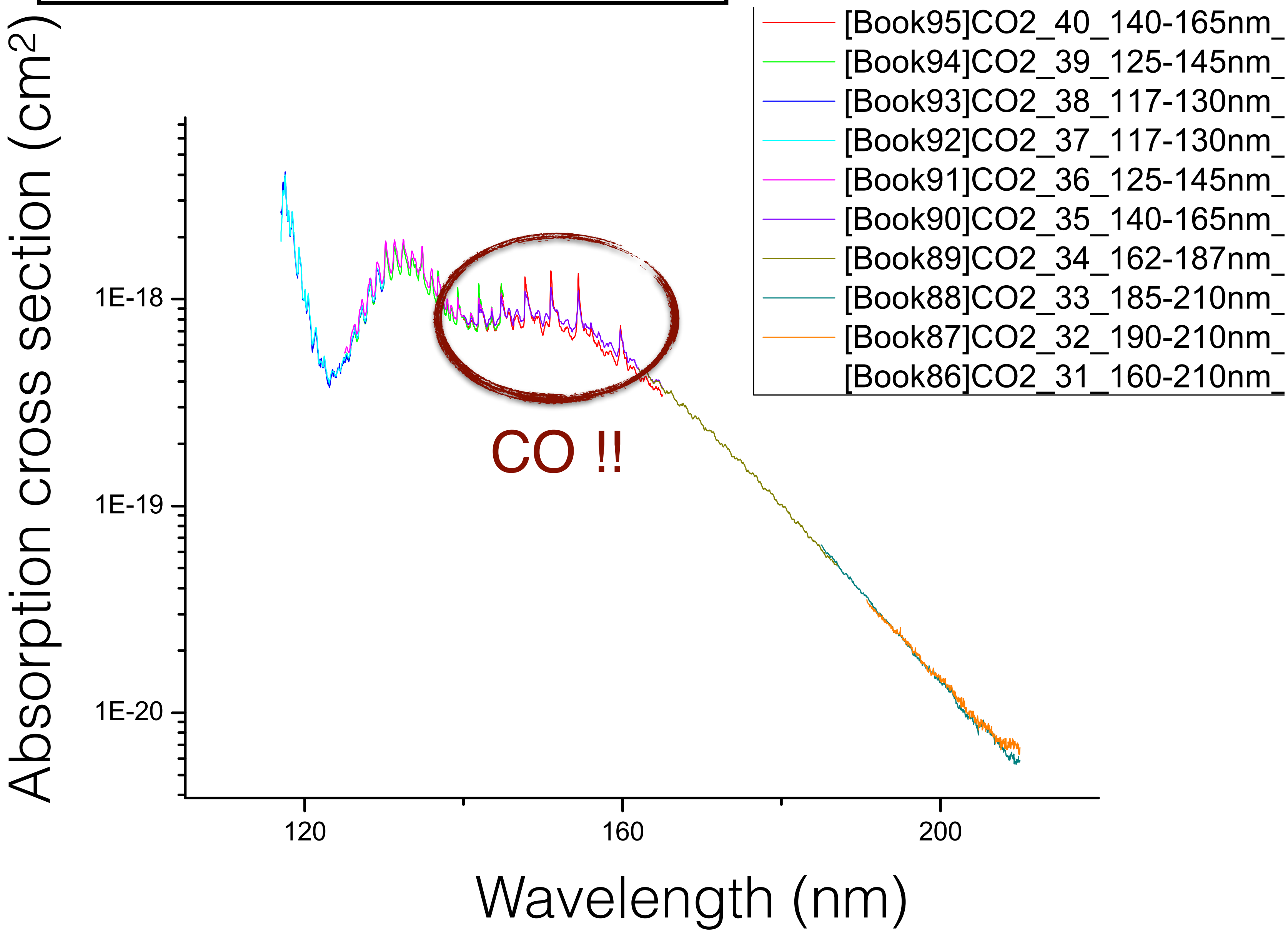

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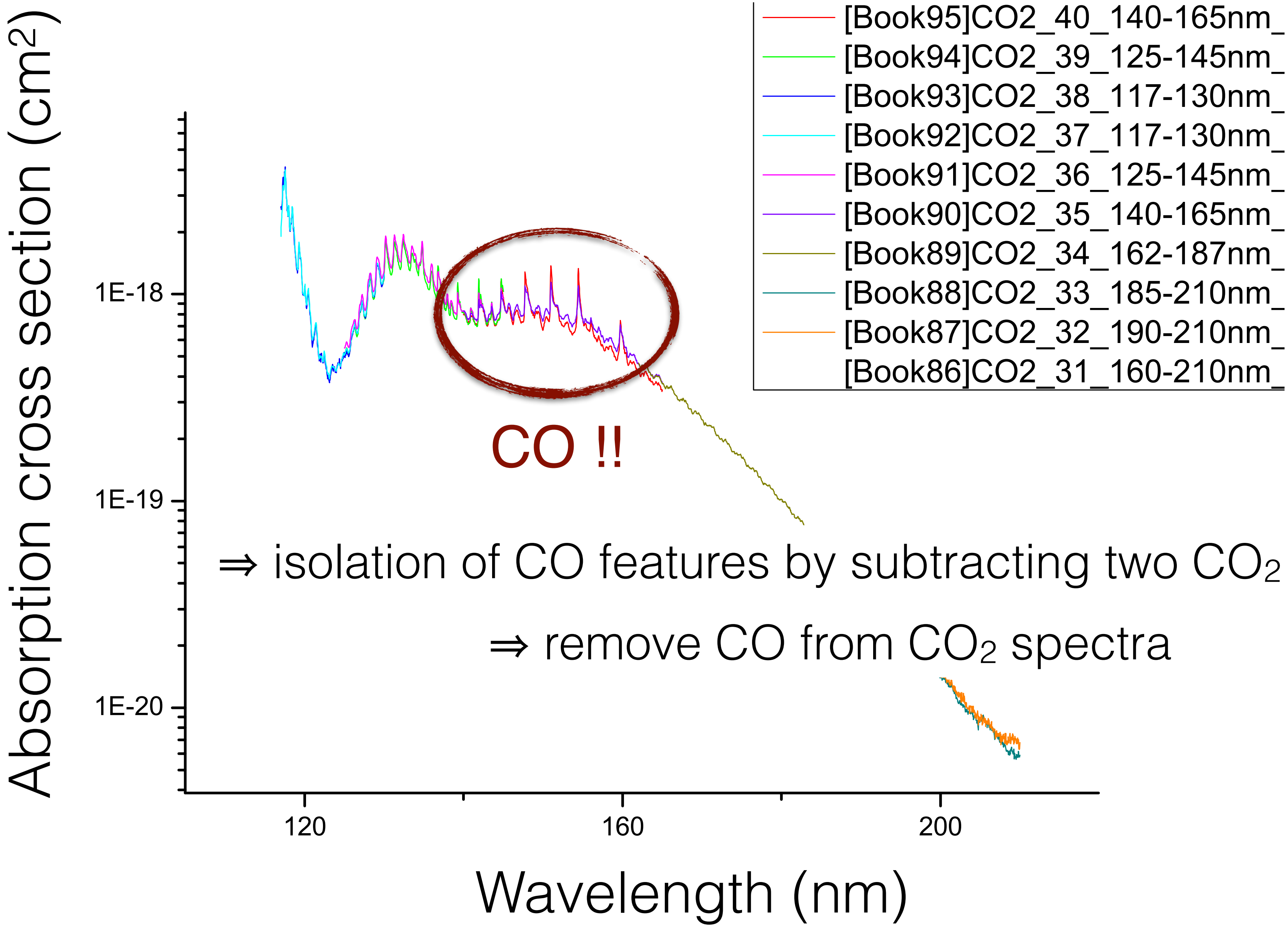

⇒ isolation of CO features by subtracting two CO_2 spectra

⇒ remove CO from CO_2 spectra

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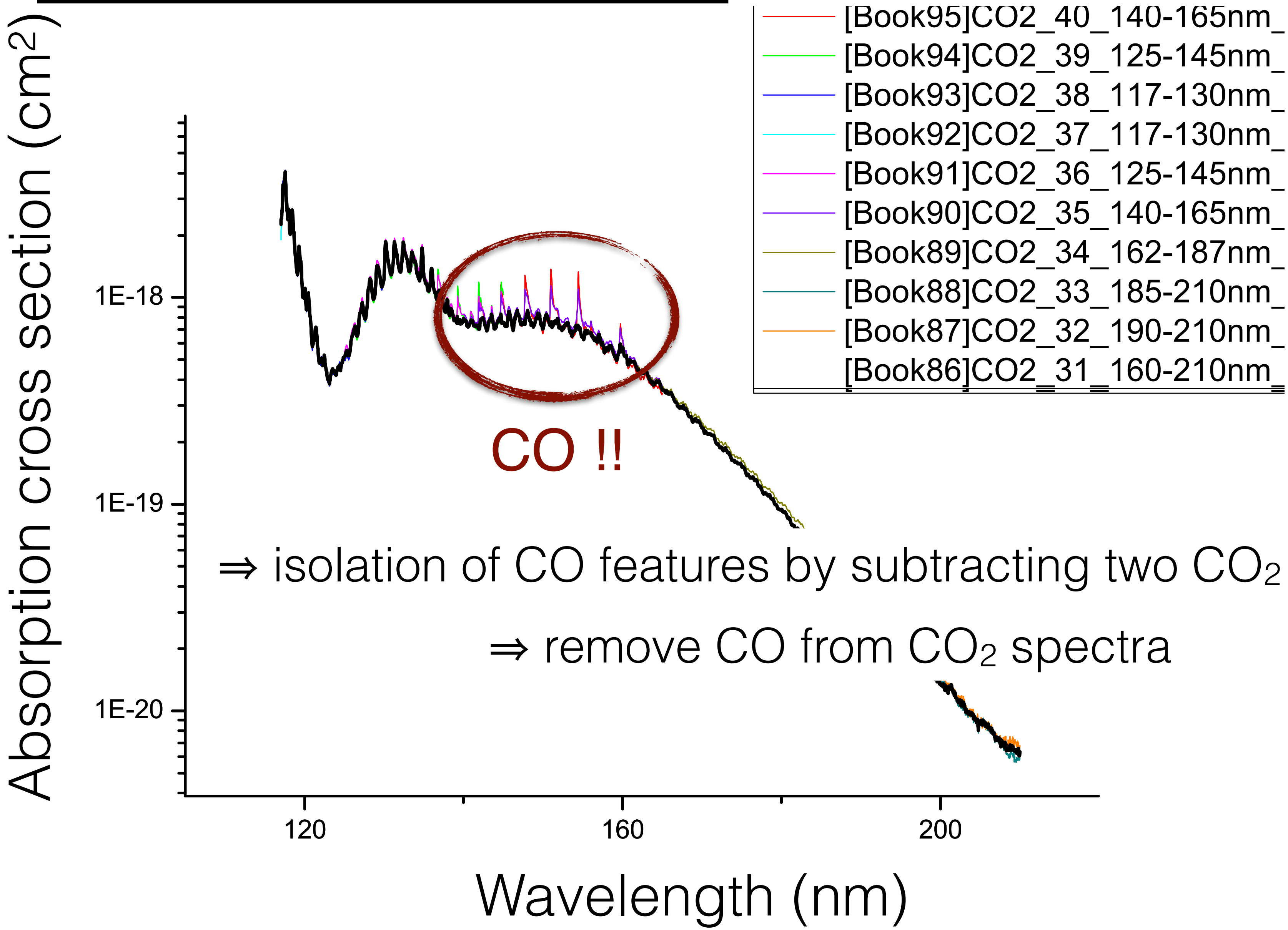

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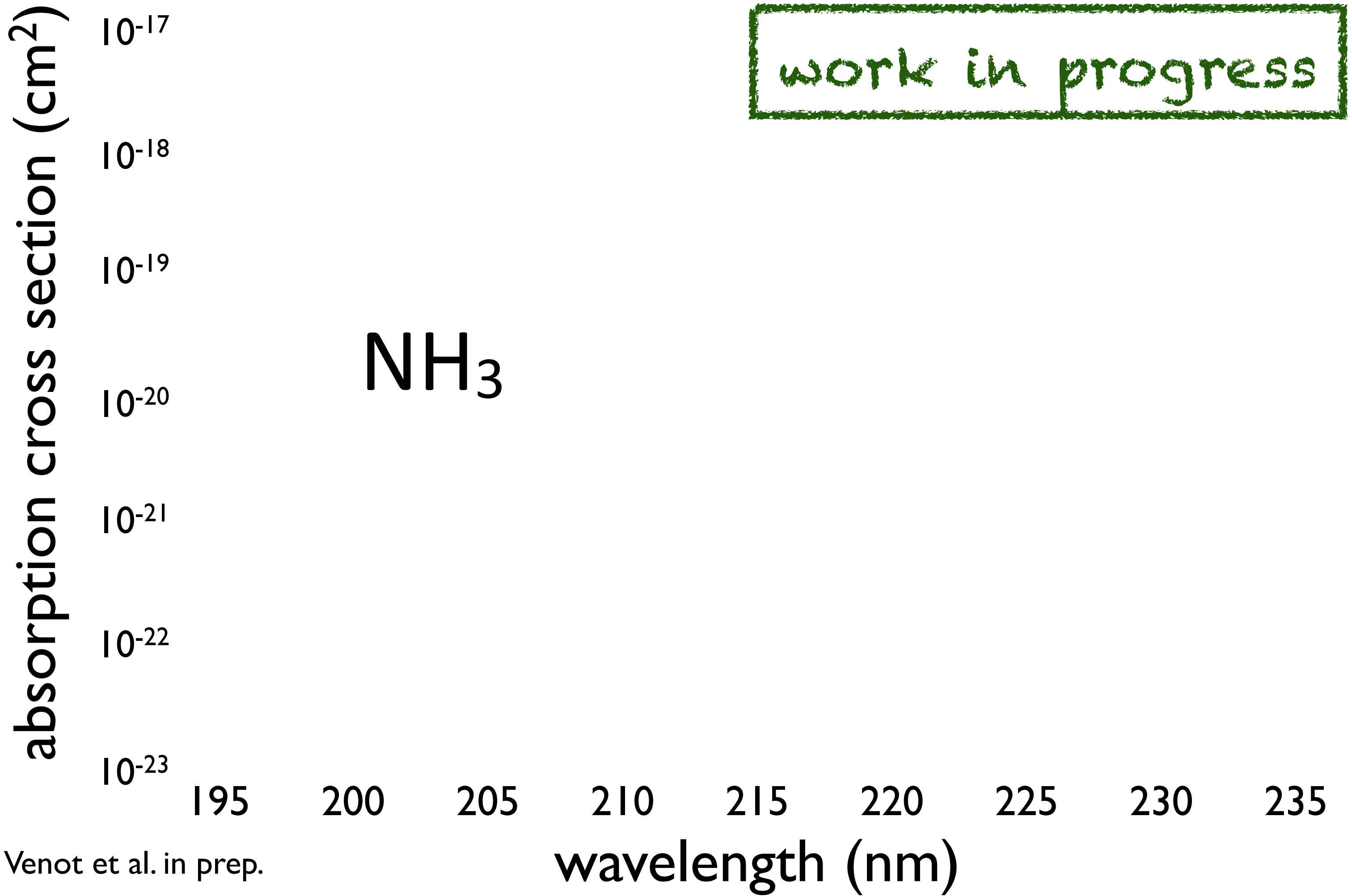
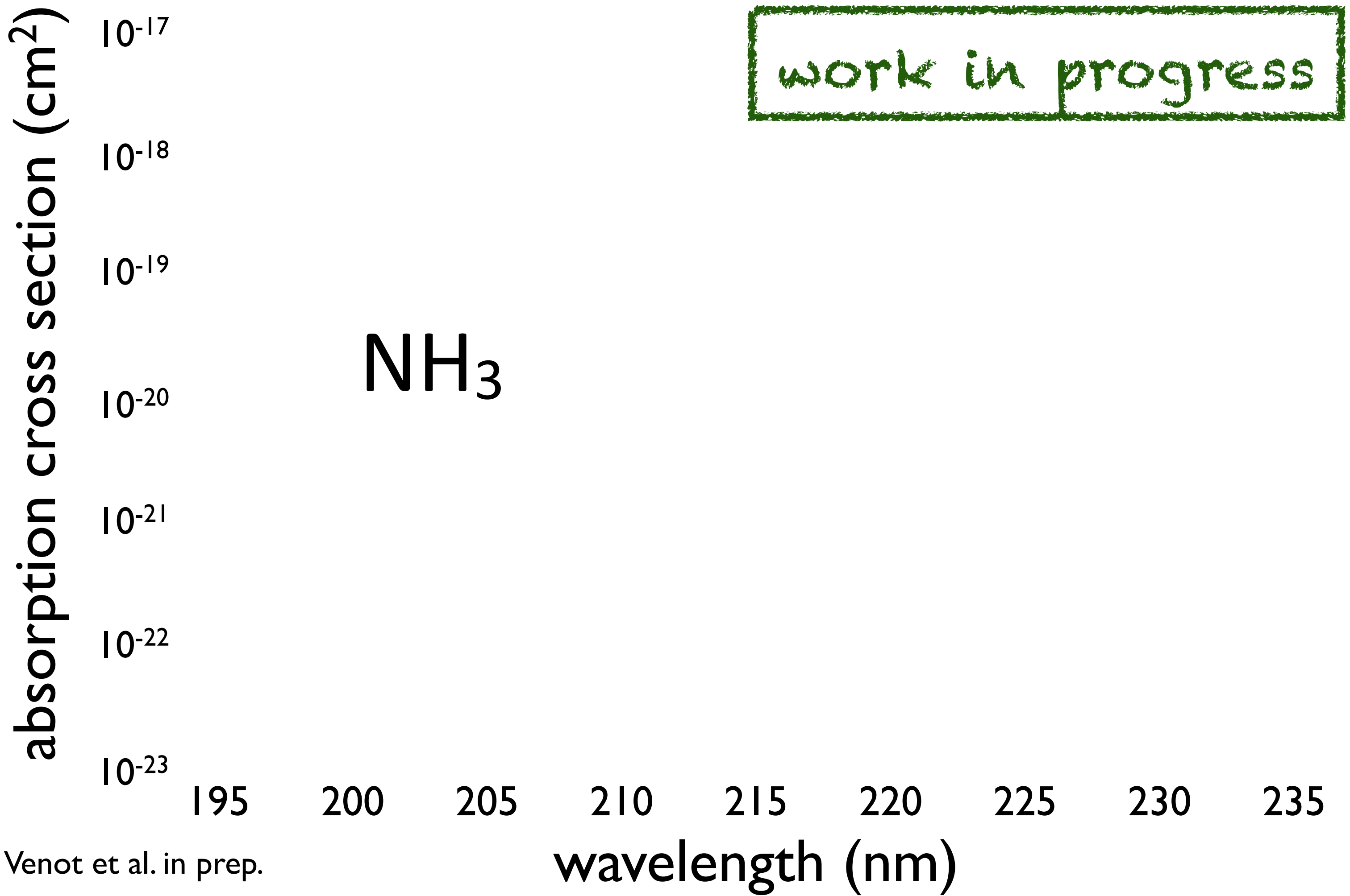


Venot et al. in prep.

Experimental issues

but....

$NH_3 \rightarrow NH_2 + H$



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Experimental issues

⟹ solution: measurements at SOLEIL SYNCHROTRON in May 2015

but....

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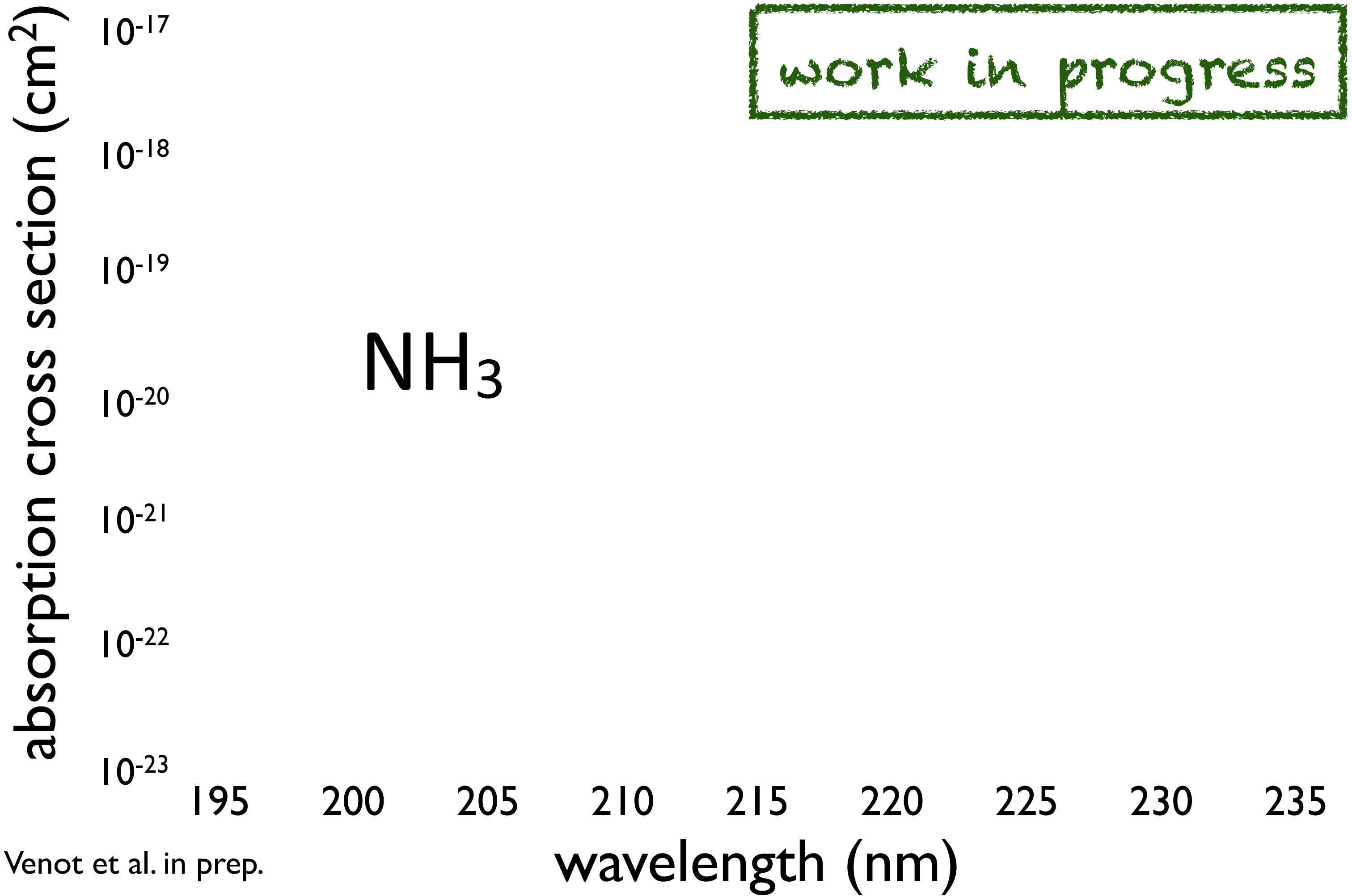
Beamline with a FT spectrometer and a mass spectrometer - (DESIRS) - polychromatic acquisition



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Conclusions & Perspectives

- 2 chemical schemes valid at high temperature

➡ warm exoplanets, brown dwarfs (Tremblin et al. 2015), deep atmosphere of giant planets (Cavalié et al. 2014)

➡ next improvement: addition of sulfur species/reactions

- For photolysis : important need of data at T > 300K !

- Dependency of CO_2 VUV absorption cross section measured between 150 and 800 K (Venot et al. 2013, Venot et al. in prep)

- May 2015: NH_3, C_2H_2 at SOLEIL SYNCHROTRON line DESIRS with a FT spectrometer: will allow us to overcome the thermal dissociation issue (PI: O. Venot)

- And more in the coming years….(HCN, C_2H_4, CO,… ask for specific request…)

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Thank you for your attention…