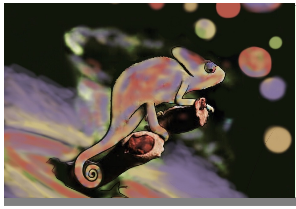
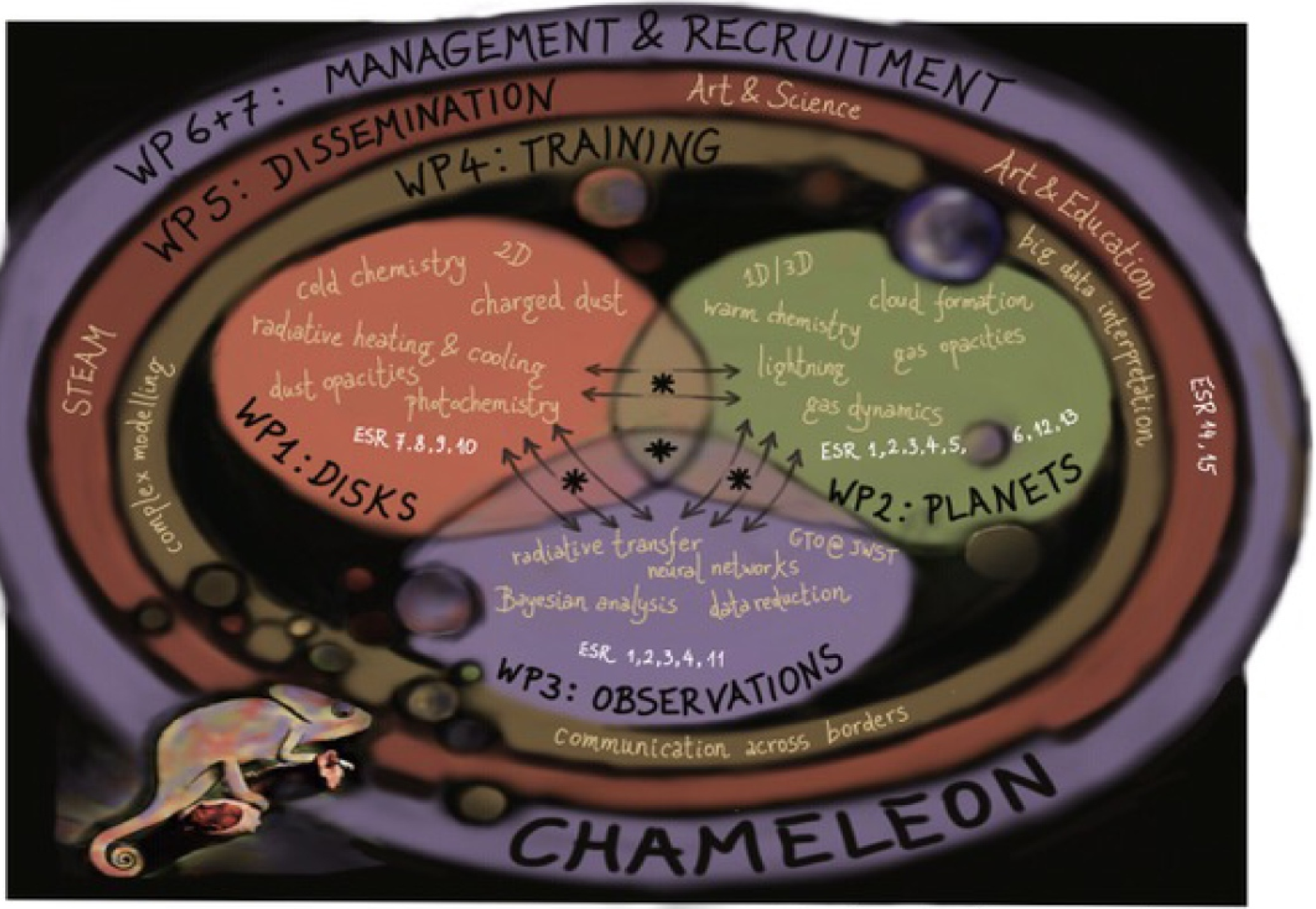
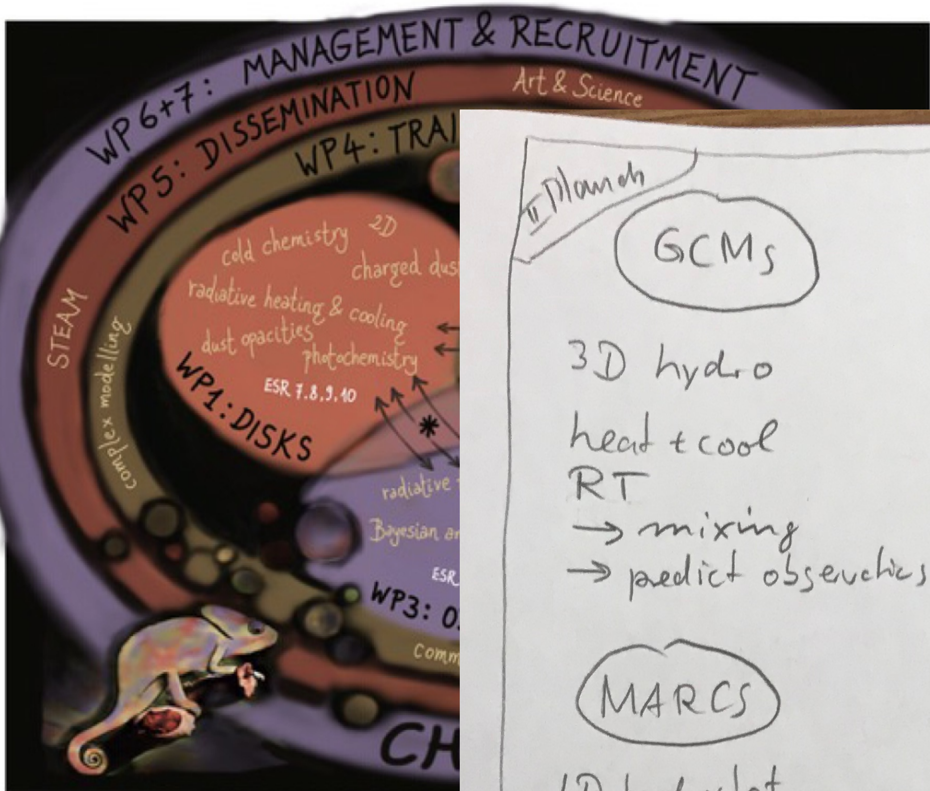


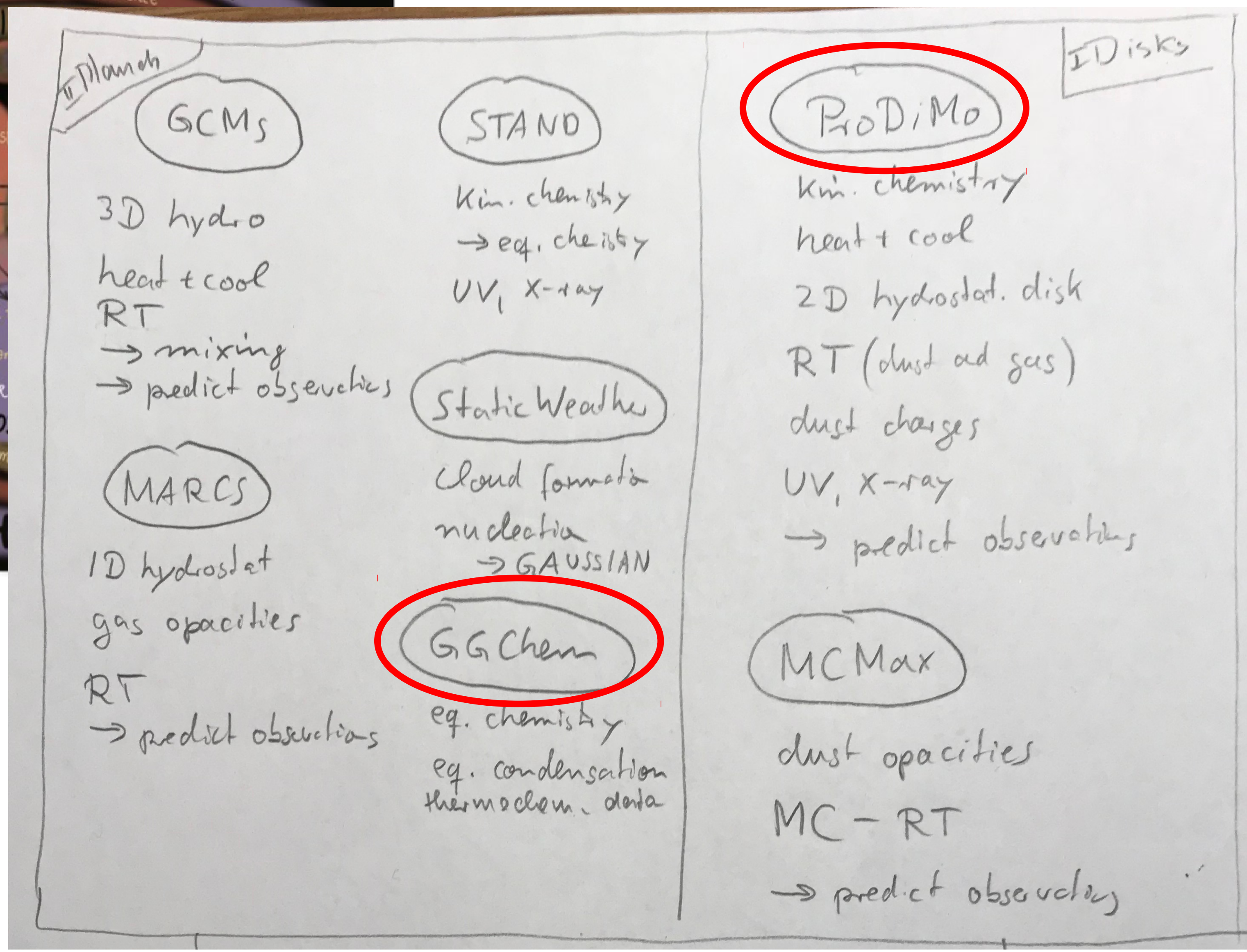
CHAMELEON: *Virtual Laboratories for Exoplanets and Planet-forming Discs*

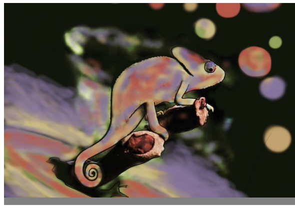


CHAMELEON: *Topics & Tools*



Virtual Laboratories





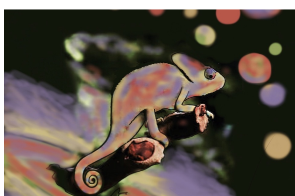
ESR 7: Grain charges and lightning in discs

- ***Thorsten Balduin***, start 27/10/2020, St Andrews (→P. Woitke)
- **secondment:** Copenhagen (→U. Joergensen)

→ **ESR 6:** *Charge conservation and cloud formation in planet atmospheres → Nanna Bach-Moeller*

→ **ESR 8:** *The warm chemistry in the inner disk → Jayatee Kanwar*

→ **ESR 13:** *Modelling lightning in 3D GCMs and the detection of biosignatures → Marrick Braam*



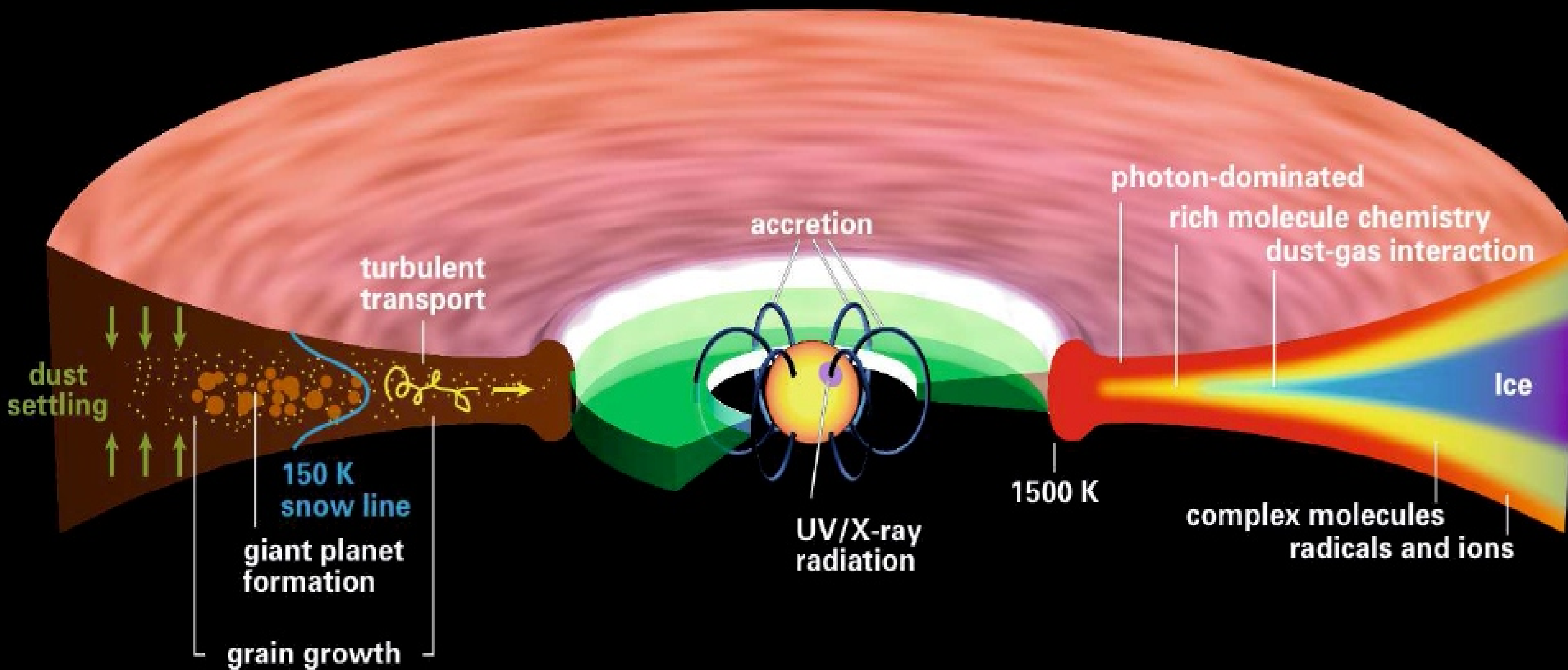
ESR 9: Machine Learning from complex disc models

- ***Till Käufer***, start 27/09/2020, St Andrews (→P. Woitke)
- **secondment:** SRON/Groningen (→M. Min)

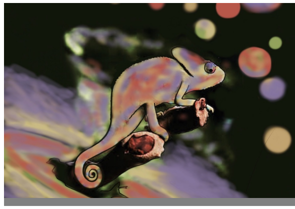
→ **ESR 11:** *Machine learning for inferring physical and chemical parameters from exoplanet observations → Francisco Ardevol*

→ **ESR 10:** *The disk-planet connection: exoplanet composition informed by disc models → Areli Castrejon*

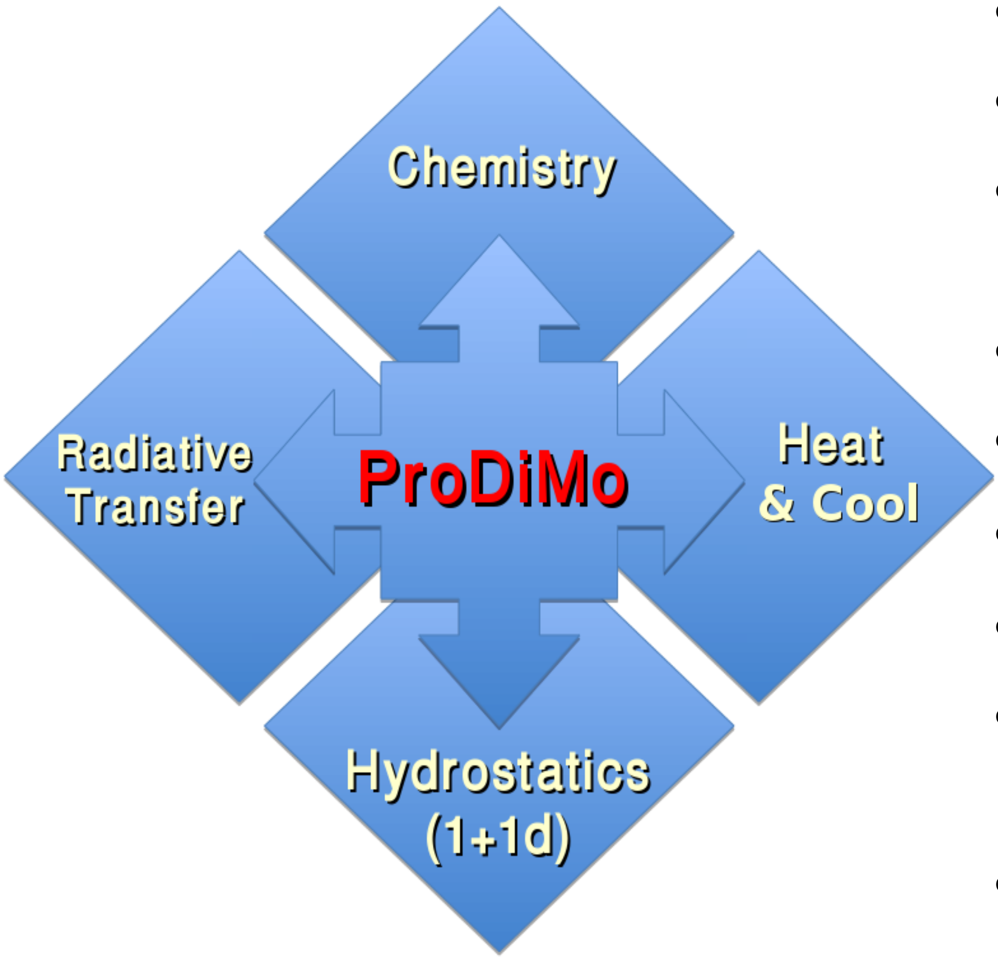
Protoplanetary Discs



© Henning & Semenov (2013)

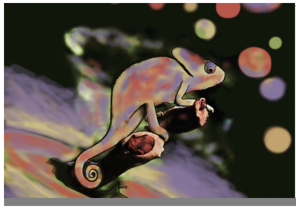


ProDiMo: A modular framework for disc research

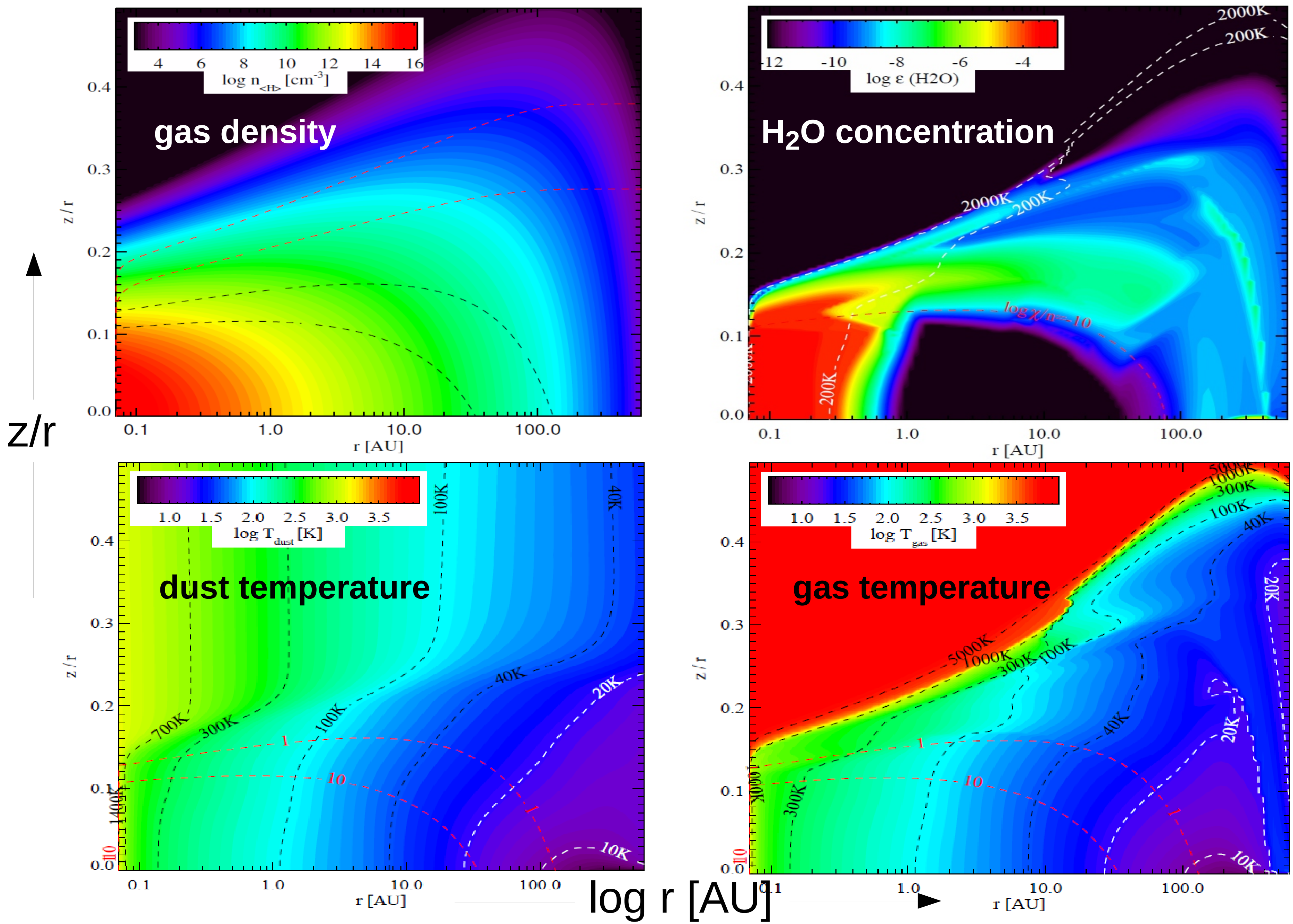


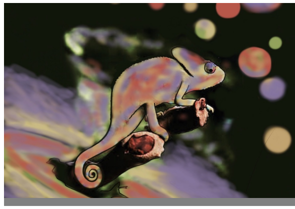
main papers: Woitke, Kamp, Thi (2009),
Kamp et al. (2010),
Thi et al. (2011),
Woitke et al. (2016)

- ***stellar parameters***
- ***2D hydrostatic disc structure***
- ***UV & X-ray irradiation***
  (from star and ISM)
- ***dust/gas, grain material, opacities***
- ***dust size distribution, settling***
- ***detailed continuum RT*** → $T_{dust}(r,z)$
- ***kinetic chemistry & ice formation***
- ***non-LTE gas heating/cooling***
  → *chemical composition,* $T_{gas}(r,z)$
- ***prediction of observations***
  → spectral energy distribution (SED)
  → continuum images, visibilities
  → line fluxes IR – mm
  → line velo-profiles, channel maps



ProDiMo: example disc modelling results



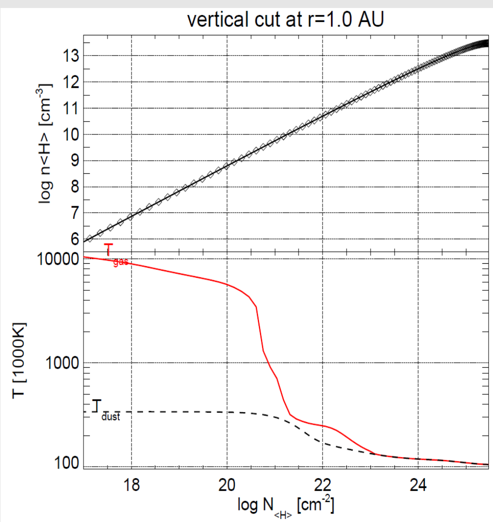


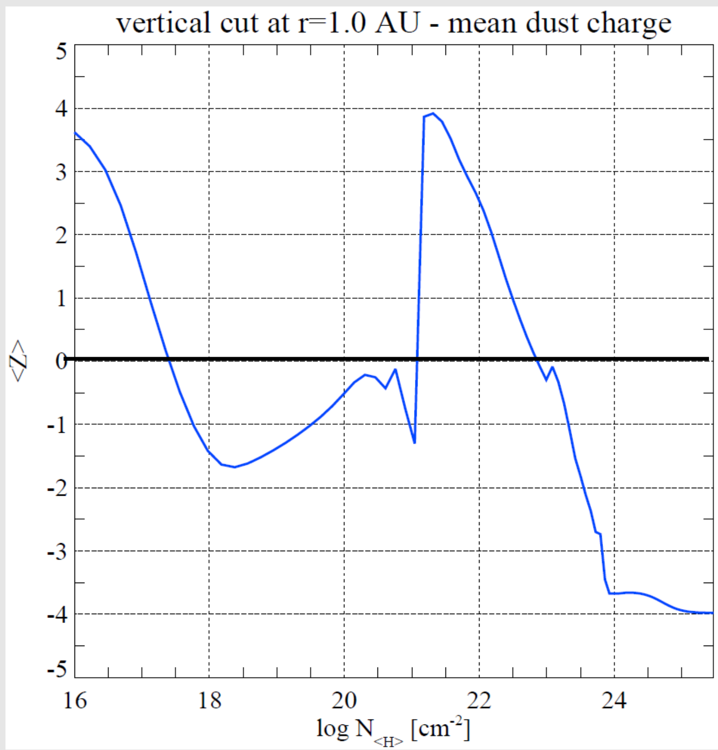
Charged grain chemistry

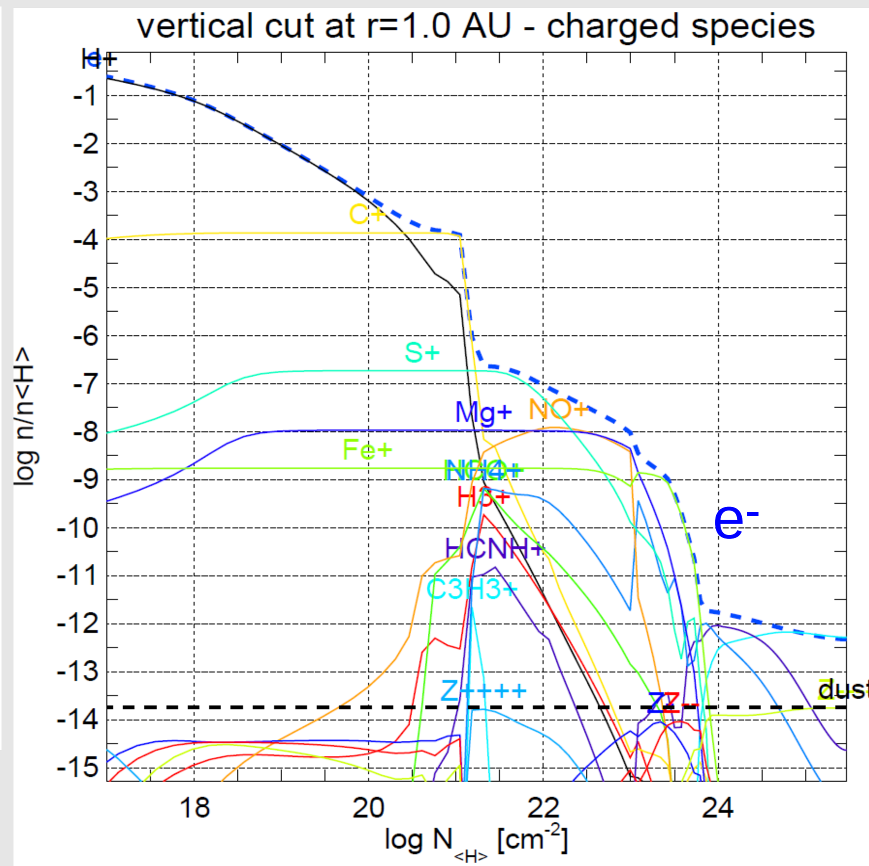
$Z + h\nu \rightarrow Z^+ + e^-$	photoelectric / photodetachment
$Z + e^- \rightarrow Z^-$	electron attachment
$Z + A^+ \rightarrow Z^+ + A$	charge exchange
$Z + AB^+ \rightarrow Z^+ + A + B$	dissociative charge exchange
$Z \rightarrow Z^+ + e^-$	thermionic emission
$Z + M \rightarrow Z^+ + e^- + M$	collisional electron detachment
$Z + Z \rightarrow Z^+ + Z^-$	*tribo-electric changing (missing)*

included species

$Z^{----}, Z^{---}, Z^{--}, Z^{-},$
$Z,$
$Z^{+}, Z^{++}, Z^{+++}, Z^{++++}$

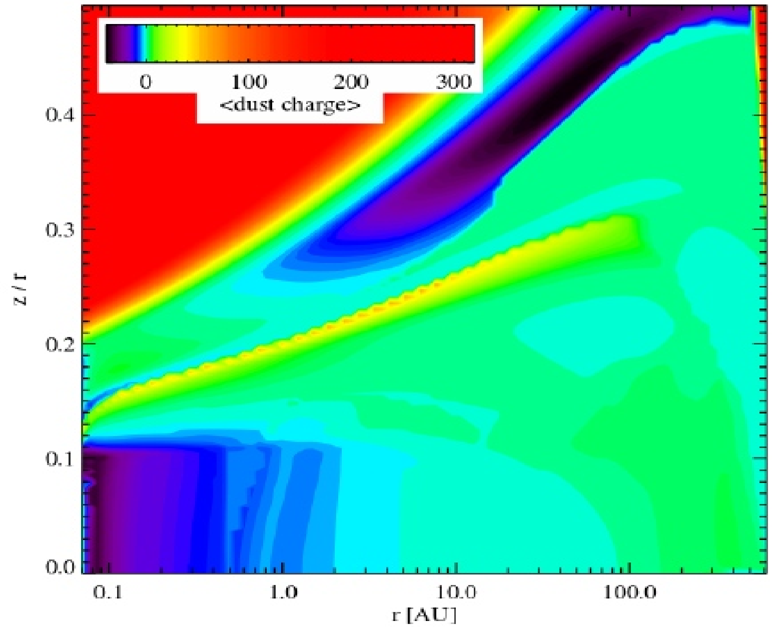


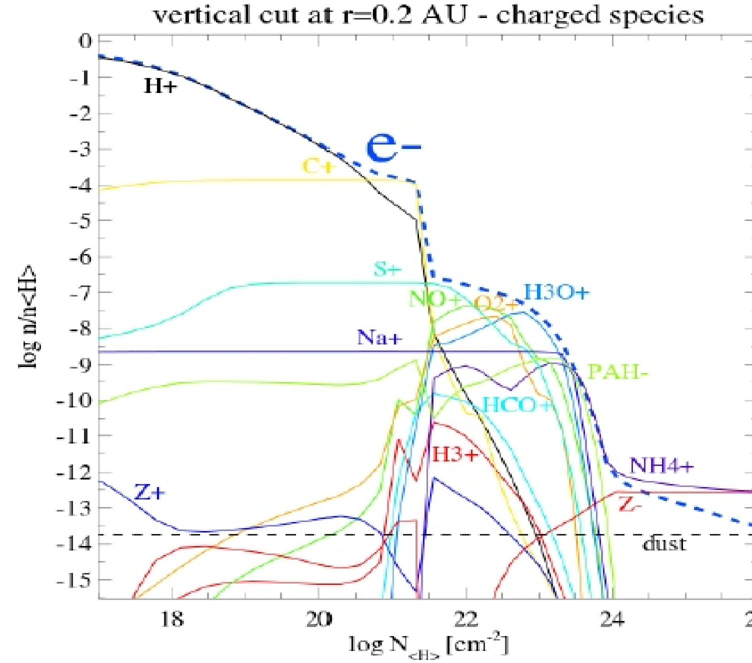


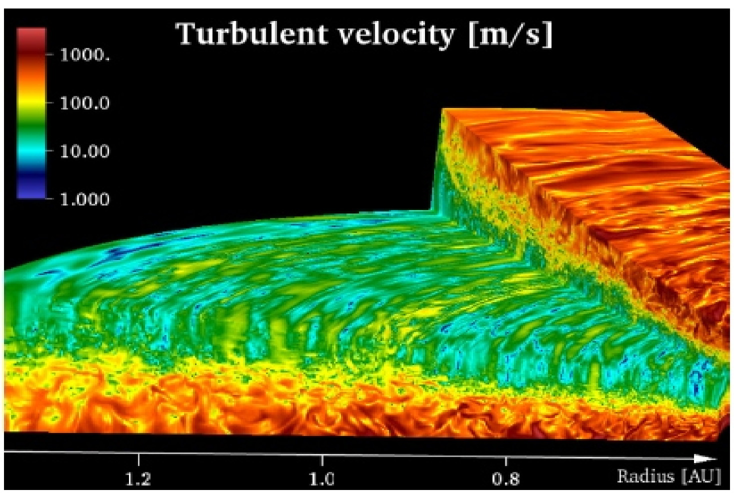


new: charge moments

$$[Z^+] = n_d \sum_{1}^{Z_{max}} Z_d f(Z_d)$$



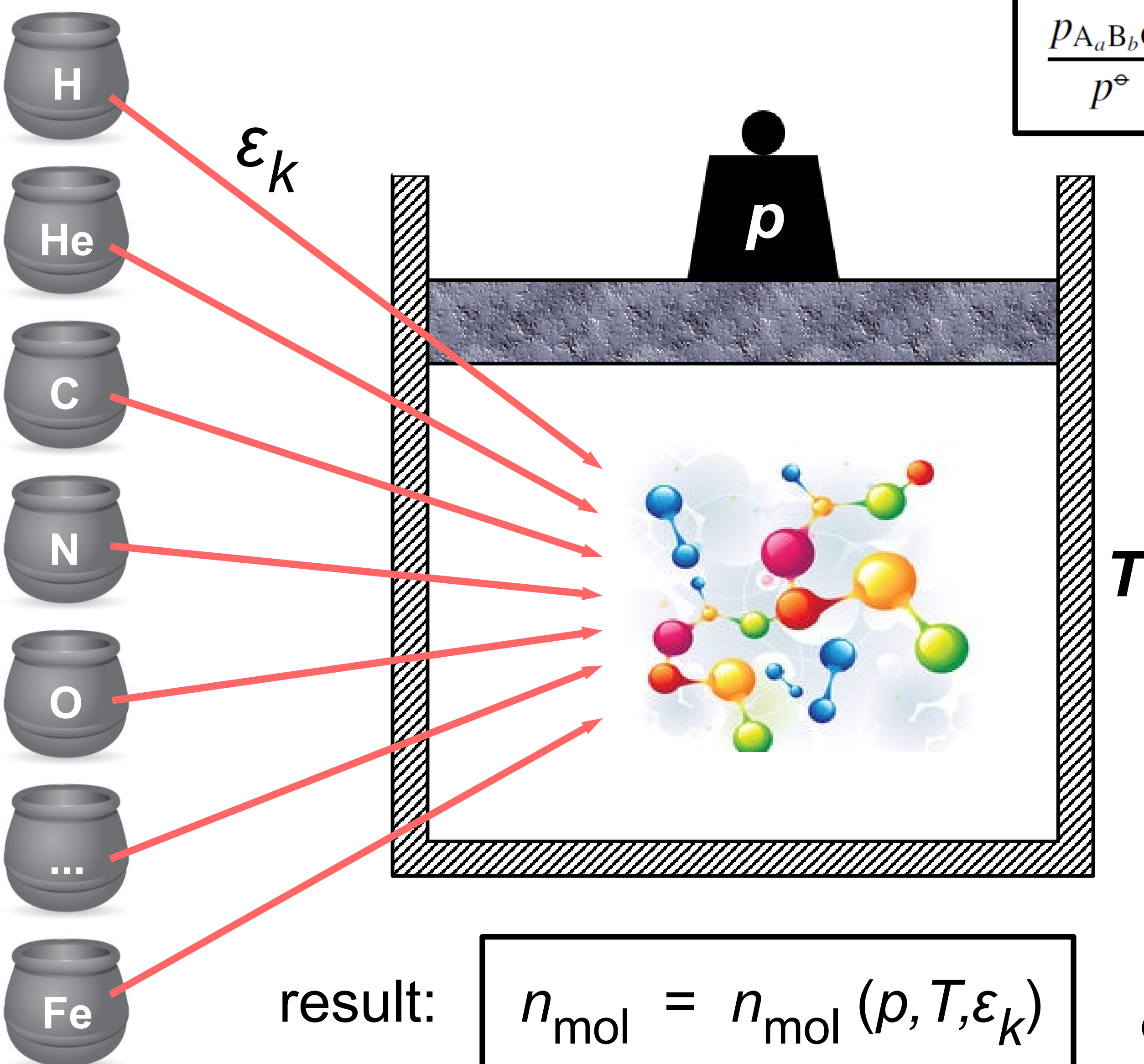




	dusty plasma	dust in dead zone	dust in insulating gas
charge carriers	$n_{\rm el} \approx n_{\rm ions} \gg n^+_{\rm dust}, n^-_{\rm dust}$	$n^-_{\rm dust} \approx n_{\rm ions} \gg n_{\rm el}$	$n^-_{\rm dust} \approx n^+_{\rm dust} \gg n_{\rm el}, n_{\rm ions}$
electron concentration	$10^0 \ldots 10^{-13}$	$\lesssim 10^{-13}$	$\lesssim 10^{-13}$
dust motions can build up an electric field?	no	no	yes

GGchem: chemical Equilibrium in the Gas Phase

$$\frac{p_{\mathrm{A}_a\mathrm{B}_b\mathrm{C}_c}}{p^{\ominus}} = \left(\frac{p_{\mathrm{A}}}{p^{\ominus}}\right)^a \left(\frac{p_{\mathrm{B}}}{p^{\ominus}}\right)^b \left(\frac{p_{\mathrm{C}}}{p^{\ominus}}\right)^c \exp\left(-\frac{\Delta G_{\mathrm{f}}^{\ominus}}{RT}\right)$$



minimisation of system Gibbs free energy
<=>
solution of Guldberg's law of mass action

atom partial pressures

elements

molecule $\mathrm{A}_a\mathrm{B}_b\mathrm{C}_c$

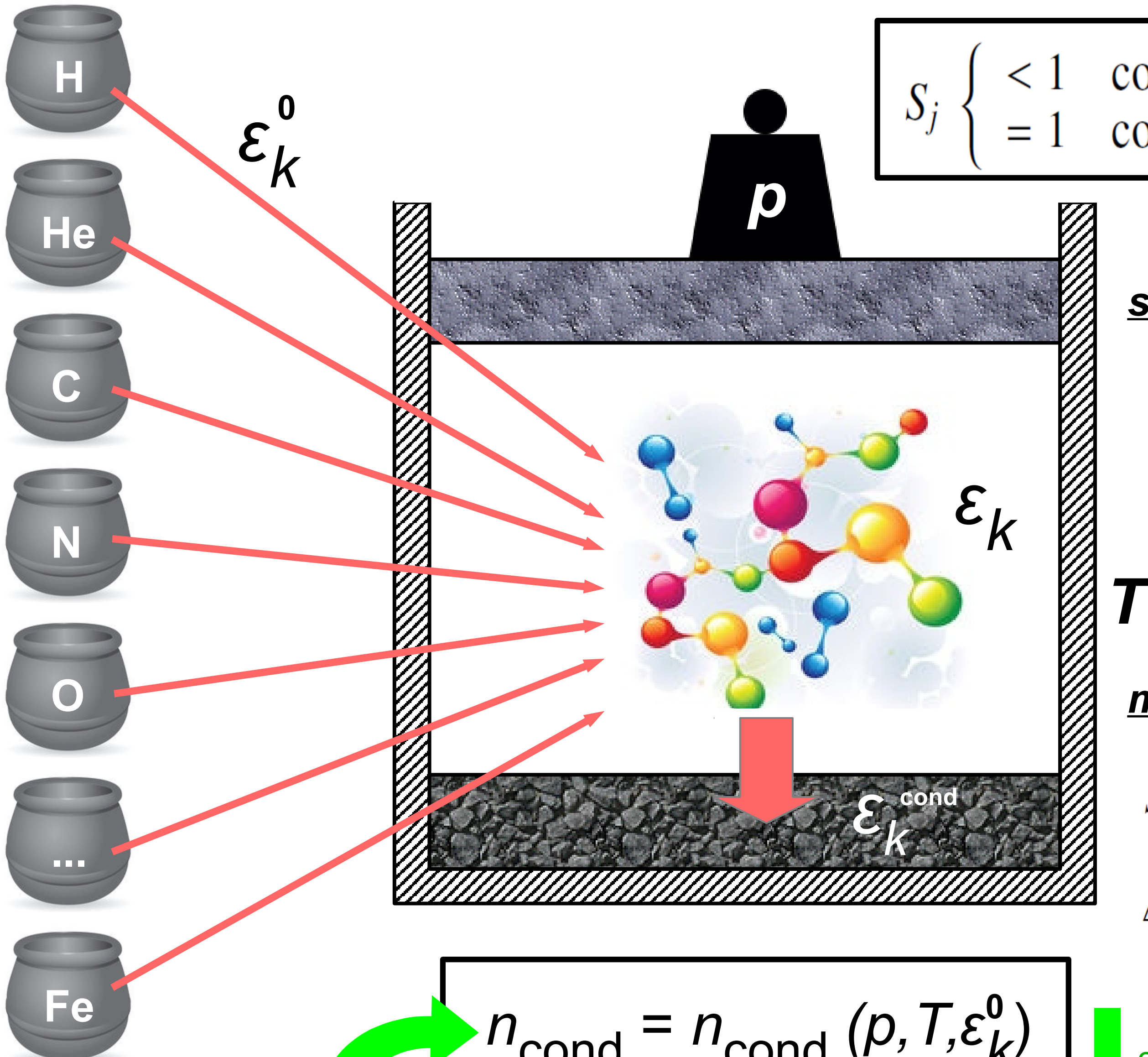
stoichiometric factors

result: $\boxed{n_{\mathrm{mol}} = n_{\mathrm{mol}}(p, T, \varepsilon_k)}$

Gibb's free energy

$$\Delta G_{\mathrm{f}}^{\ominus} = G^{\ominus}(\mathrm{A}_a\mathrm{B}_b\mathrm{C}_c, T) - a\,G^{\ominus}(\mathrm{A}, T) - b\,G^{\ominus}(\mathrm{B}, T) - c\,G^{\ominus}(\mathrm{C}, T)$$

Equilibrium condensation (phase equilibrium)



$$S_j \begin{cases} < 1 & \text{condensate is unstable and not present,} \\ = 1 & \text{condensate is stable and present,} \end{cases}$$

species stable as free a molecule

$$S_j = \frac{p_j}{p_j^{\mathrm{vap}}(T)}$$

$$p_j^{\mathrm{vap}}(T) = p^\circ \exp\left(\frac{G^\circ(j[\mathrm{cond}],T) - G^\circ(j,T)}{RT}\right)$$

molecule does not exist

$$S_{\mathrm{A}_a\mathrm{B}_b\mathrm{C}_c} = \left(\frac{p_\mathrm{A}}{p^\circ}\right)^a \left(\frac{p_\mathrm{B}}{p^\circ}\right)^b \left(\frac{p_\mathrm{C}}{p^\circ}\right)^c \exp\left(-\frac{\Delta G_\mathrm{f}^\circ}{RT}\right)$$

$$\Delta G_\mathrm{f}^\circ = G^\circ(\mathrm{A}_a\mathrm{B}_b\mathrm{C}_c[\mathrm{cond}],T) - a\,G^\circ(\mathrm{A},T) - b\,G^\circ(\mathrm{B},T) - c\,G^\circ(\mathrm{C},T)$$

supersaturation ratios & selection of condensates

$$n_{\mathrm{cond}} = n_{\mathrm{cond}}\,(p,T,\varepsilon_k^0)$$

$$\varepsilon_k = \varepsilon_k^0 - \varepsilon_k^{\mathrm{cond}}$$

$$n_{\mathrm{mol}} = n_{\mathrm{mol}}\,(p,T,\varepsilon_k)$$

computation of gas-phase chem. equil.

The GGchem code

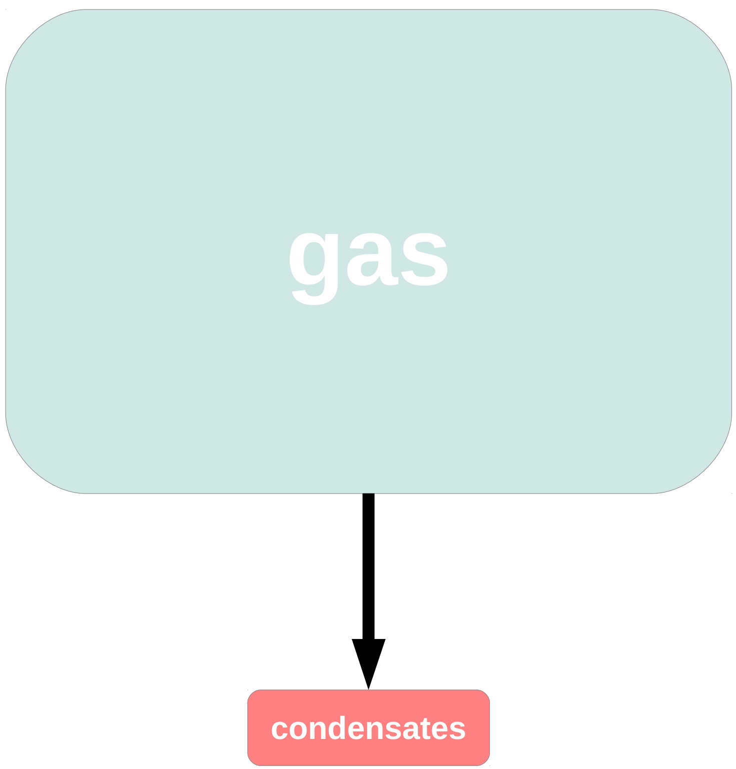
- up to **40 elements** (H, … , Zr, and W)
- up to **1155 molecules**
- up to **251 condensates** (solids & liquids) from **NIST-JANAF** and **SUPCRTBL**
- **customised selection** of elements, molecules, and condensates
- thermo-chemical data **down to 100 K** carefully checked
- **ultra-fast Fortran code**, about 40 ms / call for K=24 elements, scales ~ K^3
  - stable iterative solution scheme based on Newton-Raphson
  - fast real*8 (T > 1000 K) and stable real*16 (T→100 K)
- **benchmarked** against TEA code (Blecic 2016)
- optionally include **ions and free electrons, condensates**
- specify gas density (ρ,T) or gas pressure (p,T)

→ Woitke, Helling, Hunter, Millard, Turner, Worters, Blecic, Stock **(A&A 2018, 614,1)**

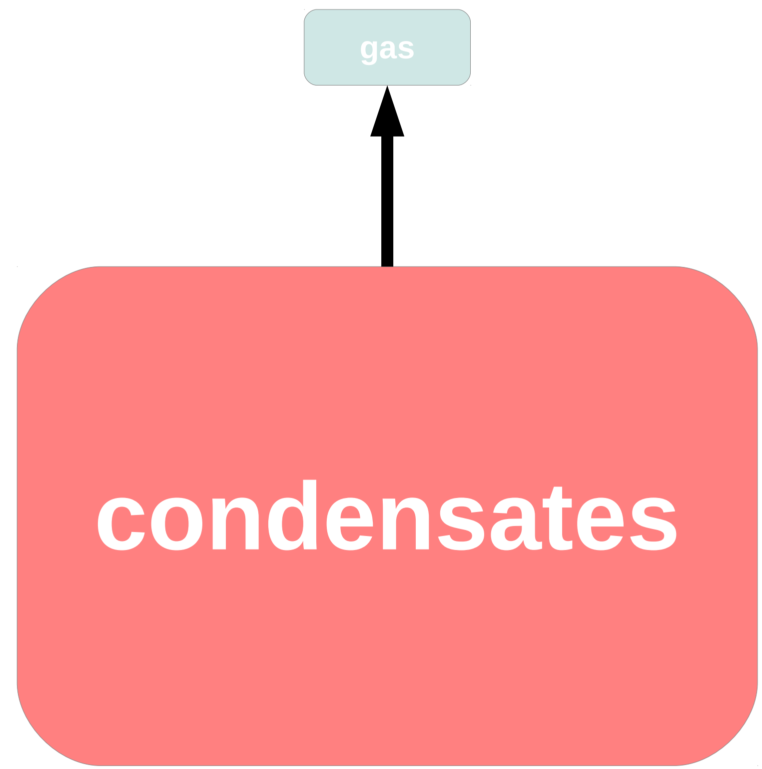
→ ***public code:*** **https://github.com/pw31/GGchem**

> git clone https://github.com/pw31/GGchem
(includes all thermo-chemical data)

Astro-Chemistry



Geology



Classification of exoplanet atmospheres based on H-C-N-O abundances

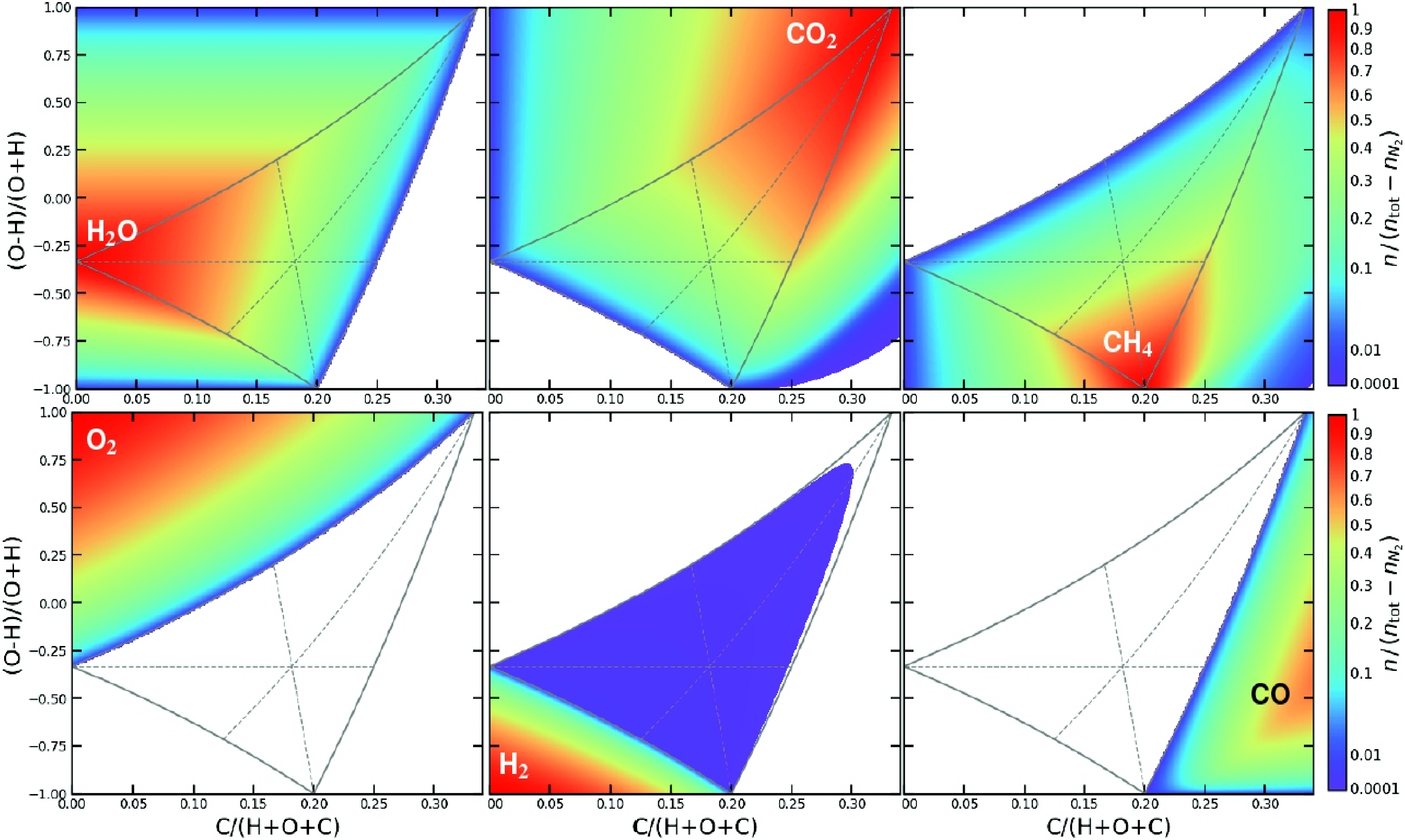


Fig. 1. Molecular particle concentrations in chemical equilibrium as function of hydrogen, carbon, and oxygen element abundances, calculated for $T = 400\,\mathrm{K}$ and $p = 1\,\mathrm{bar}$. The central gray triangle marks the region within which H_2O, CH_4 and CO_2 coexist in chemical equilibrium. The dashed lines indicate where the concentrations of two molecules are equal: H_2O and CO_2, CO_2 and CH_4, and CH_4 and H_2O. Blank regions have concentrations $< 10^{-4}$. In order to enhance the colour contrasts, a colourmap was chosen that is linear in $(n/n_{tot})^{1/2}$ from 0.01 to 1.

Table 2. Trace gas concentrations in chemical equilibrium with element abundances $N = 2/13$, $H = 6/13$, $O = 3/13$ and $C = 2/13$, where main constituents are 25% N_2, 25% H_2O, 25% CO_2 and 25% CH_4.

	200 K	300 K	400 K	500 K	600 K	700 K
H_2	2 ppb	5.8 ppm	390 ppm	0.52%	2.9%	9.5%
CO	< 1 ppb	< 1 ppb	260 ppb	39 ppm	0.11%	1.2%
NH_3	205 ppb	4.7 ppm	23 ppm	58 ppm	101 ppm	130 ppm

→ ***very pure gas at low temperatures***
→ ***effect of mixing entropy with increasing temperature***

Effect of water and graphite condensation

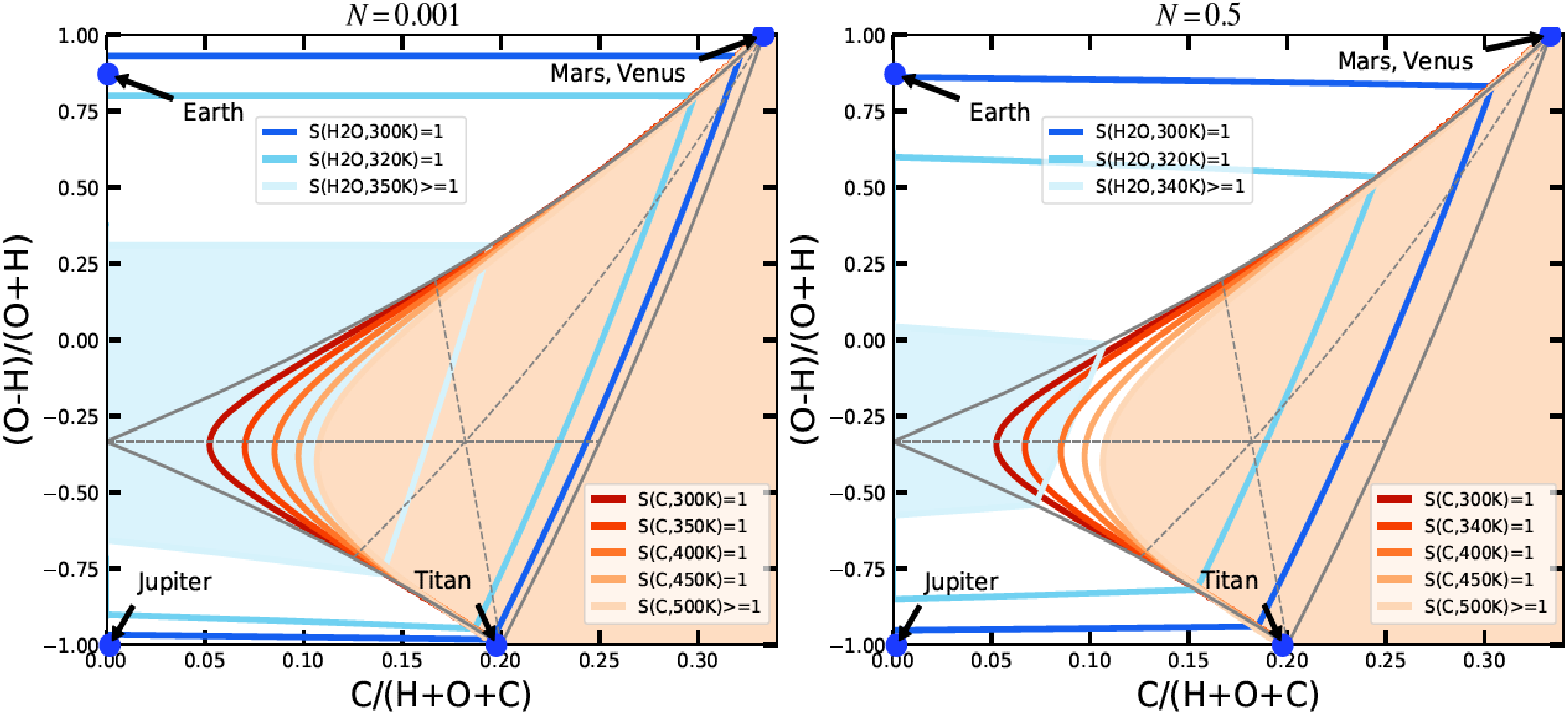
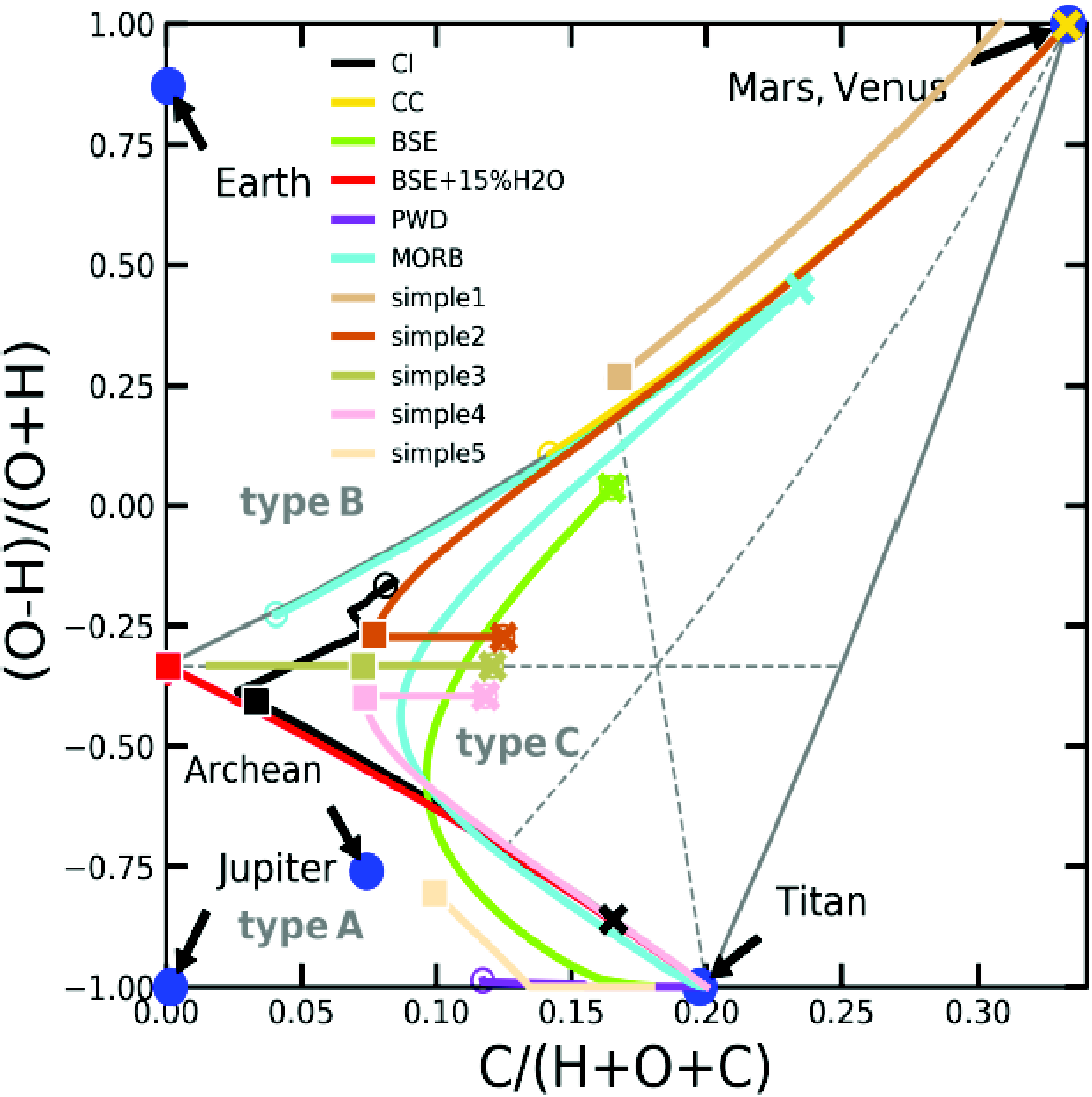


Fig. 2. Impact of liquid water (H_2O) and graphite (C) condensation. The blue and orange contour lines mark where the supersaturation ratio equals one for water and graphite, respectively, at selected temperatures. Inside of the light blue and light orange shaded regions, the gas is supersaturated with respect to water at 350 K and graphite at 500 K, respectively. For higher temperatures, the shaded areas shrink and eventually vanish. The atmospheric compositions of Earth, Mars, Venus, Jupiter and Titan are marked. Earth (assuming 1.5% water content) sits right on top of the $S(H_2O, 300\,K) = 1$ line. A constant pressure of $p = 1$ bar is assumed.

Equilibrium condensation models



type A: **H_2**-containing atmospheres made of **CH_4, H_2O** and **NH_3**, but no CO_2 and no O_2.

type B: **O_2**-containing atmospheres made of **N_2 , CO_2** and **H_2O**, but no CH_4 and no NH_3.

type C: Atmospheres made of **H_2O, CO_2, CH_4 and N_2**, but no H_2, no O_2 and no NH_3.

Type C exoplanet atmospheres are not found in the solar system, however, slightly warmer exoplanets may well host such atmospheres.

The equilibrium condensation models show that type C atmospheres can naturally be created by the outgassing from common rock materials such as carbonaceous chondrites (CI)

CI = Carbonaceous Chondrites
MORB = Mid Oceanic Ridge Basalt
CC = Continental Crust,
BSE = Bulk Silicate Earth
PWD = Polluted White Dwarf observations.

The points where the trajectories start to have graphite are marked by crosses, and the points where liquid water starts to occur are marked by squares.

Summary & Conclusions

- **H_2O, CO_2, CH_4, N_2** are the thermodynamically most favourable molecules in the H – C – N – O system at low temperatures
- in chemical equilibrium, we find 3 types of atmospheres 200K – 600K:
  type A: **H_2, H_2O, CH_4, NH_3, N_2** – but no CO_2, no O_2
  type B: **O_2, H_2O, CO_2, N_2** – but no CH_4, no H_2, no NH_3
  type C: **H_2O, CH_4, CO_2, N_2** – but no H_2, no O_2, no NH_3
- ***%-molecules are in chemical equilibrium:*** Their concentrations are constrained by stoichiometry & element abundances – only the identification of what are the most stable molecules must be correct
- ***non-equilibrium markers:***
  a combination of (i) a molecule that reacts exothermic with one of (ii) H_2O, CH_4 or CO_2 – both need to be detected simultaneously
- ***a biosignature*** should be a non-equilibrium marker. Krissansen-Totton+2019 proposed **CH_4 and CO_2 without CO**. This works well in type A and type B atmospheres, but it does not work in type C atmospheres, likely producing many false positives