Self-consistent modelling of stellar and sub-stellar atmospheres

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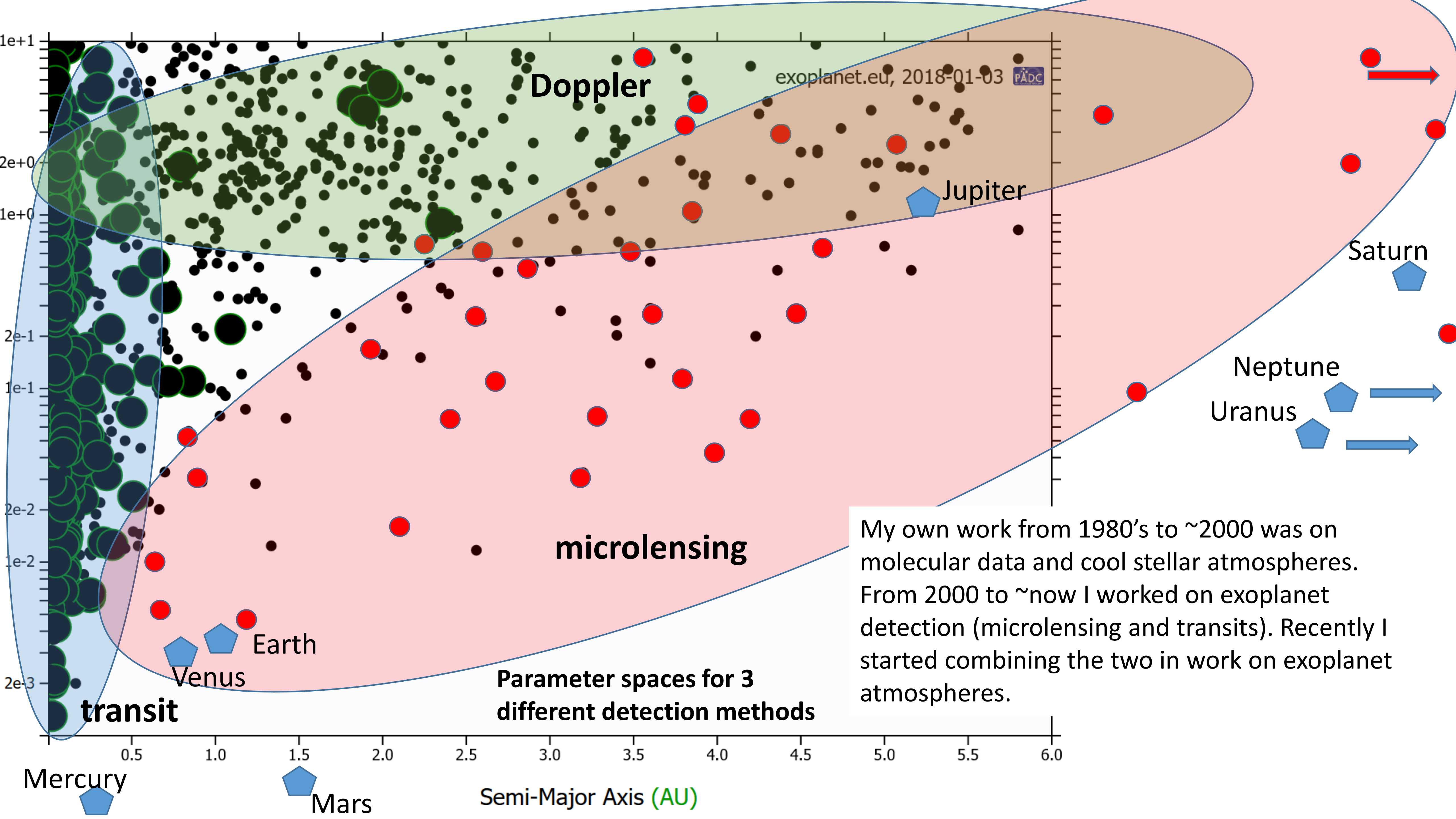
Major challenges to Progress:

- combine the strengths of different type of exoplanet modelling methods
- assure the still missing molecular data
- understand the microphysics of cloud formation

Questions we eventually would like to answer:

Which types of exoplanets are common in our Galaxy?
Are Earth-like exoplanets habitable (do they have water)?
Can we recognize the existence of life in the spectra?
(half a century of very detailed measurements from Mars didn't reveal whether there is life on Mars)



My own work from 1980's to ~2000 was on molecular data and cool stellar atmospheres. From 2000 to ~now I worked on exoplanet detection (microlensing and transits). Recently I started combining the two in work on exoplanet atmospheres.

Quantitative interpretation of observed exoplanet spectra requires detailed input data and **model atmospheres. D**etection of biology requires time dependent chemistry (**life includes** local entropy reduction, which requires out of equilibrium chemistry).

A numerical code could build on development of:

- Spectral retrieval models (with some free parameters)
- Earth climate models (Global Circulation Models)
- Models of Jupiter and other planets (tuned to types of exoplanets that we do not see yet)
- Cool stellar and brown dwarf models (this work)
- A combination of some of the above (which is our future aim)

Stellar atmosphere codes have the advantage of being very well tested. Compared to **planetary and GCM models** they usually have more advanced radiative transfer and are self-consistent, but they often lack advanced dynamics and cloud-formation.

Together with Christiane Helling, St.Andrews, and PhD student Diana Juncher we constructed a grid of self-consistent dust-gas DRIFT-MARCS models (Juncher et al, A&A, 2017) based on a combination of the MARCS atmospheric code (Gustafsson et al 2008) and the DRIFT cloud formation code (Helling et al 2008, 2016).

Nucleation and condensation species

Nucleation and condensate considerations

- refractory
- gas phase abundancy
- thermal stability of monomers

Nucleation species and growth monomers are two different things.

Nucleation candidates

Al_2O_3	$CaTiO_3$	TiO_2
Fe		SiO

Solids

TiO_2 [s]	Mg_2SiO_4 [s]	SiO_2 [s]
Fe [s]	$MgSiO_3$ [s]	Al_2O_3 [s]
MgO [s]	$CaTiO_3$ [s]	FeO [s]
FeS [s]	Fe_2O_3 [s]	SiO [s]

While we adopt TiO2 as the most important nucleation seed, other people find $CaTiO_3$ to have the highest nucleation rate, and metallic W to have the highest condensation temperature.

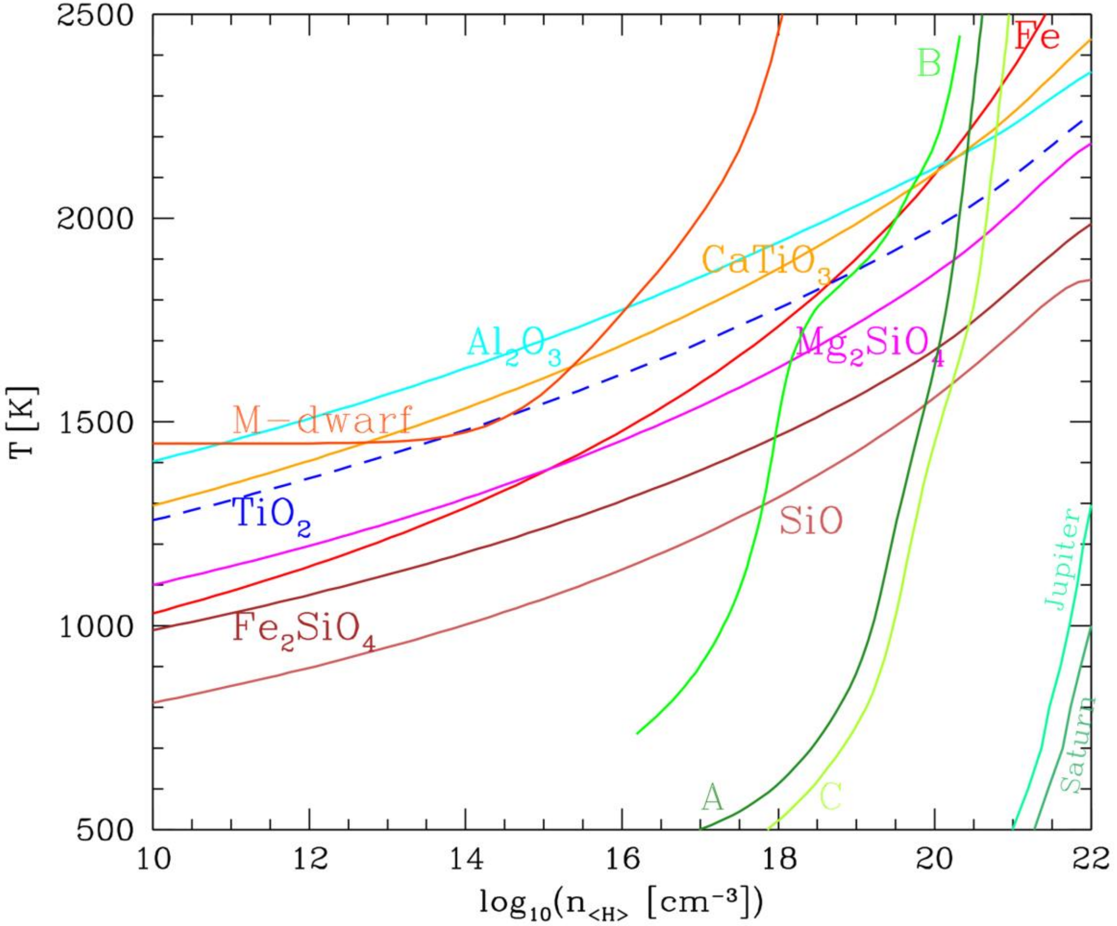
Cloud formation

Earth:

- collections of droplets of liquid water or ice crystals
- form when humid air cools down enough for the water vapor to condensate on pre-existing nucleation seeds (dust)

Ultra cool dwarfs and exoplanets:

- very different conditions!
- composed of minerals such as rutile (TiO_2), olivine ($(Mg,Fe)_2SiO_4$) and corundrum (Al_2O_3)



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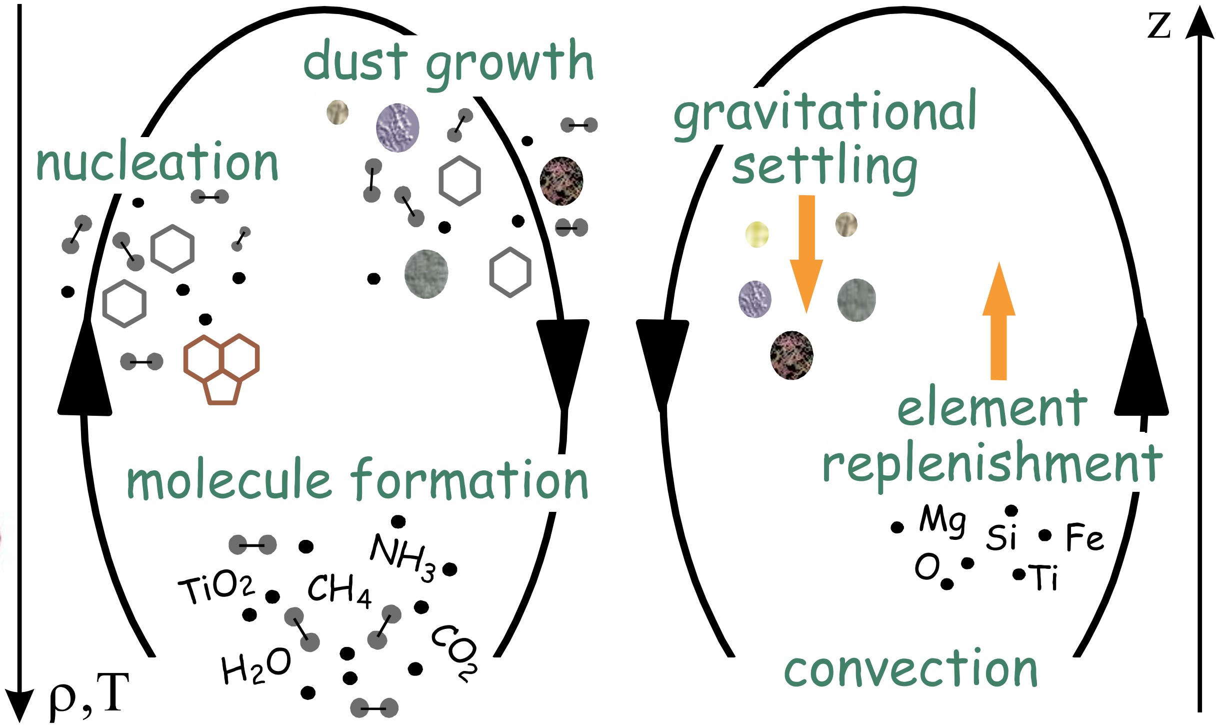
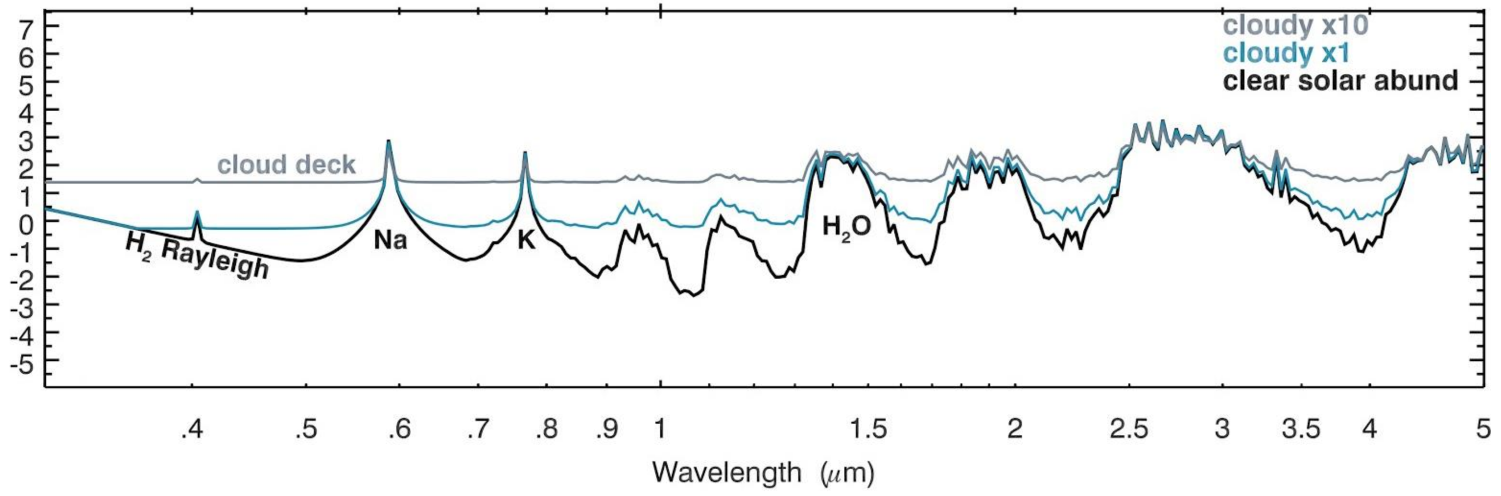
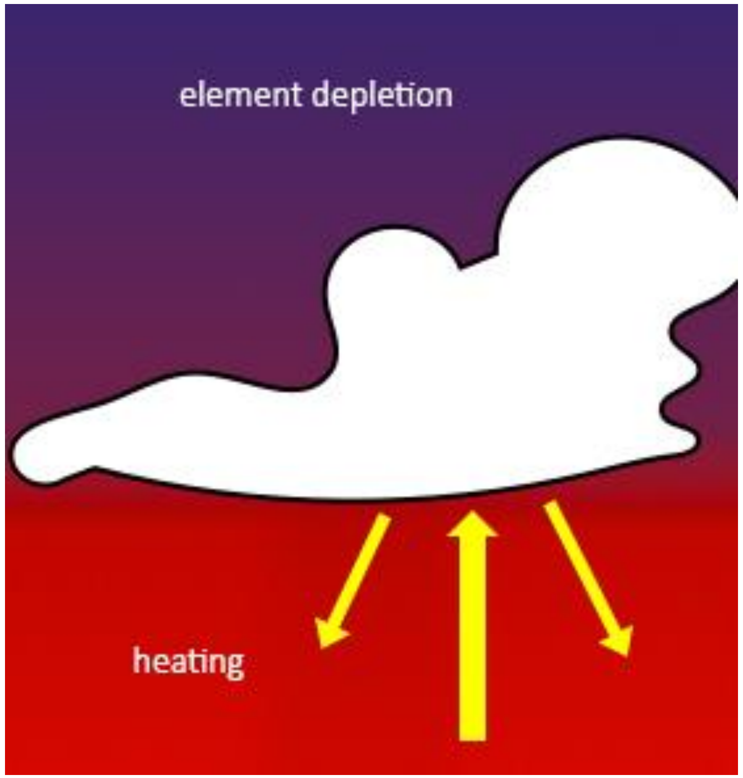
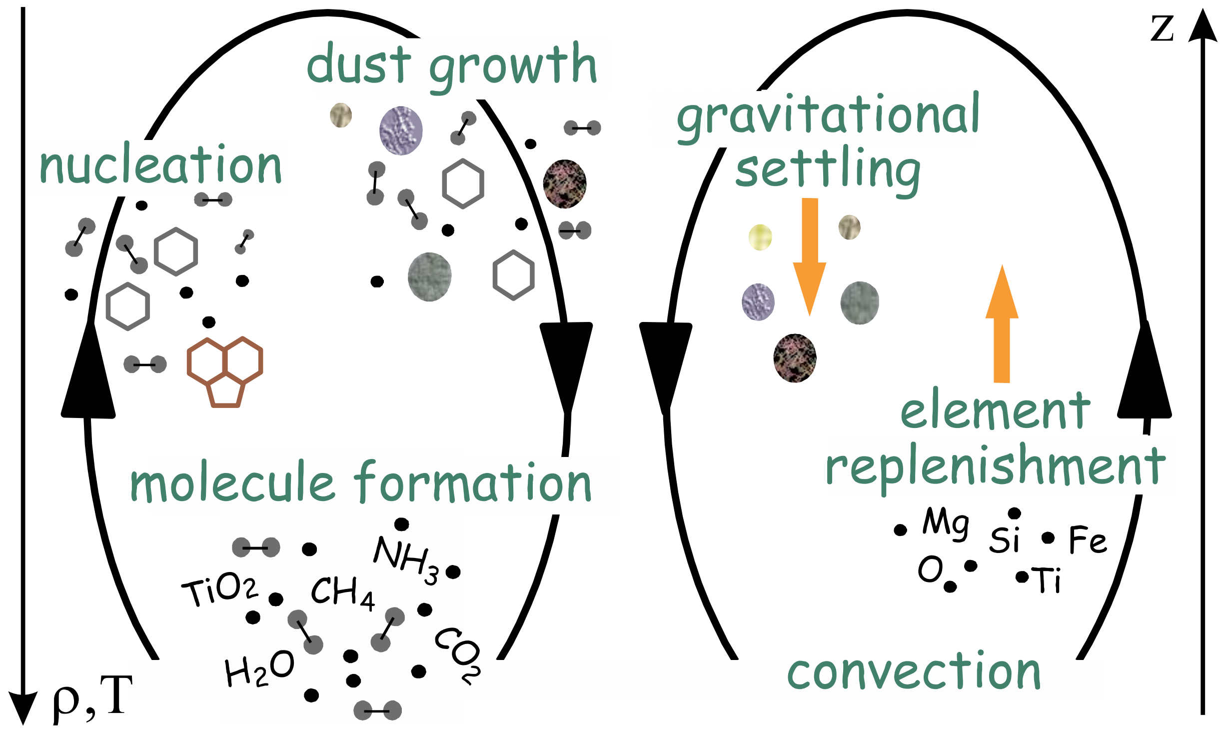


Clouds are essential for the energy balance but often very different from Earth-like clouds

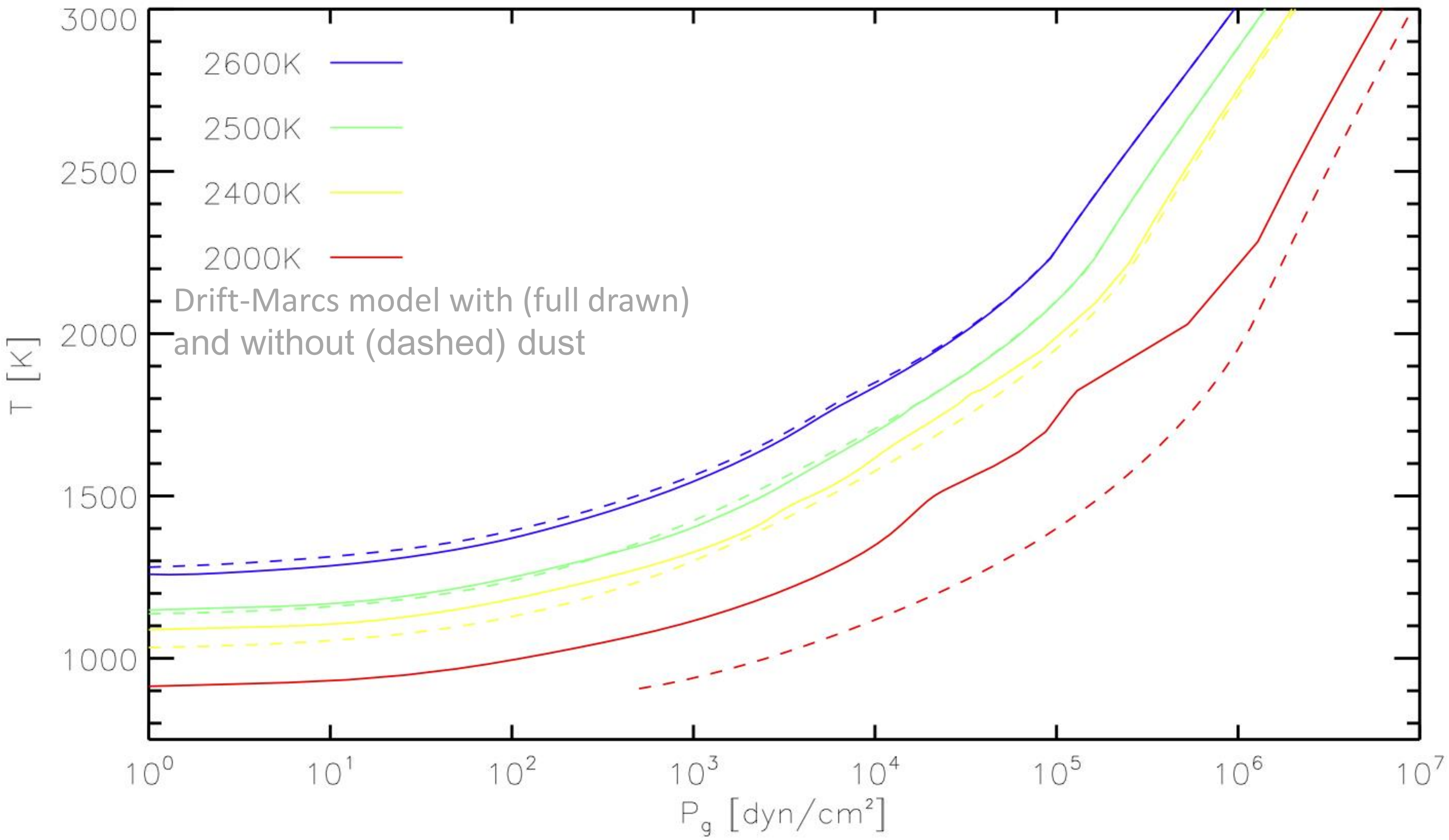
In objects with energy coming from below (i.e. stars, brown dwarfs, some exoplanets) clouds will heat the lower atmosphere.
From a numerical point of view this complicates the convergence.
From an observational point of view, molecular abundances are lowered and the clouds smooth out the remaining gas absorption bands.



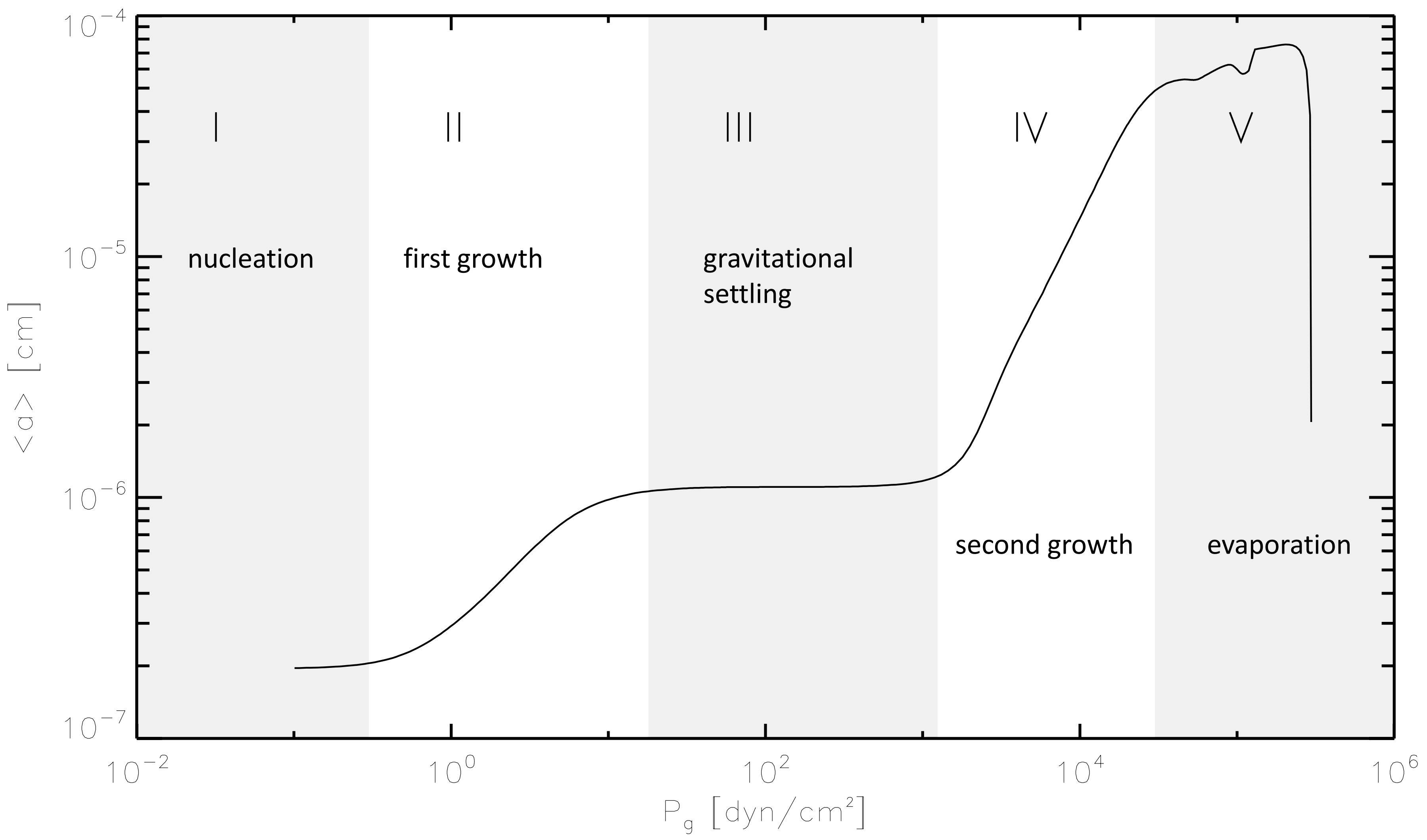


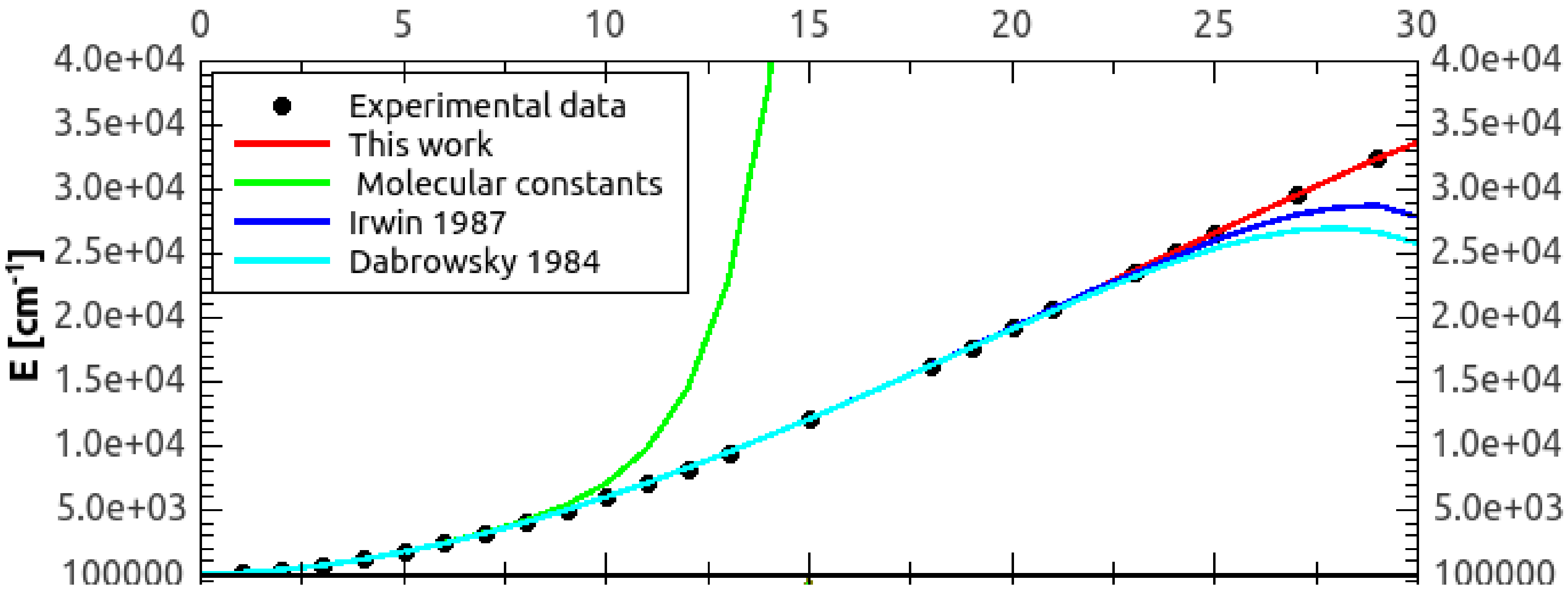


Warmer models are slightly cooled because on decreasing gas opacities, while cooler models are strongly heated by cloud back-warming.
Irradiated exoplanets may cool or heat depending on details of where the clouds are, just like on Earth.



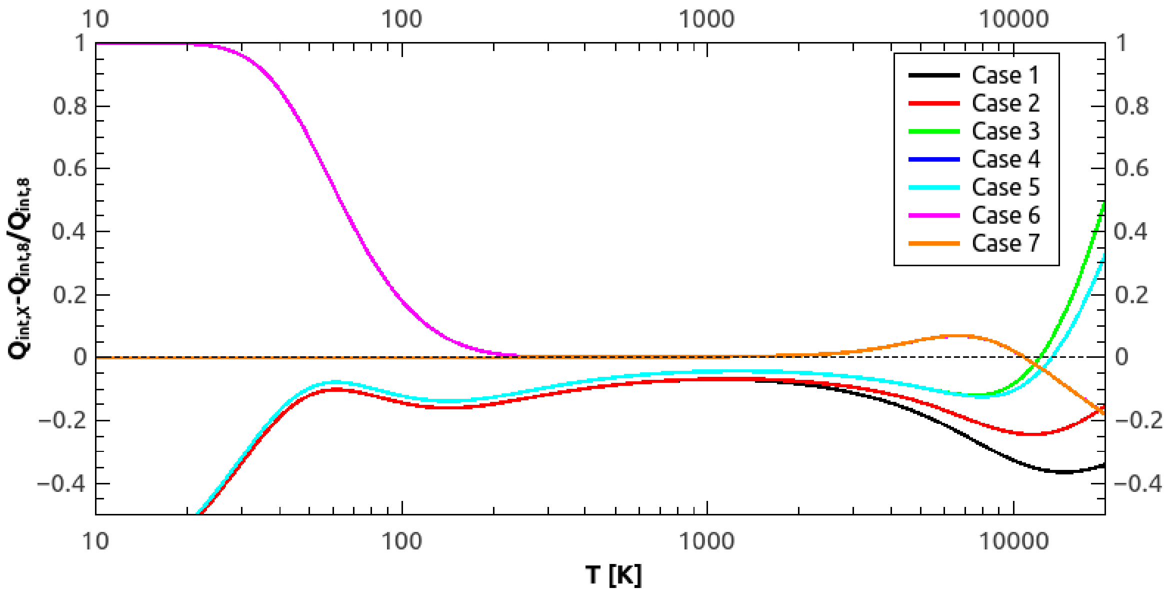
Cloud regions





Partition functions: Dunham coefficient fits and careful evaluation of upper boundary of the energy is recommended.

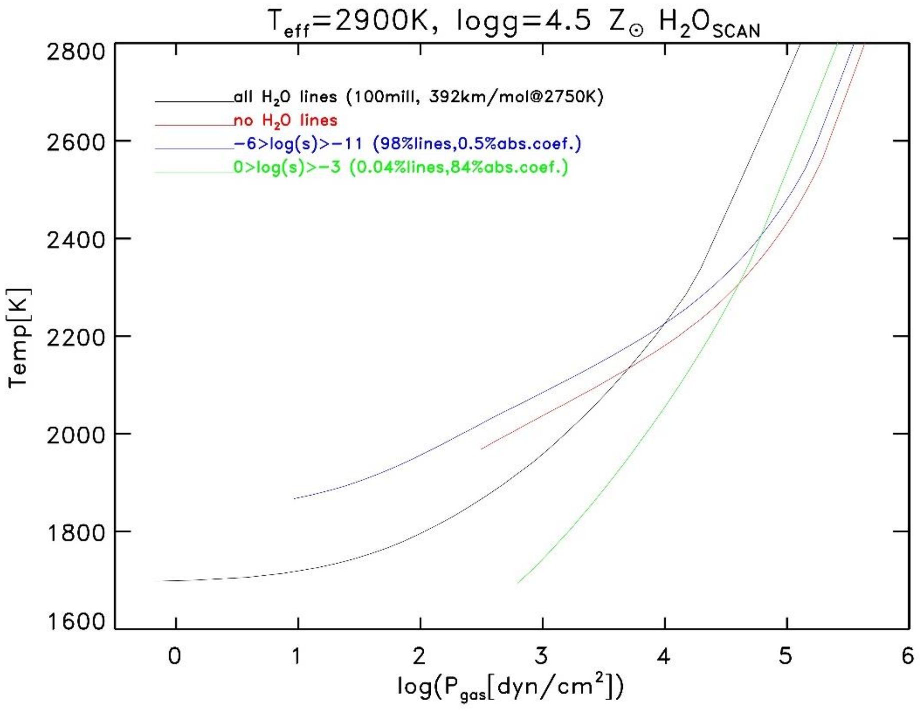
Analysis of the H2 molecule from Popovas&Jørgensen A&A 595, 130, 2016. Independent of the atmospheric modelling method, the fundamental data have to be correct. The line intensities scale directly with the value of the partition functions, and hence roughly also the obtained abundances. Line lists and partition functions must be mutually consistent.



Various polynoimial fits and upper cut offs have been applied in the literature. We use Dunham coefficient fits, which still uses the concept of quantum numbers, but are less rooted in the classical diffuse image of atoms on a vibrating-rotating spring as forming the molecule. Dunham polynomia fits the higher energy levels better, but are still erroneously describing the degeneration multiplicity as being determined by the assigned quantum number. It further has the same basic problem with the upper boundary being unknown. We sum to the minimum of either the dissociation energy or where deltaE(v,j) < 0. In reality Q is pressure dependent since the upper energy is determined by the available space to the surrounding molecules. Also the inclusion of quasistable electronic states into the partition function is in principle an undefined issue, but of less importance than the quality of the fits to the upper levels and the cut off value. The subsequent polynomial fit to the value of Q as function of temperature is often what introduces the largest error into the value of Q and should be avoided. Together the various approximations applied in the literature (case 1 – 7 in previous slide) can introduce 40% or larger errors in Q (for H_2) at the highest temperatures of interest.

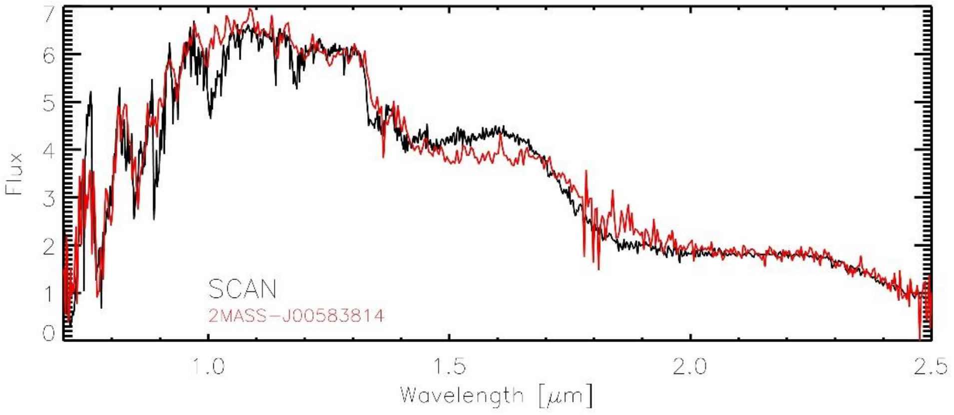
How many lines at which accuracy should a line list have?

My early work was among the first to demonstrate the importance of the many weak molecular lines for the atmospheric structure (e.g. Jørgensen et al 1985, JChPh,83,3034 about HCN). The strong lines can be measured as function of temperature in the lab. The weak lines can only be calculated, and how to do this "correct" can only be estimated from stellar spectra.

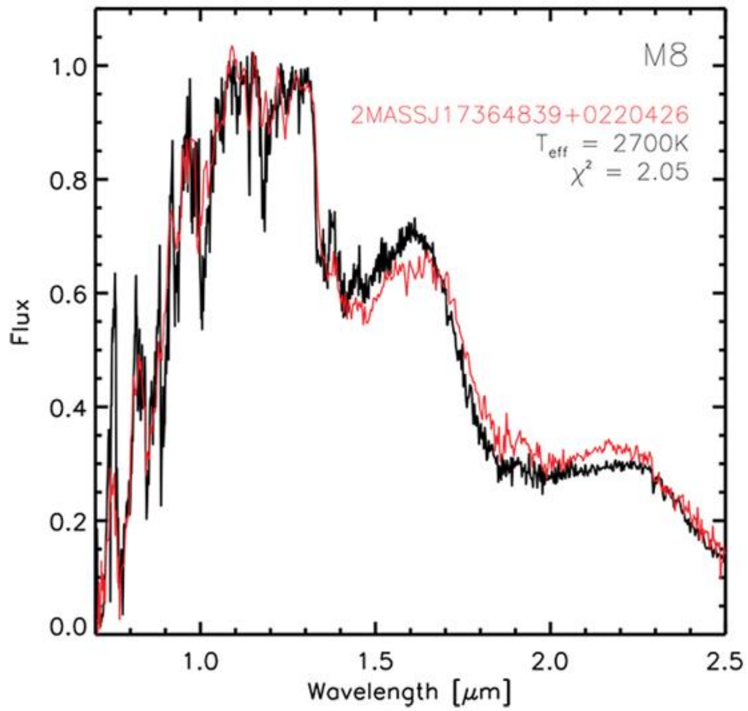


Strong/weak line example: the 100 million lines absorption coefficient of the water molecule

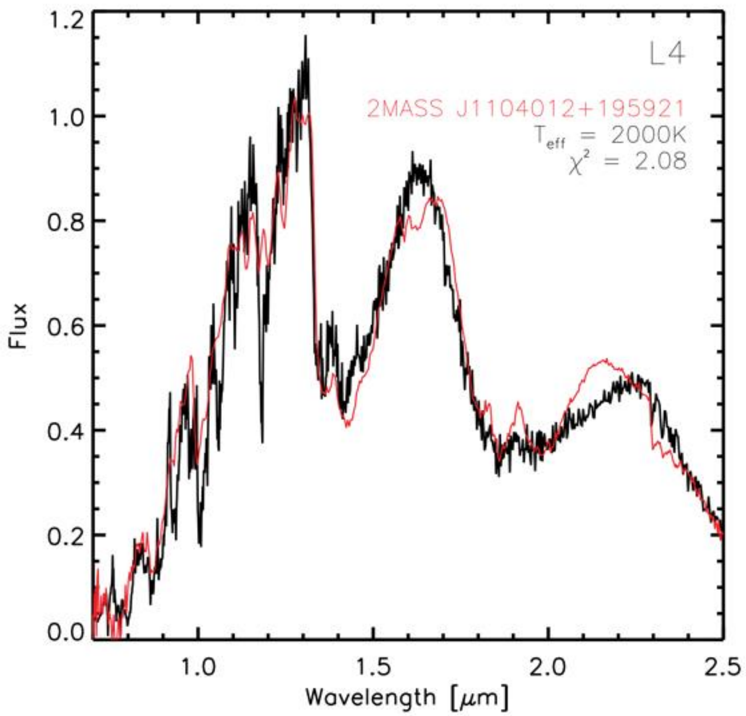
Observed (black) and computed (red) spectrum of a Teff~2900K M dwarf based on 100 million lines H2O SCAN list.
Some of the strong lines fit poorly to 2900 K laboratory measurements in the 1.4 to 2.3 micron region, but reproduce the stellar spectrum (and structure) correctly.



Laboratory experiments measure the strong lines only, while the atmospheric structure is most sensitive to the weak lines. 1.e8 lines per 1.e4 Å is 30.000 lines per line width!

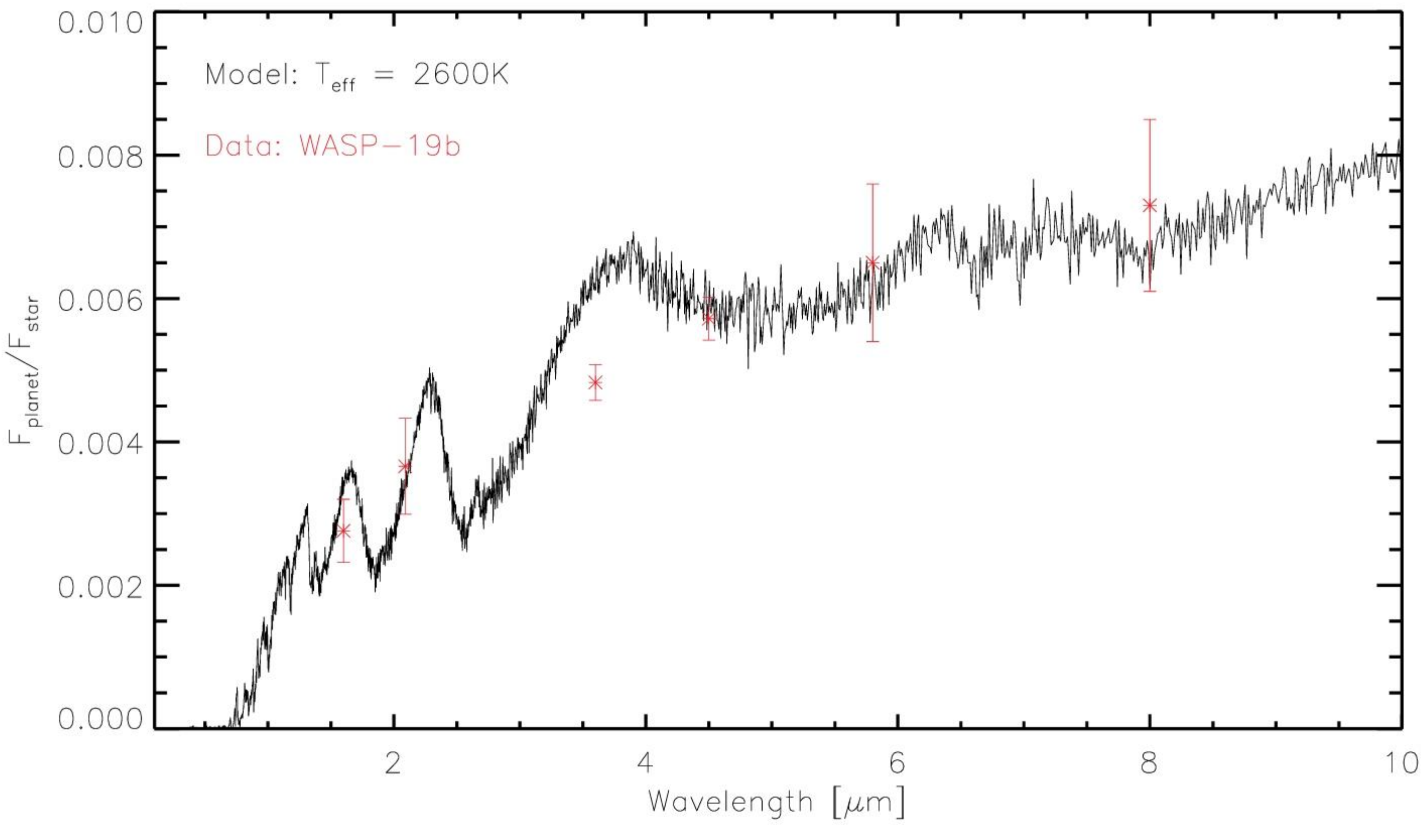


Synthetic DRIFT-MARCS spectra of cool stars and brown dwarfs fit observed spectra well
– i.e. the code, the input data and the methods are now well tested and reliable in the temperature range down to hot-jupiters.



WASP-19b is a hot Jupiter orbiting a solar type star. With teff=2600K it has some, but very little, dust. It is to a first approximation heated into deep layers by visual stellar light (like Earth's troposphere), that re-emits in IR. It can therefore as a test be approximated by a non-radiated model atmosphere. Our DRIFT-MARCS atmosphere of 2600 K fits IR photometric data well, except for the 3.6 micron point.

WASP-19b can be approximated with a carbon- or oxygen-rich atmosphere of Teff = 2600 K, log =4, and solar metallicity, and has only little dependence on gravity.



Conclusions:

We have combined a well tested radiative-convective 1D self-consistent stellar atmosphere code (MARCS) with a well tested dust formation code (DRIFT) to compute non-irradiated atmospheres with clouds.

Various methods to compute the partition functions give widely different results, and we warn against inconsistent use of partition functions.

The weak lines of extensive line lists cannot easily be compared with laboratory data. The quality of the weak-line veil is best tested by comparing observed and self-consistent synthetic spectra.

Work in progress: include irradiation, lower temperature gas chemistry, combine with GCM dynamics, more complete partition functions and dust species ---
-- *and to figure out where the extra-terrestrials live……..*

Note added during upload, following the discussion:

I was very pleased by a lively discussion following my talk, where it was stressed that comparing computed and measured line intensities is an essential part of a complete and accurate line list calculation. I completely agree with this point. Fortunately, good and very important progress has been obtained during a number of years on this issue. However, there is still a problem concerning the veil of weak lines, which plays a most central role for the atmospheric structure (and hence for the spectrum), and which is not easily solved in the laboratory. I touched upon some of the still unsolved issues about this in my presentation, including the incomplete description of the very upper most states in traditional quantum mechanics, as well as the difficulty in using laboratory experiments at fixed pressure or cell volume to account for the veil.

Another point raised during the discussion was that it is not possible to compute complete and accurate exoplanet atmospheres without irradiation, exactly as I stressed it in my slides, but which had seemingly not been clear. My presentation is a progress report about inclusion of cloud formation into existing well-tested stellar model atmospheres as a step toward high quality exoplanet modelling, including a discussion about why such first steps can give a reasonable fit to low resolution spectra of some hot-jupiter exoplanets, and what we can learn from that. The models presented here are not the final DRIFT-MARCS exoplanet atmospheres, which are yet to be computed.