# Atoms and molecules in stellar atmospheres

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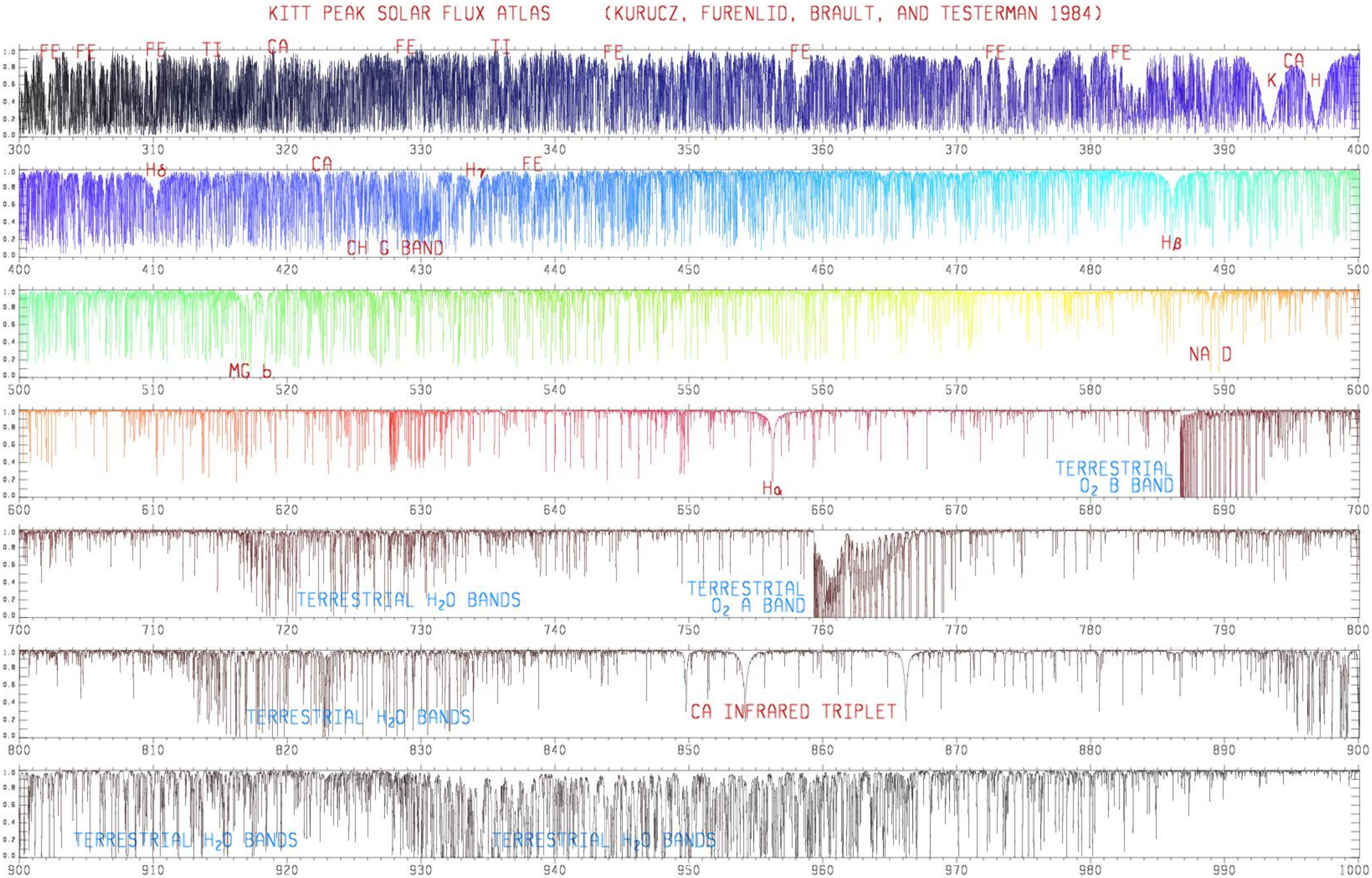
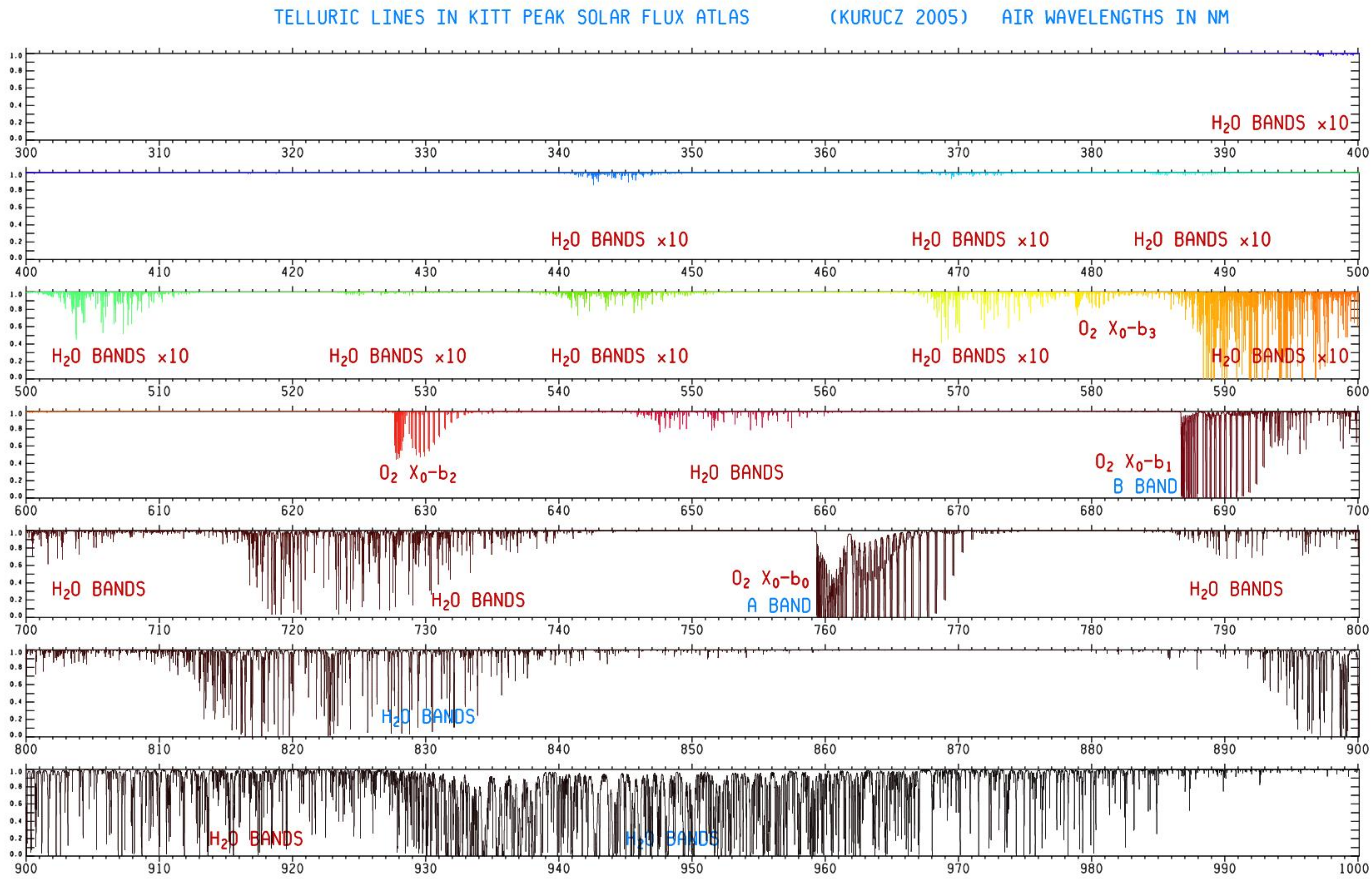
example stellar spectra
model atmospheres
model spectra
progress and challenges, esp. regarding molecular lines
The CH story

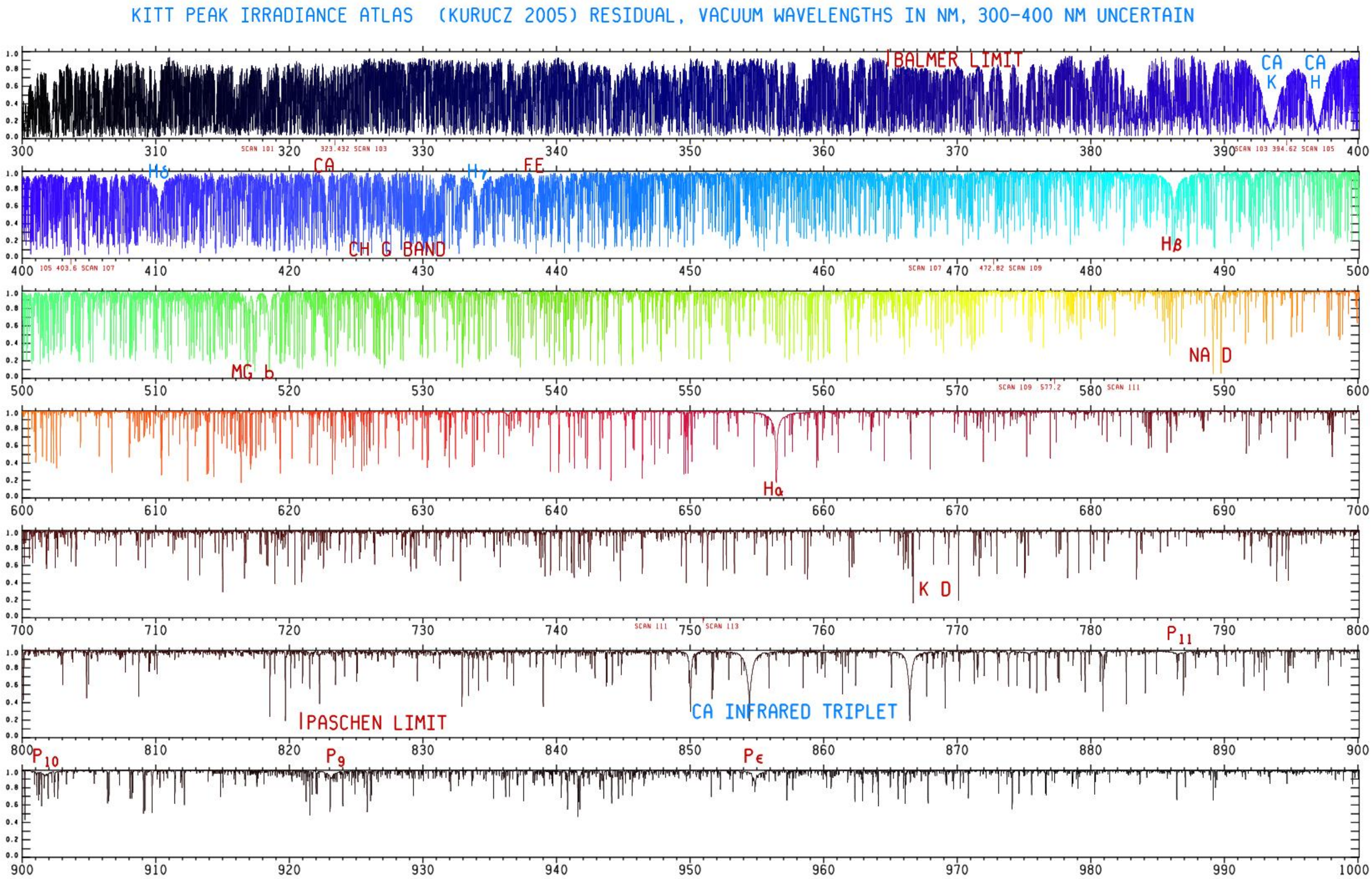
# The solar spectrum (with telluric absorptions)



# Telluric absorptions

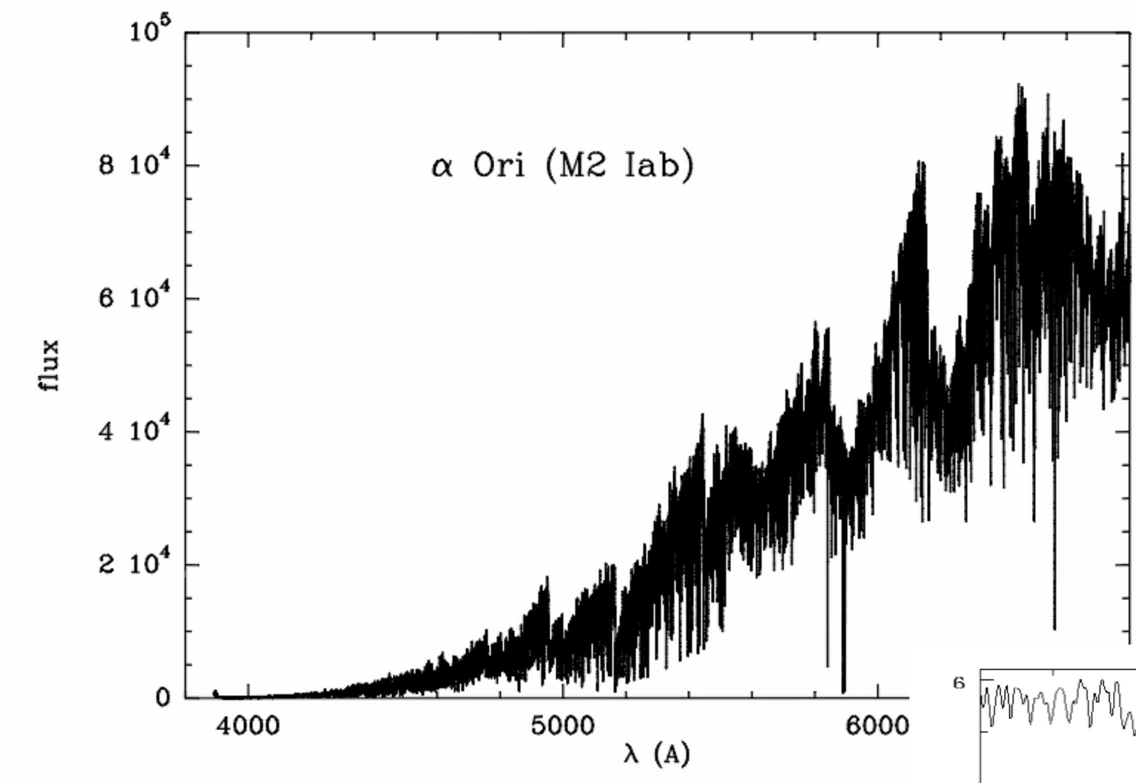


# The solar spectrum (withOUT telluric absorptions)



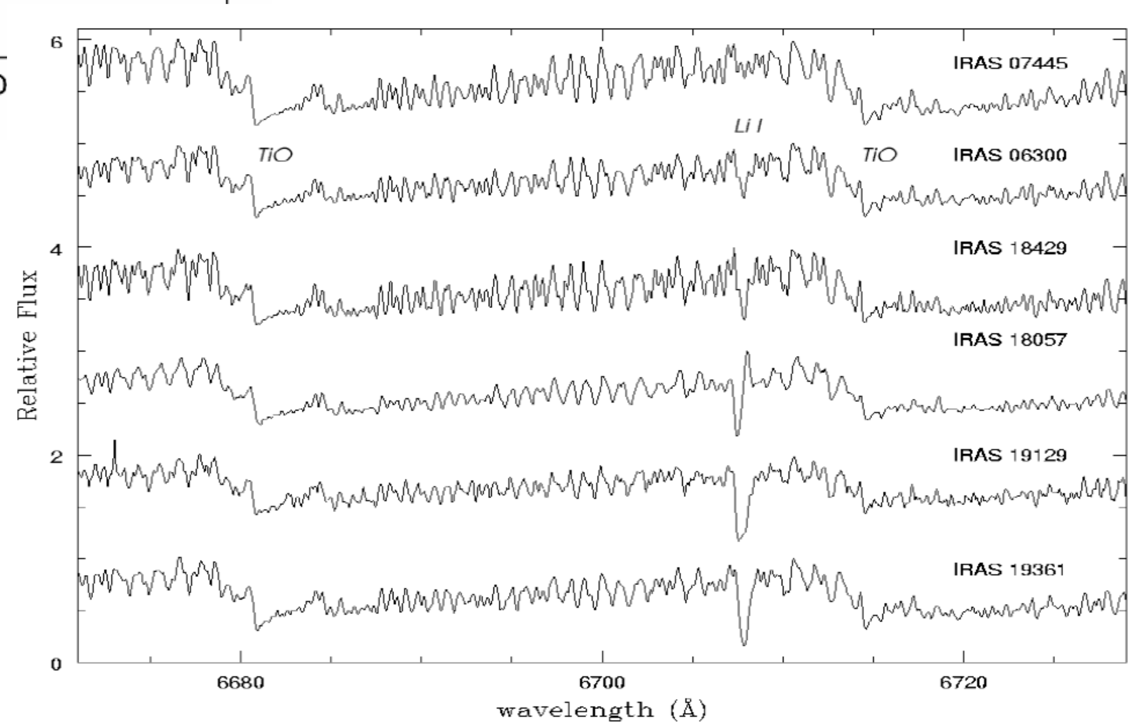

**Many lines! => Large amount of data needed to correctly model this**

# Other spectacular examples




These are high S/N spectra.
All wiggles are lines!

**spectra of red giant stars in the 671nm Li I line region**



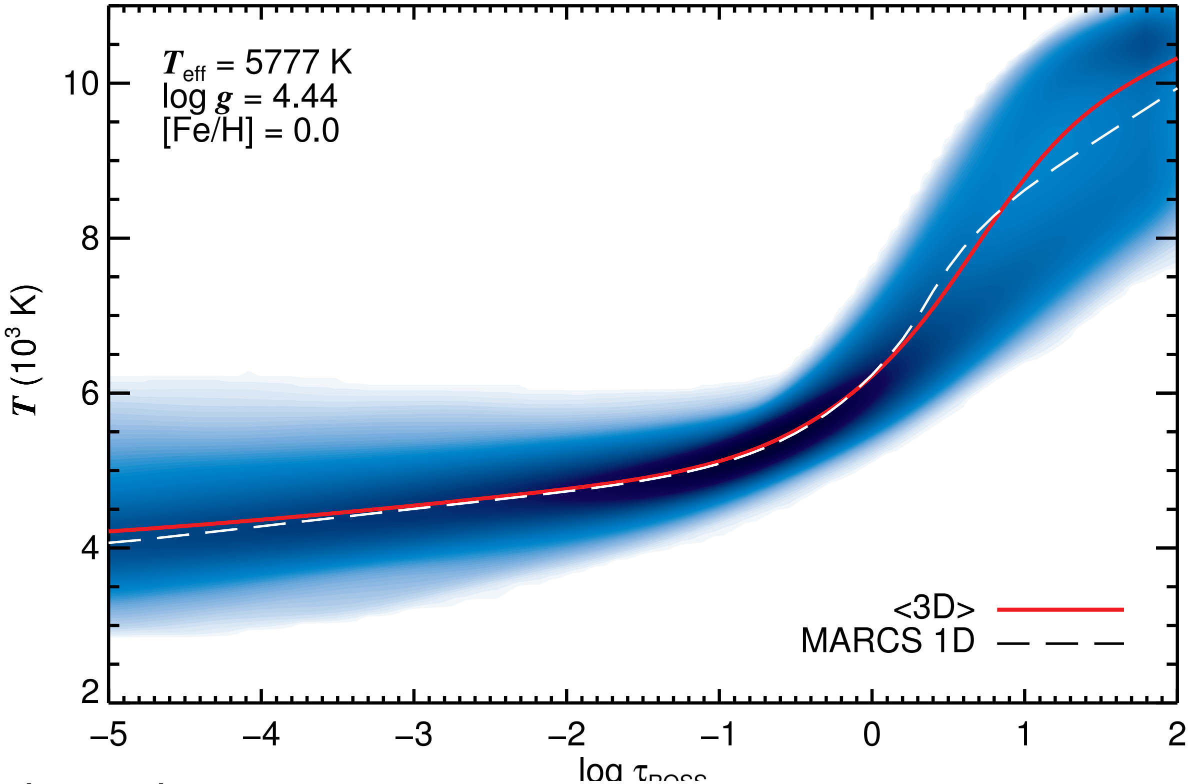

**Betelgeuse, a red supergiant star. Large absorption bands are mostly due to TiO**

# Deriving stellar parameters

How do we model these spectra, in order to derive stellar parameters, in particular chemical composition?

=> Compute a model atmosphere and compare the emergent spectrum with observations.

Atomic and molecular lines being ubiquitous in stellar spectra, we need lots of (good) data




We need :

- models with a realistic T, P (**v**, …) structure
- accurate physical data, e.g., detailed line lists with accurate line positions, strengths, broadening parameters, partition functions, etc
- methods and codes to efficiently compute spectra at various approximation levels, e.g., 1D LTE or 3D NLTE
- and, be clever in choosing the spectral domain, which may not be possible when dealing with special lines (e.g. Li I , Pb I , U II, …). The IR is a domain of choice with new instruments coming-up and less line blending. *(see talk by Henrik Hartman)*

# Model atmospheres

Illustration with *classical models:*

- 1D
- homogeneous
- hydrostatic
- Local Thermodynamic Equilibrium (LTE)
- convection: mixing-length theory
- **detailed radiative transfer with > $10^5$ wavelengths**

opacities affect the thermal structure (line blanketing)

*For 3D models see talk by Martin Asplund*

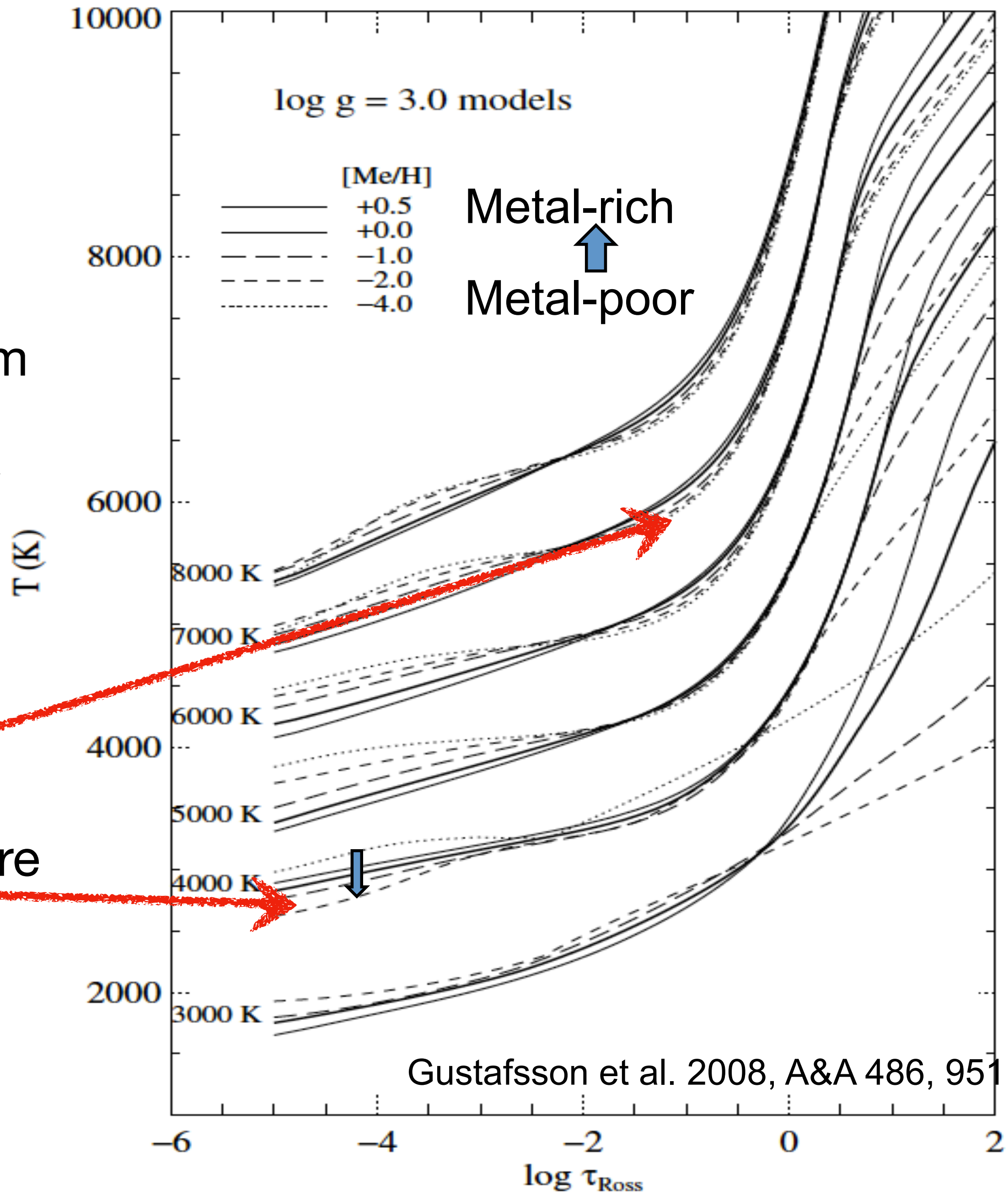
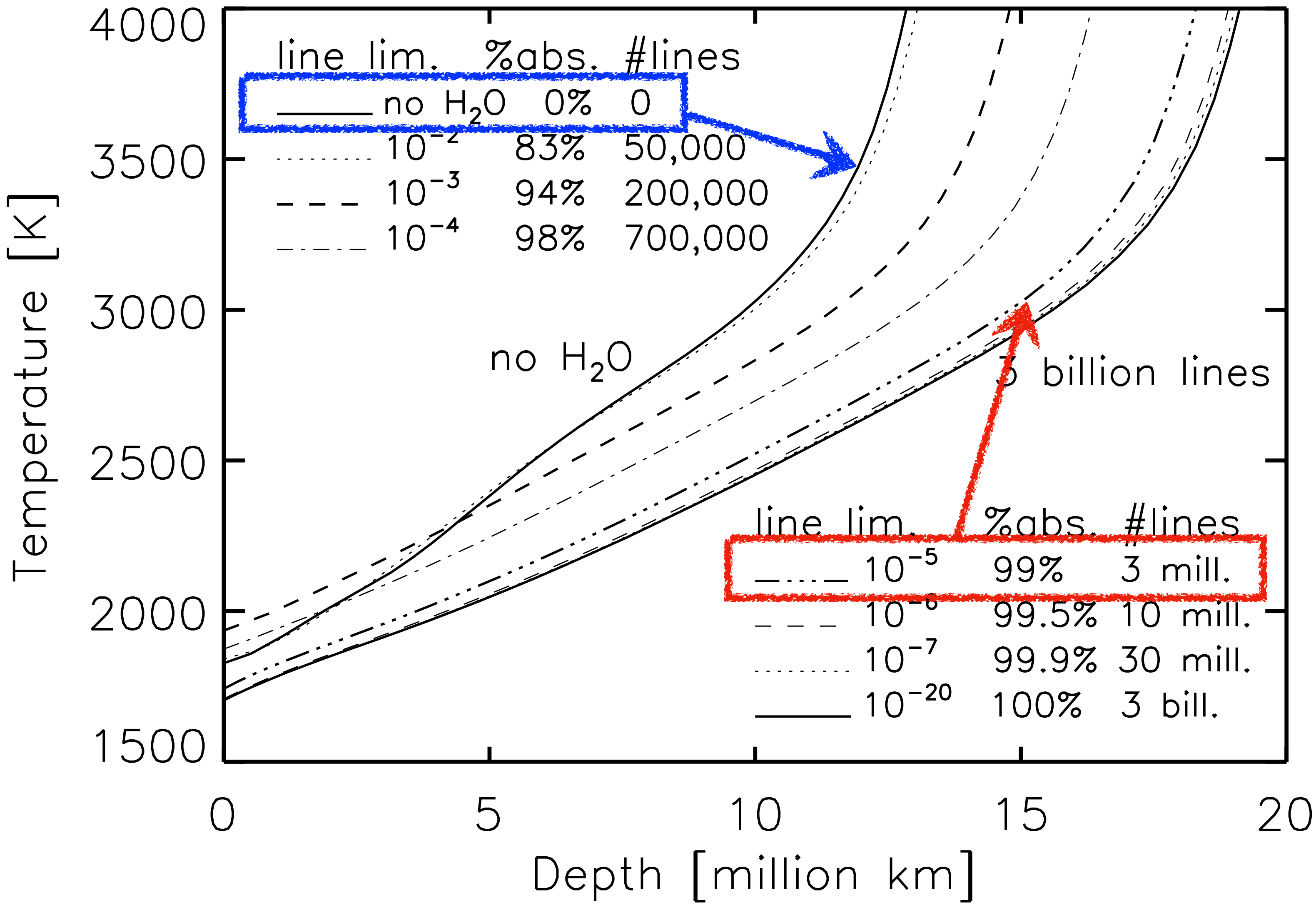



**Fig. 2.** The temperature structures for a set of model atmospheres with different $T_{\rm eff}$, $\log g = 3$ and different metallicities.

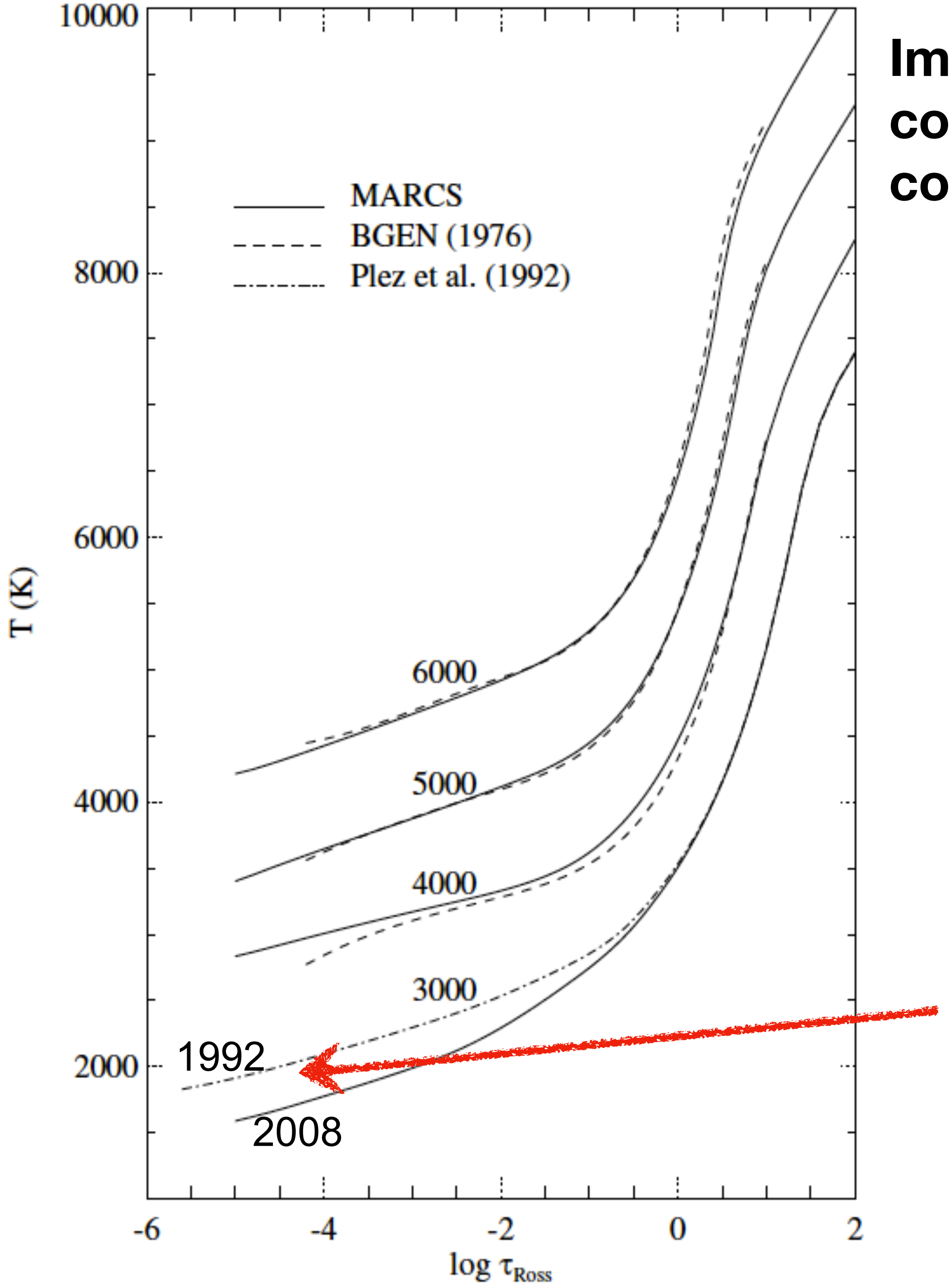
# Importance of using sufficiently complete line lists when computing stellar atmospheres




NB: line limit is in km/mol @ 3500K

*Jørgensen et al. 2001, A&A 372, 249*

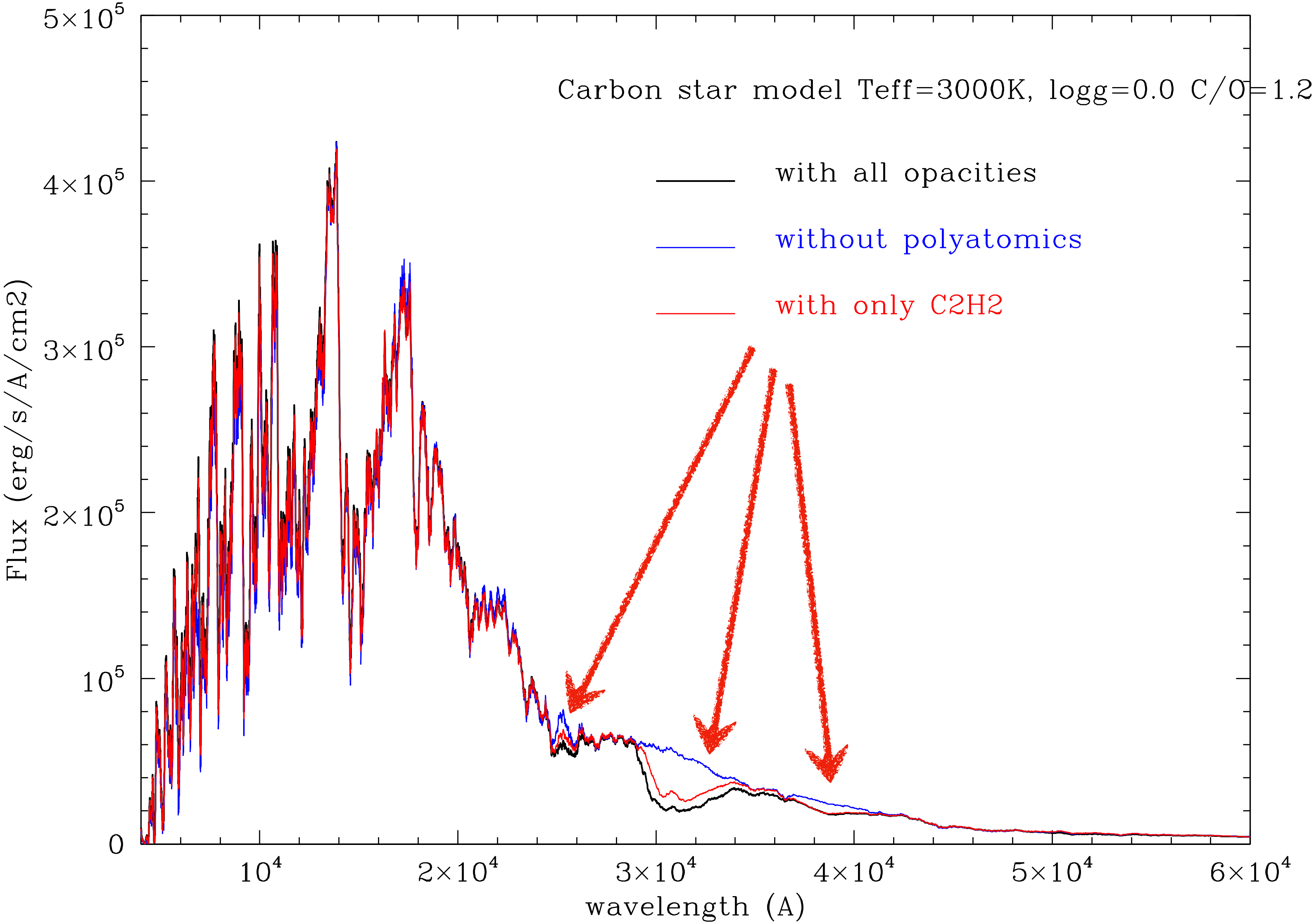
## Importance of using sufficiently complete line lists when computing stellar atmospheres



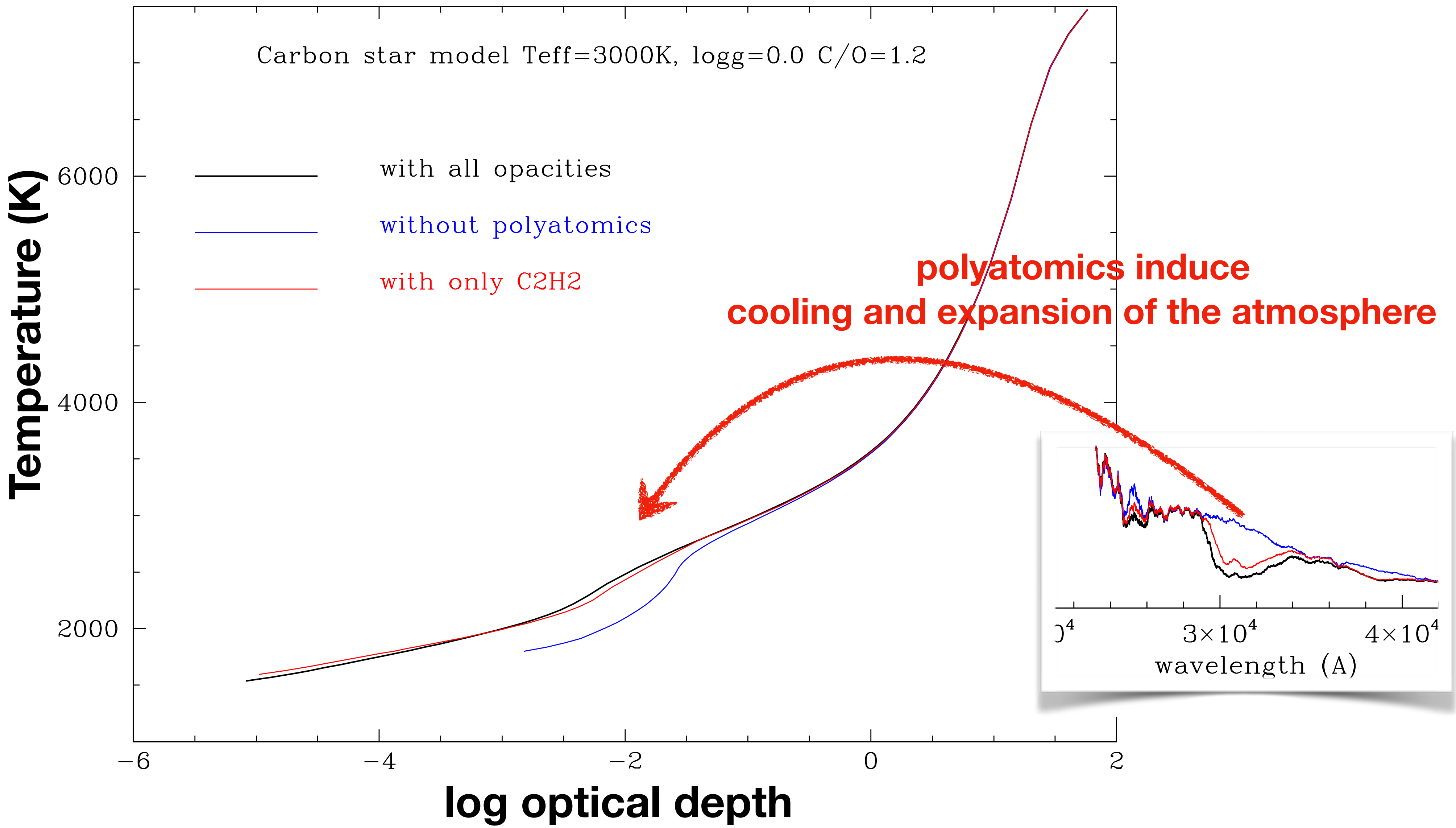

In 1992 MARCS models, $H_2O$ opacity was *underestimated*, resulting in *hotter* surface layers (300K).

*Gustafsson et al. 2008*

# Importance of including all contributing species when calculating spectra



# Impact on the model structure



# Opacities

Continuum and line opacities impact the thermal structure and the spectrum

=> For the thermal structure we need to include all sources, at least in a statistical way. Very accurate line positions are not necessary.

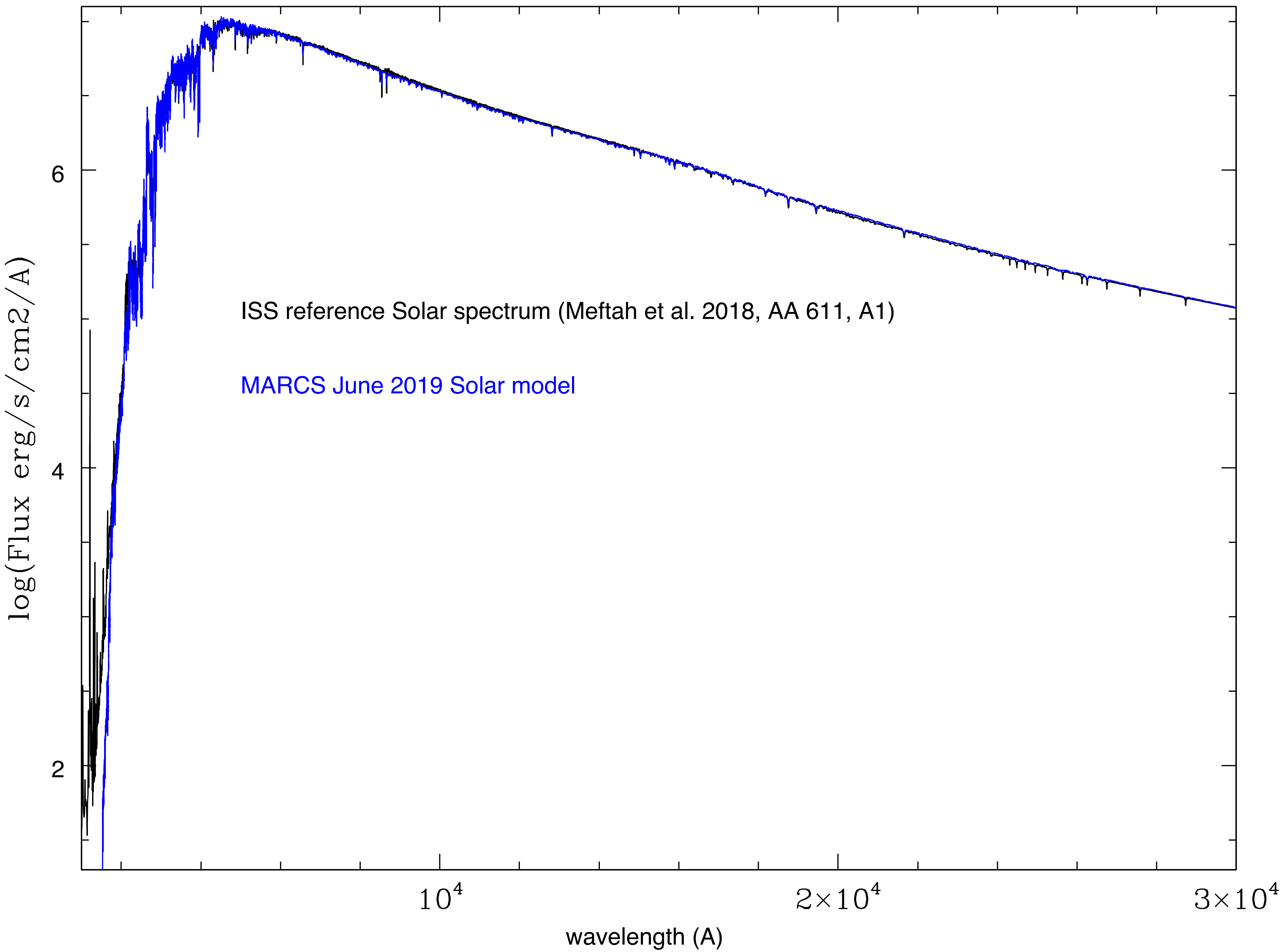
=> For the spectrum we need accurate line positions

In addition : line broadening (collisions with e, H, …), hfs, isotopic shifts, …

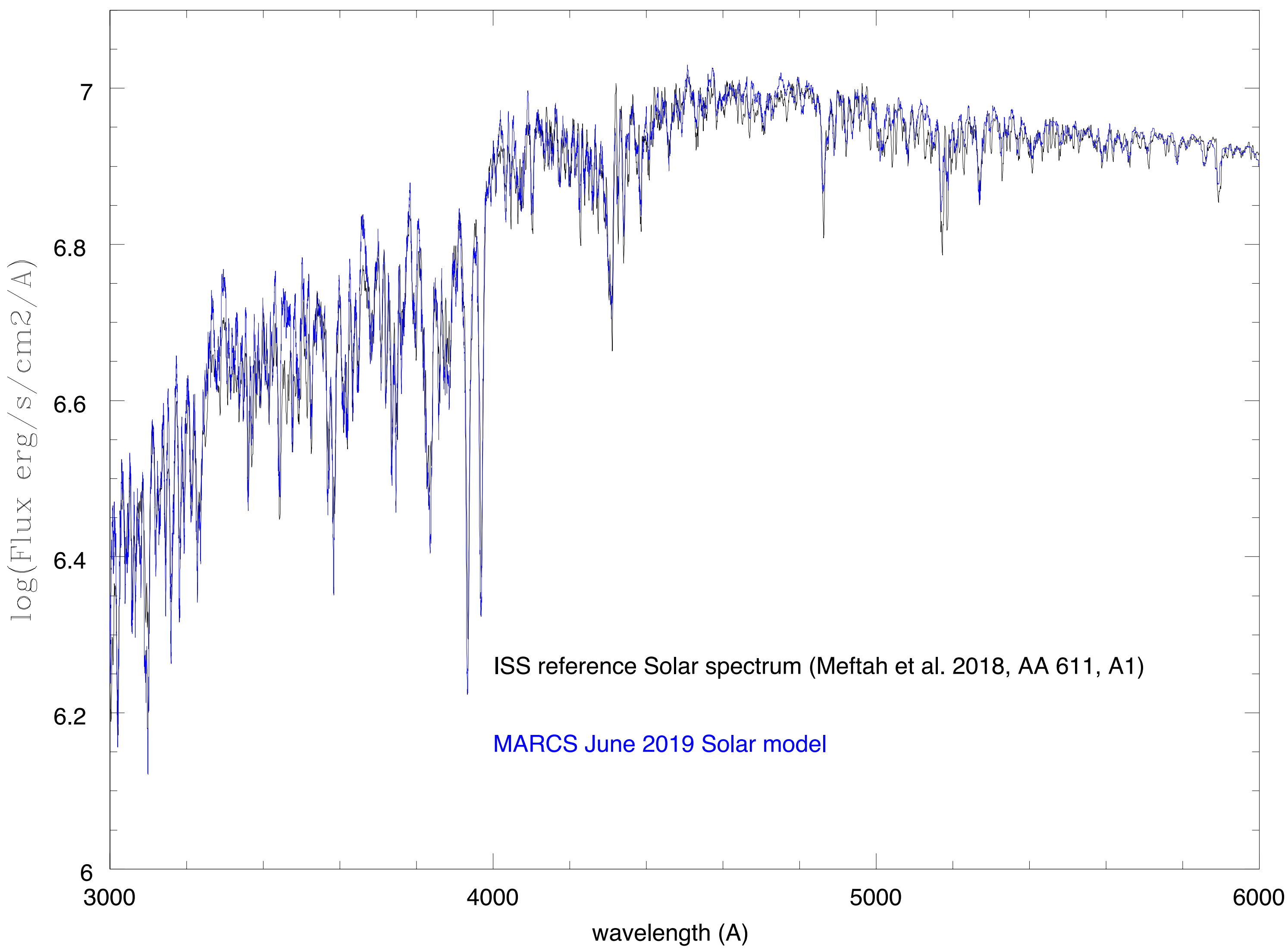
For cool stars : many molecules, possibly dust

And now … a few illustrations of the **importance of securing the best and most complete opacities**

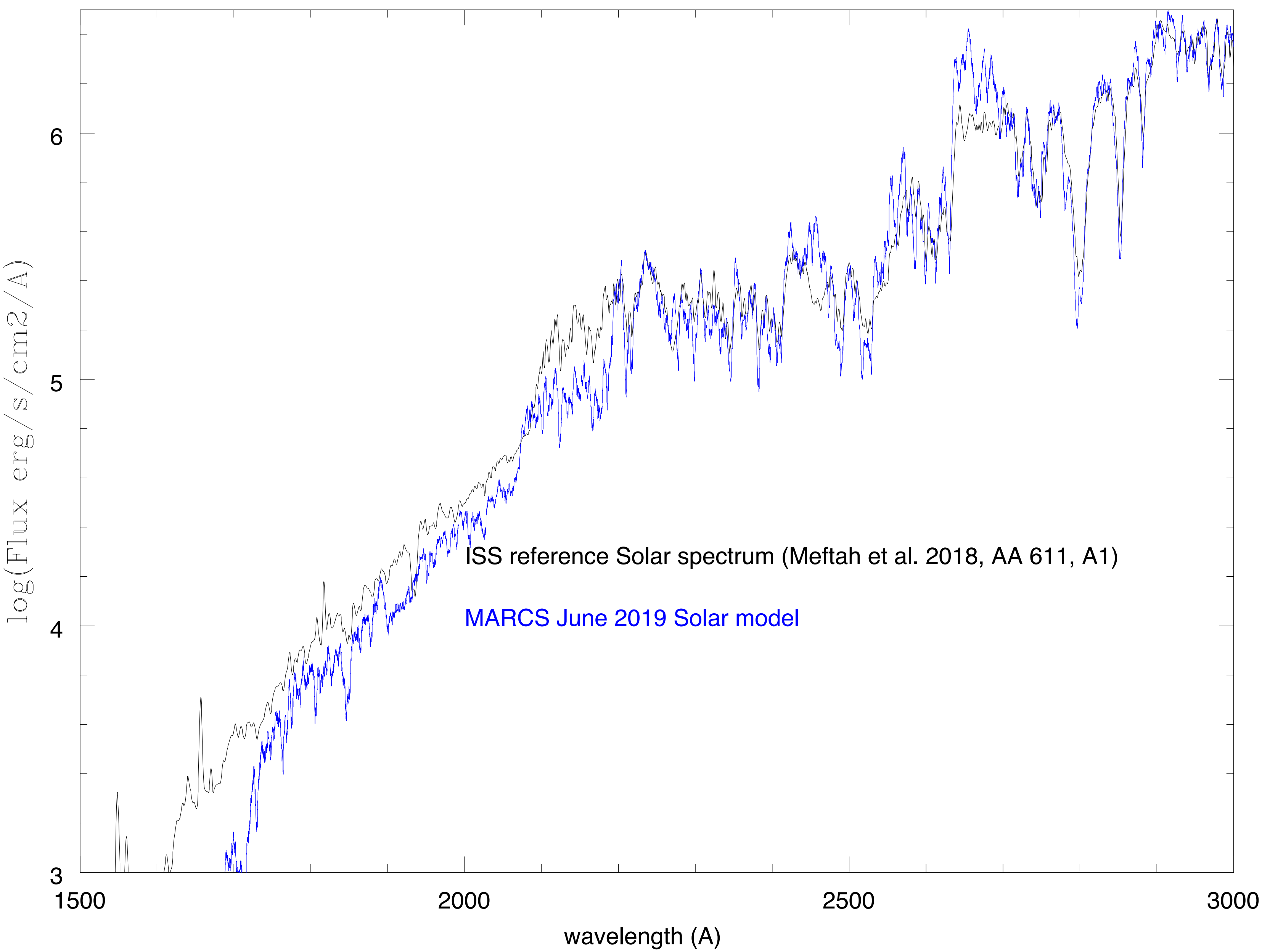
# MARCS model of the solar spectrum



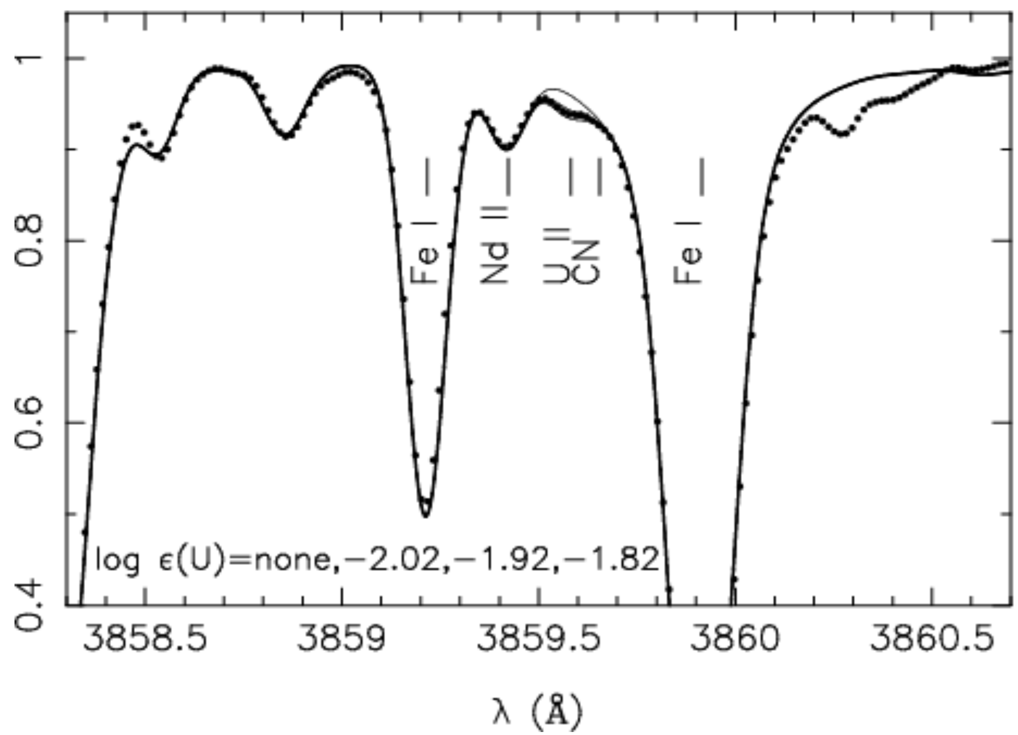
# Quite good at some places

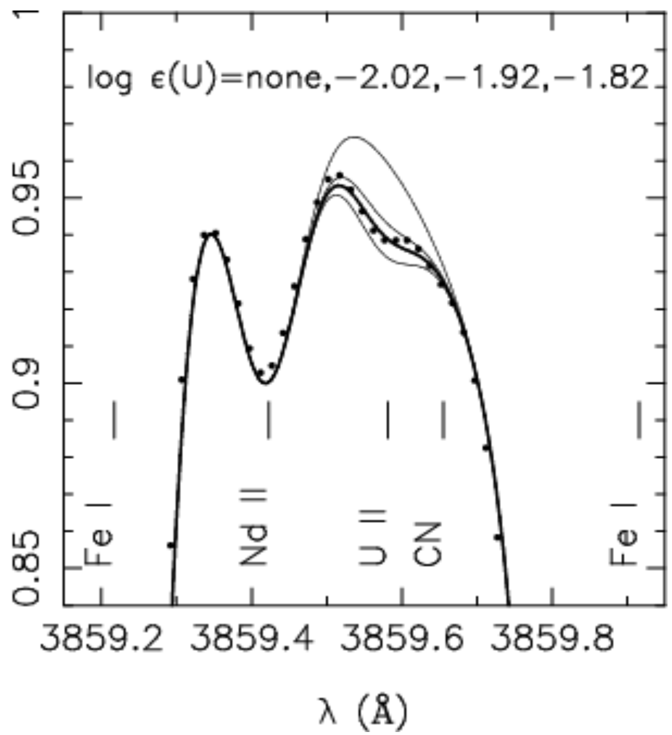


# In need of improvement at some other places



# The art/science of deriving detailed abundances

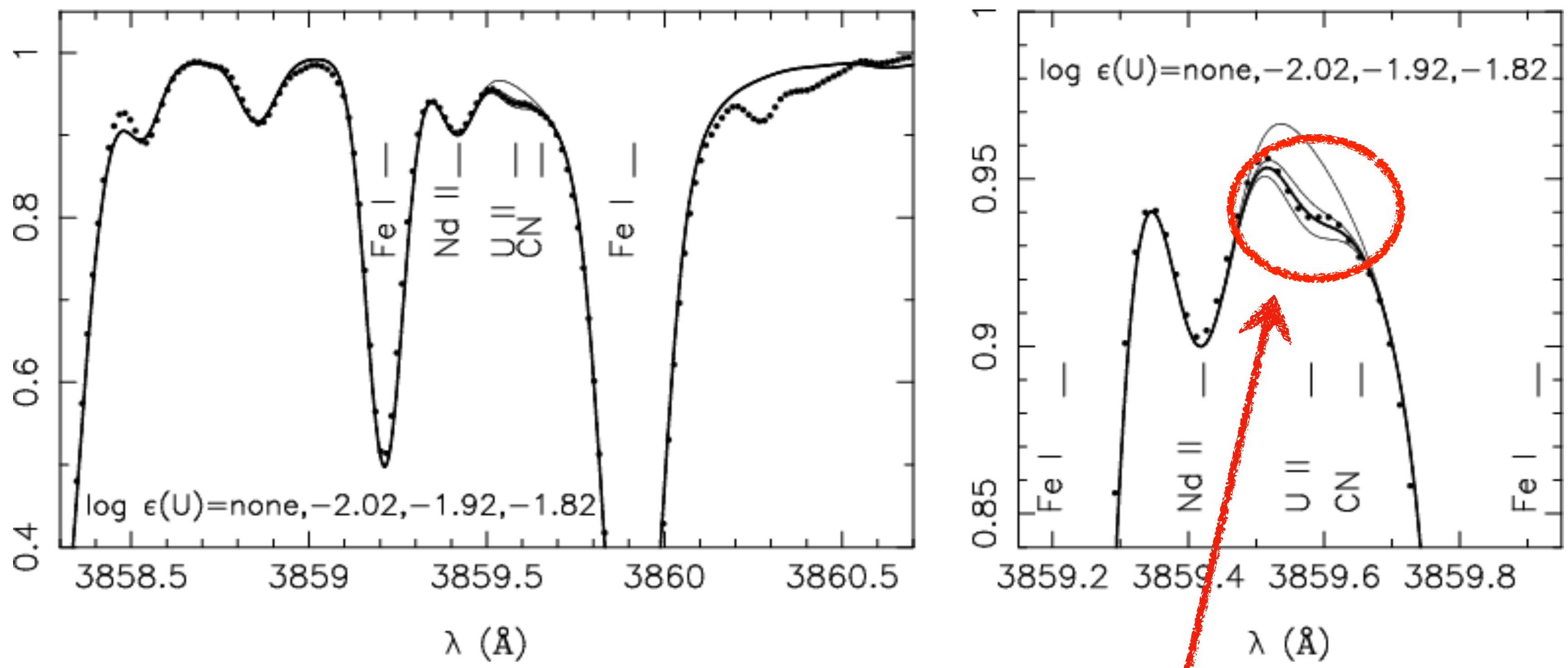



**Uranium abundance** in CS31082-001:

*Cayrel et al. 2001, Nature 409, 691*

# The art/science of deriving detailed abundances



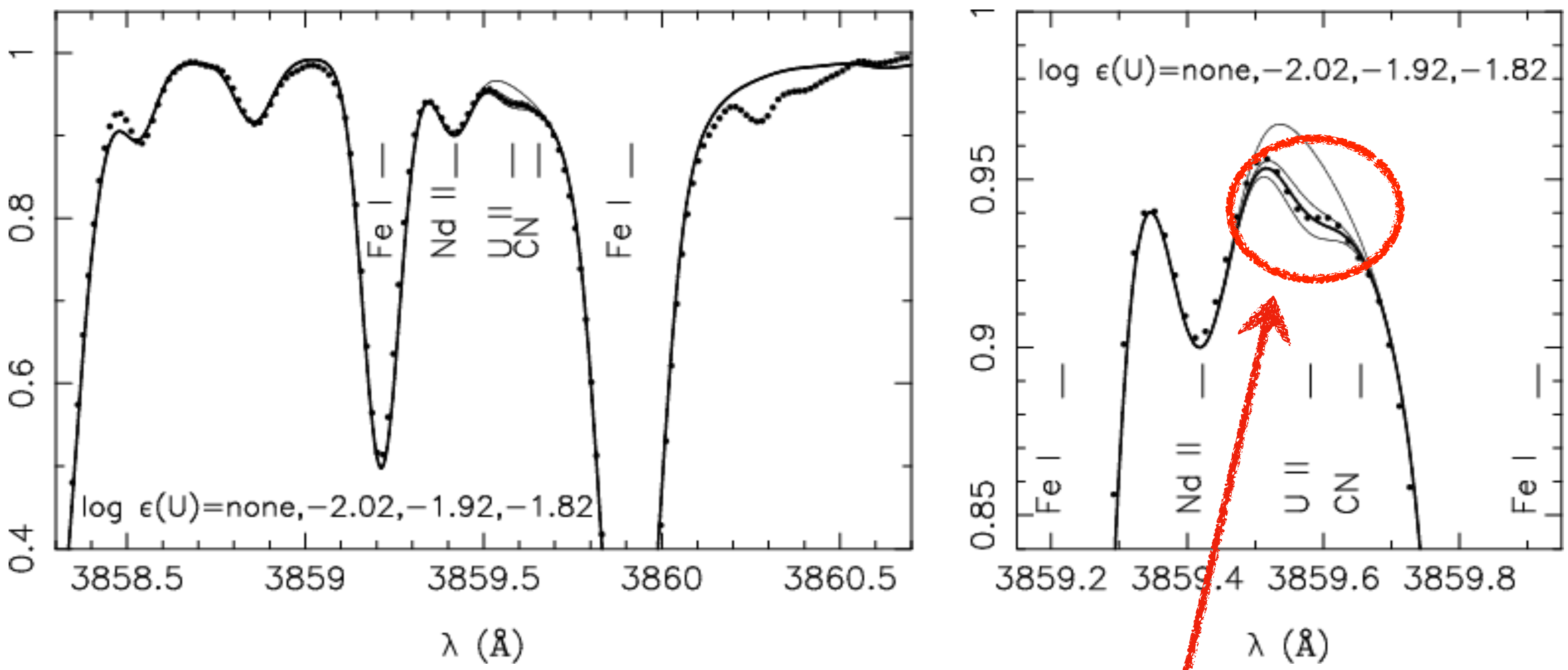

**Uranium abundance** in CS31082-001:

**0.1 dex difference in abundance corresponds to sub-percent variations of the flux level,**

and *over 1 Gyr of uncertainty on the age*.

*Cayrel et al. 2001, Nature 409, 691*

# The art/science of deriving detailed abundances




**Uranium abundance** in CS31082-001:
**0.1 dex difference in abundance corresponds to sub-percent variations of the flux level,**
and *over 1 Gyr of uncertainty on the age*.

=> Importance of completeness of line lists with **accurate line positions, gf-values, partition functions, broadening and line formation mechanism,** …
in addition to a good model atmosphere (i.e. T, P, (**v**) in the line forming region) !

*Cayrel et al. 2001, Nature 409, 691*

# Huge progress in the past decades concerning the knowledge of spectral lines

**However:**

Heiter et al. (2015) find problems when comparing calculated spectra with Gaia-ESO survey spectra.

- master line list built from databases (VALD) + molecules
- specific laboratory work for some lines
- careful selection of gf-values (lab or calculated), collisional broadening, with quality flags

=> still unidentified lines in the optical spectrum of FGK stars!

Heiter et al. 2015
3 iron lines with different quality flags :
Y = yes
U = undecided
N = no

Black line is observation
red and blue calculations

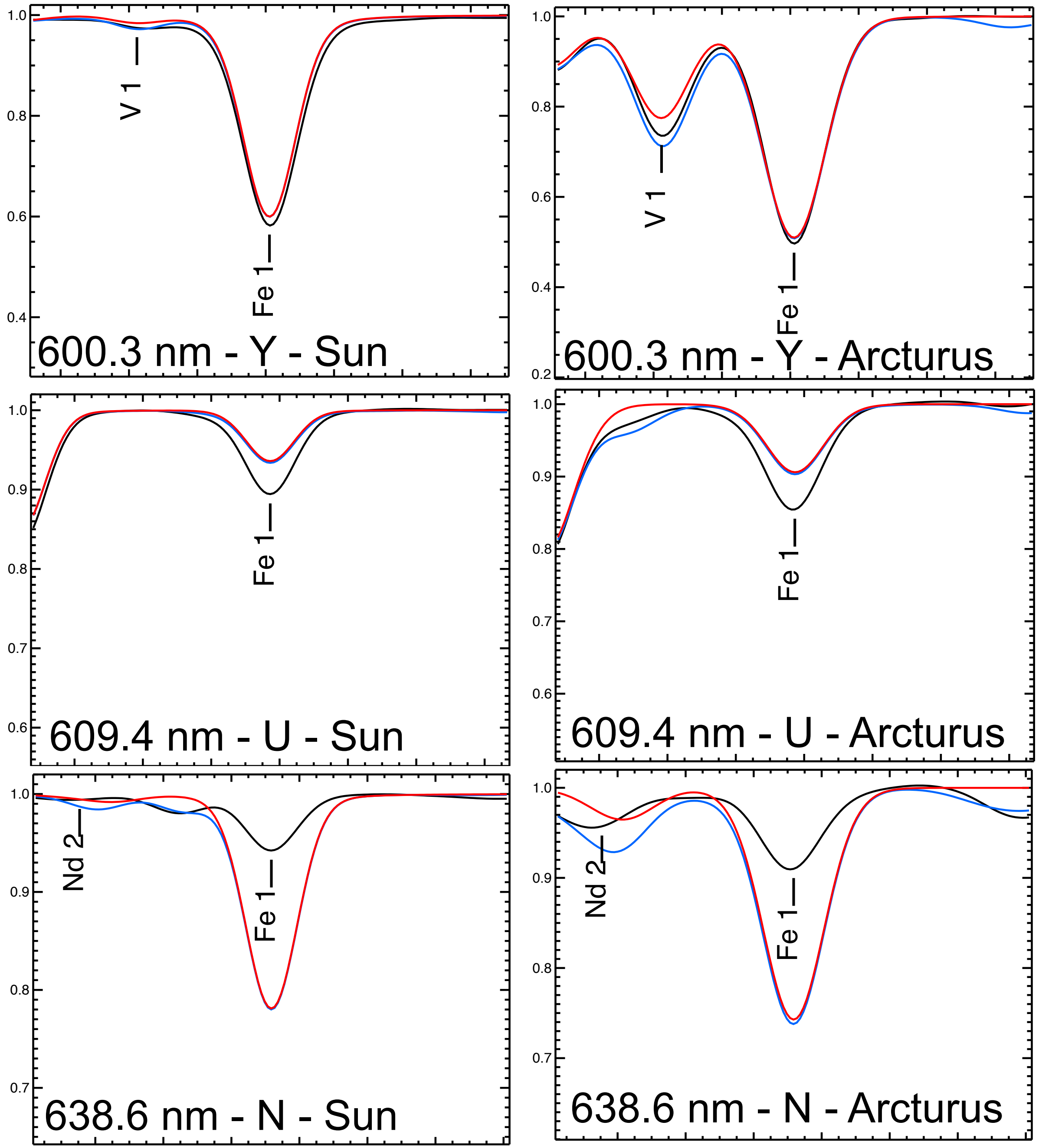


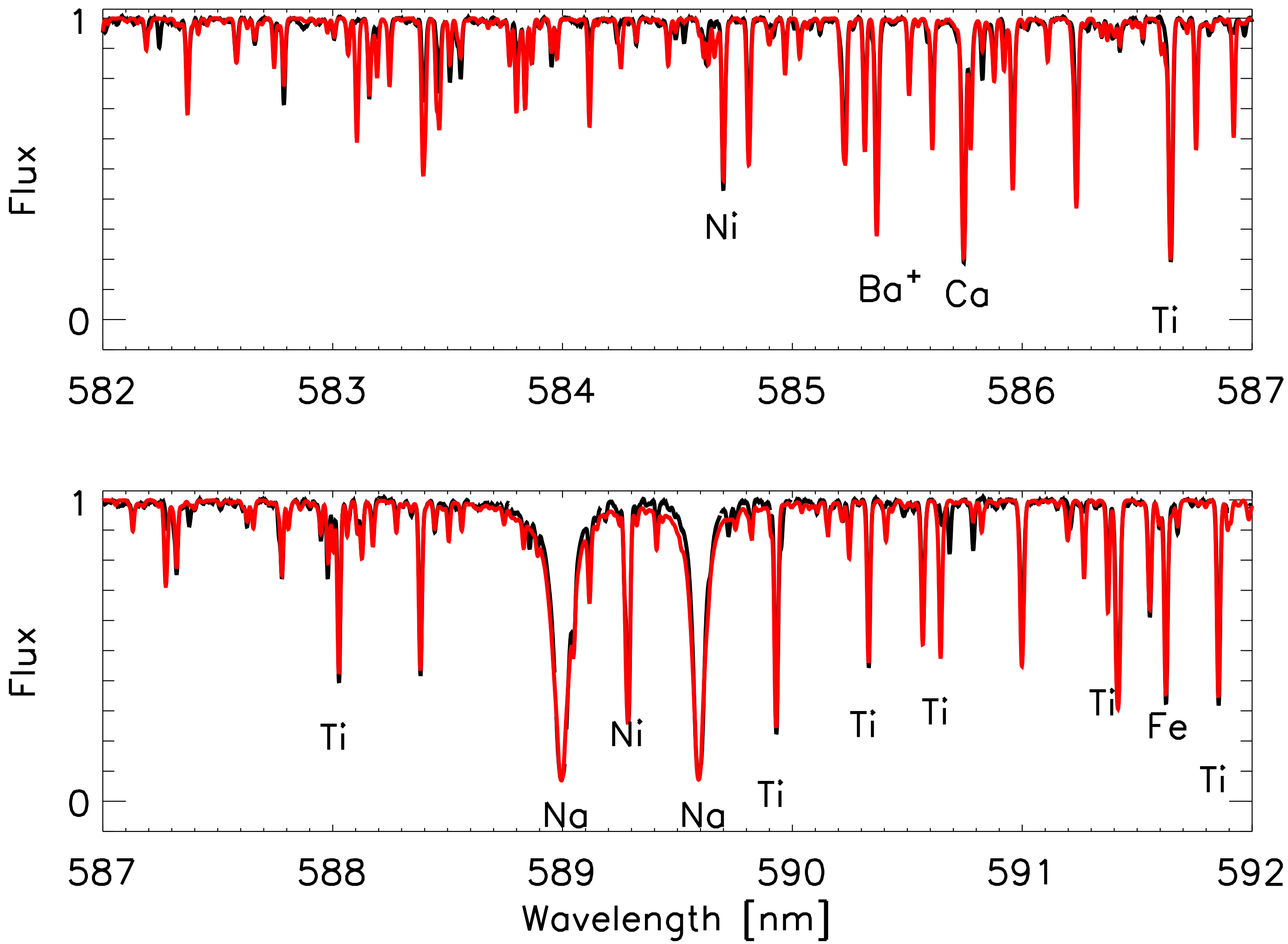

**Figure 3.** Comparison of observed and synthetic spectra around three Fe lines with different flags (Y for *Yes*, U for *Undecided*, N for *No*) for the Sun (left) and Arcturus (right). Black lines: observations, red lines: calculations including preselected spectral lines only, blue lines: calculations including blends.

*see also the BRASS effort: talk by Alex Lobel and poster by Mike Laverick*

# Completeness of line data

A number of lines are still missing, or have insufficiently accurate data, even for FGK stars!

**observed and calculated spectrum of Arcturus**




*Heiter et al. 2015, Phys. Scr 90, 054010*

**Figure 4.** Observed (black) and calculated (red) spectra for Arcturus around the Na doublet lines at 589 nm. The calculations include the full Gaia-ESO line list.

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=> still unidentified lines in the optical spectrum of FGK stars!

**Need laboratory work, and calculations.**

**And use stellar spectra, where higher levels may get excited:**

E.g. Peterson and Kurucz (2015): identification of high-lying FeI energy levels using stellar spectra.

See also Masseron et al. (2014): same thing for CH.

**Table 2**

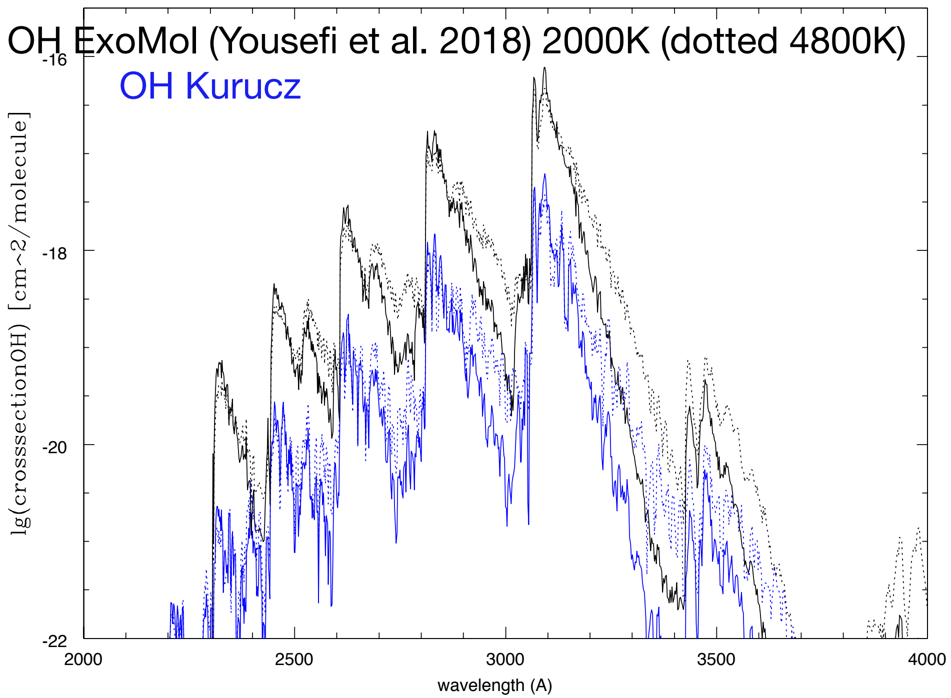
New Fe I Levels and Energies

| Expanded Label | Label | $J$ | $E$ (cm$^{-1}$) | $\sigma$ (cm$^{-1}$) |
|---|---|---|---|---|
| *23 Even Levels:* | | | | |
| 3d6 4s(6D)4d e7F | 4s6D4d e7F | 0 | 51143.92 | 0.03 |
| 3d7(4F)4d 5D | (4F)4d 5D | 0 | 54304.21 | 0.02 |
| 3d6 4s(6D)4d 5D | 4s6D4d 5D | 0 | 58428.17 | 0.03 |
| 3d6 4s(4D)4d 5P | 4s4D4d 5P | 1 | 58628.41 | 0.03 |
| 3d7(4P)5s 3P | (4P)5s 3P | 1 | 59300.54 | 0.03 |
| 3d6 4s(4D)4d 3D | 4s4D4d 3D | 2 | 58779.59 | 0.02 |

# Molecules

**Large scale efforts**, esp. **ExoMol** (J. Tennyson et al.): calculations and compilations of **line lists for many molecular species**

- targeted towards planets and (very) cool stars
- mostly for opacities, i.e. aiming at completeness in terms of levels and transitions
- not always accurate for spectroscopy.




**metal hydrides**

- MgH
- NaH
- NiH
- AlH
- CrH
- CaH
- BeH
- TiH
- FeH
- LiH
- ScH

**ions**

- $LiH^+$
- $H_2^+$
- $HeH^+$
- $H_3^+$
- $OH^+$

**other diatomics**

- PN
- KCl
- NaCl
- LiCl
- CN
- $C_2$
- $H_2$
- CS
- CP
- PS
- NS
- SiS
- NaF
- AlCl
- AlF
- KF
- LiF
- CaF
- MgF

**other hydrides**

- NH
- CH
- OH
- HCl
- SiH
- SH
- HF
- PH

**other oxides**

- CO
- NO
- PO

**metal oxides**

- VO
- AlO
- MgO
- TiO
- SiO
- CaO

**triatomic molecules**

- $H_2O$
- $CO_2$
- $SO_2$
- HCN
- $N_2O$
- $H_2S$
- OCS

**larger molecules**

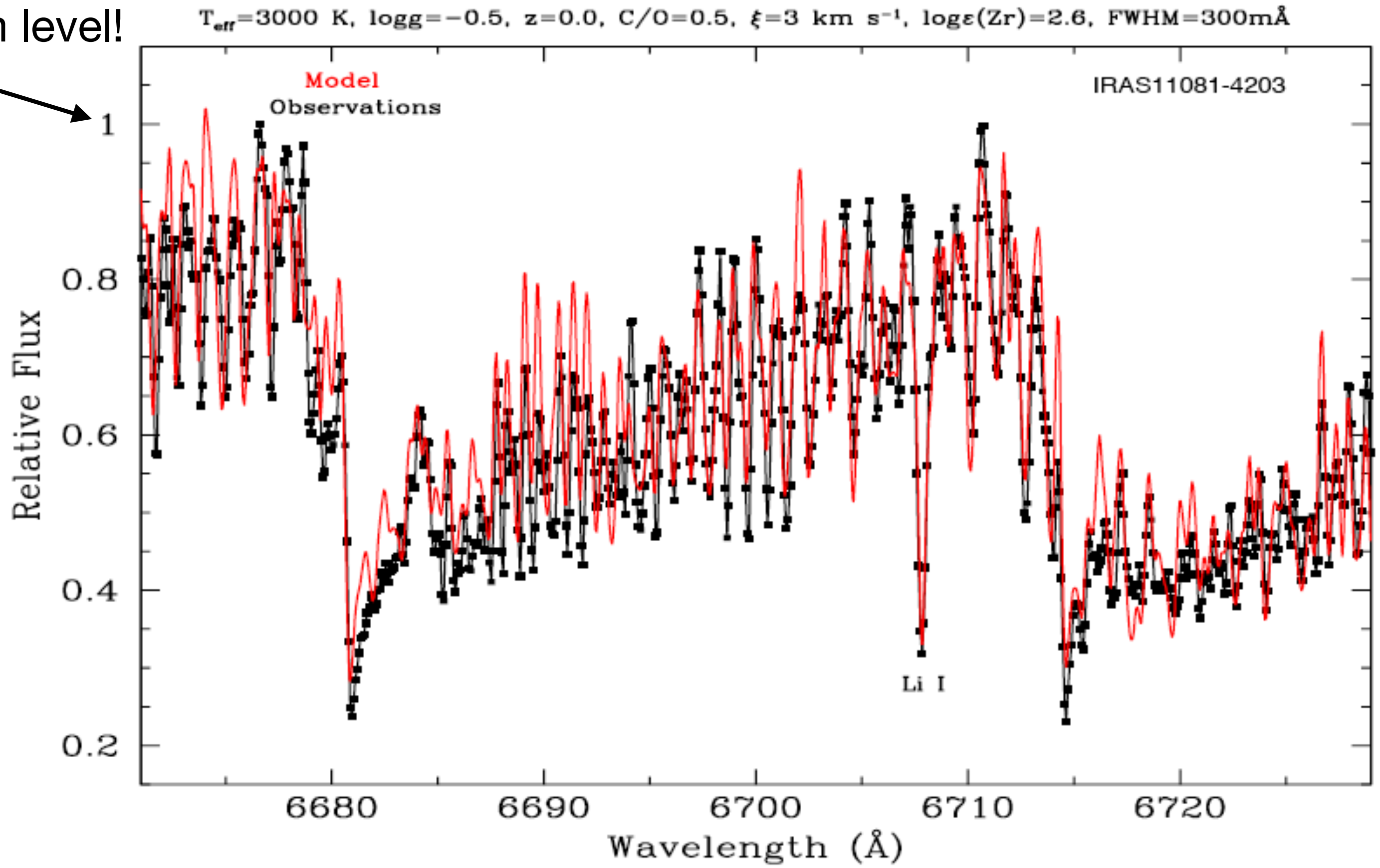
- $CH_4$
- $NH_3$
- $HNO_3$
- $H_2O_2$
- $H_2CO$
- $SO_3$
- $SiH_4$
- $CH_3F$
- $CH_3Cl$
- $C_2H_4$
- $C_2H_2$
- $AsH_3$
- $P_2H_2$
- $PF_3$
- $PH_3$
- $CH_3$

Other theoretical and experimental efforts going on, thanks to a number of dedicated groups in atomic and molecular physics

# Fitting the Li line of a cool red giant

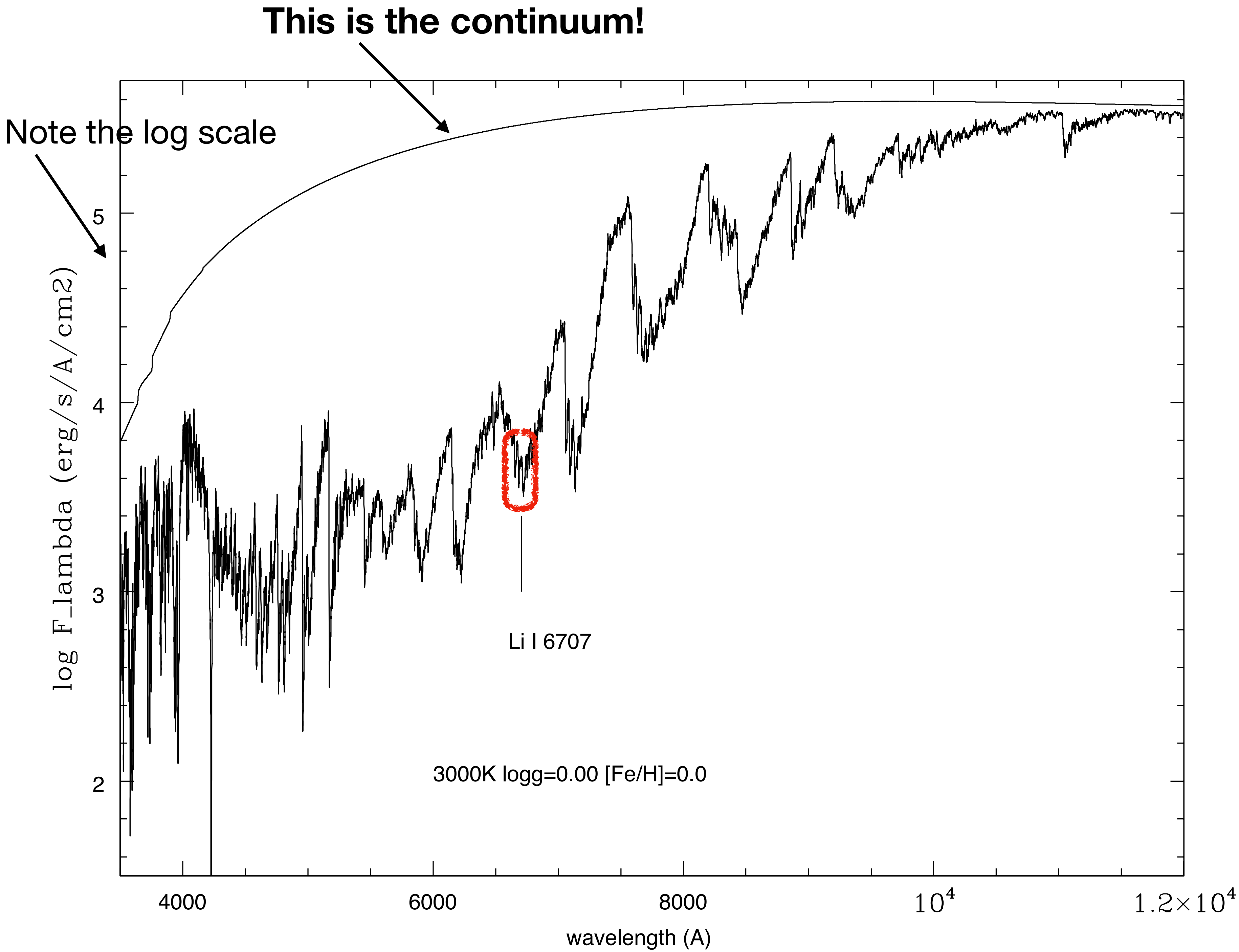
$T_{eff}$ = 3000K
Absorption veil mostly due to TiO.
**The Li line is far below the continuum!**

This is **not** the continuum level!



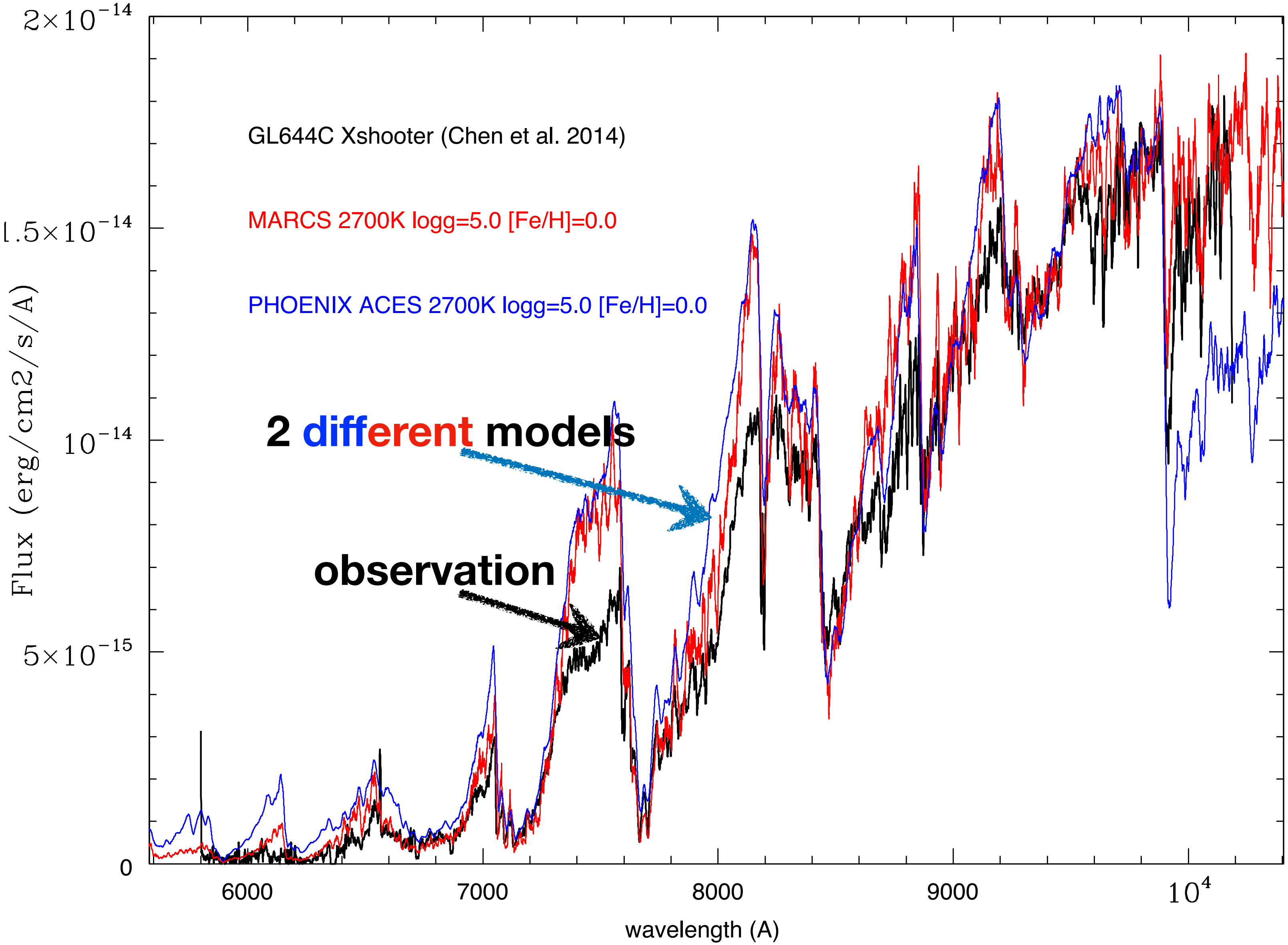

*García-Hernández et al. 2007, A&A 462, 711*

# Li in red giants



# Another example: cool M dwarf

**Improvements needed** in terms of line list completeness and line strengths



# The CH story, the tale of a successful collaboration between quantum chemists and astrophysicists*

** There are many such stories, but you will soon understand why I picked that one,*
*… or you probably already did !*

# The CH story, the tale of a successful collaboration between quantum chemists and astrophysicists*

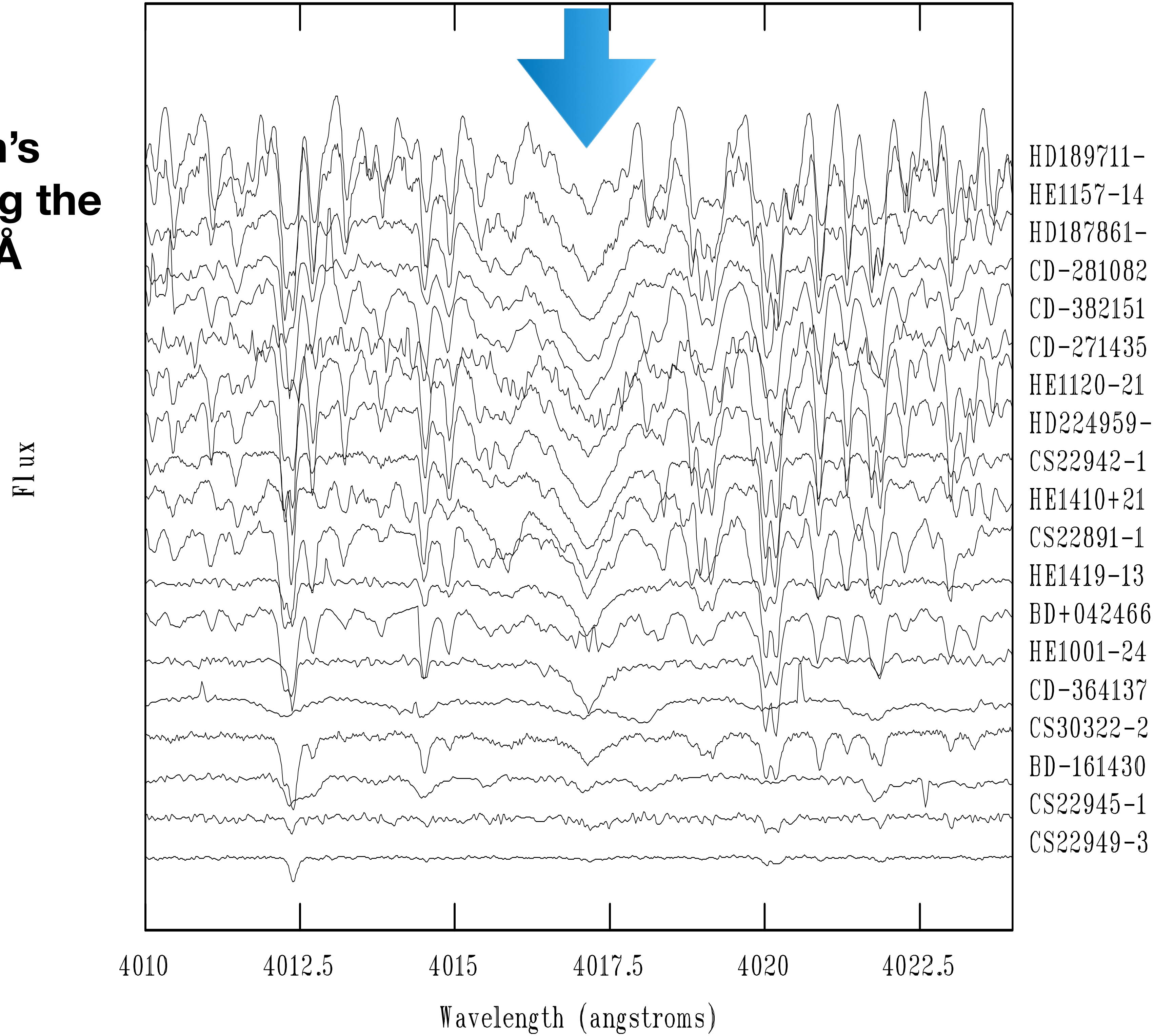
## Late 2003:

- Mike Bessell finds unidentified lines in metal-poor stars HE0107-5240 {halo giant with [Fe/H]=-5.3, C & N/Fe=+4, +2.5} from about 3693 to 4110A.
- Most are broader than other lines.
- Finds correlation of strength with CH lines, but not present in any molecular band catalog.
- Detection in CS22957-027 as well

No progress during 2 years.

**** There are many such stories, but you will soon understand why I picked that one, … or you probably already did !***

**T. Masseron's plot showing the line at 4017Å**



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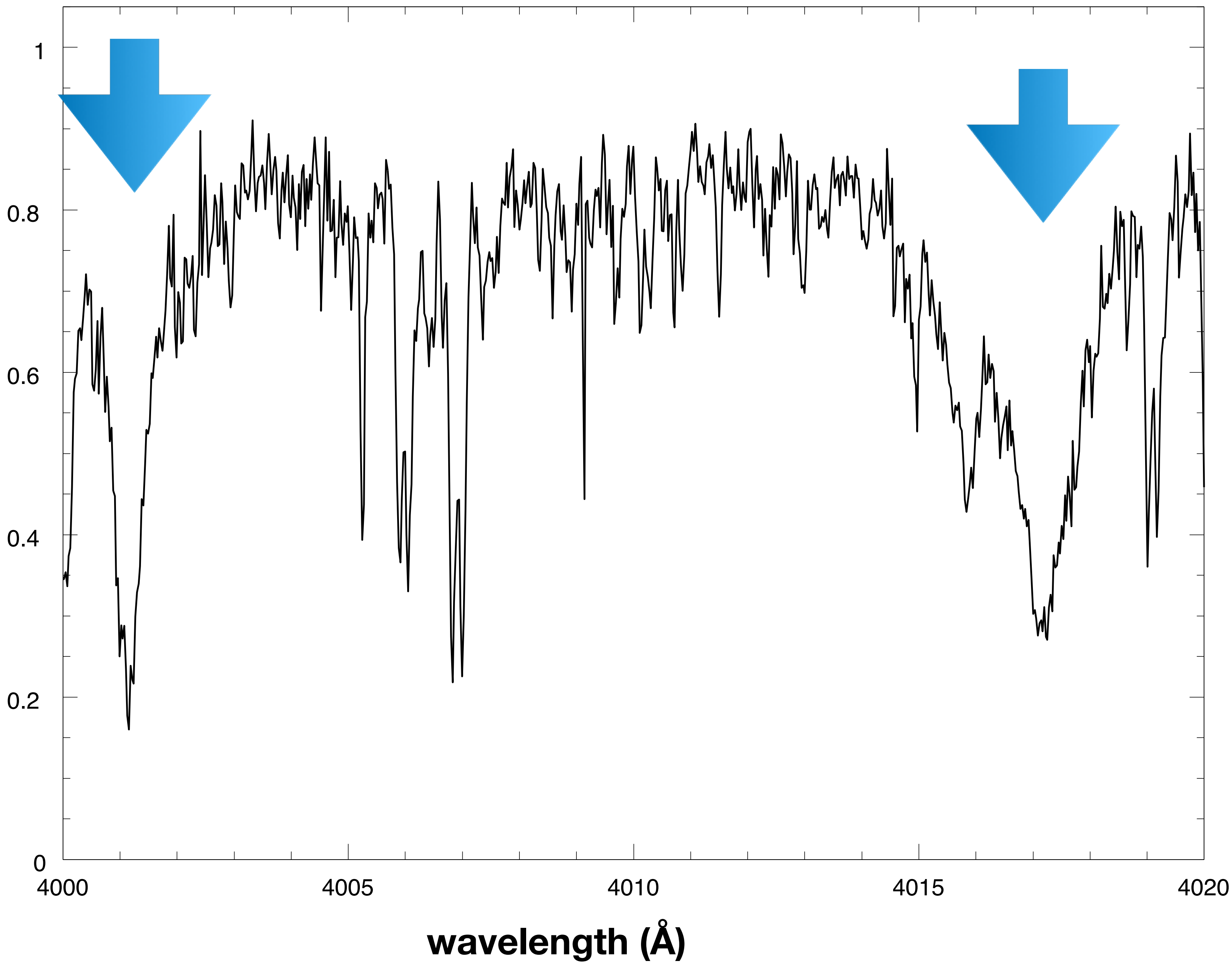
No progress during 2 years.

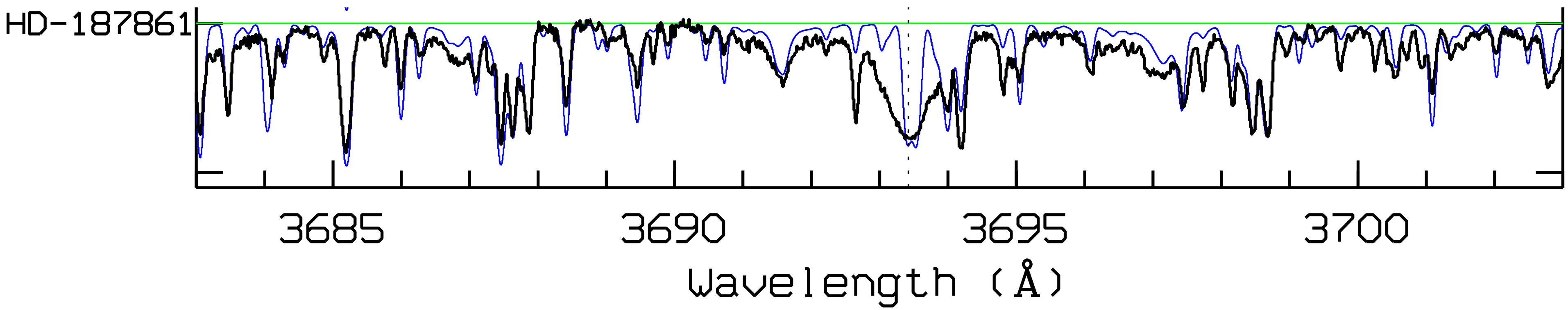
**Then independently:**

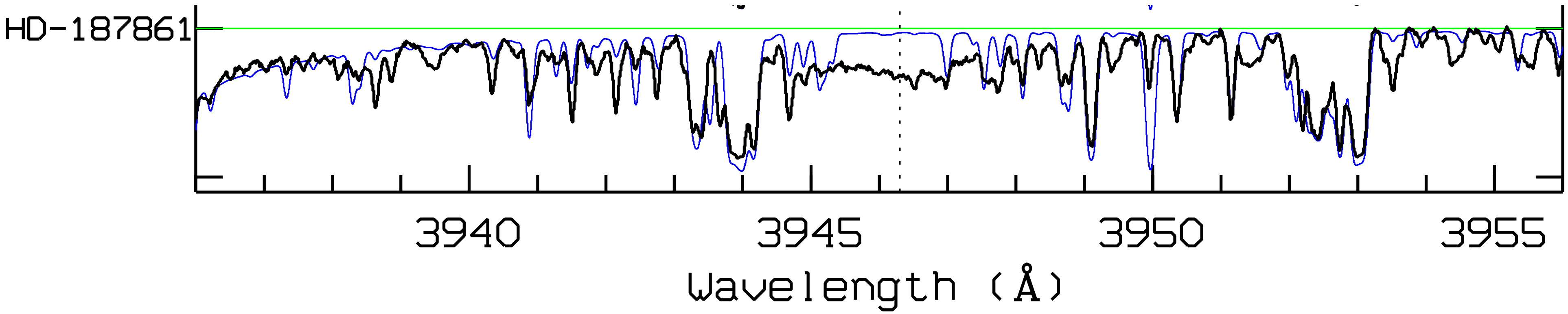
- Thomas Masseron, my PhD student, finds strong lines in many carbon-rich metal-poor stars.
- I look back and realize I had also found the same very strong lines in the spectrum of G77-61, a cool very metal-poor carbon- and nitrogen-rich dwarf. These lines couldn't be fit by existing CN, CH or $C_2$ line lists, which otherwise dominate the spectrum of G77-61.

# And in G77-61!



# Observations vs. spectral synthesis with existing line lists in early 2006



# The searches merge, and more get involved

**December 2005:**

- Discussion between Norbert Christlieb and Thomas Masseron at the CRUMPS* meeting in December 2005.
- Sophie van Eck and Alain Jorissen get involved.
- Pierre-François Coheur and … Michel are invited to help

** Carbon-Rich Ultra Metal-Poor Stars*

# The searches merge, and more get involved

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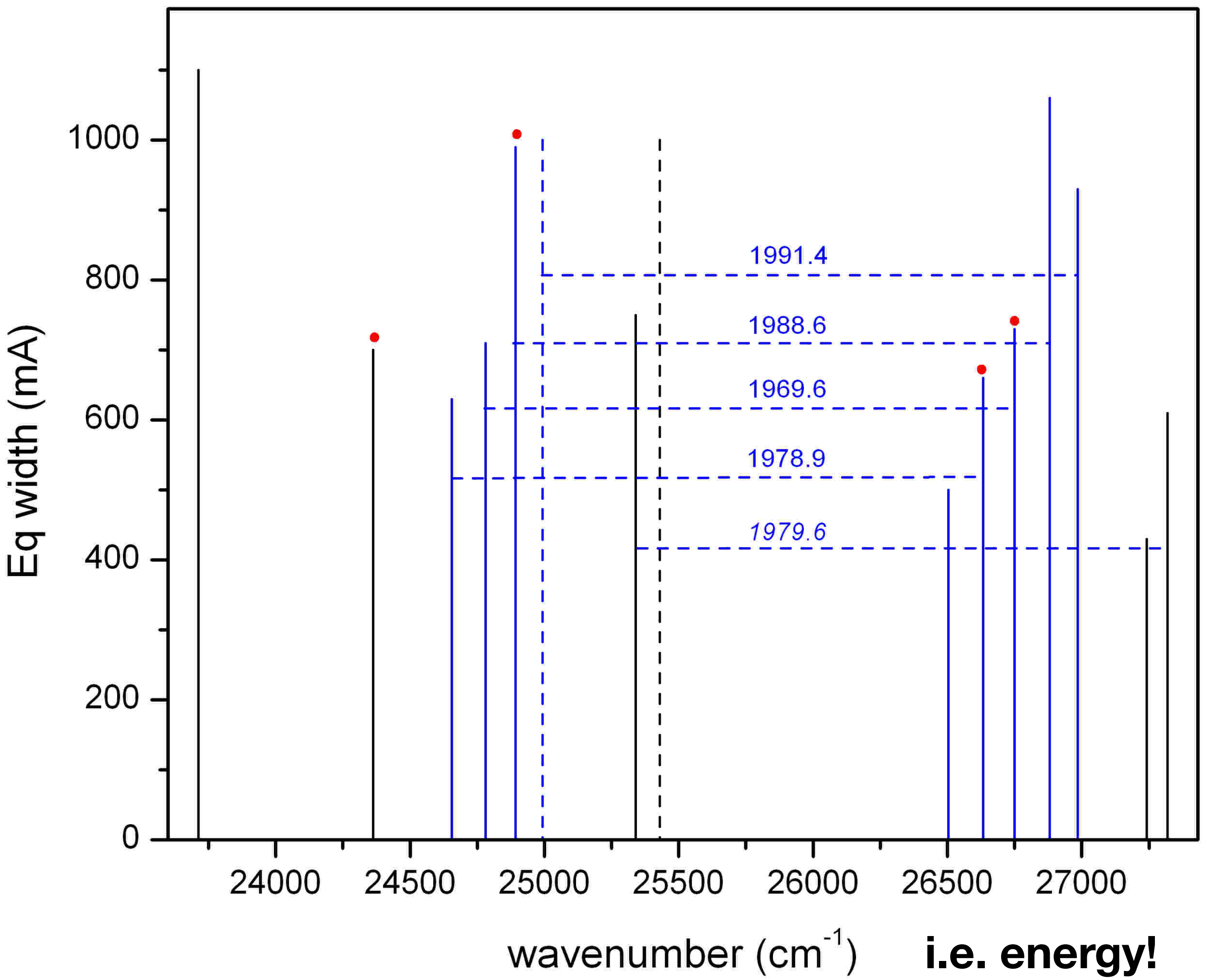
- Pierre Coheur and … Michel Godefroid are invited to help

- We look at correlations with temperature, surface gravity, C, N, O, Fe, or heavy-element abundance.
- We check the stability and relative abundances of molecular species, some quite exotic,…
- Find that some white dwarfs (DQ type) seem to show similar lines.
- think of C2H, CH2, C60, …

* *Carbon-Rich Ultra Metal-Poor Stars*

**The quantum chemists idea. Plot like this!**
**Or, why energy is better.**




**i.e. energy!**

=> This is definitely due to a molecular species
=> Typical energy separation of vibrational levels

One week later we secure the **identification** !

Noting, that

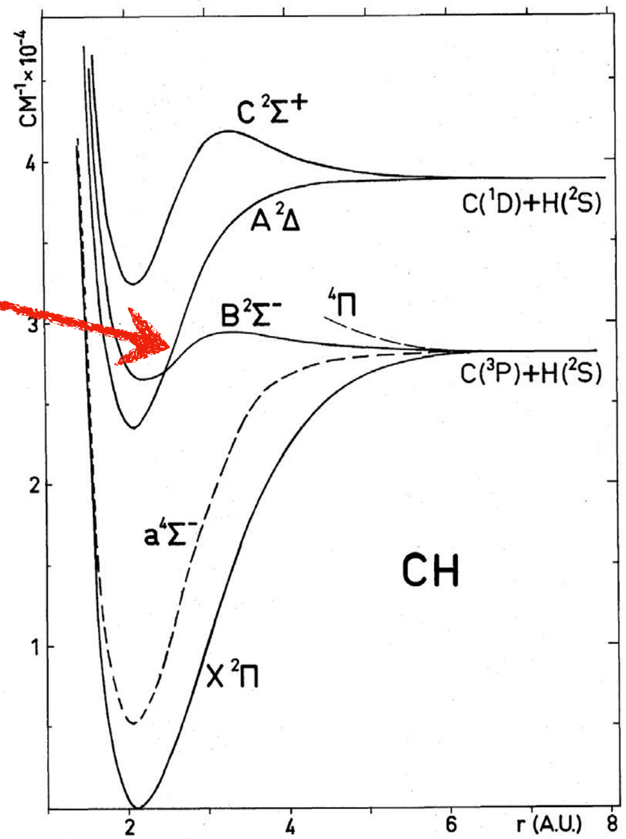
1) the bluest lines are at 3600A -> 27700cm-1 -> 3.44eV, which is D00 of CH
2) $\omega_e$=1795cm$^{-1}$
3) bandhead at the right place for being CH
4) CH very abundant in these stars

In our earlier line list (Plez & Jorissen) assembled from laboratory data + calculated levels, we had suppressed lines with the upper level lying above dissociation, … but:

=> When including these levels again, lines are predicted at the position of the broad features!!

Their width can be explained by the short lifetimes of the levels, due to predissociation.

**Pre-dissociation lines in the CH B-X transition !!**



# Michel's molecular career*

In the 80's, Michel contributed to the writing of codes used for the derivation of molecular constants from FTS spectra taken in Brussels by e.g. Michel Herman and Jean Vander Auwera ($HNO_3$, OCHCHO, $CH_3CHO$, $HNO_2$, $C_2H_2$, etc).

He then got interested in molecular torsion and wrote with Isabelle Kleiner the BELGI code**. He worked with Jon Hougen, and they published a well-cited paper on $CH_3CHO$: Hougen et al. 1994, JMS 163, 559. The code kept being used after that, but by then Michel was back working on atoms.

… Except for a short interlude with us, which resulted in a quite well-cited paper as well!

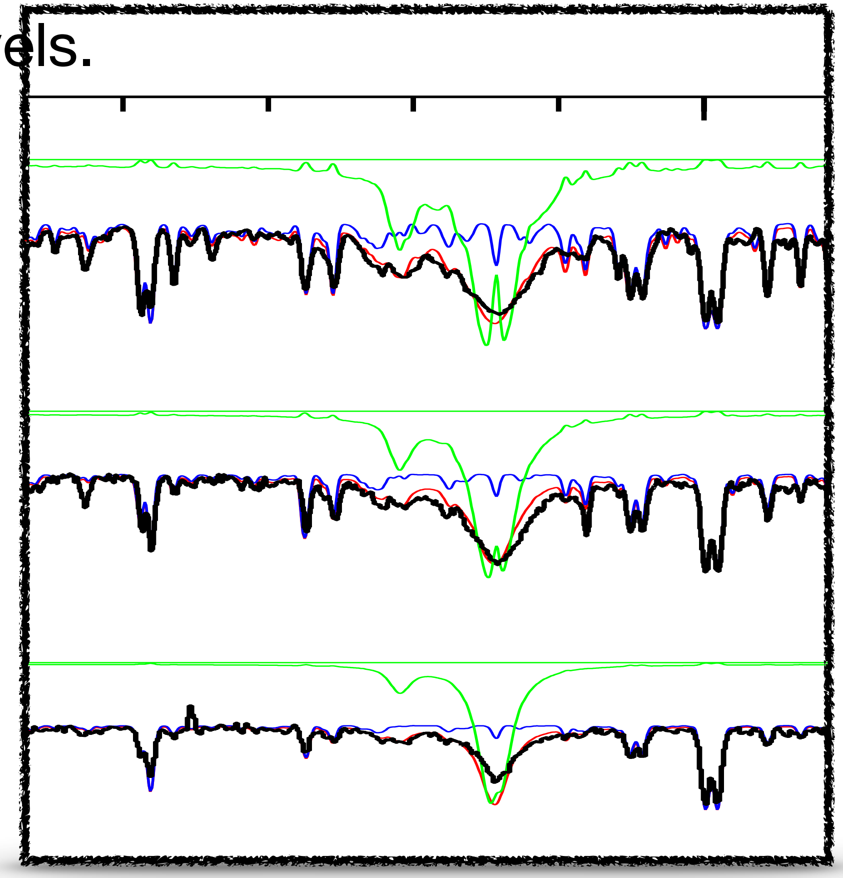
** This is very condensed, and most probably not fully accurate*

** *http://www.ifpan.edu.pl/~kisiel/introt/belgi/belgi_references.htm*

# Michel glanced back on molecules in 2005

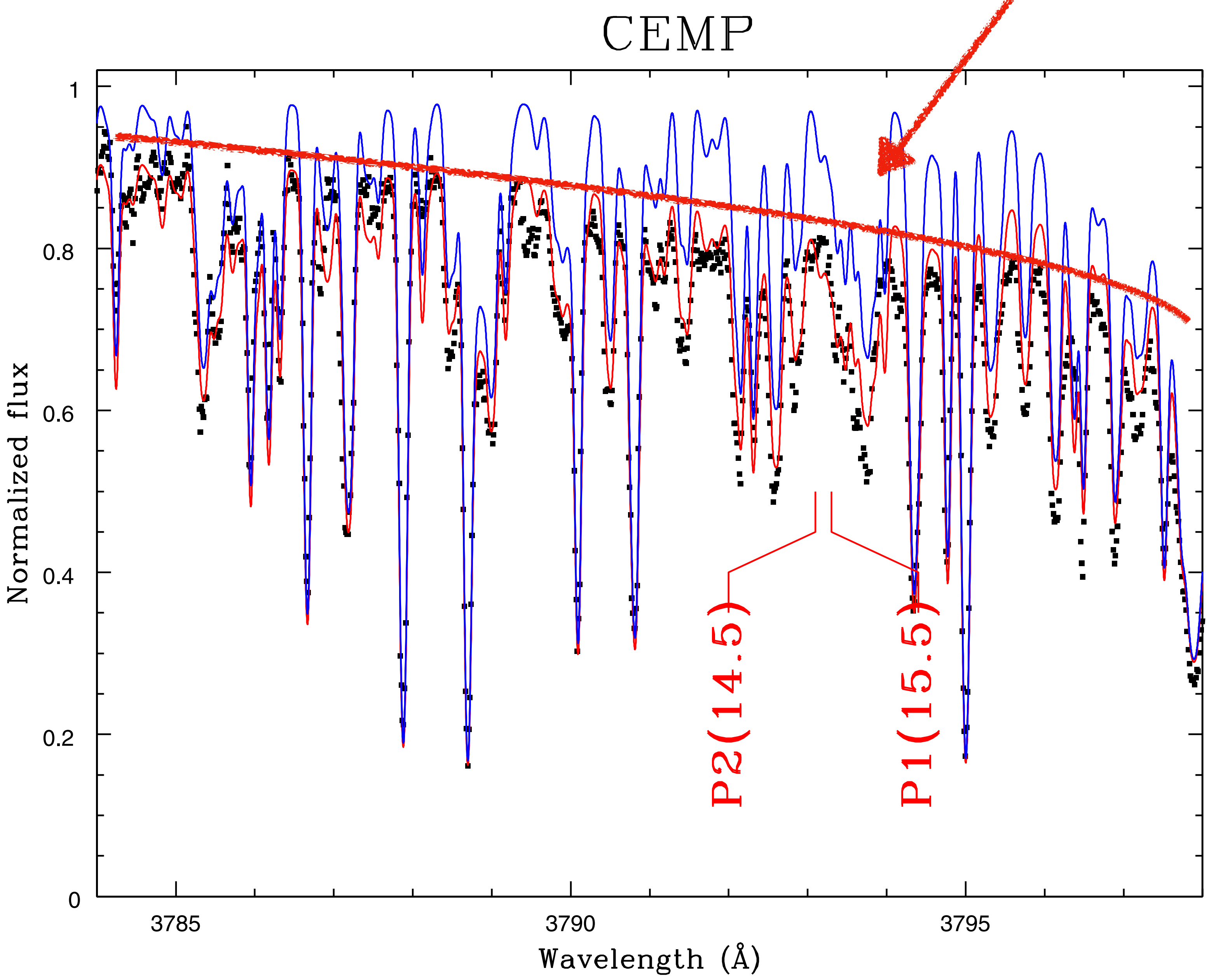
Thanks to Michel's knowledge of molecular quantum calculations we could set up PGopher and use it to compute a new line list including high lying levels, **and using stellar observations to derive better molecular constants**. We also extrapolated lifetimes using observed line widths

=> line list expanded to higher rotational levels.
=> fit the strong lines

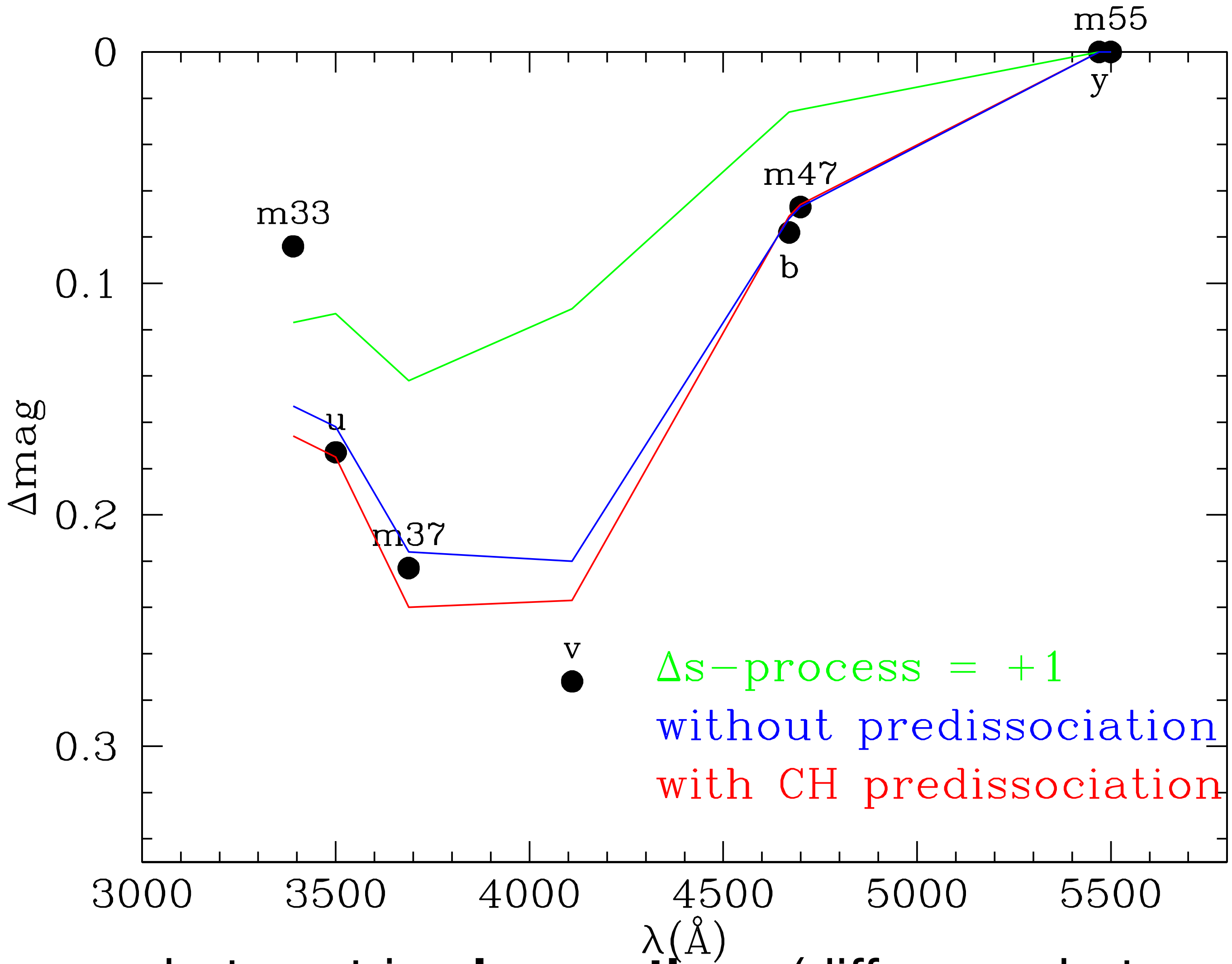


**The 4017Å line is matched by one of our predicted lines, both in position, strength, and width**

**CS22942-019**
**The haze of CH lines acts as a pseudo-continuum**



# The Bond-Neff (1969) depression in Barium stars is explained




**Black dots** are photometric **observations** (difference between a Ba and non-Ba star).

**Red line** is the **calculated** photometry using our full line list for CH.

A&A 571, A47 (2014)
DOI: 10.1051/0004-6361/201423956


Astronomy & Astrophysics

# CH in stellar atmospheres: an extensive linelist★

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[3] Service de Chimie quantique et Photophysique, Université Libre de Bruxelles, CP160/09, avenue F.D. Roosevelt 50, 1050 Bruxelles, Belgium
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## ABSTRACT

The advent of high-resolution spectrographs and detailed stellar atmosphere modelling has strengthened the need for accurate molecular data. Carbon-enhanced metal-poor (CEMP) stars spectra are interesting objects with which to study transitions from the CH molecule. We combine programs for spectral analysis of molecules and stellar-radiative transfer codes to build an extensive CH linelist, including predissociation broadening as well as newly identified levels. We show examples of strong predissociation CH lines in CEMP stars, and we stress the important role played by the CH features in the Bond-Neff feature depressing the spectra of barium stars by as much as 0.2 mag in the $\lambda = 3000-5500$ Å range. Because of the extreme thermodynamic conditions prevailing in stellar atmospheres (compared to the laboratory), molecular transitions with high energy levels can be observed. Stellar spectra can thus be used to constrain and improve molecular data.

**Key words.** molecular data – techniques: spectroscopic – stars: carbon

**And Howard Bond writes to Thomas Masseron:**

-------- Forwarded Message --------
From: Howard E. Bond <bond@stsci.edu>
To: tpm40@ast.cam.ac.uk
Subject: Bond-Neff feature
Date: Wed, 29 Oct 2014 18:40:20 -0400

Hello,

Just wanted to say I very much enjoyed your recent posting in astro-ph, in which you seem to have provided an excellent explanation for the Bond-Neff depression in barium stars.

I had always thought that the feature must be due primarily to CH...partly because there is a class of red-giant stars that lack CH (due to carbon deficiency...sometimes they are called "weak-G-band stars"). The same type of photometry that shows the B-N depression in barium and CH stars reveals an effective flux excess in the weak-CH stars, instead of a depression, when compared to red giants of normal composition. So it was pretty clear that the depression must be closely linked to the presence of CH.

regards,
Howard

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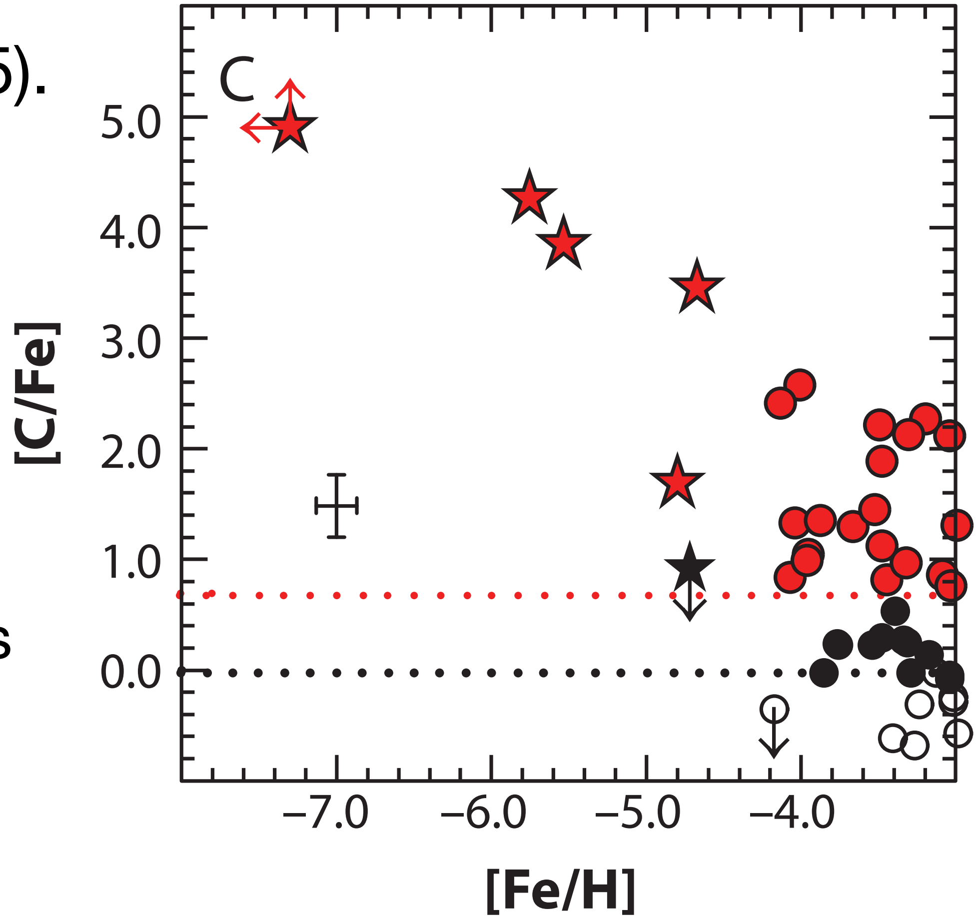
# CH in CEMP stars

## The origin of carbon-rich metal-poor stars (CEMP)

Large fraction of metal-poor stars are carbon-rich (7 out of 8 at [Fe/H]<-4.5).

Many posibilities for their origin

- they form more easily
- supermassive fast rotating stars
- mixing and fallback SN II
- zero-metallicity rotating massive stars
- binary evolution
- …and a number of other scenarios

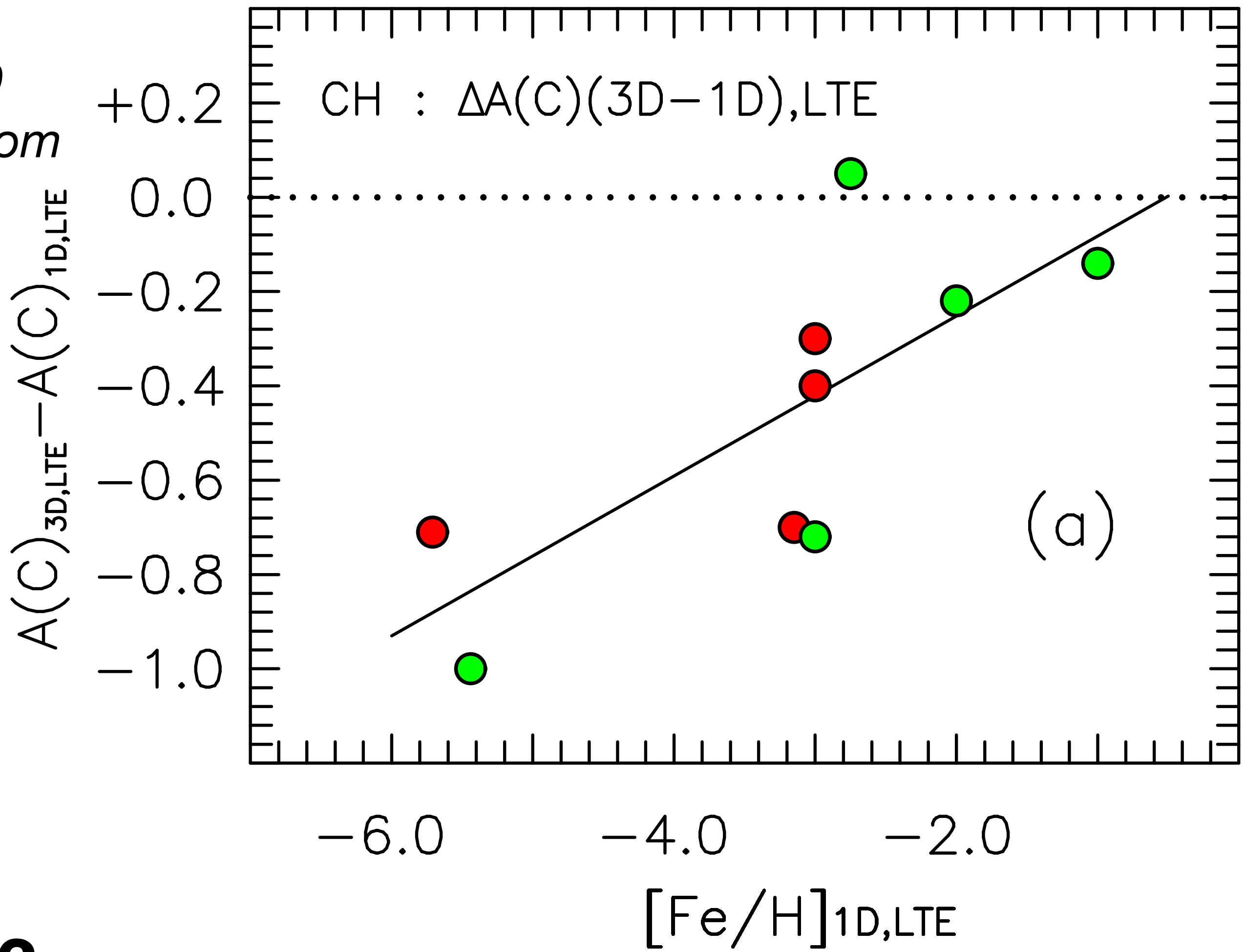



**First thing to do: make sure we got the abundances right.**

*Frebel & Norris 2015*

# 3D effects in CH line formation in Fe-poor stars

*Norris & Yong 2019 compilation of data from various sources*




**What about NLTE effects?**

**This is our next step. For that we need:**

- levels energies + gf-values
- photoionization + photodissociation
- collisional excitation / ionization / dissociation (H and e)

# As conclusion: Challenges for line lists

In order to compute the **thermal structure of models,** we need:

- line lists complete up to high lying energy levels
- medium accuracy on line positions, sufficient for lines to appear in the right frequency domain
- good accuracy on line strength

For the **computation of spectra,** for e.g. abundance analysis

- line list complete in the calculated frequency interval
- laboratory precision on line positions (<< 1km/s)
- line strengths in the 1-10% precision range

**Atoms**: there are still unidentified lines in stellar spectra !

**Molecules**: good quality and/or complete line lists still lack for some species: LaO, $C_3$, FeH, $C_2$, …

The demand is moving more and more to the IR (less blends, more flux in cool stars, …)

# Other challenges

For **detailed abundance analyses**, we are shifting to 3D, NLTE
This requires:

- inelastic collision cross-sections for electron and hydrogen collisions
- photo-ionization cross-sections
- and for molecules, photo-dissociation, and excitation and dissociation collisional cross-sections (H and e)

For magnetic fields, Landé factors, also for molecules (FeH, TiO, …)

Progress is fast in all these domains.

! The demand is increasing, with many large instruments and surveys being designed and in operation. Analyses are turning large-scale, fully automatic, and for a science requiring small errors !

Keep going!

# Abstract

Atomic and molecular lines make a strong imprint on stellar spectra, and are ubiquitous at all wavelengths in cool star spectra. They also have a profound impact on the thermal structure of cool star atmospheres. Large efforts have been devoted in recent years to compute and assemble line lists for model atmosphere and spectra calculations. I will show a few illustrative examples, including CH where Michel Godefroid contributed to creating a line list which in particular solved the enigma of the Bond-Neff depression in Ba stars.