Chemical abundances from stellar spectra

Arthur Alencastro Puls

Goethe University Frankfurt

ECR Astronuclear School on ELEMENTS - July 2024

Contents

- Using 1D LTE model atmospheres to calculate **stellar abundances**.
- **Equivalent widths** and **spectral synthesis** from a practical point of view. How to assemble good **line lists**.
- Constraining the models -- how to calculate **stellar parameters**:
  - **Excitation and ionisation balance** method. Advantages and limitations.
  - Alternative methods: using **photometry**, **astrometry**, and **asteroseismology**.
- (In the afternoon) How to interpret **MOOG output**.

Some definitions

Equivalent Width (EW) - width of a box of unit height with the same area of the measured spectral line.

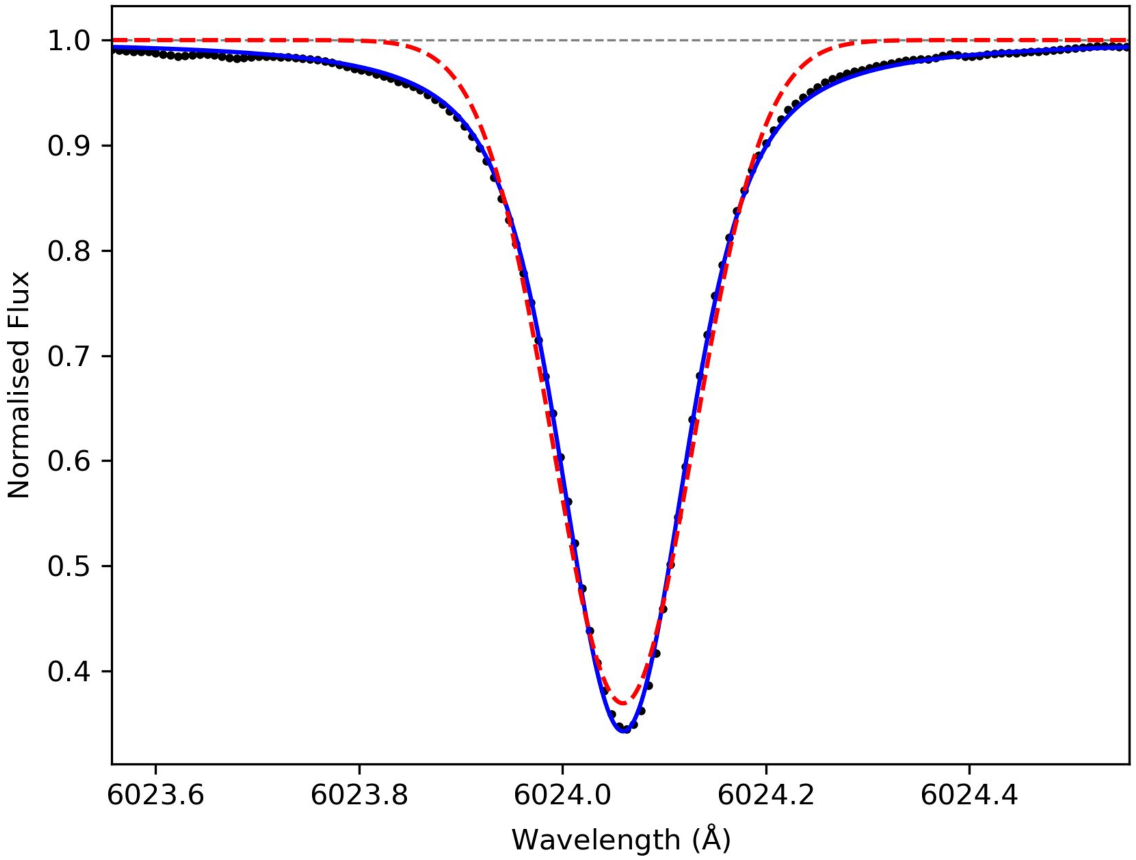
Reduced Width (RW) - the base-10 logarithm of the EW, normalised by the wavelength of the spectral line.

Abundance (A(X)) - logarithm of the number density of the element X relative to H in the stellar photosphere.

Stellar parameters - **Effective Temperature** T_{eff}, **surface gravity** log g, **metallicity** [M/H], **microturbulence** v_t.

Curve of growth - function relating A(X) and RW.

Equivalent Widths - Voigt profile

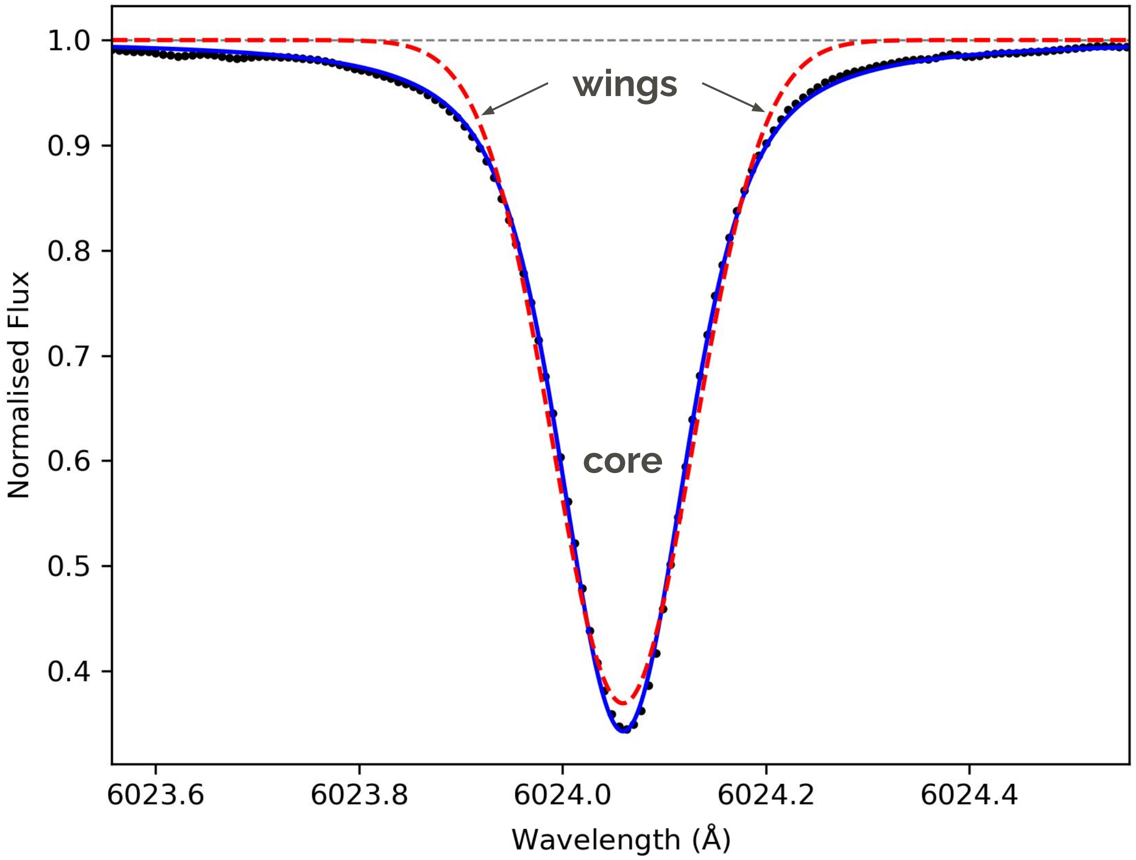


The process of line formation includes processes that enlarge the spectral line, each one resulting in line broadening with either **Gaussian** or **Lorentzian** profiles.

The resulting shape of a spectral line is the so-called **Voigt profile**.

The Voigt profile is a **convolution** between a Gaussian and a Lorentzian.

Equivalent Widths - Voigt profile



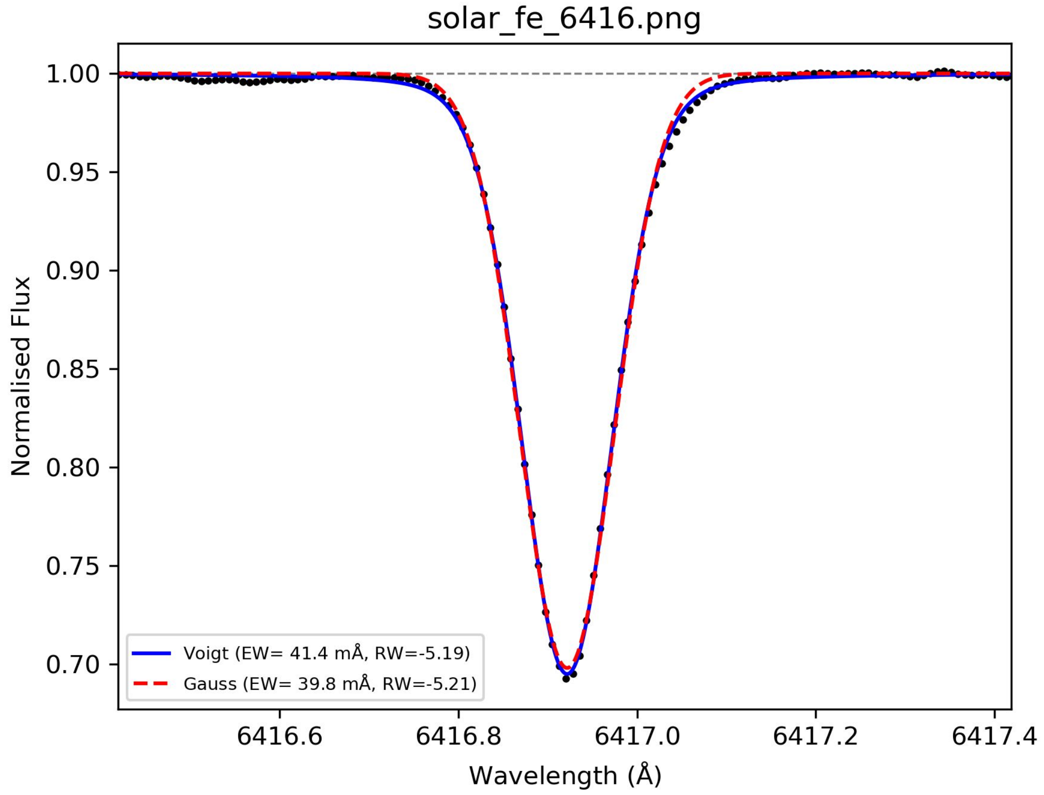
The process of line formation includes processes that enlarge the spectral line, each one resulting in line broadening with either **Gaussian** or **Lorentzian** profiles.

The resulting shape of a spectral line is the so-called **Voigt profile**.

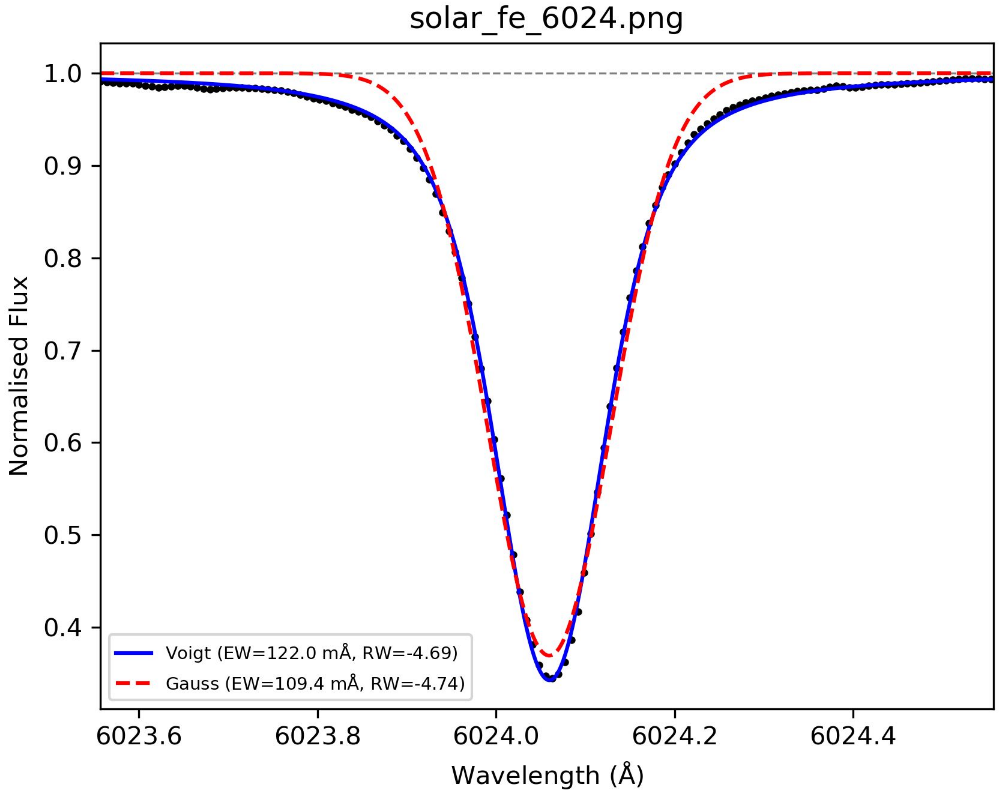
The Voigt profile is a **convolution** between a Gaussian and a Lorentzian.

Equivalent Widths

Weaker line (more Gaussian)

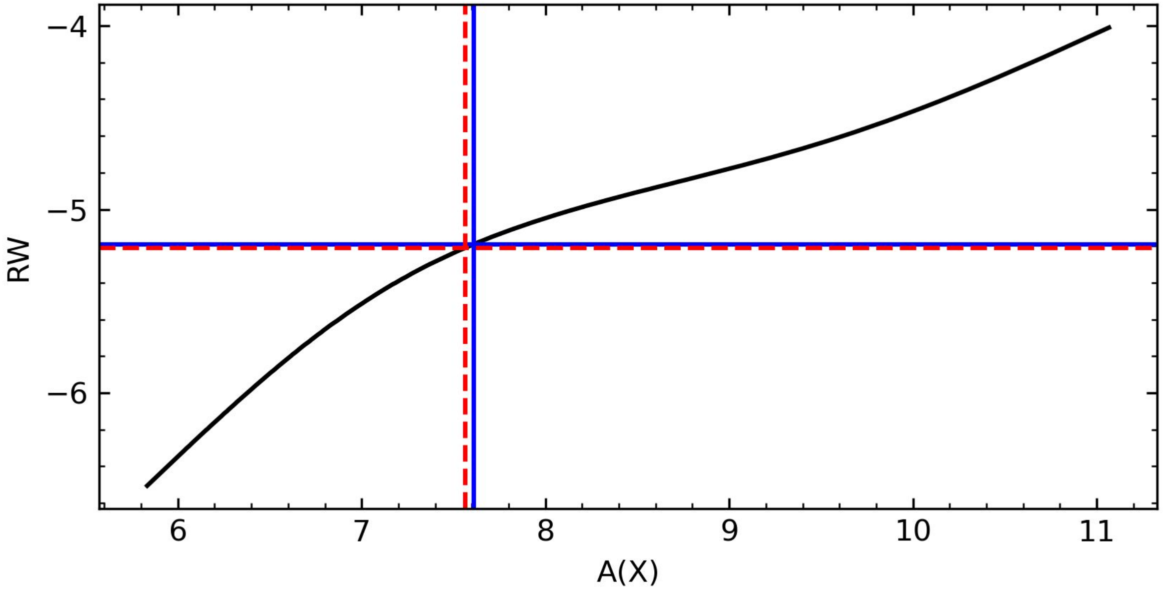


Stronger line (approaching saturation)

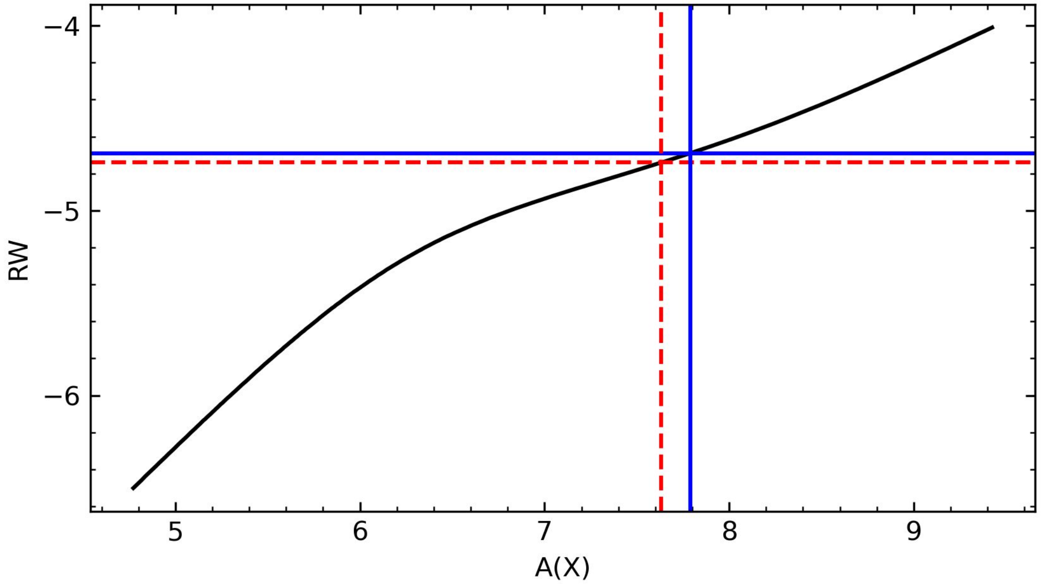


Equivalent Widths

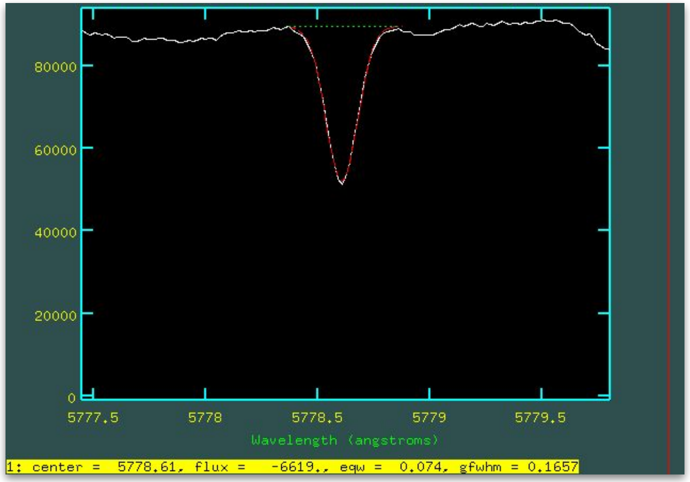
Weaker line (more Gaussian)



Stronger line (approaching saturation)



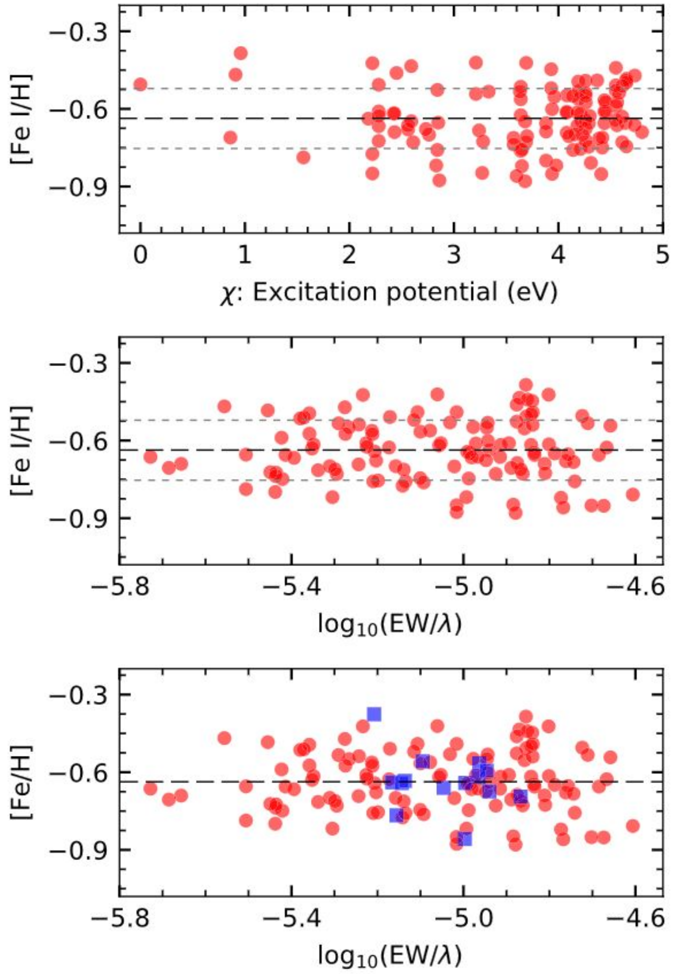
How to fit EW?



There are several options. Among them:

- Using IRAF's task *splot*.
- Using ARES (Sousa et al. 2007, 2015) - https://github.com/sousasag/ARES
- Writing your own routine! (e.g., using `scipy.optimize.curve_fit`)

Stellar parameters - excitation/ionisation method



Puls et al. 2018

Uses the spectral lines themselves to derive the stellar parameters.

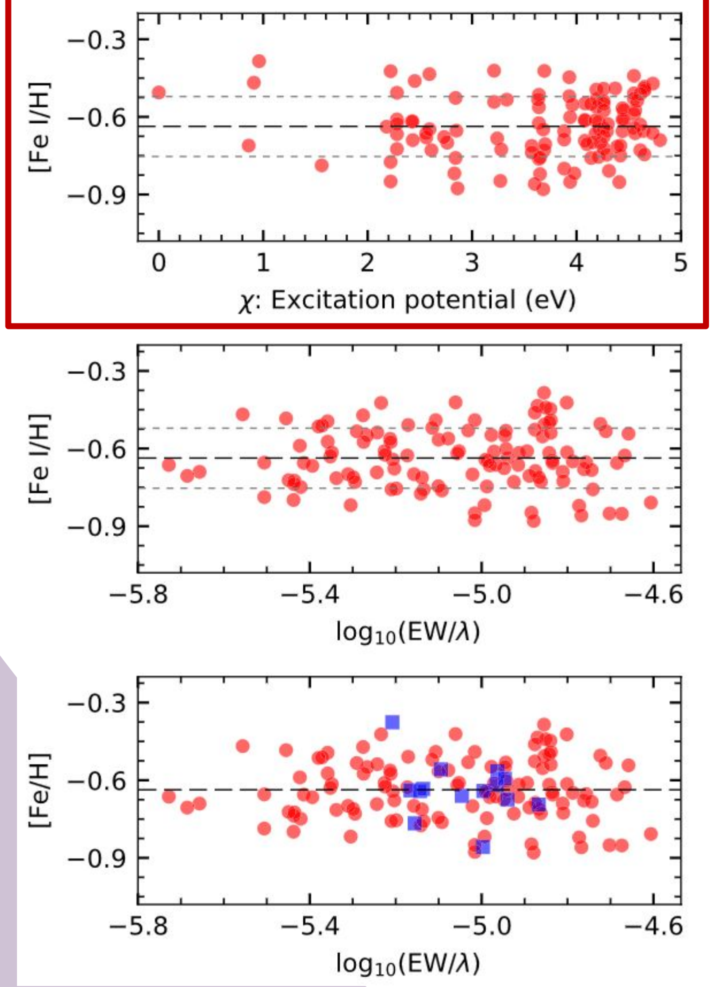
According to the Boltzmann's (excitation) equation, the number of absorbers producing a spectral line depends on both the **lower excitation potential** (LEP) and temperature.

$$\frac{N_j}{N} = \frac{\varpi_j e^{-E_j/(kT)}}{\sum \varpi_i e^{-E_i/(kT)}}.$$

→ The denominator is the partition function!

Thus, spectral lines with **LEP approaching zero** (ground state) will have a larger number of atoms in the state required to absorb a photon in their particular wavelength, and **will be stronger** (if all other variables are the same).

Stellar parameters - excitation/ionisation method



Puls et al. 2018

Uses the spectral lines themselves to derive the stellar parameters.

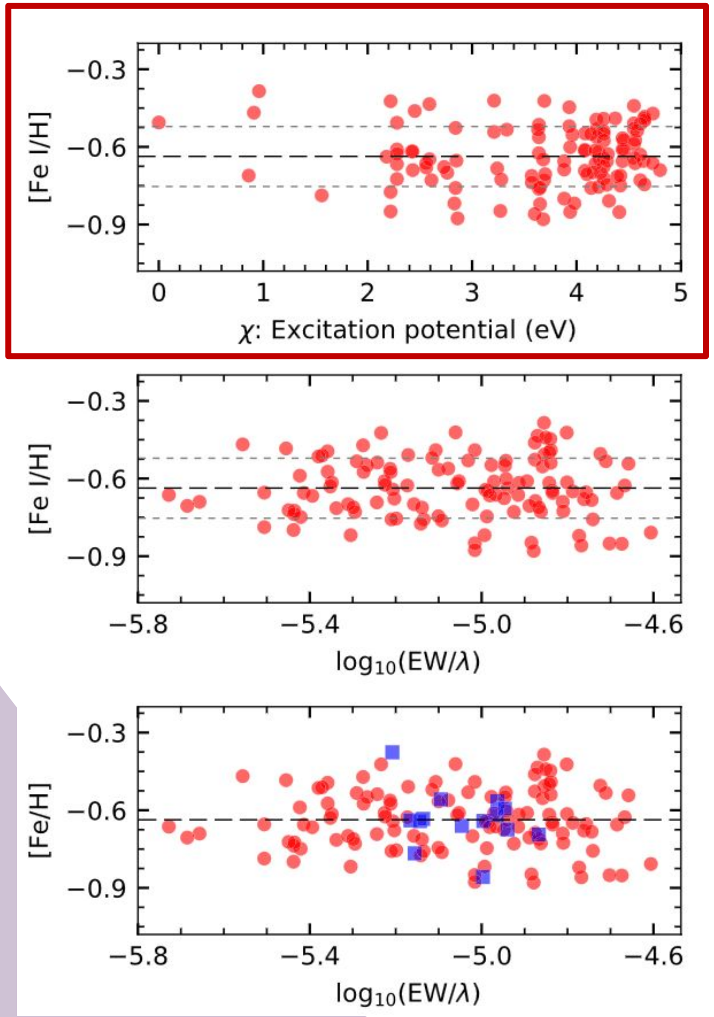
According to the Boltzmann's (excitation) equation, the number of absorbers producing a spectral line depends on both the **lower excitation potential** (LEP) and temperature.

$$\frac{N_j}{N} = \frac{\varpi_j e^{-E_j/(kT)}}{\sum \varpi_i e^{-E_i/(kT)}}.$$

→ The denominator is the partition function!

Hence, by measuring spectral lines of different values of LEP we can constrain the temperature scale of the model atmosphere and its **effective temperature**. We do that by ensuring that all lines of the same species have the same abundance (plus some scatter). Thus, the **slope of a linear fit** of the abundances wrt to LEP **must be zero**.

Stellar parameters - excitation/ionisation method

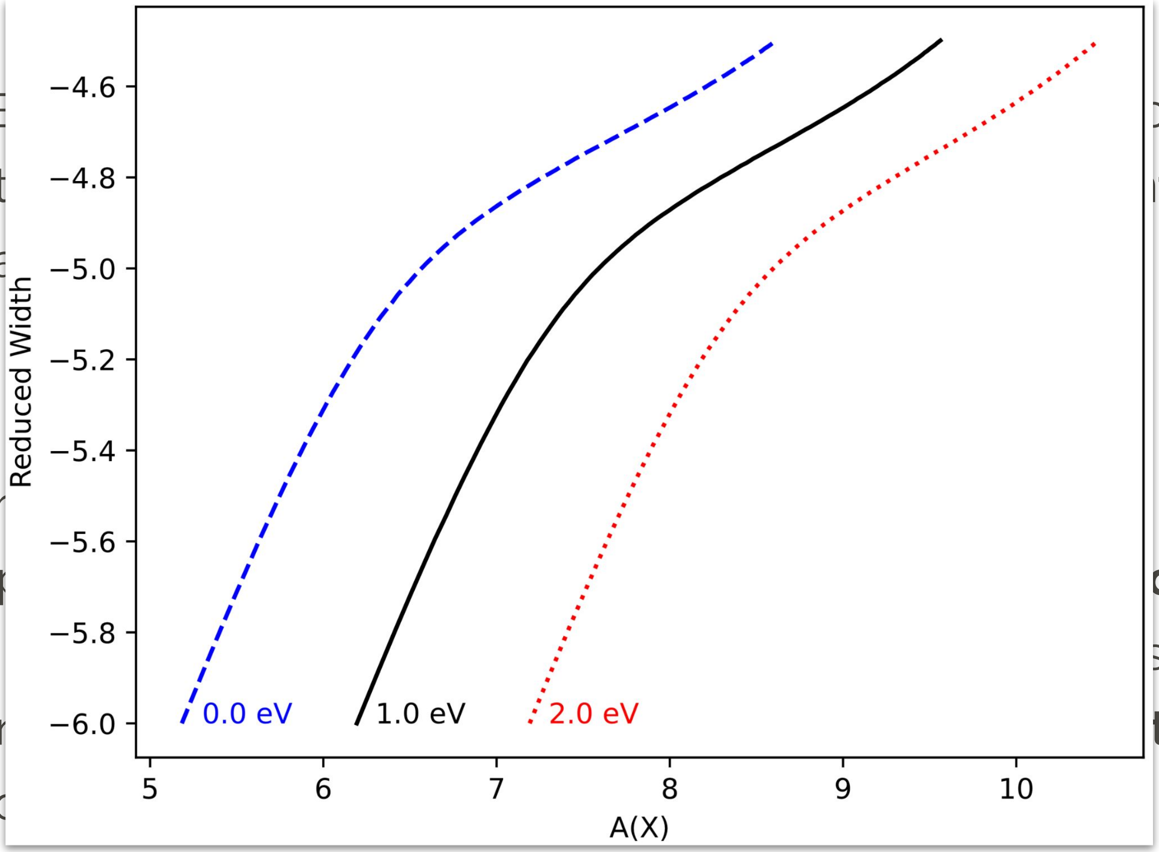


Puls et al. 2018

Uses the spectral lines themselves to derive the stellar parameters.

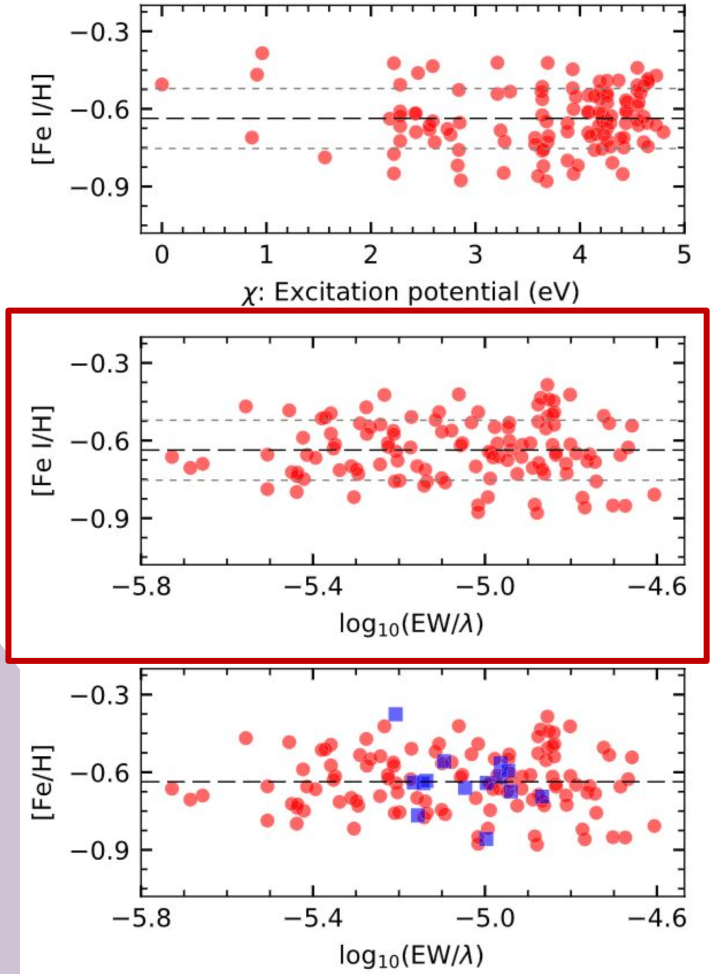
According to the E … orbers producing a spect … **tial** (LEP) and tempera…

Hence, by measur… constrain the temp… **ctive temperature**. We … s have the same abundar… **t** of the abundances wrt to…



Alencastro Puls PhDT 2023

Stellar parameters - excitation/ionisation method



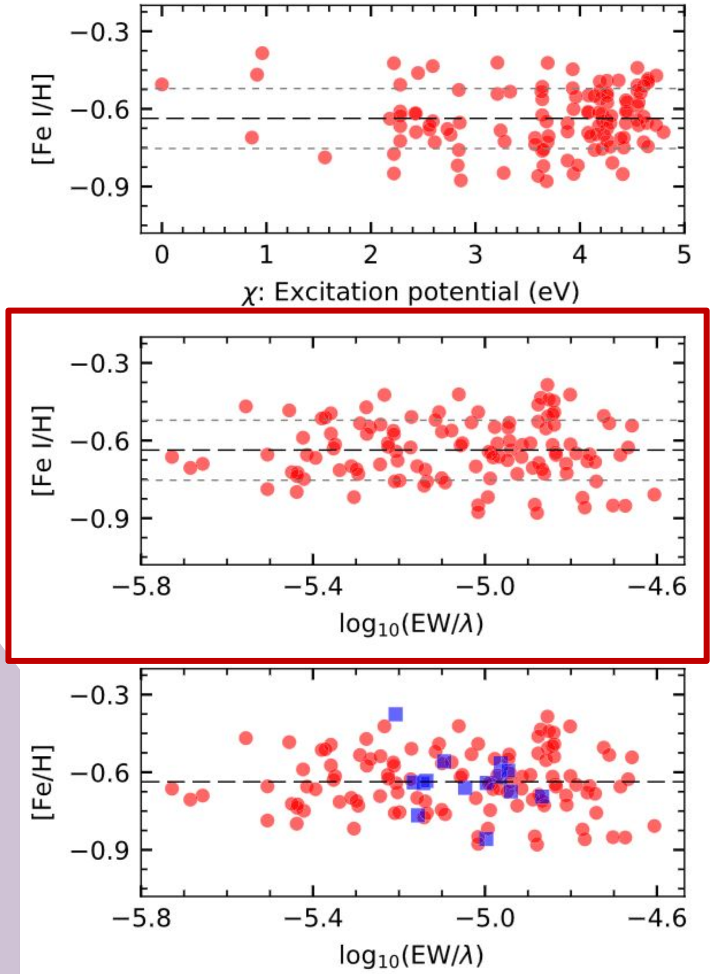
Puls et al. 2018

Uses the spectral lines themselves to derive the stellar parameters.

Stronger lines are more sensitive to changes in microturbulence than weaker lines. This can be visualised by inspecting curves of growth for the same line formed in atmospheres with different values of microturbulence.

Hence, by measuring spectral lines in a large range of **EW (~1.0-1.5 dex in RW scale)** we can constrain the **microturbulence** of the model atmosphere. Again, we do that by ensuring that all lines of the same species have the same abundance (plus some scatter). Thus, the **slope of a linear fit** of the abundances wrt to RW **must be zero**.

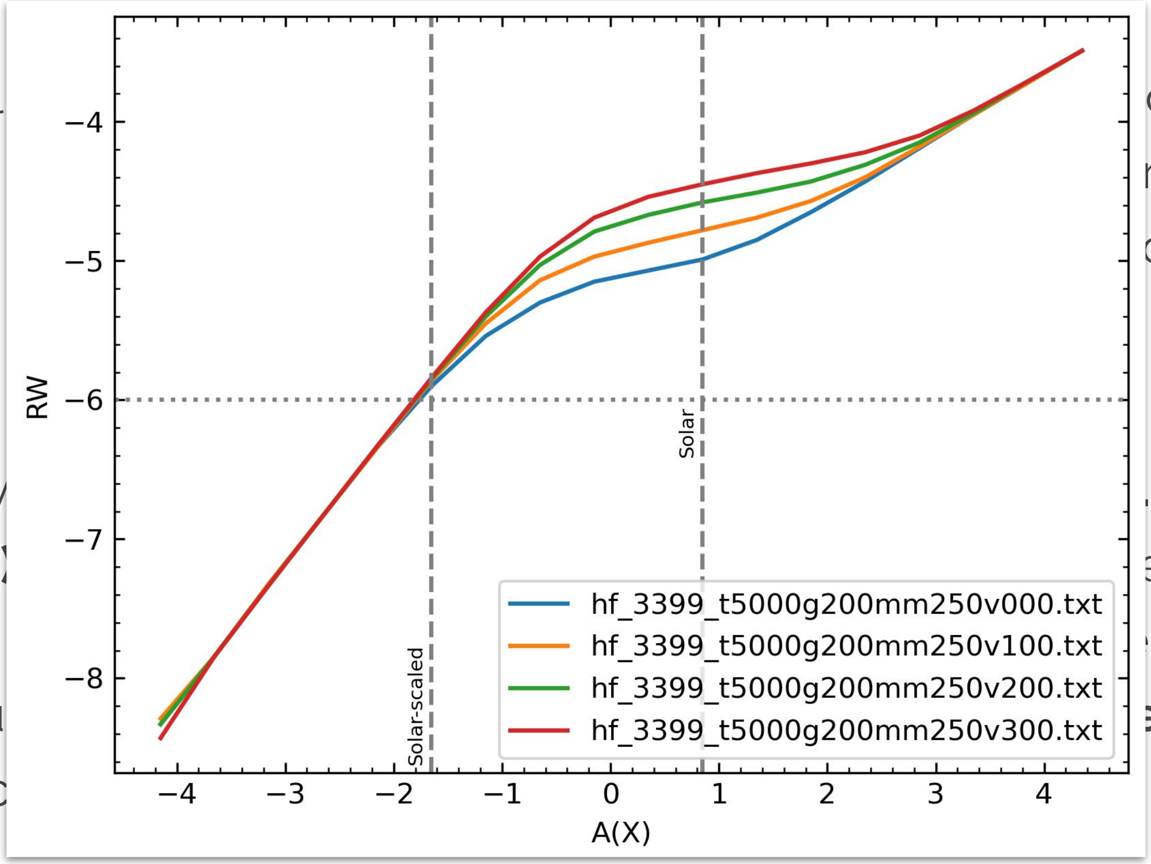
Stellar parameters - excitation/ionisation method



Puls et al. 2018

Uses the spectral lines themselves to derive the stellar parameters.

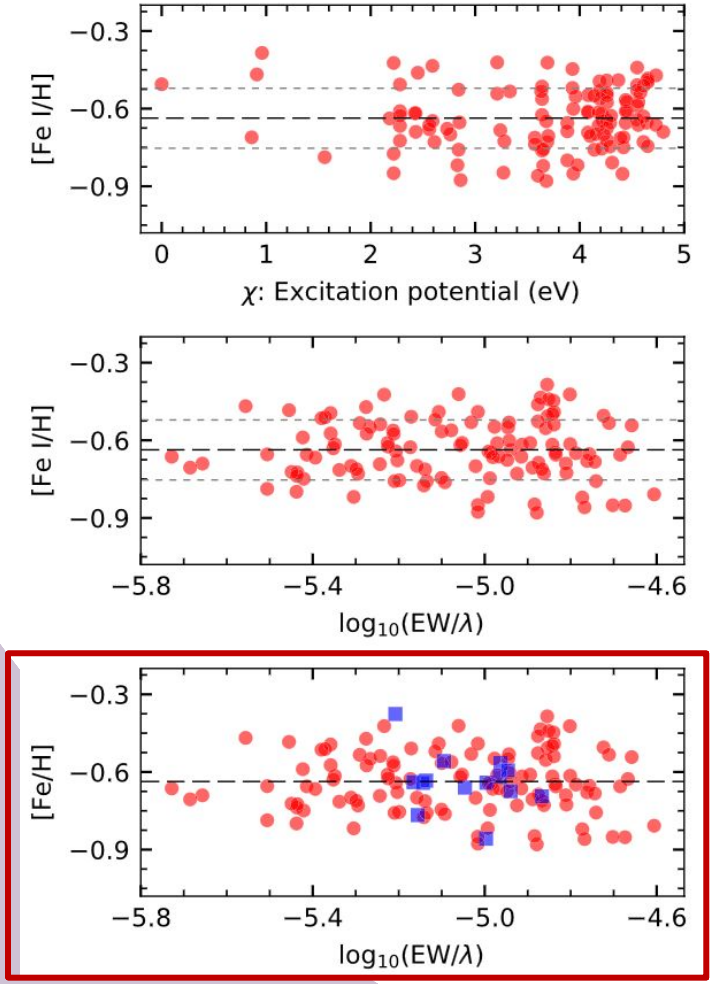
Stronger l … ce than weaker lines. This … r the same line formed in … ce.



Hence, by … **.0-1.5 dex in RW scale** … el atmosphere.

Again, we … s have the same abu … **ear fit** of the abundanc

Stellar parameters - excitation/ionisation method



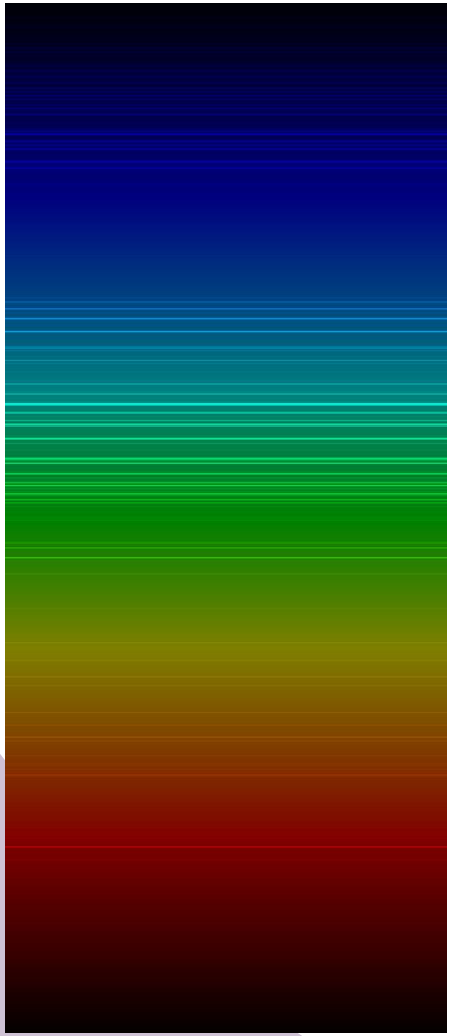
Puls et al. 2018

Uses the spectral lines themselves to derive the stellar parameters.

Lines if the same element in different **ionisation states** present different sensitivities to pressure. In the model atmosphere, pressure is linked to **surface gravity**.

Hence, by measuring spectral lines of the same element, but from different ionisation states, we can constrain the surface gravity of the star. Thus, the **difference of the average/median abundance** of lines from different ionisation states **<u>must be zero</u>**.

Stellar parameters - excitation/ionisation method



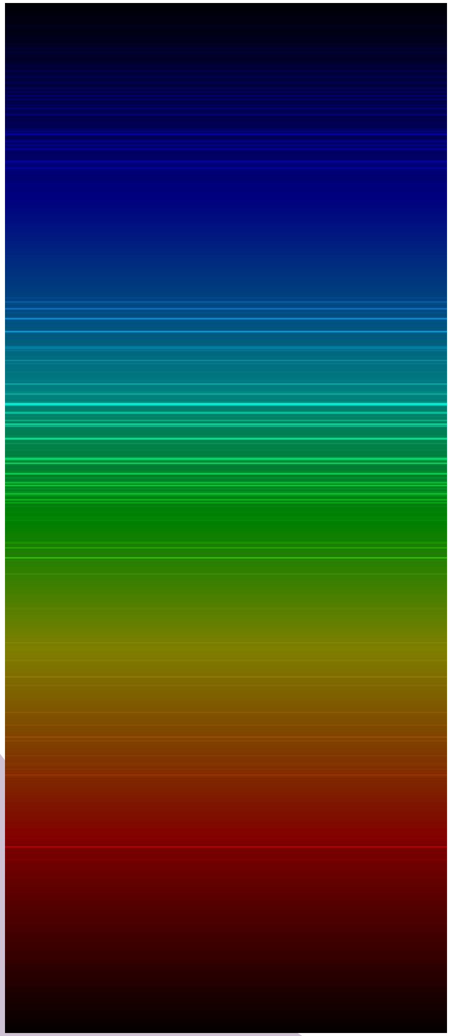
Uses the spectral lines themselves to derive the stellar parameters.

The element **Fe** is usually employed to derive stellar parameters.

The main reasons are:

- The rich variety of Fe lines in the optical region of the electromagnetic spectrum;
- The relatively high abundance of Fe compared to other metals in the universe;
- The photospheres of late type stars (FGK-types) being in the “goldilocks zone” for formation of both **Fe I (neutral)** and **Fe II (singly ionised)** lines.

Stellar parameters - excitation/ionisation method



Uses the spectral lines themselves to derive the stellar parameters.

- Pros:
  - Self consistency with the spectrum under study.
  - Does not require further observations.
  - Allows differential analysis.

- Cons:
  - Model dependence.
  - Fe I and Fe II abundances are not consistent in lower metallicities due to differential LTE effects.
  - Suboptimal choice of line list may bias the derived parameters.

The line list

Lambda,	sp,	EP,	loggf,	C6,	FP,	EW
5560.21	26.0	4.43	-1.120	0.0	0.0	69.7
5576.09	26.0	3.43	-1.000	0.0	0.0	146.8
5633.95	26.0	4.99	-0.180	0.0	0.0	79.5
5638.26	26.0	4.22	-0.800	0.0	0.0	99.8
5651.47	26.0	4.47	-1.850	0.0	0.0	33.1
5662.52	26.0	4.18	-0.573	0.0	0.0	119.0
5679.02	26.0	4.65	-0.810	0.0	0.0	73.4
5731.76	26.0	4.26	-1.110	0.0	0.0	82.5
5775.08	26.0	4.22	-1.230	0.0	0.0	83.0
5778.45	26.0	2.59	-3.430	0.0	0.0	69.1
5853.15	26.0	1.49	-5.260	0.0	0.0	63.8
5902.47	26.0	4.59	-1.880	0.0	0.0	24.6
6078.49	26.0	4.79	-0.400	0.0	0.0	85.1
6093.64	26.0	4.61	-1.430	0.0	0.0	38.4
6096.67	26.0	3.98	-1.900	0.0	0.0	64.9
6098.24	26.0	4.56	-1.810	0.0	0.0	32.2
6120.25	26.0	0.92	-5.970	0.0	0.0	66.3
6187.99	26.0	3.94	-1.690	0.0	0.0	78.1
6240.65	26.0	2.22	-3.320	0.0	0.0	118.3
6322.69	26.0	2.59	-2.426	0.0	0.0	135.1
6392.54	26.0	2.28	-4.070	0.0	0.0	73.5
6518.37	26.0	2.83	-2.570	0.0	0.0	121.3
6574.23	26.0	0.99	-5.004	0.0	0.0	129.1
6703.57	26.0	2.76	-3.080	0.0	0.0	90.7
6726.67	26.0	4.61	-1.140	0.0	0.0	59.8
6842.69	26.0	4.64	-1.200	0.0	0.0	54.3
6857.25	26.0	4.08	-2.190	0.0	0.0	40.1
6858.15	26.0	4.61	-0.930	0.0	0.0	63.6
7114.55	26.0	2.69	-4.070	0.0	0.0	43.7
7421.56	26.0	4.64	-1.680	0.0	0.0	26.4
7531.15	26.0	4.37	-0.590	0.0	0.0	111.0
7547.90	26.0	5.10	-1.080	0.0	0.0	25.6
4491.40	26.1	2.86	-2.700	0.0	0.0	93.3
4576.34	26.1	2.84	-2.820	0.0	0.0	75.4
5234.62	26.1	3.22	-2.150	0.0	0.0	86.7
5264.81	26.1	3.23	-3.130	0.0	0.0	45.0
5425.26	26.1	3.20	-3.220	0.0	0.0	44.9
6247.56	26.1	3.89	-2.300	0.0	0.0	33.9
6369.46	26.1	2.89	-4.110	0.0	0.0	22.2

Before choosing the lines that will compose the line list, we must know what's the purpose of the analysis.

Defining stellar parameters? Fe lines are recommended. The other elements will depend on your aims.

Also:

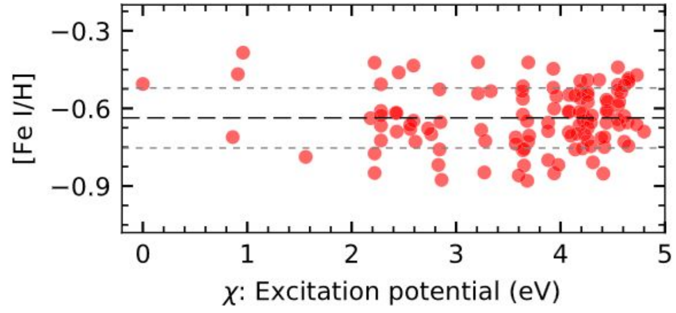
- What's the **wavelength coverage** of the spectrum/spectra?
- What's the expected metallicity? Compare with a **spectral atlas**!
- What are the Teff and evolutionary states of the star(s)? Where is/are the star(s) in a **colour-magnitude diagram**?

The line list

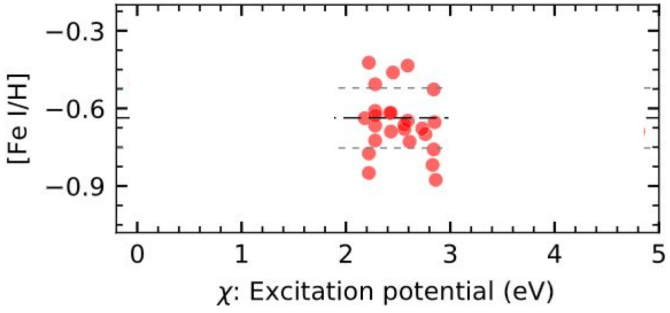
Lambda,	sp,	EP,	loggf,	C6,	FP,	EW
5560.21	26.0	4.43	-1.120	0.0	0.0	69.7
5576.09	26.0	3.43	-1.000	0.0	0.0	146.8
5633.95	26.0	4.99	-0.180	0.0	0.0	79.5
5638.26	26.0	4.22	-0.800	0.0	0.0	99.8
5651.47	26.0	4.47	-1.850	0.0	0.0	33.1
5662.52	26.0	4.18	-0.573	0.0	0.0	119.0
5679.02	26.0	4.65	-0.810	0.0	0.0	73.4
5731.76	26.0	4.26	-1.110	0.0	0.0	82.5
5775.08	26.0	4.22	-1.230	0.0	0.0	83.0
5778.45	26.0	2.59	-3.430	0.0	0.0	69.1
5853.15	26.0	1.49	-5.260	0.0	0.0	63.8
5902.47	26.0	4.59	-1.880	0.0	0.0	24.6
6078.49	26.0	4.79	-0.400	0.0	0.0	85.1
6093.64	26.0	4.61	-1.430	0.0	0.0	38.4
6096.67	26.0	3.98	-1.900	0.0	0.0	64.9
6098.24	26.0	4.56	-1.810	0.0	0.0	32.2
6120.25	26.0	0.92	-5.970	0.0	0.0	66.3
6187.99	26.0	3.94	-1.690	0.0	0.0	78.1
6240.65	26.0	2.22	-3.320	0.0	0.0	118.3
6322.69	26.0	2.59	-2.426	0.0	0.0	135.1
6392.54	26.0	2.28	-4.070	0.0	0.0	73.5
6518.37	26.0	2.83	-2.570	0.0	0.0	121.3
6574.23	26.0	0.99	-5.004	0.0	0.0	129.1
6703.57	26.0	2.76	-3.080	0.0	0.0	90.7
6726.67	26.0	4.61	-1.140	0.0	0.0	59.8
6842.69	26.0	4.64	-1.200	0.0	0.0	54.3
6857.25	26.0	4.08	-2.190	0.0	0.0	40.1
6858.15	26.0	4.61	-0.930	0.0	0.0	63.6
7114.55	26.0	2.69	-4.070	0.0	0.0	43.7
7421.56	26.0	4.64	-1.680	0.0	0.0	26.4
7531.15	26.0	4.37	-0.590	0.0	0.0	111.0
7547.90	26.0	5.10	-1.080	0.0	0.0	25.6
4491.40	26.1	2.86	-2.700	0.0	0.0	93.3
4576.34	26.1	2.84	-2.820	0.0	0.0	75.4
5234.62	26.1	3.22	-2.150	0.0	0.0	86.7
5264.81	26.1	3.23	-3.130	0.0	0.0	45.0
5425.26	26.1	3.20	-3.220	0.0	0.0	44.9
6247.56	26.1	3.89	-2.300	0.0	0.0	33.9
6369.46	26.1	2.89	-4.110	0.0	0.0	22.2

For stellar parameters, a large range in LEP is necessary for the neutral species.

States with LEP ≳ 5 eV are usually not populated enough to form spectral lines in FGK-type stars.



Good!



Avoid!

The line list

Lambda,	sp,	EP,	loggf,	C6,	FP,	EW
5560.21	26.0	4.43	-1.120	0.0	0.0	69.7
5576.09	26.0	3.43	-1.000	0.0	0.0	146.8
5633.95	26.0	4.99	-0.180	0.0	0.0	79.5
5638.26	26.0	4.22	-0.800	0.0	0.0	99.8
5651.47	26.0	4.47	-1.850	0.0	0.0	33.1
5662.52	26.0	4.18	-0.573	0.0	0.0	119.0
5679.02	26.0	4.65	-0.810	0.0	0.0	73.4
5731.76	26.0	4.26	-1.110	0.0	0.0	82.5
5775.08	26.0	4.22	-1.230	0.0	0.0	83.0
5778.45	26.0	2.59	-3.430	0.0	0.0	69.1
5853.15	26.0	1.49	-5.260	0.0	0.0	63.8
5902.47	26.0	4.59	-1.880	0.0	0.0	24.6
6078.49	26.0	4.79	-0.400	0.0	0.0	85.1
6093.64	26.0	4.61	-1.430	0.0	0.0	38.4
6096.67	26.0	3.98	-1.900	0.0	0.0	64.9
6098.24	26.0	4.56	-1.810	0.0	0.0	32.2
6120.25	26.0	0.92	-5.970	0.0	0.0	66.3
6187.99	26.0	3.94	-1.690	0.0	0.0	78.1
6240.65	26.0	2.22	-3.320	0.0	0.0	118.3
6322.69	26.0	2.59	-2.426	0.0	0.0	135.1
6392.54	26.0	2.28	-4.070	0.0	0.0	73.5
6518.37	26.0	2.83	-2.570	0.0	0.0	121.3
6574.23	26.0	0.99	-5.004	0.0	0.0	129.1
6703.57	26.0	2.76	-3.080	0.0	0.0	90.7
6726.67	26.0	4.61	-1.140	0.0	0.0	59.8
6842.69	26.0	4.64	-1.200	0.0	0.0	54.3
6857.25	26.0	4.08	-2.190	0.0	0.0	40.1
6858.15	26.0	4.61	-0.930	0.0	0.0	63.6
7114.55	26.0	2.69	-4.070	0.0	0.0	43.7
7421.56	26.0	4.64	-1.680	0.0	0.0	26.4
7531.15	26.0	4.37	-0.590	0.0	0.0	111.0
7547.90	26.0	5.10	-1.080	0.0	0.0	25.6
4491.40	26.1	2.86	-2.700	0.0	0.0	93.3
4576.34	26.1	2.84	-2.820	0.0	0.0	75.4
5234.62	26.1	3.22	-2.150	0.0	0.0	86.7
5264.81	26.1	3.23	-3.130	0.0	0.0	45.0
5425.26	26.1	3.20	-3.220	0.0	0.0	44.9
6247.56	26.1	3.89	-2.300	0.0	0.0	33.9
6369.46	26.1	2.89	-4.110	0.0	0.0	22.2

The **log gf**, or the oscillator strength *f*, is a quantity related to the probability of the photon being absorbed by the atom. It is proportional to the Einstein coefficients.

In the linear part of the curve of growth, **the difference (log gf - LEP [eV])** is a good approximation to compare the strength of lines **of the same species**.

Hence, the range of RW necessary to constrain microturbulence can be predicted by the combination of the **atomic parameters** LEP and log gf.

$$B_{12} = \frac{e^2}{4\varepsilon_0 m_e h\nu} f_{12},$$

$$B_{21} = \frac{e^2}{4\varepsilon_0 m_e h\nu} \frac{g_1}{g_2} f_{12},$$

$$A_{21} = \frac{2\pi\nu^2 e^2}{\varepsilon_0 m_e c^3} \frac{g_1}{g_2} f_{12}.$$

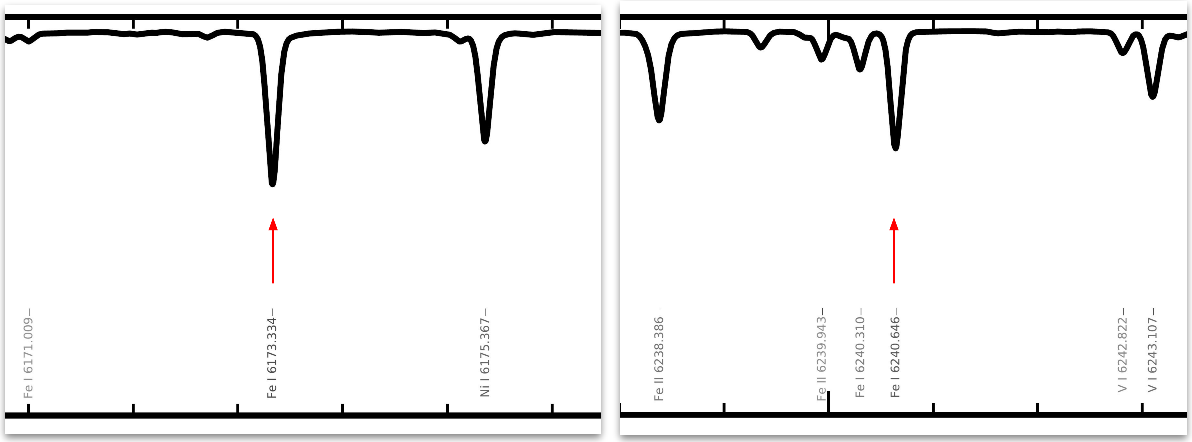
The line list

The **log gf**, or the oscillator strength *f*, is a quantity related to the probability of the photon being absorbed by the atom. It is proportional to the Einstein coefficients.

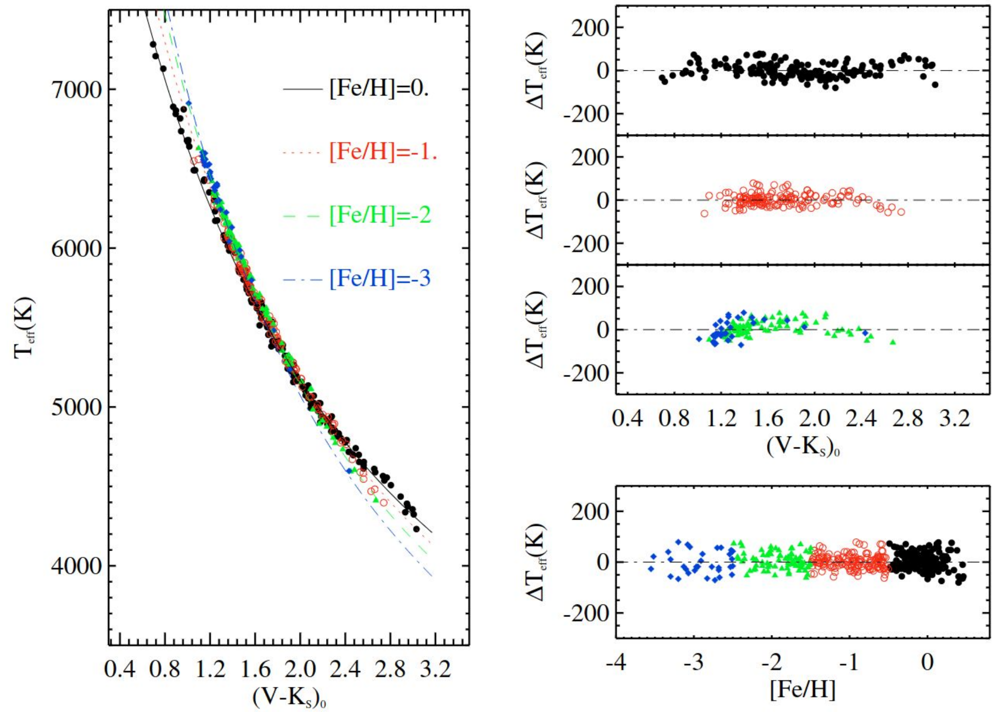
In the linear part of the curve of growth, **the difference (log gf - LEP [eV])** is a good approximation to compare the strength of lines **of the same species**.

Strassmeier+ 2018

For instance: Fe I lines at 6173.334 Å and 6240.646 Å have the same excitation energy, but the transition probability is larger for the former, resulting in a stronger line.



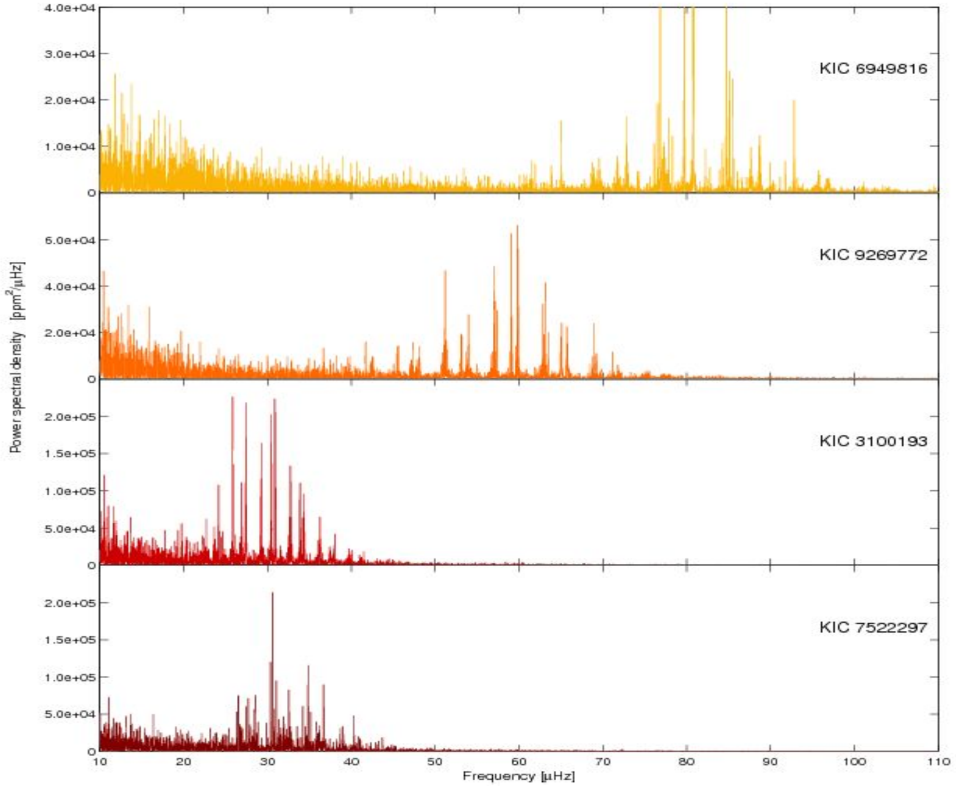
Stellar parameters - other methods



Gonzalez Hernandez & Bonifacio 2009

Colour-Teff relations.

Asteroseismology



$$\log \frac{g}{g_\odot} = \log \frac{M}{M_\odot} + 4\log \frac{T}{T_\odot} - \log \frac{L}{L_\odot}$$

$$\log g \simeq \log \frac{\nu_{\max}}{\nu_{max,\odot}} + \frac{1}{2}\log \frac{T_{\rm eff}}{T_{\rm eff,\odot}} + \log g_\odot$$

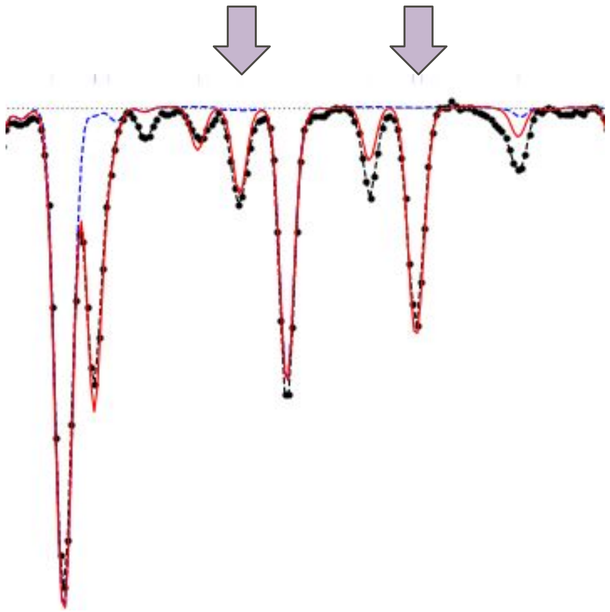
Chaplin & Miglio 2013

Measuring stellar abundances

More equivalent widths

Remember:

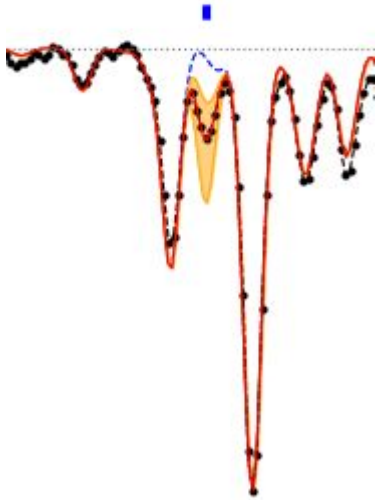
Lines must be clean!



For lines with heavy blending

or hyperfine structure:

Spectral synthesis!



Measuring stellar abundances

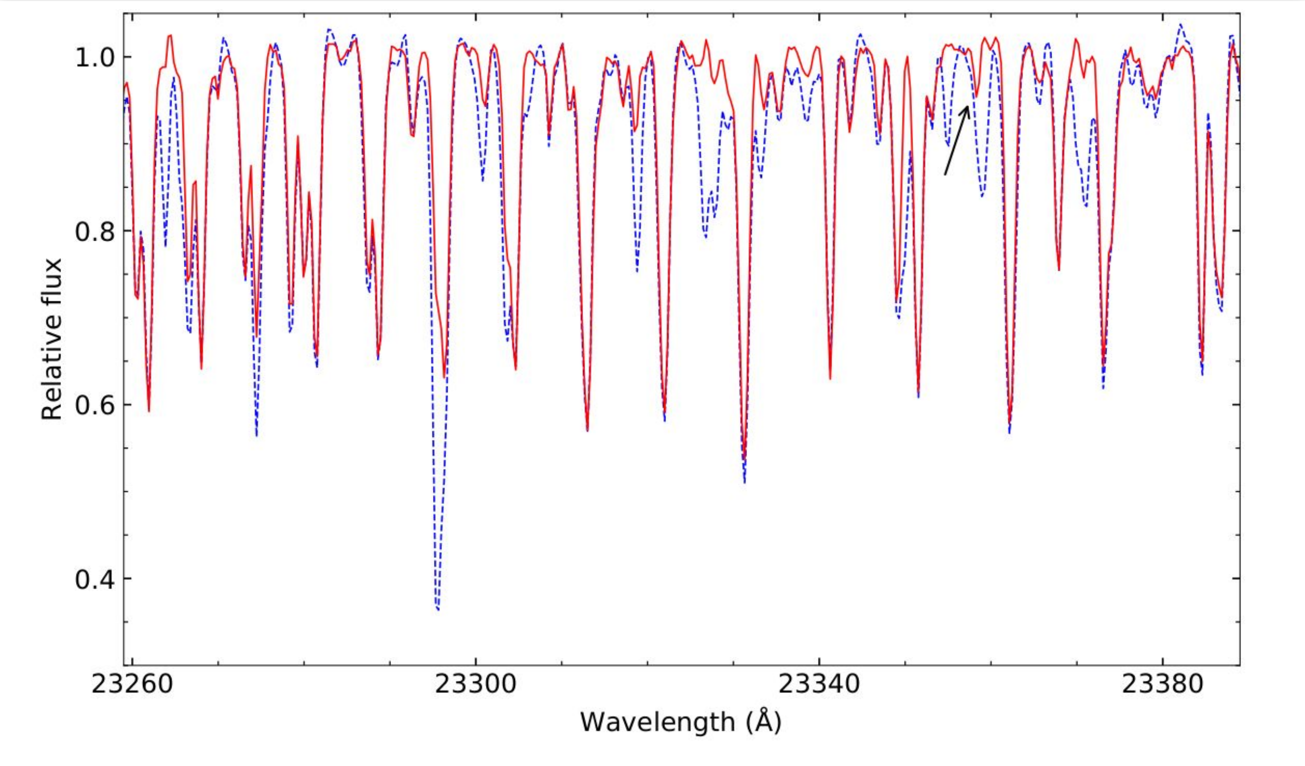
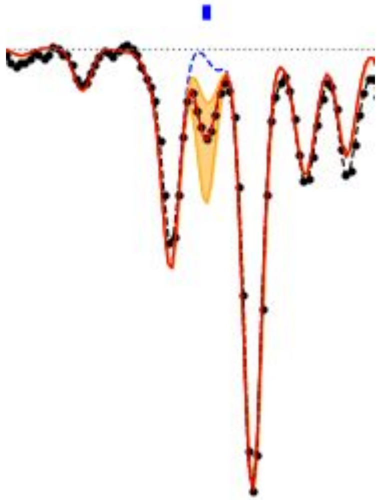


Figure 12 – A portion of the spectra of the star HD 5223. *Blue dashed line*: (doppler corrected) spectrum with telluric features. *Red solid line*: telluric subtracted spectrum. For this object – with observed radial velocity of -211.7 km s^{-1} – the 1-0 R9 HF line, marked with an arrow, fell inside a telluric feature. Its presence was revealed only after the subtraction.

Alencastro Puls MsCT 2018

For lines with heavy blending
or hyperfine structure:
Spectral synthesis!



Some applications: origin of the elements

Studies on detailed stellar composition give hints on the sites of formation of different elements.

For instance, detailed chemical analysis of old, metal-poor stars helps to constrain the astrophysical sites of the r-process elements.

Hansen+ 2014 ApJ 797 123

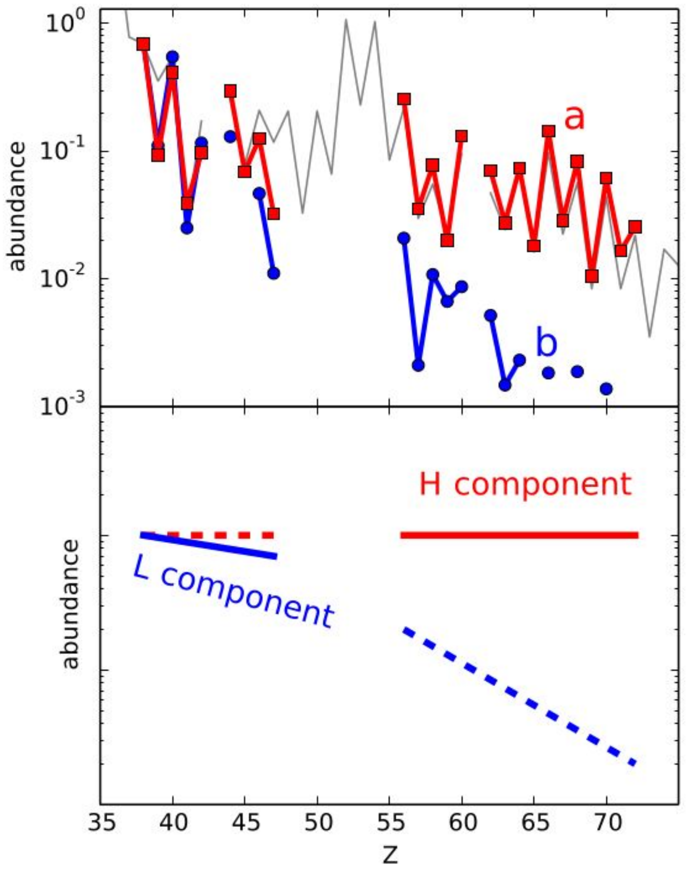


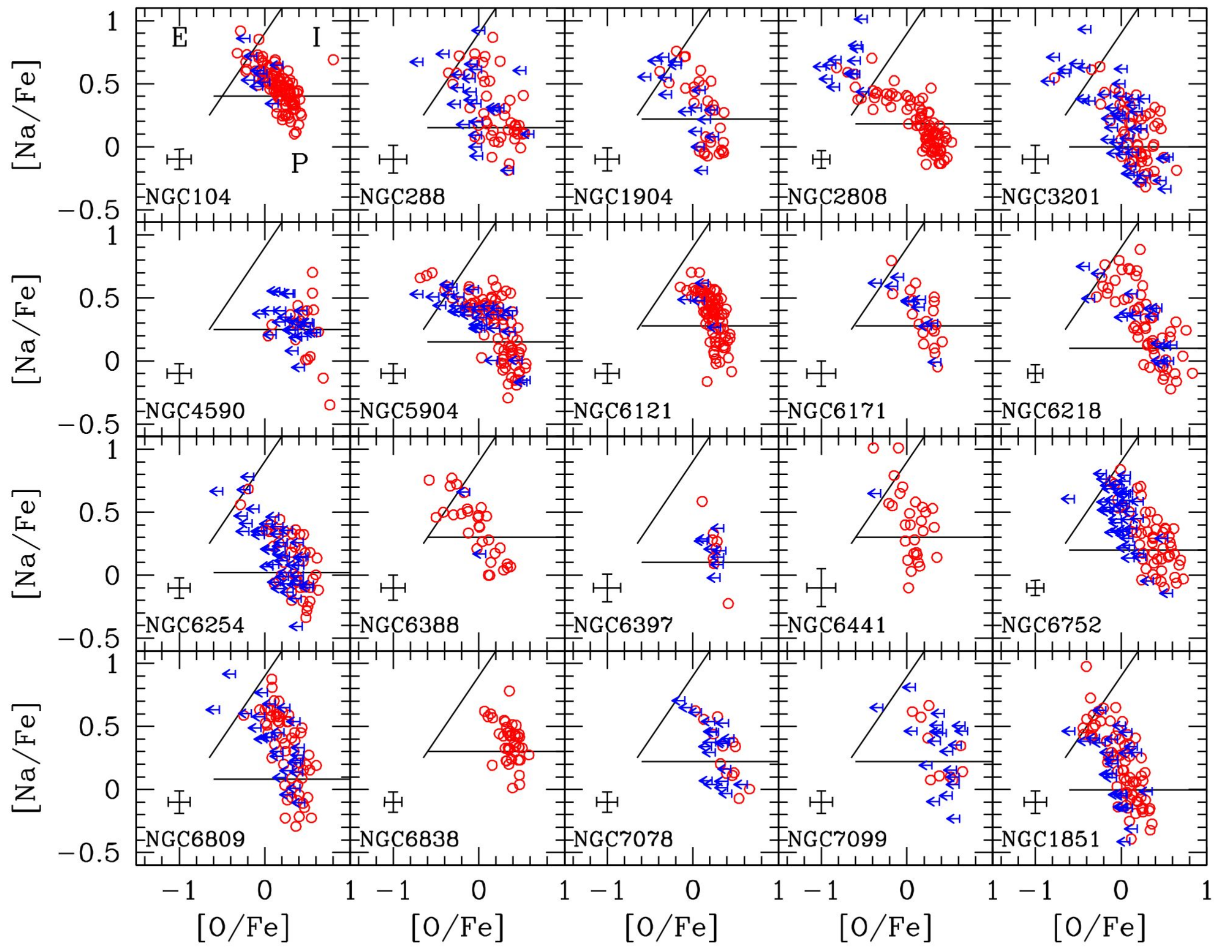
Figure 1. Two metal-poor stellar abundance patterns are shown in the upper panel compared to the solar *r* process (gray thin line). The pattern "a" (red line and squares) corresponds to CS 22892-052, and the "b" pattern (blue line and circles) to HD 122563. All abundances are normalized to Sr. The bottom panel

Some applications: stellar clusters

Globular clusters were traditionally thought to be formed by the same progenitor cloud, but detailed chemical analysis has challenged that scenario.

Any theory of formation of globular clusters has to take those differences into account.

Gratton+ 2012 A&ARv 20 50



Some applications: stellar clusters

Gratton+ 2012 A&ARv 20 50

Globular clu

be formed by

detailed cher

scenario.

Any theory of

to take those

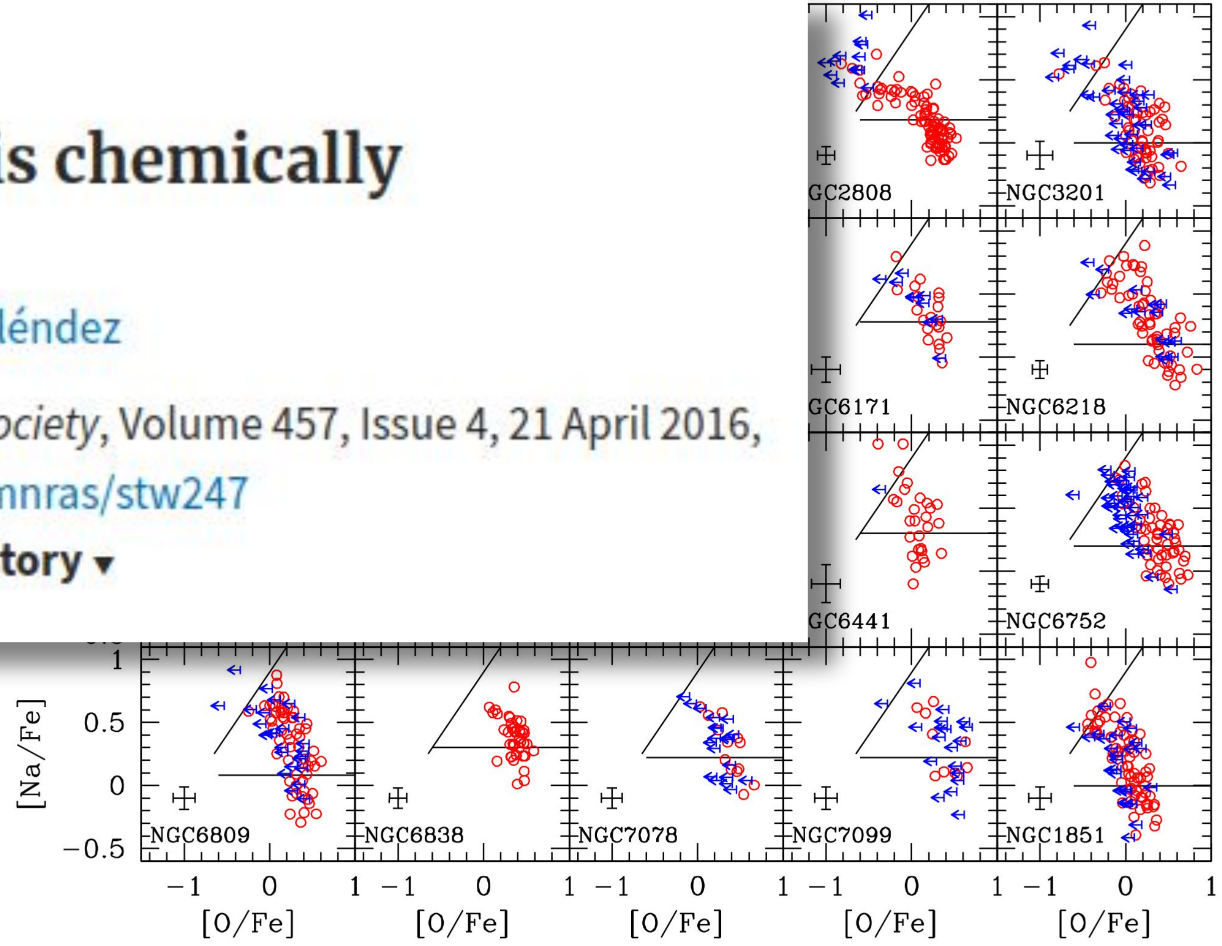
JOURNAL ARTICLE

The Hyades open cluster is chemically inhomogeneous FREE

F. Liu, D. Yong, M. Asplund, I. Ramírez, J. Meléndez

Monthly Notices of the Royal Astronomical Society, Volume 457, Issue 4, 21 April 2016, Pages 3934–3948, https://doi.org/10.1093/mnras/stw247

Published: 29 January 2016 **Article history ▾**



Some applications: Galactic archaeology

Large scale surveys also give hints on the formation of large structures in the Milky Way.

For instance, two substructures of the Milky Way disc have different chemical profiles.

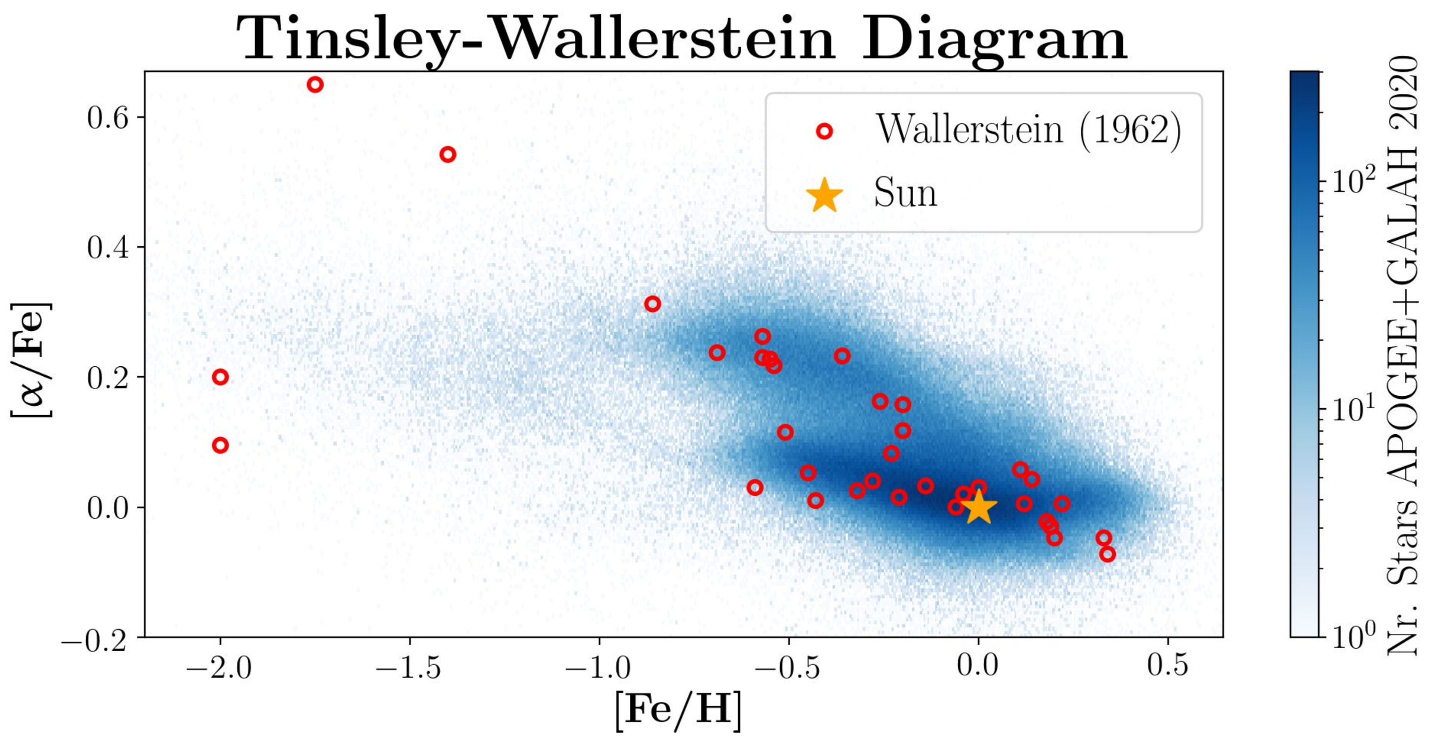
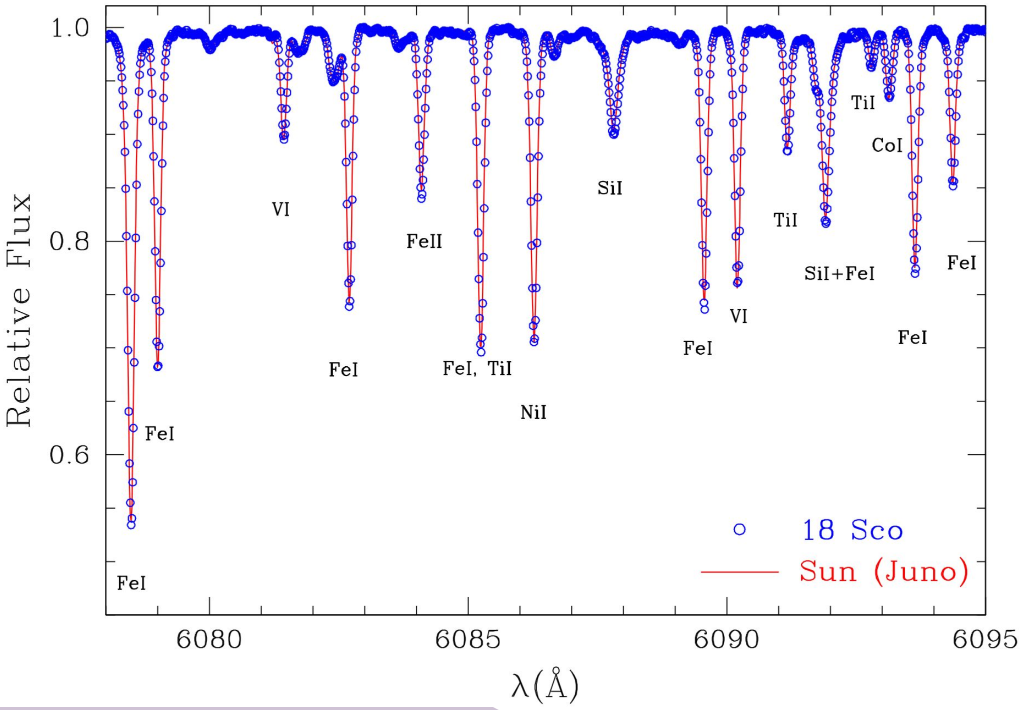


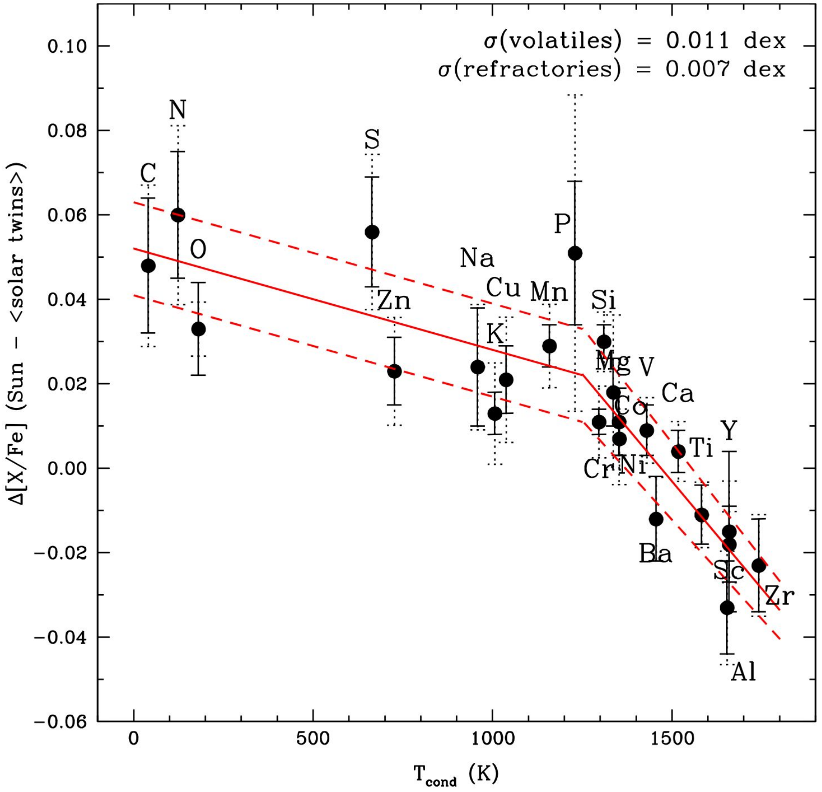
Image: GingerLemon@Wikipedia

Some applications: the origin of the Sun

The search and study of solar twins can shed light on the origin of the Sun in the Galaxy, as well as how it differs (or not) from the average star, and a better understanding of Sun-like exoplanet hosts.

Melendez+ 2014 ApJ 791 14





Melendez+ 2009 ApJ 704 66