



BETWEEN THE LINES
A Stellar Spectroscopy Workshop

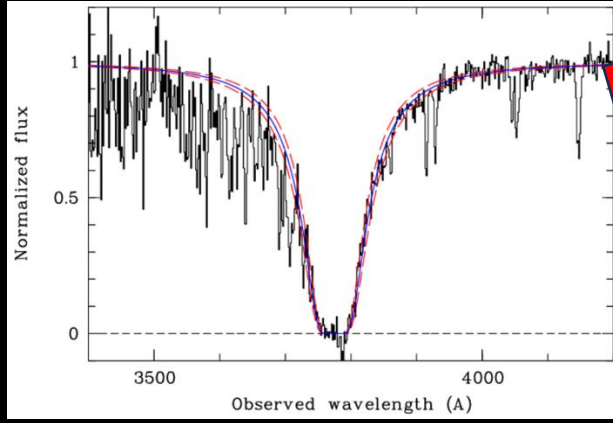
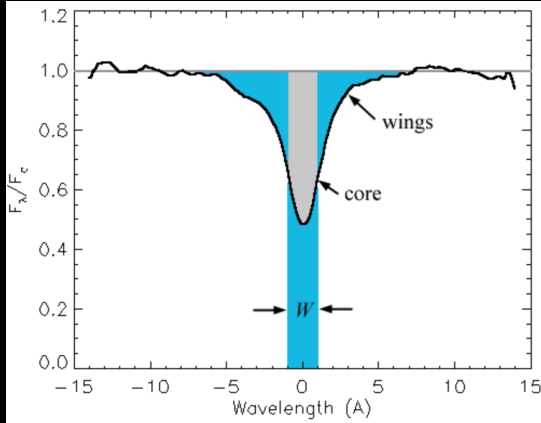
<https://www.astronomersdoitinthedark.com/index.php?c=152&p=427>

Techniques for stellar parameter determination

Chris Sneden
Department of Astronomy & McDonald Observatory
University of Texas at Austin
csneden

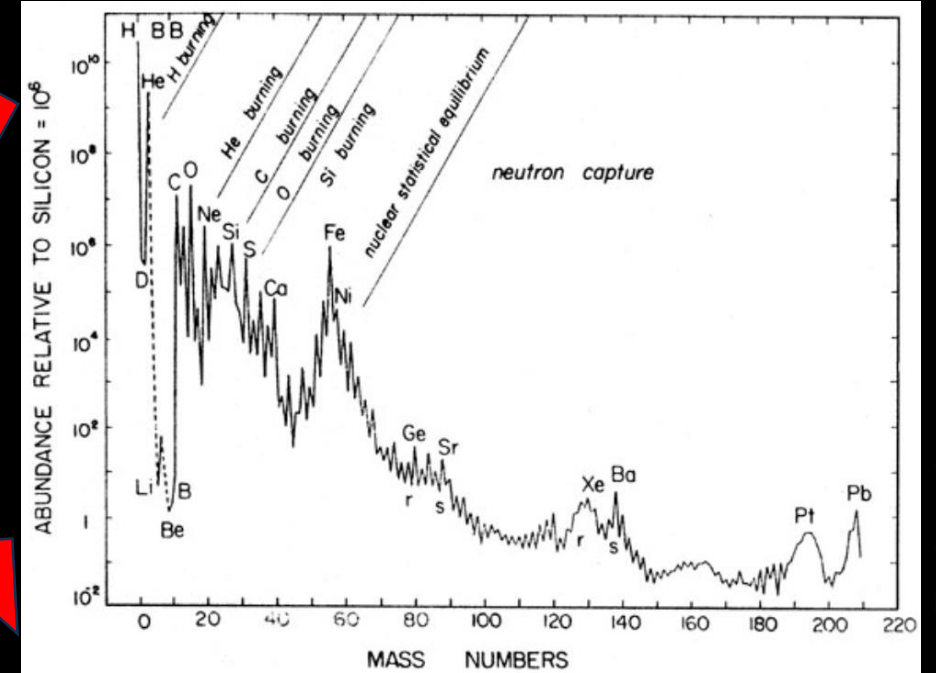
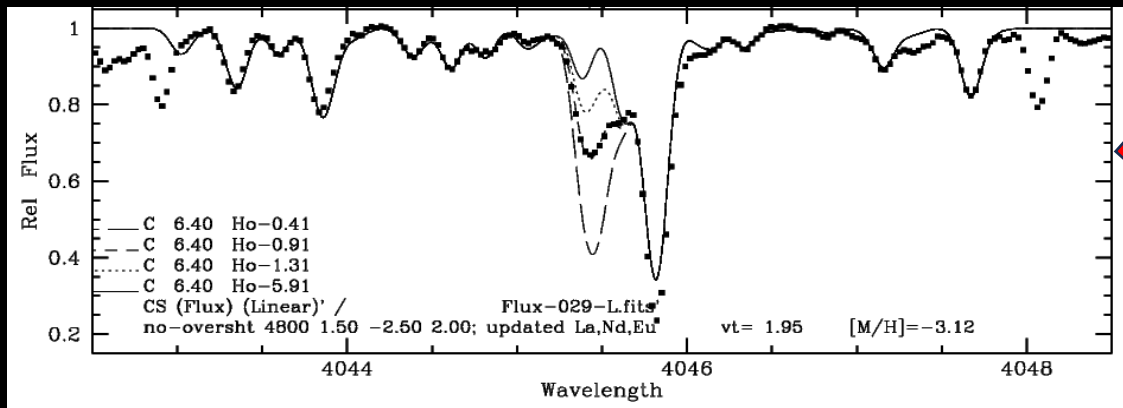
the overall goal is to extract reliable abundances from observed spectra

either by measuring the “equivalent width”(EW)
absorption of single isolated absorption lines

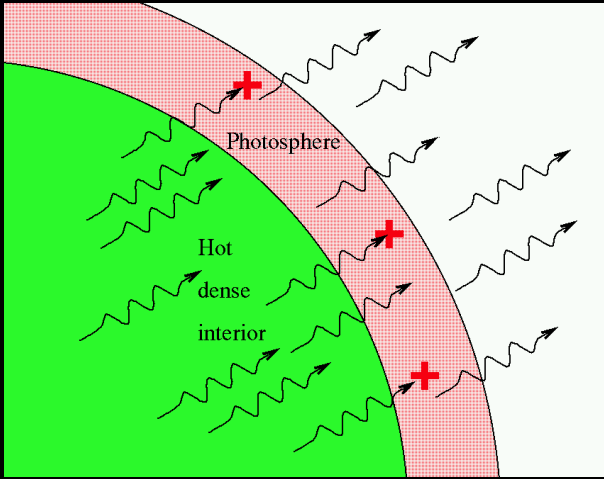


Rau et al. (2010)

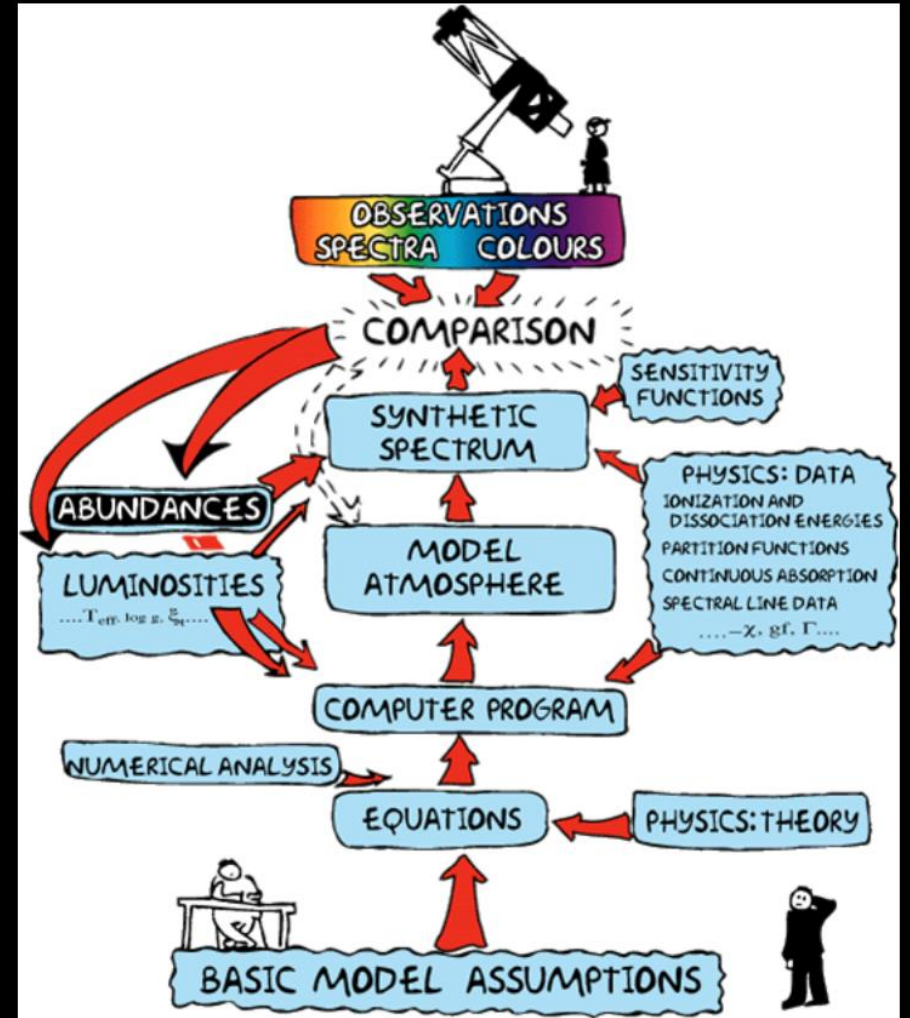
or by extracting the contributions of individual
elements in complex blended spectra



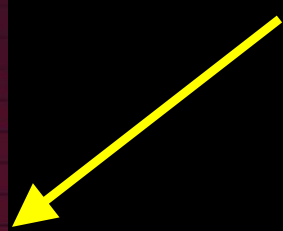
which can be
interpreted in terms of
stellar nucleosynthesis



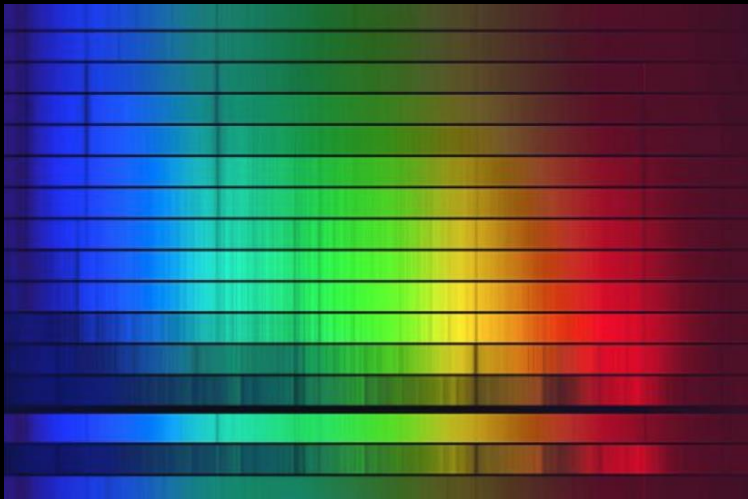
how do we execute this ...



to approximate this ...



"good enough"??



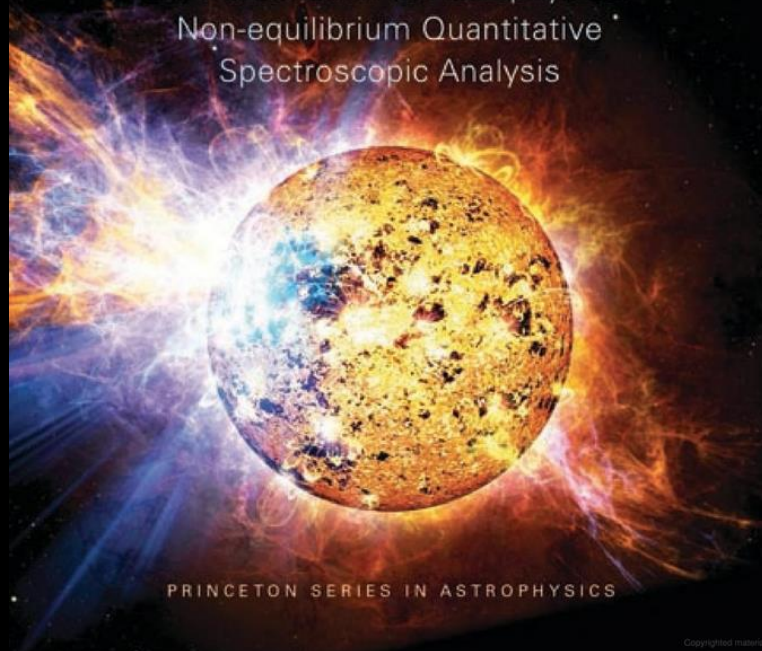
comprehensive texts

Thorough, detailed, mathematical from a theoretical modeling point of view

Ivan Hubeny & Dimitri Mihalas

THEORY OF STELLAR ATMOSPHERES

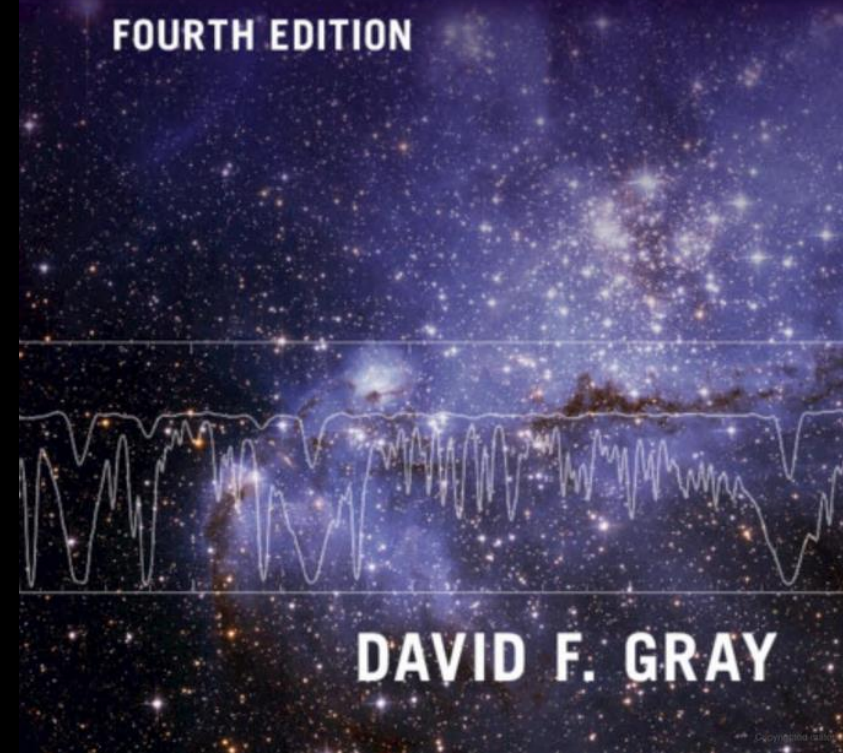
An Introduction to Astrophysical
Non-equilibrium Quantitative
Spectroscopic Analysis



pragmatic, easily applicable, from an observer's point of view; excellent figures

The Observation and Analysis of STELLAR PHOTOSPHERES

FOURTH EDITION



minimum requirements for a spectroscopic analysis

- line analysis code for EWs or synthetic spectra
- stellar model atmosphere (τ , T , P_g , P_e , (turbulent velocities, ...))
- line list (λ , species, χ_{lower} or EP_{lower} , gf , (damping, EW, ...))
- observed spectrum for EW measurements or syntheses
 - my discussion of course will be based on my own code MOOG (Snedden 1973)
 - MOOG has its particular assets and liabilities
 - but so do all line analysis codes
 - your job is to first understand the peculiarities of the code that you adopt/write
 - and then to stay in command of what you do
 - it is a poor user who blames the code! If a code has unhappy limits, find another code

NOTATION

- $[X/Y] = \log_{10}(N_X/N_Y)_{\text{star}} - \log_{10}(N_X/N_Y)_{\text{Sun}}$
where N is an elemental number density;
These are abundances relative to the Sun
- $A \equiv \log \epsilon(X) = \log_{10}(N_X/N_H) + 12.0$ (spectroscopy)
these are “absolute” without reference to the Sun
- $\log N(X) = \log_{10}(N_X/N_{\text{Si}}) + 6.0$ (meteorites)
- Metallicity \rightarrow $[\text{Fe}/\text{H}] \rightarrow$ sometimes labeled $[\text{M}/\text{H}]$
- Most metal-rich? $[\text{Fe}/\text{H}] \sim +0.5$ (proven)
- Most metal-poor? $[\text{Fe}/\text{H}] < \sim -8$ (probably not the limit)
- Metallicity labels (watch out! these vary greatly from paper to paper)
 - metal-poor: $[\text{Fe}/\text{H}] \leq -2$
 - very metal-poor: $[\text{Fe}/\text{H}] \leq -2$
 - extremely metal-poor: $[\text{Fe}/\text{H}] \leq -3$
 - NATURE paper metal-poor: $[\text{Fe}/\text{H}] \leq -6$ or -7 or ...

WATCH OUT! [X/Y] quantities have ASSUMPTIONS

This is the only careful treatment that has been published

THE ASTRONOMICAL JOURNAL, 164:256 (12pp), 2022 December




<https://doi.org/10.3847/1538-3881/ac9bfa>

© 2022. The Author(s). Published by the American Astronomical Society.

OPEN ACCESS



A Concise Treatise on Converting Stellar Mass Fractions to Abundances to Molar Ratios

Natalie R. Hinkel¹ , Patrick A. Young² , and Caleb H. Wheeler III³ 

¹ Southwest Research Institute, 6220 Culebra Rd, San Antonio, TX 78238, USA; natalie.hinkel@gmail.com

² School of Earth and Space Exploration, Arizona State University, Tempe, AZ 85287, USA

³ Simons Foundation, Center for Computational Astrophysics, 162 5th Ave, New York, NY 10010, USA

Received 2022 August 8; revised 2022 October 17; accepted 2022 October 18; published 2022 November 18

Abstract

Understanding stellar composition is fundamental not only to our comprehension of the Galaxy, especially chemical evolution, but it can also shed light on the interior structure and mineralogy of exoplanets, which are formed from the same material as their host stars. Unfortunately, the underlying mathematics describing stellar mass fractions and stellar elemental abundances is difficult to parse, is fragmented across the literature, and contains vexing omissions that makes any calculation far from trivial, especially for nonexperts. In this treatise, we present a clear mathematical formalism and clarification of inherent assumptions and normalizations within stellar composition measurements, which facilitates the conversion from stellar mass fractions to elemental abundances to molar ratios, including error propagation. We also provide an example case study of HIP 544 to further illustrate the provided equations. Given the important chemical association between stars, as well as the interdisciplinary relationship between stars and their planets, it is vital that stellar mass fractions and abundance data be more transparent and accessible to people within different subfields and scientific disciplines.

stellar line formation

there are many good sources, especially in texts by Hubeny & Milahas (2014), Gray (2021), LeBlanc (2010), Crivellari et al. (2012)

all discuss the pathways from: $\mu \frac{dI_\nu}{d\tau_\nu} = I_\nu - S_\nu.$

to:

$$I_\nu^+(0, \mu) = \int_0^\infty S_\nu(\tau_\nu) e^{-\tau_\nu/\mu} d\tau_\nu/\mu$$
$$\mathcal{F}_\nu^+(0) = 2\pi \int_0^\infty S_\nu(\tau_\nu) E_2(\tau_\nu) d\tau_\nu$$

using quantities that you might be able to measure:

$$[\alpha_\nu^l]_{\text{LTE}} = \frac{\pi e^2}{m_e c} n_l^{\text{LTE}} f_{lu} \varphi(\nu - \nu_0) [1 - e^{-h\nu_0/kT}]$$

See DETAILS: slides 1-8

line analysis codes: a partial list of popular ones

Line analysis code:

- Kurucz WIDTH: <http://kurucz.harvard.edu/programs/WIDTH>
- Kurucz SYNTHE: <http://kurucz.harvard.edu/programs/SYNTHE>
- Hubeny TLUSTY: <http://nova.astro.umd.edu>
- Plez TURBOSPECTRUM: <http://www.pages-perso-bertrand-plez.univ-montp2.fr>
- Masseron BACCHUS: <https://ui.adsabs.harvard.edu/abs/2016ascl.soft05004M/abstract>
- Sneden MOOG: <http://www.as.utexas.edu/~chris/moog.html>
- Wheeler KORG: <https://github.com/ajwheeler/Korg.jl>
- Other personal programs not generally available to public

WHICH CODE TO USE? **WHO CARES!** KEEP FOCUSED ON WHAT YOU WANT AND BE HONEST ABOUT WHAT YOU REPORT

These codes all have tradeoffs between convenience, speed, and sophistication of basic physics:

- Allowance for scattering in continuum opacities & source functions
- LTE or “better”
- How much atomic/molecular information comes with code
- Plane-parallel or spherical geometry
- User friendliness
- Common-sense outputs that help user avoid stupidities

MOOG was written to try to mimic Edmonds (1969)


J. Quant. Spectrosc. Radiat. Transfer. Vol. 9, pp. 1427–1446.

RADIATIVE TRANSFER WITHIN A STELLAR ABSORPTION LINE. THE CONTRIBUTION CURVES OF FINE-ANALYSIS METHODS

FRANK N. EDMONDS, JR.

Department of Astronomy, The University of Texas at Austin, Austin, Texas 78712

local thermodynamic equilibrium (LTE), plain-parallel geometry, no spots, magnetic fields, simple microturbulence description, ...

Don't be a coward! It is simple FORTRAN coding meant to be available for modification by users, so look "under the hood" to find where these equations live: 

This is a good paper to understand "contribution curves"

$$D(\Delta\lambda) = \int_{-\infty}^{\infty} C_D(\Delta\lambda, x) dx. \quad (13)$$

When pure absorption or equation (4) is assumed, equations (1)–(3) and (5)–(7) give

$$C_R(\Delta\lambda, x) = \frac{2\tau(x)}{0.4343 F_\lambda(0)} \frac{\kappa_\lambda(x)}{\kappa(x)} B_\lambda(T[x]) \left\{ 1 + \frac{\kappa_v(x)}{\kappa_\lambda(x)} \right\} E_2(\tau_\lambda[x] + \tau_v[x]), \quad (14)$$

where $\kappa(x)$ is the opacity associated with the reference optical depth;

$$\begin{aligned} C_D(\Delta\lambda, x) &= \frac{2\tau(x)}{0.4343 F_\lambda(0)} \frac{\kappa_\lambda(x)}{\kappa(x)} B_\lambda(T[x]) \\ &\times \left[E_2(\tau_\lambda[x]) - \left\{ 1 + \frac{\kappa_v(x)}{\kappa_\lambda(x)} \right\} E_2(\tau_\lambda[x] + \tau_v[x]) \right] \\ &= \frac{C_\lambda(x)}{F_\lambda(0)} - C_R(\Delta\lambda, x) \end{aligned} \quad (15)$$

for the F-S method, where $C_\lambda(x)$ is the continuum contribution curve at the wavelength of the line;

$$C_D(\Delta\lambda, x) = \frac{2}{F_\lambda(0)} \frac{dB_\lambda(T[x])}{dx} [E_3(\tau_\lambda[x]) - E_3(\tau_\lambda[x] + \tau_v[x])] \quad (16)$$

for the P-G method; and

$$C_D(\Delta\lambda, x) = \frac{2\tau(x)}{0.4343 F_\lambda(0)} \frac{\kappa_v(x)}{\kappa(x)} \int_x^\infty \frac{dB_\lambda(T[x'])}{dx'} E_2(\tau_\lambda[x'] + \tau_v[x]) dx' \quad (17)$$

for the W-S method.

In these equations,

$$\tau_v(x) = \frac{1}{0.4343} \int_{-\infty}^x \tau(x') \frac{\kappa_v(x')}{\kappa(x')} dx', \quad (18)$$

$$\kappa_v(x) = N(x) \frac{\pi e^2}{mc} \frac{f}{\Delta\nu_D(x)} [1 - e^{-hc/\lambda kT(x)}] U(a[x], v[x]), \quad (19)$$

$$\Delta\nu_D(x) = \frac{1}{\lambda} \left[\frac{2kT(x)}{M} + \xi^2(x) \right]^{1/2}, \quad (20)$$

$$v(x) = \Delta\lambda \left/ \frac{\lambda}{c} \left[\frac{2kT(x)}{M} + \xi^2(x) \right]^{1/2} \right., \quad (21)$$

and

$$a(x) = \frac{\Gamma_n(x) + \Gamma_s(x) + \Gamma_w(x)}{2\pi\lambda^{-1} \left\{ [2kT(x)/M] + \xi^2(x) \right\}^{1/2}}. \quad (22)$$

Requirement for chemical composition analyses:

A grid of model stellar photospheres:

- Kurucz ATLAS: <http://kurucz.harvard.edu/grids.html>
- Gustafsson MARCS: <http://marcs.astro.uu.se>
- Hauschildt PHOENIX: <https://www.physik.uni-hamburg.de/en/hs/group---hauschildt.html>

Typical model atmosphere output: Kurucz ATLAS

```
TEFF 3500. GRAVITY 0.00000 LTE
TITLE SDSC GRID [+0.0] VTURB 0.0 KM/S L/H 1.25
OPACITY IFOP 1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 0 0 0 0
CONVECTION ON 1.25 TURBULENCE OFF 0.00 0.00 0.00 0.00
ABUNDANCE SCALE 1.00000 ABUNDANCE CHANGE 1 0.91100 2 0.08900
READ DECK6 72 RHOX,T,P,XNE,ABROSS,ACCRAD,VTURB
1.92081317E-02 2162.9 1.918E-02 3.953E+05 6.942E-06 1.304E-03 0.000E+00
2.55242080E-02 2185.4 2.549E-02 5.259E+05 7.141E-06 1.219E-03 0.000E+00
3.37376143E-02 2204.8 3.370E-02 6.928E+05 7.301E-06 1.118E-03 0.000E+00
4.44603299E-02 2223.3 4.441E-02 9.084E+05 7.451E-06 1.024E-03 0.000E+00
5.84449198E-02 2243.2 5.838E-02 1.191E+06 7.631E-06 9.457E-04 0.000E+00
7.66163984E-02 2264.8 7.653E-02 1.561E+06 7.847E-06 8.769E-04 0.000E+00
1.00122149E-01 2288.2 1.000E-01 2.047E+06 8.106E-06 8.122E-04 0.000E+00
1.30562972E-01 2308.0 1.304E-01 2.662E+06 8.320E-06 7.329E-04 0.000E+00
1.70060206E-01 2328.6 1.699E-01 3.462E+06 8.564E-06 6.653E-04 0.000E+00
...
```

construction of model atmospheres is a long subject for textbooks

$RHOX = \rho x$
where x is physical depth

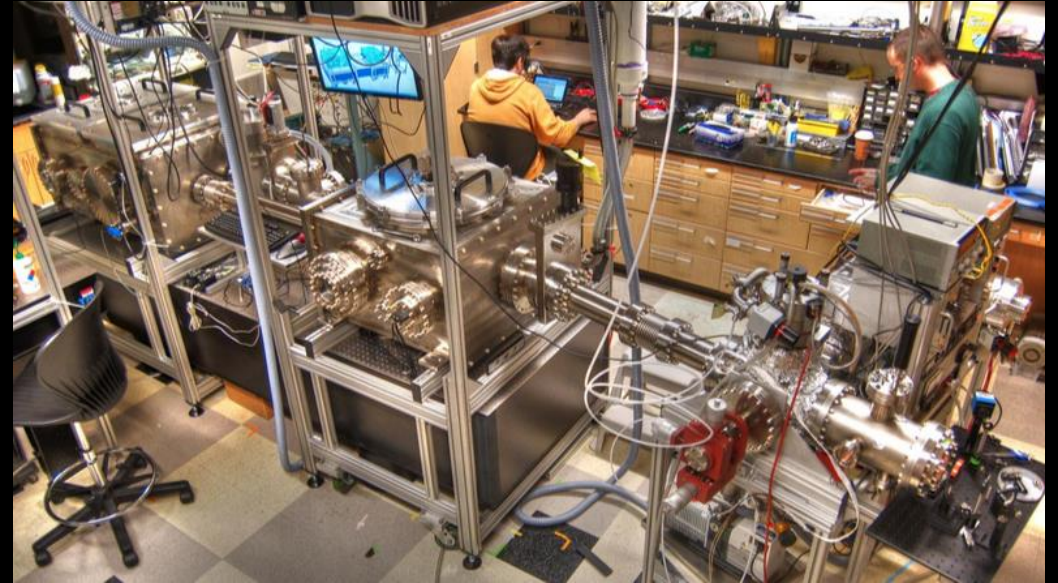
$$d\tau = \kappa \rho dx$$

ABROSS = Rosselan mean opacity

See DETAILS: slides 9–18

Requirement for chemical composition analyses: input line lists

- input atomic *and* molecular line lists
- at a fundamental level, abundance $\propto Nf$,
where “N” is number density of absorbers and
“f” is the oscillator strength
- if oscillator strength “f” is wrong, every
other sophistication in your analysis is
utterly useless
- recent lab improvements make neglect
of this issue a serious analysis flaw

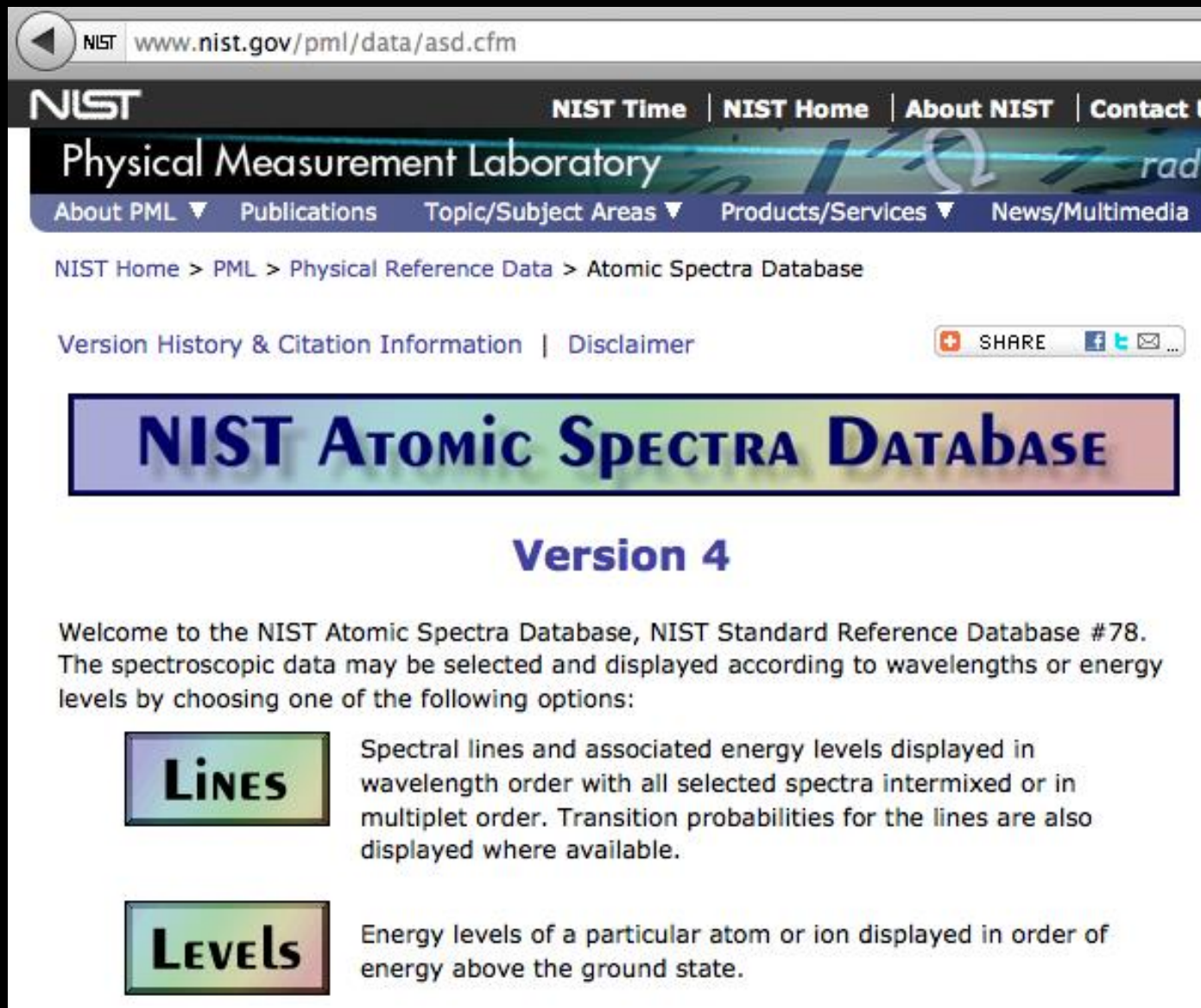


<https://physics.osu.edu/research/atomic-molecular-and-optical-physics/agostini-dimauro-atomic-physics-research-group/lab>

See DETAILS: slides 19–33

I am very interested (obsessed) with this issue

A good summary site for lab atomic data



www.nist.gov/pml/data/asd.cfm

NIST Time | NIST Home | About NIST | Contact Us

Physical Measurement Laboratory

About PML | Publications | Topic/Subject Areas | Products/Services | News/Multimedia

NIST Home > PML > Physical Reference Data > Atomic Spectra Database

Version History & Citation Information | Disclaimer

SHARE

NIST ATOMIC SPECTRA DATABASE

Version 4

Welcome to the NIST Atomic Spectra Database, NIST Standard Reference Database #78. The spectroscopic data may be selected and displayed according to wavelengths or energy levels by choosing one of the following options:

LINES Spectral lines and associated energy levels displayed in wavelength order with all selected spectra intermixed or in multiplet order. Transition probabilities for the lines are also displayed where available.

LEVELS Energy levels of a particular atom or ion displayed in order of energy above the ground state.

Warning: the transition probabilities at NIST are “curated”

this means that they have been often renormalized in individual NIST papers

NIST ASD Team

Principal Developers (Currently Active):

Alexander Kramida, Yuri Ralchenko, and Joseph Reader

Data Compilers (Currently Active):

Alexander Kramida, Edward B. Saloman

Database Developers (Currently Active):

Alexander Kramida, Yuri Ralchenko, and Karen Olsen

NIST entries for Fe I near 4045Å: 6 lines

Observed Wavelength Air (Å)	Ritz Wavelength Air (Å)	Rel. Int. (?)	A_{ki} (s ⁻¹)	$\log(g_i f_{ik})$	Acc.	E_i (eV)	E_k (eV)
	4 043.88486	m				2.7275443	- 5.7926458
4 043.8964	4 043.89713	2690	8.69e+06	-0.826	D+	3.2409689	- 6.3060611
4 043.9767	4 043.97712	660				3.2409689	- 6.3060005
4 044.4906	4 044.4920	166				4.1033735	- 7.1680148
4 044.5444	4 044.5449	398				3.2671124	- 6.3317137
4 044.6089	4 044.60883	6800	8.17e+06	-1.221	B	2.8315910	- 5.8961438
4 045.1116	4 045.1122	510				4.2604530	- 7.3246244
4 045.5936	4 045.59336	3470	7.39e+06	-0.896	C	3.2111892	- 6.2749962
4 045.8122	4 045.81193	1000000	8.62e+07	0.280	A	1.4848643	- 4.5485058
4 046.0620	4 046.06181	1620	6.85e+06	-1.297	C+	3.2657059	- 6.3291582
4 047.3037	4 047.3025	288	2.15e+05	-2.800	C	2.2786045	- 5.3411178

Acc. = their estimated accuracies for lab values; the way of "C" and worse

But line lists for spectrum syntheses has 30 Fe I lines;
they often come from semi-empirical line databases

Robert L. Kurucz

**Harvard-Smithsonian Center for Astrophysics
60 Garden Street
Cambridge, MA 02138, USA**

Telephone 617-495-7429

Fax 617-495-7049

Email RKURUCZ@CFA.HARVARD.EDU

This is a combined Web/outgoing-FTP site, KURUCZ.HARVARD.EDU or CFAKU5.CFA.HARVARD.EDU. It provides up-to-date public access to my data and programs. These are the same programs and files that I use in my research. Many bugs and problems have been corrected but there are still many more errors remaining to be found. Programs and data that I would not use myself because they are still under development are not on this computer. Many of the files are large and are also available on CDs or DVDs, and I am willing to write DVDs on demand. Some files taken from Kurucz CD-ROMs 1-26 are given for historical checks although many have been replaced by new versions. Binary versions will eventually be replaced by (much larger) ASCII versions. I am willing to rewrite them in ASCII on demand. Neither the programs nor data are "black boxes". You should not be using them if you do not have some understanding of the physics and of the programming in the source code.

the Kurucz line database has all sorts of transition data

Table of Contents

1. [News](#)
2. [Vita and Bibliography](#)
3. [Papers](#)
4. [Atoms](#)
5. [Molecules](#)
6. [Linelist](#)s
7. [Opacities](#)
8. [Grids of model atmospheres](#)
9. [Sun](#)
10. [Stars](#)
11. [Programs](#)
12. [CD-ROMs](#)
13. [Temporary files](#)

There are more data than anonymous FTP can digest. Instead there is a user account with username GUEST and password CFAGUEST that can be accessed by FTP and TELNET. Simple OpenVMS commands like "TYPE file", "SEARCH file string", and "HELP" will work. The directories [NEWS], [VITABIB], [PAPERS], [ATOMS], [MOLECULES], [LINELISTS], [PROGRAMS], and [CDROMS] are on disk KU5E. [OPACITIES],[GRIDS] ,[SUN], and [STARS], are on KU5D, [TEMP] is on KU5C. and other directories and disks may be added. FTP does not execute the login so the logical names are not defined, but TELNET does. To go to a new directory "SET DEFAULT [name]". Case does not matter.

Kurucz/Linelist

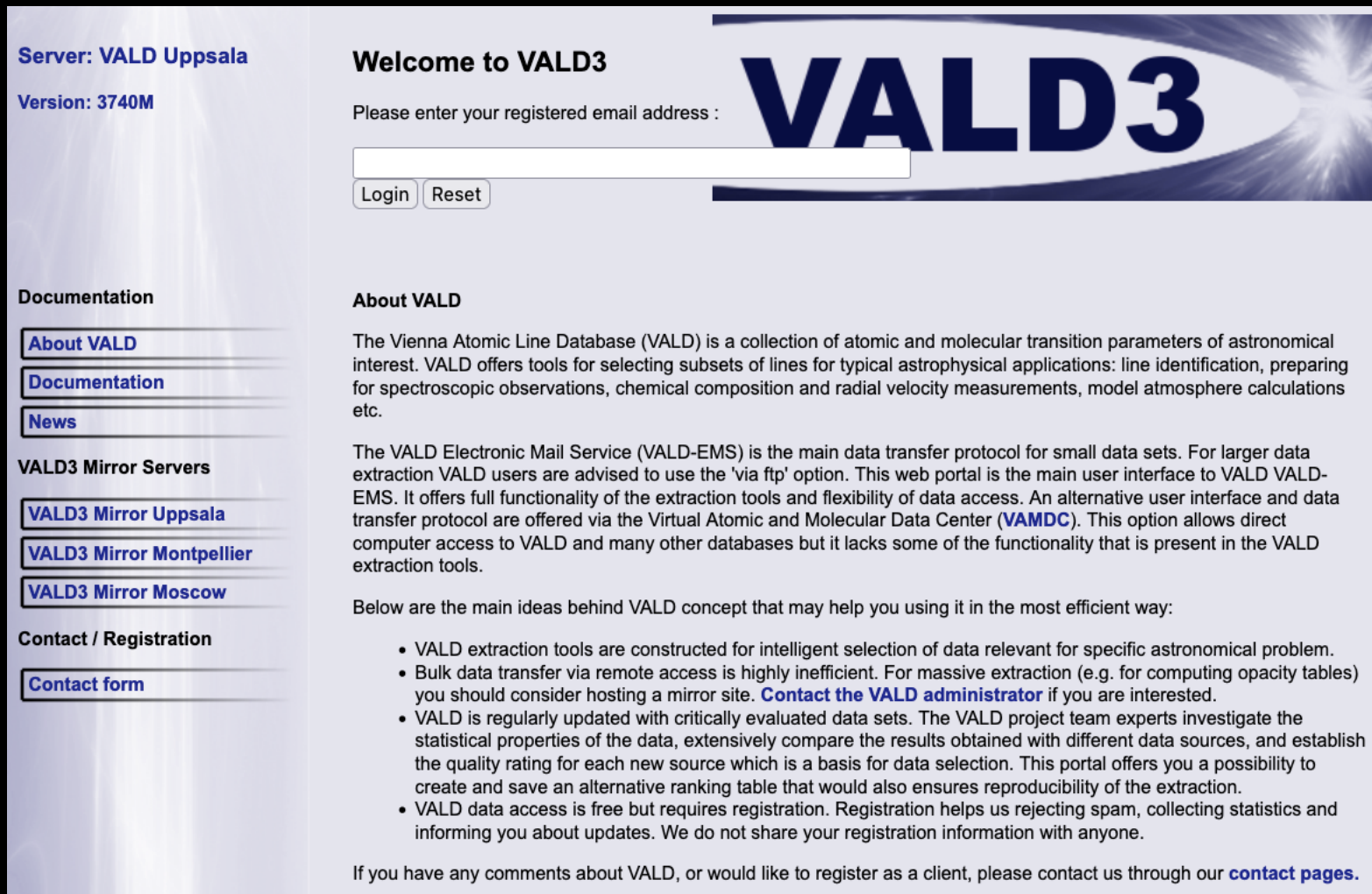
*** See /ATOMS or /MOLECULES for new calculations (now underway).

At the time these gf files were made all the laboratory data in the literature were considered and laboratory data were substituted for computed data when they appeared to be better than the computed. All of the files, atomic and molecular, need to be updated.

- [GF10:](#) wavelength-sorted atomic lines in 10 nm intervals
- [GF100:](#) wavelength-sorted atomic lines in 100 nm intervals
- [GFALL:](#) wavelength-sorted atomic lines in one file per spectrum and also all merged into one file
- [GFHYPER10:](#) wavelength-sorted atomic lines in 10 nm intervals with hyperfine splitting for levels that have been measured
- [GFHYPER100:](#) wavelength-sorted atomic lines in 100 nm intervals with hyperfine splitting for levels that have been measured
- [GFHYPERALL:](#) wavelength-sorted atomic lines in one file per spectrum with hyperfine splitting for levels that have been measured and also all merged into one file
- [LINES:](#) Sample programs for reading the files. References.
- [LINESCD:](#) binary files from CD-ROMs 1 and 15 that have 58 million atomic and diatomic linss packed 16 bytes per line
- [LINESMOL:](#) wavelength sorted diatomic molecular lines in various large files with extension .ASC . The same data also are given divided into smaller wavelength intervals in files with extension .100 .

<http://kurucz.harvard.edu/>

the dominant “compilation” transition data site



Server: VALD Uppsala
Version: 3740M

Welcome to VALD3

Please enter your registered email address :

Login Reset

Documentation

- About VALD
- Documentation
- News

VALD3 Mirror Servers

- VALD3 Mirror Uppsala
- VALD3 Mirror Montpellier
- VALD3 Mirror Moscow

Contact / Registration

- Contact form

About VALD

The Vienna Atomic Line Database (VALD) is a collection of atomic and molecular transition parameters of astronomical interest. VALD offers tools for selecting subsets of lines for typical astrophysical applications: line identification, preparing for spectroscopic observations, chemical composition and radial velocity measurements, model atmosphere calculations etc.

The VALD Electronic Mail Service (VALD-EMS) is the main data transfer protocol for small data sets. For larger data extraction VALD users are advised to use the 'via ftp' option. This web portal is the main user interface to VALD VALD-EMS. It offers full functionality of the extraction tools and flexibility of data access. An alternative user interface and data transfer protocol are offered via the Virtual Atomic and Molecular Data Center (**VAMDC**). This option allows direct computer access to VALD and many other databases but it lacks some of the functionality that is present in the VALD extraction tools.

Below are the main ideas behind VALD concept that may help you using it in the most efficient way:

- VALD extraction tools are constructed for intelligent selection of data relevant for specific astronomical problem.
- Bulk data transfer via remote access is highly inefficient. For massive extraction (e.g. for computing opacity tables) you should consider hosting a mirror site. **Contact the VALD administrator** if you are interested.
- VALD is regularly updated with critically evaluated data sets. The VALD project team experts investigate the statistical properties of the data, extensively compare the results obtained with different data sources, and establish the quality rating for each new source which is a basis for data selection. This portal offers you a possibility to create and save an alternative ranking table that would also ensure reproducibility of the extraction.
- VALD data access is free but requires registration. Registration helps us rejecting spam, collecting statistics and informing you about updates. We do not share your registration information with anyone.

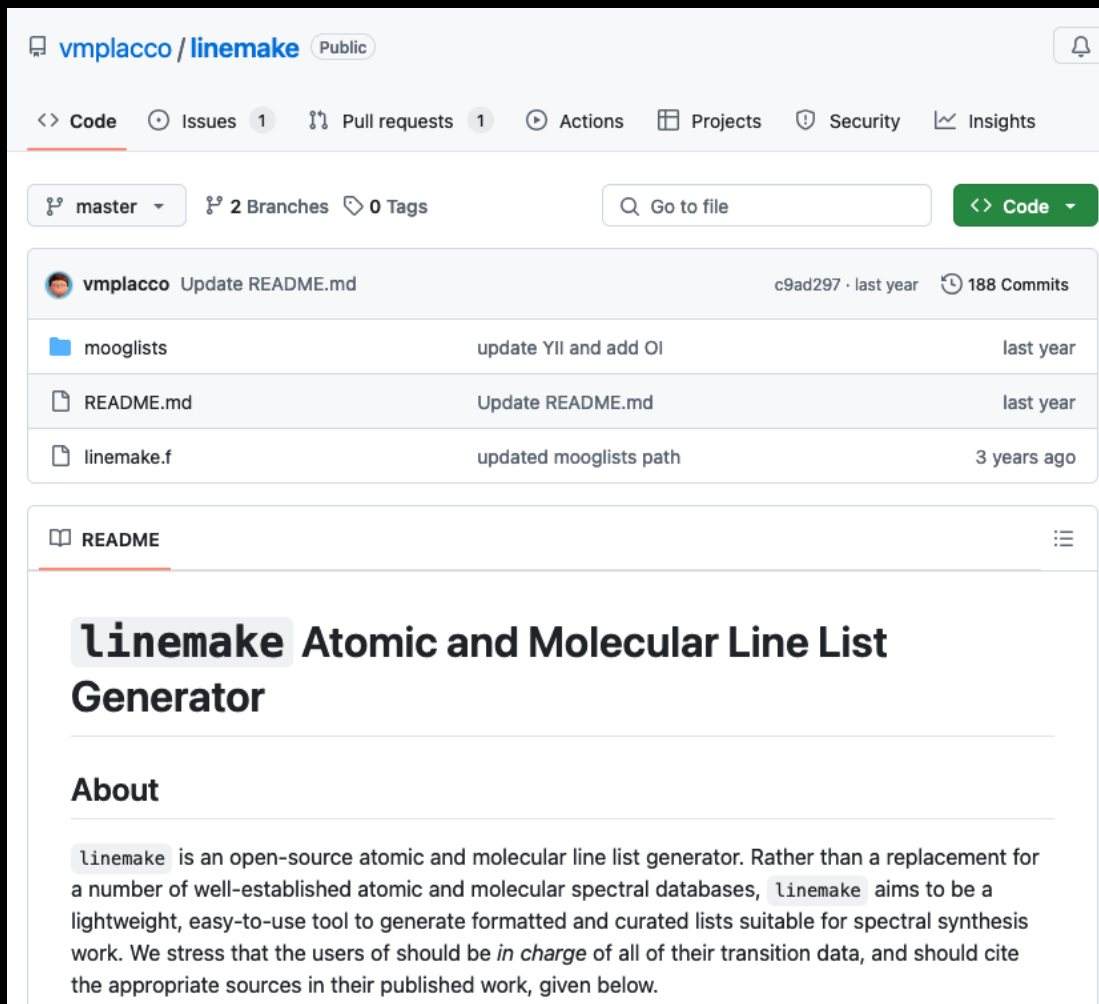
If you have any comments about VALD, or would like to register as a client, please contact us through our [contact pages](#).

- ❖ it is excellent!
- ❖ the biggest concern is casual application by users
- ❖ VALD has all the necessary information to make critical assessment of line lists
- ❖ users need to take the time to understand from where line parameters have been taken
- ❖ users must assess the uniformity of transition data for individual species

<http://vald.astro.uu.se/>

linemake: a simple curated line database

<https://github.com/vmplacco/linemake>



vmplacco / linemake Public

<> Code Issues 1 Pull requests 1 Actions Projects Security Insights

master 2 Branches 0 Tags

Go to file Code

vmplacco Update README.md c9ad297 · last year 188 Commits

mooglists	update YII and add OI	last year
README.md	Update README.md	last year
linemake.f	updated mooglists path	3 years ago

README

linemake Atomic and Molecular Line List Generator

About

linemake is an open-source atomic and molecular line list generator. Rather than a replacement for a number of well-established atomic and molecular spectral databases, linemake aims to be a lightweight, easy-to-use tool to generate formatted and curated lists suitable for spectral synthesis work. We stress that the users of should be *in charge* of all of their transition data, and should cite the appropriate sources in their published work, given below.

- + simple to download compile and execute
- + lab data sources are clearly labeled, and controlled in transparent ways
- + create synthetic spectrum lists or examine files for individual species
- +/- for syntheses, lines without trustworthy lab data are adopted from the Kurucz database
- output line lists are specifically for MOOG input (but one can modify the FORTRAN source code)
- almost always the choice is one lab source per species

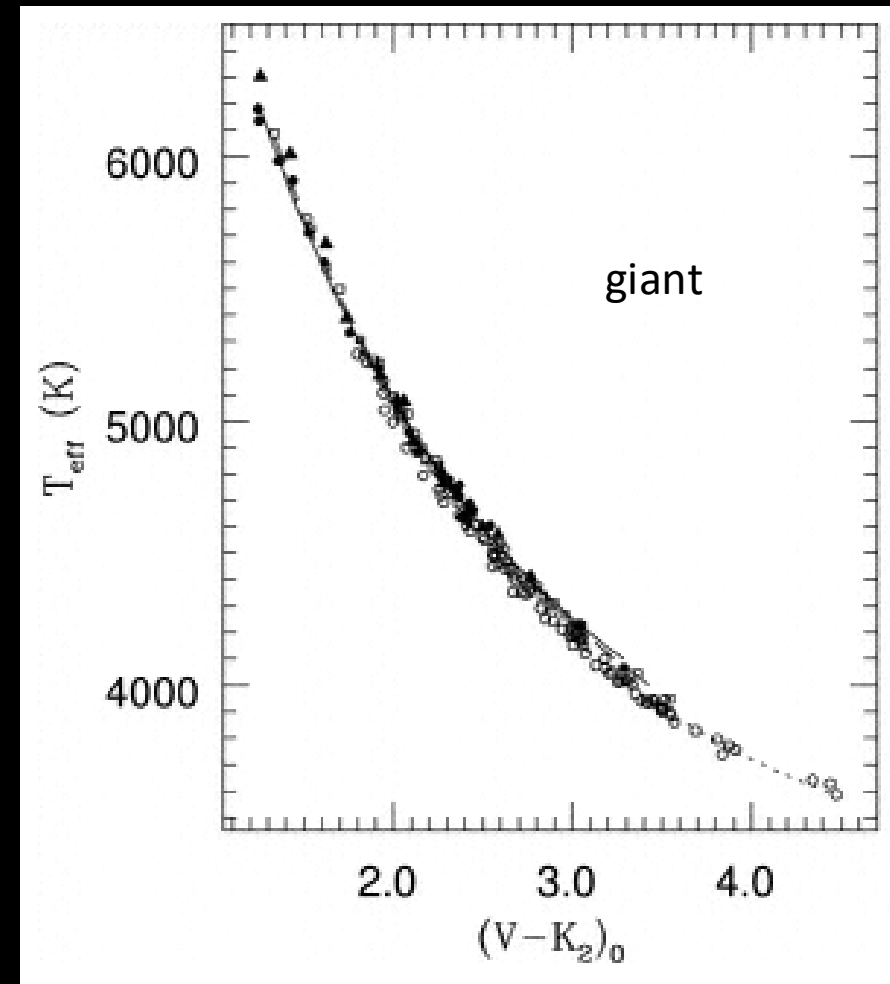
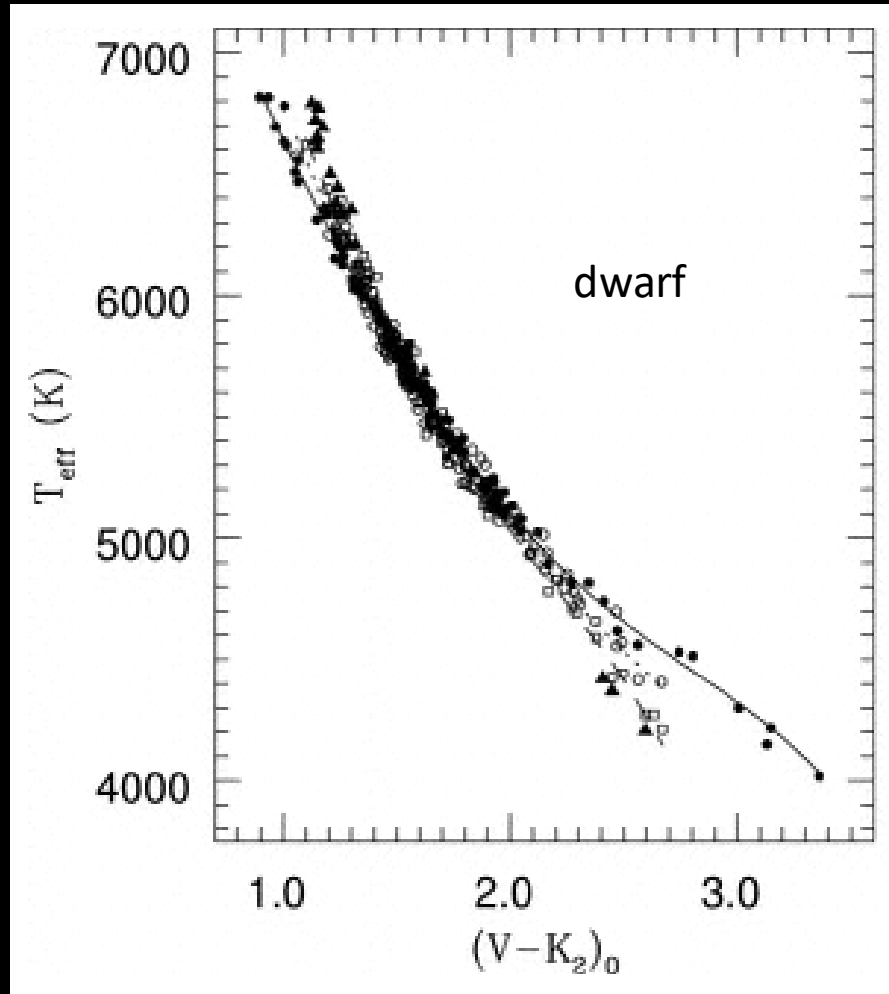
Requirement for chemical composition analyses: “reliable” model atmosphere parameters

Effective temperature T_{eff} : colors and/or spectral line data

- Colors: often B-V, V-I, V-K, J-K
 - Calibrated with “infrared flux method”
 - Gaia colors now contribute heavily to T_{eff}
- spectral lines
 - “traditional” abundance vs excitation energy
 - requires well understood transition probabilities
 - done while deriving abundances in line analysis
 - becoming more common: line depth ratios (calibrated)
 - preselected and calibrated line depths sensitive to T_{eff}
 - somewhat empirical approach

T_{eff} estimated from calibrated photometry

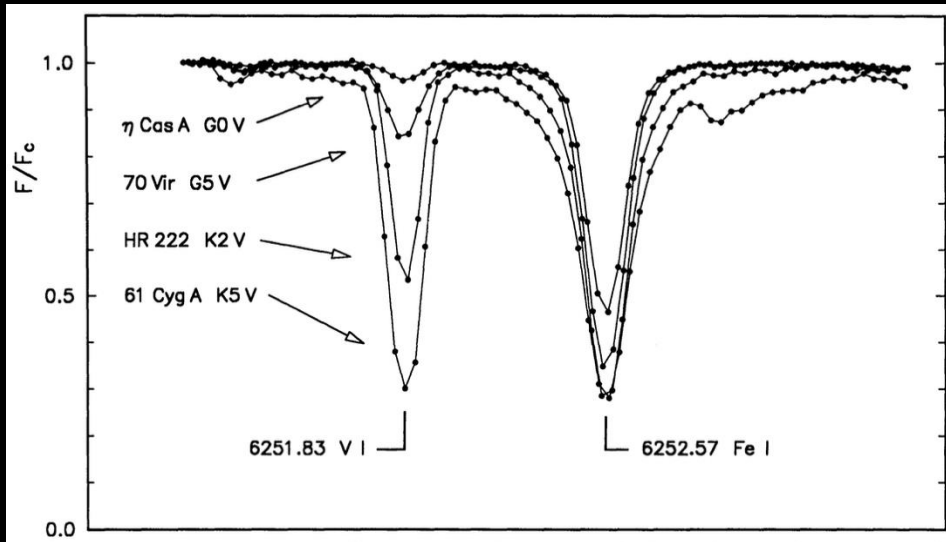
Ramirez & Melendez 2005



works best with long color baseline extending into the near-IR
sensitive to metallicity and dust obscuration effects

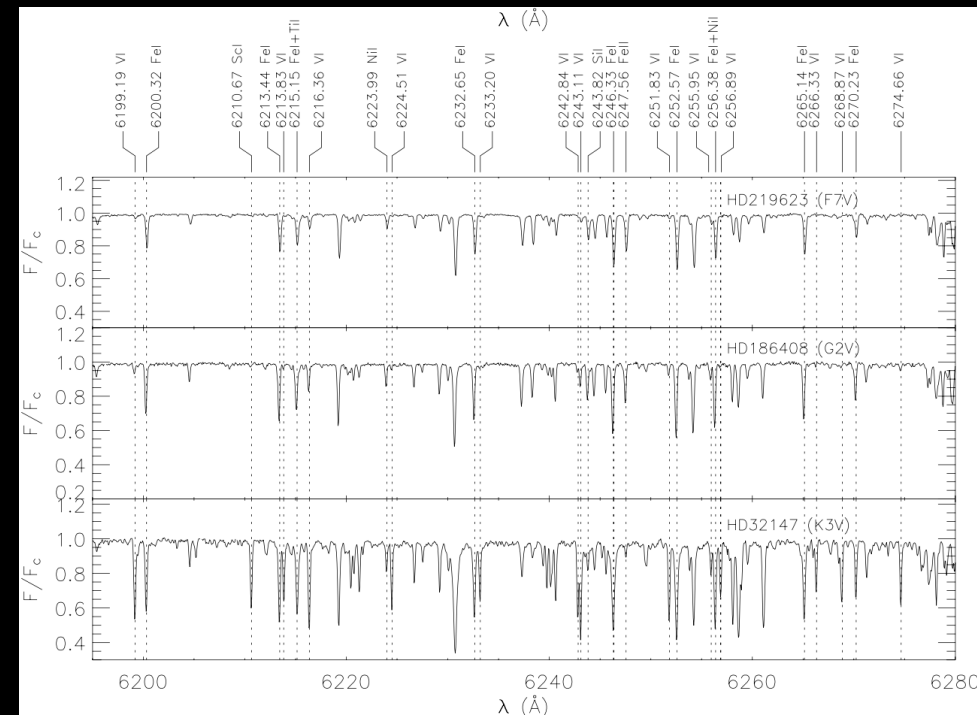
an empirical T_{eff} method: absorption line depth ratios

Gray & Johanson 1991



- this is Boltzmann/Saha at work as T_{eff} decreases from spectral type goes from G0 V to K5 V
- V I 6251Å (E.P.=0.3eV) **grows** as V gets less ionized and as electrons go to lower excitation states
- Fe I 6252.6Å (E.P.=2.4eV) gets less ionized (more slowly than V!) but the higher excitation state loses electrons to lower states, so the absorption line depth changes more slowly
- **NET**: a big change in the line depth ratio – very sensitive T_{eff} probe

- an empirical method; no detailed line parameters needed
- look for wavelength regions with “good” line pairs
- useful T_{eff} limits for a line pair:
 - too warm: one/both lines become too weak
 - too cool: both lines become hopelessly saturated
- between these limits good line ratios are very sensitive
- translation to T_{eff} is a question of calibration

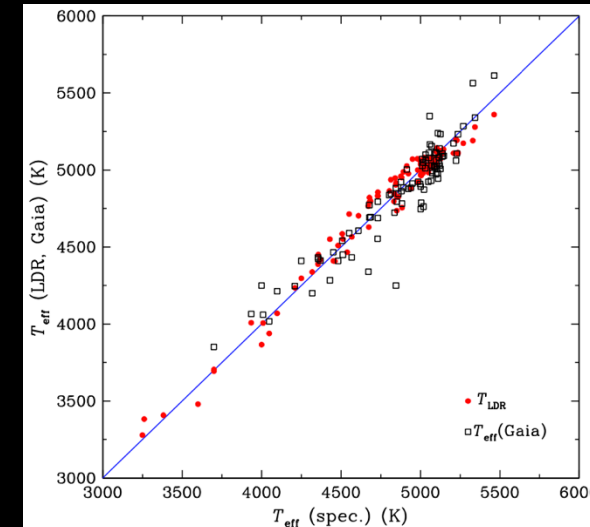
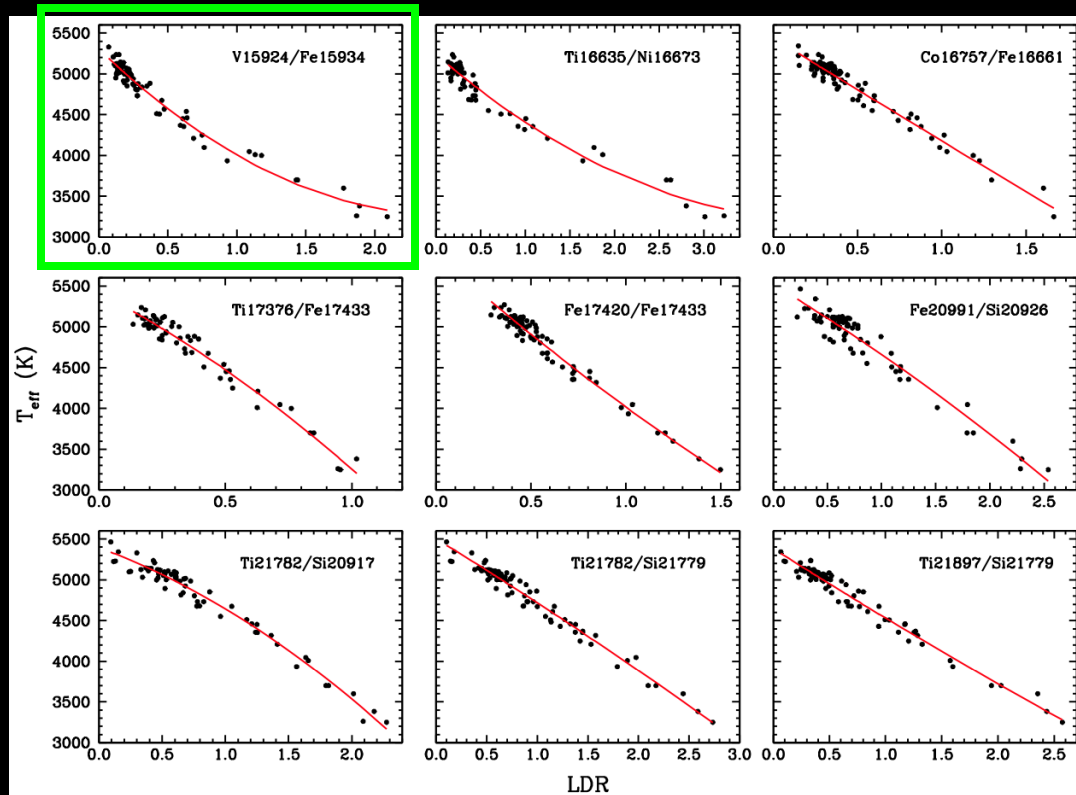
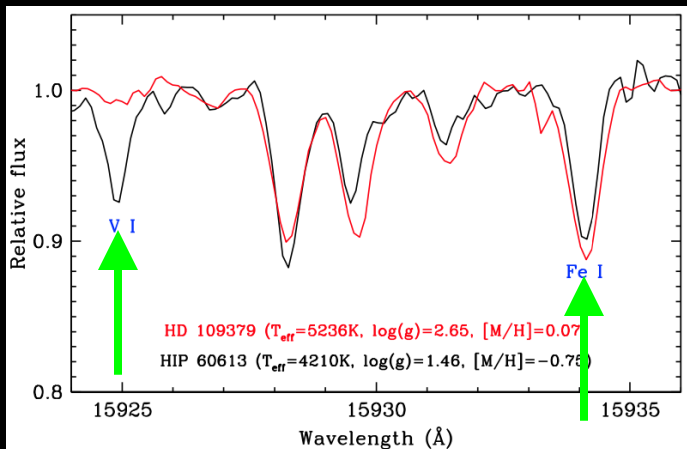


Biazzo 2007

good line depth ratios can be found in any region

In this paper identified 21 useful line ratios

Alas!! this method cannot really be used in the near-IR for gravity-sensitive line pairs ... because there are very few ionized-species lines!



Here is one example: IGRINS spectra of 2 red horizontal branch stars

Work out *without* calculations just why the spectra are similar & different

The listed model parameters, the line data, aided by Boltzmann & Saha, are all you need here

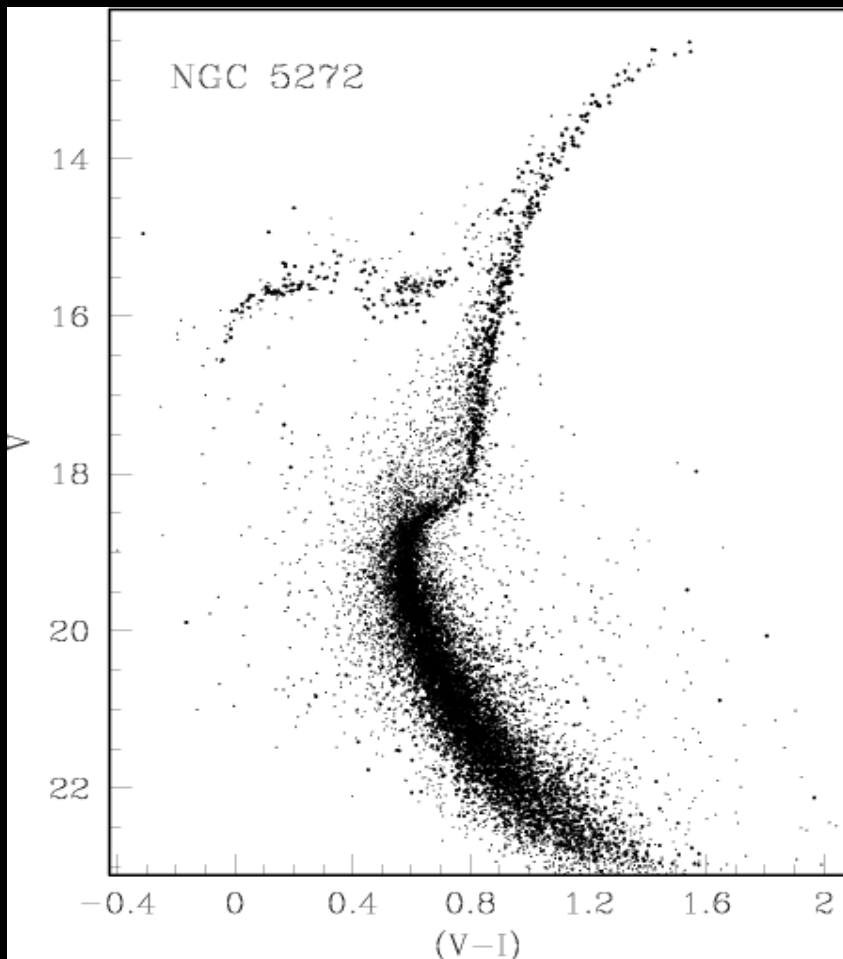
the star-to-star scatter in dominated by the LDR- T_{eff} calibration relationship (usually linear or quadratic)

The big bonus: ability to estimate T_{eff} values in regions too dust-obscured to obtain optical spectra

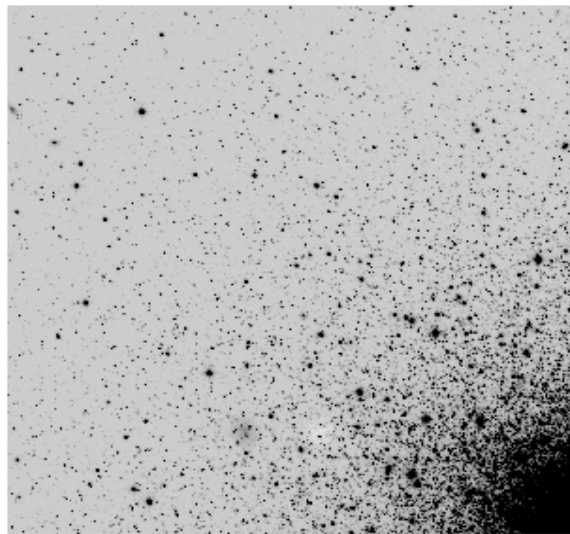
Requirement for chemical composition analyses: “reliable” model atmosphere parameters

Surface gravity $\log g$: cluster, physical, and/or spectral line data

Cluster:



- Easiest method in theory
- Want L/L_{sun}
- Need good reddening $E(B-V)$
- Usually must assume $R_V = A_V/E(B-V)$
- Must derive true distance modulus $V-M_V$



Rosenberg et al. 2000

to be more explicit on physical gravity

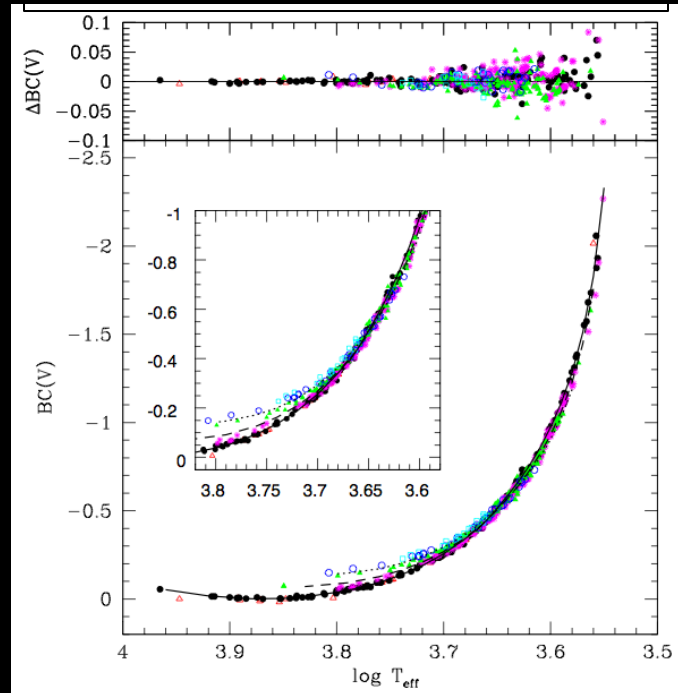
$$\log g_{\star} = 0.4(M_{V\star} + BC - M_{\text{Bol}\odot}) + \log g_{\odot} + 4\log\left(\frac{T_{\text{eff}\star}}{T_{\text{eff}\odot}}\right) + \log\left(\frac{m_{\star}}{m_{\odot}}\right)$$

cluster color-mag;
parallax (Gaia hopefully);
spectral type;
guesses from colors

$$BC = M_{\text{bol}} - M_V$$

from photometry (IR flux method)
or rough estimate (good enough)

assumed (guessed);
Stellar isochrones



IDEALLY: determined previously
BUT OFTEN determined iteratively
at the same time as T_{eff}

Alonso et al 1999

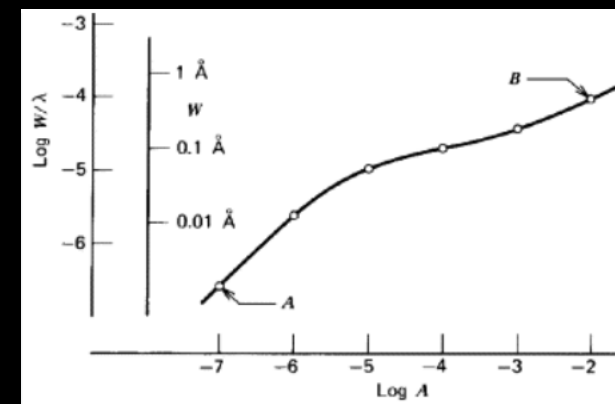
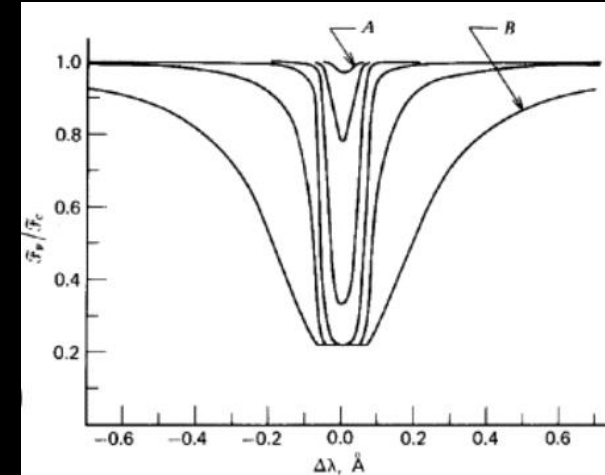
Requirement for chemical composition analyses: what we call “microturbulence”

sources of observed broadening of spectral lines:

- ❑ spectrograph instrumental broadening (you should know this)
- ❑ thermal but slowly changing $(2kT/m)^{1/2}$
- ❑ microturbulence (affects total absorption of strong saturated lines)
- ❑ “damping”: natural, Stark, van der Waals (affects strong lines)
- ❑ macroturbulence (large-scale motions; “no effect” on line strengths)
- ❑ rotation (can’t easily be disentangled from macroturbulence)
- ❑ magnetic fields
- ❑ starspots and other atmospheric complications

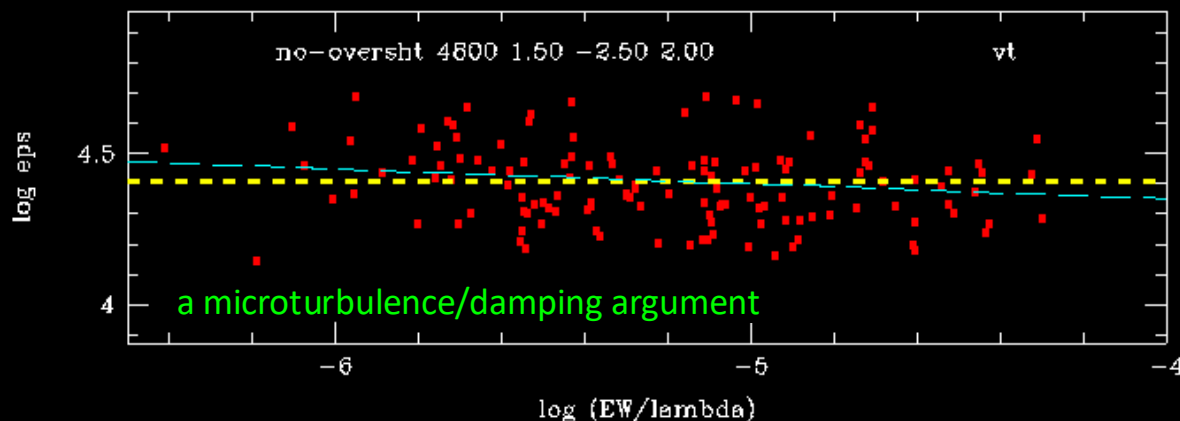
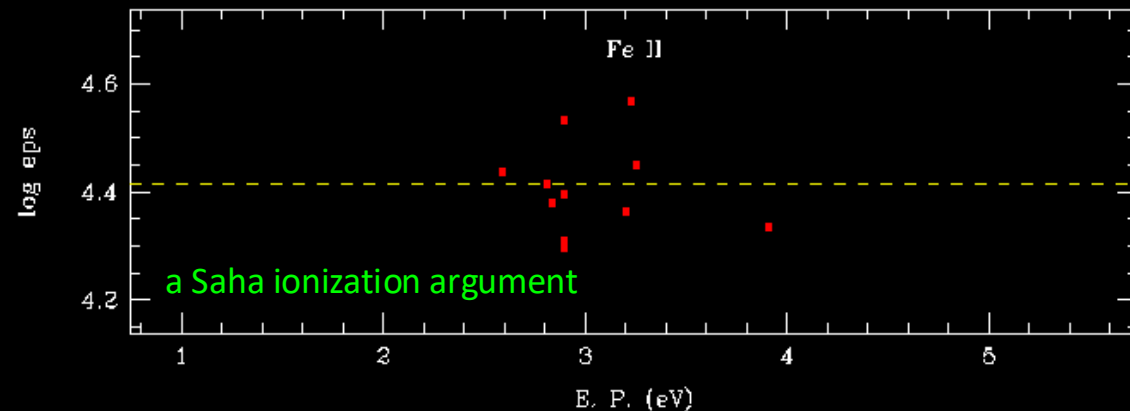
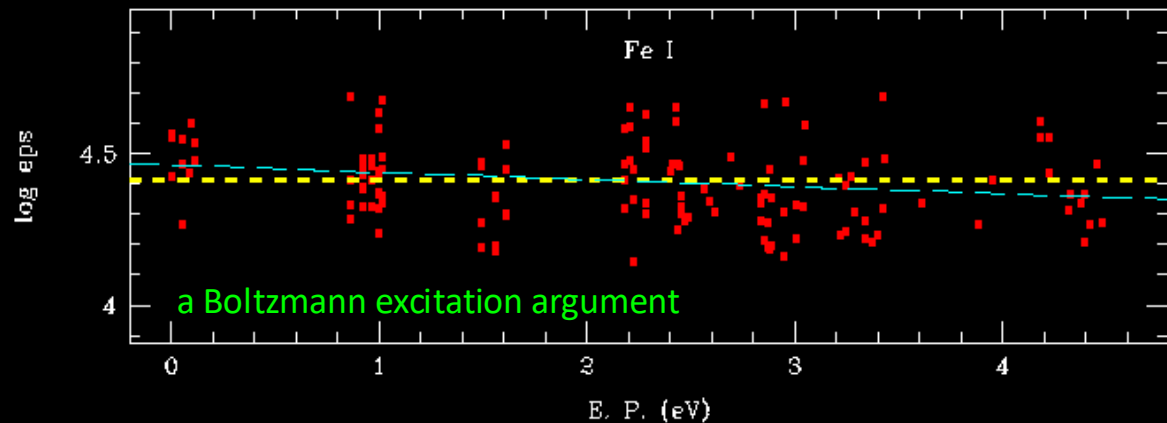
The microturbulent velocity is defined as the microscale non-thermal component of the gas velocity in the region of spectral line formation. Convection is the mechanism believed to be responsible for the observed turbulent velocity field, both in low mass stars and massive stars.

<https://en.wikipedia.org/wiki/Microturbulence>



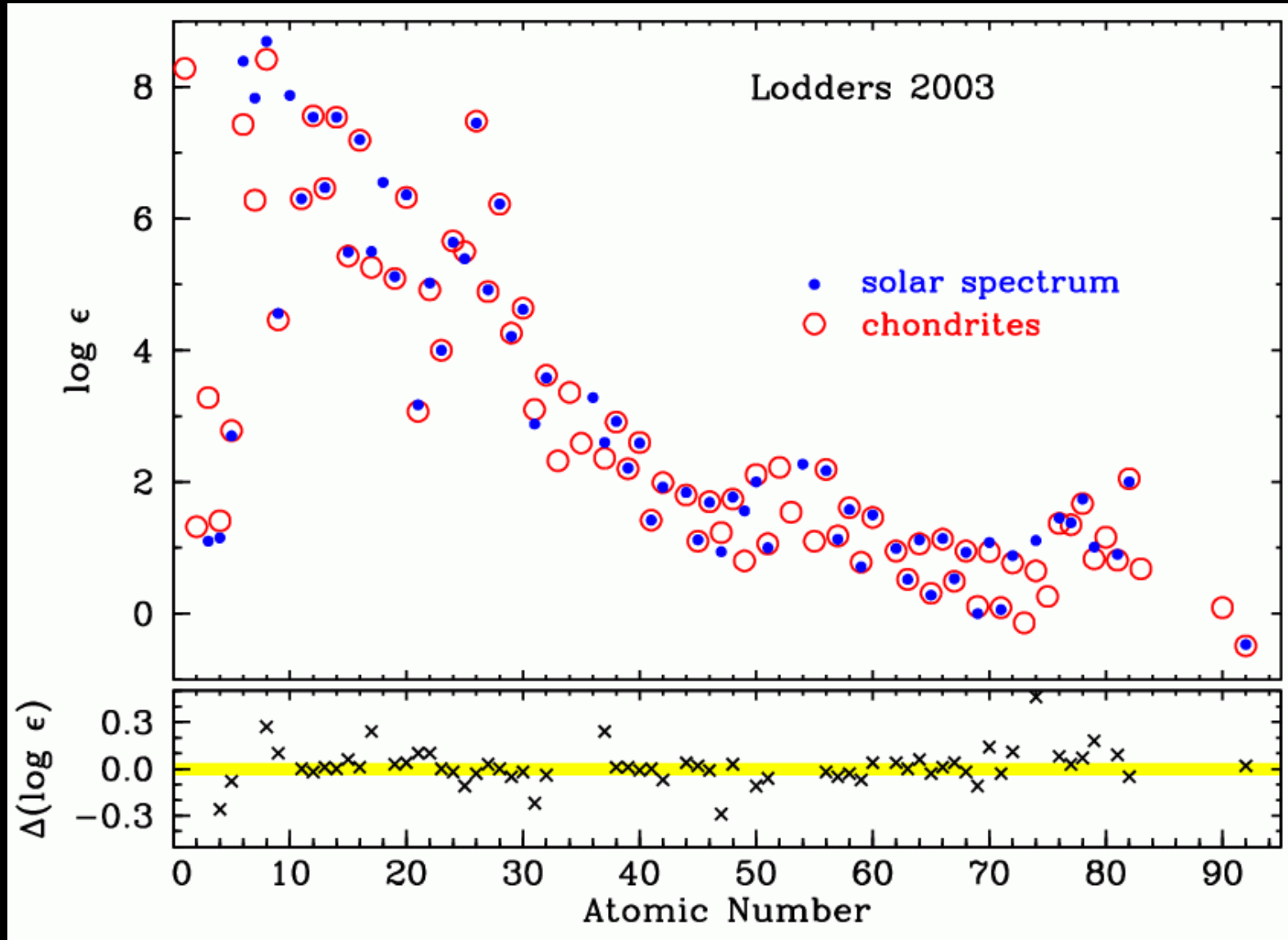
<https://www.sciencedirect.com/topics/physics-and-astronomy/stellar-abundances>

T_{eff} , $\log(g)$, v_{micro} , $[\text{Fe}/\text{H}]$ metallicity, $[\text{X}/\text{Y}]$ “all at once”: iterative abundance calculations



- ✓ trying to change parameters to satisfy all on average
- ✓ YOU should explain the “arguments” to yourself
- ✓ but parameter choices are rarely independent!
 - ✓ e.g. the strong lines are usually the low excitation lines
 - ✓ e.g. in metal-rich K-M giants most lines are strong!
- ✓ all this discussed in detail by Martina Baratella

Some support for standard LTE stellar abundance analyses



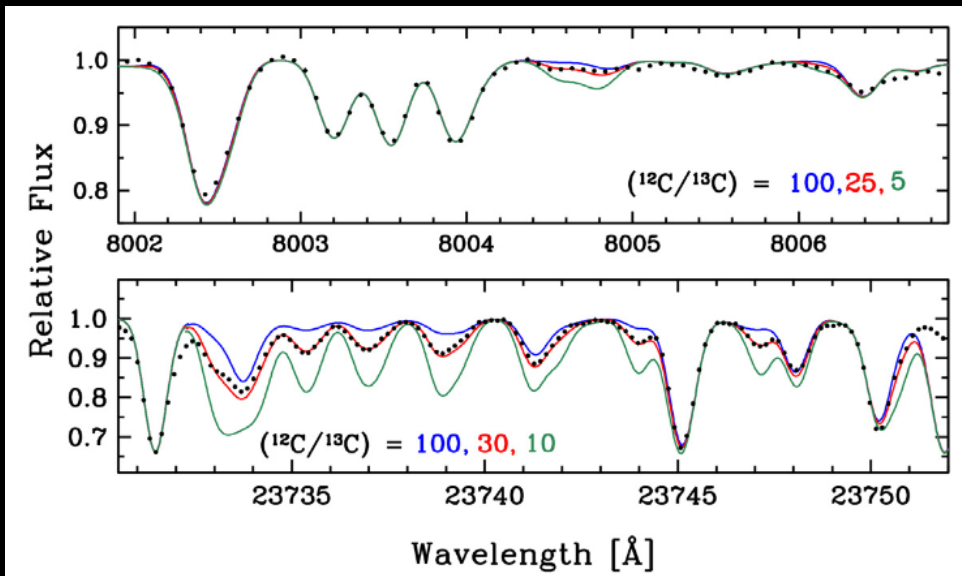
updates by, e.g. Asplund et al. 2009 do not change the basic agreement

Snedden & Lawler 2005

What about the critical CNO abundances?

- Carbon: C I, C₂ blue/yellow, CH blue, CN blue, red, near-IR, CO near-IR
 - lots of transitions; can you make them all agree?
- Nitrogen: CN from blue through near-IR
 - very dependent on first deriving C and O abundances
- Oxygen: O I, [O I], O-rich molecules in special cases
 - most abundances depend on ONLY the [O I] 6300.3Å line

When $T_{\text{eff}} < 6000\text{K}$, these are coupled and need molecular equilibrium calculations



The Equilibrium Constant (K_c)



$$K_c = \frac{[C]^c [D]^d}{[A]^a [B]^b}$$



$$K_c = \frac{[\text{CH}_4][\text{H}_2\text{O}]}{[\text{CO}][\text{H}_2]^3}$$

simplified molecular equilibrium: H-C-N-O

$$P(H) = p(H) + 2p(H_2) + p(CH) + p(NH) + p(OH) + 2p(H_2O) + \dots \text{very coupled equations}$$

$$P(C) = p(C) + p(CH) + 2p(C_2) + p(CN) + p(CO) + p(CO_2) + \dots$$

$$P(N) = p(N) + p(NH) + p(CN) + 2p(N_2) + p(NO) + \dots$$

$$P(O) = p(O) + p(OH) + p(CO) + p(NO) + 2p(O_2) + 2p(CO_2) + \dots$$

But (happily!) the importance of each depends on abundance of the element(s) and the molecular dissociation energy

$$\frac{p(AB)}{p(A)p(B)} = \text{const} \frac{M(AB)^{-3/2}}{M(A)M(B)} \frac{\exp(-U(AB)/kT)}{\exp(-U(A)/kT)\exp(-U(B)/kT)} \exp(-D_0/kT)$$

$$P(H) = p(H) + 2p(H_2) + \dots \quad (\text{H cares only about itself})$$

$$P(C) = p(C) + p(CO) + \dots \quad (\text{C cares only about O})$$

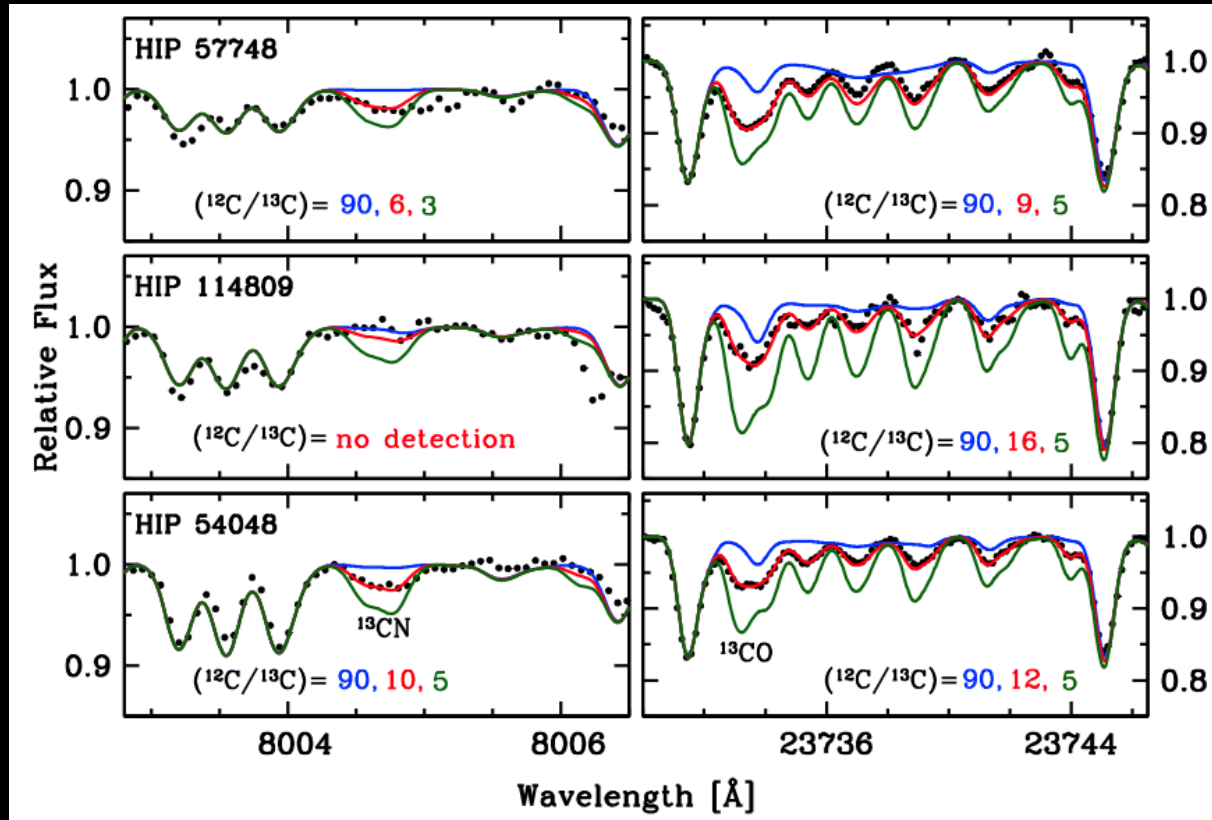
$$P(N) = p(N) + 2p(N_2) + \dots \quad (\text{N cares only about itself})$$

$$P(O) = p(O) + p(CO) + \dots \quad (\text{O cares only about C})$$

many codes quietly do this in the background... but YOU must be aware

isotopic abundances: can be “easy” for molecular features

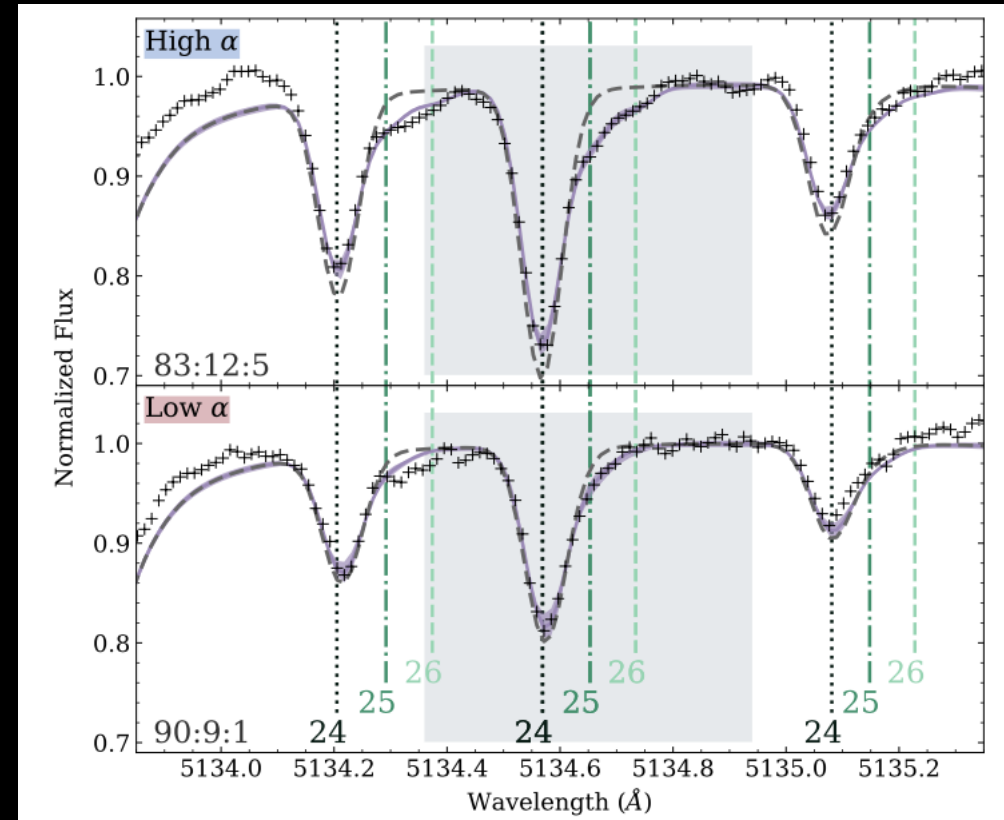
Carbon



Afşar et al 2018

Sun: $^{12}\text{C}/^{13}\text{C} \approx 90$
 can use C_2 , CH, CN, CO

Magnesium

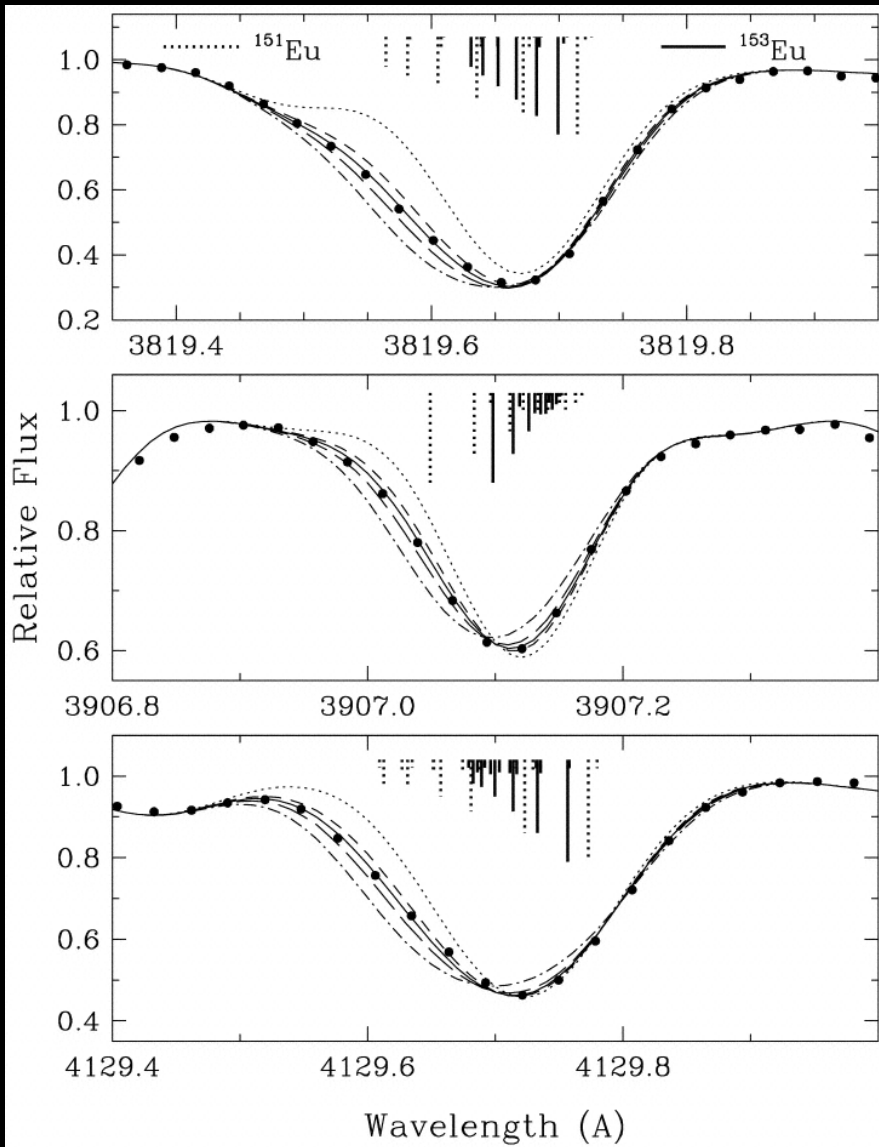


McKenzie et al 2024

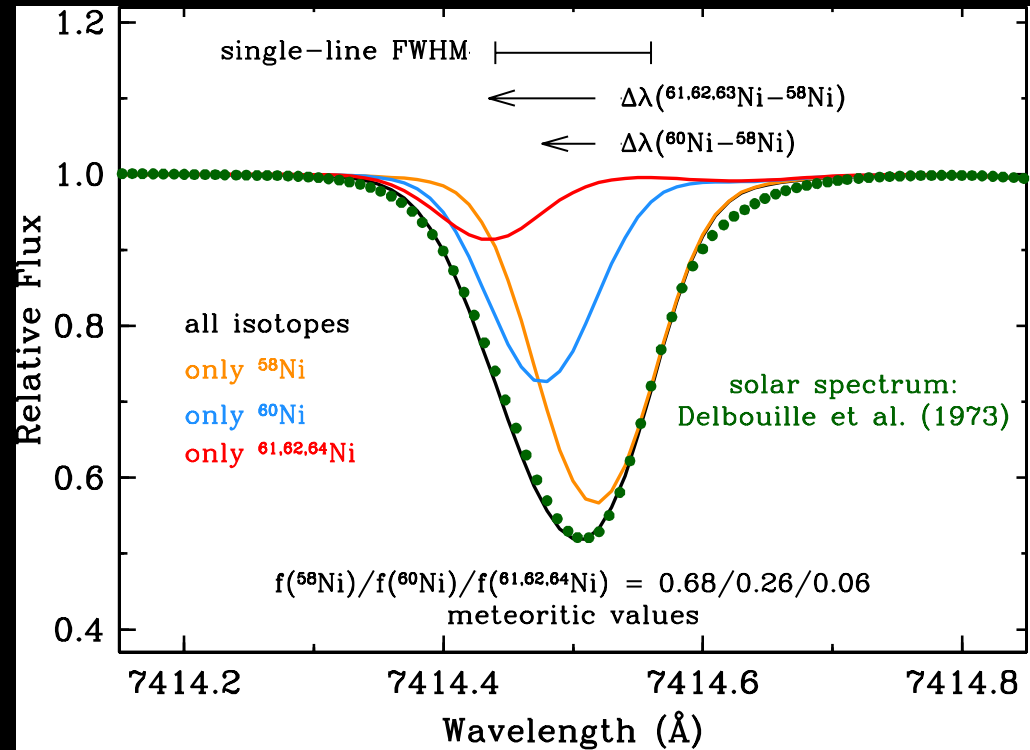
Sun: $^{24}\text{Mg}:^{25}\text{Mg}:^{26}\text{Mg} \approx 79\%:10\%:11\%$

much harder for atoms but not impossible

Europium



Nickel



Sneden et al. 2014

See DETAILS: slides xx-xx
for more good & bad examples

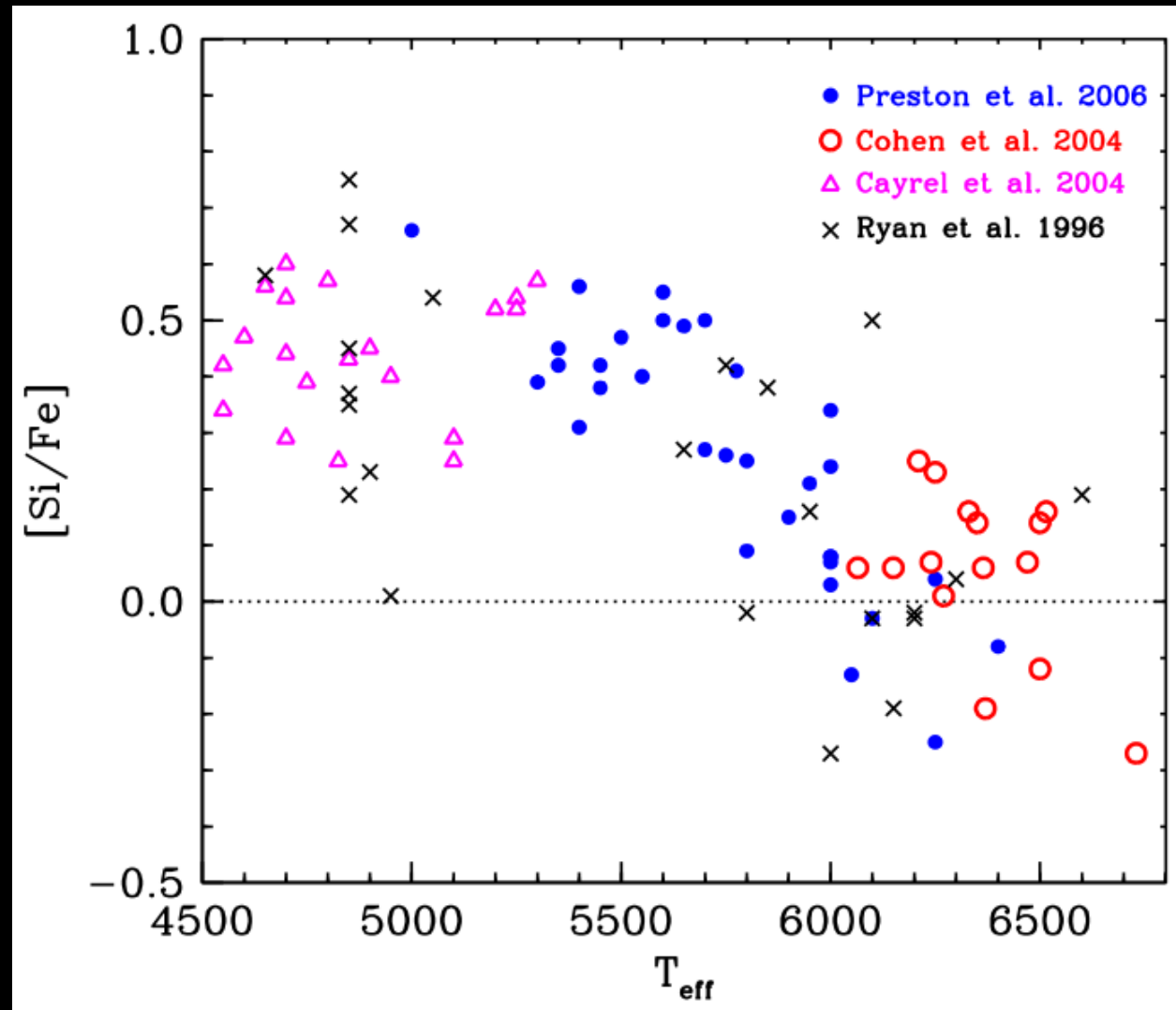
final comments: pointing to where LTE simply fails

here is a plot of $[\text{Si}/\text{Fe}]$ abundances in metal-poor stars using the dominant 3905Å Si I lines

Wait a minute: a temperature-dependent Si/Fe ratio simply cannot be right!

Given the claimed importance of Si in cosmic chemical evolution, we must do better

See DETAILS: slides 33–47



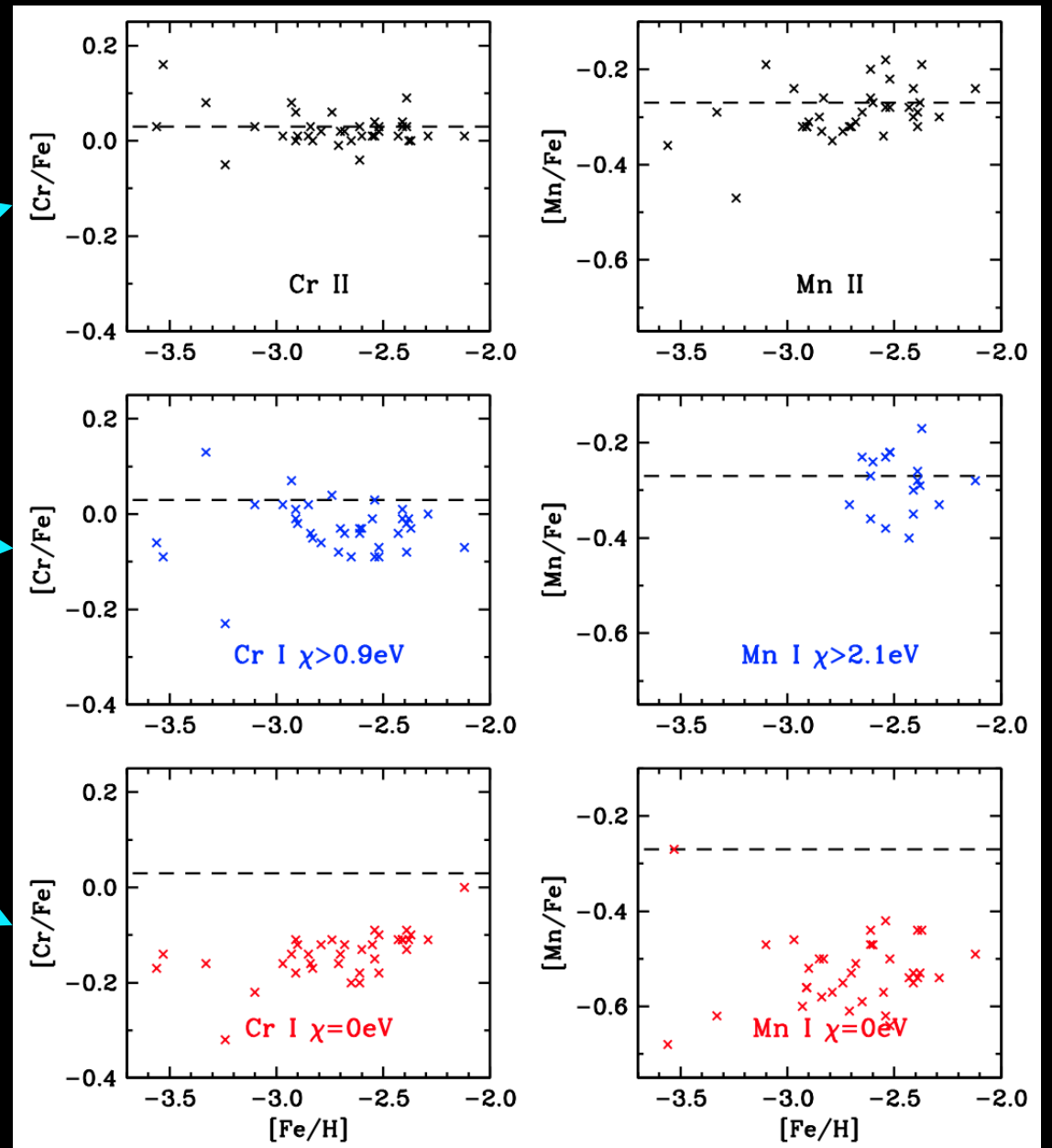
another warning sign: neutral resonance lines in metal- poor stars

I argue that the Cr II & Mn II lines give
“correct” [Si/Fe] abundance ratios

and higher-excitation Cr I & Mn I essentially
are in agreement

but the Cr I & Mn I lines are uniformly “low”
by factors of at least 2

Here’s the pragmatic problem: most
published Cr and Mn abundances for metal-
poor stars rely on the resonance lines



This just scratches the surface!

Don't forget that abundances are supposed to tell us about stellar & Galactic chemical evolution

Thanks, and further contacts are welcome: chris@verdi.as.utexas.edu