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Atomic data for stellar spectroscopy

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Abstract. High-precision spectroscopy of large stellar samples plays a crucial role for several topical issues in astrophysics, such as studying the chemical evolution of the Milky Way Galaxy. Data are accumulating from instruments that obtain high-quality spectra of stars in the ultraviolet, optical and infrared wavelength regions on a routine basis. The interpretation of these spectra is often based on synthetic stellar spectra, either calculated on the fly or taken from a spectral library. One of the most important ingredients of these spectra is a set of high-quality transition data for numerous species, in particular neutral and singly ionized atoms. We rely heavily on the continuous activities of laboratory astrophysics groups that produce and improve the relevant experimental and theoretical atomic data. As an example, we briefly describe the efforts done in the context of the Gaia-ESO Public Spectroscopic Survey to compile and assess the best available data in a standard way, providing a list of recommended lines for analysis of optical spectra of FGK stars. The line data, together with specialised analysis methods, allow different surveys to obtain abundances with typical precisions of ∼0.1 dex on an industrial scale for ∼10 chemical elements. Several elements with urgent need for better atomic data have been identified.

Keywords. atomic data, stars: late-type, techniques: spectroscopic, surveys

1. Introduction

High-precision spectroscopy of large numbers of stars provides a good basis for studying the chemical and dynamical structure and evolution of the *Milky Way*, deriving the *origin of chemical elements*, and characterizing *planetary host stars*. In recent years, high-quality spectra have been accumulating from surveys and individual programs. The interpretation of these data using synthetic stellar spectra requires high-quality atomic transition data.

The wavelength regions that are mainly used for the above science cases span from the UV – mostly relying on Hubble Space Telescope spectra – to the optical and infrared, where spectra are obtained by ground-based 2- to 10-m telescopes around the world (e.g. ESO/Chile, France, USA, Australia, China). The relevant species are mainly neutral and singly ionized atoms, as well as diatomic and triatomic molecules, as most targets for galactic and planetary studies are F-, G-, or K-type stars.

The types of atomic and molecular data needed for a transition between two states (corresponding to a spectral line) can be broadly divided into two categories: 1) *transition probabilities* (oscillator strengths, gf-values), which can either be measured by laboratory astrophysics groups or calculated by atomic physics groups, and 2) parameters for *line-broadening by collisions* with neutral or charged particles, for which experimental data are very scarce, and the majority of which are therefore calculated by atomic physics groups (Barklem 2016).

† and the Gaia-ESO line list group (Karin Lind, Maria Bergemann, Martin Asplund, Paul S. Barklem, Šarunas Mikolaitis, Thomas Masseron, Patrick de Laverny, Laura Magrini *et al.*)

Data published by different laboratory astrophysics and atomic phsics groups have been collected and are being distributed by a number of databases, each with a different specialisation, although there is considerable overlap in data content. A few examples are the NIST Atomic Spectra Database (Kramida *et al.* 2018), the VALD database (Ryabchikova *et al.* 2015), and the STARK-B database (Sahal-Bréchot *et al.* 2017). The Virtual Atomic and Molecular Data Centre (Dubernet *et al.* 2016 and this conference, VAMDC, http://www.vamdc.eu) is an electronic infrastructure providing access to ∼30 databases simultaneously, both via a web interface (the VAMDC portal) and via various Virtual Observatory tools.

2. Stellar spectroscopic surveys and their line lists

A handful of surveys are currently collecting or processing stellar spectroscopic data on an industrial scale, and several more are planned for the near future. The common goal of these surveys is to provide a homogeneous overview of the distributions of motions and chemical abundances in the Milky Way. Each of the surveys is approaching this goal in a somewhat different way. We give three examples in chronological order, all of which are obtaining spectra with a resolution of $\lambda/\Delta\lambda \gtrsim 20\,000$ and are targeting on the order of 10^5 to 10^6 stars.

The APOGEE survey (Majewski *et al.* 2017, USA) is working at infrared wavelengths (H-band), with a focus on the dust-obscured parts of Galaxy. The line list (Shetrone *et al.* 2015) comprises ∼130 000 lines for 36 atoms and 6 molecules, with the "best" atomic data from the literature, and astrophysical atomic data calibrated on the Sun and Arcturus for ∼20 000 lines. The Gaia-ESO Public Spectroscopic Survey (Gilmore *et al.* 2012; Randich *et al.* 2013, ESO) covers a considerable part of the optical spectral region and was designed to complement the ESA space mission Gaia by obtaining high-resolution spectra for faint stars. Also the GALAH survey (De Silva *et al.* 2015; Buder *et al.* 2018, Australia) is operating at optical wavelengths, and has its focus on chemical tagging.

Within the Gaia-ESO consortium a large effort has been put into the construction of a common line list which is being used throughout the survey (involving up to 14 abundance analysis groups). The Gaia-ESO line list has also constituted the starting point for the GALAH line list. In brief, ∼1300 transitions were preselected in the relevant wavelength ranges (475 nm to 685 nm and 850 nm to 895 nm), which were presumed to allow accurate determination of stellar parameters, and of abundances for many elements for FGK-type stars. A compilation of the best atomic data for these lines defined the standard line list, comprising 44 neutral and singly ionised species (atomic numbers 3, 6, 8, 11–14, 16, 20–30, 38–42, 44, 56–60, 62–64, and 66). The preferred sources for gf-values were accurate laboratory measurements (usually from more recent publications, i.e. 1980s onwards), which were supplemented by less accurate laboratory gf-values (usually from older publications), and by theoretical data. We emphasise that no astrophysical gf-values were included or derived. A simple flag for recommended use was assigned to each line, according to the quality of the transition probabilities: *gf-flag* = **Y**es / **U**ndecided / **N**o, often (but not always) corresponding to the three levels of sources mentioned above.

The preselected lines were complemented with available data for all lines in the observed spectral range of the target stars, extracted from the VALD database in the case of atoms, and calculated and compiled by T. Masseron for 12 diatomic molecules. These data are needed to identify blends for the preselected lines, and as "background" for synthetic spectrum calculations. They were used to assign a second flag to each preselected line, according to blending properties: *syn-flag* = Y / U / N. Hence, the best lines to use in an abundance analysis would be those for which both *gf-flag* and *syn-flag* are equal to "Y". This is the case for about 15% of the preselected lines. The remainder

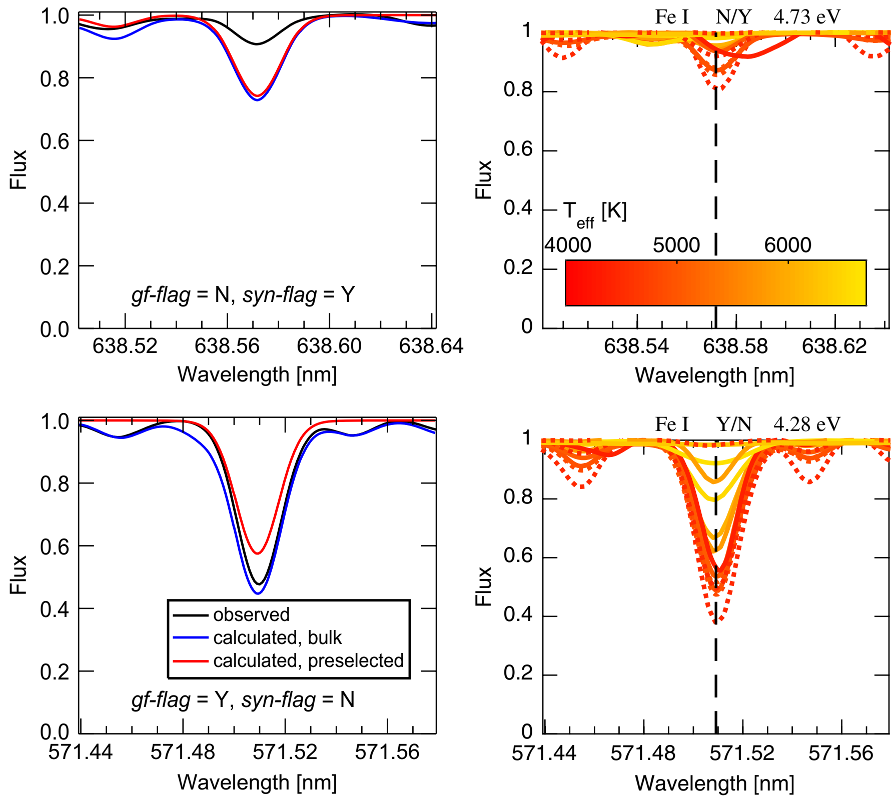

Figure 1. *Left:* Comparison of observed and calculated line profiles for Arcturus around two of the preselected Fe I lines with different combinations of *gf-flag* and *syn-flag*, convolved to a uniform spectral resolution of R =47000. Black lines: observations, red lines: calculations including preselected spectral lines only, blue lines: calculations including blends from background line list. *Right:* Observed line profiles for selected Gaia FGK benchmark stars (Heiter *et al.* 2015; Blanco-Cuaresma *et al.* 2014) for the same lines at the same resolution. Quality flags and lower level energy are indicated at the top of each panel. The vertical dashed line indicates central wavelength. Colour coding indicates effective temperature, solid lines are dwarfs, and dotted lines are giants.

should be regarded with care (different combinations of Y/U/N values for the two flags) or completely discarded (N/N case). An example for the giant star Arcturus is given in Fig. 1, which shows a line with inaccurate gf-value which is blend-free (upper panels) and a line with good gf-value which is blended (lower panels). The reason for this assessment becomes apparent only when observed line profiles are compared to calculated ones (left panels). The right panels show the same lines for several stars with different effective temperatures, surface gravities, and metallicities. For similar temperatures and gravities (e.g. red dotted lines representing cool giants) the variation in line strength is due to the difference in metallicity.

More examples and an extensive description and discussion of the Gaia-ESO line list is to be found in Heiter *et al.*, to be submitted to A&A.

3. Line list impact and data needs

One way to evaluate the impact of atomic data is to investigate the abundance precisions achieved by the different surveys. However, we caution that the significance of this approach is limited, since the abundance precisions also depend on stellar parameters,

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analysis methods, and the definition of "precision". For example, in the Gaia-ESO survey the method-to-method dispersion or line-to-line scatter is used, while the APOGEE survey refers to the star-to-star scatter within clusters. With this caveat the general picture emerging within the Gaia-ESO survey (Smiljanic *et al.* 2014; Mikolaitis *et al.* 2014; Lanzafame *et al.* 2015; Jofré *et al.* 2015) is that high precision abundances (uncertainties <0.15 dex) can be obtained for up to ten elements, including Al, Si, and Ca, while the least reliable abundances are obtained for Co, Ni, Zn, and Y. There are also problems for V at low metallicities. As a second example, the abundances obtained by the APOGEE survey (Holtzman *et al.* 2015; Mészáros *et al.* 2015; see also Holtzman *et al.* 2018; Jönsson *et al.* 2018) appear to achieve the highest precision (their uncertainties <0.05 dex) for α-elements, Fe, and Ni, and the lowest precision for V. Problems for Al, Ca, and Ti are encountered at low abundances.

The flags in the Gaia-ESO line list can be used to assess future data needs and to compile a wish list for new experimental gf-values in the *optical* wavelength region. Focussing on lines which are more or less unblended (*syn-flag* = Y or U), high priority should be given to species which have *gf-flag* = U or N for $>50\%$ of these lines. This concerns $\sim$240 Fe I lines, $\sim$50 Ni I lines (whith high excitation energies), and some Fe II, Na I, Si I, and Ca II lines. However, there are a few species for which all of the few available "unblended" lines have uncertain gf-values, and these should be given even higher priority: Al I, S I, and Cr II.

In summary, we argue that accurate atomic data in the optical and IR are an important ingredient of large-scale stellar spectroscopic surveys. For recent progress in laboratory astrophysics see the latest report by the IAU Working Group on High-Accuracy Stellar Spectroscopy (Barklem *et al.* 2018). The Gaia-ESO survey provides a list of recommended lines for analysis of optical spectra of FGK stars. Abundances with typical precisions of $\sim$0.1 dex are today being obtained on an industrial scale for $\sim$10 chemical elements. Several elements with urgent need for better atomic data have been identified.

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