# DIVISION B / COMMISSION B5 / WORKING GROUP HIGH-ACCURACY STELLAR SPECTROSCOPY

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# 1. Introduction

While the measurement of stellar properties such as chemical compositions, masses and ages is a fundamental problem in astrophysics, the problem has become even more relevant in the era of large astrometric surveys such as SEGUE, Gaia, LSST and Skymapper, complimented by large, high-resolution and high-signal-to-noise ratio spectroscopic surveys such as 4MOST, WEAVE, GALAH and Gaia-ESO (e.g. Heiter *et al.* 2015). This WG was initiated in 2016 within the commission for Laboratory Astrophysics with the main goal to promote better coordination of activities between laboratory spectroscopists, theorists and stellar spectroscopists, in the field of high-accuracy stellar spectroscopy.

Various meetings provide important forums for such exchanges between laboratory spectroscopists, theorists and stellar spectroscopists, especially the ICAMDATA and ASOS meetings on alternating years, and to a lesser extent meetings such as APS-DAMOP, ICSLS, and ICPEAC. The "Workshop on Astrophysical Opacities" held in Western Michigan University during Aug 1–4, 2017 aimed at evaluating the current status on the atomic and molecular opacities, giving an overview of methodologies, and discussing the ongoing recalculation of data for resolving the existing discrepancies. The proceedings of the workshop (Editor-in-Chief Claudio Mendoza, Astronomical Society of the Pacific Conference Series) will be available in later 2018. We note that in 2018 there will be a special session of the European Week of Astronomy and Space Science EWASS meeting in Liverpool on "Atomic and molecular data needs for astronomy and astrophysics", with particular emphasis on data for spectroscopic surveys. The focus of the meeting will be knowledge transfer with astronomers highlighting their data needs, and spectroscopists and theorists presenting new data of astronomical interest and the capabilities of their facilities for future collaborations.

The advent of the internet and social media as a possible channel for interaction has also been explored by our working group. In particular the ASTROATOM blog (https://astroatom.wordpress.com/, Luridiana *et al.* 2011), started in 2010 as forum for news, comments and general discussions on the production of atomic data and their astrophysical applications, has been revived. The blog has an attached twitter feed (https://twitter.com/AstroAtom), and we note the existence of a complimentary twitter feed on precision stellar spectroscopy (https://twitter.com/PrecisionSpec).

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## 2. Developments within the past triennium

In this section we discuss a small selection of results from the past triennium, with the note that of course this discussion cannot be exhaustive, and certainly reflects the biases of the authors.

#### 2.1. Atomic structure

For meaningful interpretation of high resolution stellar spectra, accurate atomic data are vital: laboratory measured wavelengths (atomic energy levels), to at least a part in  $10^7$  ( $30 \text{ ms}^{-1}$ , 0.15 mÅ at 1500 Å),  $\log(gf)$ s ('f-values') accurate to a few %, and line broadening effects like hyperfine structure (HFS). We summarise here efforts by key groups, particularly for line rich iron group spectra. Accurate energy levels and wavelengths are reported: by NIST for Cu II (Kramida *et al.* 2017), with critical evaluations of data for CI (Haris & Kramida 2017), VI (Saloman & Kramida 2017a), and VII (Saloman & Kramida 2017b); Co III (Smillie *et al.* 2016) important in hot star analysis, and progress in finding new energy levels for Fe I was made using stellar spectra (Peterson *et al.* 2017). New data for VI (Basar *et al.* 2017) and Mn II (Townley-Smith *et al.* 2016). Progress in ongoing analyses for singly ionised iron group element wavelengths, energy levels and HFS was reviewed (Nave *et al.* 2017).

Improvements in f-values included accurate laboratory measurements of level lifetimes and branching ratios, and where this was not possible theoretical calculation. Highlights of new f-value measurements include: Cr II (Lawler *et al.* 2017a), VI (Wood *et al.* 2018; Holmes *et al.* 2016), Sc II (Rhodin *et al.* 2017b), Fe I (Belmonte *et al.* 2017), Mg I (Rhodin *et al.* 2017a), Ni II (Hartman *et al.* 2017), and a review (Lawler *et al.* 2017b). New fvalues from combined experiment and theory include Y II, Co II, Ti II (Palmeri *et al.* 2017; Quinet *et al.* 2016; Lundberg *et al.* 2016). Theoretically calculated f-values for allowed and forbidden lines included the significant work on Ni II (Cassidy *et al.* 2016), and doubly ionised iron group f-values (Fivet *et al.* 2016). Other calculations gave data for Fe III for plasma diagnostics (Laha *et al.* 2017), and for highly excited ions for studies of hot white dwarfs (Rauch *et al.* 2017a). Significant progress review reports include those by Quinet (2017) and Jonsson *et al.* (2017). The experimental methodology used for intensity calibration for laboratory f-value measurements is being checked, to ensure confidence in accuracy (Lawler & Den Hartog 2018).

# 2.2. Astrophysical Opacity

While photo-excitation is the most common source of line formation and the corresponding transition probabilities are needed for spectral analysis, the intrinsic resonances in photoionization can appear as absorption lines (e.g. Pradhan 2000) and in electron-ion recombination as dielectronic satellite lines in emission spectra (Nahar & Pradhan 2006). The resonant lines are detectable for few electrons systems. However, resonances in photoionization contribute considerably to plasma opacities (Nahar *et al.* 2011) and hence to the radiating flux distribution of a star. Opacity ( $\kappa_{\nu}$ ) of a plasma measures the amount of radiation absorbed through photo-excitations and photoionizations as

$$\kappa_{\nu}(\mathbf{i} \to \mathbf{j}) = \frac{\pi \mathbf{e}^2}{\mathbf{mc}} \mathbf{N}_{\mathbf{i}} \mathbf{f}_{\mathbf{i}\mathbf{j}} \phi_{\nu}, \quad \kappa_{\nu} = \mathbf{N}_{\mathbf{i}} \sigma_{\mathbf{PI}}(\nu)$$
(2.1)

where  $f_{ij}$  is the oscillator strength and  $\sigma_{PI}(\nu)$  is photoionization cross section. Determination of total  $\kappa_{\nu}$  requires inclusion of all possible transitions, both bound-bound and bound-free, of all ionization stages of all elements that exist in the plasma. A lack of accurate atomic data is the reason for the uncertainties in the opacities. The latest *ab*  *initio* calculations using the *R*-matrix method for photoionization and electron-ion recombination of large number excited states (n=10) were obtained for P II, including benchmarking of the observed features in the Advanced Light Source experiment (Nahar 2017a,b; Nahar *et al.* 2017), Ca XV (Nahar 2017b), Ti I (Nahar 2016), and Fe XVII (Nahar & Pradhan 2016).

Opacities required for modelling the solar interior have been studied extensively in the past under the Opacity Project (The Opacity Project Team 1995, 1997) by calculating large-scale bound-bound transition strengths and bound-free photoionization cross sections with precise delineation of the autoionizing resonance profiles. However, the often dominant inner-shell transitions could not be considered owing to constraints on the available computers at the time. This is one main possible source for discrepancy between the current solar abundances derived from spectroscopic observations, and those abundances  $(N_i)$  required in opacities for solar structure models to reproduce helioseismic observations. The 3D non-LTE (non-local thermodynamical equilibrium) analysis of the solar spectrum gives solar elemental abundances up to 50% lower for common volatile elements such as C, N, O and Ne (Asplund et al. 2009). It was suggested that an enhancement of up to 30% in opacities in solar structure models could resolve the discrepancy (e.g. Bahcall et al. 2005). The recent experimental measurement of iron opacity at the Sandia Z-pinch inertial confinement fusion device, under stellar interior conditions prevalent at the base of the solar convection zone shows 30-400% higher monochromatic opacity than that of the Opacity Project (Bailey et al. 2015). The follow-up study on photoionization of Fe XVII found that resonances due to inner shell excitations were much stronger and increased its opacity by 35% (Nahar & Pradhan 2016).

#### 2.3. Cool stars

For cool stars (F-, G- and K- type), a particularly pressing problem over recent decades has been the need for data on inelastic processes due to electron and hydrogen atom impacts. These data are needed for accurate non-LTE modelling of cool star spectra, and the state of affairs in 2016 was reviewed in Barklem (2016). For electron collisions, the main advances have been the systematic exploitation of the existing method, especially the *R*-matrix, *B*-spline *R*-matrix, and CCC methods (e.g. Zatsarinny et al. 2016; Taval & Zatsarinny 2016; Barklem et al. 2017) The situation for hydrogen atom collisions has been particularly poor, and the main development during the last triennium has been the extensive application of model approaches to providing reasonable estimates for these data, with sufficient scope for astrophysical applications. In particular, data have become available for Be (Yakovleva et al. 2016), O (Barklem 2018b), K and Rb (Yakovleva et al. 2018), Ca (Belyaev et al. 2016, 2017; Mitrushchenkov et al. 2017) (and applied in Mashonkina et al. 2017), Mn (Belyaev & Voronov 2017), and Fe (Barklem 2018a). A further simplified general theoretical model, which can in principle be used to produce estimates for any atom, has been developed and applied to K (Belyaev & Yakovleva 2017b) and Ba (Belyaev & Yakovleva 2017a). A semi-empirical approach based on existing calculations was developed by Ezzeddine et al. (2016). Presently, the accuracy of these data is mostly assessed by examining the effect on modelling spectra of standard stars in comparison with observations, including spatially resolved spectra on the Sun (e.g. Lind *et al.* 2017). Similar studies should be carried out for the cases described above. At least some of the data will hopefully also be able to be compared with experiments, e.g. with DESIREE (Thomas et al. 2011), which is expected to start producing results on low-energy mutual neutralisation in the very near future.

#### 2.4. Hot stars

Many spectral features of neutral and ionized species that are strong in cool stars persist in hotter stars. Important lessons can be learned concerning non-LTE line-formation when studying these features across spectral borders. Such an approach was followed by Sitnova *et al.* (2016) who employed recently determined *ab-initio* photoionization crosssections to build up an improved model atom for Ti I/II and tested it for stars through spectral ranges K to A. In order to remove remaining discrepancies between models and observations accurate collisional data will be required. In a similar fashion Alexeeva *et al.* (2016) studied C I/II non-LTE line-formation in A- and B-type stars, finding that the photospheric C I emission lines in the near-IR are reproduced well only when accurate electron-impact excitation rates are applied. Carbon is also of high interest as a tracer for the action of the CNO cycles in hot, massive stars. Carneiro *et al.* (2018) provided a comprehensive model atom for C II-V for O star analyses. The status of the quantitative spectroscopy of mass outflows from massive (supergiant) stars was reviewed recently by Martínez-Núñez *et al.* (2017) considering spectral diagnostics in the UV/optical and at X-ray wavelengths, which relies heavily on the provision of *ab initio* data.

End stages of low-mass stars can provide objects with hotter atmospheres than usually found among massive stars. In a number of papers Rauch et al. (2016a,b, 2017b,a) calculated oscillator strengths for several high-ionization stages (usually in the range IV-VI) of the heavy elements Se, Kr, Zr, Mo, Te, I and Xe, and applied them to non-LTE analyses of the UV spectra of hot white dwarfs. Some exotic evolution channels can lead to the formation of hot helium stars without Wolf-Rayet characteristics, i.e. with visible photospheres. One class are the so-called (super-)giant extreme helium (EHe) stars, which have atmospheres dominated by helium ( $\gtrsim 95\%$  mass fraction) and carbon (a few percent). These generate test environments for atomic data that are very complementary to stars with conventional chemical composition, because of reduced continuum opacities and much harder radiation fields due to the absence of the hydrogen Lyman jump. Kupfer et al. (2017) investigated the prototype of this object class for the first time in detailed non-LTE. It became clear that our knowledge of atomic data even for such a simple element like helium is very incomplete. Radiative data and Stark-broadening data for transitions involving levels with principal quantum number  $n \ge 20$  are urgently required, and eventually even data for inelastic collisions with neutral helium atoms.

### 2.5. Databases of A&M line parameters

Atomic parameters of spectral lines are collected in different spectroscopic databases (see e.g. Ryabchikova 2017). Below is a short list of the databases most important for spectroscopic analysis, with a brief description of the improvements over the past triennium.

**R.Kurucz collection** (kurucz.harvard.edu/atoms.html). This is an online collection that contains a huge amount of laboratory and theoretical data for atomic and molecular lines. Kurucz's collection is frequently updated. The most significant contribution over the past years consists of the extended sets of energy levels and wavelengths of Fe I lines potentially detectable in stellar spectra (Peterson & Kurucz 2015; Peterson *et al.* 2017). At present more than 1100 classified levels are known with ten levels having energies above the Fe I ionization potential. Classification of new levels and line identification study were based on the high-resolution high signal-to-noise stellar spectra in UV, visible and near-IR spectral regions. Although the average uncertainty of the theoretical calculations is still as large as  $\pm 0.35$  dex on a logarithmic scale, they play an important role for spectral synthesis, and, in particular, for flux calculations where completeness of the line data is crucial. NIST Atomic Spectra Database Version 5.5 (Kramida *et al.* 2018). NIST ASD contains critically evaluated atomic data: energy levels of a particular atom or ion, level classification, line wavelengths (observed and Ritz), transition probabilities and their evaluated accuracy, and bibliography. Different options are provided for data extraction. Additions, corrections, and improvements in data and interface are given in Version History (https://physics.nist.gov/PhysRefData/ASD/Html/verhist.shtml). Over the last three years the largest revision of energy levels and transition probabilities were made for C I (Haris & Kramida 2017), V I and II (Saloman & Kramida 2017a,b), and Cu II (Kramida *et al.* 2017). Critical compilations are carried out by the Atomic Spectroscopy group at the National Institute of Standards and Technology (NIST), USA.

The Vienna Atomic Line Database (VALD). VALD is a collection of atomic and molecular line parameters primarily designed for astrophysics and offers special tools for data extraction, including the popular 'request stellar', where the user gets data merged from different VALD linelists, to synthesize line spectra for a particular object. A brief description of the latest version, VALD3, is given in Ryabchikova *et al.* (2015). VALD has three mirror sites: in Uppsala (vald.astro.uu.se/~vald3), in Moscow (vald.inasan.ru/~vald3) and in Vienna (vald.astro.univie.ac.at/~vald3/php/vald.php). Data evaluation is carried out by VALD project experts and is based on investigation of statistical properties of the data and comparison with high-quality stellar spectra. New features for high resolution spectroscopy are being developed in VALD3: accounting effects of isotopic composition and hyperfine splitting. At present VALD contains parameters for several isotopes of Li, Ca, Ti, Cu, Ba, Eu, and hyperfine splitting of 35 isotopes from Li to Eu (Pakhomov *et al.* 2017).

High-resolution transmission molecular absorption database (HITRAN – www.hitran.org). The new HITRAN2016 edition (Gordon *et al.* 2017) represents a compilation of spectroscopic parameters to predict and simulate the transmission and emission of light in the atmosphere of the Earth and in atmospheres beyond the Earth. HITRAN is composed of five major components: traditional line-by-line parameters, experimental IR cross-sections for almost 300 molecules for atmospheric studies, collision-induced absorption data, aerosol indices, and general tables such as partition sums that apply globally to the data. The new structure enables the incorporation of an extended set of fundamental parameters per transition, provides user-defined output formats, convenient searching, filtering, etc.

**ExoMol database** (www.exomol.com). ExoMol is a database of molecular line lists that can be used for spectral characterisation and simulation, and as input to atmospheric models of exoplanets, brown dwarfs and cool stars (Tennyson & Yurchenko 2012). The new data structure described in Tennyson *et al.* (2016) includes energy levels and Einstein A coefficients as well as other key properties, including lifetimes of individual states, temperature-dependent cooling functions, Landé *g*-factors, partition functions and cross-sections. At present ExoMol contains information on more than 50 diatomic, triatomic and larger molecules, including the recent experimental data and calculations for C<sub>2</sub> (Furtenbacher *et al.* 2016), SiH (Yurchenko *et al.* 2018), VO (McKemmish *et al.* 2016) as well as H<sub>2</sub><sup>18</sup>O and H<sub>2</sub><sup>17</sup>O (Polyansky *et al.* 2017), etc.

Virtual Atomic and Molecular Data Centre (VAMDC – vamdc.eu). The main goal of VAMDC was to create a well-documented interoperable interface to the differently organised existing Atomic and Molecular databases. At present it functions in the form of the VAMDC consortium (Dubernet *et al.* 2016) that consists of 17 full members, full member candidates and associated member candidates from 16 countries of Europe, North and South America, Africa, and the Asia-Pacific region. Currently, 29

databases are running in VAMDC. Software tools are developed to help data providers create and manage a VAMDC node (Regandell *et al.* 2018).

# 3. Closing remarks

The above suggests that considerable progress has been made over the last triennium, and bodes well for the period now leading up to the spectroscopic surveys in the post-Gaia era. Going forwards we stress the need for continued good communication between atomic data providers and astronomers, to ensure important data needs can be met into the future, particularly for new astronomical facilities. We also note that the need for atomic and molecular data for stellar spectroscopy, overlap considerably with those of other astrophysical objects. The astrophysical highlight of the reporting period was without doubt the identification of r-process nucleosynthesis in the double neutron-star merger that gave rise to the gravitational-wave event GRB 170817A (Pian *et al.* 2017). Quantitative analysis of the resulting 'kilonova' spectrum will require knowledge of detailed atomic data for numerous r-process elements, which will have considerable overlap with those needed in stars, creating unique chances for a prosperous future development of our field. In particular, this discovery is likely to give new impetus to the study of the spectra of the lanthanide elements.

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