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

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TRIENNIAL REPORT 2018–2021

1. Introduction

The role of this working group, initiated in 2016 within the commission for Laboratory Astrophysics, has been to promote work on the high-accuracy atomic and molecular data required for accurate stellar spectroscopy, especially through encouraging the interplay between theoretical atomic physics, laboratory spectroscopy, and astrophysical observations. 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. Jofré *et al.* 2019), as well as the need to understand the host stars in the study of exoplanets (e.g. Teske *et al.* 2019; Carrillo *et al.* 2020) and their atmospheres.

2. Meetings during the past triennium

Several conferences and workshops have promoted these themes, either being entirely devoted to or having sessions related to these topics:

- Special Session “SS4 STARS: Atomic and molecular data needs for astronomy and astrophysics” at the April 2018 European Week of Astronomy and Space Science (EWASS) meeting, held in Liverpool, UK.
- IAU Symposium 350, “Laboratory Astrophysics: from Observations to Interpretation”, April 2019, Cambridge, UK (`http://www.astrochemistry.org.uk/IAU_S350/`)
- 50th Annual Meeting of the APS Division of Atomic, Molecular and Optical Physics, Session: “N09 Atomic and Molecular Databases and Data Applications”, May 2019, Milwaukee, Wisconsin, USA (`http://meetings.aps.org/Meeting/DAMOP19/Session/N09`)
- ASOS2019, “13th International Colloquium on Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas”, June 2019, Fudan, China (`https://asos2019.fudan.edu.cn/`)
- XXI Mendeleev Congress on General and Applied Chemistry, symposium ”The Periodic Table through Space and Time”, September 2019, St. Petersburg, Russia (`http://mendeleev2019.ru/index.php/en/`)

• Solvay Workshop, "New Frontiers in Atomic, Nuclear, Plasma and Astrophysics" November 2019, Brussels, Belgium
(`http://www.solvayinstitutes.be/event/workshop/new_frontiers_2019/new_frontiers_2019.html`)

3. Example scientific developments within the past triennium

Pleasingly, the last triennium has seen extensive activity in the field. Here we discuss a small selection of results from the past triennium (and late in the previous triennium), with the note that of course this discussion cannot be exhaustive, and certainly reflects the biases of the authors.

3.1. *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 ($30\,\mathrm{ms}^{-1}$, 0.15 mÅ at 1500Å), log(*gf*)s ('f-values') accurate to a few %, and line broadening effects like hyperfine structure (HFS) and isotope shifts. We summarise here efforts by key groups, particularly for line rich iron group spectra and heavy element spectra.

Based on laboratory experiments, large scale analyses have given accurate energy levels, new levels and wavelengths, reported for Mn II (Liggins *et al.* 2021b), and Ni V and Fe V (Ward *et al.* 2019). The levels of La II have been revised (Guzelcimen *et al.* 2018). Selected levels have been found for species such as La I (e.g. Ozturk *et al.* 2020), Nb I (e.g. Kroger *et al.* 2018), Ho I, II & III (e.g. Ozdalgic *et al.* 2019b,c; Furmann *et al.* 2019).

Selected accurate wavelengths for possible time variation of the fine structure constant investigations using quasar spectra were also reported for Si II, C II, Fe I and Ni II (Nave & Clear 2021), and isotope shift data for Ca I & II (Kramida 2020).

New laboratory data for HFS is important for accurate abundance determinations. A large scale study of HFS data for Co II (Ding & Pickering 2020) was published. Studies of selected HFS have been published also for: Mn II (Glowacki *et al.* 2020), V I (Basar *et al.* 2018), Lu II (Den Hartog *et al.* 2020), Nb I (e.g. Faisal *et al.* 2020), Ho I & II (e.g. Ozdalgic *et al.* 2019a; Furmann *et al.* 2019), and Ta I (Windholz *et al.* 2019).

Progress in ongoing analyses for neutral, singly and doubly ionised iron group element wavelengths, energy levels and HFS was reviewed (Pickering *et al.* 2020). The importance of theoretical calculations for analysis of experimental data was discussed in a paper looking at the significance of the Cowan code (Kramida 2019).

Improvements in f-values ($\log gf$s and transition probabilities) 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: Sc I & II (Lawler *et al.* 2019), Fe II (Den Hartog *et al.* 2019), V II (Nilsson *et al.* 2019b), weak Co II lines (Lawler *et al.* 2018), Ir I (Zhou *et al.* 2018), Nb I & II (Gao *et al.* 2019; Nilsson *et al.* 2019a), and Re I (Li *et al.* 2020b). An impressive, very detailed line list, the result of a large international effort, containing critically assessed $\log gf$s with uncertainties for use in the Gaia ESO survey was reported (Heiter *et al.* 2021).

Theoretically calculated transition probabilities include data for: Ti II (Li *et al.* 2020a), Ce II-IV (Gallego *et al.* 2021) for kilonovae studies, La I (Gamrath *et al.* 2019), Th II and U II for cosmochronology applications (Gamrath *et al.* 2020), excited ions Cu IV-VII for hot white dwarf studies (Rauch *et al.* 2020), Si III & IV for plasma investigations (Atalay *et al.* 2019), and for the lanthanides (Radziute *et al.* 2020). New $\log gf$ and wavelength data for forbidden lines of Mn II is useful for plasma diagnostics (Liggins *et al.* 2021a).

Significant progress review reports include atomic data for solving stellar spectroscopy problems (Sneden *et al.* 2018), and a look to the future for experimentally measured transition probabilities (Lawler *et al.* 2020). The experimental methodology used for intensity calibration for laboratory f-value measurements was reviewed to ensure confidence in accuracy (Lawler & Den Hartog 2019).

3.2. *Astrophysical Opacity*

3.2.1. *Astrophysical Iron Opacity for Sun*

Determination of the chemical composition of the Sun has remained a long standing problem. The abundances of elements are relevant to the plasma opacity (κ_ν) which mainly depends on the two radiative atomic processes, photo-excitations and photoionization as

$$\kappa_\nu(\mathbf{i} \rightarrow \mathbf{j}) = \frac{\pi \mathbf{e^2}}{\mathbf{mc}} \mathbf{N_i f_{ij}} \phi_\nu, \quad \kappa_\nu = \mathbf{N_i} \sigma_{\mathbf{PI}}(\nu) \tag{3.1}$$

where f_{ij} is the oscillator strength and $\sigma_{PI}(\nu)$ is the photoionization cross section. Determination of total κ_ν requires inclusion of all possible transitions, both bound-bound and bound-free, of all ionization stages of all elements that exist in the plasma. The problem of accurate opacity persists. Its measure and importance for solution for abundances can be depicted by the recent statements of two well-known researchers in the field (e.g. Asplund *et al.* 2009). Recently Nicholas Grevesse said "I am now tempted to give a new name, 'the solar opacity problem', to the 'solar abundance problem' as it was erroneously called then better rephrased as the 'solar modelling problem' !!!! Of course part of the solution will come from better modelling the Sun but I do believe that the largest part of the solution will come from the new opacities" (private communication, 2021), and Martin Asplund writes "I realise it is probably impossible to say at this stage but would you be able to take a punt on how long it will take to overcome the remaining hurdles and make the computations to unequivocally say whether the increased Rosseland opacities in the relevant region will be sufficient?" (private communication, 2021).

The Ohio State University (OSU) team has been investigating the radiative atomic processes of elements, particularly iron (e.g. Nahar & Pradhan 1994; Nahar 1995), to determine accurate opacity under the Opacity Project (The Opacity Project Team 1995, 1997) since its inception in the eighties. The accuracy of the calculated opacity can be estimated by use of it in determining the distance of the boundary between the radiative and convective zones, R_{RC}, inside the Sun which is known with high accuracy from helioseismology observations. Iron is known as one of the most important sources of opacity and Fe XVII – Fe XIX are the most abundant iron ions near R_{RC}. While the OSU team has studied Fe XVII extensively for oscillator strengths (Nahar *et al.* 2003) and photoionization and opacity (Nahar *et al.* 2011; Nahar & Pradhan 2016), new findings on the photoionization that cause higher absorption of radiation are still being revealed. The latest findings show that fine structure splittings of resonances increase absorption (to be presented at APS 2021 meeting in May). The computational challenges have now been overcome for photoionization of Fe XVII and Fe XVIII and the analysis of results are in the process. The challenge of Fe XIX has led computation of photoionization to use LS coupling (Nahar 2019a) without fine structure.

The other complex issue is on how to deal the plasma broadening of the detailed resonances which requires extensive computational time even for testing. Pradhan has been working on a large code for the broadening as described in Pradhan & Nahar (2018). Transition rates for diagnostics and modelings were also carried out for some iron-peak elements by Çelik *et al.* (2020).

3.2.2. *Spectral analysis for bio-signature elements in exoplanetary systems*

Chemical elements, such as, carbon, nitrogen, oxygen, phosphorus, and sulfur form the basis of human life on the earth. The search for crucial atoms and molecules that can sustain life has been on the rise as more exoplanets are being discovered. Among all of these, phosphorus has been the least studied element, except for its energies by Martin *et al.* (1985), until recently. Phosphorus lines had been missing and linked to not finding extra-terrestrial life forms. With the latest observatories launched or to be launched soon, such as JWST, the scope for searching for P lines in exoplanets has increased. The recent studies include photoionization of P II for many levels (Nahar 2017b) and benchmarking of them (Nahar *et al.* 2017), electron-ion recombination of P II (Nahar 2017a), collision strengths of P III (Naghma *et al.* 2018), photoionization of P III and P IV (Hernández *et al.* 2015). Most other studies have been on oscillator strengths for a limited number of transitions and a limited number of lifetime measurements. Recently Nahar *et al.* (2020) reported in an APS conference the predicted spectra of all 15 ions of phosphorus, from x-ray to infrared, to illustrate the regions of wavelengths with strong lines that can be used to search for the element.

3.2.3. *Photoabsorption of lanthanides for interpretation of kilonova*

Since the observation of the electromagnetic spectrum of lanthanides followed by the detection of gravitational waves created during the merger of two neutron stars in a kilonova event in 2017, study of these heavy elements has become crucial to interpret the broad feature in the wavelength range of about 3000 - 7000 . Study has been carried out by a number of investigators, such as, Kasen *et al.* (2017), transition rates of singly ionized lanthanides, Pr-Gd by Radžiūtė *et al.* (2020), Kobayashi *et al.* (2020), Tanaka *et al.* (2020), and (Nahar 2021a).

3.2.4. *Atomic data for planetary nebulae and supernova remnants*

For the spectral analysis of the planetary nebulae and on the recent finding on calcium abundance in supernova remnant SN2016hnk, R-matrix calculations for photoionization cross sections for the ground and many excited levels have been carried out for Cl II (Nahar 2021c), for Ne III (Nahar 2019b) which was benchmarked by Nahar *et al.* (2019). Photoionization cross sections for Li- and He-like calcium for many levels were reported in a recent APS meeting (Nahar 2021b).

It may be noted that the database NORAD-Atomic-Data provides details of its data for various atomic processes; see Nahar (2020).

3.3. *Cool stars*

In cool stars, the predominant needs for accurate modelling and interpretation of spectra beyond those directly connected to atomic structure and spectral lines (reviewed above, energy levels, f-values, HFS and isotope splitting), are those needed for atmospheric modelling, including in non-LTE. This encompasses other radiative processes and sources of opacity (e.g. photoionisation), and collisional processes. Other data such as Landé factors are needed when magnetic fields are important. Heiter (2020) presents a review of atomic data for abundance determinations and Kochukhov (2021) a review on magnetic field measurements in cool stars.

Very significant progress has been made in the field, and pleasingly there has been often collaboration between theory, experiment and stellar spectroscopy, leading to some significant advances in precision of derived properties, especially chemical abundances. One particular example is that there continues to be good progress on inelastic collision processes involving hydrogen atoms and electrons, for a long time a major uncertainty in all non-LTE spectral modelling. A particularly noteworthy advance has been the first final-state resolved experiments for mutual neutralisation involving hydrogen, $X^+ + H^- \rightarrow X^* + H$, where usually the hydrogen is replaced with deuterium in the experiments due to advantages of higher mass in merged-beams experiments. Studies of Li^+/D^- and Na^+/D^- have been carried out in Louvain (Launoy *et al.* 2019) and in Stockholm at DESIREE (Eklund *et al.* 2020, 2021). Such processes are important in the statistical equilibrium of Li and Na in cool stellar atmospheres, and these experiments allow the accuracy of abundances for these elements to be further improved and constrained. This has been done, including in 3D-non-LTE modelling, by Barklem *et al.* (2021), and it is concluded that inelastic collisions with hydrogen are no longer a significant source of uncertainty for these simple atoms. Additional calculations for Li+H have been performed during the period using the quantum probability current method based on accurate adiabatic potentials (Belyaev & Voronov 2018), thus obtaining an extensive data set for modelling with high accuracy and complementing existing full quantum and asymptotic model calculations. The importance of accurate UV opacities, due to coincidences between spectra of different elements, reminiscent of the Bowen mechanism, has also been demonstrated for Li by Wang *et al.* (2020a)

Further, hydrogen collision processes on C and N have also been calculated (Amarsi & Barklem 2019), and used to improve abundance determinations in the Sun (Amarsi *et al.* 2020, 2019a), and previously calculated data on hydrogen collisions with O has also be applied to the Sun (Amarsi *et al.* 2018). C and O have also been studied in metal-poor stars with the new models (Amarsi *et al.* 2019b). Again, improved data have also been calculated using alternate methods to complement earlier calculations (Belyaev *et al.* 2019b; Mitrushchenkov *et al.* 2019). Data for hydrogen collisions with K and Rb were provided by Yakovleva *et al.* (2018), and applied to non-LTE modelling in a study that also included improved electron collision calculations from both B-spline R-matrix and convergent close-coupling calculations (Reggiani *et al.* 2019). Non-LTE modelling of Ca has been performed by Osorio *et al.* (2019) using recent hydrogen collision data and improved electron collision data. Alternate calculations for Ca+H processes have also been performed (Belyaev *et al.* 2018, 2019a).

Progress has also been significant regarding heavier elements, including the iron group. Bergemann *et al.* (2019) apply new Mn+H collision data and photoionisation calculations in non-LTE modelling. Grumer & Barklem (2020) have calculated hydrogen collision data for Mn and Ti. Data for electron collisions on Ti II have been calculated by Tayal & Zatsarinny (2020b) and on Cr II by Tayal & Zatsarinny (2020a), as well as some radiative processes in both cases. A particularly important advances are detailed calculations for electron collisions on neutral Fe (Wang *et al.* 2018), as well as photoionisation processes (Zatsarinny *et al.* 2019).

Broadening of spectral lines due to collisions is also very important in a number of contexts, both for atmospheric modelling and abundance determinations. Calculations for line broadening by He collisions, prevalent in DZ white dwarfs, have been performed for Ca (Blouin *et al.* 2019) and Mg (Allard *et al.* 2018). A study of the line profiles of Na perturbed by H_2 (Allard *et al.* 2019) will be very important for determining surface gravities and abundances in M-dwarf stars.

The study of molecular spectra has also seen very significant advances, to a large degree driven by the study of planetary atmospheres, and the possibility to resolve transit spectra of the atmospheres of exoplanets orbiting M-dwarfs. The ExoMol project (Tennyson *et al.* 2020) has made substantial progress. As an example, the study of TiO is particularly important, and during the last triennium has included laboratory study (Bittner & Bernath 2018; Breier *et al.* 2019), a new calculated linelist and partition function

(McKemmish *et al.* 2019), and applications in modelling (Pavlenko *et al.* 2020). Other efforts are being made to provide partition functions, including complex molecules (e.g. Gamache *et al.* 2017). Empirical linelists for 22 molecules, including FeH and MgH, have been provided by Wang *et al.* (2020b), noting molecules such as FeH are very important in the study of M-dwarfs (Lindgren & Heiter 2017).

3.4. *Hot stars*

Spectral line formation in hot stars of spectral types A, B and O is known to be prone to deviations from detailed equilibrium, up to point where the atmospheres of the hottest stars are completely dominated by non-LTE effects. In this field, the main focus in the past triennial laid on investigations of non-LTE effects based on model atoms employing existing atomic data (energy level data, oscillator strengths, photoionization cross sections, collisional excitation and ionization data, line-broadening data). Often, the investigations extended in scope over previous work, facilitated by the availability of refined atomic data and improved computing facilities.

Non-LTE effects in line-formation computations for main-sequence A- and B-type stars were investigated for He I lines (Korotin & Ryabchikova 2018), Ne I/II (Alexeeva *et al.* 2020), Mg I/II (Alexeeva *et al.* 2018), Si I-III (Mashonkina 2020) and Ca I/II (Sitnova *et al.* 2018). In particular photospheric emission lines can only be explained via non-LTE effects, such that an emphasis was given in explaining their formation mechanisms. A study of C I-IV in B- and O-type stars concentrated on this aspect (Alexeeva *et al.* 2019). C II-IV line-formation in hydrodynamic non-LTE atmospheres of more luminous O stars, covering also supergiant stars, was investigated by Carneiro *et al.* (2018).

The Belgrade group continued to provide data on Stark shifts and widths of relevance for hot stars, e.g. for Ar II (Hamdi *et al.* 2018) or Co II (Majlinger *et al.* 2020). Investigations on the impact of such data on the comparison between model computations and HST/STIS spectroscopy were performed for the case of Cr III (Chougule *et al.* 2020).

Hot stars as the progeny of the evolution of low-mass stars also require non-LTE methods for a reliable quantitative analysis. The Tübingen group continued their investigations of abundances of heavy elements in hot white dwarfs, from first detections of Br VI and Sb VI lines (Werner *et al.* 2018), and for Cu IV-VI and In V (Rauch *et al.* 2020). Non-LTE modelling of spectral lines of the isotope ^{3}He in subluminous B-type stars was reported by Schneider *et al.* (2018), with atomic diffusion in the extremely stable atmospheres of these stars yielding the highly non-solar isotope ratio relative to ^{4}He.

4. Closing remarks

The above suggests that considerable progress has been made over the last triennium, and provides a much improved platform for future spectroscopic surveys, as well as new instruments in the near and more distant future. A general trend towards M dwarfs and the infrared, largely driven by the study of exoplanets and their atmospheres, is noted.

It should be stated that it has of course not been possible to include all the new research in this field in this brief summary. Going forwards we stress the need for continued good communication between astronomers and atomic data providers, to ensure important data needs can be met into the future, particularly for new astronomical facilities (Belmonte *et al.* 2018). Consideration of funding for the necessary experimental measurements and theoretical calculations of the atomic data should be given greater emphasis when planning new astronomical facilities and surveys. On this theme, white papers in the American Astronomical Society decadal survey Astro2020 (Nave *et al.* 2019; Savin *et al.* 2019) discuss the needs and challenges in this and related fields, both scientifically and professionally.

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