

Atomic Data for the Gaia-ESO Chemo-Dynamical Survey (GCDS)

Final Report for GREAT/ESF short visit grant 5435

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1. Purpose of the Visit

This GREAT/ESF funded short visit (grant number 5435, and hereafter referred to as SV5435) had two key objectives; the first to discuss the atomic data requirements of the Gaia-ESO (GES) project, and the second to provide Dr. Ruffoni with basic training in modelling stellar atmospheres. Full details of the aims are given in the original grant application [1].

2. Work carried out

2.1 Discussion of deficiencies in the atomic database

The first aim of SV5435 was to discuss the atomic spectroscopy data requirements of the GES Chemo-Dynamical Survey (GCDS) – one of the GREAT/ESF initiatives in connection with WGA3. Particular focus was placed on the need for accurate atomic oscillator strengths (f -values, usually expressed as $\log(gf)$ where g is the statistical weight of the lower level) that are required to extract chemical abundances from GES spectra. While compiling atomic data for GES Data Release 1 (DR1), the GES line list team – part of Working Group 11 – identified a large number of important metal lines for which laboratory data are inadequate.

From a total of 1313 potential target lines within the GES observation windows (475 nm to 685 nm and 850 nm to 895 nm) [2], 545 originate from Fe I; by far the most numerous of all observable chemical species. Of these, 449 are sufficiently strong and unblended to be good candidates for inclusion in the analysis of GES spectra. However, upon examining the literature to obtain accurate, experimentally measured $\log(gf)$ s for these lines, the GES line list team discovered that only 162 are accompanied by such atomic data. By contrast, 167 have reported $\log(gf)$ s that are of questionable accuracy and 120 are altogether absent from the experimental atomic database. Clearly, new, accurately measured, experimental $\log(gf)$ s are required by the GES project in order to extract the greatest amount of data from measured spectra¹.

During SV5435, Dr. Ruffoni and Dr. Bergemann discussed these deficiencies in the atomic database, and examined possible ways to rectify them. During this discussion, it was noted that of the 167 experimental $\log(gf)$ s of questionable accuracy, 49 originate from May et al. [3].

In this paper, more than 1000 Fe I $\log(gf)$ s were measured from the emission of a low current arc. This technique exploits the fact that “the occupation numbers of the excited Fe I levels follow a Boltzmann distribution with an excitation temperature, T , which is a function of the radius of the arc”. The intensities of observed emission lines depend on the upper level population and are thus

¹ Similar deficiencies also exist for other chemical species, particularly Si I and Ti I, but due to the lower number of observable lines originating from them, new measurements of Fe I $\log(gf)$ s should take precedent.

very sensitive to variations in the source conditions. Consequently, in the recent critical compilation of experimental $\log(gf)$ s by Fuhr & Weise [4], the $\log(gf)$ s from [3] were graded E for their accuracy, indicating experimental uncertainties of greater than 50 %.

This suggests they should be re-examined using modern techniques, and so, during SV5435, it was decided that the $\log(gf)$ s in [3], in particular, should be targeted as part of a new measurement campaign at Imperial College London (IC).

Today, $\log(gf)$ s are typically obtained in the laboratory from measurements of atomic transition probabilities, A [5].

$$\log(g_{lf}) = \log \left[A_{ul} g_u \lambda^2 \times 1.499 \times 10^{-14} \right] \quad (1)$$

where the subscript u denotes a target upper energy level, and ul , a transition from this level to a lower state, l , that results in emission of photons of wavelength λ (nm). g_u is the statistical weight of the upper level. The A_{ul} values are found by combining experimental branching fractions, BF_{ul} , with radiative lifetimes, τ_u [6].

$$A_{ul} = \frac{\text{BF}_{ul}}{\tau_u} \quad (2)$$

At IC, the laboratory spectroscopy team operates two Fourier transform (FT) spectrometers [7], with which it is possible to measure high-resolution ($R = 2,000,000$ at 200 nm), Doppler resolved line profiles of atomic emission spectra in the GES observation windows. By calibrating the intensity of these lines, BFs can be measured by comparing the relative intensity, I , of all the lines from a given upper level [8, 9].

$$\text{BF}_{ul} = \frac{A_{ul}}{\sum_l A_{ul}} = \frac{I_{ul}}{\sum_l I_{ul}} \quad (3)$$

Unlike the technique adopted by May et al. [3], this approach does not depend on any form of equilibrium in the population distribution over different levels. However, it is essential that all significant transitions from u be included in the sum over l .

For the 49 lines from [3] that are of interest to GES, corresponding values of τ_u have been published by Corliss & Tech [10]. However, this paper offers little quantitative analysis of experimental uncertainties. The authors instead conclude that “the general scale” of their lifetimes “may be small by about 30 +/- 10 %”, and that in some cases, uncertainties “may be about 50 %”. A revision published some years later [11] removes a “systematic error in the transition probabilities, which propagated also into the calculation of lifetimes”, but still the probable uncertainty in individual values of τ_u remains high. These too must therefore be remeasured using a modern technique, such as Laser Induced Fluorescence (LIF) [12].

LIF lifetimes combined with FT measured BFs can provide $\log(gf)$ s accurate to a few percent for strong lines [8]. Discussion during SV5435 therefore concluded that this should be our preferred approach to measuring new $\log(gf)$ s for GES. However, Dr. Ruffoni has noted in previous work [9] that the experimental requirements for FT spectroscopy and LIF lifetime measurements can often become mutually exclusive when studying $\log(gf)$ s in the near infra-red and at longer wavelengths. This also applies to $\log(gf)$ measurements for some lines of interest to GES.

In these cases, Equation 2 cannot be solved by combining experimental BFs with experimental lifetimes. The solution is to derive “effective lifetimes” for the upper levels not accessible by LIF. This can be achieved by adopting a calculated lifetime for each upper level [13], inserting these into Equation 2 with FT measured BFs to generate “initial” $\log(gf)$ s, and then fitting the intensity of synthetic line profiles modelled with these $\log(gf)$ s to stellar spectra. The result is a small correction, $\delta\log(gf)$, for each line, which can be averaged over all lines from an upper level to obtain a refined, semi-empirical value for τ_u [9].

However, for this technique to be applied more widely in our future work, the laboratory astrophysics team at IC must learn how to generate synthetic stellar spectra, and, though fitting them to data from astronomical observations, extract values for $\delta\log(gf)$. Training in this area thus formed the second part of SV5435.

2.2 Training in the modelling of stellar spectra

The GES line list team analyses stellar spectra with the Spectroscopy Made “Easy” (SME) code [14], which adopts a general non-linear least squares algorithm to fit synthetic stellar spectra to astronomical observations, and so extract key atomic and atmospheric parameters. These include atomic data, such as $\log(gf)$ s and van der Waals damping constants; atmospheric parameters, such as the effective stellar temperature, T_{eff} , and local gravity; elemental abundances; and radial, turbulent, and rotational velocities.

Radiative transfer is modelled with the assumption of local thermodynamic equilibrium (LTE), plane parallel geometry, no bulk flows, no molecular line opacity, and negligible magnetic field. The resulting atomic line profile fits are thus not strictly as accurate as would be obtained from state-of-the-art three-dimensional non-LTE (NLTE) models, but for simple fits of $\log(gf)$ s, as required here to obtain $\delta\log(gf)$ s and refined values of τ_u , these assumptions are reasonable.

During SV5435 the use of SME was discussed in detail, with Dr. Bergemann demonstrating all the key features of SME that would be required to fit $\log(gf)$ s to stellar spectra. In particular, Dr. Bergemann explained how to specify lists of target lines, define line fitting masks, include astronomical spectra, and run the fitting algorithms. Use of the SME graphical interface was also explained as a means to assessing the quality of both input fit parameters, and output line profiles.

The importance of examining the same target absorption lines in different types of stars, including, for example, metal-rich dwarves (e.g. the Sun), metal-poor dwarves (e.g. Mu Cassiopeiae), metal-rich giants (e.g. Mu Leonis), and metal-poor giants (e.g. Arcturus), was also emphasised. Various stellar parameters, particularly uncertainties in chemical abundances for different stars, affect the intensity of a line observed in a given spectrum. If errors in atomic data are to be identified and used to refine upper level lifetimes, systematic variations in $\delta\log(gf)$ s should be sought not just across different lines from the same upper level, but also across the same sets of lines in different stars.

Following this tuition, Dr. Ruffoni is now equipped with the latest version of SME, and stellar spectra of 16 different stars in the GES observation windows. Work began during SV5435 on modelling the profiles of Fe I lines of interest to GES, for which LIF upper level lifetime measurements are unavailable. This will continue at IC in conjunction with FT spectroscopy BF measurements.

Outcome of the visit

During SV5435, Dr. Ruffoni and Dr. Bergemann discussed key deficiencies in experimental $\log(gf)$ s in the atomic database. A campaign of measurements will take place at IC in the near future to ensure that these are addressed, allowing a more complete analysis of GES spectra in the future. Initially, this work will focus on providing new $\log(gf)$ s for the Fe I lines that were originally studied by May et al. [3]. Other Fe I lines of interest to GES will then be included in subsequent measurements, followed by measurements of lines from other chemical species, such as Si I and Ti I.

In the more distant future, measurements of hyper-fine structure (HFS) splitting of lines in the GES observation windows will further aid the analysis of GES spectra. Such measurements can also be conducted on the IC FT spectrometers [15].

In addition to this, Dr. Ruffoni is now able to model stellar line profiles with the SME code and fit $\delta\log(gf)$ s to observed absorption lines. This will allow the laboratory astrophysics team at IC to obtain experimental $\log(gf)$ s for lines where FT measured BFs are available, but LIF measurements of upper level lifetimes are not possible.

Future collaboration

Dr. Ruffoni and Dr. Bergemann are both co-investigators on the GES project and members of the GES line list team, and will continue to work together, and in collaboration with the rest of the GES community, on improving the GES line lists.

Specifically, we will continue to support the project by supplying high-precision, experimentally measured atomic data for the analysis of GES spectra. Initially, this will focus on providing accurate $\log(gf)$ s for Fe I, but will then be expanded to include other important elements; particularly Ti and Si. If further data requirements arise from the work of the GES community, these will be considered, and new measurements planned, where possible.

Projected Publications

- 1) Experimental Fe I $\log(gf)$ s derived from measurements of atomic transition probabilities [6]. This first paper will focus on improving data in May et al. [3]
- 2) A second paper will provide further experimental Fe I $\log(gf)$ s derived from experimental BFs and astronomically determined effective lifetimes. This publication will explicitly require the use of the SME code and the modelling techniques studied by Dr Ruffoni during SV5435.
- 3) Upon completion of the above, $\log(gf)$ measurements will be expanded to include other elements. At present, Ti and Si hold the greatest importance to GES after Fe I, and will therefore be targeted first. Additional publications will therefore be produced to report the $\log(gf)$ s obtained from these data.

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