Laboratory Astrophysics: from Observations to Interpretation
Proceedings IAU Symposium No. 350, 2019
F. Salama & H. Linnartz, eds.
doi:10.1017/S1743921320000642

Recent advances in experimental laboratory astrophysics for stellar astrophysics applications and future data needs

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Abstract. Accurate atomic data for line wavelengths, energy levels, line broadening such as hyperfine structure and isotope structure, and f-values, particularly for the line rich iron group elements, are needed for stellar astrophysics applications, and examples of recent measurements are given. These atomic data are essential for determination of elemental abundances in astronomical objects. With modern facilities, telescopes and spectrographs, access to under-explored regions (IR, UV, VUV), and improved stellar atmosphere models (3D, NLTE), and extremely large datasets, astronomers are tackling problems ranging from studying Galactic chemical evolution, to low mass stars and exoplanets. Such advances require improved accuracy and completeness of the atomic database for analyses of astrophysical spectra.

Keywords. atomic data, line: identification, line: profiles, instrumentation: spectrographs, Sun: abundances, stars: abundances, infrared: stars, ultraviolet: stars

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1. Introduction

The last few decades have seen a dramatic advance in the capabilities of ground and space based telescopes, giving astronomical, particularly stellar, spectra of unprecedented resolution and wavelength coverage from cutting edge spectrographs. These advances are only set to continue with new telescopes planned, such as ELT (Extremely Large Telescope). Examples of projects requiring a wide range of accurate atomic data are current and planned Galactic Surveys (Belmonte *et al.* 2018b) aimed at understanding galaxy evolution, analysing vast numbers of stars. These include the ongoing Gaia-ESO survey measuring spectra of 10^5 stars with the VLT (Very Large Telescope) (Heiter *et al.* 2015), APOGEE (Majewski *et al.* 2017) part of the Sloan Digital Sky Survey, WEAVE (Dalton *et al.* 2016) using the William Herschel Telescope, GALAH (Martell *et al.* 2017) at the AAT (Anglo-Australian Telescope) and 4MOST (de Jong *et al.* 2016) planned at the VISTA telescope in the Southern Hemisphere.

There has been, and continues to be, increasing demand from astronomers for atomic data of accuracy and completeness required for the interpretation of the astrophysical spectra that have been acquired at such great expense and effort. The atomic data used by astronomers (e.g. wavelengths, atomic energy levels and transition probabilities) were typically measured for the first time in laboratories using grating spectrographs in the decades of the 1930s-50s, and were sufficient at the time for astronomical purposes because of the limitations of astronomical instrumentation, particularly in terms of resolving power. However, the new instrumentation available to astronomers over the last couple of decades has led to exciting new high resolution spectra of astronomical objects, and to interpret these spectra a leap forward in resolution and accuracy of

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the atomic data was, and in many cases, still is required. In this Talk and Proceedings Review paper we take stock of the achievements of Laboratory Astrophysics in terms of the advances made in the new atomic data now available to astronomers for iron group element neutral, singly and doubly ionised species, and also look to future data needs.

2. The atomic data "wish list" of astronomers

In attending astronomy conferences over the years around the world, we have talked with many astronomers about what atomic data they need. The most common request has been 'everything' and 'now'. The Imperial College London Spectroscopy Group has over the past few decades focussed our research particularly on the relatively highly abundant line-rich iron-group (3d) elements (Belmonte *et al.* 2018a). The reason for this has been that these iron group elements are responsible for the majority of stellar opacity. The task facing the Imperial Group was immense. Astronomers wanted at least an order of magnitude, if not two orders of magnitude, improvement in accuracy of wavelengths, with corresponding improvement in atomic energy levels. Astronomers seek to identify lines in spectra, disentangle blends, and perform synthetic spectral fits to astrophysical spectra using state-of-the-art stellar atmosphere models and need an atomic data base that includes everything that might contribute to the spectrum. It was rather a shock, for example, 20 years ago in the case of the Hubble Space Telescope (HST), when many of the UV spectral lines were unidentified in stellar spectra, because the key atomic data was missing (Leckrone *et al.* 1999). This led to a large scale effort in laboratory and theoretical studies of the atomic data needed in the UV. But this situation of lack of atomic data is not a thing of the past (Pickering *et al.* 2011). The same scenario is repeating itself with missing data needed for interpretation of IR spectra, also still for VUV spectra, or recently also for fitting of lanthanide element lines in spectra of kilonovae, where laboratory measurements will allow improvement of the theoretical calculations needed for these large numbers of lines (J. Grumer, private comm. at IAU350S).

Accurate atomic data allow correct interpretation of complex line structures in astronomical spectra, and underpin reliable spectrum synthesis and chemical elemental abundance estimates. It is not possible to theoretically calculate atomic data with sufficient precision for analyses of high resolution astrophysical spectra.

3. The challenge

We began our contribution to the vast undertaking to improve the atomic database for astrophysics in the early 1990s. At that time the atomic data available to astronomers for the iron group elements had been recorded mainly in the 1930s and 40s up to 1970s and 80s, on grating spectrographs, and was commonly less accurate than the astronomical spectra they were being used to interpret (Kurucz 2002). The development of Fourier Transform (FT) spectroscopy, and the advent at Imperial College (IC) of the push to the first UV and then VUV FT spectrometers (Pickering 2002), together with suitable light sources, meant that we could meet the challenge of improving this atomic data base. The vast improvement in resolution between a grating and FT spectrum is seen in Figure 1.

At Imperial College we have been improving the accuracy and completeness of the atomic database by using our unique High Resolution VUV Fourier Transform Spectrometer (FTS), with world record short wavelength cut-off of 135 nm in the VUV. This spectrometer offers the ability to measure atomic spectra of resolving power up to 2 million at 200 nm. We are thus able to resolve the atomic emission lines we observe, and are limited by their Doppler width alone.

Our visible-VUV FTS provides wavelengths and energy levels accurate to at least a part in 10^7 (30 ms^{-1}, 0.15 mÅ at 1500 Å), loggfs (transition probabilities or 'f -values')

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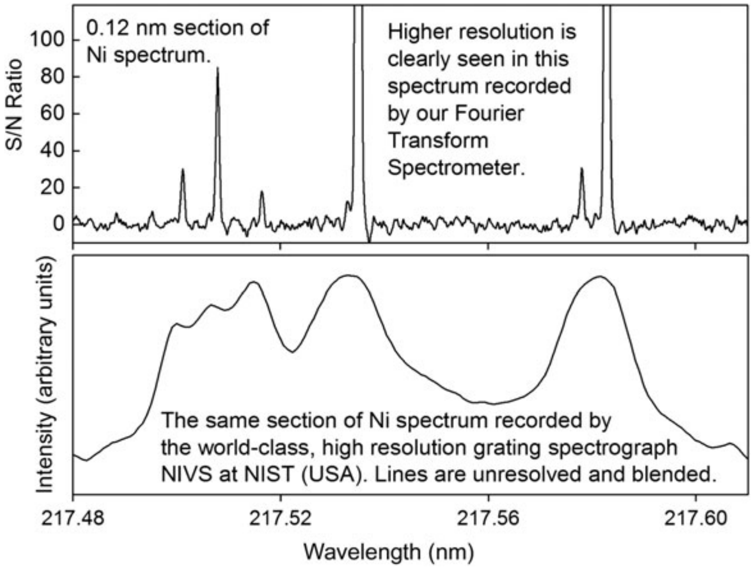

Figure 1. Improvement in resolution of FT spectroscopy over grating spectroscopy.

accurate to a few %, and resolved line broadening effects like isotope structure (IS) and hyperfine structure (HFS) (see Fig. 2), (Belmonte *et al.* 2018a; Pickering 2002). For readers less familiar with astrophysics applications it should be noted that $\log gf$, commonly used by astronomers is the $\log_{10}(g_i f_{ik})$, where $g_i = 2J_i + 1$ the statistical weight of the initial state, and f_{ik} is the transition oscillator strength..

The IC VUV FTS has a spectral range that is unique for an instrument of its kind 135 - 800 nm. This range covers most of the spectra of neutral, singly and doubly ionised iron group elements. We collaborate with other laboratories (e.g. NIST, USA, and Lund University, Sweden) to extend the spectral range we can measure at high resolution beyond our wavelength cut-offs in both the IR and VUV, for example, measuring with Gillian Nave at NIST for FT spectra in the IR, and beyond 135 nm at shorter wavelengths with grating spectroscopy which remains the best tool for that region. A stable light source is required for FT spectroscopy to avoid source noise, and we use water cooled hollow cathode lamps and a Penning discharge lamp (Belmonte *et al.* 2018a) with cathodes of the metal under investigation. Careful wavelength calibration (Ruffoni & Pickering (2010), Pickering 2002) and intensity calibration yield spectral linelists for a particular atomic species that we then use to improve the known atomic energy levels and also to search for new, previously unknown, energy levels.

In addition we can measure atomic transition probabilities (e.g. Pickering *et al.* 2001b; Ruffoni *et al.* 2014; Rhodin *et al.* 2017), but this was not the main topic of the lead author's talk at this Symposium, and is covered by Invited Speaker Prof Jim Lawler (see contribution by Lawler, this volume). We therefore do not cover the important topic of transition probabilities for astrophysics here in detail.

The wavelength and intensity calibrated linelists for a particular atomic species being investigated may contain many thousands of measured spectral emission lines, fully resolved. By a process known as 'Term Analysis' (Pickering & Thorne 1996; Liggins 2018) we systematically work through previously published energy levels, 'known levels', correcting their energies using a least squares fitting method. The previous energy levels may need very significant correction, commonly because of inaccuracies in calibration of the older grating spectra and their poorer resolution. In some cases incorrect energy levels are discarded, or their label descriptions need assignment or correction (see egs

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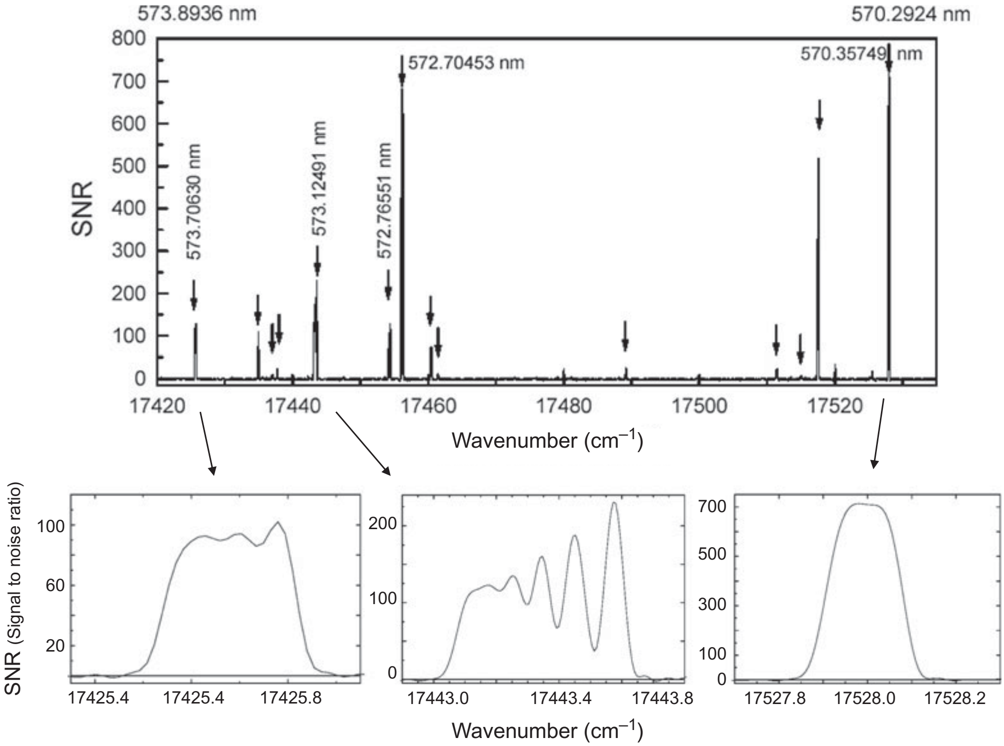

Figure 2. Examples of hyperfine structure seen in line profiles in the FT spectrum of vanadium, recorded at Imperial College.

in Pickering *et al.* 1998). We search for new atomic levels using our unidentified spectral lines and using theoretical calculations such as those of Kurucz (2019) as a guide. On finding new energy levels we assign atomic configuration and term ‘labels’ based on appropriate coupling descriptions, such as LS coupling or JK coupling. In some cases the number of known energy levels and identified lines can as much as double compared with previous studies (e.g. Pickering *et al.* 1998).

Where an atomic species exhibits hyperfine structure (HFS) in its spectrum, the high resolution of the FT spectrometers allows us to analyse the recorded line profiles to measure the hyperfine structure A splitting factors. This can be done for many hundreds of line profiles observed in an FT spectrum to give splitting factors for most known levels. These HFS data are very important for accurate estimates of stellar abundances (Bergemann *et al.* 2010; Lawler *et al.* 2018). Examples of transitions recorded using FT spectroscopy exhibiting a range of hyperfine splitting can be seen in Figure 2.

Our fundamental atomic data: wavelengths, atomic energy levels, information on relative line intensities, are then published and passed on to atomic data bases (such as NIST, VALD, Kurucz) for use by astronomers, often with the astronomers entirely unaware of the origin of these datasets and almost certainly not considering citing the original atomic data papers on which they are based.

4. Progress

There has been a sea change in the quality and quantity of atomic data available to astronomers for the iron group elements. We give here some highlights for the neutral, singly and doubly ionised species we have studied. For all species the studies listed below, undertaken by FT spectroscopy, represent an improvement in accuracy of wavelengths

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and energy levels of at least an order of magnitude, with typical wavelength and energy level uncertainties better than 1 part in 10^7, or a few mK (1 mK = 0.001 cm^{-1}), 0.1 mÅ.

4.1. *Cobalt*

Co I - 300 previously known energy levels were revised, and 64 new levels found, and the published linelist included 2442 classified lines (Pickering & Thorne 1996). The first very large scale investigation of HFS for a particular iron group element species using FT Spectroscopy led to new measurements, most for the first time, of HFS A splitting factors for 297 levels (Pickering 1996). These measurements involved the analysis of 1020 line profiles in the wavelength range 222 - 3000 nm.

Co II - 215 of the previously known energy levels were revised, and we found 222 new levels with the number of identified lines doubled (Pickering *et al.* 1998, Pickering 1998a; Pickering 1998b). Many of the new line identifications were particularly in the UV spectral region (Morton 2003). Our study of Co II HFS is in progress, but our measurements of HFS of key energy levels allowed new NLTE analyses of Co I and Co II lines in the spectra of cool stars, giving more accurate stellar cobalt abundance estimates (Bergemann *et al.* 2010).

Co III - our recent large scale term analysis (Smillie *et al.* 2016) used spectra recorded by FTS from 156 - 256 nm, yielding 514 accurate (0.2 mÅ at 2000 Å) classified lines, and with grating spectroscopy in the 131 - 250 nm region adding a further 240 classified lines. All these lines were used to optimise and improve the 287 known energy levels. Ritz wavelengths and calculated loggfs were also published.

4.2. *Manganese*

Mn I - the term analysis is almost completed, using the FT spectra recorded in the 152 - 5327 nm range (Blackwell-Whitehead (2003)), at IC in the visible - VUV and in the IR at NIST. The linelist currently contains 1284 classified lines, and we are finding new energy levels. Our large scale analysis of HFS in Mn I gave HFS A splitting factors for 106 levels, of which 67 were measured for the first time (Blackwell-Whitehead *et al.* 2005a). We measured new loggfs in the IR - UV (Blackwell-Whitehead *et al.* 2005b), and these, together with more accurate wavelengths and HFS information led to improved abundance determinations, for example a new Solar manganese abundance (Blackwell-Whitehead & Bergemann 2007). Further new atomic data in the IR were part of a project to allow atomic lines, rather than molecular lines, to be used to determine parameters such as effective temperature and metallicity in ultra cool dwarf stars and sub-stellar objects (Blackwell-Whitehead *et al.* 2011; Lyubchik *et al.* 2004).

Mn II - term analysis has been completed (Liggins 2018), with 477 levels revised, and 27 new levels, as well as 56 levels that had previously been found using stellar spectra now found accurately using high resolution FT laboratory spectra. Our results are in preparation for publication, to also include a linelist of 2360 classified lines, of which 1219 are measured by FTS at IC, with the remainder from grating measurements at NIST (Liggins *et al.* 2019). HFS splitting A factors for 47 levels were found using line profiles observed in our FT spectra (Townley-Smith *et al.* 2016).

Mn III - we have undertaken preliminary tests of Mn with a Penning light source, and are investigating how best to excite the spectrum for observation with FT Spectroscopy.

4.3. *Vanadium*

V I - FT spectra were recorded in the range 149 - 2860 nm, giving 3130 classified spectral lines. The subsequent term analysis led to 544 accurate energy levels, of which

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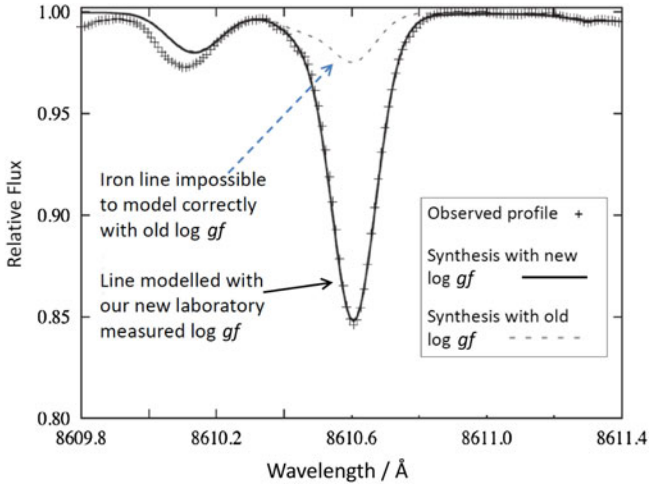

Figure 3. Example of the impact of new accurate laboratory loggfs for the Gaia GES survey, tested in the Solar spectrum. The new atomic data is now in the Gaia GES linelist.

89 were new, found for the first time (Thorne *et al.* 2011). We also measured transition probabilities for 208 lines in the range 304-2000 nm from 39 upper levels by combining our FTS measured relative line intensities and atomic level lifetimes, measured at Lund laser centre, (Holmes *et al.* 2016), increasing the number of laboratory loggfs available at longer wavelengths.

V II - our published linelist includes 1242 classified lines in the 149-580 nm range from FT spectra. We revised 409 energy levels and found 5 new levels (Thorne *et al.* 2013).

4.4. *Iron*

Fe I and Fe II - FT spectra measured at Imperial College were combined with iron spectra measured at Kitt Peak (USA) in a large analysis undertaken by Gillian Nave and Sveneric Johannson (Nave & Johansson 2013, Nave *et al.* 1994). This huge study gave revised and new energy levels of these important species.

At IC for iron we concentrated on measuring loggfs in challenging spectral regions, at long and short wavelengths. We measured the first loggfs to cover the large and key gap between 160 and 240 nm in Fe II (Pickering *et al.* 2001a; Pickering *et al.* 2002a), needed for HST spectral analyses in the UV and VUV. We also measured loggfs in the H band (Ruffoni *et al.* 2013), where few data exist, needed for the APOGEE project, and other previously unmeasured loggfs for the Gaia ESO survey (Ruffoni *et al.* 2014). An example of the impact of improved loggfs is seen in Figure 3. The APOGEE and Gaia ESO surveys include large scale chemical abundance measurements of thousands of stars to understand Galactic evolution. Our work, in collaboration with the groups of Gillian Nave (NIST) and Jim Lawler (Wisconsin), was highlighted in a Nature Editorial, where the Editors comment *'Some physicists are now pointing out the irony that multimillion-dollar projects, such as the SDSS, are producing data that cannot be analysed because of a failure to support much cheaper lab work on the ground'* (Nature 2013).

Fe III - spectra have been recorded with the IC FTS (see e.g. Fig. 4), and are supplemented with grating spectra recorded at NIST. We are using the resulting linelists from IR to VUV in ongoing term analysis to improve the atomic energy levels.

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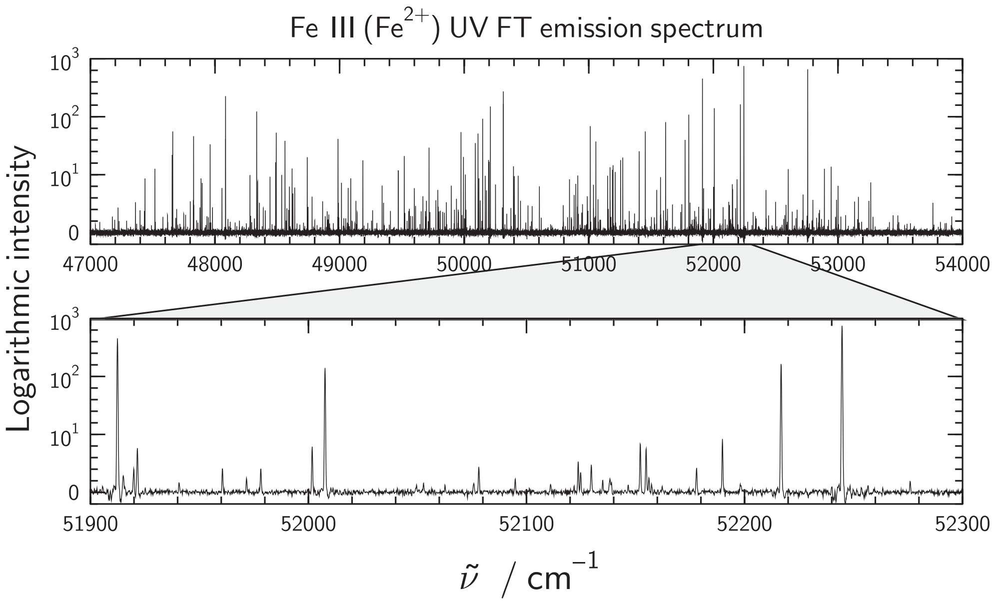

Figure 4. A broadband UV-VUV FT spectrum of Fe III, with a 1.4 nm section expanded, recorded at Imperial College London.

4.5. *Chromium*

Cr I - FT spectra recorded at IC in range 178 - 5590 nm are being used in term analysis of Cr I in collaboration with NIST, with new energy levels being found.
Cr II - term analysis was published by NIST (Sansonetti & Nave 2014).
Cr III - we measured the first high resolution spectrum in the VUV and have published an accurate linelist that can be used for calibration of VUV spectra (Smillie *et al.* 2008).

4.6. *Titanium*

Ti I - early FTS measurements at Kitt Peak (NSO, USA) from 300 - 5500 nm were used, supplemented by grating measurements at shorter wavelengths, in a term analysis undertaken in the Lund group in 1991 and later (Saloman 2012).
Ti II - this spectrum was also studied by the Lund Group, and their linelist has been included in a NIST compilation, however a full analysis of FTS spectra is still needed (Nave *et al.* 2017).
We made novel measurements in collaboration with NIST and Lund University of IR Ti I loggfs for applications in analyses of cool star spectra (Blackwell-Whitehead *et al.* 2006). We also made large scale measurement of transition probabilities in Ti II, publishing 624 measured loggfs for lines in range 187 - 602 nm (Pickering *et al.* 2001b, 2002b).

4.7. *Nickel*

Ni I - this was the earliest iron group element term analyses using FT spectroscopy from UV-IR 180 - 5500 nm. It was an international effort, using Kitt Peak IR-visible spectra, supplemented with UV FT spectra recorded at IC on the new instrument at the time, and the subsequent term analysis was done at Lund University (Litzen *et al.* 1993).

Ni II - our term analysis has recently been completed (Clear 2018) using newly recorded FT spectra in the 147 - 5555 nm range, and is in preparation for publication. We improved

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357 energy levels, and the linelist contains 1456 accurate FT measured lines. We are currently searching for new energy levels, with 22 levels found recently.

4.8. *Forbidden lines*

Our atomic data can also be used to improve the data for forbidden lines, that cannot be observed in the laboratory with our light sources, but are seen in astrophysical spectra, for example of supernovae and nebulae. We have published wavelengths with calculated loggfs for forbidden transitions for Co II and V II (Ruffoni & Pickering 2013), with similar data for Ni II, Mn I and Mn II in preparation.

5. Summary

There has been a sea change in the available atomic data for astronomers for the iron group element neutral, singly and to some extent doubly ionised, spectra. Our data are used by countless astronomers, often without their knowledge, in their stellar spectrum fits, be it for cool, hot, chemically peculiar or low mass stars, and in their abundance analyses from their studies of Galactic evolution to abundance analyses of host stars of exoplanets. Our work continues, often in collaboration, with NIST in particular. Similar atomic data advances are needed for higher ionisation stages, and for other elements, such as the lanthanides. Very importantly we need astronomers to tell us what atomic data they need, in detail, rather than *'everything'*. We welcome requests for atomic data. We thank STFC (UK) and The Royal Society (UK) for supporting this research.

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