



Article

The Belgian Repository of Fundamental Atomic Data and Stellar Spectra (BRASS) Identifying Fruitful Methods for Producing Atomic Data

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Abstract: The Belgian repository of fundamental atomic data and stellar spectra (BRASS) aims to provide the largest systematic and homogeneous quality assessment to-date of input atomic data required for stellar spectral synthesis. In addition to quality-assessed atomic data, BRASS shall also provide of a range of extremely high-quality benchmark stellar spectra spanning late B-type stars to early K-type stars. In this paper, we summarise the project's progress and available results to-date. We provide a brief comparison between our results and the BRASS project's compiled and cross-matched atomic literature, with the goal of providing useful feedback to the atomic community on which methods may produce more reliable and accurate atomic data. We hope that the examples presented here stimulate further investigation by the atomic physics community.

Keywords: atomic data; stellar spectra; oscillator strengths; atomic and molecular databases

1. Introduction

The Belgian repository of fundamental atomic data and stellar spectra (BRASS) aims to take the first, crucial steps towards constraining and removing systematic input errors from quantitative stellar spectroscopy [1]. The BRASS project shall perform a large-scale, homogeneous quality assessment of the atomic literature data by comparing state-of-the-art theoretical spectra against extremely high-quality observed stellar spectra. These comparisons will help to simultaneously constrain rest-wavelengths and oscillator strengths for a large number of neutral and ionic atomic transitions, spanning the optical wavelength range of 4200–6800 Å, which appears in the spectrum of late B-type to early K-type stars. In addition to quality-assessing atomic data, BRASS shall also provide a range of high-quality stellar spectra, of resolution $R \sim 85,000$ and signal–noise ratios of 200–1000, for the public to use. Both quality-assessed atomic data and high-quality stellar spectra will be combined together in a new interactive online database, currently under development at brass.sdf.org, which shall help astronomers and atomic physicists alike to identify spectral features and which atomic data are available.

To date, BRASS has retrieved, cleaned, and cross-matched atomic data from a number of atomic repositories (see Laverick et al. 2018a, henceforth Paper 1 [2]), and critically evaluated the literature data against the spectra of several G-type dwarf stars including the Sun (see Laverick et al. 2018b, henceforth Paper 2 [3]). Out of the 1099 investigated spectral lines, 383 were found to be reliable for spectral synthesis, and for these lines BRASS was able to evaluate the quality of available literature data, with the goal of improving input line lists for astronomers and providing valuable feedback to atomic physicists on which literature data performs better compared to stellar spectra. In this paper, we summarise the currently available results of the BRASS project so far (Section 2), and present a brief comparison of the literature data $\log(gf)$ values compared with benchmark $\log(gf)$ values for the 383 spectral lines (Section 3). We hope that the brief investigation presented here will encourage further, more in-depth study by atomic physicists into which data production methods lead to more accurate and reliable atomic data.

2. Availability of Results To-Date

2.1. Cross-Matched Literature

In 2016, in preparation for our quality assessment work, BRASS retrieved a “snapshot” of the available atomic literature from several atomic databases such as VALD [4], NIST [5], and providers within the VAMDC [6]. An input atomic data line list was compiled for BRASS in 2012, using older versions of VALD and NIST, and we also have access to the SpectroWeb line list, compiled in 2008. The retrieved atomic data was homogenised, cleaned, and cross-matched, as described in Paper 1, to compare the data of multiple literature occurrences of the same physical transition. The cross-match results revealed a general consensus on transition wavelengths and energy levels, but $\log(gf)$ values were shown to vary by as much as 2 dex for a number of transitions. The results of this literature cross-match are available to view at brass.sdf.org via the “line” tab. The data can be queried per species per wavelength interval, and can be presented either as a table of atomic data, or plotted as $\log(gf)_{brass}$ against $\Delta \log(gf)_{brass-database}$ for each retrieved database.

2.2. High-Quality Stellar Spectra

As implied by the project acronym, BRASS shall provide a significant number of high-quality stellar spectra for the community to use. The spectra are divided into two categories: *benchmark spectra* and *reference spectra*. The *benchmark spectra* are extremely high-quality observations of over 20 stellar objects, spanning late B-type stars to early K-type stars. These spectra were obtained through a dedicated observation program using the HERMES spectrograph mounted on the Mercator 1.2 m telescope, La Palma [7]. Through co-addition of multiple exposures taken throughout a single night, the merged spectra were able to reach a signal-to-noise ratio of $S/N \sim 800-1000$, which, when taken at the HERMES spectral resolution of $R \sim 85,000$, produces exquisite spectra with measurable spectral lines down to less than 1% of the normalised continuum. These benchmark spectra are used in the BRASS project to quality-assess the atomic literature. The *reference spectra* are a larger set of around 100 stellar spectra that sample the stellar parameter-space more finely than the benchmark stars. The majority of the reference spectra are taken using the MERCATOR-HERMES spectrograph with a small number extracted from the UVES-POP archive [8]. As a trade-off for their increased parameter-space coverage, the reference spectra have lower signal-to-noise ratios of $S/N \sim 200-500$.

Substantial work is currently under way to produce and publish online the science-ready, normalised benchmark and reference spectra. As of June 2018, several benchmark spectra are available to download via the website “download spectra” tab. The benchmark spectra are available in three forms: the extremely high-quality observed spectra, and the corresponding theoretical spectra in both broadened (to the resolution of the benchmark spectra) and unbroadened format. The benchmark spectra will be released progressively, and thus far, the benchmark spectra of stars with effective temperatures of $\sim 5000-6000$ K are available: *Eps Eri*, *70 Oph A*, *70 Vir*, *51 Peg*, *10 Tau*, and *Beta Com*.

2.3. Interactive Online Viewing

In addition to simply providing both quality-assessed atomic data and stellar spectra, BRASS aims to combine both aspects together in an online interactive interface. The coupling of such datasets in an online format has previously been implemented by SpectroWeb, the BRASS project's spiritual predecessor, as well as a similar line identification implementation by the NIST ASD, albeit aimed at reproducing laboratory spectra rather than stellar spectra. The completed website will allow users to view the available wavelength range for any benchmark or reference spectrum, alongside interactive labels for identified spectral features, investigated spectral lines, and quality-assessed transitions, that will provide additional atomic information. Our goal is that the BRASS website becomes a quick and reliable reference tool for astronomers to use to identify transitions in their own stellar spectra without requiring lengthy data downloads or software package installation.

The online spectra interface is currently under development, but a preliminary version is available via the website "spectra" tab. As of June 2018, several benchmark spectra are available to view interactively: the seven benchmark spectra used in our recent Paper 2 line analysis, the Neckel and Labs KPNO solar spectrum [9], and Mercator-HERMES benchmark spectra (currently unavailable for download) of *Arcturus*, *Procyon*, *68 Tau*, and *HR 7512*. An example of the spectral labelling is implemented for atomic lines that are theoretically deeper than 2% of the normalised continuum (blue labels) and for 1099 lines investigated as part of Paper 2 (red labels). It is important to emphasise that the spectra interface is still a work-in-progress and that we expect to implement a number of substantial changes in the coming year. For functionality and usage help, we refer readers to the "help" tab of the website which will provide the most up-to-date information.

2.4. Quality-Assessed Atomic Data

Undoubtedly, the most important aspect of the BRASS project are the quality assessments of the atomic literature data. Our recent quality assessment work and results for lines in G-type stellar spectra were presented at the EWASS 2018 special session: atomic and molecular data needs for astronomy and astrophysics, and details of our methods and results can be found in Paper 2. Almost 1100 atomic lines were investigated and 383 lines were found to be suitable for quality assessment and are thus recommended for stellar spectral synthesis work. The quality-assessment data are available in ascii-format via Paper 2 and the brass website via dedicated webpages for each of the 1099 investigated lines. Two examples can be found at the following links: [one link for a quality-assessed Fe I line](#), and [for a Fe I line that was not suitable for quality-assessment](#).

3. Comparisons Between the BRASS Results and Previously Retrieved Literature

By comparing the 383 quality assessed, best fitting $\log(gf)$ values from Paper 2 against literature $\log(gf)$ values, it is possible to gain knowledge into which atomic data measurements and calculations lead to more accurate and reliable $\log(gf)$ values. To demonstrate the how the project results can be utilised, we have briefly investigated the quality assessment results for any insights into which methodologies could potentially be exploited. Table 1 lists all the references for which we have two or more occurrences within our 383 quality-assessed lines. To quantify how well each reference set performed, we calculated a median from the absolute values of $\Delta \log(gf)_{lit-best}$ of all relevant lines the standard deviation of the $\Delta \log(gf)_{lit-best}$ values. Taking the median of the absolute values allows us to probe the general agreement between the literature dataset and the Paper 2 results, and thus we have ordered the table in ascending order with respect to this value.

We find that some of the best performing literature sets within the cross-matched data are actually sets of experimental data, producing accurate relative transition probabilities via branching fractions, that have later been rescaled using absolute oscillator strengths determined from newer, more accurate lifetime measurements. One clear example of such a correction are the oscillator strengths of Si I lines provided by Garz (1975) [10], which were later rescaled by O'Brian and Lawler (1991) [11]. Not only

do the majority of rescaled values produce great agreement with the Paper 2 results, but they also show substantial improvements in the median offsets compared to the unscaled sources. It is also worth noting that the unscaled sources exhibited a sizeable median offset but have relatively small standard deviations, suggesting that the distribution of relative $\log(gf)$ values is accurate, and a simple rescaling is appropriate. The re-scalings were all experimentally justified, thus it is promising that the astrophysically-derived values also detected similar offsets with respect to the unscaled sources, and could potentially be used to indicate other offsets in experimental data. We do, however, emphasise that our work entirely relies on the solar abundances of Asplund et al. (2009) [12], and as such it is possible that offsets could arise from these abundance values. Careful examination of the atomic data used in the solar abundance determinations, such as those listed by Scott et al. (2015) [13], is required before our detected offsets can truly be used to rescale experimental datasets. It is also worth noting the excellent agreement between the Paper 2 results and those of Melendez and Barbuy (2009) [14]. Melendez and Barbuy combined theoretical gf -values, for which multiplet line ratios are often reliable, with either: (a) experimental life-time measurements when available; or, failing that, (b) line profile measurements of the Hinkle et al. (2000) KPNO solar flux spectrum [15] to derive absolute gf -values for a large number of Fe II lines.

A somewhat surprising result is the agreement with the astrophysically-derived $\log(gf)$ values of Kostyk (1981, 1982a, 1982b) [16–18]. Both Kostyk and Paper 2 make use of equivalent widths to derive $\log(gf)$ values, but the implementation of the methods was expected to produce significant systematic differences. The works of Kostyk only employ one benchmark spectrum, the Liege solar spectrum atlas, whereas the Paper 2 analysis employs several benchmark spectra, including the Sun. Additionally, Kostyk makes use of the Holweger-Müller solar model using a solar micro-turbulence value of 0.8 km/s, whereas BRASS adopts the ATLAS9 atmospheric models using a solar micro-turbulence value of 1.1 km/s. Finally, Kostyk (1982a) determines a solar titanium abundance of $\log \epsilon_{Ti} = 4.83$, whereas Paper 2 adopts the Asplund et al. (2009) solar titanium abundance of $\log \epsilon_{Ti} = 4.93$, leading us to expect at least a systematic offset of roughly 0.1 dex between our results and the Kostyk (1982a) values. Despite the differences in implementation, we found the two sets of results to be in very good agreement, leading us to conclude that the multiple systematic differences between the methods have effectively cancelled each other out, leading to the derivation of the same absolute $\log(gf)$ values.

A polar opposite of the previous situation, we found that the calculations of fine-structure theoretical $\log(gf)$ values performed in Paper 1, derived from the TIPbase and TOPbase $\log(gf)$ values, performed poorly relative to the best-fitting $\log(gf)$ values. This is no doubt due to the fact that the original ab-initio single-configuration calculations of TIPbase and TOPbase made no attempt to account for fine-structure effects. More recent theoretical calculations make use of the multi-configuration Hartree–Fock method (MCHF), which accounts for configuration mixing that can lead to significant revision in $\log(gf)$ values on the order of a few dex. Given our findings, we do not recommend that fine-structure atomic data produced in the simplistic manner of Paper 1 be used for detailed spectral synthesis. It is worth noting that, due to the absence of any other alternative atomic data, the Asplund et al. (2009) solar abundance determinations of magnesium, aluminium, potassium, and calcium relied upon such calculations for the species Mg I, Al I, K I, and Ca II (detailed in [13]). Fortunately, the recent work of Pehlivan Rhodin et al. (2017) has produced new experimental measurements and theoretical calculations for a number of Mg I lines [19].

Table 1. Literature sources with data for two or more of the 383 recommended atomic lines present in G-type stellar spectra. References are sorted in ascending order according to the median of the absolute $\Delta \log(gf)$ between the given literature values and the best overall atomic data values. References with lines belonging to several species are denoted with *.

Literature Source	Species	N	Median $ \Delta \log(gf) $	Standard Deviation
Bard et al. (1991) rescaled using Den Hartog et al. (2014) [20,21]	Fe I	3	0.010	0.014
Sobeck et al. (2007) [22]	Cr I	14	0.020	0.055
Kostyk (1982a) [17]	Ti I	7	0.020	0.018
Garz (1973) rescaled using O'Brian and Lawler (1991) [10,11]	Si I	7	0.020	0.033
Blackwell et al. (1986) rescaled using Grevesse et al. (1989) [23,24]	Ti I	3	0.020	0.037
Kostyk (1982b) [18]	Ni I	30	0.025	0.034
Melendez and Barbuy (2009) [14]	Fe II	5	0.030	0.035
Lawler et al. (2013) [25]	Ti I	26	0.030	0.048
Blackwell et al. (1982) rescaled using O'Brian et al. (1991) [26,27]	Fe I	6	0.030	0.028
Bridges priv. comm. with NIST (1976) [5]	Cr I	12	0.040	0.036
Blackwell et al. (1982) [26]	Fe I	10	0.040	0.037
Bard and Kock (1994) [28]	Fe I	12	0.045	0.039
Blackwell et al. (1984) [29]	Cr I	2	0.050	0.050
Rescaled values of Lennard et al. (1975) [30]	Ni I	3	0.050	0.087
Kostyk (1981) [16]	Cr I	6	0.050	0.016
Smith and O'Neill (1975) [31]	Ca I	3	0.050	0.026
Blackwell et al. (1979) [32]	Fe I	3	0.050	0.029
Ryabchikova et al. (1999) [33]	Fe II	3	0.050	0.049
Martin et al. (1988) [34]	Cr I/Ti I/Mn I	22	0.055	0.070
Den Hartog et al. (2014) [21]	Fe I	12	0.055	0.095
Wood et al. (2014) [35]	Ni I	21	0.060	0.082
Bard and Kock (1994) rescaled using O'Brian et al. (1991) [27,28]	Fe I	3	0.060	0.025
Ruffoni et al. (2014) [36]	Fe I	11	0.070	0.083
O'Brian et al. (1991) [27]	Fe I	29	0.070	0.130
Bard et al. (1991) rescaled using O'Brian et al. (1991) [20,27]	Fe I	2	0.070	0.040
Raassen and Uylings (1998a) [37]	Fe II	7	0.070	0.049
Wood et al. (2013) [38]	Ti II	9	0.070	0.039
Bard et al. (1991) [20]	Fe I	3	0.070	0.037
Pickering et al. (2002) [39]	Ti II	8	0.075	0.129
Hannaford et al. (1982) [40]	Y II	2	0.075	0.045
Wickliffe and Lawler (1997) [41]	Ni I	3	0.080	0.038
Blackwell et al. (1986) [23]	Ti I	12	0.080	0.037
May et al. (1974) [42]	Fe I	82	0.080	0.096
Kostyk and Orlova (1983) [43]	Cr II/Ti II	3	0.090	0.074
Blackwell et al. (1980) [44]	Fe II	9	0.100	0.131
Kurucz and Bell (1995) [45]	Si I	7	0.100	0.033
Garz (1973) [10]	Si I	7	0.100	0.033
Wiese and Martin (1990) [46]	*	25	0.100	0.243
Fuhr et al. (1988) [47]	Fe I/Ni I	112	0.100	0.116
Raassen and Uylings (1998b) [48]	Cr II/Fe II	6	0.105	0.059
NIST (online values before 2004) [5]	*	63	0.110	0.119
Blackwell et al. (1982) [49]	Ti I	2	0.110	0.020
Kurucz (1999-2014) [50]	*	153	0.120	0.229
Schnabel et al. (2004) [51]	Fe II	4	0.125	0.183
Lobel (2011) [52]	*	212	0.130	0.212
Blackwell et al. (1983) [53]	Ti I	3	0.140	0.017
Biémont et al. (2011) [54]	Y II	2	0.140	0.010
Lennard et al. (1975) [30]	Ni I	2	0.145	0.145
Doerr and Kock (1985) [55]	Ni I	9	0.160	0.141
Fuhr and Wiese (1998) [56]	Ca I	3	0.190	0.179
Laverick et al. (2018a) [2]	*	64	0.340	1.232

4. Summary and Future Plans

In this paper, we summarise the status of the BRASS project to-date and we discuss a number of data-products already available to the astronomy and atomic physics communities. The cross-matched atomic literature, compiled in Paper 1, is available to query and view online at brass.sdf.org, with high-quality benchmark spectra and quality assessment results of Paper 2 are now available to download via the BRASS website. BRASS is currently developing an interactive online interface that will allow users to view stellar spectra alongside atomic data, of which a preliminary version can already be found online. To help users understand, interpret, and exploit the quality assessment results of Paper 2, we have developed a set of 1099 dedicated webpages for the spectral lines investigated.

We hope that by providing such information both astronomers and atomic physicists alike can fully comprehend and make use of the project results.

We also present a very brief literature comparison with the Paper 2 results to infer possible data production methods that may lead to improved atomic data in the future, and to stimulate further, more in-depth investigations by the atomic community. We summarise our findings and note that the combination of reliable relative line strengths and accurate absolute scaling seems to produce consistent results with the Paper 2 stellar derivations. The brief comparison presented here does not attempt to take into account uncertainties associated with the literature atomic data, but we do acknowledge the substantial efforts put into producing such values, especially for recent theoretical calculations (for a review on theoretical uncertainties, see Chung et al. 2016 [57]). To truly exploit the results of the project, and to use the quality assessment results to benchmark both experimental and theoretical methodologies, one should compare entire datasets against each other. Unfortunately, due to the compilation nature of the line lists and repositories such as VALD and NIST, the cross-matched atomic data do not contain multiple complete sources of atomic data. We hope that further, more in-depth investigations by the atomic data community can provide beneficial and valuable feedback on how to further improve atomic data.

In the coming year, BRASS aims to extend the work to cover a wider range of spectral types and atomic lines, and to investigate potential NLTE effects in hotter A- and B-type stars. A significant number of high-quality, science-ready, normalised stellar spectra will also be made publicly available through a new online interactive spectral database coupled with atomic data. Development will continue on the BRASS website and we aim for a full, working release by the end of 2019.

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