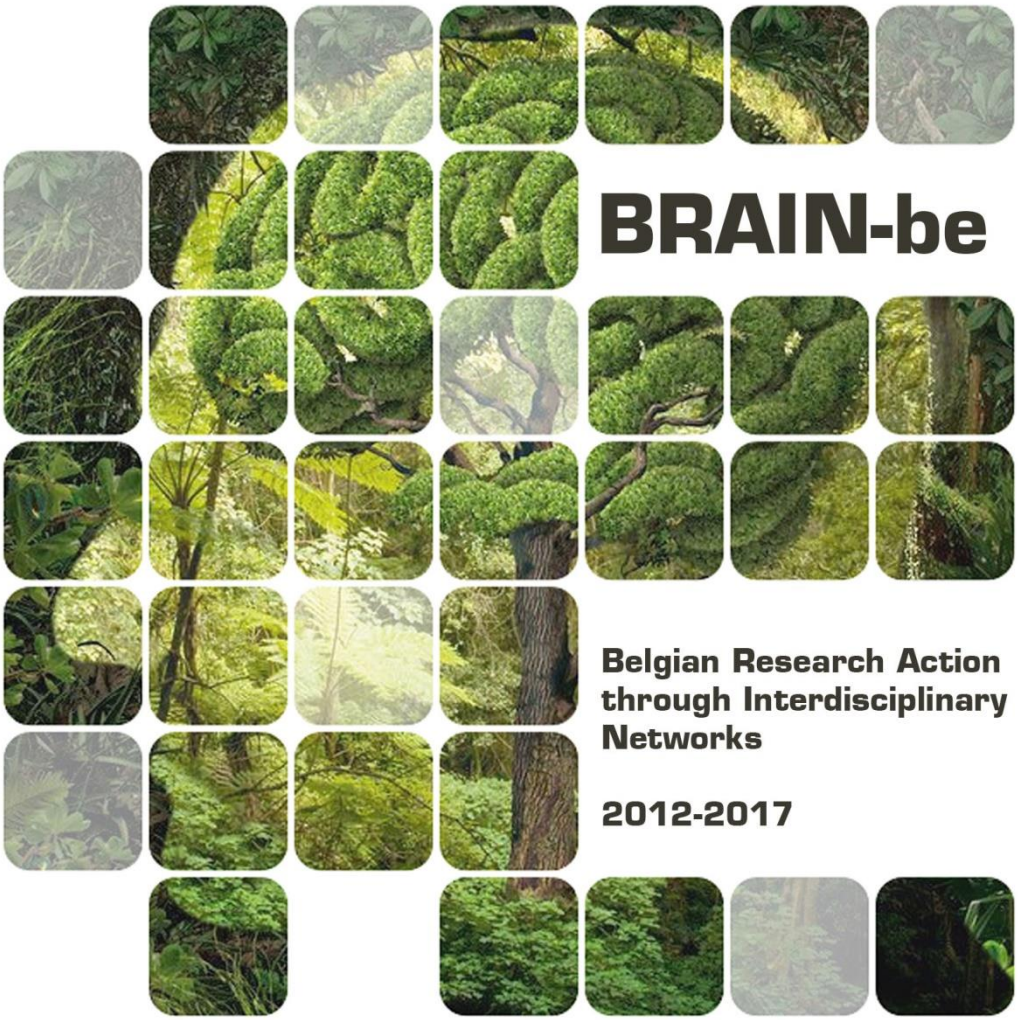

BRASS

The Belgian Repository of fundamental Atomic data and Stellar Spectra

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NETWORK PROJECT

BRASS

The Belgian Repository of fundamental Atomic data and Stellar Spectra

Contract - BR/143/A2/BRASS

FINAL REPORT

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TABLE OF CONTENTS

ABSTRACT

Context

Accurate atomic line transition data are fundamental input parameters in astrophysics. Spectrum synthesis calculations are of central importance for the development of complex models that describe, analyze and explain stars and planets, their internal structures, atmospheres, and evolution in relation to their environments. Uncertainties and errors in adopted fundamental atomic data may systematically propagate throughout all fields of astrophysics, from star-planet formation to large-scale galactic evolution. It is very difficult to obtain accurate fundamental atomic data of astrophysical interest from laboratory measurements. There are only a limited number of repositories that offer these important atomic data values. The atomic repositories are often complementary rather than redundant, and can provide incomplete or inaccurate information. Important quality assessments of the provided atomic data values are scarce (and mostly absent), which very much complicates the validation of results that follow from their application.

Conclusions

The BRASS project has produced important new results with the development of novel methods for the quality assessment of atomic line data central in modern astrophysical spectroscopic research. It provided accuracy assessment results of atomic log(*gf*)-values required for theoretical modelling of high-resolution stellar spectra using seven FGK-type benchmark stars including the Sun. Astrophysical log(*gf*)-values have been calculated for 1091 carefully selected un-blended line transitions between 420 nm and 680 nm using two different methods. The agreement between both methods selected 845 lines suitable for the atomic quality assessments. An investigation of mean Δlog(*gf*)-values revealed large differences for lines with limited atomic data quality offered in the literature for $-3 \leq \log(gf) \leq -0.5$.

The BRASS results showed that ~53% of the quality-assessable lines have at least one literature log(*gf*)-value in agreement with astrophysical values, while values for other lines can differ by more than 0.5 dex. Only ~38% of the investigated Fe I lines have sufficiently accurate literature log(*gf*)-values, while ~70%-75% for other Fe-group element lines. The large percentage of theoretical Fe I log(*gf*)-values with low quality offered in the literature mainly results from medium-strong and weak lines in atomic multiplets having lower transition levels above 4 eV, likely due to strong level mixing and inaccurate/incomplete energy levels. The results also revealed that the majority of $\Delta\lambda$-values are below ±0.01 Å, comparable to the high accuracy of the HERMES spectra wavelength scale.

The cross-matched atomic line datasets and the observed and theoretical stellar spectra have been incorporated in the online BRASS Data Interface (BDI). Users of the BRASS repository can query the Lines and Spectra BDI for atomic data downloading, including the corresponding literature references, with interactive display of dynamic plots for comparisons of database log(*gf*)-values. The Spectra BDI offers interactive display tools for the (observed and theoretical) benchmark spectra, combined with line identifications and atomic data values and line properties for user downloading. The BDI offers interactive atomic data quality assessment pages for the 1091 investigated spectral lines. It also offers tools for

interactive line equivalent width measurements and comprehensive help pages and tutorial videos to its users.

Keywords

Atomic transition data; Stars; Spectroscopy; Spectral lines; Databases

1. INTRODUCTION

Fundamental atomic transition data, such as line oscillator strength values are of central importance for determining the physical conditions in stellar atmospheres and for measuring their chemical compositions. In this report the atomic oscillator strengths or atomic transition probabilities are denoted as 'log(*gf*)-values'. Despite the significant work underway to produce these atomic data values for many astrophysically important ions, the uncertainties in these parameters remain large and can propagate throughout the entire field of astronomy.

The importance of accurate atomic data in astrophysical spectroscopy for understanding the chemical composition of the Universe cannot be overstated. Problems due to the limited quality of atomic data are frequently subject of intense scientific debate (Przybilla 2006; Bigot & Thevenin 2008; Lobel 2011; Pehlivan et al. 2015; Rauch et al. 2015). For example, improvements in both atomic data and spectral synthesis methods have led to significant revisions of the solar chemical composition with far-reaching impact for astronomical research (Grevesse & Sauval 1998; Caffau et al. 2008; Asplund et al. 2009; Caffau et al. 2011; Scott et al. 2015a; Scott et al. 2015b; Grevesse et al. 2015). Persistent uncertainties in these atomic data compilations have recently led to a variety of efforts for improving the atomic data quality of many ions with much-needed experimental data required for quantitative stellar spectroscopy (Wood et al. 2013; Lawler et al. 2015; Ruffoni et al. 2014; Belmonte et al. 2017).

With the fast advancements in scientific computing of the past few decades many more 'theoretical' (as opposed to laboratory or empirical) log(*gf*)-values have also become available, resulting from increasingly more complex atomic quantum physics calculations (Deb & Hibbert 2014; Ruczkowski et al. 2014; Bouazza et al. 2015; Castelli et al. 2015; Quinet et al. 2016). Online atomic data repositories developed over the last decades, such as the Vienna Atomic Line Database (VALD; Ryabchikova et al. 2015), the National Institute of Standards and Technology Atomic Spectra Database (NIST; Kramida et al. 2015), and providers within the Virtual Atomic and Molecular Data Centre (VAMDC; Dubernet et al. 2016) have considerably facilitated the user-retrieval of large amounts of atomic line data. However, despite the continual efforts for centralizing huge quantities of atomic data of interest to astrophysical spectroscopy, important information about the reliability and quality of the offered atomic data values remain poor and are mostly absent in the repositories and literature.

The Belgian Repository of fundamental Atomic data and Stellar Spectra (BRASS) project aims to provide a large systematic and homogeneous quality assessment of atomic line data required for quantitative stellar spectroscopy. BRASS compares theoretical spectrum calculations to very high-quality observed spectra of FGK-type stars in order to critically evaluate the atomic data of over a thousand atomic lines. In this report we discuss the detailed analysis of Mercator-HERMES benchmark spectra of FGK-type stars and the KPNO-FTS spectrum of the Sun. We present the results obtained in BRASS with the development of novel methods for assessing the quality of atomic log(*gf*)-values and line rest-wavelengths we have collected and combined for advanced theoretical spectrum calculations of the BRASS benchmark spectra. § 3 discusses new cross-matching methods for the atomic line data retrieved from a variety of databases and the literature for the

development of the Lines BRASS Data Interface (BDI). In § 3 we also present the BRASS benchmark spectrum modelling results of 1091 investigated atomic lines for the log(*gf*) accuracy assessment pages offered in the Spectra BDI. § 4 provides an overview of all BRASS results and its added value for astrophysical spectroscopy research. § 5 discusses the dissemination and valorisation of the BRASS project results. An overview of the BRASS publications is provided in § 6.

2. STATE OF THE ART AND OBJECTIVES

The main objective of BRASS was to properly assess the quality of input atomic data required in astrophysics research. In particular, atomic line transition data are fundamental parameters for quantitative stellar spectroscopy. Spectrum synthesis calculations are of central importance for the development of complex models that describe, analyze and explain stars and planets, their internal structures, atmospheres, and evolution in relation to their environments. Uncertainties and errors in adopted fundamental atomic data may systematically propagate throughout all fields of astrophysics, from star-planet formation to large-scale galactic evolution. Emphasis was set on the development and application of new methods for removing and reducing systematic errors in fundamental atomic datasets offered in the literature and the largest online repositories by comparing very high-quality observed stellar spectra with state-of-the-art theoretical spectra.

The importance of high-quality atomic data in astrophysics cannot be overstated. It is the subject of periodic international science symposia and workshops. Multiple authors have insisted on persistent issues with inaccurate fundamental atomic data and the lack of reference stars for validating the analysis methods over large stellar parameter spaces (Lee et al. 2008; Siebert et al., 2011; Jofré et al., 2014). Previous efforts to constrain errors in atomic data typically employ a few reference stellar spectra of comparable spectral types mostly observed with different instruments. They are also limited in wavelength coverage and spectral line types (Ryabchikova et al., 2008; Bautista et al., 2015). The objective of BRASS is to provide the largest systematic and homogeneous quality assessment of fundamental atomic data to date in terms of wavelengths and atomic species.

The objective of BRASS was to combine very high-quality stellar spectra, observed with modern high-resolution spectrographs, with carefully selected fundamental atomic data required for computing accurate theoretical stellar spectra. We compared the observed and theoretical spectra in detail on a line-by-line basis to assess the validity and quality of the selected atomic input data. The theoretical spectra were computed with state-of-the-art radiative transfer codes that utilize atmosphere models of stars of the K, G, F, A, & B spectral types. An important goal of BRASS was also to deliver an open dynamic data platform with standardized data representations allowing user-interaction with the integrated (hyper-linked) investigated atomic data, in combination with advanced graphics display tools that can offer powerful new functionalities for stellar spectroscopic research.

To achieve these goals the following questions were addressed:

(1) Can fundamental atomic data of central importance to astrophysical spectroscopic research, but scattered across a large variety of online data repositories and in the scientific literature, be combined in a single open access database? What methods are required for uniformly combining these datasets? This goal has been accomplished by developing two methods for ordering atomic line data according the traditional cross-matching method using transition wavelengths, and a more advanced novel approach that can account for unique electronic transition configuration information.

(2) Can fundamental atomic data available in the repositories and literature we combined be quality-assessed as they are mainly produced in laboratory measurements and/or

theoretical atomic structure and transition probability calculations with limited accuracies inherent to these (historical) production methods? This goal has been accomplished by offering atomic line data we thoroughly tested by comparing theoretical and observed stellar spectra. We performed extensive quality assessments of the selected atomic input data using advanced radiative transfer spectrum synthesis calculations we compare in detail to high-resolution Mercator-HERMES and ESO-VLT-UVES spectra of FGK-type stars observed with very large signal-to-noise ratios.

(3) Can the quality analysis results of the tested atomic data be comprehensively provided in a user-friendly open access way? This goal has been accomplished with the development of advanced online access infrastructure offering the quality assessment results together with all input data. The validated datasets, combined with the observed and theoretical spectra, are interactively offered at brass.sdf.org. The combination of stellar spectra and atomic line data is a novel approach for its development providing a universal reference for advanced stellar spectroscopic research.

By combining the atomic and spectroscopic data analyses for BRASS (i.e., using spectral line lists and high-quality benchmark stars) this project has established an extensive list of reference spectral lines suitable for the quality assessment of all retrieved atomic datasets. The objectives of the project have been accomplished by performing a systematic analysis of selected spectral lines for each benchmark star. This resulted in a final list of 1091 spectral lines that have been scrutinized and quantitatively compared between the various atomic data repositories and the stellar benchmark spectrum observations.

3. METHODOLOGY

3.1 BRASS Work-packages

The BRASS networking project was divided in four major Work Packages (WPs). The research work for WP1 and WP2 started early 2015. Preparatory work for WP3 and WP4 also started mid 2015 with an investigation of the various formats for atomic line data offered in a variety of online data repositories. The retrieval and archive compilation of all atomic data for BRASS required the definition of a standard protocol for collecting and storing the atomic datasets together with all available metadata. Algorithms for retrieving the atomic datasets from the providers (including some molecular-data providers) have been developed, implemented and tested. The processing of the atomic data updates continued in the course of project and was used for detailed synthetic stellar spectrum calculations. This research work was performed in preparation of the detailed line-by-line comparisons to observed Mercator-HERMES benchmark spectra for assessing the quality of the atomic input data which began to be incorporated in the online BRASS database early 2017.

BRASS was organized in four WPs (Figure 1) with full or partial contributions from the project partners, collaborators, and the members of the follow-up committee according their scientific and/or technical expertise.

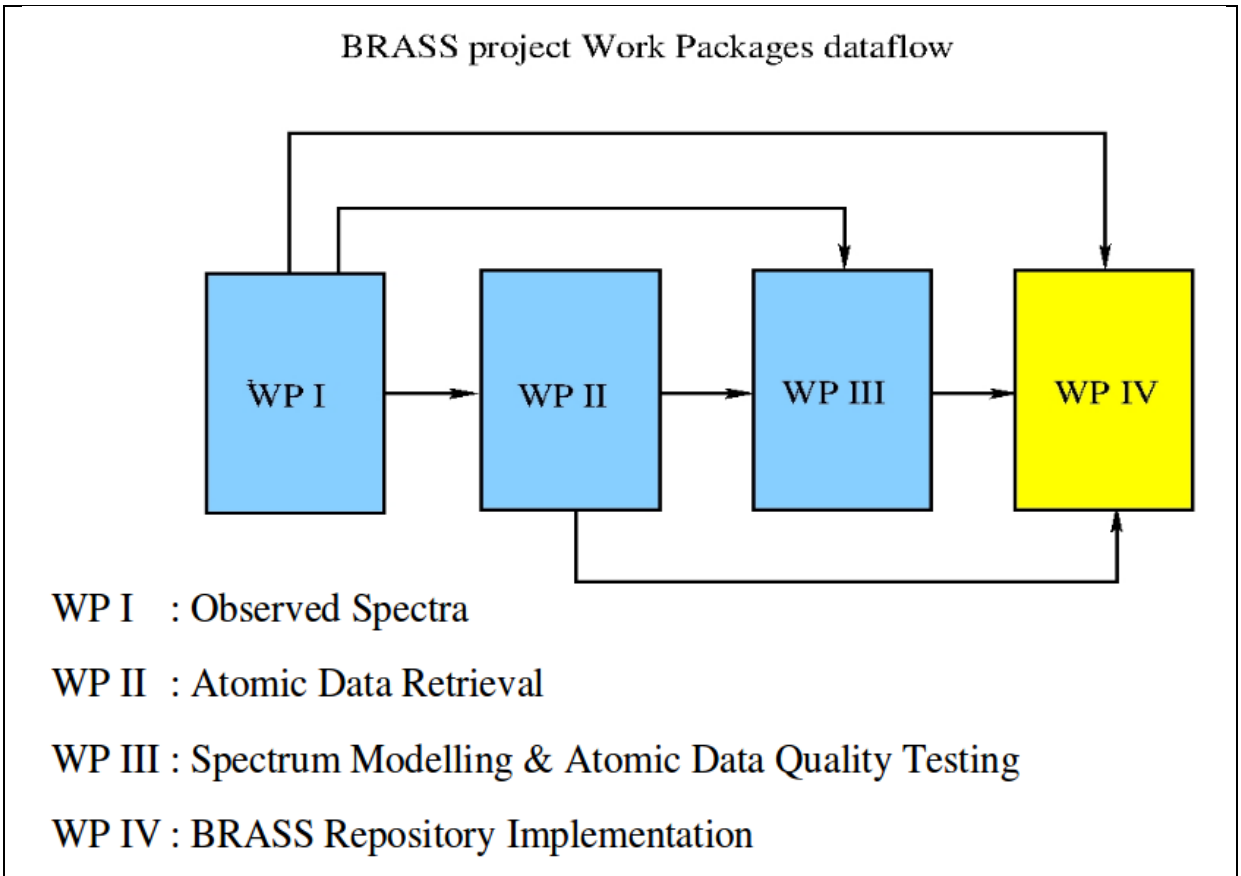


Figure 1. Daisy-chained dataflow between the four BRASS Work Packages (WP I - IV). Tasks within some of the WPs sequentially overlap in time. Only WP IV (yellow panel) received input data from all WPs.

3.2 WP I: Observed Spectra

The BRASS project relied on the availability of very high-quality stellar spectra previously observed with the HERMES spectrograph of the Mercator telescope at La Palma, and with the UVES spectrograph of the ESO-Very Large Telescope in Chile. Advanced calibration pipelines have been developed for producing the final HERMES and UVES spectra. For this purpose a number of instrumental effects had to be removed from the final data products. Only after completing these processing steps the final HERMES and UVES spectra could be fully exploited for BRASS.

An important challenge of the BRASS project was the development of automated procedures for each processing step in the four WPs. Reliable data-processing methods have been developed and efficient procedures were implemented for adequate quality assessments of all intermediate and final BRASS data products.

The main tasks accomplished for WP I encompass:

(i) *Selection of appropriate observations*
The selection was mainly based on the spectral S/N ratios. Saturated spectral regions have been masked out and only observations with large S/N ratios in at least a part of the wavelength range were retained. For bright stars, it was possible to combine one part of a long exposure that was partially saturated with another wavelength portion of a shorter, but unsaturated, exposure.

(ii) *Removal of cosmic rays*
The HERMES calibration pipeline is known to leave a large number of CCD cosmic ray hits, not properly removed from the final 1D-spectra. The BRASS project developed special software tools for removing the remaining cosmic ray flux spikes in the final spectra.

(iii) *Response correction*
The spectral response function of the HERMES spectrograph exhibits strong wavelength dependence but also some time-variability. However, spectra with regular and smooth continuum flux shapes are required for performing automatic spectrum continuum normalization calculations (see § 3.7). Consequently, all signatures of the instrument's response had to be removed from the spectra. However, the time-dependence of the response function also introduced a considerable degree of complexity. For the BRASS project new pipeline algorithms were developed for determining the response correction curve at every point in time from previous calibration observations.

(iv) *Identification of spectra that can be merged, per target and per spectral type*
The BRASS project has created an inventory of spectra of sufficiently large S/N ratios for co-addition into template spectra. Statistical methods for calculating the templates using spectra from different observing epochs were developed to ensure the final co-added spectra are comparable within given tolerance values.

3.3 Re-calibration of VLT-UVES spectra for BRASS

The BRASS spectra also incorporated stars observed with the ESO-VLT-UVES in the Southern Hemisphere. Calibrated UVES spectra are offered in the ESO Data Archive (Paranal Observatory Project - POP Archive). However, many ESO-UVES Archive products have been previously processed using non-optimal (outdated) calibration images from a database of calibration frames. In the best cases the archive offers sub-optimal quality spectra, and for worse cases, the used calibration frames introduce spurious artefacts and incorrect wavelength shifts in the provided spectra.

For the re-calibration research of UVES-POP spectra for BRASS, the international partner Dr. C. Martayan of ESO first retrieved all un-calibrated (raw) POP observations from the ESO Data Archive. He also collected all calibration frames observed closest in time to the POP observations. It is important to note that the retrieved calibration files may not be the best for re-calibration as at the time of the actual POP observations a properly defined UVES calibration pipeline did not (yet) exist. Moreover, it remains uncertain if these files contain the same calibration data used for the subsequent POP calibrations because no further information was provided in the ESO-POP publication (Bagnulo et al., 2003).

Next Dr. Martayan re-calibrated the raw POP science data using the latest UVES pipeline version (v5.5.7). He compared the results with the spectra of the POP Archive which used UVES pipeline version v1.2.0. The detailed comparison considered the signal-to-noise ratios of the final UVES spectra, the wavelength scale, the amplitude of spurious flux ripples, and the quality of merging the échelle orders. He also compared the results with spectra of the ESO External Data Product Archive which were more recently calibrated by ESO's QC/Archive Group using the Basic Master Database of basic parameters. The EDP spectra have been provided by ESO as "science-ready" spectra to the scientific community.

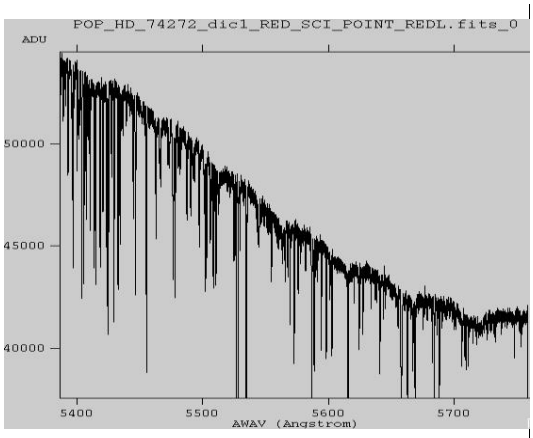
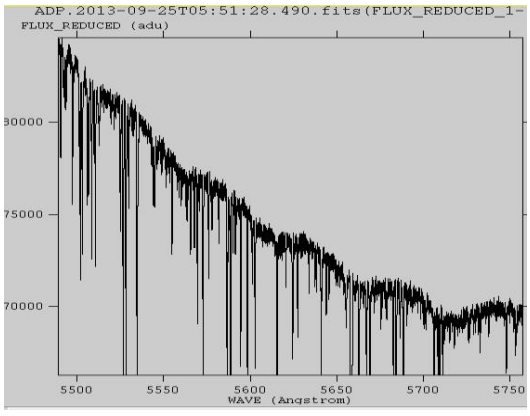
Comparing the resulting signal-to-noise ratios Dr. Martayan found that using the same calibration algorithms as POP, a small improvement of up to 5% could be obtained for the BRASS re-calibrations. However, major improvements were observed for the UVES flux ripples and échelle order-merging. The flux ripples in the re-calibrated spectra are ~5 times weaker. This allowed him to calculate order-merged spectra, while the ESO-POP Archive spectra can only be used order-by-order. The comparison of radial velocities revealed a difference of 13-15 km/s between the re-calibrated spectra and the POP spectra because the heliocentric velocity was not applied. After heliocentric correction the radial velocities are identical. The RMS error of the BRASS UVES wavelength solution was 106 m/s.

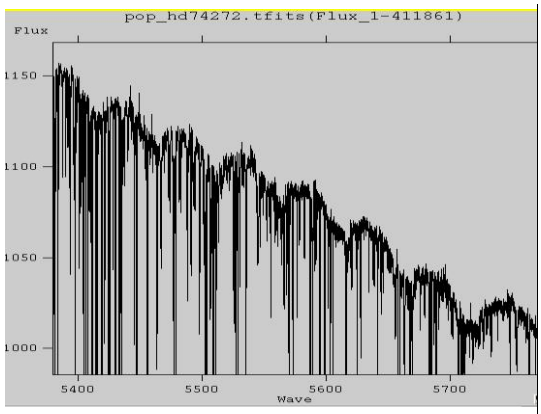
The comparison of the manually re-calibrated UVES-POP spectra with those provided in the ESO External Data Products Archive showed that the spurious flux ripples were properly corrected in both cases but that the S/N ratios were 15% - 50% smaller compared to the BRASS results. The BRASS re-calibration results for the spectrum of n Vel are shown in Figure 2 and compared to the ESO-ADP calibration and the original ESO-UVES-POP calibration.

3.4 Wavelength calibration of UVES spectra for BRASS

Dr. Martayan is an ESO instrument specialist. He provided re-calibrations of selected UVES stellar spectra for BRASS by correcting for many of the problems observed in the standard ESO-UVES reduction pipeline. To reach sufficiently large S/N ratios each star was observed

multiple times and he performed new calibrations of each individual spectrum. Next Dr. P. van Hoof of the Royal Obs. of Belgium further investigated these datasets. He first co-added the spectra and next compiled an assessment of the quality of the resulting sum spectra. This consisted of a measurement of the S/N ratios in each of the spectra as well as an extensive analysis of the quality of the wavelength calibration by comparing the observed wavelengths of telluric (Earth) lines with laboratory wavelengths in the HITRAN database (see bottom panels of Figure 3). The S/N ratios in the combined spectra typically ranged between 400 and 500 with some outliers in each direction.

	BRASS calibration
	ESO-Advanced Data Products calibration



ESO-UVES-POP calibration

Figure 2. The top panel shows the BRASS calibration of the ESO-UVES-POP spectrum of n Vel using the latest version of the UVES reduction pipeline and the best calibration frames. It considerably decreased the flux ripples observed in the ESO-ADP (*middle panel*) and original POP calibrations (*bottom panel*). The latter spectra show larger flux variations using older UVES pipeline versions and unknown (un-adapted) and ADP master calibration frames. The BRASS calibrations provided the best S/N ratios, 15% - 50% better than the available ESO-ADP calibrations.

The analysis results of Dr. van Hoof of the wavelength scale accuracy showed standard deviations between 70 and 240 m/s which were satisfactory for BRASS. Dr. van Hoof also conducted a literature study of the stars in the sample to search for possible anomalies. Based on this research work two stars were excluded from the initial UVES sample; one because it was a SB2 type spectroscopic binary, and another because it revealed an HgMnSi chemical abundances anomaly.

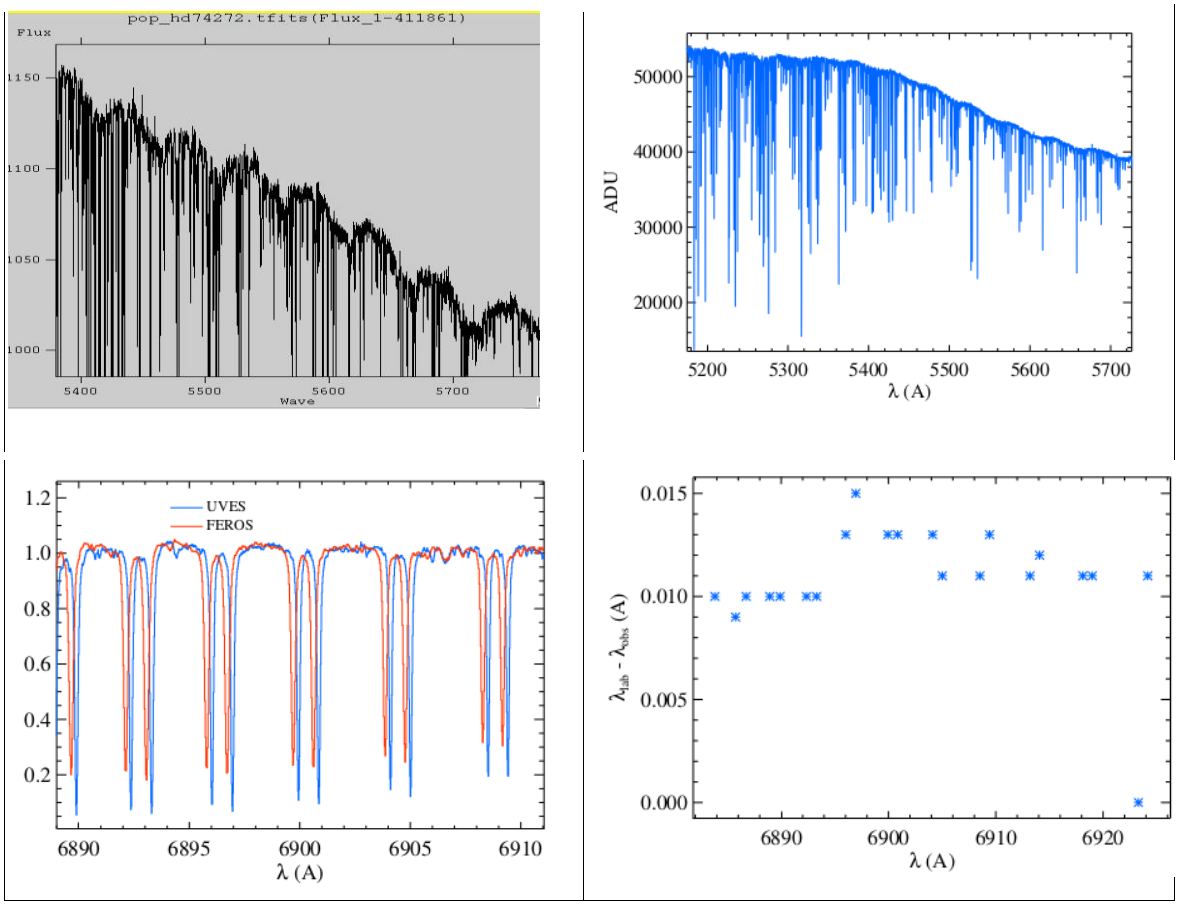


Figure 3. The top right-hand panel shows the BRASS re-calibration of the ESO-VLT-UVES POP spectrum of the star e Vel using the latest version of the UVES reduction pipeline and the best calibration frames. The top left-hand panel shows the spectrum of n Vel calibrated with the older ESO UVES pipeline. It reveals large flux variations (continuum rippling) using older UVES pipeline versions. The BRASS re-calibrations of the UVES spectra considerably reduce these disturbing flux ripples. The BRASS UVES calibrations provide the best SNRs, 15% to 50% better than the available ESO UVES spectrum calibrations. The bottom panels show an example of the analysis of the quality of the BRASS wavelength re-calibrations by comparing the observed wavelengths of telluric lines (i.e., the sharp near-IR O_2 doublets in ESO-UVES and ESO-FEROS spectra of L Car in the bottom left-hand panel) with their laboratory wavelengths provided in the HITRAN database. The observed wavelength differences stay below 0.015 Å as is shown in the bottom right-hand panel.

3.5 HERMES response curve for BRASS spectra

In 2017 Dr. T Merle of Univ. Libre de Bruxelles started an investigation of the instrumental response curve of the Mercator-HERMES spectrograph with the goal of enhancing the calibration of spectra merged for BRASS by recovering the continuum shape of each spectrum. This facilitated the next step of flux continuum normalizing the selected spectra. In summary, the merged spectrum of a HERMES science target was corrected for:

1. effects of the flat-field lamp continuum,
2. earth's atmospheric absorption,
3. instrumental response or CCD detector sensitivity curve.

Items 1 and 2 were straightforward to achieve, while 3 required more consideration of additional reference A- and B-type stars observed the same night as the science target. The research work of Dr. Merle is illustrated in Figure 4 for the merged spectra (top panel) and the spectra corrected for the instrumental response (two bottom panels). More details are provided in the figure caption. The method for modelling the instrumental response curve was crucial for performing the spectrum continuum normalization of sufficiently good quality including in small wavelength regions (see Merle et al. 2018).

In 2017 Dr. M. Van der Swaelmen of Univ. Libre de Bruxelles investigated the co-addition of Mercator-HERMES spectra of F-, G-, and K-type stars for BRASS. Figure 5 shows an example of the spectrum co-addition results for the F-type star 95 Virgo. Six HERMES observations have been co-added for calculating the black drawn spectrum. The procedure of spectrum “stacking” consisted of discarding outliers by sigma-clipping at a given wavelength, and next by averaging the selected fluxes. While the S/N ratios of individual spectra remained below 200 in most cases, the S/N ratios of the stacked spectrum can reach 340, or the large S/N ratios required for BRASS. Moreover, this sigma-clipping method allowed Dr. Van der Swaelmen to remove all remaining hot pixels due to cosmic ray hits on the CCD and to obtain a high-quality final product suited for advanced spectroscopic applications (such as the determination of stellar parameters, chemical abundance values, etc). These tests also showed that it is possible to successfully apply the ESO-developed software tool molecfit for removing telluric lines and features from HERMES spectra. This is important for producing science-ready spectra (400 nm to 680 nm) without introducing altered flux levels at telluric line wavelengths in the BRASS spectra.

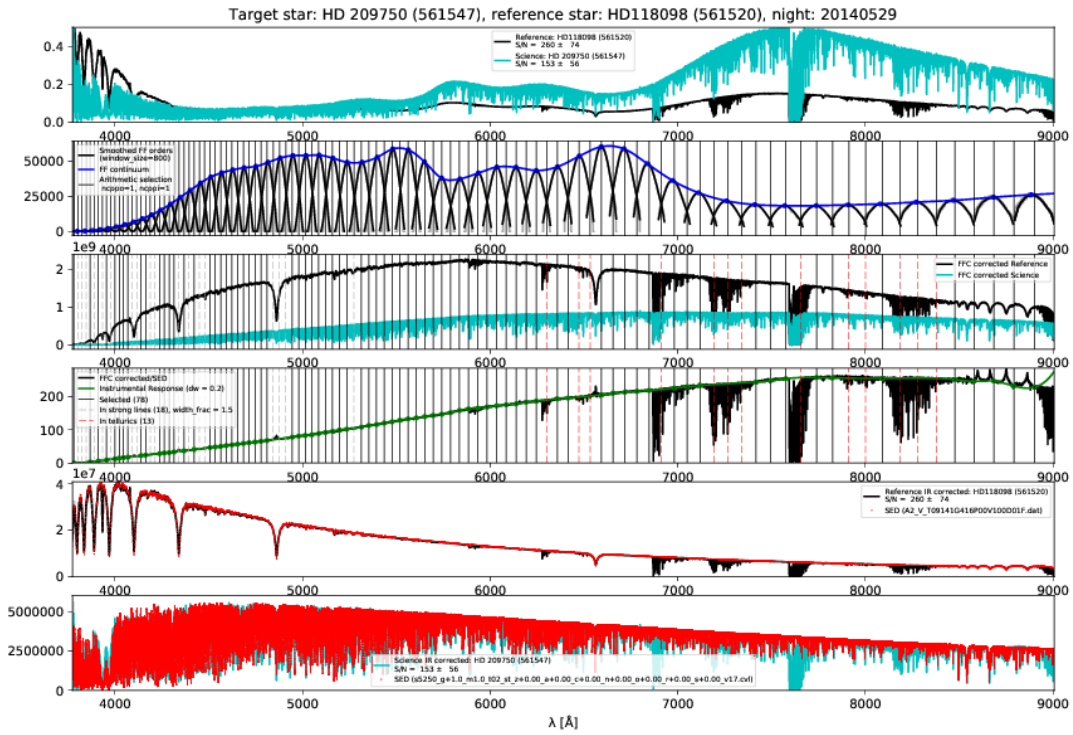


Figure 4. The top panel shows for a given night, the science (*cyan drawn line*) and the reference (*black*) HERMES spectra. The second panel from the top shows the flat-fields (*grey*) and a smoother version of them (*black*) for each HERMES échelle order. The maximum values of each order are used for modelling the global shape of the flat-field continuum (*blue line*). The third panel shows the science and reference spectra corrected for the flat-field continuum. By dividing the reference spectrum in the third panel, with a synthetic spectrum of it (*red curve in the fifth panel*), the black curve in the fourth panel is calculated. By using a criterion based on the HERMES orders (one point per order and inter-order marked with vertical lines in the second panel) continuum points were selected by excluding the ones falling in strong and broad Hydrogen lines (*vertical dashed drawn grey lines*) and in telluric lines (*vertical dashed red*). A spline interpolation was used to model the instrumental response curve (*green line*). The reference (*black drawn*) and science (*cyan*) spectra corrected for the instrumental response curve are displayed in panels five and six, respectively. For assessing the quality of this correction the science spectrum was compared to a synthetic one of similar spectral resolution (*red curve in bottom panel*).

3.6 Development of automatic spectrum flux spike removal tool

An automatic removal tool of spurious flux spikes was developed by Mr. M. Laverick PhD student of KU Leuven and Royal Obs. of Belgium as part of the processing required for the HERMES spectra in BRASS. The removal tool `BRASSGLITCH` was designed to accurately remove bad data with minimal damage to the true stellar spectra. `BRASSGLITCH` operates on re-sampled, order-merged spectra, however it could be expanded to operate on individual orders in pixel-space for greatly improving its detection efficiency. The tool has been

implemented in the latest HERMES data reduction pipeline to help improving the quality of all Mercator-HERMES spectra.

Large-scale testing of BRASSGLITCH has been performed for over 3500 HERMES spectra of objects with spectral types ranging from O to M, and with S/N ratios ranging from 50 to 350. The test database provided adequate diversity for assessing the performance and limitations of BRASSGLITCH, including possible damage to spectra and spike detection efficiency. The testing was performed for a range of spectral types (O to M), for spectra containing few to many glitches. It was extensively tested on spectra with average S/N ratios above 100 in accordance with the BRASS goals.

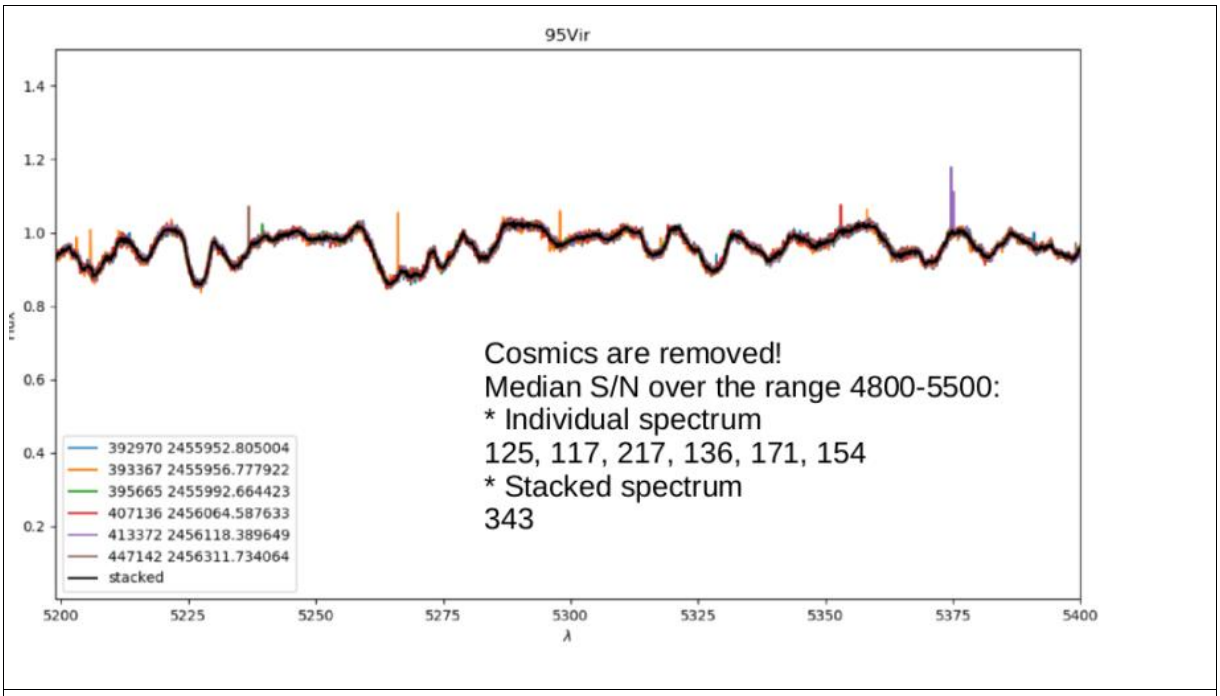


Figure 5. Example of spectrum co-addition for BRASS around 5300 Å of 95 Vir. Observations at different epochs are shown in legend with coloured lines, while the black drawn line is the stacked final spectrum. The stacking procedure also removed remaining cosmic hits that could not be removed by preceding spectrum cleaning operations. The noise level clearly decreases in the final sum spectrum compared to the individual epoch observations.

It was found that BRASSGLITCH performed exceptionally well on the hot stars of spectral types O to F, and reasonably well on cooler stars of spectral types G to M. The hotter stars usually contain fewer metallic and molecular absorption bands hence the local statistics of the flux tend to vary much less. The stability of the local statistics makes it much easier for a sharp flux spike to be identified. Hotter stars tend to flag more glitches than cool stars because of this. The flux spikes were correctly detected despite their close proximity to absorption lines/features demonstrating the quality of the new spike removal tool. The tests also showed that the impact on true stellar spectra stayed negligible and the detection of cosmic glitches was thorough.

3.7 Spectrum continuum normalization procedure for BRASS

The observed BRASS spectra have been automatically continuum flux normalized using a special 'template normalization' procedure Dr. A. Lobel of the Royal Obs. of Belgium developed for BRASS. It searches for variable wavelength points over sufficiently continuous flux regions close to the stellar continuum level in the theoretical spectra for folding the observed spectra to these (continuum anchor) points. The re-normalization step repeats each time the astrophysical parameters (APs) are updated during the best fit iteration procedure. It ensures that local flux normalization effects become minimized and the continuum normalization around the lines selected for evaluating the quality of atomic line data is consistent with the APs determined from the diagnostic spectral lines set.

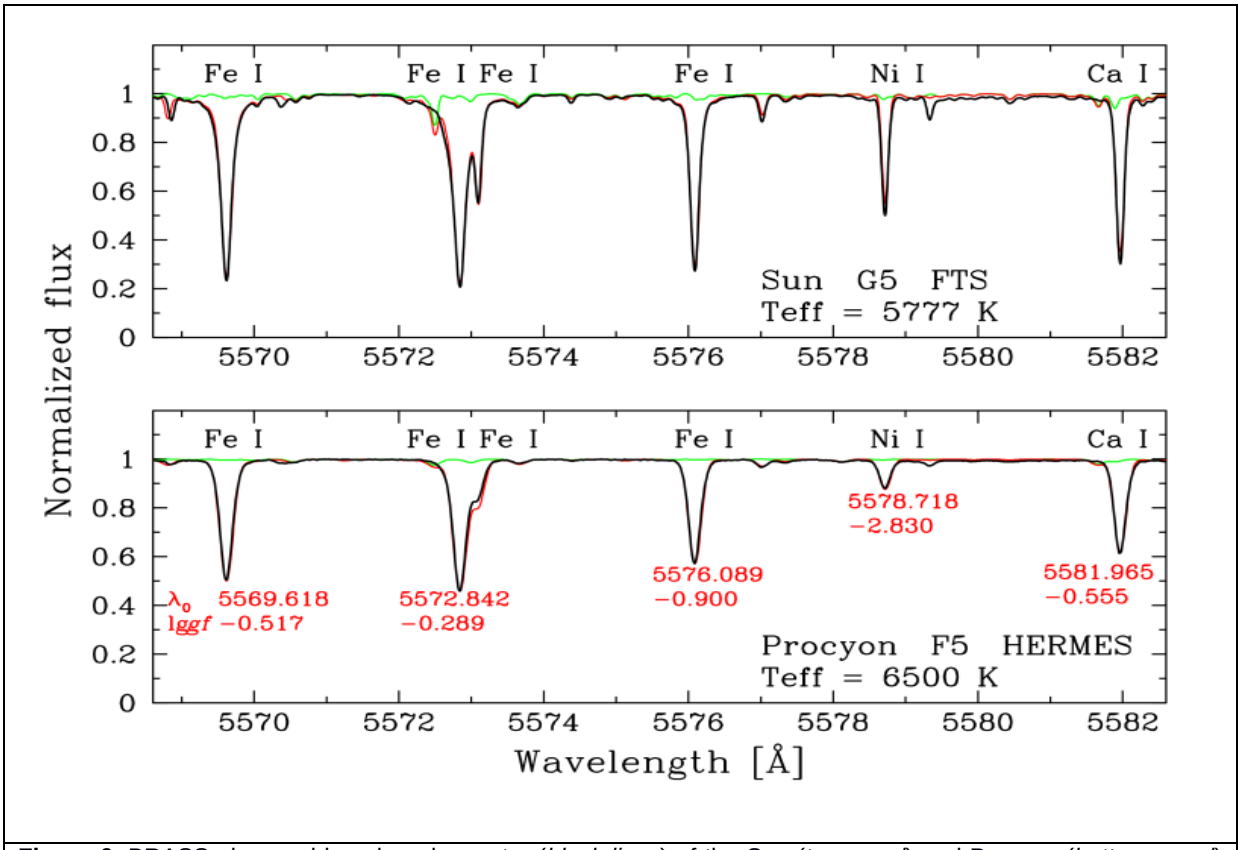


Figure 6. BRASS observed benchmark spectra (*black lines*) of the Sun (*top panel*) and Procyon (*bottom panel*) are shown over ~15 Å with marked respectively medium-strong and weak neutral metal absorption lines. The theoretical spectra calculated with published atomic line data values of λ_0 and log*gf* are listed in red below the lines in the bottom panel and provide the best fit (*red lines)* to the observed spectra. The green drawn lines show the synthetic spectra calculated without these neutral lines. They reveal the lines are not significantly blending together with strong background lines that can complicate the best line fit procedure and the proper selection of atomic input data.

Dr. H. Hensberge of the Royal Obs. of Belgium also continuum normalized five HERMES spectra of the star DV Cam using the ESO-Midas software. He installed the package for interactively normalizing the spectra and to investigate the quality of this procedure. The goal was to compare with the automatic normalization procedure for BRASS reference spectra. His investigation was also useful to test if the ESO-POP spectra re-calibrations using the ESO-UVES pipeline could be further improved.

Dr. M. David of the Univ. of Antwerp and Dr. Hensberge of the BRASS follow-up committee also provided important scientific feed-back for the preparation of BRASS publications. For example, in connection with the FGK spectra for BRASS they advised that: “The possibility of co-adding spectra of the same object was mentioned during the BRASS annual meeting. This should be approached with the utmost care, lest the nominally increased S/N ratio creates a false sense of security. In fact, co-addition will truly improve the quality of the spectrum only if the flux difference between co-added spectrum bins consists of a continuum difference and “pure noise”. Often in high-S/N spectra, noise is the least of our worries (since we have statistical tools to deal with it properly) while other errors (e.g., some slight wavelength shift or difference in wavelength calibration between the spectra to be used) are better detectable if the spectra are kept separate. In any case, even though tests (to verify that co-addition is safe) probably require the spectra to be normalized.” They advised to perform the actual co-addition on the non-normalized spectra because each normalization may add some weak low-frequency flux error of its own.

3.8 WP II Atomic Data Retrieval

3.8.1 Astrophysical Parameters

Dr. Lobel of Royal Obs. of Belgium developed a suite of computer codes (called `BRASSAPS`) for the semi-automatic determination of astrophysical parameters (APs) and chemical composition of BRASS benchmark spectra. It requires three subsequent major computational steps. First the pre-processor estimates the APs using a limited number of diagnostic H Balmer, Fe, and Mg absorption lines. The second pipeline step iterates over Teff, surface gravity (log*g*), microturbulence velocity (ζμ), and mean metallicity [*M*/H] until the best fit is found to the detailed shapes of a set of diagnostic photospheric lines having reliable atomic data values of line log(*gf*), energy levels (χ), rest wavelength (λ_0) (and Einstein coefficient A_{ki}). The final step uses the iterated APs as input for measuring individual element abundances ([*X*/H]) from selected sets of sufficiently clean, mostly medium-strong unsaturated, lines on the curve-of-growth (c-o-g).

Figure 6 shows the best fit to the spectrum of the Sun and Procyon observed between 5569 Å and 5583 Å (*solid black drawn lines*). The marked medium-strong neutral metal lines are best fit (*red lines*) with the atomic data values listed below the lines in the bottom panel. The atomic data values are selected from the literature and/or retrieved in atomic databases for calculating the best fit to the line depths and shapes. The best fits with these values are good to excellent (e.g., ≤ 0.01 in normalized line depths). The green lines mark the spectra calculated without the neutral lines. The lines are blended with weak atomic or molecular background lines below 5% of the line equivalent widths.

3.8.2 Atomic line data retrieval

For the BRASS project Mr. Laverick and Dr. Lobel retrieved atomic line data values from the literature and online atomic databases such as NIST and various databases offered in VAMDC. The VAMDC portal offers important research infrastructure for querying and retrieving atomic line data according to user-defined selection criteria from a large variety of repositories of astrophysical interest. The BRASS project retrieved atomic data values of ~400,000 line transitions from six online repositories. The atomic data were systematically queried, cross-matched and organized per spectral line and used for the state-of-the-art

synthetic spectrum calculations in BRASS. Mr. Laverick developed a novel procedure for cross-matching the databases, searching for identical atomic line transitions, with a sophisticated method that compares the upper and lower electronic state configurations and angular momenta *J*. The new method yielded multiple occurrences of atomic data values of identical lines offered by the different data providers.

Next Mr. Laverick developed a novel method for BRASS to ensure that cross-matching of atomic line transitions is 'exact'. This is based on the precise electronic state configurations. It eliminated possible errors of so-called 'inexact' cross-matching methods limited to the line rest-wavelengths and energy levels (hence ignoring the detailed electronic configuration and atomic term information when available). The new cross-matching method was also very useful for removing duplicate occurrences of the same spectral lines from the heterogeneous linelist compilations required for the advanced synthetic spectrum calculations in BRASS.

3.8.3 Molecular line data retrieval

The BRASS spectrum synthesis calculations included important line broadening effects for strong resonance lines and opacities due to molecular lines and bands important in the spectra of late-type stars. The used equation of state incorporates abundant di-atomic molecules with updated partition functions for important hydrides such as CH, AlH, CaH, SiH, FeH, CrH, NH, OH, MgH, carbon bearing molecules C_2, CN, CO, and the oxides TiO, ZrO, and VO. Dr. Lobel retrieved extensive molecular line data values in more recent literature and in the online ExoMol database providing several millions of extra lines. These data have been incorporated in the input line lists for detailed synthetic benchmark spectrum calculations and the systematic atomic line data quality testing in BRASS.

3.9 WP III: Spectrum Modelling & Atomic Data Quality Testing

In order to assess the quality of log(*gf*)-values (oscillator strengths) of important (so-called 'graded') lines provided in the literature it was important to assess how much blended the lines are with respect to the rest of the spectrum. The symmetry of a line in an observed spectrum is a strong indicator whether it is actually a blend of two or more lines. However, in some cases where there is little difference between the wavelengths of both (overlapping) spectral lines, the symmetry is not sufficient for identifying line blending. For each graded line two synthetic spectra were calculated, one including the transition and another excluding it. They have been compared to quantify how much the lines blend together. The difference between both spectra determined the total area, depth, and equivalent line width (W_λ). A line was considered to be blended if more than 10% of the total absorption in the complete spectrum was present in the incomplete spectrum, within the wavelength range $\lambda_{line} \pm 0.5 \times W_\lambda$ (see Figure 7).

Mr. M. Laverick performed two spectral synthesis calculations for each of the 2647 graded lines in five different BRASS benchmark stars of spectral types BAFGK. The calculations were performed in LTE using the `TurboSpectrum` spectrum synthesis code, combined with ATLAS9 1-D atmosphere models. The amount of line core blending (Ω_{core}) was calculated for ~82,000 lines of the BRASS input atomic lines list. For the FTS spectra of the Sun and the HERMES spectrum of 51 Peg spectral resolutions of respectively R~350,000 and R~85,000 were used. To reduce the impact of the line blending on the quality assessment (discussed below) a cut-off of $\Omega_{core} \leq 10\%$ was used. This cut-off value was selected as a balance

between Ω_{core} and the number of investigated lines. An additional cut-off on the central line depth $d \geq 0.02$ was also imposed to ensure that the observed line profiles are actually measurable and less affected by noise in the observed spectra.

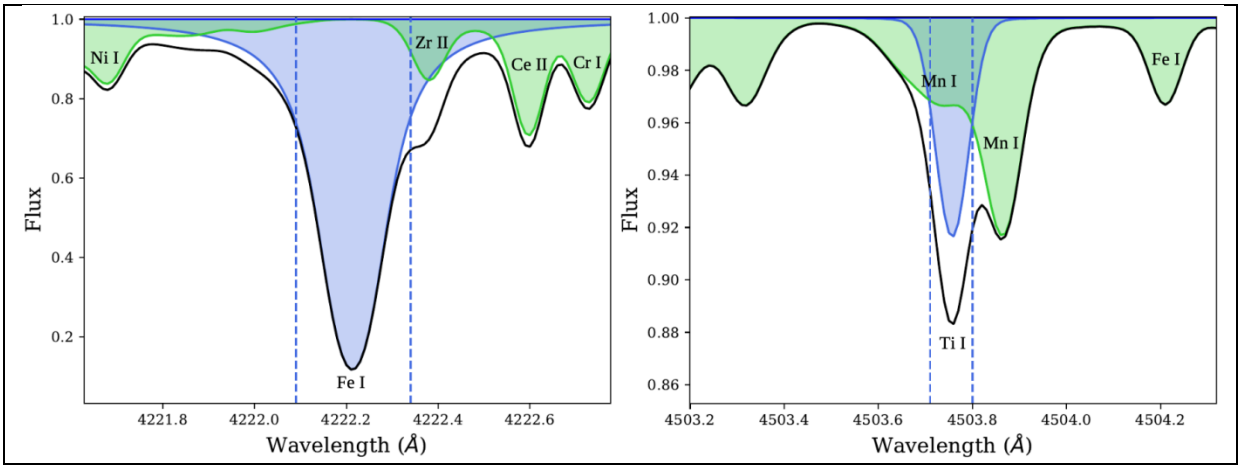


Figure 7. The left-hand panel shows an un-blended spectral line of Fe I suitable for quality assessment in BRASS. Right-hand panel: a spectral line of Ti I that is too blended for accurate analysis of its log(*gf*)-value. The black line shows the total theoretical spectrum synthesized with all atomic and molecular lines in the BRASS input line lists. The blue shaded areas depict the line profiles of interest, and the green shaded areas show the background lines, i.e., the remaining flux after subtracting the line of interest.

In the following step Dr. Lobel and Mr. Laverick expanded the selection of (graded) lines for detailed quality assessing of atomic lines in FGK-type stars. The graded lines were selected from the full retrieved literature atomic data (over 82,000 lines instead of the previous subset of 2647 lines) by evaluating the degree of theoretical line blending. Once the theoretically unblended lines were selected, the observed spectra counterparts were measured using a Gaussian fit function for producing equivalent width values per star and per line. The quality of fit to the observed profiles was used to further refine these line selections, resulting in 1091 theoretically unblended and observationally measurable atomic lines.

The suitability of the 1091 lines for the modelling and quality assessment work was further analyzed using a novel method developed for BRASS. The W_λ-values measured for a spectral line observed in seven FGK-type benchmark stars were compared against the theoretically calculated curves-of-growth (i.e., one per atomic line, per ionic species, and per benchmark star). These values were compared to the log(*gf*)-values measured from detailed line shape fits. An example of detailed line profile fits to an optical Fe II line observed in the benchmark spectrum of the solar-like star 51 Peg is shown in Figure 8.

The mean log(*gf*)-values were next compared for internal consistency so the selected values accurately reproduce the line profiles in the FGK benchmark spectra. Hence, two complementary quality assessment methods have been explored: one using the theoretical curves of growth in conjunction with measured equivalent widths (called the COG method), and the other employing a detailed iterative line profile modelling approach (called the GRID method). Both methods were used in each of the seven FGK benchmark stars for producing mean log(*gf*)-values per method. Extra effort went into the determination of systematic errors and uncertainties associated with the final log(*gf*)-values, leading to substantial and expanded analysis.

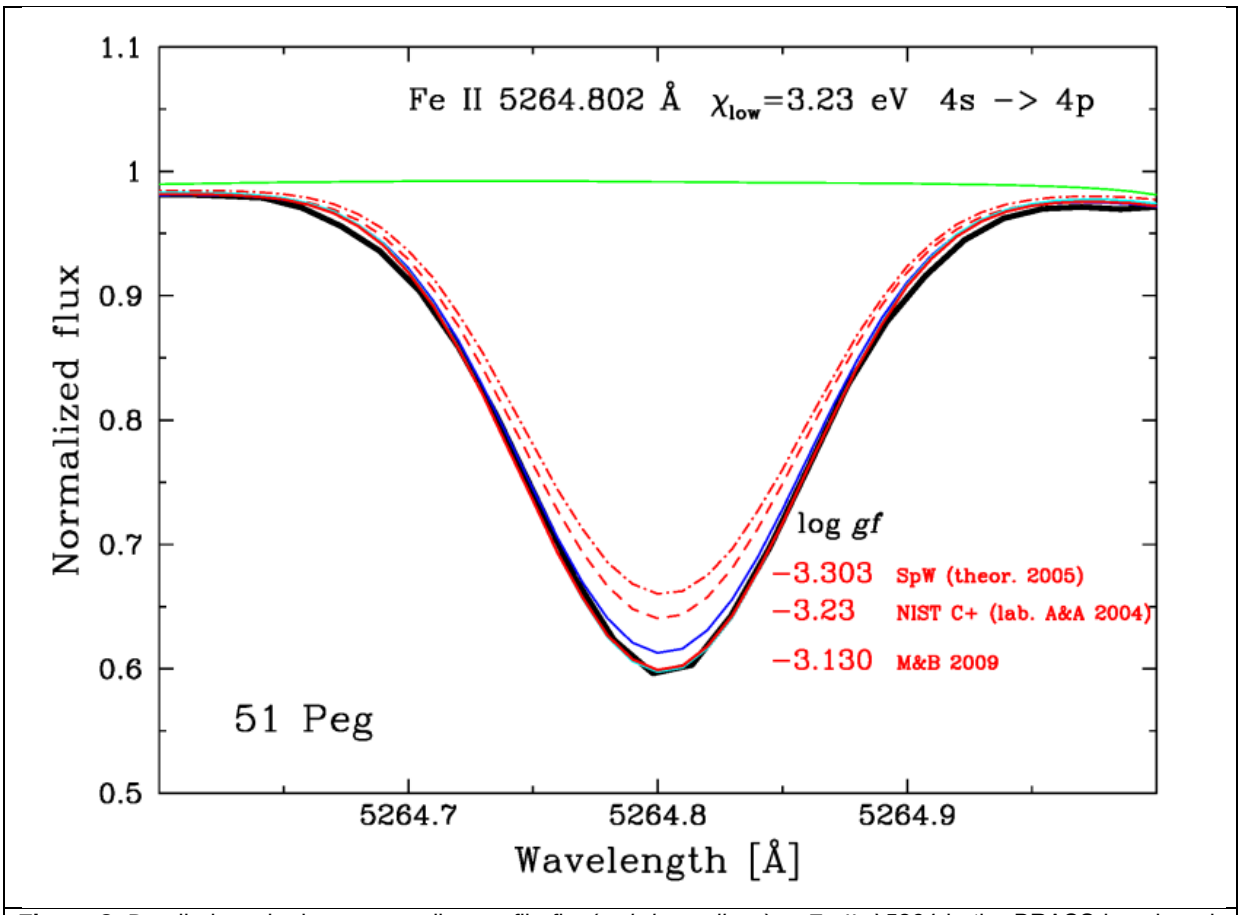


Figure 8. Detailed synthetic spectrum line profile fits (*red drawn lines*) to Fe II λ5264 in the BRASS benchmark spectrum of solar-like star 51 Peg observed with HERMES (*black line*). The broken lines are calculated for literature log(*gf*)-values of −3.303 (*dash-dotted line*) from SpectroWeb and −3.23 (*dashed line*) from NIST. For the larger log(*gf*)=−3.130 published in 2009 the theoretical profile (*solid red line*) correctly matches the observed line width and depth. The red drawn spectra are calculated for Teff=5804 K while the blue drawn spectrum for Teff=5858 K.

The agreement between the two measurement methods was used for determining whether or not a spectral line is reliable for quality assessments. 845 of the 1091 spectral lines were determined to be quality assessable, of which 408 were robust against the systematic differences arising from the two different measurement methods. The previously retrieved literature data of the 845 selected lines were next evaluated against the log(*gf*)-values of the GRID method. Using the grid log(*gf*)-value uncertainties as a criteria for agreement, it was found that ~53% of the investigated atomic lines had sufficiently accurate atomic data, the value rising to around 60% to 70% for non-iron group elements, and down to ~38% for the investigated Fe I lines.

3.10 WP IV: BRASS Repository Implementation

From the start of the project Dr. Lobel and Mr. Thienpont developed a new user interface (BRASS Data Interface - BDI) for online querying and visualization of BRASS spectra combined with atomic line data. The BDI at brass.sdf.org loads in every modern internet browser. User interactions combine fast spectrum display and atomic data listing using modern integrated HyperText (HT Markup Language), JavaScript, `JQuery` (Cascading Style Sheets), and `Dygraphs` software technology. The BDI developments have been targeted at user-friendliness, ensuring easy visualization, selection and retrieval of any desired subset offered in the BRASS database. The BDI functionality was expanded from `SpectroWeb` at spectra.freeshell.org/spectroweb.html, for example also allowing synchronized wavelength zooming on four spectral segments of 30 Å for two user-selected spectra from a list of stars. Eleven benchmark HERMES spectra have been incorporated in the BDI together with the FTS spectrum of the Sun.

Mr. Thienpont of the follow-up committee contributed to the WP IV preparations with important expertise in the field of development and implementation of large databases in the public domain. He is a data analyst of the Flemish Government and advised that for making the online BRASS database safe and user accessible with the modern advances of internet technology, and also given the scope of the BRASS database, the choice of Javascript libraries and `Dygraphs` was most appropriate. The BRASS repository is offered online through a publicly accessible data server at SDF (Super Dimension Fortress). The Javascript libraries have been installed on the hosting SDF server and will remain permanently available. For the implementation of the BRASS repository Mr. Thienpont also emphasized the need of the JavaScript Library & Frameworks for the fast online operation of BRASS as an open Internet application. This also required a specialized graphics Javascript (open-source) library `Dygraphs` for displaying high-resolution BRASS spectra in dynamical graphs combined with various specific graphics display options for the BRASS end-users.

The BRASS Spectra BDI required the implementation of six components:

1. Synchronized zooming of user-selected spectral regions.
2. Line labels lifting and dropping for enhancing the clarity of the spectral graphs.
3. Saving of atomic data of graded lines marked by users.
4. Downloading of observed and theoretical BRASS spectra.
5. Advanced tools for interactive line equivalent width measurements.
6. Help pages for use-cases with video tutorials.

The atomic datasets collected from various atomic data providers have been also incorporated in the Lines BDI (LBDI). The atomic lines have been cross-matched and offered for user retrieval. This includes all literature references for the provenance of the atomic datasets, together with the full electronic configuration information used in the lines cross-matching procedure. Older data from the TIPbase and TOPbase databases have been incorporated as well. The LBDI can be queried for a given (or all) element(s) in a user-defined wavelength interval, and the query results sorted by increasing values of the wavelength or standard deviation σlog(*gf*)-values. The results can be saved in extensive line lists or per selected line to machine-readable (ASCII) tables. The online interface can also display the Δlog(*gf*)-values in interactive plots for all atomic data sources (ordered by neutral,

singly-, and multiply-ionized species), offering a comprehensive overview of all log(*gf*) data available to BRASS users.

The BRASS Lines BDI user queries required the implementation of four components:

1. The storage and analysis of over a hundred thousand records with modern database technology. The MySQL evironment has been implemented as a popular powerful open source database.

2. Receiving requests and delivering data to the end-users by means of easy front-end Web forms have been implemented using the Java Server Pages (JSP) technology.

3. Coupling between the BRASS database and Web requests has been implemented using the Spring Java-based Framework configured with the TomCat server of SDF.

4. Graphical representation of differences between different providers of the oscillator strengths has been implemented using the Google Charts technology.

The BRASS benchmark observed and theoretical (broadened and un-broadened) spectra can be displayed using the BDI in combination with clickable line labels. The spectra are offered together with the atomic data of graded and un-graded lines having central core depths exceeding 2% (*red and blue line labels*). All cross-matched atomic data have been ingested in the BDI and are accessible via dynamic tabs with interactive line graphs of theoretical graded line profile calculations and best fits, also offering quality assessment information and flags for the associated atomic line data. It also includes the observed and theoretical W_λ-values, the atomic data sources, and Δlog(*gf*)- and $\Delta\lambda$-values providing the best fit to the observed line profiles in the benchmark spectra.

4. SCIENTIFIC RESULTS AND RECOMMENDATIONS

4.1 Atomic lines compilation results

An important source of uncertainty in stellar spectrum synthesis calculations is the accuracy of atomic data of permitted transitions. It is crucial to constrain atomic data uncertainties for reliable measurements of the thermal conditions and chemical composition of stellar atmospheres. For BRASS we retrieved ~400,000 transition entries from various online atomic databases: VALD-3, NIST, Spectr-W^3, TIPbase, TOPbase, CHIANTI, and SpectroWeb (see acronyms in § 4.11). We collected the atomic transition data of neutral species and ions up to the fifth ionization stage for wavelengths between 420 and 680 nm. The datasets were homogenized and cross-matched against the initial BRASS atomic line list compilation. The initial BRASS list is composed of Kurucz and NIST V4.0 lines containing for each transition the species (element and ionization stage), line rest-wavelength, log(*gf*)-value, upper and lower electronic configurations and energy levels, *J*-values, and the corresponding literature references.

The BRASS atomic lines cross-matching has been performed in two different ways: the *parametric cross-match* method is based on wavelength- and level energy-values for finding the same transition of a given species. On the other hand, the *non-parametric cross-match* method is based on detailed electronic configuration information for finding transitions that are physically identical between the datasets. The cross-matching accounts for atomic fine structure, the provided isotopic information, and the type of transition. It however does not account for currently missing hyperfine structure information.

The BRASS atomic lines compilation was initially tested with theoretical spectrum calculations of the solar flux spectrum (Neckel & Labs, 1984) and using Mercator-HERMES (Raskin et al., 2011) spectra of selected B-, A-, F-, G-, and K-type stars (see Lobel et al., 2017). The BRASS list has been also cleaned from numerous un-observed lines, spurious atomic and molecular background features, and duplicated lines were excluded. Note that the SpectroWeb atomic lines list was previously compiled from VALD-2 and NIST data (V2.0 through V4.0), and was also extensively tested similar to the BRASS list with theoretical spectrum calculations of high-quality hot and cool star spectra (Lobel, 2011). TABLE I lists the number of retrieved lines, source databases, dates of retrieval, and various atomic data values collected from each database. We made extensive use of the online VAMDC portal offering homogenized datasets that expedited the comparison and cross-matching of the datasets we retrieved for BRASS. We partly incorporate data from TIPbase and TOPbase and included some of our expansions into fine-structure transitions (Laverick et al., 2018). We also calculated line log(*gf*)-values for the Spectr-W^3 datasets, using the f_{ik} -values the online repository is offering.

Atomic databases for BRASS

Repository	Origin	No. lines	Date	Ion	λ	A_{ki}	f_{ik}	$\log(gf)$	$E_{low/up}$	$J_{low/up}$
BRASS	-	82337	2012 [b]	✓	✓			✓	✓	✓
SpectroWeb	-	62181	2008 [b]	✓	✓			✓	✓ [f]	
VALD3	VALD	158861	26/05/2016	✓	✓			✓	✓	✓
NIST	NIST	36123	14/03/2016	✓	✓ [c]	✓	✓	✓	✓	✓
Spectr-W^3	VAMDC	5515	14/03/2016	✓	✓	✓	✓		✓	✓
TIPbase[a]	NORAD	33108	28/02/2017	✓	✓	✓	✓		✓ [g]	
TOPbase[a]	VAMDC	33462	24/05/2016	✓	✓			✓ [e]	✓ [g]	
CHIANTI	VAMDC	3587	18/03/2016	✓	✓ [d]	✓		✓ [e]	✓ [f]	✓

TABLE I. Overview of the retrieved number of lines for BRASS from various atomic databases, including the retrieval dates and types of atomic data per source. Sub- and superscripts *a-g* are explained in Laverick et al. (2018).

4.2 Atomic lines cross-matching results

For the BRASS project Laverick et al. (2018) used the non-parametric cross-match method to explore differences between multiple occurrences of identical transitions in the retrieved datasets (see § 4.1). Detailed comparisons of λ vs. ∆λ, E vs. ∆E, ∆λ vs. ∆E, and ∆λ vs. ∆log(*gf*)-values mainly reveal the presence of small-scale conversion precision differences. Large-scale systematic correlations were detected for a few cases only. However, the comparison of the line log(*gf*)-values revealed differences in excess of 2 dex (decimal exponent), which has important implications for quantitative stellar spectroscopy. An investigation of duplicated transitions (also accounting for hyperfine-, isotopic-, and E2-M1 forbidden-transitions) in the retrieved datasets showed a significant number of almost 2% in the VALD-3 lists. These duplicates could be sourced back to the original work in 99% of cases, hence they were not produced by the databases from which the BRASS datasets are retrieved. The duplicated transitions, for example, were not detected in the line datasets retrieved from NIST.

The cross-matched atomic datasets, including the BRASS atomic lines compilation, have been incorporated in the online Lines BRASS Data Interface (LBDI) at brass.sdf.org.

Figure 9 shows the online LBDI page that can be queried for a given element in a user-defined wavelength interval. In case a cross-match listing for every element is requested the users can set the Element input field to 'all'. The query results can be sorted by increasing rest-wavelengths or σlog(*gf*)-values (standard deviations) marked in blue in Figure 10.

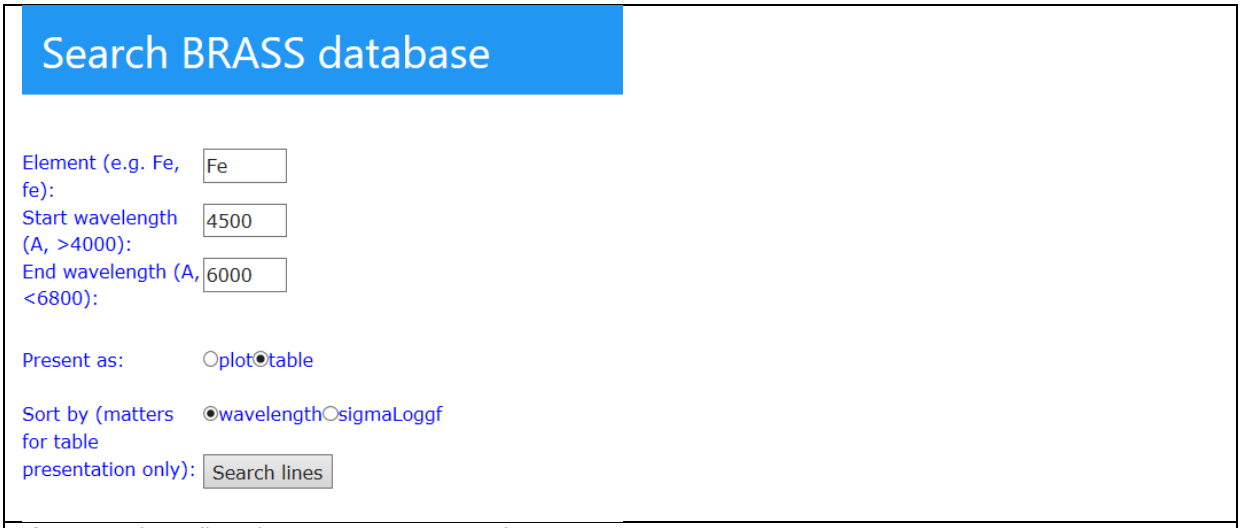


Figure 9. The online Lines BRASS Data Interface query page.

The query results can be exported and saved in extensive line lists or per user-selected line to machine-readable (tab-separated ASCII) tables. Figure 10 shows for example the cross-matched atomic data of a S II line retrieved from seven atomic data sources providing five different log(*gf*)-values ranging from −0.341 dex to −0.059 dex. The literature references of the log(*gf*)-values are offered together with the upper and lower electronic configurations and level energies. Figure 11 also shows a subset of LBDI dynamic plots of the BRASS compilation log(*gf*)-values vs. log(*gf*)-difference values for VALD3-BRASS and NIST-BRASS of cross-matched Fe I and Fe II lines, and of the doubly and higher ionization species of Fe. These dynamic plots can be interactively zoomed and the data of individual lines marked and displayed by mouse interaction. The log(*gf*)-difference plots are provided per query for all atomic data sources and are ordered by neutral, singly, and multiply ionized species (from left to right). It provides users with an interactive and comprehensive overview of all cross-matched log(*gf*) datasets offered in BRASS.

The lists of duplicated spectral lines resulting from the cross-matching are also offered in the BDI in a variety of data formats (HTML, ASCII, and PDF) shown in Figure 12. Two lists of non-S I duplicated lines and S I duplicated lines have been compiled. Each pair of lines in the lists represents two transitions for which it was determined they are duplicated according the atomic electronic configuration information and *J*-values. The duplicates have been manually checked for hyperfine structure and isotopic transitions according to their respective References.

Note that the BRASS Data Interface also offers comprehensive Help pages (under the main green tab) for a number of BRASS use-cases and corresponding tutorial videos (see § 4.8).

Figure 10. BRASS query results page for singly-ionized Sulfur lines (Element S) sorted by transition Wavelength. The lines data are cross-matched in BRASS using various atomic databases and the corresponding literature References are also offered.

4.3 BRASS Data Interface spectral implementation results

For the BRASS project we observed benchmark spectra of a variety of bright stars ($V < 7^m$) with the HERMES and ESO-VLT-UVES high-resolution spectrographs. We investigated HERMES benchmark spectra of 6 dwarf stars of F, G, and K spectral types observed with very high signal-to-noise ratios (SNR) of ~800-1000: 51 Peg, 70 Oph, 70 Vir, 10 Tau, Eps Eri, and β Com (having Teff values between 5000 K and 6000 K). The spectra have been modelled in detail with advanced Local Thermodynamic Equilibrium synthesis calculations using 1-D hydrostatic atmosphere models (see Lobel et al., 2017). The detailed spectrum modelling determines atmospheric Teff-, log(*g*)-, [*M*/H]-, ζμ-, *v*sin*i*-, and [α/Fe]-values we also compared to published stellar parameters measured using high-resolution spectra. The BRASS benchmark stars exclude binaries and have been selected for non-variability and non-peculiarity. They are normal dwarf stars with narrow absorption lines having small rotational velocities below ~6 km/s and metallicities very close to solar values. Metal-poor stars were excluded to avoid non-LTE effects in the theoretical spectrum calculations for BRASS.

The spectra of eleven BRASS benchmark stars (including the solar FTS spectrum) and the theoretical spectra have been incorporated in the Spectra BRASS Data Interface (SBDI) shown in Figure 13. Users can interactively display up to four spectral Regions in two benchmark stars selected from the left-hand menus. The wavelengths of identified atomic lines are marked with red and blue labels. The red label numbers mark investigated lines. The red (and blue) labels can be clicked for displaying BRASS atomic data (log(*gf*)- and Elow-values in a red 'graded list' in the right-hand panels), together with measured line properties such as the observed line equivalent widths (W_λ and W_λ-uncertainty), and the type of quality assessment we performed for the accuracy of the line log(*gf*)- and rest-wavelength-values. By double-clicking the red line labels users can build up lists of BRASS line data values (marked in green) for saving to their local computer disc. Clicking the 'View data quality' link in the red (or green) tables populates the 'Atomic Data Quality' tab in the

central SBDI panel for a complete overview of the atomic line data quality assessment results BRASS offers for each investigated line.

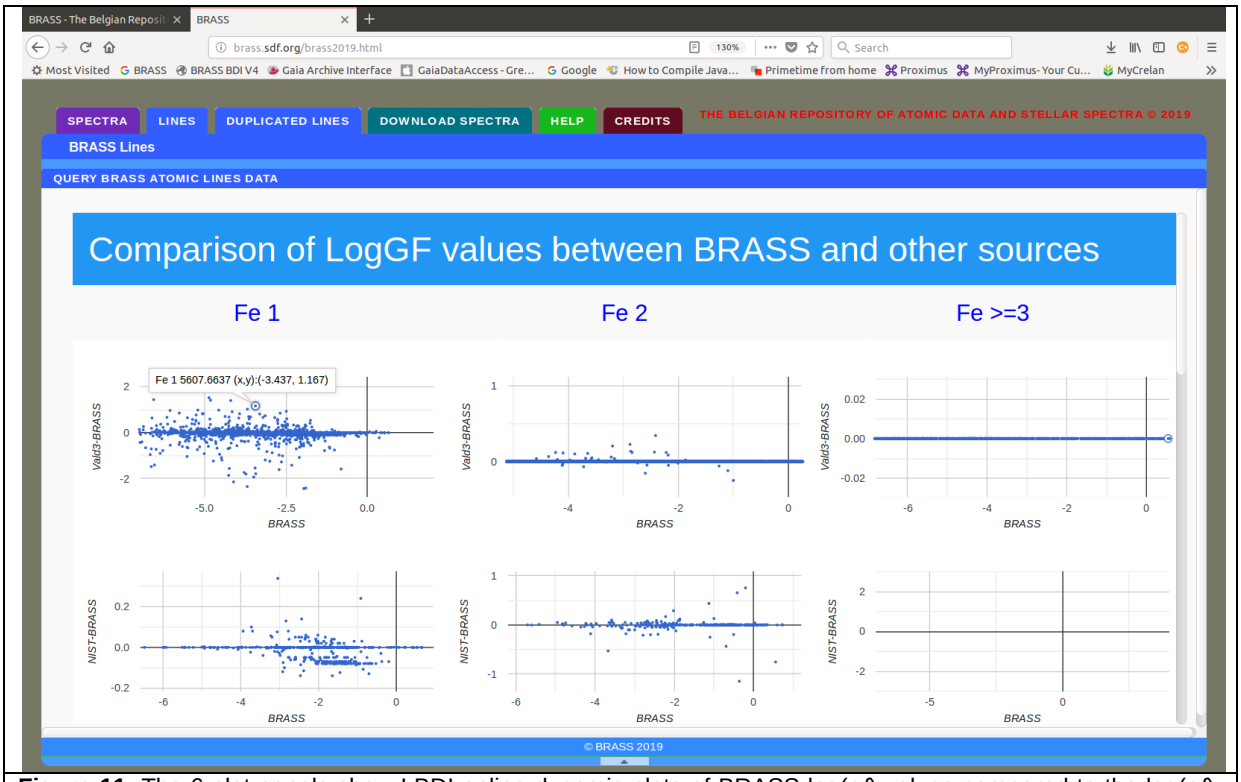


Figure 11. The 6 plot panels show LBDI online dynamic plots of BRASS log(*gf*)-values compared to the log(*gf*)-differences for VALD3-BRASS (*top plot panels*) and NIST-BRASS (*bottom panels*) of cross-matched Fe I lines (*left-hand panels*), of Fe II lines (*middle panels*), and of the higher Fe ions (*right-hand panels*).

The BRASS benchmark spectra are offered in the SBDI under the DOWNLOAD SPECTRA tab in Figure 13. The observed spectra are offered for both continuum-normalized and un-normalized flux values. The benchmark spectra have been normalized using an advanced template normalization procedure developed in BRASS that can select continuum normalization anchor-points in (or close within 1% of) the theoretical stellar continuum flux levels. The local density of the anchor-points in fixed wavelength-intervals, typically void of strong spectral lines, determines if they are useful for folding the observed spectrum to the detailed template spectrum. The un-broadened and broadened template spectra are also offered in the SBDI. For the broadened template spectra the individual rotational velocity and instrumental resolution of the benchmark star was used in the line broadening calculations. The un-broadened theoretical spectra are drawn with red lines in the middle panel of Figure 13, while the broadened spectra are shown in blue colour.

4.4 Atomic line data quality assessment results

A large-scale homogeneous selection of atomic lines has been performed by Laverick et al. (2019) for BRASS by calculating the theoretical spectra of the six FGK benchmark HERMES spectra and the solar FTS spectrum. A selection of 1091 theoretically deep and sufficiently un-blended lines in the wavelength range 420 nm to 680 nm proved to be suitable for advanced quality assessments of the accuracy of the atomic datasets collected in BRASS (see § 4.1). For BRASS we determined astrophysical (semi-empiric) log(*gf*)-values for these

1091 transitions using two commonly employed analysis methods. The agreement of the measured log(*gf*)-values was used for selecting well-behaving lines for the quality assessment research work. A total of 845 atomic lines were found to be suitable for quality assessment, of which 408 are robust against any systematic differences between both analysis methods. We determined the value of ±0.04 dex as a constraint on the lines selection for limiting the impact of systematic differences between both methods on the atomic data quality assessment results. Around 53% of the quality-assessed lines were found to have at least one literature log(*gf*)-value in agreement with the calculated values, although the remaining values can disagree by as much as 0.5 dex (see § 4.5).

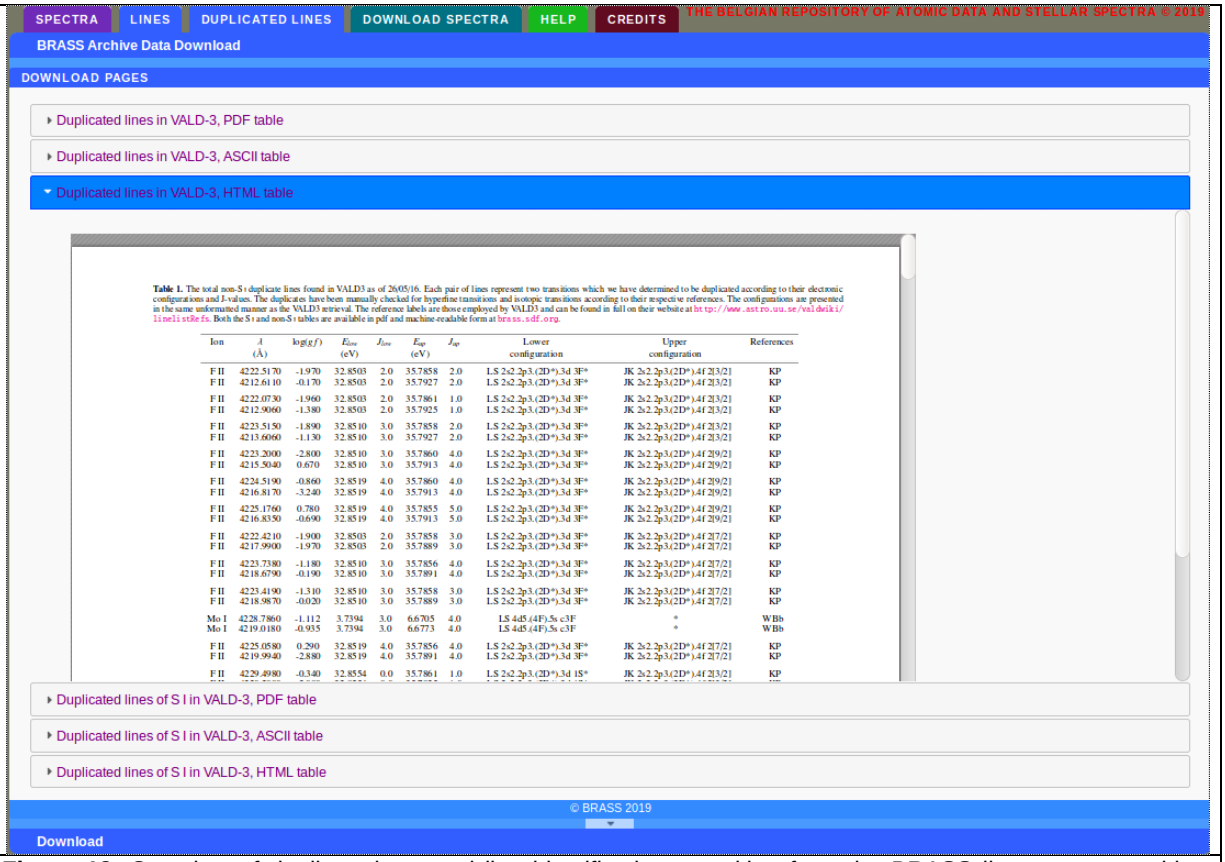


Figure 12. Overview of duplicated spectral line identifications resulting from the BRASS lines cross-matching analysis offered in the LBDI in three data formats.

For selecting atomic lines we calculated the amounts of blending in 82,337 BRASS lines of the solar and 51 Peg benchmark spectra. To reduce the impact of the line blending amounts on the atomic data quality assessment work a cut-off for blending of less or equal than 10% was used, selected as a good balance between blending of the line core and the number of investigated lines. An additional cut-off on the central line core depth equal or above 0.02 was also used to ensure the observed line profiles can be measured with sufficient accuracy. A total of 1515 atomic lines were initially selected as 'un-blended' lines in both benchmark stars. The lines selection procedure does not place limits on the atomic species. The equivalent line widths of the 1515 un-blended lines have been automatically measured in all seven benchmark spectra using a single Gaussian fit profile. The line fit procedure has been optimized using Gauss-Newton non-linear regression, or Nelder-Mead minimization in the case of slow convergence (for a detailed analysis overview see Lobel et al., 2018). The best

fit to the observed line fluxes has been limited to the wavelength interval between two local flux maxima in both line wings exceeding 2% of the normalized continuum flux level. Beyond the local flux maxima the W_λ integration is extended for Gaussian line wings. A goodness-of-fit value of $\chi^2 \leq 0.95$ was used to remove poorly fitted (in addition to visual inspection), non-existent, too blended, or Earth line contaminated absorption features.

Figure 13. Screen copy of the SBDI for the solar FTS spectrum (*central top panel*) and the BRASS benchmark HERMES spectrum of solar-like star 51 Peg (*central bottom panel*). The red and blue interactive labels mark identified absorption lines with atomic and line property data tables shown in the right-hand sub-panels. Atomic quality assessment pages are displayed under the central Atomic Data Quality tab by clicking on the View data quality link in the red or green line data tables.

The astrophysical log(*gf*)-values have been determined with two commonly employed methods. The measured line equivalent widths are converted into log(*gf*)-values using the theoretical curve-of-growth calculated for the line in each benchmark star (called the COG method). The other method varies the log(*gf*)-values in detailed radiative transfer calculations for determining the best-fit value to the observed line profile. The latter method is called GRID because it involves an iterative line modelling procedure for which a grid of spectra is calculated and the best fitting spectrum for a range of log(*gf*)- and λ-values is obtained with χ^2-minimization by interpolating in steps of $\Delta\lambda$ (0.005 Å) and Δlog(*gf*) (0.01 dex) using a bivariate cubic spline fit. Both methods introduce assessable uncertainties resulting from the accuracy of the best fit procedures to the observed W_λ-value and the continuum normalized line flux distribution. The uncertainties can be attributed to the spectral S/N ratio, specific atmosphere modelling assumptions, the continuum flux level normalization procedure, and blending with the observed line unaccounted for in the theoretical spectrum calculations.

BRASS Benchmark Spectra Table

LINES | DUPLICATED LINES | DOWNLOAD SPECTRA | HELP | CREDITS | SPECTRA — THE BELGIAN REPOSITORY OF ATOMIC DATA AND STELLAR SPECTRA © 2019

BRASS Data Download

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for accessing BRASS data files in these Tables

BRASS BENCHMARK STAR SPECTRA

Spectral Type	Instrument	Star name	Spectrum	Spectrum	Spectrum	Spectrum
			OBSERVED	OBSERVED	MODEL	MODEL
			NORMALIZED	NOT NORMALIZED	UNBROADENED	BROADENED
K	Hermes	Arcturus	Arcturus_OBN.ascii Arcturus_OBN.fits	Arcturus_OBU.ascii Arcturus_OBU.fits	Arcturus_MUB.ascii Arcturus_MUB.fits	Arcturus_MBR.ascii Arcturus_MBR.fits
K	Hermes	Eps Eri	Eps_Eri_OBN.ascii Eps_Eri_OBN.fits	Eps_Eri_OBU.ascii Eps_Eri_OBN.fits	Eps_Eri_MUB.ascii Eps_Eri_OBN.fits	Eps_Eri_MBR.ascii Eps_Eri_OBN.fits
G	Hermes	70 Oph	70-Oph_OBN.ascii 70-Oph_OBN.fits	70-Oph_OBU.ascii 70-Oph_OBN.fits	70-Oph_MUB.ascii 70-Oph_OBN.fits	70-Oph_MBR.ascii 70-Oph_OBN.fits
G	Hermes	70 Vir	70-Vir_OBN.ascii 70-Vir_OBN.fits	70-Vir_OBU.ascii 70-Vir_OBN.fits	70-Vir_MUB.ascii 70-Vir_OBN.fits	70-Vir_MBR.ascii 70-Vir_OBN.fits
G	Hermes	51 Peg	51-Peg_OBN.ascii 51-Peg_OBN.fits	51-Peg_OBU.ascii 51-Peg_OBN.fits	51-Peg_MUB.ascii 51-Peg_OBN.fits	51-Peg_MBR.ascii 51-Peg_OBN.fits
F	Hermes	10 Tau	10-Tau_OBN.ascii 10-Tau_OBN.fits	10-Tau_OBU.ascii 10-Tau_OBN.fits	10-Tau_MUB.ascii 10-Tau_OBN.fits	10-Tau_MBR.ascii 10-Tau_OBN.fits
F	Hermes	Beta Com	Bet_Com_OBN.ascii Bet_Com_OBN.fits	Bet_Com_OBU.ascii Bet_Com_OBN.fits	Bet_Com_MUB.ascii Bet_Com_OBN.fits	Bet_Com_MBR.ascii Bet_Com_OBN.fits
F	Hermes	Procyon	Procyon_OBN.ascii Procyon_OBN.fits	Procyon_OBU.ascii Procyon_OBN.fits	Procyon_MUB.ascii Procyon_OBN.fits	Procyon_MBR.ascii Procyon_OBN.fits
A	Hermes	68 Tau	68-Tau_OBN.ascii 68-Tau_OBN.fits	68-Tau_OBU.ascii 68-Tau_OBN.fits	68-Tau_MUB.ascii 68-Tau_OBN.fits	68-Tau_MBR.ascii 68-Tau_OBN.fits
B	Hermes	HR 7512	HR_7512_OBN.ascii HR_7512_OBN.fits	HR_7512_OBU.ascii HR_7512_OBN.fits	HR_7512_MUB.ascii HR_7512_OBN.fits	HR_7512_MBR.ascii HR_7512_OBN.fits
More to come	Other	Other	Other	Other	Other	Other

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Download

TABLE II. Overview of observed and theoretical BRASS benchmark spectra offered in the online BRASS Data Interface.

For the seven BRASS benchmark spectra we measured an intrinsic scatter between both methods of ±0.04 dex (1-σ standard deviation) for line blending levels below 3% - 4%. The value of ±0.04 dex is therefore used as a constraint on the lines selection for limiting the impact of systematic differences between both methods on the atomic data quality assessment results. In the analysis method the close agreement between the COG and GRID log(*gf*)-values is required for quality assessing the literature log(*gf*)-values retrieved for BRASS. The COG log(*gf*)-value was calculated for a given transition with the observed W_λ-value of an absorption feature we can attribute to the line, while the GRID log(*gf*)-value results from complete theoretical spectrum calculations that fit the observed spectrum incorporating the (sufficiently un-blended) line profile.

The Spectra BDI offers atomic data quality assessment pages showing plots and data values for the 1091 investigated lines. Figure 14 shows a screen copy of the SBDI Atomic Data Quality tab for the Ni I λ6598 line observed in the BRASS benchmark spectra (solid *black line with dots*) over-plotted with the theoretical profiles we calculated for the atomic data values retrieved from four atomic databases. The line profiles calculated for log(*gf*)-values we determined from the GRID and COG analysis methods are over-plotted in blue and green colours, respectively. Users can interactively zoom-in, pan, and reset these line profile plots for each benchmark star. By clicking the check boxes above the plots the theoretical line profiles calculated with the log(*gf*)-values in the atomic databases are also over-plotted for user inspection.

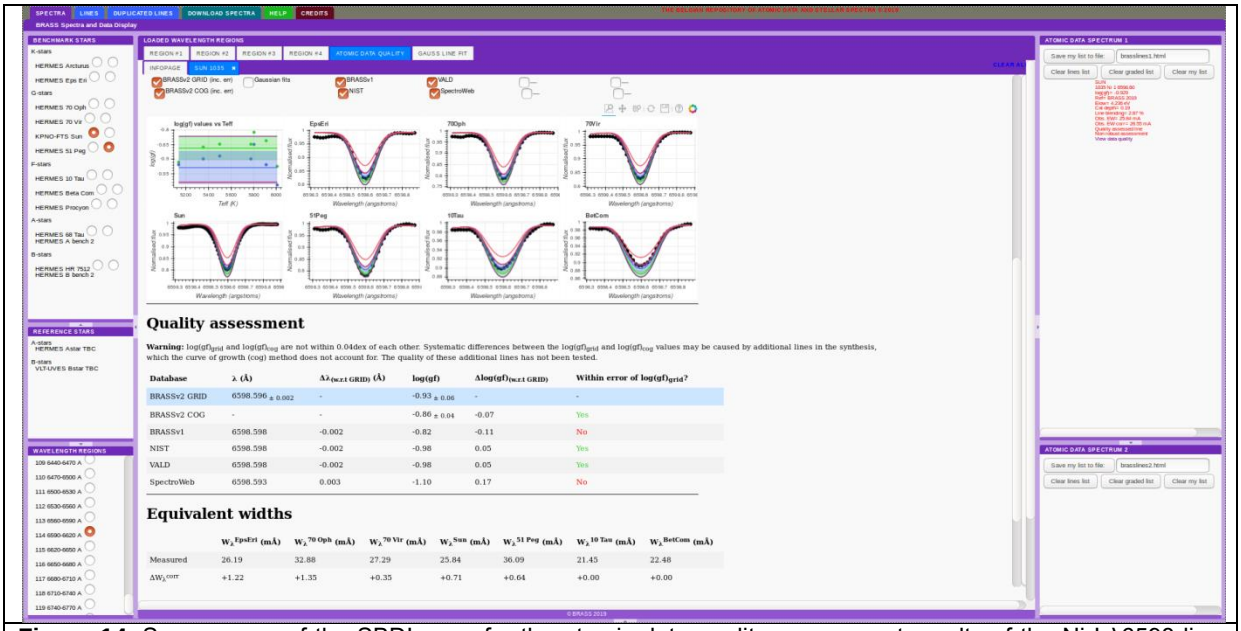


Figure 14. Screen copy of the SBDI page for the atomic data quality assessment results of the Ni I λ6598 line observed in seven BRASS benchmark spectra. The observed and theoretical line profiles shown in the top sub-panels can be displayed with user interaction. The SBDI pages offer an overview of all atomic data quality results for each investigated line, together with the observed and theoretical line equivalent width values.

The Quality assessment table shown below the line profile plots lists the GRID and COG line log(*gf*)- and rest-wavelength (λ)-values, together with the differences (Δlog(*gf*) and Δλ) with respect to the GRID values. The last column of this table offers a Yes/No flag indicating if the Δlog(*gf*)-value is within the errors of the GRID log(*gf*)-value. The flags and Δ-values are useful for determining if the log(*gf*)-values retrieved from the databases for BRASS are sufficiently accurate for detailed spectrum synthesis calculations. For example, for Ni I λ6598 we determined GRID log(*gf*)- and COG log(*gf*)-values within errors of each other (hence having quality-assessable atomic data), but not within ±0.04 dex of each other, signalling the line is not robust against the analysis method. The bottom table with Equivalent widths offers the observed (Measured) and theoretical W_λ-values (in mÅ) we calculated for the investigated line per database in all the benchmark stars. Note that we also add small corrections listed for ΔW_λ^{corr} to the observed line equivalent width values in case the line saturates on the curve-of-growth and Voigt-profile corrections were introduced in our best Gaussian spectral line fit procedure.

The SBDI also offers an interactive W_λ measurement tool under the Gauss line fit tab of the central panel in Figure 13. Users can select lines in observed BRASS spectra and display the single Gaussian best fit result together with the list of measured line properties for saving to their computer's disc (see § 4.7).

The BDI employs interactive line labels for marking individual features in a displayed spectrum (the blue and red boxes shown in Figure 13). The BRASS lines compilations, however, did not always correspond to actual lines (or features) in the observed benchmark spectra, mainly in case of strongly overestimated predicted line strengths. To address this problem a new version of the BDI line label database was created using the observed 51 Peg spectrum. The first step of the process was to scan this spectrum and mark 'blended' regions. This was done by measuring the width of any wavelength region where the

normalized spectrum continually stayed below 0.98. If the width was larger than expected for a single line the region was marked as 'blended'. This qualification was used for the line selection process. The line blending is more prevalent towards the shorter wavelengths. The next step was to process a database of 69,160 BRASS lines. Individual spectra for each line were calculated for 51 Peg (or each theoretical spectrum contains a single line). A fit of a Gaussian absorption line superimposed on a linear continuum was calculated for each theoretical spectrum. The linear continuum has both the level and slope as free parameters. The Gaussian has the central wavelength, width, and depth as free parameters. The best fit was determined by minimizing the fit χ^2 using the `Amoeba` algorithm. It was found to be slower than other algorithms, but also more stable and therefore deemed more appropriate. If the fit failed (typically indicating an extremely weak line), or the line depth was less than 2%, the line was rejected. After this selection procedure, a database of 7114 viable lines remained. The final step was to fit each selected line observed in 51 Peg using the same best fit method. Each line was given a score, where (0) flagged the line as detected, (1) the line was possibly present, and (2) that the line remained undetected and was rejected. A total of 2936 lines were detected (0), 1648 lines were possible (1), and 2530 lines were rejected (2). A visual inspection of the line regions in the 51 Peg spectrum showed that this selection procedure yielded good results.

4.5 Comparison of atomic data quality assessment results

We found 845 of the 1091 investigated lines to be quality-assessable, and 408 are also analysis-independent lines. Nearly half of the investigated and quality-assessable lines are of Fe I, while another ∼10% belong to singly-ionized species. The retrieved literature log(*gf*)-values of a quality-assessable line are considered in agreement with our results and can be recommended in theoretical spectrum calculations only in case they agree within the uncertainties of the mean (averaged over all benchmarks) GRID log(*gf*)-value and its standard deviation. We did not consider any literature error-bars because they are not available for the vast majority of investigated lines. In most cases we adopted the mean GRID log(*gf*)-value as the BRASS reference value because the GRID method yields smaller χ^2-values than the COG method. About 53% of the quality-assessable lines have literature log(*gf*)-values in agreement with the mean GRID log(*gf*)-values. A similar percentage of the 408 analysis-independent lines had sufficiently accurate atomic data. The majority of Fe-group species (V I , Cr I , Mn I , Co I , Ni I , Ti I , and Sc II , Ti II , Fe II) had a good number of lines with accurate atomic data for 70-75% of the lines. The Fe I lines, however, have only ∼38% with sufficiently accurate atomic data (see § 4.7).

The right-hand panel of Figure 15 shows mean GRID log(*gf*)-values (*blue dots*) and mean COG log(*gf*)-values (*black dots*) compared to the log(*gf*)-values in the BRASS (input) dataset for the 408 analysis-independent lines (where both COG and GRID astrophysical values agree within ±0.04 dex). We found sizable differences with the BRASS log(*gf*)-values for a considerable number of lines. Difference log(*gf*)-values in excess of ±0.5 dex have been observed. The inset panel shows lines with smaller log(*gf*) differences (below 0.2 dex), although many are not in agreement within the derived error-bars.

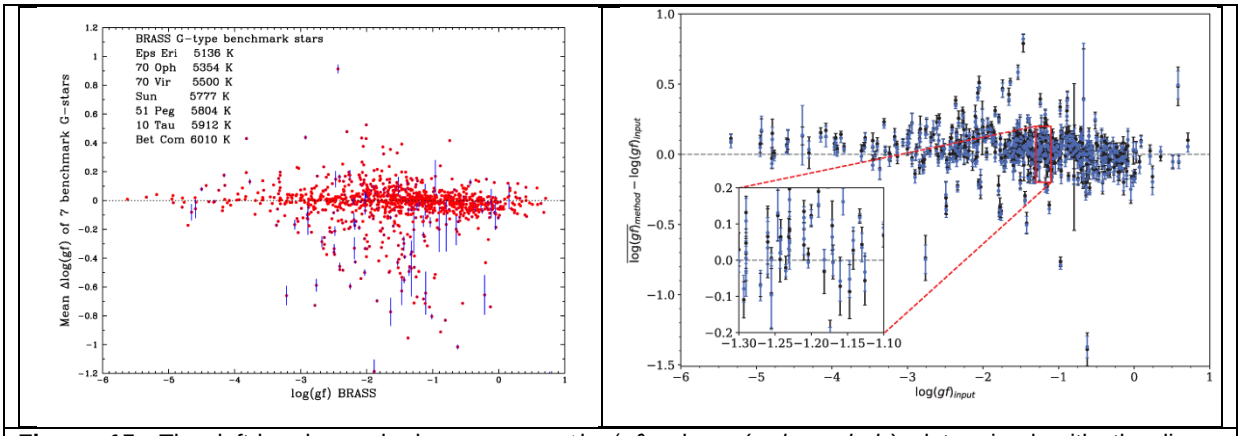


Figure 15. The left-hand panel shows mean Δlog(*gf*)-values (*red symbols*) determined with the linear approximation method against the literature log(*gf*)-values retrieved for BRASS. The standard deviations (*blue lines*) for the 7 benchmark stars stay below 0.02 dex for the vast majority of investigated lines. The right-hand panel shows a similar difference plot for astrophysical log(*gf*)-values of 408 analysis-independent lines from the GRID (*blue symbols*) vs. COG (*black symbols*) atomic data quality assessment method.

It is important to point out that the large differences between the literature log(*gf*)-values we retrieved for BRASS and the mean astrophysical log(*gf*)-values calculated with the FGK BRASS benchmark spectra were also detected using a linear approximation method. Absorption lines on the linear part of the curve-of-growth follow a linear relationship between W_λ- and log(*gf*)-values. For these lines the difference between observed and theoretical log(*gf*)-values equals $\log(W_\lambda^{obs} / W_\lambda^{mod})$, where W_λ^{mod} is the line equivalent width we calculated with the theoretical log(*gf*)-value.

The left-hand panel of Figure 15 shows the mean of the Δlog(*gf*)-values we calculated for the seven BRASS benchmark stars against the retrieved BRASS log(*gf*)-values. The largest mean Δlog(*gf*)-values can also exceed 0.5 dex, although the standard deviations are ≤ 0.02 dex for the majority of investigated lines (*blue error-bars*) (see Lobel et al., 2018). Similar to the GRID vs. COG quality assessment method the mean log(*gf*)-differences we calculated with this linear approximation method remain typically below ±1 dex and are chiefly observed for the medium-strong lines having −3 ≤ log(*gf*) ≤ −0.5. The lines with negative log(*gf*)-differences were also found in a separate analysis of Fe-group element lines in the solar FTS spectrum and in HERMES and UVES spectra of Procyon and Eps Eri (Lobel, 2011). For these lines the literature log(*gf*)-values are overestimated yielding theoretical W_λ-values that exceed the observed values. Similar to the full-fledged GRID vs. COG analysis method smaller Δlog(*gf*)-values are also found towards the weakest (log(*gf*) < −3.5) and strongest (log(*gf*) > 0) investigated lines.

4.6 Interactive BDI overview of atomic data quality assessment results

The atomic data quality assessment results have been incorporated in the online Spectra BDI shown in TABLE III. All investigated atomic lines are listed in elemental and ionic order from lightest to heaviest, beginning with the neutral species of each element. Users can click on the red left-hand line numbers for populating the INVESTIGATED LINE DATA tab at the top of the table. It provides for each line the overview of atomic data quality results shown in Figure 14 and discussed in § 4.4.

TABLE III lists for each investigated line transition:

Column 1: The line number of the transition used to identify 1091 investigated lines with red labels in the BRASS benchmark spectra.

Column 2: The input wavelength of the transition.

Column 3: The derived mean λ_{grid} value including 1-σ error.

Column 4: The lower energy Elow of the transition.

Columns 5 and 6: The mean $\log(gf)_{cog}$ and mean $\log(gf)_{grid}$ values derived by BRASS including 1-σ errors.

Columns 7 and 8: Whether the transition is considered Quality-Assessable and Independent of Analysis methods used in BRASS.

BRASS Investigated Lines Table

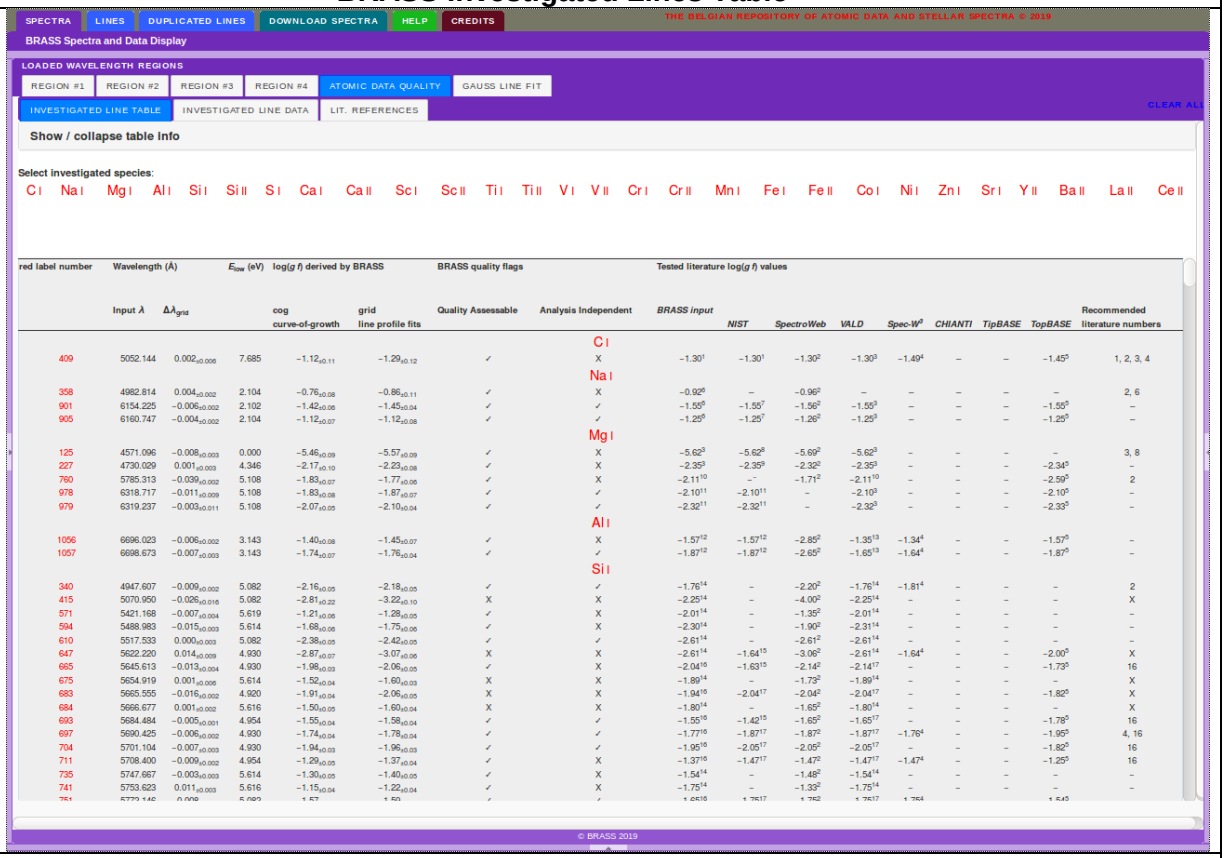


TABLE III. Interactive table in the Spectra BRASS Data Interface of all investigated and quality assessed atomic lines.

Columns 9 to 16: The available literature log(*gf*)-values of a transition with superscripted literature references provided in the LIT. REFERENCES tab at the top of TABLE III, where each column lists the database of origin for the given literature value.

Column 17: Which literature references, if any, reproduce the mean $\log(gf)_{grid}$ values within the σ_{grid}-errors and are recommended by BRASS. If a line cannot be quality-assessed then the "Recommended literature numbers" column will display an "X", and if the line can be quality-assessed but has no recommended literature values it displays a "−".

4.7 Multiplet analysis results of Fe I transitions in BRASS

The rather small percentage of only ~38% of sufficiently accurate atomic data for the Fe I lines in BRASS called for an investigation of its origin. Figure 16 shows the curve-of-growth for Fe I lines we observed in the solar benchmark spectrum. The black dots show observed (reduced) W_λ/λ -values against log(*gf*) (co-added with other terms), for log(*gf*)-values in the (input) BRASS compilation of TABLE I. We found considerable scatter for the transitions on the linear part of the curve, or mainly for the weak and medium-strong Fe I lines. The large scatter is due to the limited accuracy of the literature log(*gf*)-values for these lines. We found that this scatter across the curve substantially reduces after replacing the literature log(*gf*)-values with the ones we calculated from the linear approximation method presented in § 4.5 and shown with red symbols in Figure 16. By replacing the log(*gf*)-values with the ones we calculated from the COG vs. GRID method the scatter nearly vanishes and the curve assumes the smooth (and narrow) shape required for atomic lines belonging to the same species in stellar spectra. The large percentage we found of over 60% of literature Fe I atomic data with limited quality mainly results from medium-strong (and weak) lines having $-3 \leq \log(gf) \leq -0.5$ in Figure 15 (see also Lobel et al., 2019).

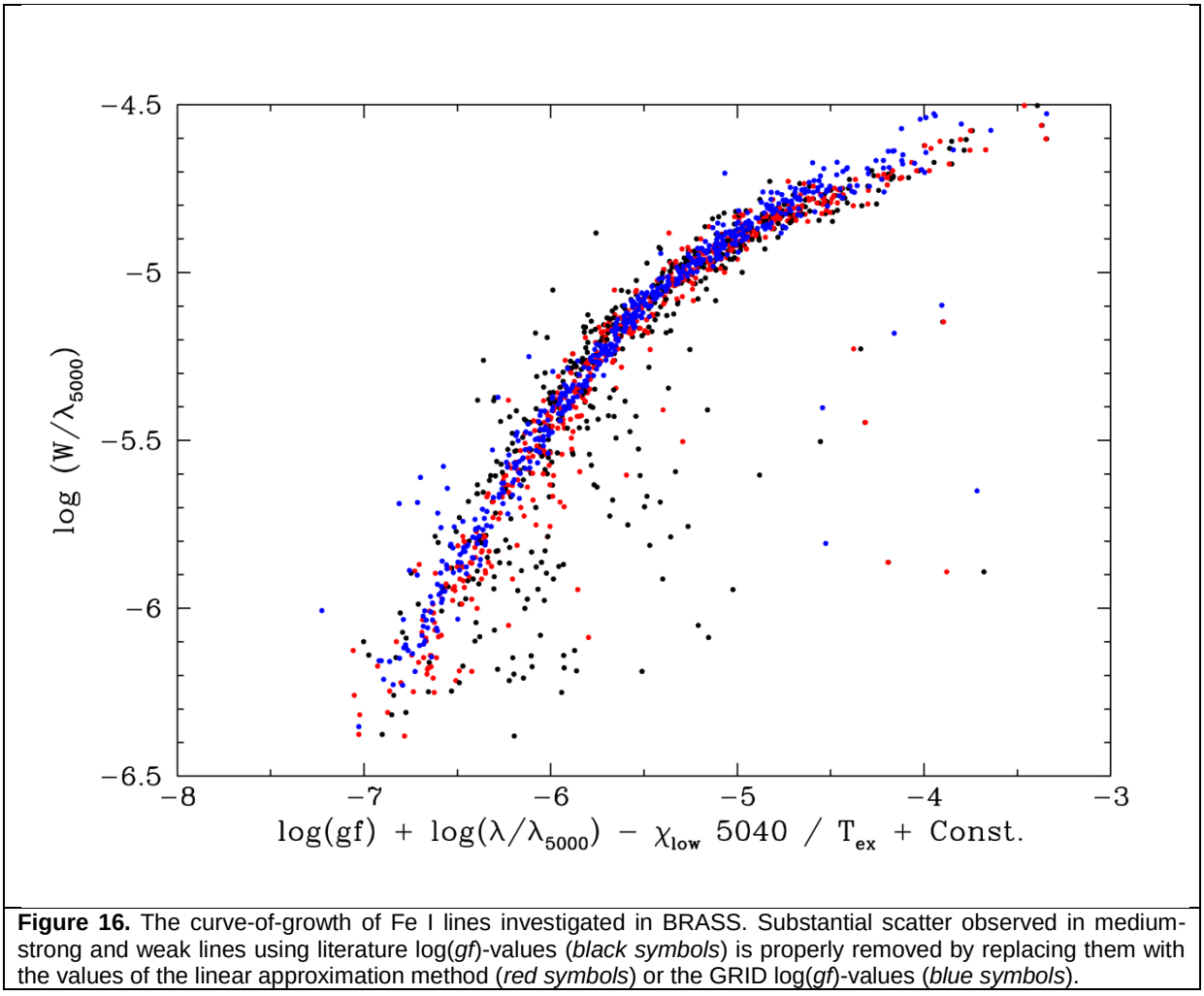


Figure 16. The curve-of-growth of Fe I lines investigated in BRASS. Substantial scatter observed in medium-strong and weak lines using literature log(*gf*)-values (*black symbols*) is properly removed by replacing them with the values of the linear approximation method (*red symbols*) or the GRID log(*gf*)-values (*blue symbols*).

A more extensive analysis of the Fe I fine structure data we retrieved for BRASS revealed that the lines with limited/poor log(*gf*) quality mostly have transition Elow in excess of 4 eV.

We compiled 25 electric dipole multiplets of 69 Fe I lines in BRASS, also shown Figure 17. For each line of these multiplets we calculated the relative line strength ratios assuming single-configuration Russell–Saunders (LS) coupling and obeying the selection rules for these permitted transitions. The calculated multiplet line strengths (using detailed Wigner 6j-symbol calculations) are normalized by scaling the LS-coupling log(*gf*)-values to the strongest available principal line (marked with x1 or x2 in Figure 17), or the largest log(*gf*)-value we calculated with the GRID method using the BRASS benchmark spectra. For a number of multiplets we found reasonable to good agreement between the LS and GRID relative log(*gf*)-values. For example multiplet a5P → y5D (Elow =2.17-2.23 eV) shows very similar distributions across its principal (x) and satellite (y and z) transitions. For multiplet y3D → y3F (Elow =4.73-4.84 eV) the relative log(*gf*) distributions agree less, but also show differences between the literature and GRID log(*gf*)-values of ~1.0 dex. This is also the case for x5F → 5F (Elow = 4.9-5.1 eV) and y5D → e5P (Elow = 4.1-4.23 eV) multiplets for which the relative LS and GRID log(*gf*)-distributions across the x, y, and z line series are dissimilar and a re-normalization cannot remove the large differences above 0.5-1.0 dex for individual lines. Figure 17 shows that the differences between the normalized LS and the (best) BRASS GRID log(*gf*)-values increase towards larger transition Elow-values. For lines having Elow above 4 eV in the 25 studied Fe I multiplets the differences can increase above 0.5-1.0 dex mainly for the satellite transitions (marked y).

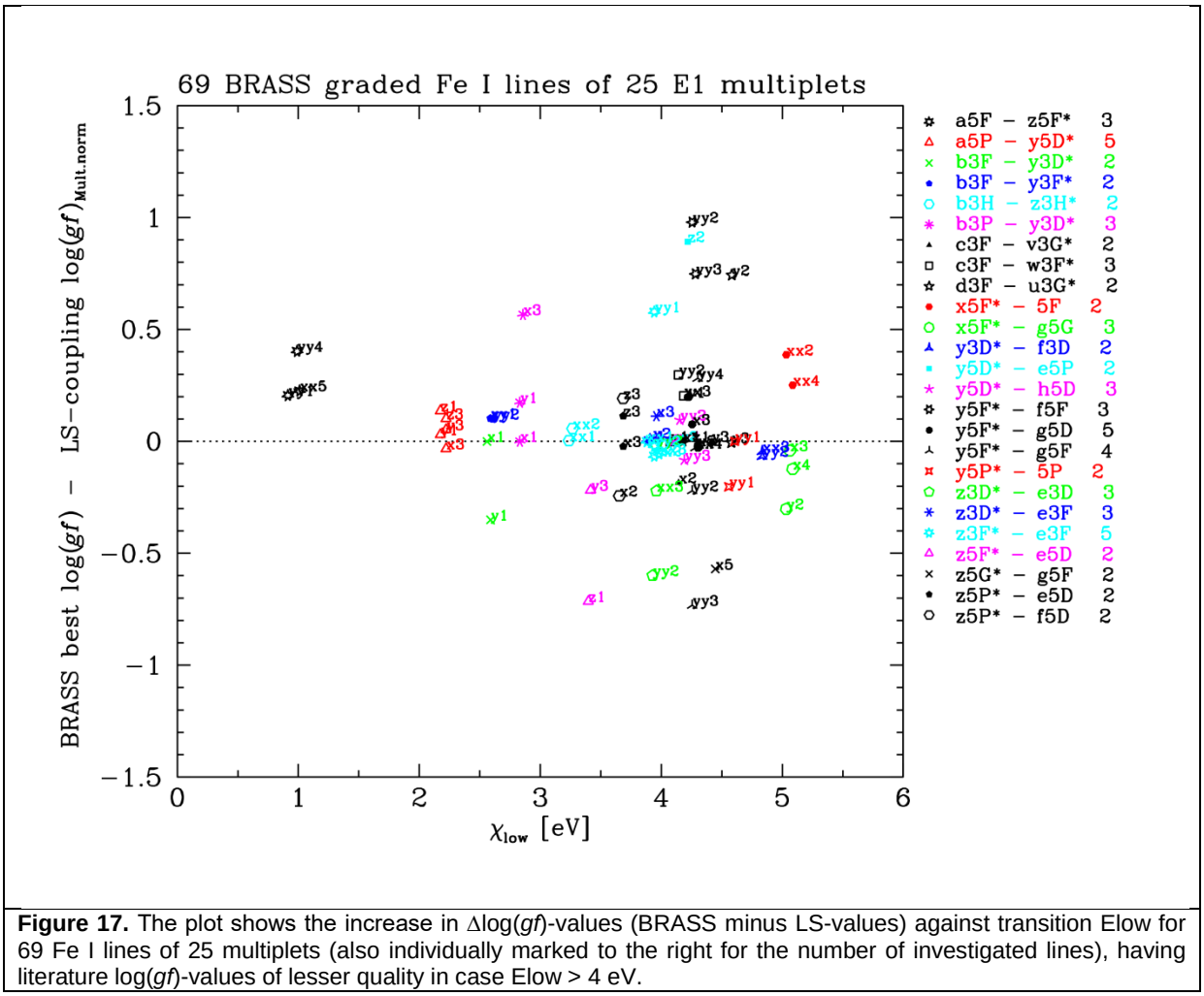


Figure 17. The plot shows the increase in Δlog(*gf*)-values (BRASS minus LS-values) against transition Elow for 69 Fe I lines of 25 multiplets (also individually marked to the right for the number of investigated lines), having literature log(*gf*)-values of lesser quality in case Elow > 4 eV.

Using the interactive NIST Grotrian diagrams we found that the x5F multiplet energy levels have level components that lie very close in energy to neighbouring high energy levels of other atomic terms. For example the x5F (J = 2) level at 5.085 eV falls next to another energy level at 5.070 eV corresponding to the x5S (J = 2) level. The proximity of other nearby energy levels for multiplet lower levels yields significant configuration interaction between the levels. The LS-coupling calculations cannot accurately predict the relative line strengths assuming single electronic configuration interaction. The increasing differences between the literature, LS and GRID log(*gf*)-values towards larger Elow results from inaccurate theoretical Fe I log(*gf*)-values due to poorly constrained configuration mixing coefficients and inaccurate or incomplete theoretical energy levels for the large number of close energy levels above ~4 eV in the neutral Fe atom.

4.8 BRASS Help pages implementation results

4.8.1 Use-cases and video tutorials

For interactive queries of the BDI we also developed online help pages. Eight use-cases have been identified for the LBDI, SBDI, and for the downloading of BRASS datasets:

Lines BDI: *How do I query BRASS for atomic line data?*

How do I make a plot of BRASS cross-matched log(gf)-values?

Spectra BDI: *How do I interactively display BRASS stellar spectra?*

How do I make a plot of investigated BRASS lines?

How do I display atomic BRASS atomic data quality information of investigated lines in the benchmark spectra?

How do I display atomic BRASS atomic data quality information in the list of investigated lines?

Save Data: *How do I save a list of investigated BRASS lines?*

How do I measure equivalent line widths?

The use-cases are provided under the HELP tab. Detailed user instructions are offered by following a point-by-point actions list (see Figure 18). The written instructions have been supplemented with tutorial videos. These short videos of maximum 10 min. have been embedded in a movie player so users do not require external video software for watching them.

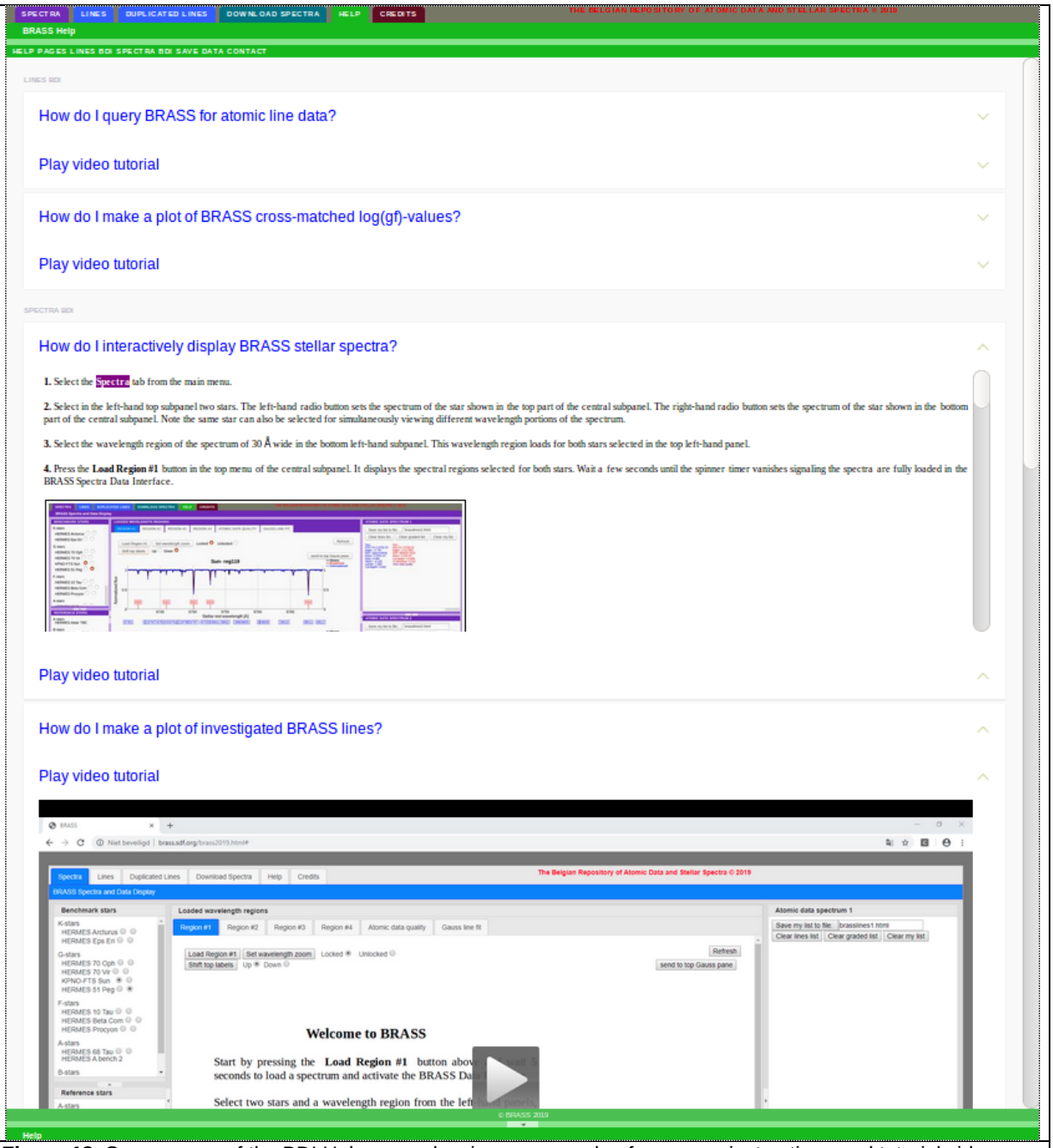


Figure 18. Screen copy of the BDI Help page showing an example of use-case instructions and tutorial video.

4.8.2 Example use-case: interactive equivalent line width measurements

The Spectra BDI also offers an advanced interactive tool for measuring the equivalent widths of identified spectral lines (blue labels) in the benchmark spectra. The interactive best fit procedure employs a single-Gaussian line profile. The implemented minimization procedure varies the wavelength position and depth of the line core, together with the line width ('Gauss sigma' result). Since every benchmark spectrum has been continuum normalized using theoretical (template) spectra (see § 4.3) the 'Background flux level' of the best line profile fit is also measured and listed in the interactive results table (red list to the right of the central plot panel). Users can interactively modify the starting and ending line wavelength boundaries, and hence the number of 'Used fit points' for calculating the 'Fit quality'. The line equivalent width value ('Eqv. Width') is being calculated by extending the best fitting Gauss

profile beyond the boundaries to infinity. The measured background level is used to calculate the uncertainty of the equivalent line width ('Eqv. width error') and added to the results list. The results list is updated by pressing the run top/bottom fit buttons and can be saved to the user's computer disc in the SBDI right-hand sub-panels.

Below we provide an example page of the use-case: *How do I measure equivalent line widths?* Detailed instructions are provided in 12 steps for facilitating user interaction with the measurement tool and for the results downloading.

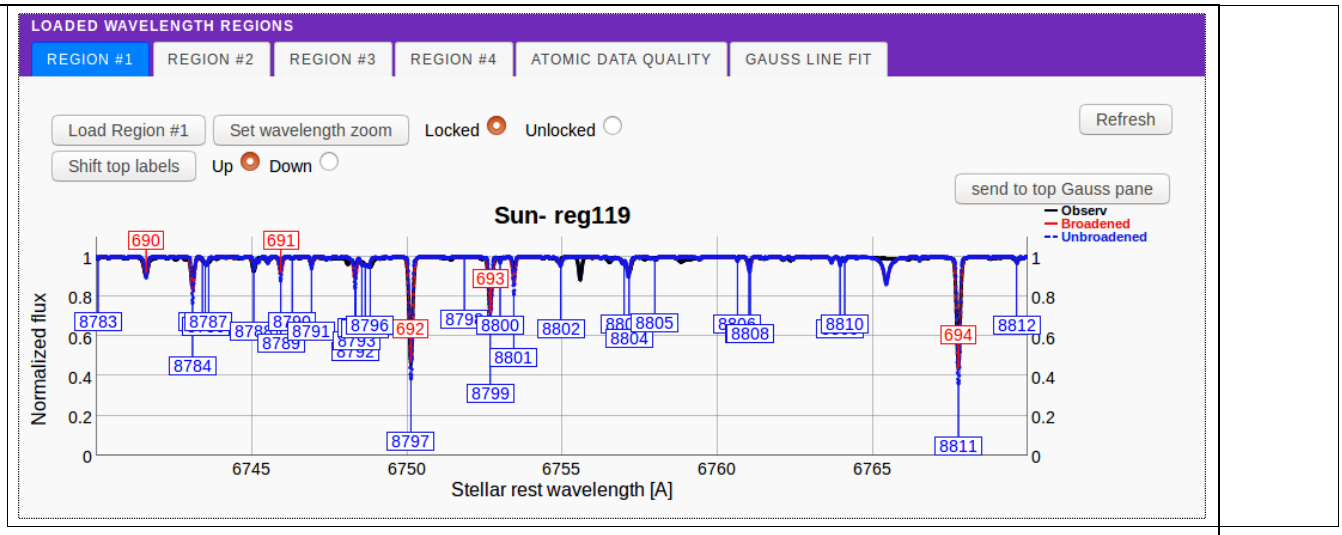
1. Select the **Spectra** tab from the main menu.

2. Select in the left-hand top sub-panel two stars. The left-hand radio button sets the spectrum of the star shown in the top part of the central sub-panel. The right-hand radio button sets the spectrum of the star shown in the bottom part of the central sub-panel. Note the same star can also be selected for simultaneously viewing different wavelength portions of the spectrum.

3. Select the wavelength region of the spectrum of 30 Å wide in the bottom left-hand sub-panel. This wavelength region loads for both stars selected in the top left-hand panel.

4. Press the **Load Region #1** button in the top menu of the central sub-panel. It displays the spectral regions selected for both stars. Wait a few seconds until the spinner timer vanishes signalling the spectra are fully loaded in the BRASS Spectra Data Interface.

5. The red and blue line labels marked on the wavelength axis can be lifted onto the stellar spectrum by checking the **Up** radio button and pressing the **Shift top labels** button next to it.



6. The selected wavelength region can be enlarged. Press the left-hand mouse button for marking the starting wavelength region on the spectrum display. Hold down while sliding along the spectrum wavelength scale and release at the endpoint of the region for enlargement. The mouse zooming function can also be applied along the vertical direction of the spectrum for enlarging the Normalized flux region.

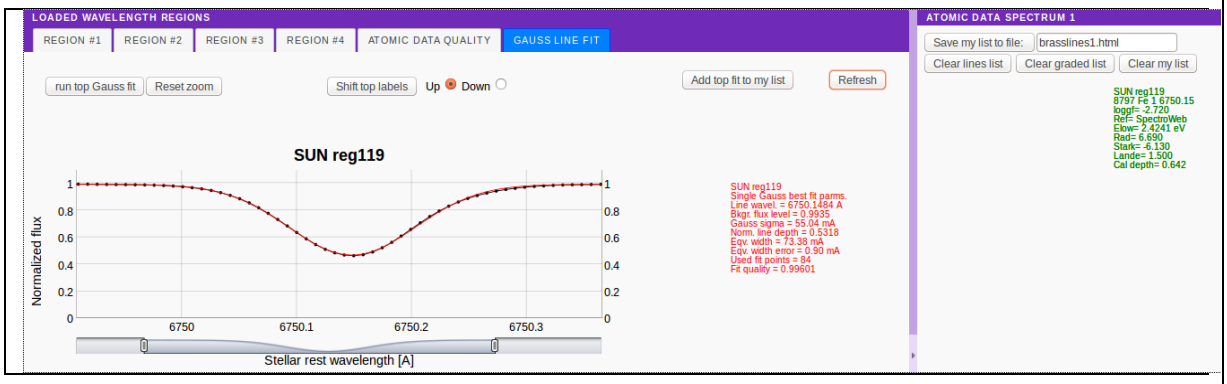
7. The loaded spectral regions can be used for measuring the equivalent line width values of lines selected by the user. The spectral region displayed in the top central sub-panel can be sent to the **Gauss Line fit** tab by pressing the **send to top Gauss pane** button in the top right-hand corner. The spectral region displayed in the bottom central sub-panel can also be sent this tab by pressing the

send to bottom Gauss pane button in the bottom right-hand corner. The Gauss fitting page can be displayed by clicking on the **Gauss Line fit** tab.

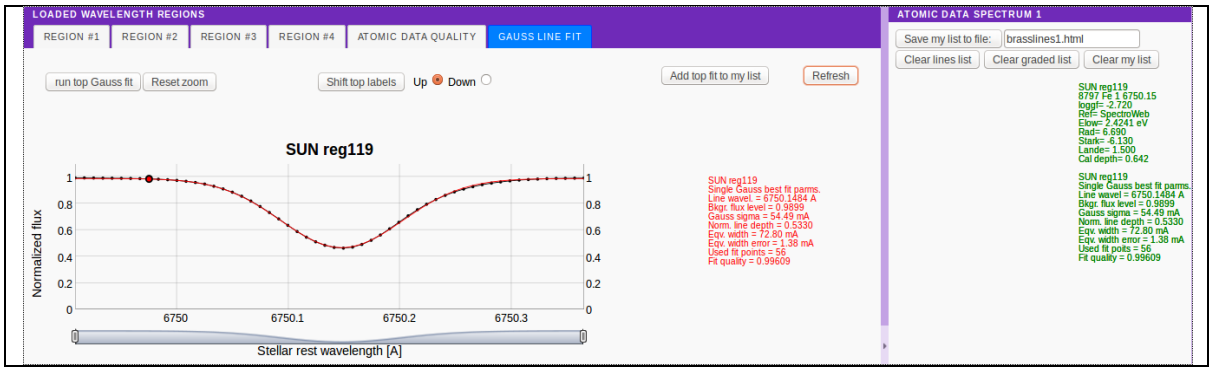
8. For measuring line equivalent widths zoom in on one spectral line with the mouse, for example in the observed spectrum shown in the top central sub-panel. The interactive sliders shown below the spectrum can be moved for enlarging the wavelength region around the selected line. By clicking the blue label the line identification information will populate the green coloured **my list** in the right-hand top (or bottom) sub-panels. The line information in this table can be saved to the user's disc (see point 12. below).

9. By pressing the run **top Gauss fit** button in the top left-hand corner the Gaussian best fit to the observed line fluxes is calculated and over-plotted with the solid red line. The line equivalent width values (**Eqv. width**) are listed in red colour to the right-hand side of the central sub-panel. Other fit parameters are listed in this table as well.

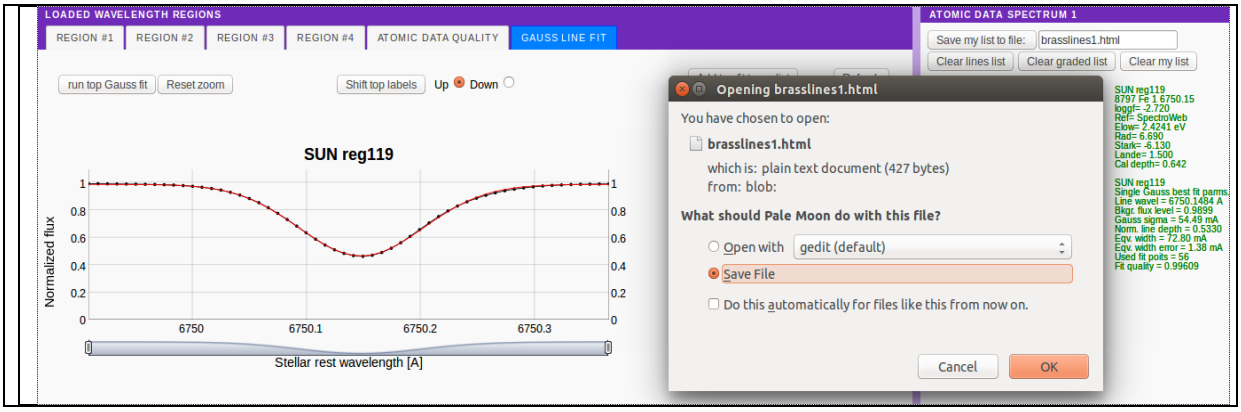
10. By moving the interactive sliders below the spectrum the wavelength region for the line equivalent width calculation can be modified.



11. Next press once more the run **top Gauss fit button** to re-calculate the best fit shown with the red over-plotted line. It also updates the best-fit line values listed in the red right-hand table for the wavelength region set by the user. The final best fit line values can be added to the green colored table in the right-hand sub-panel by pressing the **Add top fit to my list** button.



12. The green table with the line identification, equivalent line width, and more information in the right-hand sub-panel can be exported to the user's disc by pressing the **Save my list to file:** button at the top side of the top or bottom right-hand sub-panels. Additional lines can be added to the list green lists for user saving by selecting and Gauss fitting more lines in point 7.



4.9 References

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4.10 Acronyms

LBDI	Lines BRASS Data Interface
SBDI	Spectra BRASS Data Interface
NIST	National Institute of Standards and Technology
VALD	Vienna Atomic Line Database
VAMDC	Virtual Atomic and Molecular Data Centre
TIPbase	The Iron Project database
TOPbase	The Opacity Project database
CHIANTI	The CHIANTI atomic database
SpectroWeb	The SpectroWeb database
Spec-W^3	The Spectr-W^3 database
HERMES	High Efficiency and Resolution Mercator Echelle Spectrograph
FTS	Fourier Transform Spectrograph
SNR	Signal to Noise Ratio
FWHM	Full-Width Half-Maximum

5. DISSEMINATION AND VALORISATION

5.1 Products

The dissemination has been done through publication of the results in international peer reviewed journals, conference proceedings, oral and poster presentations at scientific meetings, annual network meetings, PhD commission meetings, popular lectures and interview. An overview of activities is provided in § 5.2-5.3. The list of publications in which the project is acknowledged, is provided in § 6.

For the BRASS project a new online database has been developed at brass.sdf.org.The BRASS Data Interface offers atomic datasets combined with advanced tools for the interactive display (zooming, panning, comparing, etc.) of stellar spectra. The spectra and atomic datasets can be interactively selected, displayed, and downloaded through database queries and line marking procedures. User support is offered with help pages and tutorial videos.

The BRASS database will become a standard reference for quality tested atomic data in astrophysics research. For example, Larsen et al. (2018) and Swan et al. (2019) cite very recent BRASS publications for recognizing the importance of discrepancies found between atomic datasets and its impact for contemporary astrophysics research.

5.2 Outreach activities

5.2.1 Presentations on BRASS research

Oral at international and national scientific conferences:

1. A. Lobel & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra,* oral at Solvay Workshop on "New Frontiers in Atomic, Nuclear, Plasma and Astrophysics", 25-27 Nov 2019, Univ. Libre de Bruxelles, Belgium.

   The workshop and presentation were important for providing an oral overview of BRASS research results and the most recent developments of the networking project to an international audience of researchers in atomic physics and astrophysics.
   Presentation published online:
   http://www.solvayinstitutes.be/event/workshop/new_frontiers_2019/slides_cts/Lobel.pdf

2. A. Lobel & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra*, oral at The 13th International Colloquium on “Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas - ASOS13”, 23-27 Jun 2019, Univ. of Fudan, Shanghai, China.

   The colloquium and presentation were important for providing an oral overview of BRASS research results. The meeting at the Univ. of Fudan was important for stimulating interest for the BRASS results with the international atomic physics and astrophysics communities.

3. A. Lobel & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra: Radial Velocity Standards for Hot Stars,* poster talk at International Astronomical Union 30, General Assembly, 20-31 Aug 2018, Univ. of Vienna, Austria.

   The GA meeting and presentation were important for providing an overview of BRASS progress results to an international assembly of astronomers interested in observational and theoretical astronomical spectroscopy.

4. A. Lobel & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra: Atomic Line Data Validation*, oral at Workshop on "Astrophysical Opacities", 3 Aug 2017, Univ. of Western Michigan, Kalamazoo, USA.

   The workshop and presentation were important for providing an overview of BRASS progress results to an international audience of atomic and stellar atmospheric physics researchers. The meeting at Univ. of W-Michigan focused on atomic and molecular opacities for stellar spectroscopy investigated in BRASS.

5. A. Lobel & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra: Status Update 2015-2016*, oral at 12th International Colloquium on "Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas – ASOS12", 4 Jul 2016, Univ. of São Paulo, Brazil.

   The colloquium and presentation at Univ. of São Paulo were important for providing an oral overview of BRASS progress results to an international audience of researchers in atomic physics and astrophysics.

6. M. Laverick & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra: quality assessment of atomic lines*, oral at European Week of Astronomy and Space Science, Royal Astronomical Society, National Astronomy Meeting, Special Session 4 - Stars: "Atomic and molecular data needs for astronomy and astrophysics", 3-6 Apr 2018, Liverpool, UK.

7. T. Merle & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra (BRASS)*, oral at French Society of Astronomy and Astrophysics (SF2A), PNPS Workshop S05, 3-6 Jul 2018, Univ. of Bordeaux, France.

8. N. Gorlova, *BRASS - a new interactive website for analysis of stellar spectra*, oral at 4th Super-VOSS meeting: "The Search for Extra-Astronomical Life", Vatican Observatory Summer School, 3-7 Sep 2019, Vatican Obs., Castel Gandolfo, Italy.

9. M. Laverick & BRASS Team, *The Belgian Repository of fundamental Atomic Data and Stellar Spectra*, oral at FNRS Contact Group meeting, 19 Sep 2017, Planetarium of the Royal Observatory of Belgium.
   Presentation published online: http://www.planetarium.be/cg/files/Laverick2017.pdf

10. T. Merle & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra*, oral at Post-doctoral research projects seminar, 13 Nov 2016, Solvay Room of Univ. Libre de Bruxelles, Belgium.

Posters at international and national scientific conferences:

11. M. Laverick & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra,* poster at Solvay Workshop on "New Frontiers in Atomic, Nuclear, Plasma and Astrophysics", 25-27 Nov 2019, Univ. Libre de Bruxelles, Belgium

12. M. Laverick & BRASS Team, *The Belgian Repository of fundamental Atomic data and Stellar Spectra*, poster at The 13th International Colloquium on "Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas - ASOS13", 23-27 Jun 2019, Shanghai, China.

13. M. Laverick & BRASS Team, *The Belgian Repository of Fundamental Atomic Data and Stellar Spectra*, poster at XXIX Canary Islands Winter School of Astrophysics, 13-17 Nov 2017, La Laguna, Tenerife, Spain.

14. M. Laverick & BRASS Team, *The Belgian Repository of Fundamental Atomic Data and Stellar Spectra: an insight into systematic line selection*, poster at Workshop on "Astrophysical Opacities", 1-4 Aug 2017, Univ. of Western Michigan, Kalamazoo, USA.

15. M. Laverick & BRASS Team, *The Belgian Repository of Fundamental Atomic Data and Stellar Spectra*, poster at 72nd Dutch Astronomy Conference, 22-24 May 2017, Nijmegen, The Netherlands.

16. M. Laverick & BRASS Team, *The Belgian Repository of Fundamental Atomic Data and Stellar Spectra*, poster at FNRS Contact Group Astronomie & Astrophysique, 11 Oct 2016, Planetarium of the Royal Observatory of Belgium.

17. M. Laverick & BRASS Team, *The Belgian Repository of Fundamental Atomic Data and Stellar Spectra*, poster at 12th International Colloquium on "Atomic Spectra and Oscillator Strengths for Astrophysical and Laboratory Plasmas – ASOS12", July 4-7 2016, Univ. of São Paulo, Brazil.

5.2.2 Annual BRASS network meetings

The annual meetings of the BRASS networking project have been organized by the coordinator at the Royal Observatory of Belgium, Nadir Room. The participants delivered oral presentations (including via teleconferencing) on research progress for BRASS. The annual meetings between partners, collaborators and the follow-up committee were important for providing overview of research results, progress reporting, and new developments within the networking project. The meetings reinforced the networking collaboration efforts and provided ample opportunity for scientific discussion. It also offered the BRASS PhD student (ML) an opportunity to orally present results to an audience of international experts involved in the project.

- First annual meeting of 4 Nov 2015
  Participants: A. Lobel (ROB, chair), P. Royer (KUL), C. Martayan (ESO), M.Laverick (KUL & ROB), M. David (UA), H. Hensberge (ROB), E. Thienpont (VVS), D. Cox (Belspo)

- Second annual meeting of 23 Nov 2016
  Participants: A. Lobel (chair), P. Royer, C. Martayan, M. Laverick, T. Merle (ULB), M. David, H. Hensberge, E. Thienpont, D. Cox

- Third annual meeting of 4 Dec 2017
  Participants: A. Lobel (chair), P. Royer, C. Martayan, M. Laverick, P. van Hoof (ROB), T. Merle, M. Van der Swaelmen (ULB), M. David, H. Hensberge, E. Thienpont
  Presentations online: http://brass.sdf.org/ann2017/

- Fourth annual meeting of 7 Dec 2018
  Participants: A. Lobel (chair), P. Royer, C. Martayan, M. Laverick, P. van Hoof, T. Merle, M. Van der Swaelmen, M. David, H. Hensberge, E. Thienpont

5.2.3 PhD meetings for BRASS

The BRASS networking project has supported the doctoral research work of M. Laverick at the KU Leuven and the Royal Observatory of Belgium between 15 Sep 2015 and 15 Sep 2019. Annual PhD Committee meetings have been organized at the KU Leuven, Inst. voor Sterrenkunde, Van Hoof Room. The meetings between BRASS Team members and the KUL PhD Commission were important for providing an overview of new PhD research results for BRASS and the PhD project progress evaluation.

- Supervisory PhD Committee Meeting of 17 Jun 2016: Mr. M. Laverick, Research progress evaluation & PhD project endorsement on BRASS.

- Supervisory PhD Committee Meeting of 23 Jun 2017: Mr. M. Laverick, PhD project mid-term research progress evaluation.

- Supervisory PhD Committee Meeting of 4 Sep 2018: Mr. M. Laverick, PhD project research progress evaluation.

- Supervisory PhD Committee Meeting of 24 May 2019: Mr. M. Laverick, Internal PhD defence evaluation, KU Leuven Arenberg Doctoral School. Invited external PhD jury member: Dr. H. Hartman, Univ. of Malmö, Sweden.

PhD Dissertation published online: *Fundamental atomic data deduced using stellar spectroscopy*, Mike Laverick, Arenberg Doctoral School, Faculty of Science, KU Leuven, Belgium, Sep 2019: http://brass.sdf.org/docs/Mike_Laverick_PhDthesis_Sep2019.pdf

5.2.4 Popular lecture on BRASS

A. Lobel, Invited lecture: *Spectroscopisch Onderzoek te Koninklijke Sterrenwacht van België*. Vereniging voor Sterrenkunde “Spectroscopiedag” of 24 Nov 2018 at Sterrenwacht Tivoli, Oudenburg, The Netherlands.

Popular lecture for amateur astronomers including a presentation on the BRASS Data Interface developments.

5.2.5 Interview on BRASS

On 23 Dec 2019 the BRASS coordinator A. Lobel was interviewed by Mr. F. Meeus of the Volkssterrenwacht Mira in Grimbergen. The interview: *2020-01 MIRA Ceti sprak met... Alex Lobel* also focused on the BRASS research results and Data Interface developments.

Interview published online: https://www.mira.be/artikels/2020-01-mira-ceti-sprak-met-alex-lobel

5.3 Research visitor for BRASS

Research visit of Dr. M. Safronova of Univ. of Delaware, USA to ROB (A. Lobel) in the context of atomic physics research collaboration for BRASS. Seminar on *Variation of fundamental constants and the current status of atomic theory*, 11 Sep 2019, Meridian Room, ROB.

5.4 Researcher employments for BRASS

The networking project has provided salary for the employment of a post-doctoral researcher at ROB and a PhD student at the KUL. These employments have helped the timely realization of the BRASS research goals.

- PhD student KUL, Mr. M. Laverick, full-time employment for BRASS at KU Leuven from 15 Sep 2015 to 15 Sep 2019.

- Post-doctoral researcher ROB, Dr. P. van Hoof, full-time employment for BRASS at ROB from 1 Sep 2017 to 1 Mar 2019.

6. PUBLICATIONS

6.1 Refereed Science Journals

2019

Lobel, A., Royer, P., Martayan, C., Laverick, M., Merle, T., Van der Swaelmen, M., van Hoof, P.A.M., David, M., Hensberge, H., Thienpont, E. 2019, Atoms, 7, 105
The Belgian Repository of Fundamental Atomic Data and Stellar Spectra (BRASS)
https://doi.org/10.3390/atoms7040105

Laverick M., Lobel A., Royer P., Merle T., Martayan C., van Hoof P. A. M., Van der Swaelmen M., David M., Hensberge H., Thienpont E. 2019, Astronomy & Astrophysics, 642, A60
The Belgian repository of fundamental atomic data and stellar spectra (BRASS). II. Quality assessment of atomic data for unblended lines in FGK stars
https://doi.org/10.1051/0004-6361/201833553

2018

Laverick M., Lobel A., Merle T., Royer P., Martayan C., David M., Hensberge H. and Thienpont E. 2018, Astronomy & Astrophysics, 612, A60
The Belgian repository of fundamental atomic data and stellar spectra (BRASS) I. Cross-matching atomic databases of astrophysical interest
http://dx.doi.org/10.1051/0004-6361/201731933

Laverick, M., Lobel A., Royer P., Martayan C., Merle T., van Hoof, P. A. M., Van der Swaelmen, M., David M., Hensberge H., Thienpont E. 2018, Galaxies, 6, 78
The Belgian Repository of Fundamental Atomic Data and Stellar Spectra (BRASS) Identifying Fruitful Methods for Producing Atomic Data
https://doi.org/10.3390/galaxies6030078

2017

Lobel A., Royer P., Martayan C., Laverick M., Merle T., David M., Hensberge H., Thienpont E. 2017, Canadian Journal of Physics, 10.1139/cjp-2016-0750
The Belgian repository of fundamental atomic data and stellar spectra
https://doi.org/10.1139/cjp-2016-0750

Laverick M., Lobel A., Royer P., Martayan C., Merle T. 2017, Canadian Journal of Physics, 10.1139/cjp-2016-0754
BRASS: Cross-match of atomic repositories and spectral line blending investigations
https://doi.org/10.1139/cjp-2016-0754

6.2 Conference Proceedings

Lobel A., Royer P., Martayan C., Laverick M., Merle T., van Hoof, P. A. M., Van der Swaelmen, M., David M., Hensberge H., Thienpont E. 2018, ASPCS, 515, 255, Eds. Claudio Mendoza, Sylvaine Turck-Chiéze, and James Colgan. San Francisco.
The Belgian Repository of Fundamental Atomic Data and Stellar Spectra: Atomic Line Data Validation
http://aspbooks.org/custom/publications/paper/515-0255.html

Laverick, M., Lobel A., Royer P., Martayan C., Merle T., van Hoof, P. A. M., Van der Swaelmen, M., David M., Hensberge H., Thienpont E. 2018, ASPCS, 515, 263, Eds. Claudio Mendoza, Sylvaine Turck-Chiéze, and James Colgan. San Francisco.
The Belgian Repository of Fundamental Atomic Data and Stellar Spectra: An Insight into Systematic Line Selection
http://aspbooks.org/custom/publications/paper/515-0263.html

Merle, T., Laverick, M., Lobel, A., Royer, P., Van der Swaelmen, M., Frémat, Y., Sekaran, S., Martayan, C., van Hoof, P. A. M., David, M., Hensberge, H., Thienpont, E. 2018 SF2A-2018: Proceedings of the Annual meeting of the French Society of Astronomy and Astrophysics. Eds.: P. Di Matteo, F. Billebaud, F. Herpin, N. Lagarde, J.-B. Marquette, A. Robin, O. Venot, pp.153-156
The *Belgian Repository of fundamental Atomic Data and Stellar Spectra (BRASS)*
http://adsabs.harvard.edu/abs/2018sf2a.conf..153M

6.3 BRASS Network Internal Reports

- Van Hoof, P.A.M., *UVES Spectra in BRASS*, Royal Observatory of Belgium, 18 Dec 2017.
- Laverick, M., *Automatic glitch removal tool: Technical Note*, KU Leuven, 18 Jan 2016.
- Laverick, M., *Automatic glitch removal tool*, KU Leuven, 10 Jan 2016.
- Lobel, A. & the Partners of the BRASS Networking Project, *A new method for determining radial velocity values of A-type stars in BRASS*, Royal Observatory of Belgium, 1 Nov 2015.

6.4 Progress Reports

A. Lobel and the BRASS Team, *BRASS Annual Network Report to Belspo*,
Intital Report of 2015 and Annual Reports of 2016, 2017, & 2018.

6.5 PhD Dissertation

Mike Laverick, PhD Dissertation, Arenberg Doctoral School, Faculty of Science, KU Leuven, Belgium, September 2019
Fundamental atomic data deduced using stellar spectroscopy
http://brass.sdf.org/docs/Mike_Laverick_PhDthesis_Sep2019.pdf

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Members of the BRASS follow-up committee:

Prof. Dr. M. David, University of Antwerp, Faculty of Science

Dr. H. Hensberge, Brazil and Royal Observatory of Belgium, Dpt. Astronomy & Astrophysics

Mr. E. Thienpont, Vereniging voor Sterrenkunde