Summary

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.

Methodology

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. Emphasis was set on the development and application of new methods for removing and reducing systematic errors in 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 objective of BRASS was to provide the largest systematic and homogeneous quality assessment of fundamental atomic data to date in terms of wavelengths and atomic species. We have combined 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 advanced radiative transfer codes that utilize modern 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 offer powerful new functionalities for stellar spectroscopic research.

To achieve these goals the following questions were addressed:

(1) Can fundamental atomic data required for 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 KPNO-FTS spectra of FGK-type stars observed with very large signal-to-noise ratios.

(3) Can the quality analysis results of tested atomic data comprehensively be 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.

Our detailed comparisons of line transition data (or log(*gf*)-values) retrieved from various atomic data repositories and the literature revealed remarkably large differences of up to 3 dex or more. The values can considerably change over time, sometimes within a few years, showing the importance of providing an external assessment of their accuracy (quality) by comparing to values obtained from contemporary high-quality astrophysical spectroscopic observations.

By combining the atomic and spectroscopic data analyses of BRASS (i.e., using spectral line lists and high-quality benchmark stars) the project compiled an extensive list of reference spectral lines suitable for the quality assessment of the retrieved atomic datasets. The results of these complementary analysis methods determined the reliability of the atomic line data. In case the methods produced similar values within errors the retrieved atomic data were considered reliable, otherwise one or more complicating factors could exclude them from further analysis.

The objectives of the project were accomplished by performing a systematic analysis of the selected spectral lines in each FGK benchmark star. It resulted in the final list of 1091 spectral lines that were scrutinized and quantitatively compared between the various atomic data repositories and the observed stellar benchmark spectra. A subset of 845 atomic lines was retained having log(*gf*)-values internally consistent with our astrophysical selection criteria. The 'astrophysical' values therefore have been used as benchmark values for quality assessing against those retrieved from the repositories and literature. In case the latter values were in agreement with the benchmark values they are recommended as reliable for advanced spectroscopic research.

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 (difference between literature and BRASS astrophysical log(*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 Δλ-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.