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# Benchmarked atomic data for astrophysics

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**Abstract.** The recent calculations of atomic data for ions of astrophysical interest are reviewed with a focus on work performed in Cambridge. The calculations have been benchmarked against high-resolution laboratory and astrophysical spectra. A framework for assessing uncertainties in atomic data has also been developed. Long-standing discrepancies in predicted spectral line intensities have been resolved, and a significant number of levels in coronal ions have finally been identified, improving the modelling of the extreme-ultraviolet and soft X-ray spectral regions. Recent improvements based on collisional-radiative modelling are presented. They are relevant for the modelling of satellite lines in the X-rays and for solving the long-standing problems in the chromosphere-corona transition in stellar atmospheres.

**Keywords.** atomic data,atomic processes, line: identification, techniques: spectroscopic

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## 1. Atomic data calculation, benchmark and distribution

The need to improve atomic data for the extreme ultraviolet (EUV: 150–900 Å) became very obvious once the first high-resolution (60 mÅ) solar spectra from the Hinode Extreme-ultraviolet Imaging Spectrometer (EIS) were produced in 2006. Within the 175–200 Å range, dominated by transitions from highly ionized Fe ions, about half of the observed spectral lines in active region spectra were not identified or had a dubious identification. Departures between observed and predicted radiances in some ions (especially Fe XI) were significant, about a factor of two. This included even the strongest lines in the observed spectra.

In preparation for the Hinode mission, a laboratory astrophysics programme was started in 2002 at the Atomic Astrophysics group at DAMTP. The focus was to improve and benchmark the atomic data for the Iron ions, from Fe VII to Fe XXIV. The method, described in Del Zanna *et al.* (2004), is to assess for each ion all available experimental data, to improve atomic structure and scattering calculations, and compare all the main line intensities to those observed in laboratory and astrophysical plasma. The atomic calculations have been carried out within the Iron Project and later the UK RMAX and UK APAP network (apap-network.org). The workhorses are AUTOSTRUCTURE and a set of $R$-matrix codes, developed for the Iron Project by a largely UK-based team. For a review of such atomic calculations and benchmark studies see Del Zanna & Mason (2018), while for a review of the UK APAP network studies see Badnell *et al.* (2016).

Over a period of 25 years, the Culham group produced a a significant amount of laboratory plates, used for line identifications in the XUV, as decribed in the review by Fawcett (1990). Some of the original plates were rescued and used for the benchmark project. Results from beam-foil spectroscopy (in a series of papers, see, e.g. Träbert (2005)) and several studies using Electron Beam Ion Traps (EBIT, see e.g. Träbert *et al.* (2014)) have also been extremely useful.

In several cases, standard semi-empirical corrections to the atomic structure were necessary. In some cases, corrections within the scattering calculations were also introduced. They produced significant improvements, as described e.g. in Del Zanna & Badnell (2014).

The benchmark work has resulted in a large number of new identifications. For some ions such as Fe XI, the energies of more than half of the lower 3d levels were unknown. The new identifications have recently been confirmed with large-scale calculations using GRASP2K by Wang *et al.* (2018). GRASP2K is an extension of the original general-purpose relativistic atomic structure program and is capable of obtaining nearly spectroscopic accuracy (uncertainties in level energies of a few hundreds of Kaisers), as reviewed in Jönsson *et al.* (2017).

The benchmark work ultimately resulted in the identification of all the strongest lines in the Hinode EIS spectra, although many weaker unidentified lines remain, as shown e.g. in Brown *et al.* (2008), Del Zanna (2009) and Del Zanna (2012b).

The NASA Solar Dynamics Observatory (SDO), launched in 2010, carried a suite of instruments, two of which have been used to study the solar corona: the Atmospheric Imaging Assembly (AIA) with its seven EUV broad-band images, and the Extreme ultraviolet Variability Experiment (EVE) instrument which produced until May 2014 medium-resolution (1Å) irradiance spectra in the 50–1050 Å range. A benchmark of the most recent atomic data against EVE quiet Sun irradiances is described in Del Zanna (2019), after a significant revision of the EVE radiometric calibration (see Del Zanna & Andretta (2015)). Very good agreement (within 20% or so) between predicted and observed EUV irradiances was found, indicating that the accuracy of the atomic data is now better than the accuracy in the radiometric calibration of EUV space instruments.

**Soft X-rays**

There was excitement in the community when the soft X-ray AIA bands at 94 and 131 Å provided, for the first time, high-cadence imaging in hot emission, due to Fe XVIII and Fe XXI, respectively. However, it became very clear that the atomic data at these wavelengths, dominated by $n = 4 \rightarrow n = 3$ transitions in highly ionised Fe ions, was very poor and incomplete. The hot lines were blended with unidentified transitions. The first soft X-ray studies are Edlén's pioneering ones in the 1930s, later extended by Fawcett *et al.* (1972). As only cross-sections for $n = 4$ levels in Fe X were available (and turned out to be incorrect), a series of large-scale scattering calculations for all the coronal Fe ions was necessary. The new atomic data led to several new identifications, summarised in Del Zanna (2012a). The most significant one is a revision of the identification of the Fe XIV $3s^2$ 3d $^2D_{3/2}$–$3s^2$ 4p $^2P_{1/2}$ transition with the 93.61 Å line, which turns out to be the strongest contribution to the SDO AIA 94 Å band in quiescent solar active regions. However, most of the weaker transitions in the soft X-rays still await identifications, as also evidenced by the EBIT measurements.

It is not necessarily the case that a large-scale atomic calculation is better than a smaller one. But in this case, three surprising results were found for all the ions. The first surprising result was that in several cases (e.g. the $3s^2$ $3p^4$ 4s levels in Fe X), Distorted-Wave (DW) scattering calculations significantly underestimated the cross-sections. The second surprising result was the large cross sections for the forbidden transitions to the 3s $3p^q$ 4s levels. Such levels decay via dipole-allowed transitions which turn out to be stronger than the transitions identified by Edlén and Fawcett. The third surprising result is the most important one: the addition of $n = 4, 5$ levels resulted in increased excitation and extra cascading for the lower $n = 3$ levels. Single cross-sections to $n = 3$ levels only increase by 10% or so, but the cumulative effect is significant: for some ions (e.g. Fe X, Fe XII), the populations of the lower ground-configuration levels changed by 30–50%. This change in the populations has modified the predicted intensities of the famous forbidden lines by up to a factor of two, and all the density diagnostics related to the ground-configuration levels.

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**CHIANTI**

The CHIANTI atomic data and programs (www.chiantidatabase.org) are now widely used in astrophysics for the modelling of collisional plasma. CHIANTI has over 3000 citations, but its data are also included in many other widely-used modelling packages (e.g. CLOUDY, XSTAR, MOCASSIN, ATOMDB). The main programs are written in IDL and are available as a stand-alone or via SolarSoft, a programming environment for the solar physics community, although Python versions are also available. A review of CHIANTI is available at Young *et al.* (2016), while the latest versions are described in Zanna *et al.* (2015) and Dere *et al.*(2019).

## 2. Ion charge state distributions and non-equilibrium effects

Now that we have accurate atomic rates within the main ions, the next challenge is to improve the modelling of the ion charge states. Most of the charge states are calculated assuming ionisation equilibrium and zero electron density, i.e. all ions in their ground states. We recently started a new project, to include processes often neglected in the literature to calculate ion charge states. The main ones are density-dependent recombination rates and photoionisation-recombination. To include them, a collisional-radiative modelling needs to be implemented. A first step in this direction is described in Dufresne & Del Zanna (2019) for carbon. The typical density of the quiet Sun transition region affects the rates so that the C IV intensity is increased by nearly a factor of three, compared to the zero-density case. C IV is one of the so-called anomalous ions, i.e. those that have predicted radiances typically a factor of 3–5 lower than observed. The most affected ions are those of the Li- and Na-like isoelectronic sequences, and the problem is also present in stellar atmospheres, see e.g. Del Zanna *et al.* (2002). In general, all lower charge states are affected, see e.g. Polito *et al.* (2016).

Other effects that we have studied in our group over the years is how non-Maxwellian distributions affect spectral line intensities, and how time-dependent ionisation affect the hydrodynamic modelling of magnetically-closed structures. For a review, see Dudík *et al.* (2017) and Del Zanna & Mason (2018).

## 3. Outlook for the future

Now that the atomic rates for several ions have been calculated several times with different approximations and codes, the next challenge is to provide some estimates of uncertainties in the rates. It is even more important to assess how uncertainties in the atomic rates affect the spectral line intensities and the derived quantities, such as electron temperatures and densities. If we take for example the Be-like N IV, it has been found that three calculations produce cross-sections that differ typically by one order of magnitude for the weaker transitions. They were all produced by large-scale $R$-matrix codes (ICFT, DARC and B-spline), but with different approaches and different configuration-interaction and close-coupling expansions. The reasons for such discrepancies have been discussed in the literature, but their relevance for astrophysical applications was not studied. The scatter in the atomic rates was used in Del Zanna *et al.* (2019) as a measure of uncertainty in each rate. A Monte-Carlo approach showed that for all the observable transitions the variations in the emissivities were small (less than 20%), despite the large variations in the rates of the weaker transitions. A similar approach, described in Yu *et al.* (2018) and Yu *et al.* (this volume), was applied to Fe XIII EUV lines, used to measure the electron density in the solar corona (see e.g. Young *et al.* (2009)).

In future astrophysical missions, high-resolution spectroscopy featurs prominently. Therefore, we can expect further challenges to laboratory astrophysics, especially in unexplored spectral regions. For example, SIRIUS is a mission proposed to ESA to study stellar coronae, white dwarfs and the interstellar medium at high resolution in the 170–260 Å range. Most of this range is now well known thanks to Hinode EIS spectra, but the 210–245 Å region, rich in spectral diagnostics, is almost unexplored, with the exception of some slitless Skylab spectra.

Aside from the need to complete the Table of the astrophysical elements with large-scale calculations of atomic rates, there is also a need for renewed efforts in laboratory spectroscopy, using e.g. EBIT or ECR/plasma traps (cf. Giarrusso *et al.*, this volume) which are producing plasma similar to that found in astrophysical sources.

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