Atomic Data for Astrophysics

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Abstract. Some recent calculations of basic atomic data which are of importance for astrophysical applications are briefly reviewed. A few issues concerning the derivation of chemical abundances from remote-sensing XUV measurements are then introduced. Atomic data storage and distribution are also discussed. An on-going long-term project on benchmarking atomic data for astrophysics is described.

1. Introduction

In optically-thin plasmas, spectral line intensities are directly proportional to $N_j\ A_{ji}$, where A_{ji} is the spontaneous transition probability, $N_j(X^{+r})$ is the number density of the upper level j of the emitting ion (X^{+r}). In low density plasmas the collisional excitation processes are generally faster than ionization and recombination timescales, therefore the collisional excitation is dominant over ionization and recombination in populating the excited states. The intensity $I(\lambda)$ of a spectral line is normally expressed as an integral along the line-of-sight h:

$$I(\lambda) = \int_h A_{ji} \frac{N_j(X^{+r})}{N(X^{+r})}\ \frac{N(X^{+r})}{N(X)}\ \frac{N(X)}{N_{\rm H}} \frac{N_{\rm H}}{N_{\rm e}}\ N_{\rm e}\, dh \quad = \int_h N_{\rm e}\, N_{\rm H}\, A(X)\, G(N_e, T, \lambda)\, dh \tag{1}$$

where $\frac{N_j(X^{+r})}{N(X^{+r})}$ is the fractional population of ions $\mathrm{X}^{+\mathrm{r}}$ lying in the state j; $N(X^{+r})/N(X)$ is the ionization ratio of the ion X^{+r} relative to the total number density of element X; $A(X) = N(X)/N_{\rm H}$ is the elemental abundance relative to Hydrogen; $N_{\rm H}/N_{\rm e}$ is the Hydrogen density relative to the free electron density (often assumed equal to 0.83 whenever H, He are fully ionised). The fraction $\frac{N_j(X^{+r})}{N(X^{+r})}$ can be calculated once all the important collisional and radiative excitation and de-excitation rates between all important levels are known. Similarly, the ionization ratio can be calculated once all the ionization and recombination rates are known.

The product $\epsilon_{ji} = A_{ji}\ \frac{N_j(X^{+r})}{N(X^{+r})}$ is the *line emissivity* and expresses the number of photons emitted per unit time by the transition $j \rightarrow i$. The line emissivity depends on both the temperature and the density of the emitting plasma. The ionization ratio is strongly dependent on the temperature with some density dependence.

A comparison between observed and predicted emissivities / intensities can provide 'direct' measurements of electron densities, temperatures, as well as chemical abundances.

2. Calculations of basic atomic data

A significant amount of new atomic data have been produced in the last few years. A few notable cases are mentioned here. Dere (2007) has calculated ab-initio cross-sections for direct ionization of ions by impact with electrons and compared them with available experimental data for a large number of ions. A new set of radiative recombination rates has been produced by Badnell (2006). Badnell, with a number of collaborators, has produced, with a series of papers (the first being Badnell et al. 2003), a large dataset of dielectronic recombination rates. The above rates have produced new ionization tables, published in Dere et al. (2009). For some ions, these are significantly different from previous ones. It is important to keep in mind that high densities and time-dependent ionization can significantly affect ion abundances. Over the years, a large amount of accurate radiative and excitation data have been produced, for a number of ions, by the Iron Project [1] and UK Rmax.

2.1. APAP

The APAP (Atomic Processes in Astrophysical Plasmas: *http://www.apap-network.org*) collaboration is a follow-up of UK Rmax. Currently, active members are N.Badnell, P.Storey, G.Liang, G.Del Zanna and H.Mason. One important APAP aim is the calculation of electron excitation and radiative rates for a few entire isoelectronic sequences, for ions important for astrophysics, from hydrogen up to krypton.

The work on the F-like ions was published in Witthoeft et al. (2007), and the data for some important ions was included in the CHIANTI database version 6. The work on the Na-like ions was described in Liang et al. (2009b). For the Ne-like (Liang & Badnell 2010), a large-scale calculation with 209 levels close-coupling expansion was done. The calculation for the Li-like (Liang & Badnell 2011) iso-electronic sequence includes core- and valence-excitations. The inclusion of Auger and radiation damping significantly reduce the resonance enhancements for core-excitations. Detailed comparisons along the sequence have been done to check the accuracy for each sequence calculation. They included comparisons between theoretical energies and those from previous calculations and with experimental energies. Also, of line strengths and excitation rates. The new calculations include larger targets and configuration interaction, and for many ions are the most sophisticated ones. For a number of ions, they are the first such calculations.

Specific work on some ions has also been done. For example, the Si x model ion was improved with new excitation data, calculated with a large-scale model. Some new lines have been identified with these resultant excitation data (Liang et al. 2009a). The Fe xiv model ion was also improved over previous calculations by Liang et al. (2010). As a by-product of a new large-scale calculation, it was found that significant inconsistencies are present between the theoretical and experimental cross-section near threshold for the important green coronal forbidden line. This and other discrepancies between observations and models for other ions suggest that at the moment there are large uncertainties associated with excitation rates of forbidden lines at low temperatures, typical of nebulae and photoionized plasmas in general.

[1] http://www.usm.uni-muenchen.de/people/ip/iron-project.html

The APAP collisional-radiative data are released via our web pages in the form of one kind of 'adf04' format, used within ADAS. These are ascii files which contain the target energies, the A-values, the excitation rates, and a number which is used to know the high-energy limit for the transition.

3. Chemical abundances

Direct in-situ measurements of the solar wind clearly show that the slow wind has variable chemical abundances and an first ionization potential (FIP) bias of 2–3, i.e. with high-FIP elements depleted by factors of 2-3, compared to the low-FIP (and their 'photospheric' abundances). On the other hand, fast wind emanating from the coronal holes has less-varying chemical abundances, which are close to the 'photospheric' abundances. It is important to keep in mind that for some important elements such as helium, neon and argon, only in-situ or remote-sensing XUV measurements can directly provide the 'photospheric' abundances.

Following on from the pioneering work of Pottasch (1963), a large literature now exists on measurements of chemical abundances in the solar corona using some form of emission measure (EM) analysis (see Del Zanna 1999 for a review). One way, for example, is to consider the loci of the $I(\lambda)/\left(A(X)\,G(T)\right)$ curves, which represent the upper limits to the column emission measure $EM_{\rm h} = \int_h N_e\,N_H\,dh$ at each temperature.

Unfortunately, in a number of cases, incorrect modelling or assumptions have led to over- or under-estimations of the chemical abundances of some elements by large (2–10) factors. For example, Widing & Feldman (1992) used an approximation which assumes that there is a continuous distribution of plasma at different temperatures along the line of sight, and found an FIP bias of a factor of 10 for a solar plume. Del Zanna et al. (2003) showed that instead the plasma is likely to be isothermal and explained the same observations with no FIP bias. Fig. 1 shows an update of the Del Zanna et al. (2003) results using the latest CHIANTI v.6 ion abundances and 'photospheric' abundances (Asplund et al. 2009). A similar problem was found in active region observations (see Del Zanna 2003).

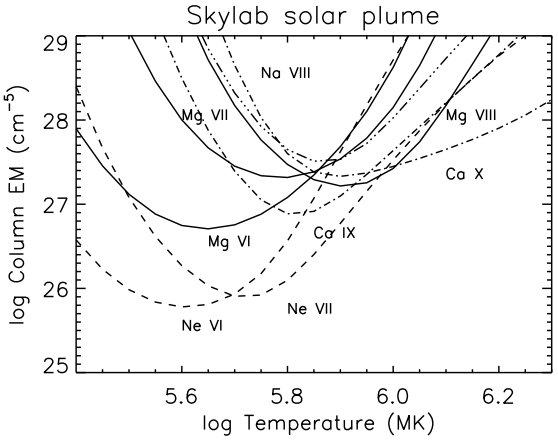

Figure 1. The EM loci curves for a solar plume observed by Skylab.

Anomalous EM for lines of the Li and Na isoelectronic sequences has been present in all the EUV observations (including those of Pottasch 1963), however this issue has been noted only occasionally in the literature (the first mention was from Burton et al. 1971). A revision of older measurements (Del Zanna 1999; Del Zanna et al. 2001) has found that ions of the Li-like sequence such as N v and C iv can be underestimated by factors of up to 10, while those like Ne viii and Mg x are often overestimated by factors of 5 to 10. Ions of the Na-like sequence also show emission measures with significant departures. The problem was discovered to be general, indeed it also applies to stellar coronae as shown by Del Zanna et al. (2002), and therefore casts some doubts into the use of remote sensing and EM analyses for studies of chemical abundances. It has to be pointed out, however, that in the majority of cases results are in close agreement with those obtained from the use of photospheric absorption lines (which involves much more significant modeling, and is therefore subject to large uncertainties) and with 'direct' in-situ sampling. In any case, the ion abundances are the major source of uncertainty in the derivation of chemical abundances.

4. Atomic data storage and distribution

One of the reasons why the CHIANTI (*www.chiantidatabase.org*) database (Dere et al. 1997, 2009) has become so successful (more than 1000 citations) is the inclusion of observed wavelengths, and of all the necessary rates to calculate line emissivities. All the atomic data are properly assessed and referenced. There is no other ion database which is as complete as CHIANTI. But most of all, the CHIANTI database has become widely used because of the inclusion of IDL programs to perform all necessary calculations with user-friendly graphic user interfaces, written mostly by myself and P.Young.

For each ion CHIANTI has a set of three minimum ascii files that contain: 1) level energies (theoretical, observed) 2) transition probabilities, absorption oscillator strengths (gf values), theoretical and observed wavelengths; 3) spline fits to Maxwellian-averaged electron collision strengths. The fits are done in the Burgess & Tully (1992) domain. This allows a proper extrapolation of the rates at very low or very high temperatures. Additional files/data are included for many ions. They include spline fits to proton collision rates. In version 6 (Dere et al. 2009), new ionization and recombination (radiative and dielectronic) rates have been included.

One limitation of the CHIANTI package is the use of proprietary software (IDL). Another one is the limited number of rates provided for each ion. Normally we include only excitation rates from the ground state and to/from metastable levels. The model ions are therefore valid only until some values of the electron densities. The current limit is however beyond densities even of large solar flares, so mainly applies to some laboratory plasmas. The reason why only a limited set of excitation data are included is because each transition is assessed visually, to make sure that the rates are consistent with the high-energy limits, and see if the spline fits well reproduces the original rates. We are currently in the process of designing a new format for the CHIANTI database and new software to overcome various current limitations. This will be implemented in version 8. The next version 7 includes important updates for various ions important in the EUV and the X-rays.

CHIANTI emissivities are currently calculated for plasmas in ionization equilibrium and in stationary conditions. The effects of photo-excitation to the level balance

of an ion can be included. There is currently a correction factor applied to level populations which takes into account the effect of ionization and recombination to the ground state. This will be improved. There are ways to estimate emissivities for non-Maxwellian electrons, but this has not been implemented yet.

CHIANTI data and programs are distributed via: 1) tar files (available from the web pages); 2) web pages; 3) SolarSoft (IDL packages for Solar Physics); 4) Astrogrid (see below); 5) VAMDC (see below); 6) a Python interface, written by K.Dere.

One important issue for any atomic database or package concerns the various limitations for their use, which the users must always be aware. In the case of CHIANTI, many restrictions are described on the web pages and in the user guides (mostly written by myself). Another important issue is the need to propagate references to any original atomic physics calculation or measurement. Once atomic data are ingested into CHIANTI, for example, references easily become lost. This is very common. Indeed, CHIANTI atomic data are included in many other databases or modeling codes such as: XSTAR, APED/ATOMDB, XSPEC, ISIS, PINTofALE, CLOUDY, MOCASSIN.

The CHIANTI database supplies the references to the original sources and comments, elucidating the details of experimental measurements or calculations. Data are extracted from the literature, provided from the authors, or calculated by us. Each CHIANTI release is accompanied by a refereed publication, unlike other databases.

4.1. VOTADA

The VOTADA project aimed at providing accurate basic atomic data and tools for astrophysical applications, within the Astrogrid (*http://www2.astrogrid.org/*) (UK funded) and the Virtual Observatory. A subset of CHIANTI data were imported into a MySQL database in 2006. A Table named **SpectralLines** containing all information for each spectral line in the database has been created. This includes ion, observed and theoretical wavelengths, transition probability, weighted oscillator strength, full spectroscopic notation together with observed and theoretical energies of initial and final levels, and finally full reference to original publications, with comments. The table **SpectralLines** can easily be accessed and queried via the AstroGrid Workbench. The output results of the query can be saved as a Votable and browsed with e.g. TOPCAT. As a second step, the idea was to make derived products such as line emissivities available. Instead of writing wrapper scripts which would then call the existing software, it seemed best to make line emissivities directly available. This has been done by creating a Table named **LineEmissivities** which contains the values of the spectral line emissivities calculated for a grid of electron temperatures and densities. The table can be queried via the AstroGrid Workbench. CHIANTI-VOTADA atomic data were made easily accessible to VOSpec via a SLAP (Simple Line Access Protocol) interface.

4.2. VAMDC

The Virtual Atomic and Molecular Data Centre (VAMDC, see *www.vamdc.eu*) aims at building an interoperable e-infrastructure for the exchange of atomic and molecular data. VAMDC involves 15 administrative partners representing 24 teams from 6 European Union member-states, Serbia, the Russian Federation and Venezuela. The VAMDC is being built upon the expertise of existing databases, data producers and service providers with the specific aim of creating an infrastructure that is easily tuned to the requirements of a wide variety of users in academic, governmental, industrial or public communities.

In collaboration with H.Mason (DAMTP), the IoA (Cambridge University) and MSSL/UCL, we are incorporating CHIANTI data following a similar procedure as in VOTADA. We are extending upon it by making most CHIANTI data available. We are also planning to replicate some of the functions of the CHIANTI programs.

5. Benchmarking atomic data

Now that large amounts of atomic data can be calculated, there is a need to assess / benchmark them against observations, so the best calculations can be chosen. In the last few years, I have embarked in a long-term project of benchmarking atomic data. Work started with Fe x (Del Zanna et al. 2004), then extended to Fe vii, Fe viii, Fe xi, Fe xii, Fe xiii, Fe xiv, Fe xvii, Fe xviii, Fe xx, Fe xxiii, Fe xxiv. All previous identifications have been reviewed and assessed by comparing not only predicted wavelengths and gf-values (as mostly done in previous literature), but also by comparing line intensities with observations. In this way, a large number of new lines and energy levels have been identified and *given uncertainties*.

The most complete database of observed wavelengths and energy levels for ions is the NIST[2] compilation. This compilation in turn relies on original work mostly done in the 70's (in the EUV and X-rays with the pioneering work by researchers such as B. Edlen and B.C. Fawcett), based on laboratory measurements and 'simple' (for that time) atomic structure calculations. The benchmark work showed that many identifications and wavelengths needed to be revised. Transition probabilities have also been benchmarked with lifetimes measured with beam-foil spectroscopy. The estimates of line intensities for each laboratory or astrophysical source also allows to point out when lines are blended. Many new diagnostic line ratios to measure electron densities and temperatures have been discovered.

The benchmark work is a direct way to provide an estimate on the accuracy of the atomic data. The use of large-scale atomic structure and R-matrix scattering calculations has improved significantly accuracy. In general terms it is evident that for the strongest lines relative accuracies for A-values are better than 10%, and for excitation data better than 20%. Two examples of ions important for the X-rays and EUV are now provided, Fe xviii and Fe xi.

Fe xviii produces, in the X-ray and extreme ultraviolet, L-shell ($n = 2, 3, 4 \rightarrow 2$) spectral lines which are among the brightest ones. There has always been a discrepancy of factors 2-3 between observed and predicted intensities for the very bright $3s \rightarrow 2p$ transitions. The first large-scale R-matrix scattering calculations of Witthoeft et al. (2006) have finally resolved this puzzle. In this case, it turned out that the effect of the resonances was very important. A benchmark work (Del Zanna 2006) showed excellent agreement between observed and predicted intensities for the first time. Also, it provided new important diagnostics to measure electron temperatures and densities. Fig. 2 shows the emissivity ratio curves:

$$F_{ji}(T_{\rm e}) = C \ \frac{I_{\rm ob} N_{\rm e}}{N_j(N_0, T_{\rm e})\, A_{ji}} \qquad (2)$$

[2]http://physics.nist.gov/PhysRefData/ASD/index.html

calculated at a fixed density N_0 (and with a scaling constant C), using the R-matrix results (right) and spectroscopic observations by Chandra of Capella (Phillips et al. 2001). The curves intersect at log T[K] =6.65, meaning that the line intensities can be explained, to with a few percent accuracy, by an isothermal plasma at a temperature well below that of peak abundance in ionization equilibrium (T[K] =6.85). On the other hand, previous distorted-wave (DW) atomic data (Sampson et al. 1991) show a very large scatter (i.e. discrepancy).

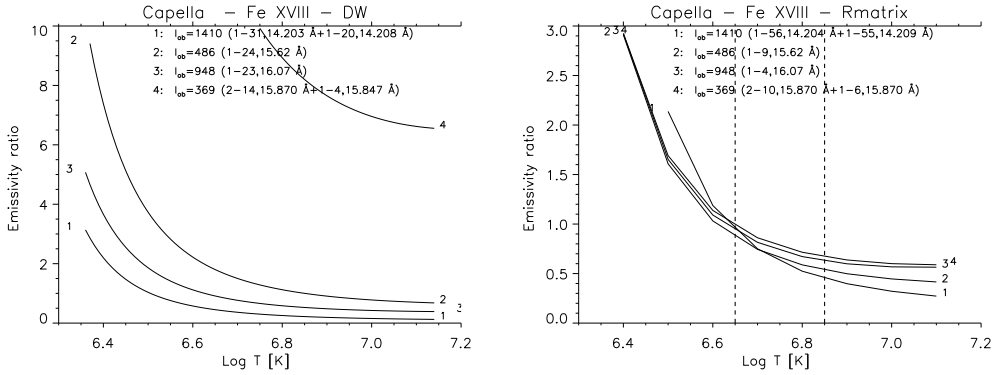

Figure 2. The emissivity ratio curves for the strongest Fe XVIII X-ray lines. Left, previous DW calculations; right: first R-matrix calculations.

After six years of benchmark work on the ions along the S-like sequence, the mysteries about some among the strongest lines in Fe XI have been unveiled. Three $J = 1$ levels in the $3s^2\ 3p^3\ 3d$ electron configuration give rise to strong lines in the EUV spectrum and their energies and identifications have been the source of much confusion in the literature. All previous atomic calculations produced discrepancies of factors 2-3 for these lines. A new R-matrix scattering calculation for electron collisional excitation of Fe XI was performed using an optimal target by Del Zanna et al. (2010). The energies of most of the $3s^2\ 3p^3\ 3d$ levels, some giving rise to important forbidden lines have now been firmly identified Del Zanna (2010). New and important temperature diagnostics have been found.

There is still a large amount of work needed to finalise the atomic data just for the iron ions.

Acknowledgments. Support from STFC (UK) via the Advanced Fellowship programme is acknowledged. Support from VAMDC and the LOC to participate at the workshop is acknowledged. VAMDC is supported by the EU in the framework of the FP7 "Research Infrastructures-INFRA-2008-1.2.2 - Scientific Data Infrastructures" initiative. It started on the 1st of July for a duration of 42 months. The VOTADA project was carried in collaboration with S. Dalla (now in University of Central Lancashire UK) and K. Benson (UCL/MSSL UK). The work of the UK APAP Network is funded by the UK STFC under grant no. PP/E001254/1 with the University of Strathclyde. CHIANTI is a collaborative project involving the NRL (USA), RAL (UK), and the following Univerisities: Cambridge (UK), George Mason (USA), and Florence (Italy).

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