Journal of Physics: Conference Series **635** (2015) 052035 doi:10.1088/1742-6596/635/5/052035

Advances in atomic data for plasma diagnostics

L. Fernández-Menchero*[1], G. del Zanna†[2] and N. R. Badnell*[3]

* Department of Physics, University of Strathclyde. Glasgow G4 0NG, United Kingdom

† Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 0WA, United Kingdom

Synopsis We present sets of new atomic data for astrophysical and fusion plasma diagnostics. We calculate electron-impact excitation collision strengths and effective collisions strengths for the Be- and Mg-like isoelectronic sequences up to Kr^{q+}. We use the R-Matrix Intermediate-Coupling Frame Transformation method. We also study the accuracy of calculations for highly-excited states and give extrapolation rules to estimate the effective collision strengths and their error at high n. We demonstrate the importance of a well converged CI/CC expansion in the R-matrix calculation to get good quality results, mainly for highly-excited states.

Atomic data requirements for modeling of fusion or astrophysical plasmas are becoming more and more demanding. Data bases, such as CHIANTI (www.chiantidatabase.org) or OPEN-ADAS (open.adas.ac.uk), require continual advancement as the demands of plasma modelers and observations grow.

Observations from several missions, such as SKYLAB and SOHO, detected spectral lines from ions in highly excited states ($n \geq 4$). To guarantee a good description of those levels, we require a good convergence of the Configuration Interaction (CI) basis set expansion of the target and the Close Coupling (CC) calculation.

We have carried-out Intermediate Coupling Frame Transformation (ICFT) R-Matrix calculations. The CI basis set for the Be-like sequence includes a total of 238 intermediate coupling levels from the configurations $1\mathrm{s}^2\,\{2\mathrm{s}^2, 2\mathrm{s}2\mathrm{p}, 2\mathrm{p}^2\}$, and $1\mathrm{s}^2\,2\{\mathrm{s},\mathrm{p}\}\,nl$, with $n = 3-7$ and $l = \mathrm{s},\mathrm{p},\mathrm{d},\mathrm{f},\mathrm{g}$ for $n = 4,5$ and $l = \mathrm{s},\mathrm{p},\mathrm{d}$ for $n = 6,7$. For the Mg-like sequence, a total of 283 levels arising from the configurations $1\mathrm{s}^2\,2\mathrm{s}^2\,2\mathrm{p}^6\,\{3\mathrm{s}^2, 3\mathrm{s}3\mathrm{p}, 3\mathrm{s}3\mathrm{d}, 3\mathrm{p}^2, 3\mathrm{p}3\mathrm{d}, 3\mathrm{d}^2\}$ and $1\mathrm{s}^2\,2\mathrm{s}^2\,2\mathrm{p}^6\,3\{\mathrm{s},\mathrm{p},\mathrm{d}\}\,nl$, with $n = 4,5$ and $l = \mathrm{s},\mathrm{p},\mathrm{d},\mathrm{f},\mathrm{g}$.

We present new data for the electron-impact excitation collision strengths Ω and Maxwell integrated effective collision strengths Υ for the Be-like isoelectronic sequence from B^{+} to Kr^{32+} [1], and for the Mg-like isoelectronic sequence from Al^{+} to Kr^{24+} [2]. We show data for non-Maxwellian velocity distributions too.

We also investigate extrapolation rules to estimate the electron-impact excitation effective collision strengths for highly excited states [3]. We focus in the H- and He-like isoelectronic sequences as a benchmark. Calculations for highly excited states are strongly limited by the quality of the atomic structure and the close coupling expansion for such terms/levels. Eventually, extrapolation from good-quality data for lower states gives a more accurate result than an unconverged calculation. We give an estimation of the error associated with the extrapolation too.

We look at differences between the R-matrix method and the distorted wave one for weak one-photon forbidden transitions ($J - J' = 0 - 0$). These differences are due to the transformation from the reactance matrix K to the transmission matrix T in an exact fashion, conserving the unitarity (AS-UDW), or in an approximate non unitary one (AS-DW) [4].

The completeness of the basis set in the CI/CC expansion of the target is the main source of error, mostly for the higher excited states. Other effects produce considerably smaller inaccuracies, like the method used to include relativistic effects in the Hamiltonian [5].

The present advances in atomic data for plasma modeling and diagnostics are available in CHIANTI and OPEN-ADAS data bases.

References

[1] L. Fernández-Menchero *et al* 2014 *Astron. and Astroph.* **566** A104

[2] L. Fernández-Menchero *et al* 2014 *Astron. and Astroph.* **572** A115

[3] L. Fernández-Menchero *et al* 2015 *Astron. and Astroph. in progress.*

[4] L. Fernández-Menchero *et al* 2015 *Astron. and Astroph. submitted.*

[5] L. Fernández-Menchero *et al* 2015 *Mon. Not. R. Astr. Soc. submitted.*

[1]E-mail: luis.fernandez-menchero@strath.ac.uk
[2]E-mail: gd232@cam.ac.uk
[3]E-mail: badnell@phys.strath.ac.uk