Data Evaluation for Atomic, Molecular and Plasma-Material Interaction Processes in Fusion

Evaluation of electron-impact excitation data along iso-electronic sequences

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The advent of high-quality high-resolution laboratory and astrophysical X-ray and EUV spectra requires correspondingly accurate electron−atom/ion interaction data (including electron-impact excitation, EIE) to utilize fully their potential diagnostic modelling capability for celestial objects. A program — the Atomic Processes for Astrophysical Plasmas network[†] — was setup in the UK to generate accurate atomic data (including electron-impact excitation) along iso-electronic sequences and to assess the reliability of the final product. These data and their evalution method are also applicable for the magnetic fusion community.

The intermediate-coupling framework transformation (ICFT) *R*-matrix approach [1] was used to calculate EIE data. The R-matrix method efficiently includes resonances usually omitted by the distorted-wave method. The ICFT variant is less resource (time/memory) demanding than the full Breit-Pauli *R*-matrix method, without reduction of accuracy. So far, calculations for the He-like, Li-like, F-like, Ne-like and Na-like iso-electronic sequences [2, and references therein] have been completed and an assessment of the resultant data has been carried-out. Calculations for another three iso-electronic sequences (including Be-like, B-like and Mg-like) and some urgently important ions are planned in the 2nd APAP program.

A detailed accuracy assessment was done for four/five/six selected ions spanning the iso-electronic sequence and which poses insight into the behaviour of the whole sequence of ions. For each ion, we adopt the following procedures: (1) firstly, the target structure was assessed by comparing the calculated level energies with available experimental data and previous calculations with different methods. (2) secondly, weighted oscillator strengths or line strengths or radiative decay rates were compared with various available theoretical works for several transitions. Usually a 'survey' comparison with another database has been done for all available transitions by way a scatter plot. (3) thirdly, direct comparison for the excitation (effective) collision strength is done with available measurements or with previous published data. A 'survey' comparison with another database is usually presented to investigate the widespread of consistency or inconsistency among the different calculations. In conclusion, the resultant excitation data along the iso-electronic sequences were assessed to be reliable and were incorporated into astrophysical and fusion database/modelling codes, such as CHIANTI, ADAS, AtomDB etc.

[1] Griffin D C, Badnell N R and Pindzola M S, *J. Phys. B: At. Mol. Opt. Phys.* **31,** 3713 (1998)
[2] Liang G Y and Badnell N R, *Astron. Astrophys.* **528**, A69 (2011)

[†] http://www.apap-network.org