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Benchmark calculations for electron collisions with complex atoms: accuracy, convergence and completeness[1]

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Over the past decade, we have developed a highly flexible B-spline R-matrix (BSR) method [1] that has some advantages compared to the standard R-matrix (close-coupling) approach. The two essential refinements are i) the capability for using the flexible term-dependent one-electron orbitals, and ii) the use of B-splines as a universal and effectively complete basis to generate the R-matrix basis. These features allow us to achieve a high accuracy in the target description, as well as a truly consistent treatment of the scattering system. The BSR code was successfully applied to many problems of electron collisions from atoms and ions, with special emphasis was placed on complex, open-shell targets. Often considerable *improvement* was obtained in comparison with previous calculations. Many examples can be found in a recent Topical Review [2]. More recently, the BSR complex has been extended to i) the fully relativistic Dirac scheme and ii) intermediate energies using the continuum pseudo-state approach. These extensions allow for an accurate treatment of *heavy targets* as well as a fully non-perturbative way to handle electron-impact *ionization*, including such highly correlated processes as ionization plus simultaneous excitation. During the last years we developed parallel versions of our BSR and DBSR codes. They made it possible to carry out large-scale $R-$matrix with pseudo-states (RMPS) calculations and thereby provide *converged* (with respect to the number of coupled states) results for electron impact excitation of individual target states. For many systems our calculations revealed dramatic reductions of the predicted excitation cross-sections at intermediate energies, due to the strong influence of coupling to the target continuum. These results raise questions about the absolute normalization in several published measurements. Our RMPS calculations represent the extensive and *complete* sets of electron scattering data ready for applications.

[1] Zatsarinny O 2006 *Comput. Phys. Commun.* **174** 273
[2] Zatsarinny O and Bartschat K 2013 *J. Phys. B: At. Mol. Opt. Phys.* **46** 112001

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