

Generation of Atomic Data for Complex Many-Electron Atoms and Ions

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Domain : Fusion

The universal method of generation of fairly accurate atomic data (wave functions, energy spectra, wavelengths of electric and magnetic multipole electronic transitions, oscillator strengths, transition probabilities and lifetimes of excited levels) for complex atoms and ions of various ionisation degrees is presented. It is based on the angular momentum theory, graphical methods, second quantisation in coupled tensorial form, irreducible tensors in three spaces (orbital, spin and quasispin) and completely reduced matrix elements of irreducible tensorial operators [1]. The efficiency of the methods of accounting for correlation and relativistic effects is analysed. This approach is implemented in the form of fairly universal special mathematical software for atomic calculations, allowing to generate the fairly accurate atomic data in principle for any atom of Periodical Table, ions with open f-shells included. The accuracy of the data generated for various complex atoms and ions of various ionisation degrees is evaluated and its high efficiency is demonstrated.

[1] Z. Rudzikas, *Theoretical Atomic Spectroscopy*, Cambridge University Press, Cambridge, 1997, 448 p.