Extended Calculations of Spectroscopic Data for Highly-Charged Ions Comparison study using MCDHF and RMBPT methods

Chong-Yang Chen*[1], Kai Wang†, Ran Si*, Chun-Yu Zhang*, Yao-Wu Liu*, Shuang Li‡, Xue-Ling Guo§, Jun Yan‡, Ya-Ming Zou*

* Shanghai EBIT Lab, Institute of Modern Physics, Department of Nuclear Science and Technology, Fudan University, Shanghai 200433, China

† Hebei Key Lab of Optic-electronic Information and Materials, The College of Physics Science and Technology, Hebei University, Baoding 071002, China

‡ Institute of Applied Physics and Computational Mathematics, Beijing 100088, China

§ Department of Radiation Oncology, Changhai Hospital, Second Military Medical University, Shanghai 200433, China

Synopsis Employing two state of the art approaches, multiconfiguration Dirac–Hartree–Fock (MCDHF) method and second-order relativistic many-body perturbation theory (RMBPT), a large amount of energies, transition probabilities, and lifetimes for highly-charged ions, partically for K-, L-, M-, and N-shell ions, have been calculated. Through the comparisons of our two datasets and further with the observed ones, the accuracies of our results are assessed. In general, the present calculated energies of L-shell ions deviate from experiment on the order of 0.01% while they differ from the observed ones by about 0.1% for M- and N-shell ions. The lifetimes calculated from the two methods are in good agreement on the order of 1%. The amount of data at high accuracy is significantly increased for many ions of astrophysics and fusion interest, where experimental data are largely scarce.

Atomic data such as energy levels, wavelengths, and transition probabilities, as well as processes of photoionisation, collisional broadening and inelastic collisions, are required for the modelling of a variety of plasmas, including solar, astrophysical, laser-produced and fusion. These data are also needed for determining plasma parameters, viz. spectroscopic diagnostics, and the measurement of chemical abundances in solar and other astrophysical plasmas. Due to the paucity of experimentally measured data, one heavily relies on theoritical calculation.

Recently, we have performed a series of large-scale calculations on atomic data (including energies, wavelengths, transition probabilities, etc) for highly-charged ions by using two state of the art approaches, multiconfiguration Dirac–Hartree–Fock (MCDHF) method and second-order relativistic many-body perturbation theory (RMBPT). Many-body and relativistic effects, as well as small corrections for finite nuclear size, nuclear recoil, vacuum polarization, and self-energy correction, have been taken into accout. Extensive comparisons with experiments show our results are highly accurate. More details can be found in [1, 2, 3] for H- and He-like ions, [4, 5, 6, 7, 8, 9] for Be-, C-, N-, O-, F- and Ne-like ions, [10, 11] for Mg-like ions, [12] for Al-like ions, [13, 14] for $3d^k$ ($k = 1 - 9$) ions, and [15] for Kr-like ions. In the presentation, we'll discuss the new large-scale calculations on B-like, Al-like, Si-like, Ar-like ions.

The present complete dataset provides the possibility to point out a number of lines for which the experimental identifications were be questioned, and should be helpful in analyzing new observations from the solar and other astrophysical sources, and is also likely to be useful for modeling and diagnosing a variety of plasmas including astronomical and fusion plasma.

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[1]E-mail: chychen@fudan.edu.cn