Accurate calculations of atomic properties for boron- and carbon-like ions of astrophysical interest

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Information about physical processes in astrophysical and fusion plasmas can be inferred from high resolution spectra. The X-ray spectra from iron L-shell ions are particularly important for astrophysics as they are in the wave length range covered by telescopes on board the space observatories Chandra and XMM-Newton. The analysis of high-resolution X-ray spectra requires knowledge of a large number of accurate transition data and transition probabilities, both from theory and experiment, to identify spectral lines, produce synthetic spectra, and carry out plasma diagnostics.

During the last years a number of calculations have been undertaken to provide more complete sets of energies and transition data for highly charged ions. Although theoretical data are available it is still very difficult to analyse spectra, unambiguously identify transitions, and deduce energy levels with the proper labels.

Looking at the NIST Atomic Spectra Database [1] there remain large gaps that need to be filled. Also there are misidentifications. This work reports from a long term theoretical effort to attain "spectroscopic accuracy", i.e. calculated transition energies that are accurate enough to confirm or revise experimental identifications. The basis for the work is large scale relativistic multiconfiguration methods [2] with hundreds of thousands of configuration states functions. By accurately balancing electron correlation effects it now is possible to compute transition energies with an inaccuracy of fractions of a per mille [3]. As an application, calculations were performed for the 290 lowest states in boron-like ions belonging to the configurations $1s^22s^22p$, $1s^22s2p^2$, $1s^22p^3$, $1s^22s^23l$,$1s^22s2p3l$, $1s^22p^23l$, $1s^22s^24l'$, $1s^22s2p4l'$, $1s^22p^24l'$ (l = 0, 1, 2 and l' = 0, 1, 2, 3). Calculations were also performed for the 230 lowest states in carbon-like ions belonging to the configurations $1s^22s^22p^2$, $1s^22s2p^3$, $1s^22p^4$, $1s^22s^22p3l$, $1s^22s2p^23l$, $1s^22p^33l$ (l = 0, 1, 2) . Results are presented and discussed in relation to other works with special attention to boron- and carbon-like iron.

References:
[1] A. Kramida *et al.*, NIST Atomic Spectra Database (ver. 5.0), National Institute of Standards and Technology, Gaithersburg, MD. (2012).
[2] P. Jönsson *et al.,* Computer Physics Communications, in press (2013).
[3] P. Jönsson, P. Bengtsson, J. Ekman *et al.,* At. Data Nucl. Data Tables, in press (2013).