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Isotope shifts in beryllium-, boron-, carbon-, and nitrogen-like ions from relativistic configuration interaction calculations

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ABSTRACT

Energy levels, normal and specific mass shift parameters as well as electronic densities at the nucleus are reported for numerous states along the beryllium, boron, carbon, and nitrogen isoelectronic sequences. Combined with nuclear data, these electronic parameters can be used to determine values of level and transition isotope shifts. The calculation of the electronic parameters is done using first-order perturbation theory with relativistic configuration interaction wavefunctions that account for valence, core–valence, and core–core correlation effects as zero-order functions. Results are compared with experimental and other theoretical values, when available.

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Contents

1. Introduction

High resolution solar and stellar spectra reveal isotope shifts (IS) and hyperfine structures of many spectral lines. These small structures are not always completely resolved and instead they shift and broaden the atomic lines. To correctly interpret the spectra it is often necessary to include isotope shifts and hyperfine structures in a theoretical modeling of the line profiles [1,2]. Hyperfine and isotope data are also needed for generating synthetic spectra to study isotope anomalies in astronomical objects [3] and for understanding nucleosynthesis mechanisms [4,5]. In the last decade, several studies have shown that the typical isotope shifts may be of the same order of magnitude as the effects of the possible temporal and spatial variation of the fine-structure constant. In this framework, Kozlov et al. [6] proposed a method to exclude systematic effects caused by changes in the isotope abundances during the evolution of the universe, but there is a need to develop methods that can accurately estimate isotope shifts [7]. Isotope shifts of spectral lines are also used in nuclear physics to estimate the root-mean-square nuclear charge radii and mean-square radii changes $\delta\langle r^2\rangle^{A,A'}$ for which the electronic factors play a crucial role (see for example Refs. [8–12]).

Relativistic effects on the electronic structure are expected to increase with the nuclear charge. Shabaev [13,14] and, in an independent way, Palmer [15], derived relativistic corrections to the mass shift. Since then several papers have shown the importance of relativistic effects on isotope shifts [16–20]. The development of experimental techniques allowing the accurate measurement of line IS enhances the need for accurate calculations of the relevant electronic parameters that account for both electron correlation and relativistic effects, especially for medium and heavy open-shell atoms [21,22]. Amongst these techniques, the storage ring measurement of isotope shifts in the spectrum of resonant electron–ion recombination of heavy few-electron ions gives access to nuclear charge radii changes involving heavy stable and unstable nuclides, as demonstrated for three-electron Nd^{57+} isotopes produced at GSI's storage ring ESR [8]. Dielectronic recombination (DR) measurements have also been performed at the heavy-ion storage ring TSR in Heidelberg for Be-, B-, and C-like ions relevant to astrophysics and plasma physics [23,24], although no IS in the DR spectra have been reported so far. DR experiments are also envisaged at ISOLDE [25] where the availability of radioisotopes together with the TSR electron collision facilities will open up new opportunities.

GRASP2K [26] is a fully relativistic code based on the multiconfiguration Dirac–Hartree–Fock (MCDHF) method. Its latest release [27] includes a module, RIS3 [28], that evaluates the isotope shift parameters including the relativistic corrections to the recoil operator as derived by Shabaev [13,14]. The purpose of the