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Hyperfine structures and Landé g_J-factors for $n = 2$ states in beryllium-, boron-, carbon-, and nitrogen-like ions from relativistic configuration interaction calculations

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ABSTRACT

Energy levels, hyperfine interaction constants, and Landé g_J-factors are reported for $n = 2$ states in beryllium-, boron-, carbon-, and nitrogen-like ions from relativistic configuration interaction calculations. Valence, core–valence, and core–core correlation effects are taken into account through single and double-excitations from multireference expansions to increasing sets of active orbitals. A systematic comparison of the calculated hyperfine interaction constants is made with values from the available literature.

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Contents

1. Introduction

The hyperfine interaction, i.e. the interaction between the electrons and the non-spherical part of the electromagnetic field produced by the nucleus, is important in a number of applications. The hyperfine interaction breaks the J symmetry of the atom and may open forbidden transitions that can be used for diagnostic purposes in plasmas [1,2]. Combined with accurate measurements of hyperfine structure splittings, calculated atomic parameters can be used to extract nuclear quadrupole moments Q [3]. In a different setting the hyperfine interaction is a key factor in determining excited state nuclear g-factors from recoil-in-vacuum experiments [4]. Hyperfine interaction is also important in astrophysics, and high resolution solar and stellar spectra reveal isotope shifts and hyperfine structures of many spectral lines. To correctly interpret the spectra it is necessary to include isotope shifts and hyperfine structures in a theoretical modeling of the line profiles [5,6]. Hyperfine interaction is also of theoretical interest and is a valuable and sensitive probe of both electron correlation and QED effects [7–9].

Strong magnetic fields have been detected in hot stars of types O, B, and A. Investigations of these magnetic fields require knowledge of accurate Landé g_J-factors [10]. There is also a need for data to support polarization measurements of the coronal magnetic field [11]. Some experimental g_J-factors have been published in successive NIST compilations, but data for many levels are still lacking. From a more theoretical point of view Landé g_J-factors give valuable information about coupling conditions in atomic systems, and they can also be used to identify and label states [12].

A number of computer codes have modules for computing hyperfine structures and Landé g_J-factors, e.g. CIV3 [13], MCHF [14], ATSP2K [15]. The former codes are non-relativistic with relativistic corrections in the Breit–Pauli approximation. Hyperfine interaction is an inner property and is very sensitive to relativistic effects [16]. For this reason the calculations in this work rely instead on the fully relativistic GRASP2K code [17,18], which has modules both for hyperfine structure [19] and Landé g_J-factors [20]. The purpose of the present work is to complement the data sets on the isotope shift electronic factors [21] along the beryllium, boron,