CAPABILITIES OF THE ELECTRONIC ENERGY STRUCTURE CALCULATION SOFTWARE

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Due to the insufficient amount of data to perform accurate calculations of the energy structure of arsenic, antimony and bismuth atoms, the investigation of the analogous radial parameter values shift within the 15-th group of the periodic table will be performed. As the first step of this research the fine structure and hyperfine structure calculations of the even-parity configuration of the atomic nitrogen were carried out. The system of even configurations of the nitrogen has a similar structure, therefore it is purposeful to determine the two-body contributions to the fine and the hyperfine structures, resulting from the excitations from electronic closed shells to open shells and from closed shells to empty shells for this element first.

On the basis of experimental data [1, 2], a multi-configuration fit of 170 even configurations ($2s2p^4$, $2p^43d$, $2p^45g$, $2s2p^23s^2$, $2s2p^23d^2$, $\sum_{n=3}^{80} 2s^22p^2ns$, $\sum_{n=4}^{80} 2s^22p^2nd$, $\sum_{n=5}^{14} 2s^22p^2ng$) was carried out. The present report is the application of our many-body parametrization method allowing the analysis of a complex electronic system composed of a configuration of up to four open shells, presented in general terms in the first work of the series under the common title *Construction of the energy matrix for complex atoms* [3]. The contributions from the second-order perturbation theory originating from electrostatically correlated spin-orbit interactions in the fine structure, as well as electrostatically correlated hyperfine interactions (core polarization effects) in the hyperfine structure, were considered. Calculations of the nitrogen system was performed on personal computer (PC) due to the sufficiently low number of matrix elements describing the system.

The calculations of the enormous fine- and hyperfine structure matrices required high-performance computing (HPC), concerning both CPU (Central Processing Unit) speed and memory allocation. For the purpose of the huge matrix diagonalization in the case of terbium atom, the methods utilizing the personal computer clusters and, alternatively, the Microsoft Azure cloud computing, have been proposed by us in the papers [4]. Recently our program package was launched in Poznan Supercomputing and Networking Center (PSNC) and calculations of holmium atom are carried out using the resources of the Poznan Supercomputing and Networking Center.

For unknown electronic levels predicted values of the level energies and hfs constants are given, which can facilitate further experimental investigations.

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