



## New Double Zeta Bases Sets for Boron and Carbon Obtained by HF<sup>Gauss</sup> – GSA

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### ABSTRACT

In previous work [1] were constructed new atomic 3G and 6G minimal bases for the first row atoms of the Periodic Table applying a stochastic method, the Generalized Simulated Annealing. Using this approach new Double Zeta (DZ) atomic bases for the Lithium and Beryllium atoms [2], were obtained recently. These new bases were used to calculate Hartree-Fock (HF) and full CI energies, and to calculate the permanent electric dipole [2, 3] and quadrupole [4] moments using the Multi-Reference Hartree-Fock Configuration Interaction (MRHF-CI) method. These results were obtained for some molecules formed with first row atoms of the periodic table.

The procedure, designated HF<sup>Gauss</sup>-GSA method, consists in the direct optimization of the HF functional of the atom, taking simultaneously as variational parameters the coefficients of the atomic orbital expansions in the basis functions and the coefficients and the exponents of the Gaussian functions which define the basis functions set.

By other side the HF equation is not linear and has, in principle, several solutions [5]. So, for each system, can be determined several HF solutions with the adequate point and spin symmetry. With each of the HF extreme we can construct a base of the full CI space in adequate symmetry class. In the MRHF-CI method are employed several HF extremes as references to expand the state function.

In this work we are using the HF<sup>Gauss</sup>-GSA method to obtain new DZ bases for the Boron and Carbon atoms. Were implemented modifications in the HF<sup>Gauss</sup>-GSA FORTRAN code and in the present stage we are adjusting the best GSA parameters ( $q_A$ ,  $q_V$  and  $q_T$ ) for the procedure. The new bases obtained with this approach will be used in MRHF-CI calculations for systems involving Boron and Carbon atoms.

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