MRHFCI Calculations for BH molecule in the DZ base

A. M. de C. Sobrinho (PQ), M. D. de Andrade (PQ), L. A. C. Malbouisson (PQ)

Instituto de Física da UFBa – Depto. de Física do Estado Sólido, Salvador – Ba, Brasil
e-mail: moreira@ufba.br

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ABSTRACT

The Hartree-Fock (HF) equation is not linear and has, in principle, several solutions [1]. In former works [2, 3] we introduced a multi-reference configuration interaction method based on HF multiples solutions (MRHFCI). In this method, are employed several HF extremes as references to expand the state function. So, for each system, are determined several HF solutions with the adequate point and spin symmetry. With each of the ω^{th} HF extreme we can construct a base of the full CI space. With the ω^{th} HF extreme is construct the $\mathbf{B}^{\omega}$ base and the set of the $\mathbf{B}^{\omega}$ bases is a generator system, **G**, of the full CI space. Although the $\mathbf{B}^{\omega}$ bases generates the same space, the correspondent configurations of these bases have distinct quantum-mechanical information contents (QMIC). Then, we can use mixed bases to formulate the CI problem, i. e., multi-reference HF bases (MRHF) that include vectors of **G** originated of different $\mathbf{B}^{\omega}$ bases [2 – 5], to calculate the energy and properties of molecules using reduced MRHF bases. In this work we have nineteen $^1\sum^+$ HF solutions obtained for the BH molecule in the double zeta (DZ) base. Were construct several bases MRHF and in the present stage we are performing the corresponding MRHFCI calculations. Some initial results for the permanent electrical dipole moment are displayed in the table below.

Table I. MRHFCI calculations for BH with the DZ basis.*

*CSF*s	*HF* solutions	*MRHFCI* Energy	μ
139	A,F	-25.1268543	1.2686
63	A,E	-25.1210269	1.2803
213	A,B,C,D	-25.1234686	1.2745
171	A,B,C,D	-25.1191880	1.2889
265	A,B,C,D	-25.1265645	1.2717
184	A,H	-25.1359379	1.3012
241	A,G	-25.1252752	1.2791
302	A,F	-25.1405398	1.2537
Full CI: 2575 CSF's		-25.1740150	1.5246

* Energies of the used HF References (a.u.): A = -25.1133953; B = -24.2866430; C = -23.1832873; D = -22.8364870; E = -22.3616984; F = -21.0350312; G = -8.2243947; H = -6.5179617; Exp. Dipole Value: μ = 1.270 debye; Interatomic distance: R = 2.329 bohr.

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