

Development of Octave functions for quantum chemistry methods using Gaussian type orbitals

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Synopsis A suite of functions is being developed in Octave for performing different kinds of quantum chemistry computations aiming at generalized oscillator strengths evaluation

The main objective of this work is to obtain a simple to use platform to evaluate molecular properties not available on quantum chemistry packages (Gaussian, GAMESS, etc.). This will be done by providing the user with a set of functions to be called on by the Octave package.

The Octave package is a clone of the commercial package Matlab and is part of the GNU Project, therefore it has a very permissive license.

The evaluation of molecular integrals over Cartesian Gaussian functions are a fundamental challenge and the most time demanding part of most quantum chemistry computations. Several methods for that kind of integrals exists but this work is mainly based on the efficient recurrence relations of Obara and Saika [1].

So far we have achieved a satisfactory result in the overall formulation of the problem as an algorithm for the main operations of Gaussian type basis set. It is left for the user to import or to define at his will the basis set which is placed as an object (as in object oriented languages) and

he is therefore able to call functions that operates on this object in a straightforward manner.

Based on the overlap, kinetic energy, nuclear-electron attraction and electron-electron repulsion integrals a simple Hartree-Fock program was developed as a guide to validate the code and to help the user develop their own codes.

Evaluating other integrals, such as electric dipole moment, based on hartree-fock computations from other packages are also straightforward by using the basis set, geometry and the optimized coefficients. For other methods, such as CI, a very fast procedure was obtained using natural orbitals for the evaluation of molecular properties.

The same procedure is being extended to two states properties: transition moment and generalized oscillator strength.

References

- [1] S. Obara, A. Saika 1986 *J. Chem. Phys.* **84** 3963

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