

## Quantum Chemistry

edited by  
William F. Coleman  
Wellesley College  
Wellesley, MA 02481

Edward W. Fedosky  
University of Wisconsin–Madison  
Madison, WI 53715

### Restricted Hartree-Fock SCF Calculations Using Microsoft Excel

by Taylor R. Page, Courtney A. Boots, and Mark A. Freitag,\* Department of Chemistry, Creighton University, Omaha, NE 68178; \*freitag@creighton.edu

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Requires Microsoft Excel

Courses in computational chemistry are increasingly common at the undergraduate level. Excellent user-friendly programs, which make the execution of ab initio calculations quite simple, are available. However, there is a danger that the underlying SCF procedure (usually coupled with contracted Gaussian atomic orbital basis sets) can become a 'black box' for the student. We have attempted to rectify this situation by creating a Microsoft Excel spreadsheet that contains all the essential elements of far more complicated ab initio calculations, but on the simplest possible molecular system.

This submission performs Restricted Hartree-Fock (RHF) self-consistent field (SCF) calculations on a two-body, two-electron system. In addition, the spreadsheet makes use of standard minimal Gaussian basis sets for hydrogen and helium. Therefore, one can perform the following ab initio single-point energy calculations for  $H_2$ ,  $HeH^+$ , or  $He_2^{2+}$ :

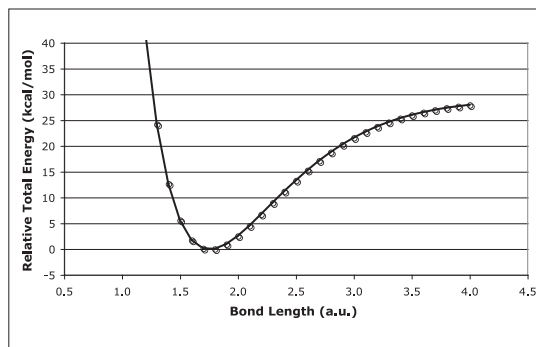
RHF/STO-1G

RHF/STO-2G

RHF/STO-3G

To fulfill the above pedagogical objectives, *all* the calculations are carried out using standard Excel cell formulas to make the entire procedure more transparent to the student. Specifically, the spreadsheet contains:

- contracted Gaussian atomic orbital basis sets
- calculation of one- and two-electron integrals
- the construction of a Hamiltonian core initial molecular orbital (MO) guess, or the option for the student to provide their own initial MO guess
- calculation of the orthogonalized Fock matrix
- diagonalization of the Fock matrix to generate new MOs, the density matrix, and the total energy of the system
- use the new MOs to recalculate the Fock matrix, generate new MOs, and calculate the new energy.



The potential energy surface of  $HeH^+$  at the RHF/STO-3G level of theory. Energies are relative to the minimum, and are calculated at intervals of 0.1 Bohr (a.u.).

This process is then repeated until self-consistency in the energy is achieved. The student is able to step through the SCF procedure one iteration at a time, or step through each *part* of *one* iteration; in the latter case, built-in macros walk the student through each step of the SCF cycle and highlight the relevant parts of the spreadsheet to show where a particular calculation is carried out.

The spreadsheet makes use of these features:

- The student can plot the highest occupied molecular orbital ( $\psi_1$ ), lowest unoccupied molecular orbital ( $\psi_2$ ),  $|\psi_1|^2$ ,  $|\psi_2|^2$ , or any combination of the four *during the SCF cycle*. This allows the student to easily see how the wave function is being improved.
- The contraction coefficients and Gaussian exponents can be changed to demonstrate the variational principle.
- The electronic energy convergence threshold can be changed.

The spreadsheet described here is accompanied by a manuscript that summarizes the RHF SCF method and presents the full form of all the working equations used in the spreadsheet.

### Supporting JCE Online Material

<http://www.jce.divched.org/Journal/Issues/2008/Jan/abs159.html>

Full text (HTML and PDF)

### Supplement

Find *Restricted Hartree-Fock SCF Calculations Using Microsoft Excel* in the JCE Digital Library at <http://www.JCE.DivCHED.org/JCEDLib/WebWare/collection/reviewed/JCE2008p0159WW/index.html>