CALIFORNIA STATE SCIENCE FAIR
2010 PROJECT SUMMARY

Name(s)
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Project Number
S1918

Project Title
Calculation of Atomic Energies Using Mathematica

Abstract

Objectives/Goals
The purpose of this experiment was to calculate the energies of the hydrogen atom, the helium ion He+ , doubly ionized lithium Li2+ , and the helium atom and to determine the most accurate wave function for the different atoms using Mathematica. The energies were computed using trial wave functions and minimizing the energy with respect to the parameters of the trial wave functions. These energies give information about the interactions between the electron and the nucleus and also give the ionization energy of the atom.

Methods/Materials
The energy of the atom was expressed as a volume integral of the wave function and its derivatives. Then, a trial wave function with a few adjustable parameters was chosen. Using Mathematica, the integral expression for the energy based on the trial wave function was minimized by adjusting the parameters. The trial wave function that gave the lowest energy was the closest to the actual wave function.

Results
The energies of the hydrogen atom, the helium ion He+ , doubly ionized lithium Li2+, and the helium atom were computed using the variational method. When psi(r) = e^(-ar) was used as a trial wave function, the minimum energy was -1 Rydbergs when a = 1. This calculation gives an ionization energy for hydrogen of 1 Rydberg or 1312.75 kJ/mol, which agrees very well with the measured value of 1312 kJ/mol. The energy of He+ was found to be -4 Rydbergs, and of Li2+ to be -9 Rydbergs. The helium atom energy was found to be -5.70 Rydbergs. The helium atom computation was considerably more complicated than the one for the hydrogen atom because there are two electrons in this atom. The Li+ ion also is a two electron system. The energy of this ion was found to be -14.4453 Rydbergs.

Conclusions/Discussion
The numerical variational method gives accurate results for the energies of the atoms studied. The ionization energies of the atoms studied were in good agreement with the experimentally measured values. The variational method gives a very accurate determination of the energies of atoms and of their ionization potentials. In the one electron systems, the atomic energies calculated were identical to the theoretical values. For the two electron systems, the atomic energies calculated were in very good agreement with the theoretical values, but did not match them exactly due to the fact none of the trial wavefunctions used were the exact solution for the wavefunction.

Summary Statement
The atomic energies of atoms were computed in Mathematica using the variational principle method.

Help Received
My father provided the references on the variational method.