1014-Q1-119 **Ronald E Mickens*** (rohrs@math.gatech.edu), Clark Atlanta University, Box 172, Physics Department, Atlanta, GA 30314. *Calculation of Molecular Configurations for Identical Atoms.*

A fundamental issue in chemistry is the determination of possible stable molecular structures given a fixed number of various atoms. In general, this is a difficult computational problem and is usually not considered until the senior undergraduate year and/or in graduate programs. However, there are advantages for students if they can see how this process works within the context of a general chemistry course. With only a knowledge of the elements of calculus and a basic knowledge of the properties of the atom-atom interaction, we show that all the essential features of molecular structure determination can be given within the framework of a "toy" universe consisting of a single type atom. From the a priori principle that the most stable state of a collection of n-atoms corresponds to the configuration having lowest energy, we explicitly calculate the ground states for the case $n = 3, 4, 5, 6$. The examples discussed can also be presented in a standard calculus course as illustrations of the concepts of minimization of functions of either a single- or multi-variables. (Received July 29, 2005)