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Computer-Assisted Molecular Modeling

**Introduction:**

Through exploration of various features of programs offered in computational chemistry, characteristics such as electrostatic forces, bond strengths, bond angles, bond lengths, and general molecular shape can be observed and analyzed [1]. In order to simplify the electron-electron approximations and wavefunction component of the Schrodinger equation in the self-consistent field theory model, Hartree-Fock theory approximates wavefunction [4].

The Born-Oppenheimer Approximation assumes “electronic motion and the nuclear motion in molecules can be separated” [3]. This basically gives a shortcut that can be used to give an accurate approximation of the energy values of the particles and electrons. Since the nuclei are so much more massive than the electrons, and it is experiencing a force that is the average of the forces from each electron, rather than an individual force from each electron. This is part of the self-consistent field theory, which creates an average force of all the electrons exerted on the nucleus, instead of overtly distinct electron-electron interactions of single electrons. It accounts for the electron-electron correlation, which is the interaction of electrons with other electrons. We can also assume that the nucleus is stationary so that the nuclei are point charges that are the center for the electrons. This allows the Schrodinger’s equation to be solved with these simplifications.

The self-consistent field theory is performed, and the wavefunctions and energies of the electrons can be determined from the nuclear positions. The Slater determinant uses matrices and eigenvalues to account for the antisymmetric nature of electron systems [4]. Finally, the Roothan equations give a way to solve these equations with basis sets that are repeated until the self-consistent field theory requirements are attained [5]. For example, though the bond lengths and bond angles do not precisely remain at constant values due to the molecular vibrations of subatomic particles and quantum theory, the equilibrium bond lengths and angles can be calculated and the molecular vibrations are assumed to cause divergences. The interactive program *Spartan* uses HF theory and molecular mechanics to predict these characteristics and allows scientists to study them. We will compare the results of the Hartree-Fock theory of the simulation to VSEPR, or Valence shell electron pair repulsion, theory. Molecular mechanics, unlike Hartree-Fock, estimates the shape, bond lengths, and bond angles of molecules using classic principles such as electromagnetism. It is much less time-consuming than Hartree-Fock and provides an accurate depiction of proteins.

**Procedure:**

The optimal structural orientation of molecules was determined by geometry optimizations performed at the Hartree-Fock and Molecular Mechanics levels of theory. By means of stretching, twisting, rotating, bending, and other motions, the equilibrium value of these structural features can be determined through each energy from each motion can be computed and viewed in order to minimize the potential energy. Calculations form the Hartree-Fock theory also determined dipole moments and atomic charges were also determined through these methods using vector geometry to account for the size and direction of each dipole moment from each atom in order to give the molecule an electrostatic map and dipole moment as a whole.

**Conclusion:**

Computational chemistry can test theory based off experimental evidence. VSEPR theory takes into account the repulsion of lone electron pairs when determining the molecular geometry of different molecules. The calculations agreed with the VSEPR predictions. The results that were the most compelling were the dipole moment of acrylonitrile due to the high electronegativity of nitrogen and the electrostatic map of this molecule. It took into account the electron densities and electronegativities in order to create these models.

References:

[1]Iyengar, Srinivasan. Lab Lecture.

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[5] "The Hartree-Fock Self- Consistent-Field Method." *Eastern Michigan University Community*. Eastern Michigan University, n.d. Web.

[6]Tuckerman, Mark. "The Born-Oppenheimer Approximation." New York University, 17 Mar. 2008. Web.