Introduction

The electronic structure of a molecule determines much of its reactivity. If a description of the most probable locations of electrons and their energies is available, one may be able to predict useful properties such as the molecular dipole moment, polarizability, vibrational frequencies, probability of absorption of visible light, and tendency to donate electrons in a reaction.

The wavefunctions for electrons in molecules are known as molecular orbitals. It is only possible to analytically describe wavefunctions for single atoms with a single electron. For more complex molecules, only approximations can be made. The variational principle allows us to approximate true wavefunctions with sums (linear combinations) of trial wavefunctions. We write the wavefunction as

where is a trial wavefunction and ci is its contribution to . The goal is to find values of ci so that the electron has the lowest energy. Expectation values of the energy are also calculated since the trial wavefunctions are not eigenfunctions of the Hamiltonian. In order to accurately predict electronic energy, one searches for the best arrangement, geometry optimization calculation, of atoms until the energy is lowest. To efficiently perform enough calculations to accurately predict energy and geometry, computers are utilized with advance software. Other calculations of the studied molecules were data of dipole moments, vibrational peaks and UV-Vis peaks.

Molecules that were studied in this experiment were Hydrogen chloride, Sulfur dioxide, p-dichlorobenzene.

Experimental

The program wxMacMolPlt was used to build a simple model of each molecule. A molecular mechanics optimization was performed on each structure in the program Jmol. wxMacMolPlt was used to generate AM1 and PM3 geometry optimization input files for GAMESS computation package. The software GAMESS calculated geometries for each level of theory. Upon completion of the calculation from GAMESS, the resultant file (.log) was checked if it exited gracefully. The results from lower levels of theory were used as input files for higher levels of theory. Jmol was used to view the molecular orbitals and compare geometries. wxMacMolPit was used to generate input files for vibrational frequency calculations from optimized geometry results. The calculations were completed using GAMESS. The dipole moment was extracted from the resulting files with TextEditor and searched for “Debye.” Generated the potential energy surface versus bond length for the diatomic molecule. The best *ab initio* results were the starting point and the calculations were performed at 6-21G, 6-31G and DZV level. A UV-Vis spectrum of the aromatic compound was calculated by using optimized results at each level of theory. Jmol was used to visualize and obtain data of molecular vibrations and UV-Vis spectra data**.** The data was compared with the calculated transition energies with those observed in experimental spectra. After each step, the files were saved with appropriate title filenames. After completion of all calculations, Jmol was use to develop website of the molecules studied. Jmol was used to export data of molecules and web browser SeaMonkey was used to edit website.

Conclusion

Computational results are useful to predict general patterns of activity in molecules, but do not always provide exact values that match experimental evidence. Also useful for knowing how different structures affect various properties. Computational results are not useful when exact values are needed.