**Abstract**

Using several different computer software programs, the molecular geometries, bond lengths, bond angles, electrostatic potentials, dipole moments, vibrational frequencies, energy levels, and partial atomic charges of three separate molecules were found. These three include the small polar molecule Chlorine Monofluoride (FCl), the nonpolar molecule carbon dioxide (CO2), and the aromatic compound O-Xylene. The different calculations run on each molecule include AM1, PM3, 6-21G, 6-31G, and DZV. Interestingly, the best level used to find geometry and dipole moments of FCl was AM1. O-Xylene and CO2 geometry was best found using *ab initio* level 6-21G.

**Introduction**

In determining the electronic structure of a molecule, much of the molecule’s reactivity is also known. Additionally, by observing different energy levels and where the electrons are most likely to be, different properties of the molecule may be estimated. These predicted properties include molecular dipole moments, vibrational frequencies, polarizability, absorption of visible light probabilities, and a molecule’s tendency to donate electrons.

In calculating basic wave functions and molecular orbitals, according to the variational principle, the wavefunction with the lowest energy is the best approximation of the true wavefunction. Using this principle, the optimized geometry of a molecule can be predicted, as it is the most stable in its lowest energy form. In calculating an optimized geometry of a molecule, finding the arrangement that forms a system of minimal energy is needed. Preferably, a large basis set wavefunctions is used to find the trial wavefunction and then it is normalized. A larger basis set will most likely lead to a more accurate energy estimate. Large basis sets could not be used until the rise and common use of computers; they are almost impossible to calculate by hand due to their complexity and the amount of time it would take to do so.

The computer program used to initially guess the correct molecular structure is Avogadro1. This program “treats molecules as a collection of harmonic oscillators,” and “adjusts atom positions to minimize stress on the molecule.”2 The method for calculation depends on the number of atoms and not number of electrons, making it easier to use for large systems. AM1 and PM3 are two Hamiltonian choices that need semi-empirical data used for two electron overlap integrals. Because only two overlap integrals are being calculated, AM1 and PM3 are the quickest method used. The methods in which all integrals are calculated is *ab initio*- the best level of theory. Steven K Burger and Weitao Yang in their study of *Linear-scaling quantum calculations using non-orthogonal localized molecular orbitals* go into more detail about non-orthogonal orbitals in particular. They state, “conventional semi-empirical and ab initio methods are constrained by nonlinear-scaling operations associated with constructing the one-electron Hamiltonian.”3

The basis sets used in order of increasing size are: 6-21G, 6-31G, and double zeta valence (DZV).

The three molecules FCl, CO2, and O-Xylene (C6H4(CH3)2) were made in Avogadro. To refine the geometries, the program wxMacMolPlt was used. Then, the file created in Avogadro and run through wxMacMolPlt was put into the software GamessQ to perform the integral calculations at AM1, PM3, and the three *ab initio* levels. Jmol was used to model the calculations and values to add to this website. The following hyperlinks are where properties of each molecule can be observed:

**Conclusion**

The best level of theory used to find geometries and dipole moments overall was AM1. However, because the basis set used only 2 overlap integrals, it could not be utilized as much. Therefore, the *ab initio* theory of 6-21G was the main level used. Our percent error for the FCl molecule’s dipole moment was 28.5% and 3.79% for bond length using the 6-21G level. Using the 6-21G level of theory our percent error for O-Xylene’s dipole moment was 1.1%. For CO2 6-21G was also used to yield a percent error of 1.81% for its optimized geometry.

The DZV level of theory was used to calculate the wavelengths of the vibrational frequencies that would absorb energy. The calculated wavelengths were compared to an IR spectrum of each molecule, if there was one available. These can be observed in their respective webpages. Although DZV was used for vibrational frequencies, note that for most calculations the DZV level of theory was not the most accurate. The inconsistency in all the levels of theory when calculating values for each molecule may present a problem for anyone wanting to obtain these values using this software.

**References**

1. Avogadro software. <http://sourceforge.net/projects/avogadro/> (accessed February 17, 2015).
2. Gutow, J. *Molecular Orbital (MO) Calculations* **2014**, p 1-3.
3. Burger, Steven K.; Yang, Weitao. *Journal of Physics: Condensed Matter* **2008***, Volume 20, Issue 29*, 294209.
4. NIST Website: Constants, Units, and Uncertainty. <http://physics.nist.gov/cuu/Constants/index.html> (accessed February 17, 2015)
5. NIST Website: NIST Chemistry WebBook <http://webbook.nist.gov/chemistry/> (accessed February 15, 2015).
6. *CRC HANDBOOK of CHEMISTRY and PHYSICS;* 68TH ed; Weast, Robert C., Ed.; CRC Press, Inc.: Boca Raton 1987-1988.
7. Electrostatic Potential Maps. <http://chemwiki.ucdavis.edu/Theoretical_Chemistry/Chemical_Bonding/General_Principles/Electrostatic_Potential_maps> (accessed March 7, 2015).
8. Kaye & Laby Tables of Physical and Chemical Constants: 3.8.7 UV-visible spectroscopy. <http://www.kayelaby.npl.co.uk/chemistry/3_8/3_8_7.html> (accessed March 9, 2015).