

CHM 1213 University Chemistry 1 - Prof. Appleby

University Chemistry 1 (CHM 1213) is a freshmen level course that is taken by all chemistry, nursing, and engineering majors. Students study the laws and concepts of chemistry and their application to chemical systems. They also study the liquid and solid states, phase changes and phase diagrams, oxidation-reduction chemistry, electrochemistry, chemical thermodynamics, gas-phase equilibrium, atomic and molecular structure.

Students often have a difficult time comprehending and visualizing molecular structure. The current molecular structure models, such as VSEPR (Valence Shell Electron Pair Repulsion) theory and the Lewis Electron Dot Structure have many limitations. One of these limitations include the accurate depiction of how lone pair electrons affect molecular geometry. Our research project will explore the molecular structure of small molecules and determine how lone pair electrons affect the molecular structure. This research project will use the Spartan Wavefunction software to perform ab initio and semi-empirical calculations.

The first week of the project, students will be introduced to the Lewis Electron Dot Structure and the VSEPR models. They will also be introduced to the Spartan program. The second week students will perform ab initio and semi-empirical calculations to determine the electron density and electrostatic potential to locate the lone pair electrons on small molecules. The third week, students will analyze the data collected to determine the molecular structure and demonstrate how lone pair electrons effect the molecular structure.