Introducing Quantum Mechanics into General Chemistry

IWONA POPKOWSKI, HAFED BASCAL, University of Findlay — Periodicity has long been recognized as the tool that chemists can use to bring some order to investigating the chemistry of more than one hundred elements. Such studies provide useful tools for understanding a wide array of chemical principles. The advances in computational chemistry make it possible to study and teach such trends with hands on approach. In this study we utilize recently acquired software Spartan Pro to illustrate theoretical measurements of bond length, bond angle and dipole as compared to experimental data. We constructed a matrix of values obtained from the theoretical calculations and obtained trends in bond length, bond angle and dipoles for the several periodic groups.