Abstract

Understanding the distribution of electric charge within a molecule is essential for comprehending chemical reactivity, molecular interactions, and structure-activity correlations. This is where molecular electrostatic potential, or MESP, comes into play. Additional chemical applications of MESP, such as bonding, covalent radii, resonance, and the inductive effect, have also been studied. Later on, this scalar field was rigorously treated quantitatively by topographical analysis. In my work I have calculated and visualized the molecular elctrostatic potential of H_2^- by varying the bond lengths of anion along with the topological analysis. Other part of my work includes the optimization calculations of alkyl amines at different level of theories.