DFT STUDY OF THE C–Cl BOND DISSOCIATION ENTHALPIES AND ELECTRONIC STRUCTURE OF SUBSTITUTED CHLOROBENZENE COMPOUNDS

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UDC 539.19;547.539

Quantum chemical calculations were used to estimate the bond dissociation energies (BDEs) for 13 substituted chlorobenzene compounds. These compounds were studied by employing the hybrid density functional theory methods (B3LYP, B3PW1, B3P86) with 6-31G** and 6-311G** basis sets. It was demonstrated that B3P86/6-311G** method is the best method for computing the reliable BDEs for substituted chlorobenzene compounds which contain the C–Cl bond. It was found that the C–Cl BDE depends strongly on a computational method and basis set used. Substitution effect on the C–Cl BDE of substituted chlorobenzene compounds is further discussed. It is shown that the effects of substitution on the C–Cl BDE of substituted chlorobenzene compounds are very insignificant. Frontier orbital energy gap of studied compounds was also investigated. From the data on frontier orbital energies gap, we estimated the relative thermal stability of substituted chlorobenzene compounds.

Keywords: density functional theory; bond dissociation enthalpy; substituent effect; substituted chlorobenzene compounds.