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Application of Hammett Constant for Prediction of Acidity Properties of Substituted Benzoic Acid

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Abstract

Hammett constants (σ) can be important factor to understanding substitution and position effects on benzoic acid. This report describes a computational study of ΔG◦ and σ for six substituted benzoic acid (X= F,Cl ,OH ,NH_2,CN,NO_2)and phenylacetic acid substituted (X=OH ,NH_2) at para and meta positions ingas and aqueousphases by DFT method and comparesit to available experimental and theoretical results.

Keywords. *Hammett Constant, Benzoic acid,Phenylacetic acid substituted, Aqueous phases.*

Introduction

The development of correlation between UV-Vis. absorption and Hammett substituent constants is one of the major achievements of physical chemistry (Hansch et al. 1991). Hammett substituent coefficients (σ) are used to evaluate the effect of the substituents upon the rate of a chemical reaction for which mechanism is known. Several studies were reported the correlation between UV absorption frequencies with substituent parameters [1].The effects of substituent on the electronic absorption spectra of substituted Benzoic acid are investigated by correlations between absorption maximum wavelengths (nm) and the Hammett substituent parameters. The scopes of λ_{max} as a function of the σ(sum of Hammett substituent constant), indicating the applicability of the Hammett equation in the form [1]:

$$(\lambda_{max})X = (\lambda_{max}) \text{ without substitutent} + \rho\ (\sigma)\ X \quad (1)$$

Computational chemistry is playing the role of a real partner in applied chemistry research where theory and experimental are mutually complementary tools.The present workexamines the applicability of quantum chemical parametersas descriptors for substituent effects onthe pK_as of substituted benzoic acids. The linear free energy relationship and values of Hammett constants (σ) of substituted benzoic acid are

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