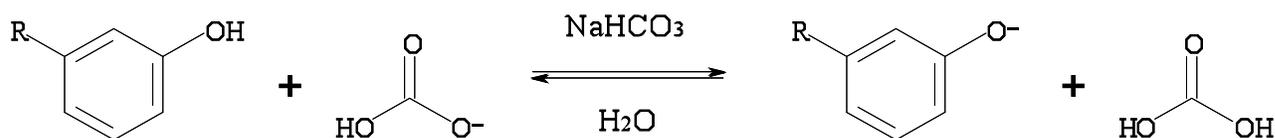


Computational Analysis of Solvation Methods in Acid-Base Reactions of Substituted Phenols

Benjamin T. Hanf and Justin B. Houseknecht*

Department of Chemistry, Wittenberg University, Springfield, OH

The interaction between solute and solvent is essential when describing the energy of many molecules within polar reactions. Further examination of these interactions is important both because they occur frequently in biochemistry and because there have not been extensive computational studies in this field. The purpose of this project is to determine how to best model the acidity of substituted phenols. Previous research on the gas phase acidity of phenol and acetic acid has shown that the most efficient method for modeling this reaction has been MPW1K/6-31+G*. This level of theory has now been applied to different solvation methods including PCM and SM6 for the first step of the reaction where an acid-base reaction occurs between phenol and bicarbonate. The SM8 method has also been used to model the reaction with the density functional method B3LYP/6-31+G**. In addition to implicit solvation methods, one or two water molecules were explicitly added to the solutes and underwent the same solvation methods as the solutes with no water molecules. All of these solvation methods were used to determine which is most efficient in determining the change in Gibbs free energy of the first step of this reaction as it occurs in water. Analysis of the Gibbs free energy change of the reaction with phenol gives no indication of which solvation method is more accurate, but most methods became more accurate with the addition of explicit water molecules to the solutes. When comparing the change in Gibbs free energy of the reaction using phenol to the change in Gibbs free energy of the reaction using different meta-substituted phenols, the difference in calculated energies is closer to the actual differences using the PCM and SM8 solvation methods.



R=F, Cl, CN, NO₂, CH₃