Arene-Arene Binding Energies: Correlation with Hammett Substituent Constants

Mike Lewis
Department of Chemistry
Saint Louis University

Non-covalent interactions of aromatics are important in a wide array of chemical biological fields. Work in our group is focused on predicting non-covalent binding energies of aromatics based on the substitution pattern of the aromatic. Recent work in our group on face-to-face arene-arene interactions of benzene and substituted aromatics showed an excellent correlation between the face-to-face arene-arene binding energies and the sum of the Hammett substituent constants σ_p ($\Sigma\sigma_p$) of the substituted aromatics. The results of these computational studies correlate with the types of arene-arene 1:1 co-crystals in the Crystal Structure Database. We will discuss the results and explore some explanations for why arene-arene binding energies should correlate with Hammett substituent constants.