Are the molecular non-covalent interactions of alkali cation-benzene (M^+-XC_6H_5) complexes confined to a specific carbon atom or propagated through space effects of the substituents? An intense reinvestigation using LFER

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The importance of potential use of Linear Free Energy Relationships (LFER, both Hammett and Taft equations) is explored by applying to the binding/interaction energies of the cation-benzene molecular complexes. An intense study of the application of both Hammett and Taft correlations in their various forms in the present study reveals that the substituent effect is not confined to a particular carbon atom of the π-system of benzene but propagated through the entire moiety of the π-system. Possible explanations are provided based on the magnitude of several Hammett and Taft reaction constants (ρ and ρ^*).

Keywords: Hammett equation, Taft equation, Binding energies, Interaction energies

Strong non-covalent molecular interactions or binding