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**SYMMETRY-ADAPTED PERTURBATION THEORY AS A TOOL FOR STUDYING  
AND DIAGNOSING NON-COVALENT INTERACTIONS**

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**Abstract**

Non-covalent interactions (NCIs) are central to many chemical transformations, but the prediction and diagnosis of NCIs in chemical systems remains underexplored due to their weak strength and complexity. In order to explore the effect of arene-substitution on cation- $\pi$ , anion- $\pi$ , CH- $\pi$ , and  $\pi$ - $\pi$  interactions, a computational data library of 810 interactions was built using 54 arenes and 15 different interaction types. Symmetry-adapted perturbation theory (SAPT) reports electrostatic, repulsive, inductive, and dispersive components of the total interaction energy between two interacting fragments and therefore lends a deeper understanding to trends in NCIs. We hypothesized that by understanding individual NCI substituent effect trends we would be able to diagnose their presence in chemical systems. Characteristic features of each NCI were determined by comparing trends within and between interaction types. Cation- $\pi$  and anion- $\pi$  interactions are composed mainly of electrostatic forces by percent contribution, while CH- $\pi$  and  $\pi$ - $\pi$  interactions are largely dispersive in nature. Unlike the dispersion-driven CH- $\pi$  interactions, however, changes in  $\pi$ - $\pi$  interaction energies with differing arene substitution patterns are governed by electrostatics. Having gained an understanding of substituent effects on NCIs, we turned our focus to demonstrating the utility of this library in chemical transformations by selecting three case studies in asymmetric catalysis and supramolecular chemistry. Alongside correlation ( $R^2$ ) analysis, residual and rank-order analysis were employed to analyze and diagnose an NCI as present in a particular system. This process has been automated, allowing our data library functions as a descriptive tool that can be used to analyze NCI-driven processes.