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Deconstructing Cation-pi Interactions: Understanding the Binding Energies Involved with Metal and Aromatic Amino Acid Residues

Jen E. Werner, Lyudmila V. Slipchenko, and Yen Bui
Department of Chemistry, Purdue University

ABSTRACT

The Effective Fragment Potential (EFP) method is a computationally efficient technique for describing non-covalent interactions, such as hydrogen bonding and van der Waals forces. Cation-pi interactions are a type of non-covalent interactions and are thought to be important in biological processes, such as permittivity of ion channels. The goal of our work is to establish that the EFP method reliably describes the strength, directionality, and composition of cation-pi interactions. Optimal geometries were found for a series of biologically relevant cations (K^+, Li^+, Na^+, Ca^{2+}, and Mg^{2+}) and aryl moieties appearing as residue groups in natural amino acids (3-methyl-1h-indole, p-cresol, phenylalanine, toluene, and tyrosine) using the MP2 level of theory and the cc-pVTZ basis set. The cation was then displaced along a line normal to the aromatic compound with EFP calculations performed for every 0.2 angstroms between 1 and 7 angstroms along the trajectory. The obtained binding energies and relative energy components were compared against Symmetry-Adapted Pertubation Theory (SAPT) calculations at 0.4 angstrom increments along the same trajectory. SAPT has been previously used to test the accuracy of EFP for a variety of systems. Preliminary results indicate that the EFP method accurately predicts equilibrium geometries in cation-pi complexes. The low computational cost of EFP against SAPT provides promise in expansion on the research of cation-pi interactions to larger systems using EFP.

KEYWORDS

EFP, cation-pi interactions, non-covalent interactions, SAPT, amino acid residues