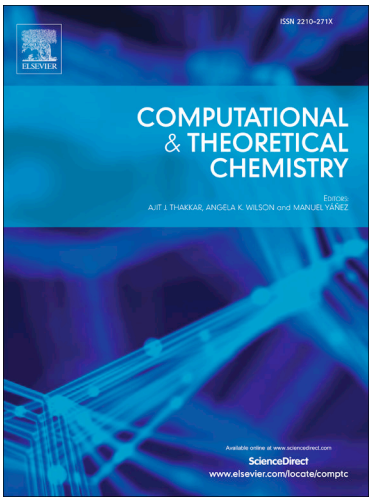

Non-covalent Interaction in Benzene and Substituted Benzene: A Theoretical Study

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Non-covalent Interaction in Benzene and Substituted Benzene: A Theoretical Study

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ABSTRACT

Non-covalent interaction is believed to play a vital role in stabilizing various complex chemical species. Herein, we have undertaken a theoretical study to understand the nature and extent of non-covalent interaction between the aromatic surfaces of benzene and its substituted derivatives with hydrogen bond donors as well as lone pair containing molecules. Molecular electrostatic potential (MESP) calculation has been used to identify the attractive zones of the aromatic surface. Symmetry adopted perturbation theory (SAPT) calculations reveal that the stability of these interactions is dominated by both electrostatic as well as dispersion interaction. Non-covalent interaction plot (NCI) analysis provided the qualitative visualization of the interaction while quantum theory of atoms in molecules (QTAIM) proved the existence of this interaction through the formation of bond and cage critical points.

Keywords: Non-covalent interaction; MESP; SAPT; NCI; QTAIM

1. INTRODUCTION

The role of non-covalent interaction in various physical, chemical and biochemical processes are well known and hence, have attracted many researchers towards their nature [1-5]. This has become one of the recent and major interest for computational chemistry to understand and characterizing varieties of non-covalent interaction. Among these noncovalent interactions, hydrogen bond is mostly analyzed due its critical role in stabilizing various supramolecular framework, in proton transfer reactions, crystal engineering and others [6-9]. However, recently halogen substituted (mostly fluorine) molecules have been found to increase the role of other types of interaction and is becoming an expanding area of both experimental and theoretical research [10-13]. While the interaction of benzene with water takes place via the hydrogen atom of water and the π cloud of benzene, the interaction of water with fluorinated benzene takes place via the lone pair of the oxygen atom of water and π cloud of benzene of benzene (Scheme 1). This lone pair-π interaction has recently been verified both theoretically and experimentally [12]. The first experimental proof of the lone