COMPUTATIONAL INVESTIGATION OF INTERMOLECULAR INTERACTIONS OF PYRENE AND AMINOPYRENE WITH PHENOTHIAZINE AND PROMAZINE

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Pyrene and its derivatives are polyaromatic hydrocarbons which cause environmental pollution (ie. petrolium wastes). They can also enter the human body by various ways and may interact with some biologically important molecules. Some drugs (i.e. promazine and paracetamol) have aromatic structures consisting of π-electron systems. Phenothiazine is an aromatic molecule which contains π-electrons. Its derivatives are a pharmaceutically important class of heterocycles, known as pharmacophores in sediatives, antitumor agents, etc. Promazine and fluphenazine (phenothiazine derivatives) are frequently used with psychotic patients in psychiatric practice. Previous studies on phenothiazine and promazine tranquilizers suggested that these compounds act as good electron donors and can function as a charge transfer or electron transfer donor at drug receptor sites[1]. This hypothesis is consistent with the observation of the formation of charge transfer complexes of phenothiazine and its derivatives with a variety of acceptor compounds[1]. Pyrene and its derivative 1-aminopyrene are fluorescent probes frequently used for solvent polarity studies in different media[2].

Determining molecular complexation and their geometries are among the most important tasks in biological systems [3]. In this study, possible complex formations in the ground state between pyrene and aminopyrene (as acceptors) and phenothiazine and promazine (as donors) have been investigated by utilizing computational quantum chemical methods. In particular, all the geometries were optimized and characterized using DFT-PBE1PBE method as implemented Gaussian 98 program suite [4]. Single point TD-DFT calculations for determining vertical excitation energies of the complexes were also performed utilizing their ground state DFT geometries.

The major finding of this study is that the pyrene-phenothiazine, pyrene-promazine, aminopyrene-phenothiazine and aminopyrene-promazine complexes have thermodynamic stabilities at the ground state in gas phase. Additionally, the TD-DFT calculations revealed that the $S_0 \rightarrow S_1$ transitions for all complexes are pure charge transfer transitions from donor to acceptor molecules between HOMO – LUMO of the complexes.

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