Investigation of Complex Formation between Pyrene and Selected Drug Molecules by Spectroscopic and Semiempirical Methods

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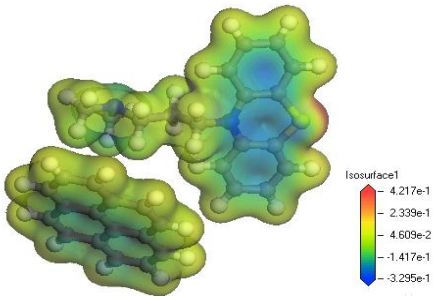
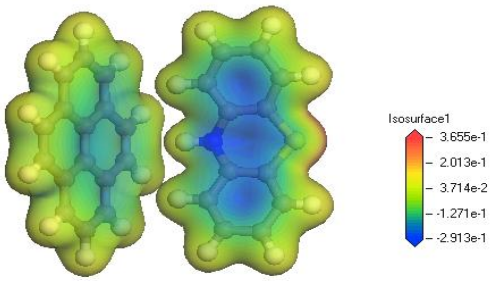
Pyrene and its derivatives are natural or synthetic aromatic hydrocarbons that are found in the environment in large quantities. Because of their amounts in the environment, they could easily enter the metabolism of living organisms. Their π-electronic system allows them to interact with several molecules in metabolism.

Phenothiazine and its derivative promazine are drug molecules especially used as antidepressants. Due to the presence of heteroatoms (especially nitrogen) in their structure, they may interact in many reactions in biological systems.

In this study, possible interactions between pyrene and the drugs phenothiazine and promazine have been investigated in ground and excited states. In addition to experimental methods like UV and fluorescence spectroscopy, semiempirical calculations have also been performed by using the VAMP module [1] as implemented in Materials Studio package [2].



Py-Prom



Py-Pheno

The results indicate that there is no complex formation in the ground state, thus there are no interactions. On the other hand, fluorescence quenching has been observed in the excited state and it has been concluded that these interactions show weak charge/electron transfer processes. Experimental and semiempirical methods used in the study are in qualitative agreement.

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[1] T. Clark, A. Alex, B. Beck, F. Burkhardt, J. Chandrasekhar, P. Gedeck, A. Horn, M. Hutter, B. Martin, G. Rauhut, W. Sauer, T. Schindler and T. Steinke, VAMP 8.1 Build 32, Erlangen (2003).
[2] Materials Studio 4.1, Accelrys Inc. (2006).

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