# Computational investigation of the exciplexes formed between pyrene and selected monoamines

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Intermolecular electron transfer processes were investigated computationally. Pyrene (Py) was used as acceptor and some aliphatic amines trimethylamine (TEA), tripropylamine (TPA), and 1-azabicyclo[2.2.2]octane (ABCO) were used as donors. Calculations were performed by density functional theory (DFT) with the ωB97XD functional, where 6-311++G(d,p) basis set employed for molecules. Time-dependent density functional theory (TDDFT) with the B3LYP functional and same basis set was used for excited state calculations. 40 lowest singlet excited states were calculated for each molecule. Molecular orbital energies and the UV-Vis spectra of the studied molecules were illustrated with the same method using the Gaussview5 program [1] using the ground state geometries. The total electron density surface of pyrene and its derivatives mapped with the electrostatic potential values in gas state and various solvents for the excited state. All calculations were performed using Gaussian09 software [2].

HOMO   LUMO
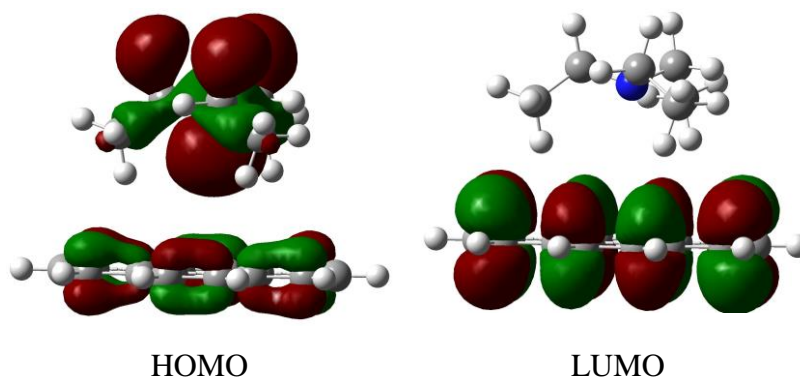
Analyses of first excited singlet states have revealed that there are charge transfers between Pyrene and investigated amines. Figure shows charge transfer between Pyrene (Py) and trimethylamine (TEA) in gas phase. $S_0 \rightarrow S_1$ transition (376 nm) between H→L orbitals for Py-TEA system has a CT character from TEA to Py.

[1] GaussView, Version 5, R. Dennington, T. Keith, J. Millam, Semichem Inc., Shawnee Mission, KS, 2009.
[2] Gaussian 09, Revision **C.**01, M. J. Frisch, Gaussian, Inc., Wallingford CT, 2009.