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Prediction of charge transfer transition energies of the molecular complexes of PMDA with a series of methylbenzenes by TDDFT

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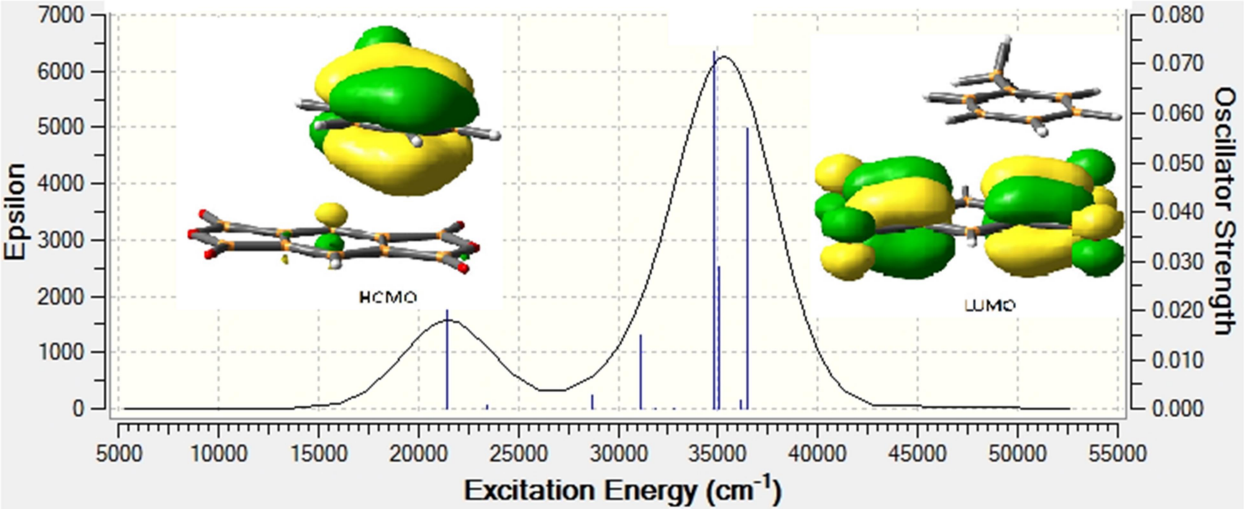

Abstract:
The functionals M06, M06-L, M06-2X and B3LYP were used to establish molecular complex formation and to calculate CT transition energies of the molecular complexes of PMDA with benzene, toluene, *p*-xylene, mesitylene and durene in CCl_4 medium by a TDDFT calculation under the PCM formalism. Using the ground state optimized geometries as starting points, attempts were made to calculate the CT transition energies of the molecular complexes by TDDFT/6-31++G(d,p). The calculated values obtained by the different functionals were compared among themselves and also with experimentally reported values. Agreement of the calculated CT transition energies with experimental values is reasonably good, M06 results being closest. The lowest energy CT absorption bands as calculated by TDDFT were found to abide by the theory of charge transfer complexes given by Mulliken (*J. Am. Chem. Soc.,* 1952, **74**, 811).

Key words: TDDFT, Charge transfer, PMDA complex, M06 functionals, Mulliken's theory