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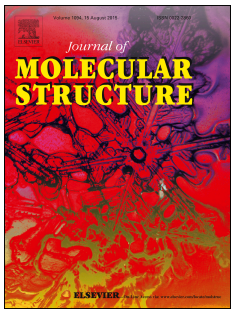

Linear, non-linear optical properties and reorganization energies of D- π-A star shaped triazine derivatives: A DFT study

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Linear, Non-linear Optical Properties and Reorganization energies of D- π-A star shaped Triazine Derivatives: A DFT Study

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Abstract:

We have theoretically investigated two series of D-π-A star shaped octupolar triazine derivatives by using density functional theory (DFT) and time dependent density functional theory (TDDFT) calculations employing B3LYP methods with 6-31G (d, p) basis set. One series of triazine derivatives has furan as the π bridge, while the other series has thiophene as the π bridge between donor and acceptor moieties. The photophysical, charge transfer, non-linear optical properties and reorganization energy studies were carried out focusing on the effect of varying substitution on the central triazine core of the molecules under study. The charge transfer properties of the molecules are studied by using VMOdes software.

Key words: Donor/Acceptor; Charge Delocalization; First Hyperpolarizability; Organic Push-Pull Molecules; Reorganization energy.

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