

Accepted Manuscript

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

V.M. Vidya, Anuj Tripathi, Chetti Prabhakar



PII: S0022-2860(18)31108-6

DOI: [10.1016/j.molstruc.2018.09.025](https://doi.org/10.1016/j.molstruc.2018.09.025)

Reference: MOLSTR 25659

To appear in: *Journal of Molecular Structure*

Received Date: 28 May 2018

Revised Date: 3 September 2018

Accepted Date: 11 September 2018

Please cite this article as: V.M. Vidya, A. Tripathi, C. Prabhakar, Linear, non-linear optical properties and reorganization energies of D- π -A star shaped triazine derivatives: A DFT study, *Journal of Molecular Structure* (2018), doi: <https://doi.org/10.1016/j.molstruc.2018.09.025>.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Vidya V. M., Anuj Tripathi and Chetti Prabhakar*

Department of Chemistry, National Institute of Technology, Kurukshetra-136119, India.

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.

To whom correspondence should be addressed:

*Email: chetty_prabhakar@yahoo.com

Download English Version:

<https://daneshyari.com/en/article/11032227>

Download Persian Version:

<https://daneshyari.com/article/11032227>

[Daneshyari.com](https://daneshyari.com)