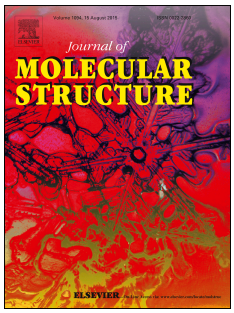
Accepted Manuscript



Theoretical investigation of the photophysical properties of donor-acceptor dyes containing coumarin and naphthoquinone moieties linked by an aminomethylene bridge

Mikaelly O.B. Sousa, Maria D. Vargas, Fabio S. Miranda

PII: S0022-2860(18)30341-7

DOI: 10.1016/j.molstruc.2018.03.052

Reference: MOLSTR 24991

To appear in: *Journal of Molecular Structure*

Received Date: 30 August 2017

Revised Date: 12 March 2018

Accepted Date: 13 March 2018

Please cite this article as: M.O.B. Sousa, M.D. Vargas, F.S. Miranda, Theoretical investigation of the photophysical properties of donor-acceptor dyes containing coumarin and naphthoquinone moieties linked by an aminomethylene bridge, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.03.052.

Theoretical investigation of the photophysical properties of donor-acceptor dyes containing coumarin and naphthoquinone moieties linked by an aminomethylene bridge

Mikaelly O. B. Sousa, Maria D. Vargas, Fabio S. Miranda*

Instituto de Química, Universidade Federal Fluminense, Niterói, RJ 24020-141, Brazil

**e-mail: fsmiranda@id.uff.br*

Highlights

- Synthesis of novel naphthoquinone-coumarin hybrids
- Quenching of the coumarin fluorescence by a charge transfer process
- TD-DFT calculations of donor-acceptor systems
- Challenges involved in the description of CT systems by TD-DFT

Abstract

Mannich bases **HL1** and **HL2** derived from lawsone, heptylamine and 3-formylcoumarins have been synthesized for the investigation of their photophysical properties. The cyclic voltammetry data showed a charge transfer (CT) process from the coumaryl to the naphthoquinonoid group, in spite of the absence of conjugation between these two fragments, with the nitrogen atom playing an important role. Photophysical studies by UV-Visible and fluorescence spectroscopy in acetonitrile revealed low emission quantum yield (Φ), thus