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

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1 **Theoretical investigation of the photophysical properties of donor-**  
2 **acceptor dyes containing coumarin and naphthoquinone moieties linked**  
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10 Highlights

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

16

17 Abstract

18

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

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