



Computational studies on linear, second and third-order nonlinear optical properties of novel styrylquinolinium dyes

Submitted by Régis Barille on Fri, 03/10/2017 - 10:06

Titre	Computational studies on linear, second and third-order nonlinear optical properties of novel styrylquinolinium dyes
Type de publication	Article de revue
Auteur	Karakas, Asli [1], Karakaya, M. [2], Taser, M. [3], Ceylan, Y. [4], Gozutok, A. [5], Arof, A.K. [6], El Kouari, Y. [7], Sahraoui, Bouchta [8]
Editeur	Elsevier
Type	Article scientifique dans une revue à comité de lecture
Année	2016
Langue	Anglais
Date	16 Mars 2016
Pagination	47-52
Volume	648
Titre de la revue	Chemical Physics Letters
ISSN	0009-2614
Résumé en anglais	<p>The electric dipole moments (μ), static dipole polarizabilities (α) and first hyperpolarizabilities (β) of styrylquinolinium dyes, D8 and D21, have been computed by density functional theory (DFT). The one-photon absorption (OPA) characterizations have been investigated using UV-vis spectroscopy and further interpreted using computational chemistry. The time-dependent Hartree-Fock (TDHF) method has been used to describe the dynamic dipole polarizabilities, dynamic second-order and also static and dynamic third-order nonlinear optical (NLO) properties. D8-D21 have rather high β and second hyperpolarizabilities (γ). The highest occupied molecular orbitals (HOMO), the lowest unoccupied molecular orbitals (LUMO) and the HOMO-LUMO band gaps for D8-D21 have been evaluated by DFT.</p>
URL de la notice	http://okina.univ-angers.fr/publications/ua15720 [9]
DOI	10.1016/j.cplett.2016.01.075 [10]
Lien vers le document	http://www.sciencedirect.com/science/article/pii/S0009261416300070 [11]
Titre abrégé	Chem. phys. lett.

Liens

- [1] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=20813>
- [2] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=4157>
- [3] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=20818>
- [4] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=20798>
- [5] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26462>

- [6] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26454>
- [7] <http://okina.univ-angers.fr/publications?f%5Bauthor%5D=20861>
- [8] <http://okina.univ-angers.fr/bouchta.sahraoui/publications>
- [9] <http://okina.univ-angers.fr/publications/ua15720>
- [10] <http://dx.doi.org/10.1016/j.cplett.2016.01.075>
- [11] <http://www.sciencedirect.com/science/article/pii/S0009261416300070>

Publié sur *Okina* (<http://okina.univ-angers.fr>)