Electronic and optical properties of new synthesized TTF-based azine derivatives – Experimental and theoretical study

Titre	Electronic and optical properties of new synthesized TTF-based azine derivatives – Experimental and theoretical study
Type de publication	Article de revue
Auteur	Ayadi, Awatef [1], Mydlova, Lucia [2], Zouari, Nabil [3], Makowska-Janusik, Malgorzata [4], Sahraoui, Bouchta [5], El-Ghayoury, Abdelkrim [6]
Editeur	Elsevier
Type	Article scientifique dans une revue à comité de lecture
Année	2016
Langue	Anglais
Date	Juin 2016
Pagination	27-35
Volume	56
Titre de la revue	Optical Materials
ISSN	1873-1252
Mots-clés	Crystal structure [7], DFT [8], Electron density [9], hydrogen bonds [10], N ligands [11], Tetrathiafulvalene [12]
Résumé en anglais	The synthesis and detailed characterization of two tetrathiafulvalene-appended azine derivatives, namely 2-([2,2′-bi(1,3-dithiolylidene)]-4-yl)-6-((2,4-dimethylphenyl)hydrazono) methyl)pyridine (L1) and 5-([2,2′-bi(1,3-dithiolylidene)]-4-yl)-2-((2,4-dimethylphenyl)hydrazono) methyl)pyridine (L2) are described. The crystal structure of ligand L2 indicates that the mentioned molecule is completely planar with the presence of a strong intramolecular N1 [single bond] H1⋯N3 hydrogen bonding. The quantum chemical calculations show that the intermolecular interaction in crystal structure does not affect the HOMO and LUMO orbitals present in isolated molecule. The optical properties of these ligands indicate the presence of intramolecular charge transfer band in the case of ligand L2 while the electrochemical behavior of the two compounds indicates that they are valuable candidates for the construction of crystalline radical cation salts.
URL de la notice	http://okina.univ-angers.fr/publications/ua15715 [13]
DOI	10.1016/j.optmat.2016.01.054 [14]
Lien vers le document	http://www.sciencedirect.com/science/article/pii/S0925346716300544 [15]
Titre abrégé	Opt. mater.

Liens

[1] http://okina.univ-angers.fr/aayadi/publications

[2] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26451

[3] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=26452
[4] http://okina.univ-angers.fr/publications?f%5Bauthor%5D=4147
[5] http://okina.univ-angers.fr/bouchta.sahraoui/publications
[6] http://okina.univ-angers.fr/a.elghayoury/publications
[7] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=4795
[8] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=20189
[9] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=22517
[10] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=5394
[11] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=5546
[12] http://okina.univ-angers.fr/publications?f%5Bkeyword%5D=4788
[13] http://okina.univ-angers.fr/publications/ua15715
[14] http://dx.doi.org/10.1016/j.optmat.2016.01.054
[15] http://www.sciencedirect.com/science/article/pii/S0925346716300544