Research paper

A Comprehensive Study of the Optoelectronic Properties of Donor-Acceptor Based Derivatives of 1,3,4-oxadiazole

Ankita Joshi, C.N. Ramachandran

PII: S0009-2614(17)30419-0
DOI: http://dx.doi.org/10.1016/j.cplett.2017.04.088
Reference: CPLETT 34777

To appear in: *Chemical Physics Letters*

Received Date: 15 February 2017
Accepted Date: 26 April 2017

Please cite this article as: A. Joshi, C.N. Ramachandran, A Comprehensive Study of the Optoelectronic Properties of Donor-Acceptor Based Derivatives of 1,3,4-oxadiazole, *Chemical Physics Letters* (2017), doi: http://dx.doi.org/10.1016/j.cplett.2017.04.088

A Comprehensive Study of the Optoelectronic Properties of Donor-Acceptor Based Derivatives of 1,3,4-oxadiazole

Ankita Joshi, C.N. Ramachandran*
Department of Chemistry, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, India-247667
E-mail: ramcnfcy@iitr.ac.in

Abstract

A variety of 1,3,4-oxadiazole derivatives based on electron- donor pyrrole and -acceptor nitro groups are modelled. Various isomers of pyrole-oxadiazole-nitro unit and its dimer linked to substituted and unsubstituted phenyl group are studied using the dispersion corrected density functional theoretical method. The electron density distribution in frontier orbitals of the phenyl-spacer compounds bearing amino and phenylamino groups indicates the possibility of intramolecular charge transfer. The isomers of phenyl-spacer compounds absorb in visible region of electromagnetic spectrum. The compounds show high values of light harvesting efficiency, despite the weak anchoring nature of nitro groups.