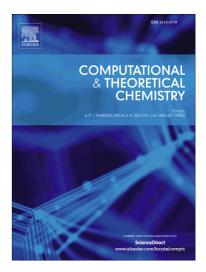
Accepted Manuscript

A DFT Study on reactivity, aromaticity and absorption spectra of Perylo[1,12b,c,d] thiophene tetraester doped with B, N, O, Se and BN

Pradip Kr. Bhattacharyya

PII:	S2210-271X(16)30060-3
DOI:	http://dx.doi.org/10.1016/j.comptc.2016.03.003
Reference:	COMPTC 2072
To appear in:	Computational & Theoretical Chemistry
Received Date:	10 December 2015
Revised Date:	26 February 2016
Accepted Date:	2 March 2016



Please cite this article as: P.K. Bhattacharyya, A DFT Study on reactivity, aromaticity and absorption spectra of Perylo[1,12-b,c,d] thiophene tetraester doped with B, N, O, Se and BN, *Computational & Theoretical Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.comptc.2016.03.003

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

ACCEPTED MANUSCRIPT

A DFT Study on reactivity, aromaticity and absorption spectra of Perylo[1,12-b,c,d] thiophene tetraester doped with B, N, O, Se and BN.

SCRIF

Pradip Kr. Bhattacharyya Department of Chemistry, AryaVidyapeeth College, Guwahati, Assam-781016, India Email: <u>prdpbhatta@yahoo.com</u>

Abstract:

Reactivity, aromaticity and absorption spectra of Perylo[1,12-b,c,d] thiophene tetraester doped with B, N, O Se and BN have been discussed in the light of Density Functional Theory (DFT) and Time Dependent Density Functional Theory (TDDFT). Doping with electron rich and electron deficient centres affects the reactivity and aromaticity of the thiophene tetraesters. A significant shift in the absorption spectra is observed in case of B and BN doped species. Aromaticity of the species is gauged by nucleus independent chemical shift (NICS). Results show that the doped species vary in their reactivity and aromaticity. N, O or Se doped species exhibit almost comparable excitation energies and absorption peaks.

Keywords: Reactivity, absorption spectra, thiophene tetraester, excitation energy, aromaticity, NICS.

Download English Version:

https://daneshyari.com/en/article/5392887

Download Persian Version:

https://daneshyari.com/article/5392887

Daneshyari.com