

Low Band Gap Donor-Acceptor Phenothiazine Copolymer with Triazine Segment: Design, Synthesis and Application for Optical Limiting Devices

Sona Narayanan, Anshad Abbas, C. Sudha Kartha, Rani Joseph, K.S. Devaky, Krishnapillai Sreekumar



PII: S0022-2313(17)31411-4
DOI: <https://doi.org/10.1016/j.jlumin.2018.01.044>
Reference: LUMIN15329

To appear in: *Journal of Luminescence*

Received date: 13 August 2017
Revised date: 3 December 2017
Accepted date: 21 January 2018

Cite this article as: Sona Narayanan, Anshad Abbas, C. Sudha Kartha, Rani Joseph, K.S. Devaky and Krishnapillai Sreekumar, Low Band Gap Donor-Acceptor Phenothiazine Copolymer with Triazine Segment: Design, Synthesis and Application for Optical Limiting Devices, *Journal of Luminescence*, <https://doi.org/10.1016/j.jlumin.2018.01.044>

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 galley proof before it is published in its final citable 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.

Low Band Gap Donor-Acceptor Phenothiazine Copolymer with Triazine Segment: Design, Synthesis and Application for Optical Limiting Devices

Sona Narayanan,^a Anshad Abbas,^b C. Sudha Kartha,^b Rani Joseph,^c K. S. Devaky,^a Krishnapillai Sreekumar^{d*}

^aSchool of Chemical Sciences, MG University, Kottayam, India

^bDepartment of Physics, Cochin University of Science and Technology, Cochin-22, India

^cDepartment of Polymer Science and Rubber Technology, Cochin University of Science and Technology, Cochin-22, India

^dDepartment of Applied Chemistry, Cochin University of Science and Technology, Cochin-22, India

Abstract

Soluble conjugated donor-acceptor phenothiazine-N-piperidine substituted triazine copolymer (P(PZ-TN)) has been designed and synthesized via Suzuki coupling reaction. To investigate the variation in band structure of the copolymer, quantum-chemical calculation using DFT theory was carried out in the periodic boundary condition (PBC) formalism at HSE06 and B3LYP correlation function using 6-31G basis set. The insertion of triazine unit as an alternating monomer in the copolymer of phenothiazine and triazine lowers the HOMO and LUMO energy levels. The optical band gap of the copolymer was calculated to be 2.5 and 2.3 eV in THF solution and as thin film, respectively from the onset of low energy optical transition. In thin film, the energy gap tends to narrow and the absorption and emission peaks are red shifted to longer wavelengths owing to the better interaction and increase in planarity of the copolymer in thin film. Theoretical studies along with photophysical and electrochemical studies confirmed that the copolymer exhibited relatively low band gap than that of homopolymer. The absorption and emission spectra of the copolymer, in solvents of varying polarity showed positive solvatochromism. The third-order nonlinear optical properties of copolymer, P(PZ-TN) were investigated by Z-scan technique at 532 nm. The copolymer showed strong third-order nonlinear optical susceptibility and low optical limiting threshold values of 1.27×10^{-11} esu and 0.22 GW/cm², respectively.

Keywords: Phenothiazine-triazine copolymer, DFT theory, Solvatochromism, Z-scan technique

Download English Version:

<https://daneshyari.com/en/article/7840283>

Download Persian Version:

<https://daneshyari.com/article/7840283>

[Daneshyari.com](https://daneshyari.com)