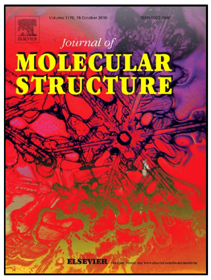

Effect of bromination on the optical limiting properties at 532 nm of BODIPY dyes with *p*-benzyloxystyryl groups at the 3,5-positions

Bokolombe P. Ngoy, Aviwe K. May, John Mack, Tebello Nyokong

PII: S0022-2860(18)30956-6

DOI: 10.1016/j.molstruc.2018.08.012

Reference: MOLSTR 25533

To appear in: *Journal of Molecular Structure*

Received Date: 27 February 2018

Accepted Date: 05 August 2018

Please cite this article as: Bokolombe P. Ngoy, Aviwe K. May, John Mack, Tebello Nyokong, Effect of bromination on the optical limiting properties at 532 nm of BODIPY dyes with *p*-benzyloxystyryl groups at the 3,5-positions, *Journal of Molecular Structure* (2018), doi: 10.1016/j.molstruc.2018.08.012

Effect of bromination on the optical limiting properties at 532 nm of BODIPY dyes with *p*-benzyloxystyryl groups at the 3,5-positions

Bokolombe P. Ngoy,† Aviwe K. May,† John Mack and Tebello Nyokong*

Centre for Nanotechnology Innovation, Department of Chemistry, Rhodes University, Grahamstown 6140, South Africa

Corresponding Author
*E-mail: j.mack@ru.ac.za, Tel&Fax: +27-46-603-7234.
† These authors contributed equally to this study.

ABSTRACT

The optical limiting (OL) properties of 3,5-di-*p*-benzyloxystyrylBODIPY dyes that contain both protons and bromine atoms at the 2,6-positions have been investigated by using the Z-scan technique at 532 nm on the nanosecond timescale. There is relatively weak absorbance at 532 nm under ambient light conditions, because the incorporation of *p*-benzyloxystyryl groups at the 3,5-positions results in a ca. 140 nm red shift of the main BODIPY spectral band to the 640–670 nm range. Reverse saturable absorbance (RSA) profiles that are consistent with an excited state absorption (ESA) mechanism involving the T_1 and/or S_1 states are observed in CH_2Cl_2 solution. Second order hyperpolarizability values of ca. 8×10^{-30} esu are obtained and this demonstrates that the dyes are potentially suitable for use in OL applications at 532 nm. There is a slight enhancement of the OL properties upon bromination, due to increased intersystem crossing to the triplet manifold, but the enhancement of the OL properties is less significant than has been observed with metal phthalocyanine complexes.

KEYWORDS: BODIPY dyes; Knoevenagel condensation; Optical limiting; Z-scan; Photophysics; TD-DFT calculations.

1. Introduction

Optical limiting (OL) materials can protect the human eye and sensitive optical devices from intense incident laser beams [1-3]. An ability to effectively absorb intense pulses of laser light at 532 nm is particularly important in this regard [4-7], since it is the second harmonic of Nd:YAG laser systems that are widely used in laser pointers. Ideally, there should be high transmittance of low-intensity light, along with the attenuation of the incident laser beam, in a manner that limits the output fluence [1-3]. Optical limiting can be achieved through nonlinear absorption (NLA), nonlinear refraction and nonlinear light scattering [8,9]. The focus of this study is on the use of the NLA processes of molecular dyes in OL applications. Materials with positive NLA coefficients result