



Diode effect caused by sequence of benzothiazole on optical properties



Chaoqun Luo, Hao Chen, Kang Cao, Wenbiao Wang, Jianrong Gao, Jianhong Jia*

College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, 310014, Zhejiang, China

ARTICLE INFO

Article history:

Received 2 March 2017

Received in revised form

7 April 2017

Accepted 10 April 2017

Available online 13 April 2017

Keywords:

Fluorescent

Benzothiazole derivatives

Third-order nonlinear

DFT

TDDFT

ZINDO calculations

ABSTRACT

In this work, two kinds of benzothiazole derivatives were synthesized. The third-order nonlinear optical properties of the benzothiazole derivatives in minimal curative dose (DCM) were analyzed using the Z-scan measurement at 532 nm with a 120 fs pulse laser. The largest third-order nonlinear susceptibility ($\chi^{(3)}$) and second-order hyperpolarizability of the complexes (γ) were estimated at 1.4×10^{-13} esu and 0.86×10^{-30} esu, respectively. The results showed that the sequence of 2- and 6-position in benzothiazole has served as a “diode,” linking to the other groups that had great influence on the optical properties such as fluorescence and nonlinear optical absorption, and the increase of the polarity and the extension of the conjugate structure had benefits to the third-order nonlinearity. The experimental findings were confirmed with the use of DFT, TDDFT, and ZINDO calculations.

© 2017 Elsevier Ltd. All rights reserved.

1. Introduction

Among the different classes of compounds analyzed, the sequences connecting to 2- and 6-position in benzothiazole were scarcely evaluated for the third nonlinear optical properties, leaving alone the CIS-reverse connection, whereas many of its derivatives were widely examined for the other various photophysical applications. The benzothiazole derivatives have a wide range of applications and have a vital role in the pharmaceutical industry,^{1–5} as related literature reported. The thiazole ring consisted of S and N, which was easy to coordinate with. Also, the thiazole derivatives could be used to design the ion probe,^{6,7} while DNA probe could spare more time for treatment. Today, the problem of modern society resources has become more serious. The benzothiazole could also be used to separate the elements rhenium (III)^{8,9} to save the resources. Also, the derivatives were easy to polarize, making the molecular orbital electrons more liable for transfer with a critical role in photochemistry.¹⁰

The nonlinear materials were valuable components necessary for the development of the optoelectronic and photonic devices. Several approaches were noted to improve the nonlinear optical

features.¹¹ Since the development of such strategies in the early 1960s,^{12,13} none had yet been found as a universal solution to regulate the nonlinear optical (NLO) device fabricators.¹⁴ Many molecular systems had managed to get satisfactory results in the thermal, mechanical, and chemical stability such as transparency and nonlinear optical coefficients.^{15,16} The analysis of the connecting sequence in this paper has a guiding role in the nonlinear polymer molecular design and synthesis. The benzothiazole consisted of the thiazole full of electrons and benzenes. As previously thought, its connection sequence would have a tremendous influence on the optical properties, especially for the fluorescence and nonlinear optical absorption. Most of the third-order nonlinear designs were based on symmetry, but seldom could be found an asymmetric molecular bridge like benzothiazole, which was part of the study.^{24,25} So our work has revolved around this concept.

The benzothiazole derivatives were synthesized to explore their effects such as diode about the 2- and 6-position in the benzothiazole on the optical properties. So the two structures were devised (Fig. 1), which selected the triphenylamine as a donor. Also, the different factors on Structure 1 were analyzed by NLO and fluorescence, such as the length of π bridge and molecular polarity. The preparation of the benzothiazole derivatives and the measurements of optical properties, such as fluorescence, the nonlinear optical absorption, and refraction effects, were discussed in these compounds by the Z-scan. It was found that Structure 2 was better

* Corresponding author.

E-mail address: zgdjjh@163.com (J. Jia).

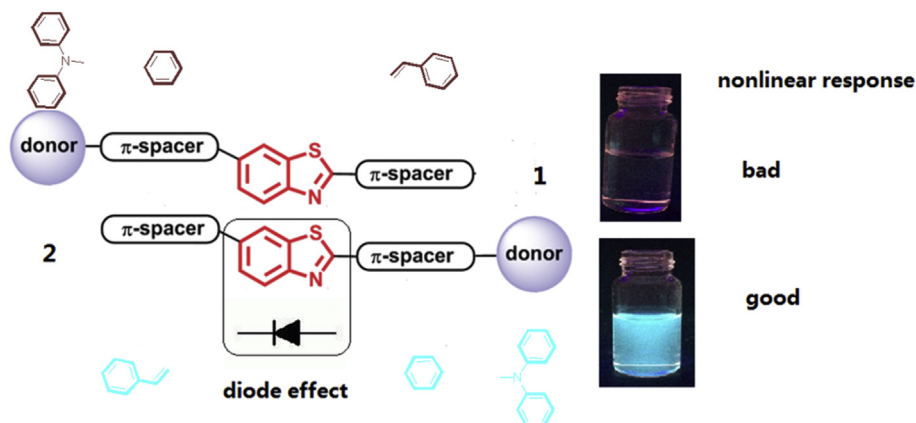


Fig. 1. Cis-reverse connection to 2,6 position in benzothiazole.

than Structure 1 over the fluorescence and the nonlinear optical absorption. To support the analysis, the experimental results have been confirmed with DFT and TDDFT calculations.

2. Results and discussion

2.1. UV–vis absorption spectra and fluorescence

The UV–vis absorption spectrum of all compounds in DCM was shown in Fig. 2.1A. The difference between **6-1** and **6-2** was that in the latter it contained a nitro substituent, which was an electron

withdrawing group. This led to the absorption peak of the **6-2** red shift to 310 nm for electron cloud density decreased (Fig. 2.2C), and the molar extinction coefficient increased to $8 \times 10^5 \text{ M}^{-1} \text{ cm}^{-1}$. However, when changing the sequence linked to the benzothiazole that made **7** to get a peak absorption at 370 nm and **6-1** did not. Both **7** and **8** showed a similar peak. The 300 nm absorption peak originated from $\pi \rightarrow \pi^*$ electronic transition absorption (see Fig. 2.1A). When **8** was added a styryl, the conjugate length extended, **7** got the red shift to 380 nm.

The fluorescence emission spectra of the compounds in DCM were shown in Table 1 and Fig. 2.1B. The fluorescence emission

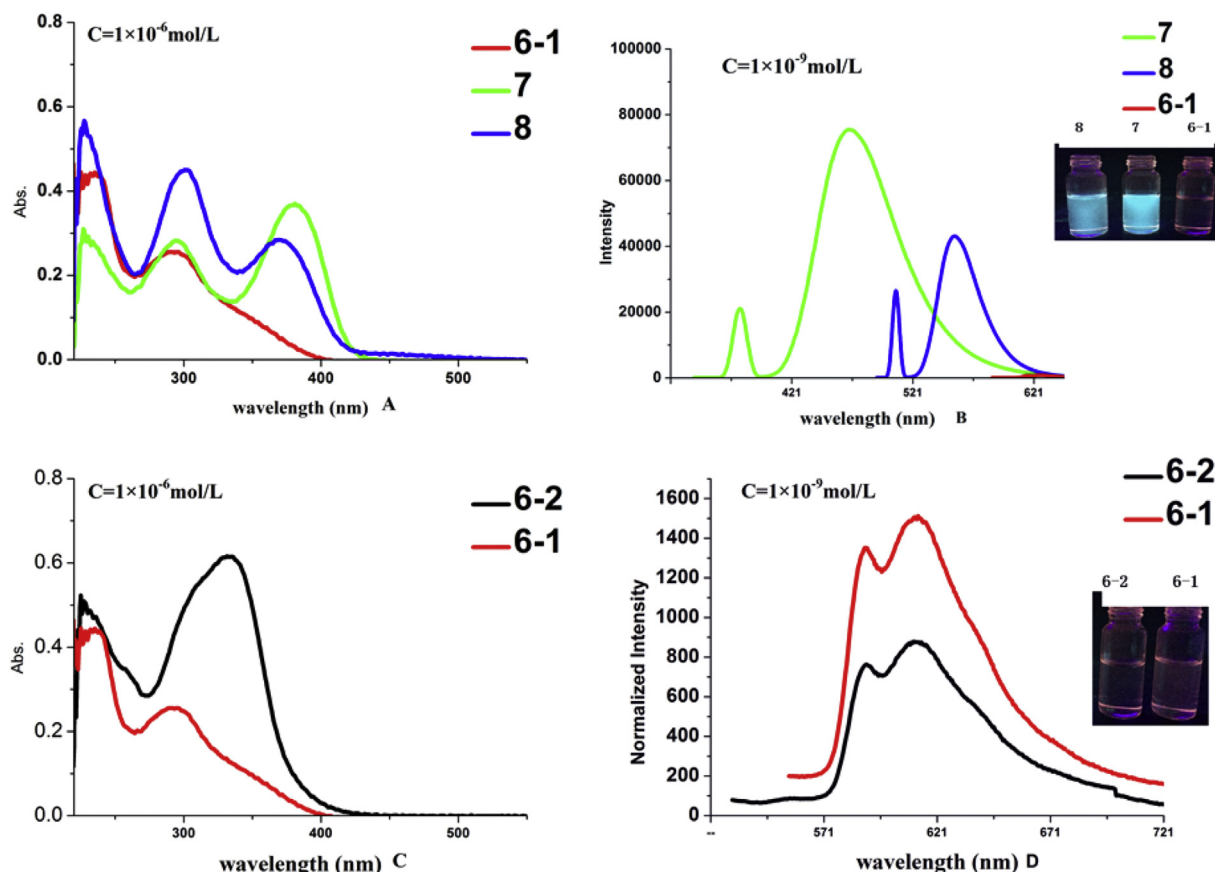


Fig. 2. 1 UV-absorption spectra (A), fluorescence spectra (B) for **6-1-7** and **8** in CH_2Cl_2 . 2 UV-absorption spectra (C), fluorescence spectra (D) for **6-1** and **6-2** in CH_2Cl_2 .

Download English Version:

<https://daneshyari.com/en/article/5212583>

Download Persian Version:

<https://daneshyari.com/article/5212583>

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