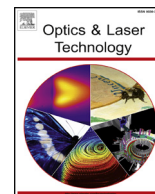




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Full length article

Synthesis of four pyrene-containing chalcone derivatives: Achieving excellent third-order nonlinear optical properties by optimizing halopyridines

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HIGHLIGHTS

- Four chalcone derivatives based on pyrenyl and halopyridyl were synthesized.
- A novel and unique method, 4f phase coherent imaging technology, was used to test the optical nonlinearity.
- Four compounds can respond quickly to 4 ns laser pulses.
- The structure-activity relationship was discussed in detail.

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ABSTRACT

Four chalcone derivatives **3a–3d** based on pyrenyl donor and different halopyridyl acceptors were synthesized successfully. The resultant chromophores **3a–3d** were characterized by nuclear magnetic resonance (NMR), high resolution mass spectra (HR-MS) and ultraviolet (UV) spectra. The theoretical calculations and thermal properties of the materials **3a–3d** were systematically studied to illustrate structure-performance relationship. Further, a novel and unique method, 4f phase coherent imaging technology, was introduced to investigate the third-order nonlinear optical properties of title compounds **3a–3d** with 4 ns laser pulses at 460 nm. The thermal properties, the theoretical calculations and the experimental results consistently indicate that the compound **3b**, namely 3-(5-bromopyridin-2-yl)-1-(pyren-1-yl) prop-2-en-1-one, is a more promising candidate for optoelectronic and nonlinear optical devices. Its third-order nonlinear absorption coefficient (β), refraction index (n_2) and polarization ($\chi^{(3)}$) are found to be up to such order of magnitude as 10^{-9} m/W, 10^{-16} m²/W and 10^{-11} esu, respectively.

1. Introduction

Nonlinear optical (NLO) materials are of high scientific significance due to their potential applications in optical switching, optical communications, optical limiting, data storage, dynamic holography, harmonic generator, etc. [1–8]. NLO properties of organic compounds, as a wide category of materials, have been studied for a few decades [9–11]. Compared with inorganic materials, organic NLO materials have many advantages such as large NLO absorption coefficients, large molecular hyperpolarizabilities, fast intrinsic response time, ease of processing, lower cost and so on [12–14]. On the other hand, organic compounds used as NLO materials can more easily be modified by tuning the intrinsic donors and/or acceptors in their parent molecules to obtain desired NLO properties [15–17]. Because it may not be possible in most

of the inorganic compounds for donor and acceptor functional groups to combine within the same molecules. Since the early 1990s, a large number of studies on the NLO properties of such organic NLO materials as chalcone derivatives have been carried out [18–22], but there is only few work upon pyrene-containing chalcone derivatives reported [23–29].

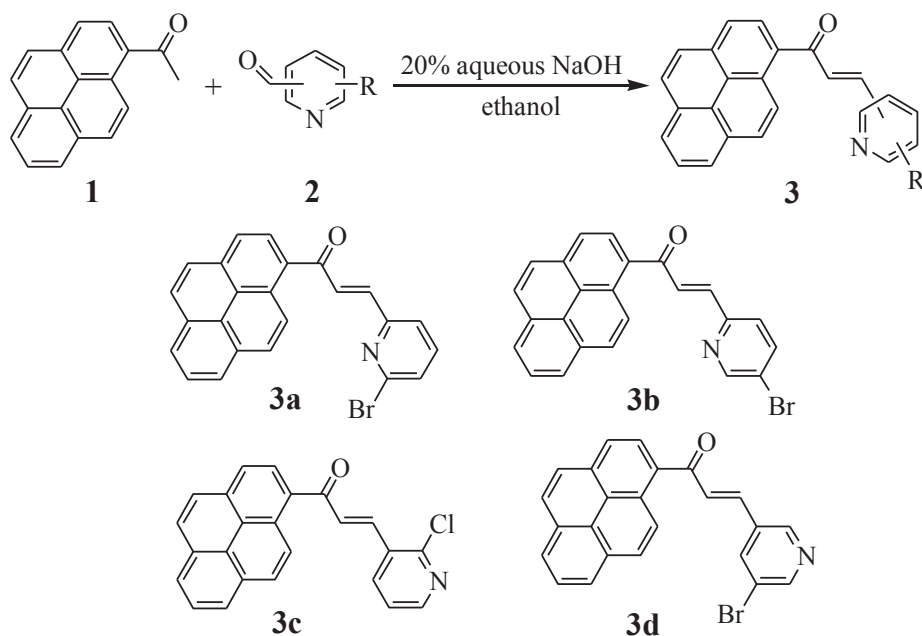
Pyrene is considered as one of the most promising nonlinear functional units with both a larger π -conjugated system and a larger electron density, which makes pyrene-containing chalcone derivatives be able to exhibit excellent NLO properties [23]. It is known that the NLO response of materials depends on various parameters, such as pulse duration, input wavelength, light polarization, etc. Hence, a considerable research efforts have been devoted to investigating the NLO response of pyrene and its derivatives, especially on femtosecond or

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Scheme 1. Synthetic route and chemical structures of pyrene-containing chalcone derivatives **3a–3d**.

picosecond time regime [24–29]. It is reported that introducing different donor/acceptor functional groups at the end position within a chalcone molecule can regulate the size and the electronic density of the π -conjugated system [17,29]. So modifying the π -conjugated system and the surrounding environment could be the reasonable way to achieve more excellent performances such as a larger absorption coefficient, a larger molecular hyperpolarizability, faster intrinsic response time, etc.

In view of the fact that pyridine is a good electron acceptor and halogen atoms are able to conjugate with the pyridine ring via p- π conjugation, we designed, synthesized and systematically characterized four chalcone derivatives **3a–3d** with both pyrenyl and halopyridyl units in order to select an organic material with excellent third-order NLO properties from them by optimizing halopyridines and explore the structure-activity relationship between the molecular composition and the NLO properties of **3a–3d** (Scheme 1). Theoretically, the frontier molecular orbitals of **3a–3d** were calculated by quantum chemical methods. Experimentally, a novel and unique method, 4f phase coherent imaging technology, was introduced to investigate the third-order NLO properties of the materials **3a–3d** with 4 ns laser pulses at 460 nm.

There are many common methods to measure the third-order NLO properties of electro-optic materials such as nonlinear interferometry, third harmonic generation, degenerate four-wave mixing, Z-scan, etc. [30–33]. By comparison, 4f phase coherent imaging technology, as a new method to measure the third-order optical nonlinearity by using 4f phase coherent imaging system, has many advantages such as single laser shot, simple optical path, no sample movement, easy manipulation of spatial frequencies and lower sensitivity to statistical fluctuations of the laser beam, which raises people's interest and promotes the in-depth study [34–37]. Therefore, a lot of research upon 4f phase coherent imaging technology has been made to characterize the third-order NLO properties of materials [34–46]. However, to our best information, the third-order NLO properties of synthesized organic compounds have not been measured by means of 4f phase coherent imaging technology in order to select better third-order NLO materials.

2. Experimental section

2.1. Apparatus and reagents

Melting point data were obtained using a WRD-1B digital melting point instrument. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker Advanced III-NMR spectrometer with TMS as internal standard and DMSO- d_6 as solvent, with 600 MHz or 400 MHz for ^1H NMR and 150 MHz for ^{13}C NMR, respectively. High resolution mass spectra (HR-MS) data were obtained on an APEX-QE Fourier transform ion cyclotron resonance mass spectrometer. Differential scanning calorimetry (DSC) analyses were performed by using a DCS 200 F3 differential scanning calorimeter.

All chemicals were purchased from commercial sources and used without further purification. All of the reactions were monitored by thin-layer chromatography (TLC). 1-Acetyl pyrene was prepared according to the literature [47].

2.2. General procedure for the preparation of **3a–3d**

To a mixture of 1-acetyl pyrene (0.35 g, 1.4 mmol) and substituted pyridyl aldehyde (1.4 mmol) in 1,4-dioxane (15 mL), 10% aqueous sodium hydroxide (2 mL) was added. The mixture was stirred for about 20 h. After completion of the reaction (monitored by TLC), the reaction mixture was poured into ice-cold water (60 mL). The solid-liquid mixture was filtered, washed with ethanol, and then every of the resultant solids was recrystallized with ethanol to obtain pure products **3a–3d**. All products were dried under vacuum for 12 h.

2.3. Structural characterization of **3a–3d**

The chemical structures of the title compounds **3a–3d** were characterized by nuclear magnetic resonance (^1H NMR and ^{13}C NMR), high resolution mass spectrum (HR-MS), and ultraviolet (UV) absorption spectra, respectively. All ^1H NMR, ^{13}C NMR and HR-MS spectra are given in Supplementary data (from Figs. S1–S12).

2.3.1. 3-(6-Bromopyridin-2-yl)-1-(pyren-1-yl) prop-2-en-1-one (**3a**)

Pale yellow solid powder, 70% (0.40 g). m.p.: 159.6–160.6 °C; ^1H NMR (400 MHz, DMSO- d_6) δ /ppm: 8.67–8.64 (d, 1H, J = 12.0 Hz, H-

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