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Synthesis and Study on Laser Photophysical Properties of Benzhydrenyl Modified Trans-Diphenylvinylbenzene Derivatives

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Abstract: *Organic π-conjugated laser materials have attracted much attention in the fields of optoelectronic devices and biosensing due to their tunable optical physical properties and low-cost processability. Among them, the trans-diphenylenyloxybenzene not only has a high fluorescence quantum yield, excellent stability and threshold laser emission performance, but also is a high-quality organic laser gain medium. This study, based on the molecular engineering strategy, synthesized three new DSB derivatives modified with phenyleneacetylene using dimethoxybenzene and bromobenzaldehyde as raw materials, explored the regulatory mechanism of molecular structure on the luminescence performance, and clarified the influence laws of conjugation length and substituents. The research results provide important theoretical and experimental support for the precise design of DSB functional materials and their applications in lasers, sensing, and optoelectronic devices.*

Keywords: *Distyrylbenzene Derivatives; Optical Properties; Fluorescence Lifetime; Laser Performance*

1. Introduction

With the iterative upgrading of organic synthesis technology, structurally controllable π-π conjugated molecular systems have developed rapidly, significantly promoting the research and application of organic optoelectronic materials. The trans-diphenylvinylbenzene (DSB) derivatives possess excellent fluorescence quantum efficiency and are a type of highly performing photonic functional framework materials. Their luminescent properties can be directionally regulated through side group modification [1]. Organic laser materials are unsaturated organic compounds capable of generating stimulated radiation under optical pumping or electrical excitation. They possess high fluorescence quantum yields, favorable chemical stability and broad gain bandwidth. Compared with inorganic counterparts, organic laser materials feature tunable molecular structures, easy processability, low cost, and their emission wavelengths can cover the entire visible spectral region [2]. Their luminescence mechanism relies on large conjugated π-systems. Upon photoexcitation, π-electrons transition to excited singlet states. After internal conversion and vibrational relaxation, population inversion is achieved, thereby generating stimulated radiation. At present, organic laser materials are diverse, including host materials, small-molecule laser dyes and conjugated polymers. Considerable progress has also been made in near-infrared organic laser materials, which have been applied in fields such as biological imaging and optical communication [3-4]. DSB-based materials are mainly utilized in organic solid-state lasers, tunable lasers, flexible optoelectronic devices, fluorescent sensors and biomedical detection [5]. Trans-stilrylbenzene is a conjugated molecule with high solid-state photoluminescence performance. Its maximum absorption wavelength is approximately 400 nm in hexane, and it emits blue-violet fluorescence at around 450 nm. This compound was first synthesized in the mid-19th century. It was systematically developed alongside the industrial advancement of fluorescent whitening agents from the 1950s to the 1960s. In the 1990s, driven by the demand for blue organic electroluminescent devices, it emerged as a promising candidate material [6], and a series of derivatives such as 4,4'-bis(2,2-diphenylvinyl)-1,1'-biphenyl were subsequently developed [7]. Since the 21st century, DSB derivatives have been further extended to nanocomposites, nonlinear optical materials and photoresponsive smart materials. In recent years, research has focused on their applications as biological probes. Given the wide variety of existing DSB derivatives, the design and synthesis of novel derivatives are of great research significance [8]. In this work, several trans-stilrylbenzene derivatives with newly introduced substituents were designed and synthesized. The chemical structures and high fluorescence quantum yield of the target products were verified via multiple characterization techniques. Finally, the research achievements and existing

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limitations were summarized.

2. Design and Synthesis of Trans-Distyrylbenzene Derivatives

DSB-based fluorescent materials possess excellent optical properties and favorable laser performances, holding promising application prospects in organic lasers, fluorescent probes, optoelectronic devices and other fields. Molecular modification of DSB is generally realized by introducing diverse substituents (such as electron-donating or electron-withdrawing groups) on the central benzene ring and styryl moieties to regulate energy level structures and luminescence behaviors. Meanwhile, conjugated side chains can be incorporated to adjust solubility and solid-state stacking modes. In this study, a synthetic strategy combining Sonogashira coupling reaction and Horner-Wadsworth-Emmons (HWE) reaction was adopted [9-10]. Firstly, aromatic halides were used as starting materials. Alkynyl groups were introduced via Sonogashira coupling to construct rigid conjugated frameworks. Subsequently, aromatic aldehyde fragments underwent condensation with phosphonates under alkaline conditions through HWE reaction to form vinylene linkages. This synthetic route features mild reaction conditions, simple operation and high stereoselectivity, which exclusively yields trans-vinylene structures, and the target products can be easily purified. The conjugation length of DSB molecules can be systematically tuned by selecting different bromobenzaldehyde substrates. In this work, three novel molecules, namely DSB-1, DSB-2 and DSB-3, were successfully designed and synthesized.

2.1. Synthesis of precursor: 1,4-bis(diethoxyphosphorylmethyl)-2,5-dimethoxybenzene

The synthesis was carried out in a two-step sequence. In the first step, 1,4-dimethoxybenzene (6.35 g) and paraformaldehyde (6.75 g) were charged into a round-bottom flask equipped with a reflux condenser. To this mixture, 50 mL of glacial acetic acid was added as the solvent. The reaction mixture was then heated to reflux at 70 °C under a continuous nitrogen atmosphere to prevent oxidation. Subsequently, 18 mL of 48% aqueous hydrobromic acid was carefully introduced to the system, and the reaction was allowed to proceed under stirring for 5 hours. Upon completion, the reaction mixture was quenched by pouring it into crushed ice water. The resulting precipitate was collected via suction filtration and thoroughly washed sequentially with deionized water and methanol to remove residual acids and solvents, affording the intermediate as a solid.

In the second step, the isolated intermediate was transferred to a reaction vessel and mixed with 30 mL of triethyl phosphite. The mixture was heated to 150 °C and maintained at this temperature for 12 hours to ensure complete conversion. After the reaction time elapsed, the system was cooled to room temperature and quenched with n-hexane to induce precipitation. The crude product was then collected by suction filtration and rinsed extensively with n-hexane to remove any unreacted reagents and byproducts. Finally, the solid was dried under vacuum to yield the desired precursor as a pale yellow powder.

2.2. Synthesis of DSB-1

Into a 250 mL two-necked flask, 1 g 3-bromobenzaldehyde, 102.7 mg copper(I) iodide, 190 mg bis (triphenylphosphine) palladium(II) dichloride and 20 mL triethylamine were charged under nitrogen atmosphere. Afterwards, 0.9 mL phenylacetylene and 30 mL *N,N*-dimethylformamide (DMF) were injected, and the reaction was carried out at 50 °C for 12 h. The reaction was terminated with saturated ammonium chloride solution, and the mixture was extracted with ethyl acetate. The organic phase was washed with deionized water and dried over anhydrous sodium sulfate. After removing the solvent under reduced pressure, the residue was purified by column chromatography (petroleum ether/dichloromethane = 40:1) to obtain 3-(phenylethynyl) benzaldehyde.

Then 0.44 g the as-prepared precursor, 0.52 g 3-(phenylethynyl) benzaldehyde, 0.39 g sodium *tert*-butoxide and 15 mL tetrahydrofuran (THF) were added into a 50 mL flask under nitrogen protection. The mixture was heated at 70 °C for 12 h. The solvent was evaporated under reduced pressure, and the residue was triturated with acetone/water (2:1, v/v). The solid was collected by suction filtration and washed with deionized water, then purified by column chromatography using pure dichloromethane as eluent to yield DSB-1.

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2.3. Synthesis of DSB-2

2g 3,5-dibromobenzaldehyde, 457.9 mg tetrakis (triphenylphosphine) palladium(0), 144.3 mg copper(I) iodide and 20 mL triethylamine were placed in a 100 mL two-necked flask under nitrogen protection. 0.9 mL phenylacetylene and 20 mL DMF were added subsequently, and the reaction was maintained at 76 °C for 12 h. The reaction mixture was quenched with saturated ammonium chloride solution and extracted with dichloromethane. The organic layer was washed with deionized water and dried over anhydrous sodium sulfate. Column chromatography (petroleum ether/dichloromethane = 4:1) was performed to obtain 3,5-bis (phenylethynyl) benzaldehyde.

A 50 mL flask was loaded with 0.44 g precursor, 0.77 g 3,5-bis(phenylethynyl) benzaldehyde, 0.39 g sodium *tert*-butoxide and 20 mL THF under nitrogen atmosphere. The mixture was reacted at 70 °C for 12 h. After solvent removal under reduced pressure, the residue was triturated with acetone/water (2:1, v/v). The solid was filtered, washed with deionized water and methanol in sequence, and then purified by column chromatography (petroleum ether/dichloromethane = 2:1) to give DSB-2. ^{1}H NMR ($CDCl_3$): δ 7.69 (d, 4H), 7.63–7.52 (m, 12H), 7.38 (m, 12H), 7.16–7.08 (m, 4H), 3.96 (s, 6H). The results matched well with the theoretical structure.

2.4. Synthesis of DSB-3

Under an inert nitrogen atmosphere to prevent moisture and oxygen interference, a 50 mL round-bottom flask was charged with 0.44 g of the precursor, 0.52 g of 4-(phenylethynyl) benzaldehyde, and 0.39 g of sodium tert-butoxide (NaOtBu) serving as the base. Subsequently, 15 mL of anhydrous tetrahydrofuran (THF) was added to the mixture as the reaction solvent. The resulting suspension was stirred and heated to 70 °C, and the reaction was allowed to proceed for 12 hours to ensure complete conversion. Upon completion, the reaction mixture was cooled to room temperature, and the solvent was carefully removed under reduced pressure using a rotary evaporator. The resulting residue was then subjected to trituration with an acetone/water mixture (2:1, v/v) to facilitate the precipitation of the target compound. The solid was collected via suction filtration and thoroughly washed with deionized water to remove residual inorganic salts and excess base, yielding the crude product.

To achieve high purity, the crude sample was dissolved in a minimal volume of dichloromethane (DCM). Anti-solvent recrystallization was then performed by the dropwise addition of n-hexane until a persistent turbidity was observed, indicating the onset of precipitation. The pure product, DSB-3, was subsequently isolated and further purified through rotary evaporation and recrystallization. The chemical structure of the synthesized DSB-3 was unambiguously confirmed by ^{1}H NMR spectroscopy ($CDCl_3$), which displayed the following characteristic peaks: δ 7.59–7.48 (m, 14H), 7.35 (q, 6H), 7.13 (d, 4H), and 3.94 (s, 6H). The spectral data were in excellent agreement with the anticipated molecular structure, confirming the successful integration of the desired functional groups.

3. Characterization of Trans-Distyrylbenzene Derivatives

Derivatives of 1,4-distyrylbenzene (DSB) have garnered significant attention in the fields of organic photonics and optoelectronics due to their exceptional chemical and photostability, alongside superior optical and electronic properties. These favorable characteristics make them highly promising candidates for a wide range of advanced applications, including organic solid-state lasers, organic light-emitting devices (OLEDs), and highly sensitive fluorescence sensing platforms. In this chapter, we present a comprehensive and systematic investigation into the photophysical performances of three specifically designed DSB derivatives, namely DSB-1, DSB-2, and DSB-3. To elucidate the structure-property relationships and evaluate their potential as optical gain media, their optical behaviors were thoroughly characterized through a series of spectroscopic analyses. Specifically, the study encompasses ultraviolet-visible (UV-Vis) absorption spectroscopy to determine their electronic transition characteristics, steady-state fluorescence emission spectroscopy to assess their radiative properties and emission profiles, and time-resolved fluorescence decay measurements to determine their excited-state lifetimes. Furthermore, the amplified spontaneous emission (ASE) properties of these derivatives were systematically evaluated under optical pumping to determine their lasing thresholds and optical gain capabilities, thereby providing critical insights into their suitability for next-generation organic laser applications.

ISSN 2616-5880 Vol. 7, Issue 1: 115-120, DOI: 10.25236/AJMC.2026.070116

3.1. Reagents

The three DSB derivatives, toluene, acetonitrile, tetrahydrofuran, chloroform, and dichloromethane were all purchased from Beijing Innochem Technology Co., Ltd.

3.2. Instruments

The photophysical properties of the synthesized compounds were systematically investigated using a series of advanced spectroscopic instruments. Ground-state absorption spectra were recorded on a HITACHI U-3900 UV-Vis spectrophotometer. Steady-state and transient fluorescence measurements were conducted using a HITACHI F-7000 fluorescence spectrophotometer and an Edinburgh Instruments FLS920 steady-state and transient fluorescence spectrometer, respectively. Furthermore, amplified spontaneous emission (ASE) properties were evaluated utilizing a custom-built optical setup, which was pumped by a 400 nm femtosecond laser source to provide high-intensity excitation.

To thoroughly explore the solvatochromic effects and understand the nature of the excited states, the solubility and optical behaviors of all three target compounds were examined across a diverse set of solvents with varying polarities. It was found that all three compounds exhibit excellent solubility in toluene, acetonitrile, tetrahydrofuran (THF), chloroform, and dichloromethane (DCM). Consequently, their UV-Vis absorption and fluorescence emission spectra were meticulously measured in each of these five solvents. By comparing the spectral shifts in different solvent environments, the solvent-dependent photophysical properties and the extent of solvatochromism were comprehensively analyzed.

3.3. Test Results

3.3.1. UV-Vis absorption spectroscopy

UV-Vis absorption spectroscopy was used to test the optical performance of the samples, the results are shown in Table 1. During the test process, trace amounts of samples were dissolved in the five solvents respectively by fixing the concentration with a constant. Then the sample was put into the machine and the scaaning procedure was set to scan the sample to determine the UV spectra of samples. The scanning range is from 300 to 600 nm, with the scanning rate at 1 nm s^{-1}. As shown in **Table 1**, DSB-1 have three typical adsorption peaks at 300 nm, 320 nm and 395 nm. DSB-2 showed major absorption peaks at 305 nm and 395 nm, along with a shoulder peak at 325 nm (Table 1). For DSB-3, prominent absorption bands appeared at 340 nm and 415 nm (Table 1).

The absorption near 300 nm originates from the π→π* transition of the extended conjugated system, such as benzene moieties. The conjugation between two phenyl rings and the central C=C reduces the energy gap and can occupied the molecular orbital and the lowest unoccupied molecular orbital. The peaks at around 320 nm correspond to the primary K-band transitions. The presence of electron-donating groups, such as methoxy or hydroxyl groups, on the benzene rings can stabilize the excited state. The peak at 395 nm of DSB-1 indicates a significantly narrow energy gap is due to an extended conjugation length or the intramolecular charge transfer effect, which driven by the strong substituents. Furthermore, the trans-isomer also allows the phenyl rings to remain coplanar with the central C=C, which can minimize the steric hindrance and maximize the effective conjugation. The planar conformation can lead longer wavenumber and higher molecule absorption.

DSB-2 has a larger conjugated system, which dilutes the electron-donating effect of methoxy groups, thus the intramolecular charge transfer peak at 325 nm weakens into a shoulder peak (Table 1). This characteristic peak is absent in DSB-3 due to its longer molecular long axis. The absorption around 400 nm is assigned to the long-wavelength π→π* transition of rigid conjugated structures, and a slight red shift occurs in DSB-3 owing to its extended molecular skeleton (Table 1). Obvious solvatochromism was only observed for DSB-3 in acetonitrile: the absorption band near 400 nm underwent a blue shift, while the absorbance at 340 nm increased. This phenomenon is attributed to the high polarity of acetonitrile and the extended molecular conformation of DSB-3, which disrupts intermolecular stacking.

3.3.2. Fluorescence emission spectroscopy

To further investigate the photophysical properties of the synthesized compounds, fluorescence emission spectroscopy was also used to characterized samples. Consistent with the UV-Vis absorption studies, the samples were also dissolved in five solvents with varying polaritiesa and then each solutions were excited at a wavelength of 400 nm. As summarized in Table 1, all three derivatives display strong fluorescence emission with insignificant solvatochromic effects (Table 1). The fluorescence emission

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spectra show a mirror-image relationship with their corresponding UV-Vis absorption spectra. The spectra feature is characteristic of systems where the vibrational structures of the ground and the excited states are similar, conforming to the principle for vibration-coupled electronically resolved spectra.

3.3.3. Fluorescence lifetime measurement

The microcrystalline samples of the synthesized derivatives were successfully prepared via a solvent evaporation method. To investigate their photophysical properties in the solid state, the fluorescence lifetimes were systematically evaluated using the time-correlated single-photon counting technique, which is renowned for its high temporal resolution and accuracy. As shown in Table 1, the decay curves were well-fitted, revealing that DSB-1 and DSB-2 possess fluorescence lifetimes of approximately 1.575 ns, 1.573 ns, suggesting that minor structural modifications between these two derivatives have negligible effects on their excited-state relaxation processes. In contrast, DSB-3 exhibited a noticeably shorter lifetime of 1.073 ns (Table 1). All three derivatives exhibit relatively long fluorescence lifetimes on the nanosecond scale. This prolonged excited-state lifetime is highly advantageous, as it provides sufficient time for radiative transitions to compete effectively with non-radiative decay pathways, thereby indicating their promising potential for optoelectronic applications.

3.3.4. Amplified spontaneous emission (ASE) measurement

The powder microcrystalline samples of the three compounds were optically pumped using a 400 nm femtosecond laser. The evolution of their emission spectra was systematically recorded across a range of pump energy densities. Remarkably, all three compounds exhibited amplified spontaneous emission (ASE) bands (Table 1) characterized by exceptionally narrow full widths at half maximum (FWHM). This pronounced spectral narrowing serves as a definitive indicator of excellent laser monochromaticity and high optical gain within the microcrystalline medium (Table 1). Furthermore, the observation of low ASE thresholds across all samples demonstrates that the lasing action can be readily achieved under moderate excitation conditions, highlighting their promising potential for low-threshold laser applications.

The three DSB derivatives display characteristic UV-Vis absorption peaks in the 300–500 nm spectral range, indicating strong light-harvesting capabilities. Beyond their optical absorption, these compounds possess favorable fluorescence emission properties and notably long fluorescence lifetimes, which are crucial for efficient radiative transitions. Furthermore, they demonstrate outstanding laser performances, making them highly promising candidates for advanced photonic and optoelectronic applications.

Table 1. Optical characteristic parameters of DSB derivatives

Characterization	DSB-1	DSB-2	DSB-3
UV-Vis absorption	300 nm, 320 nm, 395 nm	305 nm, 395 nm, 325 nm (shoulder peak)	340 nm, 415 nm
Fluorescence emission	Exhibits strong fluorescence emission with insignificant solvatochromic effect.	Exhibits strong fluorescence emission with insignificant solvatochromic effect.	Exhibits strong fluorescence emission with insignificant solvatochromic effect.
Fluorescence lifetime	τ_1 = 1.575335 ns	τ_1 = 1.573308 ns	τ_1 = 1.073308 ns
Amplified spontaneous emission (ASE)	Narrow ASE full width at half maximum (FWHM) and low threshold.	Narrow ASE full width at half maximum (FWHM) and low threshold.	Narrow ASE full width at half maximum (FWHM) and low threshold.

4. Conclusions and Perspectives

In this work, a systematic investigation on the synthesis and photophysical properties of trans-distyrylbenzene (DSB) derivatives was carried out. Three phenylethynyl-modified DSB derivatives (DSB-1, DSB-2, and DSB-3) with distinct conjugated architectures were successfully synthesized via a combined Sonogashira coupling and Horner-Wadsworth-Emmons (HWE) synthetic strategy. This protocol features mild reaction conditions and high stereoselectivity, and the chemical structures of all target compounds were unambiguously verified by H NMR spectroscopy. Based on comprehensive spectroscopic measurements and amplified spontaneous emission (ASE) characterization, the photophysical behaviors and structure–property relationships of the DSB derivatives were elucidated. The extension of the molecular conjugated skeleton effectively induces bathochromic shifts in absorption and emission spectra. Benefiting from its enhanced conjugation degree and elongated molecular

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backbone, DSB-3 exhibits prominent solvatochromic effects in polar solvents, demonstrating that molecular configuration plays a dominant role in modulating the optical performances of DSB-based materials. This study establishes an efficient synthetic route for structurally tailored DSB derivatives and clarifies their fundamental photophysical characteristics, which verifies the great potential of such compounds as promising gain media for organic lasers. Future research will focus on molecular structure optimization, device fabrication improvement, and functional group modification to further enhance their laser performances and broaden their applications in optoelectronic devices, fluorescence sensing, and bioimaging. This work provides credible experimental support and theoretical guidance for the rational design and practical development of high-performance DSB-based organic laser materials.

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