

Pressure-induced remarkable luminescence-changing behaviours of 9, 10-distyrylanthracene and its derivatives with distinct substituents

Aisen Li^{a,b}, Yingjie Liu^a, Lu Han^b, Shuping Xu^a, Chongping Song^a, Yijia Geng^a, Lingyun Pan^b, Bin Xu^a, Wenjing Tian^a, Houyu Zhang^a, Weiqing Xu^{a,*}, Haining Cui^{b,**}

^a Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, 130012, PR China

^b College of Physics, Jilin University, Changchun, 130012, PR China

ARTICLE INFO

Keywords:

High pressure
Piezochromism
Fluorescent spectra
Raman
Reversibility

ABSTRACT

Piezochromic luminescence behaviours of 9, 10-distyrylanthracene (DSA) derivatives with different substituents based on their single crystal structures were investigated under hydrostatic pressure via a diamond anvil cell (DAC), compared with the anisotropic force produced from grinding. Upon grinding, three single crystals show identifiable blue-shifts in fluorescent spectra because of the disturbance for ordered crystal structure to amorphous state, but nearly sightless color changes. The high-pressure fluorescent experiments applied by DAC reveal three DSA crystals all show large red-shifts. High pressure absorption spectra display that a new charge transfer state appears when $-CH_3$ or $-2CN$ is introduced to DSA and all of them show obvious red-shifts. Once the pressure was relieved gradually to the ambient pressure, the fluorescence and absorption spectra both entirely recovered, indicating this geometric change is reversible in a certain pressure region, which is further confirmed by Raman spectra. The relationships between molecular structures and spectroscopic behaviours were further discussed by their single crystal data. This work provides deep insights into the relationship between molecular structure and photo-physical properties of practical mechanochromic luminescent materials, and is significant in the potential applications of pressure transducers.

1. Introduction

The altering fluorescence of the π -conjugated organic molecules have attracted considerable interests because of their potential applications as active components for optical and electronic devices such as organic light-emitting diodes (OLEDs) [1–3]. So far, the preparations of various and switchable organic solid materials that exhibit dynamic fluorescence responses upon external stimuli (e.g. acid-base, solvent polarity, heating, and pressure, etc.) have obtained considerable attention [4–7]. Among them, pressure is one of the most common natural external stimuli. There are many mechanochromic materials reported, which display obvious color-changing upon grinding [8–10] or using nanoindentation technique [11–14]. Different from the pressure produced by grinding and nanoindentation that is nonhydrostatic, limited and uncontrollable, the DAC device gives the hydrostatic force, which can be used to further study on how the intermolecular interaction changed with the pressure. In general, the optical properties of piezochromic materials, which can be used for pressure-sensing and optical-recording systems [15,16], are strongly influenced by their

intramolecular configurations and staking modes along with the hydrostatic pressure [17–19], or the modulation of charge transfer (CT) [20–25]. Besides, the supramolecular interactions between molecules including C-H/ π and C-H/N(O) can also induce the molecules becoming rigid and restrict the intramolecular motions to maintain molecular conformations [26,27]. Thus, tuning the intermolecular packing and intramolecular configuration could availably alter the optical properties of piezochromic materials. In 2012, Tian and Zou's group reported that 9,10-bis((E)-2-(pyrid-2-yl)vinyl)anthracene (BP2VA) showed color-changing via the variation of aggregation states [19]. And Yang's group prepared a highly efficient electrofluorescent material 4-(2-(4-(diphenylamino)-[1,1-biphenyl]-4-yl)-1Hphenanthro[9,10-d]imidazol-1-yl)benzotrile (TBPMCN), which achieved the change of excited state property from a CT-dominated state to a hybridized locally excited and charge-transfer state resulting from the rehybridization of nitrogen atom with increasing external pressure [26]. Although a large number of piezochromic materials have been reported in the past years to reveal the variable optical properties and unique piezochromic mechanisms accompanied by simultaneous changes in molecular arrangements and

* Corresponding author.

** Corresponding author.

E-mail addresses: xuwq@jlu.edu.cn (W. Xu), cuihn@jlu.edu.cn (H. Cui).

<https://doi.org/10.1016/j.dyepig.2018.09.041>

Received 21 August 2018; Received in revised form 18 September 2018; Accepted 18 September 2018

Available online 19 September 2018

0143-7208/ © 2018 Elsevier Ltd. All rights reserved.

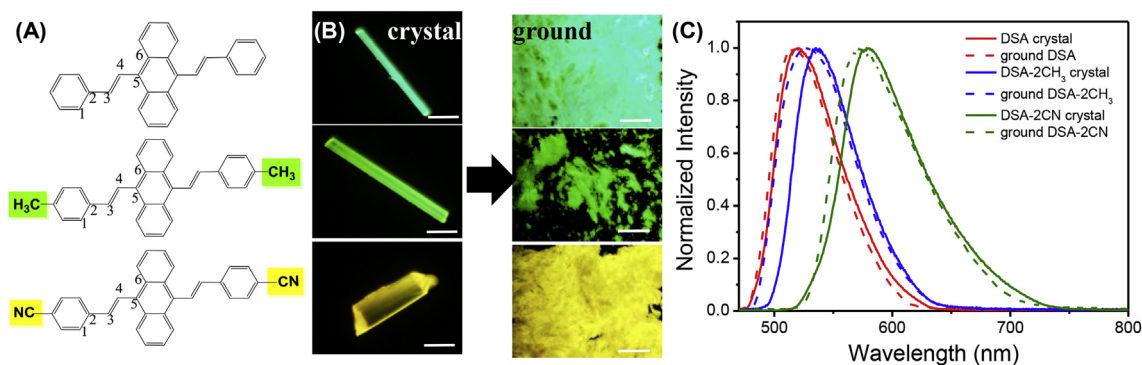


Fig. 1. (A) Molecular structures of DSA, DSA-2CH₃, DSA-2CN, respectively. (B) Corresponding photographs of single crystals and ground powders of DSA, DSA-2CH₃, DSA-2CN under the illumination of 365 nm light. (C) Fluorescent spectra of these three DSA derivatives before and after grinding. The scale of photos is 100 μ m.

configurations [16–27], it is still inadequate to accurately explain the relationship between the photo-physical properties and their corresponding changes in molecular assemblies or packing modes owing to the absence of an effective mechanism. It is well-known that the photophysical processes of a given molecular system would show significant variation according to the molecular aggregation states or conformations by means of altering intermolecular interactions [19]. Therefore, investigations on how to control the molecular stacking modes and the consequent intermolecular interactions are still of importance for further developing novel piezochromic materials.

9,10-Distyrylanthracene (DSA) and its derivatives were firstly synthesized by Shuzo Akiyama and Walter Fabian in 1991, and their absorption and luminescence properties were studied systematically [28]. Since then, DSA derivatives have attracted the wide attentions of researchers and the investigations are further carried out. So they become star molecules because of their simple molecular structure, convenient synthesis steps, excellent optical and electrical properties. Herein, we studied three DSA derivatives for the investigations of high-pressure fluorescence, UV-Vis and Raman spectroscopies connected with a diamond anvil cell (DAC), and compared with the results upon grinding. Our study is of significance in the control of the photoluminescence features *via* molecular structures. This force-sensing switching property makes this material useful in many applicable fields, e.g. sensing and data storage devices.

2. Experimental section

2.1. Materials

9,10-Distyrylanthracene (DSA), methyl-substituted 9,10-distyrylanthracene (DSA-2CH₃), cyano-substituted 9,10-distyrylanthracene (DSA-2CN) were obtained from Prof. Wenjing Tian's group and their single crystals were developed from appropriate solvents of dichloromethane solutions.

2.2. Materials characterizations

The results of single-crystal X-ray were recorded on a Japan Science R-Axis RAPID X-ray single crystal diffractometer. And the fine structures were solved via SHELXS-97 and refined on F². Subsequently, the stacking structures of DSA derivatives were analysed by diamond software. High-pressure fluorescent, UV-Vis and Raman experiments at room temperature were performed on a small piece of DSA derivatives loaded into a T301 stainless steel gasket ($d = 5.00$ mm) with the thickness of 0.25 mm, which was drilled to make a hole with a diameter of 0.2 mm as the sample chamber. Silicone oil was added as a pressure-transmitting medium (PTM) for obtaining the hydrostatic pressure according to the Pascal's principle [29,30], and the pressure was calibrated according to monitoring the fluorescent band shift of the ruby

R1 line [31,32]. The measurement of the ruby chip were performed on a triplemate Jobin Yvon spectrometer (T64000) equipped with a CCD system and excited with a 514.5 nm line of an Argon ion laser working at 7 mW. The high-pressure fluorescent spectra and photos under nonhydrostatic and hydrostatic conditions were received by a fluorescent microscope (IX71, Olympus 20 \times , numerical aperture = 0.4) equipped with a spectrometer (Horiba JobinYvon iHR320), and the radiation illuminant of which was a mercury lamp with an excitation wavelength of 365 nm [33]. High-pressure UV-Vis absorption spectra were attained through an optical fibre spectrometer (Ocean Optics, QE65 Pro) with a deuterium-halogen light source. The high-pressure Raman spectra under hydrostatic conditions were acquired using a confocal Raman system (LabRAM Aramis, Horiba Jobin Yvon) equipped with an excitation source laser of 785 nm with power of 25 mW. The laser was directed into the microscope and focused on the sample by a 50 \times /0.75 NA objective with an integration time of 10 s.

2.3. Computational methods

Geometries of the 9,10-Distyrylanthracene (DSA), methyl-substituted 9,10-distyrylanthracene (DSA-2CH₃), cyano-substituted 9,10-distyrylanthracene (DSA-2CN) crystal were optimized via Becke's LYP (B3LYP) exchange-correlation functional with 6-31G (d, p) basis set based on density functional theory (DFT) [34,35]. All the calculations were performed with the Gaussian 09 package.

3. Results and discussion

3.1. Phase transformation of DSA, DSA-2CH₃ and DSA-2CN induced by grinding

Fig. 1A shows the chemical molecular structures of DSA, methyl-substituted 9,10-distyrylanthracene (DSA-2CH₃) and cyano-substituted 9,10-distyrylanthracene (DSA-2CN) [36–39]. The DSA derivatives own twisted molecular configurations and can form single crystals with high quality and high fluorescence efficiency, which have potential applications of optoelectronic devices and fluorescent sensors. The fluorescent photos and corresponding emission spectra of three compounds are shown in Fig. 1B and C. The fluorescent spectra of DSA, DSA-2CH₃ and DSA-2CN exhibit identifiable peaks at 512, 528 and 570 nm, respectively, indicating the molecular constitution-adjusted photophysical properties. Once these crystals were ground, different degrees of blue-shifts in fluorescent spectra were respectively observed (dashed curves in Fig. 1C, 2, 7 and 5 nm shifts for red, blue and green ones), due to the destruction of long-term ordered crystal structures [40,41]. Moreover, their remarkable differences in intramolecular conformations are summarized in Table 1 and the dihedral angle $\theta(1,2,3,4)$, $\theta(2,3,4,5)$ and $\theta(3,4,5,6)$ (marked in Fig. 1A) were compared in detail. $\theta(1,2,3,4)$ represents the twist degree between phenyl (Ph) and vinyl

Download English Version:

<https://daneshyari.com/en/article/11024388>

Download Persian Version:

<https://daneshyari.com/article/11024388>

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