



Experimental and theoretical study of photo- and electroluminescence of divinyldiphenyl and divinylphenanthrene derivatives

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ABSTRACT

Electronic absorption and luminescence spectra of four new compounds of divinyldiphenyl and divinylphenanthrene derivatives are investigated experimentally in tetrahydrofuran solutions and thin films obtained by thermal vacuum deposition and by spin coating of these substances embedded into polyvinylcarbazole matrix. Molecular geometry optimizations and electronic spectra have been calculated in the framework of XMC-QDPT2/6-31G (d, p) and TDDFT/B3LYP/6-31G (d, p) levels of theory. We have fabricated and studied OLED devices with the structure ITO/PEDOT:PSS/NPD/L/Ca/Al and ITO/PEDOT:PSS/PVK + L/Ca, where L is the luminophore. It is demonstrated that the photo- and electroluminescence spectra of divinyldiphenyl are not identical and undergo strong changes depending on the method of sample preparation.

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1. Introduction

Since the publication of the material on the first light-emitting diode based on 8-hydroxyquinoline aluminum (Alq₃) [1], organic luminophores have been studied intensively for their application as a material emitting light in OLED devices under the action of applied voltage. One of the tasks of OLED application is fabrication of white-color displays and lighting devices [2] for which a mixture of blue, green, and red colors is required. For green and red spectral ranges, effective and stable compounds are now available [3]. The blue range remains the problem even at present [4]. Organic luminophores emitting in this range are either inefficient or unstable [5]. In this regard, interest in investigation of organic luminophores emitting in the blue and blue-green spectral ranges is high.

Earlier our group investigated a series of molecules with linear configuration belonging to the class of divinyldiphenyl thiophene sulfones and detected strong blue electroluminescence of one of them [6]. It was also noted that the compounds of this class are prone to aggregation in amorphous films [6–9]. Indeed, luminophores in OLED devices are in the solid state phase formed either by thermal vacuum deposition or by incorporation into a current-conducting polymer, for example, polyvinylcarbazole (PVK). For close packing of molecules, strong intermolecular interactions are possible both between the molecules of the

luminophore itself and molecules of different species at the boundaries of the OLED layers. In these cases, the emission spectrum of the OLED luminophore can differ significantly from the photoluminescence spectrum unperturbed by intermolecular interaction. Emitted radiation can belong either to a dimer or to higher-order aggregate formed in the ground state, to excimer formed in electronically excited state by two the same molecules, to exciplex of different species in electronically excited state, or by emission of different species simultaneously. The spectral discrepancy of the electroluminescence and photoluminescence was described in a number of works [10–20].

In the present work, the results of experimental and quantum-chemical study of the spectral properties of four recently synthesized linear compounds – divinyldiphenyl and divinylphenanthrene derivatives are presented. The luminescence is studied under photo- and electrical excitation in tetrahydrofuran (THF) solutions, polyvinylcarbazole (PVK) films, and films prepared by thermal vacuum deposition (TVD). Quantum-chemical modeling is carried out using ab initio and density functional levels of theory.

2. Experimental and computational details

2.1. Experimental

The compounds under study were synthesized and purified at the Institute of New Materials Chemistry of the National Academy of

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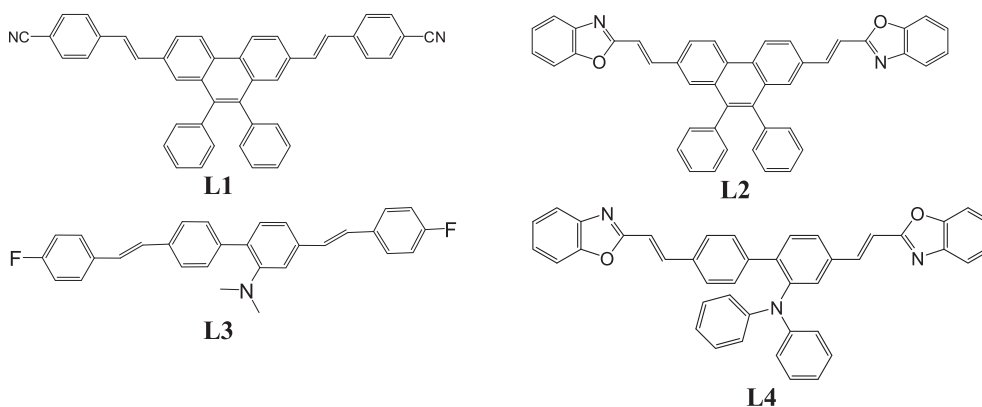


Fig. 1. The chemical structures of L1, L2, L3 and L4 compounds.

Sciences of Belarus. The chemical structures of investigated compounds are shown in Fig. 1. The vinyl units present in all compounds. They connect phenanthrene moiety for L1, L2 compounds and diphenyl moiety for L3 and L4 with the benzonitrile for L1, benzoxazole for L2, L4 and fluorobenzene for L3.

The absorption and fluorescence spectra of compounds in THF solutions, PVK films, and films prepared by the TVD method on a glass substrate were investigated using a CM2203 fluorometer (“SOLAR,” Belarus) and a Carry Eclipse spectrofluorometer (“Varian”).

The fluorescence quantum yield of the compounds in solutions was determined by means of a comparison with the etalon [21]. Coumarin102 ethanol solution with a known quantum yield equals to 0.95 was used as an etalon [22]. The polymer-based films were prepared by the spin coating method from a PVK solution in THF with addition of luminophore with initial concentration of 10^{-3} M. The films thickness was ~100 nm. The TVD films were prepared in an AUTO-306 vacuum evaporator.

Samples of two types: ITO/PEDOT:PSS/NPD/L/Ca/Al (structure I) and ITO/PEDOT:PSS/PVK + L/Ca/Al (structure II) were prepared to study the electroluminescent properties. Here L is the luminophore. ITO denotes indium and tin oxide deposited on the glass substrate that served as an anode in these sandwich-structures. PEDOT:PSS (AI 4083 HeraeusClevios) denotes 2.8 mass% aqueous solution of poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (Aldrich) deposited on ITO by the spin coating method with a velocity of 4000 rpm during

30 s and dried at a temperature of 120 °C. This substance was used both to smooth the anode surface and to emit holes. Films prepared from PVK solutions were deposited with a velocity of 2000 rpm and dried at a temperature of 80 °C. The thicknesses of the PEDOT:PSS films and of the radiating layer were 30 and 40 nm, respectively. NPD – N4,N4’-di(naphthalen-1-yl)-N4,N4’-diphenylbiphenyl-4,4’-diamine – was deposited by the TVD method. The layer thickness was 30–40 nm. This compound in sandwich-structures was used to transport holes. Ca protected from oxidation by the Al layer served as a cathode. Ca and Al were also deposited by the TVD method.

The substrates with ITO were carefully washed before the deposition of layers in an aqueous ammonia solution with subsequent ultrasonic washing in acetone and isopropyl alcohol. In the final stage, the substrates were treated by oxygen plasma using an ATTO installation (Diener, Germany). All subsequent operations were performed in a DELLIX glove box (China) in a dry nitrogen atmosphere with water and oxygen contents on levels of several ppm units.

The rates of deposition of the organic layers were 0.2 Å/s; those of the cathodes were 2 Å/s for vacuum of 10^{-5} mbar in the working volume. Film thicknesses in the process of deposition were controlled using a quartz gauge and measured on control substrates using a KLA TENCOR Micro Xam-100 profilometer.

Electroluminescence characteristics were measured using the setup comprising a source – KEITHLEY237 high voltage unit – and an AvaSpec 2048 fiber optic spectrometer. The volt-ampere and volt-brightness

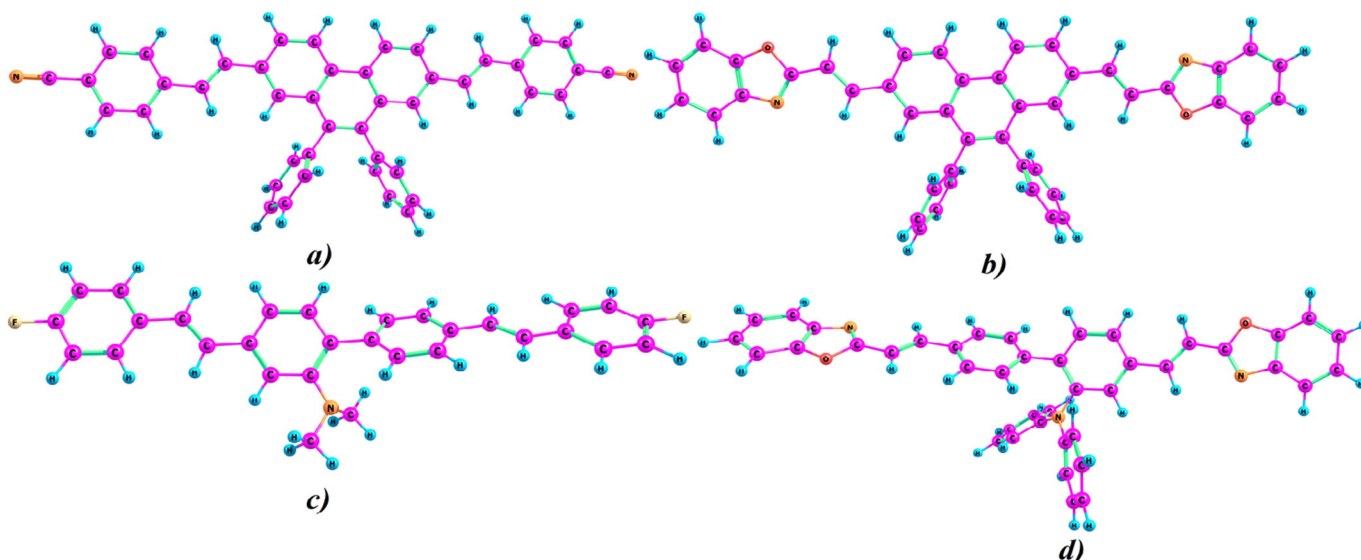


Fig. 2. Equilibrium geometries of the S_0 state of a) L1, b) L2, c) L3, and d) L4 molecules.

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