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# Novel dipyrazolopyridine derivatives as deep blue emitters for polymer based organic light emitting diodes

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#### ABSTRACT

Paper reports synthesis and spectroscopic properties of four newly synthesized dipyrazolo[3,4-*b*; 3',4'*e*]pyridine (DPP) derivatives. The spectroscopic studies are supplemented by quantum-chemical calculations using DFT/TDDFT/PCM method at the B3LYP/6-31+G(d,p) level of theory. The optical absorption and fluorescence emission processes appear to be weakly dependent on attached side phenyl and/or methyl groups exhibiting in cyclohexane solution the first absorption band (00' transition) in the region of 386– 401 nm and the fluorescence band (0'0 transition) in the range of 412–425 nm. The electroluminescence devices (OLEDs) with an active PVK layer doped by DPP dyes have been designed. All the devices exhibit deep blue electroluminescence with the emission maximum being rather weakly dependent on the type of the fluorescent dopant. The obtained results demonstrate that a series of newly synthesized DPP dyes may be considered as perspective blue fluorescent emitters for electroluminescent applications.

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SPECTROCHIMICA ACTA

## Introduction

Heterocyclic dyes have attracted a considerable interest in the past decade due to a number of optoelectronic applications among which organic light emitting diodes and electroluminescent displays (OLEDs) may be considered as dominant. Relevant technologies have already been transferred from laboratories to the industry [1,2] and due to obvious advantages OLEDs over the traditional LCD/LED displays they are expected to become competitive on the world markets in nearest perspective. Despite spectacular commercial success of OLEDs, there is still an aspiration to improve their electroluminescent characteristics such as quantum efficiency, color purity and stability as being required by full-color display technology [1,3,4]. A key element in OLED structure is a dye doped polymer layer. Among variety of potentially suitable fluorescent molecules, a special attention were paid to pyrazologinoline (PQ) dyes. The core molecule was synthesized long time ago and since then a lot of its derivatives have been studied in different applications [5]. At the beginning of the last decade due to remarkable fluorescence found for a number of PQ derivatives [6] these heterocyclic organic dyes have been successfully employed in many OLED structures [7,8]. However, their crystallization inside the active layer decreased significantly the efficiency and lifetime

of the fabricated devices. This drawback was eliminated by further modifications of PQ derivatives [9–11]. Relevant molecules incorporated in OLED architecture featured in efficient electroluminescence, preferably in blue, blue-green or green spectral regions [12–15].

In the current work we further developed the concept started in PQs and proposed four new dipyrazolopyridine (DPP) chromophores. Several other DPP derivatives have been originally synthesized by Danel and coworkers [16]. The core of newly synthesized dyes represents dipyrazolo[3,4-*b*; 3',4'-*e*]pyridine molecule consisting of pyridine substituted with two pyrazole rings on both sides opposite to the hetereoatom as shown in the scheme below.

The structures of that type should provide a better and more symmetrical charge distribution than in the case of PQs. Moreover, a rule-of-thumb, established during developing the PQ chromophores, predicts that the presence of aryl moieties attached to PQ rings prevents the molecule from unwanted crystallization. This concept is also applied here to DPP derivatives. As one may see in the scheme above, the studied molecules, abbreviated as DPP1 through DPP4, were built up of DPP core surrounded by aryl and/ or methyl ligands in different geometries. Particular arrangement of aryl and methyl groups attached to pyrazole does not vary significantly the molecule's overall dipole moment [17], which remains rather small, ranging from c.a. 2.0 to 2.5 D. We expected, that this property would enable solubility of DPP derivatives in

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the case of less polar solvents, what would be a benefit from practical point of view.

In this brief report we give the optical spectroscopy characterization of DPP dyes and demonstrate their applicability in polymer based electroluminescent devices as dopant emitters in deep blue region of the visible spectra. The optical absorption, fluorescence and electroluminescence spectra are supplemented by the quantum-chemical analysis based on DFT/TDDFT/PCM calculations.

#### Synthesis

# 4-tert-Butylphenyl-3,5-dimethyl-1,7-diphenyl-bis-pyrazolo[3,4-b; 3',4'-e]pyridine (DPP1)

A mixture of 5-amino-3-methyl-1-phenylpyrazole (3.4 g; 0.02 mol), *p-tert*-butylbenzaldehyde (1.62 g; 0.01 mol) and 10 ml of sulfolane were heated together in a round bottomed flask (50 ml) equipped with air condenser at 140–150 °C for 45 min and at 240–250 °C for 2 h. After cooling the reaction mixture was diluted with ethanol (25 ml) and the precipitate was filtered off. The compound was purified on column packed with silica gel (Merck 60, 70–230 mesh) using toluene as eluent. White crystals, 42%, mp. 231–2 °C (toluene). Anal. calcd. for:  $C_{31}H_{29}N_5$ : C 78.95; H 6.20%; N 14.85%. Found: C 78.65; H 6.01; N 14.82%. <sup>1</sup>H NMR(CDCl<sub>3</sub>,  $\delta$  ppm): 8.40(d, *J* = 8.1 Hz, 4 H); 7.50(m, 4 H); 7.33(s, 4 H); 7.20(m, 2 H); 2.05(s, 6 H); 1.33(s, 9 H).

### 5-Methyl-1,3,7-triphenyl-bis-pyrazolo[3,4-b; 3',4'-e]pyridine (DPP2)

Equimolar amounts (0.01 mol) of 5-methyl-2-phenylpyrazol-3amine and 5-chloro-1,3-diphenyl-pyrazole-4-carbaldehyde were heated together at 140–180 °C for 60 min. After cooling the reaction mixture was digested with ethanol (25 mL), boiled and filtered. The precipitate was purified on column packed with silica gel (Merck 60, 70–230 mesh) using toluene as eluent. Light yellow crystals, 33%, mp. 215–216 °C (toluene). Anal. calcd. for: C<sub>26</sub>H<sub>19</sub>N<sub>5</sub>: C 77.79; H 4.77; N 17.44. Found C 77.47; H 5.03; N 17.51. <sup>1</sup>H NMR(CDCl<sub>3</sub>,  $\delta$  ppm): 2.72(s, 3 H, Me); 7.26–7.36(m, 2 H); 7.48– 7.62(m, 6 H); 8.08(d, 2 H, *J* = 6.9 Hz); 8.40(d, 2 H, *J* = 6.9 Hz); 8.40(d, 2 H, *J* = 7.6 Hz); 8.50(d, 2 H, *J* = 7.6 Hz); 8.61(s, 1 H).

## 1,3,4,5,7-Pentaphenyl-bis-pyrazolo[3,4-b; 3',4'-e]pyridine (DPP3)

Light yellow crystals, 23%, mp. 284–286 °C (toluene). Anal. calcd. for:  $C_{37}H_{25}N_5$ : C 82.35; H 4.67; N 12.98. Found C 82.41; H 4.54; N 13.06. <sup>1</sup>H NMR(DMSO- $d_6$ ,  $\delta$  ppm): 6.79–6.89(m, 4 H); 6.99–7.18(m, 11 H); 7.32–7.37(m, 2 H), 7.55–7.61(m, 4 H); 8.52–8.59(m, 4 H).

### 1,7-Dimethyl-3,5-diphenyl-bis-pyrazolo[3,4-b; 3',4'-e]pyridine (PP4)

Yellow powder, 31%, 143 °C (toluene). Anal. calcd. for C<sub>21</sub>H<sub>17</sub>N<sub>5</sub>: C 74.32; H 5.05; N 20.63. Found 74.36; H 5.14; N 20.72. <sup>1</sup>H NMR(CDCl<sub>3</sub>,  $\delta$  ppm): 4.21(s, 6 H, N-Me); 7.42–7.57(m, 6 H); 7.96(d, 4 H, *J* = 6.9 Hz); 8.83 (1 H).

### **Results and discussion**

The optical absorption and fluorescence spectra were measured using spectrophotometer Oriel MS125 equipped with CCD array. The measurements were performed by means of a standard 1 cm path length quartz cuvette for absorption spectrometry. Fig. 1 shows the steady state optical absorbance and normalized fluorescence spectra of DPP dyes being recorded in cyclohexane (CHX) solution (mass concentration of about 0.1%). The low-energy part



**Fig. 1.** Steady state optical absorbance (blue color) and normalized fluorescence (green color) spectra of DPP dyes: (a) DPP1; (b) DPP2; (c) DPP3; (d) DPP4. Vertical broken bars correspond to spectral positions of 00' vibronic band (optical absorption, blue online color) and 0'0 vibronic band (fluorescence emission, green online color) being determined from the measured spectra by second derivative method. Solid vertical bars (red color) are the excitation spectra calculated by TDDFT/PCM method (CHX solution) with B3LYP *xc*-potential. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

of the optical absorption spectra is characterized by two partially superimposed bands being at room temperature practically unstructured due to strongly overlapped broad vibronic bands. The first absorption maximum only weakly depends on the position of side methyl and/or phenyl groups and is centered for the studied DPP dyes in the spectral region of 370-385 nm. Similar comment may be addressed also to the absorption threshold position which in these dyes is slightly different depending on the positions of the attached radicals, namely it corresponds to the excitation energies in the range of 2.95-3.06 eV. The first absorption band exhibits smooth shape thus the position of its 00' vibronic band, associated particularly with the HOMO  $\rightarrow$  LUMO transition, cannot be precisely determined from the measured absorption spectra. Its rough evaluation, applying the second derivative method, gives the HOMO-LUMO gap for the excitation processes in the range 3.09-3.21 eV (386-401 nm). Relevant spectral positions corresponding to 00' vibronic band are listed in Table 1 and marked by blue dash vertical bars for each particular dye in Fig. 1.

In the following we compare the measured optical absorption spectra with the excitation spectra evaluated by DFT/TDDFT method at B3LYP/6-31+G(d,p) level of theory. The calculations have been carried out within the quantum chemical package of programs Gaussian-09 [18]. To account the solvation the DFT/TDDFT methods were combined with polarizable continuum model (PCM) applying the linear-response approach. Fig. 2 shows the equilibrium molecular geometry of DPP dyes optimized by DFT/ PCM method in CHX solution. All the DPP dyes are characterized by the planar symmetry of its dipyrazolopyridine skeleton whereas the phenyl rings take twisted orientation with different torsion angles. The first absorption band is mainly formed by the HOMO– LUMO transition, relevant molecular orbitals (calculated by the program Gabedit, version 2.3.6 [19]) and their energies (see labeled) are shown in Fig. 2. The excitation process is evidently



**Fig. 2.** Equilibrium ground state molecular geometry, HOMO and LUMO orbitals and their energies (see labeled) for DPP dyes as calculated by DFT/PCM method (CHX solution) with B3LYP *xc*-potential. The orbitals have been calculated using the program Gabedit [19]. Red and blue indicate opposite orbital phases. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

accompanied by a certain relocation of the electron density from the electron-donating phenyl group to the electron-accepting dipyrazolopyridine moiety. However, the dipole moments of both ground or excited states are characterized either by moderate (as e.g. for DPP1-DPP3 dyes), or rather small (DPP4 dye) values as one can see in Table 1. This finding suggests that solvatochromic effect on the absorption or emission energies is expected to be not large for DPP molecules. The spectra measured in solvents of different polarity may prove this assumption however relevant investigations appear out of scope of actual study and will be published elsewhere soon. Depending on lateral substituents the DFT calculations give the HOMO energy in the range  $-5.80 \div -5.74$  eV and the LUMO energy in the range  $-2.16 \div -1.93$  eV. Accordingly, the HOMO-LUMO gap of  $3.6 \div 3.8$  eV appears to be somewhat larger comparing to the one determined from the optical absorption spectra (3.1–3.2 eV). It turns to be typical for DFT methods which indeed deal with occupied and virtual molecular orbitals thus electron correlation effects, which accompany the excitation process [20], obviously cannot be accounted there. For this reason its time-dependent counterpart, TDDFT method, which typically mixes several pairs of the ground state molecular orbitals due to correlation effects, usually provides much more accurate evaluation of the excitation energies and is more suitable for comparison with optical spectra. The DPP derivatives are not exception in this respect as one can see from Fig. 1 and Table 1. Here the TDDFT excitation spectra are presented by the vertical solid red bars.

The spectral position of the first absorption band (00'-transition) is predicted in most cases with an excellent accuracy, better than 0.02 eV, and only in the case of DPP4 dye the discrepancy between the experiment and theory is somewhat larger,  $\sim$ 0.09 eV.

The fluorescence emission has been excited by means of mercury lamp at the wavelength  $\lambda_{ex}$  = 365 nm. Relevant spectra were recorded in CHX solution (mass concentration of about 0.1%). The normalized fluorescence spectra for DPP dyes are shown in Fig. 1. Basic features of the fluorescent emission appear to be similar for all the dyes. The asymmetric fluorescent bands are slightly structured due to vibronic coupling and are characterized by the emission maxima in the range 425-435 nm exhibiting thus rather weak changes depending on lateral positions of substituted methyl and/ or phenyl groups. Here again, the spectral positions corresponding to 0'0 electronic transition, as determined by the second derivative method, are marked by green dash vertical bars in Fig. 1 and listed in Table 1. Their comparison with the spectral positions of reverse 00' transitions (blue dash vertical bars) gives the Stokes shift,  $\sim$ 17– 40 nm. Its relatively small magnitude may be an evidence that conformational reorganization of the solute in the excited state (solute relaxation) is indeed weak. Making such conclusion we rely on the solvatochromic Liptay-Mataga equation [21,22] according to which the molecular reorganization (solvent relaxation) in weakly polar solvents, as e.g. CHX, has practically no impact on the Stokes shift.

In order to explore the electroluminescence properties of DPP dyes, relevant molecules were incorporated into the active layer of a simple sandwich-type OLED structure, see insert in Fig. 3. It consists of the glass substrate covered by indium tin oxide (ITO) transparent electrode, 5 nm layer of poly(3,4-ethylene dioxythiophene)-poly-(styrene sulfonate) (PEDOT:PSS), 80 nm of DPP doped (1 wt%) polyvinylcarbazole (PVK) layer, 10 nm of Ca layer and capping 100 nm protective aluminum layer. The active layer was deposited on substrates by spin-coating in argon atmosphere using PVK and DPP dissolved in tetrahydrofurane. Following such route the EL devices of ITO/PEDOT:PSS/PVK:DPP/Ca/Al configuration have been designed. Fig. 3 shows the electroluminescence emission intensity versus the biasing voltage for these OLEDs. Since the devices were not optimized, the turn-on voltage appears to be higher than 12 V. Nevertheless this graph may serve for qualitative analysis to compare the efficiency of the studied dyes. The lowest turn-on voltage and the strongest electroluminescence intensity are observed in the case of DPP2 and DPP3 based devices. The EL emission spectra, shown in Fig. 4, have been recorded at forward-bias voltages of about 18-24 V. All the devices exhibit blue electroluminescence with the emission maximum being rather weakly dependent on the type of the fluorescent dopant. In comparison to the fluorescence spectra, the electroluminescence of PVK:DPP based OLEDs exhibits either nearly the same spectral position of the emission band, as e.g. in the case of DPP1 or DPP4 dyes, or it is red shifted by about 10 or 25 nm for the PVK layer doped by DPP2 or DPP3, respectively. However, in all the cases the electroluminescence is characterized by the emission band

#### Table 1

The spectroscopy characteristics of DPP dyes.  $\lambda_{abs}^{00'}$  is the spectral position of the first absorption band (00' transition);  $\lambda_{fl}^{0'0}$  is the spectral position of the fluorescence 0'0 band;  $\mu_g$  and  $\mu_e$  are the ground and excited state dipole moments for the equilibrium ground state molecular geometry;  $\lambda_{el}^{max}$  is the electroluminescence emission peak position for OLEDs with configuration ITO/PEDOT:PSS/PVK:DPP/Ca/Al (DPP = DPP1-DPP4); X, Y and Z are the color coordinates of DPP emitters according to CIE(1931) standard; exp – experiment; calc – calculated by DFT/TDDFT/PCM method at B3LYP/6-31+G(d,p) level of theory.

Compound	$\lambda_{abs}^{00'}$ (exp)	$\lambda_{fl}^{0'0}$ (exp)	$\lambda_{abs}^{00'}$ (exp)	$\mu_g$ (calc)	$\mu_e$ (calc)	$\lambda_{el}^{max}$ (calc)	CIE(1931) (	CIE(1931) (exp)		
	[nm]	[nm]	[nm]	[D]	[D]	[nm]	X	Y	Ζ	
DPP1	386	425	383.3	4.5	3.4	432	0.1489	0.0832	0.7679	
DPP2	401	424	398.7	2.3	3.3	442	0.1472	0.1057	0.7471	
DPP3	401	417	403.6	2.9	3.6	451	0.1526	0.1214	0.7260	
DPP4	398	412	386.7	0.36	0.43	431	0.1506	0.0922	0.7572	



**Fig. 3.** Luminance-voltage characteristics of the electroluminescence devices with OLED structure ITO/PEDOT:PSS/PVK:DPP/Ca/Al (DPP  $\equiv$  DPP1-DPP4). The insert shows schematically the configuration of OLED.



**Fig. 4.** Electroluminescence spectra of DPP based OLEDs with structure ITO/ PEDOT:PSS/PVK:DPP/Ca/AI: (a) DPP  $\equiv$  DPP1; (b) DPP  $\equiv$  DPP2; (c) DPP  $\equiv$  DPP3; (d) DPP  $\equiv$  DPP4.

being somewhat narrower than the fluorescence one. It means that mutual coupling of dye molecules resulting in excimers formation, which is likely presented in the CHX solution, appears considerably reduced in DPP doped PVK layer due to essential dispersion of guest dye molecules in the host polymer matrix. Based on the electroluminescence spectra (Fig. 4) we give appropriate characterization of the luminance color. Relevant color coordinates, *X*, *Y* and *Z*, determined within the CIE(1931) standard are given in Table 1. Evidently, the designed OLEDs emit light of deep blue color, the most deeper blue emission exhibits DPP1 dye.

# Conclusion

In conclusion we report here the synthesis aspects and spectroscopic properties of four newly synthesized dipyrazolopyridine derivatives. The steady state optical absorption and fluorescence spectra were recorded in CHX solution and compared with the results of quantum-chemical calculations using DFT/TDDFT/PCM method at the B3LYP/6-31+G(d,p) level of theory. The absorption and fluorescence processes appear to be weakly dependent on the position of side methyl radicals exhibiting the first absorption band (00' transition) in the region of 386–401 nm and the fluorescence band (0'0 transition) in the range of 412-425 nm. The quantumchemical analysis based on DFT/TDDFT/PCM with B3LYP xc-potential quite accurately predicts the excitation energies. The absorption-emission cycle is accompanied by relatively small Stokes shift (17–40 nm) what may be an evidence that the solute relaxation in the excited state is indeed weak for all the DPP dyes. We demonstrate also the OLEDs being constructed according to the scheme with the polymer PVK layer doped by DPP fluorescence emitters. All the devices exhibit deep blue electroluminescence with the emission maximum being rather weakly dependent on the type of the fluorescent dopant. Based on the electroluminescence spectra the emission color is characterized by the color coordinates according to the CIE(1931) standard. The obtained results show that a series of newly synthesized DPP dyes may be considered as perspective blue fluorescent emitters for electroluminescent applications.

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