Tayloring of molecular materials for organic electronics

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Received: 25 October 2010 / Received in revised form: 13 August 2011, Accepted: 25 August 2011, Published: 25 October 2011 © Sevas Educational Society 2011

Abstract

An example of targeted modification of chemical structure in order to extent utilisation of diketo–pyrrolo–pyrroles in organic electronics is presented. The introduction of solubilising groups opens solution–based techniques for device preparation and therefore reduces the manufacturing cost. The influence of the substitution on the optical activity is discussed.

Keywords: Organic electronics, diketo-pyrrolo-pyrroles

Introduction

Diketo-pyrrolo-pyrroles (DPPs) comprise one of the promissing classes of materials suitable for organic electronics. Nowadays, the DPPs are mainly used as high performance industrially important pigments. This requires excelent photostability, high absorption coeficients but also low solubility. However, the ability to solubilize these materials would open the possibility to use solution-based techniques (spin-coating, drop-casting, inject printing, etc.) to prepare devices from DPPs. One of the reason for the insolubility is the existence of hydrogen bonds between the -NH group and oxygen. Since the basic DPP core is perfectly planar, a π - π electrons overlap occurs in solid state and also contributes to their insolubility. These interactions can be so strong, that cause colour change between solid and dissolved form and influence also other properties, e.g. fluorescence and Stokes shift (Song et al. 2007). It is therefore clear, that to modify the solubility one has to introduce the N-substituion and/or break the molecule planarity (Potrawa and Langhals 1987). In this contribution, we will discuss the influence of such substitution on the optical properties of the DPPs with respect to the utilization in organic electronics and possibly in bielectronics in future.

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Materials and Methods

All of the studied derivatives (Fig 1) were synthesised by Research institute of organic synthesis (RIOS, a.s.). The samples were dissolved in dimethylsulfoxide (Aldrich).

Results and Discussion

Substitution of an alkyl group on the nitrogen on the DPP core decreases molar absorption coefficient (hypochromic shift) and simultaneously the longer wavelength maximum is shifted towards higher energy region (hypsochromic shift). Furhermore, the vibration structure is less pronounced. As was pointed out in our previous paper reporting different structures (Vala et al. 2008), this is caused by torsion between pyrrolinone central part and phenyl adjacent to the alkyl group and consequently, is caused by loss of molecule planarity which is in turn responsible for loss of effective conjugation. Since the addition of second alkyl rotates also the second phenyl group, this effect is even more pronounced. The loss of vibration structure can be attributed to the increased dipole moment interacting with polar DMSO solvent. The dipole-dipole interaction of bi-substituted derivatives with the completely nonplanar structure is the most pronounced. No dependency on the length of the alkyl used was found.



Figure 1: The studied derivaties of diphenyl-diketopyrrolo- pyrrole

Conclusions

It was found, that the N-alkylation only does not significantly influence the fluorescence quantum yield. On the other hand the Stokes shift is gradually increased going from the monoalkylated to dialkylated derivatives. The observed spectra are characteristic by graduate loss of mirror symmetry of absorption–fluorescence and vibronic structure. The phenyl torsion due to the N-alkylation is the main mechanism for this behaviour in polar DMSO.

Acknowledgement

The work was supported by Grant Agency of the Czech Republic via project No. P205/10/2280.

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