

Summary of doctoral thesis

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“Reactions of coupling, cycloaddition and condensation in the synthesis of new materials for organic electronics”

The research problem undertaken in the doctoral dissertation is the synthesis of new acetylene, benzene, naphthalene and pyridine derivatives and study their electrochemical properties. Comprehensive electrochemical studies, as well as knowledge gained in DFT calculations allow for a detailed discussion of the construction of the resulting compounds and their properties. An important aspect of the research was also verification, whether these compounds could be applied as emission materials in organic light-emitting diode.

The first stage of doctoral thesis was to develop methods of obtaining, purification, and verification the structure of compounds. Scheduled molecules were synthesized by Sonogashira coupling, [4+2] Diels-Alder cycloaddition and condensation reaction. Construction of the synthesized compounds was verified by ^1H , ^{13}C NMR spectroscopy (for selected derivatives: ^1H - ^1H COSY, ^1H - ^{13}C HMQC i ^1H - ^{13}C HMBC), HRMS and elemental analysis. In the case of compounds obtained as solids, the melting points were measured.

In the second stage of doctoral thesis, the synthesized compounds were investigation to electrochemical methods by cyclic voltammetry (CV) and differential pulse voltammetry (DPV). These measurements enabled the determination of potentials of oxidation and reduction. The electrochemical oxidation and reduction potentials were used for estimation of the HOMO, LUMO energies and energy gap. To better understand the results, they were compared with the DFT calculations. Finally, for selected compounds, a detailed research has been carried out for their use in organic light-emitting diode (OLED). The above mentioned studies have allowed us to determine the basic properties of the materials, which determine their practical applications.