

## Abstract

The 21<sup>st</sup> century is a time of vigorous development in various fields of science related to innovative energy harvesting and processing, among which organic electronics deserve special attention. In the era of combating climate change, combined with soaring energy demands, it is undeniably important to search for efficient sources of sustainable energy. However, it should be recognized that only some energy sources are capable of providing very large amounts of power, while others (e.g., organic electronics) serve only as complementary sources. To meet the requirements of science world, synthetic chemists continually offer access to a range of new chemical compounds, exhibiting desirable properties that can serve as functional organic materials. In this context, derivatives of perylene – a polycyclic aromatic hydrocarbon (PAH) consisting of five fused aromatic rings – play an extremely important role. The interesting physicochemical properties of perylene and its derivatives, as well as the possibility of modifying their structure by attaching various motifs to the aromatic core, mean that these compounds can be considered as promising molecular materials, especially in the field of organic electronics. One possible synthesis route for perylene derivatives is the annulative  $\pi$ -extension (APEX) of the aromatic core, through which a new compound, enriched by at least one aromatic ring, can be obtained in one step. An excellent tool in this process is one of the fundamental reactions of organic chemistry – the Diels-Alder cycloaddition (DAC). This work is dedicated to the synthesis of new functionalized nanographenes based on the perylene structure obtained *via* DAC reactions. As part of the conducted research, a series of experiments were carried out aimed at selecting the most favorable conditions for the cycloaddition of various dienophiles, both to perylene and its derivatives. The Diels-Alder cycloaddition reactions to the *bay regions* of perylene diimides are known in the literature. However, when it comes to other perylene derivatives, such as those described in this doctoral thesis, namely perylenetetracarboxylate (PTE) derivatives and aminoperylene derivatives, knowledge about the possibilities of applying DAC to their extension at the *bay* position is limited. Therefore, the work presents the possibilities of extending the core of such perylene derivatives through the annulative  $\pi$ -extension (APEX) reaction, along with an in-depth analysis of the results of quantum chemical calculations. These calculations provided many important informations about the activation energies of the reactions and the structure-property relationships of the newly obtained functionalized nanographenes. The work yielded compounds dedicated to potential applications, such as in the manufacture of devices like OLEDs or solar cells. The new knowledge in the area of chemistry and organic synthesis – including the Diels-Alder cycloaddition to the cavities of perylene and its derivatives, APEX strategies, and the regioselectivity of electrophilic substitution and the cycloaddition itself is also very important.