

NEW POSSIBILITIES OF 3,9-DIAMINOSUBSTITUTED PERYLENES CORE EXTENSION VIA DIELS-ALDER CYCLOADDITION TO BAY REGION

Aneta Kurpanik, Stanisław Krompiec, Marek Matussek

Faculty of Chemistry, Department of Inorganic, Organometallic Chemistry and Catalysis, University of Silesia, ul. Bankowa 12 40-007 Katowice

Perylene and its derivatives has attracted a great deal of interest over last few decades. Due to excellent photophysical properties (high absorption coefficient and high fluorescence quantum yield) of these compounds, they are widely used in the area of organic electronics, mainly as active components in organic light-emitting diodes (OLEDs). Their optical properties could be tuned by functionalizing *peri*, *orto* or *bay* position of perylene with different substituents. Perylene belongs to a group of polycyclic aromatic hydrocarbon molecules with extended π -conjugated system and the application of wide variety of substituents to the *bay* position is highly favorable, because the extension of π -conjugation affects the electroluminescent properties. A few literature reports show that the chemistry of *bay* region of perylene derivatives is not well developed, so far. In view of this, new perylene derivatives with arynes (benzyne, naphthyne), *p*-benzoquinone, acetylenedicarboxylates, maleic anhydride (with further transformation into imide) and one of the most reactive dienophile – 4-phenyl-1,2,4-triazole-3,5-dione attached at the *bay* region of perylene core were synthesized. Moreover, the naphtho[1,2,3,4-*ghi*]perylene reaction conditions have been optimized. A variety of experimental conditions, including temperature, reaction time, solvent, amount of substrates, were tested – the most effective ones have been applied to further reactions using 1-(trimethylsilyl)-2-naphthyl trifluoromethanesulfonate and 3-(trimethylsilyl)-2-naphthyl trifluoromethanesulfonate as dienophiles in [4+2] cycloaddition.

Optical properties of the obtained compounds were characterized by UV-Vis spectroscopy (absorption and emission spectra were recorded). Experimental studies were enriched with quantum mechanical calculations made at the DFT level (the energies of HOMO and LUMO were determined). Moreover, absorption and emission spectra were predicted by TDDFT calculations. All the calculations were carried out using the program package GAUSSIAN09 and the hybrid-correlation B3LYP functional in conjunction with 6-31G(d,p) basis set. Molecular structures have been confirmed by ¹H NMR and ¹³C NMR spectroscopy and mass spectrometry (MS).

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