

Theoretical Insights into the Impact of Pyrrole and Imidazole Substituents on the BODIPY Chromophore

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Streszczenie

This paper concerns the *in silico* studies of the influence of heterocyclic substituents as well as their protonated and deprotonated forms on the spectral characteristics of BODIPY (4,4-difluoro-4-bora-3a,4a-diaza-s-indacene) dyes. Computational studies were carried out in order to reveal the most effective method of modeling of the spectral features of fluorescent BODIPY dyes. To perform these studies, the pyrrole and imidazole derivatives of BODIPY dyes were selected, and their spectral features were investigated with DFT and TD-DFT calculations. The calculations showed that the deprotonation of the substituents leads to a bathochromic shift of the calculated absorption wavelength, while the protonation (imidazole derivative) brings about a hypsochromic shift with respect to the neutral form of the dye. The calculated spectral characteristics, considering the influence of the solvent polarity (PCM model), were correlated with the ENTETN solvatochromic parameter. These correlations show that the increase in the solvent polarity causes a hypsochromic shift of the calculated absorption and emission wavelengths, whereas the bathochromic shift of the wavelengths is observed for the protonated form.

Słowa kluczowe

BODIPY dye, protonation, deprotonation, DFT, TD-DFT

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