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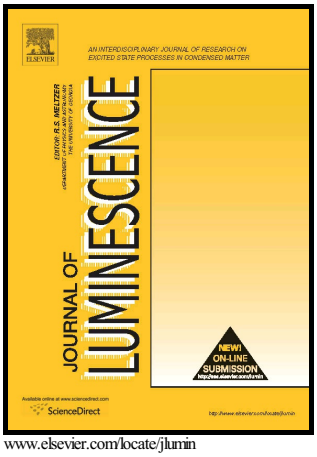

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Influence of the spatial substituents on self organization and spectral properties of diketopyrrolopyrrole derivatives

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Abstract

Two diketopyrrolopyrrole derivatives (DPPs) with spatial substituents (di-*tert*-butylbenzyl groups) and alkyl chains have been synthesized and investigated using DFT and TD-DFT calculations, vibrational (IR and Raman), electronic (absorption, fluorescence) spectroscopies, and electrochemical methods. Moreover, the creation of Langmuir layers was also investigated. The most of spectral investigations show only small differences between the investigated species as well as the electrochemical data. The electronic spectra show a small shift of the Soret and Q bands while the vibrational spectra in comparison with DFT calculation results suggest the presence of additional interactions involving the thiophene rings in one of the samples. The significant difference is observed in the formation of Langmuir layers of the mentioned molecules. The DPPs with spatial substituents form more densely packed layer in comparison with alkyl chain-substituted DPPs. Moreover, substitution with di-*tert*-butylbenzyl groups enhances the fluorescence quantum yields (up to 0.77) and slightly prolonging the fluorescence lifetimes (to over 5 ns). Spectroscopic studies of varied polarity solutions indicates J type aggregation of DPPs.