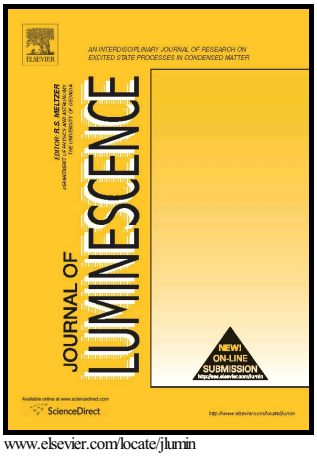

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Photophysics of an unsymmetrical Zn(II) phthalocyanine substituted with terminal alkynyl group

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Abstract

This paper examines photophysical properties of an unsymmetrical zinc phthalocyanine substituted with a terminal alkynyl group. The studies were concentrated on absorption (in the UV-vis-IR range) and fluorescence (steady-state and time resolved) in chloroform of unsymmetrical 9(10),16(17),23(24)-tri-*tert*-butyl-2-(pent-4-yloxy)phthalocyaninato zinc(II) of different concentrations. Moreover, dye photodegradation studies were also done. Besides, a laser-induced optoacoustic spectroscopy was also used to determine thermal deactivation as well as singlet oxygen generation yield. The Langmuir layers of the dye were formed and the *in-situ* absorption technique was applied to follow ability of the dye to aggregate formation. The experimental data were supported by the quantum chemical calculations with the use of the time-dependent density functional theory (TD-DFT) to obtain information on the distribution of electron density and electronic transitions in the molecular systems. The spectroscopic results of the unsymmetrical zinc phthalocyanine were confronted with the data of the symmetric zinc phthalocyanine.

Keywords: UV-vis absorption, *in-situ* light absorption, fluorescence quantum yield, fluorescence quantum lifetime, singlet oxygen generation, quantum chemical calculations

Abbreviations: ZnPc – zinc phthalocyanine, Pc – phthalocyanine, bromocresol purple – BCP, laser induced optoacoustic spectroscopy – LIOAS, time-dependent density functional theory – TD-DFT