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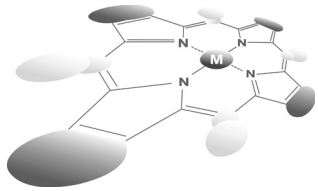

Pyridone substituted phthalocyanines: Photophysicochemical properties and TD-DFT calculations

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This paper is dedicated to Professor Kazuchika Ohta on the occasion of his retirement.

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ABSTRACT: A 4-(6-methyl-3-nitro-2-oxo-1,2-dihydropyridin-4-yloxy)phthalonitrile has been used to prepare a novel Zn(II) phthalocyanines with four peripheral pyridone substituents. The compound has been characterized by UV-visible absorption, FT-IR and ^{1}H-NMR spectroscopy, elemental analysis and MALDI-TOF mass spectroscopy. The fluorescence, triplet quantum and singlet oxygen quantum yields have been determined and TD-DFT calculations have been used to identify trends in the electronic structure.

KEYWORDS: phthalocyanines, pyridones, TD-DFT calculations, singlet oxygen, photophysics.

INTRODUCTION

Phthalocyanines are an important class of dyes and pigments that have been the focus of ongoing intense research since their first synthesis at the beginning of the last century. Because of their unique spectroscopic and electrochemical properties, metallophthalocyanines (MPc) have found applications as semiconductors, nonlinear optical and optical limiting materials, chemosensors, organic photovoltaics, catalysis and photosensitizers for photodynamic therapy and photodynamic inactivation [1–13]. Pyridone derivatives are heterocyclic intermediates used for the synthesis of arylazo dyes. Azo pyridone dyes display bright hues and are used as dye colorings for polyester fabrics [14]. Recently, the synthesis and quartz crystal microbalance (QCM) based ion sensors properties of free base and cobalt Pcs with four 4-(6-methyl-3-nitro-2-oxo-1,2-dihydropyridin-4-yloxy) substituents at the peripheral positions have been reported [15]. The aim of this study was to synthesize a Zn(II) phthalocyanine with a similar set of peripheral pyridone substituents (Scheme 1) and investigate their photophysicochemical properties to assess their possible utility as photosensitizers in singlet oxygen applications such as photodynamic therapy (PDT). ZnPcs are particularly important in this regard since generally they have high singlet oxygen quantum yield values due to the heavy atom effect, making these compounds suitable for use as photosensitizers in photodynamic therapy [16].

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EXPERIMENTAL

Materials

All chemicals were reagent grade. Solvents were dried, purified and stored over molecular sieves.

Instrumentation

Electronic absorption spectra were obtained on a Shimadzu UV-2450 UV–visible spectrophotometer. Infrared spectra (IR) were recorded on a Perkin Elmer Spectrum 100 FT-IR spectrometer. Elemental analyses were performed by the Instrumental Analysis Laboratory of the TUBITAK Marmara Research Center. The ^{1}H-NMR