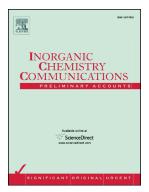
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Synthesis, spectroscopy and singlet oxygen quantum yield of a non-aggregating hexadecamethyl-substituted phthalocyanine silicon(IV) derivative



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ACCEPTED MANUSCRIPT

Title

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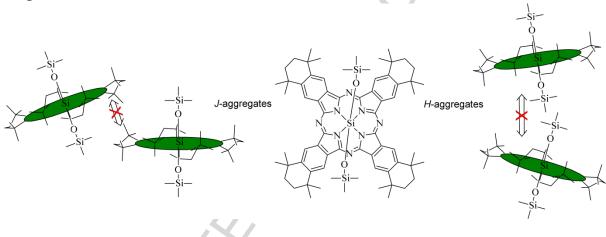
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Graphical Abstract



Abstract

A rigid hexadecamethyl substituted phthalocyanine (Pc*) silicon(IV) dichloride was synthesized by template cyclization of corresponding 1,3-diiminoisoindoline derivative with SiCl₄. Attempts to prepare the same compound by insertion of HSiCl₃ into preformed H₂Pc* in the presence of bases were unsuccessful. Exchange of the axial chloride ligands with trimethylsiloxy groups made the molecular complex Pc*Si(OTMS)₂ very soluble and non-aggregating, as shown by UV-Vis experiments. The effect of such peripheral alkyl substitution on the singlet oxygen quantum yield of the Pc*Si(OTMS)₂ complex was determined and found to be 0.28; significantly lower than that for unsubstituted parent PcSi(OTMS)₂. The merit of improving solubility over reduced singlet oxygen quantum yields is discussed.

Keywords: silicon, phthalocyanine, singlet oxygen, photosensitiser

Photodynamic therapy is a well established method for the treatment of cancer that reduces unwanted side-effects by using light, typically tissue-penetrating IR-laser light, to activate a photosensitiser (PS) in a specific region where activity is desired[1]. Therapeutic activity is achieved by the excitation of triplet oxygen present in the cell to singlet oxygen, which then oxidizes the surrounding biomolecules; the effectiveness of a compound to do this is measured as its singlet oxygen quantum yield, Φ_{Δ} . Whereas the first generation of compounds consisted mainly of porphyrins, such as photofrin,

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