

# Silicon octaphenoxypthalocyanines: photostability and singlet oxygen quantum yields

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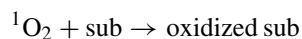
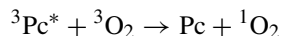
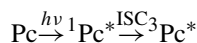
## Abstract

Photochemical properties of series of axially substituted silicon octaphenoxypthalocyanines with aryloxy, siloxy, aminoalkoxy, esters of carboxylic acids and sulphonic acid esters residues as axial ligands were studied in dimethylsulfoxide (DMSO) solution. It was found, that under Q-band excitation axial ligands in compounds studied have the propensity to be changed by hydroxyl groups with quantum yields in the range  $10^{-5}$  to  $10^{-2}$  depending on the nature of the axial ligand. Axial substituent phototransformation was followed by slow photobleaching of dihydroxysilicon octaphenoxypthalocyanine (photoproduct) in self-sensitized singlet oxygen mediated oxidation of the macrocycle. Singlet oxygen quantum yields were found to be in the range 0.15–0.20 for majority of the phthalocyanines (Pc) studied. © 2001 Elsevier Science B.V. All rights reserved.

**Keywords:** Silicon phthalocyanine; Phototransformation; Singlet oxygen; Quantum yields

## 1. Introduction

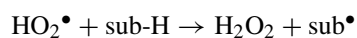
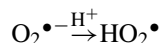
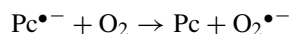
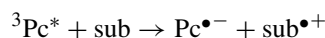
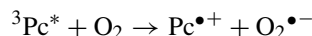
There is considerable interest in phthalocyanines (Pc) containing non-transition metals for use as photosensitizers in the relatively new method of cancer treatment called photodynamic therapy (PDT) [1–3]. The mode of operation in PDT is based on visible light excitation of a tumor-localized photosensitizer. After excitation, energy is transferred from the photosensitizer (in its triplet excited state) to ground state oxygen ( $^3\text{O}_2$ ), forming singlet oxygen ( $^1\text{O}_2$ ). This process is the dominating initial elementary step of PDT, and it is followed by oxidation of cellular targets (sub) by  $^1\text{O}_2$ ; the so-called type II mechanism [3–5]



where ISC is intersystem crossing from the singlet to the triplet excited state.

In addition to the singlet oxygen pathway, the formation of radicals by photoinduced electron transfer and radical oxida-

tion of biological substrates can occur through the so-called type I mechanism [4,5]



$\text{sub}^{\bullet+}$ ;  $\text{sub}^{\bullet}$ ;  $\text{H}_2\text{O}_2 \rightarrow$  further reactions, oxidized sub

The route via singlet oxygen is considered to be the main process in photosensitized tumor cell inactivation.

The study of the photochemical properties of Pc complexes is of importance for their use in PDT and other applications based on their photosensitizing abilities, such as in photovoltaic devices [6,7], light harvesting coatings [8] and non-linear optics [9]. To date, several reports can be found in the literature on the influence of the central metal and the structure of the macrocycle on the photostability and efficiency of singlet oxygen photogeneration by Pc and their analogs [10–13]. However, some Pc complexes such as SiPc possess covalently bound axial substituents, which further influence the molecule's physico-chemical properties. Furthermore, axially ligated SiPc exist as single isomers if both the available axial positions are substituted [14].

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