

INTERACTION OF PALLADIUM PORPHYRIN WITH DIOXYGEN MOLECULE. THE PERSPECTIVE FROM THEORETICAL CALCULATIONS

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The formation of singlet oxygen in the presence of palladium complexes has applications in photodynamic therapy and in the determination of oxygen concentration, among others of biological importance. The elucidation of the electronic factors involved in the formation of singlet oxygen is of great importance.

DFT, TDDFT and NEVPT2 calculations were performed for palladium porphyrin complex, Pd(II)Por. The ground and low-lying, electronic excited states of palladium porphyrin were characterised. Energy curves of electronic states as function of the porphyrin ring distortion were determined. The photophysical processes of palladium porphyrin such as fluorescence, phosphorescence and intersystem crossing (ISC) were studied, and rate constants were calculated.

The palladium(II) porphyrin interaction with molecular oxygen was investigated. The energy curves as function of dioxygen – Pd(II)Por distance were constructed. Based on obtained results, the mechanism of transforming oxygen to the singlet state in the presence of the porphyrin palladium(II) complex was proposed. Products of palladium porphyrin oxidation as a result of the action of oxygen have also been investigated. This is important from the point of view of the stability of the Pd(II)Por system in the process of singlet oxygen formation.