INTERACTIONS OF DICLOFENAC WITH IRON OCTACARBOXYPHTHALOCYANINE. EXPERIMENTAL AND DFT STUDY

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Phthalocyanines have a conjugated system of 18 delocalized π-electrons. The inner part of the macrocycle can accomodate almost all metal ions from the periodic table [1]. For better solubility in water we used iron octacarboxyphthalocyanines (FePcOC, fig. 1).



Fig. 1. Structure of iron octacarboxyphthalocyanine.

The subject of our research was the interaction of diclofenac (DNF) with iron octacarboxyphthalocyanine under oxidizing conditions. The most energy-efficient arrangement of FePcOC with DNF has been found. UV-Vis spectra of the complex have been calculated and compared with experimental data. All DFT and TDDFT calculations were carried out using the Gaussian 16 program [2]. Fully optimized structures in the gas phase were obtained at B3LYP/6-31G(d) level of theory. The UV-Vis adsorption spectra have been computed using the long-range corrected CAM-B3LYP functional [3].

**References**

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