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Research of the sorption activity of copper phthalocyanine

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Abstract

In the work a research the sorption capacity of copper phthalocyanine with respect to polars sorbats by the method of quantum-chemical modeling. The theory of the density functional with the hybrid functional B3LYP5 and basic sets 6-31G(d,p) (optimization of geometry) and cc-pVDZ (single point calculation) was chosen as the calculation method. The purpose of this work was theoretical prediction of the effectiveness of surfactants in the hydrophobization of the copper phthalocyanine surface (necessary for the flushing process).

Modeling of sorption activity was carried out on a single molecule of copper phthalocyanine and bimolecular complex with a geometry of the crystal grid of the β-modification.

Prediction of sorption activity was carried out by the methods of dipole moments, molecular electrostatic potential and the frontier molecular orbital theory.

As a result of modeling, the electrophilic characteristics of the entire surface of copper phthalocyanine were established, but the sorption of nucleophilic molecules is possible only on surfaces containing indole rings. On other surfaces possible sorption of small electrophilic particles, such as OH^-.

The most probable centers of sorption are the nitrogen atoms of the indole ring (confirmed by all three methods).

To the results of the research, the most effective surfactants for hydrophobizing the surface of copper phthalocyanine are nucleophilic molecules that give an acidic or neutral medium.

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