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Quantum-chemical modeling of photoreduction of copper acetate

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Abstract

Aqueous solution for photoselective activation of dielectric material based on cupric acetate(II) was investigated as photopromoter. Sodium salt of anthraquinone-2-sulfonic acid was investigated as optical sensitizer. Sorbitol and ethanol were introduced in the composition of the photoactivator as the secondary reductant.

The mechanism of the photoreduction process of copper(II) was developed on the basis of quantum-chemical modeling.

It was shown the determining role of long-lived excited triplet electronic states anthraquinone and polarization fluctuations on the mechanism of transfer electron density from anthraquinone to the vacant orbitals of copper. These states provide alignment of the energy levels of the donor and the electron density acceptor.

It was found that the cuprous ion is an intermediate product of photoreduction of copper(II). This ion turns into metallic copper by dark reactions or disproportionation.