

The article is published on the materials of speech at the XX All-Russian Conference

"The structure and dynamics of molecular systems." Yalchik 2013.

Publication is available for discussion in the framework of the on-line Internet conference "Butlerov readings".

<http://butlerov.com/readings/>

Contributed: July 12, 2013.

Modeling of nonlinear optical materials on the basis Of composite polymers with binary chromophore groups

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Keywords: *nonlinear optical activity, composite materials, molecular modeling, quantum-chemical calculations, oligomers, chromophores.*

Abstract

With the use of molecular modeling we studied the structure of a new type of composite material, wherein the guest chromophores contain tricyanoethenyl electron-acceptor group, and the host polymer matrix is modeled by epoxyamine oligomers with multichromophoric dendritic fragments. Electrical characteristics (dipole moment μ and molecular polarizability α , β) of the researched molecular systems are calculated quantum-chemically at the level of TDHF//AM1. It has been shown that introduction of additional chromophores-guests leads to spatial organization of the chromophore groups and an increase in the quadratic nonlinear-optical activity of molecular systems under investigation. The optimal ratio between the number of additional chromophores attributable to the dendritic segment has been defined.