

Molecular structure of the new photochromic 3,4-di-(1,2-dimethylindolyl-3)-2,5-dihydrothiophen

© Valeriy V. Tkachev,^a Andrey N. Utenyshev,
Sergey M. Aldochin, and Konstantin V. Bozhenko^{b*,+}

Institute for problems of chemical physics at RAS. Acad. Semenov Ave., Chernogolovka, 1142432. Russia.

Phone: ^{a)} +7 (49652) 21563. E-mail: ^{a)} vatka@icp.ac.ru ; ^{b)} bogenko@icp.ac.ru

^{*}Supervising author; ⁺Corresponding author

Keywords: *X-ray structural analysis, dihetarylethene, photochromic compounds, quantum-chemical calculations.*

Abstract

X-ray structural investigation of the new photochromic dihetarylethene – 3,4-di-(1,2-dimethylindolyl-3)-2,5-dihydrothiophen was carried out. It has been shown that in crystalline stage the investigated compound has antiparallel arrangement of indole fragments with intramolecular distance of 3.479 Å between the indicated reactionary carbons, which is a satisfactory condition for the process of photocyclization. Quantum-chemical calculations were performed on the initial compound and its photoproduct, as a result of which it has been shown that the initially discovered form is energy-wise more beneficial than the photo product by 22.5 kcal/mol.