Quantum-Chemical Simulation of Charge-Transfer Complexes of 2,4,7-Trinitro-9*H*-fluoren-9-one with Donor Molecules. Crystal and Molecular Structure of the 1 : 1 Complex of 2,4,7-Trinitro-9*H*-fluoren-9-one with Anthracene

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Abstract—Quantum-chemical simulations of charge-transfer complexes of 2,4,7-trinitro-9*H*-fluoren-9-one with eight donor molecules differing in size and structure of the π-aromatic system have been performed in the scope of the density functional theory approximation, and data on the structure and properties of the complexes have been obtained. The electronic and energy characteristics of the acceptor, donors and the complexes, the average interplanar distances, and the values of charge transfer in the complexes have been obtained, and regularities in the change of these quantities have been elucidated. The crystal and molecular structure of the 1 : 1 complex of 2,4,7-trinitro-9*H*-fluoren-9-one with anthracene ($C_{13}H_5N_3O_7 \cdot C_{14}H_{10}$) have been determined by means of X-ray diffraction analysis.

Keywords: 2,4,7-trinitro-9,10-fluorenone, anthracene, charge-transfer complexes, quantum-chemical simulation, X-ray diffraction analysis

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