МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
СУМСЬКИЙ ДЕРЖАВНИЙ УНІВЕРСИТЕТ

ФІЗИКА, ЕЛЕКТРОНІКА, ЕЛЕКТРОТЕХНІКА

ФЕЕ: 2016

МАТЕРІАЛИ
та програма

НАУКОВО-ТЕХНІЧНОЇ КОНФЕРЕНЦІЇ

(Суми, 18–22 квітня 2016 року)

Суми
Сумський державний університет
2016

Potential Surface of Polymethine Dye Molecule in the optimized state

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Polymethine dyes (PMD) is widely used as sensitizers and as a convenient object for studying properties of chromophore systems. For research of PMD and the processes occurring in them, in this paper are applied quantum chemistry methods that are implemented using software package MOPAC2016, a well-established themselves with studies of complex molecules.

In this paper, the calculation of the potential surfaces of the ground and excited states of the dioksazoltrimetintsianin molecule in the optimized state is made. It was confirmed the phase transition found in previous work, in which the singlet ground state was replaced by a triplet (Fig.1). Inability in previous studies to optimize the molecules at each step of increasing the bond length between the carbon atoms in the chromophore chain, not allowed telling with confidence about the presence of this condition.

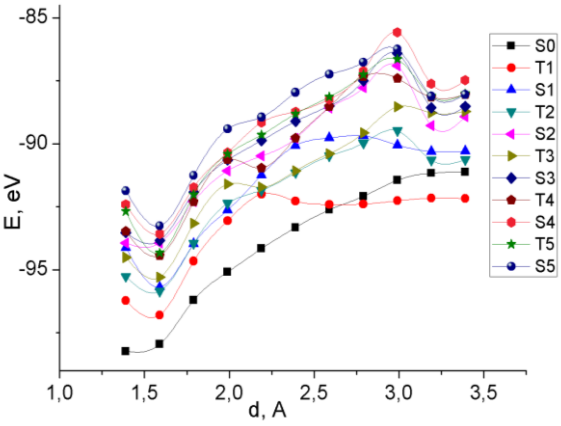

Figure 1 – Dependence of potential surfaces on the bond length in the chromophore chain of the PMD molecule

Furthermore, with increasing the bond length, as expected, there was a general decreasing of energy of the potential surfaces.