Thematic Section: Quantum-Chemical Study. **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 12-30-5-47
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: June 5, 2012.

X-ray and quantum-chemical study of new luminophors derivatives of 2-tosyl -3-fenilakrilonitril.

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Keywords: *organic luminophores, derivatives of 2-tosyl-3-phenylacrylonitrile, a luminescence, fluorescence, X-ray diffraction analysis, critical points, the topological analysis of electronic density.*

Abstract

Performed X-ray diffraction analysis of new organic luminophores 2-tosyl-3-(2,3-dimethoxyphenyl)-acrylonitrile (**I**) and 2-tosyl-3-(1,2-dimethoxyphenyl)acrylonitrile (**II**). Compounds **I** and **II** in a crystal condition possess an intensive luminescence in the visible part of a spectrum, disappearing in a solution, that, apparently it is caused by influence of a crystal field. With objective of an explanation of this fact, for compounds **I** and **II** has been performed comparative cristallochemical analysis of a crystal and molecular structure. Quantum-chemical calculations at B3LYP/6-311G (d) level has been executed and the topological analysis of distribution of electronic density, using QTAIM of Bader for the specified compounds has been performed. It has been shown, that some intermolecular and intramolecular not valent interactions are somewhat caused by formation in intermolecular and intramolecular spaces of very weak covalent bindings.