Thematic Section: Physico-Chemical Research._____ **Full Paper**
Subsection: Organic Chemistry. *Registration Code of Publication:* 13-35-8-1
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: May 4, 2013.

Phylloquinone. Excited electronic states and intersystem conversion.

© **Svetlana N. Tseplina**,[+] **Evgeny E. Tseplin**,* and **Olga G. Khvostenko**
Institute of Molecular and Crystal Physics. Ufa Research Centre of Russian Academy of Sciences.
Octyabrskiy Prospect, 151. Ufa, 450075. Russia. Phone: +7 (347) 292-14-17. E-mail: sn_tseplina@mail.ru

*Supervising author; [+]Corresponding author

Keywords: *singlet-triplet intersystem conversion, phylloquinone, excited states.*

Abstract

The optical absorption, emission and excitation spectra of phylloquinone (Vitamin K1) were recorded. On the basis of TDDFT B3LYP/6-31+G(d,p) calculations we carried out the assignment of the absorption bands to specific singlet transitions. It has been revealed that two different excitation spectra are registered in phylloquinone depending on the registration length wave where one of the spectra is related to fluorescence and the other corresponds to phosphorescence, also in agreement with the appropriate attribution of the luminescence bands. On the basis of the complex analysis of absorption, luminescence and excitation spectra in accordance with the selection rule, it has been shown that the intersystem crossing mainly occurs between S_1 and T_2 states.