Full Paper _____ *Thematic Section:* Physoco-Chemical Research.
Registration Code of Publication: 13-33-3-130 *Subsection:* Physical Chemistry of Explosives.
Publication is available for discussion in the framework of the on-line Internet conference "*Butlerov readings*".
http://butlerov.com/readings/
Contributed: February 21, 2013.

Features of molecular interactions in the binary system of cellulose nitrate-filler

© **Rinat O. Almashev**,* **Tatiana A. Eneykina**, **Lilia Selivanov**, **Nadezhda A. Romanko**, **Anna V. Kiprova**,+ **Elvira N. Tarazova**, **Roza F. Gatina**, and **Yury M. Mikhailov**
State Scientific-Research Institute of Chemical Products. Svetlaya St., 1. Kazan, 420033. Tatarstan Republic. Russia. E-mail: anekolab@mail.ru

*Supervising author; +Corresponding author

Keywords: *IR spectroscopy, filler, cellulose nitrate, molecular interactions, octogen, hexogen.*

Abstract

Using IR-spectrometry we studied intermolecular interaction in systems cellulose nitrate (CN) – octogen (hexogen). It has been established that the stability of the molecular complexes CN-octogen (hexogen) depends on the properties of CN, the type and the content of the filler and the characteristics of hydrogen bonds (E) in the interval 12.1-33.2 kJ/mol. The strongest intermolecular interactions in the considered range of the input of fillers (0-80 % weight.) is observed in the compositions hexogen- colloxylin, starting with the component ratio 60:40 due to the great number of the molecular complexes being formed (E = 33.2 kJ/mol). For compositions octogen – colloxylin the similar dependence is preserved, but at the lower energies of hydrogen bonds (E = 16.1-25.1 kJ/mol). In the compositions of hexogen (octogen) – pyroxylin the optimal compositions, from the point of view of steady molecular complexes, are those with the filler content ~60 % weight (E = 27.1 and 25.1 kJ/mol, accordingly).