Thematic Section: Kinetics Research. **Full Paper**
Subsection: Physical Chemistry. *Registration Code of Publication:* 14-40-12-133
The article is published on the materials of report presented at the "International Scientific Forum Butlerov Heritage – 2015". http://foundation.butlerov.com/bh-2015/ *(English Preprint)*
Contributed: December 27, 2014.

Mechanically stressed structures and thermal degradation kinetics of zinc and cobalt acetylenedicarboxylates dehydrates

© **Vitaly A. Shershnev**,[1]*+ **Nina N. Volkova**,[2]*+
Gulzhian I. Dzhardimalieva,[1]* and **Boris E. Krisyuk**[3,4]*+
[1] *Laboratory of Metallopolymers.* [2] *Laboratory of Filtration Combustion.* [3] *Laboratory of Kinetic of Thermal Transformation. The Institute of Problems of Chemical Physics of the Russian Academy of Sciences. Academician Semenov St., 1. Chernogolovka, 142432. Moscow Region., Russia.*
E-mail: femtos@mail.ru, nvolkova@icp.ac.ru, bkris@mail.ru
[4] *Department of Chemistry and Physics. Plekhanov Russian University of Economics. Stremyanny per., 36. Moscow, 117997. Russia.*

*Supervising author; +Corresponding author

Keywords: crystalline hydrates of acetylenedicarboxylate zinc and cobalt, the kinetics of mass loss, a critical value of the mass loss, mechanochemical destruction of crystals and initiation reactions, quantum chemical calculation of strain energy.

Abstract

The mass loss kinetics of Zn and Co acetylenedicarboxylates was investigated in the temperature range of 263-313 K and at residual pressure of 1.3 Pa. It was shown that mass loss observed was due to dehydration that had only lasted until special critical value of residual water was reached. With a small change in that value during further dehydration the rapid collapse of ZnAC and CoAC took place involving chemical bonds destruction and formation of active particles that initiated solid state polymerization. Dehydration enthalpy was calculated using DFT methods. Model clusters of different size were considered and in every case substantial enthalpy values of 70-100 kJ/mole for each molecule of water removed were obtained. Such considerable values indicate mechanochemical activation for observed collapse of ZnAC and CoAC structures.