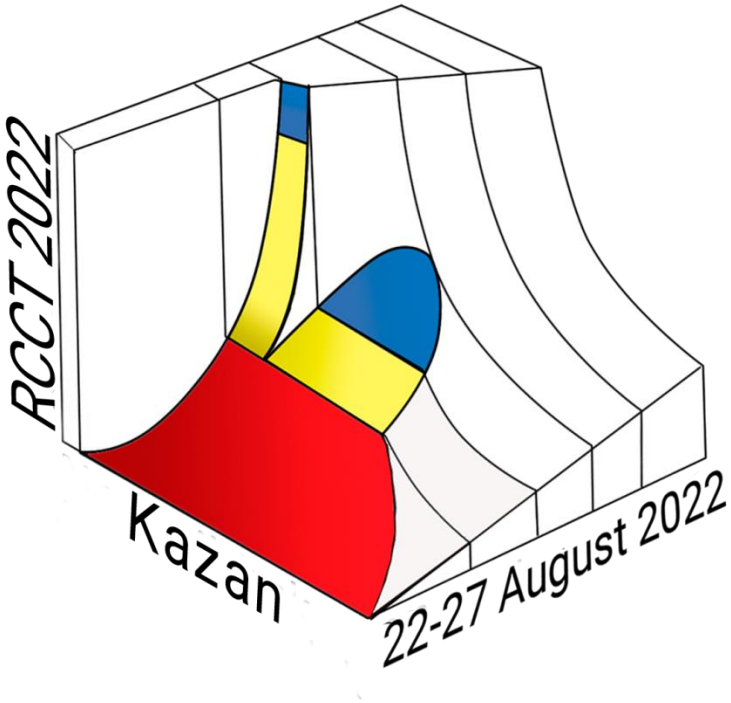
XXIII International Conference on Chemical Thermodynamics in Russia

August 22-27, 2022
Kazan, Russia



RCCT – 2022

BOOK OF ABSTRACTS

Kazan Federal University

Kurnakov Institute of General and Inorganic Chemistry of Russian Academy of Sciences

Kazan Scientific Center of Russian Academy of Sciences

Mendeleev Chemical Society of Russia

PREFACE

XXIII International Conference on Chemical Thermodynamics in Russia, RCCT-2022 August 22-26, 2022, Kazan, Russia: Abstracts. – Kazan, 2022. - 361 p.

This book contains the scientific program and the abstracts of presentations at the XXIII International Conference on Chemical Thermodynamics in Russia (RCCT-2022). The conferences on Chemical Thermodynamics are among the largest held in Russia since 1961. RCCT is an important scientific event not only for Russian but also for the international research community, being among the largest conferences on Chemical Thermodynamics. The conference traditionally covers all aspects of chemical thermodynamics from fundamentals to applications, including multidisciplinary approaches and related fields of science.

Until 1977 a conference of this series was called “All-Union Conference on Calorimetry" and later, until 1992, "All-Union Conference on Calorimetry and Chemical Thermodynamics". Today the RCCT International Conferences are organized every two years by large Russian scientific centers that have included Moscow (2005, 2013), Saint Petersburg (2002, 2019), Ivanovo (2007), Kazan (2009), Samara (2011), Nizhny Novgorod (2015) and Novosibirsk (2017).

This year the conference brings together more than 250 scientists from 32 cities and 15 countries; many of them are young researches, including undergraduate and graduate students. Two junior poster awards have been established by the organizers for the best poster presentations: the RCCT-2022 junior poster award “Excellence in Chemical Thermodynamics” and “Lev G. Berg award”, a special award is dedicated to the founder of theory of Differential Thermal Analysis, the first president of the International Confederation for Thermal Analysis (ICTA), professor Lev G. Berg.

The scientific program of RCCT2019 includes plenary and keynote lectures, 4 parallel sessions of oral presentations and 3 poster sessions. These contributions reflect the latest trends in Chemical Thermodynamics, including the development and application of theory, new experimental techniques and computer simulation for various systems. It is our pleasure to thank all the participants of RCCT-2022 and to welcome you in Kazan.

On behalf of the organizers,

Boris N. Solomonov, RCCT-2022 Vice-chair

KINETIC AND THERMODYNAMIC CONTROLS OF ZINK CYAMELURATE CRYSTAL FORMATIONS

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The dynamic combinatorial library (DCL) of cyamelurates consists of 17 tautomers of cyameluric acid and their ions, as well as metal aquacomplexes. That leads to a variety of compounds in the $Zn(NO_3)_2$ – $K_3(C_6N_7O_3)$ – H_2O system. All compounds are obtained with impurity amorphous and crystalline phases, which complicates their study. In this work, metastable phases of zinc, nickel and iron cyamelurates were obtained and their crystal structures were determined for the first time. Kinetic control of chemical reactions allowed us to isolate two zinc cyamelurate metastable phases. The metastable compound $K_2Zn(C_6N_7O_3H)_2 \cdot 8H_2O$ is formed immediately after mixing the precursor solutions, and after two hours it is converted to another metastable compound $Zn(C_6N_7O_3H) \cdot 5H_2O$. Due to hydrate isomerization, after 12 hours in the mother liquor the latter transforms into a thermodynamically stable compound of the same composition. The features of the synthesis and crystalline structure of zinc cyamelurates can be interpreted from the standpoint of the non-classical nucleation theory. The crystal structures of the synthesized compounds $K_2Zn(C_6N_7O_3H)_2 \cdot 8H_2O$, $Zn(C_6N_7O_3H) \cdot 5H_2O$ and $Zn(C_6N_7O_3H_2)_2 \cdot 8H_2O$ allowed us to conclude that decomposition of supersaturated zinc solution lead to formation of double electric micelles. They can be considered as nanoreactors playing an important role in crystal nucleation.

The features of synthesis and crystal structure of zinc cyamelurates, indicating a nonclassical nucleation, allowed us to propose the stages of crystal formation. Colloidal particles with an electric double layer, formed due to the concentration decay, play an important role in crystal nucleation. Inside such particles, the precursors transform into building blocks, which generate crystal nuclei through self-assembly process. The chemical composition of the crystal nucleus depends on the composition of the colloidal particle. Isolation of metastable phases by means of kinetic control has demonstrated its significance in obtaining crystalline substances, which make it possible to draw a conclusion regarding the process of crystal nucleation, provided that the object of study is successfully selected.

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