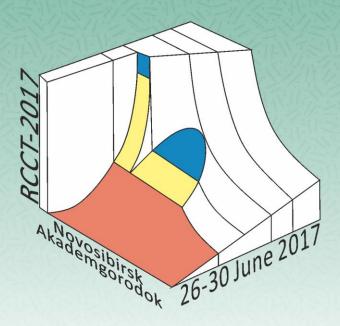


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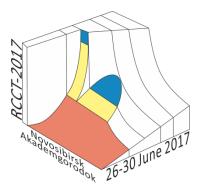
## ABSTRACTS

XXI International Conference on Chemical Thermodynamics in Russia

School-Conference on Chemical Thermodynamics for Young Scientists



June 26-30, 2017, Akademgorodok, Novosibirsk, Russia



### XXI International Conference on Chemical Thermodynamics in Russia (RCCT-2017)

School-Conference on Chemical Thermodynamics for Young Scientists

## ABSTRACTS

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XXI International Conference on Chemical Thermodynamics in Russia (RCCT-2017) (June 26-30, 2017, Novosibirsk, Russia): Abstracts. – Novosibirsk: NIIC SB RAS, 2017. – 401 pp.

ISBN 978-5-90168-841-0

This book presents abstracts of the participants of the XXI International Conference on Chemical Thermodynamics in Russia (RCCT-2017). The conferences on chemical thermodynamics are among the largest conferences held in Russia since 1961. Till 1977 the conference was called "All-Union conference on calorimetry", further, till 1992 - "All-Union conference on calorimetry", then after a long break the tradition of holding the conference was revived in 2001.

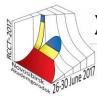
At present the RCCT International Conferences take place every two years in various large Russian scientific centers such as Moscow, St. Petersburg, Nizhny Novgorod, Novosibirsk, Kazan, Samara and others. At present the RCCT International Conferences take place every two years in various large Russian scientific centers such as Moscow, St. Petersburg, Nizhny Novgorod, Novosibirsk, Kazan, Samara and others. Every RCCT is unique and significant event both for Russian and for world thermodynamic community as a whole. The conference traditionally covers all the aspects of chemical thermodynamics: from fundamental to applied areas, including multidisciplinary approaches and related areas of science.

RCCT-2017 scientific program includes plenary and invited lectures, oral presentations, poster sessions and virtual contributions

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26-30 June 2017, Akademgorodok, Novosibirsk

#### EFFECTS OF pH AND COMPOSITION OF AQUEOUS BIPHASIC SYSTEMS CONTAINING NONIONIC SURFACTANT TRITON X-114 ON PARTITION BEHAVIOR OF THE BIOCOMPOUNDS

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Aqueous biphasic systems are applied in liquid-liquid extraction (LLE) of organic and bioactive compounds, ions of metals [1], [2]. One of the techniques of biphasic partitioning is a cloud point extraction (CPE) based on nonionic surfactant (NIS). The extract (i.e. micellar or surfactant rich) and raffinate (i.e. aqueous or surfactant poor) phases in NIS system are formed at the cloud point temperature (CPT). The CPE method is carried out at the temperature above the CPT or in the presence of certain additives limiting solubility of NIS in aqueous solution. In comparison with the traditional organic solvents for LLE, NISs are biocompatible and provide mild conditions, which are especially important for extraction processes of biomolecules sensitive to the organic media and to the high temperatures. The CPE has been successfully applied to provide the biocatalytic reaction by a continuous mode [3].

It is known that an addition of some additives (salt or other surfactant) impact on CPT and on the partition coefficient  $(lgP^{\alpha\beta})$  of some solutes in biphasic micellar system [4]. Furthermore, some additives affect the density and the viscosity of both liquid phases what determines velocity of the phase separation. Hence, density and viscosity data of both phases are particularly important for a design of the extraction process.

In the present work, the aqueous solutions of NIS Triton X-114 with salt additives (NaCl and  $K_2HPO_4/KH_2PO_4$ ) were considered as the systems for CPE of the compounds of penicillin G hydrolysis i.e. penicillin G (PenG), 6-aminopenicillinic (APA) acid and phenylacetic acid (PAA) [3]. The effects of pH, salt additives and component concentrations on phase behavior, physicochemical properties of coexisting phases (density and viscosity) and partitioning of the solutes are under study. The temperature of the measurements (310.2 K) was chosen as provided the highest velocity of the bioreaction. The  $lgP^{\alpha\beta}$  values of the solutes were determined by phase separation followed by HPLC analysis.

The study of the phase behavior shows that the CPT of Triton X-114 micellar systems without solutes do not sensitive to a change in pH value from 6.8 to 2.7. An addition of NaCl or  $K_2HPO_4/KH_2PO_4$  reduces expectably the CPT of the Triton X-114 solutions with and without solutes. An addition of APA has no effect on CPT, while the presence of PAA leads to a significant decrease of the CPT.

Moreover, it was found, that an addition of the organic compounds has almost no effect on density of both phases. The viscosity of micellar phase containing APA is close to that of surfactant-rich phase of Triton X-114 system without any additives. The additive of PAA highly decreases the viscosity of the micellar phase. The viscosity values of the aqueous phases are practically the same for all the systems and are close to the viscosity of the pure water. The  $lgP^{\alpha\beta}$  data show that NaCl as additive or decrease of pH improves the extraction of PAA.

Chromatographic researches were carried out on the equipment of the Research park of St. Petersburg State University, Center for Chemical Analysis and Materials Research.

This study was financially supported by RFBR according to the research project # 16-53-12029 HHI/O\_a.

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