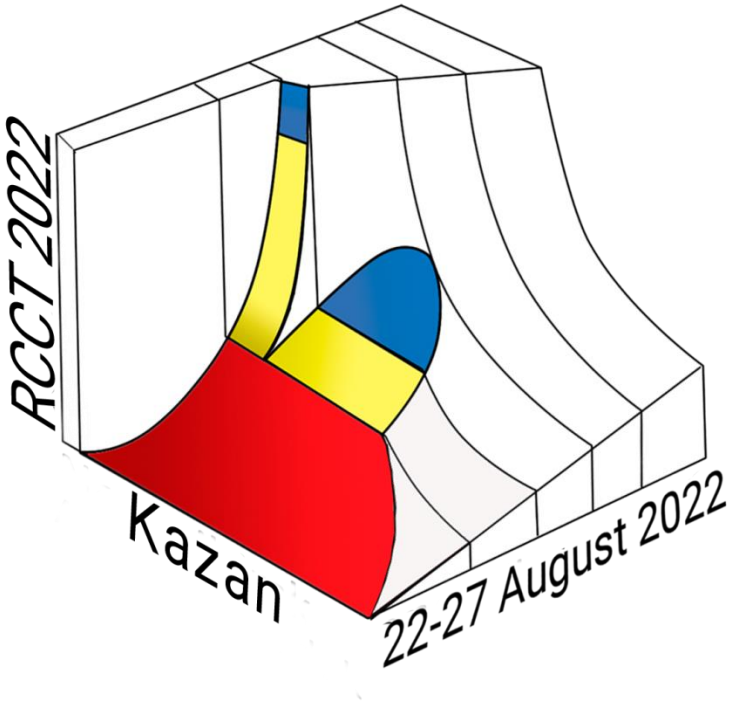
XXIII International Conference on Chemical Thermodynamics in Russia

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

Organizing Committee

Chairs
Oleg G. Sinyashin (Kazan)
Konstantin S. Gavrichev (Moscow)

Vice-Chairs
Boris N. Solomonov (Kazan)
Alexey I. Victorov (St. Petersburg)

Members
A.I. Rusanov (St. Petersburg)
A.Yu. Tsivadze (Moscow)
F.V. Grechnikov (Samara)
M.F Churbanov (Nizhni Novgorod)
N.T. Kuznetsov (Moscow)
V.N. Parmon (Novosibirsk)
V.L. Stolyarova (Saint-Petersburg)
A.B. Yaroslavtsev (Moscow)
A.K. Shchekin (Saint-Petersburg)
O.L. Kuskov (Moscow)
V.P. Fedin (Novosibirsk)
V.V. Gusarov (Saint-Petersburg)
K.V. Zherikova (Novosibirsk)
L.N. Zelenina (Novosibirsk)
A.A. Goryunkov (Moscow)
A.A. Pimerzin (Samara)
A.M. Kolker (Ivanovo)
A.M. Toikka (Saint-Petersburg)
A.S. Alikhanyan (Moscow)
A.V. Knyazev (Nizhni Novgorod)
A.V. Markin (Nizhni Novgorod)
A.Y. Manakov (Novosibirsk)
E.G. Osadchiy (Chernogolovka)
I.A. Uspenskaya, Moscow (Moscow)
I.A. Zvereva (Saint-Petersburg)
M.G. Kiselev (Ivanovo)
N.N. Smirnova (Nizhni Novgorod)
N.V. Gelfond (Novosibirsk)
P.P. Fedorov (Moscow)
S.I. Lopatin (Saint-Petersburg)
S.V. Stankus (Novosibirsk)
Y.G. Galyametdinov (Kazan)

International Scientific Committee
A. Blokhin (Belarus)
S. Enders (Germany)
I. Smirnova (Germany)
E. Voutsas (Greece)
J. N. Jaubert (France)
A. Navrotsky (USA)
A. Galindo (United Kingdom)
S.P. Verevkin (Germany)
N. Koga (Japan)
M. Monte (Portugal)
S. Vyazovkin (USA)
S. Vecchio Ciprioti (Italy)

Sponsor
ANO eNano “Electronic Education for Nanoindustry” (Rusnano Group of Companies)

eНано

Local Committee
M.A. Ziganshin
V.V. Gorbatchuk
I.A. Sedov

KEYNOTE LECTURES

PARTITIONING OF N-OCTANOL IN MIXED MICELLAR SOLUTIONS OF TRITON WITH 1-METHYL-3-OCTYLIMIDAZOLIUM CHLORIDE: EXPERIMENT AND MODEL PREDICTIONS

A.I. Victorov, P.O. Sorina, E.A. Safonova, Yu.G. Dobryakov, E.A. Iakovleva
Saint-Petersburg State University, St. Petersburg, Russia
e-mail: victorov_a@yahoo.com

Micelle-mediated separation is an attractive noninvasive technique, particularly for the biocomponents having fragile molecules. The design of the separation processes requires knowledge of the equilibrium distribution of species between the solution and the multicomponent micellar aggregates. Measurement of this distribution and its modeling are both quite challenging. The properties of the aggregates, including their shape and polydispersity typically respond to the variation of the solution composition, and partitioning of a component between the aggregates and their environment depends, in turn, on the aggregate characteristics.
A molecular-thermodynamic model has been proposed recently [1,2] that describes aggregation equilibrium and partitioning of components for mixtures of nonionic and ionic surfactants and an organic additive. We continue this work here, performing experimental studies of aqueous mixtures of Triton TX-114 and 1-methyl-3-octylimidazolium chloride (surface active ionic liquid) with/without added n-octanol (model biocomponent). Experimental data on n-octanol partition coefficients (head-space chromatography) and 2D NOESY NMR spectra are reported. For varying composition of the system, the calculated distribution of n-octanol between the polydisperse aggregates and aqueous environment is compared with experimental data. The results are discussed in light of predicted structural details of the aggregates (the number of hydrogen bonds in corona and hydration numbers, etc.).

Acknowledgements We thank RSF (project No. 20-13-00038) for financial support. The NMR measurements were carried out at the Research park of St. Petersburg State University (Center for Magnetic Resonance).

[1] E.A. Iakovleva, P.O.Sorina, E.A.Safonova, A.I.Victorov, *Fluid Phase Equilib*., 2022, 556, 113376.
[2] E.A. Iakovleva, E.A. Safonova, Al.I. Victorov, *Fluid Phase Equilib*., 2021, 546, 113134.