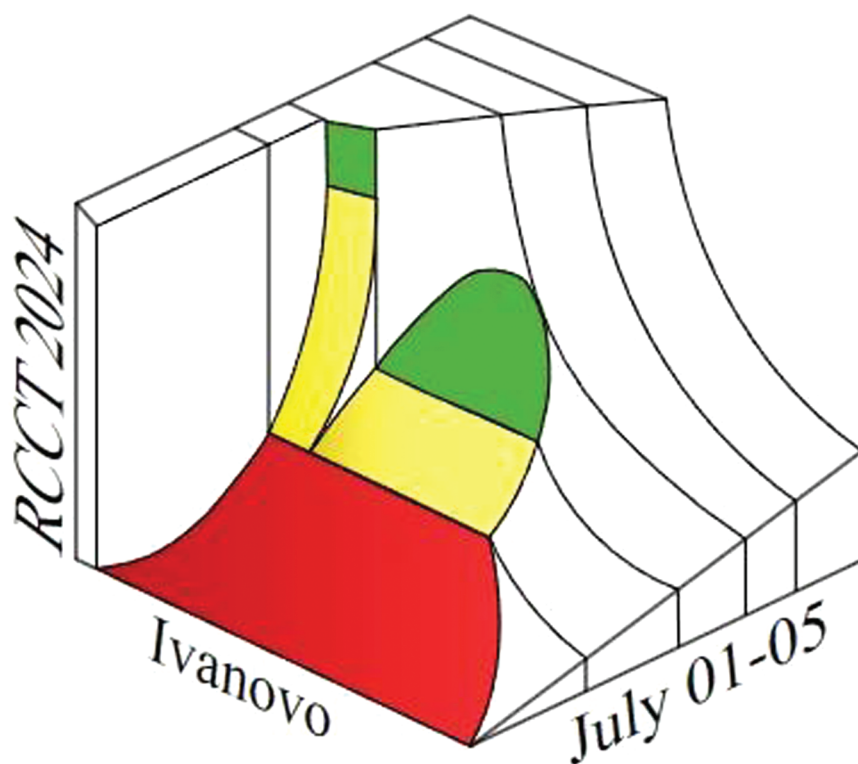


XXIV International Conference on Chemical Thermodynamics in Russia

**July 1-5, 2024
Ivanovo, Russia**

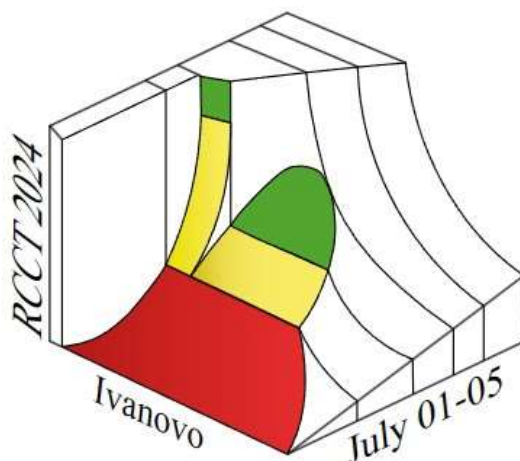


RCCT-2024

BOOK OF ABSTRACTS

XXIV International Conference on Chemical Thermodynamics in Russia

**July 1-5, 2024
Ivanovo, Russia**



RCCT-2024

BOOK OF ABSTRACTS

G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences

Ivanovo State University of Chemistry and Technology

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

Ministry of Science and Higher Education

Russian Academy of Sciences

Mendeleev Russian Chemical Society

Scientific Council for Physical Chemistry of the Russian Academy of Sciences

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THE EVAPORATION STUDY AND THERMAL STABILITY OF SOME IMIDAZOLIUM-BASED IONIC LIQUIDS

K.D. Semavin, N.S. Chilingarov, O.V. Dorofeeva, A.I. Druzhinina,
V.Yu. Markov, E.V. Skokan

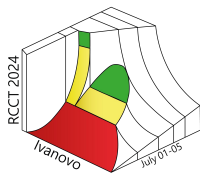
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Ionic liquids (ILs) are the hot topic in the last decades. The unique physicochemical properties of these compounds, such as low volatility, non-combustibility and resistance to many chemical agents, offer a tantalizing perspective. The ILs was applied as a solvents, catalytic environment, lubricants and heat-transfer agents. Unfortunately, information about thermodynamics and thermostability data of ILs often is not available. But reliable information about thermodynamics properties is needed to predict the properties of ILs in different application and useful for the development of the theory of liquid phase.

In this study, the determination of thermodynamic parameters of evaporation of the following ILs: [EtMIm][MS], [BuMIm][MS], [EtMIm][Cl], and [BuMIm][Cl] was carried out. The thermodynamics information about evaporation of methanesulfonates, [EtMIm][MS] and [BuMIm][MS], such as saturated vapor pressure and enthalpy of vaporization $\Delta_{vap}H_T^0$ was presented in the literature fragmentally^{1,2}. The information about their thermal stability is not available. The determination of vapor pressure and $\Delta_{vap}H_T^0$ was carried out by the method of Knudsen effusion mass-spectrometry (KEMS). Commercial MI1201 magnetic mass spectrometer ($r = 200$ mm, $R = 500$) with original high temperature ion source (EI, $E_{ion} = 70$ eV) was used. The $\Delta_{vap}H_T^0$ was determined by “Second Law Treatment” and “Third Law Treatment” procedures. To calculate the thermodynamic functions of liquid state the heat capacities of ionic liquids were obtained by high vacuum calorimetry. Thermodynamics functions of ideal gas state were calculated with quantum chemistry methods. Under the KEMS conditions, [EtMIm][MS] and [BuMIm][MS] are not thermally stable. In the case of [EtMIm][MS] the quantitative description of the thermolysis process was carried out. The kinetic curves for thermolysis reactions were obtained and the pseudo-zero order regions were found. The thermolysis proceeds by a typical S_N2 -mechanism. The possible products of [BuMIm][MS] thermolysis were described. The thermodynamic activity of both methanesulfonates is equal 1 under the experiments: MALDI and APCI mass spectra of initial samples and residues in the cells after evaporation were similar.

The evaporation study of chlorides, [EtMIm][Cl] and [BuMIm][Cl], was presented early^{3,4}. In this work, the thermostability and chemical transformation of [BuMIm][Cl] have been investigated more thoroughly. It was found that in addition to the thermolysis of [BuMIm][Cl] by the S_N2 -mechanism, a new ionic liquid [BMMIm][Cl] was formed by the C2-methylation of [BuMIm][Cl]. The methylating reagent is chloromethane formed by [BuMIm][Cl] thermolysis.

- [1] D. Zaitsau, A. Yermalayeu, A. Pimerzin and S. Verevkin, *J. Chem Eng Res Des*, 2018, 137, 164-173.
- [2] F. Heym, W. Korth, J. Thiessen, C. Kern and A. Jess, *J. Chem Ing Tech (Weinh)*, 2015, 87, 791-802.
- [3] D. Zaitsau, R. Siewert, A. Pimerzin at al., *J. Mol. Liq.*, 2021, 323, 114998.
- [4] K. Semavin, N. Chilingarov, O. Dorofeeva at al., *J. Mol. Liq.*, 380, 121733.



2024

July 1-5

**XXIV International
Conference on Chemical
Thermodynamics in Russia
(RCCT-2024)**

Program of

**XV Russian School-Conference
of Young Scientists
"Supercritical Fluid
Technologies in Solving
Environmental
Problems (SCF)"**

Ivanovo Russia

The Organizers of XXIV International Conference on Chemical Thermodynamics in Russia (RCCT-2024):

- G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences
- Ivanovo State University of Chemistry and Technology
- Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences
- Ministry of Science and Higher Education
- Russian Academy of Sciences
- Mendeleev Russian Chemical Society
- Scientific Council for Physical Chemistry of the Russian Academy of Sciences

The Organizers of XV Russian School-Conference of Young Scientists "Supercritical Fluid Technologies in Solving Environmental Problems (SCF):

- Ministry of Science and Higher Education
- Russian Academy of Sciences
- G.A. Krestov Institute of Solution Chemistry of the Russian Academy of Sciences
- M.V. Lomonosov Northern (Arctic) Federal University
- Kurnakov Institute of General and Inorganic Chemistry of the Russian Academy of Sciences
- Journal of "Supercritical Fluids: Theory and Practice"

Спонсоры:

- ООО «Техноинфо»
- ООО «Современные лаборатории»
- ЗАО «ШАГ»

**Short program of XXIV International Conference on Chemical Thermodynamics in Russia (RCCT)
and XV Russian School-Conference of Young Scientists "Supercritical Fluid Technologies in
Solving Environmental Problems (SCF)**

Ivanovo State University of Chemistry and Technology, Ivanovo, Sheremetevsky prospect, 10

MONDAY (1.07.2024)	
11.00 – 15.00	RCCT&SCF Registration (Flask hall)
15.00 – 15.20	Opening ceremony (Conference hall)
15.20 – 18.00	Plenary session (Conference hall), <i>4 reports</i>
18.30 – 20.30	Welcome party at Sheremetev Park Hotel, Naumova Street 1
TUESDAY (2.07.2024)	
9.00 – 11.00 (RCCT&SCF)	Plenary session <i>3 reports RCCT</i> (Conference hall) <i>4 reports SCF</i> (Co-working hall)
11.00 – 11.15	Coffee break
11.15 – 13.00	Oral reports
RCCT, section 3	<i>6 orals</i> (Conference hall)
RCCT, section 1	<i>6 orals</i> (B204)
RCCT, section 5	<i>6 orals</i> (B203)
SCF	<i>2 plenary reports and 2 orals</i> (Coworking)
13.00 – 14.00	Lunch
14.00 – 16.00	Oral reports
RCCT, section 3	<i>7 orals</i> (Conference hall)
RCCT, section 1	<i>6 orals</i> (B204)
RCCT, section 5	<i>7 orals</i> (B203)
SCF	<i>6 orals</i> (Co-working hall)
16.00 – 16.15	Coffee break
16.15 – 18.00	Oral reports
RCCT, section 2	<i>5 orals</i> (Conference hall)
RCCT, section 1	<i>7 orals</i> (B204)
RCCT, section 6	<i>5 orals</i> (B203)
SCF	<i>3 orals</i> (Co-working hall)
18.00 – 19.30 (RCCT&SCF)	Poster session (sections 1, 3, 5), SCF
19.30	Quiz

WEDNESDAY (3.07.2024)	
09.00 – 11.40 (<i>RCCT&SCF</i>)	Plenary session (<i>4 reports</i>)
11.40 – 12.15	Lunch
12.30 – 20.30	Excursion RCCT
8.30-17.30	Excursion SCF
THURSDAY (4.07.2024)	
9.00 – 11.00	Plenary session RCCT (<i>3 reports</i>)
11.00 – 11.15	Coffee break
11.15 – 13.00	Oral reports
<i>RCCT, section 2</i>	<i>5 orals</i> (Conference hall)
<i>RCCT, section 4</i>	<i>6 orals</i> (B203)
<i>RCCT, section 1</i>	<i>6 orals</i> (Co-working hall)
<i>RCCT, section of young scientists</i>	<i>10 orals</i> (B204)
13.00 – 14.00	Lunch
14.00 – 16.00	Oral reports
<i>RCCT, section 2</i>	<i>7 orals</i> (Conference hall)
<i>RCCT, section 4</i>	<i>6 orals</i> (B203)
<i>RCCT, Jubilee section</i>	<i>8 orals</i> (Co-working hall)
<i>RCCT, section of young scientists</i>	<i>12 orals</i> (B204)
16.00 – 16.15	Coffee break
16.15 – 18.00	Oral reports
<i>RCCT, sections 1-4</i>	<i>7 orals</i> (Conference hall)
<i>RCCT, section 4</i>	<i>5 orals</i> (B203)
<i>RCCT, section 6</i>	<i>6 orals</i> (Co-working hall)
<i>RCCT, section of young scientists</i>	<i>6 orals</i> (B204)
18.00 – 19.30 <i>RCCT</i>	Poster session (<i>sections 2, 4, 6</i>)
19.45	Table tennis tournament
FRIDAY (5.07.2024)	
9.00 – 11.00	Plenary session (Conference hall) <i>3 reports</i>
11.00 – 12.40	Oral reports
<i>RCCT, section 1</i>	<i>4 orals</i> (Conference hall)
12.00 – 12.15	RCCT-204 Conference closing ceremony

Program of the XXIV International Conference on Chemical Thermodynamics in Russia

MONDAY (1.07.2024) **RCCT&SCF**

11.00 – 15.00	Registration (<i>Flask hall</i>)
15.00 – 15.20	Opening ceremony (<i>Conference hall</i>)
15.20 – 18.00	Plenary session RCCT&SCF (Conference hall) Chairs: <u>Stolyarova V.L., Gavrichev K.S.</u>
15.20 – 16.00	Prof. <u>Solomonov B.N.</u> , M.I. Yagofarov (<i>KFU, Kazan</i>) COMPENSATION RELATIONSHIP IN SOLVATION THERMODYNAMICS OF ORGANIC NON-ELECTROLYTES
16.00 – 16.40	Prof. <u>Markin A.V.</u> , S.S. Sologubov, A.I. Tkachuk, N.N. Smirnova (<i>UNN, Nizhny Novgorod</i>) THERMODYNAMIC PROPERTIES OF C ₆₀ AND C ₇₀ FULLERIDES AND REDOX-ISOMERIC COMPLEXES OF THE TRANSITION METALS
16.40 – 17.20	Prof. <u>Zvereva I.A.</u> (<i>SPbU, Saint Petersburg</i>) PARTICULARITIES OF THE FORMATION MECHANISM OF AND THERMODYNAMIC PROPERTIES OF LAYERED MATERIALS CONSTRUCTED ACCORDING TO THE BLOCK PRINCIPLE
17.20 – 18.00 (on-line)	Prof. <u>Petraccone L.</u> (<i>University of Naples "Federico II", Naples, Italy</i>) THE INTERACTION BETWEEN MODEL BIOMEMBRANES AND THERAPEUTIC PEPTIDES THROUGH THE LENS OF PHYSICAL CHEMISTRY
18.30 – 20.30	Welcome party at Sheremetev Park Hotel, Naumova Street 1

TUESDAY (2.07.2024)

9.00 – 11.00	Plenary session RCCT (Conference hall) Chairs: <u>Verevkin S.P., Kiselev M.G.</u>
9.00 – 09.40	Prof. <u>Victorov A.I.</u> (<i>SPbU, Saint Petersburg</i>) MODELING OF SOFT MESOSCOPIC STRUCTURES: OVER THE 30 YEARS OF MOLECULAR-THERMODYNAMIC LANDSCAPE
9.40 – 10.20 (on-line)	Prof. <u>Idrissi A.</u> (<i>University of Lille, Lille, France</i>) UNRAVELING LOCAL STRUCTURE DYNAMICS IN IONIC LIQUID-SOLVENT MIXTURES: INSIGHTS FROM SPECTROSCOPY, SIMULATION, AND QUANTUM CALCULATIONS
10.20 – 11.00 (on-line)	Prof. <u>Pál Jedlovsky</u> (<i>Eszterházy Károly Catholic University, Eger, Hungary</i>) SURFACE AFFINITY OF SIMPLE IONS IN AQUEOUS SOLUTIONS
11.00 – 11.15	Coffee break (RCCT&SCF)

Oral reports (11.15 – 13.00)

Section 3 «Thermochemistry and Databases», Conference hallChairs: Markin A.V., Usacheva T.R.

11.15 – 11.45 (on-line)	<u>Stefano Vecchio Cipriotti</u> (<i>Italy, Rome</i>) AN EFFUSION AND CALORIMETRIC STUDY ON SIX 5-SUBSTITUTED PHENANTHROLINES (keynote lecture)
11.45 – 12.00	<u>V.A. Vorozhtcov</u> , S.I. Lopatin, V.L. Stolyarova (<i>Saint Petersburg</i>) CALCULATION OF THE THERMODYNAMIC PROPERTIES IN THE SrO-TiO ₂ -ZrO ₂ SYSTEM BASED ON THE SEMI-EMPIRICAL APPROACHES USING THE HIGH TEMPERATURE MASS SPECTROMETRIC DATA

12.00 – 12.15	<u>A.K. Koryttseva</u> , A. Navrotsky, K.E. Smetanina (<i>Nizhny Novgorod</i>) THERMOCHEMISTRY OF SODIUM, IRON, NIOBIUM PHOSPHATE NASICON SOLID SOLUTIONS
12.15 – 12.30	<u>M.A. Bespyatov</u> (<i>Novosibirsk</i>) THERMODYNAMIC AND MAGNETIC PROPERTIES OF YTTERBIUM TRIFLUORIDE AT LOW TEMPERATURES
12.30 – 12.45 (on-line)	Riccardo Testa, Lorenza Romagnoli, Alessandro Latini, <u>Andrea Ciccioni</u> (<i>Italy, Rome</i>) VAPORIZATION BEHAVIOR AND THERMODYNAMIC PROPERTIES OF BaS AND BaZrS ₃
12.45– 13.00 (on-line)	<u>L. Romagnoli</u> , A.R.R.P. Almeida, J.M.S. Ferraz, A. Latini, V.L.S. Freitas, M.D.M.C. Ribeiro da Silva, S. Vecchio Cipriotti, A. Ciccioni (<i>Italy, Rome</i>) THERMODYNAMIC STUDY OF SnI ₄ SUBLIMATION IN A LOW TEMPERATURE RANGE (313 K – 340 K) BY EFFUSION TECHNIQUES

Section 1 «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», B 204

Chairs: Zvereva I.A., Budkov Yu.A.

11.15 – 11.45	<u>S.M. Pestov</u> , A.I. Krasnopyorov (<i>Moscow</i>) THERMODYNAMIC ANALYSIS OF SYSTEMS CONTAINING LIQUID CRYSTALS (keynote lecture)
11.45 – 12.00	<u>A.Y. Zavrazhnov</u> , I.N. Nekrylov, S.S. Berezin, N.Y. Brezhnev, V.Y. Zavaluev, A.V. Kosyakov (<i>Voronezh</i>) PHASE DIAGRAMS FOR THE Ga – S AND Mn – Ga – S SYSTEMS
12.00 – 12.15	<u>O.V. Grineva</u> (<i>Moscow</i>) CAN WE CALCULATE WITH EXPERIMENTAL ACCURACY VOLUMETRIC THERMODYNAMIC PROPERTIES FOR AQUEOUS SOLUTIONS OF NONELECTROLYTES USING MOLECULAR DYNAMICS?
12.15 – 12.30	<u>M.I. Yagofarov</u> , B.N. Solomonov (<i>Kazan</i>) COMPENSATION RELATIONSHIP IN VAPORIZATION THERMODYNAMICS OF ORGANIC NON-ELECTROLYTES AND HEAT CAPACITIES OF LIQUID AND GASEOUS PHASES
12.30 – 12.45	<u>V.D. Kulikov</u> , M.Yu. Belyakov (<i>Moscow</i>) WIDOM LINES IN TRADITIONAL AND “COMPLETE” SCALING MODELS
12.45 – 13.00	<u>V.E. Podnek</u> , Yu.F. Kiyatchenko, I.K. Yudin, B.A. Grigoriev (<i>Moscow</i>) A NEW FULLY INSTRUMENTAL OPTICAL METHOD FOR DETERMINING PARAMETERS OF THE LIQUID-GAS CRITICAL POINT OF MIXTURES

Section 5 «Thermodynamics of Interfacial and Confined Phenomena», B 203

Chairs: Cherkasov D.G., Agafonov A.V.

11.15 – 11.45	<u>D.G. Cherkasov</u> , V.V. Danilina, K.K. Ilin (<i>Saratov</i>) PHYSICO-CHEMICAL SUBSTANTIATION OF THE METHOD OF EXTRACTIVE CRYSTALLIZATION OF SALTS BASED ON THE ANALYSIS OF PHASE DIAGRAMS OF TERNARY SALT – WATER – ANTISOLVENT SYSTEMS (keynote lecture)
11.45 – 12.00	<u>O.Yu. Milyaeva</u> , A.R. Rafikova, K.Yu. Rotanova, B.A. Noskov (<i>Saint Petersburg</i>) SILK FIBROIN ADSORPTION FILMS ON AIR-WATER INTERFACE
12.00 – 12.15	<u>A.V. Akentiev</u> , B.A. Noskov (<i>Saint Petersburg</i>) DYNAMIC SURFACE ELASTICITY OF DISPERSIONS OF BOVINE SERUM ALBUMIN FIBRILS
12.15 – 12.30	<u>A.M. Makarenko</u> , K.V. Zherikova, N.B. Morozova (<i>Novosibirsk</i>) METAL β-DIKETONATES AS PRECURSORS IN MOCVD PROCESSES: THE THERMODYNAMICS OF THEIR EVAPORATION

12.30 – 12.45	M.P. Smotrov , S.N. Balaban (Saratov) INFLUENCE OF TEMPERATURES ON THE SALTING-OUT OF BUTYRIC ACID FROM ITS AQUEOUS SOLUTIONS BY POTASSIUM DIHYDROGEN PHOSPHATE
12.45 – 13.00	K.V. Zherikova (Novosibirsk) PHASE TRANSITION THERMODYNAMICS OF β -DIKETONATE METAL COMPLRXES FOR GAS-PHASE DEPOSITION PROCESSES

Lunch (13.00 – 14.00)

Oral reports (14.00 – 16.00)

Section 3 «Thermochemistry and Databases», B 203

Chairs: Uspenskaya I.A., Barannikov V.P.

14.00 – 14.30	S.I. Lopatin , S.M. Shugurov, O.Yu. Kurapova, A.A. Selyutin (<i>Saint Petersburg</i>) VAPORIZATION AND THERMODYNAMIC PROPERTIES OF $\text{La}_2\text{Zr}_2\text{O}_7$, $\text{Nd}_2\text{Zr}_2\text{O}_7$ AND $\text{Eu}_2\text{Zr}_2\text{O}_7$ STUDIED BY KNUDSEN EFFUSION MASS SPECTROMETRY (keynote lecture)
14.30 – 14.45	I.N. Melnikov , V.G. Kiselev, N.V. Myravyev, A.N. Pivkina (<i>Moscow</i>) PREDICTION OF GAS-PHASE FORMATION ENTHALPIES USING MODERN SEMI-EMPIRICAL METHODS FOR HIGH-THOROUGHPUT SCREENING OF PROMISING ENERGETIC MATERIALS
14.45 – 15.00	D.S. Tsvetkov , M.O. Mazurin, D.A. Malyshkin, V.V. Sereda, I.L. Ivanov, A.A. Zaslavsky (<i>Yekaterinburg</i>) EXPERIMENTAL THERMOCHEMICAL STUDY OF PEROVSKITE-TYPE CsPbX_3 (X – Cl, Br, I) HALIDES AND THERMODYNAMIC MODELLING OF BINARY PHASE DIAGRAMS INVOLVING THESE COMPOUNDS
15.00 – 15.15	A.K. Koryttseva , A. Navrotsky (<i>Nizhny Novgorod</i>) ANALYSIS OF ACID-BASE RELATIONS OF OXIDES BASED ON HIGH TEMPERATURE OXIDE MELT SOLUTION CALORIMETRY
15.15 – 15.30	Yu.A. Sarmini , S.S. Sologubov, N.N. Smirnova, A.V. Markin (<i>Nizhny Novgorod</i>) THERMODYNAMIC STUDY OF SOME REPRESENTATIVES OF THE SYNTHETIC GLUCOCORTICOIDS
15.30 – 15.45	G.V. Vasiliev , V.A. Tikhanova, L.T. Denisova (<i>Krasnoyarsk</i>) STUDY OF THE INFLUENCE ON THE STRUCTURE AND THERMAL PROPERTIES OF ISOVALENT SUBSTITUTION OF BISMUTH FOR EUROPIUM IN TITANATE $\text{Bi}_4\text{Ti}_3\text{O}_{12}$
15.45 – 16.00	A.K. Gatiatulin , M.A. Ziganshin, V.V. Gorbachuk (<i>Kazan</i>) 4D STRUCTURE-PROPERTY STUDIES OF NATIVE CYCLODEXTRINS

Section 1 «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», B 204

Chairs: Pestov S.M., Khodov I.A.

14.00 – 14.30	Yu.K. Tovbin (<i>Moscow</i>) THE SECOND BEGINNING AND CURRENT STATE OF THERMODYNAMICS (keynote lecture)
14.30 – 14.45	V.V. Turovtsev (<i>Tver</i>) CONFORMATIONAL ANALYSIS AS THE BASIS FOR THERMODYNAMIC CALCULATION
14.45 – 15.00	F.N. Bedretdinov , T.V. Chelyuskina (<i>Moscow</i>) ANALYSIS OF THE PHASE BEHAVIOR OF A MULTICOMPONENT SYSTEM IN THE PRESENCE OF A SEPARATING AGENT
15.00 – 15.15	S.V. Pavlova, N.V. Sviridenkova, Yu.M. Artemkina, V.V. Shcherbakov (<i>Moscow</i>) DETERMINATION OF ENTHALPIES OF COMBUSTION OF IONIC LIQUIDS

15.15 – 15.30	V.N. Kuryakov (<i>Moscow</i>) WATER PURITY CONTROL: RESEARCH OF NANOSCALE IMPURITIES AND EVALUATION OF WATER PURIFICATION METHODS USING ULTRAMICROSCOPY
15.30 – 15.45	N.D. Kondratyuk , V.I. Deshchenya, O.V. Kashurin (<i>Moscow</i>) PREDICTING SHEAR VISCOSITIES OF BINARY ORGANIC MIXTURES BY MOLECULAR DYNAMICS METHODS

Section 5 «Thermodynamics of Interfacial and Confined Phenomena», Conference hall

Chairs: **Viktorov A.I., Fedotova M.V.**

14.00 – 14.30 (on-line)	A.N. Khlyupin (<i>Moscow</i>) UNRAVELING THE INFLUENCE OF SURFACE MORPHOLOGY ON PHYSICOCHEMICAL PHENOMENA IN CONFINED FLUIDS: FROM LENNARD-JONES MIXTURES TO ELECTROLYTE SOLUTIONS (keynote lecture)
14.30 – 14.45	I.V. Talyzin, V.M. Samsonov , S.A. Vasilyev, V.V. Puytov, A.A. Romanov (<i>Tver</i>) CONTACT MELTING IN METAL NANOSYSTEMS: MOLECULAR DYNAMICS SIMULATION
14.45 – 15.00	R.D. Oparin (<i>Ivanovo</i>) NEAR-INFRARED SPECTROSCOPY AS AN EFFECTIVE TECHNIQUE TO STUDY CONFORMATIONAL EQUILIBRIA OF LIDOCAINE MOLECULES IN A HIGHLY CONCENTRATED LIDOCAINE SOLUTION IN SUPERCRITICAL CO ₂
15.00 – 15.15	V.V. Danilina , D.G. Cherkasov, V.F. Kurskiy, K.K. Il'in (<i>Saratov</i>) PHASE EQUILIBRIA, SALTING-IN–SALTING-OUT EFFECTS AND EXTRACTIVE CRYSTALLIZATION IN THE TERNARY POTASSIUM IODIDE–WATER–DIISOPROPYLAMINE SYSTEM IN THE RANGE 0–60 °C
15.15 – 15.30	R.A. Babkin , E.A. Vasilieva, F.G. Valeeva, D.M. Kuznetsov, A.P. Lyubina, A.D. Voloshina, L.Ya. Zakharova (<i>Kazan</i>) SELF-ASSEMBLY AND BIOLOGICAL ACTIVITY OF HOMOLOGOUS SERIES OF PYRROLIDINIUM AMPHIPHILES
15.30 – 15.45	P.O. Sorina , A.I. Victorov (<i>Saint Petersburg</i>) DESCRIPTION OF INTERFACIAL BOUNDARIES AND AGGREGATES IN NONIONIC FLUIDS WITH THE AID OF MULTILAYER QUASICHEMICAL MODEL
15.45 – 16.00	S.F. Petrova , S.P. Ivanov, Ed.M. Khamitov (<i>Ufa</i>) LIPOPHILICITY AND SOLUBILITY OF 5-HYDROXY-6-METHYLURACIL AND ITS METHYL DERIVATIVE
16.00 – 16.15	Coffee break (RCCT&SCF)

Oral reports (16.15 – 18.00)

Section 2 «Thermodynamics of Solvation and Complex Formation in Solutions», Conference hall

Chairs: **Kolker A.M., Safonova L.P.**

16.15 – 16.45	R.N. Nagrimanov , A.R. Ibragimova, A.R. Italmasov, A.A. Samatov, B.N. Solomonov (<i>Kazan</i>) THERMOCHEMISTRY OF SOLVATATION AND VAPORIZATION OF MOLECULAR AND IONIC LIQUIDS (keynote lecture)
16.45 – 17.15	I.V. Terekhova (<i>Ivanovo</i>) NON-COVALENT INTERACTIONS OF DRUGS WITH BIORELEVANT MEDIA COMPONENTS (keynote lecture)
17.15 – 17.30	G.I. Egorov , A.A. Kruglyakova, M.E. Nikitin (<i>Ivanovo</i>) STRUCTURAL-THERMODYNAMIC CHARACTERISTICS AND INTERMOLECULAR INTERACTIONS IN GLYCEROL MIXTURES
17.30 – 17.45	V.N. Agieienko , O.V. Kazarina, R. Buchner (<i>Nizhny Novgorod</i>) WHY ETHALINE CANNOT BE REGARDED AS A DEEP EUTECTIC SOLVENT?
17.45 – 18.00	M.D. Chekunova , E.Yu. Tyunina (<i>Ivanovo</i>) ELECTROCHEMICAL CHARACTERISTICS OF LiAsF ₆ SOLUTIONS IN PROPYLENE CARBONATE – DIMETHYLSULFOXIDE

Section 1. «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», B 204

Chairs: Pestov S.M., Khodov I.A.

16.15 – 16.30	<u>T.A. Mukhametzyanov</u> (<i>Kazan</i>) INTERMEDIATE STATES IN PROTEIN FOLDING: EXPERIMENTAL OBSERVATION AND THERMODYNAMIC CONSTRAINTS
16.30 – 16.45	<u>S.M. Orakova</u> , S.M. Rasulov, R.G. Batyrova, I.A. Isaev, I.M. Abdulagatov (<i>Makhachkala</i>) ABRUPT BEHAVIOR OF THE P-T AND C_V -T ISOCHORES TO PRECISELY MEASUREMENT OF THE PHASE TRANSITION AND CRITICAL PROPERTIES OF THE COMPLEX THERMODYNAMIC SYSTEMS
16.45 – 17.00	<u>N.I. Ilinykh</u> , S.A. Lelyukh, B.R. Gelchinskii, A.A. Rempel (<i>Yekaterinburg</i>) INVESTIGATION OF THE POSSIBILITY OF FORMING OF LOW-MELTING HIGH-ENTROPY ALLOYS
17.00 – 17.15	<u>A.A. Osipenko</u> (<i>Yekaterinburg</i>) METHODS OF DEFINING THE DECOMPOSITION TEMPERATURE OF RUTHENIUM TRICHLORIDE DISSOLVED IN LiCl-KCl-CsCl MELT
17.15 – 17.30	<u>A.M. Kut'in</u> , A.D. Plekhovich (<i>Nizhny Novgorod</i>) DYNAMIC CALORIMETRY AS A RESULT OF THEORETICAL PROCESSING OF THERMAL ANALYSIS DATA USING THE EXAMPLE OF SYNTHESIS OF BORATE GLASS-CERAMICS
17.30 – 17.45	<u>T.A. Mukhametzyanov</u> , R.A. Andrianov (<i>Kazan</i>) EXPERIMENTAL ASSESSMENT OF THE PROPERTIES OF CRYSTAL NUCLEI IN THE SUPERCOOLED MELT
17.45 – 18.00	<u>D.M. Makarov</u> , Yu.A. Fadeeva, V.A. Golubev, A.M. Kolker (<i>Ivanovo</i>) A DATA-DRIVEN APPROACH TO DESIGNING DEEP EUTECTIC SOLVENTS AS EFFICIENT CO ₂ ABSORBERS

Section 6 «Thermodynamics of Functional Materials and Engineered Self-Assembly», B 203

Chairs: Toikka A.M., Usoltseva N.V.

16.15 – 16.45	<u>K.V. Pochivalov</u> , A.V. Basko, T.N. Lebedeva, A.N. Ilyasova, M.Y. Yurov (<i>Ivanovo</i>) A NEW LOOK AT THE PHASE EQUILIBRIA IN TERNARY SYSTEMS COMPOSED OF SEMICRYSTALLINE POLYMER, SOLVENT AND NONSOLVENT (keynote lecture)
16.45 – 17.00	<u>V.V. Vasilevskaya</u> (<i>Moscow</i>) ON SOME SPECIFIC FEATURES OF SELF-ASSEMBLY OF AMPHIPHILIC HOMOPOLYMERS
17.15 – 17.30	<u>E.A. Balabanova</u> , S.I. Lopatin, S.M. Shugurov, N.G. Tyurnina, Z.G. Tyurnina (<i>Saint Petersburg</i>) THERMODYNAMIC PROPERTIES OF THE SrO-Al ₂ O ₃ -SiO ₂ SYSTEM STUDIED BY HIGH TEMPERATURE MASS SPECTROMETRY
17.30 – 17.45	<u>A.S. Toikka</u> , M.E. Ilin, N.V. Kamanina (<i>Gatchina</i>) THE METHODS OF CONTROL SURFACE FREE ENERGY IN LASER-ORIENTED DEPOSITED ITO THIN FILMS
17.45 – 18.00	<u>G.A. Buzanov</u> , G.D. Nipan (<i>Moscow</i>) CONCENTRATIONAL TETRAHEDRON OF Li-Mn-Eu-O SYSTEM

18.00 – 19.30 **Poster session (RCCT sections 1, 3, 5 & SCF)**

19.30

Quiz

WEDNESDAY (3.07.2024)

9.00 – 11.00 Plenary session **RCCT&SCF** (Conference hall)Chairs: Viktorov A.I., Uspenskaya I.A.

9.00 – 9.40	Dr. <u>Batalin O.Yu.</u> , N.G. Vafina (<i>Oil and Gas Research Institute RAS, Moscow</i>) ATTRIBUTES OF SUPERCRITICAL FLUID
9.40 – 10.20	Prof. <u>Budkov Yu.A.</u> (<i>HSE University, Moscow</i>) A NEW APPROACH TO CALCULATING MECHANICAL STRESSES IN MOLECULAR SYSTEMS FROM THE FIRST PRINCIPLES OF STATISTICAL PHYSICS. FROM GENERAL THEORY TO SPECIFIC PROBLEMS
10.20 – 11.00	Prof. <u>Toikka A.M.</u> (<i>SPbU, Saint Petersburg</i>) ALTERNATIVE APPROACHES TO THE ANALYSIS OF THERMODYNAMIC STABILITY CONDITIONS AND THEIR FORMULATIONS
11.00 – 11.40	TechnoInfo (<i>Moscow</i>) TIME-RESOLVED FLUORESCENCE SPECTROSCOPY IN RUSSIA THESE DAYS

Lunch (11.40 – 12.15)

Excursion (12.30 – 20.30)

THURSDAY (4.07.2024)

9.00 – 11.00 Plenary session (Conference hall)

Chairs: Zvereva I.A., Kolker A.M.

09.00 – 09.40	Prof. <u>Uspenskaya I.A.</u> (<i>MSU, Moscow</i>) TO THE 100 ANNIVERSARY OF CHEMICAL THERMODYNAMICS LABORATORY AT MSU: PROGRESS IN EXPERIMENTAL AND COMPUTATIONAL METHODS
09.40 – 10.20	Dr. <u>Ksenofontov A.A.</u> , E.V. Antina (<i>ISC RAS, Ivanovo</i>) MOLECULAR COMPLEXES WITH PHOTOINDUCED ENERGY TRANSFER BASED ON DIPYRROMETHENE SERIES COMPOUNDS
10.20 – 11.00	Dr. <u>Rychkov D.A.</u> (<i>ISSCM SB RAS, Novosibirsk</i>) WHY IS IT IMPORTANT TO COMPLEMENT EXPERIMENTS WITH COMPUTATIONAL METHODS FOR MOLECULAR CRYSTALS: CRYSTAL STRUCTURES, THERMODYNAMIC AND MECHANICAL PROPERTIES OF VARIOUS POLYMORPHS

11.00 – 11.15 Coffee break

Oral reports (11.15 – 13.00)

Section 2 «Thermodynamics of Solvation and Complex Formation in Solutions», Conference hallChairs: Nagrimanov R.N., Antina E.V.

11.15 – 11.45	<u>P.A. Nikolaychuk</u> , E. Kozeschnik (<i>Kurgan</i>) THERMODYNAMIC ESTIMATION OF THE PHASE AND CHEMICAL EQUILIBRIA IN THE SYSTEMS Al – Mg – Si – O AND Al – Mg – Si – H ₂ O (keynote lecture)
11.45 – 12.00	<u>M.V. Vener</u> , A.V. Shishkina, A.A. Ksenofontov, N.V. Penkov (<i>Moscow</i>) DICLOFENAC ION HYDRATION: EXPERIMENTAL AND THEORETICAL SEARCH FOR ANION PAIRS
12.00 – 12.15	<u>E.V. Ivanov</u> , D.V. Batov, A.V. Kustov, A.F. Syschenko (<i>Ivanovo</i>) ENTHALPY- HOMOTACTIC PARAMETERS OF INTERACTION FOR UROTROPINE AND SOME

	OTHER BIOACTIVE NITROGEN-CONTAINING CYCLIC NON-ELECTROLYTES AS SOLUTES IN D ₂ O AND H ₂ O AT 298.15 K
12.15 – 12.30	<u>T.Yu. Ivanenko</u> , E.V. Morozov, I.V. Peterson (Krasnoyarsk) PFG NMR STUDY OF LOCAL DYNAMICS AND PHASE BEHAVIOR OF IONIC LIQUIDS RELEVANT TO PETROLEUM ASPHALTENE DISPERSION
12.30 – 12.45	<u>N.A. Bumagina</u> , E.V. Antina, M.B. Berezin (<i>Ivanovo</i>) CHROMO-FLUOROGENIC DIPYRROMETHENE CHEMOSENSORS FOR ZINC IONS DETECTION
12.45 – 13.00	<u>M.S. Gruzdev</u> , U.V. Chervonova, D.V. Starichenko, V.E. Vorobeve, N.G. Bichan (<i>Ivanovo</i>) DENDRIMERIC AZOMETHINE Fe ³⁺ COORDINATION COMPOUNDS CONTAINING CARBAZOLE UNITS

Section 4 «Thermal Analysis and Calorimetry of Substances for Advanced Materials», B 203

Chairs: **Zelenina L.N., V.G. Shevchenko**

11.15 – 11.45	<u>K.S. Gavrichev</u> , V.N. Guskov, P.G. Gagarin, A.V. Khoroshilov, A.V. Guskov (<i>Moscow</i>) THERMODYNAMIC PROPERTIES OF RE TITANATES RE ₂ Ti ₂ O ₇ WITH PYROCHLORE STRUCTURE (keynote lecture)
11.45 – 12.00	<u>L.N. Zelenina</u> , T.P. Chusova, T.V. Rodionova, A.Yu. Manakov, A.V. Sartakova (<i>Novosibirsk</i>) DIFFERENT STATES OF WATER IN α - AND β -CYCLODEXTRIN HYDRATES
12.00 – 12.15	<u>A.S. Kurlov</u> (<i>Yekaterinburg</i>) THERMAL ANALYSIS OF NANOCRYSTALLINE POWDERS OF TRANSITION METAL CARBIDES
12.15 – 12.30	<u>A.E. Musikhin</u> , M.A. Bespyatov, E.F. Miller (<i>Novosibirsk</i>) LOW-TEMPERATURE HEAT CAPACITY OF CADMIUM TUNGSTATE
12.30 – 12.45	<u>N.V. Muravyev</u> (<i>Moscow</i>) MACHINE LEARNING FOR THERMAL STABILITY PREDICTION OF ORGANIC COMPOUNDS
12.45 – 13.00	<u>T.E. Lomakina</u> , O.V. Tolochko (<i>Saint Petersburg</i>) SOL-GEL SYNTHESIS AND CHARACTERIZATION OF 10Gd ₂ O ₃ -90CeO ₂ (MOL.%) PRECURSORS AND CERAMICS

Section 1 «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», Co-working hall

Chairs: **Turovtsev V.V., Kiselev M.G.**

11.15 – 11.45	<u>S.P. Verevkin</u> (<i>Samara</i>) THERMOCHEMISTRY IN 21ST CENTURY – QUO VADIS? IN SILICO ASSISTED DIAGNOSTICS OF AVAILABLE THERMOCHEMICAL DATA (keynote lecture)
11.45 – 12.00	<u>I.A. Velmuzhova</u> (<i>Nizhny Novgorod</i>) CALCULATION OF GERMANE ISOTOPOLOGUES THERMODYNAMIC FUNCTIONS FROM HIGH-RESOLUTION IR SPECTRA
12.00 – 12.15	<u>I.A. Khodov</u> (<i>Ivanovo</i>) INVESTIGATING STRUCTURAL MODIFICATIONS IN MODEL LIPID MEMBRANES WITH DRUGS VIA MAS NMR SPECTROSCOPY
12.15 – 12.30	<u>A.N. Manin</u> , G.L. Perlovich (<i>Ivanovo</i>) APPLICATION OF HYDROGEN BOND PROPENSITY CALCULATIONS TO PREDICT THERMODYNAMIC PARAMETERS OF COCRYSTAL FORMATION
12.30 – 12.45	<u>V.N. Kuryakov</u> , E.G. Gudkova, D.A. Mrachkovskaya, D.D. Ivanova (<i>Moscow</i>) COMPARISON OF THE CAPABILITIES OF DSC AND THE OPTICAL METHOD FOR STUDYING THE PHASE BEHAVIOR OF NANO-SIZED AQUEOUS DISPERSIONS OF N-ALKANES

12.45 – 13.00	<u>D.L. Gurina</u> , Y.A. Budkov (<i>Ivanovo</i>) MOLECULAR DYNAMICS SIMULATION OF SELF-ASSEMBLY OF WATER REVERSE MICELLES WITH IMIDAZOLIUM IONIC LIQUIDS IN SUPERCRITICAL CARBON DIOXIDE
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Section of young scientists, B 204

Chairs: Makarov D.M. Ksenofontov A.A.

11.20 – 11.30	<u>S.P. Tyukina</u> , J.A. Velmiskina, A.O. Dmitrienko, M.G. Medvedev (<i>Moscow</i>) BINOMIAL UNCERTAINTY IN MOLECULAR DYNAMICS-BASED REACTIONS ANALYSIS
11.30 – 11.40	<u>V.S. Safronova</u> , E.N. Korosteleva, A.G. Knyazeva, O.N. Kryukova (<i>Tomsk</i>) TRANSFORMATION MECHANISMS IN POWDER COMPRESSED TI-CUO UNDER CONTROLLED HEATING CONDITIONS
11.40 – 11.50	<u>O.V. Miloshevskaya</u> , A.A. Ksenofontov, E.V. Antina (<i>Ivanovo</i>) TWO-CHANNEL DYE BASED ON BODIPY-CYANINE 7.5 CONJUGATE
11.50 – 12.00	<u>I.I. Bryzgalov</u> , P.S. Bocharov, A.A. Ksenofontov, E.V. Antina (<i>Ivanovo</i>) STUDY OF SUPRAMOLECULAR COMPLEXES FORMED BY BODIPYS AND SERUM ALBUMINS
12.00 – 12.10	<u>V.A. Kalinkina</u> , L.A. Antina, M.B. Berezin, E.V. Antina, V.V. Sharoyko (<i>Ivanovo</i>) NOVEL WATER-SOLUBLE FORMS OF RED-EMITTING BODIPY LUMINOPHORES BASED ON PLURONIC F127: SPECTRAL, STRUCTURAL CHARACTERISTICS AND APPLICATION POSSIBILITIES IN BIOIMAGING
12.10 – 12.20	<u>M.A. Korobov</u> , V.B. Motalov, A.M. Dunaev, L.S. Kudin (<i>Ivanovo</i>) INVESTIGATION OF THERMODYNAMIC PROPERTIES OF RACEMATES OF PROTEINOGENIC AMINO ACIDS
12.20 – 12.30	<u>D.O. Patrushev</u> , A.M. Kut'in, A.D. Plekhovich, A.P. Velmuzhov (<i>Nizhny Novgorod</i>) INVESTIGATION OF STANDART CALORIMETRIC AND VOLUMETRIC PROPERTIES OF GLASSES $(\text{Ge}_{0.21}\text{Te}_{0.79})_{1-x}(\text{AgI})_x$ ($x = 0.1 - 0.5$) WITH A VARYING CONTENT OF SILVER IODIDE
12.30 – 12.40	<u>A.A. Smirnov</u> , M.A. Toikka (<i>Saint Petersburg</i>) SEPARATION EFFICIENCY OF THE 1-BUTANOL – 1-BUTYL FORMATE SYSTEM BY DES BASED ON CHOLINE CHLORIDE
12.40 – 12.50	<u>M.E. Ilin</u> , E.S. Zaikina, A.S. Toikka, Yu.A. Zubtcova, N.V. Kamanina (<i>Saint Petersburg</i>) STUDY OF SPECTRAL, REFRACTIVE, MECHANICAL AND WETTING PROPERTIES OF GRAPHENE OXIDE CONTACTS FOR DISPLAY APPLICATIONS
12.50 – 13.00	<u>S.V. Kuzovchikov</u> , I.A. Bajenova, A.V. Khvan, M.S. Gusakov, A.G. Beresnev, V.V. Cheverikin (<i>Moscow</i>) PHASE EQUILIBRIA OF ALLOYS BASED ON THE CR-TA-W-V SYSTEM

Lunch (13.00 – 14.00)

Oral reports (14.00 – 16.00)

Section 2 «Thermodynamics of Solvation and Complex Formation in Solutions», Conference hall

Chairs: Solomonov B.N., Mamardashvili N. G.

14.00 – 14.30	<u>G.A. Gamov</u> (<i>Ivanovo</i>) INTERACTION OF GOLD(III) WITH SERUM ALBUMINS AND DNA IN AQUEOUS SOLUTION (keynote lecture)
14.30 – 14.45	<u>V.P. Barannikov</u> , V.I. Smirnov, I.N. Mezhevoi, E.Yu. Tyunina (<i>Ivanovo</i>) PATTERNS OF INTERACTION BETWEEN PEPTIDES OF VARIOUS STRUCTURES AND PYRIMIDINE NUCLEIC BASES IN A BUFFERED SALINE MEDIUM ACCORDING TO THE THERMODYNAMIC PARAMETERS OF THE PROCESS

14.45 – 15.00	<u>L.A. Antina</u> , A.A. Kalyagin, V.A. Kalinkina, S.A. Dogadaeva, M.B. Berezin, E.V. Antina (<i>Ivanovo</i>) BODIPY PHOTOSENSITIZERS DELIVERY SYSTEMS: STRUCTURAL AND PHOTOPHYSICAL PROPERTIES
15.00 – 15.15	<u>Yu.V. Ereemeeva</u> , I.R. Gilfanov, G.B. Guseva, L.E. Nikitina, E.V. Antina (<i>Ivanovo</i>) THE EFFECT OF STRUCTURAL AND SOLVATION FACTORS ON SPECTRAL CHARACTERISTICS, STABILITY, AFFINITY TO BIOSTRUCTURES OF α -BODIPY CARBOXYLIC ACID AND ITS CONJUGATES WITH MONOTERPENOIDS
15.30 – 15.45	<u>T.V. Volkova</u> , O.R. Simonova (<i>Ivanovo</i>) SOLUBILITY THERMODYNAMICS AND PERMEABILITY OF RILUZOLE WITH CYCLODEXTRINS AND POLYMERS
15.45 – 16.00	<u>G.B. Guseva</u> , E.V. Antina (<i>Ivanovo</i>) BODIPY CARBOXYLIC ACIDS AND THEIR ETHERS AS FLUORESCENT MARKERS FOR BIOIMAGING

Section 4 «Thermal Analysis and Calorimetry of Substances for Advanced Materials», B 203

Chairs: **Shugurov S.M., Usacheva T.R.**

14.00 – 14.30	<u>V.G. Shevchenko</u> , D.A. Eselevich, A.V. Konyukova, V.N. Krasilnikov (<i>Yekaterinburg</i>) THERMAL ANALYSIS AT THE BASIS OF DEVELOPMENT OF METAL FUEL (keynote lecture)
14.30 – 15.00	<u>S.M. Shugurov</u> , S.I. Lopatin, E.A. Balabanova, D.A. Repin, O.A. Zhinkina (<i>Saint Petersburg</i>) THERMODYNAMIC STUDY OF MULTICOMPONENT OXIDE SYSTEMS ON BASE OF CERIUM OXIDE BY KEMS METHOD (keynote lecture)
15.00 – 15.15	<u>E.Yu. Anikina</u> , V.N. Verbetsky, E.V. Belova, A.V. Gracheva, I.S. Tereshina (<i>Moscow</i>) THERMODYNAMIC ASPECTS OF THE INTERACTION OF HYDROGEN WITH R_2Fe_{17}
15.15 – 15.30	<u>V.G. Matveeva</u> , M.G. Sulman, O.V. Manaenkov, M.E. Grigor'ev, L.Zh. Nikoshvili (<i>Tver</i>) DESIGN OF BIFUNCTIONAL NANOSYSTEMS FOR CATALYTIC PROCESSING OF PLANT BIOMASS
15.30 – 15.45	<u>A.A. Churakova</u> (<i>Ufa</i>) ANALYSIS OF CALORIMETRIC CURVES OF TINI ALLOY WITH MULTIPLE MARTENSITIC TRANSFORMATIONS
15.45 – 16.00	<u>A.E. Musikhin</u> , E.F. Miller (<i>Novosibirsk</i>) LOW-TEMPERATURE HEAT CAPACITY OF ZINC TUNGSTATE

Jubilee section devoted to 100 Anniversary of Chemical Thermodynamics

Laboratory at MSU (Co-working hall)

Chairs: **Uspenskaya I.A., S.P. Verevkin**

14.00 – 14.15	<u>A.V. Khvan</u> , V.V. Cherverikin, S.V. Kuzovchikov, I.A. Bajenova, A.S. Ivanov (<i>Moscow</i>) DATABASES FOR ALLOYS WITH REFRACTORY ELEMENTS: PROBLEMS OF STABLE AND METASTABLE EQUILIBRIA
14.15 – 14.30	<u>I.A. Bajenova</u> , A.V. Khvan, A.V. Kondratiev (<i>Moscow</i>) THIRD-GENERATION CALPHAD ASSESSMENT OF SiO_2 - GeO_2 AND Si - Ge SYSTEMS AT ATMOSPHERIC PRESSURE
14.30 – 14.45	<u>E.G. Kabanova</u> , A.S. Pavlenko, E.A. Ptashkina, V.N. Kuznetsov (<i>Moscow</i>) INFLUENCE OF UNCERTAINTY OF PHASE MODELS' PARAMETERS OF BINARY Au - Pd ON CALPHAD CALCULATION OF THE Au - Ag - Pd TERNARY
14.45 – 15.00	<u>S.V. Kurdakova</u> , Y.Luo (<i>Moscow</i>) SOLID-LIQUID PHASE EQUILIBRIA IN THE K^+ , H^+ Ox^{2-} , Cit^{3-} – H_2O SYSTEM AT 298.15 K
15.00 – 15.15	<u>A.L. Voskov</u> , S.V. Kuzovchikov, A.V. Khvan (<i>Moscow</i>) DEVELOPMENT OF THE COMPUTER PROGRAM FOR CALCULATION OF PHASE EQUILIBRIA IN MULTICOMPONENT SYSTEMS

15.15 – 15.30	E.V. Belova , A.S. Kapelushnikov, A. A. Novikov, I.A. Uspenskaya (<i>Moscow</i>) MODELING OF PHASE EQUILIBRIA AND THERMODYNAMIC PROPERTIES OF PHASES IN WATER-SALT SYSTEMS CONTAINING METHANESULFONATE
15.30 – 15.45	A.A. Novikov , G.A. Knyazhenko, E.V. Belova (<i>Moscow</i>) THERMODYNAMICS AND PHASE EQUILIBRIA IN THE Na^+ , K^+ // H_2PO_4^- , Cl^- – H_2O SYSTEM
15.45 – 16.00	A.S. Arkhipin , A. Pisch, G.M. Zhomin, I.A. Uspenskaya (<i>Moscow</i>) EXPERIMENTAL STUDY AND MOLECULAR DYNAMICS SIMULATION OF PHYSICO-CHEMICAL PROPERTIES OF GLASSES IN THE $\text{CaO-MgO-Al}_2\text{O}_3\text{-TiO}_2$ SYSTEM

Section of young scientists, B 204

Chairs: Mukhametzyanov T.A., Manin A.N.

14.00 – 14.10	I.K. Bakulin (<i>Dolgoprudny</i>) MOLECULAR-LEVEL INSIGHTS TO STRUCTURE AND HYDROGEN BONDS NETWORK OF 1,4-DIOXANE AQUEOUS SOLUTION
14.10 – 14.20	E.K. Kosareva (<i>Moscow</i>) APPLICATION OF ATOMIC FORCE MICROSCOPY TO THE ENERGETIC MATERIALS SUBLIMATION STUDY
14.20 – 14.30	I.S. Nesterova , A.N. Khlyupin, N.M. Evstigneev, O.I. Ryabkov, K.M. Gerke (<i>Moscow</i>) HOW MOLECULAR SCALE ELECTRODE SURFACE STRUCTURE INFLUENCES ELECTRIC DOUBLE LAYER PROPERTIES
14.30 – 14.40	A.D. Radina , A.G. Kvashnin (<i>Moscow</i>) THE DOPING OF $\text{WB}_{(5-x)}$ WITH TRANSITION METALS FOR CATALYTICAL APPLICATION
14.40 – 14.50	K.V. Nikiforova , I.Yu. Gotlib, A.I. Victorov (<i>Saint Petersburg</i>) EFFECTS OF ION charge ASYMMETRY IN MODELING STRUCTURE AND THERMODYNAMIC PROPERTIES OF LINEAR POLYELECTROLYTE SOLUTIONS
14.50 – 15.00	E. Kofanova , M. Deminsky, S. Vasilievskii, D. Shirabaikin, E. Lozben, V. Plaksin, B. Potapkin (<i>Moscow</i>) FLUID WORKBENCH: SOFTWARE TOOL FOR CALCULATION OF THERMO-PHYSICAL AND OPTIC PROPERTIES OF GASES AND PLASMA. APPLICATION FOR ACCURATE CALCULATION OF TRANSPORT AND RADIATION PROPERTIES OF LOW-TEMPERATURE PLASMA OF NOBLE GASES
15.00 – 15.10	P.S. Bocharov , A.A. Ksenofontov, E.V. Antina (<i>Ivanovo</i>) THE INFLUENCE OF THE MOLECULAR STRUCTURE OF BODIPY ON THEIR AFFINITY FOR BLOOD TRANSPORT PROTEINS
15.10 – 15.20	M.G. Nikitina , I.V. Terekhova (<i>Ivanovo</i>) THERMODYNAMICS OF FORMATION OF METHOTREXATE INCLUSION COMPLEXES WITH MODIFIED β -CYCLODEXTRINS
15.20 – 15.30	A.S. Sherudillo , M.M. Lukanov, A.A. Kalyagin, L.A. Antina, M.B. Berezin, E.V. Antina (<i>Ivanovo</i>) HALOGEN-FREE BIS(BODIPY) BICHROMOPHORE PHOTSENSITIZERS: INFLUENCE OF BODIPY UNITS LINKING POSITIONS ON SPECTRAL PROPERTIES AND AGGREGATION BEHAVIORS
15.30 – 15.40	A.A. Garibyan , I.V. Terekhova (<i>Ivanovo</i>) THERMODYNAMICS OF COMPLEX FORMATION OF NATIVE, MODIFIED, DIMERIC AND POLYMERIC CYCLODEXTRINS WITH THE IMMUNOMODULATOR BARICITINIB
15.40 – 15.50	G.Kh. Misikov , A.A. Samarov, M.A. Trofimova (<i>Saint Petersburg</i>) TEMPERATURE VARIATION OF THE CHEMICAL EQUILIBRIUM FOR THE ETHYL ACETATE SYNTHESIS REACTION: EXPERIMENTAL DATA, THERMODYNAMIC ANALYSIS AND CALCULATIONS

Coffee break (16.00 – 16.15)

Oral reports (16.15 – 18.00) Sections 1-4, Conference hall
Chairs: M.I. Yagofarov, G.A. Gamov

16.15 – 16.30 (on-line)	<u>Federica D'Aria</u> , C. Giancola (<i>Naples, Italy</i>) THERMODYNAMIC STUDIES OF NON-CANONICAL NUCLEIC ACID STRUCTURES (section 1)
16.30 – 16.45	A.S. Dubok, <u>D.A. Rychkov</u> (<i>Novosibirsk</i>) STUDY OF MECHANICAL PROPERTIES OF POLYMORPHIC MODIFICATIONS OF 2-PYRAZINCARBOXAMIDE USING COMPUTATIONAL METHODS (section 1)
16.45 – 17.00 (on-line)	<u>D. Alister</u> , F. Villapiano, F. D'Aria, T. Usacheva, L. Mayol, M. Biondi, C. Giancola (<i>Naples, Italy</i>) THERMODYNAMICS OF THE COMPLEXATION OF RUTIN WITH HYDROXYPROPYL- β -CYCLODEXTRIN (section 2)
17.00 – 17.15	<u>A.A. Samarov</u> , S.V. Vostrikov, S.P. Verevkin (<i>Saint Petersburg</i>) A COMBINED APPROACH INCLUDING QUANTUM-CHEMICAL CALCULATIONS AND THE GROUP CONTRIBUTION METHOD FOR PREDICTING THE ENTHALPY OF FORMATION OF ORGANIC COMPOUNDS (section 3)
17.15 – 17.30	<u>K.V. Drozd</u> , D.E. Boycov, O.R. Simonova, A.G. Ramazanova, A.N. Manin, T.V. Volkova (<i>Ivanovo</i>) FORMATION THERMODYNAMICS OF CARBAMAZEPINE COCRYSTALS (section 2)
17.30 – 17.45	<u>A.V. Agafonov</u> , A.V. Noskov, O.V. Alekseeva, V.D. Shibaeva (<i>Ivanovo</i>) THERMAL BEHAVIOR OF IONIC LIQUID/ALUMINOSILICATE IONOGELS (section 2)
17.45 – 18.00	<u>M.D. Kaplina</u> (<i>Moscow</i>) EXPERIMENTAL STUDY ON THE PHASE EQUILIBRIA OF THE PB-SM SYSTEM (section 4)

Section 4 «Thermal Analysis and Calorimetry of Substances for Advanced Materials», B 203
Chairs: Shugurov S.M., Usacheva T.R.

16.15 – 16.30	<u>S.S. Sologubov</u> , A.V. Markin (<i>Nizhny Novgorod</i>) A CALORIMETRIC STUDY OF THE PHASE TRANSFORMATIONS IN THE FUNCTIONAL COMPOUNDS
16.30 – 16.45	<u>K.S. Gavrichev</u> , V.N. Guskov, P.G. Gagarin, A.V. Guskov, A.V. Khoroshilov (<i>Moscow</i>) HEAT CAPACITY AND THERMODYNAMIC PROPERTIES OF REMgAl ₁₁ O ₁₉ (RE=La,Pr,Nd, Sm) HEXALUMINATES WITH MAGNETOPLUMBITE STRUCTURE
16.45 – 17.00	<u>B.A. Rusanov</u> , V.E. Sidorov, J.K. Bukreeva, V.A. Perevyshin, A.A. Sabirzyanov, A.I. Rusanova (<i>Yekaterinburg</i>) DSC, DENSITY, ELECTRICAL RESISTIVITY AND MAGNETIC SUSCEPTIBILITY OF Al-Ni-Co-Cu-Zr HIGH-ENTROPY ALLOYS IN SOLID AND LIQUID STATES
17.00 – 17.15	<u>E.V. Suslova</u> , M.O. Karimova, D.A. Shashurin (<i>Moscow</i>) SYNTHESIS AND THERMOPHYSICAL PROPERTIES OF ONION-LIKE CARBON NANOPARTICLES
17.15 – 17.30	<u>A.D. Plekhovich</u> , A.M. Kut'in, K.V. Balueva, E.E. Rostokina, M.E. Komshina, K.F. Shumovskaya, S.D. Plekhovich (<i>Nizhny Novgorod</i>) STUDY OF THE CONDITIONS FOR THE SYNTHESIS OF GLASS-CERAMICS FROM ULTRADISPERSE PRECURSORS BASED ON Bi ₂ O ₃ -B ₂ O ₃ -BaO GLASS AND YAG BY THERMAL ANALYSIS METHOD

Section 6 «Thermodynamics of Functional Materials and Engineered Self-Assembly», Co-working hall
Chairs: Tkachev N. K, Gorbachuk V.V

16.15 – 16.30	<u>M.N. Gabdulkhaev</u> , V.V. Gorbachuk, M.A. Ziganshin (<i>Kazan</i>) METHOD FOR PREPARING METASTABLE FORMS OF DRUGS
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16.30 – 16.45	<u>I.Sh. Khabriev</u> , V.F. Khairutdinov, I.M. Abdulagatov (<i>Kazan</i>) OBTAINING A COMPOSITE MATERIAL FROM THERMODYNAMICALLY INCOMPATIBLE POLYCARBONATE AND POLYETHYLENE TEREPHTHALATE THROUGH THE DISPERSION PROCESS USING THE METHOD OF SEDS
16.45 – 17.00	<u>A.P. Voronin</u> , A.G. Ramazanova, G.L. Perlovich (<i>Ivanovo</i>) POLYMORPHISM IN MULTICOMPONENT CRYSTALS OF RILUZOLE WITH HYDROXYBENZOIC ACIDS
17.00 – 17.15	<u>N.A. Gribchenkova</u> , A.S. Smirnov, A.S. Alikhanyan (<i>Moscow</i>) EXTRANEIOUS INTERACTIONS IN HIGH-TEMPERATURE MASS SPECTROMETRY STUDIES OF METAL OXIDES
17.15 – 17.30	<u>A.S. Smirnov</u> , N.A. Gribchenkova, K.G. Smorchkov, A.S. Alikhanyan (<i>Moscow</i>) A MASS SPECTROMETRIC INVESTIGATION OF THE VAPORIZATION THERMODYNAMICS OF THE WO ₃ -ZnO SYSTEM
17.30 – 17.45	<u>Yu.F. Kiyatchenko</u> , V.M. Malyshev, V.E. Podnek, V.P. Voronov (<i>Moscow</i>) ADIABATIC CALORIMETRIC STUDY OF PHASE BEHAVIOR OF A BINARY METHANE–PENTANE MIXTURE WITH AN EQUAL WEIGHT FRACTION OF COMPONENTS

Section of young scientists, B 204

Chairs: Mukhametzyanov T.A., Manin A.N.

16.20 – 16.30	<u>A.R. Abdullin</u> , T.A. Mukhametzyanov, I.A. Sedov (<i>Kazan</i>) CRYSTALLIZATION KINETICS OF CROSS-LINKED POLYMERS
16.30 – 16.40	<u>N.A. Isakov</u> , B.A. Noskov, M.V. Belousov, A.A. Nizhnikov (<i>Saint Petersburg</i>) PROPERTIES OF SPREAD LAYERS OF PLANT PROTEIN AGGREGATES
16.40 – 16.50	<u>K.V. Belov</u> , D. Huster, H.A. Scheidt, I.A. Khodov (<i>Ivanovo</i>) SPATIAL STRUCTURE OF FENAMATE MOLECULES IN LIPID BILAYERS: INSIGHTS FROM MAS NOESY
16.50 – 17.00	<u>Y.S. Klimova</u> , N.I. Suvorova, K.E. Zubarev, D.G. Cherkasov (<i>Saratov</i>) SALTING-OUT OF POLYETHYLENE GLYCOL-1500 (PEG-1500) FROM AQUEOUS SOLUTIONS BY CESIUM CHLORIDE AND NITRATE IN THE RANGE OF 10-100°C
17.00 – 17.10	<u>N.U. Volodina</u> , I.V. Prihodko, A.A. Samarov (<i>Saint Petersburg</i>) PHASE EQUILIBRIUM IN PSEUDOTERNARY SYSTEMS OF DEEP EUTECTIC SOLVENTS WITH ESTERS AND ALCOHOLS FOR THE SEPARATION OF AZEOTROPIC MIXTURES
17.10 – 17.20	<u>A.I. Larionov</u> , N.A. Sirotkin (<i>Ivanovo</i>) PLASMA-CHEMICAL SYNTHESIS AND PHYSICO-CHEMICAL PROPERTIES OF NANOSTRUCTURED MXENES OF COMPOSITION TiC _n Cl _x
17.20 – 17.30	<u>K.D. Semavin</u> , N.S. Chilingarov, O.V. Dorofeeva, A.I. Druzhinina, V.Yu. Markov, E.V. Skokan (<i>Moscow</i>) THE EVAPORATION STUDY AND THERMAL STABILITY OF SOME IMIDAZOLIUM-BASED IONIC LIQUIDS

Poster session RCCT, Section 2, 4, 6 (18.00 – 19.30)

19.45	Table tennis tournament
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Friday (5.07.2024)

9.00 – 11.00

Plenary session (Conference hall)

Chairs: Solomonov B.N., Toikka A.M.

09.00 – 9.40	Prof. <u>Samsonov V.M.</u> , I.V. Talyzin, S.A. Vasilyev, V.V. Puytov (<i>TSU, Tver</i>) ON APPLICABILITY OF THE THERMODYNAMIC PHASE AND PHASE TRANSITION CONCEPTS TO NANOPARTICLES AND NANOSYSTEMS
09.40 – 10.20	Dr. <u>Tkachev N.K.</u> , N.P.Kulik, D.A.Rozhentsev, N.I.Shurov (<i>IHTE UB RAS, Ekaterinburg</i>) PREPARATION OF NANOPOROUS METALS BY MEANS OF HIGH-TEMPERATURE ELECTROCHEMICAL DEALLOYING
10.20 – 11.00	Prof. <u>Gorbachuk V.V.</u> , M.N. Gabdul Khaev, K.V. Gataullina, A.K. Gatiatulin, M.A. Ziganshin (<i>KFU, Kazan</i>) THERMODYNAMICS OF DRUG POLYMORPHISM

Oral reports (11.00 – 12.00)

Section 1 «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», Conference hall

Chairs: Malyshev V.M., Kiselev M.G.

11.00 – 11.30	<u>I.A. Sedov</u> , I.Y. Ibraev, T.I. Magsumov (<i>Kazan</i>) EQUILIBRIUM CONFORMATIONAL ENSEMBLES OF A MISFOLDING PEPTIDE UNDER VARIOUS CONDITIONS FROM ATOMISTIC SIMULATIONS (keynote lecture)
11.30 – 11.45 (on-line)	<u>J.M. Silva Ferraz</u> , Lorenza Romagnoli, Marco Magi, Bruno Brunetti, Andrea Ciccioli, Stefano Vecchio Cipriotti (<i>Rome, Italy</i>) DESIGN, CONSTRUCTION AND TESTING OF A NEW DUAL QCM BASED APPARATUS FOR THE DETERMINATION OF VAPORIZATION AND SUBLIMATION ENTHALPIES
11.45 – 12.00	<u>V.G. Kiselev</u> , N.V. Muravyev, K.A. Monogarov, A.N. Pivkina (<i>Novosibirsk</i>) MODERN PREDICTIVE QUANTUM CHEMICAL CALCULATIONS FOR THERMOCHEMISTRY AND DECOMPOSITION KINETICS OF ENERGETIC MATERIALS
12.00 – 12.15 (on-line)	<u>TechnoInfo</u> (<i>Moscow</i>) APPLICATION OF SPUTTERING SYSTEMS TO IMPROVE IMAGE QUALITY IN ELECTRON MICROSCOPY STUDIES

12.15 – 12.30 (RCCT) Conference closing ceremony

**Программа XV Всероссийской школы-конференции молодых учёных «Сверхкритические флюидные технологии в решении экологических проблем» (СКФ),
01-03 июля, Иваново, Шереметьевский проспект, 10**

1 ИЮЛЯ, ПОНЕДЕЛЬНИК

11.00 – 15.00	Регистрация участников
15.00 – 15.20	Открытие конференций RCCT и СКФ
15.20 – 18.00	Совместная пленарная сессия RCCT/СКФ

18.30 – 20.30 Вечер встречи в Шереметьев парк отеле, Наумова, 1

2 ИЮЛЯ, ВТОРНИК

Пленарное заседание СКФ

Коворкинг (9.00 – 11.00)

Председатель заседания: Паренаго Ольга Олеговна

9.00 – 9.30	<u>Проф. Д.А. Леменовский</u> СОВРЕМЕННОЕ СОСТОЯНИЕ ИССЛЕДОВАНИЙ В ХИМИИ СОЕДИНЕНИЙ ЭЛЕМЕНТОВ – «ИНЕРТНЫХ ГАЗОВ» <i>Москва, Московский государственный университет имени М.В. Ломоносова</i>
9.30 – 10.00	<u>Проф. М.Ю. Синев</u> ВОДА ПРИ ВЫСОКИХ ПАРАМЕТРАХ СОСТОЯНИЯ: НА ПУТИ К ФИЗИКО-ХИМИЧЕСКОМУ ОСМЫСЛЕНИЮ <i>Москва, Федеральный исследовательский центр химической физики им. Н.Н. Семенова РАН</i>
10.00 – 10.30	<u>М.О. Костенко</u>, О.О. Паренаго ЭКСПЕРИМЕНТАЛЬНЫЕ АСПЕКТЫ ИЗУЧЕНИЯ ФАЗОВЫХ РАВНОВЕСИЙ В УСЛОВИЯХ ПОВЫШЕННЫХ ДАВЛЕНИЙ <i>Москва, Институт общей и неорганической химии имени Н. С. Курнакова РАН</i>
10.30 – 11.00	<u>А.М. Воробей</u>, М.О. Костенко, Я.И. Зуев, О.О. Паренаго ОЦЕНКА РАСТВОРИМОСТИ МИКРОНИЗУЕМЫХ ВЕЩЕСТВ В СМЕСЯХ CO ₂ -РАСТВОРИТЕЛЬ ПРИ ОСАЖДЕНИИ МЕТОДОМ SAS <i>Москва, Институт общей и неорганической химии имени Н.С. Курнакова РАН</i>
11.00 – 11.20	Перерыв на кофе

Пленарные доклады СКФ

Коворкинг (11.20 – 12.20)

Председатель заседания: проф. Синев Михаил Юрьевич

11.20 – 11.50	<u>Проф. М.Г. Киселев</u>, Р.Д. Опарин, Д.В. Ивлев, Ю.А. Будков, И.А. Ходов КОНФОРМАЦИОННЫЕ РАВНОВЕСИЯ НА ГРАНИЦЕ РАЗДЕЛА ФАЗ КРИСТАЛЛ-СВЕРХКРИТИЧЕСКИЙ ФЛЮИД <i>Иваново, ИХР РАН им. Г.А. Крестова</i>
11.50 – 12.20	<u>А.М. Чибиряев</u> Прогресс в использовании суб- и сверхкритических спиртов в органическом синтезе <i>Новосибирск, Институт катализа им. Г.К. Борескова, СО РАН</i>

Секционные доклады молодых ученых

Коворкинг (12.20 – 13.00)

Председатель заседания: проф. Синев Михаил Юрьевич

12.20 – 12.40	<u>Е.О. Якушина</u> , Т.Р. Билалов ПРИМЕНЕНИЕ СКФ ТЕХНОЛОГИЙ В ОЧИСТКЕ ФАРМАЦЕВТИЧЕСКИХ СУБСТАНЦИЙ <i>Казань, Казанский национальный исследовательский технологический университет</i>
12.40 – 13.00	<u>Е.А. Иванова</u> , В.Г. Меркулов, М.Н. Жарков, С.Г. Злотин РАЗРАБОТКА МЕТОДА ОКИСЛЕНИЯ СУЛЬФИДОВ МОЛЕКУЛЯРНЫМ КИСЛОРОДОМ В ПРИСУТСТВИИ $g\text{-C}_3\text{N}_4$ В СРЕДЕ СВЕРХКРИТИЧЕСКОГО ДИОКСИДА УГЛЕРОДА <i>Москва, ИОХ РАН им. Н.Д. Зелинского</i>
13.00 – 14.00	Обед

Секционные заседания школы СКФ

Коворкинг (14.00 – 16.00)

Председатель заседания: проф. Леменовский Д.А.

14.00 – 14.20	<u>А.А. Онучина</u> , А.В. Фалёва, Д.В. Овчинников, Н.В. Ульяновский НОВЫЙ ПОДХОД К ВЫДЕЛЕНИЮ ЦЕННЫХ БИОЛОГИЧЕСКИ АКТИВНЫХ ЛИГНАНОВ ПРИ ПОМОЩИ ПРЕПАРАТИВНОЙ СВЕРХКРИТИЧЕСКОЙ ФЛЮИДНОЙ ХРОМАТОГРАФИИ <i>Архангельск, Северный (Арктический) Федеральный Университет</i>
14.20 – 14.40	<u>П.Р. Васютин</u> , Ю.А. Гордиенко, М.Ю. Синев, Ю.Д. Ивакин, Е.А. Лагунова, В.Ю. Бычков СИНТЕЗ СМЕШАННЫХ ОКСИДНЫХ Ln-Al ($\text{Ln} = \text{La}, \text{Ce}, \text{Pr}$) КАТАЛИЗАТОРОВ ВЫСОКОТЕМПЕРАТУРНОГО СЕЛЕКТИВНОГО ОКИСЛЕНИЯ ЛЁГКИХ АЛКАНОВ С ИСПОЛЬЗОВАНИЕМ ОБРАБОТКИ ИХ ПРЕДШЕСТВЕННИКОВ ВО ФЛЮИДНЫХ СРЕДАХ <i>Москва, ФИЦ ХФ им. Н.Н. Семенова РАН, г. Москва</i>
14.40 – 15.00	<u>Я.И. Зуев</u> , А.М. Воробей, Я.П. Рубцов, О.О. Паренаго МНОГОКРАТНОЕ ДИСПЕРГИРОВАНИЕ УГЛЕРОДНЫХ НАНОТРУБОК МЕТОДОМ RESS <i>Москва, ИОХ РАН им. Н.Д. Зелинского</i>
15.00 – 15.20	<u>С.А. Алехин</u> , С.В. Морозов, А.А. Востриков, О.Н. Федяева ИНТЕНСИФИКАЦИЯ ОКИСЛЕНИЯ КУРИНОГО ПОМЕТА В СВЕРХКРИТИЧЕСКОЙ ВОДЕ ПРИ ДОБАВЛЕНИИ МЕТАНА <i>Новосибирск, ИОХ им. Н.Н. Ворожцова СО РАН</i>
15.20 – 15.40	<u>А.У. Аетов</u> , Ф.М. Гумеров, Р.А. Усманов, С.В. Мазанов ОКИСЛЕНИЕ ПРОМЫШЛЕННОГО СТОКА ЗАВОДА "БИСФЕНОЛ А" ПАО "КАЗАНЬОРГСИНТЕЗ" В ПЕРИОДИЧЕСКОМ РЕЖИМЕ ПРИ ВЫСОКОМ ДАВЛЕНИИ. <i>Казань, ФГБОУ ВО «Казанский национальный исследовательский технологический университет»</i>
15.40 – 16.00	<u>К.В. Белов</u> , А.А. Дышин, М.А. Крестьянинов, М.Г. Киселев, И.А. Ходов КОНФОРМАЦИОННЫЕ РАВНОВЕСИЯ ФЕНАМАТОВ В СВЕРХКРИТИЧЕСКИХ

	ФЛЮИДАХ НА ГРАНИЦЕ РАЗДЕЛА ФАЗ ФЛЮИД-КРИСТАЛЛ: ИССЛЕДОВАНИЕ МЕТОДОМ NOESY <i>Иваново, ИХР РАН им. Г.А. Крестова</i>
16.00 – 16.20	Перерыв на кофе
Секционное заседание молодых ученых Коворкинг (16.20 – 17.20) <i>Председатель заседания: к.х.н. Паренаго Ольга Олеговна</i>	
16.20 – 16.40	<u>В.Г. Меркулов</u> , С.П. Русаков, Е.А. Иванова, М.Н. Жарков, С.Г. Злотин ОРГАНОКАТАЛИТИЧЕСКОЕ ФОТООКИСЛЕНИЕ КИСЛОРОДОМ В СРЕДЕ ДИОКСИДА УГЛЕРОДА — КЛЮЧ К БЕЗОПАСНЫМ ПРОЦЕССАМ С-Н АКТИВАЦИИ ОРГАНИЧЕСКИХ СОЕДИНЕНИЙ <i>Москва, Институт органической химии им. Н.Д. Зелинского</i>
16.40 – 17.00	<u>Е.И. Перепелкин</u> , И.С. Чащин, В.Г. Васильев, М.А. Синолиц, Г.А. Бадун, М.Г. Чернышева, Н.М. Анучина, Н.П. Бакулева НАНОЧАСТИЦЫ ХИТОЗАНА С ВАНКОМИЦИНОМ, ПОЛУЧЕННЫЕ В БИФАЗНОЙ СИСТЕМЕ ВОДА-УГЛЕКИСЛЫЙ ГАЗ КАК ОСНОВА ПОКРЫТИЯ ДЛЯ БИОПРОТЕЗОВ <i>Москва, ИНЭОС РАН им. А.Н. Несмеянова</i>
17.00 – 17.20	<u>Т.А. Семёнов</u> , Н.М. Ашарчук, Е.О. Епифанов, Н.В. Минаев, Е.И. Мареев РАЗРАБОТКА СИСТЕМЫ КОМПЛЕКСНОЙ IN-SITU ВРЕМЯ-РАЗРЕШЕННОЙ ОПТИЧЕСКОЙ ДИАГНОСТИКИ ОБРАЗОВАНИЯ МИКРО- И НАНОЧАСТИЦ В СВЕРХКРИТИЧЕСКИХ ФЛЮИДАХ <i>Москва, ИФТ, КККиФ, НИЦ "Курчатовский Институт"</i>
17.20 – 18.00	Подведение итогов, Заккрытие школы СКФ
18.00 – 19.30	Стендовая сессия (РССТ&СКФ)
3 ИЮЛЯ, СРЕДА Экскурсия Палех-Шуя 8.00 – 17.30	

Section 1. Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation

ISOTHERMAL TITRATION CALORIMETER FOR STUDYING THE PROCESSES OF DISSOLUTION, MIXING AND COMPLEXATION IN SOLUTIONS D.V. Batov , A.V. Kustov, P.K. Morshnev, A.F. Syshchenko, A.A. Emel'yanov (<i>Ivanovo</i>)	1.1
THE STABILITY OF N-BUTYL ALCOHOL UNDER TEMPERATURE T. A-G. Dzhabbarov , A.R. Bazaev, B.K. Osmanova, E.A. Bazaev (<i>Makhachkala</i>)	1.2
ESTIMATION OF THERMAL PROPERTIES OF ALKYLAMMONIUM HYDROGEN SULFATES USING QUANTUM CHEMICAL DESCRIPTORS K.A. Fedorov , I.V. Fedorova, L.P. Safonova (<i>Ivanovo</i>)	1.3
PREDICTING THE VISCOSITY OF DEEP EUTECTIC SOLVENTS USING MACHINE LEARNING METHODS K.A. Fedorov , A.A. Garibyan, S.D. Galibin, D.M. Makarov (<i>Ivanovo</i>)	1.4
CHEMICAL THERMODYNAMICS ON POST STAMS P.P. Fedorov , E.V. Chernova (<i>Moscow</i>)	1.5
QUATERNARY BIAZEOTROPY IN THE ACETONITRILE + CHLOROFORM + CYCLOHEXENE + WATER SYSTEM A.V. Frolkova , V.I. Zhuchkov, A.K. Frolkova (<i>Moscow</i>)	1.6
PHASE BEHAVIOR FEATURES OF BINARY MIXTURES WITH PRESSURE VARYING A.K. Frolkova , A.V. Frolkova (<i>Moscow</i>)	1.7
A CLASSICAL FORCEFIELD FOR SELENIUM OXYANIONS A.A. Glushak , G.S. Smirnov (<i>Moscow</i>)	1.8
POLY(DIALLYLDIMETHYLAMMONIUM) CATION MOBILITY AND COUNTERION DISTRIBUTION IN WATER AND AQUEOUS SALT SOLUTION FROM MD SIMULATION AND EXPERIMENT I.Yu. Gotlib , E.A. Safonova, P.A. Korchak (<i>Saint Petersburg</i>)	1.9
QSPR-METHOD OF PREDICTION OF VAPORIZATION ENTHALPIES OF ALKYL BENZENES E.L. Krasnykh , A.K. Kazakov, V.S. Sarkisova (<i>Samara</i>)	1.10
INTERACTIONS IN MIXTURES OF CHOLINE CHLORIDE WITH UREA, FORMAMIDE, ETHANOLAMINE AND 1-AMINO-2-PROPANOL OF COMPOSITION 1:2 ACCORDING TO QUANTUM CHEMICAL CALCULATIONS M.A. Krestyaninov , A.M. Kolker (<i>Ivanovo</i>)	1.11
DATA EXCHANGE FILE FORMAT FOR GATHERING THERMOPHYSICAL AND THERMOCHEMICAL EXPERIMENTAL OF MATERIALS S.V. Kuzovchikov , A.V. Khvan, M.I. Nezhurina, I.A. Uspenskaya (<i>Moscow</i>)	1.12
THERMODYNAMIC PROPERTIES AND PHASE EQUILIBRIA OF THE CITRIC ACID – OXALIC ACID – WATER SYSTEM Y. Luo (<i>Moscow</i>)	1.13
MOLECULAR DYNAMICS SIMULATION OF ELECTROLYTES UNDER CONDITIONS OF CONFINED GEOMETRY OF NANOPORES E.G. Odintsova , D.L. Gurina, Yu. A. Budkov (<i>Ivanovo</i>)	1.14
COMPARISON OF THE REDLICH-KISTER-MUGGIANU AND ASSOCIATED SOLUTION MODELS FOR DESCRIBING MELTS WITH STRONG SHORT-RANGE ORDERING IN THE SYSTEMS (Ag, In)–Pd–Sn A.S. Pavlenko , E.G. Kabanova, E.A. Ptashkina, V.N. Kuznetsov (<i>Moscow</i>)	1.15

THEORETICAL MODELING OF THE HEAT CAPACITY IN CoV_2O_4 NEAR PHASE TRANSITIONS: A NEW APPROACH S.V. Pavlov (<i>Moscow</i>)	1.16
STUDY OF THE STABILITY OF THE β -CYCLODEXTRIN/NAPROXEN INCLUSION COMPLEX IN A SUPERCRITICAL SOLVENT USING COMPUTER MODELING METHODS M.L. Antipova, E.G. Odintsova, V.E. Petrenko (<i>Ivanovo</i>)	1.17
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POSTER PRESENTATIONS (RCCT-2024)

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