



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
<i>RCCT, section 3</i>	<i>6 orals</i> (Conference hall)
<i>RCCT, section 1</i>	<i>6 orals</i> (B204)
<i>RCCT, section 5</i>	<i>6 orals</i> (B203)
<i>SCF</i>	<i>2 plenary reports and 2 orals</i> (Coworking)
13.00 – 14.00	Lunch
14.00 – 16.00	Oral reports
<i>RCCT, section 3</i>	<i>7 orals</i> (Conference hall)
<i>RCCT, section 1</i>	<i>6 orals</i> (B204)
<i>RCCT, section 5</i>	<i>7 orals</i> (B203)
<i>SCF</i>	<i>6 orals</i> (Co-working hall)
16.00 – 16.15	Coffee break
16.15 – 18.00	Oral reports
<i>RCCT, section 2</i>	<i>5 orals</i> (Conference hall)
<i>RCCT, section 1</i>	<i>7 orals</i> (B204)
<i>RCCT, section 6</i>	<i>5 orals</i> (B203)
<i>SCF</i>	<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 <i>SCF</i>
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 (<i>on-line</i>)	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 (<i>on-line</i>)	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 (<i>on-line</i>)	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 hall**Chairs: Markin A.V., Usacheva T.R.**

11.15 – 11.45 (<i>on-line</i>)	<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	A.K. Koryttseva , A. Navrotsky, K.E. Smetanina (<i>Nizhny Novgorod</i>) THERMOCHEMISTRY OF SODIUM, IRON, NIOBIUM PHOSPHATE NASICON SOLID SOLUTIONS
12.15 – 12.30	M.A. Bespyatov (<i>Novosibirsk</i>) THERMODYNAMIC AND MAGNETIC PROPERTIES OF YTTERBIUM TRIFLUORIDE AT LOW TEMPERATURES
12.30 – 12.45 (<i>on-line</i>)	Riccardo Testa, Lorenza Romagnoli, Alessandro Latini, Andrea Ciccioli (<i>Italy, Rome</i>) VAPORIZATION BEHAVIOR AND THERMODYNAMIC PROPERTIES OF BaS AND BaZrS ₃
12.45– 13.00 (<i>on-line</i>)	L. Romagnoli , 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. Ciccioli (<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	S.M. Pestov , A.I. Krasnopyorov (<i>Moscow</i>) THERMODYNAMIC ANALYSIS OF SYSTEMS CONTAINING LIQUID CRYSTALS (keynote lecture)
11.45 – 12.00	A.Y. Zavrazhnov , 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	O.V. Grineva (<i>Moscow</i>) CAN WE CALCULATE WITH EXPERIMENTAL ACCURACY VOLUMETRIC THERMODYNAMIC PROPERTIES FOR AQUEOUS SOLUTIONS OF NONELECTROLYTES USING MOLECULAR DYNAMICS?
12.15 – 12.30	M.I. Yagofarov , 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	V.D. Kulikov , M.Yu. Belyakov (<i>Moscow</i>) WIDOM LINES IN TRADITIONAL AND “COMPLETE” SCALING MODELS
12.45 – 13.00	V.E. Podnek , 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	D.G. Cherkasov , 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	O.Yu. Milyaeva , 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	A.V. Akentiev , B.A. Noskov (<i>Saint Petersburg</i>) DYNAMIC SURFACE ELASTICITY OF DISPERSIONS OF BOVINE SERUM ALBUMIN FIBRILS
12.15 – 12.30	A.M. Makarenko , 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 (Saint Petersburg) 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 (Moscow) 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. Malyskin, V.V. Sereda, I.L. Ivanov, A.A. Zaslavsky (Yekaterinburg) 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 (Nizhny Novgorod) 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 (Nizhny Novgorod) THERMODYNAMIC STUDY OF SOME REPRESENTATIVES OF THE SYNTHETIC GLUCOCORTICOIDS
15.30 – 15.45	G.V. Vasiliev , V.A. Tikhanova, L.T. Denisova (Krasnoyarsk) 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 (Kazan) 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 (Moscow) THE SECOND BEGINNING AND CURRENT STATE OF THERMODYNAMICS (keynote lecture)
14.30 – 14.45	V.V. Turvtsev (Tver) CONFORMATIONAL ANALYSIS AS THE BASIS FOR THERMODYNAMIC CALCULATION
14.45 – 15.00	F.N. Bedretdinov , T.V. Chelyuskina (Moscow) 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 (Moscow) 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

BINARY MIXTURES

Section 1. «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», B 204Chairs: 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 ISOCHOES 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 203Chairs: 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. Batalin O.Yu., N.G. Vafina (*Oil and Gas Research Institute RAS, Moscow*) ATTRIBUTES OF SUPERCRITICAL FLUID
- 9.40 – 10.20 Prof. Budkov Yu.A. (*HSE University, Moscow*) 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. Toikka A.M. (*SPbU, Saint Petersburg*) ALTERNATIVE APPROACHES TO THE ANALYSIS OF THERMODYNAMIC STABILITY CONDITIONS AND THEIR FORMULATIONS
- 11.00 – 11.40 **TechnoInfo** (*Moscow*) 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. Uspenskaya I.A. (*MSU, Moscow*) TO THE 100 ANNIVERSARY OF CHEMICAL THERMODYNAMICS LABORATORY AT MSU: PROGRESS IN EXPERIMENTAL AND COMPUTATIONAL METHODS
- 09.40 – 10.20 Dr. Ksenofontov A.A., E.V. Antina (*ISC RAS, Ivanovo*) MOLECULAR COMPLEXES WITH PHOTOINDUCED ENERGY TRANSFER BASED ON DIPYRROMETHENE SERIES COMPOUNDS
- 10.20 – 11.00 Dr. Rychkov D.A. (*ISSCM SB RAS, Novosibirsk*) 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 P.A. Nikolaychuk, E. Kozeschnik (*Kurgan*) THERMODYNAMIC ESTIMATION OF THE PHASE AND CHEMICAL EQUILIBRIA IN THE SYSTEMS Al – Mg – Si – O AND Al – Mg – Si – H₂O (**keynote lecture**)
- 11.45 – 12.00 M.V. Vener, A.V. Shishkina, A.A. Ksenofontov, N.V. Penkov (*Moscow*) DICLOFENAC ION HYDRATION: EXPERIMENTAL AND THEORETICAL SEARCH FOR ANION PAIRS
- 12.00 – 12.15 E.V. Ivanov, D.V. Batov, A.V. Kustov, A.F. Syschenko (*Ivanovo*) ENTHALPY-HOMOTACTIC PARAMETERS OF INTERACTION FOR *UROTOPINE* 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	T.Yu. Ivanenko , 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	N.A. Bumagina , E.V. Antina, M.B. Berezin (<i>Ivanovo</i>) CHROMO-FLUOROGENIC DIPYRROMETHENE CHEMOSENSORS FOR ZINC IONS DETECTION
12.45 – 13.00	M.S. Gruzdev , U.V. Chervonova, D.V. Starichenko, V.E. Vorobeva, 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	K.S. Gavrichev , 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	L.N. Zelenina , 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	A.S. Kurlov (<i>Yekaterinburg</i>) THERMAL ANALYSIS OF NANOCRYSTALLINE POWDERS OF TRANSITION METAL CARBIDES
12.15 – 12.30	A.E. Musikhin , M.A. Bespyatov, E.F. Miller (<i>Novosibirsk</i>) LOW-TEMPERATURE HEAT CAPACITY OF CADMIUM TUNGSTATE
12.30 – 12.45	N.V. Muravyev (<i>Moscow</i>) MACHINE LEARNING FOR THERMAL STABILITY PREDICTION OF ORGANIC COMPOUNDS
12.45 – 13.00	T.E. Lomakina , 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	S.P. Verevkin (<i>Samara</i>) THERMOCHEMISTRY IN 21ST CENTURY – QUO VADIS? IN SILICO ASSISTED DIAGNOSTICS OF AVAILABLE THERMOCHEMICAL DATA (keynote lecture)
11.45 – 12.00	I.A. Velmuzhova (<i>Nizhny Novgorod</i>) CALCULATION OF GERMANE ISOTOPOLOGUES THERMODYNAMIC FUNCTIONS FROM HIGH-RESOLUTION IR SPECTRA
12.00 – 12.15	I.A. Khodov (<i>Ivanovo</i>) INVESTIGATING STRUCTURAL MODIFICATIONS IN MODEL LIPID MEMBRANES WITH DRUGS VIA MAS NMR SPECTROSCOPY
12.15 – 12.30	A.N. Manin , G.L. Perlovich (<i>Ivanovo</i>) APPLICATION OF HYDROGEN BOND PROPENSITY CALCULATIONS TO PREDICT THERMODYNAMIC PARAMETERS OF COCRYSTAL FORMATION
12.30 – 12.45	V.N. Kuryakov , 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 **D.L. Gurina**, Y.A. Budkov (*Ivanovo*) MOLECULAR DYNAMICS SIMULATION OF SELF-ASSEMBLY OF WATER REVERSE MICELLES WITH IMIDAZOLIUM IONIC LIQUIDS IN SUPERCRITICAL CARBON DIOXIDE

Section of young scientists, B 204

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

11.20 – 11.30 **S.P. Tyukina**, J.A. Velmiskina, A.O. Dmitrienko, M.G. Medvedev (*Moscow*) BINOMIAL UNCERTAINTY IN MOLECULAR DYNAMICS-BASED REACTIONS ANALYSIS

11.30 – 11.40 **V.S. Safronova**, E.N. Korosteleva, A.G. Knyazeva, O.N. Kryukova (*Tomsk*) TRANSFORMATION MECHANISMS IN POWDER COMPRESSED TI-CUO UNDER CONTROLLED HEATING CONDITIONS

11.40 – 11.50 **O.V. Miloshevskaya**, A.A. Ksenofontov, E.V. Antina (*Ivanovo*) TWO-CHANNEL DYE BASED ON BODIPY-CYANINE 7.5 CONJUGATE

11.50 – 12.00 **I.I. Bryzgalov**, P.S. Bocharov, A.A. Ksenofontov, E.V. Antina (*Ivanovo*) STUDY OF SUPRAMOLECULAR COMPLEXES FORMED BY BODIPYS AND SERUM ALBUMINS

12.00 – 12.10 **V.A. Kalinkina**, L.A. Antina, M.B. Berezin, E.V. Antina, V.V. Sharoyko (*Ivanovo*) 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 **M.A. Korobov**, V.B. Motalov, A.M. Dunaev, L.S. Kudin (*Ivanovo*) INVESTIGATION OF THERMODYNAMIC PROPERTIES OF RACEMATES OF PROTEINOGENIC AMINO ACIDS

12.20 – 12.30 **D.O. Patrushev**, A.M. Kut'in, A.D. Plekhovich, A.P. Velmuzhov (*Nizhny Novgorod*) 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 **A.A. Smirnov**, M.A. Toikka (*Saint Petersburg*) SEPARATION EFFICIENCY OF THE 1-BUTANOL – 1-BUTYL FORMATE SYSTEM BY DES BASED ON CHOLINE CHLORIDE

12.40 – 12.50 **M.E. Ilin**, E.S. Zaikina, A.S. Toikka, Yu.A. Zubtcova, N.V. Kamanina (*Saint Petersburg*) STUDY OF SPECTRAL, REFRACTIVE, MECHANICAL AND WETTING PROPERTIES OF GRAPHENE OXIDE CONTACTS FOR DISPLAY APPLICATIONS

12.50 – 13.00 **S.V. Kuzovchikov**, I.A. Bajenova, A.V. Khvan, M.S. Gusakov, A.G. Beresnev, V.V. Cheverikin (*Moscow*) 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 **G.A. Gamov** (*Ivanovo*) INTERACTION OF GOLD(III) WITH SERUM ALBUMINS AND DNA IN AQUEOUS SOLUTION (**keynote lecture**)

14.30 – 14.45 **V.P. Barannikov**, V.I. Smirnov, I.N. Mezhevoi, E.Yu. Tyunina (*Ivanovo*) 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 PHOTSENSITIZERS 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	<u>E.V. Belova</u> , 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	<u>A.A. Novikov</u> , 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	<u>A.S. Arkhipin</u> , 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	<u>I.K. Bakulin</u> (<i>Dolgoprudny</i>) MOLECULAR-LEVEL INSIGHTS TO STRUCTURE AND HYDROGEN BONDS NETWORK OF 1,4-DIOXANE AQUEOUS SOLUTION
14.10 – 14.20	<u>E.K. Kosareva</u> (<i>Moscow</i>) APPLICATION OF ATOMIC FORCE MICROSCOPY TO THE ENERGETIC MATERIALS SUBLIMATION STUDY
14.20 – 14.30	<u>I.S. Nesterova</u> , 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	<u>A.D. Radina</u> , A.G. Kvashnin (<i>Moscow</i>) THE DOPING OF $\text{WB}_{(5-x)}$ WITH TRANSITION METALS FOR CATALYTICAL APPLICATION
14.40 – 14.50	<u>K.V. Nikiforova</u> , 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	<u>E. Kofanova</u> , 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	<u>P.S. Bocharov</u> , 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	<u>M.G. Nikitina</u> , I.V. Terekhova (<i>Ivanovo</i>) THERMODYNAMICS OF FORMATION OF METHOTREXATE INCLUSION COMPLEXES WITH MODIFIED β -CYCLODEXTRINS
15.20 – 15.30	<u>A.S. Sherudillo</u> , M.M. Lukanov, A.A. Kalyagin, L.A. Antina, M.B. Berezin, E.V. Antina (<i>Ivanovo</i>) HALOGEN-FREE <i>BIS</i> (BODIPY) BICHROMOPHORE PHOTSENSITIZERS: INFLUENCE OF BODIPY UNITS LINKING POSITIONS ON SPECTRAL PROPERTIES AND AGGREGATION BEHAVIORS
15.30 – 15.40	<u>A.A. Garibyan</u> , 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	<u>G.Kh. Misikov</u> , 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. Gabdulkaev</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. Abdulgatov (<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 Ciccioi, 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 **Проф. Д.А. Леменовский**
СОВРЕМЕННОЕ СОСТОЯНИЕ ИССЛЕДОВАНИЙ В ХИМИИ СОЕДИНЕНИЙ ЭЛЕМЕНТОВ – «ИНЕРТНЫХ ГАЗОВ»
Москва, Московский государственный университет имени М.В. Ломоносова
- 9.30 – 10.00 **Проф. М.Ю. Синев**
ВОДА ПРИ ВЫСОКИХ ПАРАМЕТРАХ СОСТОЯНИЯ: НА ПУТИ К ФИЗИКО-ХИМИЧЕСКОМУ ОСМЫСЛЕНИЮ
Москва, Федеральный исследовательский центр химической физики им. Н.Н. Семенова РАН
- 10.00 – 10.30 **М.О. Костенко, О.О. Паренаго**
ЭКСПЕРИМЕНТАЛЬНЫЕ АСПЕКТЫ ИЗУЧЕНИЯ ФАЗОВЫХ РАВНОВЕСИЙ В УСЛОВИЯХ ПОВЫШЕННЫХ ДАВЛЕНИЙ
Москва, Институт общей и неорганической химии имени Н. С. Курнакова РАН
- 10.30 – 11.00 **А.М. Воробей, М.О. Костенко, Я.И. Зуев, О.О. Паренаго**
ОЦЕНКА РАСТВОРИМОСТИ МИКРОНИЗУЕМЫХ ВЕЩЕСТВ В СМЕСЯХ CO₂-РАСТВОРИТЕЛЬ ПРИ ОСАЖДЕНИИ МЕТОДОМ SAS
Москва, Институт общей и неорганической химии имени Н.С. Курнакова РАН
- 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 **Проф. М.Г. Киселев, Р.Д. Опарин, Д.В. Ивлев, Ю.А. Будков, И.А. Ходов**
КОНФОРМАЦИОННЫЕ РАВНОВЕСИЯ НА ГРАНИЦЕ РАЗДЕЛА ФАЗ КРИСТАЛЛ-СВЕРХКРИТИЧЕСКИЙ ФЛЮИД
Иваново, ИХР РАН им. Г.А. Крестова
- 11.50 – 12.20 **А.М. Чибиряев**
Прогресс в использовании суб- и сверхкритических спиртов в органическом синтезе
Новосибирск, Институт катализа им. Г.К. Борескова, СО РАН

Секционные доклады молодых ученых

Коворкинг (12.20 – 13.00)

Председатель заседания: проф. Синев Михаил Юрьевич

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| 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.

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| 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 (Ln = La, Ce, 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

Иваново, ИХР РАН им. Г.А. Крестова

16.00 – 16.20

Перерыв на кофе

Секционное заседание молодых ученых

Коворкинг (16.20 – 17.20)

Председатель заседания: к.х.н. Паренаго Ольга Олеговна

16.20 – 16.40

В.Г. Меркулов, 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

Москва, Институт органической химии им. Н.Д. Зелинского

16.40 – 17.00

Е.И. Перепелкин, 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

Москва, ИНЭОС РАН им. А.Н. Несмеянова

17.00 – 17.20

Т.А. Семёнов, 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

Москва, ИФТ, КККиФ, НИЦ "Курчатовский Институт"

17.20 – 18.00

Подведение итогов, Закрытие 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. Dzhapparov , 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
MODEL FOR MOLECULAR DYNAMICS SIMULATION OF LIGNIN DEPOLIMERIZATION AND SELF-ASSEMBLY IN WATER-ETHANOL MIXTURE T.V. Bogdan, E.G. Odintsova, M.L. Antipova, K.V. Bogdan, V.E. Petrenko (<i>Ivanovo</i>)	1.18
PAIRWISE ENTROPY AS A STRUCTURE PARAMETER FOR THE DESCRIPTION OF THE GLASS TRANSITION IN MOLECULAR SIMULATIONS V.V. Pisarev , J. Grossi (<i>Moscow</i>)	1.19
QUANTUM CHEMICAL MODELING MOLEKULES OF Bi_2O_3 - B_2O_3 - BaO AND $\text{Re}:\text{YAG}$ COMPONENTS OF GLASS CERAMICS S.D. Plekhovich , A.D. Plekhovich, A.M. Kut'in, K.V. Balueva, E.E. Rostokina, M.E. Komshina, K.F. Shumovskaya (<i>Nizhny Novgorod</i>)	1.20
IN SILICO EXPLORATION OF DRUG-CANDIDATE CONFORMATIONAL SPACE IN SOLVATED ENVIRONMENTS: A COMBINED ATOMISTIC SIMULATION AND MACHINE LEARNING APPROACH D.O. Potapov , V.I. Deshchenya, N.D. Kondratyuk (<i>Dolgoprudny</i>)	1.21
INVESTIGATION OF THE SELECTIVE PROPERTIES OF IONIC LIQUIDS V. I. Zhuchkov, D.A. Ryzhkin , V.M. Raeva (<i>Moscow</i>)	1.22
THE EFFECT OF AN EXTERNAL HOMOGENEOUS AGNETIC FIELD ON THE SYNTHESIS OF Fe_2O_3 NANOPARTICLES IN A PULSED UNDERWATER DISCHARGE PLASMA A.S. Sarapulov , V.V. Korolev, N.A. Sirotkin, O.V. Balmasova (<i>Ivanovo</i>)	1.23
A NEW ALGORITHM FOR CALCULATING THE CONTACT ANGLE OF BINARY MIXTURES IN SLIT PORES A.A. Semenchuk , I.V. Kopanichuk, N.D. Kondratyuk (<i>Moscow</i>)	1.24
ENTHALPIES OF FORMATION OF SOME IONIC LIQUIDS Yu.M. Artemkina, S.V. Pavlova, N.V. Plechkova, V.V. Shcherbakov (<i>Moscow</i>)	1.25
STUDY OF THE INFLUENCE OF TEMPERATURE ON THE CONFORMATIONAL EQUILIBRIA OF LIDOCAINE IN SUPERCRITICAL CARBON DIOXIDE USING 2D NOESY V.V. Sobornova , K.V. Belov, I.A. Khodov (<i>Ivanovo</i>)	1.26
SOLUBILITY OF AFm PHASES AS A FUNCTION OF PAIR ENTROPY E.V. Tararushkin , G.S. Smirnov (<i>Moscow</i>)	1.27
THERMODYNAMIC PROPERTIES OF CALCIUM STANNATE PHASES FROM COMPUTER ATOMISTIC SIMULATIONS T.V. Bogdan, E.V. Tararushkin , Yu.D. Ivakin, N.V. Mashchenko, V.I. Bogdan (<i>Moscow</i>)	1.28
CALCULATION OF THE CHEMICAL POTENTIAL OF WATER IN THE LIQUID FILM ON THE SPHERICAL HYDROPHILIC NANOPARTICLE N.A. Volkov (<i>Saint-Petersburg</i>)	1.29
PREDICTION ENTHALPIES OF VAPORIZATION OF ESTERS OF HYDROXYCARBOXYLIC ACIDS BY QSPR METHOD Y.F. Yamshchikova , E.L. Krasnykh, S.V. Portnova (<i>Samara</i>)	1.30
THE THERMODYNAMIC MODELING OF THE FORMATION OF HIGH-ENTROPY PHASES O.V. Zaitseva , A. Ostovari Moghaddam, K.S. Litvinyuk, E.A. Trofimov (<i>Chelyabinsk</i>)	1.31
VAPOR PHASE AND HETEROGENEOUS EQUILIBRIA IN THE $\text{Ga}-\text{I}$ ($\text{Ga}-\text{Cl}$) SYSTEMS ACCORDING TO THE HT-SPECTROPHOTOMETRIC DATA A.Y. Zavrzhnov , I.N. Nekrylov, S.S. Berezin, N.Y. Brezhnev, V.Y. Zavaluev, A.V. Kosyakov (<i>Voronezh</i>)	1.32

Section 3. Thermochemistry and Databases

THERMODYNAMIC CHARACTERISTICS OF THE ACID-BASE EQUILIBRIUM OF SOME URACIL DERIVATIVES IN WATER A.A. Akhiyarov , S.P. Ivanov (<i>Ufa</i>)	3.1
THE INVESTIGATION OF THE FORMATION ENTHALPY OF RARE-EARTH HAFNATES I.A. Bajenova , A.V. Khvan, A.V. Guskov, P.G. Gagarin, K.S. Gavrichev (<i>Moscow</i>)	3.2
HEAT CAPACITY AND THERMODYNAMIC FUNCTIONS OF CRYSTALLINE URIDINE FROM 0 TO 320 K M.A. Bespyatov (<i>Novosibirsk</i>)	3.3
THERMOCHEMICAL PROPERTIES OF BULKY BENZOQUINONE-TYPE DERIVATIVES AT $T = 298.15$ K P.E. Goryunova , N.N. Smirnova, L.V. Kolesnikova, A.V. Markin (<i>Nizhny Novgorod</i>)	3.4
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