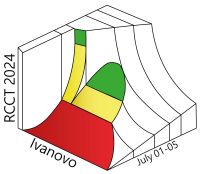

2024 July 1-5

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 Nothern (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), *4 reports*
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 *3 reports RCCT* (Conference hall) *4 reports SCF* (Co-working hall)
11.00 – 11.15	Coffee break
11.15 – 13.00	Oral reports
RCCT**, section 3* ***RCCT**, section 1* ***RCCT**, section 5* ***SCF	*6 orals* (Conference hall) *6 orals* (B204) *6 orals* (B203) *2 plenary reports and 2 orals* (Coworking)
13.00 – 14.00	Lunch
14.00 – 16.00	Oral reports
RCCT**, section 3* ***RCCT**, section 1* ***RCCT**, section 5* ***SCF	*7 orals* (Conference hall) *6 orals* (B204) *7 orals* (B203) *6 orals* (Co-working hall)
16.00 – 16.15	Coffee break
16.15 – 18.00	Oral reports
RCCT**, section 2* ***RCCT**, section 1* ***RCCT**, section 6* ***SCF	*5 orals* (Conference hall) *7 orals* (B204) *5 orals* (B203) *3 orals* (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 *(RCCT&SCF)*	Plenary session (*4 reports)*
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 (*3 reports*)
11.00 – 11.15	Coffee break
11.15 – 13.00	Oral reports
***RCCT**, section 2*	*5 orals* (Conference hall)
***RCCT**, section 4*	*6 orals* (B203)
***RCCT**, section 1*	*6 orals* (Co-working hall)
***RCCT**, section of young scientists*	*10 orals* (B204)
13.00 – 14.00	Lunch
14.00 – 16.00	Oral reports
***RCCT**, section 2*	*7 orals* (Conference hall)
***RCCT**, section 4*	*6 orals* (B203)
***RCCT**, Jubilee section*	*8 orals* (Co-working hall)
***RCCT**, section of young scientists*	*12 orals* (B204)
16.00 – 16.15	Coffee break
16.15 – 18.00	Oral reports
***RCCT**, sections 1-4*	*7 orals* (Conference hall)
***RCCT**, section 4*	*5 orals* (B203)
***RCCT**, section 6*	*6 orals* (Co-working hall)
***RCCT**, section of young scientists*	*6 orals* (B204)
18.00 – 19.30 ***RCCT***	**Poster session (*sections 2, 4, 6)***
19.45	Table tennis tournament
FRIDAY (5.07.2024)	
9.00 – 11.00	Plenary session (Conference hall) *3 reports*
11.00 – 12.40	Oral reports
***RCCT**, section 1*	*4 orals* (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 (*Flask hall*)
15.00 – 15.20	Opening ceremony (*Conference hall*)

15.20 – 18.00 Plenary session *RCCT&SCF* (Conference hall)

Chairs: Stolyarova V.L., Gavrichev K.S.

15.20 – 16.00	Prof. **Solomonov B.N., M.I. Yagofarov** *(KFU, Kazan)* COMPENSATION RELATIONSHIP IN SOLVATION THERMODYNAMICS OF ORGANIC NON-ELECTROLYTES
16.00 – 16.40	Prof. **Markin A.V., S.S. Sologubov, A.I. Tkachuk, N.N. Smirnova** (*UNN, Nizhny Novgorod)* THERMODYNAMIC PROPERTIES OF C_{60} AND C_{70} FULLERIDES AND REDOX-ISOMERIC COMPLEXES OF THE TRANSITION METALS
16.40 – 17.20	Prof. **Zvereva I.A.** (*SPbU, Saint Petersburg*) 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. **Petraccone L.** (*University of Naples "Federico II", Naples, Italy*) 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: Verevkin S.P., Kiselev M.G.

9.00 – 09.40	Prof. **Victorov A.I.** (*SPbU, Saint Petersburg)* MODELING OF SOFT MESOSCOPIC STRUCTURES: OVER THE 30 YEARS OF MOLECULAR-THERMODYNAMIC LANDSCAPE
9.40 – 10.20 ***(on-line)***	Prof. **Idrissi A.** (*University of Lille, Lille, France*) UNRAVELING LOCAL STRUCTURE DYNAMICS IN IONIC LIQUID-SOLVENT MIXTURES: INSIGHTS FROM SPECTROSCOPY, SIMULATION, AND QUANTUM CALCULATIONS
10.20 – 11.00 ***(on-line)***	Prof. **Pál Jedlovszky** (*Eszterházy Károly Catholic University, Eger, Hungary*) 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 ***(on-line)***	**Stefano Vecchio Ciprioti** (*Italy, Rome*) AN EFFUSION AND CALORIMETRIC STUDY ON SIX 5-SUBSTITUTED PHENANTHROLINES **(keynote lecture)**
11.45 – 12.00	**V.A. Vorozhtcov**, S.I. Lopatin, V.L. Stolyarova (*Saint Petersburg*) 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 (*Nizhny Novgorod*) THERMOCHEMISTRY OF SODIUM, IRON, NIOBIUM PHOSPHATE NASICON SOLID SOLUTIONS
12.15 – 12.30	**M.A. Bespyatov** (*Novosibirsk*)THERMODYNAMIC AND MAGNETIC PROPERTIES OF YTTERBIUM TRIFLUORIDE AT LOW TEMPERATURES
12.30 – 12.45 ***(on-line)***	Riccardo Testa, Lorenza Romagnoli, Alessandro Latini, **Andrea Ciccioli** (*Italy, Rome*) VAPORIZATION BEHAVIOR AND THERMODYNAMIC PROPERTIES OF BaS AND $BaZrS_3$
12.45– 13.00 ***(on-line)***	**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 Ciprioti, A. Ciccioli (*Italy, Rome*) 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 (*Moscow*) THERMODYNAMIC ANALYSIS OF SYSTEMS CONTAING 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 (*Voronezh*) PHASE DIAGRAMS FOR THE Ga – S AND Mn – Ga – S SYSTEMS
12.00 – 12.15	**O.V. Grineva** (*Moscow*) 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 (*Kazan*) 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 (*Moscow*) WIDOM LINES IN TRADITIONAL AND "COMPLETE" SCALING MODELS
12.45 – 13.00	**V.E. Podnek**, Yu.F. Kiyatchenko, I.K. Yudin, B.A. Grigoriev (*Moscow*) 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 (Saratov) 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 (*Saint Petersburg*) SILK FIBROIN ADSORPTION FILMS ON AIR-WATER INTERFACE
12.00 – 12.15	**A.V. Akentiev**, B.A. Noskov (*Saint Petersburg*) DYNAMIC SURFACE ELASTICITY OF DISPERSIONS OF BOVINE SERUM ALBUMIN FIBRILS
12.15 – 12.30	**A.M. Makarenko**, K.V. Zherikova, N.B. Morozova (*Novosibirsk*) 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 $La_2Zr_2O_7$, $Nd_2Zr_2O_7$ AND $Eu_2Zr_2O_7$ 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. Malyshkin, 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 $Bi_4Ti_3O_{12}$
15.45 – 16.00	**A.K. Gatiatulin**, M.A. Ziganshin, V.V. Gorbatchuk (*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. Turovtsev** (*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** (*Moscow*) 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 (*Moscow*) 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** (*Moscow*) 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 (*Tver*) CONTACT MELTING IN METAL NANOSYSTEMS: MOLECULAR DYNAMICS SIMULATION
14.45 – 15.00	**R.D. Oparin** (*Ivanovo*) 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 (*Saratov*) 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 (*Kazan*) SELF-ASSEMBLY AND BIOLOGICAL ACTIVITY OF HOMOLOGOUS SERIES OF PYRROLIDINIUM AMPHIPHILES
15.30 – 15.45	**P.O. Sorina**, A.I. Victorov (*Saint Petersburg*) 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 (*Ufa*) 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 (*Kazan*) THERMOCHEMISTRY OF SOLVATATION AND VAPORIZATION OF MOLECULAR AND IONIC LIQUIDS **(keynote lecture)**
16.45 – 17.15	**I.V. Terekhova** (*Ivanovo*) NON-COVALENT INTERACTIONS OF DRUGS WITH BIORELEVANT MEDIA COMPONENTS **(keynote lecture)**
17.15 – 17.30	**G.I. Egorov**, A.A. Kruglyakova, M.E. Nikitin (*Ivanovo*) STRUCTURAL-THERMODYNAMIC CHARACTERISTICS AND INTERMOLECULAR INTERACTIONS IN GLYCEROL MIXTURES
17.30 – 17.45	**V.N. Agieienko**, O.V. Kazarina, R. Buchner (*Nizhny Novgorod*) WHY ETHALINE CANNOT BE REGARDED AS A DEEP EUTECTIC SOLVENT?
17.45 – 18.00	**M.D. Chekunova**, E.Yu. Tyunina (*Ivanovo*) 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 204

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

16.15 – 16.30	**T.A. Mukhametzyanov** (*Kazan*) INTERMEDIATE STATES IN PROTEIN FOLDING: EXPERIMENTAL OBSERVATION AND THERMODYNAMIC CONSTRAINTS
16.30 – 16.45	**S.M. Orakova**, S.M. Rasulov, R.G. Batyrova, I.A. Isaev, I.M. Abdulagatov (*Makhachkala*) 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	**N.I. Ilinykh**, S.A. Lelyukh, B.R. Gelchinskii, A.A. Rempel (*Yekaterinburg)* INVESTIGATION OF THE POSSIBILITY OF FORMING OF LOW-MELTING HIGH-ENTROPY ALLOYS
17.00 – 17.15	**A.A. Osipenko** (*Yekaterinburg*) METHODS OF DEFINING THE DECOMPOSITION TEMPERATURE OF RUTHENIUM TRICHLORIDE DISSOLVED IN LiCl-KCl-CsCl MELT
17.15 – 17.30	**A.M. Kut'in**, A.D. Plekhovich *(Nizhny Novgorod)* 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	**T.A. Mukhametzyanov**, R.A. Andrianov (*Kazan*) EXPERIMENTAL ASSESSMENT OF THE PROPERTIES OF CRYSTAL NUCLEI IN THE SUPERCOOLED MELT
17.45 – 18.00	**D.M. Makarov**, Yu.A. Fadeeva, V.A. Golubev, A.M. Kolker (*Ivanovo*) 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	**K.V. Pochivalov**, A.V. Basko, T.N. Lebedeva, A.N. Ilyasova, M.Y. Yurov (*Ivanovo*) A NEW LOOK AT THE PHASE EQUILIBRIA IN TERNARY SYSTEMS COMPOSED OF SEMICRYSTALLINE POLYMER, SOLVENT AND NONSOLVENT **(keynote lecture)**
16.45 – 17.00	**V.V. Vasilevskaya** (*Moscow*) ON SOME SPECIFIC FEATURES OF SELF-ASSEMBLY OF AMPHIPHILIC HOMOPOLYMERS
17.15 – 17.30	**E.A. Balabanova**, S.I. Lopatin, S.M. Shugurov, N.G. Tyurnina, Z.G. Tyurnina (*Saint Petersburg*) THERMODYNAMIC PROPERTIES OF THE SrO-Al_2O_3-SiO_2 SYSTEM STUDIED BY HIGH TEMPERATURE MASS SPECTROMETRY
17.30 – 17.45	**A.S. Toikka**, M.E. Ilin, N.V. Kamanina (*Gatchina*) THE METHODS OF CONTROL SURFACE FREE ENERGY IN LASER-ORIENTED DEPOSITED ITO THIN FILMS
17.45 – 18.00	**G.A. Buzanov**, G.D. Nipan (*Moscow*) 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, Novosibirk*) 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 hall

Chairs: 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 – H_2O **(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 *UROTROPINE* AND SOME

	OTHER BIOACTIVE NITROGEN-CONTAINING CYCLIC NON-ELECTROLYTES AS SOLUTES IN D_2O AND H_2O 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 (*Ivanovo*) 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 (*Ivanovo*) 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 (*Moscow*) THERMODYNAMIC PROPERTIES OF RE TITANATES $RE_2Ti_2O_7$ WITH PYROCHLORE STRUCTURE **(keynote lecture)**
11.45 – 12.00	**L.N. Zelenina**, T.P. Chusova, T.V. Rodionova, A.Yu. Manakov, A.V. Sartakova (*Novosibirsk*) DIFFERENT STATES OF WATER IN α- AND β-CYCLODEXTRIN HYDRATES
12.00 – 12.15	**A.S. Kurlov** (*Yekaterinburg*) THERMAL ANALYSIS OF NANOCRYSTALLINE POWDERS OF TRANSITION METAL CARBIDES
12.15 – 12.30	**A.E. Musikhin**, M.A. Bespyatov, E.F. Miller (*Novosibirsk*) LOW-TEMPERATURE HEAT CAPACITY OF CADMIUM TUNGSTATE
12.30 – 12.45	**N.V. Muravyev** (*Moscow*) MACHINE LEARNING FOR THERMAL STABILITY PREDICTION OF ORGANIC COMPOUNDS
12.45 – 13.00	**T.E. Lomakina**, O.V. Tolochko (*Saint Petersburg*) SOL-GEL SYNTHESIS AND CHARACTERIZATION OF $10Gd_2O_3$-$90CeO_2$ (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** (*Samara*) THERMOCHEMISTRY IN 21ST CENTURY – QUO VADIS? IN SILICO ASSISTED DIAGNOSTICS OF AVAILABLE THERMOCHEMICAL DATA **(keynote lecture)**
11.45 – 12.00	**I.A. Velmuzhova** (*Nizhny Novgorod*) CALCULATION OF GERMANE ISOTOPOLOGUES THERMODYNAMIC FUNCTIONS FROM HIGH-RESOLUTION IR SPECTRA
12.00 – 12.15	**I.A. Khodov** (*Ivanovo*) INVESTIGATING STRUCTURAL MODIFICATIONS IN MODEL LIPID MEMBRANES WITH DRUGS VIA MAS NMR SPECTROSCOPY
12.15 – 12.30	**A.N. Manin**, G.L. Perlovich (*Ivanovo*) 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 (*Moscow*) 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 $(Ge_{0.21}Te_{0.79})_{1-x}(AgI)_x$ (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	**L.A. Antina**, A.A. Kalyagin, V.A. Kalinkina, S.A. Dogadaeva, M.B. Berezin, E.V. Antina (*Ivanovo*) BODIPY PHOTOSENSITIZERS DELIVERY SYSTEMS: STRUCTURAL AND PHOTOPHYSICAL PROPERTIES
15.00 – 15.15	**Yu.V. Eremeeva**, I.R. Gilfanov, G.B. Guseva, L.E. Nikitina, E.V. Antina (*Ivanovo*) 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	**T.V. Volkova**, O.R. Simonova (*Ivanovo*) SOLUBILITY THERMODYNAMICS AND PERMEABILITY OF RILUZOLE WITH CYCLODEXTRINS AND POLYMERS
15.45 – 16.00	**G.B. Guseva**, E.V. Antina (*Ivanovo*) 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	**V.G. Shevchenko**, D.A. Eselevich, A.V. Konyukova, V.N. Krasilnikov (*Yekaterinburg*) THERMAL ANALYSIS AT THE BASIS OF DEVELOPMENT OF METAL FUEL **(keynote lecture)**
14.30 – 15.00	**S.M. Shugurov**, S.I. Lopatin, E.A. Balabanova, D.A. Repin, O.A. Zhinkina (*Saint Petersburg*) THERMODYNAMIC STUDY OF MULTICOMPONENT OXIDE SYSTEMS ON BASE OF CERIUM OXIDE BY KEMS METHOD **(keynote lecture)**
15.00 – 15.15	**E.Yu. Anikina**, V.N. Verbetsky, E.V. Belova, A.V. Gracheva, I.S. Tereshina (*Moscow*) THERMODYNAMIC ASPECTS OF THE INTERACTION OF HYDROGEN WITH R_2FE_{17}
15.15 – 15.30	**V.G. Matveeva**, M.G. Sulman, O.V. Manaenkov, M.E. Grigor'ev, L.Zh. Nikoshvili (*Tver*) DESIGN OF BIFUNCTIONAL NANOSYSTEMS FOR CATALYTIC PROCESSING OF PLANT BIOMASS
15.30 – 15.45	**A.A. Churakova** (*Ufa*) ANALYSIS OF CALORIMETRIC CURVES OF TINI ALLOY WITH MULTIPLE MARTENSITIC TRANSFORMATIONS
15.45 – 16.00	**A.E. Musikhin**, E.F. Miller (*Novosibirsk*) 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	**A.V. Khvan**, V.V. Cherverikin, S.V. Kuzovchikov, I.A. Bajenova, A.S. Ivanov (*Moscow*) DATABASES FOR ALLOYS WITH REFRACTORY ELEMENTS: PROBLEMS OF STABLE AND METASTABLE EQUILIBRIA
14.15 – 14.30	**I.A. Bajenova**, A.V. Khvan, A.V. Kondratiev (*Moscow*) THIRD-GENERATION CALPHAD ASSESSMENT OF SIO2-GEO2 AND SI-GE SYSTEMS AT ATMOSPHERIC PRESSURE
14.30 – 14.45	**E.G. Kabanova**, A.S. Pavlenko, E.A. Ptashkina, V.N. Kuznetsov (*Moscow*) INFLUENCE OF UNCERTAINTY OF PHASE MODELS' PARAMETERS OF BINARY Au–Pd ON CALPHAD CALCULATION OF THE Au–Ag–Pd TERNARY
14.45 – 15.00	**S.V. Kurdakova**, Y.Luo (*Moscow*) SOLID-LIQIUD PHASE EQUILIBRIA IN THE K^+, H^+ || Ox^{2-}, Cit^{3-} – H_2O SYSTEM AT 298.15 K
15.00 – 15.15	**A.L. Voskov**, S.V. Kuzovchikov, A.V. Khvan (*Moscow*) 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 (*Moscow*) 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 (*Moscow*) 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 (*Moscow*) EXPERIMENTAL STUDY AND MOLECULAR DYNAMICS SIMULATION OF PHYSICO-CHEMICAL PROPERTIES OF GLASSES IN THE CaO-MgO-Al_2O_3-TiO_2 SYSTEM

Section of young scientists, B 204

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

14.00 – 14.10	**I.K. Bakulin** (*Dolgoprudny*) MOLECULAR-LEVEL INSIGHTS TO STRUCTURE AND HYDROGEN BONDS NETWORK OF 1,4-DIOXANE AQUEOUS SOLUTION
14.10 – 14.20	**E.K. Kosareva** (*Moscow*) 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 (*Moscow*) HOW MOLECULAR SCALE ELECTRODE SURFACE STRUCTURE INFLUENCES ELECTRIC DOUBLE LAYER PROPERTIES
14.30 – 14.40	**A.D. Radina**, A.G. Kvashnin (*Moscow*) THE DOPING OF $WB_{(5-x)}$ WITH TRANSITION METALS FOR CATALYTICAL APPLICATION
14.40 – 14.50	**K.V. Nikiforova**, I.Yu. Gotlib, A.I. Victorov (*Saint Petersburg*) 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 (*Moscow*) 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 (*Ivanovo*) 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 (*Ivanovo*) 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 (Ivanovo)* HALOGEN-FREE *BIS*(BODIPY) BICHROMOFORE PHOTOSENSITIZERS: INFLUENCE OF BODIPY UNITS LINKING POSITIONS ON SPECTRAL PROPERTIES AND AGGREGATION BEHAVIORS
15.30 – 15.40	**A.A. Garibyan**, I.V. Terekhova (*Ivanovo*) 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 (*Saint Petersburg*) TEMPARATURE VARIATION OF THE CHEMICAL EQUILIBRIUM FOR THE ETHYL ACETATE SYNTHESIS REACTION: EXPERIMENTAL DATA, THEMODYNAMIC 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)***	**Federica D'Aria**, C. Giancola (*Naples, Italy*) THERMODYNAMIC STUDIES OF NON-CANONICAL NUCLEIC ACID STRUCTURES **(section 1)**
16.30 – 16.45	A.S. Dubok**, D.A. Rychkov** (*Novosibirsk*) STUDY OF MECHANICAL PROPERTIES OF POLYMORPHIC MODIFICATIONS OF 2-PYRAZINCARBOXAMIDE USING COMPUTATIONAL METHODS **(section 1)**
16.45 – 17.00 ***(on-line)***	**D. Alister**, F. Villapiano, F. D'Aria, T. Usacheva, L. Mayol, M. Biondi, C. Giancola (*Naples, Italy*) THERMODYNAMICS OF THE COMPLEXATION OF RUTIN WITH HYDROXYPROPYL-β-CYCLODEXTRIN **(section 2)**
17.00 – 17.15	**A.A. Samarov**, S.V. Vostrikov, S.P. Verevkin (*Saint Petersburg*) 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	**K.V. Drozd**, D.E. Boycov, O.R. Simonova, A.G. Ramazanova, A.N. Manin, T.V. Volkova (*Ivanovo*) FORMATION THERMODYNAMICS OF CARBAMAZEPINE COCRYSTALS **(section 2)**
17.30 – 17.45	**A.V. Agafonov**, A.V. Noskov, O.V. Alekseeva, V.D. Shibaeva (*Ivanovo*) THERMAL BEHAVIOR OF IONIC LIQUID/ALUMINOSILICATE IONOGELS **(section 2)**
17.45 – 18.00	**M.D. Kaplina** (*Moscow*) 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	**S.S. Sologubov**, A.V. Markin (*Nizhny Novgorod*) A CALORIMETRIC STUDY OF THE PHASE TRANSFORMATIONS IN THE FUNCTIONAL COMPOUNDS
16.30 – 16.45	**K.S. Gavrichev**, V.N. Guskov, P.G. Gagarin, A.V. Guskov, A.V. Khoroshilov (*Moscow*) HEAT CAPACITY AND THERMODYNAMIC PROPERTIES OF $REMgAl_{11}O_{19}$ (RE=La,Pr,Nd, Sm) HEXALUMINATES WITH MAGNETOPLUMBITE STRUCTURE
16.45 – 17.00	**B.A. Rusanov**, V.E. Sidorov, J.K. Bukreeva, V.A. Perevyshin, A.A. Sabirzyanov, A.I. Rusanova (*Yekaterinburg*) 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	**E.V. Suslova**, M.O. Karimova, D.A. Shashurin (*Moscow*) SYNTHESIS AND THERMOPHYSICAL PROPERTIES OF ONION-LIKE CARBON NANOPARTICLES
17.15 – 17.30	**A.D. Plekhovich**, A.M. Kut'in, K.V. Balueva, E.E. Rostokina, M.E. Komshina, K.F. Shumovskaya, S.D. Plekhovich (*Nizhny Novgorod*) STUDY OF THE CONDITIONS FOR THE SYNTHESIS OF GLASS-CERAMICS FROM ULTRADISPERSE PRECURSORS BASED ON Bi_2O_3-B_2O_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	**M.N. Gabdulkhaev**, V.V. Gorbatchuk, M.A. Ziganshin (*Kazan*) METHOD FOR PREPARING METASTABLE FORMS OF DRUGS

16.30 – 16.45	**I.Sh. Khabriev**, V.F. Khairutdinov, I.M. Abdulagatov (*Kazan*) OBTAINING A COMPOSITE MATERIAL FROM THERMODYNAMICALLY INCOMPATIBLE POLYCARBONATE AND POLYETHYLENE TEREPHTHALATE THROUGH THE DISPERSION PROCESS USING THE METHOD OF SEDS
16.45 – 17.00	**A.P. Voronin**, A.G. Ramazanova, G.L. Perlovich (Ivanovo) POLYMORPHISM IN MULTICOMPONENT CRYSTALS OF RILUZOLE WITH HYDROXYBENZOIC ACIDS
17.00 – 17.15	**N.A. Gribchenkova**, A.S. Smirnov, A.S. Alikhanyan (*Moscow*) EXTRANEOUS INTERACTIONS IN HIGH-TEMPERATURE MASS SPECTROMETRY STUDIES OF METAL OXIDES
17.15 – 17.30	**A.S. Smirnov**, N.A. Gribchenkova, K.G. Smorchkov, A.S. Alikhanyan (*Moscow*) A MASS SPECTROMETRIC INVESTIGATION OF THE VAPORIZATION THERMODYNAMICS OF THE WO_3-ZnO SYSTEM
17.30 – 17.45	**Yu.F. Kiyatchenko**, V.M. Malyshev, V.E. Podnek, V.P. Voronov (*Moscow*) 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	**A.R. Abdullin**, T.A. Mukhametzyanov, I.A. Sedov (*Kazan*) CRYSTALLIZATION KINETICS OF CROSS-LINKED POLYMERS
16.30 – 16.40	**N.A. Isakov**, B.A. Noskov, M.V. Belousov, A.A. Nizhnikov (*Saint Petersburg*) PROPERTIES OF SPREAD LAYERS OF PLANT PROTEIN AGGREGATES
16.40 – 16.50	**K.V. Belov**, D. Huster, H.A. Scheidt, I.A. Khodov (*Ivanovo*) SPATIAL STRUCTURE OF FENAMATE MOLECULES IN LIPID BILAYERS: INSIGHTS FROM MAS NOESY
16.50 – 17.00	**Y.S. Klimova**, N.I. Suvorova, K.E. Zubarev, D.G. Cherkasov (*Saratov*) 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	**N.U. Volodina**, I.V. Prihodko, A.A. Samarov (*Saint Petersburg*) PHASE EQUILIBRIUM IN PSEUDOTERNARY SYSTEMS OF DEEP EUTECTIC SOLVENTS WITH ESTERS AND ALCOHOLS FOR THE SEPARATION OF AZEOTROPIC MIXTURES
17.10 – 17.20	**A.I. Larionov**, N.A. Sirotkin (*Ivanovo*) PLASMA-CHEMICAL SYNTHESIS AND PHYSICOCHEMICAL PROPERTIES OF NANOSTRUCTURED MXENES OF COMPOSITION TiC_nCl_x
17.20 – 17.30	**K.D. Semavin**, N.S. Chilingarov, O.V. Dorofeeva, A.I. Druzhinina, V.Yu. Markov, E.V. Skokan (*Moscow*) 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**

Friday (5.07.2024)

9.00 – 11.00 Plenary session (Conference hall)

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

09.00 – 9.40	Prof. **Samsonov V.M., I.V. Talyzin, S.A. Vasilyev, V.V. Puytov** (*TSU, Tver*) ON APPLICABILITY OF THE THERMODYNAMIC PHASE AND PHASE TRANSITION CONCEPTS TO NANOPARTICLES AND NANOSYSTEMS
09.40 – 10.20	Dr. **Tkachev N.K., N.P.Kulik, D.A.Rozhentsev, N.I.Shurov (***IHTE UB RAS, Ekaterinburg*) PREPARATION OF NANOPOROUS METALS BY MEANS OF HIGH-TEMPERATURE ELECTROCHEMICAL DEALLOYING
10.20 – 11.00	Prof. **Gorbachuk V.V., M.N. Gabdulkhaev, K.V. Gataullina, A.K. Gatiatulin, M.A. Ziganshin** (*KFU, Kazan*) 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	**I.A. Sedov**, I.Y. Ibraev, T.I. Magsumov *(Kazan)* EQUILIBRIUM CONFORMATIONAL ENSEMBLES OF A MISFOLDING PEPTIDE UNDER VARIOUS CONDITIONS FROM ATOMISTIC SIMULATIONS **(keynote lecture)**
11.30 – 11.45 ***(on-line)***	**J.M. Silva Ferraz**, Lorenza Romagnoli, Marco Magi, Bruno Brunetti, Andrea Ciccioli, Stefano Vecchio Ciprioti (*Rome, Italy*) DESIGN, CONSTRUCTION AND TESTING OF A NEW DUAL QCM BASED APPARATUS FOR THE DETERMINATION OF VAPORIZARION AND SUBLIMATION ENTHALPIES
11.45 – 12.00	**V.G. Kiselev**, N.V. Muravyev, K.A. Monogarov, A.N. Pivkina (*Novosibirsk*) MODERN PREDICTIVE QUANTUM CHEMICAL CALCULATIONS FOR THERMOCHEMISTRY AND DECOMPOSITION KINETICS OF ENERGETIC MATERIALS
12.00 – 12.15 ***(on-line)***	**TechnoInfo** (*Moscow*) 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 CO_2-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

12.20 – 12.40	***Е.О. Якушина**, Т.Р. Билалов* ПРИМЕНЕНИЕ СКФ ТЕХНОЛОГИЙ В ОЧИСТКЕ ФАРМАЦЕВТИЧЕСКИХ СУБСТАНЦИЙ *Казань, Казанский национальный исследовательский технологический университет*
12.40 – 13.00	***Е.А. Иванова**, В.Г. Меркулов, М.Н. Жарков, С.Г. Злотин* РАЗРАБОТКА МЕТОДА ОКИСЛЕНИЯ СУЛЬФИДОВ МОЛЕКУЛЯРНЫМ КИСЛОРОДОМ В ПРИСУТСТВИИ g-C_3N_4 В СРЕДЕ СВЕРХКРИТИЧЕСКОГО ДИОКСИДА УГЛЕРОДА *Москва, ИОХ РАН им. Н.Д. Зелинского*
13.00 – 14.00	**Обед**

Секционные заседания школы СКФ

Коворкинг (14.00 – 16.00)

Председатель заседания: проф. Леменовский Д.А.

14.00 – 14.20	***А.А. Онучина**, А.В. Фалёва, Д.В. Овчинников, Н.В. Ульяновский* НОВЫЙ ПОДХОД К ВЫДЕЛЕНИЮ ЦЕННЫХ БИОЛОГИЧЕСКИ АКТИВНЫХ ЛИГНАНОВ ПРИ ПОМОЩИ ПРЕПАРАТИВНОЙ СВЕРХКРИТИЧЕСКОЙ ФЛЮИДНОЙ ХРОМАТОГРАФИИ *Архангельск, Северный (Арктический) Федеральный Университет*
14.20 – 14.40	***П.Р. Васютин**, 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 *Москва,* ФИЦ ХФ им. Н.Н. Семенова РАН, г. Москва
14.40 – 15.00	***Я.И. Зуев**, А.М. Воробей, Я.П. Рубцов, О.О. Паренаго* МНОГОКРАТНОЕ ДИСПЕРГИРОВАНИЕ УГЛЕРОДНЫХ НАНОТРУБОК МЕТОДОМ RESS *Москва, ИОХ РАН им. Н.Д. Зелинского*
15.00 – 15.20	***С.А. Алехин**, С.В. Морозов, А.А. Востриков, О.Н. Федяева* ИНТЕНСИФИКАЦИЯ ОКИСЛЕНИЯ КУРИНОГО ПОМЕТА В СВЕРХКРИТИЧЕСКОЙ ВОДЕ ПРИ ДОБАВЛЕНИИ МЕТАНА *Новосибирск, ИОХ им. Н.Н. Ворожцова СО РАН*
15.20 – 15.40	***А.У. Аетов**, Ф.М. Гумеров, Р.А. Усманов, С.В.Мазанов* ОКИСЛЕНИЕ ПРОМЫШЛЕННОГО СТОКА ЗАВОДА "БИСФЕНОЛ А" ПАО "КАЗАНЬОРГСИНТЕЗ" В ПЕРИОДИЧЕСКОМ РЕЖИМЕ ПРИ ВЫСОКОМ ДАВЛЕНИИ. *Казань, ФГБОУ ВО «Казанский национальный исследовательский технологический университет»*
15.40 – 16.00	***К.В. Белов**, 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 (RCCT&СКФ)**

3 ИЮЛЯ, СРЕДА

Экскурсия Палех-Шуя

8.00 – 17.30

POSTER PRESENTATIONS (*RCCT&SCF*) **July 2, 2024** **18.00-19.30**

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 *(Ivanovo)*	**1.1**
THE STABILITY OF N-BUTYL ALCOHOL UNDER TEMPERATURE **T. A-G. Dzhapparov**, A.R. Bazaev, B.K. Osmanova, E.A. Bazaev *(Makhachkala)*	**1.2**
ESTIMATION OF THERMAL PROPERTIES OF ALKYLAMMONIUM HYDROGEN SULFATES USING QUANTUM CHEMICAL DESCRIPTORS **K.A. Fedorov**, I.V. Fedorova, L.P. Safonova *(Ivanovo)*	**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 *(Ivanovo)*	**1.4**
CHEMICAL THERMODYNAMICS ON POST STAMS **P.P. Fedorov**, E.V. Chernova *(Moscow)*	**1.5**
QUATERNARY BIAZEOTROPY IN THE ACETONITRILE + CHLOROFORM + CYCLOHEXENE + WATER SYSTEM **A.V. Frolkova**, V.I. Zhuchkov, A.K. Frolkova *(Moscow)*	**1.6**
PHASE BEHAVIOR FEATURES OF BINARY MIXTURES WITH PRESSURE VARYING **A.K. Frolkova**, A.V. Frolkova *(Moscow)*	**1.7**
A CLASSICAL FORCEFIELD FOR SELENIUM OXYANIONS **A.A. Glushak**, G.S. Smirnov *(Moscow)*	**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 *(Saint Petersburg)*	**1.9**
QSPR-METHOD OF PREDICTION OF VAPORIZATION ENTHALPIES OF ALKYLBENZENES **E L. Krasnykh**, A.K. Kazakov, V.S. Sarkisova *(Samara)*	**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 *(Ivanovo)*	**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 *(Moscow)*	**1.12**
THERMODYNAMIC PROPERTIES AND PHASE EQUILIBRIA OF THE CITRIC ACID – OXALIC ACID – WATER SYSTEM **Y. Luo** *(Moscow)*	**1.13**
MOLECULAR DYNAMICS SIMULATION OF ELECTROLYTES UNDER CONDITIONS OF CONFINED GEOMETRY OF NANOPORES **E.G. Odintsova**, D.L. Gurina, Yu. A. Budkov *(Ivanovo)*	**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 *(Moscow)*	**1.15**

THEORETICAL MODELING OF THE HEAT CAPACITY IN CoV_2O_4 NEAR PHASE TRANSITIONS: A NEW APPROACH **S.V. Pavlov** *(Moscow)*	**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** *(Ivanovo)*	**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** *(Ivanovo)*	**1.18**
PAIRWISE ENTROPY AS A STRUCTURE PARAMETER FOR THE DESCRIPTION OF THE GLASS TRANSITION IN MOLECULAR SIMULATIONS **V.V. Pisarev**, J. Grossi *(Moscow)*	**1.19**
QUANTUM CHEMICAL MODELING MOLEKULES OF Bi_2O_3-B_2O_3-BaO AND Re: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 *(Nizhny Novgorod)*	**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 *(Dolgoprudny)*	**1.21**
INVESTIGATION OF THE SELECTIVE PROPERTIES OF IONIC LIQUIDS V. I. Zhuchkov, **D.A. Ryzhkin**, V.M. Raeva *(Moscow)*	**1.22**
THE EFFECT OF AN EXTERNAL HOMOGENEOUS AGNETIC FIELD ON THE SYNTHESIS OF FE2O¬¬3 NANOPARTICLES IN A PULSED UNDERWATER DISCHARGE PLASMA **A.S. Sarapulov**, V.V. Korolev, N.A. Sirotkin, O.V. Balmasova *(Ivanovo)*	**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 *(Moscow)*	**1.24**
ENTHALPIES OF FORMATION OF SOME IONIC LIQUIDS Yu.M. Artemkina, S.V. Pavlova, N.V. Plechkova, **V.V. Shcherbakov** *(Moscow)*	**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 *(Ivanovo)*	**1.26**
SOLUBILITY OF AFm PHASES AS A FUNCTION OF PAIR ENTROPY **E.V. Tararushkin**, G.S. Smirnov *(Moscow)*	**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 *(Moscow)*	**1.28**
CALCULATION OF THE CHEMICAL POTENTIAL OF WATER IN THE LIQUID FILM ON THE SPHERICAL HYDROPHILIC NANOPARTICLE **N.A. Volkov** *(Saint-Petersburg)*	**1.29**
PREDICTION ENTHALPIES OF VAPORIZATION OF ESTERS OF HYDROXYCARBOXYLIC ACIDS BY QSPR METHOD **Y.F. Yamshchikova**, E.L. Krasnykh, S.V. Portnova *(Samara)*	**1.30**
THE THERMODYNAMIC MODELING OF THE FORMATION OF HIGH-ENTROPY PHASES **O.V. Zaitseva**, A. Ostovari Moghaddam, K.S. Litvinyuk, E.A. Trofimov *(Chelyabinsk)*	**1.31**
VAPOR PHASE AND HETEROGENEOUS EQUILIBRIA IN THE Ga – I (Ga – Cl) SYSTEMS ACCORDING TO THE HT-SPECTROPHOTOMETRIC DATA **A.Y. Zavrazhnov**, I.N. Nekrylov, S.S. Berezin, N.Y. Brezhnev, V.Y. Zavaluev, A.V. Kosyakov *(Voronezh)*	**1.32**

Section 3. Thermochemistry and Databases

Section 5. Thermodynamics of Interfacial and Confined Phenomena

UNSUBSTITUTED SUBPHTHALOCYANINE: THERMODYNAMICS OF SUBLIMATION **A.V. Eroshin**, Yu.A. Zhabanov, O.G. Krasnova, G.V. Girichev *(Ivanovo)*	**5.1**
RETENTION INDICES AND ENTHALPY OF SORPTION OF ESTERS OF 3,5-DI-TERT-BUTYL-4-HYDROXYBENZYL ALCOHOL AND DIBASIC CARBOXYLIC ACIDS **D.A. Fetisov**, E.L. Krasnykh, A.S. Kanashin *(Samara)*	**5.2**
SELF-CONSISTENT FIELD THEORY OF POLYELECTROLYTE SOLUTIONS IN CHARGED NANOPORES **N.N. Kalikin**, Y.A. Budkov *(Ivanovo)*	**5.3**
ELUCIDATION OF BICALUTAMIDE CONFORMERS IN DMSO-D6: A COMBINED NMR AND COMPUTATIONAL STUDY **A.A. Mololina**, K.V. Belov, I.A. Khodov *(Ivanovo)*	**5.4**
COMPUTER SIMULATION OF AEROGEL IMPREGNATION WITH MEFENAMIC ACID IN A SUPERCRITICAL CO_2 ENVIRONMENT **R.D. Oparin**, D.V. Ivlev, M.G. Kiselev *(Ivanovo)*	**5.5**
THERMAL STABILITY OF 1-BUTYL-3-METHYLIMIDAZOLIUM DICYANAMIDE IONIC LIQUID TRAPPED IN AN INORGANIC MATRIX SiO_2 **L.M. Ramenskaya**, E.P. Grishina, N.O Kudryakova *(Ivanovo)*	**5.6**
THERMODYNAMIC CHARACTERISTICS OF PHASE TRANSITIONS OF BMImDCA IONIC LIQUID CONFINED IN NANO-POROUS SILICA GEL **L.M. Ramenskaya**, E.P. Grishina, N.O Kudryakova *(Ivanovo)*	**5.7**
POLYMER COMPOSITE MEMBRANES BASED ON meta-POLYBENZIMIDAZOLE AND DIETHYLAMMONIUM MESYLATE PROTIC IONIC LIQUID **N.M. Stelmakh**, I.M. Klimentsov, Yu.A. Fadeeva, L.E. Shmukler, L.P. Safonova *(Ivanovo)*	**5.8**
THERMODYNAMIC ANALYSIS OF HIGH-ENTROPY ALLOYS MELTS OXIDATION S.N. Veselkov, **E.A. Trofimov**, O.V. Zaitseva *(Chelyabinsk)*	**5.9**
THEORY OF ELECTROLYTE SOLUTIONS IN A SLIT CHARGED PORE TAKING INTO ACCOUNT THE STRUCTURAL INTERATIONS OF IONS AND SPECIFIC ION ADSORPTION **V.A. Vasileva**, D.A. Mazur, Y.A. Budkov *(Moscow)*	**5.10**
COARSE-GRAIN DESCRIPTION OF FLUID INTERFACES APPLYING MULTILAYER QUASICHEMICAL MODEL P.O. Sorina, **A.I. Victorov** *(Saint Petersburg)*	**5.11**
LIQUID-LIQUID EQUILIBRIUM OF QUATERNARY SYSTEM LACTIC ACID - N-BUTANOL - N-BUTYL LACTATE – WATER AT 298.15 K **Y.F. Yamshchikova**, E.L. Krasnykh, S.V. Portnova *(Samara)*	**5.12**
ENTHALPY OF SUBLIMATION OF VO-ETIOP-III PETROPORPHYRIN **Yu.A. Zhabanov**, A.V. Eroshin, G.L. Pakhomov *(Ivanovo)*	**5.13**

XV Всероссийская школа-конференция молодых учёных «Сверхкритические флюидные технологии в решении экологических проблем»

АНАЛИЗ ГИДРАЗИНА, МЕТИЛГИДРАЗИНА И 1,1-ДИМЕТИЛГИДРАЗИНА МЕТОДОМ СВЕРХКРИТИЧЕСКОЙ ФЛЮИДНОЙ ХРОМАТОГРАФИИ-ТАНДЕМНОЙ МАСС-СПЕКТРОМЕТРИИ ПОСЛЕ ДЕРИВАТИЗАЦИИ 5-НИТРО-2-ФУРАЛЬДЕГИДОМ **С.А. Вахрамеев**, Д.В. Овчинников, Д.С. Косяков, Н.В. Ульяновский *(Архангельск)*	**СКФ1**
СИНТЕЗ И ДОПИРОВАНИЕ АЭРОГЕЛЕЙ НА ОСНОВЕ НАНОКРИСТАЛЛИЧЕСКОЙ ЦЕЛЛЮЛОЗЫ **М.С. Кузьмиков**, А.А. Дышин, М.Г. Киселев *(Иваново)*	**СКФ2**
ПОЛУЧЕНИЕ БИОЛОГИЧЕСКИ АКТИВНЫХ СОЕДИНЕНИЙ ИЗ ЭКСТРАКТОВ	**СКФ3**

КОМПРЕССИОННОЙ ДРЕВЕСИНЫ ОСИНЫ С ПРИМЕНЕНИЕМ ПРЕПАРАТИВНОЙ СВЕРХКРИТИЧЕСКОЙ ФЛЮИДНОЙ ХРОМАТОГРАФИИ **А.А. Онучина**, А.В. Фалёва, Э.В. Данилова, Н.В. Ульяновский *(Архангельск)*	
ОПЫТ ПРИМЕНЕНИЯ СВЕРХКРИТИЧЕСКИХ ФЛЮИДНЫХ ТЕХНОЛОГИЙ ДЛЯ ОЧИСТКИ НЕФТЕЗАГРЯЗНЕННЫХ ПОЧВ **А.З. Попова**, Д.И. Панюкова, Т.А. Марютина *(Долгопрудный)*	**СКФ4**
ИССЛЕДОВАНИЕ ПРОЦЕССОВ СОРБЦИИ КОМПОЗИТНЫХ МАТЕРИАЛОВ НА ОСНОВЕ АЭРОГЕЛЯ И МЕФЕНАМОВОЙ КИСЛОТЫ $СКСО_2$ ПРИ ПОМОЩИ СПЕКТРОСКОПИИ ЯМР **В.В. Соборнова**, К.В. Белов, И.А. Ходов *(Иваново)*	**СКФ5**

POSTER PRESENTATIONS (*RCCT-2024)* **July 4, 2024** **18.00-19.30**

Section 2. Thermodynamics of Solvation and Complex Formation in Solutions

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FEATURES OF HYDRATION AND COMPLEX FORMATION OF PROTEIN TYROSINE PHOSPHATASE 1B S.E. Kruchinin, E.E. Kislinskaya, **M.V. Fedotova** *(Ivanovo)*	**2.3**
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PHOTOACTIVE β-DIKETONATE COMPLEXES. SYNTHESIS AND CHARACTERISATION U.V. Chervonova, Ksenofontov A.A., Viushin A.A., **Gruzdev M.S.** *(Ivanovo)*	**2.5**
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MIXED LIGAND COMPLEX FORMATION OF ZINC AND NICKEL(II) IONS WITH HISTIDINE, LYSINE AND ARGININE IN AQUEOUS SOLUTION **Y.E.Karaseva**, D.F.Pyreu *(Ivanovo)*	**2.10**
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SPECTRAL FEATURES OF INTERACTION OF HEMIN AND ZINC PORPHYRIN WITH SODIUM HEXAMOLYBDENICELATE **I.V. Klimenko**, E.V. Kitushina, A.V. Oreshkina, A.V. Lobanov *(Moscow)*	**2.12**

SPECTRAL PROPERTIES OF SUPRAMOLECULAR COMPLEXES BASED ON CYCLODEXTRIN AND 5,10,15,20-TETRAPHENYLPORPHYRIN **I.V. Klimenko**, E.S. Nersesyan, A.V. Lobanov *(Moscow)*	**2.13**
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