

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)

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)
SCF	<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)
SCF	<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)
SCF	<i>3 orals</i> (Co-working hall)
18.00 – 19.30 (RCCT&SCF)	Poster session (sections 1, 3, 5), SCF
19.30	Quiz

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

**Program of the XXIV International Conference on Chemical Thermodynamics
in Russia**

MONDAY (1.07.2024)

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

RCCT&SCF

11.00 – 15.00 Registration (*Flask hall*)

15.00 – 15.20 Opening ceremony (*Conference hall*)

Plenary session *RCCT&SCF* (Conference hall)

15.20 – 18.00

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 C₆₀ AND C₇₀ 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 Prof. Petraccone L. (*University of Naples "Federico II", Naples, Italy*) THE INTERACTION BETWEEN MODEL BIOMEMBRANES AND THERAPEUTIC PEPTIDES THROUGH THE LENS OF PHYSICAL CHEMISTRY
(on-line)

Welcome party at Sheremetev Park Hotel, Naumova Street 1

18.30 – 20.30

TUESDAY (2.07.2024)

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

Plenary session *RCCT* (Conference hall)**9.00 – 11.00****Chairs: Verevkin S.P., Kiselev M.G.**

9.00 – 09.40	Prof. Victorov A.I. (<i>SPbU, Saint Petersburg</i>) MODELING OF SOFT MESOSCOPIC STRUCTURES: OVER THE 30 YEARS OF MOLECULAR-THERMODYNAMIC LANDSCAPE
9.40 – 10.20 (on-line)	Prof. Idrissi A. (<i>University of Lille, Lille, France</i>) UNRAVELING LOCAL STRUCTURE DYNAMICS IN IONIC LIQUID-SOLVENT MIXTURES: INSIGHTS FROM SPECTROSCOPY, SIMULATION, AND QUANTUM CALCULATIONS
10.20 – 11.00 (on-line)	Prof. Pál Jedlovsky (<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 (on-line)	Stefano Vecchio Cipriotti (<i>Italy, Rome</i>) 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 (<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 (on-line)	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 (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 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	<u>S.M. Pestov</u> , A.I. Krasnopyorov (<i>Moscow</i>) THERMODYNAMIC ANALYSIS OF SYSTEMS CONTAINING LIQUID CRYSTALS (keynote lecture)
11.45 – 12.00	<u>A.Y. Zavrazhnov</u> , I.N. Nekrylov, S.S. Berezin, N.Y. Brezhnev, V.Y. Zavaluev, A.V. Kosyakov (<i>Voronezh</i>) PHASE DIAGRAMS FOR THE Ga – S AND Mn – Ga – S SYSTEMS
12.00 – 12.15	<u>O.V. Grineva</u> (<i>Moscow</i>) CAN WE CALCULATE WITH EXPERIMENTAL ACCURACY VOLUMETRIC THERMODYNAMIC PROPERTIES FOR AQUEOUS SOLUTIONS OF NONELECTROLYTES USING MOLECULAR DYNAMICS?
12.15 – 12.30	<u>M.I. Yagofarov</u> , B.N. Solomonov (<i>Kazan</i>) COMPENSATION RELATIONSHIP IN VAPORIZATION THERMODYNAMICS OF ORGANIC NON-ELECTROLYTES AND HEAT CAPACITIES OF LIQUID AND GASEOUS PHASES
12.30 – 12.45	<u>V.D. Kulikov</u> , M.Yu. Belyakov (<i>Moscow</i>) WIDOM LINES IN TRADITIONAL AND "COMPLETE" SCALING MODELS
12.45 – 13.00	<u>V.E. Podnek</u> , Yu.F. Kiyatchenko, I.K. Yudin, B.A. Grigoriev (<i>Moscow</i>) A NEW FULLY INSTRUMENTAL OPTICAL METHOD FOR DETERMINING PARAMETERS OF THE LIQUID-GAS CRITICAL POINT OF MIXTURES

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

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

11.15 – 11.45	<u>D.G. Cherkasov</u> , V.V. Danilina, K.K. Ilin (<i>Saratov</i>) PHYSICO-CHEMICAL SUBSTANTIATION OF THE METHOD OF EXTRACTIVE CRYSTALLIZATION OF SALTS BASED ON THE ANALYSIS OF PHASE DIAGRAMS OF TERNARY SALT – WATER – ANTISOLVENT SYSTEMS (keynote lecture)
11.45 – 12.00	<u>O.Yu. Milyaeva</u> , A.R. Rafikova, K.Yu. Rotanova, B.A. Noskov (<i>Saint Petersburg</i>) SILK FIBROIN ADSORPTION FILMS ON AIR-WATER INTERFACE
12.00 – 12.15	<u>A.V. Akentiev</u> , B.A. Noskov (<i>Saint Petersburg</i>) DYNAMIC SURFACE ELASTICITY OF DISPERSIONS OF BOVINE SERUM ALBUMIN FIBRILS

12.15 – 12.30	<u>A.M. Makarenko</u> , K.V. Zherikova, N.B. Morozova (<i>Novosibirsk</i>) METAL β -DIKETONATES AS PRECURSORS IN MOCVD PROCESSES: THE THERMODYNAMICS OF THEIR EVAPORATION
12.30 – 12.45	<u>M.P. Smotrov</u> , S.N. Balaban (<i>Saratov</i>) INFLUENCE OF TEMPERATURES ON THE SALTING-OUT OF BUTYRIC ACID FROM ITS AQUEOUS SOLUTIONS BY POTASSIUM DIHYDROGEN PHOSPHATE
12.45 – 13.00	<u>K.V. Zherikova</u> (<i>Novosibirsk</i>) 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	<u>S.I. Lopatin</u> , S.M. Shugurov, O.Yu. Kurapova, A.A. Selyutin (<i>Saint Petersburg</i>) VAPORIZATION AND THERMODYNAMIC PROPERTIES OF $\text{La}_2\text{Zr}_2\text{O}_7$, $\text{Nd}_2\text{Zr}_2\text{O}_7$ AND $\text{Eu}_2\text{Zr}_2\text{O}_7$ STUDIED BY KNUDSEN EFFUSION MASS SPECTROMETRY (keynote lecture)
14.30 – 14.45	<u>I.N. Melnikov</u> , V.G. Kiselev, N.V. Myravyev, A.N. Pivkina (<i>Moscow</i>) PREDICTION OF GAS-PHASE FORMATION ENTHALPIES USING MODERN SEMI-EMPIRICAL METHODS FOR HIGH-THOROUGHPUT SCREENING OF PROMISING ENERGETIC MATERIALS
14.45 – 15.00	<u>D.S. Tsvetkov</u> , M.O. Mazurin, D.A. Malyshkin, V.V. Sereda, I.L. Ivanov, A.A. Zaslavsky (<i>Yekaterinburg</i>) EXPERIMENTAL THERMOCHEMICAL STUDY OF PEROVSKITE-TYPE CsPbX_3 (X – Cl, Br, I) HALIDES AND THERMODYNAMIC MODELLING OF BINARY PHASE DIAGRAMS INVOLVING THESE COMPOUNDS
15.00 – 15.15	<u>A.K. Koryttseva</u> , A. Navrotsky (<i>Nizhny Novgorod</i>) ANALYSIS OF ACID-BASE RELATIONS OF OXIDES BASED ON HIGH TEMPERATURE OXIDE MELT SOLUTION CALORIMETRY
15.15 – 15.30	<u>Yu.A. Sarmini</u> , S.S. Sologubov, N.N. Smirnova, A.V. Markin (<i>Nizhny Novgorod</i>) THERMODYNAMIC STUDY OF SOME REPRESENTATIVES OF THE SYNTHETIC GLUCOCORTICOIDS
15.30 – 15.45	<u>G.V. Vasiliev</u> , V.A. Tikhanova, L.T. Denisova (<i>Krasnoyarsk</i>) STUDY OF THE INFLUENCE ON THE STRUCTURE AND THERMAL PROPERTIES OF ISOVALENT SUBSTITUTION OF BISMUTH FOR EUROPIUM IN TITANATE $\text{Bi}_4\text{Ti}_3\text{O}_{12}$

15.45 – 16.00	A.K. Gatiatulin , M.A. Ziganshin, V.V. Gorbachuk (<i>Kazan</i>) 4D STRUCTURE-PROPERTY STUDIES OF NATIVE CYCLODEXTRINS
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Section 1 «Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation», B 204

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

14.00 – 14.30	Yu.K. Tovbin (<i>Moscow</i>) THE SECOND BEGINNING AND CURRENT STATE OF THERMODYNAMICS (keynote lecture)
14.30 – 14.45	V.V. Turovtsev (<i>Tver</i>) CONFORMATIONAL ANALYSIS AS THE BASIS FOR THERMODYNAMIC CALCULATION
14.45 – 15.00	F.N. Bedretdinov , T.V. Chelyuskina (<i>Moscow</i>) ANALYSIS OF THE PHASE BEHAVIOR OF A MULTICOMPONENT SYSTEM IN THE PRESENCE OF A SEPARATING AGENT
15.00 – 15.15	S.V. Pavlova, N.V. Sviridenkova, Yu.M. Artemkina, V.V. Shcherbakov (<i>Moscow</i>)_DETERMINATION OF ENTHALPIES OF COMBUSTION OF IONIC LIQUIDS
15.15 – 15.30	V.N. Kuryakov (<i>Moscow</i>) WATER PURITY CONTROL: RESEARCH OF NANOSCALE IMPURITIES AND EVALUATION OF WATER PURIFICATION METHODS USING ULTRAMICROSCOPY
15.30 – 15.45	N.D. Kondratyuk , V.I. Deshchenya, O.V. Kashurin (<i>Moscow</i>) PREDICTING SHEAR VISCOSITIES OF BINARY ORGANIC MIXTURES BY MOLECULAR DYNAMICS METHODS

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

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

14.00 – 14.30 (on-line)	A.N. Khlyupin (<i>Moscow</i>) UNRAVELING THE INFLUENCE OF SURFACE MORPHOLOGY ON PHYSICOCHEMICAL PHENOMENA IN CONFINED FLUIDS: FROM LENNARD-JONES MIXTURES TO ELECTROLYTE SOLUTIONS (keynote lecture)
14.30 – 14.45	I.V. Talyzin, V.M. Samsonov , S.A. Vasilyev, V.V. Puytov, A.A. Romanov (<i>Tver</i>) CONTACT MELTING IN METAL NANOSYSTEMS: MOLECULAR DYNAMICS SIMULATION
14.45 – 15.00	R.D. Oparin (<i>Ivanovo</i>) NEAR-INFRARED SPECTROSCOPY AS AN EFFECTIVE TECHNIQUE TO STUDY CONFORMATIONAL EQUILIBRIA OF LIDOCAINE MOLECULES IN A HIGHLY CONCENTRATED LIDOCAINE SOLUTION IN SUPERCRITICAL CO ₂
15.00 – 15.15	V.V. Danilina , D.G. Cherkasov, V.F. Kurskiy, K.K. Il'in (<i>Saratov</i>) PHASE EQUILIBRIA, SALTING-IN–SALTING-OUT EFFECTS AND EXTRACTIVE

	CRYSTALLIZATION IN THE TERNARY POTASSIUM IODIDE–WATER–DIISOPROPYLAMINE SYSTEM IN THE RANGE 0-60 °C
15.15 – 15.30	<u>R.A. Babkin</u> , 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	<u>P.O. Sorina</u> , 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	<u>S.F. Petrova</u> , 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 (<i>RCCT&SCF</i>)

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	<u>R.N. Nagrimanov</u> , 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	<u>I.V. Terekhova</u> (<i>Ivanovo</i>) NON-COVALENT INTERACTIONS OF DRUGS WITH BIORELEVANT MEDIA COMPONENTS (keynote lecture)
17.15 – 17.30	<u>G.I. Egorov</u> , A.A. Kruglyakova, M.E. Nikitin (<i>Ivanovo</i>) STRUCTURAL-THERMODYNAMIC CHARACTERISTICS AND INTERMOLECULAR INTERACTIONS IN GLYCEROL MIXTURES
17.30 – 17.45	<u>V.N. Agieienko</u> , O.V. Kazarina, R. Buchner (<i>Nizhny Novgorod</i>) WHY ETHALINE CANNOT BE REGARDED AS A DEEP EUTECTIC SOLVENT?
17.45 – 18.00	<u>M.D. Chekunova</u> , 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 204**

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

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

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

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

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

Poster session (*RCCT&SCF*), 18.00 – 19.30

Sections 1, 3, 5

19.30

Quiz

WEDNESDAY (3.07.2024)

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

Plenary session (Conference hall)

RCCT&SCF

9.00 – 11.00

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)

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

Plenary session (Conference hall)

9.00 – 11.00

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

09.00 – 09.40	Prof. Uspenskaya I.A. (<i>MSU, Moscow</i>) TO THE 100 ANNIVERSARY OF CHEMICAL THERMODYNAMICS LABORATORY AT MSU: PROGRESS IN EXPERIMENTAL AND COMPUTATIONAL METHODS
09.40 – 10.20	Dr. Ksenofontov A.A., E.V. Antina (<i>ISC RAS, Ivanovo</i>) MOLECULAR COMPLEXES WITH PHOTOINDUCED ENERGY TRANSFER BASED ON DIPYRROMETHENE SERIES COMPOUNDS
10.20 – 11.00	Dr. Rychkov D.A. (<i>ISSCM SB RAS, Novosibirsk</i>) WHY IS IT IMPORTANT TO COMPLEMENT EXPERIMENTS WITH COMPUTATIONAL METHODS FOR MOLECULAR CRYSTALS: CRYSTAL STRUCTURES, THERMODYNAMIC AND MECHANICAL PROPERTIES OF VARIOUS POLYMORPHS
11.00 – 11.15 Coffee break	

Oral reports (11.15 – 13.00)

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

Chairs: Nagrimanov R.N., Antina E.V.

11.15 – 11.45	P.A. Nikolaychuk , E. Kozeschnik (<i>Kurgan</i>) THERMODYNAMIC ESTIMATION OF THE PHASE AND CHEMICAL EQUILIBRIA IN THE SYSTEMS Al – Mg – Si – O AND Al – Mg – Si – H ₂ O (keynote lecture)
11.45 – 12.00	M.V. Vener , A.V. Shishkina, A.A. Ksenofontov, N.V. Penkov (<i>Moscow</i>) DICLOFENAC ION HYDRATION: EXPERIMENTAL AND THEORETICAL SEARCH FOR ANION PAIRS
12.00 – 12.15	E.V. Ivanov , D.V. Batov, A.V. Kustov, A.F. Syschenko (<i>Ivanovo</i>) ENTHALPY-HOMOTACTIC PARAMETERS OF INTERACTION FOR UROTROPINE AND SOME OTHER BIOACTIVE NITROGEN-CONTAINING CYCLIC NON-ELECTROLYTES AS SOLUTES IN D ₂ O AND H ₂ O AT 298.15 K
12.15 – 12.30	T.Yu. Ivanenko , E.V. Morozov, I.V. Peterson (<i>Krasnoyarsk</i>) 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	<u>M.S. Gruzdev</u> , U.V. Chervonova, D.V. Starichenko, V.E. Vorobeva, N.G. Bichan (<i>Ivanovo</i>) DENDRIMERIC AZOMETHINE Fe^{3+} COORDINATION COMPOUNDS CONTAINING CARBAZOLE UNITS
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Section 4 «Thermal Analysis and Calorimetry of Substances for Advanced Materials», B 203

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

11.15 – 11.45	<u>K.S. Gavrichev</u> , V.N. Guskov, P.G. Gagarin, A.V. Khoroshilov, A.V. Guskov (<i>Moscow</i>) THERMODYNAMIC PROPERTIES OF RE TITANATES $\text{RE}_2\text{Ti}_2\text{O}_7$ WITH PYROCHLORE STRUCTURE (keynote lecture)
11.45 – 12.00	<u>L.N. Zelenina</u> , T.P. Chusova, T.V. Rodionova, A.Yu. Manakov, A.V. Sartakova (<i>Novosibirsk</i>) DIFFERENT STATES OF WATER IN α - AND β -CYCLODEXTRIN HYDRATES
12.00 – 12.15	<u>A.S. Kurlov</u> (<i>Yekaterinburg</i>) THERMAL ANALYSIS OF NANOCRYSTALLINE POWDERS OF TRANSITION METAL CARBIDES
12.15 – 12.30	<u>A.E. Musikhin</u> , M.A. Bespyatov, E.F. Miller (<i>Novosibirsk</i>) LOW-TEMPERATURE HEAT CAPACITY OF CADMIUM TUNGSTATE
12.30 – 12.45	<u>N.V. Muravyev</u> (<i>Moscow</i>) MACHINE LEARNING FOR THERMAL STABILITY PREDICTION OF ORGANIC COMPOUNDS
12.45 – 13.00	<u>T.E. Lomakina</u> , O.V. Tolochko (<i>Saint Petersburg</i>) SOL-GEL SYNTHESIS AND CHARACTERIZATION OF $10\text{Gd}_2\text{O}_3$ - 90CeO_2 (MOL.%) PRECURSORS AND CERAMICS

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

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

11.15 – 11.45	<u>S.P. Verevkin</u> (<i>Samara</i>) THERMOCHEMISTRY IN 21ST CENTURY – QUO VADIS? IN SILICO ASSISTED DIAGNOSTICS OF AVAILABLE THERMOCHEMICAL DATA (keynote lecture)
11.45 – 12.00	<u>I.A. Velmuzhova</u> (<i>Nizhny Novgorod</i>) CALCULATION OF GERMANE ISOTOPOLOGUES THERMODYNAMIC FUNCTIONS FROM HIGH-RESOLUTION IR SPECTRA
12.00 – 12.15	<u>I.A. Khodov</u> (<i>Ivanovo</i>) INVESTIGATING STRUCTURAL MODIFICATIONS IN MODEL LIPID MEMBRANES WITH DRUGS VIA MAS NMR SPECTROSCOPY
12.15 – 12.30	<u>A.N. Manin</u> , G.L. Perlovich (<i>Ivanovo</i>) APPLICATION OF HYDROGEN BOND PROPENSITY CALCULATIONS TO PREDICT THERMODYNAMIC PARAMETERS OF COCRYSTAL FORMATION

12.30 – 12.45	<u>V.N. Kuryakov</u> , E.G. Gudkova, D.A. Mrachkovskaya, D.D. Ivanova (<i>Moscow</i>) COMPARISON OF THE CAPABILITIES OF DSC AND THE OPTICAL METHOD FOR STUDYING THE PHASE BEHAVIOR OF NANO-SIZED AQUEOUS DISPERSIONS OF N-ALKANES
12.45 – 13.00	<u>D.L. Gurina</u> , Y.A. Budkov (<i>Ivanovo</i>) MOLECULAR DYNAMICS SIMULATION OF SELF-ASSEMBLY OF WATER REVERSE MICELLES WITH IMIDAZOLIUM IONIC LIQUIDS IN SUPERCRITICAL CARBON DIOXIDE

Section of young scientists, B 204

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

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

12.50 – 13.00	<u>S.V. Kuzovchikov</u> , I.A. Bajenova, A.V. Khvan, M.S. Gusakov, A.G. Beresnev, V.V. Cheverikin (<i>Moscow</i>) PHASE EQUILIBRIA OF ALLOYS BASED ON THE CR-TA-W-V SYSTEM
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Lunch (13.00 – 14.00)

Oral reports (14.00 – 16.00)

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

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

14.00 – 14.30	<u>G.A. Gamov</u> (<i>Ivanovo</i>) INTERACTION OF GOLD(III) WITH SERUM ALBUMINS AND DNA IN AQUEOUS SOLUTION (keynote lecture)
14.30 – 14.45	<u>V.P. Barannikov</u> , V.I. Smirnov, I.N. Mezhevoi, E.Yu. Tyunina (<i>Ivanovo</i>) PATTERNS OF INTERACTION BETWEEN PEPTIDES OF VARIOUS STRUCTURES AND PYRIMIDINE NUCLEIC BASES IN A BUFFERED SALINE MEDIUM ACCORDING TO THE THERMODYNAMIC PARAMETERS OF THE PROCESS
14.45 – 15.00	<u>L.A. Antina</u> , A.A. Kalyagin, V.A. Kalinkina, S.A. Dogadaeva, M.B. Berezin, E.V. Antina (<i>Ivanovo</i>) BODIPY PHOTSENSITIZERS DELIVERY SYSTEMS: STRUCTURAL AND PHOTOPHYSICAL PROPERTIES
15.00 – 15.15	<u>Yu.V. Eremeeva</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 CERIU 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

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 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 BIS(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)	Federica D'Aria , C. Giancola (<i>Naples, Italy</i>) THERMODYNAMIC STUDIES OF NON-CANONICAL NUCLEIC ACID STRUCTURES (section 1)
16.30 – 16.45	A.S. Dubok, D.A. Rychkov (<i>Novosibirsk</i>) 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 (<i>Naples, Italy</i>) 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 (<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	K.V. Drozd , 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	A.V. Agafonov , 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	M.D. Kaplina (<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	S.S. Sologubov , A.V. Markin (<i>Nizhny Novgorod</i>) 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 (<i>Moscow</i>) HEAT CAPACITY AND THERMODYNAMIC PROPERTIES OF $\text{REMgAl}_{11}\text{O}_{19}$ (RE=La,Pr,Nd, Sm) HEXALUMINATES WITH MAGNETOPLUMBITE STRUCTURE

16.45 – 17.00	<u>B.A. Rusanov</u> , V.E. Sidorov, J.K. Bukreeva, V.A. Perevyshin, A.A. Sabirzyanov, A.I. Rusanova (<i>Yekaterinburg</i>) DSC, DENSITY, ELECTRICAL RESISTIVITY AND MAGNETIC SUSCEPTIBILITY OF Al-Ni-Co-Cu-Zr HIGH-ENTROPY ALLOYS IN SOLID AND LIQUID STATES
17.00 – 17.15	<u>E.V. Suslova</u> , M.O. Karimova, D.A. Shashurin (<i>Moscow</i>) SYNTHESIS AND THERMOPHYSICAL PROPERTIES OF ONION-LIKE CARBON NANOPARTICLES
17.15 – 17.30	<u>A.D. Plekhovich</u> , A.M. Kut'in, K.V. Balueva, E.E. Rostokina, M.E. Komshina, K.F. Shumovskaya, S.D. Plekhovich (<i>Nizhny Novgorod</i>) STUDY OF THE CONDITIONS FOR THE SYNTHESIS OF GLASS-CERAMICS FROM ULTRADISPERSE PRECURSORS BASED ON Bi ₂ O ₃ -B ₂ O ₃ -BaO GLASS AND YAG BY THERMAL ANALYSIS METHOD

Section 6 «Thermodynamics of Functional Materials and Engineered Self-Assembly», Co-working hall

Chairs: Tkachev N. K, Gorbachuk V.V

16.15 – 16.30	<u>M.N. Gabdulkhaev</u> , V.V. Gorbachuk, M.A. Ziganshin (<i>Kazan</i>) METHOD FOR PREPARING METASTABLE FORMS OF DRUGS
16.30 – 16.45	<u>I.Sh. Khabriev</u> , V.F. Khairutdinov, I.M. Abdulagatov (<i>Kazan</i>) OBTAINING A COMPOSITE MATERIAL FROM THERMODYNAMICALLY INCOMPATIBLE POLYCARBONATE AND POLYETHYLENE TEREPHTHALATE THROUGH THE DISPERSION PROCESS USING THE METHOD OF SEDS
16.45 – 17.00	<u>A.P. Voronin</u> , A.G. Ramazanov, 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
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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 PHYSICOCHEMICAL PROPERTIES OF NANOSTRUCTURED MXENES OF COMPOSITION TiC_nCl_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 (18.00 – 19.30)

Section 2, 4, 6

19.45	Table tennis tournament
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Friday (5.07.2024)

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

Plenary session (Conference hall)

9.00 – 11.00

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. Gabdulkhaev , 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 Ciccio, 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

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 $g\text{-C}_3\text{N}_4$ 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 ($\text{Ln} = \text{La}, \text{Ce}, \text{Pr}$) 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	<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. Казань, ФГБОУ ВО «Казанский национальный исследовательский технологический университет»
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	<u>В.Г. Меркулов</u> , С.П. Русаков, Е.А. Иванова, М.Н. Жарков, С.Г. Злотин ОРГАНОКАТАЛИТИЧЕСКОЕ ФОТООКИСЛЕНИЕ КИСЛОРОДОМ В СРЕДЕ ДИОКСИДА УГЛЕРОДА — КЛЮЧ К БЕЗОПАСНЫМ ПРОЦЕССАМ С-Н АКТИВАЦИИ ОРГАНИЧЕСКИХ СОЕДИНЕНИЙ Москва, Институт органической химии им. Н.Д. Зелинского
16.40 – 17.00	<u>Е.И. Перепелкин</u> , И.С. Чащин, В.Г. Васильев, М.А. Синолиц, Г.А. Бадун, М.Г. Чернышева, Н.М. Анучина, Н.П. Бакулева НАНОЧАСТИЦЫ ХИТОЗАНА С ВАНКОМИЦИНОМ, ПОЛУЧЕННЫЕ В БИФАЗНОЙ СИСТЕМЕ ВОДА-УГЛЕКИСЛЫЙ ГАЗ КАК ОСНОВА ПОКРЫТИЯ ДЛЯ БИОПРОТЕЗОВ Москва, ИНЭОС РАН им. А.Н. Несмеянова
17.00 – 17.20	<u>Т.А. Семёнов</u> , Н.М. Ашарчук, Е.О. Епифанов, Н.В. Минаев, Е.И. Мареев РАЗРАБОТКА СИСТЕМЫ КОМПЛЕКСНОЙ IN-SITU ВРЕМЯ-РАЗРЕШЕННОЙ ОПТИЧЕСКОЙ ДИАГНОСТИКИ ОБРАЗОВАНИЯ МИКРО- И НАНОЧАСТИЦ В СВЕРХКРИТИЧЕСКИХ ФЛЮИДАХ Москва, ИФТ, КККиФ, НИЦ "Курчатовский Институт"
17.20 – 18.00	Подведение итогов, Закрытие школы СКФ
18.00 – 19.30	Стендовая сессия (RCST&СКФ)

3 ИЮЛЯ, СРЕДА

Экскурсия Палех-Шуя

8.00 – 17.30

POSTER PRESENTATIONS (*RCCT&SCF*)

July 2, 2024

18.00-19.30

Ivanovo, Sheremetevsky prospect, 10

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	1.15

A.S. Pavlenko , E.G. Kabanova, E.A. Ptashkina, V.N. Kuznetsov (<i>Moscow</i>)	
THEORETICAL MODELING OF THE HEAT CAPACITY IN CoV_2O_4 NEAR PHASE TRANSITIONS: A NEW APPROACH	1.16
S.V. Pavlov (<i>Moscow</i>)	
STUDY OF THE STABILITY OF THE β -CYCLODEXTRIN/NAPROXEN INCLUSION COMPLEX IN A SUPERCRITICAL SOLVENT USING COMPUTER MODELING METHODS	1.17
M.L. Antipova, E.G. Odintsova, V.E. Petrenko (<i>Ivanovo</i>)	
MODEL FOR MOLECULAR DYNAMICS SIMULATION OF LIGNIN DEPOLIMERIZATION AND SELF-ASSEMBLY IN WATER-ETHANOL MIXTURE	1.18
T.V. Bogdan, E.G. Odintsova, M.L. Antipova, K.V. Bogdan, V.E. Petrenko (<i>Ivanovo</i>)	
PAIRWISE ENTROPY AS A STRUCTURE PARAMETER FOR THE DESCRIPTION OF THE GLASS TRANSITION IN MOLECULAR SIMULATIONS	1.19
V.V. Pisarev , J. Grossi (<i>Moscow</i>)	
QUANTUM CHEMICAL MODELING MOLEKULES OF Bi_2O_3 - B_2O_3 -BaO AND Re:YAG COMPONENTS OF GLASS CERAMICS	1.20
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>)	
IN SILICO EXPLORATION OF DRUG-CANDIDATE CONFORMATIONAL SPACE IN SOLVATED ENVIRONMENTS: A COMBINED ATOMISTIC SIMULATION AND MACHINE LEARNING APPROACH	1.21
D.O. Potapov , V.I. Deshchenya, N.D. Kondratyuk (<i>Dolgoprudny</i>)	
INVESTIGATION OF THE SELECTIVE PROPERTIES OF IONIC LIQUIDS	1.22
V. I. Zhuchkov, D.A. Ryzhkin , V.M. Raeva (<i>Moscow</i>)	
THE EFFECT OF AN EXTERNAL HOMOGENEOUS AGNETIC FIELD ON THE SYNTHESIS OF Fe_2O_3 NANOPARTICLES IN A PULSED UNDERWATER DISCHARGE PLASMA	1.23
A.S. Sarapulov , V.V. Korolev, N.A. Sirotkin, O.V. Balmasova (<i>Ivanovo</i>)	
A NEW ALGORITHM FOR CALCULATING THE CONTACT ANGLE OF BINARY MIXTURES IN SLIT PORES	1.24
A.A. Semenchuk , I.V. Kopanichuk, N.D. Kondratyuk (<i>Moscow</i>)	
ENTHALPIES OF FORMATION OF SOME IONIC LIQUIDS	1.25
Yu.M. Artemkina, S.V. Pavlova, N.V. Plechkova, V.V. Shcherbakov (<i>Moscow</i>)	
STUDY OF THE INFLUENCE OF TEMPERATURE ON THE CONFORMATIONAL EQUILIBRIA OF LIDOCAINE IN SUPERCRITICAL CARBON DIOXIDE USING 2D NOESY	1.26
V.V. Sobornova , K.V. Belov, I.A. Khodov (<i>Ivanovo</i>)	
SOLUBILITY OF AFm PHASES AS A FUNCTION OF PAIR ENTROPY	1.27
E.V. Tararushkin , G.S. Smirnov (<i>Moscow</i>)	
THERMODYNAMIC PROPERTIES OF CALCIUM STANNATE PHASES FROM COMPUTER ATOMISTIC SIMULATIONS	1.28
T.V. Bogdan, E.V. Tararushkin , Yu.D. Ivakin, N.V. Mashchenko, V.I. Bogdan (<i>Moscow</i>)	
CALCULATION OF THE CHEMICAL POTENTIAL OF WATER IN THE LIQUID FILM ON THE SPHERICAL HYDROPHILIC NANOPARTICLE	1.29
N.A. Volkov (<i>Saint-Petersburg</i>)	
PREDICTION ENTHALPIES OF VAPORIZATION OF ESTERS OF HYDROXYCARBOXYLIC ACIDS BY QSPR METHOD	1.30
Y.F. Yamshchikova , E.L. Krasnykh, S.V. Portnova (<i>Samara</i>)	
THE THERMODYNAMIC MODELING OF THE FORMATION OF HIGH-ENTROPY PHASES	1.31
O.V. Zaitseva , A. Ostovari Moghaddam, K.S. Litvinyuk, E.A. Trofimov (<i>Chelyabinsk</i>)	

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 (<i>Voronezh</i>)	1.32
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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. Gavrichiev (<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
THERMOCHEMICAL AND IR SPECTRAL STUDY OF THE INTERACTION OF ASYMMETRIC WATER-SOLUBLE PORPHYRINS WITH BLOOD SERUM ALBUMIN S.S. Guseinov , I.A. Vedernikova, N.S. Lebedeva, E.S. Yurina (<i>Ivanovo</i>)	3.5
THERMODYNAMICS OF THREE-COMPONENT LAVES PHASES FORMED BY IRON, CHROMIUM, SILICON, NIOBIUM AND MOLYBDENUM A.S. Ivanov , I.A. Bazhenova, A.V. Khvan, V.V. Cheverikin, A.V. Yanilkin, E.A. Meshkov (<i>Moscow</i>)	3.6
1-BUTYL-3-METHYLIMIDAZOLIUM METHANESULFONATE: LOW-TEMPERATURE HEAT CAPACITY AND STANDARD THERMODYNAMIC FUNCTIONS OF FORMATION. PART II D.A. Kalinyuk , A.I. Druzhinina, L.A. Tiflova, K.D. Semavin, Ya.V. Golubev, N.S. Chilingarov (<i>Moscow</i>)	3.7
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