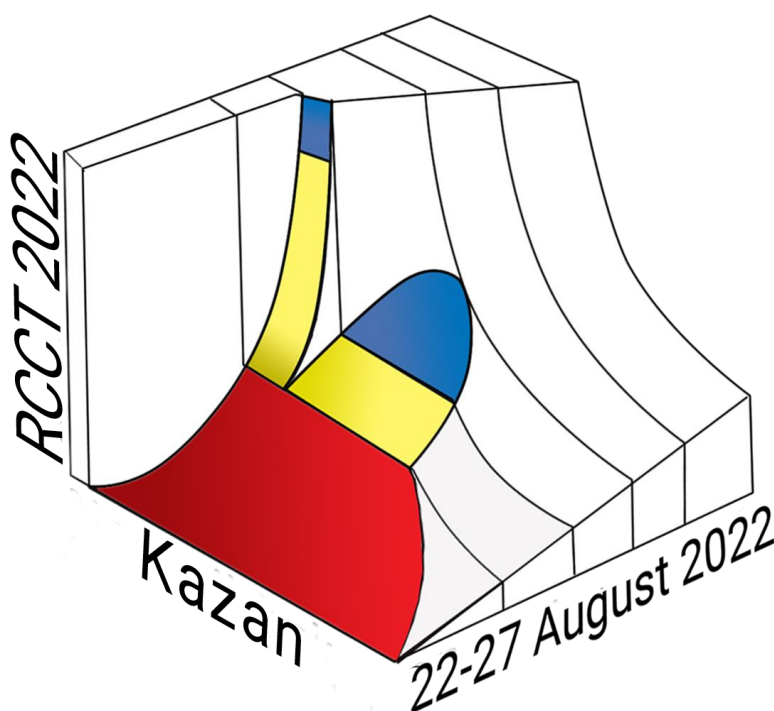


XXIII International Conference on Chemical Thermodynamics in Russia

**August 22-27, 2022
Kazan, Russia**



RCCT – 2022

PROGRAM

CONFERENCE TIMETABLE

Sunday, 21.08.2022.					
9.00-20.00	Check in. Registration				
Monday, 22.08.2022					
8.00-9.00	Check in. Registration				
Opening ceremony and plenary session					
9.00-9.20	Opening ceremony				
9.20-10.00	Kiselev M.G., TOWARDS SCREENING OF POLYMORPHISM AT SUPERCRITICAL PARAMETERS OF STATE				
10.00-10.40	Shchekin A.K., EFFECTS OF CONFINEMENT FOR SMALL AGGREGATES				
10.40-11.20	Verevkin S.P., GIBBS–HELMHOLTZ EQUATION: PRACTICAL APPLICATIONS IN THERMOCHEMISTRY				
11.20-11.50	Coffee break				
11.50-14.00 – Section reports					
Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation		Thermodynamics of Functional Materials, Interfacial and Confined Phenomena		Supramolecular systems	
11.50-12.10 (keynote lecture)	Victorov A.I. Partitioning of n-octanol in mixed micellar solutions of triton with 1-methyl-3-octylimidazolium chloride: experiment and model predictions	11.50-12.20 (keynote lecture)	Basova T.V. Fluorosubstituted metal phthalocyanines: physicochemical properties and thin films	11.50-12.20 (keynote lecture)	Ustinov E.A. External fields method in molecular simulation and thermodynamics of 2D crystals

12.10-12.30	Pisarev V.V. Molecular dynamics study of viscosity and excess entropy of hydrocarbons	12.20-12.40	Malakhov A.O. Selectivity of gas separation membranes: an approximate predictive model	12.20-12.40	Ziganshin M.A. Self-assembly, sorption and thermal properties of short-chain oligopeptides
12.30-12.50	Mokshin A.V. Crystal Nucleation in Amorphous Systems: Universal Scaling Relations	12.40-13.00	Okhotnikova E.S. Study of the bitumen phase composition by calorimetric method	12.40-13.00	Oparin R.D. Role of an intramolecular hydrogen bond in lidocaine conformer distribution and polymorph stability
12.50-13.10	Polkovnikova N.A. National challenges in material informatics	13.00-13.20	Zvereva I.A. Particularities of structure and thermodynamic properties of layered perovskite photocatalysts	13.00-13.15	Gatiatulin A.K. The role of water in guest inclusion by native cyclodextrins
13.10-13.25	Olhin A.S. Non-equilibrium thermodynamics of Enceladus ice shield: how Lattice-Boltzmann modeling helps us establish what's inside	13.20-13.40	Samsonov V.M. Nanothermodynamics: difficulties, advances and prospects		
13.25-13.40	Akhmetshina E.S. Homodesmotic method for determining the enthalpy of formation of free alkyl radicals	13.40-13.55	Davydov N.A. Photocatalytic activity of layered perovskite-like oxide $H_2La_2Ti_3O_{10}$ intercalated with n-octylamine		
13.55-15.30	Dinner				
15.30 -17.30 – Plenary session					
15.30-16.10	Navrotsky A., ORGANICS MATTER: COMMON FEATURES IN ENERGETICS OF POLYMER DERIVED CERAMICS, METAL ORGANIC FRAMEWORKS, AND OTHER HYBRID MATERIALS				
16.10-16.50	Chickos J. S., ESTIMATIONS OF THE LIQUID AND SOLID HEAT CAPACITY OF LARGE MOLECULES BY GROUP ADDITIVITY				

16.50-17.30	Vecchio Cipriotti S. THERMODYNAMIC STUDY OF FORMAMIDINIUM LEAD IODIDE (CH ₅ N ₂ PbI ₃) FROM 5 TO 357 K
17.30-18.30	Poster session (Participants in an alphabetical order from A to Ж)
19.30-22.00	Buffet

Tuesday, 24.08.2022					
9.00 – 10.20 – Plenary session.					
9.00-9.40	Gavrichev K.S., THERMODYNAMIC PROPERTIES OF MIXED OXIDES FOR THERMAL BARRIER COATINGS: RE ZIRCONATES, HAFNATES, TANTALATES				
9.40-10.20	Zherikova K.V., METAL-ORGANIC COMPOUNDS FOR GAS-PHASE DEPOSITION: HOW DO WE TINKER WITH THERMODYNAMIC AND THERMOCHEMICAL DATA POOL?				
10.20-10.40 – Oral report					
10.20-10.40	Malyshev V.M. COMPUTERIZED MEASURING DEVICES IN ADIABATIC CALORIMETRY (p. 154)				
10.40-11.30	Coffee break				
11.30 - 13.50 – Section reports					
Thermochemistry and Databases. Organic and organometallic compounds.		Modern Thermal Analysis and Calorimetry (dedicated to L.G. Berg). Fast scanning calorimetry.		Phase Equilibria: Molecular and Ionic Compounds. Ionic liquids	
11.30-12.00 (keynote lecture)	Markin A.V. Experimental calorimetry for study of materials based on organic, organoelement and polymeric compounds	11.30 -12.00 (keynote lecture)	Cangialosi D. Insights on glass dynamics from aging far below the glass transition	11.30 - 12.00 (keynote lecture)	Sedov I.A. Novel approaches for characterizing nanoheterogeneity in ionic liquids
12.00-12.20	Freitas V.L.S. Thermodynamic properties of an organic single crystal scintillator: 9-	12.00-12.20	Minakov A.A. Thermal perturbations at crystal nucleation in glasses and	12.00-12.20	Makarov D.M. QSPR models for phase transition and decomposition temperature of

	phenylcarbazole		polymers		ionic liquids
12.40-13.00	Yagofarov M.I. Temperature dependence of phase transition enthalpies of organic non-electrolytes	12.20-12.40	Gerasimov A.V. Crystallization kinetics and glass-forming ability of drugs from fast scanning calorimetry data	12.20-12.40	Postnikov E.B. Predicting thermodynamic properties of ionic liquids at high pressures based on the reference data at ambient pressure
13.00-13.20	Makarenko A.M. Scandium(III) β -diketonates as MOCVD precursors: thermodynamic and “structure-property” relationships	12.40-12.55	Andrianov R.A. The stability of poly-L-lactide nuclei according to the classical nucleation theory and fast scanning calorimetry	12.40-13.00	Safonova E.A. Polymerized ionic liquids for the enhanced bioextraction
13.20-13.35	Yurkshtovich Ya.N. Experimental and theoretical thermodynamic study of 1-benzyl-4-phenyl-1H-1,2,3-triazole and 1,3-bis(1-methyl-1H-tetrazol-5-yl)propane in gaseous and condensed aggregate states	12.55-13.10	Abdullin A.R. FSC study of crystallization kinetics of cross-linked poly(butylene terephthalate)	13.00-13.20	Kalinyuk D.A. Thermodynamic functions of formation of 1-ethyl- and 1-butyl-3-methylimidazolium chlorides
13.35-13.50	Karakovskaya K.I. Relations between structure and thermal behavior of MOCVD precursors: iridium (I) complexes with cyclooctadiene-1,5 and beta-diketonate derivatives			13.20-13.35	Korchak P.A. Liquid-liquid equilibrium and partitioning of biocomponent in aqueous mixtures of ionic liquid of different structure and kosmotropic salt
				13.35-13.50	Shelepova E.A. Empty volume in ionic liquids and its connection with the solubility of gases
13.50-15.00	Dinner				

15.00-17.00 – Section reports					
Thermochemistry and Databases. Inorganic compounds.		Phase Equilibria: Molecular and Ionic Compounds		Modern Thermal Analysis and Calorimetry (dedicated to L.G. Berg). Fast scanning calorimetry.	
15.00-15.30 (keynote lecture)	Khvan A.V. Experimental and theoretical investigation and critical assessment of thermodynamic data for pure in, cu and some binary systems from 0K	15.00-15.30 (keynote lecture)	Toikka A. M. Liquid phase splitting and critical states in quaternary systems with chemical reactions: new experimental data	15.00-15.30 (keynote lecture)	Zhuravlev E.A. Polymer and metal powders for additive manufacturing guided by differential fast scanning calorimetry
15.30-15.50	Blokhin A.V. Heat capacity in the interval 80-370 K and parameters of phase transitions of barium doped strontium ferromolybdate	15.30-15.50	Pestov S.M. Thermodynamic modelling of systems containing liquid crystals	15.30-15.50	Tropin T.V. Modeling of DSC curves of polystyrene during glass transition: from conventional to fast cooling rates
15.50-16.10	Shtenberg M.V. Calculation of temperature dependences of heat capacity of alkaline borates	15.50-16.05	Kuzovchikov S.V. Phase stability and thermodynamic modelling of alloys based on the Co-Cr-Mn system	15.50-16.10	Buzyurov A.V. New approach for vapor pressure determination by means of fast scanning calorimetry
16.10-16.30	Ostroushko A.A. Complex thermal analysis of oxide materials synthesis processes via combustion reactions taking into account charge generation	16.05-16.20	Brezhnev N.Yu. Phase diagram for the In-Se system according to the data of the thermal, structural and vapor-pressure investigations	16.10-16.25	Bolmatenkov D.N. Vaporization enthalpy of organic non-electrolytes in a wide temperature range: pencil and paper vs experimental measurements
16.30-16.45	Tolmacheva N.N. Thermodynamic properties of the Na ₂ O-BaO-B ₂ O ₃ system	16.20-16.40	Bazaev E.A. Phase transitions, critical and supercritical phenomena in	16.25-16.40	Larionov R.A. Thermal and supramolecular properties of oligopeptides

16.45-17.00	Osipenko A.A. Thermodynamic behaviour of palladium in LiCl–KCl–CsCl eutectic melt		ternary mixture of water +1-propanol+n-hexane		
17.00-18.30	Poster session (Participants in an alphabetical order from 3 to II)				

Wednesday, **24.08.2022**

9.00 - 11.00 – Plenary session.

9.00-9.40	Solomonov B.N., THE DISSOLUTION THERMODYNAMICS AS THE KEY TO UNDERSTANDING VARIOUS PHYSICO-CHEMICAL PHENOMENA
9.40-10.20	Mukhametzyanov T.A., FAST SCANNING CALORIMETRY: NEW OPPORTUNITIES FOR CHEMICAL THERMODYNAMICS
10.20-11.00	Varfolomeev M.A., THERMOCHEMISTRY OF NATURAL GAS STORAGE
11.00-11.30	Coffee break

11.30-13.00 – Section reports

Applied Thermodynamics and Biothermodynamics (dedicated to A.A. Pimerzin)		Thermochemistry and Databases. Organic and organometallic compounds.		Thermodynamics of solutions	
11.30-12.00 (keynote lecture)	Bykov A.G. Proteins, polyelectrolytes and copolymers for pulmonary surfactants	11.30 -12.00 (keynote lecture)	Smirnova N.N. The dependence of thermodynamic properties of polyphenylenes on their structure	11.30-12.00 (keynote lecture)	Kustov A.V. Solvophobic and solvophilic effects in urea and tetramethylurea solutions
12.00-12.20	Maksimov E.G. Control of hydrogen bonding in photoactive orange carotenoid protein by noncanonical amino acid substitutions of tyrosine-201	12.00-12.20	Dávalos J.Z. Thermochemical and structural properties of the new sulphur-containing compounds with relevance on atmospheric chemistry	12.00-12.20	Kononova E.G. Research of the systems amino-alcohol - water

12.20-12.40	Manin A.N. Study of the cocrystallization effect on the carbamazepine thermal stability	12.20-12.40	Samarov A.A. Alkyl-substituted biphenyls as potential candidates for liquid organic hydrogen carriers	12.20-12.40	Gamov G.A. Dependence of formal electrode potential on ionic strength
12.40-13.00	Portnova S.V. Influence of the structure of esters of natural hydroxycarboxylic acids on thermodynamic and thermophysical property	12.40-12.55	Sarmini Yu.A. Study of the thermodynamic properties of organosilicon dendrimers and their corresponding nanogels with different nature terminal groups		
13.00-14.00	Dinner				
14.00-18.00	Excursion				
19.00-22.00	Banquet				
Thursday, 25.08.2022					
9.00-11.00 – Plenary session.					
9.00-9.40	Budkov Yu.A. MEAN-FIELD THEORY OF MACROSCOPIC FORCES IN INHOMOGENEOUS IONIC FLUIDS				
9.40-10.20	Fedorov P.P. APPLICATION OF THE THIRD LAW OF THERMODYNAMICS TO THE STUDY OF PHASE DIAGRAMS				
10.20-11.00	Baidakov V.G. LIMITS OF STABILITY OF METASTABLE PHASES AND METASTABLE PHASE EQUILIBRIA IN SIMPLE ONE-COMPONENT SYSTEM				
11.00-11.30	Coffee break				

11.30 - 13.50 – Section reports							
Amphiphilic compounds: thermodynamics of self-organization, physicochemical properties and practical application.		Applied Thermodynamics and Biothermodynamics (dedicated to A.A. Pimerzin). Biothermodynamics		Development of General Methods and Tools of Chemical Thermodynamics: New Experimental Techniques, Theory and Computer Simulation. Quantum Chemical Methods.		Phase Equilibria: Molecular and Ionic Compounds	
11.30-12.00 (keynote lecture)	Derkach S.R. Gelatin as a stabilizer for emulsions: molecular modification	11.30-12.00 (keynote lecture)	Noskov B.A. Protein microgel layers at the liquid-gas interface	11.30-12.00 (keynote lecture)	Khursan S.L. Homodesmotic method for studying the molecular energetics of organic compounds	11.30-12.00 (keynote lecture)	Gorbachuk V.V. Thermodynamics of molecular recognition and polymorphism
12.00-12.20	Gainanova G.A. Ammonium – phosphonium – isothiuronium amphiphiles: CMC, solubilizing capability and catalytic effect	12.20-12.40	Milyaeva O.Yu. The impact of thrombine on dynamic surface properties of fibrinogen solutions	12.00-12.30 (keynote lecture)	Medvedev N.N. Voronoi-Delaunay method. Applications to solutions	12.00-12.20	Almeida A.R.R.P. Pressure-temperature phase diagrams near the triple point of four benzaldehydes
12.20-12.40	Burilov V.A. New macrocyclic amphiphiles for sensing and green micellar&metal/photocatalysis	12.20-12.40	Magsumov T.I. Influence of organic solvents on thermal stability and denaturation mechanism of lysozyme	12.30-12.50	Agienko V.N. Monoethanolamine hydration as seen by dielectric relaxation spectroscopy and quantum chemical calculations	12.20-12.40	Golikova A.D. Heat effects of phase and chemical processes in a multicomponent system with chemical interaction
12.40-12.55	Pavlov R.V. Aggregation of carbamate gemini	12.40-	Akentieva A.V. Films of lysozyme fibrillar	12.50-	Rychkov D.A. Comparison of	12.40-	Kabanova E.G. Experimental study

	surfactants and their potential as liposome modifiers	13.00	aggregates on the water surface	13.10	different computational techniques for evaluation of quercetin conformers	13.00	and CALPHAD modeling of the Ag-In-Pd ternary
12.55-13.10	Radaev D.D. Amphiphilic NHC precursors based on imidazole-4,5-dicarboxylic acid: synthesis and aggregation in aqueous media.	13.00-13.20	Bazhin N.M. Helmholtz energy: is it energy or not?	13.10-13.30	Chuev G.N. A new approach to the calculation of solvation effects in biomolecular solutions in the framework of the classical density functional theory	13.00-13.20	Guskov V.Yu. Thermodynamic features of enantiomer adsorption on the surfaces with supramolecular chirality
13.10-13.25	Faria B.F. Simulation of surfactant adsorption at liquid-liquid interface	13.20-13.35	Khaibrakhmanova D.R. Evaluation of the binding properties of drugs to albumin from DSC thermograms	13.30-13.45	Maltsev M.A. Quantum chemical study of the interatomic interaction of diatomic argides	13.20-13.35	Lyubichev D.A. Separation of azeotropic mixtures: novel approaches of using choline chloride based deep eutectic solvents
13.25-13.40	Oselskaya V.Yu. Hydration effect on encapsulation of indometacin by solid cyclodextrins	13.35-13.50	Fatkhutdinova A.A. Step-scan differential scanning calorimetry for investigation of protein denaturation			13.35-13.50	Smirnov A.A. Investigation of the efficiency of the ethanol – ethyl formate system separation by various DESs based on choline chloride

13.40-13.55	Chirkov N.S. Formation of mixed DNA/polyelectrolyte layers at the water–air interface						
13.50-15.00	Dinner						
15.00-16.40 – Section reports							
Amphiphilic compounds: thermodynamics of self-organization, physicochemical properties and practical application.		Thermochemistry and Databases. Inorganic compounds.		Thermochemistry and Databases. Organic and organometallic compounds.		Thermodynamics of solutions	
15.00-15.30 (keynote lecture)	Zakharova L.Ya. Structural factor controlling self-assembly behavior and functional activity of surfactant systems	15.00-15.30 (keynote lecture)	Kurapova O.Yu. The use of the thermodynamic approach for advanced ceramics development	15.00-15.20	Ribeiro da Silva M.D.M.C. (An experimental insight on the thermochemistry of naphthalene diols)	15.00-15.20	Tkachev N.K. Thermodynamic perturbation theory for molten alkali halides
15.30-15.50	Ziganshina A.Yu. Stimuli-responsive nanocarriers for substrate binding and release	15.30-15.50	Semerikova A.N. Thermodynamic characteristics of cesium dimolybdate and lithium monomolybdate doping by 10% cesium	15.20-15.40	Nagrimanov R.N. New relationship between enthalpies of vaporization and solution for molecular and ionic liquids	15.20-15.40	Khodov I.A. Conformational preferences of fenamates in supercritical state parameters of the solvent based on NOESY data

15.50-16.10	Volkov N.A. Modelling micelles in polar and non-polar solvents: from single aggregate to aggregates size distribution	15.50-16.10	Silyukov O.I. Inorganic-organic derivatives of layered perovskite-like oxides thermal stability and photocatalytic activity	15.40-16.00	Chernyaikin I.S. Heat capacity and thermodynamic functions of crystalline copper(II) dipivaloylmethanate from 0 to 430 K	15.40-16.00	Anashkin I.P. Molecular simulation of the pervaporation process
16.10-16.25	Belov R.N. Reductive cleavage of C-O bonds in p-tert-butylcalix[4]arene derivatives in the presence of hydrazine.	16.10-16.25	Kutuzova V.E. Study of Al ₂ O ₃ - ZrO ₂ -Yb ₂ O ₃ precursors by the differential scanning calorimetry	16.00-16.20	Miroshnichenko E.A. Rearrangement energy of framework radicals	16.00-16.20	Kadtsyn E.D. Volumetric properties of aqueous alcohol solutions: a Voronoi analysis
16.25-16.40	Makarov E.G. Novel tetra-azide and triazole derivatives of thia- and calix[4]arene with free phenolic hydroxyls	16.25-16.40	Vorozhtsov V.A. Mass spectrometric study and modeling of the thermodynamic properties of the Al ₂ O ₃ -SiO ₂ -ZrO ₂ system				
16.40-18.10	Poster session (Participants in an alphabetical order from P to Я)						

Friday, 26.08.2022.	
9.00-10.40 – Oral reports	
9.00-9.20	Sun L.-X. ENERGY STORAGE MATERIALS AND SENSORS
9.20-9.40	Sineva S.I. HIGH-TEMPERATURE PHASE EQUILIBRIA IN THE Fe-Sn-S SYSTEM
9.40-10.00	Lőrinczy D.M. APPLICATION OF DSC FOR STUDYING THE DOSE DEPENDENT EFFECT OF CYCLOPHOSPHAMIDE TREATMENT ON ACTIN
10.00-10.20	Meier R. GROUP CONTRIBUTION REVISITED: THE ENTHALPY OF FORMATION OF ORGANIC COMPOUNDS WITH “CHEMICAL ACCURACY”
10.20-11.00	Coffee break
11.00-12.20 – Plenary session	
11.00-11.40	Turovtsev V.V. APPLICABILITY OF POPULAR FUNCTIONALS IN CALCULATIONS OF THE ENERGY, THERMODYNAMIC AND SPECTROSCOPIC PROPERTIES OF SUBSTANCES
11.40-12.20	Tovbin Yu.K. EQUILIBRIUM DROPS: A DIFFERENCE BETWEEN THERMODYNAMICS BY CLAUSIUS AND GIBBS IN TASKS OF THE PHASE EQUILIBRIUM
12.20	Closing ceremony
Saturday, 27.08.2022	
10.00-13.00	Training Seminar on Fast Scanning Calorimetry

POSTER PRESENTATIONS
Monday, 22.08.2022 17.30-18.30
DEPENDENCE OF THE STANDARD THERMODYNAMIC PROPERTIES OF POLYOXIMES ON THE COMPOSITION <i>N.V. Abarbanel, N.N. Smirnova, A.V. Markin</i>
THERMODYNAMIC PROPERTIES OF PHASE TRANSITION OF 2-METHYLQUINOLINE, 2-CHLOROQUINOLINE AND 2-PHENYLQUINOLINE <i>R.S. Abdullah</i>
KINETIC AND THERMODYNAMIC CONTROLS OF ZINK CYAMELURATE CRYSTAL FORMATIONS <i>N.V. Avramenko, L.A. Aslanov</i>
THERMODYNAMIC MODELING OF LAYERED STRUCTURES BASED ON GRAPHITE OXIDE <i>N.V. Avramenko, A.T. Rebrikova, A.M. Parfenova, M.V. Korobov</i>
THERMODYNAMIC CALCULATION OF BOUNDARIES OF SOLID SOLUTIONS IN SYSTEMS PbTe–Bi ₂ Te ₃ –Sb ₂ Te ₃ AND PbTe–SnTe–Bi ₂ Te ₃ <i>A.I. Aghazade, A.N. Mammadov, M.B. Babanly</i>
ACCELERATION OF METHANE HYDRATE NUCLEATION BY CRYSTALS OF HYDRATED SODIUM DODECYL SULFATE <i>T.P. Adamova, D.A. Strukov, A.Y. Manakov</i>
SOME FEATURES OF THE PROCESS OF HYDRATE FORMATION ON AQUEOUS FOAM STABILIZED BY SURFACTANTS <i>T.P. Adamova, A.Yu. Manakov, A.A. Chernov</i>
THERMODYNAMICS OF SORPTION OF SODIUM OLEATE ONTO COPPER-MOLYBDENUM ORE <i>Sh.K. Amerkhanova, R. Shlyapov, A.S. Uali</i>
ELECTROFLOTATION IN WASTEWATER TREATMENT FROM CHROMIUM (VI) IONS: THERMODYNAMIC ANALYSIS <i>Sh.K. Amerkhanova, D. Belgibayeva, R. Shlyapov, A.S. Uali</i>
MOLECULAR SIMULATION OF THE PERVAPORATION PROCESS <i>I.P. Anashkin, A.V. Klinov, S.G. Dyakonov</i>
CALVE CALORIMETRY AND P-C ISOTHERMS: COMPARATIVE ANALYSIS OF THERMODYNAMIC DATA <i>E.Yu. Anikina, V.N. Verbetsky, N.Ul.Yorov</i>
CALORIMETRIC STUDY OF HYDROGEN INTERACTION WITH Dy ₂ Fe ₁₇ <i>E.Yu. Anikina, V.N. Verbetsky, N.Ul.Yorov</i>
TESTING CARNAHAN–STARLING AND RUSANOV EQUATIONS OF STATE FOR HARD SPHERES IN DENSITY FUNCTIONAL CALCULATIONS OF PROFILES AND SURFACE TENSION OF DROPLETS AND BUBBLES <i>K.D. Apitsin, A.K. Shchekin, D.V. Tatyanyenko, L.A. Gosteva</i>
THERMODYNAMIC STUDY OF THE Cu ₂ Si(Ge)S ₃ AND Cu ₈ Si(Ge)S ₆ COMPOUNDS BY EMF AND DSC METHODS <i>K.N. Babanly, U.R. Bayramova, L.F.Mashadiyeva, I.J. Alverdiyev, Yu.A. Yusibov</i>
ESTIMATION OF VAPORIZATION AND SUBLIMATION ENTHALPIES OF TERPENES AND TERPENOIDS AT 298.15 K <i>R.A. Babkin, A.A.Samatov, R.N. Nagrimanov</i>

<p>THERMODYNAMIC CHARACTERISTICS OF DYES SORPTION ON COAL SORBENTS FROM TEXTILE PRODUCTIONS WASTEWATER AFTER THEIR CHEMICAL TREATMENT WITH A COAGULANT ON THE BASIS OF DICYANDIAMIDE <i>M.Yu. Babkin, D.V. Filippov, O.V. Zakharov</i></p>
<p>THERMODYNAMIC PARAMETERS OF POSITIVE AND NEGATIVE IONS IN THE GAS AND LIQUID PHASES AND THEIR CHANGE DURING SOLVATION <i>N. M. Bazhin</i></p>
<p>THIRD GENERATION CALPHAD ASSESSMENT OF DATA FOR PURE SI AND GE AND THE BINARY SI-GE SYSTEM <i>I. Bajenova, A. Khvan, A. Dinsdale, A. Kondratiev</i></p>
<p>PHASE TRANSITIONS AND CRITICAL PROPERTIES OF C₃H₇OH+C₈H₁₈ SYSTEM <i>E.A. Bazaev, A.R. Bazaev, I.M. Abdulagatov, B.K. Osmanova, T.A. Dzhapparov</i></p>
<p>VAPORIZATION AND THERMODYNAMIC PROPERTIES OF THE SrO-Al₂O₃ SYSTEM STUDIED BY KNUDSEN EFFUSION MASS SPECTROMETRY <i>E.A. Balabanova, S.I. Lopatin, S.M. Shugurov, N.G. Tyurnina, Z.G. Tyurnina, I.G. Polyakova</i></p>
<p>ESTIMATION OF THE TEMPERATURE DEPENDENCE OF THE SUBLIMATION ENTHALPIES OF AROMATIC COMPOUNDS <i>I.S. Balakhontsev, M.I. Yagofarov</i></p>
<p>EFFECT OF COMPLEX FORMATION ON VOLUME PROPERTIES OF URACIL IN BUFFER SOLUTIONS WITH GLYCYL-L-TYROSINE AT VARIOUS TEMPERATURES <i>B.P. Barannikov, E.Yu. Tyunina, G.N. Tarasova, A.A. Stavnova</i></p>
<p>THERMODYNAMICS OF INTERACTION BETWEEN SOME PEPTIDES AND NUCLEIC ACID BASES: URACIL AND CYTOSINE <i>V.P. Barannikov, D.R. Koltyshev, V.I. Smirnov, I.N. Mezhevoi</i></p>
<p>THE PHENOMENON OF PARTIAL ISOBARIC COMPRESSIBILITY (“NEGATIVE EXPANSIBILITY”) OF UREA AS A SOLUTE IN TERT-BUTANOL AND METHANOL MEDIA: A COMPARATIVE ANALYSIS <i>D.V. Batov, E.V. Ivanov, E.Yu. Lebedeva, A.V. Kustov, A.A. Pakina, N.G. Ivanova</i></p>
<p>COMPARATIVE CHARACTERISTICS OF THE ENTHALPY PARAMETERS OF THE INTERMOLECULAR INTERACTION OF UREA AND TETRAMETHYL UREA IN WATER, ETHYLENE GLYCOL AND FORMAMIDE AT T = 288 - 328 K <i>D.V. Batov, E.V. Ivanov, N.L. Smirnova, A.V. Kustov</i></p>
<p>ANALYSIS OF VARIOUS ISO-MANIFOLDS IN MULTICOMPONENT SYSTEMS WITH BIAZEOTROPIC CONSTITUENTS <i>F. Bedretdinov, T. Chelyuskina</i></p>
<p>EFFICIENT REMOVAL IONS CR (VI) ON WASTEWATER BY ANION EXCHANGE MATERIAL BASED ON PVC <i>D. Bekchanov, G. Babajonova, M. Mukhamediev</i></p>
<p>ON COALESCENCE TIME OF FREE DROPLETS IN VAPOR: MOLECULAR DYNAMICS APPROACH <i>D. Beloborodov, A. Vishnyakov</i></p>
<p>LIDOCAINE CONFORMATIONAL PREFERENCES UNDER ISOTHERMAL CONDITIONS <i>K.V. Belov, A.A. Dyshin, M.G. Kiselev, M.A. Krestyaninov, I.A. Khodov</i></p>
<p>PHASE EQUILIBRIA IN Me(CH₃SO₃)₂-H₂O (Me=CO, Ni, Mn) SYSTEMS <i>E.V. Belova, J. D. Shakirova, K. A. Lyssenko, I. A. Uspenskaya</i></p>

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<p>THE PATTERN OF CHANGES IN THE THERMAL PROPERTIES OF COMPOUNDS IN THE SERIES $SrLnCuSe_3$ ($Ln = La - Lu$) <i>A.M. Peterikov, N.N. Habibullayev, O.V. Andreev</i></p>
<p>DEVELOPMENT OF APPROACHES TO THE EVALUATION OF INTERMOLECULAR INTERACTIONS IN BINARY AZEOTROPIC SYSTEMS <i>Petrov A.A., Rakipov I.T., Solomonov B.N.</i></p>
<p>TYPING OF NEAR-CRITICAL RESERVOIR FLUIDS BY INTENSITY OF CRITICAL OPALESCENCE ON THE DEW-BUBBLE BOUNDARY CURVE <i>V.E. Podnek, Y.F. Kiyachenko, A.S. Sirota, B.A. Grigoriev</i></p>
<p>WIDE-RANGING PREDICTION OF PHASE BEHAVIOUR IN THE SYSTEMS OF $[Cxmim][BF_4]$ AND $[Cxmim][PF_6]$ ($2 \leq x \leq 12$) IONIC LIQUIDS BY CP-PC-SAFT WITH UNIVERSAL kij VALUE <i>I. Polishuk</i></p>
<p>STUDY OF TRANSPORT PROPERTIES OF SOLUTIONS WITH INVERSE PREMICELLAR AGGREGATES VIA MOLECULAR DYNAMICS SIMULATIONS <i>M.S. Polovinkin, N.A. Volkov, L.Ts. Adzhemyan, A.K. Shchekin</i></p>
<p>ASSIGNMENT OF THE ENAMEL INSULATION GLASS TRANSITION TEMPERATURE BY DSC <i>E.I. Popova, K.I. Karezin, A.V. Sokovishin, R.E. Nevskiy</i></p>
<p>EQUILIBRIUM AND THERMODYNAMIC PARAMETERS FOR ESTERIFICATION OF SUCCINIC, MALIC AND CITRIC ACID WITH ETHANOL <i>S.V. Portnova, Y.F. Yamshchikova, S.V. Moiseeva</i></p>
<p>SURFACE FREE ENERGY OF CRITICAL CRYSTAL NUCLEI AND CAVITIES: MOLECULAR DYNAMICS SIMULATION <i>K.R. Protsenko, V.G. Baidakov</i></p>
<p>NUCLEATION IN LENNARD-JONES SOLUTIONS WITH COMPLETE AND PARTIAL SOLUBILITY OF THE COMPONENTS: MOLECULAR DYNAMIC SIMULATION <i>S.P. Protsenko, V.G. Baidakov, V.M. Bryukhanov</i></p>
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<p>THE EFFECT OF ORANGE OT IONIZATION ON SOLUBILIZATION BY CATIONIC MORPHOLINIUM SURFACTANTS <i>E.A. Romanova, R.V. Pavlov, F.G. Valeeva, G.A. Gaynanova, D.M. Kuznetsov, L.Ya. Zakharova</i></p>
<p>SELF-ASSEMBLY OF CATIONIC SURFACTANTS IN THE PRESENCE OF ATP AS A BIOLOGICAL HYDROTROPE <i>E.A. Romanova, E.A. Vasilieva, F.G. Valeeva, D.M. Kuznetsov, D.A. Kuznetsova, G.A. Gaynanova, L.Ya. Zakharova</i></p>

NONLOCAL ELECTROSTATIC APPROACH TO STABILIZATION OF MONOVALENT CATIONS IN AQUEOUS CAVITY OF ION CHANNEL <i>A.A. Rubashkin, P. Iserovich, O.S. Ostroumova</i>
NONLOCAL ELECTROSTATIC CALCULATION OF ION SOLVATION ENERGY. EFFECT OF THE DISTRIBUTION OF A PART OF THE ELECTRONIC CHARGE OUTSIDE OF THE ION FOR THE CATION AND ANION <i>A.A. Rubashkin, M.A. Vorotyntsev</i>
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ALTERNATIVE METHOD FOR ESTIMATION OF PHASE TRANSITION ENTHALPIES OF ALIPHATIC COMPOUNDS <i>A.A. Samatov, R.N. Nagrimanov, B.N. Solomonov</i>
ON THE PROBLEM OF THE PREDICTION OF STABILITY/INSTABILITY FOR NANOCLUSTERS AND NANOALLOYS: THEORETICAL APPROACH AND COMPUTER SUMULATION <i>V.M. Samsonov, N.Yu. Sdobnyakov, A.N. Bazulev, S.S. Bogdanov</i>
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STUDY OF THE BEHAVIOR OF DIOXADET MOLECULES IN WATER BY MOLECULAR DYNAMICS METHODS

E. Yakush, A. Kim

LIQUID-LIQUID EQUILIBRIUM OF TERNARY SYSTEMS BUTANOL + WATER + BUTYL LACTATE AND BUTANOL + WATER + BUTYL GLICOLATE

Y.F. Yamshchikova, S.V. Portnova

POPULAR THERMODYNAMICS

CHEMICAL THERMODYNAMICS ON POST STAMPS

P.P. Fedorov, E.V. Chernova