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## 25 June

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17.30 – 19.00 Registration, ICKC lobby

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19.00 – 21.00 Welcome Get-Together, ITC lawn

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## 26 June

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08.15 – 08.45 Registration, ICKC lobby

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### Joint Session 1, ICKC, Chair: Yuri Tsvetkov

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08.45 – 08.55 Opening of the Conference

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08.55 – 09.00 Voevodsky Prize Awarding Ceremony

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09.00 – 09.45 **Jack Freed**, Modern ESR at ACERT and applications in biophysics

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09.45 – 10.30 **Renad Sagdeev**, Magnetic resonance and spin chemistry

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10.30 – 11.00 **Andrei Vorobiev**, Molecular alignment and mobility in partially ordered media as determined by EPR of nitroxide spin probes

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11.00 – 11.30 Coffee break

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### Joint Session 2, ICKC, Chair: Andrei Vorobiev

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11.30 – 12.00 **Elena Bagryanskaya**, Distance measurements in nucleic acids using advanced SDSL with nitroxide and trityl radicals

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12.00 – 12.30 **Alexander Kokorin**, Influence of polarity and ionic strength on intramolecular spin exchange in nitroxide biradicals

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12.30 – 13.00 **Sylvain Marque**, Persistent radical effect: From fundamental chemistry to nitroxide mediated polymerization and material sciences

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13.00 – 13.30 **Maxim Yulikov**, Recent progress in RIDME spectroscopy with paramagnetic metal centers

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13.30 – 15.00 Lunch

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## 26 June

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**Parallel session ICKC1: “ESR One”, Chair:  
Alexander Maryasov**

**Parallel session ITC1: “Spin One”, Chair:  
Edward Fel'dman**

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15.00 – 15.25 **Matvey Fedin**, EPR study of MOF-based functional systems

**Konstantin Ivanov**, Parahydrogen allows ultra-sensitive indirect NMR detection of catalytic hydrogen complexes

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15.25 – 15.50 **Olesya Krumkacheva**, EPR studying of codon-anticodon interaction of mRNA with tRNAs in human ribosome

**Denis Sosnovsky**, The role of the level anti-crossings of the spin energy levels for the formation of hyperpolarization in the solid state

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15.50 – 16.15 **Leonid Kulik**, Structure and spin-dependent recombination of charge-separated state in polymer/fullerene composites

**Vladimir Verkhovlyuk**, Detection of hyperfine structure in the OD ESR spectra of radical ions in polymer matrices

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16.15 – 16.40 **Mikhail Uvarov**, Relaxation-induced coherence transfer within triplet states and origin of the narrow line in the EPR spectrum of triplet C<sub>70</sub>

**Anatoly Melnikov**, X-ray generated exciplexes of diphenylacetylenes with -CF<sub>3</sub> or -OMe substituent group

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16.40 – 17.10 Coffee break

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## 26 June

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**Parallel session ICKC2: “ESR Two”, Chair:  
Matvey Fedin**

**Parallel session ITC2: “NMR One”, Chair:  
Konstantin Ivanov**

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17.10 – 17.35 **Alexander Maryasov**, Coherence transfer processes in EPR spectroscopy of free radicals in liquids: The role of forbidden transitions

**Edward Fel’dman**, Investigations of quantum correlations and decoherence of quantum states with magnetometry and methods of magnetic resonance

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17.35 – 18.00 **Andrey Komarovskikh**, EPR of germanium-vacancy defect in diamond: Experiment and DFT calculation

**Sergey Babajlov**, Kinetics of reversible photochemical processes by NMR under photostationary and nonstationary conditions: State of the art and prospects of application for therapy

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18.00 – 18.25 **Sergei Anishchik**, Level anti-crossing spectra of nitrogen-vacancy centers in diamond detected by using modulation of the external magnetic field

**Daniil Kolokolov**, Tailoring rotational dynamics by a rational design of the octacarboxylate linkers in Cu-based Metal-Organic Frameworks

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18.25 – 18.50 **Sergey Veber**, Optical properties of magnetoactive compounds based on copper(II) ions and stable nitroxide radicals

**Olga Morozova**, Indirect NMR detection of reversible protonation of guanosyl radical in neutral aqueous solution

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## 27 June

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### Joint Session 3, ICKC, Chair: Alexander Volodin

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- 9.00 – 9.30 **Anatoly Vanin**, Dinitrosyl iron complexes with thiol-containing ligands as a "working form" of nitric oxide in living systems: Physico-chemical and biological evidence
- 9.30 – 10.00 **Michael Bowman**, Energy transduction: What cytochrome *bc1* tells us
- 10.00 – 10.30 **Anton Savitsky**, The magic of trehalose: Coupling between matrix properties and protein function
- 10.30 – 11.00 **Vladimir Nadolinny**, EPR investigations of external influences (light, pressure, temperature and atmospheric components) on the magnetic properties of transition metal compounds
- 11.00 – 11.30 Coffee break
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### Joint Session 4, ICKC, Chair: Anton Savitsky

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- 11.30 – 12.00 **Alexander Volodin**, EPR spectroscopy for the study of solid catalytic materials
- 12.00 – 12.30 **Oleg Martyanov**, Development and application of EPR methods to study the structure and evolution of multicomponent catalytic systems *in situ* including sub and supercritical fluids
- 12.30 – 13.00 **Željko Knez**, Thermodynamic and transport data for the systems polymer/dense gases
- 13.00 – 13.30 **Elena Boldyreva**, From reactivity of solids to high-pressure crystallography and back: response of molecular crystals to mechanical stress
- 13.30 Conference Photo, ICKC
- 13.30 – 15.00 Lunch
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## 27 June

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**Parallel session ICKC3: “Photo One”, Chair:  
Anatoly Metelitsa**

**Parallel session ITC3: “Biology One”, Chair:  
Victor Bagryansky**

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15.00 – 15.25 **Pavel Frantsuzov**, Role of the electron-phonon interaction in single semiconductor quantum dot blinking

**Vitaliy Berdinskiy**, Quantum theory of spin dependent biological magnetosensitivity

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15.25 – 15.50 **Artem Smolentsev**, Modulation of chromenes fluorescence *via* photochromic reaction and solvent polarity

**Victoria Syryamina**, The dynamics of spin label surroundings probed by <sup>2</sup>H Electron Spin echo Envelope Modulation spectroscopy

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15.50 – 16.15 **Evgeny Mostovich**, Novel thieno[3,4-b]pyrazines for organic optoelectronics

**Olga Snytnikova**, Metabolomic profiling of biological tissues by NMR spectroscopy

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16.15 – 16.40 **Michael Shestopalov**, Comparative study of optical properties and X-ray induced luminescence of octahedral molybdenum and tungsten cluster complexes

**Aleksandra Kim**, Penetration of nifedipine molecule through DOPC lipid bilayer in the presence of glycyrrhizic acid

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16.40 – 17.10 Coffee break

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## 27 June

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**Parallel session ICKC4: “Photo Two”, Chair:  
Pavel Frantsuzov**

**Parallel session ITC4: “Structure One”, Chair:  
Nikolai Uvarov**

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17.10 – 17.35 **Vladimir Razumov**, Principle of detailed balance  
in the luminescence of complicated systems

**Svetlana Yashnik**, The effects of ammonia crystallization on  
ZSM-5 zeolite structural transformation and ESR spectra of copper  
ammines

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17.35 – 18.00 **Evgeniy Chesnokov**, Zero-area optical pulses – how it  
can be used in chemical kinetics

**Stanislav Chizhik**, Following the kinetics of solid state  
photochemical reaction by measurement of macroscopic mechanical  
response in crystals

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18.00 – 18.25 **Alexandra Pyryaeva**, The impact of oxygen encounter  
complexes on photophysics of molecular oxygen in gas  
and liquid phases

**Boris Zakharov**, X-Ray diffraction studies for understanding  
mechanical effects on solid-state transformations

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18.25 – 19.00 Coffee break

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19.00 VVV Memorial meeting, ICKC

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## 28 June

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### Joint Session 5, ICKC, Chair: Vladimir Polshakov

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9.00 – 9.30 **Geoffrey Bodenhausen**, Dynamic Nuclear Polarization coupled with rapid Dissolution: from technology to new science

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9.30 – 10.00 **Fridrikh Dzheparov**, Basic processes of spin dynamics in disordered solids and magnetic resonance and relaxation of polarized beta-active nuclei

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10.00 – 10.30 **Igor Koptug**, Parahydrogen-based signal enhancement in NMR and MRI

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10.30 – 11.00 **Svetlana Kozlova**, Self-diffusion of aromatic chiral molecules in external magnetic fields. <sup>1</sup>H NMR

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11.00 – 11.30 Coffee break

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### Joint Session 6, ICKC, Chair: Igor Koptug

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11.30 – 12.00 **Vladimir Polshakov**, NMR studies of yeast telomerase

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12.00 – 12.30 **Nikolay Polyakov**, The role of weak non-covalent interactions in drug delivery – NMR and EPR study

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12.30 – 13.00 **Alexandra Yurkovskaya**, Competition of singlet and triplet recombination of radical pairs in photoreactions of 3,3',4,4'-tetracarboxy benzophenone and biologically important molecules

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13.00 – 13.30 **Robert Griffin**,  $\beta$ -Amyloid, subterahertz microwaves, and the magic angle

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13.30 – 15.00 Lunch

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15.00 – 18.30 **Poster session, ICKC**

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19.00 – 21.00 Conference Dinner, NSU

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## 29 June

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### Joint Session 7, NSU, Chair: Victor Nadtochenko

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9.00 – 9.30 NSU Welcome Address

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9.30 – 10.00 **Günter Grampp**, Are the current theories of electron transfer applicable to reactions in ionic liquids? A dynamic ESR study

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10.00 – 10.30 **Nikolay Uvarov**, Ionic transport in orientationally disordered phases

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10.30 – 11.00 **Gonzalo Angulo**, Influence of the excitation light intensity on the rate of fluorescence quenching reactions

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11.00 – 11.30 Coffee break

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### Joint Session 8, NSU, Chair: Gertz Likhtenshtein

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11.30 – 12.00 **Victor Nadtochenko**, Mechanism of ultrafast electron transfer in Photosystem I: Femtosecond spectroscopy with excitation of Reaction Center chlorophylls in the far-red edge of the Q<sub>Y</sub> band

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12.00 – 12.30 **Victor Plyusnin**, Photochemistry of dithiolate Cu(II) and Ni(II) complexes

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12.30 – 13.00 **Anatoly Metelitsa**, Photomodulated chromogenic systems on the basis of photochromic spiropyrans

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13.00 – 13.30 **Arnulf Rosspeintner**, How good is the generalized Langevin equation to describe the dynamics of photo-induced electron transfer in fluid solution?

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13.30 – 15.00 Lunch

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## 29 June

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**Parallel session ICKC5: “Kinetics One”, Chair:  
Andrei Shmakov**

**Parallel session ITC5: “Spin Two”, Chair:  
Sergey Veber**

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15.00 – 15.25 **Zinfer Ismagilov**, Study on spectral characteristics of laser ignition of fossil coals. Comparison with ignition of benzene in model porous matrices

**Tatyana Leshina**, Spin effects and chiral drugs stereoselectivity

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15.25 – 15.50 **Denis Knyazkov**, Combustion chemical kinetics of biodiesel surrogates

**Egor Nasibulov**, Theoretical treatment of pulsed Overhauser DNP

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15.50 – 16.15 **Olga Shkoda**, The influence of preliminary mechanical activation of silicon and niobium powders on thermal explosion

**Marina Petrova**, Quantum chemical study of magnetic coupling in “breathing crystals”  $\text{Cu}(\text{hfac})_2\text{L}^{\text{R}}$

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16.15 – 16.40 **Maruf Kabilov**, Analytical solution of the nonstationary problem of filtration combustion of gases

**Irina Mirzaeva**, Parity violation energy difference between rotosymmetric isomers of DABCO molecule

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16.40 – 17.10 Coffee break

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## 29 June

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**Session ICKC6: “Kinetics Two”, Chair:  
Victor Plyusnin**

**Parallel session ITC6: “Structure Two”, Chair:  
Petr Purtov**

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17.10 – 17.35 **Evgenii Stoyanov**, Stable dialkyl halonium ions ( $R_2Hal^+$ ) and their chemical properties

**Igor Lomonosov**, Physical chemical properties of matter at extreme conditions

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17.35 – 18.00 **Ivan Sorokin**, Radical cations of small heterocycles at low temperatures: Patterns in phototransformations

**Alexander Doktorov**, The influence of the “cage effect” on the mechanism of reversible bimolecular multistage chemical reaction in solutions

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18.00 – 18.25 **Peter Sherin**, Photoinduced reactions of eye lens chromophores with proteins under anaerobic conditions

**Nikolai Medvedev**, A global view on the structure of solutions

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18.25 – 18.50 **Ivan Pozdnyakov**, Mechanistic study of micropollutants photooxidation by Fe(III) species and humic substances

**Vladimir Zyryanov**, From mechanism of mechanochemical reactions to design of nanomaterials

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## 30 June

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### Joint Session 9, ICKC, Chair: Roman Morgunov

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- 9.00 – 9.30 **Gerd Kothe**, Creating a multitude of entangled nuclear spin qubits in hyperpolarized molecular solids
- 9.30 – 10.00 **Nikita Lukzen**, A novel technique for conversion of spin pair singlet state into observable spin hyperpolarization by means of adiabatic switching of spin-locking magnetic field
- 10.00 – 10.30 **Kiminori Maeda**, Precise analysis of the time resolved MARY in photo excitation of Flavin Adenine Dinucleotide
- 10.30 – 11.00 **Daniel Kattnig**, Magnetic field effects on radical pair recombination: Unexpected consequences of chemical reactivity
- 11.00 – 11.30 Coffee break
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### Joint Session 10, ICKC, Chair: Nikita Lukzen

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- 11.30 – 12.00 **Hans-Martin Vieth**, Nuclear spin hyperpolarization at variable magnetic field
- 12.00 – 12.30 **Roman Morgunov**, Quantum bits in  $^{29}\text{Si}$  enriched crystals
- 12.30 – 13.00 **Alexander Okotrub**, Electronic structure and magnetic properties of half fluorinated graphene
- 13.00 – 13.30 **Olga Lapina**, NMR Crystallography as a new tool for characterization of active sites of solid catalysts
- 13.30 – 15.00 Lunch
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## 30 June

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### Joint Session 11, ICKC, Chair: Vladimir Razumov

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15.00 – 15.30 **Vsevolod Borovkov**, New horizons for applying the method of the Time-Resolved Magnetic Field Effects in recombination fluorescence of spin-correlated radical ion pairs

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15.30 – 16.00 **Kev Salikhov**, Minor interactions with major consequences in chemical reactions

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16.00 – 16.30 **Gertz Likhtenshtein**, Multielectron and optimum distance electron transfer processes in biology. 47 Years of history

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16.30 – 17.00 Closing of the Conference

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## Poster Session, 28 June

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**Ekaterina Afanasyeva**, An alternative membrane-modifying mechanism of the antimicrobial peptides action

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**Aleksandra Ageeva**, Influence of substituents on the lappaconitine derivatives photophysics and reactivity

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**Sergei Anishchik**, Action of ionizing irradiation on carbon nanotubes

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**Sergey Babajlov**, NMR investigation of iron(II) sulfate complex with 4-amino-1,2,4-triazole possessing spin crossover

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**Irina Beregovaya**, Radical anion dimers of decafluorobiphenyl and 4-amino-nonafluorobiphenyl. Two more to a small family

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**Boris Bol'shakov**, Sorption enthalpy of oxygen and argon in glassy poly(ethyl methacrylate)

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**Mark Bushuev**, Kinetics of spin crossover with thermal hysteresis

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**Mark Bushuev**, Reinvestigation of spin crossover in prototypical iron(II) complex with 4-amino-1,2,4-triazole

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**Nikolay Dozmorov**, Modelling of the femtosecond intramolecular dynamics in the high-lying electronic states of molecular iodine

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**Nikolay Dozmorov**, Modelling of the femtosecond dynamics of the photoinduced desolvation of rubidium atoms from helium nanodroplets

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**Galina Dultseva**, Free radicals in the atmospheric photonucleation of aromatic aldehydes

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**Kirill Ershov**, Generation of Ti and W atoms and their oxides in the molecular beam

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**Lydia Fedenok**, Mechanism of CH-cyclization of 1-alkynylantraquinones into thienoanthraquinones with the participation of Na<sub>2</sub>S

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**Natalya Fishman**, Effect of pH on sensitized photo-oxidation of thymine and thymidine in aqueous solution: CIDNP study

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**Alexander Germov**, NMR study of Co nanoparticles encaged in carbon nanocapsules

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**Yuriy Glazachev**, Study of physicochemical properties of insect internal environment with L-band EPR spectroscopy

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**Evgeni Glebov**, Photochemistry of 2,3-diarylcyclopentenones: Photochromism and skeletal rearrangement

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**Elena Golysheva**, Dynamical transition in proteins observed by spin-probe relaxation

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**Andrei Gurinov**, Solvent-free synthesis of metal sulfides by thiourea decomposition and probing the surrounding by DNP SENS NMR spectroscopy

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**Mikhail Ivanov**, Peculiarities of ZnTPP spin dynamics in C2-methylated Ionic Liquids studied by Time-Resolved EPR

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**Evgenii Kadtsyn**, The structure of TMAO and TBA water solutions

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**Evgeny Kalneus**, Some practical aspects of registering signal with long relaxation times in Magnetic Resonance Sounding

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**Maria Kardash**, Lipid-mediated clusters of spin-labeled molecules in model membranes and their dissolving in presence of lipid rafts

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**Anastasiya Khlichkina**, Metabolomic profiling of human blood plasma and aqueous humor

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**Alexandr Khudozhnikov**, The mobility of the framework linker in MIL-53 (Al) in the presence of different xylene isomers

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**Alexander Kipriyanov**, Many-particle aspects in the theory of association dissociation reaction

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**Alexander Kipriyanov**, Exciplex formation in non-polar solutions

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**Alexander Kokorin**, Photoaccumulating systems based on thin films of TiO<sub>2</sub>-MoO<sub>3</sub>-V<sub>2</sub>O<sub>5</sub> oxides

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**Vitaliy Kozinenko**, A new method for robust filtering of hyperpolarized multiplet spin order

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**Yaroslav Kraft**, Influence of coal dust particles sizes on laser ignition threshold

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**Denis Kuleshov**, Study of the mechanism of sodium 2,3-disulfanylpropane-1-sulfonate (unithiol) soft oxidation by mass spectrometry with electrospray ionization

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**Arkady Kupryakov**, Photophysical processes for  $\text{Eu}^{3+}$  complexes with a chiral ligand containing 1,10-phenanthroline and (-)-menthol

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**Ivan Kurganskii**, Fullerenes C60 and PCBM as spin probes for investigation of inhomogeneities in ionic liquids

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**Nina Kurus**, Investigation of the energy profile of helix unwinding in DNA by means of atomic force spectroscopy

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**Andrey Kuzhelev**, Trehalose as immobilizer of biopolymers for room temperature pulsed dipolar EPR spectroscopy

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**Diana Kuzmina**, Spin probe study of  $\text{CO}_2/\text{O}_2/\text{N}_2$  gas sorption in ZIF-8

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**Nikolay Lavrik**, Estimation of the molar absorption coefficient of copper salicylate within the spectral range 300-350 nm

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**Nikolay Lavrik**, The effect of recrystallization of aqueous solutions of metal sulfates on the acid-base balance

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**Sofia Lazareva**, Photochromism of diarylethenes in solutions and polymer matrices

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**Ilya Magin**, Stereoselectivity of photo-CIDNP in chiral systems

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**Alexander Marchuk**, Influence of an outer-sphere anion on the crystal structure of photosensitive complexes  $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{XNO}_3$ , (X = Cl, Br, I)

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**Nadezhda Masiuk**, The possibility to operate the homogeneous propane pyrolysis by  $\text{CO}_2$ -laser radiation

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**Anna Matveeva**, Analytical solution of the PELDOR inverse problem using the integral Mellin transform

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**Svetlana Matveeva**, Primary photochemical processes for Hexachloroosmate(IV) in aqueous solutions

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**Makich Musayelyan**, DMSO action on hydrogen atom abstraction reaction from  $\text{Zn}^{\text{II}}(3,5\text{-di-iso-propylsalicylate})_2$  by *tert*-butylperoxyl radicals

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**Yuri Naberukhin**, Collective vortex-like patterns of the diffusive motion in liquid argon. Computer modeling

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**Victor Nadtochenko**, Ultrafast exciton dynamics and photocatalytic activity of Ni promoted CdS nanocrystals stabilized with polymeric shell

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**Eugenia Nemova**, Spin trapping studies of conformation changes in albumin induced by the terahertz radiation: Interaction with NO

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**Maria Oplachko**, Photochromic properties of a 2,3-diarylcyclopentenone

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**Dmitry Pavlov**, Free radical diallyl disulfide rearrangement in the KOH/DMSO system

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**Artem Poryvaev**, EPR spin probe approach for MOF investigation

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**Pavel Potashov**, Manipulation of quantum dots using optical trap

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**Andrey Pravdivtsev**, Complete description of photo initiated Para-Hydrogen Induced Polarization

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**Svetlana Pylaeva**, AIMD of radicals in frozen solutions and its relation to Overhauser-DNP in insulating solids

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**Bogdan Rodin**, Generating long-lived order in multi-spin systems by adiabatically ramped RF-fields

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**Alexey Romanov**, Extending the lifetime of hyperpolarized propane gas through reversible dissolution

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**Victoria Salomatova**, UV-degradation of some bisphenols and their complexes with  $\beta$ -cyclodextrin

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**Olga Selyutina**, The NMR and MD study of glycyrrhizin membrane-modifying activity

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**Veronica Semionova**, Photochromic materials based on metal-organic coordination polymers

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**Kirill Sheberstov**, Nuclear long-lived state in  $^{15}\text{N}$ -enriched azobenzenes

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**Ekaterina Shelepova**, Investigation of glycyrrhizic acid influence on a lipid bilayer

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**Alena Sheveleva**, EPR spectroscopy for gas adsorption study in Metal-Organic Frameworks

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**Olga Shkoda**, Mechanochemical synthesis of titanium nitride in an energy-intensive mill

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**Anna Shlotgauer**, Non-covalent associates of statins with novel drug-delivery system – glycyrrhizic acid

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**Anton Shushakov**, Photophysics and photochemistry of mixed diazide Pt<sup>IV</sup> complexes

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**Oleg Shushakov**, Magnetic-resonance sounding of pore-space microstructure

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**Irina Slepneva**, Dual effect of nitric oxide on the enzyme-mediated melanization

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**Alexey Solovyev**, Quantum chemical calculations of the optical spectra of intermediates: Photochemical reactions of nickel and copper dithiolate complexes

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**Ekaterina Sormacheva**, Mechanisms of aromatic amino acid modifications in anaerobic photolysis sensitized by kynurenic acid

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**Alexandra Svyatova**, Study of singlet oxygen O<sub>2</sub> (<sup>1</sup>Δ<sub>g</sub>) formation *via* photoexcitation of contact complexes X-O<sub>2</sub> (X = TiO<sub>2</sub>, WO<sub>3</sub> and all trans-retinal)

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**Victoria Syryamina**, The Alamethicin self-assembling in membrane at low concentrations by EPR spectroscopy

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**Ivan Timofeev**, Pulse and CW EPR study of triarylmethyl radicals in glassy trehalose

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**Sergey Tumanov**, EPR study of light-induced metastable states in two spin Cu(hfac)<sub>2</sub>L<sup>R</sup> compounds

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**Timofey Tyugashev**, Impact of the active site amino acid residues on the lesion recognition by human 8-oxoguanine DNA glycosylase 1

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**Igor Valuev**, The influence of magnetic solution on the magnitude of zero-field splitting in a cobalt(II) complex

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**Sergey Veber**, Magnetic properties of Co<sup>II</sup> with large ZFS: Experimental and computational study

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**Maxim Zelikman**, Investigation of the formation of CnEm dimers in water by the molecular dynamics method

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**Yuliya Zhuravleva**, Quenching of kynurenic acid in triplet state by biological compounds

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