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Magnetic resonance and its applications

Book of Abstracts

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30 March — 3 April 2026

Saint Petersburg, Russia

SAINT PETERSBURG STATE UNIVERSITY
Department of Nuclear Physics Research Methods

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Lectures

Elasticity of the magnon Bose-Einstein condensate

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In most experiments magnons are treated as a weakly interacting gas of incoherent quasiparticles. In contrast, a magnon Bose–Einstein condensate (BEC) represents a distinct phase characterized by a macroscopic coherent order parameter and spontaneous breaking of U(1) symmetry. This transition qualitatively changes the nature of low-energy excitations, giving rise to collective phase dynamics and an effective elastic response of the condensate.

In the long-wavelength limit, spatial and temporal variations of the condensate phase propagate as Goldstone modes. These collective excitations are a direct consequence of phase rigidity and are analogous to sound modes in superfluids. Such modes were first observed in a magnon BEC in superfluid ^{3}He-B [1, 2] and subsequently in the antiferromagnet $MnCO_3$ [3]. Their observation provides unambiguous evidence of spontaneous symmetry breaking and distinguishes a true magnon condensate from an incoherent magnon gas.

Previous attempts to detect Goldstone modes in Yttrium Iron Garnet (YIG) film at room temperature were hindered by external phase locking imposed by continuous RF pumping, which suppresses intrinsic phase dynamics of the condensate. Since a defining signature of Goldstone modes is low-frequency modulation of the condensate phase, the dominance of the pump frequency masks the corresponding spectral features in the emitted signal.

Here we demonstrate a regime of self-generated magnon Bose–Einstein condensation in YIG, in which the condensate phase is not externally fixed. In this regime, we observe intrinsic low-frequency oscillations of the emitted microwave signal, interpreted as Goldstone modes of the magnon condensate. These results provide direct dynamical evidence for magnon BEC in YIG, complementing recent optical observations [4, 5].

The work was supported by the Russian Science Foundation. Grant No.22-12-00322-p.

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Magnon Laser and its applications

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The concept of an atom laser emerged in 1997, by analogy with an optical laser [1]. The coherence in conventional photon lasers is formed through the stimulated photon emission process that requires population inversion in the incoherent gain medium, which sets a lower bound for the energy threshold. In contrast, a coherent matter wave can form as the ground state, rather than the inverted state, of a multi-particle quantum system. While an optical laser generates a coherent beam of photons, an atom laser generates a beam of coherent atoms in a Bose-Einstein condensate state. The lifetime of atomic Bose condensates in an optical trap is limited by atomic evaporation. By directing a beam of coherent atoms into the trap, it is possible to compensate for atomic evaporation and significantly increase the lifetime of the Bose condensate [2].

In the case of magnetic resonance, the magnetization deflection angle and consequently magnon density increases with increasing RF pump power. It has been shown theoretically that for Yttrium Iron Garnet (YIG) film magnetized perpendicular, at room temperature, the critical magnon density for the formation of Magnon Bose Einstein Condensate (MBEC) at room temperature corresponds to the angle of deviation of the magnetization 2.5° [3].

In this presentation, we experimentally demonstrate the flow of coherent magnons beyond their excitation region, which is consistent with the concept of a quasiparticle laser. Furthermore, since coherent magnons emit photons, we were able to observe coherent photon emission [4,5]. Various applications of this new coherent state of magnons will be discussed.

The work was supported by the Russian Science Foundation. Grant No. 22-12-00322 - p.

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RECENT APPLICATIONS OF NMR FOR STUDIES OF NANOSTRUCTURED AND BULK METALS AND ALLOYS

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Since long time NMR has been successfully used to study bulk solid and liquid metals and their alloys. Here we present short review of recent results obtained by NMR for nanostructured and bulk low-melt metals and alloys.

NMR was suggested to prove the impact of magnetic field on orientation of crystalline axes upon solidification. The unambiguous evidences of the directional solidification were obtained for bulk tin and gallium metals.

The structural transformation in the supercooled melt (the liquid-liquid phase transition) was found by NMR for bulk and nanostructured gallium and for some nanostructured gallium alloys.

NMR was suggested to be used to study alterations caused by nanoconfinement in the phase diagrams of metallic alloys.

Strong changes in the hyperfine coupling of conduction electrons with nuclei were observed in nanostructured metals and metallic alloys through measurements of the temperature evolution of the Knight shift.

Ionic mobility in many metals and alloys was shown by NMR to be remarkably affected by nanoconfinement.

NMR was used to observe unusual phenomena upon freezing and melting of confined metals as well as to reveal size effects on polymorph transitions.

MECHANISM OF ASYMMETRIC AUTOAMPLIFYING SOAI REACTION STUDIED BY COMBINATION OF NMR EXPERIMENTS AND DFT COMPUTATIONS

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Since the first report on the Autoampifying Autocatalitic Asymmetric catalysis observed in the reactions of pyrimidinc aldehydes with disopropyl zinc (later called "Soai Reaction") [1-4], this unusual transformation received vigorous attention of the researchers attempting to undercover its mechanistic details. Although neither mechanistic suggestion can be considered as the final solution, any conscientious effort in this field has a certain value, since it implies modeling the consequence of processes that must result in amplification of the catalyst's own chirality. After three decades of concentrated efforts, it becomes clear this is not an easy task. Nevertheless, even incomplete or limited success in this route can provide insights useful for the adjacent fields. In this talk the origins and the early mechanistic studies of the Soai reaction are summarized [5-11] together with the most recent developments.

This research was financially supported by Russian Science Foundation through Grant 22-13-00275П

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GUEST MOBILITY AND MOLECULAR SIEVING MECHANISM OF C3-C4 HYDROCARBONS IN POROUS METAL-ORGANIC FRAMEWORKS PROBED BY SOLID STATE 2H NMR AND MOLECULAR DYNAMICS

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The current sustainable development strategy requires new, energy-efficient ways to separate industrially valuable hydrocarbons. One of the most demanded processes in practice is the separation of C3-C4 hydrocarbons – propane and propylene, as well as butane isomers. One of the promising directions for the separation of these mixtures is the use of microporous sorbents capable of either selectively absorbing one of the isomers or selectively delaying due to differences in diffusion coefficients (the so-called kinetic separation). Due to the proximity of the molecular structure and size of propane and propylene, this is a complex task that requires materials with a molecular structure adapted to interact with one of the isomers. This report presents data on the molecular mobility and separation of C3-C4 hydrocarbons new porous metal-organic frameworks based on imidazole, carboxylate and amino acid linkers. By combining the results of measurements of solid-state 2H NMR spectroscopy and modeling by molecular dynamics methods, it was possible to establish the mechanism of molecular adsorption and mobility of guest molecules in the pores of these frameworks and to show the mechanism of separation selectivity in this framework. The also discuss the potential directions of linker modification to optimize guest-host intermolecular interactions to increase selectivity.

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NMR GUIDED STRATEGIES FOR TARGET ORIENTED DRUG DISCOVERY

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A major objective of contemporary biomedical research is the target-oriented discovery of new therapeutics. Among the biophysical techniques supporting this goal, NMR spectroscopy occupies a prominent position, as it provides detailed information on molecular structure, dynamics, and intermolecular interactions that are critical for understanding drug mechanisms and identifying novel bioactive compounds.

NMR spectroscopy is widely applied to the structural characterization of biologically active natural products and to the analysis of highly specific interactions between small molecules and biomolecular targets [1]. These capabilities have enabled the development of fragment based and NMR guided screening strategies. This presentation reviews current NMR screening approaches and fragment based methods for the rational design of bioactive compounds, including both target observed techniques such as SAR-by-NMR and ligand observed experiments such as STD and WaterLOGSY.

The concepts are illustrated by examples of clinically approved drugs discovered using NMR based approaches, as well as by our own studies on potential inhibitors of bacterial enzymes. We investigated inorganic pyrophosphatase from *Mycobacterium tuberculosis* and NAD^+ dependent formate dehydrogenase from *Staphylococcus aureus*, both essential for bacterial survival and lacking close human counterparts. Using uniformly isotope labeled proteins and complementary ligand and protein observed NMR experiments, we identified and optimized compounds that bind functional sites and inhibit enzymatic activity with micromolar IC_{50} values. These inhibitors are structurally distinct from known compounds and represent promising leads for the development of new antibiotics.

The study was supported by the Russian Science Foundation grant No. 24-14-00081.

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PROBLEMS WITH SAMPLE SHAPES AND SIZES IN NMR EXPERIMENTS

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Magnetic resonance experiments are generally designed assuming ideal equipment and samples. But this is not reality and non-linear static ($\mathbf{B}_0$) and oscillating ($\mathbf{B}_1$) magnetic fields and non-constant magnetic gradients (**g**) present major problems. Indeed, the hardware can never be perfect (e.g., $\mathbf{B}_0$ should have spatial homogeneity and time stability exceeding 10^{-8} T) and the problems are worsened when the magnetic susceptibility interfaces of the sample result in large background magnetic gradients. In Diffusion NMR and MRI this results in incorrect estimates of diffusion coefficients and distorted images with unexpected intensities.

This lecture includes a personal historical perspective and includes considerations of steps that can be taken to reduce these deleterious effects including bespoke sample holders and sample preparation. These techniques have particular relevance when one wants to precisely correlate MR datasets of deformable samples with other measurements (e.g., pathology).

Alternative Calculation of EPR Spectra: Collective Modes in Spectral Diffusion

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Abstract

An alternative approach to the calculation and interpretation of EPR spectra based on the collective dynamics of quantum coherence in an ensemble of spins whose interactions change randomly over time is described. In contrast to the traditional phenomenological representation of the spectrum as a sum of independent Lorentzian lines of individual subensembles, the EPR spectrum is considered as a response of a set of independent “orthogonal” collective modes of spin magnetization motion, formed as a result of coherence transfer between subensembles.

It is shown that spectral diffusion, which includes various mechanisms such as spin exchange during random collisions and changes in the dipole-dipole interaction due to mutual diffusion of interacting spins, plays an active role in shaping the response of an ensemble of spins to an external microwave field. Different mechanisms of spectral diffusion contribute additively to the rates of elementary spin decoherence processes (the contributions of different mechanisms add up) and the rates of quantum coherence transfer to the interaction partner (in this process, the contributions of different mechanisms can even be subtracted!). So different mechanism of spectral diffusion jointly determine the observed shape of the EPR spectrum.

The spectrum is represented as a sum of contributions from collective modes characterized by complex resonant frequencies. It is shown that the presence of collective modes of the evolution operator does not guarantee their manifestation in the observed spectrum. The observability of the modes is determined by the excitation conditions of the microwave field. Each collective mode has its own "oscillator strength" for excitation by a microwave field. In the region of sufficiently fast spectral diffusion, one of the collective modes tends to the most symmetric form, and it is this mode that contributes significantly to the observed EPR spectrum. This circumstance allows us to consistently explain the absence of the expected additional lines in the fast spin exchange limit case and to revise the traditional interpretation of the exchange narrowing of the spectrum.

The proposed approach sets a different methodological level for calculating EPR spectra and provides a description and interpretation of the shape of individual resonance lines and the entire EPR spectrum at arbitrary spectral diffusion rates.

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BRIDGING PROTON DELOCALIZATION IN SHORT HYDROGEN BONDS: EFFECTS IN ^{1}H NMR SPECTRA

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In this report we discuss how the bridging proton delocalization in strong (short) hydrogen bonds affects the observed averaged ^{1}H NMR chemical shift. Several origins of proton delocalization are discussed:

a) delocalization due to zero-point energy vibrations (proton wave function delocalization),

b) dynamic delocalization due to thermal fluctuations of the surrounding medium (solvent motion or phonon vibrations) and

c) delocalization due to the mutual influence of several coupled hydrogen bonds.

The content of the presentation is based on several recently published papers: ref. [1] deals with an isolated H-bonded complex with OHO bond in vacuum; ref. [2] focuses on several crystals with chains of coupled OHO hydrogen bonds; ref. [3] as well as earlier published papers [4] and [5] are dedicated to short OHO, FHF, OHN and NHN hydrogen bonds both in vacuum and in thermally fluctuating media. Most of these results are based on quantum-chemical calculations cross-checked in several cases with the results of experimental low-temperature liquid-state NMR spectroscopy.

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Oral Reports

A MAGNETOCALORIC MODEL FOR THE MAGNETIC HYSTERESIS IN DYSPROSIUM TETRAFLUORIDE

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Lithium–rare-earth double fluorides $LiRF_4$ (R = Y, Gd-Lu) attract interest as model objects in physics of dipolar magnets. $LiDyF_4$ is a dipolar antiferromagnet, magnetic moments of Dy^{3+} ions order in the (001) plane, T_N =610(15) mK; crystal structure belongs to $I4_1/a$ symmetry [1, 2]

Previously, there was a magnetic hysteresis effect detected in crystalline samples (a micro-sized powder and a single crystal) in the temperature range of 2-10 K [3, 4]. This work develops a magnetocaloric approach [5] to describe this paramagnetic-phase phenomenon, involving the exchange-charge framework for calculations of magnetic properties [1, 3] and *ab initio* simulations of phonon thermodynamics within the density functional theory framework [6], achieving both qualitative and quantitative agreement for the $LiDyF_4$ single-crystal magnetization data collected in the magnetic field applied along its [100] axis.

The financial support of the Russian Science Foundation (grant No. 22-12-00259-П) is gratefully acknowledged.

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INFLUENCE OF NONTRIVIAL TOPOLOGY ON ^{125}Te NMR SPECTRA IN THE *Td*-WTe_2 SINGLE CRYSTAL

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WTe_2 grown in the *Td* phase is a non-centrosymmetric crystal. The lack of inversion symmetry allows a nontrivial topology in Weyl semimetals. WTe_2 was the first material suggested as a type-II Weyl semimetal [1]. Nevertheless, its nature was questionable for a long time. Sufficiently convincing evidence was obtained by the transport measurements and scanning tunneling microscopy. But some ambiguity remains.

Our first NMR studies of *Td*-WTe_2 [2,3] revealed an additional line in ^{125}Te NMR spectra at low frequencies, which did not belong to the tellurium sites in the crystal structure.

In the present work we focus on the room-temperature measurements of *Td*-WTe_2 single crystal to study the angular dependence of ^{125}Te NMR line positions, especially, of the additional line at low frequencies. We report the evolution of the ^{125}Te NMR spectra at the rotation of the single crystal about the *a* axis by an angle from 0 to 150°. The main components in the ^{125}Te NMR spectra are ascribed to four non-equivalent tellurium positions. The strong angular dependence of the additional low-frequency line is observed for the first time. This line is treated as the manifestation of topological electronic states in the non-centrosymmetric *Td*-WTe_2.

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NMR STUDY OF FAST ANION REORIENTATIONS IN $Y(BH_4)_3 \cdot xNH_3$ (x = 3 AND 7)

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Metal borohydrides are intensively studied due to their potential applications in hydrogen storage and solid-state ionics. Their functional properties are strongly influenced by the dynamics of complex anions [1]. Ammine borohydrides $Y(BH_4)_3 \cdot xNH_3$ form a versatile family of compounds in which the introduction of neutral NH_3 ligands significantly modifies both structure and atomic dynamics [2 – 4].

In order to find out the effect of the introduction of a neutral NH_3 ligand on the dynamics of anions in $Y(BH_4)_3 \cdot xNH_3$ (x = 3 and 7) we have measured ^1H and ^{11}B nuclear magnetic resonance (NMR) spectra and spin-lattice relaxation rates over the temperature range of 6 – 300 K. Our results indicate that the anions $[BH_4]^-$ in both compounds exhibit unusually fast reorientations down to low temperatures, indicating enhanced mobility compared to pristine $Y(BH_4)_3$ [5]. According to the NMR data, in $Y(BH_4)_3 \cdot 3NH_3$, two reorientational processes for BH_4 groups with low activation energies are observed; the fastest process is characterized by the average activation energy of 69 meV. In contrast, in $Y(BH_4)_3 \cdot 7NH_3$, there are four reorientation processes for BH_4 groups, and the fastest of these processes has the average activation energy of 18 meV. This exceptional mobility is related to the coordination environments of $[BH_4]^-$ anions: while in $Y(BH_4)_3 \cdot 3NH_3$, a BH_4 group is coordinated by a single Y^{3+} ion via a tetrahedron face, BH_4 groups in $Y(BH_4)_3 \cdot 7NH_3$ have no Y^{3+} ions in their nearest-neighbor environment, being coordinated only via relatively weak dihydrogen bonds.

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FEATURES OF DENDRIMER DIFFUSION IN MELT: FULL-ATOMISTIC SIMULATION

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This report examines the mobility characteristics of carbosilane dendrimer macromolecules of generations G2-G4 in melts. Using molecular dynamics simulations with full-atomistic resolution, it was established that subdiffusion, related to processes commonly referred to as "anomalous diffusion," is observed in melts of dendrimers of all generations. It is important to note that the same dendrimers were examined in a solvent environment in [1], which revealed a complete absence of subdiffusion.

To determine the influence of the dendrimer environment, we studied the mechanism of atomic mobility in the macromolecule and found that the atoms randomly walk across the geometric surface corresponding to the dendrimer's shape, which is spherical [2, 3]. In [4], it was shown that dendrimer molecules have an impermeable core, leading to a crowded environment effect in the melt. Moreover, for the generation of G4, this effect even influences mechanical relaxation. We demonstrate that the resulting subdiffusion in melts is a consequence of the crowded environment effect (which is absent in the solvent environment) combined with the walking of atoms on a sphere. We also demonstrate that subdiffusion can be described with high accuracy within the fractional Brownian motion (fBm) theory.

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IMPACT OF ENVIRONMENT ON QUANTUM CORRELATIONS IN TWO-SPIN SYSTEMS WITH DIPOLE-DIPOLE INTERACTIONS

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The influence of the environment on quantum correlations (entanglement [1] and quantum discord [2,3]) is studied in a two-spin-1/2 system with the dipole-dipole interactions on the basis of the Lindblad equation [4], which is of fundamental importance in this case since it describes quantum dynamics in the most general way [5,6]. We consider a simple case when the environment leads to dephasing of the system spins only [7].

We obtained an exact solution of the Lindblad equation for two-spin systems with dephasing relaxation. The dependencies of entanglement and the quantum discord on the relaxation rate and the evolution time are also obtained. The temperature dependencies of entanglement and the quantum discord are investigated. We also compare the influence of the environment on entanglement and the quantum discord.

The experimental verification possibilities of the obtained results in NMR experiments in solids are also discussed.

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Molecular and magnetic relaxation processes during Hemoglobin S aggregation.

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Experimental data obtained using three independent methods— ^{1}H magnetic relaxation (4MHz) [1], electron paramagnetic resonance (classical spectrum and ST EPR) [2], and ^{1}H magnetic resonance dispersion (at 20 KHz to 60 MHz) [4,5] —have been used to evaluate proton magnetic relaxation in hemoglobin (Hb) solutions and during hemoglobin S (HbS) polymerization process. The dominant role of the macromolecular rotational correlation time in the modulation of the spin- lattice and spin-spin magnetic relaxation mechanisms was demonstrated after the consideration of the following factors [1-6]: i) the changes of the relative contributions of the various magnetically nonequivalent states (monomers, dimers, microtubules, defective microtubules, and finally domains) [3] during HbS polymerization; ii) the gradual increase of the paramagnetic sites from oxyHbS (diamagnetic) to deoxyHbS (paramagnetic) during macromolecular aggregation; iii) the increasing in the anisotropy of the HbS solutions as a result of the emergence of paramagnetic centers and the rising in the dimensions of the molecular aggregates; iv) the appearance of new magnetic relaxation mechanism, such as Spin-Curie interaction and the magnetic susceptibility anisotropy, as a consequence of the increasing of the magnetic field strength and the molecular correlations times [4] as well as v) the changes in the spectral density function due to a change in the resonant frequency.

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Quantitative descriptors space: a basic platform for qMRI.

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In the vast majority of MRI procedures performed in hospitals, the images are interpreted visually by specialists, limiting the richness of the information contained. A similar situation occurs in preclinical studies [1-7]. Concepts and procedures are combined in a relative new field of quantitative MRI (qMRI). This term is defined differently depending on the approach and area of application [5-7].

Information in MRI essentially comes solely from measuring the intensity of image pixels, which is affected by physical and technical factors that determine image quality. Defining and determining quantitative descriptors of MRI equipment performance, including its temporal stability, constitutes an essential platform for qMRI [1-7].

This paper discusses physical and technological aspects of MRI that limit quantification. It addresses methods for compensating for and correcting these limitations by constructing a space of quantitative descriptors used in the design and execution of qMRI experiments, and in the processing and post-processing of MRI images, as a complement to phase and image spaces [4].

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TIME-DOMAIN NMR DETECTION OF APPLE JUICE ADULTERATION

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Fruit juices are so popular due to their natural constituents and high nutritional value that they are frequently adulterated for profit (usually by blending them with cheaper fruit juices, diluting them with water, or adding sugars). Apple juice, in particular, is regarded as one of the fruit juices most susceptible to diluting with water because of its comparatively low scent intensity and high natural water content. Water adulteration increases product volume while disrupting the balance of fruit-specific ingredients and viscosity. This leads to serious issues with legislation and consumer confidence. Fruit juice adulteration can be detected using techniques such as near-infrared spectroscopy (NIRS) [1], Raman spectroscopy (RS) [2], Fourier transform infrared spectroscopy (FT-IR) [3], and hydrogen nuclear magnetic resonance spectroscopy (^{1}H NMR) [4]. In this context, Time-Domain Nuclear Magnetic Resonance (TD-NMR) is considered a powerful and, at the same time, low-cost tool, because it can directly probe the behavior of water molecules in food systems.

In this work, TD-NMR was used to detect adulteration of apple juice by water dilution. T_1 (spin-lattice) and T_2 (spin-spin) relaxation times, as the parameters both sensitive to chemical environment and dynamics of liquid molecules, were measured using TD-NMR in both pure apple juice and samples diluted with varying water ratios. It was established that the addition of water significantly increased both T_1 and T_2 times. According to TD-NMR data, shorter T_1 and T_2 relaxation times were observed in pure juice due to the higher content of saccharides and the higher acidity of apple juice. On the other hand, dilution of apple juice with water results in a gradual increase of relaxation constants as a result of the higher mobility of molecules of the liquid mixture. Thus, our study reveals the potential of TD-NMR as an efficient method for detecting water and other juice adulterants in apple juice and other juices by probing their effect on relaxation parameters. We plan to extend these studies to other types of juices, particularly those with higher costs, to examine the effects of additional additives (e.g., sugars).

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PROTON DYNAMICS IN THE COUPLED OHO(–) AND OHN(+) BONDS IN COMPLEXES OF PHOSPHINIC ACID WITH PYRIDINES

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This report is focused on the discussion of mutual influence of the coupled OHO and OHN bonds in non-equimolar molecular complexes formed by homoconjugated anions of dimethylphosphinic acid and substituted pyridines. It is assumed that they are present as structural motifs in proton-conducting membranes of fuel cells based on polyphosphoric acids [1], as well as in intermediates of stereoselective hydrogenation reactions with chiral organophosphorus acids [2] and of proton-coupled electron transfer reactions [3].

The formation of the adjacent OHN bond leads to asymmetrization of the OHO bond with a concomitant redistribution of the negative charge between the acid residues. This means that their ability to donate and accept protons, *i.e.* their nucleophilicity in chemical reactions, can be controlled by tuning the strength of the N-base. We have experimentally addressed this largely unexplored issue by low-temperature ^{1}H and ^{31}P NMR spectroscopy in a liquified mixture of deuterated freon gases. Comparison of positions and relative integral intensities of signals in the ^{1}H and ^{31}P{^{1}H} spectra of samples with varying acid-to-base ratio allowed us not only to establish the stoichiometry of neutral and charged complexes, but also to capture a gradual change in the geometry of the coupled OHO and OHN bonds with an increase in the strength of the N-base. Furthermore, it allowed to draw a counterintuitive inference about the change in partial negative charges on the oxygen atoms depending on the strength of the N-base. A decrease in the strength of the N-base leads to a shortening of the OHN bond with a simultaneous increase in the negative charge on the central acid residue at the expense of decreased negative charge of the terminal acid molecule.

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Probing Anion Basicity Effects on Cation Dynamics and Hydrogen Bonding in Phosphonium Ionic Liquids via ²H NMR

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Ionic liquids (ILs) based on trialkylphosphonium cations offer a unique platform for probing structure-property relationships due to the accessible phosphonium P–H proton, a potential hydrogen bond (H-bond) donor. While anion basicity is known to influence macroscopic properties like viscosity and conductivity in ammonium ILs, its specific role in governing ion dynamics and interionic interactions in phosphonium systems remains insufficiently understood at the molecular level. Analogous trialkylammonium ILs with methanesulfonate anion ($[OMs]^-$) form stronger hydrogen bonds than triflate ($[OTf]^-$) or bis(trifluoromethanesulfonyl)imide ($[NTf2]^-$) anions. The in-depth study on the microscopic level is required to determine the validity of this correlation for trialkylphosphonium ILs.

This study presents a comparative investigation of a homologous series of triethylphosphonium ($[P_{222}\text{-}D]^+$) ILs with anion of varying basicity ($[OMs]^-$, $[OTf]^-$, and $[NTf2]^-$). The choice of triethylphosphonium cation is dictated by the lowest melting temperature of resulting ILs compared to ILs with $[P_{111}\text{-}D]^+$ and $[P_{444}\text{-}D]^+$ cations. We employ ^2H NMR spectroscopy as a powerful, cation-selective probe to elucidate microscopic dynamics both in the solid and liquid state. The ^2H NMR spin relaxation in the liquid state characterizes the cation dynamics and allows to probe the microscopic viscosities of ILs. The ^2H NMR spectrum line shape provides insight on the interaction between ions, as well as the phase transition phenomena in these ILs.

The most unexpected finding is anomalous temperature dependence of spin relaxation in the liquid state was observed. The T_1 and T_2 spin relaxation times are known to become equal in the high temperature limit. However, this is not the case for ILs under study. We propose motional model that explains such phenomenon and allows determining mobility of cationic species.

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Ion Transport in Liquid Crystal Electrolytes: Molecular Insights from NMR Spectroscopy

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Optimizing ion mobility in electrochemical devices requires balancing efficient charge transport with a stable electrochemical environment. Functionalizing electrolytes with liquid crystals (LCs) has emerged as a promising strategy to fine-tune ion transport by introducing mesoscale order and anisotropic dynamics [1,2]. Incorporating LCs adds a dynamic structural component that modifies the local environment of ions, enabling active control over their transport pathways.

In this work, we investigate how LC doping influences ion dynamics in bulk electrolytes, providing a model system for locally variable LC environments that may arise near solid interfaces. LiTFSI-based electrolytes functionalized with the nematic mesogen 4-cyano-4'-pentylbiphenyl (5CB) were studied using a range of solution and solid-state NMR techniques. Molecular-level miscibility and spatial proximity of the components were examined using the HOESY technique. Ion diffusion and electric-field-induced mobility were probed via pulsed-field gradient NMR and electrophoretic NMR (eNMR) [3,4]. We show that even at low LC concentrations, local 5CB enrichment markedly modifies ion mobility under electrochemical conditions. The LC medium restricts ion hopping, while specific ion–LC interactions further immobilize charge carriers, generating localized mobility-retardant zones. These findings demonstrate how small mesogen fractions can exert disproportionately large control over ion transport, offering a framework for designing adaptive compositionally self-tuned electrolytes for electrochemical devices.

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MULTICHANNEL NMR MAGNETOMETER FOR LOW-FIELD MRI SYSTEMS. SCHEMATIC DESIGN

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Low-field MRI is a developing and promising technology [1-3]. The high homogeneity of static magnetic field is required. Passive and active shimming is used to achieve this, based on iterative field mapping (via spherical harmonic decomposition using data from a ROI boundary [4]). While commercial solutions exist for high-field systems (1.5 T, 3 T) [5], there is a lack of such specialized instruments in a low-field range. The efficiency of shimming critically depends on measurement accuracy and speed, affected by sensor positioning accuracy. An effective solution in this sense is in development of a multi-channel measurement system. NMR sensors provide the required accuracy [6]. Their integration into a multi-channel array ensures high speed and ease of use.

This work presents the results of a circuit design simulation of a multi-channel NMR magnetometer for low fields, particularly for 0.07T application. A circuit was designed and simulated where multiple sensors are connected via a common coaxial cable. Sensors sequential activation is controlled by a shift register and MOSFETs operating in switching mode. This device has potential of integration into a standard low-field MRI setup: magnetometer could be used together with MRI transceiver instead of Tx/Rx coil, so additional RF transceiver is not required. The proposed solution aims to reduce time and efforts required for passive shimming of low-field MRI systems.

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SYNTHESIS AND PROPERTIES OF CATIONIC IONIC LIQUID MONOMER

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In modern times, the volume of research work is constantly increasing in order to create environmentally friendly "green chemistry" technologies and production processes based on the application of these technologies in order to reduce the amount of volatile, toxic compounds that pollute the environment and atmosphere.Ionic liquids (ILs), known as solvents that meet the requirements of ecologically harmless or "green" chemistry are of particular practical importance in the creation of new ecologically harmless chemical technologies [1].

Taking into account the above, the presented thesis material reflects the results of the synthesis, structural structure, and study of the physicochemical properties of an ionic liquid monomer containing N,N-diethyl-(2-hydroxyethyl)-N-(2-methacryloxyethyl)ammonium bromide based on the quaternization reaction. The synthesis process of the monomer was carried out in two stages. In the first stage, the intermediate product 2-bromomethylmethacrylate was obtained in the form of a basic liquid from the interaction of dibromoethane and methacrylic acid under the intended reaction conditions; in the second stage, the corresponding ionic liquid-containing complex salt was obtained in 95% yield from the interaction reaction of the said intermediate product with diethylaminoethanol.

The structure of the synthesized ionic liquid monomer was studied by IR-, ^{1}H NMR-spectral analysis methods, the composition was studied by elemental analysis, and the physical-thermal parameters were studied by Derivotographic and Differential Scanning Calorimetry methods. Thus, the IR spectrum of this ionic liquid monomer is characterized by the presence of absorption bands related to the C-N bond and ammonium group in the cation fragment, along with the valence vibrations of the C=O bond of the ether fragment. In the ^{1}H NMR spectrum of the sample, the signals of protons specific to the methyl groups of the ethyl fragment connected to the nitrogen atom were observed in the form of a triplet (1.42-1.47 ppm), and the methylene groups of the ethyl fragment connected to the nitrogen atom were observed in the form of a quartet (3.26-3.34 ppm).

The composition of the synthesized ionic liquid monomer was determined using the elemental analysis method on a PERKIN ELMER-2400 device according to the instructions. The amount of C, H, N elements in the sample was determined, and the result (C-46.48; H-7.80; N-4.51) was consistent with theoretical calculations (C-46.45; H-7.74; N-4.52). It was determined that the electrical conductivity of the synthesized ionic liquid monomer is ($3.1\cdot10$-3 $Sm\cdot cm^{-1}$), and the melting temperature is 91-93 ^{0}C.

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DEVELOPMENT AND TESTING OF GRADIENT POWER AMPLIFIERS FOR A LOW-FIELD MRI SYSTEM

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Portable low-field MRI systems [1] require compact, cost-effective gradient power amplifiers (GPAs). Known open-source projects (e.g., GPA-FHDO [2]) provide a limited value of output current. To achieve higher gradient strength values with a coil efficiency of approximately 0.1–0.2 mT/m/A, a drive current up to 90 A is needed. This current is applied to a load with resistance of 40 – 90 mΩ and inductance of 90-150 µH.

This work shows the design, simulation and experimental validation of 90 A GPA. The H-bridge design uses PWM switching with MOSFETs and SiC diodes on an aluminum substrate for optimal heat dissipation. To provide the requirements of the amplitude current pulse rise time ≤1 ms and the ripple of the steady-state current ≤0.1 A, given the parameters of the load, a DC bus voltage level of 24 V and a PWM frequency of 200 kHz were selected. To control an amplifier the TMS320F28379D is, utilizing its 16-bit ADC. UDP/Ethernet (100 Mbps) facilitates console communication, supporting 10 µs trajectory loading, sync-pulse execution, diagnostics, and protection.

Three identical GPAs were implemented and tested while connected to solenoid loads at each channel. Current measurements were performed using current probes and built-in GPA current sensors. The test methodology included calibration across the entire current range up to 90A to determine a calibration coefficient. Pulses of various amplitude, duration, and duty cycle were sequentially generated to assess the correspondence between the measured current waveform and the set trajectory. The areas under identical pulses were compared to evaluate reproducibility. The measured signal data was filtered to suppress high-frequency noise.

The results confirm that the proposed amplifiers demonstrate required properties for GPA in low-field MRI applications. Further work includes evaluating the gradient pulse shape using a solenoid probe and confirmation of acquired properties together with gradient coils.

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NMR SPECTROSCOPY IN THE STUDY OF COMB-LIKE POLYELECTROLYTES

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The report discusses the features of surface-active monomers polymerization based on n-bromoalcanol derivatives with 11, 9, 6, 3 methylene spacers between cationic and acryloyloxy groups. The polymerization products of these substances are comb-like polyelectrolytes that have proven themselves in carrying out organic reactions in water that is green and environmentally friendly solvent. Compounds with different lengths of the methylene spacer between the polymerized and polar groups of the molecule were synthesized to study the effect of micelle formation on the polymerization kinetics of surface-active monomers by in-situ NMR technique. Polar groups that are potentially capable to stabilize the surfactant micelle due to additional interactions (pyridinium and quinolinium cations) were introduced in the monomer molecular structure. It was found that the monomer micelles act as a kind of reservoir with surfactant molecules and practically do not participate in the propagation of polyelectrolyte during micellar polymerization. The impossibility of topological polymerization of these monomers is substantiated; as a result of micellar polymerization, a high-molecular products with a significant dispersion index (Đ) are formed. The resulting comb-like polyelectrolytes form hydrophobic aggregates in aqueous solution. Diffusion coefficients of individual macromolecules and their aggregates were determined using two-dimensional DOSY NMR spectroscopy and dynamic light scattering. The report compares the results of these two methods.

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SPIN KINETICS OF ^{3}He IN CONTACT WITH NANOSIZED POWDER PrF_3.

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PrF_3 is a dielectric Van Vleck paramagnet with Pr^{3+} ($4f^{12}$) ions. The crystal field splits the ground state multiplet of $^3H_4$ into nine singlets. The nucleus of this rare earth element has a nuclear spin of 5/2, and compounds of this element exhibit nuclear magnetism. PrF_3 can be used for the dynamic polarization of the nuclear spins of ^{3}He [1].

PrF_3 nanoparticles measuring 56 × 34 nm were obtained by hydrothermal synthesis using a nitrate reaction with treatment in a classic autoclave. Their composition and structure were confirmed by X-ray diffraction (Bruker D8 Advance), and their morphology and size were confirmed by transmission electron microscopy (Hitachi HT Exalens).

NMR spectroscopy and relaxometry of ^{3}He in contact with nanosized PrF_3 particles were studied. Measurements were performed on a laboratory-made NMR spectrometer [2]. The effect of nanosized powder of PrF_3 magnetic particles on the rate of longitudinal and transverse relaxation of helium-3 nuclei in an adsorbed layer, gas, and liquid, as well as with adsorbed helium-4, was studied. Measurements were performed at a temperature of 1.5 K in fields of 0–800 mT. The mechanisms of nuclear magnetic relaxation are considered. A model describing the nuclear magnetic relaxation of helium-3 in contact with PrF_3 nanoparticles is proposed.

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ANTIRADICAL ACTIVITY OF CATECHOLAMINES: INSIGHTS FROM KINETIC EPR MEASUREMENTS

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In this work, the antiradical properties of catecholamines, in particular dopamine and norepinephrine, were investigated. Catechol and caffeic acid were used as reference (structural) analogues. The studied compounds belong to the class of biologically active substances that function in the organism as hormones and neurotransmitters and are involved in the regulation of a wide range of physiological processes [1].

The aim of the study was to determine the anti-peroxyl radical capacity of catecholamines and to analyze the relationship between their chemical structure and antiradical activity (SAR). The anti-peroxyl radical capacity was determined using the kinetic electron paramagnetic resonance (EPR) method with pulse reagent injection [2].

The experimentally obtained values of anti-peroxyl radical capacity indicate that catecholamines are capable of efficiently neutralizing peroxyl radicals, confirming their pronounced antiradical properties. A dependence of the anti-peroxyl radical capacity on the structure of the investigated compounds was established. The capacity values of catecholamines were comparable to those of the reference antioxidants—catechol and caffeic acid—and ranged from 1.8 to 2.5. The observed differences in anti-peroxyl radical capacity are attributed to the number of hydroxyl groups capable of participating in reactions with peroxyl radicals.

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DIFFUSION PROPERTIES OF MELT OF POLY(PROPYLENE IMINE) DENDRIMERS

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Poly(propylene imine) (PPI) dendrimers represent a class of highly branched macromolecules with a dense core, which makes them distinct from poly(amidoamine) (PAMAM) systems. [1] One of the primary advantages of PPI dendrimers for fundamental research is the absence of internal hydrogen bonding sites, as polar NH_2 groups are located exclusively at the periphery. In this work, we performed atomistic molecular dynamics (MD) simulations of PPI dendrimer melts (generations G=2–4) at temperature 600K to investigate their diffusion properties. To evaluate accuracy of determining the diffusion coefficient simulation cells of various linear sizes L were analyzed. The simulations were carried out using the OPLS-AA force field in the Gromacs package. The translational diffusion coefficient D was calculated from the mean square displacement (MSD) using the Einstein relation. To compare the simulation results with experimental data, one may refer to NMR techniques. It is interesting to note that the evaluation of the experimental temperature dependence of the diffusion coefficient in [2] gives a value quite close to our results. Additionally, we investigated the rotational diffusion of PPI dendrimers. In our MD model, the rotational diffusion was estimated by analyzing the autocorrelation functions of the vectors directed from the core to the terminal groups. It is interesting to note that even in the case of dendrimers in solution (see [1] and [3]) an exact match of the P_1^{rot} functions is not observed, although the τ_{rot} values are very close.

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NMR RELAXATION TIME T_2 AS A MEASURE OF ENTROPY

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The report overviews various types of molecular systems including liquids with different viscosities, colloidal suspensions, rubbery materials and polymers with more complex structural organization, to reveal the correlation between NMR relaxation times and such a fundamental thermodynamic parameter as entropy.

Since the observed dephasing period of spin coherences, named T_2 is generally inversely proportional to the multiplication of the static second moment M_{2stat} and the correlation time τ_c, the static spin-spin relaxation time T_{2stat} can be considered as a measure of system ergodicity or as the period when the system can take all its possible microstates. For the T_2 of liquids (a few seconds range) with fast motions or short τ_c, this number of microstates is huge, while when the correlation time is of the same order as T_{2stat}, the measured T_2 values are falling down to tens of microseconds. Within this approach the entropy should follow the logarithmic dependence on spin-spin relaxation time according to the Boltzmann formula.

We then perform the comparative analysis of the experimental NMR data for the enumerated types of samples with their known entropy values, coming to the confirmation of mentioned logarithmic dependence. Possible exceptions and special cases are discussed as well.

FERROMAGNETIC RESINANCE AND INVERSE SPIN-HALL EFFECT IN $Ni_{80}Fe_{20}/Mn_xPt_{1-x}$ BILAYER

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Antiferromagnets of the MnMe class, where Me is Pd, Ir, and Pt, have remained a promising research object for a long time due to the effects of spin-charge transformations found in them. For example, in the equiatomic configuration, the MnIr and MnPt systems exhibit significant exchange bias effects and classical spin-Hall effects, and the Mn_3Pt and Mn_3Ir systems are promising for switching the direction of magnetization of ferromagnets with perpendicular magnetic anisotropy (PMA) due to the magnetic spin-Hall effect. Also $L1_0$-MnMe antiferromagnets are characterized by sufficiently high Neel temperatures. Among the presented Mn_xMe_{1-x} class compounds, the system where Me = Pt: θ_{SHE} (MnPt) = 0.06±0.01 has the largest Hall angle. The Hall angle for connecting MnPt with the equal content of elements is closest in magnitude to the Hall angle Pt θ_{SHE} (Pt) ≈ 0.082.

Due to the increasing attention to antiferromagnetic materials in spintronics, the study of spin-Hall effects in systems containing the MnxPt1-x layer remains an urgent task today.

In this study, we investigated ferromagnetic resonance and the inverse spin-Hall effect (ISHE) in $Ni_{80}Fe_{20}/Mn_xPt_{1-x}$ bilayer systems under spin pumping conditions. The voltage signals of the ISHE were obtained using the resonator technique of the FMR experiment. Based on the received voltage signals, the Hall angles for the Mn_xPt_{1-x} layers were estimated, where x=49-61. The dependence of the spin-Hall angle in the $L1_0$-Mn_xPt_{1-x} system on the content of heavy normal metal – Pt is demonstrated. The dependence of the magnitude of the contribution of the ISHE signal on the crystallinity of the heterostructure is also shown using the example of synthesized polycrystalline bilayer systems.

SIMULATION OF RABI OSCILLATIONS IN LOW-SCALE SPIN MODELS

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Different modifications of carbon, such as fullerene arrays, have electrical, optical and mechanical properties that are valuable for practical applications [1]. The properties of these materials can be controlled by introducing metal cores into the shells or by depositing magnetic ions on the carbon surface. In addition, the described materials can find applications in the development of new systems for storing, processing and transmitting information using spin magnetic moments [2].

We improved our numerical method to perform calculations in a rotating frame system and supplemented by the construction of Fourier spectra of obtained magnetization signals. Calculations were performed for ordered (chain, square lattice) and disordered (magnetic particles randomly located on the surface of a nanosphere and nanotube) structures in rotating and non-rotating frames.

At our spectra graphs for disordered structures in rotating frame we observed additional peaks which are close to zero. At spectra of a rectangular and other ordered structures without rotating we cannot see the same thing. In this work we are conducting a theoretical analysis to understand the nature of additional peaks. In our work [3] we observed different random spin structures in rotating frame and obtained additional peaks in their spectra. Also in [3] we made the analytical estimate of two interacting spins free conduction decay. In described analytical calculations [3] we did not find any low-frequency terms. Now we assume that low-frequency dynamics can be found in higher dimensions and in this work we are considering other theoretical models with higher number of spins and different arrangements in space.

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Proposal for Detection of Axion-Induced Spin Precession by Earth's Field Continuous NMR Technique

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The search for ultralight axions and axion-like particle dark matter has motivated a wide range of high-precision experiments based on nuclear magnetic resonance (NMR). In experiments such as CASPEr [1], the axion field is expected to manifest itself as an extremely weak oscillating pseudo-magnetic field (the so-called "axion wind"), producing tiny perturbations in nuclear spin precession. Over the past decade, systematic searches have been carried out across a broad frequency range using various NMR-based techniques, including zero- and ultralow-field NMR (CASPEr-ZULF) [2] at sub-hertz to tens-of-hertz frequencies, as well as high-field continuous-wave NMR experiments probing the kHz-MHz regime.

By contrast, the frequency range corresponding to Larmor precession in the Earth's magnetic field (approximately 1–10 kHz for protons) has received little attention so far. This intermediate area lies between the conventional zero-field and high-field domains. It remains experimentally challenging due to magnetic-field noise, stringent stability requirements, and the limited sensitivity of standard detection schemes.

In this work, we propose to initiate an axion search in this regime using a custom-built Earth-field (low-field) NMR (EF-NMR) spectrometer. We present preliminary sensitivity estimates and compare them with the levels required for axion detection reported in the literature. Our initial estimates indicate that a sensitivity improvement of roughly two to three orders of magnitude for EFNMR is needed to make axion detection feasible in the targeted frequency range. We outline several realistic, incremental routes to improving sensitivity. They include optimized impedance matching of the pickup coil, the use of lower-noise front-end amplifiers, differential signal readout to suppress common-mode interference, and bandwidth optimization for narrowband detection. Among the possible alternatives, we analyze the use of an improved Skrypov-type continuous-flow NMR generator [3]. Owing to its continuous, phase-coherent output and the absence of dead time, this approach looks suitable for detecting slow phase and frequency modulations. It may provide a promising path toward enhanced sensitivity to axion-induced effects in the frequency range of Earth-field NMR.

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Use of the Hückel Method for Calculating Carbon Structures and Problems of Predicting NMR Chemical Shifts

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One of the preliminary steps in creating carbon structures with desired functional properties is predicting the electronic structure using theoretical methods. Quantum mechanical methods (QMM) are the most reliable, providing appropriately selected electric field potentials are chosen [1]. However, selecting the desired structures requires varying the material's composition. Given the significant time required, the use of QMM methods becomes problematic. In the context of two-dimensional carbon materials, the π-electron system plays a key role, determining both the electronic and topological properties. Analysis shows that the Hückel method effectively describes the π-electron structure of planar carbon systems due to the orthogonality of the σ and π orbitals and qualitatively reproduces edge states and topological features [2,3]. This paper presents the results of using the extended Hückel method for a number of model carbon structures, parameterized by comparison with DFT data. The calibrated EHM method qualitatively reproduces key features of electron density, allowing for the estimation of magnetic anisotropy and the nuclear chemical shift tensor, as well as ring currents. The method has been applied to explain the anomalously strong diamagnetic shielding in synthesized carbon structures intended for anodes.

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NMR analysis of surfactants characteristics based on methacrylic acid.

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Introduction

There is a growing trend in chemistry to perform important and widely used organic reactions, especially synthetic transformations, in water. Using surfactants for this purpose is a powerful strategy that advances the principles of Green Chemistry. Micellar catalysis allows reactions to be carried out in a pseudo-homogeneous aqueous environment. Among the most effective systems are micelles formed from amphiphilic polyelectrolytes. We have synthesized a new surfactant based on methacrylic acid. NMR spectroscopy, a key analytical technique in organic synthesis, is essential here to evaluate critical parameters of the micelles.

Method

To obtain the target methacrylic acid based cationic monomer with a methoxypolyethylene glycol fragment a 4 stage synthesis was carried out. Each stage was characterized by 1-H NMR spectroscopy analysis, including different synthesis methodic as well as a number of impurities. Based on the obtained products, polyelectrolytes were synthesized. After that, we performed a series of model Suzuki reactions to evaluate the catalytic properties of the obtained compounds. The kinetic activity of the polymers was also confirmed the by 1-H NMR spectroscopy analysis.

Conclusion

New cationic surfactants derived from methacrylic acid were successfully synthesized and characterized via ^{1}H NMR. The resulting polyelectrolyte micelles efficiently catalyzed Suzuki cross-coupling reactions in water, with reaction progress quantitatively monitored using ^{1}H NMR kinetics.

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PRECISE CALIBRATION OF THE 180° PULSE BASED ON THE FREE INDUCTION DECAY SHAPE UNDER STRONG RADIATION DAMPING CONDITIONS

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Radiation damping in nuclear magnetic resonance spectroscopy has been recognized since the early days of magnetic resonance. It occurs in experiments where the detected signal is an induced current in a receive coil and can have a direct impact on measured signals. Radiation damping is typically undesirable, as it causes effects such as line broadening and line shape distortions, as well as alterations of the effective radio-frequency pulse shape. Mechanistically, a strong transverse macroscopic magnetization (for example, from bulk water protons) generates an electromagnetic field in the receiver coil, which induces a current; the coil current in turn produces a secondary magnetic field at the Larmor frequency that acts back on the magnetization and can rotate it toward the static field on a timescale shorter than intrinsic relaxation [1].

In addition to the aforementioned effects, radiation damping can cause an initial rise in the free induction decay (FID) and lead to the formation of an Echo-FID–like signal. Such an FID waveform occurs for nominal flip angles between 90° and 270° [2]. The FID shape is particularly sensitive to small deviations of the flip angle near 180°, which motivated us to investigate the hypothesis that FID shape analysis could be used for precise calibration of the 180° pulse. Experimental studies have demonstrated that this approach enables calibration accuracy on the order of tenths of a degree. Accurate 180° pulse calibration and more complete inversion of radiation-damped signals can be beneficial in many applications requiring precise control over the magnetization trajectory, such as water suppression or magnetization transfer techniques.

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A multi-model analysis of proton magnetic relaxation in hemoglobin solutions.

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The longitudinal proton magnetic relaxation (PMR) dispersions profiles (^{1}HMRD) obtained in hemoglobin (Hb) solutions, under physiological conditions, are used to determine the most proper physical model to describe the PMR in these macromolecular solutions [1]. The Hb samples were obtained from samples of venous whole blood donated by healthy volunteers, using centrifugation, decanting and freeze and thawing cycles [1-3]. The ^{1}HMRD profiles were obtained, utilizing the inversion-recovery radiofrequency (RF) pulse sequence, in a Fast Field Cycling NMR relaxometer (FFC 2000, Spinmaster) operating from 20 kHz to 10 MHz; additional points were obtained at 20 MHz and 60 MHz using the Mq20 and Mq60 NMR analyzers (BRUKER Minispec) [1,3]. These profiles were fitted employing the phenomenological equations of Koenig, as well as the water exchange models betwen two sites (2SWEM) and among three sites (3SEM), considering spherical and ellipsoidal geometries for the protein molecule. New theoretical models were proposed to describe the longitudinal and transversal PMR in samples of Hb considering ellipsoidal geometry for the macromolecule [3]. The most proper physical model to describe the PMR in Hb solutions was the 3SEM considering an ellipsoidal geometry for the protein molecule [1]. It was posible, using this result, to develop a new PMR-based method to determine the dynamic viscosity of Hb solutions with potential medical applications [2].

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STUDY OF THE HELIUM-3 NUCLEAR POLARIZATION PROCESS BY THE PAMP METHOD AT VARIOUS TEMPERATURES AND RF PLASMA FREQUENCIES

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Hyperpolarization of noble gases (helium-3 and xenon-129) is a promising and in-demand field. Hyperpolarized noble gases are used as probes for lung MRI and studies of porous media using NMR. In addition, hyperpolarized helium-3 is used in spin filters and polarized targets for neutron polarization and detection. The most widely used methods for gas hyperpolarization are those utilizing optical pumping: SEOP and MEOP (for helium-3 only). Recently, a new method for producing helium-3 nuclear polarization, called PAMP (Polarization of Atoms in a Magnetized Plasma), has been introduced [1]. In this method, polarization induces in a magnetized, low-pressure (~10 mbar) pure (~1 ppm of impurities) helium-3 plasma in strong magnetic fields.

To study the capabilities of this polarization method, the following experimental equipment was assembled: a helium-3 gas purification and polarization cell system providing the required degree of purity, equipment for detecting the NMR signal from helium-3, and an RF pumping system for creating a helium-3 plasma [2].

Using the assembled equipment, the new PAMP method for polarizing helium-3 nuclei was reproduced. When investigating the efficiency of this method, the following features were discovered: the magnitude and rate of the polarization process increase with the power of the RF plasma pumping and polarization strongly depends on gas purity. During the experiments, a polarization of ~8% and a polarization rate of ~1 s^{-1} were achieved. Furthermore, a strong correlation was found between the polarization magnitude and the temperature of the polarization cell; polarization increases significantly with temperature in the range of 300–500 K [3]. The dependence of the polarization magnitude and rate on the RF plasma pumping frequency within the range of 12–55 MHz was investigated. It was found that at the same applied power, increasing the frequency leads to an increase in both the polarization magnitude and rate.

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Detection of concealed energetic materials by nuclear quadrupole resonance

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The detection of energetic and dangerous objects in luggage, transport means, and under clothes is one of the most actual problems in civil security. Now, easy access to improvised and military substances increases the potential danger to life. The solid dangerous substances usually contain nitrogen-14 and can be detected by the nuclear quadrupole resonance (NQR). The application of NQR has several advantages, including high discrimination ability, non-ionizing radiofrequency radiation, and a simple sensor. The NQR applications for security scanners have been studied for the past 40 years [1,2,3]. Regarding the NQR applications of security checkpoints, several important limitations exist: the influence of metal objects that persist in baggage and their partial shielding effect, the presence of containers containing liquids, radiofrequency interference from electronic devices, and the effect of the position of targeted substances within the scanned volume. For that reason, it remains a non-trivial task to design RF probes specific to a given application and targeted substance list, as well as to develop efficient NQR approaches for practical use.

In this work, we present various sensor designs developed for NQR scanners of luggage and electronic devices. We study the minimum detectable quantity of the probed substance in conditions close to real application cases. Some specific technical solutions for NQR detection applications are discussed. We also demonstrate the detection of NQR signals of a reference nitrogen-containing sample concealed in a small electronic device in switch-off and switch-on modes.

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HYPERPOLARIZATION OF NITRATE BY PHIP-SAH

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Introduction.

The spin hyperpolarization of the nuclei makes it possible to increase the signal by several orders of magnitude in NMR and MRI methods. One of the widely used approaches to create a nonequilibrium population of spin energy levels is parahydrogen-induced polarization (PHIP), this technique is based on the pairwise addition of a stable nuclear spin isomer of molecular hydrogen, parahydrogen, to the substrate.[1]

Relevance.

The greatest interest to the PHIP technique arises in the context of obtaining polarized metabolites for various biomedical applications, however, a number of substrates that can be polarized by direct parahydrogen addition is limited. One of the possible solutions to this problem is the use of carboxylic acid esters, which include an unsaturated moiety (propargyl or allylic). To obtain a polarized product, it is necessary to transfer the polarization to the magnetically active nuclei and hydrolyze the ester.[2,3]

In this work, this approach is extended to the inorganic nitrate anion. The production of polarized nitrate by the PHIP-SAH method using propargyl nitrate with natural abundance of ^{15}N isotope as a precursor is demonstrated. We have established optimal conditions for hydrogenation of propargyl nitrate on a homogeneous rhodium catalyst $[Rh(NBD)(dppb)]BF_4$ in terms of conversion to the final product (**40±2%**) and observable ^{1}H signal enhancement (**P_{1H} = 33±2%**). The polarization transfer to ^{15}N nuclei was carried out using the magnetic field sweep in the range of 0-1μT. After the field sweep optimization, the highest observed polarization for ^{15}N nuclei was estimated as **8.6±0.6%** for allyl nitrate. We have selected the optimal system for the alkaline hydrolysis of allyl nitrate into a nitrate anion and we demonstrate that the ^{15}N hyperpolarization is retained during the hydrolysis and the hyperpolarization on nitrate anion is estimated as **>2%**. In addition, experimental results were accompanied by calculation of nuclear spin-hamiltonian correlation diagram in low magnetic field and simulation of polarization transfer by numerical solution of **Liouville-von Neumann equation.**

Keywords: propargyl nitrate, nitrate, PHIP-SAH, parahydrogen, catalytic hydrogenation

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Effect of paramagnetic additive on chemical shifts of NMR spectral lines (^{1}H, ^{13}C, ^{14}N) and ion mobility in the system $Co(NO_3)_2{\cdot}6H_2O$– $BmimNO_3$.

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Mixtures of ionic liquids (IL) with inorganic salts have become a popular object of research, primarily as electrolytes in metal-ion batteries, as well as mixtures with low eutectic (DES). NMR methods are widely used to analyze particles dynamics and the microstructure of mixtures of IL's with inorganic salts [1]. Of particular importance is the study of mixtures containing metal salt crystalline hydrates: NMR methods make it possible to study the immediate environment of a metal ion, as well as to monitor the state of water molecules in such mixtures and structural rearrangements when the concentration of the inorganic component changes. It was previously shown that the introduction of an inorganic salt component into IL can cause a line position in NMR spectra. In the case of a diamagnetic additive (for example, lithium, magnesium, calcium, aluminum salts), there are no significant shifts in the ^{1}H NMR lines [2]. In the case of a paramagnetic additive, there is a clear change in the shape and shifts of the NMR lines [3]. This is a consequence of restructuring of IL's – changes in the local environment of the organic cation and the inorganic anion, which affects the physical and chemical properties of the ionic liquid. The question of the effect of a paramagnetic additive on changes in the local structure of IL and the mobility of particles remains poorly understood, and the dependences of the shift of spectral lines with a change in the concentration of the paramagnetic component in IL are practically not represented in the literature.

Therefore, in this work, the effect of the addition of $Co(NO_3)_2{\cdot}6H_2O$ on the chemical shifts of NMR spectral lines on ^{1}H, ^{13}C, and ^{14}N nuclei in a mixture with BmimNO3 in the range of cobalt salt concentrations of 0 – 0.08 mol/l (0.02 mol/l apart) and on diffusion coefficients of ions (on ^{1}H nuclei) in the range temperatures of 25^{0} – 75^{0}C (10^{0}C apart).

Acknowledgments

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NMR ^{133}Cs IN $CsPbBr_3$+Ag PEROVSKITES CRYSTALS

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Complex lead halides $APbX_3$ (where A is a monovalent organic or inorganic cation and X is a halogen anion) with a perovskite structure have excellent electronic and optical characteristics, which determines their effective use as photoactive materials in solar cells in the field of solar energy conversion, as well as as signal converters for digital equipment [1, 2]. Previously, we investigated $CsPbBr_3$+Bi [3]. In this paper, we present the results of the study of perovskite $CsPbBr_3$+Ag crystals by ^{133}Cs NMR. The use of Ag as an alloying impurity instead of Bi has led to the identification of new features.

$CsPbBr_3$ structures with low Ag concentrations up to 4% were studied as samples. MAS NMR and non–spinning ^{133}Cs NMR spectra at natural abundance for 5 samples with Ag concentrations from 0.0032 to 3.7% were were acquired.

It was found that with an increase in the Ag concentration, starting from 1,07 % , a deviation of the measured sample rotation speed appears at a magic angle compared to the set speed value in the installation. The difference between the peaks of the lines from rotation gives a frequency less than that specified in the experiment. As the Ag concentration increases, this difference increases rapidly. We associated this effect with the appearance of Foucault currents. The effect is strongly manifested at high rotational speeds.

According to the results of processing the spectra without rotation, a shift of the maximum of the central line of the spectra was found, which is about 1.8 ppm per change in Ag concentration from 0.0032 to 3.7% on average.

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EPR MONITORING OF THE CATALYTIC MICHAEL ADDITION REACTION

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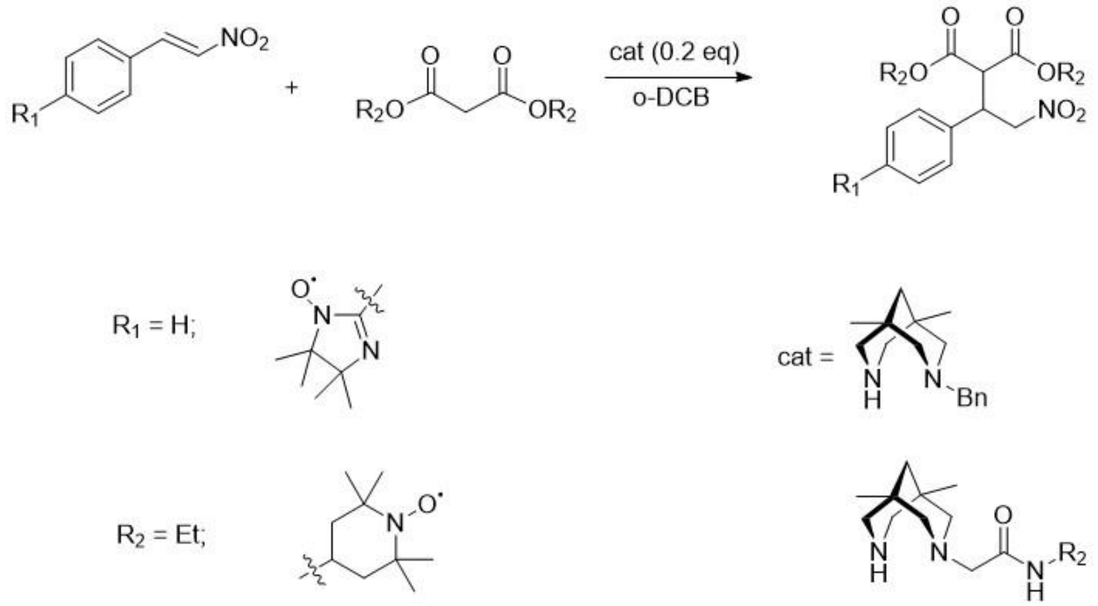
The Michael addition reaction between nitrostyrene (and its substituted derivatives) and malonate (and its substituted derivatives) was investigated using electron paramagnetic resonance (EPR) spectroscopy. Both spin labeled (nitroxide) and diamagnetic catalysts were employed in this study.



The reaction mechanisms were examined in two distinct systems: 1) catalysts with nitroxide spin labels when substituted bispidines served as catalysts; 2) substrates with nitroxide groups when the Michael addition was performed using nitrostyrene and malonate derivatives in which a nitroxide group was incorporated as a substituent.

EPR monitoring of these reactions was carried out. In the case of diamagnetic malonate, the EPR spectra showed no significant changes. However, when spin-labeled malonate was reacted with either spin-labeled or diamagnetic nitrostyrene, pronounced alterations in the EPR spectra were observed. From the acquired spectra, key magnetic resonance parameters – including the exchange interaction parameters – were determined.

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Cylindrical Metasurface for Efficient Travelling-wave MRI at 7T

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This research focuses on a compact and lightweight metasurface designed to increase transmit efficiency and improve radiofrequency field homogeneity, critical factors for achieving high-quality MR-images in traveling-wave MRI [1]. The metasurface is designed to replace the state-of-the-art dielectric waveguide [2] for radiofrequency field focusing in traveling-wave MRI. By carefully engineering the metasurface properties, we achieved performance equivalence between the metasurface and the dielectric waveguide. The metasurface design was based on a grid of copper strips loaded with parallel-plate capacitors [3], demonstrated improved RF field homogeneity and transmit efficiency compared to the dielectric waveguide. Optimized for radiofrequency field focusing in human brain applications for 7T traveling-wave MRI, the proposed metasurface showed similar performance in travelling wave MRI to that of the dielectric waveguide, while utilizing a simple, robust and lightweight design. The proposed metasurface can be used for both research and clinical applications in traveling-wave MRI systems.

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EFFECT OF ISOTOPIC SUBSTITUTION ON DALFAMPRIDINE HYPERPOLARIZATION VIA THE SABRE TECHNIQUE

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SABRE (Signal Amplification by Reversible Exchange) is a parahydrogen-based hyperpolarization technique that allows to boost the sensitivity of NMR and MRI. In SABRE, parahydrogen and substrate molecules reversibly bind to an iridium complex, which mediates polarization transfer from hydrides to the substrate spins via the J-coupling network. Hyperpolarization of heteronuclei like ^{15}N and ^{13}C offers the advantages of longer polarization lifetime and background-free detection. It can be achieved via the SABRE-SHEATH (SABRE in SHield Enables Alignment Transfer to Heteronuclei) approach, in which spin order is transferred at ultra-low magnetic field. An alternative approach is the use of dedicated RF pulse sequences (e.g., SLIC-SABRE) for polarization transfer at high field. The optimization of conditions is necessary for achieving the maximum polarization for both heteronuclear SABRE variants.

Dalfampridine (4-aminopyridine, FAM) is a drug used for treating multiple sclerosis. Previously, single labelled (in the pyridine ring) [^{15}N]FAM was hyperpolarized via both SABRE-SHEATH [1] and SLIC-SABRE [2] approaches. It is known that the presence of quadrupolar nuclei such as ^{14}N may accelerate spin-lattice relaxation of nearby scalar-coupled spin-1/2 nuclei at low magnetic fields, leading to hyperpolarization losses [3]. In this work, we investigated the effect of ^{14}N-to-^{15}N isotopic substitution in amino group on the hyperpolarization efficacy of FAM by SABRE-SHEATH and SLIC-SABRE. Magnetic field of 0.6 μT and temperature of 38 °C were identified as the optimal conditions for SABRE-SHEATH of FAM. Contrary to the expectations, the replacement of ^{14}N for ^{15}N in the amino group accelerate relaxation of heterocyclic ^{15}N nucleus in submicrotesla fields, leading to the polarization level decrease by 1.5–2-fold. Thus, it can be concluded that only essential scalar-coupling between ^{15}N and quadrupolar ^{14}N nuclei is deleterious in the context of SABRE-SHEATH.

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Invistegation of complexation of fullerenols with Lys2Gly peptide dendrimer provided via MD simulation

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Abstract

Fullerenes are promising for biomedical applications; however, they are poorly soluble in water. Solubility can be improved by attaching OH groups to them or encapsulating them in various nanocontainers, such as dendrimers. Using molecular dynamics (MD) simulations in the Gromacs package with the AMBER-99SB-ILDN force field, we studied the complexation of fullerenols ($C_{60}(OH)_n$, where n=12, 24 and 36 is the number of OH groups) with the Lys2Gly peptide dendrimer in aqueous solution.

It was shown that a stable complex forms within 10-100 ns for all the initial conditions and numbers of OH groups in fullerenols considered. The radius of gyration of the dendrimer doesn't changed upon complex formation with either fullerenol or fullerene. Furthermore, the distance between the centers of mass of the fullerenol and dendrimer is in all cases close to the distance in the complex with the fullerene. At the same time, their density profile distributions differ. A typical fullerene is located practically at the center of mass of the dendrimer. Fullerenols are also located near the center of mass of the dendrimer, but slight fluctuations in their position within it are possible. Fullerenol (like fullerene) partially displaces some of the dendrimer's atoms and water molecules with counterions from the center of the dendrimer. This leads to an increase in the zeta potential of Lys2Gly in the complex by more than 1.5 times compared to the single dendimer.

Using MD calculations, we found that increasing the number of OH groups in fullerenol from n = 12 to 36 does not influence on the formation of its complex with the dendrimer or its location near the dendrimer center, but it significantly change the complexation mechanism. We demonstrated that a decrease in the number of hydrophobic contacts between the dendrimer and fullerenol with an increase in the proportion of hydroxylated groups of fullerenol is compensated for by an increase in the number of hydrogen bonds between these two molecules. Thus, we demonstrated that the Lys2Gly peptide dendimer can be a good nanocarrier for both fullerenes and fullerenols. Overall, simultaneous partial hydroxylation of the fullerene and its encapsulation in a dendrimer nanocarrier allows for its solubility while maintaining high biological activity.

Lithium Diffusion in Intercalated Titanium Diselenides: NMR Study

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This report focuses on a research of atomic dynamics in intercalated layered dichalcogenides which are considered as materials for different practical applications [1]. In particular, lithium intercalated dichalcogenides have recently attracted an attention for creation of cathode materials [2,3]. Our research is devoted to the study of the dynamics of lithium atoms intercalated in titanium diselenides Li_xTiSe_2 (x = 0.25, 1) using different NMR methods. These methods are known as effective tools for investigation of atomic dynamics [4,5]. The measurements of ^{7}Li NMR spectra and spin-lattice relaxation rates were performed conducted in the wide temperature range (80 – 593 K), and the results were compared to various theoretical models.

The NMR study reveals that the behavior of spin-lattice relaxation rates in the temperature region T > 300 K is determined by quasi-two-dimensional diffusion of Li ions. The diffusion of Li ions in $Li_{0.25}TiSe_2$ is characterized by the activation energy of 501 meV and in $LiTiSe_2$ – by the activation energy of 509 meV. The diffusion coefficients and theoretical ionic conductivity were calculated near the room temperature. In addition, these compounds are interesting as models for study of the mechanisms of atomic mobility in layered dichalcogenides.

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STUDYING THE MECHANISM OF LITHIUM CATION TRANSFER IN SOLVATE-ION ELECTROLYTE SYSTEMS BASED ON TETRAGLYME AND LITHIUM SALT BY NMR

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Solvated ionic liquids (SILs) are a relatively new class of ionic liquids consisting of a coordinating solvent and a salt forming a chelate complex with properties very similar to those of ionic liquids [1]. Typically, SILs are formed by diffusion of cationic charge through the binding of a rigid cation, often in an ethereal solvent [2]. The use of these solvates as electrolytes for lithium-ion batteries has been described previously [3-6]. The most well-known in the literature is the dissolution of LiTFSI in triethylene glycol dimethyl ether or tetraethylene glycol dimethyl ether ([Li(G3)]TFSI or [Li(G4)]TFSI). The absence of free solvent molecules in SILs gives it properties similar to those of an ionic liquid, such as high ionic conductivity, thermal stability and viscosity, low volatility and flammability, and broad electrochemical stability. These properties make SILs suitable candidates for high-voltage lithium-ion batteries.

The mechanism of ion transport in electrolytes based on a solvate-ionic liquid of the composition LiTFSI in tetraglyme in the ratio of 1:1, 1:2, 1:4 mol was studied. NMR methods (high-resolution, pulse-gradient field and spin echo spectroscopy) in combination with quantum-chemical modeling of electrolyte compositions revealed the mechanism of ion transport in the systems LiTFSI:G4 = 1:1, 1:2, 1:4 mol. It was shown that in the LiTFSI-G4 system (1:1 mol), the translational mechanism of lithium cation transfer is realized in the system, and in the LiTFSI-G4 system (1:2 mol), the exchange-ligand transfer of the $Li+$ cation is realized. In the third composition, with an excess of tetraglyme molecules, it is released into a separate phase.

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COMPARISON OF THE MECHANISMS OF INTERACTION OF L-TRYPTOPHAN WITH GOLD AND PLATINUM NANOPARTICLES

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Functionalization of metal NPs with bioorganic molecules, such as amino acids, represents a key strategy for improving their controllability in biomedical applications. L-Tryptophan, a hydrophobic amino acid, is of special interest for NP functionalization and enhancing biological activity, and has attracted attention as a model for studying AA-NP interactions. The aim of this work is to find key differences in the mechanisms of interaction of L-trp with Pt and Au NPs using NMR methods. A comprehensive understanding of the mechanisms of interaction between metal NPs and AA will enable significant progress in molecular modeling for a variety of applications.

To elucidate the interaction mechanisms between L-Trp and NPs, a combination of NMR spectroscopic techniques was employed, including chemical shift analysis and nuclear Overhauser effect spectroscopy (NOESY).

Analysis of the ^{1}H NMR spectra of L-Trp indicates that the presence of Pt NPs alters the chemical shifts of aromatic ring protons, with minor downfield changes observed for the *d*, *c*, and *b* protons. Meanwhile, the presence of Au NPs did not affect the chemical shift of the protons of the aromatic ring.

Based on the intensity values of the cross-peaks and diagonal peaks in the NOESY spectra, cross-relaxation rates were determined for four pairs of protons in close spatial proximity. The calculated cross-relaxation times are consistent with a possible reorientation of the tryptophan side chain relative to the benzene ring in the presence of Au NPs.

The results of a comprehensive NMR-based investigation indicate that Pt NPs interact with L-tryptophan through an electron transfer mechanism. In contrast, Au NPs bind L-Trp through π-stacking of the indole ring.

Blood Viscosity: A Predictive Factor for Preeclampsia

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Abstract

In this study, the absolute dynamic viscosity of whole blood was determined in pregnant women with preeclampsia and eclampsia. For this purpose, the proton magnetic relaxation method was used to measure the viscosity of hemoglobin and plasma [1,2]. These values, together with the hematocrit, allowed the calculation of whole blood viscosity [3]. The results showed a viscosity range of 5.24 – 8.55 mPa·s, values significantly higher than those observed in healthy pregnant women. It is noteworthy that, out of the 15 pregnant women studied, 13 presented viscosity values above the upper mean between weeks 26 and 29 of gestation, subsequently developing severe forms of the disease (aggravated preeclampsia and eclampsia). This finding reinforces the predictive value of blood viscosity in the early detection of preeclampsia and suggests its clinical utility in risk assessment and follow-up of pregnant patients.

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^{13}C HYPERPOLARIZATION OF ACETOACCETATE USING PHIP-SAH

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Nuclear hyperpolarization (HP) techniques dramatically increase signal-to-noise ratio in magnetic resonance. The combination of heteronuclear MRSI with administration of HP contrast agents opens the doors to detection and quantification of metabolic flux *in vivo*. One of the promising HP methods is parahydrogen-induced polarization (PHIP) which exploits the singlet spin order of parahydrogen (pH_2) as a source of non-equilibrium polarization. Recently, PHIP by side arm hydrogenation (PHIP-SAH) approach was proposed, which expands the capabilities of PHIP technique for obtaining HP carboxylates in a biocompatible form. One of the prospective biomolecules is acetoacetate (AcAc) which converts to 3-hydroxybutyrate *in vivo*, and kinetics of this reaction is associated with mitochondria redox status. Here, we propose the PHIP-SAH based procedure for hyperpolarization of AcAc.

[1,3-$^{13}C_2$]Allylacetoacetate ($^{13}C_2$-alAcAc) was produced in hydrogenation of the corresponding propargylic precursor using pH_2. Under optimized experimental conditions, $^{13}C_2$-alAcAc (32 mM) was produced with 100% efficiency and P(^{1}H) ≈ 24% was achieved. The ^{1}H-to-^{13}C polarization transfer was performed using the B_0 linear sweep approach (B_0 field was diabatically dropped down to 25 nT and then linearly adiabatically increased to 700 nT over 4 s) and the highest observed ^{13}C polarization levels were estimated as 4.1% for 1-^{13}C and 2.7% for 3-^{13}C atoms. Next, it was found that the mild conditions (150 mM $NaHCO_3$, r.t.) typically used for hydrolysis of pyruvate esters are not sufficient to hydrolyze [1,3-$^{13}C_2$]alAcAc since a stable negatively charged enolate is formed. We demonstrate that ^{13}C hyperpolarization is retained during harsh hydrolysis conditions (1 M NaOH, T ≈ 100 °C, 30-120 s) and HP [1,3-$^{13}C_2$]AcAc is produced with P(^{13}C) of ~0.5%, although some amount of enolate remains unreacted and, moreover, partial decomposition of acetoacetate into acetone and carbonate is observed. In acidic conditions, fast decomposition of allyl [1,3-$^{13}C_2$]acetoacetate into acetone and $^{13}CO_2$ took place, no signals of HP [1,3-$^{13}C_2$]AcAc were detected.

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NONLINEAR TRANSITION UNDER SHORT TRANSVERSE PULSE IN CLASSICAL DIPOLE SIMULATION

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The magnetic resonance phenomena and spin dynamics are effectively described by a linear approach due to weakness of typical dipole interaction in crystals [1, 2]. On the other hand, the dipole ensembles with strong interaction become a bright object of interest in nonlinear dynamics. The complex long-time behavior of dipole-coupled ensembles permits to study collective modes and thermalization of the system [3]. Magnetization response on continuous electromagnetic wave exhibits a complex behavior with synchronized regimes and signatures of chaos [4-7].

This study presents a series of numerical simulations of classical spin ensembles under a short rectangular pulse of transverse magnetic field. The magnetic moments are located in finite cubic lattice of varying sizes. The initial state corresponds to an almost uniform longitudinal polarization. The effect of the pulse length and magnitude is analyzed.

During the pulse, the transverse magnetization increases to a certain value and decays fast until time T_2 since the pulse ends; this evolution is independent on the perturbation strength. The magnetization dynamics at large time exhibit two characteristic regimes. A low-field pulse produces regular oscillations with a narrow spectrum. However, above a certain pulse magnitude, a complex signal with broad spectrum is observed in simulations. The transition between these regimes and the excitation of nonlinear magnetization modes are studied.

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INFLUENCE OF DIFFERENT MAGNETIC FIELDS ON GALLIUM TEXTURE

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The production of metals and metallic alloys with specific grain orientations holds exceptional significance for technological applications [1,2]. It was shown recently that NMR is a powerful means to reveal the formation of oriented crystalline metallic phases upon solidification within the magnets of the NMR spectrometers owing to the strong angular dependence of the Knight shift of the resonance lines [3,4]. In particular, NMR was used to prove the influence of magnetic field on the orientational solidification of gallium. In the present work we report the effect on the formation of oriented crystalline α-Ga of different magnetic fields 7, 9.4, and 11.7 T. The emergence of oriented crystalline ranges was observed by the appearance of very narrow gallium resonance lines corresponded to the central and satellite transitions, similar to those in the gallium single crystal. The fraction of oriented α-Ga was found to increase with increasing magnetic field. The crystalline structure of oriented α-Ga was suggested to be perfect based on the widths of the resonance lines corresponded to satellite transitions.

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INTERRELATION OF DIPOLAR SPIN DYNAMICS AND MULTIPLE QUANTUM DYNAMICS OF TWO-SPIN SYSTEM WITH DEPHASING RELAXATION

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We consider the spin dynamics of a two-spin system governed by the secular part of the dipole-dipole interaction (due to being in a strong magnetic field) [1] and an analogous system governed by the multiple-quantum Hamiltonian [2], both systems being subject to dephasing relaxation [3]. In both cases we obtained the exact solution of the Lindblad equation [4] with the initial state obtained by applying a $\pi/2$ resonance y-pulse to the thermodynamic equilibrium state. We showed that the obtained solutions are closely related: the system's density matrix for the dipolar Hamiltonian at time t coincides with the density matrix for the multiple quantum Hamiltonian at time $3t$ if the dephasing relaxation rate for the system with the multiple quantum Hamiltonian in three times less than for the system with the dipolar Hamiltonian.

The practical advantage of the above findings is that the slower dynamics under the action of multiple quantum Hamiltonian allows investigating long time behavior more accurately. A comparison of the spin dynamics in two different cases allows one to find the dephasing relaxation rate.

The experimental possibilities of a verification of obtained results in NMR experiments in solids are also discussed.

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Theoretical study of long-lived state relaxation in trans-azobenzene with two ^{15}N nuclear isotopes

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Long lived spin states (LLS) find various applications in magnetic resonance, namely in the study of slow dynamical processes [1], ligand-protein screening by NMR [2] and nuclear hyperpolarization storage [3]. In trans-azobenzene LLS corresponds to singlet spin state of ^{15}N nuclei pair. This state demonstrates lifetime about 2 minutes at the field 16.4 T, which can be enhanced up to 20 minutes by applying spin-locking [4]. Furthermore, hyperpolarization of ^{15}N nuclei can be achieved by photo-SABRE [5]. Detailed theoretical description of the LLS relaxation may bring new ideas on extending its lifetime even more.

Dipole-dipole (DD) interaction and chemical shift anisotropy (CSA) don't lead to singlet-triplet transitions of ^{15}N nuclei spin pair and consider the closest to the pair protons is necessary. Four the closest protons were considered. To calculate relaxation, J-couplings, and DD interactions between all spin pairs, and also CSA of ^{15}N nuclei were taken into account. Moreover, cross-correlation between all DD interactions, containing at least one nitrogen nucleus, and between these interactions and CSA were considered. To compute relaxation, Redfield theory was used with approach described in [6]. Dependence of the LLS lifetime on external magnetic field was calculated and compared to experimental data.

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Low cost and low maintenance solid-state nuclear magnetic resonance applied to paramagnetic Lithium detection

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Probing the structure and molecular motion of paramagnetic materials has long remained a critical challenge in the field of solid-state nuclear magnetic resonance (ssNMR). The underlying reason stems from the dramatic amplification of paramagnetic shifts under high magnetic fields, while the magic-angle spinning (MAS) rates of conventional solid-state NMR probes are frequently inadequate to mitigate such shifts, thus impeding the acquisition of high-resolution NMR signals for diverse structures within paramagnetic materials.

As key materials in the new energy field, cathode materials for lithium-ion batteries (e.g., lithium iron phosphate and nickel-cobalt-manganese ternary materials) generally exhibit strong paramagnetism. Under high-field superconducting NMR conditions, the significant paramagnetic shifts of these materials lead to extreme broadening of their magnetic resonance signals. Even at a MAS rate of 100 kHz, it remains challenging to obtain high-resolution signals.

In this study, we developed a solid-state NMR system capable of observing high-resolution signals of multiple nuclear spins in paramagnetic materials. In this system, the paramagnetic shifts in paramagnetic materials are effectively reduced by limiting the magnetic field strength to 0.5T; meanwhile, a maximum MAS rate of 20 kHz is achieved with a novel MAS system. Our report will present the NMR spectra of lithium ions in lithium iron phosphate and lithium manganate obtained using our equipment. For comparison, the results of the same materials measured under a 7T magnetic field are also provided. The results demonstrate that our low-field solid-state high-resolution system exhibits significantly superior signal resolution compared to high-field solid-state high-resolution systems, enabling effective discrimination of different types of lithium ions in paramagnetic materials. This highlights the great application potential of the system in studying the structure and molecular motion of paramagnetic materials.

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Increased acidity of silicoaluminophosphate BSAPO-11 according to multinuclear solid-state NMR

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Reactions of hydrodeoxygenation and hydroisomerization of fatty acid esters can used for production of valuable fuels from renewable sources such as food production waste. These multi-stage reactions require the presence of a bifunctional heterogeneous catalyst, which has both metallic and acidic active sites. The latter are provided by a porous support. Several prospective supports for these catalysts are represented by the family of silicoaluminophosphates (SAPO-n). In order to finely tune the catalytic properties of SAPOs, various heteroatoms can be introduced into their frameworks. In this work, we investigate the effect of introduction of boron into the framework of SAPO-11 on its Brønsted acid sites using multinuclear NMR spectroscopy and other physical methods.

According to ^{11}B NMR, the amount of boron successfully integrated into the SAPO framework directly correlates with the amount of silicon used in the synthesis. Furthermore, ^{1}H and ^{29}Si MAS NMR measurements demonstrate the decrease of signals connected to the presence of silicon islands. Thus, introduction of boron into the SAPO-11 framework leads to a more uniform distribution of Si sites in the framework and, consequently, increase of the Brønsted acidity of the material. Such an effect of boron substitution was confirmed by NH_3 TPD measurements and tested in the model reaction of hydroisomerization of methylpalmitate. In this reaction, the boron-substituted sample demonstrated high catalytic activity and suppressed cracking, improving the quality of the reaction products.

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RELAXIVITIES OF METALLOFULLERENOLS AND THEIR COMPLEXES WITH NANODIAMONDS IN AQUEOUS DISPERSIONS

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Dispersions of endofullerenols $Fe@C_{60}(OH)_{30}$, $Gd@C_{82}(OH)_{30}$, $Ho@C_{82}(OH)_{40}$ and their complexes with detonation nanodiamonds (DNDZ+, DNDZ-, size ~5 nm) with positive (negative) potentials (30-70 mV) were studied by proton NMR spectroscopy (20°C, field 11.7 T) in heavy water with an admixture of light water. The longitudinal and transverse spin relaxation times (T_1,T_2) of protons were measured, and the relaxivities of dissolved substances $R_1 \sim 1$, $R_2 \sim 10\ s^{-1}\ mM^{-1}$ were found to characterize the influence of magnetic ions Fe^{3+}, Gd^{3+}, Ho^{3+} on protons in fullerenols and surrounding water through dipole and exchange interactions. In addition, strong electric fields of diamonds (~10^7 V/m) in the complexes modulated their characteristics due to the attraction or repulsion of metal ions. An increase in the relaxivity by an order of magnitude was achieved due to the association of Fe-fullerenols with DNDZ- diamonds, since Fe^{3+} ions are attracted to them, pressing against the inner walls of fullerenols and transferring uncompensated spin density to them and the diamond facets [1, 2]. In the case of positively charged diamonds, the repulsion of ions from them prevents diamond activation, and complexes have the relaxivites lower than that of free fullerenols. For Fe^{3+} ions, a significant positive effect was detected primarily due to their small size and ability to partially penetrate the cells of carbon cages of fullerenols. However, lanthanide ions, which are larger and located further from the carbon walls of fullerenols, failed to activate the diamonds and showed only a negative effect. The development of Fe-fullerenol complexes with DNDZ- and similar objects with magnetic ions of 3d elements promises to improve the magnetic relaxation properties of the resulting compounds for use as effective contrast agents in Magnetic Resonance Imaging.

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EFFICIENT ^{15}N HYPERPOLARIZATION AT MILLITESLA MAGNETIC FIELDS BY REVERSIBLE EXCHANGE

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Hyperpolarization techniques enable dramatic enhancement of NMR signal intensities. One of these techniques called signal amplification by reversible exchange (SABRE) uses spin order of parahydrogen (p-H_2), which is transferred to other nuclei by means of an iridium metal complex. Due to a reversible exchange it is possible to utilize this approach to produce a bolus of a hyperpolarized substance for various biomedical applications. Conventional SABRE is used to transfer polarization to protons, but in the biomedical context hyperpolarization of heteronuclei (e.g., ^{13}C, ^{15}N) is preferable because of the higher T_1 at high magnetic fields as well as almost zero background signal from tissues. There are two major approaches for heteronuclear SABRE: the utilization of submicrotesla fields for polarization transfer (SABRE-SHEATH [1]) and the application of radiofrequency pulse sequences at high field of an NMR spectrometer. Here, we present a novel approach, which uses magnetic fields in the millitesla range to transfer polarization to ^{15}N nuclei and obtain polarization levels, which may exceed those provided by SABRE-SHEATH.

In this study, we investigated a number of biocompatible ^{15}N-labeled substrates such as $^{15}N_2$-metronidazole ($^{15}N_2$-MNZ), $^{15}N_2$-fampridine ($^{15}N_2$-FAM), $^{15}N_3$-metronidazole ($^{15}N_3$-MNZ) and $^{15}N_3$-nimorazole ($^{15}N_3$-NMZ). Polarization transfer field profiles, polarization buildup, T_1 relaxation times at the maximum polarization points and at the field of an NMR spectrometer (7 T) were measured for each substrate. For $^{15}N_2$-MNZ, we additionally estimated T_1 values at different points of the field sweep. All experiments were conducted at room temperature and 7.8 atm p-H_2 pressure. Among the presented compounds the highest polarization is achieved for the ^{15}N-1 and ^{15}N-3 sites of $^{15}N_3$-NMZ (absolute values of 3.0% and 4.9%, respectively). According to simulations data, it results from the lower exchange rates of $^{15}N_3$-NMZ in comparison with $^{15}N_2$-MNZ at the same temperature. This new approach paves the way for the efficient hyperpolarization of wide range of substrates and their various biomedical applications.

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[1]H NMR SPECTROSCOPY APPLICATION FOR DETERMINATION OF THE STRUCTURE AND CATALYTIC BEHAVIOR OF POLYELECTROLYTES

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Comb-like polyelectrolytes are effective surfactants for micellar catalysis of organic reactions in water. It was shown that these polymers are able to perform as co-catalysts of hydrolysis reactions [1] and constructive reactions [2], for example, Suzuki cross-coupling reaction in water which is considered in this work. However, the influence of the co-catalyst's degree of polymerization (DP) on catalytic effect of such systems has not been studied yet, so that is the aim of the current work. The ^{1}H NMR spectroscopy was used as the main method for determination of the structure and DP of the polyelectrolytes as well as for assessment their catalytic behavior in Suzuki rection.

Polyelectrolytes were synthesized in two stages. Firstly, RAFT polymerization of 11-bromundecylacrylate was carried out and, secondly, quaternization reaction as polymeranalogous reaction was performed in DMFA. The DP of the polyelectrolytes were calculated related to the signal of the RAFT agent in ^{1}H NMR spectrum. The model Suzuki reaction of phenylboronic acid and 1-bromo-4-nitrobenzene with $PdCl_2$ as catalyst was performed in water with different concentrations of polyelectrolytes. The conversion of the functional groups was measured using ^{1}H NMR spectroscopy.

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PHASE BEHAVIOR AND IONIC MOBILITY OF THE [$C_8C_2C_2$-ND][TFSI] IONIC LIQUID, NEAT AND IMPREGNATED INTO THE MIL-100(AL) METAL-ORGANIC FRAMEWORK STUDIED BY ^{2}H NMR SPECTROSCOPY.

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Ionic liquids (ILs) are fully ionic compounds that are liquids at room temperature or below 100 °C. Due to their low vapor pressure, high thermal stability, and tunable chemistry, they are widely used in electrochemistry and energy storage, serving as promising electrolytes for batteries, supercapacitors, and other devices. Composites based on ILs embedded in a porous matrix are promising for use in power sources and energy storage devices.

The work investigates the N,N-diethyloctan-1-ammonium bis(trifluoromethanesulfonyl)imide **[$C_8C_2C_2$-ND][TFSI]** (or [N822D][TFSI]) ionic liquid with asymmetric alkylammonium cation. To develop a solid electrolyte operational over a broad temperature range, an ionic liquid was impregnated into the pores of MIL-100(Al), a metal-organic framework based on Al^{3+} and 1,3,5-benzenetricarboxylic acid (BTC). MIL-100(Al) exhibits a rigid mesoporous structure and high thermal stability.

^{2}H NMR spectroscopy was used to characterize hydrogen bond strength and ionic mobility. Spectral changes from broad anisotropic signals at low temperatures to narrow isotropic lines at high temperatures indicated a transition from solid to liquid state, corresponding to dynamic melting.

Impregnation of the ionic liquid into the MOF modified the nature of this dynamic melting without altering the activation energy of isotropic molecular rotation. It was also established that the volumetric ionic conductivity of [N822D][TFSI] is primarily governed by isotropic molecular diffusion.

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Calculation of interaction parameters of Pu^{3+} ions with spins of fluorine nuclei in CaF_2

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Experimental data obtained by ENDOR method [1] revealed that the interaction of Pu^{3+} 5f-electrons with fluorine nuclei in CaF_2 crystal differs significantly from the classical dipole-dipole interaction. There is a large isotropic electron-nucleus interaction with the A_s parameter, which was found to be negative. The reason for this anomalous phenomenon has not yet been explained.

In this work, we consider the effect of mixing the 5f-electron wave functions of the Pu^{3+} ion with the 2s- and 2p- wave functions of fluorine on the values of the electron-nuclear double resonance (ENDOR) parameters A_s and A_p. Using the technique of irreducible tensor operators, we derive expressions for the spin Hamiltonian parameters of A_s and A_p via the hybridization parameters. In addition to this generally accepted covalent approach, the virtual transfer processes of 2s- and 2p- electrons of fluorine into the empty 6d-shell of plutonium have been taken into account. All overlap integrals were calculated on the Hartree-Fock wave functions of plutonium taken from [2], which were previously approximated by Gaussian-type orbital expansions. In the numerical evaluations of A_s and A_p, the covalency parameters were assumed to be proportional to the overlap integrals. interaction with the A_s parameter, which was found to be negative. As it could be expected on the basis of transferred hyperfine interaction analysis, for rare-earth compounds (see, for example, [3]), the magnitude and sign of A_s for the Pu^{3+} ion in CaF_2 can be explained by virtual processes of transfer of 2s- and 2p-electrons of fluorine to the empty 6d-shell of plutonium. Moreover, using the experimental data of [1] we obtained the covalence parameters of 5f- and 6d-electrons of Pu^{3+} in CaF_2.

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Компания Лакопа – проводник инновационных решений, которая обеспечивает доступ к экспертным знаниям и перспективным технологиям, способствует повышению уровня научных исследований, подготовке квалифицированных кадров, способных работать с прорывными идеями и творчески мыслить.

Наша компания является официальным дистрибьютером Suzhou Niumag Analytical Instrument - ведущего производителя, специализирующееся на разработке и применении технологии «низкопольного ядерного магнитного резонанса». Компания отличается мощным научно-исследовательским потенциалом, осуществляет полный цикл производства. Благодаря постоянному накоплению технологий, новаторским решениям и разработкам в различных областях применения оборудования, Niumag быстро стало высокотехнологичным предприятием, ориентированным на привлечение в команду ведущих специалистов в отрасли, инновации и развитие.

НАСТОЛЬНЫЙ ТВЕРДОТЕЛЬНЫЙ ЯМР-СПЕКТРОМЕТР С ВРАЩЕНИЕМ ОБРАЗЦА ПОД МАГИЧЕСКИМ УГЛОМ (MAS)

Настольный твердотельный ЯМР-спектрометр MAS20 использует вращение под магическим углом для достижения высокоточного измерения химического сдвига в твердых телах или гетерогенных системах, что позволяет анализировать структурное и молекулярное движение, а также анализировать компонентный состав.

ТЕХНИЧЕСКИЕ ХАРАКТЕРИСТИКИ:

- Тип магнита: постоянный магнит, не требует охлаждения и обеспечивает крайне низкие затраты на обслуживание
- Индукция магнитного поля: 0,5 Тл
- Диаметр ротора: 3,5 мм
- Максимальная скорость: 20 кГц
- Детектируемые ядра: доступны в исполнениях 1H, 7Li, 19F и 31P
- Безопасность: магнитное поле <2 Гс на корпусе прибора
- Температура окружающей среды: 20–26 °C, температурный дрейф <2 °C/ч
- Влажность окружающей среды: менее 80%
- Питание: 220 В, 50/60 Гц
- Пользовательский интерфейс: английский

ОБЛАСТИ ПРИМЕНЕНИЯ:

MAS20 применяется для научных исследований, обучения, предварительного анализа образцов и рутинного контроля качества, особенно для изучения парамагнитных материалов. Прибор позволяет устранить значительные боковые полосы вращения (spinning sidebands) парамагнитных материалов в традиционных магнитно-резонансных системах с высоким полем, которые влияют на качественный и количественный анализ.

- Материалы для литиевых аккумуляторов: анализ дефектов, идентификация информации о связях Li-O-TM (TM = Co, Cr, Mn,Fe, Ni) и анализ искажений
- Фосфорсодержащие материалы: анализ распределения Fe^{2+}/Mn^{2+} в парамагнитных фосфатных соединениях и кислотности катализаторов
- Парамагнитные комплексы: определение структуры и дифференциация кристаллических и аморфных структур
- Фторсодержащие материалы: определение содержания фтора, участия фтора в реакциях и структурный анализ

Специалисты компании имеют большой опыт работы в области перспективных разработок и знают, как сложно прокладывать путь первопроходцам. Сотрудничая со многими ведущими экспертами, мы развиваем междисциплинарные коммуникации для обмена опытом, подбираем правильные технологии, адаптируем их для решения самых сложных задач.

Poster Session

FEATURES OF SOLID-PHASE SYNTHESIS OF Gd2-xRexTi2O7 AND Gd1-xRexTiO3 TITANATES

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Perovskite-like rare-earth metal oxides attract significant attention due to their magnetic properties and pronounced magnetocaloric effect [1]. Among these compounds, gadolinium titanate $GdTiO_3$, containing titanium in the +3 oxidation state, and gadolinium pyrochlore $Gd_2Ti_2O_7$ are of particular interest. These materials are considered promising candidates for solid-state magnetic refrigeration applications [2].

In this work, the solid-phase synthesis of titanates with the general formula $Gd_{2-x}Re_xTi_2O_7$ and $Gd_{1-x}Re_xTiO_3$ was investigated, where Re denotes a rare-earth element. The aim of the study was to determine the synthesis features and optimal conditions for obtaining single-phase products. Various starting materials were used, including metallic titanium, titanium (IV) oxide, and rare-earth oxides of gadolinium and Re. The synthesis was carried out in argon or argon–hydrogen atmospheres at temperatures of 1200–1400 °C with durations of 10–20 hours.

Phase composition and crystal structure were analyzed using X-ray diffraction combined with Rietveld refinement. The results confirm the formation of single-phase crystalline compounds with a pyrochlore structure over a wide range of synthesis conditions, largely independent of the titanium precursor and synthesis atmosphere.

The study demonstrates that the solid-phase synthesis of $Gd_{2-x}Re_xTi_2O_7$ and $Gd_{1-x}Re_xTiO_3$ titanates requires careful control of synthesis parameters, which depend on the specific composition. Future work will include first-principles calculations of the structural, spectral, and magnetic properties of these compounds within the framework of density functional theory.

The research was supported by the Russian Science Foundation grant No. #25-22-00324

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Phosphine Oxides as Probes for Hydrogen Bonding: A Solid-State Study of Complexes with Substituted Phenols Using XRD and ^{31}P NMR

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This work examines recent insights into the behavior of phosphine oxides as molecular probes for characterizing hydrogen bond interactions, with particular emphasis on the spectroscopic response of the P=O group in the solid state. Phosphine oxides provide a uniquely sensitive platform for correlating measurable NMR parameters with the underlying hydrogen bond geometries, thereby enabling a detailed assessment of interaction strength [1].

The distinctive responsiveness of the P=O group arises from the high sensitivity of the ^{31}P nucleus [2], whose chemical shift undergoes substantial changes upon formation of non-covalent interactions [3-4]. Historically, this property has been exploited to quantify Lewis acidity through the Gutmann–Beckett approach, and theoretical predictions of ^{31}P shifts further underscore the diagnostic value of this functional group [5-7]. In crystalline environments, combining solid-state NMR spectroscopy with single-crystal X-ray diffraction offers a coherent framework for establishing quantitative correlations between spectroscopic features and structural parameters.

In the present study, 1:1 crystalline complexes of triphenylphosphine oxide (Ph_3PO) with substituted phenols were prepared and examined in order to elucidate the relationship between hydrogen-bond strength and the ^{31}P chemical shift. The crystallographic data consistently demonstrate the formation of P=O···O–H hydrogen bonds, while the corresponding solid-state NMR spectra reveal systematic variations in δP. A clear inverse correlation is observed between the O···O distance and the magnitude of the chemical-shift change, whereby shorter hydrogen bonds—reflecting stronger interactions—produce higher δP values. This correlation confirms that δP represents a reliable experimental indicator of hydrogen-bond strength in these systems.

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REAL-TIME MRI OF THE ARTICULATORY ORGANS AND LUNGS DURING SPEECH PRODUCTION

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This report summarizes the experience of conducting MRI experiments on a 0.5-T clinical scanner, revealing the possibilities of real-time visualization of the articulatory organs and lungs during speech production.

Experiments on visualization of jaw structures during the pronunciation of vowel sounds [1, 2], as well as consonants in combination with vowels, are noted [3]. Attention is drawn to the possibility of visualizing not only soft organs (tongue, lips, etc.), but also teeth [4], as well as volumetric visualization of articulatory organs [5]. Experiments involving visualization of the lungs while reading fiction (prose and poetry) are also noted [6].

It has been shown that MRI can be successfully used to study the physiological processes that accompany speech production, identifying patterns characteristic of native and foreign speakers [7]. This is useful for language teaching and diction correction, especially if there are specific differences (due to illness or injury) in the structure of the articulatory organs or lung function.

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APPLICATION OF NMR METHODS TO CONTROL THE SYNTHESIS AND OPTIMIZATION OF THE STRUCTURE OF SORBENTS BASED ON MAGNETIC NANOPARTICLES MODIFIED WITH IONIC LIQUIDS

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Core-shell magnetic nanoparticles (MNPs) are promising sorbents. The choice of surface modifiers for MNPs offers broad possibilities for the selective concentration and extraction of various biologically active substances from objects with complex matrices, such as biological fluids and natural samples. Ionic liquids— an alternative to molecular solvents with tunable properties depending on the nature of their constituent cations and anions—are of particular interest as MNP modifiers. The combination of ionic liquids and MNPs opens up the possibility of creating rapid and effective materials for the microextraction of biologically active substances due to the high sorption capacity of nanoparticles and various types of interactions (ion-dipole, dipole-dipole, hydrogen bonds, π-π) between ionic liquids and analytes. However, the existing diversity of approaches to synthesizing magnetite-based nanoparticles modified with ILs requires the development of reproducible methods for producing such sorbents, as the selectivity and sorption capacity of the particles depend on this. The synthesis of such sorbents is complicated by the high viscosity of the ILs used and their susceptibility to hydrolysis, which limits the application of many physicochemical methods for their characterization. The solution to this problem is possible using NMR spectroscopy methods. Therefore, the aim of this study was to develop and optimize a method for synthesizing magnetite-based nanoparticles covalently modified with imidazolium ILs using NMR techniques. The potential of a combination of NMR spectroscopy methods (^{1}H, ^{13}C, HMBC and COSY NMR) was demonstrated for establishing the structure and purity of the intermediate compounds and assessing the degree of conversion.

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OBSERVATION OF TWINNING IN $YAlO_3$ CRYSTALS BY EPR USING TRANSITION ION AND RARE-EARTH Dy^{3+} ION SIGNALS

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Rare-earth impurity ions in $YAlO_3$ perovskite crystals are used as active centers for laser generation and as a source of scintillation photons, including the near-IR region, which is convenient for radiobiology and radiation monitoring. The $YAlO_3$ structure serves as an effective doping matrix due to its mechanical and thermal stability. Research on the spectral properties and crystal fields of impurity centers in such structures is actively underway (e.g., [1, 2]).

Here we present the results of a study of Dy-doped $YAlO_3$ crystals. The samples were grown by the Bridgman method with nominal Dy concentrations of 0.15 and 3 at%. The aim of the study was to determine the parameters of the rare-earth ion Dy^{3+} and to identify trace impurities of transition metals by electron paramagnetic resonance spectra. Measurements were performed at frequencies of 94 and 9.4 GHz at temperatures of about 6 K and at 300 K. HF EPR measurements were performed on the EPR/ODMR spectrometer [3], and X-band measurements were performed on a commercial JEOL spectrometer. Strongly anisotropic signals with well-resolved hyperfine structure belonging to the Dy^{3+} ion (configuration $4f^9$, S=1/2) at the Y^{3+} site were recorded. For the (ac) rotation plane, two signals from magnetically nonequivalent Y^{3+} positions are observed. For the (bc) rotation, two signals from the Dy^{3+} ion come from crystal regions separated by a twinning plane are visible. The presence of twins is also monitored through the signals from transition ions in the g = 2 region (presumably – unintentionally introduced Cr^{3+} and Fe^{3+} ions substituting the Al^{3+} sites). Twinning was confirmed in polarized light. The research was carried out with the support of the Ministry of Science and Higher Education of the Russian Federation (FFUG-2024-0046) (A.V. Batueva, A.S. Gurin) and the State Science Committee of Armenia (No. 1-6/23-I/IPR) (H.R. Asatryan, K.L. Hovhannesyan, A.G. Petrosyan).

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CALCULATION OF THE AMPLITUDE–FREQUENCY RESPONSE OF GRADIENT MAGNONIC CRYSTALS

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Magnonic crystals based on thin-film ferrimagnetic materials are of considerable interest for microwave magnonics as elements for signal filtering and processing [1]. In recent years, particular attention has been paid to gradient magnonic crystals, the unit-cell period of which varies along the structure. Such systems potentially enable flexible control of stop-bands making them promising for the implementation of compact band-pass and tunable filters. The aim of this work is to model the amplitude-frequency response of a gradient magnonic crystal.

The amplitude-frequency response were simulated numerically using the transfer-matrix method for a structure supporting the propagation of surface spin waves in an yttrium iron garnet (YIG) film. A periodic structure with alternating thickness was considered as an already known initial case. After that, a gradient magnonic crystal was introduced as a structure with a variable period. This “period”, i.e. length of the unit cell, was modified according to both linear and nonlinear laws by stepwise reduction of the unit-cell segment lengths. Obtained results allowed us to analyze the influence of the number of unit cells and the magnitude of the period-variation step on the resulting amplitude-frequency characteristics.

The results show that the amplitude-frequency response exhibits a band structure consisting of passbands and narrow stopbands associated with Bragg reflection for a periodic structure. When a period variation is introduced, the nature of the stop-bands changes significantly. Each unit cell produces reflection at its own characteristic frequency determined by the local period, resulting in a non-constant Bloch wavevector and a distributed stopband starting at $k \geq k_B$. Therefore, with a sufficiently large number of unit cells in a gradient magnonic crystal and an appropriately chosen period-variation profile, it is possible to achieve a transmission spectrum in which only a single effective passband remains for $0 < k < k_B$.

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The effect of solution dilution on the microstructure and molecular mobility in LiCl-CsCl-H2O ternary system by molecular dynamics simulations

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Introduction

In recent years, ternary aqueous solutions have attracted increasing attention as promising electrolytes for batteries. To optimize the selection of the ratio of solution components, it is necessary to identify the mechanisms of microstructure formation as well as the main factors affecting the molecular mobility in such systems. In the present study the molecular dynamics simulations method was employed to study the effect of solution dilution on the microstructure and molecular mobility in LiCl-CsCl-H2O ternary system.

Methodology

At all, 15 systems were considered: 13 ternary and 2 binary solutions. The simulations were carried out using the MDynaMix package. All systems were simulated in an isothermal-isobaric ensemble (25°C, 1 atm.) in a cubic cell with periodic boundary conditions. The equations of motion were solved using Verlet algorithm with a time step of 2 fs. The coulombic interactions were calculated using the Ewald method. Constant temperature and pressure were maintained using the Nose-Hoover algorithm. The equilibration time for each model system was 2 ns, simulation time – 1 ns.

Results

Based on the simulation results, the radial distribution functions between solution components as well as the coordination numbers of all ions were calculated. A special attention was given to changes in the composition and stability of the first solvation shells of the cations with decreasing salts concentration. The effect of solution dilution on the molecular mobility (self-diffusion coefficients of solution components, the average residence times of water molecules in the hydration shells of ions, the times of H_2O molecules reorientation) were considered in detail.

The Origin of Mirror Symmetry in High-Resolution NMR Spectra

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A correlation between the symmetry of high field NMR spectra, including higher order patterns, and the underlying properties of the spin system has been established. It is demonstrated that for a spectrum to be symmetric about its mid resonance frequency (ν_0), two conditions must be satisfied simultaneously: (i) the spin resonance frequencies must be arranged symmetrically about ν_0, and (ii) the spectrum must remain invariant under reflection of the J coupling matrix about its anti diagonal. In the simplest case, the latter condition is fulfilled when the J coupling matrix itself is symmetric with respect to the anti diagonal.

DIHYDROXYLATION OF THE LATERAL VINYL GROUP IN A TETRAPYRROLE FROM THE PERSPECTIVE OF A PROTON SPECTRA

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This report focuses on a tetrapyrrole which originates from a pheophorbide *a*. The tetrapyrrole is obtained after the oxidation of the pheophorbide *a* methene bridge at the C4–C5 position, then the reduction of the "western" methene bridge of the *seco*–pyropheophorbide *a*, its prototropic tautomerization and hydroxylation of the ethyl lateral group. The tetrapyrrole obtained contains four methyl, one vinyl, one hydroxyethyl, one propionyl, two carbonyl, one aldehyde and one methoxycarbonyl lateral group(s). In literature for the lateral group the words: side-chain [1], periphery [2] and peripheral substituents [3] can be met. Vinyl group is dihydroxylated to a 1,2-dihydroxyethyl lateral group. Vinyl protons and 1,2-dihydroxyethyl protons show characteristic signals in proton spectra enabling straightaway recognition of a tetrapyrrole with vinyl lateral group or its 1,2-dihydroxy derivative.

The lateral vinyl group has three characteristic *doublet of doublets* with the AMX spin splitting pattern. *trans*-Coplanar arrangement indicated is by a coupling constant of 17.9 Hz for H_M (δ 6.07) and H_X (δ 6.43) protons. The coupling constant of 11.9 Hz indicated the presence of H_A (δ 5.34) and H_X protons. The coupling constant of 2.3 Hz indicated geminal protons H_A and H_M. After dihydroxylation of the lateral vinyl group in the proton spectrum characteristic spin splitting pattern is not present. The *triplet* signal of a methine proton from –CHOH appears at δ 4.52 (*J*=5.4 Hz). The –CH_2OH group methylene protons signals appear at δ 3.80 (*J*=5.4 and 9.5 Hz) and δ 3.63 (*J*=5.6 and 9.6 Hz). The –OH signals underwent deutero exchange in CD_3OD solvent. The formed tetrapyrrole with the 1,2-dihydroxyethyl lateral group in proton spectrum does not have characteristic vinylic AMX pattern found in the range of δ 5.34–6.43. It has signals for methine proton –CHOH at δ 4.52 and methylene protons –CH_2OH at δ 3.80 and at δ 3.63.

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NUMERICAL MODELING OF SPIN-WAVE DISPERSION IN A RECTANGULAR FERROMAGNETIC WAVEGUIDE

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This work reports on theoretical investigation of spin wave (SW) dispersion characteristics in ferromagnetic rectangular waveguides. In particular, the influence of non-uniform distribution of the internal magnetic field on the SW spectrum for various directions of the external magnetic field was considered. The spatial distribution of the internal magnetic field was expressed by integral relation with the saturation magnetization, which was obtained solving the static problem for dipole-exchange SW spectrum with tensorial Green's function method [1].

The calculation results showed that the non-uniformity of the internal magnetic field depends strongly on both the width-to-thickness ratio of the waveguide and the direction of the external magnetic field. As this ratio approaches unity, the average strength of the internal magnetic field changes by almost a factor of two, with the increase or decrease being determined by the direction of the external field.

Solving the dynamic problem yielded the dispersion equation that describes the SW propagation in a ferromagnetic waveguide with defined parameters. The simulation showed that taking into account the internal magnetic field distribution leads to a frequency shift of the SW spectra, with the sign of the shift being determined by the direction of the external magnetic field. In addition, the group velocity decreases. The non-uniform magnetic field distribution across the waveguide cross-section also leads to the localization of magnetization oscillations within a confined region.

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Investigation of the Dynamic Properties of Gradient Copolymers by Brownian Dynamics simulations

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Abstract

Block copolymers self-assemble into complex nanostructures due to their ability to the microphase separation. This plays a key role in nanotechnologies. Advances in modern synthesis enable the production of copolymers with a gradual variation in chemical composition. Unlike copolymers with uniform monomer distributions, gradient copolymers have been less studied.

Coarse-grained models of polymer chains comprising 128 monomers were investigated using Brownian dynamics simulations. The chains consisted of two types of monomers—hydrophilic and hydrophobic. Reference cases were selected as those typical of regular block copolymers, featuring uniform distributions of hydrophilic and hydrophobic blocks, as well as polymer chains consisting of only one type of monomer (either hydrophilic or hydrophobic). The objects of study were chains with various gradient distributions of hydrophobic and hydrophilic monomers.

System equilibration was determined from the time dependence of the radius of gyration of a chain. Following equilibration, trajectory simulations were performed for subsequent analysis. The trajectory length was chosen to be no less than $10000\tau_{\mathrm{rot}}$, where τ_{rot} is the rotational time of the chain as a whole. Dynamic properties of the chains were calculated from the obtained trajectories. For each chain type, autocorrelation functions of the orientational mobility of the vector directed from one end of the chain to the other were computed. The rotational time of the chain as a whole, τ_{rot}, was determined from the decay of these autocorrelation functions on long timescales. Substituting the value of τ_{rot} into the Perrin-Debye relation yielded the hydrodynamic radius (from rotational diffusion).

The mean-square displacement (MSD) from the chain's centre of mass was also calculated. The diffusion coefficient was obtained from the longer linear part of MSD. Substituting the diffusion coefficient into the Einstein-Stokes relation gave the hydrodynamic radius (from translational diffusion). A comparison was made between the hydrodynamic radii obtained by both methods (via rotational and translational diffusions). It was found that gradient copolymers demonstrated, on average, lower mobility than regular block copolymers.

Computer Simulation by Brownian Dynamics of the Structural Characteristics of Gradient Copolymers

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Abstract

Copolymers are of wide interest for practical applications in industry and biotechnology. In addition to traditional block copolymers, the synthesis of gradient copolymers is possible. In such copolymers, chemical properties and composition vary gradually. Block copolymers are well studied both theoretically and experimentally. In contrast, gradient copolymers remain poorly investigated.

In our work, gradient copolymers were investigated using computer simulation by Brownian dynamics and compared with block copolymers. All chains had an identical number of hydrophobic and hydrophilic monomers but differed in their distribution along the chain. The computer simulations were conducted in two stages: equilibration and main simulations. During the main stage, snapshots of system coordinates were recorded at specified intervals into files. Subsequent analysis was performed using these trajectory files.

For each system, the chain's radius of gyration was calculated. Another characteristic considered was the end-to-end distance of the chain. For both characteristics, the average value and distribution (to measure molecular 'fluctuations') were computed. The shape of each polymer molecule was evaluated using the shape anisotropy parameter. Analysis of the internal structure was carried out via density profile distributions—for the molecule as a whole, as well as separate distributions for hydrophilic and hydrophobic monomers. The average angle between monomers was also calculated. We obtained, that the internal structure of gradient copolymers substantially differs from that of block copolymers. This arises from non-trivial intramolecular microphase separation than observed in regular block copolymers.

OPTIMIZATION OF THE DELAY TIME BETWEEN PULSES ON ^{31}P CORES TO STUDY THE FUNCTIONAL COMPOSITION OF LIGNIN

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^{31}P-NMR is successfully used for the study of the functional composition of lignin [1]. The standard protocol of the experiment was presented by Dimitris Argyropoulos, Xianzhi Meng, et al [2]. It includes quantitative analysis of OH-groups content in lignin after its phosphitylation and registration of the ^{31}P-NMR spectra. The N-hydroxy-5-norbornene-2,3-dicarboximide is used as an internal standard (152,0 ppm). The proposed protocol allows the obtaining of reliable and representative results, but the disadvantage of this approach is a long experiment time, varying from 30 minutes to 2 hours.

The spectrum registration time in this method is unacceptably long for a simple task of determining of hydroxyl groups in lignin. We therefore decided to test the possibility of the optimization of the experiment duration by reducing delay time. The remaining parameters of the spectrum registration were performed in accordance with Protocol of Dimitris Argyropoulos, Xianzhi Meng et al [2].

The analysis of the dependence of signals intensities on pulse delay allows to calculate the minimum pulse delay for representative quantitative analysis of the samples. The results demonstrate that the dependencies change their slope and become almost horizontal at pulse delay of 5 s, which means that 5 s of delay is enough for analysis. The studied polymer has very short relaxation time, and its signals do not change with delay varying, so the minimum delay depends on T_1 relaxation time of the used internal standard (low molecular compound), and the direct T_1 measurement would be not effective for the studied sample.

Instrumentation of the Core Facility Center «Arktika» of Northern (Arctic) Federal University was used in this work.

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INDUCED NONLINEAR PHASE SHIFT IN THE GRADIENT MAGNONIC CRYSTAL

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Periodic magnetic-film structures are excellent experimental media for studying of different linear and nonlinear spin waves (SW) phenomena [1, 2]. At the same time, nonlinear SW phenomena in gradient magnonic crystals (GMC) were not studied yet. This report focused on the induced nonlinear phase shift (INPS) of SW in a tangentially magnetized GMC. The investigation of the INPS of SWs in GMC is motivated by it potential application for developing novel magnonic logic gates based on the Mach-Zehnder interferometer design [3-5].

The main findings obtained as a result of the study are as follows. The dependence of the SWs INPS vs the pump wave power in the GMC initially exhibits a linear growth and then a clear saturation. This consists with the numerical model derived from a system of coupled nonlinear Ginzburg-Landau equations. Furthermore, increase in the GMC groove depth and the pump frequency results in significant suppression of the INPS. This suppression is attributed to the enhanced Bragg reflection of the pump wave from the gradient structure.

The close match between experimental data and numerical modeling confirms the reliability of the proposed theoretical model. The conducted study provides a foundation for developing new magnonic logic devices utilizing GMC-based phase shifters within a Mach-Zehnder interferometer architecture.

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Probing the water dynamics in wheat grains by relaxation and diffusion NMR

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In this study the relaxation and diffusion NMR were employed to investigate the local dynamics and transport of water in wheat grains with varying moisture content following natural, thermal, and contact drying.

Wheat grains are essential for global food security and sustainable agriculture, with their post-harvest quality largely determined by drying parameters. NMR techniques, specifically relaxometry and diffusometry, provide a powerful, non-invasive means to assess how different drying methods affect the local dynamics and transport of water within grain tissues, as well as their structural integrity. Alongside traditional convective (thermal) drying, modern approaches include natural, vacuum, infrared, freeze-drying, and an innovative contact drying technique that uses solid sorbents as desiccants [1-3]. This sorbent-based method is of particular scientific and practical interest, as it enables gentle, non-thermal moisture removal through direct contact with hygroscopic materials, thereby minimizing risks of thermal degradation. Application of relaxation and diffusion NMR is crucial for evaluating and optimizing such contact drying processes, as these methods can directly probe the states, local dynamics, and long-range diffusion of water without altering the sample.

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PHASE DIAGRAM OF THE Ga-In ALLOY UNDER NANOCONFINEMENT

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The investigation of the influence of nanoconfinement on the physical properties of gallium and its alloys is quite important because they are promising nanomaterials for soft robotics and wearable electronics [1,2]. We suggest using NMR as a perspective method for finding phase diagrams of nanostructured alloys, since it is sensitive to changes in the local structure of an alloy. Here, we present NMR studies of the impact of nanoconfinement on the phase diagram of the Ga-In alloy embedded into a porous Al_2O_3 ceramic template with the mean pore size 50 nm. The temperature dependencies of the Knight shift and integral intensities of the NMR lines of gallium and indium in nanoconfined Ga-In alloys of various compositions were used to proof the alterations in the solidus and liquidus lines on the phase diagram. NMR revealed that the eutectic composition of the nanostructured Ga-In alloy did not change compared to the bulk alloy.

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Computer Simulation of Interaction of GED and AED Peptide Molecules with KRH or KHR Dendrimer in Water

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Abstract

Abstract: - Previously, it was shown that several short bioactive peptides, containing GluAsp (ED) sequence, can modulate gene expression and promote normalization of function of different organs. In this work, we use Molecular dynamics simulations of the interaction between bioactive GlyGluAsp (GED) and AlaGluAsp (AED) peptide molecules and a second-generation lysine dendrimer containing arginine-histidine (ArgHis) spacers were performed. Unlike prior simulations involving charged double lysine or arginine (LysLys, ArgArg), neutral double hydrophobic (LeuLeu, AlaAla, GlyGly), and double pH-dependent (HisHis) spacers, this study focuses on dendrimers with ArgHis and HisArg spacers, where amino acids in spacer are different, and histidine charge vary with pH. The simulation modeled the complexation of 16 GED or 16AED molecules with the dendrimer at two pH levels: (a) pH > 7, where histidine residues remain noncharged, and (b) pH < 5, where histidines are fully protonated. Results indicate that protonated histidines enable the dendrimer to carry a higher number of GED and AED molecules, suggesting enhanced loading capacity at lower pH levels.

CYLINDRICAL DISTRIBUTION FUNCTION FOR STUDYING THE STRUCTURE OF POLYMER MELTS

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The study of the structure of melts of disordered polymer systems is a difficult challenge due to the high diffusion mobility, which does not allow the system to maintain stable long-lived symmetry. For example, in the case of molecular dynamics modeling, time averaging is used to obtain statistically reliable data. This does not allow, as a rule, to obtain local features of the mutual arrangement of neighboring macromolecules due to rapid diffusion in the system.

This paper presents a cylindrical distribution function (CDF) adopted for analysis of local structure of carbosilane dendrimers of the fourth generation (CSD G4) in a melt. This system was chosen because the presence of an impermeable core in the dendrimer leads to the formation of regions of reduced density in the interdendrimer space [1-2], which in turn leads to a dense environment effect that slows translational mobility. To calculate the function, the vector between the central atoms of adjacent dendrimers at each time point was used. The function was then averaged over all dendrimer pairs over time. To determine the cylindrical distribution function for the dendrimer atom density, it was found that a region of reduced density arises at the dendrimer periphery. Moreover, the density distribution of the dendrimer's centers of mass indicates a tetragonal packing of the dendrimers. It is important to note that this packing is not static, as diffusional movement causes displacement of the macromolecules and exchange of packing between the dendrimers. However, on average, this packing is maintained.

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BENCHMARKING OF MAGNONIC RESERVOIR COMPUTING WITH NARMA10

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The objective of this work is to evaluate the computational capability of a magnonic reservoir computer [1-2] using the standard NARMA10 benchmark [3] and to compare the obtained results with the results of other tests. This task is relevant because previously, testing of the magnonic reservoir computer was conducted exclusively using short-term memory and parity check tests, which did not allow for a comprehensive comparative analysis of the results.

The work involved numerical simulation of the reservoir computer's operation and investigation of its parameters [4]. An algorithm for testing the magnonic reservoir computer using NARMA10 was proposed, the influence of reservoir parameters on the test capacity values (STM and PC) [5] and on the Normalized Root Mean Square Error (NRMSE) value was investigated. The obtained results made it possible to find a correlation between the studied tests.

The following results were obtained in the work. The proposed method for forming the state matrix of virtual neurons for the NARMA10 task demonstrated high efficiency compared to the traditional method. The physical parameters of the system affect the results of all considered tests. This indicates the necessity of selecting optimal parameters for the reservoir's efficient operation. The correlation analysis of the tests showed that the result of processing a random sequence by the reservoir depends simultaneously on its memory and nonlinearity, and the NRMSE has a high degree of coincidence with the STM and PC capacities. All conducted studies showed that with an increase in the reservoir's memory, the Normalized Root Mean Square Error (NRMSE) for processing a random sequence decreases. The dependence of NRMSE on the PC capacity turned out to be more complex. The correlation between these tests depends on the interrelationship between the STM and PC capacities themselves.

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Determination of the structure of esters based oN dicyclopentadiene by spectral methods

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Among industrial monomers and polymers derivatives of acrylic and methacrylic acids are the most widely used. They are employed in the production of varnishes, paints, resins, oils, organic glass, liquid crystal displays for televisions and computer monitors, photographic emulsions, toothpastes, rubbers, orthopedic and filling materials, textile impregnations, packaging films, and bags. Alicyclic polyacrylates, due to their combination of excellent thermal, electrical, and physical-mechanical properties, occupy a prominent place among various classes of heat-resistant polymers[1-3].

Considering the relevance of the problem, in contrast to existing methods, we have developed an effective method for obtaining new reactive monomers – functional polycyclic (meth)acrylates – by adding (meth)acrylic acids to tri- and tetracyclic monoesters. The results of the studies showed that the most effective catalyst for the synthesis of polycyclic acrylic diesters is boron trifluoride etherate.

With a molar ratio of tricyclic unsaturated monoesters and acrylic acids equal to 1:1.5 mol, with a catalyst amount of 0.5% by weight (of the initial acid weight), a temperature of 90°C and a reaction duration of 5 hours, the yield of polycyclic acrylic monomers is 74-80%.

The physicochemical constants of the obtained esters were determined, and their structures were identified using IR, ^{1}H and ^{13}C NMR spectroscopy. IR spectra were recorded on an ALPHA İQ FTIR spectrometer (Bruker, Germany) in the 600-4000 cm^{-1} range. NMR spectra were recorded on a Bruker AV instrument (USA) at 300 MHz in acetone-d_6. The synthesized polycyclic diesters are transparent liquids with a characteristic odor. These reactive monomers can be utilized to synthesize polymeric materials of significant practical value.

NMR analysis confirmed that acrylic acids stereoregularly add to the double π-bond of tricyclodecenol and tetracyclododecenol monoesters to form exo-exo tricyclic and tetracyclic acrylic diesters.

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USING SOLID-STATE NMR SPECTROSCOPY TO STUDY OF AN UNKNOWN VESSEL FRAGMENT RECOVERED FROM THE BOTTOM OF THE BALTIC BAY.

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The use of sophisticated scientific equipment for the study of various historical objects is currently becoming more and more developed. This approach makes it possible to highlight new facets of the history of material culture. The method of solid-state NMR spectroscopy is one such technique, and his using is becomes more widespread. This paper shows an example of this technique application for the studying of a wooden fragment of an unknown vessel raised from the bottom of the Baltic Gulf.

The examined fragment is probably a knee-plate. The fragment is carefully covered on all sides with a dark substance. Several probes were taken from the fragment by drilling out wood flour from individual annual rings. The chemical composition characteristics were estimated by ^{13}C CP/MAS NMR spectroscopy as a function of the distance from the fragment surface. It is shown that the method of solid-state NMR spectroscopy is a convenient tool for rapid analysis of such objects of natural origin.

CAPACITIVE DILATOMETER FOR MEASURING MAGNETOSTRICTION

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In this report we present the construction of capacitive dilatometer and the results of measuring the magnetostriction of the Van Vleck dielectric single crystal of lithium-thulium double fluorides $LiTmF_4$ along the [100] crystallographic axis.

The capacitive dilatometer was designed and assembled according to the design proposed by G. M. Schmiedeshof et al [1] and was used with a PPMS system and a capacitive bridge [2]. The design of the capacitive dilatometer cell offers an open architecture that allows for convenient placement of samples for testing. The samples can be in the form of cylinders and rectangles with a maximum size of 6 mm along the dimension of the sample being tested, and they can also be less than perfectly shaped with selected parallel planes.

The $LiTmF_4$ single crystal was grown using the Bridgeman-Stockbarger method. After evaluating the single crystallinity and axis orientation, two parallel planes perpendicular to the crystallographic axis [100] were selected and polished using a brass mandrel and water-based abrasives.

Using a capacitive dilatometer, the magnetostriction of the $LiTmF_4$ single crystal was obtained at a temperature of T=5 K. Our data are consistent with previous studies up to 3 T [3], and also qualitatively consistent with preliminary calculation in a single crystal up to 3.5 T.

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NMR-STUDY OF STIMULI-RESPONSIVE IONIC LIQUIDS EXHIBITING CHROMISM

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Although the first ionic liquid was synthesized back in 1888 [1], the potential for their research and practical applications is still not fully realized. Among the diverse range of stimuli-responsive ionic liquids (ILs), those that display chromic behavior, particularly acidochromism, are of special interest owing to their simple and direct colorimetric response [2].

One of the most important steps of fundamental characterization of ILs based on acidochromic indicators is to evidence their form, *i.e.* to show the molar ratio between cations and anions in the composition of the IL, as well as to confirm their purity. In the case of organic ions this can be achieved using NMR-techniques as shown further.

In this work, a series of ion pairs with tetra(decyl)ammonium (TDA^{+}) as a cation was synthesized for the first time with a conventional method described in [3]. The following water-soluble acido- and metallochromic dyes served as anions: bromophenol blue (BPB^{2-}), bromothymol blue (BTB^{2-}), fluorescein (FL^{2-}), thymolphthalein (TPT^{2-}), methyl red (MR^{-}), ethyl orange (EO^{-}) and eriochrome black T (EBT^{2-}).

All the novel compounds were comprehensively characterized by methods of NMR: ^{1}H and ^{13}C relaxation, COSY and NOESY spectroscopy. In this contribution, we pay special attention to peculiarities of NMR application relative to the mentioned class of ionic liquids: acquisition and analysis of ^{1}H and ^{13}C NMR spectra, relaxation data processing, and interpretation of COSY and NOESY spectra.

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^{14}N NQR study of urea citrate and urea succinate cocrystals

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Urea is one of the most important industrial compounds. Among its numerous useful applications, it has a capacity to form complexes with many organic and inorganic molecules. One of a few applications is nonlinear optical materials [1] and advanced fertilizers [2]. Some organic cocrystals were studied by ^{14}N NQR double resonance. This study focuses on urea cocrystals of organic acids as a model object that is close to industrial applications.

Urea citrate (US) and urea succinate (US) cocrystals were prepared by slow evaporation of water solutions of 1:1 molar ratio mixture of urea and citric and succinic acids, respectively. NQR analysis showed that $\nu+$ NH_2 group frequency of urea in both cocrystals shifted up from 2.820MHz at 25C to 2.957MHz. Both cocrystals also feature drastic increase of T_1 relaxation time, as well as appearance of multimodal spin-lattice relaxation time distribution. T_1 measurements were made by saturation method. While urea has T_1 around 1s at room temperature, UC and US demonstrated increase of T_1 to around 2.5-4.2s and 47-60s, with UC having slightly lower relaxation times. Both samples also acquired a short T_1 component around 150ms, most probably attributed to amide bond vibrational mode. Both NH_2 and CO groups in urea cocrystals has hydrogen bonds, which reduce its mobility and lead to T_1 increase. Results show that NQR relaxation can be used to characterize spin dynamics in molecular cocrystals.

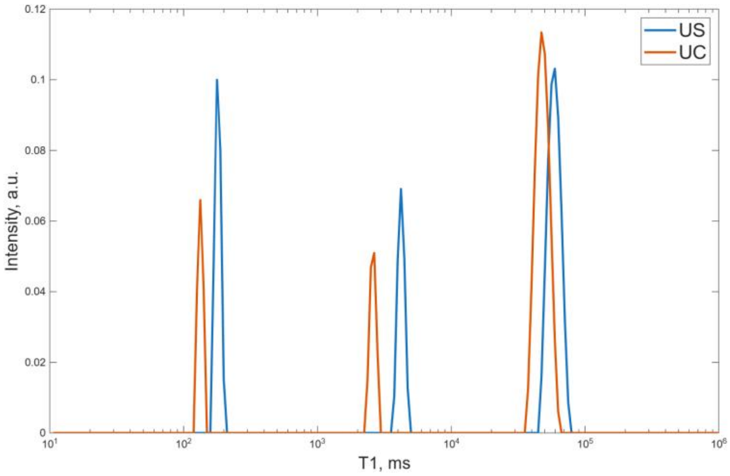

Figure 1. T_1 relaxation time distributions for urea citrate (UC) and urea succinate (US).

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The effect of hydrogen-deuterium isotopic substitution on the molecular mobility in aqueous solutions of europium nitrate by molecular dynamics simulations

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Investigation of trivalent europium ion (Eu^{3+}) interactions with water molecules is important for a large number of applications in chemistry, materials science, and biology. In the present work, the effect of hydrogen-deuterium isotopic substitution on the molecular mobility in aqueous solutions of europium nitrate is studied by molecular dynamics simulations.

Simulations were carried out using the MDynaMix software package [1]. Solutions of $Eu(NO_3)_3$ in H_2O and D_2O at 10 different concentrations (from 0.05 to 4 mol/kg) were considered. The model for heavy water was developed by merely changing the hydrogen mass in a classical concept. The calculations were performed in an NPT ensemble at 298 K and 1 atmosphere. The temperature was kept constant using a Nose-Hoover thermostat [2], and the pressure was maintained by a Hoover barostat [3]. The equations of motion were solved using the Verlet algorithm with a time step of 2 fs. The electrostatic interactions were treated using Ewald method. The geometry of the model water molecules and nitrate anions was maintained using the SHAKE algorithm [4]. For each system the equilibration time was equal to 1 ns, the following simulation run was 1 ns long.

Based on the simulation results, the changes in the composition, geometry and stability of the first solvation shell of the europium ion with increasing salt concentration were considered in detail. A special attention was given to the effect of hydrogen-deuterium isotopic substitution on the mobility of solvent molecules.

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T_1–T_2 CORRELATION FOR PROBING ACIDITY OF MICROPOROUS AND MICRO-/MESOPOROUS ZEOLITES

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Zeolites are widely used in industry as molecular sieves, ion exchangers, sorbent and catalysts. Understanding the relaxation behavior of liquids confined in a zeolite matrix is critically important for optimizing the sorption capacity and diffusion accessibility of active sites, which ultimately determines the effectiveness of an adsorption-catalytic system. According to recent studies mesoporosity is beneficial to the rational design of catalysts with controlled product selectivity and the improved catalyst lifetime due to the efficient mass-transport properties. Two-dimensional (2D) time-domain NMR have proven to be extremely useful for exploring systems with hierarchical porosity [1]. For confined liquids, the observed spin-lattice (T_1) and spin-spin (T_2) relaxation times of nuclear spins differ from their bulk values. Interaction of adsorbed molecules with the surface, which is usually inhomogeneous, results in a distribution of relaxation times, that can be used to probe the inner surface. In this contribution we report on the results of ^{1}H NMR relaxation studies of water confined in a set of zeolite samples to follow the effect of mesoporosity and pore arrangement on the surface affinity and adsorbate behavior in zeolite catalysts with different framework topology (mordenite and ZSM-5). For this purpose, T_1–T_2 correlation experiment, composed of an inversion recovery pulse sequence followed by a Carr- Purcell- Meiboom- Gill echo pulse train ware carried out at home-built relaxometer with operating ^{1}H NMR frequency of 60 MHz. 2D $T_1 - T_2$ correlation maps for 15 different zeolite samples were obtained and analyzed. The role of Si/Al ratio, zeolite framework, pore size and its mutual arrangement was discussed.

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^{31}P NMR STUDIES OF BLOOD SERUM TAKEN FROM PATIENTS WITH MULTIPLE MYELOMA

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NMR of human blood plasma and serum is wildly used to get information about different types of deceases. In particular, ^{31}P NMR spectra provide analysis of the phospholipid composition [1]. These spectra were shown to be changed for patients with renal cell carcinoma [2], acute leukemia [3], and ischemic stroke [4]. However, there are no publications concerning the phosphorus NMR applications to multiple myeloma. *Multiple myeloma* is a cancer that forms in plasma cells.

Here we report ^{31}P NMR spectra obtained for blood serum taken from 5 patients with multiple myeloma and 3 healthy donors. Measurements were carried out using a pulse Avance 500 Bruker spectrometer at room temperature. The collected blood with clotting activator was kept in test tubes and then centrifuged at 3000 rpm for 15 min. Then the samples were frozen until NMR experiments. The spectra showed a strong line relevant to phosphatidylcholine and a group of three lines shifted to high frequency. Following previous studies, we compared the relative intensities of the lines. We found unambiguous correlations between relative intensities and the diagnosis of multiple myeloma.

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APPLICATION OF ^{1}H AND ^{17}O NMRD TO HYDRATION OF METALLOPROTEINS

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Using ^{1}H and ^{17}O relaxation measurements of bulk water as a function of the applied magnetic field (Nuclear Magnetic Relaxation Dispersion - NMRD) technique, the hydration of some globular proteins (cytochrome *c*, cytochrome b_5 and rubredoxin) containing metal atoms was studied. These metals in biologically active proteins constantly change their oxidation state and transition from a paramagnetic state to a diamagnetic one and vice versa... This transition significantly affects proton spin-lattice relaxation, while for oxygen-17 relaxation the magnetic properties of metals do not have a significant effect for the proteins studied. At the same time, ^{17}O NMRD can clearly indicate the change in the property and dynamics of a limited number of water molecules within a protein during such a transition, which can shed light on the biological activity of proteins.

Potentialities and limitations of the use of ^{1}H NMRD technique for the characterization of the hydration properties of unfolded or partially folded states of proteins are discussed. The dispersion profile, analyzed with an extended relaxation matrix analysis, indicates the presence of long-lived water molecules in the folded state, that are released upon unfolding.

Facilitating Total Lineshape Analysis: FOMA & ANATOLIA-X

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Total lineshape analysis of complex multispin NMR spectra remains a challenge for conventional software. To address this, we introduce two novel computational tools: FOMA and ANATOLIA-X. FOMA (First-Order Multiplet Analyzer) performs total lineshape fitting of individual complex first-order multiplets. ANATOLIA-X is a modified version of our previous ANATOLIA program, incorporating X-factorization of the spin Hamiltonian to enable the analysis of standalone strongly coupled multiplets. Both tools are designed to analyze subspectra and generate high-quality initial parameter guess, thereby streamlining and enhancing the robustness of the overall total lineshape fitting workflow.

EPR OF MAGNETIC IRON OXIDE NANOPARTICLES FOR BIOMEDICAL DIAGNOSTICS

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Due to the increasing use of aqueous dispersions of magnetic iron oxide nanoparticles in immunomagnetic analysis [1], immunochemiluminescent analysis [2], NMR diagnostics (DMR method [3]), questions arise related to the aggregation processes of magnetic nanoparticles (MNPs) in a magnetic field, the coating properties of nanoparticles, with conjugation of various molecular compounds focused on capturing analyzed objects.

EPR studies of superparamagnetic iron oxide nanoparticles in aqueous suspensions were carried out depending on their size and concentration. A comparative analysis of the typical EPR spectra shows the following patterns. A change in the concentration of MNPs in stable homogeneous solutions does not lead to a shift in the g-factor and a broadening of the line. In aggregated samples the shape of the EPR lines may contain two components – narrow and wide signals with different g-factor. Comparison of EPR line widths and g-factors shows that when aggregating magnetic nanoparticles there is a significant broadening of the EPR lines and their displacement to the region of higher values of g-factors. An increase in the size of nanoparticles led to a significant broadening of the EPR lines. A decrease in the sample temperature from 289 K to 100 K led to a broadening of the EPR line and a shift of its g-factor to higher values.

Thus, EPR studies of aqueous dispersions of magnetic nanoparticles allow us to evaluate their stabilizing properties and aggregation ability, EPR biomedical diagnostics capabilities.

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The application of NMR spectroscopy for identification of the structures of 6-methyl-2-nitro-3-(trichloromethyl)-2,3-dihydro-4*H*-furo[3,2-c]pyran-4-one and its dehydrochlorination product

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1-Bromo-1-nitro-3,3,3-trichloropropene reacts with CH-acids via the formation of either dihydrofurans [1] or cyclopropanes [2]. The reaction with the heterocyclic CH-acid – 4-hydroxy-6-methylpyran-2-one – yields two types of products, depending on the reaction time. Investigation of the first product (shorter reaction time) by NMR methods allowed the assignment of a dihydrofuran structure characterized by doublets of the methine protons (4.95 and 6.55 ppm). The vicinal *J*-coupling constant (1.2 Hz) indicates their *trans* configuration.

The unexpected structure of the second compound (longer reaction time) was determined using one-dimensional (^{1}H; ^{13}C) and two-dimensional (HMQC, HMBC, COSY) NMR spectroscopy. It was found that a singlet at 6.89 ppm belongs to the proton of the nitromethine fragment, while the absence of the second dihydrofuran proton signal can be explained by the formation of a dichloromethylene derivative.

An interesting and important feature in the NMR spectra of both compounds is the correlation of the methyl protons with the singlet of the pyran-2-one ring in the ^{1}H-^{1}H COSY, caused by long-range *J*-coupling ($^{4}J_{HH}$).

The proposed structures were confirmed by single-crystal X-ray diffraction analysis performed for both compounds.

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INTERACTION OF LOVASTATIN WITH TRANSITION METAL IONS BY NMR SPECTROSCOPY AND MOLECULAR DYNAMICS SIMULATIONS

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Cardiovascular diseases (CVD) are the leading cause of death worldwide, strongly linked to elevated levels of low-density lipoprotein (LDL). While statins are the standard LDL-lowering therapy, their efficacy is limited in some patients, and they can cause adverse effects. Coordination compounds of statins with transition metals represent a promising avenue for developing new drugs with potentially improved properties. This work aims to elucidate the interaction mechanisms of lovastatin with metal ions using NMR spectroscopy and molecular dynamics (MD) simulations to facilitate the design of more effective and safer CVD therapeutics.

The interaction of lovastatin with Mn^{2+}, Ni^{2+}, and Zn^{2+} ions in an acetone-d_6 solution was studied by high-resolution NMR spectroscopy (^{1}H, ^{13}C, HSQC, HMBC, NOESY, DOSY) at 308 K. MD simulations of the corresponding systems were performed to validate the coordination sites and binding dynamics.

NMR data revealed distinct differences in the interaction of lovastatin with the metal ions. Zn^{2+} does not interact with lovastatin under these conditions, whereas Mn^{2+} and Ni^{2+} form stable complexes, coordinating within the same internal region of the molecule via its carbonyl functional groups. MD simulations corroborated these findings. Analysis of radial distribution functions (RDF) confirmed a high spatial probability density for Mn^{2+} and Ni^{2+} in the vicinity of specific hydrogen atoms (0.55-0.75 nm), corresponding to the identified coordination site involving the carboxylic acid group. In contrast, the RDF profile for Zn^{2+} showed no such preferential localization, confirming the absence of stable complexation.

The integrated NMR and MD study establishes a clear difference in binding affinity (Mn^{2+} and Ni^{2+} form stable complexes vs. no detectable interaction for Zn^{2+}) and identifies the specific coordination site. These findings provide a reliable basis for the targeted synthesis of new statin-based metal complexes with predictable properties.

NATURE OF ^{75}As SPIN-LATTICE RELAXATION IN A GaAs SEMI-INSULATOR SINGLE CRYSTAL

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High resistance of the order of 10^8 Ω·cm in semi-insulator GaAs crystals, both in clean undoped and in intentionally doped samples, is associated with deep electron traps. The intrinsic EL2 defects are the most known such electron centers. Interaction of electron centers with ligand nuclei combined with spin diffusion produces an effective route of nuclear spin-lattice relaxation in solids [1]. The character of this interaction specifies the rate and evolution with temperature of the contribution of electron centers to total spin-lattice relaxation of host nuclei.

Recently, it was shown for two gallium isotopes in an undoped semi-insulator GaAs crystal [2] that within the temperature range from 80 to 300 K there is a pronounced contribution to spin-lattice relaxation due to electron centers, which was comparable to the contribution of relaxation due to gallium spin-phonon coupling. Surprisingly, the obtained results unambiguously demonstrated the quadrupole character of the interaction between electron centers and gallium nuclei. Here we report the NMR studies of ^{75}As spin-lattice relaxation in the same GaAs sample. The contribution to relaxation of electron centers was segregated. In contrast to the results for gallium, the interaction of electron centers with the ligand ^{75}As nuclei was found to have a mixture character being a combination of electric quadrupole and magnetic dipole effects. This agrees with studies carried out in [3], which confirmed the more effective superhyperfine coupling between the EL2 centers and arsenic nuclei.

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SPECTRAL FEATURES OF SUBSTITUTED 2-(NITROMETHYL)PENTANONES CONTAINING AN ASYMMETRIC CARBON ATOM

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3-Nitropropenoates and -propenones react with carbo- and heterocyclic CH acids to form Michael adducts [1, 2], and the presence of a chiral atom in their structure results in diastereotopic effects in their ^{1}H NMR spectra [3]. The aim of this study was to investigate the structure adducts of 3-nitropropenoates and -propenones with the aliphatic CH acid pentane-2,4-dione obtained for the first time. Analysis of the ^{1}H NMR spectra revealed that in the case of methyl 3-acetyl-2-(nitromethyl)-4-oxopentanoate **1**, the CH_2NO_2 group protons and the methine protons H^C and H^M form an ABCM-type spin system. Thus, the signals of the methylene protons appear as two doublets of doublets at 4.71 ppm (^2J 15.0, ^3J 6.9 Hz) and 4.58 ppm (^2J 15.0, ^3J 4.0 Hz), the methine proton H^C – a doublet of doublets of doublets at 3.89 ppm (^3J 6.9, ^3J 4.0, ^3J 6.9 Hz), and the methine proton H^M forms a doublet at 4.39 ppm (^3J 6.9 Hz). In turn, differences are observed in the ^{1}H NMR spectrum of 3-acetyl-1-(4-methoxyphenyl)-2-(nitromethyl)pentane-1,4-dione **2**. Geminal coupling in methylene group is not manifested and the signal of this protons form a doublet at 4.70 ppm (^3J 5.8 Hz), the signal of the methine proton H^C appears as a doublet of triplets at 4.81 ppm (^3J 8.4, 5.8 Hz), and the methine proton H^M forms a doublet at 4.51 ppm (^3J 8.4 Hz). Probably, this change in the spectral picture is associated with the additional influence of the aromatic ring. The assignment of signals is confirmed by the results of ^{1}H-^{1}H dqf-COSY experiments obtained for compounds **1, 2**. The ^{13}C-{^{1}H} NMR spectra of adducts **1, 2** are similar and contain signals of all structural fragments of the molecule. Thus, it was shown that structurally similar 2-(nitromethyl)pentanones containing an asymmetric carbon atom, but differing in the presence of an alkoxycarbonyl or aroyl substituent, exhibit differences in the signal shapes in the ^{1}H NMR spectra.

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EXTRACTION PURIFICATION OF TRANSFORMER OIL USING A DEEP EUTECTIC SOLVENT: FTIR EVALUATION OF PROCESS EFFICIENCY

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Deep eutectic solvents (DES) are currently regarded as a promising class of compounds that are functionally close to ionic liquids, due to the similarity of their physicochemical properties. Environmentally benign DES are formed by mixing an organic salt with a hydrogen bond donor, which may include carboxylic acids, alcohols, amines, or amides.

A structural feature of these systems is the formation of large asymmetric ionic associates characterized by reduced lattice energy. This circumstance, in turn, leads to a decrease in the melting temperature of eutectic mixtures compared to their individual components [1].

It should be noted that, despite the active development of this research field, studies devoted to deep eutectic solvents are still at an earlier stage compared to those on ionic liquids. At the same time, the majority of published works focus on systems containing quaternary ammonium and imidazolium cations [2].

Meanwhile, the fields of practical application of DES are steadily expanding and include polymer synthesis, electrochemistry, biotransformations, as well as various separation processes [3]. In recent years, it has been demonstrated that the use of deep eutectic solvents as analogues of ionic liquids opens new opportunities for intensifying the extraction purification of petroleum fractions [4].

Taking the above into account, a deep eutectic solvent was obtained in the present study based on a hydrogen bond acceptor—diethylammonium acetate—and a hydrogen bond donor—ethylene glycol. The synthesized DES was applied as an extractant in the extraction purification of transformer oil.

To evaluate the efficiency of the purification process, a qualitative analysis of the initial and purified oil samples was carried out using FTIR spectroscopy. The obtained results confirmed the prospects of using deep eutectic solvents as highly selective solvents providing the removal of undesirable components from transformer oil.

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STUDY OF A MULTICOMPONENT MAGNETIC SYSTEM AT DIFFERENT TIMESCALES: ESR and ^{57}Fe MÖSSBAUER SPECTROSCOPY, MAGNETOMETRY

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This work is devoted to solving the problem of identifying the contributions of various magnetic subsystems in dilute magnets. It is known that the "apparent" magnetic state is determined by the ratio of the relaxation time to the characteristic measurement time [1]. Therefore, a multimethod approach was used, covering a measurement time range of 10^{-10}–10^{2} s. The methods used were ESR and Mössbauer spectroscopy, quasi-static magnetometry, and a.c. susceptibility χ measurements. The object of the study is artificial glass synthesized by the petrological synthesis method. Melting was carried out at 1515°C in a gas flame furnace [2].

The study established a three-level organization of the magnetic system. The ESR method showed the coexistence of isolated Fe^{3+} ions in the glass structure ($g \sim 3.98$) and ferrimagnetic, including superparamagnetic, iron oxide nanocrystals ($g \sim 2.28$). Analysis of the hysteresis parameters on the Day plot and the specific morphology of the "wasp waist" type loop indicate a bimodal distribution of particles by size with a predominance of the pseudo-single-domain state near the superparamagnetism boundary with a significant paramagnetic contribution. A fundamental paradox of time scales has been identified, whereby the system exhibits signs of stable ferrimagnetism in quasi-static measurements at 300 K, but displays paramagnetic behavior in Mössbauer spectra. The transition of the magnetic moments of superparamagnetic particles to a locked state is confirmed by the appearance of a magnetic sextet when the temperature is lowered to 77 K. The χ measurements exhibit frequency dispersion, indicating a superparamagnetic response. At the same time, there is a tendency for χ to increase with increasing magnetizing field, which is usually associated with irreversible domain boundary movements.

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LOW-FIELD BENCH-TOP NMR STUDY OF PEI-COATED MAGNETIC IRON OXIDE NANOPARTICLES

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Polyethyleneimine-coated magnetic iron oxide nanoparticles (PEI-NPs) are successfully used in magnetofection [1-4]. Bench-top NMR instruments efficiently assess magnetic properties for process control, even with low-field spectral resolution limitations.

The NPs were obtained by co-precipitation [5] and were coated with PEI. ^{1}H NMR spectra and relaxation times were measured. Relaxation times T1 and T2 were determined via inversion recovery and Carr-Purcell-Meiboom–Gill method, while T2* was estimated from spectral linewidth. The data show that PEI-NPs significantly reduce aqueous proton relaxation times. Linewidth and chemical shift increase with Fe concentration due to demagnetization effects. PEI-NPs exhibited the dephasing power close to dextran and chitosan-stabilized magnetic nanosols [6]. The dephasing proton magnetization is described by model attributed for spin refocusing in spin-echo precession period for magnetic statistically irregular ensembles of magnetic spheres [7,8].

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Blood Viscosity: A Predictive Factor for Preeclampsia

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Abstract

In this study, the absolute dynamic viscosity of whole blood was determined in pregnant women with preeclampsia and eclampsia. For this purpose, the proton magnetic relaxation method was used to measure the viscosity of hemoglobin and plasma [1,2]. These values, together with the hematocrit, allowed the calculation of whole blood viscosity [3]. The results showed a viscosity range of 5.24 – 8.55 mPa·s, values significantly higher than those observed in healthy pregnant women. It is noteworthy that, out of the 15 pregnant women studied, 13 presented viscosity values above the upper mean between weeks 26 and 29 of gestation, subsequently developing severe forms of the disease (aggravated preeclampsia and eclampsia). This finding reinforces the predictive value of blood viscosity in the early detection of preeclampsia and suggests its clinical utility in risk assessment and follow-up of pregnant patients.

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Determination of the 1-(2-nitrovinyl)-3-phenylpyrrolidine structure using NMR spectroscopy

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Nitroenamines attract considerable interest due to their potential in organic synthesis and biological activity [1]. The most convenient and widely used synthon in this group is N,N-dimethyl-2-nitroethen-1-amine, first synthesized as early as the 20th century [2]. However, information on the chemical properties and, particularly important, spectral data of its derivatives remain limited to this day. One of the most effective methods for obtaining diverse nitroenamines, varying by the substituent at the amino group, is the transamination reaction.

For the first time, the interaction of N,N-dimethyl-2-nitroethen-1-amine with 3-phenylpyrrolidine was carried out, leading to the formation of a new nitroenamine, which can exist as two geometric isomers, E and Z. In the ^{1}H NMR spectrum, a doubled set of signals from all structural fragments is observed, indicating the obtaining of a mixture of two substances with similar structures. The vicinal coupling constant of the olefinic protons in each of the sets are 10.5 and 10.7 Hz, which agrees with literature data for structures of related compounds existing in the E-form [1].

Thus, the reason for the doubling of signals in the ^{1}H NMR spectra is the existence of the obtained product as two conformers. This is related to the asymmetric structure of the 3-phenylpyrrolidine substituent, whose rotation around the C–N bond is hindered due to conjugation involving the lone electron pair of the nitrogen atom and the C=C bond of the nitroolefin fragment.

Therefore, based on two-dimensional NMR spectroscopy, the structure of the obtained conformers was confirmed by us.

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EVALUATION OF THE DEGREE OF DEAROMATIZATION OF TRANSFORMER OIL BY NMR SPECTROSCOPY

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Ionic liquids are a special class of organic compounds with a reduced melting point, the structure of which can be purposefully modified depending on the required properties. Due to the combination of ionic nature, high polarity and chemical stability, these compounds are used in catalytic and electrochemical processes, as well as in the separation and purification of multicomponent systems.

In recent years, the Institute of Petrochemical Processes has been conducting systematic research on the use of ionic liquids in the selective purification of petroleum fractions, which demonstrates the environmental and economic importance of ion-liquid extraction [1, 2].

In this work, a study of the extraction purification process of T-1500 transformer oil using an acetate-type ionic liquid as an extractant was carried out. The ^{1}H and ^{13}C NMR spectroscopy methods implemented in collaboration with St. Petersburg State University were used to estimate changes in the component composition of the oil before and after extraction.

In the recorded high-resolution ^{1}H and ^{13}C NMR spectra, the regions of the spectra from aromatic and aliphatic hydrogen and carbon nuclei do not overlap, which made it possible to analyze the relative intensities of these regions of the spectra and correlate these intensities with the number of atoms in the corresponding fragments of molecules in the mixture.

The character of the revealed changes in the component composition makes it possible to classify the ionic liquid used as one of the promising extractants for selective purification of transformer oil.

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Comparison of Gadolinium Effect on Statins by NMR spectroscopy

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Statins such as atorvastatin, pravastatin, and lovastatin are widely used hypolipidemic agents that inhibit HMG-CoA reductase and are essential in the prevention of cardiovascular diseases [1,2]. Despite their clinical importance, the molecular interactions between these drugs and gadolinium ions (Gd^{3+}) remain insufficiently explored. Given the widespread use of gadolinium-based contrast agents in MRI and growing concerns about Gd^{3+} retention in biological tissues and even in patients with normal renal function. It is crucial to understand how free Gd^{3+} may influence the structure and behavior of co-administered pharmaceuticals [3].

In this study, we employed high-resolution NMR spectroscopy to investigate the interaction of Gd^{3+} with three common statins: atorvastatin, pravastatin, and lovastatin. The addition of Gd^{3+} to statin solutions resulted in significant broadening of ^{1}H NMR signals, accompanied by reduced cross-peak intensity in HMQC spectra and loss in ^{1}H–^{13}C correlations in HMBC spectra. It is indicative of dynamic complex formation and paramagnetic relaxation enhancement for statin and Gd^{3+} ion. Despite differences in binding affinity, all three statins showed preferential coordination of Gd^{3+} to oxygen-rich regions of their molecular structures. These findings highlight both commonalities and distinctions in how structurally related statins respond to Gd^{3+} exposure, offering new insights into potential drug-contrast agent interactions at the molecular level.

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Study of the complexation of Gd^{3+}, Ni^{2+}, and Zn^{2+} Ions with Pravastatin by NMR Spectroscopy.

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The study of drug interactions with transition metal ions is a subject of interest in the fields of targeted drug delivery and pharmacology, as such interactions can affect the bioavailability and therapeutic effectiveness of pharmaceuticals [1]. Metal ions such as Zn^{2+} and Ni^{2+} (components of metal-containing drugs), as well as Gd^{3+} (the basis of MRI contrast agents), can be present in the body together with medicinal agents [2]. Pravastatin is one of the key statins used to treat primary hypercholesterolemia, hyperlipidemia, and mixed dyslipidemia [3]. Its molecular structure contains functional groups capable of coordinating with ions particularly with Gd^{3+}, Ni^{2+}, and Zn^{2+}.We investigated the complexation of pravastatin with transition metal ions (Ni^{2+}, Zn^{2+}) and a lanthanide ion (Gd^{3+}) in D_2O using high-resolution NMR spectroscopy.

The analysis of 1D and 2D NMR spectra revealed that the addition of Gd^{3+} and Ni^{2+} ions to pravastatin with D_2O solution causes selective broadening of the CH-15 and CH2-16 proton signals in the 1H NMR spectra and disrupts cross-peaks in the ^1H-^{13}C HMBC spectra. This thing indicates the spatial proximity of these ions to the C-15 and C-16 carbon atoms. In contrast the Zn^{2+} ion doesn't cause significant line broadening, leading only to minor changes in chemical shifts. The observed decrease in pravastatin's diffusion coefficient in D_2O upon addition of Gd^{3+}, Ni^{2+}, or Zn^{2+} provides clear evidence for complex formation with each metal ion.

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FEATURES OF SELF-DIFFUSION AND NUCLEAR MAGNETIC RELAXATION IN AQUEOUS SUGAR SOLUTION SYSTEMS

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The study of the characteristics of saccharides during their dissolution plays an important role in determining their structural and functional properties. The mechanisms underlying the interaction between water molecules and saccharides are still being refined [1-3], and the possibility of applying various models to describe intermolecular interactions in these systems is being discussed [4-5]. Important information about the patterns of interaction between molecules in aqueous saccharide solutions can be obtained from studies of molecular mobility [6]. The nuclear magnetic resonance method is one of the most informative methods for studying and evaluating the influence of dynamic processes on the mobility and interaction of molecules [7-9].

The goal of our study is to investigate the interaction between water molecules and saccharides in aqueous solutions using NMR method. A number of saccharides were selected as research objects in this study: the monosaccharides D-mannose and D-xylose, the disaccharides sucrose and maltose, and the trisaccharide raffinose.

It has been shown that the concentration dependencies of the self-diffusion coefficients and spin-lattice relaxation times for water molecules in aqueous saccharide solutions can be satisfactorily described within the framework of the hydration model with quite realistic values of the number of water molecules in the hydration shell of the saccharide molecule. Unlike the data on spin-lattice relaxation and self-diffusion, the behaviour of spin-spin relaxation of water molecules in aqueous solutions of saccharides, characterised by a significantly higher transverse relaxation rate compared to that of dissolved saccharide molecules, cannot be reconciled with the hydration model. It has been suggested that the effect of a significant reduction in the spin-spin relaxation time of protons in water molecules and hydroxyl groups of saccharides may be due to the chemical exchange of protons (water and -OH) between states with different resonance frequencies – different chemical shifts.

The work was carried out on the equipment of the Federal Center of Shared Facilities for physical and chemical research of substances and materials (FCSF) KFU Bruker AVANCE 400 MHz spectrometer optimized for microtomography, solid state and self-diffusion.

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Orientational mobility of ions in a solution of lithium salt TFSI in the ionic liquid BMPyrrTFSI according to NMR data.

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This work is devoted to the study of the orientational mobility of molecular groups of an ionic liquid (IL) in the BMPyrrTFSI system with lithium bistrifluoromethanesulfonylimide (LiTFSI) salt at different lithium concentrations (0 mol, 0.1 mol and 1.5 mol) [1][2]. These systems were studied using NMR relaxometry on a Bruker Avance III 500 MHz NMR spectrometer. Measurements of spin-lattice relaxation rates were carried out at various temperatures in the range from 243 to 333 K for several nuclei: ^{1}H, ^{13}C, ^{7}Li, ^{19}F. The obtained results were compared with the data presented in the literature. At a concentration of 1.5 mol (the most saturated salt solution in IL), we observed a characteristic kink in the graphs during the transition to low temperatures (about 278 K). This change in the character of the dependence possibly indicates both freezing of this system and a rearrangement of the molecular structure. At low concentrations (0.1 mol), as well as for the pure ionic liquid, this effect was not observed in the temperature range studied.

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THE INFLUENCE OF PRESENCE OF CONCOMITANT WATER ON MICROSTRUCTURE AND MOLECULAR MOBILITY IN MIXTURES OF ETHYLAMMONIUM AND ALUMINUM NITRATES BY MOLECULAR DYNAMICS SIMULATION DATA

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It is known that aluminum salts exist only in the form of crystalline hydrates. It is important to find out whether it is possible to remove water from a system after the addition of crystalline hydrate to ionic liquids, and to evaluate the effect of the concomitant water on the properties of a mixture. The mixture of ethylammonium nitrate (EAN) and aluminum nitrate ($Al(NO_3)_3$) was studied by NMR and it was shown: (i) in Refs. [1, 2] that standard drying procedure did not allow the removal of the aqueous environment near the Al^{3+} cation, and (ii) in Ref [3] that the mixture contains complexes with four and five water molecules.

The purpose of this work was to analyze by molecular dynamics simulation method how the presence of the aqua complexes near the Al^{3+} cation ($[Al(H_2O)_x]^{3+}$) affects the microstructure and molecular mobility in the mixture of EAN and $Al(NO_3)_3$. Four systems were considered: EAN, “EAN + $Al(NO_3)_3$”, “EAN + $[Al(H_2O)_5]^{3+}[(NO_3^-)_3]$” and “EAN + $[Al(H_2O)_6]^{3+}[(NO_3^-)_3]$”. Radial distribution functions, self-diffusion coefficients of mixture components and rotational reorientation times of the nitrate anion were calculated.

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OPTICALLY DETECTED MAGNETIC RESONANCE OF ERBIUM IONS IN YTTRIUM-ALUMINUM GARNET

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YAG:Er crystals are attractive for use in a wide range of applications in medicine, aerospace, energy, and communications. Erbium ions embedded in the crystals possess unique properties for quantum information processing due to their optical transition at 1.5 µm, the large magnetic moment of the ground electronic state with an effective spin of S = 1/2, and a long coherence time [1].

In this work, the EPR of Er3+ ions in erbium-doped yttrium aluminum garnet (YAG) crystals was recorded at a frequency of 94 GHz based on the intensity of infrared luminescence at a temperature of 7 K. The EPR spectrum of Er3+ ions is sharply anisotropic. In YAG crystals, Er3+ ions substitute for Y3+ at dodecahedral lattice sites. There are six magnetically nonequivalent positions, and six lines are observed for an arbitrary crystal orientation. Intense lines in the EPR spectra are surrounded by groups of lower-intensity lines, each consisting of nine components. Natural erbium, in addition to even erbium, has an odd isotope with a nuclear spin of I = 7/2. The natural abundance of these isotopes is 19.0% and 24.9%. The EPR of Er3+ in YAG was previously studied in [2, 3]. Comparison of the ODMR and EPR spectra shows that the ODMR spectrum belongs to the ground state of Er3+ ions. Previously, the EPR of the ground state of Ce3+ ions was recorded using the luminescence intensity of cerium in YAG crystals, which was explained by magnetic circular dichroism in the excitation of luminescence [4]. Luminescence excitation and recording were carried out in the direction of the magnetic field. The observation of EPR of Er3+ luminescence upon excitation by linearly polarized light in a direction perpendicular to the field in the present study is associated with the effect of magnetic linear dichroism in the excitation of luminescence.

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NMR-identification of furan/pyran heterocycles in polymeric chains of different nature

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Five and six-membered heterocycles with the oxygen atom (furan and pyran, correspondently) are widely spread in the structure of natural compounds such as sugars, simple carbohydrates (for example, inulin), polysaccharides et. al. Modern pharmacology and medicine based on biomimetic principle and principle of molecular similarity, often utilize these heterocycles as structural units for creation of novel compounds as carriers of drugs and gene material, artificial enzymes, and food additives. In the synthesis of biosimilar compounds, the applied reactions are differ from the natural processes, therefore there is a necessity to identify, to confirm distribution and to determine a number of these cycles in the product of synthesis. Many synthetic water soluble polymers today are of interest because they not only exhibit high biocompatibility, but also demonstrate a wide range of pronounced pharmacological activity. One of such compound is copolymer of the divinyl ether and maleic anhydride copoly(DE-MA) which, due to method of synthesis [1, 2], able to contain different amount of pyran and furan cycles in the backbone. A problem for structural analysis of copoly(DE-MA) besides of cycles stereoisomerity, is a possible microstructural heterogeneities. Based on NMR H1/C13 spectra of two copolymer samples, synthesized differently, and quantum chemical modeling of monomer units by means of B3LYP/6-311G**++ [3], at the present work have been developed a strategy of bands identification for pyran- and furan cycles and estimation of its average ratio. The used strategy has a universal character, and may be applied to different compounds with pyran and furan inclusions.

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NMR STUDY OF THE ANTIMICROBIAL PEPTIDE ECAMP3

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Antimicrobial peptides (AMPs) are a group of small, positively charged peptides produced by various living organisms and exhibiting a broad spectrum of antimicrobial activity [1]. Natural sources of AMPs range from prokaryotes to higher animals, and their targets include bacteria, fungi, protozoa, and viruses. Their predominant mechanism of action involves direct or receptor-mediated damage to pathogen cell membranes [2].

Among the many antimicrobial peptides (AMPs) of plant origin, a group has been identified that shares a common structural feature — a conserved cysteine motif. This motif is a region of the amino acid sequence containing cysteine residues that form disulfide bonds. Studies of one such group of peptides, called EcAMPs and isolated from barnyard grass (Echinochloa crus-galli), have shown that their molecules have a helix-loop-helix secondary structure. This structure consists of two antiparallel α-helices connected by a loop and is stabilized in the tertiary structure by two disulfide bonds (Cys1–Cys4 and Cys2–Cys3) [3].

The EcAMP3 peptide, isolated from Echinochloa crus-galli seeds and belonging to the α-hairpinin family, exhibits a broad spectrum of antimicrobial activity. It exhibits pronounced antifungal activity against phytopathogenic fungi such as F. graminearum, F. oxysporum, and A. niger, as well as unique bactericidal activity against P. syringae (IC_{50} ~10 μM). Due to its high activity, EcAMP3 is considered a promising candidate for protein engineering to create drugs for agriculture and pharmacology [4].

Despite its pronounced antimicrobial activity, the molecular targets of the EcAMP3 peptide, as well as its spatial organization, remain unknown. The main hypothesis is its possible interaction with the ribosome, leading to the suppression of transcription and translation.

The aim of this study was to determine the spatial structure of the antimicrobial peptide EcAMP3 using high-resolution NMR spectroscopy. NMR spectra were recorded on a Bruker Avance III HD™ 700 MHz spectrometer equipped with a QCI cryoprobe ($^1H/^1F$, ^{13}C, ^{15}N, ^{31}P). Signal assignment was based on the following experiments: 1H-1H TOCSY, 1H-1H NOESY, 1H-13C HMBC, 1H-13C, and 1H-15N HSQC. Spectra processing was performed using the CcpNMR Analysis package [5].

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Molecular Dynamics of Interaction of EDL/ED Oligopeptide Molecules with LysArgHis/LysHisArg Peptide Dendrimers

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Abstract

Ovagen (GluAspLeu or EDL) is a short bioactive peptide that normalizes liver and gastrointestinal tract function. In this work, we study complexes of EDL or shorter ED peptide molecules with the KRH dendrimer containing arginine-histidine (RH) spacers and the KHR dendrimer containing histidine-arginine (HR) spacers. These dendrimers can be used as a nanocontainer for the delivery of oppositely charged bioactive molecules, including peptides. The amino acid residues in the spacer (H and R) of each dendrimer are different, and the charge of the H residue depends on pH. Therefore, we performed molecular dynamics simulations of the complexation of 16EDL or 16ED molecules with the dendrimer at two different pH values: a) KRH at pH>7 with fully uncharged histidines (H) and b) KRHp at pH<5 with fully protonated (Hp) histidines; c) KHR at pH>7 with fully uncharged histidines (H) and d) KHpR at pH<5 with fully protonated (Hp) histidines in aqueous solution with explicit counterions. It was found that dendrimers with protonated histidines (KHpR and KRHp) could carry more Ovagen peptide molecules than dendrimers with neutral histidines (KHR and KRH), respectively. Moreover, Ovagen peptide molecules penetrate deeper into the dendrimer center in KHpR and KRHp dendrimers than in KHR and KRH dendrimers.

The use of NMR magnetometry to detect the remains of foundations of demolished buildings and technical underground utilities.

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Magnetic survey is one of the oldest and most effective geophysical methods, based on the study of spatiotemporal variations in the Earth's natural magnetic field. Its physical foundation lies in the differences in magnetic properties (magnetic susceptibility and remanent magnetization) of various rocks and ores. The method is applied to solve a wide range of problems: from regional geological mapping and mineral deposit exploration to engineering surveys and archaeology.

The Earth's magnetic field possesses unique characteristics that make it an ideal tool for surveying. Despite its global record homogeneity, which creates a smooth and predictable background, it permeates large volumes of subsurface, providing integral information about deeply buried objects. At the same time, its temporal variation under the influence of charged particle flux from the Sun requires special data processing to subtract the time-dependent component. Modern measurement technologies, based on hyperfine interactions in atoms, allow recording the field with the highest accuracy (up to 0.01 nT). It is precisely this combination — a powerful yet homogeneous background, the possibility of non-contact probing of large volumes, and ultra-precise measurements—that ensures a high degree of contrast even for weak magnetic anomalies, whose amplitude can be millions of times smaller than the main field.

In this work, conducted as part of the chemistry project session at the Educational Center "Sirius" a study of the Earth's magnetic field was carried out using the solution of the inverse NMR problem. For this purpose, several tasks were solved on the territory of the "Sirius" Educational Center: the first involved establishing the influence of objects with high magnetic susceptibility on the distance to the magnetometer. An analysis of Earth's magnetic field data obtained from variometric stations located on the same parallel and meridian was also conducted. Additionally, information on the diurnal variation of the Earth's magnetic field was compared both on the territory of Sirius and on the coast of the Black Sea, away from anthropogenic objects. The main task was to investigate the values of the Earth's magnetic field and compile a magnetometric map for detecting anomalies on the campus territory, where a 70×30 -meter area was selected. To reduce the influence of anthropogenic objects, such mapping was performed on the territory of the Sochi Ornithological Park, where measurements of the Earth's magnetic field values were conducted on a 30×30 -meter square area.

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