Applied Magnetic Resonance (2023) 54:891–894
https://doi.org/10.1007/s00723-023-01614-y

Applied
Magnetic Resonance

EDITORIAL

New Facets of Magnetic Resonance Applications

V. I. Chizhik[1] · **M. S. Tagirov**[2]

Published online: 9 September 2023

After the phenomena of electron paramagnetic resonance and nuclear magnetic resonance in condensed matter (in 1944 and 1946, respectively) were registered, the era of the development of their applications in a wide variety of areas has come that was even noted by several Nobel Prizes. This process continues at the present time, opening up new facets of applications, and this issue presents some of them.

This special issue of *Applied Magnetic Resonance* starts with the article "MRI of inanimate objects using fluorine-containing liquid" by Nikolay V. Anisimov, Lev L. Gervits, Arina A. Tarasova, Ivan A. Usanov, Yury A. Pirogov, in which a new MRI technique for 3D visualization of voids within solid objects is described. The authors show that the problem can be solved using a fluorine-containing liquid—the so-called "dry water"—for MRI in combination with the method of visualizing places from which there is no signal, i.e., in the method, the imaging signal comes from the fluorine-containing liquid which is used to immerse the studied objects, and the object is detected by the loss of a signal in this background. This is a very interesting approach that was not previously published. It is also shown that images of the environment, surrounding the receiving-transmitting coil, make it possible to obtain maps of the sensitivity of this coil.

The next few articles focus on heterogeneous systems, which have been investigated by NMR since the 1950s, but new motifs are still emerging in research in this area.

A. V. Uskov with co-authors presented the article "Ionic mobility in metallic sodium nanoparticles confined to porous glass". Sodium is one of the most abundant chemical element in the environment. Metallic sodium has many applications in chemistry, physics and medicine. Recently, great attention was paid to metallic sodium nanoparticles because of their wide practical applications, in particular, for enhanced oil recovery procedure. To study the impact of size reduction on the ionic

✉ V. I. Chizhik
v.chizhik@spbu.ru

M. S. Tagirov
Murat.Tagirov@gmail.com

[1] St. Petersburg State University, Saint Petersburg, Russia

[2] Kazan Federal University, Kazan, Russia

mobility in solid sodium, the authors carried out the measurements of Knigh shifts and spin–lattice relaxation times of the ^{23}Na nuclei in sodium nanoparticles embedded into porous glass with a mean pore size of 23 nm and in bulk sodium (the temperature range used: from 190 to 293 K).

The international scientific team (from Russia, México and Vietnam) published the work "Dynamics of guest water molecules in pillared mordenite studied by ^{1}H NMR relaxation" (Marina G. Shelyapina, Denis Yu. Nefedov, Anastasiia O. Antonenko, H'Linh Hmok, Andrey V. Egorov, Maria I. Egorova, Alexandr V. Ievlev, Rosario Yocupicio-Gaxiola, Vitalii Petranovskii, Joel Antúnez-García, Sergio Fuentes). The dynamics of H_2O molecules confined in mesopores of about 3.4 nm in size, formed by amorphous SiO_2 pillars separating 2D mordenite nanolayers, was probed by ^{1}H nuclear magnetic relaxation. The temperature dependences of spin–lattice relaxation T_1 and relaxation in the rotating frame $T_{1\rho}$ of protons indicate the complex behavior of nanoconfined water, which can be characterized by different activation energies for the following processes: freezing of nanoconfined water (29 kJ/mol), rotational motion (12 kJ/mol) and translational motion of water (23.6 kJ/mol). Comparison of the obtained results with the data for amorphous silica allows the authors to state that the main contribution to the water behavior in samples studied is due to the interaction with amorphous silica pillars, while there are no analogues to the water behavior in the 3D channels of alumosilicate zeolites.

The authors of the article "Time-domain NMR techniques in cellulose structure analysis" (Leonid Grunin, Maria Ivanova, Veronika Schiraya and Tatiana Grunina) discuss the possibilities of one of the actual NMR techniques on the basis of solving the problem of diagnostics of the structure of cellulose specimens. Although cellulose has a long history of use in human activities, its role in various/new applications has increased markedly in recent decades, since cellulose is a topical renewable material that can be supplied in huge quantities. The time-domain NMR method may become very attractive to measure such structural parameters, such as crystallinity degree, domain sizes, and sorption properties of different materials. The authors demonstrate their own results of cellulose study, at the same time, trying to contribute to the promotion of time-domain NMR applicability to biopolymers.

The article "Incorporation of boron into the AlPO-11 framework according to ^{11}B and ^{27}Al solid-state NMR spectroscopy and first-principles calculations" by Ilya V. Yakovlev with co-authors is devoted to the investigation of aluminophosphates (AlPO-n), which are a class of zeolite-like porous compounds built from strictly alternating AlO_4 and PO_4 tetrahedra. These substances demonstrate promising properties as catalysts and catalyst supports. Their acid–base properties can be varied by substitution of different Al and P sites with different heteroatoms among which boron is of great interest. The authors use the NMR crystallography method, which comprises a combination of NMR spectroscopy and quantum chemical calculations, supplemented by powder X-ray diffraction. In our opinion, the authors' approaches and results deserve further discussion.

Electrolyte solutions are a key component of energy storage devices, including Li-ion batteries (LIBs). Pure water was not considered as a good solvent due to narrow electrochemical window; however, during last decade, the "water-in-salt" (WIS) systems were proposed as new electrolytes for water-based LIBs. Nowadays,

WIS aqueous electrolyte investigations are in a strong progress. In particular, LiOAc–KOAc–H_2O triple systems were tested and it was shown that the mutual concentration of salts in the mixture had a significant effect on the character of ion mobility, and, consequently, on the electrical conductivity of such systems. The example of similar investigations is presented in the article "Molecular mobility in mixed "water-in-salt" solutions of LiOAc and KOAc according to NMR data" by Vladimir V. Matveev, Olga N. Pestova, Konstantin V. Tyutyukin, and Vladimir I. Chizhik.

The next several articles reflect the advances achieved by high-resolution NMR in the study of the structure of large organic molecules, including biomolecules.

Fan Liu, Bo Duan and Bin Xia presented the article "^{1} H, ^{13} C, and ^{15} N resonance assignments of the DNA-binding domain of Ler from Enteropathogenic *E. coli* in complex with DNA". LEE-encoded regulator (Ler) is encoded by a pathogenicity island (PAI) termed locus of enterocyte effacement (LEE), which is highly conserved among Pathogenic *E. coli*. The main results were achieved on the basis of the spectra: (1) 2D ^{1}H-^{15}N HSQC of 0.5 mM ^{15}N, ^{13}C-labeled Ler^{CTD} in complex with 5 mM unlabeled DNA d(CGCAAATTTGCG)2 in 50 mM sodium phosphate buffer (pH 5.7) with 100 mM NaCl and 0.2 mM EDTA (500 MHz Bruker Avance) and (2) finger print region of 2D F1, F2-^{15}N/^{13}C-filtered ^{1}H−^{1}H NOESY spectrum of 5 mM unlabeled DNA d(CGCAAATTTGCG)$_2$ in complex with 0.5 mM ^{15}N, ^{13}C-labeled Ler^{CTD} in 50 mM phosphate buffer (pH 5.7) with 100 mM NaCl and 0.2 mM EDTA (800 MHz Bruker Avance). The assignments for described protein–DNA complex are novel and they formed a good basis for further DNA binding mechanism studies of Ler.

Such compounds as hypercoordinated (or hypervalent) molecules, the central atoms of which are the elements of group 14 of the Mendeleev table (Si, Ge, Sn) have always attracted great attention of research chemists. These elements are in the same group as carbon, but their properties are significantly different. Despite the fact that there are many works devoted to the dynamic rigidity of systems with a hypervalent germanium atom, the relevance of the research remains very high. This is especially true for germatrans with a 6-coordinated germanium atom, which has not been studied in the area of stereochemical rigidity. The set of NMR methods (*J*-COSY, COSY, NOESY, HMQC and HMBC) was used to identify the signals of 20 protons and 11 carbons in the ^{1}H and ^{13}C spectra of a previously unknown and recently synthesized compound in the work "Homo- and heteronuclear NMR methods for signal assignments in ^{1}H and ^{13}C spectra of 1-aminoacyloxygermatran" by Denis V. Lezov, Tatiana. A. Kochina, Ruslan I. Baichurin, and Stanislav I. Selivanov. On the basis of their data, along with finding out the spatial structure of the molecule the authors proved the existence of the slow (in the NMR time scale) dynamic process associated with rearrangements within the atranium cycle.

The article "Diastereomers of cyclopropa[a]pyrrolizine spiro-fused with a benzo[4,5]imidazo[1,2-a]indole fragment: structure determinations using NMR methods" by Yulia Pronina and co-authors presents the results of a conformational analysis of newly synthesized compounds with potential cytotoxic activity. The authors studied the structure and dynamic properties of the diastereomers by NMR spectroscopy and molecular mechanics. As a result of the analysis of the NMR data

(chemical shifts, spin–spin coupling constants, and NOEs), an equilibrium scheme between several conformers of the studied compounds has been proposed. The symbiosis of accurate analysis and correct interpretation of NMR spectroscopy data implemented in this work is of methodological importance.

In some substances, there are electrons with an uncompensated angular momentum and, consequently, with an electronic magnetic moment. Such a molecular system or its fragment is usually called a paramagnetic (spin) center. The structure of substances containing spin centers is promising to study using electron spin resonance (ESR). A very voluminous study in this area is presented in the article "Investigation by ESR Spectroscopy of Biology Active Electron-Rich 1,10-Phenanthrocyanines of d-Elements (Soft Colloidal Glasses)" by Viktor Demidov, Stanislav Sukharzhevsky, Tatiana Pakhomova, Alexandra Ivanova, Sofia Paston, and Evgenia Bogomolova. The novel coordination compounds (synthesized and explored), with their unique structural characteristics, reveal potential applications in areas, such as tumor cell inhibition and DNA complexing agents.

One other type of magnetic resonance is presented in the article "Two magnon scattering contribution to the ferromagnetic resonance linewidth of Pt(Ir)/CoFeTaB/Ir(Pt) thin films" by M. Tokaç, S. Kazan, B. Özkal, N. Al-Jawfi, B. Rameev, B. Nicholson, A. T. Hindmarch. The work provides a quantitative analysis of magnetic resonance data in terms of intrinsic homogeneous and inhomogeneous contributions to the FMR linewidth for model samples of as-deposited and annealed Pt/CoFeTaB/Ir and Ir/CoFeTaB/Pt trilayer structures. The authors demonstrate that careful analysis of the angular and temperature dependences of the resonance field and linewidth of FMR enables one to draw conclusions about the differences in microstructure in these objects. The mother compound CoFeB is one of the widely used materials in various areas of the recent technology. The work contains a careful experimental study, combined with theoretical analysis, and has potential for contribution to the physics of spintronic phenomena.

We hope that the publications presented in this issue will attract the attention of scientific community to the prospects of new MR applications and will stimulate further progress in this area. We would like to bring our gratitude to all authors who have contributed to this special issue.

Data availability Not applicable.