Laboratory of Nuclear Magnetic Resonance Spectroscopy

HEAD:

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GROUP MEMBERS:

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RESEARCH PROFILE:

Experimental and theoretical magnetic resonance studies of fundamental interactions between the electromagnetic field and nuclear magnetic moments are aimed at the determination of the interaction parameters with ultra-high precision and the search for new and not observed yet effects.

CURRENT RESEARCH ACTIVITIES:

Experimental studies of nuclear magnetic resonance in the gas and liquid phase combined with quantum chemical computations focus on the determination of nuclear magnetic shielding, nuclear magnetic dipole moments, and indirect spin-spin coupling in small and medium-size molecules including water, molecular hydrogen, and components of the Earth's atmosphere. The goals of these studies are to examine (i) nuclear magnetic parameters of the isolated molecule and (ii) the influence of intermolecular interactions, isotopic substitution and the application of external fields on these parameters. For instance, it is anticipated that the application of the electric field induces several new magnetic resonance effects that permit to determine directly the absolute configuration of the molecule. In order to find these new effects, we study spin dynamics using quantum information processing methods and design, model, and fabricate dedicated resonance circuits.

SELECTED PUBLICATIONS:

1. W. Makulski, M. Wilczek, K. Jackowski, ^{17}O and ^{1}H NMR spectral parameters in isolated water molecules, Phys. Chem. Chem. Phys. 20 (2018) 22468-22476.

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2. P. Garbacz, W. Makulski, W-183 nuclear dipole moment determined by gas-phase NMR spectroscopy, Chem. Phys. 498 (2017) 7-11.
3. P. Garbacz, A.D. Buckingham, Chirality-sensitive nuclear magnetic resonance effects induced by indirect spin-spin coupling, J. Chem. Phys. 145 (2016) 204201.
4. B. Adrjan, W. Makulski, K. Jackowski, T.B. Demissie, K. Ruud, A. Antušek, M. Jaszuński, NMR absolute shielding scale and nuclear magnetic moment of ^{207}Pb, Phys. Chem. Chem. Phys. 18 (2016) 16483-16490.
5. P. Garbacz, Nuclear relaxation in an electric field enables the determination of isotropic magnetic shielding, J. Chem. Phys. 145 (2016) 064202-1 – 064202-10.
6. P. Garbacz, J. Cukras, M. Jaszuński, A theoretical study of potentially observable chirality-sensitive NMR effects in molecules, Phys. Chem. Chem. Phys. 17 (2015) 22642.
7. P. Garbacz, K. Jackowski, NMR shielding of helium-3 in the micropores of zeolites, Micropor. Mesopor. Mat. 205 (2015) 52-55.
8. W. Makulski, ^{83}Kr nuclear magnetic moment in terms of that of ^{3}He, Magn. Reson. Chem. 52 (2014) 430-434.
9. M. Jaszuński, A. Antušek, P. Garbacz, K. Jackowski, W. Makulski, The determination of accurate nuclear magnetic dipole moments and direct measurements of NMR shielding constants, Prog. Nucl. Magn. Reson. Spect. 67 (2012) 49-63.
10. P. Garbacz, K. Jackowski, W. Makulski, R.E. Wasylishen, Nuclear magnetic shielding for hydrogen in selected isolated molecules, J. Phys. Chem. A. 116 (2012) 11896-11904.