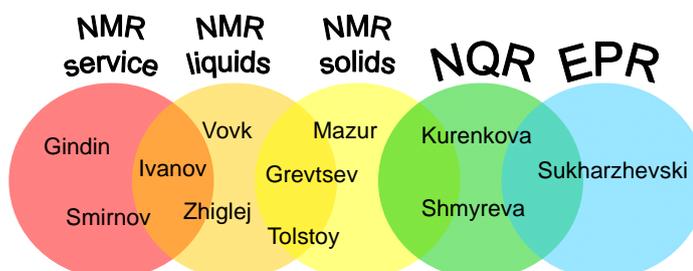




# research resources center for Magnetic Resonance St.Petersburg State University

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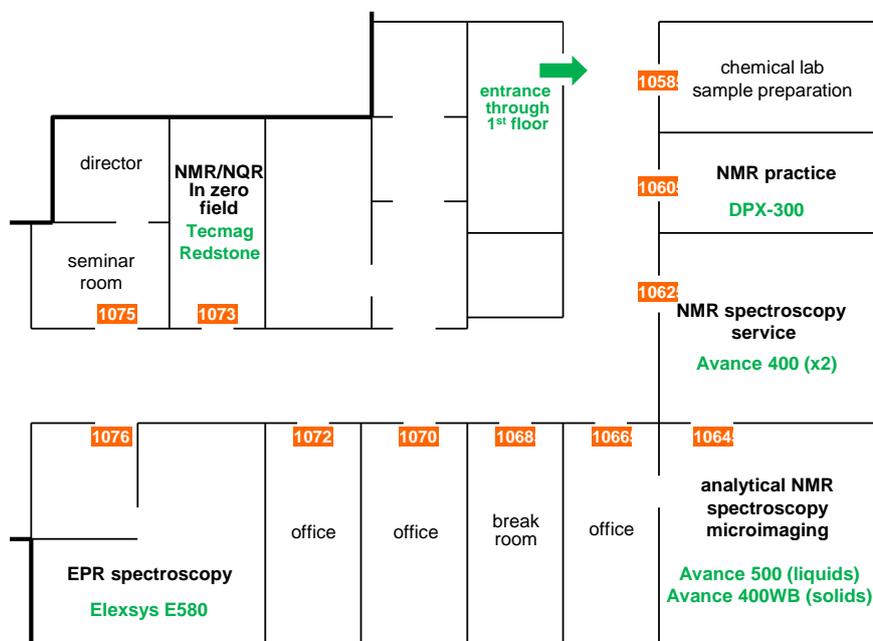
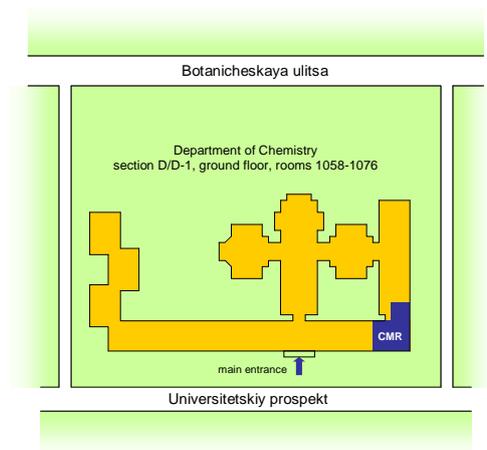
	<p><b>Peter Tolstoy</b>, director, associate professor at Physical Organic Chemistry department NMR spectroscopy of liquids, solutions and solids Research interests: cryospectroscopy, combined NMR/UV spectroscopy, optical spectroscopy, hydrogen bonding, intermolecular interactions, non-covalent interactions e-mail: <a href="mailto:peter.tolstoy@spbu.ru">peter.tolstoy@spbu.ru</a> Phone (cell): +7 (921) 430-81-91 Phone (room 1075): +7 (812) 363-68-99</p>
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	<p><b>Anna Shmyreva</b>, specialist  NMR spectroscopy of magnetically ordered systems, NQR spectroscopy  Research interests: NMR of magnetic ordered systems, spin echo method, nanostructured materials, NQR spectroscopy  e-mail: anna.shmyreva@spbu.ru  Phone (room 1073): +7 (812) 428-95-64  Phone (room 1072): +7 (812) 324-12-70, extension 5917</p>
	<p><b>Stanislav Sukharzhevskii</b>, specialist  EPR spectroscopy  spectrometers: Bruker Elexsys E580  Research interests: EPR theory, application of magnetic resonance in natural sciences, use of spectroscopic methods in geology and ecology  e-mail: stanislav.sukharzhevskii@spbu.ru  Phone (cell): +7 (921) 422-09-08  Phone (room 1076): +7 (812) 428-95-65</p>

**Location:**

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 198504 St.Petersburg, Russia



**Phones**

Room nr.	Room purpose	Phone nr.	Local phone nr.
1058	Chemical lab		
1060	NMR Service	428-43-25	4325
1062	NMR Service	428-95-63	9563
1064	Analytical NMR spectroscopy		
1066	Office	363-69-25	5915 (IP phones only)
1068	Break room		5662 (IP phones only)
1070	Office		5916 (IP phones only)
1072	Office		5917 (IP phones only)
1073	NQR and zero-field NMR spectroscopy	428-95-64	9564
1075	Director	363-68-99	5661 (IP phones only)
1076	EPR spectroscopy	428-95-65	9565

## Equipment

The Center for Magnetic Resonance provides access to the instrumentation, expertise, and infrastructure to carry out and support fundamental, applied and innovative research projects utilizing NMR, NQR and EPR spectroscopy as well as magnetic resonance microimaging. On commercial basis, all services of the Center could be provided to external users, such as medical, pharmacological and forensic organisations, as well as museums, technological and research centers, industry etc.



Bruker 300 MHz DPX and two Bruker 400 MHz Avance NMR spectrometers are dedicated to service routine measurements of 1D and 2D NMR spectra of liquids and solutions.

*Selected features:*

- Direct and inverse detection probes.
- Observed nuclei range from  $^1\text{H}$  to  $^{109}\text{Ag}$ .
- Possible  $^1\text{H}\{^{19}\text{F}\}$  and  $^{19}\text{F}\{^1\text{H}\}$  measurements.
- Possible  $^2\text{H}$  measurements with  $^{19}\text{F}$  lock.
- Temperature range from 120 to 390 K.



Bruker 500 MHz Avance NMR spectrometer is suited for measurements of 1D, 2D and 3D NMR spectra of liquids and solutions.

*Selected features:*

- Long measurements at low temperature (down to 110 K).
- Three-channel architecture (from  $^1\text{H}$  to  $^{109}\text{Ag}$ ).
- Diffusion measurements at temperatures up to 470 K.

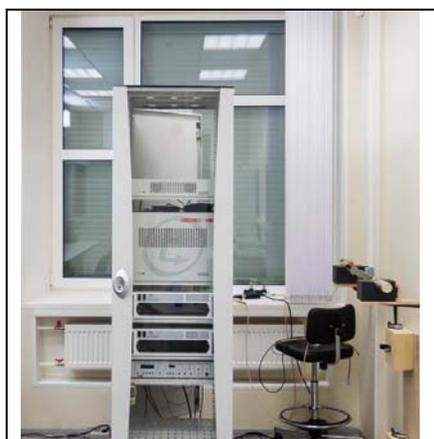


Bruker 400 MHz WB Avance NMR spectrometer is dedicated to the studies of samples in solid state: crystallines, powders, weakly ordered materials, gels, liquid crystals, amorphous compounds, nanostructures (zeolites, silicates) etc. The spectrometer allows one to study diffusion processes and obtain micro-tomographic image

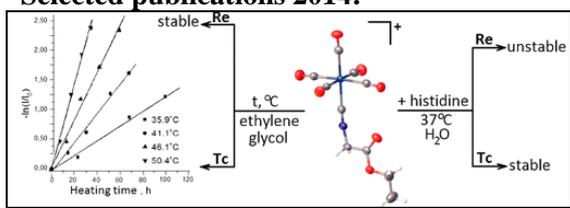
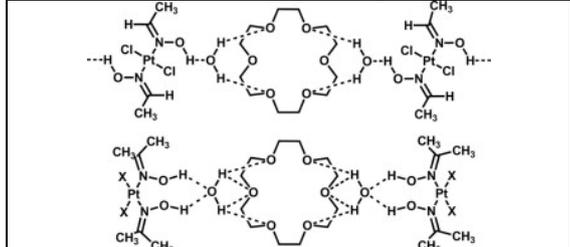
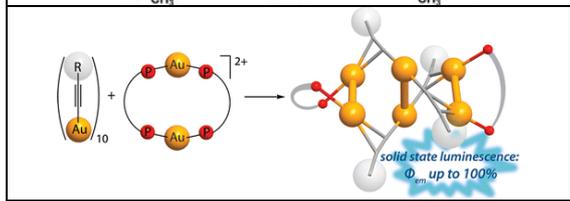
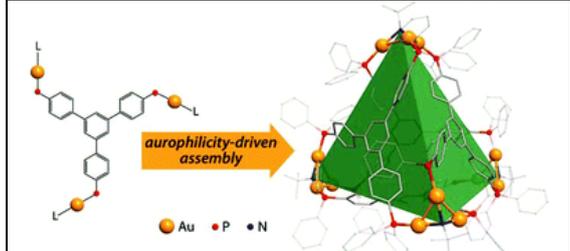
*Selected features:*

- Long measurements at temperatures from 130 K to 870 K.
- Microtomography of objects up to 30 mm in linear size.
- Magic angle spinning up to 30 kHz.
- Diffusion measurements (gradients up to 3000 G/cm).

	<p>EPR spectrometer Bruker Elexsys E580 (<math>\lambda = 3.2</math> cm, X-band) for studies of paramagnetic centers in solids, liquids, solutions, including aqueous solutions, and gases. Spectrometer is capable of measurements in CW-mode as well as in FT-mode.</p> <p><i>Selected features:</i></p> <ul style="list-style-type: none"> <li>• UV-irradiation of the samples (100 W, 200-2000 nm).</li> <li>• Temperature range from 3.7 K to 500 K.</li> <li>• ENDOR/TRIPLE measurements.</li> <li>• Planned: micro-tomographic measurements.</li> <li>• Planned: working in L-band (32 cm) and W-band (10 mm).</li> </ul>
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	<p>Tecmag Redstone NMR/NQR 1-500 MHz spectrometer allows one to obtain spectral and relaxation NMR and NQR parameters for solids, polymers, metals, glass and magnetically ordered systems.</p> <p><i>Selected features:</i></p> <ul style="list-style-type: none"> <li>• Observed frequencies in a zero external magn. field 20-120 MHz.</li> <li>• Temperature range from 4 K to 500 K.</li> <li>• Acquisition of weak NQR signals by multiple scans</li> <li>• NQR spectra of <math>^7\text{Li}</math>, <math>^{27}\text{Al}</math>, <math>^{35}\text{Cl}</math>, <math>^{63,65}\text{Cu}</math>, <math>^{75}\text{As}</math>, <math>^{93}\text{Nb}</math>, <math>^{183}\text{Ta}</math> etc nuclei.</li> <li>• NMR of <math>^{11}\text{B}</math>, <math>^{57}\text{Fe}</math>, <math>^{59}\text{Co}</math>, <math>^{61}\text{Ni}</math> etc. nuclei.</li> <li>• Investigation of orientation dependence for monocrystals.</li> </ul>
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### Selected publications 2014:

	<p>A. Miroslavov, Y. Polotskii, V. Gurzhiy, A. Ivanov, A. Lumpov, M. Tyupina, G. Sidorenko, P. Tolstoy, D. Maltsev, D. Suglobov  «Technetium and Rhenium Pentacarbonyl Complexes with C2 and C11 <math>\omega</math>-Isocyanocarboxylic Acid Esters»  <i>Inorg. Chem.</i> <b>2014</b>, 53, 7861-7869  DOI: 10.1021/ic500327s</p>
	<p>E.Yu. Bulatov, T.G. Chulkova, I.A. Boyarskaya, V.V. Kondratiev, M. Haukka, V.Yu. Kukushkin  «Triple associates based on (oxime)Pt(II) species, 18-crown-6, and water: Synthesis, structural characterization, and DFT study»  <i>J. Molec. Struct.</i> <b>2014</b>, 1068, 176-181  DOI: 10.1016/j.molstruc.2014.04.010</p>
	<p>I.O. Koshevoy, Y.-C. Chang, Y.-A. Chen, A.J. Karttunen, E.V. Grachova, S.P. Tunik, J.Janis, T.A. Pakkanen, P.-T. Chou  «Luminescent Gold(I) Alkynyl Clusters Stabilized by Flexible Diphosphine Ligands»  <i>Organometallics</i>, <b>2014</b>, 33, 2363-2371  DOI: 10.1021/om5002952</p>
	<p>Julia R. Shakirova, Elena V. Grachova, Antti J. Karttunen, Vladislav V. Gurzhiy, Sergey P. Tunik and Igor O. Koshevoy  «Metallophilicity-assisted assembly of phosphine-based cage molecules»  <i>Dalton Trans.</i>, <b>2014</b>, 43, 6236-6243  DOI: 10.1039/c3dt53645a</p>

## Cooperation partners:

### *In Russia*

International Tomographic Center, the Siberian Branch of the Russ. Acad. Sci., Novosibirsk  
A.N. Nesmeyanov Institute of Organoelement Compounds of Russ. Acad. Sci., Moscow  
Immanuel Kant Baltic Federal University, Kaliningrad  
Kazan Federal University, Kazan  
Southern Federal University, Rostov-on-Don

### *Around the world*

Institute of Biochemistry, Ernst-Moritz-Arndt University of Greifswald, Germany  
Institute of Chemistry and Pharmacology, University of Regensburg, Germany  
Institute of Chemistry and Biochemistry, Free University of Berlin, Germany  
Institute of Physics, Free University of Berlin, Germany  
Max-Born Institute of Non-Linear Optics and Short Pulse Spectroscopy, Berlin, Germany  
Department of Physics, University of Parma, Italy  
Department of Chemistry, Royal Institute of Technology, Sweden  
Martin-Luther University, Halle-Wittenberg, Germany  
Leibniz Institute of Molecular Pharmacology, Berlin, Germany  
Institute of Inorganic Chemistry, University of Zurich, Switzerland  
CIC energigune Research Center, Vitoria, Spain  
Exact Sciences and Engineering Center, University of Guadalajara, Mexico  
Department of Chemistry, University of Wroclaw, Poland  
Institute of Physical Chemistry, Polish Acad. Sci., Warsaw, Poland  
Institute for Single Crystals, Kharkiv, Ukraine