2005-2006 Annual Report

National Ultrahigh-Field NMR Facility for Solids

June 2006



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National Ultrahigh-Field NMR Facility for Solids

Centre national de RMN à ultrahaut champ pour les solides

For further information or additional copies of this report, please contact

Victor Terskikh

National Ultrahigh-Field NMR Facility for Solids

1200 Montreal Road, M-40 Ottawa, Ontario K1A 0R6

(613) 998-5552

Or visit our Website at: http://www.nmr900.ca

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National Ultrahigh-Field NMR Facility for Solids 2005-2006 Annual Report June 2006



The National Ultrahigh-Field NMR Facility for Solids has been established through a partnership between the University of Ottawa, National Research Council Canada, Canadian academic institutions, federal and provincial funding agencies, and the private sector. This facility is seen as the most cost-effective way to provide Canadian researchers with access to a worldleading NMR facility for advancing the science of materials and the innovative development of

technologically advanced products. Funding for the establishment of the facility has been arranged through CFI, provincial agencies (Ontario Innovation Trust, Recherche Québec), industry and NRC, with NRC providing a site for the facility in the newly renovated W.G. Schneider building, including office and laboratory space, test equipment and some ongoing support. The building is leased to the University of Ottawa, who manages the NMR facility. The equipment consists of a 900 MHz Nuclear Magnetic Resonance spectrometer with magnet, console, probes and ancillary equipment to acquire ultra high field static and fast spinning NMR spectra of solid materials. The uniqueness of the Facility is that it is dedicated to solid-state NMR research, where the highest magnetic fields are beneficial for quadrupolar and low-gamma nuclei such as oxygen-17, magnesium-25, and chlorine-35 among others. This type of instrument is not available elsewhere in Canada.

Objectives

- to provide Canadian researchers and their academic and industrial collaborators access to a world-leading 900 MHz NMR facility for solids and materials
- to ensure a stimulating research environment and expert assistance and training
- to contribute to the design and development of advanced equipment, including NMR probes, for solid-state NMR research at ultrahigh magnetic fields
- to enhance opportunities for collaborative and multidisciplinary research on national and international levels

Solid-State NMR Applications

Solid-state NMR spectroscopy has a wide and lasting impact especially on the development of novel materials: catalysts, battery materials, gas storage materials (fuel cells) and glasses. All have immediate applications in energy conservation and the reduction of greenhouse gas emissions. In the materials area, developments in nanotechnology also benefit tremendously from having access to a larger NMR periodic table than is now routinely available, and the capability to work with small samples. Another area that benefits greatly is the combinatorial approach to materials synthesis where the gain in sensitivity (small sample size) and application of ultra-fast spinning will lead to the rapid evaluation of new concepts and products. A high-field NMR facility thus allows the greatly enhanced use of a very powerful and discerning probe of solid-state structure to a wide range of applications, including:



- active sites in catalysts

- framework connectivities in catalysts and glasses (structure)
- semiconductors, sensors, confined clusters for novel device applications
- interfaces in nanostructured materials and nanocomposites
- combinatorial chemistry
- biomolecules, membranes and semisolids via fast spinning
- polymers and polymer blends via fast spinning
- dynamics in polymers and biomolecules (small, multiplelabelled samples)
- applications in mineral and environmental chemistry

The new knowledge generated by solidstate NMR is finding many practical and **commercial applications**, for example in the petrochemical industry (catalysts, polymers), alternative energy (battery materials, fuel cells), materials fabrication (alloys), high tech materials (glasses, ceramics, nanostructured materials), electronics (novel devices), environmental applications (catalysts, sorbents, membranes, sensor materials) and pharmaceuticals.

¹³C CP/MAS at 21.1 T of solid tetracycline (common antibiotic)



The 900 Timeline

Winter, 1997	the letter of intent is circulated among Canadian solid-state NMR researchers
May, 2001	request for funding is submitted to CFI: total cost 11.7 M\$, ten principal applicants more than 30 secondary applicants the application is supported by NRC Canada (0.9 M\$)
November, 2003	CFI approves the award (4.4 M\$)
February, 2004	Ontario Innovation Trust (2.7 M\$) and Bruker BioSpin (2.8 M\$) join the consortium
April, 2004	Recherche Québec becomes a partner (0.9 M\$)
May, 2004	the 900 instrument is ordered from Bruker BioSpin
June 1, 2005	the 900 instrument is delivered, installation begins
August, 2005	the installation phase is complete, testing begins
September, 2005	the Facility is open for users
January, 2006	the first paper featuring results from the 900 instrument is published in the Journal of the American Chemical Society
June 1, 2006	Official opening of the Facility



Official Opening of the 900 MHz NMR Facility

The National Ultrahigh-Field NMR Facility for Solids was officially inaugurated on June 1, 2006 during a well-attended opening ceremony with more than 200 invited guests representing Universities from across the country, researchers from NRC and other government labs, participants of the XeMat-III International Symposium, and many dignitaries. Among the dignitaries present was Dr. William G. Schneider, renowned for his pioneering work in high-resolution NMR and for whom the M-40 building has been named. The Grand Opening was followed by the Inaugural Solid-State NMR workshop with presentations on recent developments in the field. Celebrations were fittingly concluded with a collegial reception sponsored by Bruker Canada in the landmark 100 Sussex NRC Building.

We would like to thank everyone involved in organizing the Official Opening for their hard work and dedication, and congratulate them on what by many accounts was a very successful and becoming event.

INAUGURAL SOLID-STATE NMR WORKSHOP

Joint Session with XeMat-III International Symposium

June 1, 2006, Auditorium NRC, 100 Sussex Drive, Ottawa, ON

Sponsored by the University of Ottawa

Hosted by National Research Council Canada (NRC)

- Session 1 Chair: J. Zwanziger (Dalhousie University)14:15-14:30Introduction: R. Wasylishen (University of Alberta), C. Detellier (University of Ottawa)
- **14:30-15:15** A. Pines (University of California, Berkeley) Developments in microtesla, ex situ and remote NMR and MRI
- **15:15-15:50** P. Ellis (PNNL, WA) Low Temperature ²⁵Mg Solid-State NMR Spectroscopy of the DNA Repair Protein APE1
- 15:50-16:10 Coffee Break

Session 2 Chair: D. Bryce (University of Ottawa)

- **16:10-16:45** J.-P. Amoureux (Université des Sciences et Technologies de Lille) New solidstate NMR methods for quadrupolar nuclei
- **16:45-17:20** M. Smith (University of Warwick) Applications of High Field Solid State NMR Techniques from Water Distribution in Minerals to Hydrogen-Bonding in Biomolecules
- 17:20-17:35 Closing remarks: M. Auger (Université Laval), J. Ripmeester (SIMS NRC)
- **17:40-19:00 Reception** in the Library sponsored by Bruker BioSpin Ltd.

A Magnet for the Nation

NRC, uOttawa home to Canada's most powerful magnet

News Release

June 1, 2006, Ottawa, ON — Today, the Government of Canada in partnership with the University of Ottawa and the provinces of Quebec and Ontario officially opened the \$15M NRC W.G. Schneider Building. Named after nuclear magnetic resonance (NMR) pioneer and former NRC President, Dr. Schneider, this unique building accommodates two NMR facilities – home to a critical mass of 5 spectrometers.

The main attraction for Canadian scientists and industry is the multimillion dollar 900 MHz (21.1 Tesla) spectrometer, Canada's most powerful magnet. It will provide scientists with a new tool in their efforts to develop new battery composites, nano-materials for electronics, plastic polymers for vehicles, glasses for more sensitive sensors and faster computer processors, new materials for hydrogen storage, as well as health enhancing antibiotics.

"This new facility is a prime example of what can be achieved through collaboration." said NRC President Dr. Pierre Coulombe. "NRC believes that strategic partnerships like this one are key to building Canada's knowledge based economy."

Since 1959, magnetic resonance has evolved and led to the development of medical imaging and diagnosing equipment – Magnetic Resonance Imaging commonly known as the MRI. The partners recognize the importance of researching quantum physics and chemistry through spectroscopic measures in order to build upon the strengths of innovative materials. This characterization of new materials and elements will improve our understanding and creation of aeronautical composites for the aerospace industry as well as more selective antimicrobial therapies for more economical air travel and healthier lives.

"The National Ultra-high Field NMR Facility for Solids is the first of its kind in the world and will promote international interest and collaboration, increasing Canada's scientific prestige on the global stage," says University of Ottawa President Gilles Patry. "Our institution is committed to promoting the exciting interdisciplinary work of our researchers through partnerships like this one and we look forward to the benefits this facility will offer the uOttawa community."

This uniquely nationwide networked centre was made possible thanks to the support of its public and private partners including Canada Foundation for Innovation (CFI) funding, a codevelopment agreement with Bruker Biospin and the collaborative staffing expertise and management from the University of Ottawa and NRC.



Left to right:

Danial Wayner (Director General, NRC Steacie Institute for Molecular Sciences)

Eliot Phillipson (President and CEO, Canada Foundation for Innovation)

Henry Stronks (President, Bruker Biospin Canada)

William Schneider (Former NRC President)

Pierre Coulombe (President, NRC)

Gilles Patry (President and Vice-Chancellor, University of Ottawa)

Royal Galipeau (Member of Parliament, Ottawa-Orléans).

Photo by: Harry Turner, NRC

Our partners

Creation of the Facility was made possible by contributions from

Canada Foundation for Innovation (CFI) Ontario Innovation Trust (OIT) Recherche Québec (RQ) National Research Council Canada (NRC) Bruker BioSpin Ltd.

Ongoing operations of the Facility are funded by

Canada Foundation for Innovation (CFI) Natural Sciences and Engineering Research Council of Canada (NSERC) National Research Council Canada (NRC)

Facility is managed by

University of Ottawa

Technical support with the installation was provided by

Praxair Canada Inc. Agilent Technologies Canada Inc.

About the University of Ottawa:

The University of Ottawa is one of Canada's principal comprehensive, research-intensive, postsecondary institutions. Its campus community totals more than 35,000 full-time students, faculty and staff living, working and studying in both of Canada's official languages in a thoroughly cosmopolitan milieu. We are proud to call ourselves "Canada's university."

Media inquiries: Sophie Nadeau, Media Relations Officer, (613) 562-5800 ext 3137

About NRC:

Recognized globally for research and innovation, Canada's National Research Council (NRC) is a leader in the development of an innovative, knowledge-based economy for Canada through science and technology.

Media inquiries: Hélène Létourneau, Communications Officer, (613) 991-5419

About CFI:

The Canada Foundation for Innovation (CFI) is an independent corporation created by the Government of Canada to fund research infrastructure. The CFI's mandate is to strengthen the capacity of Canadian universities, colleges, research hospitals, and non-profit research institutions to carry out world-class research and technology development that benefits Canadians.

About Bruker BioSpin:

Bruker BioSpin, a division of Bruker, is dedicated to designing, manufacturing and distributing life science tools based on magnetic resonance. Bruker, a world leader in the manufacture and development of scientific instrumentation was incorporated in Canada in October, 1970. The company grew dramatically in the late 1970's and early 1980's and now employs over 25 people in Canada including scientists, service engineers and administrative support teams who work closely with colleagues in the U.S., Germany and Switzerland.

Management of the Facility

The management structure of the Facility consists of an International Advisory Board, a Steering Committee, and a Manager.

The International Advisory Board consists of three members, recognized experts of the international NMR community. The members are appointed jointly by the President of NRC and the Vice-Rector, Research, of the University of Ottawa. The term of membership is 3 years. The Advisory Board meets once a year. It reviews the annual report of the operations of the Facility, and provides comments, suggestions and recommendations on the efficiency of the operations, on the basis of the evaluation of the report. The mandate consists also of informing the Steering Committee of new opportunities for synergy among the users, and with external partners in different sectors. The Board appoints users to serve as members of the Steering Committee.

The Steering Committee is responsible for the operational planning. As a general responsibility, the Steering Committee maintains the state-of-the-art nature of the Facility, and takes actions to implement the necessary improvements. Its mandate consists also of establishing the criteria for access to the facility and for priority of scheduling, in managing the budget of minor upgrades, and in improving the general operations of the Facility. The Steering Committee reviews regularly the structure of user fees, oversees the budget of the Facility, and submits the Annual Report of the Facility to the Advisory Board.

The Manager is responsible for the day-to-day operations. The Manager is the liaison between the users, the technical staff and the Steering Committee. He is also the liaison with the NRC staff providing technical assistance. He prepares an Annual Report of the Facility for review by the Steering Committee before review by the Board.

International Advisory Board

J.-P. Amoureux (France) P. Ellis (U.S.A.) M. Smith (U.K.)

Steering Committee

M. Auger (Université Laval) C. Detellier (University of Ottawa) Y. Huang (University of Western Ontario) J. Ripmeester (SIMS NRC) R. Wasylishen (University of Alberta)

Operations

V. Terskikh (manager, University of Ottawa) S. Pawsey (NMR technician, University of Ottawa)

Research Facilities

NMR Instrument

The 900 MHz (21 T) Bruker AVANCE II NMR spectrometer

Magnet:	21.1 T, Ultrastabilized
	Bore size: 54 mm (SB, standard bore)
	¹ H frequency: 900.21 MHz
	Field drift: < 6 Hz/hr (1 H); < 0.5 Hz/hr with field drift compensation
	Magnet: 3.85 m x 1.88 m, ~7000 kg
	Coil temperature: 2 K
	Current: 250 A
	Liquid He volume: 700 L
	Liquid N ₂ volume: 440 L
	BMPC Bruker Magnet Pump Control Unit
	UPS (x2) + backup power generator (x2)
Console:	4-channel digital AQS/2 Bruker AVANCE II
	MAS control unit: MAS II Bruker Digital
	Temperature controller: BVT 3000 Bruker Digital
	Digital lock control unit

Gradient: GREAT 1/10 Z-gradient

- Amplifiers: BLAX1000, 6-405 MHz, 1 kW linear amplifier BLAX1000, 6-405 MHz, 1 kW linear amplifier BLAH1000, ¹H/¹⁹F, 1 kW linear amplifier BLAH300, ¹H/¹⁹F, 300 W linear amplifier
- HPPR/2 preamplifier:
 ¹H low-power

 broadband low-power

 ²H

 ¹H/¹⁹F high-power

 X broadband high-power

 Y broadband high-power

Research Facilities

Solid-state NMR probes

For magic angle spinning (MAS)

- Bruker, 2.5 mm, 35 kHz MAS, (¹H-¹⁹F) / (¹³C-³¹P), VT extended frequency range 76 372 MHz
- Bruker, 3.2 mm, 22 kHz MAS, ¹H / (¹⁵N-¹³C), VT, ²H lock extended frequency range 69 – 246 MHz
- Bruker, 4 mm, 14 kHz MAS, ¹H / (¹⁵N-¹³C), VT extended frequency range 40 321 MHz
- collaboration with Bruker BioSpin, 7 mm, low-gamma frequency range 15 – 94 MHz

Static wide-line probes, collaboration with SIMS NRC (J. Bennett)

- Static #1, single channel, 35-170 MHz
- Static #2, single channel, 40-150 MHz, variable temperature
- Static #3, double channel, ¹H/X (under construction)



³⁵Cl static NMR spectra of Glycine-HCl recorded at 88.2 MHz using the Static probe #1 : Hahn-echo (top) and QCPMG (bottom)

Research Facilities

Solid-state NMR instruments available at Partners' Institutions

The University of Ottawa

http://www.science.uottawa.ca/nmr/

Located at:

Department of Chemistry, University of Ottawa, 130 Louis Pasteur, Ottawa, Ontario, K1N 6N5, CANADA

Instruments: Bruker AVANCE 500 Wide Bore

Bruker ASX 200 Wide Bore

Steacie Institute for Molecular Sciences, National Research Council Canada

http://nmr-rmn.nrc-cnrc.gc.ca/

Located at:

1200 Montreal road, M-40, Ottawa, Ontario, K1A 0R6, CANADA

Instruments:

Bruker AVANCE 200 Wide Bore Bruker AVANCE 400 Wide Bore TecMag Discovery 500 Standard Bore

Located at:

100 Sussex Drive, Ottawa, Ontario, K1A 0R6, CANADA Instruments: Bruker AMX 300 Wide Bore TecMag Apollo 200 Wide Bore



Support Facilities at the W.G. Schneider Building (M-40)

- 1. Liquid nitrogen storage
- 2. Liquid nitrogen filling facility
- 3. Preparation laboratory
- 4. Electronic shop
- 5. Steacie Institute for Molecular Sciences NRC
 - 5a. TecMag 500 (11.7 T)
 - 5b. Bruker 400 (9.4 T)
 - 5c. Bruker 200 (4.7 T)
- 6. Cut open magnet display (4.7 T)
- 7. Institute for Biological Sciences NRC
 - 7a. Varian 600 (14.1 T)
 - 7b. MRI instrument (2 T)
- 8. National Ultrahigh-field NMR Facility Bruker 900 (21.1 T)
- 9. Magnet equipment room
- 10. Conference room and offices for visiting users

Support Facilities

Preparation laboratory (3)





Electronic shop (4)





Agilent RF Test and Measurement Equipment

Oscilloscope DSO6102A 1 GHz Spectrum Analyzer E4411B 9 kHz-1.5 GHz Network Analyzer E5061A 300 kHz-1.5 GHz Signal Generator E4428C 250 kHz-3.0 GHz Pulse Generator 8114A 100V 2A

Research Projects

From the beginning of operations in September 2005

- 15 research projects have been supported
- 18 scientists used the 900 instrument
- 8 PDF trainees and graduate students

Solid-State ^{35,37}Cl NMR Spectroscopy of Hydrochloride Salts of Amino Acids Implicated in Chloride Anion Selectivity in Ion Transport Channels

D. Bryce University of Ottawa, Ottawa, Ontario

Solid-State ¹⁷O as a New Probe to Study Biological Structures

G. Wu Queen's University, Kingston, Ontario

Solid-State NMR of Low-Gamma Nuclei in Inclusion Compounds

I. Moudrakovski Steacie Institute for Molecular Sciences, National Research Council Canada, Ottawa, Ontario

Medium-Range Order in Borate Glasses and Structural Characterization of Paramagnetic Metal Cyanides

P. Aquiar, S. Kroeker, P. Sidhu

University of Manitoba, Winnipeg, Manitoba

Solid-State NMR Characterization of Quadrupolar Nuclei in Metallocenes, Phthalocyanines and Mesoporous Solids

A. Lo, A. Rossini, R. Schurko University of Windsor, Windsor, Ontario

Solid-State ⁸⁷Rb, ⁸¹Br and ¹²⁷I NMR Studies of Chemical Shifts and Quadrupolar Interactions in Alkali Halide Solid Solutions

C. Ratcliffe Steacie Institute for Molecular Sciences, National Research Council Canada, Ottawa, Ontario

Membrane Interactions of Antiatherogenic Peptides

A. Bain, B. Berno, R. Epand McMaster University, Hamilton, Ontario

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Study of the Secondary Structure of Proteins in Recombinant and Natural Spider Silk Fibers by Natural Abundance Solid-State ¹³C NMR Spectroscopy

P. Audet, I. Cloutier, M. Auger Université Laval, Québec

Multinuclear Solid-State NMR Study of Metallacarboranes at Ultrahigh Magnetic Field Strengths

S. Borsacchi, K. Ooms, R. Wasylishen University of Alberta, Edmonton, Alberta

Ultrahigh-Field High-Resolution Solid-State ¹H MAS NMR of Supramolecular Materials

D. Brouwer Steacie Institute for Molecular Sciences, National Research Council Canada, Ottawa, Ontario

Solid-State ⁸⁷Rb NMR as a Surrogate Probe for Studying K⁺ Binding to Biological Structures

R. Ida, G. Wu *Queen's University, Kingston, Ontario*

Probing the Evolution of the Niobium Environment in Hydrothermal Synthesis from Nb_2O_5 Grains to Microporous $Na_2Nb_2O_6$ Fibers and $NaNbO_3$ Cubes by ⁹³Nb Solid-State NMR

Y. Huang, C. Kirby, J. Zhu University of Western Ontario, London, Ontario

Cation-Pi Interactions Studied by Solid-State NMR Spectroscopy

D. Bryce University of Ottawa, Ottawa, Ontario

Polymorph Identification and Characterization

J. Ripmeester Steacie Institute for Molecular Sciences, National Research Council Canada, Ottawa, Ontario

Characterization of Nanohybrid Materials from Sepiolite Minerals by ²⁵Mg NMR

C. Detellier, G. Facey University of Ottawa, Ottawa, Ontario

Publications

D.L. Bryce, G.D. Sward, and S. Adiga

Solid-State ^{35/37}Cl NMR Spectroscopy of Hydrochloride Salts of Amino Acids Implicated in Chloride Ion Transport Channel Selectivity: Opportunities at 900 MHz Journal of the American Chemical Society 128 (2006) 2121-2134

K.J. Ooms, K.W. Feindel, V.V. Terskikh, and R.E. Wasylishen

Ultrahigh-Field NMR Spectroscopy of Quadrupolar Transition Metals: ⁵⁵Mn NMR of Several Solid Manganese Carbonyls *Inorganic Chemistry 45 (2006) 8492-8499 (cover article)*

V.K. Michaelis, P.M. Aguiar, and S. Kroeker

Probing Alkali Coordination Environments in Alkali Borate Glasses by Multinuclear Magnetic Resonance Journal of Non-Crystalline Solids (2006) submitted

P.M. Aguiar and S. Kroeker

Boron Speciation and Non-Bridging Oxygens in High-Alkali Borate Glasses Journal of Non-Crystalline Solids (2006) submitted

Lectures and Conference Contributions

D.L. Bryce, G.D. Sward, and S. Adiga

Solid-state ^{35/37}Cl NMR Spectroscopy of Hydrochloride Salts of Amino Acids Implicated in Chloride Ion Transport Channel Selectivity: New Opportunities at 900 MHz Invited speaker, Institut de Biologie Structurale, CNRS, Grenoble, France (2006)

R.E. Wasylishen

Research Opportunities Using the National Ultrahigh-Field NMR Facility for Solids Invited presentation, Official Opening of the National Ultrahigh-Field NMR Facility for Solids, Ottawa, Ontario, June 1, 2006

J.A. Ripmeester

Solid-State NMR in Materials at Ultrahigh Magnetic Fields Invited presentation, Official Opening of the National Ultrahigh-Field NMR Facility for Solids, Ottawa, Ontario, June 1, 2006

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S. Kroeker

High Resolution NMR of Glasses Invited speaker, 18th Waterloo NMR Summer School: Reviews and Advances. May 31 – June 9, 2006. Waterloo ON, Canada

R.E. Wasylishen

NMR Investigations at High Magnetic Field Strengths – New Opportunities for Interrogating Quadrupolar Nuclei Invited speaker, 18th Waterloo NMR Summer School: Reviews and Advances. May 31 – June 9, 2006. Waterloo ON, Canada

R.E. Wasylishen

NMR of Non-Integer Quadrupolar Nuclei in Solids Invited speaker, 18th Waterloo NMR Summer School. May 31 – June 9, 2006. Waterloo ON, Canada

V.K. Michaelis, P.M. Aguiar, and S. Kroeker

Multinuclear Magnetic Resonance of Alkali Borate Glasses Contributed talk, 18th Waterloo NMR Summer School. May 31 – June 9, 2006. Waterloo, ON, Canada)

D.L. Bryce, G.D. Sward, and S. Adiga

Solid-state ^{35/37}Cl NMR Spectroscopy of Hydrochloride Salts of Amino Acids Implicated in Chloride Ion Transport Channel Selectivity: New Opportunities at 900 MHz *Oral presentation, 89th Canadian Chemistry Conference and Exhibition, Halifax, Nova Scotia, May 27- May 31, 2006*

C. Detellier

National Ultrahigh Field NMR Facility for Solids Invited presentation, Symposium on Large Scale Canadian Science Opportunities, 89th Canadian Chemistry Conference and Exhibition, Halifax, Nova Scotia, May 27- May 31, 2006

M. Auger, C. Detellier, J.A. Ripmeester, V. Terskikh, and R.E. Wasylishen

Research Opportunities Using the National Ultrahigh-Field NMR Facility for Solids Invited presentation, Symposium on Large Scale Canadian Science Opportunities, 89th Canadian Chemistry Conference and Exhibition, Halifax, Nova Scotia, May 27- May 31, 2006

M. Auger, I. Cloutier, J. Leclerc, M. Pézolet

Étude de Protéines de Soie d'Araignée par Spectroscopie RMN en Solution et des Solides Oral presentation, 74e Congrès de l'Acfas, Université McGill, Montréal (Québec), May 19, 2006

J. Ripmeester

Applications of NMR Spectroscopy to the Study of Materials and Processes for Gas Adsorption Invited speaker, Department of Chemical and Biological Engineering, University of B.C., Vancouver, May 2, 2006

R.E. Wasylishen

Progress in Investigating Solid Materials Using NMR Spectroscopy Invited speaker, Arrhenius Laboratory, Stockholm University, Stockholm, Sweden, April 4, 2006

J. Ripmeester

Characterizing Porous Materials with NMR Spectroscopy *Invited speaker,* Department of Chemistry, Penn State University, College Park, PA, March 3, 2006

R.W. Schurko

Observing the "Invisible" Nucleus: NMR of unreceptive nuclei in inorganic, organometallic and other solid materials Invited speaker, University of Victoria, January 30, 2006

J. Ripmeester

Characterizing Void Space and Confined Materials Invited speaker, Pacifichem 2005. December 15-20, 2005. Honolulu HI, USA

S. Kroeker and P.M. Aguiar

Experimental and Theoretical NMR Approaches to Characterizing Medium-Range Order in Borates *Contributed talk, Pacifichem 2005. December 15-20, 2005. Honolulu HI, USA*

C. Detellier

Interlamellar Grafting of Polyols in Kaolinite Invited speaker, 13th International Clay Conference, Tokyo (Japan); August 21-27, 2005

C. Detellier

National Ultrahigh-Field NMR Facility for Solids Invited presentation, Symposium on NMR Spectroscopy, 88th Canadian Chemistry Conference, Saskatoon, SK, May 28 – June 1, 2005

The Facility's Website : www.nmr900.ca



Home page

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Future Directions

Upgrades

NMR probes

- Double frequency wideline probe for a mid-frequency range (90 to 250 MHz) with exchangeable 5 mm solenoid inserts and with ¹H decoupling. With additional flat coils for ¹⁵N and ²H
- Low-gamma double frequency MAS probe, frequency range from 15 to 90 MHz with ¹H decoupling
- Triple resonance CP/MAS probehead, ¹H/¹³C/¹⁵N, for HR MAS
- Triple resonance CP/MAS probehead, ¹H/X/Y

Software upgrades

Remote access to the 900 NMR instrument

Solid-state NMR techniques implementation/development

- signal enhancement techniques for low-gamma quadrupolar nuclei
- heteronuclear correlation spectroscopy for half-integer quadrupolar nuclei
- resolution enhancement techniques for ¹H
- proton decoupling and cross-polarization in organic and *inorganic* solids at high spinning speeds
- solid-state NMR techniques in semi-solid organic matter (H/C/N probe)

Future Directions

National Solid-State NMR Network (proposal)



Main Objectives

to create and maintain a web-based information resource "Solid-state NMR in Canada" with information about Solid-State NMR facilities across Canada

- people
- projects
- available hardware

to facilitate transfer of knowledge and expertise between members at regularly organized workshops and symposia, and via quarterly bulletin "Solid-state NMR in Canada"

- news and announcements
- recent publications
- feature articles

to foster and stimulate co-operation and partnership among network members, including joint grant applications

to advance and promote Solid-State NMR among potential industrial users and the public



Left to right: Jamie Bennett (SIMS NRC), Igor Moudrakovski (SIMS NRC), John Ripmeester (member of the Steering Committee, SIMS NRC), Michèle Auger (member of the Steering Committee, Université Laval), Christian Detellier (member of the Steering Committee, University of Ottawa), Victor Terskikh (manager of the Facility, University of Ottawa), Roderick Wasylishen (member of the Steering Committee, University of Alberta)

Contact us

www.nmr900.ca

You may forward your questions and suggestions to any of the members of the Steering Committee or to

Victor Terskikh, Ph.D. C.Chem. Manager National Ultrahigh-Field NMR Facility for Solids

> 1200 Montreal Road, M-40 Ottawa, Ontario K1A 0R6

Phone: (613) 998-5552 Fax: (613) 990-1555 E-mail: Victor.Terskikh@nrc-cnrc.gc.ca