



Canadian NMR News

NRC-PBI celebrates the 25th anniversary



Our colleagues at the **NRC Plant Biotechnology Institute** in Saskatoon are celebrating the 25th anniversary of the Institute. It has also

been 60 years since the National Research Council Canada first established the NRC Prairie Regional Laboratory, which in 1983 was officially transformed into NRC-PBI. NRC-PBI is recognized worldwide for its research in agricultural biotechnology that utilizes plants to produce bioproducts, healthy foods and supplements for the benefit of environmental and human health. PBI is a major research centre for plant biosciences in Canada, with expertise in genomics, metabolic pathways, gene expression, genetic transformation, structural biology and natural product chemistry.

Read the press release by NRC Canada

http://www.nrc-cnrc.gc.ca/newsroom/news/2009/pbi09-nr_e.html

NMR spectroscopy plays a prominent role in many fundamental and applied research projects undertaken by PBI researchers and their collaborators. PBI currently houses two recently upgraded NMR instruments: a **500**



MHz Bruker Avance system (photo left) for multinuclear high-resolution studies equipped with a CryoProbe, and a **360 MHz**

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Avance wide-bore system for work in solids, including magic-angle spinning (MAS), and *in vivo* microimaging in whole plants, seeds, and plant tissues (photo right).



NMR personalities at PBI:

Sue Abrams has been recently appointed to a position of PBI's Research Director. Sue uses NMR spectroscopy in plant metabolic pathway studies.

Michèle Loewen employs high-resolution NMR along with a wide range of other techniques to learn about molecular mechanisms of membrane protein actions.

Shelley Forgeron has recently joined NRC-PBI as an NMR Facility Manager.

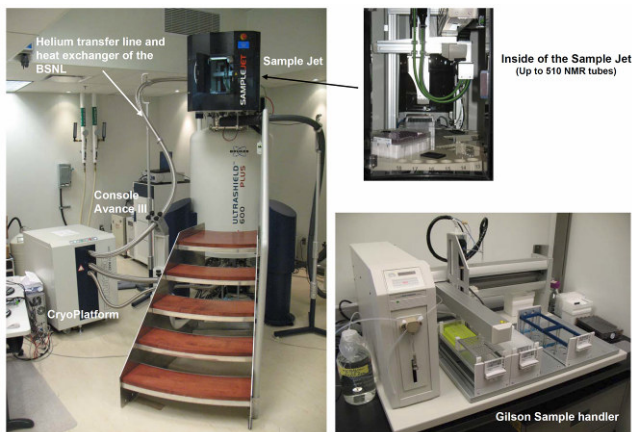
Web: <http://www.pbi.nrc.ca/>

Top photo credit: NRC Canada

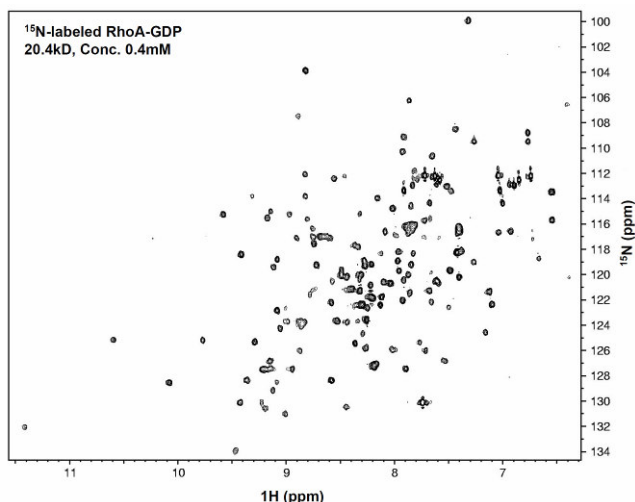
Submitted by Genevieve Seabrook (UHN-OCI)

New NMR spectrometer in Dr. Ikura's laboratory (Toronto)

In 2008 we acquired a new 600 MHz US (UltraShield Plus) Bruker Avance III spectrometer with three probes (1.7mm TCI Micro CryoProbe™, 5mm TCI CryoProbe™, 5mm Room Temperature TXI probe), with four channel (^1H , ^{15}N , ^{13}C , ^2H). Originally, the CryoPlatform was only used to provide cold helium gas to the CryoProbe. With our new high-tech system, the CryoPlatform is also being used to reliquefy the evaporating nitrogen gas coming from the magnet cryostat. As a result, the Bruker Smart Nitrogen Liquefier (BSNL) pretty much eliminates the weekly nitrogen refill. This is the first system with the BSNL installed in Canada. Our system is also equipped with a Sample Jet (NMR automation unit) mounted on the top of the magnet. The Sample Jet carousel containing up to 510 NMR samples is kept at a stable temperature of 4°C for sample stability purpose. In conjunction with the newly acquired Gilson liquid handler, this entire setup allows us to do high-throughput screening using sample volume as little as 30 μL (1.7mm NMR tubes) with the 1.7mm Micro CryoProbe.



This new spectrometer is located in the MaRS building (Toronto) and housed together with a Bruker 800 MHz US² (Ultra Stabilized, Ultra Shielded) Avance II equipped with two probes (5mm TCI CryoProbe, 5mm Room Temperature TXI probe), four channel (^1H , ^{15}N , ^{13}C , ^2H) acquired in late 2005.



^1H - ^{15}N -HSQC spectrum acquired on our new Bruker 600 MHz equipped with a 1.7mm Micro CryoProbe, 1scan, 2 min acquisition time, sample volume 30 μL .

High-resolution structures, protein interactions, protein dynamic and structure-function relationship of biologically relevant proteins correspond to our main research focus. NMR-based high-throughput screening approach of small molecules that directly interact with the protein of interest can now be done in our laboratory on a large scale.

Contacts: Genevieve Seabrook, UHN-OCI (416)-629-7391

Web: <http://nmr.uhnres.utoronto.ca/ikura/index.html>

New Biomolecular NMR Facility in the Maritimes

A new Biomolecular Magnetic Resonance Facility at the National Research Council Institute for Marine Biosciences (NRC-IMB) (Halifax, N.S.) is now officially open. The opening ceremony on February 19 was officiated by Dr. **Martha Crago**, Vice-President, Research, Dalhousie University; the Honourable **Gerald Keddy**, Parliamentary Secretary to the Minister of International Trade; and Dr. **Roman Szumski**, Vice-President, Life Sciences, NRC.

Read the news release by NRC Canada

http://www.nrc-cnrc.gc.ca/newsroom/news/2009/health-ns09-nr_e.html

This facility has been established in partnership between NRC Canada, Dalhousie University, and the Federal Government to support health-

care research in the Atlantic region. It houses a new 700 MHz Bruker Avance III NMR spectrometer equipped with the world's first 1.7 mm (40 μ L) cryoprobe for fields > 600 MHz.

Find more about the Biomolecular Magnetic Resonance Facility at NRC-IMB in the **Winter 2009** issue of the "Canadian NMR Research" news bulletin.

Web: NRC-IMB

<http://imb-ibm.nrc-cnrc.gc.ca/>

Submitted by Alex Bain (McMaster)



NMR events at CSC 2009

Two NMR symposia and a workshop will be highlights of the 92nd Canadian Chemistry Conference and Exhibition meeting in Hamilton.

Gillian Goward and Alex Bain, of McMaster University, have organized a symposium on **Materials and Magnetic Resonance**, mainly focused on Solid-State NMR.

PT7 - Materials and Magnetic Resonance, Sunday May 31 - Monday June 1, AM

<http://abstracts.csc2009.ca/vs010074.htm>

Giuseppe Melacini, also at McMaster, has put together an excellent program in **Biomolecular NMR**.

BM2 - Biomolecular NMR, Monday June 1, PM - Tuesday June 2

<http://abstracts.csc2009.ca/vs002010.htm>

Please note that this year two NMR symposia have been scheduled back-to-back. Plan your trip accordingly and don't miss this rare opportunity to attend both NMR symposia at CSC!

The conference program is now available on-line

<http://abstracts.csc2009.ca/>



4th Annual Solid-State NMR Workshop

The National Ultrahigh-Field NMR Facility for Solids and Bruker Canada are pleased to present the 4th Annual Solid-State NMR Workshop at the 92nd Canadian Chemistry Conference and Exhibition in Hamilton. The workshop will take place on **Saturday afternoon, May 30, 2009**.

http://nmr900.ca/events_e.html

Preliminary Program

Saturday, May 30, 2009, Hamilton, Ontario

Session 1

13:00 Gang Wu (Queen's) "Solid-state ¹⁷O NMR of biological samples: Progress and challenges"

13:30 Myrna Simpson (Toronto) "The Role of NMR in Environmental Chemistry"

14:00 Simon Sharpe (SickKids) "Investigating peptide and protein assemblies by solid-state NMR"

14:30 Shane Pawsey (Bruker BioSpin) "Dynamic Nuclear Polarization of Solids at 263 GHz"

15:00 Coffee Break

Session 2

15:15 Aaron Rossini (Windsor) "Characterization of metallocenes by ⁹¹Zr and ³⁵Cl solid-state NMR"

15:45 Vladimir Michaelis (Manitoba) "Structural Investigations of Germanium Oxides using Ultrahigh-Field ⁷³Ge NMR and DFT Calculations"

16:15 Igor Moudrakovski (NRC-SIMS) "²⁵Mg ultra-high field solid-state NMR and first principles calculations in magnesium salts"

16:45 The 900 NMR Facility users' meeting

17:15 Reception sponsored by **Bruker Canada**

Registration for the NMR Workshop is free but space is limited. To register please forward your name and affiliation to Victor Terskikh.

Email: terskikhv@nrc-cnrc.gc.ca

Note that the NMR Workshop registration is separate and independent from the CSC 2009 conference registration.

Magnetic Resonance Gordon Research Conference

Canadian Solid-State NMR research is front and center at the upcoming Gordon Research Conference at the University of New England, in Biddeford, Maine. Two key lectures in the "NMR of Materials" session are to be given by **Rod Wasylshen** (University of Alberta) and **Joe Zwanziger** (Dalhousie University). To register by May 24:

June 14-19, 2009, Biddeford, ME
Registration deadline May 24, 2009
<http://www.grc.org/programs.aspx?year=2009&program=magres>

Submitted by Andrew Lewis (Simon Fraser University)

VIVA III

VIVA III, the 3rd annual West Coast NMR minisymposium will take place at Simon Fraser University on Saturday and Sunday, **July 25-26, 2009**. This 1.5 day meeting, modelled after the NMR MOOT meetings in Central Canada, is designed to bring together NMR users, researchers and NMR facility managers from British Columbia, Alberta and Washington State to discuss NMR topics of general interest. Graduate Students are particularly encouraged to present papers or publications.

A preliminary announcement will be emailed shortly. Interested participants who do not receive the announcement can contact the principal organizer, **Andrew Lewis** at arl@sfu.ca

Symposium details and online registration site will be available at www.chemistry.sfu.ca

Submitted by Gang Wu (Queen's University)

ICASS 2009

The 55th International Conference on Analytical Sciences and Spectroscopy (ICASS) will be held at Queen's University (Kingston, Ontario, Canada) on **August 9-12, 2009**. The conference will feature a special NMR Symposium in honour of **Professor Rod Wasylshen**.

The conference will also have a fantastic social program including the Magical Dinner with Canada's Magic Champion Eric Leclerc and a very popular Sunset Dinner Cruise of the Thousand Islands.

The abstract submission for oral and poster presentations is now open and will last until June 1, 2009. ICASS offers a special discount for **early registration** which is available until June 1, 2009.

Please check the ICASS conference website for details
<http://www.icass.ca/2009/>

Or contact the NMR Symposium organizer, **Gang Wu**, for more information
<http://www.chem.queensu.ca/people/faculty/Wu/>

Submitted by Yves Aubin (Health Canada)

MOOT 2009 NMR minisymposium

On behalf of the organizing committee, I would like to invite all our colleagues of the NMR community to attend the 22nd edition of the MOOT NMR minisymposium in Ottawa. The meeting will be held at Carleton University on **October 17-18, 2009**. More details will be available soon via email and on the official website (coming soon)
www.mootnmr.org

For inquiries please contact **Yves Aubin**
Phone: (613) 941-6155
E-mail: yves_aubin@hc-sc.gc.ca

Submitted by Kirk Marat (Manitoba)

SpinWorks 3.1 is available for download

Version 3.1 of the SpinWorks NMR freeware processing and simulation package is now available for download at:

<ftp://davinci.chem.umanitoba.ca/pub/marat/SpinWorks>

The file is **SpinWorks_310.zip**

In addition to the usual bug fixes new features include the ability to read and display processed 2D and 3D data from NMRPipe, and a band-fitting (deconvolution) feature. The LP routines have been re-written for .NET so the code is now .NET clean, with the LP.dll Win 32 file no longer needed.

The program should run on all Windows systems from Win 2000 and up, and has been run successfully on Macs with "parallels". Being .NET clean it should also run on Linux under "mono" with all path separator issues ("\" vs "/") being resolved. I haven't been doing any Linux testing myself, so any feedback that I can get would be greatly appreciated!

Kirk Marat

<http://www.umanitoba.ca/chemistry/nmr/spinworks/index.html>

Submitted by David Bryce (Ottawa)

EFGShield 2.3 is available for download

If you use Gaussian to help interpret your solid-state NMR Sam Adiga, Dom Aebi and David Bryce (University of Ottawa) have written a computer program called "EFGShield" which parses and summarizes Gaussian output files containing shielding and EFG data. The program provides results which are directly comparable to data extracted through simulations of experimental spectra using programs such as WSOLIDS (e.g., quadrupolar coupling constants, Euler angles, etc.).

S. Adiga, D. Aebi, and D.L. Bryce, "EFGShield: A Program for Parsing and Summarizing the Results of Electric Field Gradient and Nuclear Magnetic Shielding Tensor Calculations," *Can. J. Chem.* **85** (2007) 496-505.

<http://particle.web-p.cisti.nrc.ca/rparticle/AbstractTemplateServlet?journal=cjc&volume=85&year=2008&issue=7&msno=07-009&calv1.ang=eng>

Updated **Version 2.3** includes:

1. Built-in quadrupole moments have been updated to reflect Pyykkö's most recent recommendations
P. Pyykkö, *Mol. Phys.* **106** (2008) 1965-1974.
2. The program can now handle files containing up to 900 atoms.
3. Several equivalent sets of Euler angles are outputted rather than just one representative set.
4. Minor bug fix for Euler angles in high-symmetry environments.

If you are interested, you can download the program here

<http://www.catalysis.uottawa.ca/EFGShield-download.php>

Please contact me if you have any questions or comments.

Dave Bryce

<http://www.science.uottawa.ca/~dbryc159/>

CBC reports on Quantum Computing at Waterloo

Read a feature report by CBC on quantum computing research at the University of Waterloo's Institute for Quantum Computing:

<http://www.cbc.ca/technology/story/2009/02/09/f-quantum-computing.html>

Submitted by Chris Ratcliffe (NRC-SIMS)

2011 International Year of Chemistry

The 63rd General Assembly of the United Nations has adopted a resolution proclaiming 2011 as International Year of Chemistry, placing UNESCO and the International Union of Pure and Applied Chemistry (IUPAC) at the helm of the event.

Official web-site of the International Year of Chemistry

<http://www.chemistry2011.org/>

Chris Ratcliffe is a Secretary of the Canadian National Committee for the International Union of Pure & Applied Chemistry (CNC-IUPAC). For more information about CNC-IUPAC please visit the web-site:

<http://www.cnc-iupac.ca/>

Canadian NMR blogs and news sites

Solid-State NMR Literature Blog (Rob Schurko's group, Windsor)

<http://ssnmr.blogspot.com/>

NMR Facility Blog (Glenn Facey, Ottawa)

<http://u-of-o-nmr-facility.blogspot.com/>

NMR Facility Blog (Tim Burrow, Toronto)

<http://www.chem.utoronto.ca/facilities/nmr/NMRBlog/>

NMR Facility News (Albin Otter, Alberta)

http://nmr.chem.ualberta.ca/nmr_news.htm

NMR Theses Recently Defended

Congratulate your students here!

Fu Chen (University of Alberta) March 2, 2009

Research supervisor: Roderick Wasylshen

Ph.D. thesis: "Solid-state nuclear magnetic resonance investigations of some Group 11 and Group 13 compounds"

Recognition

Two Canada Research Chairs in magnetic resonance renewed

On February 23, 2009 the Government of Canada has announced an investment of \$120.4 million to fund 134 new or renewed Canada Research Chairs in 37 Canadian universities. This includes renewal of two Tier 1 Chairs involved in magnetic resonance research.

Raymond Laflamme (University of Waterloo) Canada Research Chair Tier 1 in Quantum Information

Bruce Balcom (University of New Brunswick) Canada Research Chair Tier 1 in Materials Science and MRI. Bruce has also been awarded a complementary CFI funding under the Leaders Opportunity Fund.

Our sincere congratulations to Raymond, Bruce and their colleagues with this well-deserved recognition.

http://www.chairs.gc.ca/web/media/releases/2009/february_e.asp

Canada Research Chairs in NMR

<http://www.chairs.gc.ca/>

Cheryl Arrowsmith (Toronto) Biochemistry

Bruce Balcom (UNB) Multidisciplinary

Valerie Booth (Memorial) Biochemistry

Yining Huang (Western) Materials Science

Mitsuhiko Ikura (Toronto) Molecular Biology

Lewis Kay (Toronto) Biochemistry

Vladimir Ladizhansky (Guelph) Cell Biology

Raymond Laflamme (Waterloo) Physics

Pascale Legault (Montréal) Biochemistry

Simon Sharpe (Toronto) Biochemistry

Roderick Wasylshen (Alberta) Phys Chemistry

Josef Zwanziger (Dalhousie) Phys Chemistry

Robert Schurko (University of Windsor) was awarded a University of Windsor Award for Excellence in Research, Scholarship and Creative Activity (mid-career).

<http://uwinchemistry.blogspot.com/2009/02/university-honours-outstanding.html>

NSERC 2009 Grants Competition Results

Our sincere congratulations to all the winners of the 2009 NSERC competitions in the Discovery Grants Program (**DG**), Research Tools and Instruments Grants (**RTI**), the Major Resources Support Program (**MRS**) and Scholarship programs.

A team of six researchers from **l'Université Laval**, including Michèle Auger, Freddy Kleitz, Jean-François Morin, Thierry Ollevier, Jean-François Paquin and Anna Ritcey, have received \$132,922 in NSERC RTI funding for a triple resonance 4 mm CP/MAS $^{19}\text{F}/^1\text{H}/\text{X}$ probehead and accessories for solid-state NMR spectrometer.

David Bryce (University of Ottawa) received NSERC RTI funding for laboratory equipment (glovebox).

Becky Chapman (University of Ottawa) has been awarded a NSERC Alexander Graham Bell Canada Graduate Scholarship. She joins Cory Widdifield as the second member of Dave Bryce's group to receive this prestigious scholarship.

The National Ultrahigh-Field NMR Facility for Solids (www.nmr900.ca) has received NSERC MRS funding for the next five years.

David Bryce (University of Ottawa) has been promoted with tenure to the rank of Associate Professor. Dave joined the University of Ottawa in 2005 and has since developed an advanced program in solid-state NMR spectroscopy in materials research. While at the University of Ottawa, Dave has received several major infrastructure grants and research awards, including CFI Leaders' Opportunity Grant in 2007, Ontario Early Researcher Award in 2006, and John Charles Polanyi Prize in Chemistry in 2005. Dave also serves as a chair of the Steering Committee of the National Ultrahigh-Field NMR Facility for Solids.

<http://www.science.uottawa.ca/~dbryc159/>

Join us in congratulating Dave with this promotion!



On the move

Our NMR technician **Dr. Nadine Merkley** has recently moved to Nova Scotia to take up a position of NMR Spectroscopy Technical Officer at the National Research Council's Institute for Marine Biosciences in Halifax. We thank her excellent service to our Department at Western and to wish her the very best at her new position.

Yining Huang

Fu Chen, after finishing his Ph.D. with Roderick Wasylishen at the University of Alberta, Fu has joined the group of Prof. Joerg Matysik at the Leiden Institute of Chemistry, Leiden University in the Netherlands. Fu's postdoctoral research will involve study of CO₂ and Xe adsorption in coals, and applications of DNP NMR in these and related materials.

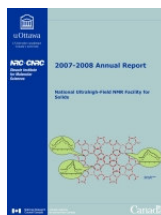
the 900 NMR Facility News

NSERC 2009 MRS Program Competition Results

The National Ultrahigh-Field NMR Facility for Solids is very pleased to announce that our application to NSERC for continued **Major Resources Support** (MRS) funding has been successful. Funding has been approved at a level of \$88,600 per year for each of the next five years. This award is critical to the ongoing operations of the facility. The funding also means that the Facility will be able to continue to provide travel grants for users, increase outreach activities, hold annual workshops, and sponsor regional NMR meetings. I would like to thank Victor Terskikh for his outstanding contributions to the operation of the Facility and also to the preparation of the grant proposal. Thanks also to all co-applicants on the proposal: John Ripmeester, Rod Wasylishen, Christian Detellier, Michèle Auger, Yining Huang, Rob Schurko, Scott Kroeker, Gillian Goward, Gang Wu, and Simon Sharpe.

David Bryce
Chair of the Facility Steering Committee

http://nmr900.ca/news_e.html



2007-2008 Annual Report

The 2007-2008 Annual Report for the National Ultrahigh-Field NMR Facility for Solids is now available in print and for download at http://nmr900.ca/annual_e.html

If you have not received a printed copy of this report and would like to receive one, please forward your mailing address to the Facility manager.

Travel support program for students and young scientists

Students and young scientists from Canadian Universities are welcome to apply for a travel stipend towards full or partial reimbursement of their travel expenses incurred while visiting the 900 Facility. All requests should be submitted by a supervisor in advance of the trip and include a cost estimate. Requests should be forwarded to the Facility manager for review and approval by the Steering Committee.

http://nmr900.ca/policies_e.html

Recent Travel Grant Recipients

Luke O'Dell (University of Windsor)

Jennifer MacDonald (Dalhousie University)

Upcoming NMR Events

Let everyone know about upcoming NMR-related events at your University or Lab. NMR conference announcements are also welcome.

5th Annual McGill Biophysical Chemistry Symposium

May 5, 2009, Otto Maass Chemistry Building, McGill University, Montreal, Quebec
<http://www.chemistry.mcgill.ca>

4th Annual Solid-State NMR Workshop at CSC 2009

May 30, 2009, Hamilton, ON
http://nmr900.ca/events_e.html

Materials and Magnetic Resonance Symposium at CSC 2009

May 31-June 1, 2009, Hamilton, ON
<http://www.csc2009.ca>



Biomolecular NMR Symposium at CSC 2009

June 1-2, 2009, Hamilton, ON
<http://www.csc2009.ca>

XeMat 2009 the 4th International Symposium on Xenon NMR of Materials

June 8-10, 2009, Ruka Fell, Kuusamo, Finland
<http://cc.oulu.fi/~nmrlab/xemat/>

Magnetic Resonance Gordon Research Conference

June 14-19, 2009, Biddeford, ME
Registration deadline May 24, 2009
<http://www.grc.org/programs.aspx?year=2009&program=magres>

AMPERE NMR School

June 21-27, 2009, Zakopane, Poland
<http://www.staff.amu.edu.pl/~school/>

EUROMAR-2009

July 5-9, 2009, Göteborg, Sweden
<http://www.euromar2009.com>

51st Annual Rocky Mountain Conference on Analytical Chemistry

July 19-23, 2009, Snowmass, Colorado
<http://www.rockychem.com/>

**VIVA III** the 3rd Annual West Coast NMR Minisymposium

July 25-26, 2009, Simon Fraser University, Vancouver, B.C.
<http://www.chemistry.sfu.ca/>

**ICASS 2009** 55th International Conference on Analytical Sciences and Spectroscopy

August 9-12, 2009, Kingston, Ontario
<http://www.icass.ca/>

**SCM 09** 11th International Spin Chemistry Meeting

August 9-11, 2009, St. Catharines, Ontario
<http://www.brocku.ca/scm09>

**NANUC NMR BootCamp** (Metabolomics)

August 28-29, 2009, Edmonton, AB
<http://www.nanucbootcamp.com/>

"Dynamic Nuclear Polarization" Second International Symposium

September 2-4, 2009, Königstein, Germany
<http://www.bio-dnp.uni-frankfurt.de/dnpsymp/>

6th Alpine Conference on Solid-State NMR

September 13-17, 2009, Chamonix, France
Registration deadline May 31st, 2009
<http://www.alpine-conference.org>

SMASH 2009 Small Molecule NMR Conference

September 20-23, 2009, Chamonix, France
Registration deadline July 31st, 2009
<http://www.smashnmr.org/>

Cryogenic NMR Symposium

September 21-22, 2009, Southampton, UK
Registration deadline August 1st, 2009
<http://cryonmr-symposium.org/>

**MOOT 22 NMR Symposium**

October 17-18, 2009, Carleton University, Ottawa, ON
<http://www.mootnmr.org>

NMR Jobs and Vacancies

You are welcome to post here your vacancies, openings, and related announcements. We can also post short "job wanted" requests.

Listings of NMR jobs and vacancies

Canadian NMR Jobs
http://nmr900.ca/nmr_jobs.html

NMR jobs on the NMR Information Server
<http://www.spincore.com/nmrjobs/>

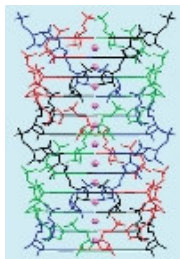
List of NMR jobs and Post-Doc positions maintained by Dror Warschawski
<https://listes.sc.univ-paris-diderot.fr/sympa/info/nmr>

NMR jobs on SpectroscopyNow.com
<http://www.spectroscopynow.com/coi/cda/list.cda?type=Job&chld=0>

Canadian NMR Research Highlights

Research highlights and most recent NMR publications by Canadian research teams.

C&EN News of the week: Nucleotide self-assembly



Recent *JACS Communication* by **Gang Wu** and **Irene Kwan** (Queen's University) has been highlighted as News of the week in *Chemical & Engineering News* as an important contribution to our understanding of self-assembly of nucleotide

monomers. In their research Gang and Irene have used a variety of liquid-state NMR techniques and computations to characterize guanosine 5'-monophosphate (5'-GMP) solutions in the presence of sodium cations. The authors have observed spontaneous formation of well-defined right-handed helical 5'-GMP structures, the finding which may have potential implications for prebiotic chemistry theories.

Read the news story in *C&EN* (picture credit) Issue February 16, 2009, p.10, **News of the week**:

<http://pubs.acs.org/cen/news/87/i07/8707notw7.html>

G. Wu and I. Kwan, "The helical structure of disodium guanosine 5'-monophosphate self-assembly in neutral solution," *Journal of the American Chemical Society* **131** (2009) 3180-3182.

<http://dx.doi.org/10.1021/ja809258y>

Review in *Biophysical Journal*

Lewis Kay and colleagues from the University of Toronto have published an article in *Biophysical Journal* reviewing recently developed NMR relaxation dispersion technique and its applications to protein folding research.

P. Neudecker, P. Lundström, L.E. Kay, "Relaxation Dispersion NMR Spectroscopy as a Tool for Detailed Studies of Protein Folding," *Biophysical Journal* **96** (2009) 2045-2054.

<http://dx.doi.org/10.1016/j.bpj.2008.12.3907>

Review in *Concepts in Magnetic Resonance*

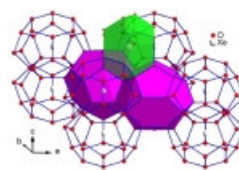


C.M. Widdifield, R.W. Schurko, "Understanding chemical shielding tensors using group theory, MO analysis, and modern density-functional theory," *Concepts in Magnetic Resonance Part A* **34A** (2009) 91-123.

<http://dx.doi.org/10.1002/cmr.a.20136>

New structure of gas hydrate: paper in *PNAS*

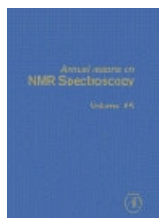
A research team from the **Steacie Institute for Molecular Sciences** (NRC Canada) and their colleagues from Oak Ridge, Stony-Brook, and Argonne, are reporting synthesis and characterization of a new structure of gas hydrate, previously known only hypothetically. Static and magic angle spinning ^{129}Xe NMR was instrumental in this research, and had provided strong confirmation of the structural analysis.



L. Yang, C.A. Tulk, D.D. Klug, I.L. Moudrakovski, C.I. Ratcliffe, J.A. Ripmeester, B.C. Chakoumakos, L. Ehm, C.D. Martin, and J.B. Parise, "Synthesis and characterization of a new structure of gas hydrate," *Proc. Natl. Acad. Sci. USA* **106** (2009) 6060-6064.

<http://dx.doi.org/10.1073/pnas.0809342106>

Review in *Annual Reports on NMR Spectroscopy*



The latest issue of *Annual Reports on NMR Spectroscopy* is dedicated to various aspects of NMR in molecular biology. The first Chapter in this six-chapter volume is written by a team from the **University of Calgary**

reviewing modern solution and solid-state NMR experiments to characterize antimicrobial peptides and mechanisms of their action.

Evan F. Haney and Hans J. Vogel, "NMR of Antimicrobial Peptides," *Annual Reports on NMR Spectroscopy* **65** (2009) 1-51.

[http://dx.doi.org/10.1016/S0066-4103\(08\)00201-9](http://dx.doi.org/10.1016/S0066-4103(08)00201-9)



Progress in Nuclear Magnetic Resonance Spectroscopy

<http://www.sciencedirect.com/science/journal/00796565>

recent reviews

B.A. Demko, R.E. Wasylshen, "Solid-State Selenium-77 NMR," *Progress in Nuclear Magnetic Resonance Spectroscopy* **54** (2009) 208-238.

<http://dx.doi.org/10.1016/j.pnmrs.2008.10.002>

R.P. Chapman, C.M. Widdifield and D.L. Bryce, "Solid-State NMR of Quadrupolar Halogen Nuclei," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2009) in press.

NMR paper in *Science Signaling*

A research team from the **Ontario Cancer Institute** and the **University of Toronto** has developed a real-time, nuclear magnetic resonance (NMR)-based assay to monitor the intrinsic GTPase activity of the small guanosine triphosphatase (GTPase) Rheb. This method can now be used to gain further understanding of the mechanisms of action of other GTPases and their GAP partners.

C.B. Marshall, J. Ho, C. Buerger, M.J. Plevin, Guang-Yao Li, Z. Li, M. Ikura, and V. Stambolic, "Characterization of the Intrinsic and TSC2-GAP-Regulated GTPase Activity of Rheb by Real-Time NMR," *Science Signaling* **2** (#55) (2009) ra3.

<http://dx.doi.org/10.1126/scisignal.2000029>

Editor's summary:

<http://stke.sciencemag.org/cgi/content/summary/sigtrans/2/55/ra3>

Special Issue of *Solid State Nuclear Magnetic Resonance*

Michael Hunger has edited a special "**Solid State NMR in Catalysis**" issue of *Solid State Nuclear Magnetic Resonance* (vol. 35, issue 2). Among authors are many renowned personae in the field including **Yining Huang** (University of Western Ontario), who is reporting their recent research in studying formation of molecular sieves.

Z. Yan, B. Chen, Y. Huang, "A solid-state NMR study of the formation of molecular sieve

SAPO-34," *Solid State Nuclear Magnetic Resonance* **35** (2009) 49-60. (**invited publication**, special issue "Solid State NMR in Catalysis")

<http://dx.doi.org/10.1016/j.ssnmr.2008.12.006>

NMR of beverages

Power-boosting and refreshing beverages are the topic dear to many reading this bulletin. Not surprisingly quite a few of us are involved in this rewarding research (think of drink leftovers after vigorous NMR tests are completed!).

André Simpson and colleagues from the University of Toronto and ACD have engaged into NMR spectroscopic studies of Red Bull Energy Drinks. Apparently these drinks are also good for an undergraduate analytical chemistry course to teach students basics of modern NMR spectroscopy. Students are introduced to solvent suppression, use of internal standards, quantitative and qualitative analysis of NMR spectra of complex mixtures.

A.J. Simpson, A. Shirzadi, T.E. Burrow, A.P. Dicks, B. Lefebvre and T. Corrin, "Use of NMR and NMR prediction software to identify components in Red Bull Energy Drinks" *Journal of Chemical Education* **86** (2009) 360.

<http://jchemed.chem.wisc.edu/Journal/issues/2009/Mar/abs360.html>

In a related story, **Chris Kirby** (Agriculture and Agri-Food Canada, P.E.I.) has teamed up with Charlottetown-based Stirling Products North America Inc and the NRC Institute for Nutrisciences and Health (NRC-INH) to develop an NMR-based technique to test yeast-based complex sugars with potential use in brewing industry for making better beer no less.

http://www.nrc-cnrc.gc.ca/highlights/2009/0904stirling_e.html

And finally, **Bruker Biospin** has recently introduced a JuiceScreener™, a fully-automated push-button fruit juice quality control system based on NMR. For example orange juice can easily be distinguished between direct juice and juice from concentrates, and even the origin of the fruit can be identified, i.e. oranges from Spain, Greece, Brazil etc. have very different NMR spectral signatures. Don't be late getting one of these instruments for your lab!

<http://www.bruker-biospin.com/juicescreener.html>

Recent NMR Publications

We are listing here most recent NMR publications by Canadian research groups as they appear on the www.nmr900.ca website. Although we are doing our best keeping track of your publications, this list should not be considered complete. You are encouraged to let us know of your recent publications as they become available.

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