



National Ultrahigh-Field NMR
Facility for Solids
Centre national de RMN à
ultrahaut champ pour les solides

Canadian NMR Research News Bulletin #4.1 Winter 2010



Guest Editorial

Gillian Goward, McMaster

In the dead of winter, such as it is in 2010, it is nice to look to summer, whether remembering the one past, or anticipating the warm months to come. From the stand point of the Canadian NMR community, early February is a good time to bring to mind CSC abstract deadline. I would like to highlight for you some of the success of the CSC 2009, and anticipated adventures of the CSC 2010. We, at McMaster, were thrilled with the results of the CSC, hosted in Hamilton, with record-breaking attendance, in spite of an economic downturn. Clearly, the Canadian chemistry community values the opportunity to network, and also recognized the high quality slate of symposia put together for last year's conference.

The 2009 meeting was held at the Hamilton Convention Center, where Hamilton put on its good face, and welcomed visitors with a combination of good weather, good food, and good drinks. I hope you had a chance to discover either Boo's Bistro & Wine Bar, or Chester's Beers of the World. On the other hand, the touristic setting was not so alluring as to extract the audience from the conference's scientific events! There were three symposia featuring a high number of magnetic resonance-based talks, including the Materials and Magnetic Resonance symposium, the Energy Conversion and Storage symposium, and the Biomolecular NMR symposium. The MMR symposium benefitted from the participation of internationally renowned speakers, including **Sharon Ashbrook**, and **Hans W. Spiess**. It was a delight to have them contribute to the meeting, and they reported to have thoroughly enjoyed the conference, and in particular, their interactions with our students and the

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Canadian NMR community, which they found to be most hospitable and engaging.

The symposium had a theme of materials, and the application of magnetic resonance techniques to study the properties of those materials. Of course, this theme was chosen due to the established strength that Canadian researchers have in this area. We heard several impressive talks, both contributed and invited, describing how the performance-governing properties of a variety of materials can be elucidated using magnetic resonance methods. Of particular note was the talk by **Bruce Balcom**, presenting the development of advanced magnetic resonance imaging which can be used in functional materials such as concrete, or even functioning devices, such as operating fuel cells. With this, Bruce picked up a theme in energy-related materials, that could be found in several of the talks and posters presented throughout the meeting. The topic is not only timely and important, but also a

good way of marketing the wide range of NMR methods for studying problems such as proton and water dynamics in fuel cells, lithium ion dynamics in battery materials, stability of nuclear storage materials, and transport efficiency in ionic liquids. Highlighting these energy-related studies taking advantage of magnetic resonance methods, we were fortunate to obtain sponsorship for the symposium from *the American Chemical Society Petroleum Research Fund*. The symposium also attracted numerous excellent student contributions, both in the oral and poster sessions, and featured a wide range of solid-state NMR research groups from across the country.

While the previous meeting was delightful, it is now time to look forward to the upcoming **93rd CSC**, which will be held in Toronto from May 29th-June 2nd, at the Metro Toronto Convention Center. The conference will be immediately preceded by the National Ultrahigh-Field NMR Facility for Solids Annual Workshop, which will take place on Saturday, May 29. The conference will feature a symposium entitled "Solid-State NMR: Methods and Applications", being organized by David Bryce and myself. This symposium will capture a broad spectrum of magnetic resonance research, from structure and dynamics in biomaterials, through polymers and macromolecules, to ceramics and oxides, underscored with the importance of methods and instrumentation developments in advancing the field. Invited speakers at this symposium will include the newly appointed members of the National Ultrahigh-Field NMR Facility for Solids International Advisory Board, namely **Timothy Cross, Arno Kentgens, and Marek Pruski**. We are also pleased to welcome **Andreas Brinkmann**, a newcomer to the Canadian NMR community, as well as several of the "usual suspects". Abstract submissions are open until **February 15th**. We look forward to another stimulating conference, and welcome your contributions to the scientific program, including particularly, student contributions. I look forward to seeing what exciting results you have to bring to the Toronto meeting this spring!

Gillian Goward

Canadian NMR News

High school students honoured with UTSC science awards

by Eleni Kanavas

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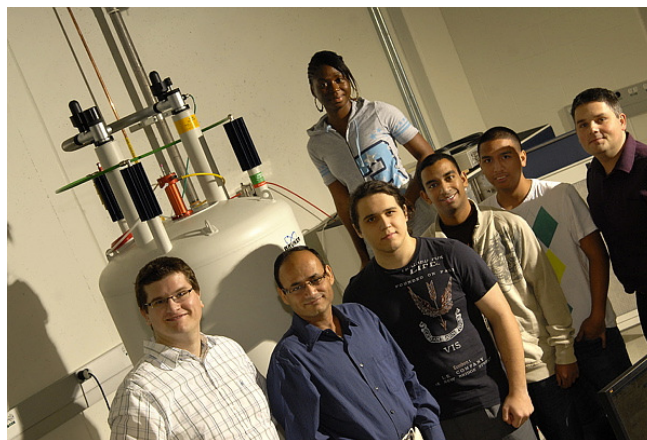
<http://webapps.utsc.utoronto.ca/ose/story.php?id=1860>

Four young people from local high schools have been recognized for their excellence in science through a new set of awards established by the University of Toronto Scarborough, in collaboration with private industry and the Ontario government.

The quartet of Grade 12 students was recently welcomed to the campus to receive the **Outstanding High School Student Science Awards**, recognizing their talent in the subject. **Celestine Sarpong** and **Patrick Polvorosa** from Jean Vanier Secondary School, along with **Abhishek Ellie** and **James Pasierbski** from Senator O'Connor Secondary School, are the inaugural recipients of the awards. All 17 years old, the students received \$250 each, an awards certificate, and a day on campus filled with exciting science and research opportunities.

"I'm so happy to receive this award because I've always been interested in science and find the subject exciting," said Sarpong, a student at Jean Vanier who hopes to become a pediatrician.

Encouraging young people to consider a career in science was the impetus behind a new set of awards founded by chemistry professor **André Simpson** of the Department of Physical and



SCIENCE AWARDS: (L to R) Prof. André Simpson (UTSC), Dr. Rajeev Kumar (Bruker BioSpin), James Pasierbski, Celestine Sarpong, Abhishek Ellie, Patrick Polvorosa, Dr. Dave McNally (UTSC).

Environmental Sciences and Director of the Environmental NMR Centre on campus. The science awards were established this past Spring with the aim of exposing the best high school students to a research and development environment and conveying excitement and enthusiasm for research to students at an early age.

"We are so pleased to welcome you to our campus, and we commend you for your achievements in science as well as your interest in research," Simpson told the visitors. "Today you can see for yourselves that science is an exciting and stimulating career and we want more young people to be aware of the opportunities available to them in this field."

Professor **Franco Vaccarino**, principal of UTSC, presented the certificates to the winners, along with **Dr. Rajeev Kumar**, representing **Dr. Henry J. Stronks**, president of Bruker BioSpin, a company specializing in the development of scientific instrumentation and a key donor of hi-tech equipment to UTSC.

"You have shown a talent and aptitude for science, and we congratulate you on being the first winners of this award," Vaccarino said in his speech to the award recipients. "I also wish to thank our donor, Bruker Canada, without whom we could not offer this program."

The awards program has been financially supported in part by the Ontario government, the University of Toronto Scarborough and Bruker BioSpin Ltd. Part of Bruker Canada, the company is a global leader in the development and manufacture of magnetic resonance technologies for both imaging and spectroscopy. In 2004, Bruker BioSpin Ltd. donated \$1.57 million to build an NMR centre at U of T Scarborough.



Students got the opportunity to use the NMR spectroscopic instrument in the Environmental Nuclear Magnetic Resonance (NMR) facility in the new Science Research Building, where they performed an imaging and magnetic resonance experiment to determine the chemical components in the Red Bull energy drink.

"The lab experiment was really interesting, and it was a great way to expose us to the field of science," said Pasierbski, a Grade 12 science student at Senator O'Connor who hopes to study life sciences at university next year.

The NMR facility is the only centre in Canada that studies the environment and is able to conduct research on environmental solids, liquids and gel samples using specially designed probes that are inserted into the NMR spectroscopic instrument. According to Dr. Kumar, "It's the most basic tool in order to conduct fundamental research in environmental science."

Organizers plan to expand the awards program in the future, offering an additional two awards (\$500 per year) to high school students in 2010 and 2011 with the help of funding from the Ontario Research Fund (Government of Ontario) as well as from additional industry partners in coming years. Only Scarborough schools participated this year, but Simpson said he hopes to expand the nomination pool through the Greater Toronto Area and Durham region.

Grades were not the sole criteria for the awards, although academic standing was important, Simpson said. An aptitude for original thinking, enthusiasm for scientific exploration, and a demonstrated interest in science as a career field were also considered by nominating schools. All students submitted an essay describing their interests and aspirations for a future career in scientific research and teaching, as well as letters of recommendation from principals and science teachers.

The selection committee included UTSC professors **André Simpson** and **Dave McNally**, **Janet Blakely** from the Department of Physical and Environmental Sciences, and **Dr. Henry Stronks** of Bruker BioSpin Ltd.

Photos by Ken Jones. For other photos from the day
http://www.utsc.utoronto.ca/~info/gallery/Outstanding_Highschool_Awards/



Contribution by Lauren Drake (ITC, Regina)

Focus on Regina

The University of Regina's International Test Centre for CO₂ Capture has been described by the US Department of Energy, among others, as one of the best-equipped research laboratories in North America. The \$12 million facility boasts four specialized analytical labs and a \$3.3 million in-house CO₂ capture pilot plant. ITC also has a \$5.2 million pre-commercial capture demonstration plant at a power plant facility located approximately two hours from the research centre.

The ITC is best known for its post-combustion capture research and development program, which entails everything from fundamental studies and solvent development to process configuration testing and pre-commercial demonstration. However, in addition to this groundbreaking capture R&D, ITC also offers commercial analytical services utilizing the facility's full array of state-of-the-art equipment.

ITC's equipment includes a number of highlights, and the particularly unique aspect of much of the equipment is the unusual couplings of certain units. For example, the 500-MHz Nuclear Magnetic Resonance (NMR) machine determines the molecular structure of most organic and some inorganic molecules, and the system configuration is highly unique in that it provides analysis of both solids and liquids. However, the NMR's rare coupling to a high performance liquid chromatograph (HPLC) permits separation of complex liquid mixtures prior to analysis, allowing for a complete breakdown of a sample's molecular

components. This set-up is ideal for studying reaction mechanisms, degradation products, proteins, drug metabolites, etc.

HPLC coupled with mass spectrometry is also used for separation and identification of mixtures of non-ionic, non-polar liquids such as hydrocarbons. To complement this, Capillary Electrophoresis is used for separation and identification of components within polar ionic liquids, such as inorganic metal ions, anions, CO₂ scrubbing solvents, and simple organic acids.

Another important coupling is the Thermo Gravimetric Analyzer – Differential Scanning Calorimeter. In this case, the DSC monitors heat flow in and out of samples while the TGA measures the accompanying weight loss. Typically coupled with Fourier Transform Infrared Spectrometry (FTIR) or Gas Chromatography (GC) for analysis of gaseous decomposition products evolving from samples, the TGA-DSC permits fundamental studies of thermal properties – oxidative stability, thermal degradation, specific heat, and reaction kinetics.

The FTIR is a particularly versatile piece of equipment. In addition to the above application, the FTIR is used for identification and quantification of organic species and some inorganic species in solids, liquids, gases, and thin films. This particular FTIR is capable of analyses over the entire infrared spectrum and is typically used in conjunction with the NMR for elucidation of molecular structure. It is equipped with a unique ATR (attenuated total reflectance) accessory, which allows study of chemical decomposition under varying pressure and temperature. It is usually used for solvent characterization.

ITC also has a suite of Gas Chromatography equipment for separation and identification of components within volatile liquids and gases. Typical applications include analysis of decomposition products and reaction intermediates. The GC family at ITC includes a GC-Mass Spectrometer, GC-Electron Capture Detector, GC-Flame Photometric Detector, and GC-Thermal Conductivity Detector.

Other interesting equipment couplings include the Scanning Electron Microscope – Energy Dispersive Spectrometer (SEM-EDS) and the

Inductively Coupled Plasma – Mass Spectrometer (ICP-MS). In the first case, the SEM provides imaging capabilities, while the EDS performs elemental mapping of the microscope images. Applications include studies of corrosion mechanisms and catalyst and membrane characterization. In the second case, the Varian ICP-MS determines elemental composition of digestible solids and liquids, including the valency of metals. This instrument is highly versatile, as it performs analysis of trace elements in materials, metals, rocks, minerals, and catalyst at the parts per million to parts per billion level.

Finally, one of our most important pieces of equipment, along with the NMR and the SEM-EDS), is the X-Ray Diffractometer. The XRD permits non-destructive identification of minerals and crystalline materials. Applications include characterization of catalysts, membranes, and packing materials, and it is also used in corrosion studies.

Taken together, this suite of equipment enables the ITC to determine the molecular and chemical composition of most organic and inorganic materials, measure chemical and molecular degradation, and identify and measure catalytic and thermal reactivity of substances. Typically, these analyses are used for chemical separation and identification; material and solvent analysis, characterization, and testing; flue gas analysis and characterization; corrosion analysis; and catalyst and membrane analysis, characterization, and testing.

However, ITC's analytical services are not restricted to carbon capture applications. ITC is capable of conducting a wide range of testing and is open to clients in any industry that can make use of this unique array of equipment. ITC has expert operators to assist with any analyses, and confidentiality is enforced by keycard security and limited/monitored laboratory access. For more information on ITC's analytical services or research and development, visit

www.co2-research.ca

or email

info.analytical@co2-research.ca

Canadian doctors hunt tiny killer – misfolded prions

A feature story about the Centre for Prions and Protein Folding Diseases at the University of Alberta by *Troy Media*.

<http://www.troymedia.com/?p=6498>

Physicists solve difficult classical problem with one quantum bit

The scientists from the Institute for Quantum Computing (Waterloo) used liquid state NMR quantum information processor based on transcrotonic acid to solve the Jones polynomial.

<http://www.physorg.com/news182165495.html>

G. Passante, O. Moussa, C.A. Ryan, R. Laflamme, "Experimental Approximation of the Jones Polynomial with One Quantum Bit," *Physical Review Letters* **103** (2009) 250501. <http://dx.doi.org/10.1103/PhysRevLett.103.250501>

Second U.S.-Canada Winterschool on Biomolecular Solid-State NMR

The second U.S.-Canada Winter School on Biomolecular Solid State NMR was held in Stowe, Vermont, January 24-29, 2010. The Winterschool was designed to be a pedagogical meeting aimed at students and postdoctorals in the field of biomolecular solid-state NMR, as well as more senior scientists who are interested in entering this field. The school featured many leading researchers in the field.

All lecture materials and notes are available for download at

<http://fbml.scripts.mit.edu/Conferences/program>

Biology group issues challenge to computing

The "eNMR" project invites the biomolecular NMR community to participate in a large-scale test of modern computing algorithms to potentially improve efficiency, reproducibility and reliability of NMR structure determination.

<http://www.isgtw.org/?pid=1002229>



Submitted by David Bryce (Ottawa)

CSC 2010: Solid-State NMR Symposium

Dear NMR colleagues,

Gillian Goward and myself are organizing a symposium entitled "**Solid-State NMR: Methods and Applications**" at the 93rd Canadian Chemistry Conference and Exhibition in Toronto. The symposium is scheduled for the afternoon of Sunday, May 30 and all day Monday, May 31.

I would like to encourage you and your students to consider submitting abstracts for 20-minute talks and/or posters through the following link:

http://www.csc2010.ca/program/submit_abstract.html

The deadline for abstract submissions is February 15.

Confirmed speakers: Alex Bain (McMaster), Andreas Brinkmann (NRC-SIMS), Arno Kentgens (Radboud University, Nijmegen), Gang Wu (Queen's), Gillian Goward (McMaster), John Ripmeester (NRC-SIMS), Josef Zwanziger (Dalhousie), Kristopher Ooms (The King's University College, Edmonton), Marek Pruski (Iowa), Megan Spence (Pittsburgh), Peter MacDonald (Toronto), Robert Schurko (Windsor), Roderick Wasylishen (Alberta), Scott Kroeker (Manitoba), Simon Sharpe (Sick Kids), Timothy Cross (National High Magnetic Field Laboratory, Tallahassee), Vladimir Ladizhansky (Guelph)

Thank you, and we look forward to seeing you in Toronto!

Dave Bryce



The National Ultrahigh-Field NMR Facility for Solids is proud to support the CSC 2010 Conference.



5th Annual Solid-State NMR Workshop

The National Ultrahigh-Field NMR Facility for Solids and Bruker Canada are pleased to present the 5th Annual Solid-State NMR Workshop at the 93rd Canadian Chemistry Conference and Exhibition in Toronto (CSC 2010). The workshop will take place on **Saturday afternoon, May 29, 2010.**

This annual Canadian Solid-state NMR event focuses on the latest developments in solid-state NMR spectroscopy with emphasis on practical aspects and applications in materials and life sciences. The workshop will be of interest not only to NMR spectroscopists, but also to students and other researchers interested in using modern NMR techniques in their research practice.

Confirmed speakers

Alex Bain (McMaster), Scott Kroeker (Manitoba), Peter Pallister (Carleton/NRC), Leigh Spencer (McMaster), Andre Sutrisno (Western), Cory Widdifield (Ottawa)

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 2010 conference registration.

Submitted by Michèle Auger (Laval)

Pacifichem 2010: Biological Solid-State NMR Symposium

We are delighted to announce a 2.5 day symposium on biological solid-state NMR at Pacifichem 2010 in Hawaii, 15-20 December 2010. www.pacifichem2010.org

Advances in Solid-State NMR of Biological Molecules (Symposium #58) in the Topic area of Biological Chemistry

Organized by: Akira Naito, Michèle Auger, Ayyalusamy Ramamoorthy, Frances Separovic

The following topics will be discussed in this symposium:

- (i) technical developments in resolution and sensitivity enhancements of solid-state NMR
- (ii) high-resolution structure determination of biomolecules by solid-state NMR
- (iii) advances in structural biology of membrane proteins and peptides
- (iv) dynamics and biomolecular function by solid-state NMR
- (v) characterization of supramolecular complexes and fibril-forming proteins

Invited Speakers: Michèle Auger (CA), Jerry Chan (TW), Timothy Cross (US), Gary Drobny (US), Toshimichi Fujiwara (JP), John Gehman (AU), Mei Hong (US), Yoshitaka Ishii (US), Yongae Kim (KOR), Vladimir Ladizhansky (CA), Gary Lorigan (US), Ann McDermott (US), Francesca Marassi (US), Isabelle Marcotte (CA), Nobuaki Matsumori (JP), Konstantin Momot (AU), Akira Naito (JP), Kaoru Nomura (JP), Eric Oldfield (US), Stanley Opella (US), Tatyana Polenova (US), William Price (AU), Ayyalusamy Ramamoorthy (US), Takeshi Sato (JP), Jacob Schaefer (US), Frances Separovic (AU), Simon Sharpe (CA), Steven Smith (US), Suzana Straus (CA), Kiyonori Takegoshi (JP), Satoru Tuzi (JP), Gianluigi Veglia (US), David Weliky (US), Katherine Wildman (US), Kurt Zilm (US)

the Organizing Committee

Submit your abstract via the Pacifichem 2010 website by **April 5, 2010**. Details are available at <http://pacifichem.abstractcentral.com/>

Submitted by Scott Kroeker (Manitoba)

Pacifichem 2010: Solid-State NMR

You are invited to participate in a symposium on "Solid-State NMR Methods and Applications in Inorganic Materials" (#228) at **Pacifichem 2010**, to be held in Hawaii from December 15-20, 2010. This four-session symposium is organized by Scott Kroeker, Jerry C.C. Chan, Sophia Hayes and Kiyonori Takegoshi.

Invited speakers include C. Bonhomme (FR), H. Eckert (GR), A. Goto (JP), G.R. Goward (CA), H.-M. Kao (TW), S.K. Lee (SK), S.-B. Liu (TW), H. Maekawa (JP), M. Murakami (JP), J.A. Reimer (US), J.A. Ripmeester (CA), K. Schmidt-Rohr (US), J.F. Stebbins (US), R.E. Wasylshen (CA)

You may also be interested in two other solid-state NMR symposia on offer at Pacifichem 2010: "NMR Spectroscopy of Polymers: Innovative NMR Strategies for Complex Macromolecular Systems" and "Advances in Solid-State NMR of Biological Molecules".

Abstract submission deadline is April 5, 2010.

For further information, see

www.pacifichem2010.org

or contact Scott Kroeker

Scott_Kroeker@UManitoba.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

NANUC Newsletters

<http://archive.constantcontact.com/fs083/1102124547477/archive/1102424169010.html>

NMR Theses Recently Defended

Congratulate your students here!

Lichi Shi (University of Guelph) December 2009

Supervisors: Leonid Brown and Vladimir Ladizhansky

Ph.D. thesis: "Solid-state NMR study of proteorhodopsin in the lipid environment: spectra assignments and structural insights"

Recognition

Tom Ziegler (University of Calgary) has been awarded **the 2010 CIC medal**. This award is presented by the Chemical Institute of Canada (CIC) as a mark of distinction and recognition to a person who has made an outstanding contribution to the science of chemistry or chemical engineering in Canada.

André Simpson (University of Toronto Scarborough) is the recipient of **the 2010 CSC Fred Beamish Award**. This award is presented to individuals who demonstrate innovation in research in the field of Analytical Chemistry, in particular, where research is anticipated to have significant potential for practical applications.

Michèle Auger (Université Laval) has been elected **Fellow of the CIC**. CIC Fellowships are granted to individuals for exceptional contributions to the chemical professions.

Robert Schurko (University of Windsor) has received **the 2009 Faculty Performance Award** by the University of Windsor for his achievements in research, service, and teaching.

On the move

Michelle Forgeron joined the Department of Chemistry at the University of Calgary in January 2010 as Manager of Instrumentation Facility and Services. Michelle is happy to be back in Alberta and close to the mountains!

Michelle can be reached at Michelle.Forgeron@UCalgary.ca or by phone at 403.220.7278

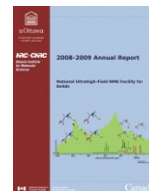
Tony Montana is the new NMR Facility Manager at the University of Lethbridge. http://www.uleth.ca/fas/phy/extra_content/nmr/index.html

Darcy Burns has joined the NMR Facility at the University of Toronto (Chemistry) as Associate Manager. Darcy managed the NMR Facility at Trent following his Ph.D. with Dr Drew Woolley at the University of Toronto. <http://www.chem.utoronto.ca/facilities/nmr/staff.html>

the 900 NMR Facility News

2008-2009 Annual Report

The 2008/09 Annual Report of the National Ultrahigh-Field NMR Facility for Solids has been finalized and 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.

NMR Facility user survey

The National Ultrahigh-Field NMR Facility for Solids is conducting the Facility user survey. Please contact Victor Terskikh if you would like to participate. The survey ends on February 28.

Major upgrades at the 900 NMR Facility

The Avance II 900 NMR spectrometer has been in service for over four years already, acquiring spectra 24/7 with virtually no downtime. To ensure the best system performance and improved reliability for many years to come the Facility Steering Committee has approved a series of upgrades which are currently being implemented.

In January the software was upgraded from TopSpin 1 to TopSpin 2, which also involved the complete workstation replacement. All user accounts and data have been successfully transferred over. The satellite data backup and archival server is in the process of replacement.

As part of this upgrade and also as preventative maintenance some hardware components in the spectrometer have been replaced with newer and more advanced versions.

Our NMR Facility strives to be at the forefront of solid-state NMR research providing the Canadian NMR community with the state-of-the-art instrumentation. Thank you for supporting our efforts!

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.

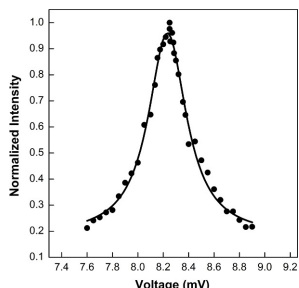
http://nmr900.ca/policies_e.html

Recent Travel Grant Recipients

Hiyam Hamaed (University of Windsor)

Margaret Hanson (University of Western Ontario)

Hall sensor for magic angle setup



Magic angle adjustment in MAS probes is commonly performed by observing ST spinning sidebands in ^{79}Br MAS NMR spectra of KBr at low spinning speeds. The magic angle is set correctly when the sidebands have the

highest intensity. A Hall effect magnetic flux sensor can be used for the same purpose, for example in low-gamma MAS probes incapable of ^{79}Br NMR.

We have recently tested this approach at the 900 NMR Facility: The figure shows the normalized intensity of the ^{79}Br ST spinning sidebands in KBr versus the Hall voltage measured. This Hall sensor will be used for magic angle setup in a 2.5 mm boron-free MAS probe which is currently under construction.

For more information see

S. Mamone, A. Dorsch, O.G. Johannessen, M.V. Naik, P.K. Madhu, M.H. Levitt, "A Hall effect angle detector for solid-state NMR," *Journal of Magnetic Resonance* **190** (2008) 135-141.

<http://dx.doi.org/10.1016/j.jmr.2007.07.012>

Upcoming NMR Events

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

Biophysical Society 54th Annual Meeting

February 20-24, 2010, San Francisco, CA
<http://www.biophysics.org/2010meeting>



Special event: Sunday, February 21, 6-7 pm, Biophysical Society of Canada Mixer



9th Chemical Biophysics Symposium

April 9-11, 2010, University of Toronto
Abstract submission deadline March 7, 2010

<http://www.chembiophys.ca>

51st ENC Experimental Nuclear Magnetic Resonance Conference

April 18-23, 2010, Daytona Beach, FL
<http://www.enc-conference.org/>

Poster abstracts deadline March 12, 2010



5th Annual Solid-State NMR Workshop

at the 93rd Canadian Chemistry Conference and Exhibition (**CSC 2010**)

May 29, 2010, Toronto, ON
http://nmr900.ca/events_e.html



"Solid-State NMR: Methods and Applications" Symposium

at the 93rd Canadian Chemistry Conference and Exhibition (**CSC 2010**)

May 30-31, 2010, Toronto, ON
Abstract submission deadline February 15, 2010
<http://www.csc2010.ca/>

EUROMAR 2010 and 17th ISMAR Conference, a World Wide Magnetic Resonance Conference (**WWMR2010**)

July 4-9, 2010, Florence, Italy
<http://www.cerm.unifi.it/wwmr2010.html>


52nd Annual Rocky Mountain Conference on Analytical Chemistry


August 1-5, 2010, Snowmass, Colorado
<http://www.rockychem.com/>

 **3rd IUPAC International Conference on Green Chemistry**, August 15-18, 2010, Ottawa, ON
Abstract submission deadline April 8, 2010
<http://www.icgc2010.ca/>

ICMRBS 2010 the XXIVth International Conference on Magnetic Resonance in Biological Systems

August 22-27, 2010, Cairns, Australia
<http://www.icmrbs2010.org/>

 **MOOT XXIII NMR Symposium**
October, 2010, Dalhousie University, Halifax
<http://www.mootnmr.org>

 **Pacificchem 2010** The International Chemical Congress of Pacific Basin Societies
December 15-20, 2010, Honolulu, Hawaii, USA
<http://www.pacificchem.org/>

Abstract submission deadline is April 5, 2010.

NMR Spectroscopy of Polymers - Innovative NMR Strategies for Complex Macromolecular Systems (Symposium #12)
Peter Macdonald, University of Toronto

Biomolecular Structure and Dynamics - Recent Advances in NMR (Symposium #43)
Mitsuhiko Ikura, Ontario Cancer Institute

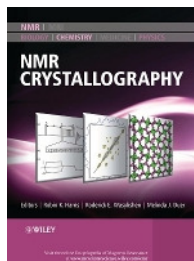
Advances in Solid-State NMR of Biological Molecules (Symposium #58) Michèle Auger, Université Laval

Solid-State NMR Methods and Applications in Inorganic Materials (Symposium #228)
Scott Kroeker, University of Manitoba

Magnetic Resonance Gordon Research Conference
June 12-17, 2011, Biddeford, ME
<http://www.grc.org/>

NMR Books

Disclaimer: For your information only. In this bulletin we are not endorsing any products or services.



NMR Crystallography

Robin K. Harris (Editor)
Roderick E. Wasylishen (Editor)
Melinda J. Duer (Editor)
Hardcover: 520 pages
Publisher: Wiley; January 2010
Language: English
ISBN: 978-0470699614

<http://www.amazon.com/dp/0470699612/>
<http://www.amazon.ca/dp/0470699612/>

Contributed by David Bryce

A new book on the subject of NMR crystallography has been published by Wiley as part of their "Encyclopedia of Magnetic Resonance Handbooks" series. While it will undoubtedly serve as a valuable reference for novices and experts alike, at 520 pages it is somewhat larger than a typical 'handbook'. Edited by our own **Rod Wasylishen**, along with the UK's **Robin Harris** and **Melinda Duer**, there are several Canadian contributors. We defer a full review until a later date; here, we provide a brief overview of the contents and highlight some Canadian contributions.

The volume is divided into six sections covering key areas including introductions to fundamental NMR interactions, crystal structure determination using NMR, properties of the crystalline state, and applications to crystalline solids. **Rod Wasylishen** (Alberta) presents the basics of dipolar and indirect coupling, and **Darren Brouwer** (Redeemer) discusses the topic of interplay between NMR and single-crystal X-ray diffraction, both areas in which these researchers have had a great impact. Following my own contribution on "Tensor Interplay", **Lindsay Cahill** and **Gillian Goward** (McMaster) examine intermolecular interactions and structural motifs within the framework of NMR crystallography. Rotational and translation dynamics, which can complicate the interpretation of NMR spectra,

particularly in the context of obtaining crystallographic information, are discussed in a subsequent chapter by the National Research Council's **Chris Ratcliffe**. The final Canadian contribution comes from **Kenneth Jeffrey** and **Glenn Penner** (Guelph), who tackle the subject of structural phase transitions.

The National Ultrahigh-Field NMR Facility for Solids in Ottawa has a copy of this wonderful volume on-hand, courtesy of Rod Wasylshen, for you to peruse during your next visit!

Canadian contributions

R.E. Wasylshen "Dipolar & Indirect Coupling: Basics," Chapter 10, *NMR Crystallography EMR Handbook*, Eds. R.K. Harris, R.E. Wasylshen, M.J. Duer, Wiley (2009) pp. 127-136.
<http://dx.doi.org/10.1002/9780470034590.emrstm1023>

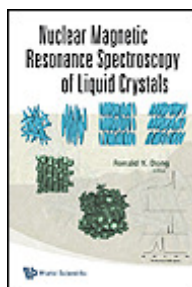
D.H. Brouwer "Interplay between NMR & Single-crystal X-ray Diffraction," Chapter 18, *NMR Crystallography EMR Handbook*, Eds. R.K. Harris, R.E. Wasylshen, M.J. Duer, Wiley (2009) pp. 263-274.
<http://dx.doi.org/10.1002/9780470034590.emrstm1041>

D.L. Bryce "Tensor Interplay," Chapter 20, *NMR Crystallography EMR Handbook*, Eds. R.K. Harris, R.E. Wasylshen, M.J. Duer, Wiley (2009) pp. 289-301.
<http://dx.doi.org/10.1002/9780470034590.emrstm1039>

L.S. Cahill, G.R. Goward "Intermolecular Interactions & Structural Motifs," Chapter 21, *NMR Crystallography EMR Handbook*, Eds. R.K. Harris, R.E. Wasylshen, M.J. Duer, Wiley (2009) pp. 305-319.
<http://dx.doi.org/10.1002/9780470034590.emrstm1074>

C.I. Ratcliffe "Rotational & Translational Dynamics," Chapter 24, *NMR Crystallography EMR Handbook*, Eds. R.K. Harris, R.E. Wasylshen, M.J. Duer, Wiley (2009) pp. 355-373.
<http://dx.doi.org/10.1002/9780470034590.emrstm1040>

K.R. Jeffrey, G.H. Penner "Structural Phase Transitions," Chapter 26, *NMR Crystallography EMR Handbook*, Eds. R.K. Harris, R.E. Wasylshen, M.J. Duer, Wiley (2009) pp. 387-413.
<http://dx.doi.org/10.1002/9780470034590.emrstm1051>



Nuclear Magnetic Resonance Spectroscopy of Liquid Crystals

edited by **Ronald Dong**
(University of British Columbia)
Hardcover: 464 pages
Publisher: World Scientific;
September 2009
Language: English
ISBN: 978-9814273664

<http://www.amazon.com/dp/981427366X>
<http://www.amazon.ca/dp/981427366X>

This book is now available to order from Amazon. *World Scientific* has made available online the Preface to this book written by **Ronald Dong**, and the First chapter.

<http://www.worldscibooks.com/materialsci/7310.html>

Contents (World Scientific):

1. Novel Strategies for Solving Highly Complex NMR Spectra of Solutes in Liquid Crystals (*E E Burnell et al.*)
2. Analytical Potentials of Natural Abundance Deuterium NMR Spectroscopy in Achiral Thermotropics and Polypeptide Chiral Oriented Solvents (*P Lesot & C Aroulande*)
3. Noble Gas Probes in NMR Studies of Liquid Crystals (*J Jokisaari*)
4. Bicelles — A Much Needed Magic Wand to Study Membrane Proteins by NMR Spectroscopy (*R Soong et al.*)
5. Advances in Proton NMR Relaxometry in Thermotropic Liquid Crystals (*P J Sebastião et al.*)
6. Deuterium NMR Study of Magnetic Field Distortions in Ferroelectric Mesogens (*R Y Dong*)
7. Deuteron NMR Study of the Effects of Random Quenched Disorder in 12CB Silica Dispersions (*D Finotello & V Pandya*)
8. Dynamics of Liquid Crystals by Means of Deuterium NMR Relaxation (*C A Veracini & V Domenici*)
9. Translational Self-Diffusion Measurements in Thermotropics by Means of Statistic Field Gradients NMR Diffusometry (*M Cifelli*)
10. Deuterium NMR Studies of Static and Dynamic Director Alignment for Low Molar Mass Nematics (*A Sugimura & G R Luckhurst*)
11. Viscoelastic Properties of Liquid Crystals: Statistical-Mechanical Approaches and Molecular Dynamics Simulations (*A V Zakharov*)
12. Carbon-13 NMR Studies of Thermotropic Liquid Crystals (*R Y Dong*)
13. A Combined DFT and Carbon-13 NMR Study of a Biaxial Bent-Core Mesogen (*A Marini et al.*)

NMR Jobs and Vacancies

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

University Health Network, Toronto

NMR Scientific Associate or Postdoctoral Fellow

Site: TDMT and Max Bell Research Center, University Health Network

Department: Research

Reports to: Dr. Cheryl Arrowsmith, Senior Scientist

Status: Permanent Full-time for Scientific Associate

<http://nmr.uhnres.utoronto.ca/arrowsmith/>

The Arrowsmith research laboratory and the Structural Proteomics in Toronto (SPiT) group, located at the University Health Network and affiliated with the University of Toronto, is one of the leading centres for genome-scale protein science in cancer structural biology. With support in place from the provincial and federal governments, U.S. National Institute of Health and the private sector, we are currently expanding our research team in the area of Nuclear Magnetic Resonance. We are seeking a Scientific Associate or Postdoctoral Fellow whose primary responsibility will be providing support to our NMR group.

We use state-of-the-art NMR instrumentation: Bruker 800, 600 and 500 MHz, all equipped with cryoprobes. We also have regular user time on Varian 600 and 500 MHz spectrometers. Specialized and qualified expertise is required for maintaining and running the instruments as well as training other members of the group. The service component of the position is estimated at 50% of the time. The successful candidate should have a solid background in biomolecular NMR and is expected to pursue independent research projects as a member of the structural proteomics team. Additional responsibilities may include the management of fee-for-service projects and academic collaborations.

The ideal candidate will be a team player, able to learn and adapt quickly and have excellent

interpersonal and communication skills. He/she will be detail-oriented, self-organized, motivated, and energetic. Computer skills (Linux and NMR related software) are required. We offer competitive salaries, commensurate with experience.

Qualifications

- PhD in Biophysics or related disciplines
- 0 to 10 years of experience post PhD
- Ability to work independently, yet be a team player
- Excellent verbal and written communication skills

Please submit your resume to **Michelle Deeton**, Manager:

E-mail: mdeeton@uhnres.utoronto.ca

or fax to (416) 340-4004

University Health Network thanks all applicants, however, only those selected for an interview will be contacted.

UHN has a diverse workforce and is an equal opportunity employer. Improving the patient's experience through patient-centred care! For additional information on patient-centred care please go to www.uhn.ca

Hospital for Sick Children, Toronto

Postdoctoral position in biological solid-state NMR

Postdoctoral positions in biomolecular solid state NMR are available at The Hospital for Sick Children. These positions will focus on structure determination and dynamic characterization of protein and peptide assemblies by solid state NMR, with an emphasis on systems relevant to human health and disease. Ongoing projects include structural studies of oligomeric states of mammalian prion proteins, membrane interactions of amyloid peptides, and structure determination of integral membrane complexes that play a key role in HIV-1 infection. These projects are highly multidisciplinary in nature, and will provide candidates with the opportunity to learn a broad range of biophysical techniques, in addition to NMR, and to collaborate with a number of other research groups.

<http://www.sickkids.ca/Research/Sharpe-lab/index.html>

Our lab is located within the Molecular Structure and Function Program at the Hospital for Sick Children and the Department of Biochemistry at the University of Toronto, providing a diverse and stimulating research environment. We are fully equipped for cloning, mutagenesis, protein expression and purification, with access to peptide synthesis, computational biology facilities and full-time use of a 500 MHz spectrometer for solids MAS and static experiments. In addition, access to the National 900 MHz NMR facility in Ottawa is also available for most projects.

Highly motivated candidates are sought, who must possess a PhD with a strong track record of scientific productivity, and who should have extensive experience in either biological NMR (solution or solid state) or protein biophysics and structure determination. The start date for this position is negotiable, but is available immediately.

Qualified candidates should send a complete CV to ssharp@sickkids.ca and arrange for 3 letters of reference to be sent to:

Simon Sharpe

Scientist, Molecular Structure and Function Program

The Hospital for Sick Children
Assistant Professor, Dept. of Biochemistry
University of Toronto
555 University Ave,
Toronto, Ontario
Canada M5G 1X8
Email: ssharp@sickkids.ca

NHMFL, Tallahassee

Two postdoctoral positions in protein solid state NMR

Dear Colleagues,

Two postdoc positions are available immediately in solid state NMR of membrane proteins in my research group at the National High Magnetic Field Laboratory. Spectroscopy is conducted on a range of instruments from 400 to 900 MHz. Applicants with experience in NMR, preferably biological solid state NMR are encouraged to apply. This NIH funded science is focused on the characterization of potential drug targets for fighting TB and Influenza.

While much of my lab's focus has been on aligned samples, I am also interested in pursuing magic angle spinning approaches for characterizing these important membrane protein targets. It has become increasingly clear that these proteins must be characterized in lipid bilayer environment. Solid state NMR is becoming the key technology for the characterization of membrane proteins. Please send a CV and the names and addresses of three references to me if you are interested. Additional information is also available upon request.

Timothy A. Cross

NMR Spectroscopy and Imaging Program
Director
National High Magnetic Field Laboratory
1800 E. Paul Dirac Dr., Tallahassee, FL 32310-3706
Tel: 850-644-0917
Fax: 850-644-1366
Email: cross@magnet.fsu.edu

<http://www.magnet.fsu.edu/search/personnel/getprofile.aspx?fname=Timothy&lname=Cross>

Earl Frieden Professor of Chemistry and Biochemistry
Florida State University
Tallahassee, FL 32306

Postdoctoral NMR positions available

http://nmr900.ca/nmr_jobs.html

CEA-Saclay, France. One fellowship is currently available to join the group of Dr. Dimitris Sakellariou.

University of Lille and CEA, France. A 3-year PhD position in Solid-State NMR & Glass is available at the University of Lille and CEA.

University of Ulster, UK. A post-doctoral research associate is required to work with Dr. Mateus Webba da Silva on control of folding of G-quadruplex nucleic acids.

University of Southern California, Los Angeles. Two postdoctoral positions are available in the group of Tobias Ulmer.

Utrecht University, The Netherlands. Immediate openings for a Ph.D. student and a postdoctoral fellow in solid-state NMR.

Iowa State University, Department of Chemistry. A postdoctoral position in biological solid-state NMR research of membrane proteins and other biomolecules.

Vanderbilt University Institute of Imaging Science. Postdoctoral position in hyperpolarized MR for in vivo and in vitro hyperpolarized and conventional multi-nuclear NMR.

Listings of NMR jobs and vacancies

Canadian NMR Jobs

http://nmr900.ca/nmr_jobs.html

NMR Wiki

<http://nmrwiki.org/wiki/index.php?title=Category:Jobs>

NMR jobs on the NMR Information Server

<http://www.spincore.com/nmrjobs/>

AMPERE mailing list

<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>

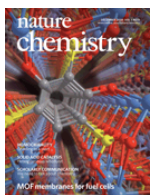
FG-MR Jobs

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

Canadian NMR Research Highlights

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

Cover article in *Nature Chemistry*



A research team from the **University of Calgary** and the **NRC Steacie Institute for Molecular Sciences** (Ottawa) has published a cover article in *Nature Chemistry*

J.A. Hurd, R. Vaidhyanathan, V. Thangadurai, C.I. Ratcliffe, I.L. Moudrakovski and G.K.H. Shimizu, "Proton Conduction at 150°C in a Nanoporous Metal-Organic Framework," *Nature Chemistry* **1** (2009) 705-710.

<http://dx.doi.org/10.1038/nchem.402>

"Materials built from metal centres and organic ligands have traditionally attracted attention for their channels' host-guest properties. Now, controlling the occupancy of the channels by guest molecules has resulted in a framework that conducts protons under anhydrous

conditions and acts as a gas-tight membrane, offering a promising approach to fuel-cell electrolytes." Solid-state NMR spectroscopy was instrumental in this research.

The paper is also accompanied by the Nature's commentary.

Hiroshi Kitagawa, "Metal-organic frameworks: Transported into fuel cells," *Nature Chemistry* **1** (2009) 689-690.
<http://dx.doi.org/10.1038/nchem.454>

Cover article in the *Journal of Physical Chemistry*



Crystalline beta-barium borate is an important nonlinear optical material often used in frequency mixing. Interestingly enough, even though beta-barium borate has been known for years, there still exists a controversy about its true

crystallographic space group. That is existed until now! In this cover article in the *Journal of Physical Chemistry C* a research team from the **University of Western Ontario** has solved this problem using ultrahigh-field solid-state NMR spectroscopy and quantum chemical calculations.

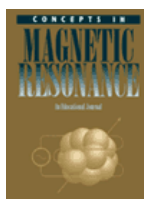
Andre Sutrisno, Cheng Lu, Robert Lipson, Yining Huang, "Combined $^{135/137}\text{Ba}$ Solid-state NMR at an Ultrahigh Magnetic Field and Computational Study of beta-Barium Borate," *Journal of Physical Chemistry C* **113** (2009) 21196-21201. **(Cover Article)**

<http://dx.doi.org/10.1021/jp9044786>



This is a **seventh cover article** featuring results obtained using resources of the National Ultrahigh-Field NMR Facility for Solids.

Concepts in Magnetic Resonance



R.M. Gregory, A.D. Bain, "The effects of finite rectangular pulses in NMR: Phase and intensity distortions for a spin-1/2," *Concepts in Magnetic Resonance Part A* **34A** (2009) 305-314.

<http://dx.doi.org/10.1002/cmr.a.20147>

Biochimica et Biophysica Acta (BBA) – Biomembranes



Special issue: "Membrane Protein Dynamics by NMR: Correlation of Structure and Function"

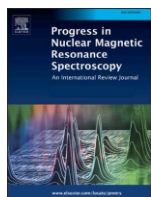
Volume 1798, Issue 2, Pages 65-302 (February 2010)

Edited by: A. Ramamoorthy and G. Veglia

T. Reddy, X. Li, L. Fliegel, B.D. Sykes, J.K. Rainey, "Correlating structure, dynamics, and function in transmembrane segment VII of the Na⁺/H⁺ exchanger isoform 1," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1798** (2010) 94-104. (**special issue**)
<http://dx.doi.org/10.1016/j.bbamem.2009.06.025>

M. Ouellet, N. Voyer, M. Auger, "Membrane interactions and dynamics of a 21-mer cytotoxic peptide: A solid-state NMR study," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1798** (2010) 235-243. (**special issue**)
<http://dx.doi.org/10.1016/j.bbamem.2009.07.029>

Progress in NMR Spectroscopy



P.T. Eles, C.A. Michal, "Two-Photon Excitation in Nuclear Magnetic and Quadrupole Resonance," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2010) in press. (**Invited Review**)

<http://dx.doi.org/10.1016/j.pnmrs.2009.12.002>

Chemical Physics Letters

Editor's choice article

A. Brinkmann, S.K. Vasa, H. Janssen, A.P.M. Kentgens, "Proton Micro-Magic-Angle-Spinning NMR Spectroscopy of Nanoliter Samples," *Chemical Physics Letters* **485** (2010) 275-280. (**Editor's Choice**)
<http://dx.doi.org/10.1016/j.cplett.2009.12.054>

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.

Memorial University of Newfoundland

T.-C. Yang, J. Rendell, W. Gulliver, V. Booth, "Peptide T exhibits a well-defined structure in fluorinated solvent at low temperature," *Journal of Peptide Science* **15** (2009) 818-823.
<http://dx.doi.org/10.1002/psc.1179>

Dalhousie University

B. Chen, U. Werner-Zwanziger, M.L.F. Nascimento, L. Ghussn, E.D. Zanotto and J.W. Zwanziger, "Structural Similarity on Multiple Length Scales and Its Relation to Devitrification Mechanism: A Solid-State NMR Study of Alkali Diborate Glasses and Crystals," *J. Phys. Chem. C* **113** (2009) 20725-20732.
<http://dx.doi.org/10.1021/jp907259e>

University of New Brunswick

J.C. García-Naranjo, P.M. Glover, F. Marica, B.J. Balcom, "Variable Bandwidth Filtering for Magnetic Resonance Imaging with Pure Phase Encoding," *Journal of Magnetic Resonance* **202** (2010) 234-238.
<http://dx.doi.org/10.1016/j.jmr.2009.11.006>

Université Laval

M. Ouellet, N. Voyer, M. Auger, "Membrane interactions and dynamics of a 21-mer cytotoxic peptide: A solid-state NMR study," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1798** (2010) 235-243. (**special issue**)
<http://dx.doi.org/10.1016/j.bbamem.2009.07.029>

McGill University

G. Kozlov, M. Ménade, A. Rosenauer, L. Nguyen, K. Gehring, "Molecular determinants of PAM2 recognition by the MLLE domain of poly(A)-binding protein," *Journal of Molecular Biology* (2010) in press.
<http://dx.doi.org/10.1016/j.jmb.2010.01.032>

J.-F. Trempe, C.X.-Q. Chen, K. Grenier, E.M. Camacho, G. Kozlov, P.S. McPherson, K. Gehring, and E.A. Fon, "SH3 Domains from a Subset of BAR Proteins Define a Ubl-Binding Domain and Implicate Parkin in Synaptic Ubiquitination," *Molecular Cell* **36** (2009) 1034-1047.
<http://dx.doi.org/10.1016/j.molcel.2009.11.021>

NRC-SIMS

H. Lu, T.D. Lorenson, I.L. Moudrakovski, J.A. Ripmeester, T.S. Collett, R.B. Hunter, C.I. Ratcliffe, "The characteristics of gas hydrates recovered from BPXA-DOE-USGS Mount Elbert Gas Hydrate Stratigraphic Test Well, Alaska North Slope," *Marine and Petroleum Geology* (2010) accepted.
<http://dx.doi.org/10.1016/j.marpetgeo.2010.01.002>

A. Brinkmann, S.K. Vasa, H. Janssen, A.P.M. Kentgens, "Proton Micro-Magic-Angle-Spinning NMR Spectroscopy of Nanoliter Samples," *Chemical Physics Letters* **485** (2010) 275-280. (Editor's Choice)
<http://dx.doi.org/10.1016/j.cplett.2009.12.054>

S. Takeya, K.A. Udachin, I.L. Moudrakovski, R. Susilo and J.A. Ripmeester, "Direct Space Methods for Powder X-ray Diffraction for Guest-Host Materials: Applications to Cage Occupancies and Guest Distributions in Clathrate Hydrates," *J. Am. Chem. Soc.* **132** (2010) 524-531.
<http://dx.doi.org/10.1021/ja905426e>

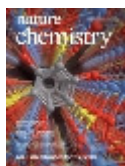
J. Seol, J.-W. Lee, D.-Y. Kim, S. Takeya, J.A. Ripmeester and H. Lee, "Molecular Cage Occupancy of Clathrate Hydrates at Infinite Dilution: Experimental Determination and Thermodynamic Significance," *Journal of Physical Chemistry B* **114** (2010) 804-808.
<http://dx.doi.org/10.1021/jp909982n>



P.G. Gordon, D.H. Brouwer, J.A. Ripmeester, "Probing the Local Structure of Pure Ionic Liquid Salts with ³⁵Cl, ⁷⁹Br and ¹²⁷I Solid- and Liquid-State NMR," *ChemPhysChem* **11** (2010) 260-268.
<http://dx.doi.org/10.1002/cphc.200900624>



I. Moudrakovski, S. Lang, S. Patchkovskii and J. Ripmeester, "High Field ³³S Solid State NMR and First-Principles Calculations in Potassium Sulfates," *J. Phys. Chem. A* **114** (2010) 309-316.
<http://dx.doi.org/10.1021/jp908206c>



J.A. Hurd, R. Vaidhyanathan, V. Thangadurai, C.I. Ratcliffe, I.L. Moudrakovski and G.K.H. Shimizu, "Proton Conduction at 150°C in a Nanoporous Metal-Organic Framework," *Nature Chemistry* **1** (2009) 705-710. (Cover article)
<http://dx.doi.org/10.1038/nchem.402>

M.Li, J. Ouyang, C.I. Ratcliffe, L. Pietri, X. Wu, D.M. Leek, I. Moudrakovski, Q. Lin, B. Yang and K. Yu, "CdS Magic-Sized Nanocrystals Exhibiting Bright Band Gap Photoemission via Thermodynamically Driven Formation," *ACS Nano* **3** (2009) 3832-3838.
<http://dx.doi.org/10.1021/nn9009455>

University of Ottawa



C.M. Widdifield and D.L. Bryce, "Solid-State ^{79/81}Br NMR and Gauge-Including Projector-Augmented Wave Study of Structure, Symmetry, and Hydration State in Alkaline Earth Metal Bromides," *Journal of Physical Chemistry A* **114** (2010) 2102-2116.
<http://dx.doi.org/10.1021/jp909106j>

G. Defontaine, A. Barichard, S. Letaief, C. Feng, T. Matsuura, C. Detellier, "Nanoporous polymer - clay hybrid membranes for gas separation," *Journal of Colloid and Interface Science* **343** (2010) 622-627.
<http://dx.doi.org/10.1016/j.jcis.2009.11.048>

S. Monfette, A.K. Crane, J.A.D. Silva, G.A. Facey, E.N. dos Santos, M.H. Araujo, D.E. Fogg, "Monitoring Ring-Closing Metathesis: Limitations on the Utility of ¹H NMR Analysis,"

Inorganica Chimica Acta **363** (2010) 481-486.
<http://dx.doi.org/10.1016/j.ica.2009.09.030>



T. Pathmalingam, F. Habib, C.M. Widdifield, F. Loiseau, T.J. Burchell, S.I. Gorelsky, A.M.

Beauchemin, D.L. Bryce, and M. Murugesu, "Combining Oximes with Azides to Create a Novel 1D Chain [NaCo^{III}₂] System: Synthesis, Structure, and Solid-State NMR," *Dalton Transactions* **39** (2010) 1504-1510.
<http://dx.doi.org/10.1039/b918082f>

D.L. Bryce, N.M. Dorval Courchesne, F.A. Perras, "Measurement of $\Delta^1J(^{199}\text{Hg}, ^{31}\text{P})$ in [HgPCy₃(OAc)₂]₂ and relativistic ZORA DFT investigations of mercury-phosphorus coupling tensors," *Solid State Nuclear Magnetic Resonance* **36** (2009) 182-191.
<http://dx.doi.org/10.1016/j.ssnmr.2009.11.004>

Queen's University

P. Gillespie, G. Wu, M. Sayer and M.J. Stott, "Si complexes in calcium phosphate biomaterials," *Journal of Materials Science: Materials in Medicine* **21** (2010) 99-108.
<http://dx.doi.org/10.1007/s10856-009-3852-8>

University of Toronto

M.J. Smith, W.R. Hardy, G.Y. Li, M. Goudreault, S. Hersch, P. Metalnikov, A. Starostine, T. Pawson, M. Ikura, "The PTB domain of ShcA couples receptor activation to the cytoskeletal regulator IQGAP1," *EMBO J.* (2010) online.
<http://dx.doi.org/10.1038/emboj.2009.399>

G.M. Gasmi-Seabrook, C.B. Marshall, M. Cheung, B. Kim, F. Wang, Y.J. Jang, T.W. Mak, V. Stambolic, M. Ikura, "A real-time NMR study of guanine nucleotide exchange and activation of RhoA by PDZ-RHOGEF," *J. Biol. Chem.* (2010) online.
<http://dx.doi.org/10.1074/jbc.M109.064691>

M.T. Mazhab-Jafari, C.B. Marshall, M. Smith, G.M. Gasmi-Seabrook, V. Stambolic, R. Rottapel, B.G. Neel, M. Ikura, "Real-time NMR study of three small GTPases reveals that fluorescent mant-tagged nucleotides alter hydrolysis and exchange

kinetics," *J. Biol. Chem.* (2010) online.
<http://dx.doi.org/10.1074/jbc.C109.064766>

A.M. Ruschak and L.E. Kay, "Methyl groups as probes of supra-molecular structure, dynamics and function," *Journal of Biomolecular NMR* **46** (2010) 75-87.
<http://dx.doi.org/10.1007/s10858-009-9376-1>

J.R. McKelvie, M. Elsner, A.J. Simpson, B. Sherwood Lollarand and M.J. Simpson, "Quantitative Site-Specific ²H NMR Investigation of MTBE: Potential for Assessing Contaminant Sources and Fate," *Environ. Sci. Technol.* **44** (2010) 1062-1068.
<http://dx.doi.org/10.1021/es9030276>

D.F. Hansen, P. Neudecker, P. Vallurupalli, F.A.A. Mulder and L.E. Kay, "Determination of Leu Side-Chain Conformations in Excited Protein States by NMR Relaxation Dispersion," *J. Am. Chem. Soc.* **132** (2010) 42-43.
<http://dx.doi.org/10.1021/ja909294n>

X. Feng, A.J. Simpson, W.H. Schlesinger, M.J. Simpson, "Altered microbial community structure and organic matter composition under elevated CO₂ and N fertilization in the duke forest," *Global Change Biology* (2010) Early View.
<http://dx.doi.org/10.1111/j.1365-2486.2009.02080.x>

Y. Xu, A.J. Simpson, N. Eyles, M.J. Simpson, "Sources and molecular composition of cryoconite organic matter from the Athabasca Glacier, Canadian Rocky Mountains," *Organic Geochemistry* **41** (2010) 177-186.
<http://dx.doi.org/10.1016/j.orggeochem.2009.10.010>

R. Soong, M.-P. Nieh, E. Nicholson, J. Katsaras and P.M. Macdonald, "Bicellar Mixtures Containing Pluronic F68: Morphology and Lateral Diffusion from Combined SANS and PFG NMR Studies," *Langmuir* (2010) ASAP.
<http://dx.doi.org/10.1021/la902795h>

N. MacKinnon, G. Guerin, B. Liu, C.C. Gradinaru, J.L. Rubinstein and P.M. Macdonald, "Triggered Instability of Liposomes Bound to Hydrophobically Modified Core-Shell PNIPAM Hydrogel Beads," *Langmuir* **26** (2010) 1081-1089.
<http://dx.doi.org/10.1021/la902423v>

F. Wang, C.B. Marshall, G.Y. Li, K. Yamamoto, T.W. Mak, M. Ikura, "Synergistic interplay between promoter recognition and CBP/p300 coactivator recruitment by FOXO3a," *ACS Chem. Biol.* **18** (2009) 1017-1027.
<http://dx.doi.org/10.1021/cb900190u>

J.M. Murphy, D.F. Hansen, S. Wiesner, D.R. Muhandiram, M. Borg, M.J. Smith, F. Sicheri, L.E. Kay, J.D. Forman-Kay, T. Pawson, "Structural Studies of FF Domains of the Transcription Factor CA150 Provide Insights into the Organization of FF Domain Tandem Arrays," *Journal of Molecular Biology* **393** (2009) 409-424.
<http://dx.doi.org/10.1016/j.jmb.2009.08.049>

McMaster University

S.K. Amini, H. Shaghghi, A.D. Bain, A. Chabok, M. Tafazzoli, "Magnetic resonance tensors in uracil: Calculation of ^{13}C , ^{15}N , ^{17}O NMR chemical shifts, ^{17}O and ^{14}N electric field gradients and measurement of ^{13}C and ^{15}N chemical shifts," *Solid State Nuclear Magnetic Resonance* (2010) accepted.
<http://dx.doi.org/10.1016/j.ssnmr.2009.12.001>

T.R. Field and A.D. Bain, "Origins of Spin Noise," *Applied Magnetic Resonance* (2010) online.
<http://dx.doi.org/10.1007/s00723-009-0107-2>

J.W. Traer and G.R. Goward, "The proton dynamics of imidazole methylphosphonate: an example of cooperative ionic conductivity," *Physical Chemistry Chemical Physics* **12** (2010) 263-272.
<http://dx.doi.org/10.1039/b917360a>

L.J.M. Davis, I. Heinmaa and G.R. Goward, "Study of Lithium Dynamics in Monoclinic $\text{Li}_3\text{Fe}_2(\text{PO}_4)_3$ using ^6Li VT and 2D Exchange MAS NMR Spectroscopy," *Chem. Mater.* (2010) ASAP.
<http://dx.doi.org/10.1021/cm901402u>

J. Milojevic, A. Raditsis, G. Melacini, "Human Serum Albumin Inhibits A beta Fibrillization through a "Monomer-Competitor" Mechanism," *Biophysical Journal* **97** (2009) 2585-2594.
<http://dx.doi.org/10.1016/j.bpj.2009.08.028>

R.M. Gregory, A.D. Bain, "The effects of finite rectangular pulses in NMR: Phase and intensity distortions for a spin-1/2," *Concepts in Magnetic Resonance Part A* **34A** (2009) 305-314.
<http://dx.doi.org/10.1002/cmr.a.20147>


R.M. Epand, R.F. Epand, B. Berno, L. Pelosi and G. Brandolin, "Phosphatidic Acid Association with the Bovine Mitochondrial ADP/ATP Carrier," *Biochemistry* **48** (2009) 12358-12364.
<http://dx.doi.org/10.1021/bi901769r>


University of Guelph

R. Janik, E. Ritz, A. Gravelle, L. Shi, X. Peng, V. Ladizhansky, "Inter-residue carbonyl-carbonyl polarization transfer experiments in uniformly ^{13}C , ^{15}N -labeled peptides and proteins," *Journal of Magnetic Resonance* **203** (2010) 177-184.
<http://dx.doi.org/10.1016/j.jmr.2009.12.014>

C. Cousins, G.H. Penner, B. Liu, P. Beckett, G. Spiers, "Organic matter degradation in paper sludge amendments over gold mine tailings," *Applied Geochemistry* **24** (2009) 2293-2300.
<http://dx.doi.org/10.1016/j.apgeochem.2009.09.009>

University of Waterloo

 **K.H. Mroué, A.-H.M. Emwas, and W.P. Power,** "Solid-state ^{27}Al Magnetic Resonance Investigation of Three Aluminum-Centred Dyes," *Canadian Journal of Chemistry* **88** (2010) 111-123.
<http://dx.doi.org/10.1139/V09-155>

 **K.H. Mroué and W.P. Power,** "High-Field Solid-State ^{67}Zn NMR Spectroscopy of Several Zinc-Amino Acid Complexes," *Journal of Physical Chemistry A* **114** (2010) 324-335.
<http://dx.doi.org/10.1021/jp908325n>


G. Passante, O. Moussa, C.A. Ryan, R. Laflamme, "Experimental Approximation of the Jones Polynomial with One Quantum Bit," *Physical Review Letters* **103** (2009) 250501(1-4).
<http://dx.doi.org/10.1103/PhysRevLett.103.250501>

J.F. Zhang, M. Ditty, D. Burgarth, C.A. Ryan, C.M. Chandrashekar, M. Laforest, O. Moussa, J. Baugh, R. Laflamme, "Quantum data bus in dipolar coupled nuclear spin qubits," *Physical Review A* **80** (2009) 012316(1-5).
<http://dx.doi.org/10.1103/PhysRevA.80.012316>

University of Western Ontario

A. Rezvanpour, J.M. Phillips, G.S. Shaw, "Design of high-affinity S100-target hybrid proteins," *Protein Science* **18** (2009) 2528–2536. <http://dx.doi.org/10.1002/pro.267>

S.A. Serniwka and G.S. Shaw, "Structure of the UbcH8-ubiquitin complex shows a unique ubiquitin interaction site," *Biochemistry* **48** (2009) 12169–12179.
<http://dx.doi.org/10.1021/bi901686j>

**A. Sutrisno, C. Lu, R. Lipson, Y. Huang,** "Combined $^{135/137}\text{Ba}$ Solid-state NMR at an Ultrahigh Magnetic Field and Computational Study of beta-Barium Borate," *Journal of Physical Chemistry C* **113** (2009) 21196–21201. **(Cover Article)**
<http://dx.doi.org/10.1021/jp9044786>

University of Windsor

J.V. Hanna, K.J. Pike, T. Charpentier, T.F. Kemp, M.E. Smith, B.E.G. Lucier, R.W. Schurko, L.S. Cahill, "A ^{93}Nb Solid-State NMR and Density Functional Theory Study of Four- and Six-Coordinate Niobate Systems," *Chemistry - A European Journal* (2010) Early View.
<http://dx.doi.org/10.1002/chem.200901581>

A. Bhattacharya, M. Revington, E.R.P. Zuiderweg, "Measurement and interpretation of ^{15}N - ^1H residual dipolar couplings in larger proteins," *Journal of Magnetic Resonance* **203** (2010) 11-28.
<http://dx.doi.org/10.1016/j.jmr.2009.11.014>

L.A. O'Dell, K.J. Harris, R.W. Schurko, "Optimized Excitation Pulses for the Acquisition of Static NMR Powder Patterns from Half-Integer Quadrupolar Nuclei," *Journal of Magnetic Resonance* **203** (2010) 156-166.
<http://dx.doi.org/10.1016/j.jmr.2009.12.016>

University of Manitoba

T. Aharen, J.E. Greedan, F. Ning, T. Imai, V. Michaelis, S. Kroeker, H. Zhou, C.R. Wiebe, and L.M.D. Cranswick, "Magnetic properties of the $S=3/2$ geometrically frustrated double perovskites $\text{La}_2\text{LiRuO}_6$ and Ba_2YRuO_6 ," *Phys. Rev. B* **80** (2009) 134423.
<http://dx.doi.org/10.1103/PhysRevB.80.134423>

University of Alberta

M. Oleszczuk, I.M. Robertson, M.X. Li, B.D. Sykes, "Solution Structure of the Regulatory Domain of Human Cardiac Troponin C in Complex with the Switch Region of Cardiac Troponin I and W7: The Basis of W7 as an Inhibitor of Cardiac Muscle Contraction," *Journal of Molecular and Cellular Cardiology* (2010) in press.
<http://dx.doi.org/10.1016/j.yjmcc.2010.01.016>

H.A. Enloe, S.A. Quideau, R.C. Graham, S.C. Sillett, S.-W. Oh, and R.E. Wasylishen, "Soil Organic Matter Processes in Old-Growth Redwood Forest Canopies," *Soil Sci Soc Am J* **74** (2010) 161–171.
<http://dx.doi.org/10.2136/sssaj2009.0031>

T. Reddy, X. Li, L. Fliegel, B.D. Sykes, J.K. Rainey, "Correlating structure, dynamics, and function in transmembrane segment VII of the Na^+/H^+ exchanger isoform 1," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1798** (2010) 94-104. **(special issue)**
<http://dx.doi.org/10.1016/j.bbamem.2009.06.025>

H.A. Taha, N. Castillo, D.N. Sears, R.E. Wasylishen, T.L. Lowary and P.-N. Roy, "Conformational Analysis of Arabinofuranosides: Prediction of $^3J_{\text{H,H}}$ Using MD Simulations with DFT-Derived Spin-Spin Coupling Profiles," *J. Chem. Theory Comput.* **6** (2010) 212-222.
<http://dx.doi.org/10.1021/ct900477x>

T.T. Nakashima, K.J. Harris, R.E. Wasylishen, "Pulse FT NMR of Nonequilibrium States of Half-Integer Spin Quadrupolar Nuclei in Single Crystals," *Journal of Magnetic Resonance* **202** (2010) 162-172.
<http://dx.doi.org/10.1016/j.jmr.2009.11.002>

B.L. Lee, X.J. Li, Y.S. Liu, B.D. Sykes, L. Fliegel, "Structural and functional analysis of extracellular loop 2 of the Na⁺/H⁺ exchanger," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1788** (2009) 2481-2488.
<http://dx.doi.org/10.1016/j.bbamem.2009.10.004>

University of Calgary

L.T. Nguyen, D.I. Chan, L. Boszhard, S.A.J. Zaat, H.J. Vogel, "Structure-function studies of chemokine-derived carboxy-terminal antimicrobial peptides," *Biochimica et Biophysica Acta (BBA) - Biomembranes* (2010) accepted.
<http://dx.doi.org/10.1016/j.bbamem.2009.11.021>

S.A. Lusceac, M.R. Vogel, C.R. Herbers, ²H and ¹³C NMR studies on the temperature-dependent water and protein dynamics in hydrated elastin, myoglobin and collagen," *Biochimica et Biophysica Acta (BBA) - Proteins & Proteomics* **1804** (2010) 41-48.
<http://dx.doi.org/10.1016/j.bbapap.2009.06.009>

University of British Columbia



P.T. Eles, C.A. Michal, "Two-Photon Excitation in Nuclear Magnetic and Quadrupole Resonance," *Progress in Nuclear Magnetic Resonance Spectroscopy* (2010) in press. **(Invited Review)**
<http://dx.doi.org/10.1016/j.pnmrs.2009.12.002>

J.K.-H. Hui, P.D. Frischmann, C.-H. Tso, C.A. Michal, M.J. MacLachlan, "Spontaneous Hierarchical Assembly of Crown Ether-like Macrocycles into Nanofibers and Microfibers Induced by Alkali-Metal and Ammonium Salts," *Chemistry - A European Journal* (2010) Early View.
<http://dx.doi.org/10.1002/chem.200902712>

P.H.W. Chan, L.L. Lairson, H.J. Lee, W.W. Wakarchuk, N.C.J. Strynadka, S.G. Withers and L.P. McIntosh, "NMR Spectroscopic Characterization of the Sialyltransferase CstII from *Campylobacter jejuni*: Histidine 188 is the General Base," *Biochemistry* **48** (2009) 11220-11230.
<http://dx.doi.org/10.1021/bi901606n>

Contact us

You are invited to forward your thoughts and suggestions about this News Bulletin to

Victor Terskikh, Manager
National Ultrahigh-field NMR Facility for Solids
1200 Montreal Road M-40
Ottawa ON, K1A 0R6
Tel. (613) 998-5552
Fax: (613) 990-1555
Email: terskikhv@nrc-cnrc.gc.ca