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

Canadian NMR Research News Bulletin #4.2
**Spring 2010**

## *Guest Editorial*

**Michèle Auger, Laval**

### Recent developments in biological solid-state NMR

The 51st ENC meeting was recently held in Daytona Beach. Unfortunately, many of our European colleagues were not able to attend the meeting due to the eruption of the unpronounceable Eyjafjallajoekull volcano. Nevertheless, thanks to technology, most of the talks by the missing speakers were still delivered via the Internet. Too bad that these "virtual" participants were not able to benefit from the vendor suites and be part of the big social event that is the ENC. The jazz band at the Bruker suite and the nightly iPad draws at the Varian suite were certainly among the highlights of the meeting.

Exciting science was presented at the ENC. It has been interesting in the last few years to witness the exchange of approaches in the areas of solution and solid-state NMR for the study of biological molecules. One recent example in protein solution NMR is the renewed interest in the detection of $^{13}C$ and $^{15}N$ nuclei to improve resolution. On the other hand, one of the new trends in biological solid-state NMR spectroscopy is the detection of $^{1}H$ nuclei, which could be particularly useful for the study of flexible loops in proteins.


**Bruker's hospitality suite at the 51st ENC**

Sensitivity enhancement was a common theme in several biological solid-state NMR presentations; significant sensitivity enhancement can be achieved with approaches such as dynamic nuclear polarization (DNP), the use of paramagnetic tags and the use of several isotopic labeling schemes, in addition to proton detection. Several groups are also using hybrid solution and solid-state NMR approaches for the study of membrane proteins. Impressive high-resolution solid-state NMR spectra can now be obtained on challenging systems such as large non-crystalline proteins and membrane proteins.

Following recent progress in DNP, *Physical Chemistry Chemical Physics* is preparing a special themed issue to be published in June

In This Issue

aptly titled "High Frequency Dynamic Nuclear Polarization - The Renaissance". Many papers from this issue, guest-edited by Robert Griffin and Thomas Prisner, are already available online.

Several other meetings featuring exciting developments in the area of biological solid-state NMR will be held before the end of the year. These include the EUROMAR/ISMAR meeting in Florence in July, the Rocky Mountain Conference in Snowmass in early August, the ICMRBS 2010 meeting in Cairns in late August and the Pacifichem Conference in Honolulu in December. In particular, a two and a half day symposium on Advances in Solid-State NMR of Biological Molecules will be held at Pacifichem, with 35 invited speakers, including 5 invited Canadian speakers. This will be a unique chance to witness the most recent developments in biological solid-state NMR. And in a nice setting!

Our research group from the Department of Chemistry at Université Laval is interested in the study of the relationship between the structure, dynamics and interactions of the components of the biological membranes and their function, and the study of silk proteins. Our research group has taken advantage of the National Ultrahigh-Field Solid-State NMR Facility for the study of the structure and dynamics of silk proteins. Future work at the 900 NMR Facility will include the investigation of the structure, topology and orientation of amyloid peptides and novel antimicrobial peptides in non-oriented and oriented lipid bilayers. In particular, recording spectra at high-field using the E-free flat-coil probehead will allow a significant gain in sensitivity and resolution for oriented samples with small quantities of $^{15}N$ labeled peptides. The increases in both sensitivity and resolution obtained with the ultrahigh field instrument will also be very beneficial for multidimensional experiments on protein nanocrystals.

It is a very exciting time for biological solid-state NMR. The combination of high-field instruments with sensitivity enhancement techniques certainly provides the tools to investigate increasingly challenging systems with interesting biomedical and pharmaceutical applications.

*Michèle Auger*

## Canadian NMR News

**NSERC 2010 Competition Results**

Natural Sciences and Engineering Research Council of Canada (**NSERC**) has announced results of the 2010 NSERC competition in the Discovery Grants Program (**DG**), Research Tools and Instruments Grants (**RTI**) and Scholarship programs.

**Michèle Auger** (Université Laval) has her NSERC Discovery Grant renewed for five years, "Biophysical studies of membrane-peptide interactions and silk proteins".

**Vladimir Michaelis** (University of Manitoba, graduate student of Scott Kroeker) has been awarded an NSERC Post-Doctoral Fellowship.

**Myrna Simpson's** (University of Toronto Scarborough) NSERC Discovery Grant was renewed. Myrna has also been awarded an NSERC Discovery Accelerator Supplement.

**Darren Brouwer** (Redeemer University College) has been awarded an NSERC Discovery Grant for five years, "New Methods for Structure Determination of Materials by Solid-State Nuclear Magnetic Resonance Spectroscopy".

**David Bryce's** (University of Ottawa) NSERC Discovery Grant has been renewed for 5 years.

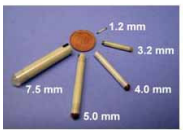
**The National Ultrahigh-Field NMR Facility for Solids** has received NSERC RTI funding for a cryogen-free cooler for the 900 MHz NMR spectrometer. Once installed, the sample cooler will provide powerful, stable and reliable cryogen-free cooling down to -80°C to samples in existing MAS and static NMR probes. This successful application to NSERC was a collaborative effort of three of the Facility users, **David Bryce** (University of Ottawa), **Roderick Wasylishen** (University of Alberta), and **John Ripmeester** (Carleton University).

Submitted by Guy Bernard (Alberta)

**Upgrade Allows Solid-State NMR at 600 MHz at the University of Alberta**

A Varian 600 MHz narrow-bore NMR spectrometer at the University of Alberta has recently been upgraded. Included in the upgrade are two solid-state NMR probes: a 3.2 mm MAS probe and a 1.2 mm UltraFast MAS

probe. Combined with the low-gamma probe kit, these probes can be tuned to frequencies as low as 10 MHz. The console, upgraded to a VNMRS system, includes a 1.0 kW broadband amplifier dedicated to solid-state NMR investigations. The instrument, capable of variable-temperature experiments, is housed in the subbasement of the U of A's Chemistry Department and is cared for by the Department's NMR Facility.




The 1.2 mm MAS probe is a triple-resonance probe capable of spinning samples at frequencies as high as 60 kHz. Applications will include $^{1}H$ (*e.g.*, transition-metal hydrides) and $^{19}F$ investigations as well as observations of nuclei in paramagnetic molecules. The 3.2 mm MAS probe, with a maximum spinning frequency of 25 kHz, is also a triple-resonance probe. With the low-gamma probe kit, all nuclei but $^{203/205}Tl$ are accessible by this probe! It will find extensive use in method development work (*e.g.*, sensitivity enhancement techniques). In addition, the relatively high magnetic field strength combined with the fast MAS capability will be very useful for ongoing investigations of quadrupolar nuclei.

Funding for the upgrade was provided through the Western Diversification Program and the Natural Sciences and Engineering Research Council. Access to the instrument for solid-state NMR experiments has been provided by the Alberta Ingenuity Centre for Carbohydrate Science (AICCS).

**Links:**

Solid-state NMR group:
http://ramsey.chem.ualberta.ca/

NMR Facility at the Department of Chemistry:
http://nmr.chem.ualberta.ca/

Western Diversification Program:
http://www.wd.gc.ca/eng/301.asp

NSERC:
http://www.nserc-crsng.gc.ca/

AICCS:
http://www.carbohydratecentre.ualberta.ca/index.cfm

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**Interview with Ronald Gillespie**

Ronald J. Gillespie, Professor Emeritus at McMaster, is a world-renowned chemist who has made many significant contributions to our understanding of the molecular structure and geometry. He was also one of the first to use NMR spectroscopy in chemical research. Read an interview with this fascinating Canadian personality in the recent issue of the *Journal of Chemical Education*.

**L. Cardellini** "Modeling Chemistry for Effective Chemical Education: An Interview with Ronald J. Gillespie," *J. Chem. Educ*. **87** (2010) 482-286. http://dx.doi.org/10.1021/ed800166f

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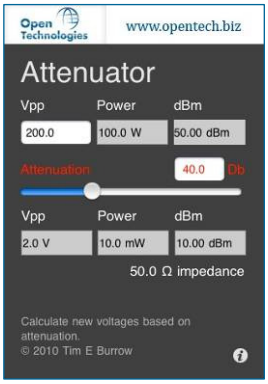
**Attenuator app for iPhone/iPod touch**




**Tim Burrow** (University of Toronto) wrote an **Attenuator** utility application for the iPhone/iPod touch that calculates attenuation values:

http://www.attenuator.ca/

**Attenuator** is a utility for anyone working with radio frequency sources and needs to know power and voltage after attenuation. You can specify an input voltage (Vpp or Vrms) and dB of attenuation to get the output voltage, power and attenuation. The impedance can be specified, typically 50 Ohm for most systems. This free application is available in English, French, Chinese and Japanese and is sponsored by *Open Technologies*.

To download the **Attenuator** app visit:
http://itunes.apple.com/ca/app/attenuator/id367216554

NMR Facility at the Department of Chemistry:
http://www.chem.utoronto.ca/facilities/nmr/nmr.html

## Solid-State NMR Best Paper Award

Dear colleagues,

we would like to draw your attention to the following new initiative of the journal of *Solid State Nuclear Magnetic Resonance*

http://www.elsevier.com/locate/ysnmr

The Editors and Publisher of *Solid State NMR* would like to stimulate research in this field by initiating the Solid-State NMR Best Paper Award. The prize will consist of a free subscription to the journal and a certificate. All authors of articles published in the journal are eligible to the Award. Starting in 2010, an international respected committee of scientists from the Editorial Advisory board will select the winner from the papers published in each calendar year, the primary selection criteria being the degree of scientific innovation and quality.

Yours sincerely,
Hellmut Eckert
Editor-in-Chief

## Bibliometrics as Weapons of Mass Citation

Dear colleagues and friends of the magnetic resonance community.

A recent paper that appeared in *Chimia*, accompanied by a post-face written by **Richard Ernst**, attracted much interest and generated some passionate responses. Since the journal is not widely accessible, I asked the Editor to provide pdf files that you can upload and forward if you wish. Our paper can be found at:

http://www.chimie.ens.fr/Resonance/bibliometrics_1.pdf

The post-face can be uploaded from

http://www.chimie.ens.fr/Resonance/bibliometrics_2.pdf

Sincerely,
Geoffrey Bodenhausen

http://www.chimie.ens.fr/Resonance/geoffrey_bodenhausen.html

## Breaking the 1 GHz barrier: *Nature*

The world-first 1 GHz NMR spectrometer is now online at the European Centre for High Field NMR (CRMN) in Lyon (France). Read the news feature about this milestone in magnetic resonance in the recent issue of *Nature*.

http://dx.doi.org/10.1038/463605a

## 2011 International Year of Chemistry

The 63rd General Assembly of the United Nations has adopted a resolution proclaiming 2011 as International Year of Chemistry (**IYC 2011**). The Chemical Institute of Canada (CIC) is leading the organization of Canadian IYC 2011 celebrations:

http://www.cheminst.ca/iyc

The CIC is pleased to announce that **Canada Post** will issue a stamp to commemorate IYC 2011. You are welcome to submit your ideas on what would be an interesting visual for the stamp by the **May 13th deadline** to

lfrigon@cheminst.ca

For more information:

http://www.cheminst.ca/media

## Plastic Money

Canada is to switch to plastic banknotes starting in 2011.

http://www.cbc.ca/money/story/2010/03/06/ott-plastic-money.html

Unconfirmed, the technology will most likely be provided by the Australian company *Securency Pty Ltd*. Read this excellent essay about history and science behind Australian plastic bills

**E.L. Prime and D.H. Solomon,** "Australias Plastic Banknotes: Fighting Counterfeit Currency," *Angewandte Chemie International Edition* **49** (2010) 3726-2736. http://dx.doi.org/10.1002/anie.200904538

## Canadian NMR blogs and news sites

Solid-State NMR Literature Blog
(Rob Schurko's group, Windsor)
http://ssnmr.blogspot.com/

NMR 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

## Dr. Donald W. Hughes (1949 – 2010)

We lost Don Hughes, an excellent NMR spectroscopist last weekend.

Everyone who passed through the NMR Facility at McMaster was impressed by his skill at running a spectrometer and solving challenging molecular structures. Even those who did not do much NMR spectroscopy usually took his excellent graduate courses. There are many reasons to remember Don, but let me give a few personal ones.

I met Don first in 1977, when he was a graduate student at McMaster and I was a postdoc. It was amazing what he could coax out of a 90 MHz iron magnet spectrometer, both in alkaloid structures and sorting out the assignments of RNA oligomers. Careful, painstaking effort yielded an impressive body of work. I can still see the look on his face when he saw the first spectra obtained on the new 400 MHz system at Guelph. That transition from 90MHz iron magnets to 400MHz supercons was a once-in-a-lifetime one.

It was around this time (1979-80) that Don, Jeremy Everett and I started our 2D-NMR work (still using the iron magnets), which launched my long collaboration with Don. He and I published 16 papers together, and he collaborated with many other people, at Mac and elsewhere. Happily, our latest paper has just been accepted for publication, so that forms part of his legacy.

After graduating from Mac, Don worked in Toronto with Charles Deber at the Hospital for Sick Children and in the NMR Facility in Chemistry Department of the University of Toronto, working partly with Bill Reynolds. He then returned to McMaster where he and the late Brian Sayer, continued to build our first-class NMR facility.

Perhaps I am biased, but I think that Don's favorite activity was running a spectrometer, from a WH90 or XL100 through to a brand-new 700 MHz instrument with a cryoprobe. He also was an excellent photographer, very interested in astronomy, and played a mean game of tennis, I hear. In all these activities, he showed his typical careful, meticulous nature. As well as us working together in the lab, I remember many trips to ENC (side trips to Palo Alto and Point Lobos), SMASH, and demo visits when we shopped for spectrometers. He was quiet and private, but did have an excellent dry sense of humour once you got to know him. I think we will all miss him.

Alex D. Bain
Professor of Chemistry
McMaster University

## NMR Theses Recently Defended

*Congratulate your students here!*

**Susan Safadi** (University of Western Ontario), December 2009
Supervisor: Gary Shaw
Ph.D. thesis: "Structure, Stability and Interactions of the Parkin Ubiquitin-like Domain"

**Nicole Marlatt** (University of Western Ontario), April 2010
Supervisor: Gary Shaw
Ph.D. thesis: "Revealing Conformational Diversity in the Multifunctional S100 Protein Family"

**Venzi Hristova** (University of Western Ontario), April 2010
Supervisor: Gary Shaw
Ph.D. thesis: "Investigating the Structural and Functional Attributes of the Parkin Ubiquitin Ligase"

**Robert Attrell** (University of Ottawa), April 2010
Supervisor: David Bryce
B.Sc. honours thesis: "A Solid-State Halogen NMR and Computational Study of Quadrupolar and Chemical Shift Tensors in Anilinium Halide Salts Exhibiting Halogen Bonding"

**Jason Traer** (McMaster University), April 2010
Supervisor: Gillian Goward
Ph.D. thesis: "Solid-State NMR Investigations of Electrolyte Materials for Hydrogen Fuel Cells"

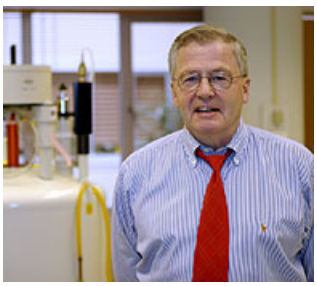
**Brandon Greer** (University of Manitoba), April 2010
Supervisor: Scott Kroeker
B.Sc. honours thesis: "Solid-State Germanium-73 NMR: Experimental and Theoretical Studies of Germanium Halides"

**Kamal Mroué** (University of Waterloo), February 2010
Supervisor: William P. Power
Ph.D. thesis: "Solid-State NMR Investeigations of $^{67}$Zn and $^{27}$Al Nuclei in Zinc-Amino Acid Complexes, Zinc-Insulin Hexamers, and Aluminum-Centered Dyes."

**Isabelle Cloutier** (Université Laval), April 2010
Supervisor : Michèle Auger
Ph.D. thesis : Études biophysiques de l'endolysine du phage Φ-KZ et de la soie d'araignée naturelle et transgénique

**Jean-François Labbé** (Université Laval), April 2010
Supervisor : Michèle Auger
Ph.D. thesis : Études biophysiques d'un peptide amyloïde et de ses interactions avec des membranes modèles

## Recognition



On April 7, 2010 **Ian Smith**, Director General of the NRC Institute for Biodiagnostics in Winnipeg, was invested as an **Officer of the Order of Canada**.

*From the citation*: "An internationally respected biophysicist, Ian Smith has contributed to Canada's reputation as a leader in state-of-the-art medical diagnostic devices. Under his leadership, the National Research Council's Institute for Biodiagnostics has garnered a reputation for world-class research. It has generated and commercialized new non-invasive diagnostic tools used in human and veterinary medicine. Moreover, he continues his cutting-edge research on the early diagnosis of cancer, using magnetic resonance imaging and spectroscopy. Over the years, he has given his support and counsel to a myriad of organizations in Canada and abroad, and served as president of the International Union of Pure and Applied Biophysics."

**Web:** NRC-IBD (Photo credit)
http://www.nrc-cnrc.gc.ca/ibd-ibd/index.html

Dr. **Mark Henkelman**, a Senior Scientist at The Hospital for Sick Children is the recipient of the **2010 Killam Prize** in health sciences.

*From the citation:* "After introducing Canada's first MRI equipment to the Ontario Cancer Institute in the early 1980's, Henkelman shifted his focus to the application of modern imaging technology to the diagnosis of cancer

and other diseases, including spearheading the development of real-time MRI for use in neurosurgery. A graduate of the University of Toronto, he also earned a Master of Science in theoretical physics at McMaster University in Hamilton, Ontario."

**Canada Research Chairs in magnetic resonance**

In March the Government of Canada has announced an investment of $165.5 million to fund 187 new or renewed Canada Research Chairs in 44 Canadian universities. This includes renewal of two Chairs involved in magnetic resonance research.

**Gary Shaw** (University of Western Ontario) Canada Research Chair Tier 1 in Structural Neurobiology

**Vladimir Ladizhansky** (University of Guelph) Canada Research Chair Tier 2 in Biophysics

http://www.chairs-chaires.gc.ca/media-medias/releases-communiques/2010/march-mars-eng.aspx

***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) Biophysics

Raymond Laflamme (Waterloo) Physics

Pascale Legault (Montréal) Biochemistry

Simon Sharpe (Toronto) Biochemistry

Gary Shaw (Western) Structural Neurobiology

Roderick Wasylishen (Alberta) Phys Chemistry

Josef Zwanziger (Dalhousie) Phys Chemistry

**2010 NSERC Strategic Project Grant**

In February **NSERC** awarded $53.5 million to 122 applications in the 2009 Strategic Project Grants competition. The competition attracted the highest number of applications in recent years (465 in total), yielding a success rate of 26 per cent.

Among successful applications was the research proposal "The development of comprehensive multiphase NMR spectroscopy to understand environmental contamination at the molecular level" by **Andre Simpson** and **Myrna Simpson** (University of Toronto Scarborough) in collaboration with Bruker BioSpin and Environment Canada. They have been awarded $450,000 over three years.

*In January Myrna and Andre Simpson have welcomed twins, Sam and Sophie. Congratulations to the happy family!*

**Vladimir Michaelis** (University of Manitoba) has been awarded an NSERC Post-Doctoral Fellowship.

## On the move

**Jason Traer** (McMaster University) has successfully defended his Ph.D. thesis on April 12th, 2010. The thesis was entitled "*Solid-State NMR Investigations of Electrolyte Materials for Hydrogen Fuel Cells*" and done under the research supervision of Gillian Goward. Jason is now working in the chemistry department at UBC, where he joined the NMR facility staff.

**Robert Attrell** and **Frédéric Perras** will begin graduate studies in David Bryce's group at the University of Ottawa in May. In addition, Fred has been awarded an NSERC scholarship to support his studies.

**Jessica Maiorino** has been awarded an NSERC Undergraduate Student Research Award to carry out summer research in the Bryce group at the University of Ottawa.

## the 900 NMR Facility News

**2008-2009 Annual Report**

The 2008/09 Annual Report of the National Ultrahigh-Field NMR Facility for Solids is available in print and for download at http://nmr900.ca/annual_e.html

To request a printed copy please forward your mailing address to the Facility manager.

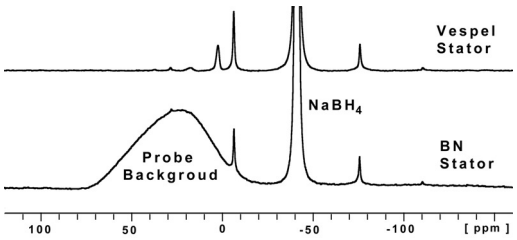
### New home-built NMR probe

One of the 900 NMR Facility objectives is to contribute to the design and development of NMR probes for solid-state NMR research at ultrahigh magnetic fields. At the moment the Facility has a dedicated NMR probe technician, **Paul Morris**, who can design and build probes to accommodate special needs of Facility users.

Two such probes have already been built and now routinely used by our users, 4 mm and 7 mm H/X NMR probes for low-gamma nuclei in stationary samples.

We are pleased to announce an addition of the third probe to this collection, a 2.5 mm MAS H/X probe for mid-gamma range. This probe has very low (none) boron background, which is important for some research projects currently underway at the Facility.

The probe is also equipped with the Hall-effect magnetic flux sensor for easy magic angle (MAS) setup.




For more information on available NMR probes visit

http://nmr900.ca/probes_e.html

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*

**Leigh Spencer** (McMaster University)

**Jianfeng Zhu** (Queen's University)

**Andre Sutrisno** (University of Western Ontario)

## Upcoming NMR Events

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

### 6th Annual McGill Biophysical Chemistry Symposium

**Thursday, May 13, 2010:** This one-day, on-site Symposium aims to bring together research groups interested in using physical/chemical tools to study biological systems. This will be a great opportunity to interact with other biophysical/biochemical labs in Eastern Canada. This year's program is very exciting, with talks from researchers at Montreal, Ottawa, Sherbrooke, and Kingston, and a plenary lecture from **Prof. Mike Summers** (HHMI).

http://www.chemistry.mcgill.ca/

Submitted by David Bryce (Ottawa)

### CSC 2010: Solid-State NMR Symposium

Dear NMR colleagues,

You are invited to take part in the "**Solid-State NMR: Methods and Applications**" symposium at the 93rd Canadian Chemistry Conference and Exhibition in Toronto. This symposium is organized by Gillian Goward and myself and it features many interesting talks and presentations.

The symposium is scheduled for the afternoon of Sunday, May 30 and all day Monday, May 31. The Symposium program is now available online (**PT7**)

http://abstracts.csc2010.ca/

We look forward to seeing you in Toronto!

*Dave Bryce*

## Solid-State NMR Workshop at CSC 2010

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** in the Metro Toronto Convention Centre (MTCC).

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.

Download the Workshop Program and Abstracts (PDF)
http://nmr900.ca/news_e.html

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**Workshop program**

**Session 1** (MTCC, room 203B)
**Chair** John Ripmeester (NRC Canada)

**13:00-13:30** Scott Kroeker (Manitoba) "Further Adventures with $^{73}$Ge NMR of Solids: Halides and Oxides"

**13:30-14:00** Andre Sutrisno (Western Ontario) "Natural Abundance Solid-State $^{73}$Ge and $^{67}$Zn Wideline NMR Studies at Ultrahigh Magnetic Field"

**14:00-14:30** Leigh Spencer (McMaster) "Materials for Lithium Ion Batteries: A Solid-State NMR Analysis"

**14:30-15:00** Fabien Aussenac (Bruker France) "Solid-State NMR Dynamic Nuclear Polarization at 263 GHz"

**15:00-15:15** Coffee Break

**Session 2** (MTCC, room 203B)
**Chair** Roderick Wasylishen (Alberta)

**15:15-15:45** Alex Bain (McMaster) "Probing Spectra of Big Quadrupoles"

**15:45-16:15** Cory Widdifield (Ottawa) "Solid-State $^{127}$I NMR Spectroscopy and GIPAW DFT Calculations of Inorganic Iodide Systems: Structure, Symmetry, and 'Beyond Second-Order" Quadrupole-Induced Shifts"

**16:15-16:45** Peter Pallister (Carleton) "$^{33}$S Ultrahigh-Field Solid-State NMR and First Principles Calculations in Various Sulfate Systems"

**16:45-17:15 Faciliy Users Meeting** David Bryce & Victor Terskikh "National Facility user survey results and overview of application procedures"

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

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

Email: Victor.Terskikh@nrc-cnrc.gc.ca

*Note that the NMR Workshop registration is separate and independent from the CSC 2010 conference registration*

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MOOT XXIII
MINI NMR SYMPOSIUM

## MOOT XXIII Preliminary Announcement

We are excited to announce that the 23rd Annual MOOT NMR Symposium will take place at Dalhousie University in Halifax, Nova Scotia on **October 16 and 17th, 2010.**

The MOOT NMR Symposium provides an informal environment for students, post-docs and faculty to present lectures and posters, discuss existing collaborations, and to establish new ones. It has traditionally been a regional gathering of NMR spectroscopists from Ontario and Quebec but has been expanding to include NMR spectroscopists from the Maritimes. As a result, MOOT XXIII will be hosted for the first time outside of its traditional region; on the East coast in beautiful Halifax, Nova Scotia!

We are currently working on getting the http://www.mootnmr.org domain name redirected, but for now we welcome you to check out and bookmark our website for the most up-to-date information:

http://structbio.biochem.dal.ca/jrainey/NMRMOOT/index.html

Preliminary Details:

(1) **Registration** along with abstract submission for posters and talks is scheduled to begin around June 1, 2010.

(2) **Accommodation** - a block of rooms has been reserved at *Atlantica* at a rate of $129 per night, including parking, and is based on 1-4 person occupancy. See the website for additional details and reservation deadlines. http://www.atlanticahotelhalifax.com

(3) **Travel** - a 10% discount has been arranged with *WestJet* for your flight to MOOT XXIII. Again, additional details are on the website.

(4) **Banquet** - to be held Saturday evening at the Halifax Citadel National Historic Site on Citadel Hill - overlooking the downtown core of Halifax and the harbour. http://www.pc.gc.ca/eng/lhn-nhs/ns/halifax/index.aspx

If you have any questions, comments or feedback about this year's MOOT and/or website, please let us know by email at

Email: mootnmr@gmail.com

We look forward to seeing you in October!

Your MOOT XXIII Organizing Committee:

Mike Lumsden
Joe Zwanziger
Jan Rainey
Ulli Werner-Zwanziger

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**2010 UK NMR BootCamp**

November 1-4, 2010, University of Birmingham, U.K.

The Canadian National High Field NMR Centre (**NANUC**) has been approached by the Biomolecular NMR Facility at the University of Birmingham to present this years training course in the United Kingdom. This will be the first NMR BootCamp to be held abroad and we're extremely excited for the opportunity to utilize new speakers and topics. Please join us in November 2010 for our latest workshop series presentation.

http://www.nanuc.ca/nmrbootcamp/2010_NMR_BootCamp/Welcome.html

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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), L. Emsley (FR), A. Goto (JP), G.R. Goward (CA), Y. Ishii (US), 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), R.E. Wasylishen (CA).

**Registration opens in June 2010.**

You may also be interested in three other NMR symposia on offer at Pacifichem 2010 (see below).

For further information, see http://www.pacifichem2010.org

or contact Scott Kroeker
Email: Scott_Kroeker@UManitoba.ca

***NMR Symposia at Pacifichem 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

**6th Annual McGill Biophysical Chemistry Symposium**
May 13, 2010, McGill University, Montreal, Quebec
http://www.chemistry.mcgill.ca

**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
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/

**Poster submission deadline** June 15, 2010

**3rd IUPAC International Conference on Green Chemistry**

August 15-18, 2010, Ottawa, ON
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 16-17, 2010, Dalhousie University, Halifax
http://www.mootnmr.org

http://structbio.biochem.dal.ca/jrainey/NMRMOOT/index.html

**2010 UK NMR BootCamp**
November 1-4, 2010, University of Birmingham, U.K.
http://www.nanuc.ca/nmrbootcamp/2010_NMR_BootCamp/Welcome.html

**Pacifichem 2010** The International Chemical Congress of Pacific Basin Societies

December 15-20, 2010, Honolulu, Hawaii, USA
http://www.pacifichem.org/

**Registration opens** in June, 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)
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**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

**Frontiers of NMR Biology** Keystone Symposium
January 8-13, 2011, Big Sky, MT, United States
Abstract Deadline: 15th September 2010
Registration Deadline: 9th November 2010
http://www.keystonesymposia.org/

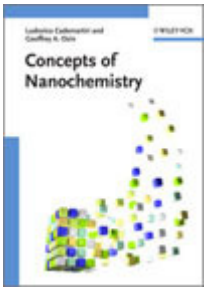
**19th ISMRM** — Scientific Meeting and Exhibition of the International Society for Magnetic Resonance in Medicine
May 7-13, 2011, Montreal, Quebec, Canada
http://www.ismrm.org

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

**7th Alpine Conference** on Solid-State NMR
September 11-15, 2011, Chamonix Mont-Blanc, France
http://www.alpine-conference.org

## New Books

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



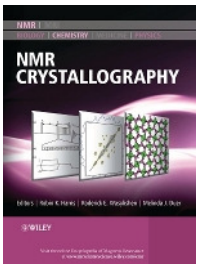

**Concepts of Nanochemistry**
Ludovico Cademartiri
Geoffrey A. Ozin
**Paperback:** 282 pages
**Publisher:** Wiley-VCH; October 2009
**Language:** English

**ISBN:** 978-3527325979

http://www.amazon.com/dp/3527325972/
http://www.amazon.ca/dp/3527325972/

This new book authored by **Ludovico Cademartiri** and **Geoffrey A. Ozin** (University of Toronto) "is ideal for interdisciplinary courses, bridging chemistry, materials science, physics and biology. Adopting a completely new and visionary approach, this is a unique learning tool, focusing on just six concepts crucial for understanding nanochemistry: surface, size, shape, self-assembly, defects and the interface of biology and nanochemistry. These concepts are elucidated through the analysis of six materials representing the real life application of the nanochemistry concepts. The teaching questions included provide real "food for thought", thus training students to think as a researcher does and so develop problem-solving skills."

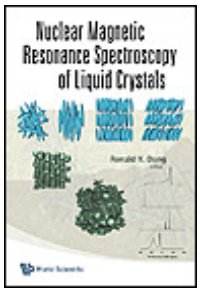
Read review of this book in *Angewandte Chemie International Edition*
http://dx.doi.org/10.1002/anie.201000743




**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/




**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

## NMR Jobs and Vacancies

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

**Department of Biochemistry and Molecular Biology, University of British Columbia**

**Assistant Professor, Tenure Track**

The Department of Biochemistry and Molecular Biology at the University of British Columbia is seeking an outstanding new investigator for a full time tenure track faculty position, at the rank of Assistant Professor. Candidates must have a Ph.D. degree, a minimum of 2 years postdoctoral research experience, and a record of accomplishment that demonstrates their potential as an independent researcher and teacher. Candidates with research and teaching interests in any area of contemporary Biochemistry or Molecular Biology are encouraged to apply. All members of the Department maintain active, well-funded research programs that encompass many areas of modern biochemistry, molecular and structural biology. Successful candidates should complement and extend the Department's expertise in research and education. Applicants should send their curriculum vitae, a record of teaching effectiveness, 3-4 relevant reprints and a brief (2-3 page) outline of their proposed research program to:

**Irene Ho**, Secretary to the Department Head
Department of Biochemistry and Molecular Biology, Faculty of Medicine
The University of British Columbia
2350 Health Sciences Mall

Vancouver, BC V6T 1Z3 Canada
Email: biochsec@interchange.ubc.ca
Website: http://www.biochem.ubc.ca

Applicants should also arrange for 3 letters of reference to be sent to the above address. **The deadline for applications is May 31, 2010**. The anticipated start date is July 1, 2010 and is negotiable. Salary will be commensurate with qualifications and experience.

UBC hires on the basis of merit and is committed to employment equity. All qualified persons are encouraged to apply. UBC is strongly committed to diversity within its community and especially welcomes applications from visible minority group members, women, Aboriginal persons, persons with disabilities, persons of any sexual orientation or gender identity, and others who may contribute to the further diversification of ideas. However, Canadian and permanent residents of Canada will be given priority.

For more information (Faculty Job Postings)
http://www.biochem.ubc.ca/department/career.html

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**Department of Chemistry, University of Alberta**

**NMR Laboratory Supervisor**

**Competition No.** - A104910984

**Closing Date** - May 31, 2010

The Department of Chemistry at the University of Alberta invites applications for a Faculty Service Officer (FSO) Level II or III position. Reporting to the Chair of the Department, the NMR Laboratory Supervisor is responsible for the management and planning of a multimillion dollar, state-of-the-art Nuclear Magnetic Resonance (NMR) Facility.

For more information visit
http://www.chem.ualberta.ca

This FSO position will oversee the day-to-day operation of the facility, coach and mentor staff and instruct users involved in NMR spectroscopic studies as the facility is used for both research and teaching purposes. The scope of NMR research is very wide; from biomolecules to inorganic complexes. The NMR facility and its staff measure approximately 2,500 research samples per year. This position will be directly involved in collaborative or independent research utilizing NMR, will work in close collaboration with key faculty members and will also have significant interactions with external users, equipment manufacturers and other related facilities on campus.

Applicants must hold a Ph.D. in Chemistry or a related field combined with six or more years of relevant experience in NMR. The candidate will have demonstrated experience and knowledge of a broad spectrum of NMR techniques and their applicability to problems that are encountered by both researchers and students. Managerial experience is considered an asset. Interested individuals should submit their Curriculum Vitae and three letters of reference by **May 31, 2010.**

All qualified candidates are encouraged to apply; however, Canadians and permanent residents will be given priority.

The University of Alberta hires on the basis of merit. We are committed to the principle of equity in employment. We welcome diversity and encourage applications from all qualified women and men, including persons with disabilities, members of visible minorities, and Aboriginal persons.

For more information and to apply online
http://www.careers.ualberta.ca/competition.aspx?id=A104910984

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**Department of Chemistry, McGill University**

**EPR Research Assistant**

Applications are invited for a research assistant in the general area of EPR spectroscopy in the Centre for Self-Assembled Chemical Structures (CSACS), McGill University, Montreal, Canada.

http://csacs.mcgill.ca/

The duties for the position are to assist in research related to materials science, free radical biology, and bioinorganic chemistry and to train students in the use of our new Bruker ELEXSYS FT-EPR. A successful candidate will have a PhD in physical chemistry with extensive hands-on EPR experience and good knowledge of pulse magnetic resonance spectroscopy. Exceptional candidates with an MSc degree and extensive EPR experience will also be considered.

The position is available immediately and will entail a year to year contract and remuneration at a level comparable to a postdoctoral position. Interested applicants should apply with a CV and arrange for three letters of reference to be sent directly to

Prof. **Dmitrii Perepichka**

Email: dmitrii.perepichka@mcgill.ca

http://perepichka-group.mcgill.ca/

Centre for Self-Assembled Chemical Structures
Department of Chemistry
McGill University
801 Sherbrooke str West
Montreal H3A 2K6

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**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&chId=0

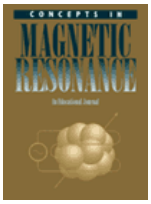
FG-MR Jobs
http://fgmrjobs.blogspot.com/

## Canadian NMR Research Highlights

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

**"Hottest 2009 Wiley article in Analytical Chemistry"**

This review by **David Hoult** (Institute for Biodiagnostics, NRC Canada, Winnipeg) in *Concepts in Magnetic Resonance* was one of the most accessed Wiley articles in Analytical Chemistry during 2009.




**D.I. Hoult** "The origins and present status of the radio wave controversy in NMR," *Concepts in Magnetic Resonance* **34A** (2009) 193-216.

http://dx.doi.org/10.1002/cmr.a.20142

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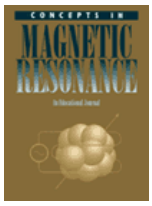
***Concepts in Magnetic Resonance***




**J. Autschbach, S. Zheng, R.W. Schurko,** "Analysis of electric field gradient tensors at quadrupolar nuclei in common structural motifs," *Concepts in Magnetic Resonance Part A* **36A** (2010) 84-126.

http://dx.doi.org/10.1002/cmr.a.20155

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**Chemistry of Energy Conversion**

The ACS's *Chemistry of Materials* special themed issue (volume 22, issue 3, 2010) highlights new directions in materials chemistry relevant to energy conversion. There are several NMR articles in this issue, including one by the **Gillian Goward**'s group (McMaster) and colleagues from Estonia on Li dynamics.

**L.J.M. Davis, I. Heinmaa and G.R. Goward,** "Study of Lithium Dynamics in Monoclinic $Li_3Fe_2(PO_4)_3$ using $^6Li$ VT and 2D Exchange MAS NMR Spectroscopy," *Chem. Mater.* **22** (2010) 769–775. (**special issue**)
http://dx.doi.org/10.1021/cm901402u

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***Biochemistry and Cell Biology***

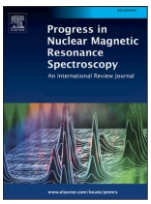

**Special issue:** papers presented at the Annual meeting of the Canadian Society for Biochemistry, Molecular & Cellular Biology (**CSBMCB**), June 1-5, 2009, Niagara-on-the-Lake, Ontario.

Volume 88, Number 2, April 2010

**T. Reddy and J.K. Rainey,** "Interpretation of biomolecular NMR spin relaxation parameters," *Biochem. Cell Biol.* **88** (2010) 131–142. **(Review)**
http://dx.doi.org/10.1139/O09-152

**D.S. Libich, M.A.M. Ahmed, L. Zhong, V.V. Bamm, V. Ladizhansky, and G. Harauz,** "Fuzzy complexes of myelin basic protein: NMR spectroscopic investigations of a polymorphic organizational linker of the central nervous system," *Biochem. Cell Biol.* **88** (2010) 143–155. **(Review)**
http://dx.doi.org/10.1139/O09-123

### *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* **56** (2010) 232-246. **(Invited Review)**

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

### NMR papers in *Nature*

**M.J. Plevin, D.L. Bryce, and J. Boisbouvier,** "Direct Detection of CH/pi Interactions in Proteins," *Nature Chemistry* (2010) online.
http://dx.doi.org/10.1038/nchem.650

**J. Chan, A.R. Lewis, M. Gilbert, M.-F. Karwaski, A.J. Bennet,** "A direct NMR method for the measurement of competitive kinetic isotope effects," *Nature Chemical Biology* (2010) online.
http://dx.doi.org/10.1038/nchembio.352

**T.D. Ladd, F. Jelezko, R. Laflamme, Y. Nakamura, C. Monroe and J.L. O'Brien,** "Quantum computers," *Nature* **464** (2010) 45-53. **(Review)**
http://dx.doi.org/10.1038/nature08812

### *Applied Magnetic Resonance*


**Special issue:** papers presented at at the 11th International Symposium on Spin and Magnetic Field Effects in Chemistry and Related Phenomena, Brock University, August 9-14, 2009.

Volume 38, Number 2, April 2010

**T.R. Field and A.D. Bain,** "Origins of Spin Noise," *Applied Magnetic Resonance* **38** (2010) 167-178. (**Special issue**).
http://dx.doi.org/10.1007/s00723-009-0107-2

### NMR paper in *Science*

**T.L. Religa, R. Sprangers, L.E. Kay,** "Dynamic Regulation of Archaeal Proteasome Gate Opening As Studied by TROSY NMR," *Science* **328** (2010) 98-102.
http://dx.doi.org/10.1126/science.1184991

### *Annular Reports on NMR Spectroscopy*

**K.V. Romanenko** "$^{129}$Xe NMR Studies of Xenon Adsorption," *Annual Reports on NMR Spectroscopy* **69** (2010) 1-38. **(Invited Review)**

http://dx.doi.org/10.1016/S0066-4103(10)69001-1

### Review: NMR in Inorganic Polymers

**A.S. Borisov, P. Hazendonk, P.G. Hayes,** "Solid-State Nuclear Magnetic Resonance Spectroscopy: A Review of Modern Techniques and Applications for Inorganic Polymers," *J. Inorg. Organomet. Polym.* **20** (2010) 183–212. **(Review)**
http://dx.doi.org/10.1007/s10904-010-9358-5

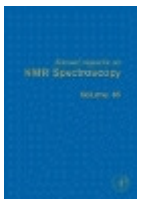
## Recent NMR Publications

*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.*

### Dalhousie University

**T. Reddy and J.K. Rainey,** "Interpretation of biomolecular NMR spin relaxation parameters," *Biochem. Cell Biol.* **88** (2010) 131–142. **(Review)**
http://dx.doi.org/10.1139/O09-152

### University of New Brunswick



**K.V. Romanenko** "$^{129}$Xe NMR Studies of Xenon Adsorption," *Annual Reports on NMR Spectroscopy* **69** (2010) 1-38. **(Invited Review)**

http://dx.doi.org/10.1016/S0066-4103(10)69001-1

### Université Laval

**D. Thibeault, M. Auger, and J.-F. Morin,** "Synthesis of Fluorine-Containing Molecular Rotors and Their Assembly on Gold Nanoparticles," *Eur. J. Org. Chem.* (2010) online.
http://dx.doi.org/10.1002/ejoc.201000252

**O. Fisette, S. Morin, P.-Y. Savard, P. Lagüe, S.M. Gagné,** "TEM-1 Backbone Dynamics—Insights from Combined Molecular Dynamics and Nuclear Magnetic Resonance," *Biophysical Journal* **98** (2010) 637-645. http://dx.doi.org/10.1016/j.bpj.2009.08.061

**M. Auger,** "Structural and Dynamics Studies of Lipids by Solid-State NMR ", *Encyclopedia of Magnetic Resonance*, Article. Online Posting Date: December 15, 2009. http://dx.doi.org/10.1002/9780470034590.emrstm1100

## McGill University

**P. Farber, H. Darmawan, T. Sprules and A. Mittermaier,** "Analyzing Protein Folding Cooperativity by Differential Scanning Calorimetry and NMR Spectroscopy," *Journal of the American Chemical Society* **132** (2010) 6214–6222. http://dx.doi.org/10.1021/ja100815a

**W. Tong, M. Gagnon, T. Sprules, M. Gilbert, S. Chowdhury, K. Meerovitch, K. Hansford, E.O. Purisima, J.W. Blankenship, N.-K.V. Cheung, K. Gehring, W.D. Lubell, H.U. Saragovi,** "Small-Molecule Ligands of GD2 Ganglioside, Designed from NMR Studies, Exhibit Induced-Fit Binding and Bioactivity," *Chemistry & Biology* **17** (2010) 183-194. http://dx.doi.org/10.1016/j.chembiol.2010.01.012

## Université de Montréal

**Z.-K. Cui, G. Bastiat, C. Jin, A. Keyvanloo, M. Lafleur,** "Influence of the nature of the sterol on the behavior of palmitic acid/sterol mixtures and their derived liposomes," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1798** (2010) 1144-1152. http://dx.doi.org/10.1016/j.bbamem.2010.02.008

**Y.J. Wang, F. Ravenelle, and X.X. Zhu,** "NMR imaging study of cross-linked high-amylose starch tablets — The effect of drug loading," *Canadian Journal of Chemistry* **88** (2010) 202-207. http://dx.doi.org/10.1139/V09-170

## NRC-SIMS

**G. Wu, J. Zhu, X. Mo, R. Wang, and V. Terskikh,** "Solid-state $^{17}$O NMR and computational studies of C-nitrosoarene compounds," *Journal of the American Chemical Society* **132** (2010) 5143–5155. http://dx.doi.org/10.1021/ja909656w

**I. Moudrakovski, R. Alizadeh, J.J. Beaudoin,** "Natural abundance high field $^{43}$Ca solid state NMR in cement science," *Physical Chemistry Chemical Physics* **12** (2010) accepted.

**A. Sutrisno, M.A. Hanson, P.A. Rupar, V.V. Terskikh, K.M. Baines, and Y. Huang,** "Exploring the limits of $^{73}$Ge solid-state NMR spectroscopy at ultrahigh magnetic field," *Chemical Communications* **46** (2010) 2817-2819. http://dx.doi.org/10.1039/b926071d

## University of Ottawa

**M.J. Plevin, D.L. Bryce, and J. Boisbouvier,** "Direct Detection of CH/pi Interactions in Proteins," *Nature Chemistry* (2010) online. http://dx.doi.org/10.1038/nchem.650

**H. Hamaed, E. Ye, K. Udachin, R. Schurko,** "Solid-State $^{137}$Ba NMR Spectroscopy: An Experimental and Theoretical Investigation of $^{137}$Ba Electric Field Gradient Tensors and Their Relation to Structure and Symmetry," *Journal of Physical Chemistry B* **114** (2010) 6014–6022. http://dx.doi.org/10.1021/jp102026m

**J.W.E. Weiss and D.L. Bryce,** "A Solid-State $^{11}$B NMR and Computational Study of Boron Electric Field Gradient and Chemical Shift Tensors in Boronic Acids and Boronic Esters," *Journal of Physical Chemistry A* **114** (2010) 5119-5131. http://dx.doi.org/10.1021/jp101416k

**P.D. Frischmann, G.A. Facey, P.Y. Ghi, A.J. Gallant, D.L. Bryce, F. Lelj and M.J. MacLachlan,** "Capsule Formation, Carboxylate Exchange, and DFT Exploration of Cadmium Cluster Metallocavitands: Highly Dynamic Supramolecules," *J. Am. Chem. Soc.* **132** (2010) 3893-3908. http://dx.doi.org/10.1021/ja910419h

## Queen's University

**G. Wu, J. Zhu, X. Mo, R. Wang, and V. Terskikh,** "Solid-state $^{17}$O NMR and computational studies of C-nitrosoarene compounds," *Journal of the American Chemical Society* **132** (2010) 5143–5155. http://dx.doi.org/10.1021/ja909656w

## University of Toronto

**G. Woods, M.J. Simpson, B.P. Kelleher, M. McCaul, W.L. Kingery, and A.J. Simpson,** "Online High-Performance Size Exclusion Chromatography-Nuclear Magnetic Resonance for the Characterization of Dissolved Organic Matter," *Environmental Science & Technology* **44** (2010) 624-630. http://dx.doi.org/10.1021/es903042s

**R. Auer, D.F. Hansen, P. Neudecker, D.M. Korzhnev, D.R. Muhandiram, R. Konrat, L.E. Kay,** "Measurement of signs of chemical shift differences between ground and excited protein states: a comparison between H(S/M)QC and R-1 rho methods," *Journal of Biomolecular NMR* **46** (2010) 205-216. http://dx.doi.org/10.1007/s10858-009-9394-z

**V. Chevelkov, Y. Xue, D.K. Rao, J.D. Forman-Kay, N.R. Skrynnikov,** "$^{15}$N-(H/D)-SOLEXSY experiment for accurate measurement of amide solvent exchange rates: application to denatured drkN SH3," *Journal of Biomolecular NMR* **46** (2010) 227-244. http://dx.doi.org/10.1007/s10858-010-9398-8

**A.A. Ogunjimi, S. Wiesner, D.J. Briant, X. Varelas, F. Sicheri, J. Forman-Kay, J.L. Wrana,** "The Ubiquitin Binding Region of the Smurf HECT Domain Facilitates Polyubiquitylation and Binding of Ubiquitylated Substrates," *Journal of Biological Chemistry* **285** (2010) 6308-6315. http://dx.doi.org/10.1074/jbc.M109.044537

**L.C. Cerchietti, A.F. Ghetu, X. Zhu, G.F. Da Silva, S. Zhong, M. Matthews, K.L. Bunting, J.M. Polo, C. Farès, C.H. Arrowsmith, S.N. Yang, M. Garcia, A. Coop, A.D. MacKerell, G.G. Privé, A. Melnick,** "A Small-Molecule Inhibitor of BCL6 Kills DLBCL Cells In Vitro and In Vivo," *Cancer Cell* **17** (2010) 400-411. http://dx.doi.org/10.1016/j.ccr.2009.12.050

**N. Ishiyama, S.-H. Lee, S.Liu, G.-Y. Li, M.J. Smith, L.F. Reichardt, M. Ikura,** "Dynamic and Static Interactions between p120 Catenin and E-Cadherin Regulate the Stability of Cell-Cell Adhesion," *Cell* **141** (2010) 117-128. http://dx.doi.org/10.1016/j.cell.2010.01.017

**T.L. Religa, R. Sprangers, L.E. Kay,** "Dynamic Regulation of Archaeal Proteasome Gate Opening As Studied by TROSY NMR," *Science* **328** (2010) 98-102. http://dx.doi.org/10.1126/science.1184991

**S.A.E. Brown, J.R. McKelvie, A.J. Simpson, M.J. Simpson,** "$^{1}$H NMR metabolomics of earthworm exposure to sub-lethal concentrations of phenanthrene in soil," *Environmental Pollution* **158** (2010) 2117-2123. http://dx.doi.org/10.1016/j.envpol.2010.02.023

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