



Canadian NMR News

Colleagues and friends gathered at Queen's University to honour Rod Wasylishen

A special NMR symposium in honour of Professor Rod Wasylishen was held during the 55th International Conference on Analytical Sciences and Spectroscopy (ICASS) at Queen's University on August 9-12, 2009. About 50 colleagues and friends attended this special symposium. Rod was accompanied by his wife, Valerie, who is originally from Kingston and used to live in a house just a stone's throw away from the Chemistry building. In the morning of August 10, Rod gave a plenary lecture "From NMR of liquids and gases to solids—reflections of an ardent fan", followed by four half-day scientific sessions. Among the invited speakers for the NMR symposium are Cynthia Jameson, Vladimir Ladizhansky, Simon Sharpe, Igor Moudrakovski, Alex Bain, Victor Terskikh, Christian Detellier, Yining Huang, Peter Macdonald, Chris Ratcliffe, and Andreas Brinkmann. Many of Rod's former group members gathered at the symposium including Sandra Mooibroek, Marco Gruwel, Glenn Penner, Glenn Facey, Bill Power, Gerry Marangoni, Gang Wu, Klaus Eichele, Aatto Laaksonen, Chris Kirby, Rob Schurko, Scott Kroeker, Guy Bernard, Dave Bryce, and Kris

In This Issue

- 1 Canadian NMR News
- 4 NMR Theses Recently Defended
- 5 Recognition
- 5 On the move
- 6 the 900 NMR Facility News
- 7 Upcoming NMR Events
- 7 NMR Books
- 8 NMR Jobs and Vacancies
- 10 Canadian NMR Research Highlights
- 12 Recent NMR Publications
- 17 Contact us

Ooms. Also in attendance were students from Gang Wu's group at Queen's University (Jianfeng Zhu, Irene Kwan, Sanela Martic, Parisa Akhshi, and Xiaoyi Ji) as well as Joseph Weiss and Andy Lo from Dave Bryce's group at the University of Ottawa.

The participants expressed great appreciation for Rod's outstanding contributions to science and education over the past 40 years. Rod has



ICASS 2009 NMR symposium participants. Photo credit: Irene Kwan

published over 330 papers during his career and given 130 invited talks in recent years. Rod is not only a world-class scientist, but also an incredible mentor. Rod has supervised 27 PhDs, 15 PDFs, 17 honours theses, and 5 visiting scientists. Nine of his former students now hold faculty positions across Canada. At the symposium, many of Rod's former students recounted how Rod's inspiration had influenced them in their career paths.

A "magical dinner" was the highlight of the event where the attendees were entertained by Canada's magic champion, Eric Leclerc, who dazzled his audience with his "hypnosis" and humor.

The symposium was organized by **Gang Wu** from the Department of Chemistry at Queen's and sponsored by the National Ultrahigh-Field NMR Facility for Solids, Bruker BioSpin, and Cambridge Isotope Laboratories.

Supervised by Rod Wasylshen

Postdoctoral Fellows and Research Associates

D.N. Sears (Killam PDF) 2004-2007
M.A.M. Forgeron (PDF) 2006-2007
T.T. Nakashima (RA) 2002 - present
R. Siegel (PDF) 2002-2005
G.M. Bernard (RA) 2001 - present
G.M. Bernard (PDF) 2000-2001
T.C. Stringfellow (Killam PDF) 1996-1997
J.C.C. Chan (PDF) 1996-1996
K. Eichele (Killam PDF) 1991-1997
G.H. Penner (Killam PDF) 1987-1988
J.F. Britten (Killam PDF) 1986-1987
M.S. McKinnon (NSERC PDF) 1985-1987
A.M. de P. Nicholas (PDF) 1984-1986
S. Peiris (PDF) 1983-1984

Graduate Students

J.R. Dwan, M.Sc., 2009, expected
R. Teymoori, Ph.D., 2010, expected
M. Wang, Ph.D., 2010, expected
F. Chen, Ph.D., 2009
K.J. Harris, Ph.D., 2009
B. Demko, Ph.D., 2008
M. Willans, Ph.D., 2008

K.J. Ooms, Ph.D., 2007
K.W. Feindel, Ph.D., 2007
M.A.M. Forgeron, Ph.D., 2006
M. Wang, M.Sc., 2005, supervised with P.Y.K. Choi
D.L. Bryce, Ph.D., 2002 (NSERC Doctoral Prize)
M. Gee, Ph.D., 2001
G.M. Bernard, Ph.D., 2000
S. Kroeker, Ph.D., 1999
R.W. Schurko, Ph.D., 1998
M.D. Lumsden, Ph.D., 1996
G. Wu, Ph.D., 1994 (NSERC Doctoral Prize)
W.P. Power, Ph.D., 1992
G.D. Marangoni, Ph.D., 1991, supervised with J.C.T. Kwak
R. Labonté, M.Sc., 1991, supervised with J.C.T. Kwak
M.R. MacIntosh, M.Sc., 1991
Z. Gao, Ph.D., 1990, supervised with J.C.T. Kwak
R.D. Curtis, Ph.D., 1990
M.L.H. Gruwel, Ph.D., 1989
S. Mooibroek, Ph.D., 1987
B.A. Pettitt, Ph.D., 1987, supervised with R.J. Boyd

Honours Students

B. Feland, 2009
W. Abdelaal, 2007
K.W. Feindel, 2000-2001
M.A.M. Forgeron, 1999-2000
G.C. Ossenkamp, 1994-1995
C.W. Kirby, 1993-1994
K. Wright, 1991-1993
A. (Ron) Dastidar, 1990-1991
M.D. Lumsden, 1990-1991
B. Fraser, 1988-1989
M.R. MacIntosh, 1988-1989
W.P. Power, 1987-1988
R. Dickson, 1985-1986
G. Facey, 1984-1985
J.O. Friedrich, 1984-1985
E. (Sabeth) Verpoorte, 1983-1984, supervised with J.C.T. Kwak
S.L. Roberts, 1983-1984, supervised with D.R. Arnold

New NMR spectrometer at Agriculture and Agri-Food Canada, Charlottetown, P.E.I.



The Government of Canada has announced funding of \$750,000 for a new NMR spectrometer for the Agriculture and Agri-Food Canada laboratory at the University of Prince Edward Island in Charlottetown. The

new spectrometer will be used primarily in plant materials, healthy foods and nutraceuticals research. The announcement was made in Charlottetown on May 22, 2009 by Parliamentary Secretary to the Minister of Agriculture **Pierre Lemieux** (photo, left) on behalf of Federal Agriculture Minister **Gerry Ritz**.

Read the news release by Agriculture and Agri-Food Canada (photo credit)

http://www.agr.gc.ca/cb/index_e.php?s1=n&s2=2009&page=n90522

Our congratulations to Chris Kirby (photo, right), a Physical Chemist and NMR Specialist with Agriculture and Agri-Food Canada!

Submitted by Tim Burrow (UoFT)

The University of Toronto Nuclear Magnetic Resonance News

The Canada Foundation for Innovation, CFI, has funded the Centre for Spectroscopic Investigation of Complex Organic Molecules and Polymers (CSICOMP) in the Department of Chemistry at the University of Toronto. The CFI award was to Professor **Mark Lautens** and many co-applicants from the Departments of Chemistry and Chemical Engineering and the Faculty of Pharmacy. The CFI contribution was \$2,588,764 with a matching contribution from the Ontario government.

Three new high-field spectrometers at 500, 600 and 700 MHz will be housed in the newly renovated NMR labs. They will be used for: highly sensitive ^{19}F NMR of environmental compounds; glycoside and glycan NMR; multiple dimensional spectra on organic compounds and proteins; highly sensitive and rapid carbon NMR of small molecules and

polymers; diffusion and solid state studies of polymers; and a wide range of multinuclear NMR.

The new NMR spectrometers will complement the extant spectrometers: one 500 MHz, four 400 MHz, one 300 MHz and two 200 MHz instruments, three of which have sample changers.

CSICOMP website

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

Canada's first 950 MHz NMR spectrometer

The Canada Foundation for Innovation, CFI, announced in June major investment in Canadian Research Infrastructure through the CFI's Leading Edge Fund and New Initiatives Fund. More than \$665 million was awarded to 133 projects at 41 Canadian research institutions. Among infrastructure projects receiving Government's support was Canada's first 950 MHz NMR spectrometer at **the University of Toronto** (Lewis Kay, Biochemistry) to enable studies of the structure and dynamics of complex biological molecules, as well as the technological development of biological NMR.

Project title: "High Field NMR Studies of Protein Molecules in Health and Disease" (CFI contribution \$4,595,843)

This very significant hardware acquisition will ensure Canada's leading role in biological NMR research.

Submitted by Yves Aubin (Health Canada)

MOOT XXII NMR Minisymposium

On behalf of the organizing committee, I would like to invite all our colleagues of the NMR community to attend the 22nd edition of the MOOT NMR minisymposium in Ottawa. The meeting will be held at Carleton University on **October 17-18, 2009**. Registration and abstract submission are now open. All details are available on the website

www.mootnmr.org

For inquiries please contact **Yves Aubin**

Phone: (613) 941-6155

E-mail: mootnmr@gmail.com

Cut-open magnet display at the University of Alberta



If you are planning on visiting Edmonton, don't miss a rare opportunity to get a glimpse inside of a cut-open NMR magnet at the University of Alberta. A well thought out and professionally arranged magnet display has been recently opened to the public in the Chemistry Department building. Not only will you have a chance to see what's inside of an NMR magnet, you will also learn a great deal about NMR from a

slide presentation that runs continuously on the overhead monitor for your enjoyment. If traveling to Edmonton is not in your plans, you can still see this presentation online, courtesy of **Albin Otter**, an NMR Facility Service Officer at the University of Alberta, who coordinated efforts in putting this wonderful educational display together (photo credit).

<http://nmr.chem.ualberta.ca/>

A cut-open 200 MHz brother of the magnet in Edmonton is on display in Ottawa, at the 900 NMR Facility. You are very welcome to drop by and see it yourself!

Perimeter Institute "Quantum to Cosmos" Festival

Canada's Perimeter Institute for Theoretical Physics (Waterloo, Ontario) celebrates its 10th anniversary by organizing a science festival "**Quantum to Cosmos: Ideas for the Future**" from October 15 to 25, 2009 at Perimeter Institute and other venues located throughout Uptown Waterloo.

An extensive program will feature more than 50 events including keynote presentations, panel discussions, exhibits, film screenings, world premieres and cultural events that will showcase a wide variety of fascinating topics such as new forms of quantum communication, scientific visualization, the future of robotics, green technologies, personal genetics, and even the possibility of life on other planets. All events, with the exception of concerts, are free. You will need advance tickets due to

space limitations. Sign up on the official Q2C website now to be ready to order your tickets starting **September 1, 2009**.

<http://www.q2cfestival.com/>

Bruker announces 1 GHz NMR Spectrometer

Bruker BioSpin has announced the launch of a breakthrough one Gigahertz Ultrahigh-field NMR spectrometer incorporating the world's first 23.5 Tesla standard-bore (54 mm) superconducting NMR magnet. The first **AVANCE 1000** system will be delivered to the Ultra-High Field European NMR Center in Lyon, France, where it will be used for research in biomolecular liquid and solid-state chemistry.

Read the press release by Bruker BioSpin

<http://www.bruker-biospin.com/pr090601.html?L=0&print=http%253A%252F%252>

Canadian NMR blogs and news sites

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

NMR Facility Blog
(Glenn Facey, Ottawa)
<http://u-of-o-nmr-facility.blogspot.com/>

NMR Facility Blog
(Tim Burrow, Toronto)
<http://www.chem.utoronto.ca/facilities/nmr/NMRBlog/>

NMR Facility News
(Albin Otter, Alberta)
http://nmr.chem.ualberta.ca/nmr_news.htm

NMR Theses Recently Defended *Congratulate your students here!*

Kristopher Harris (University of Alberta) May 22, 2009

Research supervisor: Roderick Wasylishen
Ph.D. thesis: "Solid-State Spin-1/2 NMR Studies of Disorder, Bonding, and Symmetry"

Recognition

Canadian Journal of Chemistry volume 87, number 7, 2009

<http://pubs.nrc-cnrc.gc.ca/rp-ps/inDetail.jsp?code=cjc&lang=eng&vol=87&is=7>



This special issue of *Canadian Journal of Chemistry* is dedicated to Professor **Tom Ziegler** (University of Calgary), a Tier 1 Canada Research Chair in Theoretical Inorganic

Chemistry, one of the pioneers of density functional theory (DFT). Prof. Ziegler has made many important contributions to the development of DFT calculations of NMR parameters.

We encourage you to read two wonderful tributes to Prof. Ziegler written by Arvi Rauk, Heiko Jacobsen and Tom Woo, and to browse through many excellent research papers by world-leading experts in computational chemistry.

Photo credit: University of Calgary

<http://www.ucalgary.ca/chem/pages/ziegler>



Robert Schurko (University of Windsor) has been promoted to the rank of **Professor** effective July 1, 2009. Rob started at Windsor in Fall 2000, and has developed an NSERC-funded research program focusing upon development and

application of pulse sequences for the study of spin-1/2 and quadrupolar nuclei in inorganic, organometallic and organic materials. Rob obtained funding for his NMR centre via a CFI infrastructure grant, and was recently awarded an Early Researcher Award by the Ontario Ministry of Research and Innovation. Rob is in his sixth year of service on the organizing committee for the Solid-State NMR Symposium in the Rocky Mountain Conference for Analytical Chemistry, the largest annual international conference on solid-state NMR. To find out more about his research activities, visit:

<http://mutuslab.cs.uwindsor.ca/schurko/>

Gillian Goward featured in *The Globe and Mail*

The Globe and Mail published an article "Looking for life after lithium" about recent advances by Canadian researchers and entrepreneurs in creating a new generation of batteries. **Gillian Goward** (McMaster) was prominently featured in this article for her work towards better understanding the chemistry behind extending the recharging life of lithium ion batteries.

Read the full article in *The Globe and Mail (Canada)*, April 22, 2009, Wednesday

<https://secure.globeadvisor.com/servlet/ArticleNews/story/gam/20090422/SRGREENBATTERIESART1812>

On the move

David McNally has joined the Environmental NMR Centre (Dept. of Physical and Environmental Sciences) at the University of Toronto at Scarborough on July 1, 2009. His official title with the department is research associate/lecturer and he will also manage the facility.

Andreas Brinkmann has recently joined the Materials Structure and Function group at the NRC Steacie Institute for Molecular Sciences (Ottawa) as a research officer. In 2001 he obtained his PhD from Stockholm University working in the group of Malcolm Levitt. After a postdoc in Arno Kentgens' group at the Radboud University Nijmegen and a stay with Ago Samoson at the National Institute of Chemical Physics and Biophysics in Tallinn, he became the scientific supervisor at the National Solid-State NMR Facility in Nijmegen. Andreas develops and applies new solid-state NMR methods including recoupling and decoupling sequences in magic-angle-spinning and double-rotation NMR.

Kirk Feindel has accepted a Research Associate position with the NRC Institute for Biodiagnostics and is currently located at IBD Atlantic in Halifax. Kirk was an NSERC postdoctoral fellow with Prof. Paul Callaghan at Victoria University of Wellington in New Zealand investigating the flow of complex fluids with NMR microscopy.

the 900 NMR Facility News

NMR Facility Annual Report 2008-2009

Dear NMR Facility Users:

We are preparing our 2008-2009 Annual Report, and we would like to receive the following information from you by **the end of August**:

- 1) a brief progress report for each of your research projects. Please prepare a separate report for each project, regardless of whether the project has ended or not. Each report should illustrate for non-NMR specialists major project findings and should normally not exceed one-two pages (text and figures) (preferably MS Word format, or an ASCII text + figures separately). Selected progress reports will be included in the printed version of the Annual Report;
- 2) all 2008-2009 research publications featuring results from the 900 instrument (published, accepted, submitted);
- 3) invited lectures and oral presentations in 2008-2009;
- 4) poster presentations in 2008-2009;
- 5) 2008-2009 : Honours thesis, Ph.D. thesis and similar works by your students using the 900 results (please indicate name of the student, department, title of thesis, date of the defense);
- 6) any other relevant information you may consider useful including in our report.

Let me know if any questions, and thank you for your contribution!

*On behalf of the Facility Steering Committee,
Victor Terskikh*

Previous Annual Reports

http://nmr900.ca/annual_e.html

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.

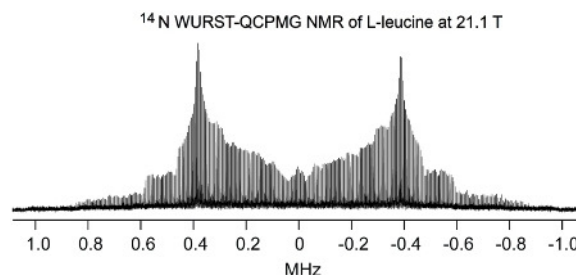
http://nmr900.ca/policies_e.html

Recent Travel Grant Recipient

Leigh Spencer (McMaster University)

WURST-QCPMG NMR

A WURST-QCPMG NMR technique has recently been introduced by **Luke O'Dell and Rob Schurko** (Windsor) to achieve uniform excitation of quadrupolar nuclei in solids across very wide bandwidth. Using this approach wide-line spectra of stationary samples can now be acquired with no need or just minimal transmitter frequency adjustment.



The spectrum shown was acquired in about 1 hour by co-adding 10 individual pieces. Experiments were performed by **Luke O'Dell**, who also kindly provided the WURST-QCPMG pulse sequence for the 900 MHz NMR instrument. This pulse program is now available to the Facility users and has already been successfully applied to ²⁵Mg, ⁶⁷Zn, and ⁷³Ge. For more information about WURST-QCPMG:

L.A. O'Dell and R.W. Schurko, "QCPMG Using Adiabatic Pulses for Faster Acquisition of Ultra-Wide-line NMR Spectra," *Chem. Phys. Lett.* **464** (2008) 97-102.

<http://dx.doi.org/10.1016/j.cplett.2008.08.095>

Upcoming NMR Events

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

NANUC NMR BootCamp (Metabolomics)

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

"Dynamic Nuclear Polarization" Second International Symposium

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

6th Alpine Conference on Solid-State NMR

September 13-17, 2009, Chamonix, France
<http://www.alpine-conference.org>

SMASH 2009 Small Molecule NMR Conference

September 20-23, 2009, Chamonix, France
<http://www.smashnmr.org/>

Cryogenic NMR Symposium

September 21-22, 2009, Southampton, UK
<http://cryonmr-symposium.org/>

DNP school

October 11-16, 2009, Safed, Israel


<http://www.weizmann.ac.il/conferences/DNP/>

 **Perimeter Institute "Quantum to Cosmos" Festival**

October 15-25, 2009, Waterloo, ON
<http://www.q2cfestival.com/>

 **MOOT 22 NMR Minisymposium**

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

 **CSC 2010** the 93rd Canadian Chemistry Conference and Exhibition

May 29 – June 2, 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, the Snowmass Conference Center, Snowmass, Colorado
<http://www.rockychem.com/>

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

August 22-27, 2010, Cairns, Australia
<http://www.icmrbs2010.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. Wasylshen (Editor)

Melinda J. Duer (Editor)

Hardcover: 496 pages

Publisher: Wiley; January 2010

Language: English

ISBN-13: 978-0-470-69961-4

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

Wiley: The term "NMR Crystallography" has only recently come into common usage, and even now causes raised eyebrows within some parts of the diffraction community. The power of solid-state NMR to give crystallographic information has considerably increased since the CPMAS suite of techniques was introduced in 1976. In the first years of the 21st century, the ability of NMR to provide information to support and facilitate the analysis of single-crystal and powder diffraction patterns has become widely accepted. Indeed, NMR can now be used to refine diffraction results and, in favorable cases, to solve crystal structures with minimal (or even no) diffraction data. The increasing ability to relate chemical shifts (including the tensor components) to the

crystallographic location of relevant atoms in the unit cell via computational methods has added significantly to the practice of NMR crystallography. Diffraction experts will increasingly welcome NMR as an ally in their structural analyses. Indeed, it may be that in the future crystal structures will be determined by simultaneously fitting diffraction patterns and NMR spectra.

This Handbook is organised into six sections. The first contains an overview and some articles on fundamental NMR topics, followed by a section concentrating on chemical shifts, and one on coupling interactions. The fourth section contains articles describing how NMR results relate to fundamental crystallography concepts and to diffraction methods. The fifth section concerns specific aspects of structure, such as hydrogen bonding. Finally, four articles in the sixth section give applications of NMR crystallography to structural biology, organic & pharmaceutical chemistry, inorganic & materials chemistry, and geochemistry.

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 of Windsor

Post-doctoral NMR position: A two-year post-doctoral position funded by NSERC and the Ontario Ministry of Research and Innovation is available in the laboratory of **Rob Schurko** at the University of Windsor. Research projects focus on development and application of pulse sequences for the acquisition of high S/N NMR spectra of quadrupolar nuclei and heavy spin-1/2 nuclei in a variety of systems, including inorganic/organometallic complexes, organic pharmaceuticals, nanoparticles and composite materials. The applicant should have a Ph.D. in Chemistry or Physics with expertise in solid-state NMR. A complete CV, including a summary of research experience and contact information for three references, can be emailed directly to Rob Schurko. Please visit website for more information <http://www.uwindsor.ca/schurko>

University of Alberta

Tenure-Track Faculty Position, Chemistry:

The Department of Chemistry at the University of Alberta invites applications for a tenure-track faculty position in Chemical Biology, Carbohydrate Chemistry or a related field including the NMR of biomolecules and biologically oriented organic chemistry. Appointment will be made at the Assistant Professor level to an individual who complements the research interests of the department; an appointment at the Associate Professor level for an outstanding candidate may be considered.

http://oraweb.aucc.ca/pls/ua/ua_re3?ADVERTISEMENT_NUMBER_IN=9684

University of Calgary

Manager, Instrumentation Facility & Services, Department of Chemistry:

The Department of Chemistry at the University of Calgary invites applications for a Manager of our Instrumentation Facility.

The appointee will have responsibilities managing the operation and maintenance of the Departmental Instrumentation Facility which includes a variety of chemical/spectroscopic techniques (e.g. NMRs, Mass Specs., EPR, FT-IR, UV-Vis, CD, Elemental Analyzer, polarimeters), scheduling of instrument usage, supervision of technical staff, manage the Facility budget, provide assistance in troubleshooting/diagnosing problems that arise, train users of the Facility, assist departmental research groups in conducting specific experiments, assist in future planning of instrument upgrades and new instrument acquisitions, maintain a high level of expertise and knowledge in the field of Chemical/Spectroscopic instrumentation techniques, assist Faculty members with the writing of grants and proposals. Candidates must have a Ph.D. in chemistry or the equivalent, hands on experience in the operation and maintenance of NMR and/or Mass Specs. Some experience in troubleshooting and basic understanding of electronics would be desirable. The appointee will be expected to remain abreast of current developments with instrumentation. Details on the Department of Chemistry can be found at <http://www.ucalgary.ca/chem/> Applications will be reviewed commencing September 15, 2009 and will be considered

until the position is filled. Qualified applicants should submit a curriculum vitae, statement of managing philosophy, evidence of experience in the operation and maintenance of instruments, and arrange for at least three letters of reference to be sent to:

Dr. Peter Kusalik
Professor and Head
Department of Chemistry
University of Calgary
2500 University Drive NW
Calgary, AB, Canada
T2N 1N4
Confidential Fax: 403-284-1372

e-mail: head@chem.ucalgary.ca

All qualified candidates are encouraged to apply; however, Canadians and permanent residents will be given priority. The University of Calgary respects, appreciates and encourages diversity.

University of Toronto

Associate NMR Manager, Department of Chemistry, Faculty of Arts and Science:

Job Number 0900545

The Department of Chemistry is seeking an Associate Manager for its state of the art NMR facility. The facility provides a wide range of NMR services to a wide user community within the Department and University as well as externally through eight NMR spectrometers; one 500, four 400, one 300 and two 200 MHz instruments. Three of the systems have sample changers. The facility is currently purchasing three new spectrometers to add to this complement: 500, 600 and 700 MHz instruments.

Under the general direction of the Facility Manager, this individual will assist with the preparation and delivery of training in the principles and practices of NMR spectrometer operations to over 300 users and in advising solution and solid state NMR users, in particular, regarding experiment selection and interpretation. This individual is also responsible for evaluating and advising on the purchase of new NMR equipment and writing grant proposals to facilitate equipment

acquisitions. This position includes maintenance of NMR instruments and associated computer systems, and supervising technical staff.

Qualifications:

An advanced chemistry degree specializing in NMR spectroscopy with a strong background in of multinuclear liquids spectroscopy and, ideally, solid state spectroscopy using Bruker and/or Varian instruments is required for this position. The applicant must have: a good understanding of NMR hardware and software design, knowledge in troubleshooting and application of NMR experiments; experience in structural elucidation, organic and inorganic chemistry; and the ability to prioritize workflow, being self-motivated. The applicant must also possess strong written, oral communication and interpersonal skills to be able to work with faculty, staff and students. This includes the ability to (i) train students at the undergraduate and graduate levels, (ii) communicate with faculty and students in research groups in chemistry and other departments, and (iii) act in an advisory role in sample preparation, experimental, design, spectrometer maintenance and other NMR related areas. Experience in RedHat Linux maintenance, writing pulse sequences, scripts and macros in C, shell languages, MAGICAL, and python are desired. The position requires some physical labour and a high level of concentration.

Compensation:

This is a full-time, continuing position and the salary range is \$64,448 per year with an annual step progression to a maximum of \$82,351 per year.

To apply:

All applicants must apply through the University of Toronto's on-line posting board at <http://www.jobs.utoronto.ca/staff.htm>

Look under "External" for job number 0900545. **This posting closes at 11:59 p.m. on August 28, 2009.**

This is a unionized position (United Steelworkers Local 1998).

University of Alberta

Research Associate, NMR, Chemistry: The Alberta Ingenuity Centre for Carbohydrate Science has a vacancy for a Research Associate specializing in the structural determination of complex carbohydrates by high resolution NMR and detailed studies of their complexes with enzymes and carbohydrate binding proteins.
http://oraweb.aucc.ca/pls/ua/ua_re3?ADVERTISEMENT_NUMBER_IN=9584

Penn State, Chemistry

NMR Spectroscopist
Job Number: 30499
https://www.ohr.psu.edu/jobs/home_EJMS/view_faculty.cfm#30499

Oak Ridge National Laboratory

Postdoctoral Research Associate in Solid State NMR
Posting # ORNL09-105-CSD
<http://www.ornl.gov/orise/edu/ornl/postneeds.htm>

PNNL, Richland, WA

NMR Postdoctoral Research Associate, two positions
Job ID# 117785
<http://jobs.pnl.gov>

Listings of NMR jobs and vacancies

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

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

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

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

Canadian NMR Research Highlights

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


PCCP themed issue
volume 11, issue 32, 2009
"Solid-State NMR spectroscopy"





This high-profile special issue of *Physical Chemistry Chemical Physics* guest-edited by **Paul Hodgkinson** (Durham, UK) and **Stephen Wimperis** (Glasgow, UK) will be presented to the participants of the upcoming **6th Alpine Conference on Solid-State NMR** in September. Among

many excellent reviews and research papers highlighting recent trends and progress in the field of solid-state NMR spectroscopy there are four by Canadian researchers, including the front cover article by **Gang Wu's** group from Queen's.

Pedro M. Aguiar, Michael J. Katz, Daniel B. Leznoff and Scott Kroeker, "Natural abundance ^{13}C and ^{15}N solid-state NMR analysis of paramagnetic transition-metal cyanide coordination polymers," *Physical Chemistry Chemical Physics* **11** (2009) 6925-6934.
<http://dx.doi.org/10.1039/b907747b>

 **Jianfeng Zhu, Amanda J. Geris and Gang Wu**, "Solid-state ^{17}O NMR as a sensitive probe of keto and gem-diol forms of alpha-keto acid derivatives," *Physical Chemistry Chemical Physics* **11** (2009) 6972-6980. **(Cover Article)**
<http://dx.doi.org/10.1039/b906438a>

 **Rebecca P. Chapman and David L. Bryce**, "Application of Multinuclear Magnetic Resonance and Gauge-Including Projector-Augmented Wave Calculations to the Study of Solid Group 13 Chlorides," *Physical Chemistry Chemical Physics* **11** (2009) 6987-6998.
<http://dx.doi.org/10.1039/b906627f>

 **Luke A. O'Dell and Robert W. Schurko**, "Static solid-state ^{14}N NMR and computational studies of nitrogen EFG tensors in some crystalline amino acids," *Physical Chemistry Chemical Physics* **11** (2009) 7069-7077.
<http://dx.doi.org/10.1039/b906114b>

PCCP themed issue
volume 11, issue 31, 2009
"Modern EPR Spectroscopy"

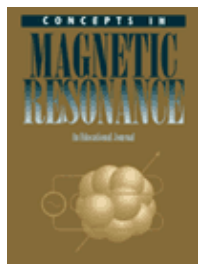
A special issue of *Physical Chemistry Chemical Physics* on modern aspects of Electron Paramagnetic Resonance (EPR) has been finalized and is now available online. This PCCP issue brings together a broad range of manuscripts dealing with novel EPR applications, new methodologies and advances in data analysis. It will be displayed at the upcoming 7th European Federation of EPR Groups conference in Antwerp, Belgium in early September 2009.

Canadian contribution in this issue is by our colleagues from the NRC Steacie Institute for Molecular Sciences collaborating with fellow EPR spectroscopists from Russia, Germany, and France.

E.G. Bagryanskaya, D.N. Polovyanenko, M.V. Fedin, L. Kulik, A. Schnegg, A. Savitsky, K. Möbius, A.W. Coleman, G.S. Ananchenko and J.A. Ripmeester, "Multifrequency EPR study of the mobility of nitroxides in solid-state calixarene nanocapsules," *Physical Chemistry Chemical Physics* **11** (2009) 6700–6707.
<http://dx.doi.org/10.1039/b906827a>

Review in Concepts in Magnetic Resonance

David Hoult (Institute for Biodiagnostics, NRC Canada, Winnipeg) presents his arguments explaining origins of the NMR free induction decay.



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>

Review in Annual Reports on NMR Spectroscopy

Cory Widdifield, Rebecca Chapman, and David Bryce from the University of Ottawa have just published a long-awaited review in

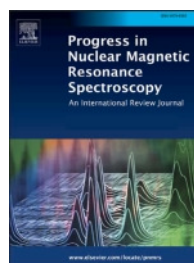
Annual Reports on NMR Spectroscopy on solid-state NMR of quadrupolar halogen nuclei. This review will be of interest not only to material scientists and NMR spectroscopists, but also to students and those just learning about solid-state NMR of half-integer quadrupolar nuclei.



Cory M. Widdifield, Rebecca P. Chapman, and David L. Bryce, "Chlorine, Bromine, and Iodine Solid-State NMR Spectroscopy," *Annual Reports on NMR Spectroscopy* **66** (2009) 195–326. **(Invited Review)**

[http://dx.doi.org/10.1016/S0066-4103\(08\)00405-5](http://dx.doi.org/10.1016/S0066-4103(08)00405-5)

Review in Progress in NMR Spectroscopy



Quadrupolar halogens find widespread use i.e. in pharmaceutical formulations. Solid-state NMR provides a direct mean to probe local halogen environment in these systems. This recent review in *Progress in Nuclear Magnetic Resonance Spectroscopy* by a

team from the University of Ottawa summarizes current advancements in the field. The most progress in recent years has been achieved due to broader availability of ultrahigh-field NMR spectrometers, including the one located in Ottawa, at the Canadian National Ultrahigh-Field NMR Facility for Solids (www.nmr900.ca).

Rebecca P. Chapman, Cory M. Widdifield and David L. Bryce, "Solid-State NMR of Quadrupolar Halogen Nuclei," *Progress in Nuclear Magnetic Resonance Spectroscopy* **55** (2009) 215–237. **(Invited Review)**

<http://dx.doi.org/10.1016/j.pnmrs.2009.05.001>

Research paper in PNAS

J.D. Dikeakos, P. Di Lello, M.J. Lacombe, R. Ghirlando, P. Legault, T.L. Reudelhuber, J.G. Omichinski, "Functional and structural characterization of a dense core secretory granule sorting domain from the PC1/3 protease," *Proceedings of The National Academy of Sciences of The United States of America* **106** (2009) 7408–7413.

<http://dx.doi.org/10.1073/pnas.0809576106>

Cover article in *Chemical Communications*



Unique instrumentation available at the 900 NMR Facility allows our users to deal with systems and nuclei inaccessible before with NMR at lower fields. One example is ^{73}Ge NMR in solids which was previously limited only to highly symmetric

environments. In this cover article just published by *Chemical Communications* a research team from the **University of Manitoba** and **NRC-SIMS** is reporting natural abundance ^{73}Ge NMR spectra in much more challenging amorphous and crystalline germanium oxides. Work continues on even more complex glasses and crystalline phases to address long-standing fundamental questions in glass science, such as the "germanate anomaly".

Vladimir K. Michaelis, Pedro M. Aguiar, Victor V. Tersikh and Scott Kroeker, "Germanium-73 NMR of Amorphous and Crystalline GeO_2 ," *Chemical Communications* (2009) 4660-4662. **(Cover Article)**
<http://dx.doi.org/10.1039/b906642j>

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, M. McDonald, M.R. Morrow, V. Booth, "The Effect of a C-Terminal Peptide of Surfactant Protein B (SP-B) on Oriented Lipid Bilayers, Characterized by Solid-State ^2H and ^{31}P NMR," *Biophysical Journal* **96** (2009) 3762-3771.
<http://dx.doi.org/10.1016/j.bpj.2009.02.027>

Dalhousie University



J.S. Hartman, B. Berno, P. Hazendonk, C. Kirby, E. Ye, J.

Zwanziger, A. Bain, "NMR Studies of Nitrogen Doping in the 4H Polytype of Silicon Carbide: Site Assignments and Spin-Lattice Relaxation," *Journal of Physical Chemistry C* **111** (2009) 15024-15036.

<http://dx.doi.org/10.1021/jp904639n>

A.S. Culf, U. Werner-Zwanziger, K.N. Robertson, B.H. Chen, M. Cuperlovic-Culf, D.A. Barnett, R.J. Ouellette, "Polymeric and polymer-ligated spirobicyclic zwitterionic Janovsky complexes," *Tetrahedron Letters* **50** (2009) 2762-2766.

<http://dx.doi.org/10.1016/j.tetlet.2009.03.136>

University of New Brunswick

L.Q. Li, H. Han, B.J. Balcom, "Spin echo SPI methods for quantitative analysis of fluids in porous media," *Journal of Magnetic Resonance* **198** (2009) 252-260.

<http://dx.doi.org/10.1016/j.jmr.2009.03.002>

E. Veliyulin, B. Egelanddal, F. Marica and B.J. Balcom, "Quantitative ^{23}Na Magnetic Resonance Imaging of Model Foods," *J. Agric. Food Chem.* **57** (2009) 4091-4095.

<http://dx.doi.org/10.1021/jf9000605>

P.F. de J. Cano-Barrita, A.E. Marble, B.J. Balcom, J.C. García, I.V. Mastikhin, M.D.A. Thomas, T.W. Bremner, "Embedded NMR sensors to monitor evaporable water loss caused by hydration and drying in Portland cement mortar," *Cement and Concrete Research* **39** (2009) 324-328.

<http://dx.doi.org/10.1016/j.cemconres.2009.01.011>

A.E. Marble, G. LaPlante, I.V. Mastikhin, B.J. Balcom, "Magnetic resonance detection of water in composite sandwich structures," *NDT & E International* **42** (2009) 404-409.

<http://dx.doi.org/10.1016/j.ndteint.2009.01.010>

M. Sankey, Z. Yang, L. Gladden, M.L. Johns, D. Lister, B. Newling, "SPRITE MRI of bubbly flow in a horizontal pipe," *Journal of Magnetic Resonance* **199** (2009) 126-135.

<http://dx.doi.org/10.1016/j.jmr.2009.01.034>

Université Laval

I. Cloutier, C. Paradis-Bleau, A.-M. Giroux, X. Pigeon, M. Arseneault, R.C. Levesque, M. Auger, "Biophysical studies of the interactions between the phage phi-KZ gp144 lytic transglycosylase and model membranes," *Eur. Biophys. J.* (2009) online.
<http://dx.doi.org/10.1007/s00249-009-0530-1>

S. Morin, S.M. Gagné, "NMR Dynamics of PSE-4 beta-Lactamase: An Interplay of ps-ns Order and us-ms Motions in the Active Site," *Biophysical Journal* **96** (2009) 4681-4691.
<http://dx.doi.org/10.1016/j.bpj.2009.02.068>

Université de Montréal

E. Brief, S. Kwak, J.T. J. Cheng, N. Kitson, J. Thewalt, and M. Lafleur, "Phase Behavior of an Equimolar Mixture of N-Palmitoyl-D-erythro-sphingosine, Cholesterol, and Palmitic Acid, a Mixture with Optimized Hydrophobic Matching," *Langmuir* **25** (2009) 7523-7532.
<http://dx.doi.org/10.1021/la9003643>

J.D. Dikeakos, P. Di Lello, M.J. Lacombe, R. Ghirlando, P. Legault, T.L. Reudelhuber, J.G. Omichinski, "Functional and structural characterization of a dense core secretory granule sorting domain from the PC1/3 protease," *Proceedings of The National Academy of Sciences of The United States of America* **106** (2009) 7408-7413.
<http://dx.doi.org/10.1073/pnas.0809576106>

T. Phoeung, L.M. Huber, M. Lafleur, "Cationic Detergent/Sterol Mixtures Can Form Fluid Lamellar Phases and Stable Unilamellar Vesicles," *Langmuir* **25** (2009) 5778-5784.
<http://dx.doi.org/10.1021/la804222w>

NRC-SIMS

Y. Seo, J.-W. Lee, R. Kumar, I.L. Moudrakovski, H. Lee, J.A. Ripmeester, "Tuning the Composition of Guest Molecules in Clathrate Hydrates: NMR Identification and Its Significance to Gas Storage," *Chemistry - An Asian Journal* **4** (2009) 1266-1274.
<http://dx.doi.org/10.1002/asia.200900087>

R. Kumar, P. Englezos, I. Moudrakovski, J.A. Ripmeester, "Structure and composition

of CO₂/H₂ and CO₂/H₂/C₃H₈ hydrate in relation to simultaneous CO₂ capture and H₂ production," *AIChE Journal* **55** (2009) 1584-1594.

<http://dx.doi.org/10.1002/aic.11844>

L.Q. Wang, D.H. Wang, J. Liu, G.J. Exarhos, S. Pawsey, I. Moudrakovski, "Probing Porosity and Pore Interconnectivity in Crystalline Mesoporous TiO₂ Using Hyperpolarized ¹²⁹Xe NMR," *Journal of Physical Chemistry C* **113** (2009) 6577-6583.
<http://dx.doi.org/10.1021/jp809740e>

R. Wang, D. Bardelang, M. Waite, K.A. Udachin, D.M. Leek, K. Yu, C.I. Ratcliffe and J.A. Ripmeester, "Inclusion complexes of coumarin in cucurbiturils," *Org. Biomol. Chem.* **7** (2009) 2435-2439.
<http://dx.doi.org/10.1039/b903057c>



V.K. Michaelis, P.M. Aguiar, V.V. Terskikh and S. Kroeker, "Germanium-73 NMR of Amorphous and Crystalline GeO₂," *Chemical Communications* (2009) 4660-4622.

(Cover Article)

<http://dx.doi.org/10.1039/b906642j>



H. Hamaed, M. Laschuk, V. Terskikh, R. Schurko, "Application of Solid-State ²⁰⁹Bi NMR to the Structural Characterization of Bismuth-Containing Materials," *Journal of the American Chemical Society* **131** (2009) 8271-8279.

<http://dx.doi.org/10.1021/ja901347k>

Queen's University



J. Zhu, A.J. Geris and G. Wu, "Solid-state ¹⁷O NMR as a sensitive probe of keto and gem-diol forms of alpha-keto acid derivatives," *Physical Chemistry Chemical Physics* **11** (2009) 6972-

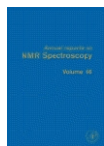
6980. **(Cover Article, Themed Issue)**

<http://dx.doi.org/10.1039/b906438a>

University of Ottawa

D.L. Bryce and J. Autschbach, "Relativistic Hybrid Density Functional Calculations of Indirect Nuclear Spin-Spin Coupling Tensors. Comparison with Experiment for Diatomic Alkali Metal Halides" *Canadian Journal of Chemistry* **87** (2009) 927-941.

<http://dx.doi.org/10.1139/V09-040>



C.M. Widdifield, R.P. Chapman, and D.L. Bryce, "Chlorine, Bromine, and Iodine Solid-State NMR Spectroscopy," *Annual Reports on NMR Spectroscopy* **66** (2009) 195-326. **(Invited Review)**

[http://dx.doi.org/10.1016/S0066-4103\(08\)00405-5](http://dx.doi.org/10.1016/S0066-4103(08)00405-5)



J.S. Hartman, B. Berno, P. Hazendonk, C. Kirby, E. Ye, J. Zwanziger, A. Bain, "NMR Studies of Nitrogen Doping in the 4H Polytype of Silicon Carbide: Site Assignments and Spin-Lattice Relaxation," *Journal of Physical Chemistry C* **111** (2009) 15024-15036.

<http://dx.doi.org/10.1021/jp904639n>

S. Letaief and C. Detellier, "Clay-Polymer Nanocomposite Material from the Delamination of Kaolinite in the Presence of Sodium Polyacrylate," *Langmuir* (2009) ASAP.

<http://dx.doi.org/10.1021/la901196f>



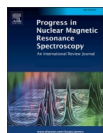
C.M. Widdifield and D.L. Bryce, "Crystallographic Structure Refinement with Quadrupolar Nuclei: a Combined Solid-State NMR and GIPAW DFT Example Using MgBr₂," *Physical Chemistry Chemical Physics* **11** (2009) 7120-7122.

<http://dx.doi.org/10.1039/b911448n>



J. Zhu, N. Trefiak, T. Woo, Y. Huang, "A ^{47/49}Ti Solid-State NMR Study of Layered Titanium Phosphates at Ultrahigh Magnetic Field," *Journal of Physical Chemistry C* **111** (2009) 10029-10037.

<http://dx.doi.org/10.1021/jp901235w>



R.P. Chapman, C.M. Widdifield and D.L. Bryce, "Solid-State NMR of Quadrupolar Halogen Nuclei," *Progress in Nuclear Magnetic Resonance Spectroscopy* **55** (2009) 215-237.

(Invited Review)

<http://dx.doi.org/10.1016/j.pnmrs.2009.05.001>



R.P. Chapman and D.L. Bryce, "Application of Multinuclear Magnetic Resonance and Gauge-Including Projector-Augmented Wave Calculations to the Study of Solid Group 13 Chlorides," *Physical Chemistry Chemical Physics* **11** (2009) 6987-6998.

(Invited Article, Themed Issue)

<http://dx.doi.org/10.1039/b906627f>

University of Toronto

R. Auer, P. Neudecker, D.R. Muhandiram, P. Lundstrom, D.F. Hansen, R. Konrat, and L.E. Kay, "Measuring the Signs of ¹H alpha Chemical Shift Differences Between Ground and Excited Protein States by Off-Resonance Spin-Lock R1-Rho NMR Spectroscopy," *J. Am. Chem. Soc.* **131** (2009) 10832-10833.
<http://dx.doi.org/10.1021/ja904315m>

A.J. Baldwin, D.F. Hansen, P. Vallurupalli, and L.E. Kay, "Measurement of Methyl Axis Orientations in Invisible, Excited States of Proteins by Relaxation Dispersion NMR Spectroscopy," *J. Am. Chem. Soc.* **131** (2009) ASAP.
<http://dx.doi.org/10.1021/ja903896p>

G.Y. Li, Y. Zhang, M. Inouye, M. Ikura, "Inhibitory mechanism of *Escherichia coli* RelE-RelB toxin-antitoxin module involves a helix displacement near an mRNA interferase active site," *J. Biol. Chem.* **284** (2009) 14628-14636.
<http://dx.doi.org/10.1074/jbc.M809656200>

B. Lam, A.J. Simpson, "Investigating Aggregation in Suwannee River, USA, Dissolved Organic Matter Using Diffusion-Ordered Nuclear magnetic Resonance Spectroscopy," *Environmental Toxicology and Chemistry* **28** (2009) 931-939.
<http://dx.doi.org/10.1897/08-441.1>


R. Soong, J.R. Brender, P.M. Macdonald, A. Ramamoorthy, "Association of Highly Compact Type II Diabetes Related Islet Amyloid Polypeptide Intermediate Species at Physiological Temperature Revealed by Diffusion NMR Spectroscopy," *J. Am. Chem. Soc.* **131** (2009) 7079-7085.
<http://dx.doi.org/10.1021/ja900285z>

P. Lundstrom, H. Lin, L.E. Kay, "Measuring ¹³C (beta) chemical shifts of invisible excited states in proteins by relaxation dispersion NMR spectroscopy," *Journal of Biomolecular NMR* **44** (2009) 139-155.
<http://dx.doi.org/10.1007/s10858-009-9321-3>

P. Walsh, J. Yau, K. Simonetti, S. Sharpe, "Morphology and Secondary Structure of Stable beta-Oligomers Formed by Amyloid Peptide


PrP(106-126)," *Biochemistry* **48** (2009) 5779–5781.
<http://dx.doi.org/10.1021/bi9007319>

McMaster University

 **J.S. Hartman, B. Berno, P. Hazendonk, C. Kirby, E. Ye, J. Zwanziger, A. Bain,** "NMR Studies of Nitrogen Doping in the 4H Polytype of Silicon Carbide: Site Assignments and Spin-Lattice Relaxation," *Journal of Physical Chemistry C* **111** (2009) 15024–15036.
<http://dx.doi.org/10.1021/jp904639n>

J. Kooistra, J. Milojevic, G. Melacini, J. Ortega, "A New Function of Human HtrA2 as an Amyloid-beta Oligomerization Inhibitor," *Journal of Alzheimers Disease* **17** (2009) 281–294.
<http://dx.doi.org/10.3233/JAD-2009-1037>

Brock University

 **J.S. Hartman, B. Berno, P. Hazendonk, C. Kirby, E. Ye, J. Zwanziger, A. Bain,** "NMR Studies of Nitrogen Doping in the 4H Polytype of Silicon Carbide: Site Assignments and Spin-Lattice Relaxation," *Journal of Physical Chemistry C* **111** (2009) 15024–15036.
<http://dx.doi.org/10.1021/jp904639n>

University of Guelph


V. Ladizhansky, "Homonuclear dipolar recoupling techniques for structure determination in uniformly ^{13}C -labeled proteins," *Solid State Nuclear Magnetic Resonance* (2009) accepted.
<http://dx.doi.org/10.1016/j.ssnmr.2009.07.003>

K.R. Jeffrey and G.H. Penner, "Structural Phase Transitions," *Encyclopedia of Magnetic Resonance*, Wiley (2009).
<http://dx.doi.org/10.1002/9780470034590.emrstm1051>

M. Aluas, C. Tripon, J.M. Griffin, X. Filip, V. Ladizhansky, R.G. Griffin, S.P. Brown, C. Filip, "CHHC and ^1H - ^1H Magnetization Exchange: Analysis by Experimental Solid-State NMR and 11-Spin Density-Matrix Simulations," *Journal of Magnetic Resonance* **199** (2009) 173–187.
<http://dx.doi.org/10.1016/j.jmr.2009.04.013>

J.H. Davis, J.J. Clair, J. Juhasz, "Phase Equilibria in DOPC/DPPE-d(62)/Cholesterol Mixtures," *Biophysical Journal* **96** (2009) 521–539.
<http://dx.doi.org/10.1016/j.bpj.2008.09.042>

University of Western Ontario


 **J. Zhu, N. Trefiak, T. Woo, Y. Huang,** "A $^{47/49}\text{Ti}$ Solid-State NMR Study of Layered Titanium Phosphates at Ultrahigh Magnetic Field," *Journal of Physical Chemistry C* **113** (2009) 10029–10037.
<http://dx.doi.org/10.1021/jp901235w>

S.Z. Qiao, C.X. Lin, Y. Jin, Z. Li, Z. Yan, Z. Hao, Y. Huang and G.Q. Lu, "Surface Functionalized Periodic Mesoporous Organosilica Hollow Spheres," *Journal of Physical Chemistry C* **113** (2009) 8673–8682.
<http://dx.doi.org/10.1021/jp810844p>

B. Chen, Y. Huang, "Dry Gel Conversion Synthesis of SAPO- and CoAPO-based Molecular Sieves by Using Structurally Related Preformed AIPO Precursors as the Starting Materials," *Microporous and Mesoporous Materials* **123** (2009) 71–77.
<http://dx.doi.org/10.1016/j.micromeso.2009.03.025>

University of Windsor

M.-H. Thibault, B.E.G. Lucier, R.W. Schurko and F.-G. Fontaine, "Synthesis and solid-state characterization of platinum complexes with hexadentate amino- and iminophosphine ligands," *Dalton Transactions* (2009) online.
<http://dx.doi.org/10.1039/b907737e>

 **L.A. O'Dell and R.W. Schurko,** "Static solid-state ^{14}N NMR and computational studies of nitrogen EFG tensors in some crystalline amino acids," *Physical Chemistry Chemical Physics* **11** (2009) 7069–7077.
(Invited Article, Themed Issue)
<http://dx.doi.org/10.1039/b906114b>

L.A. O'Dell and R.W. Schurko, "Fast and Simple Acquisition of Solid-State ^{14}N NMR Spectra with Signal Enhancement via Population Transfer," *Journal of the American Chemical Society* **131** (2009) 6658–6659.
<http://dx.doi.org/10.1021/ja901278q>



H. Hamaed, M. Laschuk, V. Terskikh, R. Schurko, "Application of Solid-State ^{209}Bi NMR to the Structural Characterization of Bismuth-Containing Materials," *Journal of the American Chemical Society* **131** (2009) 8271–8279.

<http://dx.doi.org/10.1021/ja901347k>

University of Manitoba

P.M. Aguiar, M.J. Katz, D.B. Leznoff and S. Kroeker, "Natural abundance ^{13}C and ^{15}N solid-state NMR analysis of paramagnetic transition-metal cyanide coordination polymers," *Physical Chemistry Chemical Physics* **11** (2009) 6925–6934. **(Invited Article, Themed Issue)**

<http://dx.doi.org/10.1039/b907747b>



B. Zhou, B.L. Sherriff and T. Wang, " ^{27}Al NMR spectroscopy at multiple magnetic fields and *ab initio* quantum modeling for kaolinite," *American Mineralogist* **94** (2009) 865–871.

<http://dx.doi.org/10.2138/am.2009.3142>



V.K. Michaelis, P.M. Aguiar, V.V. Terskikh and S. Kroeker, "Germanium-73 NMR of Amorphous and Crystalline GeO_2 ," *Chemical Communications* (2009) 4660–4622.

(Cover Article)

<http://dx.doi.org/10.1039/b906642j>

A.J. Lussier, P.M. Aguiar, V.K. Michalis, S. Kroeker, F.C. Hawthorne, "The occurrence of tetrahedrally coordinated Al and B in tourmaline: An ^{11}B and ^{27}Al MAS NMR study," *American Mineralogist* **94** (2009) 785–792.

<http://dx.doi.org/10.2138/am.2009.3000>

University of Alberta

F. Chen, S-W Oh, and R.E. Wasylishen, "A Solid-State ^{31}P NMR Study of 1:1 Silver-triphenylphosphine complexes - Interpretation of $^1J(^{107,109}\text{Ag}, ^{31}\text{P})$ Values," *Can. J. Chem.* **87** (2009) 1090–1101.

<http://dx.doi.org/10.1139/V09-076>

K. Huynh, A.J. Lough, M.A.M. Forgeron, M. Bendle, A.P. Soto, R.E. Wasylishen, and I. Manners, "Synthesis and Reactivity of Phosphine-Stabilized Phosphoranimine Cations,

$[\text{R}_3\text{P}\cdot\text{PR}_2][\text{NSiMe}_3]^+$ " *J. Am. Chem. Soc.* **131** (2009) 7905–7916.

<http://dx.doi.org/10.1021/ja900256g>

M.E. Halse, P.T. Callaghan, B.C. Feland and R.E. Wasylishen, "Quantitative analysis of Earth's field NMR spectra of strongly-coupled heteronuclear systems," *Journal of Magnetic Resonance* **200** (2009) 88–94.

<http://dx.doi.org/10.1016/j.jmr.2009.06.012>

B.L. Lee, X.J. Li, Y.S. Liu, B.D. Sykes, L. Fliegel, "Structural and Functional Analysis of Transmembrane XI of the NHE1 Isoform of the Na^+/H^+ Exchanger," *Journal of Biological Chemistry* **284** (2009) 11546–11556.

<http://dx.doi.org/10.1074/jbc.M809201200>

R.M.B. Hoffman and B.D. Sykes, "Structure of the Inhibitor W7 Bound to the Regulatory Domain of Cardiac Troponin C," *Biochemistry* **48** (2009) 5541–5552.

<http://dx.doi.org/10.1021/bi9001826>

M.J. Willans, R.E. Wasylishen and R. McDonald "Polymorphism of Potassium Ferrocyanide Trihydrate as Studied by Solid-State Multinuclear NMR Spectroscopy and X-ray Diffraction," *Inorganic Chemistry* **48** (2009) 4342–4353.

<http://dx.doi.org/10.1021/ic802134j>

University of Calgary

E.-J. Lee, R. Shaykhtudinov, A.M. Weljie, H.J. Vogel, P.J. Facchini, S.-U. Park, Y.-K. Kim, T.-J. Yang, "Quality Assessment of Ginseng by ^1H NMR Metabolite Fingerprinting and Profiling Analysis," *J. Agric. Food Chem.* (2009) ASAP.

<http://dx.doi.org/10.1021/jf901675y>

S.A. Lusceac, M.R. Vogel, C.R. Herbers, " ^2H and ^{13}C NMR studies on the temperature-dependent water and protein dynamics in hydrated elastin, myoglobin and collagen," *Biochimica et Biophysica Acta (BBA) - Proteins & Proteomics* (2009) online.

<http://dx.doi.org/10.1016/j.bbapap.2009.06.009>

E.F. Haney, H.N. Hunter, K. Matsuzaki, H.J. Vogel, "Solution NMR studies of amphibian antimicrobial peptides: Linking structure to function?" *Biochimica et Biophysica Acta (BBA)*

- *Biomembranes* **1788** (2009) 1639–1655.
(review)
<http://dx.doi.org/10.1016/j.bbamem.2009.01.002>

A.P. Yamniuk, K.L. Anderson, M.E. Fraser, H.J. Vogel, "Auxiliary Ca²⁺ binding sites can influence the structure of CIB1", *Protein Science* **18** (2009) 1128-1134.
<http://dx.doi.org/10.1002/pro.104>

V. Tremaroli, M.L. Workentine, A.M. Weljie, H.J. Vogel, H. Ceri, C. Viti, E. Tatti, P. Zhang, A.P. Hynes, R.J. Turner, D. Zannoni, "Metabolomic Investigation of the Bacterial Response to a Metal Challenge", *Applied and Environmental Microbiology* **75** (2009) 719-728.
<http://dx.doi.org/10.1128/AEM.01771-08>

University of Lethbridge



J.S. Hartman, B. Berno, P. Hazendonk, C. Kirby, E. Ye, J.

Zwanziger, A. Bain, "NMR Studies of Nitrogen Doping in the 4H Polytype of Silicon Carbide: Site Assignments and Spin-Lattice Relaxation," *Journal of Physical Chemistry C* **111** (2009) 15024–15036.
<http://dx.doi.org/10.1021/jp904639n>

University of British Columbia

A.C.J. Weber, X. Yang, R.Y. Dong, W.L. Meerts, E.E. Burnell, "Solute order parameters in liquid crystals from NMR spectra solved with evolutionary algorithms: Application of double Maier-Saupe Kobayashi-McMillan theory," *Chemical Physics Letters* **476** (2009) 116-119.
<http://dx.doi.org/10.1016/j.cplett.2009.06.002>

X. Li, P.T. Eles, C.A. Michal, "Water Permeability of Spider Dragline Silk," *Biomacromolecules* **10** (2009) 1270-1275.
<http://dx.doi.org/10.1021/bm900103n>

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