

### Guest Editorial

#### Gang Wu, Queen's

It appears that this summer has been full of events (personally and professionally) that are, in one way or another,

associated with Rod Wasylishen.

At the end of May, I attended the annual conference of the Canadian Society for Chemistry (CSC) in Edmonton, Alberta. Rod organized a special two-day symposium devoted to Advances in Solid-State NMR, which many of Rod's current and former students participated in (see photo). During this trip, I also had a chance to visit Rod's wife, Val, whom I had not seen after my graduation from Dalhousie - 14 years seem to have just elapsed like a second! Unfortunately, I did not see Eric, Rod's younger son, who had just left for Waterloo for his summer co-op job. In my mind, Eric is still a 5-year-old boy who enjoyed watching evaporating liquid nitrogen when Rod brought him to the laboratory on a Sunday afternoon. Now in front of my eyes is a research poster presented at the CSC conference by Eric and Brett Feland (Rod's summer student) describing "Pulse Fourier-Transform NMR Spectroscopy in the Earth's Magnetic Field". I should have thought of a project for my own 5-year-old boy, David.

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Early June brought the news that the Ultrahigh-Field NMR Facility for Solids will be able to apply for CFI LEF funding under a National Facility designation. This not only provides us with new opportunities to enhance the current capabilities of the Facility, but also reminds me of the tremendous amount of effort that Rod had put into this project. I recalled that Rod had told me his idea of



(L-R) Rod Wasylishen, Kris Ooms, David Bryce, Rob Schurko, Scott Kroeker, Glenn Penner, Gang Wu, Guy Bernard, Kris Harris, Jerrod Dwan

establishing a national solid-state NMR center as early as in 1998. Indeed Rod, together with John Ripmeester and Christian Detellier, spearheaded this national project and was instrumental in getting it funded by 2002. Now the entire Canadian solid-state NMR community is benefiting from having access to this state-of-the-art facility. However, as Alex Bain has already cautioned us in a previous Editorial, "modern spectrometers not only allow us to get beautiful spectra, but they also must be pushed to start probing systems that we would never have thought possible". I couldn't agree more. So the challenge is now on us: can we produce the best science?

Also in June, we heard another piece of good news that Rod's Canada Research Chair (CRC) in Physical Chemistry has been renewed for another seven years (in a total amount of \$1,400,000). According to the CRC citation, Rod "will address the questions surrounding the interpretation of information obtained through NMR. More specifically, he will look at how new approaches to NMR could recover information that is currently lost when an object is scanned."

In July, we were informed that the Editorial Board of the Canadian Journal of Chemistry has decided to publish a special issue in honour of Rod's outstanding contributions to Canadian chemistry. This special issue of Can. J. Chem. is scheduled to appear in 2011, and this recognition is most fitting because of Rod's commitment and service to the Journal. I am sure that Rod's students and colleagues will enthusiastically contribute to this special issue.

As I look at the picture taken at this year's CSC, I feel that a few more words need to be said about Rod and his impact on all of us. Rod is not only a fantastic scientist, but also a great educator. In fact, this particular photo displays a partial spectrum of Rod's students: Glenn Penner (PDF, 1987), Gang Wu (PhD, 1994), Rob Schurko (PhD, 1998), Scott Kroeker (PhD, 1999), Guy Bernard, (PhD, 2000), David Bryce (PhD, 2002), Kris Ooms (PhD, 2007), Kris Harris (PhD candidate), and Jerrod Dwan (MSc candidate). To date, eight of Rod's former students are on faculty in Canadian universities (Waterloo, Guelph, Ottawa, St. Francis Xavier, Queen's, Manitoba, Winnipeg, and Windsor). Others hold NMR-related positions across Canada and worldwide. It is perhaps not an

overstatement that Rod has educated, almost single-handedly, a new generation of solid-state NMR spectroscopists in Canada.

Here I am pleased to announce that a symposium in honour of Rod will be held at the 55<sup>th</sup> International Conference on Analytical Sciences and Spectroscopy (ICASS) in Kingston, Ontario (August 9-12, 2009). I hope that many of Rod's students and friends can attend this conference. Finally, as I enjoy very much recounting these events in this special summer, I would like to take this opportunity to say "Rod, thank you!"

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## Canadian NMR news

*Forward us any news of interest to the Canadian NMR community.*

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### **Thompson Rivers University to acquire a new NMR instrument**

Thompson Rivers University (Kamloops, BC) ([www.tru.ca](http://www.tru.ca)) has received federal funding via Western Economic Diversification Canada toward the purchase of nuclear magnetic resonance (NMR) equipment that will be used to train students and carry out applied research with industry. The new equipment will also provide analytical chemistry support to firms in various industry sectors in BC including mining, forestry, agriculture, nutraceuticals, and industrial biotechnology.

Read the full story here

[http://www.tru.ca/marketing/mediareleases/2008/WED\\_Release.html](http://www.tru.ca/marketing/mediareleases/2008/WED_Release.html)

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### **Magnetic Resonance at IBD**



A feature interview with Tedros Bezabeh, a physical chemist at the NRC Institute for Biodiagnostics (Winnipeg, Manitoba). Tedros applies NMR spectroscopy and MRI for the early detection and non-invasive diagnosis of cancer.

<http://www.nrc-cnrc.gc.ca/eng/education/innovations/scientists/bezabeh.html>

Photo from: <http://www.nrc-cnrc.gc.ca/>

## NMR at Cape Breton University



On May 8 the front cover of the Cape Breton Post has featured a story about NMR research at **Cape Breton University** (Sydney, Nova Scotia). A new high-field NMR spectrometer for liquids has been recently acquired by CBU to support research in the

Department of Chemistry. Matthias Bierenstiel, an assistant professor of chemistry, will be one of the primary users of this instrument. This project has been sponsored in part by Enterprise Cape Breton Corporation.

Read the full story published by the Cape Breton Post (cover credit)

<http://www.capebretonpost.com/index.cfm?sid=132773&sc=145>

The press release by CBU

<http://www.cbu.ca/cbu/newsrel/NewsDetail.asp?NewsID=419>

## Gerald Buchanan: The science of attraction



Gerald Buchanan, chancellor's professor of Chemistry at Carleton University (Ottawa), has announced his retirement. Most of his very successful research career at Carleton, since 1971, Gerald

dedicated to advancing the field of NMR spectroscopy and magnetic resonance imaging. Gerald will stay at Carleton part-time to continue his teaching and research.

Read the feature story about Gerald Buchanan in the spring issue of *EUREKA*, the Newsletter of the Carleton's Faculty of Science

<http://eureka.carleton.ca/2008-03/148.htm>

Gerald Buchanan discusses the science behind possible links between attraction and smell in the Spring 2008 issue of the *Carleton University Magazine*

[http://magazine.carleton.ca/2008\\_Spring/2034.htm](http://magazine.carleton.ca/2008_Spring/2034.htm)

Photo from: <http://www.carleton.ca/>

## MOOT 21 NMR Symposium

Windsor, Ontario, Canada - October 4-5, 2008

Submitted by Rob Schurko (University of Windsor)

### MOOT 21 NMR Symposium

The 21st annual MOOT NMR Symposium will be held at the University of Windsor in Windsor, Ontario, Canada on October 4-5, 2008. Registration and abstract submissions for talks and posters is now open.

<http://www.uwindsor.ca/moot>

For the first time in its history, the MOOT will feature NMR research groups from across Canada and the mid-western United States. Contributions from grad students, post-docs and faculty from across Canada and the U.S. are welcome.

Lectures and poster sessions will be held on campus at the Toldo Health Education Centre, Room 100. We will feature four tutorial lectures on topics including biomolecular NMR, processing of NMR spectra, CP/MAS and quadrupolar nuclei - full sets of notes will be made available to all registrants.

**Glenn Facey** (Ottawa) Spectral Processing

**Vlad Ladizhansky** (Guelph) Cross Polarization - a coherent perspective

**Giuseppe Melacini** (McMaster) Protein NMR: What it can do for you & what you can do for it

**Rod Wasylishen** (University of Alberta) NMR of Quadrupolar Nuclei

This year's banquet will be held at the Art Gallery of Windsor, in downtown Windsor, right next to all of the major hotels, and a vibrant nightlife area.

We look forward to seeing you in October!

**Chair:** Rob Schurko, University of Windsor

**Co-chair:** Philip Grandinetti, the Ohio State University



The 900 NMR Facility is a proud sponsor of the MOOT 21 NMR Symposium

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Submitted by Chris Greenwood (University of Victoria)

**VIVA II**, the West Coast NMR Users meeting, was held on June 20-21, 2008 at the University of Victoria in Victoria, B.C.

<http://chemistry.uvic.ca/viva2.html>

Over 30 participants from Canada and North-Western U.S. enjoyed a busy program of talks, a poster session with social gathering, and general discussion of NMR along with a banquet at the University Club of Victoria. After the banquet, Martin Smith (Executive VP of Bruker Canada, retired) presented a slide show "Another Vancouver Island".

Next year's VIVA will be held in June, 2009 at Simon Fraser University in Vancouver.



**VIVA II** Banquet at the University Club

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Submitted by Keith Brown (University of Saskatchewan)

### Product Operator Calculator

This is to announce the release of an open source program for the calculation of product operators, **wxProdOp**.

The current version is 0.92 and contains several features for the simplification of state expressions produced after several pulses and evolution periods. The program currently runs under both Linux and Windows and has very modest hardware requirements. Please visit

<http://chem4823.usask.ca/nmr/wxProdOp.html>

for more information and downloads. Also, there is a very detailed manual available that fully describes the current capabilities of the program.

<http://chem4823.usask.ca/nmr/wxProdOp.pdf>

Let me know what you think:

Dr. Keith Brown  
Department of Chemistry  
Saskatchewan Structural Sciences Center  
University of Saskatchewan  
Saskatoon, Saskatchewan  
306-966-1725  
<http://chem4823.usask.ca/kbrown.html>

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### Canadian NMR blogs and news sites

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



**VIVA II** At the poster session



**VIVA II** Kirk Marat demonstrates new functionalities in the SpinWorks

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 News (Albin Otter, Alberta)  
[http://nmr.chem.ualberta.ca/nmr\\_news.htm](http://nmr.chem.ualberta.ca/nmr_news.htm)

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## NMR Theses Recently Defended

*Congratulate your students here!*

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**Gang (Eric) Ye** (Department of Chemistry, McMaster University) July 10, 2008

Research supervisor: Gillian Goward

Ph.D. thesis: "Studies of Proton Conductors Based on Nafion and Sulfonated Polyether Ether Ketone (S-PEEK) Using High-resolution Solid State NMR"

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**Bryan Demko** (Department of Chemistry, University of Alberta) April 29, 2008

Research supervisor: Roderick Wasylishen

Ph.D. thesis: "A Solid-State NMR Comparison of Main Group and Transition Metal Square-Planar Complexes of the Diselenoimidodiphosphinate Anion"

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## Recognition

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### Ontario Premier's Discovery Awards

Discovery Awards celebrate the research excellence of Ontario's most accomplished researchers by highlighting their individual achievements and demonstrating Ontario's attractiveness as a global research centre. Two of the four Discovery Award Recipients in 2008 are Ontario researchers working in the field of magnetic resonance, **Lewis Kay** (University of Toronto) in the category of *Life Sciences and Medicine*, and **Raymond Laflamme** (University of Waterloo) in the category of *Natural Sciences and Engineering*.

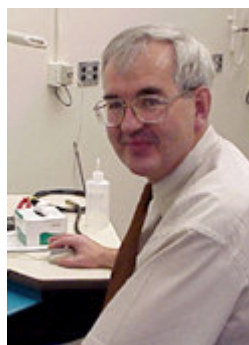
Congratulations to our colleagues!

Press release by the Government of Ontario

[http://www.mri.gov.on.ca/english/news/PIA043008\\_bd4.asp](http://www.mri.gov.on.ca/english/news/PIA043008_bd4.asp)

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### Rod Wasylishen receives Canada Research Chair



Rod Wasylishen's Tier I Canada Research Chair in Physical Chemistry has been renewed for a period of seven years. Rod's many scientific contributions are well-known to the Canadian NMR community and do not require a special introduction. Besides being a prominent world-renowned NMR researcher

and a mentor to many of us, Rod is also an active member of the 900 NMR Facility Steering Committee. Please join us in extending our warmest congratulations to Rod and his family.

Photo from: <http://www.ualberta.ca/>

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### 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

Mitsuhiro Ikura (Toronto) Molecular Biology

Lewis Kay (Toronto) Biochemistry

Vladimir Ladizhansky (Guelph) Cell Biology

Raymond Laflamme (Waterloo) Physics

Pascale Legault (Montréal) Biochemistry

Simon Sharpe (Toronto) Biochemistry

Roderick Wasylishen (Alberta) Phys Chemistry

Josef Zwanziger (Dalhousie) Phys Chemistry

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### Valerie Robertson featured in *At Guelph*



Read a feature article about Valerie Robertson, an NMR Facility Manager at the University of Guelph, in the April 2008 issue of *At Guelph*, the University of Guelph's official campus newspaper.

<http://www.uoguelph.ca/atguelph/08-04-23/focus.shtml>

Photo from: [www.uoguelph.ca](http://www.uoguelph.ca)

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**Dr. Gang Wu** (Queen's University) has been appointed to be a member of the NSERC Grant Selection Committee (GSC 26) for three years (2008-2010).

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**Pierre Harvey** (Université de Sherbrooke) has been awarded **the 2008 Gerhard Herzberg Award**. The award is presented by the Canadian Society for Analytical Sciences and Spectroscopy (CSASS) to a Canadian spectroscopist in recognition of distinguished scientific contributions to the field of spectroscopy, either fundamental or applied. It is awarded to recognize the career achievements of a prominent scientist.

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

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**Suzana Straus** (UBC) has received a **Michael Smith Career Investigator Award** to study function of cationic antimicrobial peptides and lipopeptides. The work has important implications for the design of better antibiotics.

<http://www.science.ubc.ca/news/179>

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## On the move

**Lindsay Cahill** has joined the Solid State NMR group at the Department of Physics, University of Warwick as an NSERC postdoctoral fellow. Lindsay did her Ph.D. with Gillian Goward at McMaster.

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**Kristopher Ooms**, after completing a postdoctoral fellowship with Tatyana Polenova (University of Delaware), is taking up an assistant professor position at The King's University College in Edmonton where he will be developing an NMR research program with undergraduate students.

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**Konstantin Romanenko** has recently joined Bruce Balcom's team (UNB) as a postdoctoral fellow. He is involved in development and applications of SPRITE methods. Konstantin completed his Ph.D. in solid-state NMR at the Borskov Institute of Catalysis in Novosibirsk (Russia), and then visited the Magnetic Resonance Microscopy Group at Montana State University, where he performed studies of porous media (ceramics and porous rock cores) with magnetic resonance imaging techniques and methods based on 2D Inverse Laplace Transformation.

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**Zhicheng (Paul) Xia** has settled in as a Manager of the UBC Chemistry High-Resolution NMR Analytical Services and Research Support Facility. At UBC Paul is replacing **Nick Burlinson** who is now officially retired. Before moving to Vancouver Paul has been at McGill University in Montreal.

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**Andrew Marble** has been appointed to the position of Assistant Professor in the Department of Systems and Computer Engineering at Carleton University in Ottawa. Andrew was a postdoctoral fellow with Bruce Balcom at the University of New Brunswick working on design of compact permanent magnet arrays for magnetic resonance applications.

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## the 900 NMR Facility News

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### 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.

#### *Recent Travel Grant Recipients*

**Aaron Rossini** (University of Windsor)

**Kamal H. Mroue** (University of Waterloo)

[http://nmr900.ca/policies\\_e.html](http://nmr900.ca/policies_e.html)



### Remote access NMR

Fulfilling our promise to the Canadian NMR community, we are pleased to announce that the 900 MHz NMR instrument is now accessible remotely from virtually everywhere in Canada. This exciting option for many of our users has become reality as a part of the SpectroGrid project being developed and supported by **Andre Charbonneau** and colleagues from the Information Management

Services Branch, National Research Council Canada.

**Pictured:** SpectroGrid2 client is being used from the University of Alberta in Edmonton to remotely acquire spectra on the 900 MHz NMR instrument located in Ottawa, some 2840 km apart (May 22, 2008).

More about the SpectroGrid project

<https://spectrogrid2.nrc.ca/portal/?q=node/1>

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## Upcoming NMR Events

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

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**ICASS 2008** 54<sup>th</sup> International Conference on Analytical Sciences and Spectroscopy

August 3-6, 2008, John Abbott College, St-Anne-de-Bellevue, Quebec, Canada  
<http://www.icass.ca/>

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**XXIII ICMRBS** International Conference on Magnetic Resonance in Biological Systems

August 24-29, 2008, San Diego, California  
<http://www.icmrbs2008.org/>

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**Frontiers of Magnetic Resonance**, BRSG Magnetic Resonance Group Meeting

September 15-16, 2008, University of Warwick, U.K.

[http://www.iop.org/Conferences/Forthcoming\\_Institute\\_Conferences/BRSG%20meeting/event\\_27134.html](http://www.iop.org/Conferences/Forthcoming_Institute_Conferences/BRSG%20meeting/event_27134.html)

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## MOOT 21 NMR Symposium

October 4-5, 2008, Windsor, ON  
<http://www.uwindsor.ca/moot/>

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## 50<sup>th</sup> ENC

March 29 - April 3, 2009, Asilomar, Pacific Grove, California  
<http://www.enc-conference.org/>

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## Suggestion Box for the 50<sup>th</sup> ENC

Organizers of the 50<sup>th</sup> ENC in 2009 are planning several special events/presentations to commemorate the 50<sup>th</sup> ENC. If you have some unique ideas or documents that reflect the history of the ENC and the significance to

the NMR community you are invited to share these ideas, memory items, photos, etc. through the 50<sup>th</sup> ENC Suggestion Box

<http://www.enc-conference.org/Default.aspx?tabid=136>

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**The 4<sup>th</sup> Annual Solid-State NMR Workshop** at the 92<sup>nd</sup> Canadian Chemistry Conference and Exhibition (CSC 2009)

May 30–June 3, 2009, Hamilton, ON  
[http://nmr900.ca/events\\_e.html](http://nmr900.ca/events_e.html)

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**CSC 2009** the 92<sup>nd</sup> Canadian Chemistry Conference and Exhibition

May 30–June 3, 2009, Hamilton, ON  
[http://www.cheminst.ca/index.cfm?ci\\_id=3850&la\\_id=1](http://www.cheminst.ca/index.cfm?ci_id=3850&la_id=1)

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**XeMat 2009** the 4<sup>th</sup> International Symposium on Xenon NMR of Materials

June 8-10, 2009, the Northern Finland  
<http://cc.oulu.fi/~nmrlab/xemat/>

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**VIVA III** the 3<sup>rd</sup> Annual West Coast NMR Minisymposium

June 2009, Simon Fraser University, Vancouver, B.C.  
<http://www.sfu.ca/chemistry/facilities/nmr/index.html>

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**ICASS 2009** 55<sup>th</sup> International Conference on Analytical Sciences and Spectroscopy

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

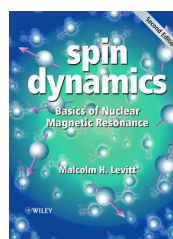
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## NMR books

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

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## Spin Dynamics: Basics of Nuclear Magnetic Resonance



Malcolm H. Levitt  
**Paperback:** 744 pages  
**Publisher:** Wiley; 2<sup>nd</sup> edition (April 25, 2008)  
**Language:** English  
**ISBN-10:** 0470511176  
**ISBN-13:** 978-0470511176

Wiley: "Completely revised and updated, the Second Edition of this successful textbook

guides the reader through the essential principles and concepts needed for a thorough understanding of NMR spectroscopy... Includes a new chapter on magic-angle-spinning and recoupling experiments, an expanded coverage of solid state NMR, and additional information on treatment of quadrupolar interaction and chemical shift anisotropy."

<http://www.amazon.ca/gp/product/0470511176/>

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## Nature Milestones in Spin



**Milestones** are special supplements published by Nature Publishing Group highlighting various fields of science and technology. The sixth such supplement **Nature Milestones in Spin** covers the story of "Spin", a topic dear to all reading these web-pages.

This very colourful and neatly arranged 48 page publication is available for free download as a PDF file.

<http://www.nature.com/milestones/milespin/digital/digital.html>

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## NMR Jobs and Vacancies

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

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### University of Guelph

**A postdoctoral NMR position** is available immediately in the area of NMR of membrane proteins and protein-protein interactions. The particular project is to study an integral 7TM protein, its interaction with its soluble transducer, and the interaction between the transducer and DNA. The project will involve both solution and solid-state NMR, conducted on a range of instruments from 500 to 800 MHz. Applicants familiar with or willing to learn protein expression and purification, and with previous experience in biological NMR are encouraged to apply. The work will be conducted in the Department of Physics, University of Guelph and will be co-supervised by Profs. V. Ladizhansky and L. Brown. Additional information is available upon request. Please send a CV and the names and addresses of three references to Leonid Brown or Vladimir Ladizhansky if you are interested.

<http://www.uoguelph.ca/~lebrown/brown.html>

<http://www.physics.uoguelph.ca/%7Evladimir/>

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## Bruker BioSpin Canada

is seeking to employ an additional **applications engineer** to support the growing activities of the AVANCE line of nuclear magnetic resonance spectrometers. In particular we seek candidates possessing M.Sc. or Ph.D. degrees. Experience in the field of nuclear magnetic resonance spectroscopy would be a distinct advantage, although candidates with a strong computer background and interest in customer support and training should not hesitate to apply.

Candidates will be Canadian citizens or permanent residents and should be prepared to offer a high degree of self motivation and demonstrate their eagerness to contribute to the company's growth in terms of scientific excellence, customer service, customer training and successfully achieved sales.

Bruker BioSpin is located in pleasant and rural surroundings in Milton, Ontario

<http://www.bruker.com/ca.html>

Our custom built facility is equipped with applications laboratories, assembly and test facilities, repair workshops and extensive employee amenities. Milton is within easy distance of Metropolitan Toronto with ready access to such outdoor pleasures such as hiking, sailing, and skiing. Bruker BioSpin offers a competitive salary and an excellent employee benefits package.

Candidates who fill these requirements are invited to apply in writing (fax or mail only please) to:

Bruker BioSpin Ltd.  
555 Steeles Avenue East  
Milton, Ontario, L9T 1Y6

Attn: Dr. Martine M. Monette, Applications Manager  
Fax: 905-876-4421

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## Listings of NMR jobs and vacancies

Canadian NMR Jobs

[http://nmr900.ca/ssnmr\\_jobs.html](http://nmr900.ca/ssnmr_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

<http://apex.ibpc.fr/wws/arc/nmr>

NMR jobs on SpectroscopyNow.com

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



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## Canadian NMR Research Highlights

Research highlights and most recent NMR publications by Canadian research teams

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### Cover article in *Phys Chem Chem Phys*



A research paper by our colleagues from NRC featuring results from the 900 instrument is on the cover of *Physical Chemistry Chemical Physics*. Congratulations!

**Darren H. Brouwer, Saman Alavi and John A. Ripmeester**, "NMR Crystallography of *p*-*tert*-Butylcalix[4]arene Host-Guest Complexes Using  $^1\text{H}$  Complexation-Induced Chemical Shifts," *Physical Chemistry Chemical Physics* **10** (2008) 3857-3860.  
<http://dx.doi.org/10.1039/b805326j>

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### Two NMR papers in *PNAS*

A research paper by **Cheryl Arrowsmith** (Ontario Cancer Institute, University of Toronto) and colleagues has been highlighted on the cover and in a commentary.



**Y. Shen, O. Lange, F. Delaglio, P. Rossi, J. M. Aramini, Gaohua Liu, A. Eletsy, Y. Wu, K.K. Singarapu, A. Lemak, A. Ignatchenko, C.H. Arrowsmith, T. Szyperki, G.T. Montelione, D. Baker, and A. Bax**,

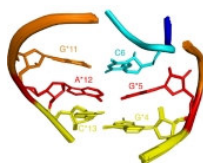
"Consistent blind protein structure generation from NMR chemical shift data," *Proc. Natl. Acad. Sci. USA* **105** (2008) 4685-4690.  
<http://dx.doi.org/10.1073/pnas.0800256105>

### *PNAS* Commentary

<http://www.pnas.org/content/105/12/4533>

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**David Bryce** (U Ottawa) has collaborated with H el ene van Melckebeke and J er me Boisbouvier (CNRS, Grenoble) to reveal the molecular origins of the high stability of HIV TAR RNA bound to its SELEX RNA aptamer. A non-canonical loop-closing GA base pair was found to be stabilized by a network of intersugar hydrogen bonds, which in turn accounts for the greatly reduced dissociation constant of the complex relative to those without the GA pair.



The structure of the "kissing complex" was determined using liquid crystal NMR spectroscopy, and represents one of the highest-resolution RNA structures determined in solution to date.

**H. Van Melckebeke, M. Devany, C. Di Primo, F. Beaurain, J.-J. Toulme, D. L. Bryce, and J. Boisbouvier**, "Liquid Crystal NMR Structure of HIV TAR RNA Bound to its SELEX RNA Aptamer Reveals the Origins of the High Stability of the Complex," *Proc. Natl. Acad. Sci. USA* **105** (2008) 9210-9215.  
<http://dx.doi.org/10.1073/pnas.0712121105>

**Press release** by CNRS (Centre national de la recherche scientifique, France)

<http://www2.cnrs.fr/presse/communiqu e/1381.htm>

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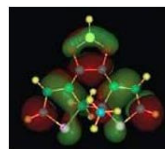
### Chemical Communications

Feature Article

**A.W. Oleman, S. Jebors, P. Shahgaldian, G.S. Ananchenko, J.A. Ripmeester**, "*para*-Acylcalix[*n*]arenes: from molecular to macroscopic assemblies", *Chemical Communications* **20** (2008) 2291-2303.  
<http://dx.doi.org/10.1039/b717495k>

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### Angewandte Chemie



An elegant work by **Neil Branda** and co-workers from Simon Fraser University studying molecular switches using  $^1\text{H}$  NMR spectroscopy among other techniques.

**V. Lemieux, M.D. Spantulescu, K.K. Baldrige, N.R. Branda**, "Modulating the Lewis acidity of boron using a photoswitch," *Angew. Chem. Int. Ed.* **47** (2008) 5034-5037.  
<http://dx.doi.org/10.1002/anie.200800869>

This work has also been highlighted by *Nature Chemistry*  
<http://www.nature.com/nchem/reshigh/2008/0608/full/nchem.23.html>

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### Trends in Analytical Chemistry

a review article by **David Wishart** (University of Alberta)

**D.S. Wishart** "Quantitative metabolomics using NMR," *Trends in Analytical Chemistry* **27** (2008) 228-237.  
<http://dx.doi.org/10.1016/j.trac.2007.12.001>

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### **Concepts in Magnetic Resonance, Part A, Bridging education and research**

Featuring an enlightening excursion into some of the basic concepts of magnetic resonance spectroscopy by **John Weil** (Professor Emeritus of Chemistry and Physics, University of Saskatchewan)

[http://www.usask.ca/chemistry/faculty\\_weil.html](http://www.usask.ca/chemistry/faculty_weil.html)

**J.A. Weil**, "The life of  $\pi$  and  $\sigma$  - A tutorial review of the ubiquitous use of these symbols in Zeeman and magnetic-resonance spectroscopy," *Concepts in Magnetic Resonance* **32A** (2008) 134-142.  
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*a teaching aid featurette, off topic and yet rather educational*

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

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