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

Canadian NMR Research News Bulletin #6.2
Spring 2012

Editorial

David Bryce
University of Ottawa

As most of the Canadian science and engineering community has heard, **NSERC** has indefinitely suspended both the Major Resources Support (**MRS**) and the Research Tools & Instruments (**RTI**) programs. If uncorrected, this will have a disastrous irreversible impact on a huge swath of Canadian science. The National Ultrahigh-Field NMR Facility for Solids is fortunate to currently hold a modest MRS grant of $88600 per year through the 2013-2014 fiscal year. Following the expiry of non-renewable Canada Foundation for Innovation Infrastructure Operating Funds (CFI IOF), the MRS represented the only source of grant funding to maintain operations of our nationally unique facility. After an initial capital investment of $11.8M, it is difficult to understand why the funding agencies would give up on facilities such as ours after such a short time. Furthermore, the loss of the RTI program means there are no dedicated funding streams for the repair or purchase of minor equipment.

I sent a letter (see next page) to The Minister of Industry, **Christian Paradis**, and to the President of NSERC, Dr. **Suzanne Fortier**, to convey the impact of the cancellation of these two core NSERC programs. The letter was **signed by 46 other scientists** from a broad range of disciplines of scientific and engineering research, and was also forwarded to several additional members of Parliament.

I have already received a response from the Honourable **Ted Hsu**, the Liberal Science and Technology Critic. Ted also holds a PhD in physics from Princeton. He has asked us to do the following in order for the issue to gain traction:

1) Ask your colleagues to write a very brief note to their local MPs. We need local MPs to hear about this issue, from all parties.

2) Ask your colleagues to send feedback to me at ted.hsu@parl.gc.ca The more I understand about the effects of cutting RTI and MRS, the better stories I can tell, the better chance we have.

Ted spoke in the House of Commons about the RTI NSERC program on May 3, 2012: http://www.youtube.com/watch?v=hMML6ixE_XE

I urge you to respond to Ted Hsu's requests.

Dave Bryce

In This Issue

May 3, 2012

Re: NSERC MRS and RTI programs

In her recent statement on *Economic Action Plan 2012*, Natural Sciences and Engineering Research Council (NSERC) president Dr. Suzanne Fortier "welcome[d] continued dialogue and exchange with the research community as we move forward". As researchers in many fields of natural sciences and engineering, we are writing to express our deep concern over the elimination of both the Major Resources Support (MRS) and the Research Tools and Instrument (RTI) programs of NSERC. This action will have drastic and irreversible effects on fundamental science and engineering research across Canada and internationally.

MRS and RTI are broad-based programs that support unique national (and international based in Canada) research facilities and the purchase of equipment critical to the discovery, innovation, and training capability of Canadian researchers. They are crucial to the support of research in many areas ranging from theoretical astrophysics, through polar research, through DNA barcoding, to materials research: in short, the full gamut of the research and innovation enterprise. These are programs so foundational to research in Canada that one would think that eliminating them was inconceivable. The funding provided enhances the training of thousands of highly qualified personnel in science and engineering.

The federal government and NSERC, through cuts to Tri-Council funding, have now killed these programs. Along with NSERC's Discovery Grant, these are the programs which supported fundamental research. There are now no funding streams dedicated to the purchase of scientific equipment or to operate nationally and internationally unique resources. The loss of the MRS program in particular means that resources built up over many years could be lost or made inaccessible due to loss of personnel needed to sustain the resource. As well, millions of dollars of equipment purchased through taxpayers' money will sit idle and gather dust due to a lack of operating funds. The negative impact on the training of the future generation of scientists cannot be overstated.

NSERC suggests that the Canada Foundation for Innovation (CFI) may pick up the slack in these two areas. However, the reality is that CFI is a different organization with different objectives and application requirements. CFI programs do not compensate for the loss of two core programs at NSERC.

Similarly, investments by the government in industrial and/or targeted research programs at NSERC do not compensate for the loss of the two core programs which enable a broad spectrum of research.

The loss of these programs is nothing short of a disaster for science in Canada. It continues the selective reduction and elimination of programs that support fundamental and discovery-driven research. This will drag down the entire research enterprise as the fundamental research of today produces the applied knowledge of tomorrow. We urge you to reconsider this direction and reaffirm NSERC's commitment to these vital programs.

Prof. David L. Bryce (on behalf of the undersigned)

Canadian NMR News

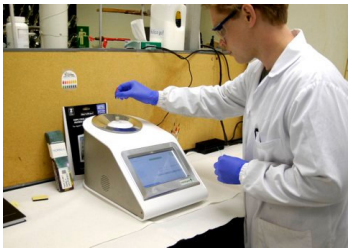
contributed by Jackie Metropolit (Nanalysis)

NMReady - 60 MHz bench-top NMR spectrometer

Nanalysis Corp. a Calgary based company has recently launched a 60MHz bench-top NMR spectrometer called the NMReady™. The Alberta Company was established in 2009 with a mandate to design and manufacture compact Nuclear Magnetic Resonance (NMR) devices. The company initially sought to commercialize Force-detected NMR (FDNMR) as realized in BOOMERANG technology, but soon transitioned to miniaturize traditional NMR to bring FT NMR technology to the bench or glovebox.

The NMReady™ debuted in March, 2012 at the American Chemical Society meeting in San Diego. Conference attendees were pleasantly surprised to find 60MHz spectroscopic resolution, running both 19F and 1H, at a fraction of the size and cost of current NMR instrumentation. The small size of the instrument allows it to fit on the benchtop, in the fume hood or even inside a glovebox. It comes equipped with a built-in touch screen display that features an easy-to-use, OneTouch NMR, operator interface. The NMReady is a cryogen-free NMR system, uses standard 3mm and 5 mm NMR tubes and has a very modest service schedule.

The NMReady has application in all types of industries, including oil & gas, chemical, pharma, biotech, and food processing, and in government and university labs. It also works as an ideal training tool in an academic setting, allowing students to gain hands-on experience with NMR. The compact NMR spectrometer can improve workflow, reduce costs of outsourcing and allow large organizations to optimize all of their spectroscopic resources.



Nanalysis has just entered into a collaborative research agreement with **Thesis Chemistry**, a Green Chemistry organization in Cambridge, Ontario. The company will integrate the analytical capability of the NMReady bench-top NMR spectrometer into their program of transforming lignocellulosic biomass into green chemicals. See the press release at http://www.accesswire.com/viewarticle.aspx?id=397349

Nanalysis will be showcasing the NMReady at **CSC 2012**, May 26-30, 2012, in Calgary. **Visit booth #222**, to get a live demo and see first-hand the capabilities of the NMReady.

For more information on the applications and functions of the NMReady, visit http://www.nanalysis.com

To watch the introduction to the NMReady 60P on YouTube
http://www.youtube.com/watch?v=PJJ9enYF6RU

EAS Faculty Award in NMR Spectroscopy: Call for Nominations

http://www.eas.org/askeas/NMR_New_faculty_award.pdf

The Eastern Analytical Symposium (EAS) establishes an EAS New Faculty Award in NMR Spectroscopy. The Inaugural Award will be presented at the 2012 Eastern Analytical Symposium. The Award, sponsored by Agilent Technologies, Inc. will recognize outstanding contributions by new faculty to the development of the field of NMR spectroscopy (broadly defined). To qualify for the award, candidates must be under the age of 40 at the time of the award and hold a position as a tenure-track Assistant Professor in an academic institution in the US or Canada. An Award winner will receive a certificate as well as $2,000 and will deliver an award lecture at a dedicated EAS session.

Persons who wish to make a nomination for the EAS New Faculty Award in NMR Spectroscopy should send complete documentation of the candidate (nominating letter summarizing achievements, curriculum vita or resume, a statement of the nominee's willingness to present an address as part of the award symposium, and at least one seconding letter). The length of the nomination packet should be commensurate with the nominee's

accomplishments, but should be limited to ten to fifteen pages. The deadline for the Inaugural 2012 Award is **June 15, 2012**. The Awardee will be selected by the EAS NMR Awards Committee and notified by August 15, 2012

Please send the nomination materials electronically (single PDF file is preferred) to:
E-mail: awards@eas.org

Andrew Teplyakov, 2012 Awards Chairman
Eastern Analytical Symposium

Visit us at: http://eas.org

100 kHz MAS in Canada

Dr. Ago Samoson (Tallinn University of Technology) was visiting the National Ultrahigh-Field NMR Facility for Solids (Ottawa) in early April. He brought along a 100 kHz MAS probe of his own built to explore the advantages of combining ultrahigh magnetic fields with very (!) fast magic angle spinning in solid-state NMR.

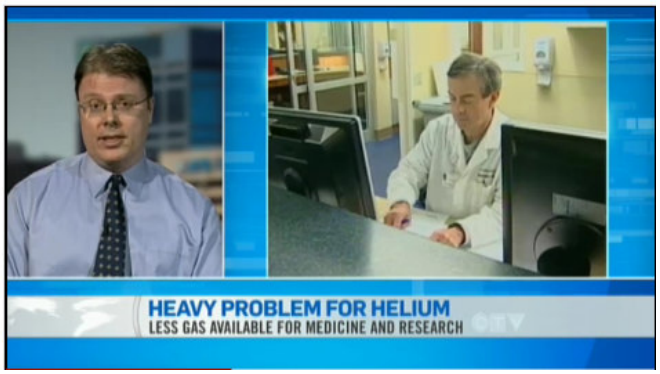
April 2012 (L-R) Leigh Spencer and Nicole De Almeida (McMaster), Ago Samoson (TTU), Andreas Brinkmann (NRC Canada).

Determining Sugar Sequence Fidelity

Chemical & Engineering News highlights research by **Todd L. Lowary** (Alberta Glycomics Centre, University of Alberta) and colleagues on enzymatic pathways in cellular carbohydrate chemistry. NMR is one of the key research tools in these studies.

http://cen.acs.org/articles/90/i18/Determining-Sugar-Sequence-Fidelity.html

Helium shortage could spell disaster



CTV News Channel interviews **Deryck Webb** (NANUC, University of Alberta) about He shortages and its impact on the MR enterprise in Canada and around the world (March 24, 2012).
http://tinyurl.com/7h89d97

Pharma firms see mixed fortunes in Québec

Canada's pharmaceutical and life sciences hub hit by cutbacks as effects of global slowdown continue to be felt, a special report by *Chemistry World* (RSC) (May 8, 2012)
http://tinyurl.com/c7lagdn

New and updated websites

NMR Facility, Faculty of Science, University of Ottawa
http://www.nmr.uottawa.ca/en/welcome.html

Université de Montréal
http://nmr900.ca/nmr_udem.html

NMR Facility, Department Chemistry & Biochemistry, Concordia University
http://chem.concordia.ca/facilities/nmr/

Nanalysis, Calgary
http://www.nanalysis.com

NMR on Twitter

New solid-state NMR papers
http://twitter.com/solidstateNMR

uOttawa NMR by Glenn Facey
http://twitter.com/uOttawaNMR

NMR Wiki http://twitter.com/nmrwiki

Canadian NMR news http://twitter.com/nmr900

Bruker http://twitter.com/bruker

Agilent http://twitter.com/agilent

International Society of Magnetic Resonance, ISMAR

In Memoriam

Sir Paul Callaghan (1947-2012)

It is with great sadness that ISMAR announces that Sir Paul Callaghan died from cancer March 24, 2012 at the age of only 64. He was an eminent figure in science in New Zealand and in NMR of materials. He is most known for his pioneering work combining rheology and NMR to unravel the flow behaviour of complex systems such as liquid crystals and polymer melts. These developments reach far beyond NMR and clearly represent landmarks of our field. His book on NMR Microscopy is a classic. His achievements have been recognized by numerous honours, prizes, and recognitions throughout the world.

Sir Paul Callaghan served as President of the International Society of Magnetic Resonance from 2008 to 2010 and did a tremendous job in this capacity. He initiated the concept of ISMAR Fellows in order to recognize eminent scientists in our field, and defined strategic goals for ISMAR's future. Though his severe illness often prevented him from travelling during his presidency, we were all extremely impressed by how much ISMAR mattered to him. Until very recently, no ISMAR action was taken without Paul's involvement and approval.

The International Society of Magnetic Resonance mourns its former President and Fellow of our Society. We feel privileged to have had the opportunity to work so closely with him for several years. On behalf of the Executive Committee and all the members of ISMAR, I express my deep gratitude.

We hold him in highest esteem and will express our appreciation at the upcoming ISMAR Conference to be held in Brazil next year.

Hans Wolfgang Spiess
ISMAR President
http://www.ismar.org/

Recognition

Canada Research Chair in magnetic resonance renewed

In March 2012 the Government of Canada has announced an investment of $124.5 million to fund 132 new or renewed Canada Research Chairs at 36 Canadian universities. This included renewal of one Chair involved in magnetic resonance research.

Simon Sharpe (University of Toronto) Canada Research Chair Tier 2 in Structural Biology of Membrane Active Proteins

Canada Research Chairs in MR

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

Cheryl Arrowsmith (Toronto) Biochemistry
Bruce Balcom (UNB) Multidisciplinary
Valerie Booth (Memorial) Biochemistry
Blaine Chronik (Western) Medical Physics
David Cory *(Waterloo) Quantum Information
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
Younès Messaddeq *(Laval) Photonics
Simon Sharpe (Toronto) Biochemistry
Gary Shaw (Western) Structural Neurobiology
Roderick Wasylishen (Alberta) Phys Chemistry
Josef Zwanziger (Dalhousie) Phys Chemistry

* Canada Excellence Research Chairs

Gary Schrobilgen (McMaster) has received the **Lifetime Achievement Award** on March 28, 2012 from SciFluor Life Sciences at the 243rd American Chemical Society National Meeting in San Diego, CA.

Professor Schrobilgen was recognized for the significant contributions he has made to the fields of synthetic and structural inorganic fluorine chemistry especially as regards the extremely challenging chemistry of the noble-gases.

Press release by McMaster
http://tinyurl.com/7vtrzqs

Anthony Mittermaier, associate professor of chemistry at McGill University (Montreal), to receive the **2012 Agilent Early Career Professor Award**. The Agilent Early Career Professor Award is presented annually to recognize and encourage excellence in measurement research.

Prof. Mittermaier has been awarded for his pioneering research in molecular biology, mutagenesis and NMR to study structure of proteins, their dynamics and function.

To read the press release by Agilent:
http://www.agilent.com/about/newsroom/presrel/2012/10may-ca12031.html

Julian Zhu – author of the week

Polymer Chemistry (RSC) profiles Prof. **Julian Zhu** (Université de Montréal) as the author of the week.

http://blogs.rsc.org/py/2012/04/27/author-of-the-week-julian-zhu/

53rd ENC Student Travel Awards

ENC has announced winners of **the 2012 Student Travel Stipends** attending the 53rd ENC, April 15-20, 2012, Miami, Florida. The stipends are funded by the ENC, the Suraj P. Manrao Science Foundation, and the generous contributions of companies. Among awardees there are several Canadian recipients, including

Andrée Gravel (Université du Québec à Montréal)

Emily Ritz (University of Guelph)

Siqi Zhu (McGill University)

Bryan Lucier (University of Windsor)

Hussain Masoom (University of Toronto)

Erick Meneses Ramirez (McGill University)

NMR Theses Recently Defended

Andre Sutrisno (University of Western Ontario), April 2012

Supervisor: Prof. Yining Huang

Ph.D. thesis: "Solid-State Nuclear Magnetic Resonance Spectroscopy of Low-Gamma Quadrupolar Nuclei in Inorganic Materials"

External Examiner: Prof. Darren Brouwer (Redeemer University College)

Cory Widdifield (University of Ottawa), February 2012

Supervisor: Prof. David Bryce

Ph.D. thesis: "Multinuclear Solid-State Magnetic Resonance Studies on 'Exotic' Quadrupolar Nuclei: Acquisition Methods, High-Order Effects, Quantum Chemical Computations, and NMR Crystallography"

External Examiner: Prof. William Power (University of Waterloo)

http://www.ruor.uottawa.ca/en/handle/10393/20722

Linda Davis (McMaster University), December 2011

Supervisor: Prof. Gillian Goward

Ph.D. thesis: "Multinuclear NMR Studies of Ion Mobility Pathways in Cathode Materials for Lithium Ion Batteries"

http://digitalcommons.mcmaster.ca/opendissertations/6692/

On the move

Eric Ye, after four years with the 900 NMR Facility Eric Ye has been transferred to work with Glenn Facey at the Chemistry Department, University of Ottawa. During his term with the 900 Facility Eric has become a real *VIP* of the 900 team. Eric's expert knowledge of NMR and his always friendly disposition will be missed by many Facility users. To contact Eric and to wish him the best at his new position

http://www.nmr.uottawa.ca/en/welcome.html

February 2012 (L-R) Dr. Eric Ye, Prof. Gillian Goward (McMaster), Dr. Michal Leskes (RA, University of Cambridge), Zoe Reeve (graduate student, McMaster).

Linda J.M. Davis, after finishing her Ph.D. with Gillian Goward in McMaster, Linda is now employed as an NSERC Industrial R&D Fellow at *Electrovaya* in Mississauga, ON.

Electrovaya designs, develops and manufactures proprietary lithium ion batteries, battery systems, and battery-related products for the clean transportation, smart grid power, consumer and healthcare markets.

the 900 NMR Facility News

2010-2011 Annual Report

the 2010/11 Annual Report of the 900 NMR Facility has been finalized and is now available for download as a PDF version at

http://nmr900.ca/annual_e.html

Upcoming NMR Events

Solid-State NMR Symposium at CSC 2012

Colleagues,

On behalf of the organizing committee for the 95th Canadian Chemistry Conference and Exhibition, it is my pleasure to invite you to attend the **"Solid-State NMR" symposium** sponsored by the Physical, Theoretical and Computational Division of the Chemical Society of Canada. CSC 2012 will be held in Calgary, **May 26-30, 2012**. Three half-day sessions will be devoted to the Solid-State NMR symposium beginning Sunday afternoon, May 27th. Please visit the conference website for a finalized schedule of talks and poster.

http://www.csc2012.ca

I am looking forward to seeing you in Calgary at the end of May,

Rod Wasylishen
University of Alberta

Web: http://ramsey.chem.ualberta.ca

Solid-State NMR Workshop at CSC 2012

The National Ultrahigh-Field NMR Facility for Solids and Bruker Canada are pleased to present the 7th Annual Solid-State NMR Workshop at the 95th Canadian Chemistry Conference and Exhibition in Calgary. The workshop will take place on **Saturday afternoon, May 26, 2012** in *the Calgary TELUS Convention Centre.*

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.

Workshop program

Session 1 (CTCC, Chinook 4)

Chair David Bryce (University of Ottawa)

13:00-13:05 David Bryce (University of Ottawa) Opening comments

13:05-13:25 Anne-Marie Thompson (NSERC) "Major Resources Support program, brief presentation and discussion"

13:25-13:50 Roderick Wasylishen (University of Alberta) "High-Field NMR Studies of Strontium-87 in Solids"

13:50-14:15 Brandon Greer (University of Manitoba) "Characterisation of chromium-bearing "yellow phase" in model nuclear waste glasses by multinuclear magnetic resonance spectroscopy"

14:15-14:40 Venkataraman Thangadurai (University of Calgary) "Evaluation of Structure, Ion-Exchange and Transport Properties of Fast Li ion Conducting Garnet-type Solid Electrolytes by Solid State Li NMR Spectroscopy and AC Impedance"

14:40-15:00 Coffee Break

Session 2 (CTCC, Chinook 4)

Chair Scott Kroeker (University of Manitoba)

15:00-15:25 Robin Stein (Bruker Canada) "Proton Solid-State NMR Crystallography"

15:25-15:50 Frédéric Perras (University of Ottawa) "^{35}Cl Solid-State NMR of Covalently-Bound, Organic,

Chlorine at 21.1 T and the use of QUEST (QUadrupolar Exact SofTware)"

15:50-16:15 Bryan Lucier (University of Windsor) "Solid-State NMR Investigations of 'Stacked' Square-Planar Pt(II) Systems"

16:15-16:40 Andreas Brinkmann (NRC Canada) "Dipolar Recoupling in Fast Magic-Angle-Spinning NMR at High Magnetic Fields"

16:40-17:05 Gillian Goward (McMaster University) "Measuring Ion Dynamics by NMR Observations from the Point of View of the Host Lattice"

17:10 Reception sponsored by **Bruker Canada**

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

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

Note that the NMR Workshop registration is separate and independent from the CSC 2012 conference registration

2012 NMR BootCamp

Biomolecular Liquids and Solids NMR Training Course will be hosted by the NMR Facility in Chemistry at the University of Toronto, June 4-9, 2012.

The Canadian National High Field NMR Centre (NANUC) is working with the Chemistry NMR Facility at the University of Toronto to present this year's training course. This will be the first NMR BootCamp held in Toronto and also our first exploration into adding bio-solids to our traditional strength of liquids biomolecular spectroscopy. We hope to see you in June.

Early registration opens March 9th to May 21st, 2012. For more information visit
http://www.nanuc.ca/nmrbootcamp/2012_NMR_BootCamp/Welcome.html

We are pleased to announce **the 2nd China Canada Systems Biology Conference and the 19th Methods in Protein Structure Analysis**, which will take place at the Ottawa Convention Centre, Ottawa, Canada from **June 25-28, 2012**. The 2012 symposium is being organized and hosted by the Ottawa Institute of Systems Biology (University of Ottawa), The International Association for Protein Structure Analysis and Proteomics, and the China-Ontario BioAnalytic Consortium (COBAC).

The goal of this meeting is to bring together internationally recognized scientists and students in the field of systems biology, protein biochemistry, and proteomics to promote scientific discussion and the development of new collaborations.

Of special interest for NMR spectroscopists will be the session "Dynamic links between protein structure and function". Invited speakers to this session include **Lewis Kay** (University of Toronto), **Katherine Henzler-Wildman** (Washington University School of Medicine), **Gianluigi Veglia** (University of Minnesota), **Kevin Gardner** (University of Texas Southwestern) and **Dorothee Kern** (Brandeis).

More information can be found at
http://www.oisb.ca/june_2012_symposium/ccsb_2012.htm

Registration is now open. Abstract submission deadline is **May 15th, 2012**.

Natalie Goto, University of Ottawa
http://mysite.science.uottawa.ca/ngoto/Welcome.html

ROCKY MOUNTAIN CONFERENCE
ON ANALYTICAL CHEMISTRY

54th Rocky Mountain Conference on Analytical Chemistry

The 54th Rocky Mountain Conference on Analytical Chemistry is taking place **July 15-19, 2012** at the Copper Conference Center in Copper Mountain, Colorado. This year's conference will feature the 35th International EPR Symposium, as well as the world-renowned Solid-State NMR Symposium.

Abstracts are now being accepted for poster presentations. Deadline to submit a poster presentation abstract is **June 15, 2012**. For information on submitting an abstract visit
http://www.rockychem.com/conference/call-for-abstracts.html

Conference registration is now open. Discounts are offered to those who are registered and paid on or before July 1, 2012
http://www.rockychem.com/conference/registration.html

You can access additional details on hotel reservations, discounted travel, area attractions and program content at

http://www.rockychem.com

12th Annual PROTEO Symposium

May 18, 2012, Sherbrooke, Québec
http://proteo.ca/en/activities_symposium.html

3rd Canadian Magnetism Meeting

May 25, 2012, Calgary, Alberta, Canada
http://nmr900.ca/events_e.html

7th Solid-State NMR Workshop at CSC 2012

May 26, 2012, Calgary, Alberta, Canada
http://nmr900.ca/events_e.html

CSC 2012, 95th Canadian Chemistry Conference and Exhibition

May 26-30, 2012, Calgary, Alberta, Canada
http://www.csc2012.ca/

NANUC 2012 Biomolecular NMR BootCamp

June 4-9, 2012, University of Toronto, Toronto, Ontario, Canada
Early registration March 9 - May 21, 2012
http://www.nanuc.ca/nmrbootcamp/2012_NMR_BootCamp/Welcome.html

24th CMSC, Canadian Materials Science Conference

June 5-8, 2012, London, Ontario, Canada
http://www.eng.uwo.ca/2012cmsc

12th Canadian Summer School on Quantum Information

June 11-16, 2012, Institute for Quantum Computing, University of Waterloo, Waterloo, Ontario, Canada
http://cssqi2012.iqc.uwaterloo.ca/

CCSB 2012, 2nd China Canada Systems Biology Conference and 19th Methods in Protein Structure Analysis

June 25-28, 2012, Ottawa, Ontario, Canada
http://www.oisb.ca/june_2012_symposium/ccsb_2012.htm

MR in Food 2012, 11th International Conference on Magnetic Resonance in Food

June 26-29, 2012, Wageningen, the Netherlands
http://www.mrfood2012.com/

XeMAT 2012, 5th International Syposium on Xenon NMR of Materials

June 27-29, 2012, Dublin, Ireland
http://euromar2012.org/xemat-2012/

AMPERE NMR School

June 24-30, 2012, Poznan, Poland
http://www.staff.amu.edu.pl/~school/

EUROMAR 2012

July 1-5, 2012, Dublin, Ireland
http://euromar2012.org/

NMRCM 2012, International Symposium and Summer School "Nuclear Magnetic Resonance in Condensed Matter"

July 9-13, 2012, St. Petersburg, Russia
http://nmr.phys.spbu.ru/nmrcm

54th Rocky Mountain Conference on Analytical Chemistry

July 15-19, 2012, Copper Mountain, Colorado
http://www.rockychem.com/

ICMRBS 2012, XXVth International Conference on Magnetic Resonance in Biological Systems

August 19-24, 2012, Lyon, France
http://www.pasteur.fr/infosci/conf/sb/ICMRBS/

SMASH 2012 Small Molecule NMR Conference

September 9-12, 2012, Providence, Rhode Island, USA
http://www.smashnmr.org/

SMARTER 3 Conference

September 10-13, 2012, Versailles, France
http://www.smarter3.uvsq.fr

IV Ibero-American NMR Meeting

September 25-28, 2012, University of Aveiro, Portugal
http://www.spq.pt/eventos/iberoanmr2012/

VIIth Symposium "Nuclear Magnetic Resonance in Chemistry, Physics and Biological Sciences"

September 26-28, 2012, Warsaw, Poland
http://www.icho.edu.pl/SympNMR2012/home.html

CSChE 2012, the 62nd Canadian Chemical Engineering Conference

October 14-17, 2012, Vancouver, BC, Canada
http://www.csche2012.ca

PANIC "Practical Applications of NMR in Industry Conference"

October 15-17, 2012, Chicago, IL
https://m360.casss.org/event.aspx?eventID=42925

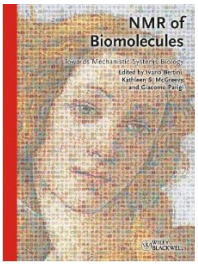
54th ENC

April 14-19, 2013, Asilomar, Pacific Grove, California
http://www.enc-conference.org/

CSC 2013, the 96th Canadian Chemistry Conference and Exhibition

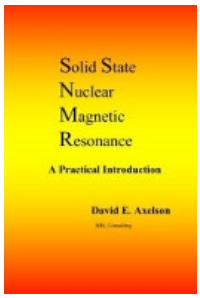
May 26-30, 2013, Québec, Québec, Canada
http://www.csc2013.ca/

New NMR Books



NMR of Biomolecules
Ivano Bertini (Editor)
Kathleen S. McGreevy (Editor)
Giacomo Parigi (Editor)
Hardcover: 650 pages
Publisher: Wiley; April 2012
Language: English
ISBN: 978-3527328505

http://www.amazon.com/dp/3527328505
http://www.amazon.ca/dp/3527328505



Solid State Nuclear Magnetic Resonance: A Practical Introduction

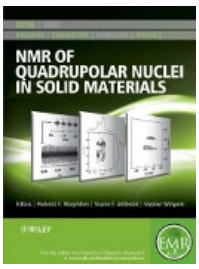
Author: David E. Axelson
Paperback: 472 pages
Publisher: CreateSpace (January 26, 2012)
Language: English
ISBN: 978-1469982274
http://www.amazon.com/dp/1469982277

"Solid state nuclear magnetic resonance now offers a wide variety of methods for characterization of materials of different compositions over a wide range of experimental conditions (temperatures, pressures, etc.). Both simple and sophisticated pulse sequences enable one to selectively probe and quantify physical properties of interest. This book mainly dwells on the practical aspects of selected topics and uses a largely non-mathematical, although extensively referenced, approach to the introduction of solid state NMR concepts."

Chapter 1 : Principles of Solid State NMR
Chapter 2 : Introduction to Pulse Sequences
Chapter 3 : Decoupling
Chapter 4 : Quantitative Analysis
Chapter 5 : Artifacts
Chapter 6 : Line Broadening Mechanisms
Chapter 7 : Resolution Enhancement
Chapter 8 : Variable Temperature

For the detailed table of contents
http://www.chemometrics-analysis.com/SSNMR.html

To contact the author, **Dr. David E. Axelson** (MRi_Consulting, Kingston, Ontario)
http://www.chemometrics-analysis.com/



NMR of Quadrupolar Nuclei in Solid Materials
Roderick E. Wasylishen (Editor)
Sharon E. Ashbrook (Editor)
Stephen Wimperis (Editor)
Hardcover: 584 pages
Publisher: Wiley; July 2012
Language: English
ISBN: 978-0470973981

http://www.amazon.com/dp/0470973986/
http://www.amazon.ca/dp/0470973986

NMR Jobs and Vacancies

Graduate student positions, University of Guelph

Graduate student positions are available in the solid state NMR group at the University of Guelph to work on the membrane protein structure determination problems. The University of Guelph NMR Centre is well equipped with an array of solid-state NMR (SSNMR) instruments operating at field strengths of 500, 600 and 800 MHz. Our facility will soon include the first in Canada Dynamic Nuclear Polarization (DNP) enhanced 600 MHz SSNMR spectrometer. We study various large membrane proteins of both bacterial and human origin. Our aim is achieve comprehensive understanding at atomic level of protein structure and functional dynamics. The research carried out in the group is highly interdisciplinary. In addition to multi-dimensional solid-state NMR, we use computational and biophysical methods, and chemical and molecular biology approaches to synthesis and purification of isotopically labeled proteins.

For more information contact **Vladimir Ladizhansky** directly.

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50 Stone Road E, Guelph,
Ontario, Canada N1G 2W1
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departmental fax: 519-836-9967
email: vladizha@uoguelph.ca
http://www.physics.uoguelph.ca/~vladimir/

PhD fellowship in Solid-State NMR
Ecole Normale Superieure, Paris, France
http://nmr900.ca/nmr_jobs.html#ens

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

Canadian NMR Research Highlights

Les secrets de Nephila

A recent special issue of *Biopolymers* focuses on **"Silks: Properties and Uses of Natural and Designed Variants"** (Volume 97, issue 6, June 2012). Two spectroscopic papers in this issue by Canadian researcher teams are from Laval. **Michel Pézolet** and colleagues use Raman spectroscopy to study the structure of silk fibers. **Michèle Auger** is involved in NMR spectroscopic studies.

T. Lefèvre, F. Paquet-Mercier, J.-F. Rioux-Dubé and M. Pézolet, "Structure of silk by Raman spectromicroscopy: From the spinning glands to the fibers," *Biopolymers* **97** (2012) 322–336. **(Review)**
http://dx.doi.org/10.1002/bip.21712

J. Leclerc, T. Lefèvre, F. Pottier, L.-P. Morency, C. Lapointe-Verreault, S.M. Gagné, M. Auger, "Structure and pH-induced alterations of recombinant and natural spider silk proteins in solution," *Biopolymers* **97** (2012) 337–346.
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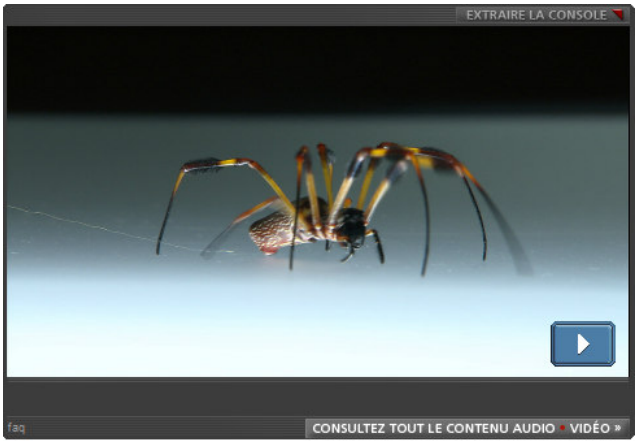
Michel Pézolet and Michèle Auger were recently featured in *Découverte*, the TV program by Radio-Canada television, were they are discussing their research. To watch the documentary "Les secrets de Nephila" (in French) http://tinyurl.com/7bz28tr



http://www.radio-canada.ca/emissions/decouverte/2010-2011/Reportage.asp?idDoc=133432

Solid-State NMR in Materials for Energy Storage and Conversion

A special issue of *Solid State Nuclear Magnetic Resonance* guest-edited by **Clare Grey** (Cambridge) and **Gillian Goward** (McMaster), Volume 42, Pages 1-98 (April 2012)
http://www.sciencedirect.com/science/journal/09262040/42

Editorial

Clare P. Grey, Gillian R. Goward, Editorial "Solid-State NMR in Materials for Energy Storage and Conversion," *Solid State Nuclear Magnetic Resonance* **42** (2012) 1.
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A. Kuhn, M. Kunze, P. Sreeraj, H.-D. Wiemhöfer, V. Thangadurai, M. Wilkening, P. Heitjans, "NMR relaxometry as a versatile tool to study Li dynamics in potential battery materials," *Solid State Nuclear Magnetic Resonance* **42** (2012) 2-8.
http://dx.doi.org/10.1016/j.ssnmr.2012.02.001

L.J.M. Davis, X.J. He, A.D. Bain, G.R. Goward, "Studies of Lithium Ion Dynamics in Paramagnetic Cathode Materials Using ^{6}Li 1D Selective Inversion Methods," *Solid State Nuclear Magnetic Resonance* **42** (2012) 26-32.
http://dx.doi.org/10.1016/j.ssnmr.2012.01.002

NMR paper in *Science*

P. Neudecker, P. Robustelli, A. Cavalli, P. Walsh, P. Lundström, A. Zarrine-Afsar, S. Sharpe, M. Vendruscolo, and L.E. Kay, "Structure of an Intermediate State in Protein Folding and Aggregation," *Science* **336** (2012) 362-366.
http://dx.doi.org/10.1126/science.1214203

Science Perspective: **David Eliezer,** "Visualizing Amyloid Assembly," *Science* **336** (2012) 308-309.
http://dx.doi.org/10.1126/science.1220356

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J.B. Ames, S. Lim and M. Ikura, "Molecular structure and target recognition of neuronal calcium sensor proteins," *Frontiers in Molecular Neuroscience* **5** (2012) 10. **(Review Article)**
http://dx.doi.org/10.3389/fnmol.2012.00010

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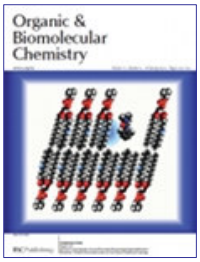

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C.J. Capicciotti, M. Leclère, F.A. Perras, D. Bryce, H. Paulin, J. Harden, Y. Liu and R.N. Ben, "Potent inhibition of ice recrystallization by low molecular weight carbohydrate-based surfactants and hydrogelators,"*Chem. Sci.* **3** (2012) 1408-1416. **(Cover Article)**
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J.L. Kitevski-LeBlanca and R.S. Prosser, "Current Applications of ^{19}F NMR to Studies of Protein Structure and Dynamics," *Progress in Nuclear Magnetic Resonance Spectroscopy* **62** (2011) 1-33. **(Invited Review)**
http://dx.doi.org/10.1016/j.pnmrs.2011.06.003

G. Wu and J. Zhu "NMR studies of alkali metal ions in organic and biological solids," *Progress in Nuclear Magnetic Resonance Spectroscopy* **61** (2012) 1-70. **(Invited Review)**
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K. Zhu, V.N. Vukotic, and S.J. Loeb, "Molecular Shuttling of a Compact and Rigid H-Shaped [2]Rotaxane," *Angewandte Chemie International Edition* **51** (2012) 2168–2172.
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This is a second publication in Angewandte Chemie featuring results obtained using resources of the National Ultrahigh-Field NMR Facility for Solids.

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http://dx.doi.org/10.1007/978-3-642-28917-0

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T. Ziegler, "A chronicle about the development of electronic structure theories for transition metal complexes," *Structure and Bonding* **143** (2012) 1-38.
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X. Tang, S. Orlicky, T. Mittag, V. Csizmok, T. Pawson, J.D. Forman-Kay, F. Sicheri, and M. Tyers, "Composite low affinity interactions dictate recognition of the cyclin-dependent kinase inhibitor Sic1 by the SCF(Cdc4) ubiquitin ligase," *Proc. Natl. Acad. Sci. USA* **109** (2012) 3287-3292.
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MetaboAnalyst 2.0 - *a comprehensive server for metabolomic data analysis*

J. Xia, R. Mandal, I.V. Sinelnikov, D. Broadhurst and D.S. Wishart, "MetaboAnalyst 2.0 - a comprehensive server for metabolomic data analysis," *Nucl. Acids Res.* **40** (2012) online. **(open access)**
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Abstract: First released in 2009, MetaboAnalyst (http://www.metaboanalyst.ca) was a relatively simple web server designed to facilitate metabolomic data processing and statistical analysis. With continuing advances in metabolomics along with constant user feedback, it became clear that a substantial upgrade to the original server was necessary. MetaboAnalyst 2.0, which is the successor to MetaboAnalyst, represents just such an upgrade. MetaboAnalyst 2.0 now contains dozens of new features and functions including new procedures for data filtering, data editing and data normalization. It also supports multi-group data analysis, two-factor analysis as well as time-series data analysis.

These new functions have also been supplemented with: (i) a quality-control module that allows users to evaluate their data quality before conducting any analysis, (ii) a functional enrichment analysis module that allows users to identify biologically meaningful patterns using metabolite set enrichment analysis and (iii) a metabolic pathway analysis module that allows users to perform pathway analysis and visualization for 15 different model organisms.

In developing MetaboAnalyst 2.0 we have also substantially improved its graphical presentation tools. All images are now generated using anti-aliasing and are available over a range of resolutions, sizes and formats (PNG, TIFF, PDF, PostScript, or SVG). To improve its performance, MetaboAnalyst 2.0 is now hosted on a much more powerful server with substantially modified code to take advantage the server's multi-core CPUs for computationally intensive tasks. MetaboAnalyst 2.0 also maintains a collection of 50 or more FAQs and more than a dozen tutorials compiled from user queries and requests. A downloadable version of MetaboAnalyst 2.0, along detailed instructions for local installation is now available as well.

Recent NMR Publications

most recent NMR publications by Canadian research groups as they appear on http://www.nmr900.ca website. 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

Z. Hu, C.M. Schneider, C.N. Price, W.M. Pye, L.N. Dawe, and F.M. Kerton, "Coordination Chemistry of *alfa-omega*-Bis(pyridylimine) Ligands Containing Flexible Linkers with Copper(I)," *European Journal of Inorganic Chemistry* **2012** (2012) 1773-1782. http://dx.doi.org/10.1002/ejic.201101414

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