



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

Canadian NMR Research News Bulletin #7.4 Fall 2013



MOOT XXVI in Kingston

After a nine-year drought, the MOOT NMR Symposium finally returned to Kingston, Ontario during the weekend of October 26-27, 2013. The symposium was held in the new Queen's Medical School building with 92 participants coming from across the country (from the Maritimes to British Columbia) and from the United States.

On Friday, October 25, a training module organized by **Dr. Sameer Al-Abdul-Wahid** (McGill) included several topics and hands-on exercises covering various aspects of NMR data processing (NMRPipe) and analysis (NMRViewJ). The workshop attracted 34 participants.

This year's MOOT keynote speaker was **Dr. Scott Prosser** from the University of Toronto

In This Issue

- 1** Canadian NMR News
- 5** Recognition
- 5** NMR Theses Recently Defended
- 5** On the move
- 7** Upcoming NMR Events
- 8** New NMR Books
- 9** NMR Software
- 10** NMR Jobs and Vacancies
- 11** Canadian NMR Research Highlights
- 14** Recent NMR Publications
- 19** Contact

at Mississauga, who spoke about the robustness of ^{19}F NMR as an atomic probe to investigate protein folding. In keeping the longstanding tradition of MOOT, over 80% of the 20 oral and 32 poster presentations were given by undergraduate and graduate students.

Of course, as the MOOT evolves, new traditions will emerge to reflect the changing dynamic of the population. This year, we introduced an



MOOT XXVI Student Award Winners (L-R): Sacha Larda (Toronto), Michael Jaroszewicz (Windsor), Anthony Sandre (Windsor), Frédéric Perras (Ottawa), Julia Meyer (Ottawa), Nick Plagos (McMaster), Kevin Burgess (Ottawa), and Avinash Ramkissoon (McMaster)

after-dinner speech at the Saturday banquet. It is most fitting that the inaugural after-dinner speech was delivered by **Dr. Alex Bain**, co-founder of the MOOT conference. This new event was one of the highlights in this year's MOOT.

Among the outstanding research contributions given by graduate students at MOOT, the volunteer judges selected the following four graduate student award winners: **Michael Jaroszewicz** from the University of Windsor (first prize in oral presentation), **Frédéric Perras** from the University of Ottawa (second prize in oral presentation), **Kevin Burgess** from the University of Ottawa (first prize in poster presentation), and **Sacha Larda** from the University of Toronto (second prize in poster presentation). In addition, we were able to offer undergraduate travel bursaries to **Julia Meyer** (University of Ottawa), **Nick Plagos** (McMaster University), **Anthony Sandre** (University of Windsor), and **Avinash Ramkissoon** (McMaster University).

MOOT XXVI would not have taken place without the generous support from Queen's University including the Office of Vice-Principal (Research), Office of Research Services, School of Graduate Studies, Faculty of Health Sciences, Faculty of Arts and Science, Department of Chemistry, and Department of Biomedical and Molecular Sciences, as well as the sponsors acknowledged below.

Next year's MOOT will be organized by **Isabelle Marcotte** (UQAM) and her colleagues in Montreal, and we look forward to seeing everyone again in 2014 !

Seth Chitayat and Gang Wu
26th MOOT NMR Symposium
<http://www.mootnmr.org>



ThermoFisher
SCIENTIFIC



GE Healthcare

Agilent Technologies



New Funding announcements

Research & Development Corporation (RDC) of Newfoundland and Labrador

<http://www.mun.ca/science/news.php?id=2558>

Robert Brown and Valerie Booth,
Department of Biochemistry, Faculty of
Science, Memorial University

*Improving cholesterol efflux by targeted
disruption of hepatic lipase interactions with
the cell surface*

The blockage of blood vessels is one of the major causes of heart disease, the leading cause of death in the Western world. Existing medications are designed to reduce bad cholesterol and other bad fats in the blood. However, medications are also needed to promote the removal of the cholesterol and bad fats from the vessel walls by good cholesterol (or HDL), and the removal of these fats from the body. This project studies an enzyme with the potential to create more HDL in the blood, and how to modulate the enzyme through the use of engineered molecules. The results of this study may yield a new beneficial treatment against the initiation of blockages in blood vessels.

RDC investment: \$68,073. Leveraged investment: \$68,073 from the Canadian Institutes of Health Research Regional Partnerships Program.

Valerie Booth and Michael Morrow, Faculty
of Science, Memorial University

NMR structural studies of surfactant protein B

This project investigates the structure of the protein SP-B, a lung protein essential for life. This knowledge will be used to improve treatments for common and frequently fatal health conditions such as Acute Respiratory Distress Syndrome, and also may be useful in developing systems for general drug delivery through the lungs. The research will generate better knowledge on the structure of SP-B and how it can improve the treatment of Acute Respiratory Distress Syndrome and general drug delivery through the lungs.

RDC investment: \$173,090. Leveraged investment: \$173,090 from the Canadian Institutes of Health Research Regional Partnerships Program.

6^{ème} COLLOQUE ANNUEL DU GRASP
6th ANNUAL GRASP SYMPOSIUM



Monday, November 25, 2013, 8:00 – 18:30

McGill New Residence Hall
3625 Avenue du Parc
Montréal, QC, H2X 3P8
514-398-3471

Dear Colleagues,

Drs. Kalle Gehring and Albert Berghuis would like to invite you to take part in the sixth scientific symposium of **GRASP** (*Groupe de Recherche Axé sur la Structure des Protéines*).

Outstanding international speakers - David Agard, Rachele Gaudet, Samir Hamdan, Mei Hong, Hongbin Li, Natalie Strynadka - poster sessions, exhibitors and short talks will be presented at this auspicious event.

For more information about this symposium, please send an email grasp.med@mcgill.ca or visit

<http://grasp.mcgill.ca/english/symposium/symposium.html>

Sincerely,

The organizing committee:

Kalle Gehring, GRASP Director
Albert Berghuis, GRASP Co-Director
Annick Guyot, GRASP Coordinator

NMR Spectroscopy in 2012

Mark Edgar summarizes main technical developments in NMR spectroscopy in 2012:

"NMR spectroscopy continues to evolve, with publications in 2012 providing an eclectic collection of applications, advances and incremental improvements. Publication highlights include: the "Prodigy" probe from Bruker, a 60 MHz benchtop NMR spectrometer, Earth-field NMR, dual receivers and dual acquisition methods, para-hydrogen enhancement by chemical-association and high-field DNP."

M. Edgar "Physical methods and techniques: NMR spectroscopy," *Annu. Rep. Prog. Chem., Sect. B* **109** (2013) 256-274. **(Review)**

<http://dx.doi.org/10.1039/c3oc90012f>



97th Canadian Chemistry Conference and Exhibition
VANCOUVER, B.C.
June 1-5, 2014
CHEMISTRY FROM SEA TO SKY



CSC 2014, the 97th Canadian Chemistry Conference and Exhibition
"Chemistry from Sea to Sky"

June 1-5, 2014, Vancouver, B.C., Canada

<http://www.csc2014.ca/>

Solid-state NMR Symposium

Organizers: Suzana Straus (UBC), Carl Michal (UBC), Rob Schurko (Windsor)

Confirmed Invited Speakers:

David Bryce (Ottawa)
Brad Chmelka (UC Santa Barbara)
Yoshitaka Ishii (Uni Illinois Chicago)
Scott Kroeker (Manitoba)
Vlad Ladizhansky (Guelph)
Rachel Martin (UC Irvine)
Len Mueller (UC Riverside)

On-line abstract submission starts
December 16th, 2013

posted on behalf of Robin Stein (Bruker Canada)

Bruker Canada will offer **NMR courses** on data processing, instrument maintenance, and automation beginning in



November 2013. The courses will be taught online by Bruker Canada so that participants can improve their NMR expertise without having to travel. All courses will provide notes and some will include exercises. The software used in the lectures will be TopSpin 3, but notes about TopSpin 1 and 2 can be provided on request.

The first course, *Introductory Processing*, will be held on Tuesday, **November 26, 2013**, from 1 PM to 4 PM EST. Topics covered are 1D processing, 2D processing, and plotting. This first class will be free, but participation is limited to 20 attendees. For more information or to register contact Shirley Galbraith at helpdesk@bruker.ca

Registration closes **November 19, 2013**.

wwPDB: 10,000 NMR structure milestone reached!

The Worldwide Protein Data Bank (wwPDB; <http://wwpdb.org>) is excited to announce that in June 2013 the number of structures available in the PDB archive determined using Nuclear Magnetic Resonance (NMR) spectroscopy has passed the 10,000 mark!

Since the first biomacromolecular NMR structure was archived in 1989, the number of NMR-derived structures in the PDB has grown steadily. Last year alone over 500 new NMR structures were deposited, more than in the first 10 years of NMR depositions combined. Today, NMR-derived structures account for more than 10% of the PDB archive which itself will reach the 100,000 structure mark in 2014.

You can read more about this milestone achievement and learn about the dedicated databases, tools and services that help make this wealth of structural information accessible to the scientific community at <http://wwpdb.org>

On behalf of the wwPDB

*Aleksandras Gutmanas
Protein Data Bank in Europe (PDBe)*

Scientific Best Practice

Wilfred F. van Gunsteren "The Seven Sins in Academic Behavior in the Natural Sciences," *Angewandte Chemie International Edition* **52** (2013) 118–122. **(Essay) (free access)**
<http://dx.doi.org/10.1002/anie.201204076>

Communication in Science: Pressures and Predators



Science's Special Issue on Communication in Science: Pressures and Predators includes free news and reviews on the lack of scrutiny at open-access journals, the rarity of published negative studies, and publishing sensitive data.

<http://www.sciencemag.org/site/special/sci-comm/>

A Life Scientist's Guide to Physical Chemistry

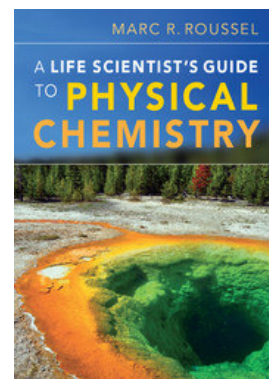
Author: Marc R. Roussel
(Department of Chemistry and Biochemistry, University of Lethbridge)

Paperback: 456 pages

Language: English

Publisher: Cambridge University Press; 1st edition (May 7, 2012)

ISBN: 978-0521186964



<http://www.amazon.com/dp/052118696X>
<http://www.amazon.ca/dp/052118696X>

Cambridge: Motivating students to engage with physical chemistry through biological examples, this textbook demonstrates how the tools of physical chemistry can be used to illuminate biological questions. It clearly explains key principles and their relevance to life science students, using only the most straightforward and relevant mathematical tools. More than 350 exercises are spread throughout the chapters, covering a wide range of biological applications and explaining issues that students often find challenging. These, along with problems at the end of each chapter and end-of-term review questions, encourage active and continuous study. Over 130 worked examples, many deriving directly from life sciences, help students connect principles and theories to their own laboratory studies. Connections between experimental measurements and key theoretical quantities are frequently highlighted and reinforced. Answers to the exercises are included in the book. Fully worked solutions and answers to the review problems, password-protected for instructors, are available at

<http://www.cambridge.org/roussel>

David P. Pursell "Review of *A Life Scientist's Guide to Physical Chemistry*," *Journal of Chemical Education* **90** (2013) 1263–1264.
<http://dx.doi.org/10.1021/ed4005744>

Call for nominations

The Russell Varian Lecture and Prize

The Russell Varian prize honors the memory of the pioneer behind the first commercial Nuclear Magnetic Resonance spectrometers and co-founder of Varian Associates. The prize is awarded to a researcher based on a single innovative contribution (a *single* paper, patent, lecture, or piece of hardware) that has proven of high and broad impact on state-of-the-art NMR technology. The prize is designed to recognize the initial contribution that laid the foundations for a specific technology of great importance in state-of-the-art NMR. It is sponsored by **Agilent Technologies** and currently carries a monetary award of 15,000 Euro. The award ceremony will take place at the **ICMRBS 2014** meeting in Dallas, Texas, USA, 24th to 29th August, 2014, with the winner delivering the Russell Varian Lecture. <http://icmrbs2014.org/>

Rules for the Russell Varian Prize

- Only single pieces of work are considered (a paper, a lecture, a patent, etc).
- In the case of multiple authorship, the prize is awarded to the author with the largest creative and innovative share of the contribution. In the exceptional case of truly equal shares in the contribution, the Prize may be split between two authors.
- No individual may receive the prize more than once.
- Prizewinners become members of the Advisory Board for the Russell Varian Prize that evaluates future nominations and makes recommendations to the Prize Committee.

Call for Nominations

Nominations must be forwarded by email to the Secretary of the Prize Committee, Gareth Morris, at g.a.morris@manchester.ac.uk. The deadline for nominations is **February 17th, 2014**. Nominations should be laid out in the format of a publishable laudatio proposal (cf. earlier laudatios, at <http://tinyurl.com/lx2ygza>

that in the case of multiple authorship must include an explanation of why the nominee is the most innovative author behind the paper. Attention is further drawn to the fact that the Russell Varian prize rewards the earliest seed paper of an important technology, rather than later more comprehensive and highly cited papers.

Prize Committee

Jean Jeener (Chairman), Krish Krishnamurthy (Agilent representative), Lucio Frydman, Gareth A. Morris (Secretary), Ole W. Sørensen, and a representative of the ICMRBS organizing committee.

Obituary

Brandon University Mourns Loss of Chemistry Professor

October 10, 2013 - BRANDON, MB
<http://www.brandonu.ca/news/2013/10/10/bu-mourns-loss-of-chemistry-professor/>

The Brandon University (BU) community is saddened by the passing of longtime professor and University supporter **Dr. Bruce James Forrest**, who lost his battle with cancer on Wednesday evening.

Born in 1950, Bruce joined the Department of Chemistry in 1986 as an associate professor. His research focused on the use of Nuclear Magnetic Resonance Spectroscopy to determine the structure of biological membrane systems, an area in which he was internationally renowned. Bruce served as Department Chair on numerous occasions, most recently from 2004 until 2010, when he took leave to care for his wife. Shortly after, he was diagnosed with cancer.

"Bruce dedicated himself to student success," says BU President and Vice-Chancellor Deborah Poff. "He established the first scholarship in Physical Chemistry at Brandon University. We are grateful for his many years of service to our students and University, and extend our sincere condolences to Bruce's family." Bruce served in other roles within the University community, including Chair of the Pension Trustees and President of the Faculty Association. An avid fan of the New York Yankees, Bruce was also a passionate wood-worker.

Donations can be made in his memory to **The Dr. Bruce and Mrs. Jane Forrest Scholarships** for Honours/Majors Chemistry which was established with his estate.

Cheques can be made payable to "Brandon University Foundation" and can be sent to:

Brandon University
Department of Institutional Advancement
270-18th Street, Brandon, MB
R7A 6A9

Bruce James Forrest Obituary

<http://www.obitsforlife.com/obituary/780926/Forrest-Bruce.php>

Recognition

Prof. David Bryce (Ottawa) has been appointed Associate Editor (**Trends**) for *Solid State Nuclear Magnetic Resonance* journal (Elsevier), effective January 1, 2014. Dave will be taking over from **Jerry Chan** (National Taiwan University).

Trends is a series of brief review articles which designed to summarize new key ideas, recent developments and important results within a chosen topical area of solid-state NMR spectroscopy. You can **access and read** each Trends article **for free** until 6 months after publication.

Some of the recent **Trends** articles <http://tinyurl.com/mtxfcxm>

Prof. David Bryce (Ottawa) has been awarded an American Chemical Society **Petroleum Research Fund** (ACS PRF) "New Directions" grant of \$100,000 over two years to study homometallic and heterometallic metal-organic frameworks using solid-state NMR.

MOOT XXVI Student Awards

Michael Jaroszewicz (Windsor) - first prize in oral presentation

Frédéric Perras (Ottawa) - second prize in oral presentation

Kevin Burgess (Ottawa) - first prize in poster presentation

Sacha Larda (Toronto) - second prize in poster presentation

MOOT XXVI Travel Awards

Julia Meyer (Ottawa)

Nick Plagos (McMaster)

Anthony Sandre (Windsor)

Avinash Ramkissoon (McMaster)

NMR Theses Recently Defended

Brian Lucier (University of Windsor)
September 2013

Supervisor: Prof. Robert Schurko

Ph.D. Chemistry: "New Directions for Solid-State NMR of Insensitive Nuclei: Applications to Metal Nuclei in Inorganic Material"

<http://scholar.uwindsor.ca/etd/4909/>

Peng He (University of Western Ontario)
September 2013

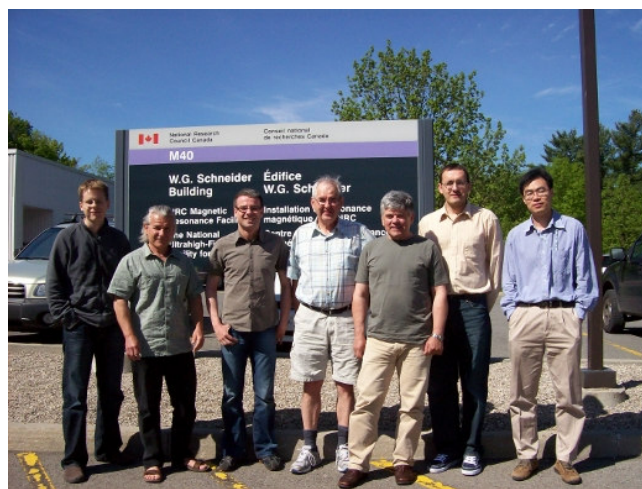
Supervisor: Prof. Yining Huang

M.Sc. Chemistry: "Solid State NMR Spectroscopic Studies of Metal-Organic Frameworks"

<http://ir.lib.uwo.ca/etd/1640/>

On the move

Dr. Randilynn Christensen (postdoctoral fellow, Kroeker group, Manitoba) has accepted a position as a Senior Materials Scientist at **3M Corporate Research and Development** in Maplewood, Minnesota.



(Summer 2011, L-R): Luke O'Dell, Jamie Bennett, Andreas Brinkmann, Rod Wasylshen, Igor Moudrakovski, Victor Terskikh, Eric Ye.

And then there was one.

NMR Events

6th Annual GRASP Symposium


November 25, 2013, McGill University,
Montréal, QC, Canada
<http://grasp.mcgill.ca/english/symposium/symposium.html>

PANIC 2014 Practical Applications of NMR in Industry Conference

February 3-5, 2014, Charlotte, NC
<http://www.panicnmr.com/>

Biophysical Society 58th Annual Meeting

February 15-19, 2014, San Francisco, CA
<http://www.biophysics.org/2014meeting>


 Biophysical Society of Canada - Travel Awards and Mixer
Sunday, February 16, 18:00-19:30

55th ENC March 23-28, 2014, Boston, MA
<http://www.enc-conference.org/>

RSC NMR Discussion Group, Spring Meeting 2014 "NMR in Structural Biology"

April 10-11, 2014, University of Cambridge,
Department of Chemistry, UK
<http://www.keeler.ch.cam.ac.uk/NMRDG/index.html>



 **CSC 2014**, the 97th Canadian Chemistry Conference and Exhibition
"Chemistry from Sea to Sky"

June 1-5, 2014, Vancouver, B.C., Canada
<http://www.csc2014.ca/>

Solid-state NMR Symposium

Organizers: Suzana Straus (UBC), Carl Michal (UBC), Rob Schurko (Windsor)

Confirmed Invited Speakers: David Bryce (Ottawa), Brad Chmelka (UC Santa Barbara), Yoshitaka Ishii (Uni Illinois Chicago), Scott Kroeker (Manitoba), Vlad Ladizhansky (Guelph), Rachel Martin (UC Irvine), Len Mueller (UC Riverside)

On-line abstract submission starts
December 16th, 2013

AMPERE NMR School

June 22-28, 2014, Zakopane, Poland
<http://www.staff.amu.edu.pl/~school/>

EUROMAR 2014

June 29 - July 3, 2014, Zürich, Switzerland
<http://www.euromar2014.org/>

56th Rocky Mountain Conference on Magnetic Resonance: Solid-State NMR Symposium & EPR Symposium

July 13-17, 2014, Copper Mountain, Colorado
<http://www.rockychem.com/symposia/solid-state-nmr-symposium.html>

ICMRBS 2014, the XXVIth International Conference on Magnetic Resonance in Biological Systems

August 24-29, 2014, Dallas, Texas
<http://icmrbs2014.org/>

MOOT XXVII NMR Symposium

Fall 2014, Montreal, Quebec
<http://www.mootnmr.org>

Pacificchem 2015 The International Chemical Congress of Pacific Basin Societies

December 15-20, 2015, Honolulu, Hawaii, USA
<http://www.pacificchem.org/>

> NMR Spectroscopy of Polymers and Biobased Materials (#12)

> Advances in Biological Solid-State NMR (#120) Michele Auger, co-chair

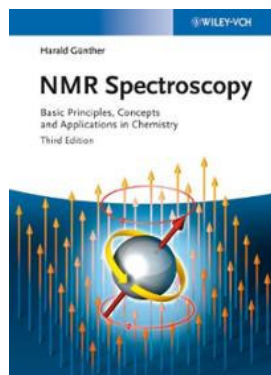
> Biomolecular Structure and Dynamics: Recent Advances in NMR (#181) Mitsuhiko Ikura, co-chair

<http://www.pacificchem.org/symposiadesc2015/>

ISMAR 2017 20th ISMAR (International Society of Magnetic Resonance) Conference

July 23-28, 2017, Québec City, Québec, Canada
<http://www.ismar.org/>

New NMR Books



NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry

Harald Günther
(Author)
Paperback: 734 pages
Language: English
Publisher: Wiley-VCH;
3 edition (November 4,
2013)
ISBN: 978-3527330003

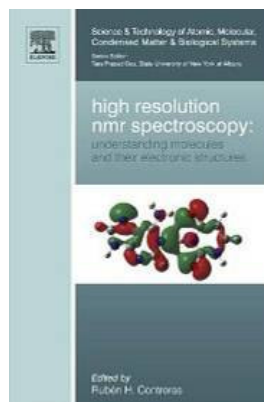
<http://www.amazon.com/dp/3527330003>
<http://www.amazon.ca/dp/3527330003>

Wiley: This third edition of the popular classic retains the clear style and excellent didactical, highly practical approach. It explains this complex topic without mathematical equations, making it ideal for those students who do not have a strong mathematical background, but want to understand the fundamentals of NMR and work with the method in an efficient and accurate way.

The contents have been completely revised and updated with approximately 25% new material, including new chapters on biological NMR and on other nuclei, outdated methods are replaced by current ones, and new developments have been added.

Many examples are taken from organic chemistry, making this an equally invaluable guide to undergraduate and graduate students from such related fields as biochemistry, medicinal chemistry, pharmaceutical chemistry and materials science.

Contains problems complete with solutions.



High Resolution NMR Spectroscopy: Understanding Molecules and their Electronic Structures

Editor: R.H. Contreras
Hardcover: 456 pages
Language: English
Publisher: Elsevier
(August 27, 2013)
ISBN: 978-0444594112

<http://www.amazon.com/dp/0444594116>
<http://www.amazon.ca/dp/0444594116>

Elsevier: The progress in nuclear magnetic resonance (NMR) spectroscopy that took place during the last several decades is observed in both experimental capabilities and theoretical approaches to study the spectral parameters. The scope of NMR spectroscopy for studying a large series of molecular problems has notably broadened. However, at the same time, it requires specialists to fully use its potentialities. This is a notorious problem and it is reflected in the current literature where this spectroscopy is typically only used in a routine way. Also, it is seldom used in several disciplines in which it could be a powerful tool to study many problems. The main aim of this book is to try to help reverse these trends.

This book is divided in three parts dealing with 1) high-resolution NMR parameters; 2) methods for understanding high-resolution NMR parameters; and 3) some experimental aspects of high-resolution NMR parameters for studying molecular structures. Each part is divided into chapters written by different specialists who use different methodologies in their work. In turn, each chapter is divided into sections. Some features of the different sections are highlighted: it is expected that part of the readership will be interested only in the basic aspects of some chapters, while other readers will be interested in deepening their understanding of the subject dealt with in them.

Shows how NMR parameters are useful for structure assignment as well as to obtain insight on electronic structures

Emphasis on conceptual aspects

Contributions by specialists who use the discussed methodologies in their everyday work

NMR Software

contributed by David Bryce (Ottawa)

EFGShield, version 4.0

New version of EFGShield with GUI now available for Gaussian, CASTEP, and ADF files



“EFGShield” is our software for the parsing and analysis of shielding and EFG data from Gaussian output files. Thanks to the work of my students **Nuiook Dicaire** and **Fred Perras**, I am pleased to announce that a new and improved version of EFGShield with a GUI is now available. There are many advantages to the new version. Most importantly, CASTEP and ADF output files can now be used in addition to Gaussian files.

The program now runs with a graphical user interface (GUI) rather than the old command line prompt. It runs under modern versions of Windows and also works in Windows emulators we have tested. The new and improved version offers many advantages compared to previous versions including:

- can now read magnetic shielding and electric field gradient output for Gaussian, ADF, and CASTEP software
- GUI functionality
- much easier to find and load files with long path names
- easier to save output files where you want them
- see results summary directly in the program window without having to open the output files
- can view results summary for different atoms and for different output files without having to restart the program
- updated quadrupole moments

New version of **EFGShield** is available for download from the “Software” link in the menu on the left on our webpage
<http://mysite.science.uottawa.ca/dbryce/>

contributed by Pierre Audet (Université Laval)

Linux GUI for Airjet XR

Hello all,

I recently bought an **Airjet XR air cooler** to run low temperature experiments. This unit has a digital temperature controller, a RS485 communication port and comes with a USB to RS485 converter.

Since RedHat has the required driver to establish the communication, I wrote a GUI to control/monitor/change the temperature setpoint from RedHat.

Before uploading my code on **Agilent Spinsights** blog and offer it to the community, I would like to find some testers ready to install it on their system to verify bugs etc.

If you are interested, please contact me directly at pierre.audet@chm.ulaval.ca

Cheers,

Pierre

Pierre Audet, Chimiste
Spécialiste résonance magnétique et spectrométrie de masse
Département de chimie, Université Laval
Tél: (418) 656-2131 x4296

contributed by Keith Brown (Saskatchewan)

Product Operator Calculator

Hi everyone,

I have worked for some time on producing a calculator that does pulse sequence analysis via product operator calculations. It has been generally available for four or five years now. The calculator will run under Linux or Windows and may be downloaded at <http://chem4823.usask.ca/nmr/wxProdOp.html>

I know that all programs have bugs in them and that this one is no different so I would much appreciate hearing from anyone who finds one. Your name will be enshrined in the source code of the next version. Suggestions for improvements are also welcome.

Cheers,

Dr. Keith Brown

<http://chem4823.usask.ca/chem112/kbrown.html>

NMR Jobs and Vacancies

PhD/MSc positions in solid-state NMR, Université du Québec à Montréal

We are looking for **two** motivated and dynamic PhD or MSc candidates to join our Laboratory of NMR of Biological Systems as early as May 2013. Candidates must be interested in membrane physico-chemistry and NMR spectroscopy with biological applications and have a background in chemistry or biochemistry or related field.

The research projects concern the in vivo NMR study of the interaction of drugs and environmental contaminants with microorganisms such as bacteria and microalgae, as well as the development of model cell membranes to study specific interactions with membrane components. Students will have full access to 400 and 600 MHz NMR spectrometers as well as infrastructure for bacterial and microalgal cell growth.

Interested students should contact Prof. Isabelle Marcotte at:
marcotte.isabelle@uqam.ca

Prof. Isabelle Marcotte, Ph.D.
Department of Chemistry
Université du Québec à Montréal
PO Box 8888, Downtown Station
Montréal (QC)
H3C 3P8 Canada
T. 1-514-987-3000 #5015
F. 1-514-987-4054
marcotte.isabelle@uqam.ca

M.Sc. or Ph.D. position in solid-state NMR at the University of Ottawa

Highly motivated candidates interested in physical chemistry and/or NMR spectroscopy are invited to apply for a M.Sc. or Ph.D. in the group of **Prof. David Bryce** at the University of Ottawa
<http://mysite.science.uottawa.ca/dbryce/>

Research in solid-state NMR in the Bryce group covers a variety of areas including the development of the spectroscopy of traditionally difficult quadrupolar nuclei, applications of double-rotation NMR, applications to weak interactions including halogen bonding, and the study of

polymorphism. Experimental work is complemented by quantum chemical studies. Interested students should contact Prof. Bryce directly at dbryce@uottawa.ca

Please note that due to budgetary constraints, the position is open only to Canadian students.

Prof. **David L. Bryce**, Ph.D.
Department of Chemistry
10 Marie Curie Private
University of Ottawa
Ottawa, Ontario K1N6N5
Phone 613-562-5800 ext 2018
Fax 613-562-5170
Email dbryce@uottawa.ca
Web <http://mysite.science.uottawa.ca/dbryce/>

The University of Ottawa invites applications for a **Tier 1 Canada Research Chair** (CRC) in Materials Chemistry
<http://www.academiccareers.uottawa.ca/node/656>

Tenure-Track, Assistant Professor Position in Biointerfacial Chemistry

The Department of Chemistry & Chemical Biology at McMaster University

http://www.mcmaster.ca/vpacademic/Biointerfases_2014.html

For new and most recent job posts follow
<https://twitter.com/nmr900>



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Expand Reply Delete Favorite More

Victor Tersikh @nmr900 2m
Assistant Professor position in Biointerfacial Chemistry, McMaster University, Hamilton, ON nature.com/naturejobs/sci... - via [@naturejobs](https://twitter.com/naturejobs)
Expand Reply Delete Favorite More

Canadian NMR Research Highlights

The Human Urine Metabolome

S. Bouatra, F. Aziat, R. Mandal, A.C. Guo, M.R. Wilson, C. Knox, T.C. Bjorndahl, R. Krishnamurthy, F. Saleem, P. Liu, Z.T. Dame, J. Poelzer, J. Huynh, F.S. Yallou, N. Psychogios, E. Dong, R. Bogumil, C. Roehring, D.S. Wishart, "The Human Urine Metabolome," *PLoS ONE* **8** (2013) e73076. (open access) <http://dx.doi.org/10.1371/journal.pone.0073076>

Abstract: Urine has long been a "favored" biofluid among metabolomics researchers. It is sterile, easy-to-obtain in large volumes, largely free from interfering proteins or lipids and chemically complex. However, this chemical complexity has also made urine a particularly difficult substrate to fully understand. As a biological waste material, urine typically contains metabolic breakdown products from a wide range of foods, drinks, drugs, environmental contaminants, endogenous waste metabolites and bacterial by-products. Many of these compounds are poorly characterized and poorly understood. In an effort to improve our understanding of this biofluid we have undertaken a comprehensive, quantitative, metabolome-wide characterization of human urine. This involved both computer-aided literature mining and comprehensive, quantitative experimental assessment/validation. The experimental portion employed **NMR spectroscopy**, gas chromatography mass spectrometry (GC-MS), direct flow injection mass spectrometry (DFI/LC-MS/MS), inductively coupled plasma mass spectrometry (ICP-MS) and high performance liquid chromatography (HPLC) experiments performed on multiple human urine samples. This multi-platform metabolomic analysis allowed us to identify 445 and quantify 378 unique urine metabolites or metabolite species. The different analytical platforms were able to identify (quantify) a total of: **209 (209) by NMR**, 179 (85) by GC-MS, 127 (127) by DFI/LC-MS/MS, 40 (40) by ICP-MS and 10 (10) by HPLC. Our use of multiple metabolomics platforms and technologies allowed us to identify several previously unknown urine metabolites and to substantially enhance the level of metabolome

coverage. It also allowed us to critically assess the relative strengths and weaknesses of different platforms or technologies. The literature review led to the identification and annotation of another 2206 urinary compounds and was used to help guide the subsequent experimental studies. An online database containing the complete set of 2651 confirmed human urine metabolite species, their structures (3079 in total), concentrations, related literature references and links to their known disease associations are freely available at <http://www.urinemetabolome.ca>

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"University of Alberta finds new metabolites in urine" **Daren Zomerman**, *the griff*, September 24, 2013, University of Alberta <http://thegriff.ca/2013/09/u-finds-new-metabolites-urine/>

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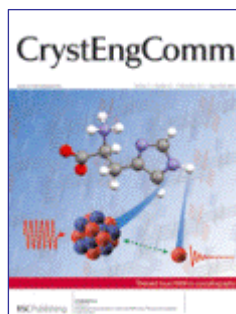
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**CrystEngComm themed issue
on NMR Crystallography**

Issue 43, 21 November 2013, pp. 8589-8850
<http://tinyurl.com/qazxr4f>




Guest-edited by **John A. Ripmeester** (NRC) and **Roderick E. Wasylishen** (Alberta)

J.A. Ripmeester and R.E. Wasylishen, "NMR crystallography," (**Editorial**) *CrystEngComm* **15** (2013) 8598-8598.


<http://dx.doi.org/10.1039/c3ce90151c>

Canadian contributions

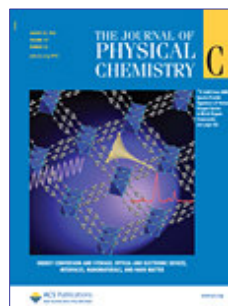
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 **P.J. Pallister, I.L. Moudrakovski, G.D. Enright and J.A. Ripmeester**, "Structural assessment of anhydrous sulfates with high field ³³S solid state NMR and first principles calculations," *CrystEngComm* **15** (2013) 8808-8822. <http://dx.doi.org/10.1039/c3ce41233d>

**Cover article in
the Journal of Physical Chemistry C**



P. He, J. Xu, V.V. Terskikh, A. Sutrisno, H.-Y. Nie, and Y. Huang, "Identification of Non-equivalent Framework Oxygen Species in Metal-organic Frameworks by ¹⁷O Solid-state NMR," *Journal of Physical Chemistry C* **117** (2013) 16953-16960.

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Abstract: ¹⁷O solid-state NMR spectra provide signatures of various oxygen species in metal-organic frameworks. We successfully prepared several prototypical ¹⁷O-enriched metal-organic frameworks (MOFs). Due to the diversity of MOF-based materials, different types of MOFs require different isotopic enrichment methods to effectively incorporate ¹⁷O from ¹⁷O-enriched H₂O. Several synthetic strategies for ¹⁷O-enrichment were discussed. Using these ¹⁷O-enriched MOFs, we were able to acquire ¹⁷O solid-state NMR spectra at a magnetic field of 21.1 T. They provide distinct spectral signatures of various key oxygen species commonly existing in representative MOFs.

This cover article features results obtained using the 21.1 T solid-state NMR spectrometer at the National Ultrahigh-Field NMR Facility for Solids (Ottawa, ON). If you are interested in using this spectrometer in your research please contact the Facility manager.

Web: <http://nmr900.ca>

**Review in
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Three Techniques - One Structure

ChemistryViews highlights research by **Robert Schurko** and his team from the University of Windsor (Canada) done in collaboration with groups from the Université Lille Nord de France (France), NRC Canada, and ESCPE Lyon (France).

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