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

Canadian NMR Research News Bulletin #3.4
Fall 2009

Canadian NMR News

MOOT XXII
MINI NMR SYMPOSIUM

Yves Aubin, Health Canada

The twenty-second edition of the MOOT NMR Mini Symposium was held at Carleton University in Ottawa on October 17-18, 2009. Among the 90 registered participants coming from Windsor, Ontario to St. John's, Newfoundland, 17 talks and 33 posters presented with enthusiasm the diversity of research programs in Canada using NMR spectroscopy. The complete MOOT XXII Scientific Program is available on the official MOOT web-site

http://www.mootnmr.org/

Three **Suraj Manrao Travel Awards** for the best three posters from graduate students were awarded to **Myriam Laneville** (Auger's lab, Laval), **Jérémie Leclerc** (Auger's lab, Laval) and **Patrick Walsh** (Sharpe's lab, Toronto). Great many thanks to **Suraj**!

The banquet was held at Al's Steakhouse and one could judge by the animated discussions and laughter that everybody and a good time and enjoyed a very good meal.

An indicator of success for a MOOT organizer is, among other things, the fact that five colleagues have volunteered to organize the next meetings. These are **Mike Lumsden**, Dalhousie, Halifax for MOOT XXIII in 2010, **Simon Sharpe**, SickKids, Toronto for MOOT XXIV in 2011, **Michèle Auger**, Université Laval, Québec for MOOT XXV in 2012. Tradition showed that MOOT usually returns to Kingston after Québec, but this needs to be confirmed, so MOOT XXVI in 2013 is a maybe, and **Isabelle Marcotte**, UQAM and **Natalie Goudreau**, Boehringer-Ingelheim, Montréal for MOOT XXVII in 2014 (or earlier).

During the poster session and the banquet I had the opportunity to discuss with a few students and all said that they found the event stimulating. Those who presented were very pleased with the opportunity to show their work to an interested and knowledgeable audience. Such opportunities are rare for students. For a couple of new professors who work isolated in departments without colleagues to discuss with, this venue was a welcome breath of fresh air.

I would like to sincerely thank all the volunteers and sponsors who made this event a scientific and networking success.

Yves

In This Issue

Dimensions: NMR research in Halifax

In previous issues of this bulletin we reported about the new Biomolecular Magnetic Resonance Facility at the NRC Institute for Marine Biosciences (NRC-IMB) in Halifax. This facility has been established in partnership between NRC Canada, Dalhousie University, and the Federal Government to support health-care research in the Atlantic region.

A feature story about this NMR Facility has been published in the first issue of ***Dimensions***, the new electronic magazine of the National Research Council of Canada, launched in October 2009.

http://www.nrc-cnrc.gc.ca/eng/dimensions/issue1/mrinstrument.html

NRC-IMB: Nadine Merkley (left), Tobias Karakach (centre) and Ray Syvitski (Photo credit: NRC Canada)

Learn more about leading-edge research at NRC by visiting *Dimensions* online
http://www.nrc-cnrc.gc.ca/eng/dimensions/index.html

"Quantum to Cosmos" Festival

Canada's Perimeter Institute for Theoretical Physics (Waterloo, Ontario) organized a science festival **"Quantum to Cosmos: Ideas for the Future"** from October 15 to 25, 2009 to celebrate its 10th anniversary.

The festival was intensively covered in media, including TVO's "The Agenda with Steve Paikin" live broadcasts. These broadcasts, along with lectures and panel discussions are now available online as stream videos for those interested in physics and its impact on modern society.

http://www.q2cfestival.com/schedule

Read the feature story about **Canada's Perimeter Institute for Theoretical Physics** in the September's issue of *Nature*

E. Hand "Physics: The edge of physics," *Nature* **461** (2009) 462-465.
http://dx.doi.org/10.1038/461462a

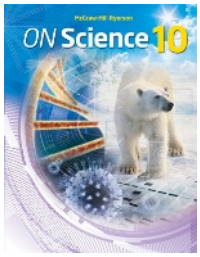
Interview with Raymond Laflamme

In July 2009, **David Johnston**, president of the University of Waterloo, sat down with **Raymond Laflamme**, director of the Institute for Quantum Computing (IQC), to discuss quantum information research at Waterloo and the recent donation to IQC of over $100 million from Mike and Ophelia Lazaridis. This conversation was filmed in Laflamme's NMR lab at IQC.

Watch the video of this interview online at IQC
http://www.iqc.ca/media/

NMR metabolomics for medical diagnostic

NMR-based profiling of metabolites is gaining momentum in medical practice as main-stream media and even high-school text-books highlight progress in this field.



The Winnipeg Free Press ran a story in September about high-resolution liquid-state NMR metabolomics in urine to identify metabolite profiles associated with acute rejection in children after renal transplantation. This research is ongoing in Winnipeg at the Manitoba Institute of Child Health (Dr. **Tom Blydt-Hansen**) and the NRC Institute for Biodiagnostics, NRC-IBD (**Ray Somorjai**). They have shown that urine metabolites (simple sugars, amino acids and waste products) detected non-invasively could help in identifying kidney rejection risks at early stages and to reduce morbidity.

To read the full story in *Winnipeg Free Press*
http://www.winnipegfreepress.com/life/making-life-easier-for-kidney-patients-58437977.html

Highlights of NMR-based metabalomic research carried out by **Tedros Bezabeh**, also from NRC-IBD in Winnipeg, have now been included in *Ontario Science 10* high-school textbook (above picture credit: McGraw-Hill Ryerson). **Tedros Bezabeh** and his colleagues from IBD apply NMR spectroscopy for the early non-invasive diagnosis of colon cancer and other bowel diseases. They just have published a

review on this subject in a special issue of *Magnetic Resonance in Chemistry* "NMR-based mixture analysis - metabolomics and beyond" :

T. Bezabeh, R.L. Somorjai and I.C.P. Smith, "MR metabolomics of fecal extracts: applications in the study of bowel diseases," *Magn. Reson. Chem.* **47** issue S1 (2009) S54-S61. **(review)**
http://dx.doi.org/10.1002/mrc.2530

This special metabolomic issue of *MRC* also includes several other papers by Canadian researchers involved in NMR metabolomic research (see below *Canadian NMR Research Highlights*).

Another recent example is an international project by a team from the University of Alberta, the University of Toronto, Australia and U.S.A. aimed at detecting pneumococcal pneumonia via urinary NMR metabolite profiling. Their research has been featured in the News section of the *Journal of Proteome Research:*

L. Cassiday "Diagnosing pneumonia with urinary metabolomics" *J. Proteome Res.* (2009) ASAP. http://dx.doi.org/10.1021/pr9009832

Scientists from the University of Alberta and the University of Calgary are leading international efforts in creating the **Human Metabolome Database** (HMDB). For more information visit www.hmdb.ca

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Submitted by Mike Lumsden (Dalhousie)

NMR^3 Fall NMR Workshop

the **Nuclear Magnetic Resonance Research Resource** (NMR^3) (Dalhousie University, Halifax) invites you to take part in the 4th Annual Fall NMR Workshop on Saturday, November 14, 2009 in the Chemistry Building.

The workshop will consist of seminars from NMR^3 staff emphasizing practical aspects of NMR, contributed oral and poster presentations from NMR^3 users, Facility tours with detailed introduction to research methods. A detailed agenda will be distributed later, but the event is planned to begin at 9:00 AM with registration and conclude by 5:00 PM. Lunch and coffee-breaks will be provided, and there is no registration fee.

http://armrc.chemistry.dal.ca/workshop.htm

NMR BootCamp 2009 – Mission Accomplished ! (+ Photos)

http://www.nanucbootcamp.com/2009photos.htm

the 2009 NANUC BootCamp took place on August 28-29, 2009 at the University of Alberta.

Professor Laurance Hall (1938-2009)

Professor **Laurance Hall**, an NMR pioneer credited with building the first clinical MRI instrument in Canada, died on August 28, 2009 in Cambridge, UK aged 71.

L.D. Hall, 1965
(photo is courtesy of the University of British Columbia Archives)

From *the Telegraph* (Oct.1, 2009): "... It was during this period that Hall began to pursue his pioneering work on NMR – an interest which he took with him, on completion of his doctorate, to Canada. An eloquent and extremely enthusiastic lecturer, he easily impressed senior professors, soon securing a research post in Ottawa, and later one in Vancouver. At the Chemistry Department of the University of British Columbia, where he spent two decades (1963-84), he built – from scratch – the first MRI instrument in Canada. Later he installed for the country its first MRI scanner large enough to examine the entire human body – in a clinic opened by the Queen."

Read the complete obituary in *the Telegraph*

http://www.telegraph.co.uk/news/obituaries/medicine-obituaries/6252025/Professor-Laurance-Hall.html

Laurance Hall had written about his early research career and his work at the University of Ottawa, NRC Canada, and the University of British Columbia, in the *Encyclopedia of Magnetic Resonance*, Volume 1 "Historical Perspectives", Eds. Grant & Harris, Wiley, 1996, p. 378-382.

Canadian NMR blogs and news sites

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

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

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

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

NANUC Newsletters
http://archive.constantcontact.com/fs083/1102124547477/archive/1102424169010.html

NMR Theses Recently Defended

Congratulate your students here!

Mumdooh Ahmed (University of Guelph) August 2009

Supervisors: George Harauz and Vladimir Ladizhansky

Ph.D. thesis: "Dynamics and Induced Structure of intrinsically disordered myelin proteins by NMR spectroscopy"

Recognition

Andrew Marble (Carleton University)

has received the **2008 NSERC Doctoral Prize** for the best Doctoral research on unilateral magnets for MRI applications done while at the University of New Brunswick.

http://www.nserc-crsng.gc.ca/Prizes-Prix/Doctoral-Doctorat/Profiles-Profils/Marble-Marble_eng.asp

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Lewis Kay (University of Toronto)

has received a **Distinguished Alumnus Award** from the University of Alberta

http://www.expressnews.ualberta.ca/article.cfm?id=10488

From the citation: "One of the world's leading biochemists, Kay is recognized for his cutting-edge research in biomolecular nuclear magnetic resonance spectroscopy. The University of Toronto professor and researcher has been instrumental in developing new three- and four-dimensional nuclear magnetic resonance methods for obtaining pictures of complex biomolecules. This revolutionary work has led to important discoveries, helping researchers understand the underlying biological characteristics of diseases. This understanding has increased the probability of finding ways to cure or prevent diseases such as cancer."

Don't miss **the video profile** of Distinguished Alumnus Lewis Kay (5 min, 23.1 MB .mov)
http://www.expressnews.ualberta.ca/media/10488_2.mov

Web: Lewis Kay's Group
http://abragam.med.utoronto.ca/UTNMR.html

CSC 2009 Student Awards

Brett Feland (R. Wasylishen, University of Alberta), **Second prize** in the Undergraduate Student Poster Competition, the Physical, Theoretical and Computational section, "Colossal Expansion: A Solid-State NMR Investigation of $Ag_3Co(CN)_6$"

Hiyam Hamaed (R. Schurko, University of Windsor), **Second prize** for oral presentation in the Graduate/Undergraduate Student Competition, the Physical, Theoretical and Computational section, "Application of Solid-State ^{209}Bi NMR to the Structural Characterization of Bismuth-Containing Materials"

MOOT XXII Awards

Suraj Manrao Travel Awards were presented for the best three posters from graduate students

Myriam Laneville (M. Auger, Université Laval)

Jérémie Leclerc (M. Auger, Université Laval)

Patrick Walsh (S. Sharpe, SickKids)

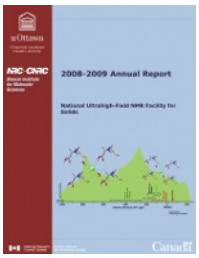
On the move

Luke O'Dell completed his PhD on solid-state NMR of nanocrystalline metal oxides under Professor Mark Smith (University of Warwick, UK) in 2007. He stayed at Warwick for an additional year as a post-doc before moving to Canada to join Rob Schurko's group at the University of Windsor. At Windsor he worked

on novel methods for the acquisition of ultra-wideline spectra from quadrupolar nuclei. In October 2009 Luke joined the Steacie Institute for Molecular Sciences (NRC Canada, Ottawa) as a Research Associate with the Materials Structure and Function Program (Dr. Chris Ratcliffe). At NRC Luke will be involved in development of the high-pressure magic angle spinning NMR technique, as well as continuing to pursue his interests in ultra-wideline NMR experiments and applying optimal control theory to quadrupolar nuclei.

the 900 NMR Facility News

2008-2009 Annual Report



The 2008/09 Annual Report of the National Ultrahigh-Field NMR Facility for Solids has been finalized and is now available for download. We will start mailing printed copies shortly.

http://nmr900.ca/annual_e.html

We would like to take this opportunity to thank all our users and clients, as well as our partners and funding agencies for continuing support.

Travel support program for students and young scientists

Students and young scientists from Canadian Universities are welcome to apply for a travel stipend towards full or partial reimbursement of their travel expenses incurred while visiting the 900 Facility. All requests should be submitted by a supervisor in advance of the trip and include a cost estimate. Requests should be forwarded to the Facility manager for review and approval by the Steering Committee.
http://nmr900.ca/policies_e.html

Recent Travel Grant Recipients

Andre Sutrisno (University of Western Ontario)

Vladimir Michaelis (University of Manitoba)

Brandon Greer (University of Manitoba)

Upcoming NMR Events

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

NMR^3 Fall NMR Workshop

November 14, 2009, Dalhousie University, Halifax
http://armrc.chemistry.dal.ca/workshop.htm

Structural Biology Keystone Symposium

January 8-13, 2010, Breckenridge, Colorado
http://www.keystonesymposia.org/

Structural Genomics: Expanding the Horizons of Structural Biology Keystone Symposium

January 8-13, 2010, Breckenridge, Colorado
http://www.keystonesymposia.org/

2nd U.S.-Canada Winter School on Biomolecular Solid State NMR

January 24-29, 2010, Stowe, Vermont

Biophysical Society 54th Annual Meeting

February 20-24, 2010, San Francisco, CA
http://www.biophysics.org/2010meeting

51st ENC Experimental Nuclear Magnetic Resonance Conference

April 18-23, 2010, Daytona Beach, FL
http://www.enc-conference.org/

Talk abstracts deadline January 12, 2010
Poster abstracts deadline March 12, 2010

CSC 2010 the 93rd Canadian Chemistry Conference and Exhibition

May 29 – June 2, 2010, Toronto, ON
http://www.csc2010.ca/

Call for papers:
Open December 1, 2009
Closed February 15, 2010

EUROMAR 2010 and 17th ISMAR Conference, a World Wide Magnetic Resonance Conference (**WWMR2010**)

July 4-9, 2010, Florence, Italy
http://www.cerm.unifi.it/wwmr2010.html

52nd Annual Rocky Mountain Conference on Analytical Chemistry

August 1-5, 2010, Snowmass, Colorado
http://www.rockychem.com/

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

August 22-27, 2010, Cairns, Australia
http://www.icmrbs2010.org/

MOOT XXIII NMR Symposium

October, 2010, Dalhousie University, Halifax
http://www.mootnmr.org

Pacifichem 2010 The International Chemical Congress of Pacific Basin Societies

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

NMR Spectroscopy of Polymers (Symposium #12) Peter Macdonald, University of Toronto

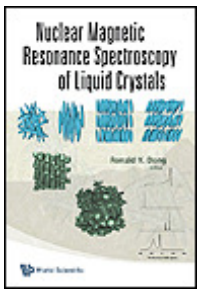
Biomolecular Structure and Dynamics - Recent Advances in NMR (Symposium #43) Mitsuhiko Ikura, Ontario Cancer Institute

Advances in Solid-State NMR of Biological Molecules (Symposium #58) Michèle Auger, Université Laval

Solid-State NMR Methods and Applications in Inorganic Materials (Symposium #228) Scott Kroeker, University of Manitoba

NMR Books

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



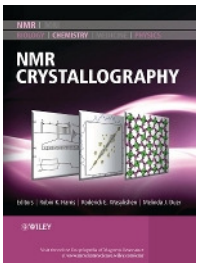
Nuclear Magnetic Resonance Spectroscopy of Liquid Crystals

edited by **Ronald Dong**
(University of British Columbia)
Hardcover: 464 pages
Publisher: World Scientific; September 2009
Language: English
ISBN: 978-9814273664

http://www.worldscibooks.com/materialsci/7310.html

http://www.amazon.com/dp/981427366X

World Scientific: "This edited volume provides an extensive overview of how nuclear magnetic resonance can be an indispensable tool to investigate molecular ordering, phase structure, and dynamics in complex anisotropic phases formed by liquid crystalline materials. The chapters, written by prominent scientists in their field of expertise, provide a state-of-the-art scene of developments in liquid crystal research. The fantastic assortment of shape anisotropy in organic molecules leads to the discoveries of interesting new soft materials made at a rapid rate which not only inject impetus to address the fundamental physical and chemical phenomena, but also the potential applications in memory, sensor and display devices. The review volume also covers topics ranging from solute studies of molecules in nematics and biologically ordered fluids to theoretical approaches in treating elastic and viscous properties of liquid crystals. This volume is aimed at graduate students, novices and experts alike, and provides an excellent reference material for readers interested in the liquid crystal research. It is, indeed, a reference book for every science library to have."

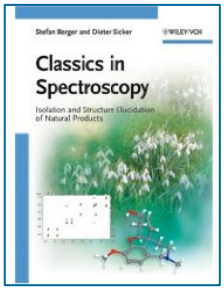


NMR Crystallography
Robin K. Harris (Editor)
Roderick E. Wasylishen (Editor)
Melinda J. Duer (Editor)
Hardcover: 496 pages
Publisher: Wiley; January 2010
Language: English

ISBN: 978-0470699614

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

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



Classics in Spectroscopy: Isolation and Structure Elucidation of Natural Products
by Stefan Berger and Dieter Sicker (Authors)
Paperback: 659 pages
Publisher: Wiley; May 2009
Language: English
ISBN: 978-3527325160

http://www.amazon.com/dp/3527325166/

This book has received the 2009 German Chemistry Industry Fund Literature Prize. Read the book review in *Angewandte Chemie International Edition* http://dx.doi.org/10.1002/anie.200904430

Wiley: "This is the first book of its kind to describe the art of NMR using everyday examples. This textbook will not only fascinate students wanting to learn about the topic, but also those experienced analytical chemists who are still inspired by their profession. The contents provide for easy reading by using natural products that everyone knows, such as caffeine, backed by an attractive layout with many pictures to visualize the topics. In addition, an in-depth analytical part makes the book a valuable teaching tool, or for self-learning using the questions and answers at the end of each chapter."

Stefan Berger *is a co-author of "100/150/200 and more basic NMR Experiments".*

NMR Jobs and Vacancies

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

University of Toronto at Scarborough

Postdoctoral Research Associate in multiphase NMR Spectroscopy

Environmental NMR Centre, Department of Chemistry, University of Toronto at Scarborough, Toronto, Ontario, Canada

http://www.utsc.utoronto.ca/~asimpson/

Project Description:

This is a unique opportunity to develop a novel application of NMR spectroscopy termed Comprehensive Multiphase NMR spectroscopy (CMP NMR).

CMP NMR is a new area of NMR spectroscopy that incorporates solid-state, semi-solids (HR-MAS) and solution-state NMR. The candidate will work with a range of unique hardware prototypes to study intact natural samples that have solid, gel and liquid components (samples may include plants, soils, sediments, tissue/bone etc.) thereby eliminating the need for drying or pre-treatment. This research aims to differentiate molecular structures in various natural phases and more importantly, to permit the study of the chemistry and transport between phases and across key interfaces by NMR spectroscopy for the first time. The successful candidate will have ample opportunities to publish in a diverse range of disciplines.

The project will be carried out in close collaboration with **Bruker BioSpin** and will involve: 1) fundamental development of the technique and preliminary applications in a range of disciplines; and 2) development of applications in environmental chemistry. Environmental applications will focus on understanding the molecular processes behind soil/sediment contamination. The costs associated with the clean-up of contaminated sites in the European Union and the United States is on the order of 1.4 trillion euro. However, current remediation strategies target only the soluble fraction of soil leaving a considerable soil-bound component, that has been linked to a variety of illnesses. Remediation of this "sequestered" fraction is presently impossible as the chemical components of soil that strongly bind contaminants as-well as the molecular mechanisms that hold the contaminants to the soil are not known. CMP-NMR will provide a detailed insight at the molecular-level of the processes that cause contaminants to be

entrapped in the soil matrix and describe the complete binding environment of the contaminant in unaltered natural samples. The results of this project will contribute directly to the development of novel soil remediation strategies.

The candidate must have an extremely strong background in NMR spectroscopy ideally with expertise in solid-state, HR-MAS and solution-state NMR. Expertise in one area is sufficient as long the candidate is willing and interesting in to learn all areas of NMR spectroscopy. The candidate must be open minded and willing to work with very complex environmental samples and be able to design novel pulse programs that combine aspects from solution-state and solid-state NMR. Candidates will need to draw upon and integrate a range of concepts including saturation transfer, diffusion editing, cross-polarization dynamics, relaxation filters, isotope filtering with 1-3D NMR spectroscopy to access specific key molecular interactions from within complex matrices. The candidate will have access to a range of state of-the-art equipment at the Environmental NMR center including prototype multiphase probes and hardware, as well as solid-state, HR-MAS, liquid-state, micro-imaging, and hyphenated (2D-HPLC-SPE-NMR-MS(Q-q-Tof) NMR spectrometers.

The candidate should have an interest in environmental chemistry and/or willingness to learn key issues in this field. *Due to the very technical nature of the project the position is specifically suited to a gifted and open-minded NMR spectroscopist rather than an environmentalist with NMR experience.* The candidate must be willing to travel and may be expected to lead visits with graduate students to Bruker BioSpin, if required.

Application: Candidates should send a complete C.V. including a publication list, a one page statement outlining their suitability and their interest in the position. Candidates should arrange to have 3 references sent directly. Applications without the appropriate references have to be considered incomplete and cannot be considered. Applications and references should be sent to

Professor **André Simpson**
Director of the Environmental NMR Center
Department of Chemistry
Division of Physical and Environmental Sciences
University of Toronto at Scarborough
1265 Military Trail, Toronto, MIC 1A4
Canada

or e-mailed as a PDF attachment to:
andre.simpson@utoronto.ca

All applications and references must be received by Nov 30th 2009.

Vanderbilt University Institute of Imaging Science, Nashville, TN

Postdoctoral position in hyperpolarized MR

Positions available for Postdoctoral Physicist, Chemist, Electrical Engineer or Biologist for in vivo and in vitro hyperpolarized and conventional multi-nuclear NMR at Vanderbilt University Institute of Imaging Science (**VUIIS**)

http://www.vuiis.vanderbilt.edu/

- Vanderbilt University is the only non-profit organization in top 100 US employer list
- Unique methods of hyperpolarization and biomedical applications
- Funded projects in area of molecular imaging of cancer
- VUIIS aims to support and integrate advances in physics, engineering, chemistry, computing and other basic sciences for the development and application of new and enhanced imaging techniques to address problems and stimulate new research directions in biology and medicine, in health and disease
- Collaborative research with other research and clinical programs
- Opportunities for independent funding
- Appointments 1-2 years with prospects
- Excellent opportunity for candidates with high resolution NMR background to enter and build career in the field on biomedical Magnetic Resonance

Requirements: PhD, demonstrated evidence of strong scientific ability and publication record, excellent written and oral communication skills and ability to execute projects independently. The successful candidate is expected to contribute to novel experimental designs, to process and analyze data, to prepare and edit manuscripts, and to assist in training and supervising graduate students. CV inquiries to **Eduard Chekmenev** at (Eduard.Chekmenev@vanderbilt.edu) and **Kevin Waddell** at (Kevin.Waddell@vanderbilt.edu)

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Assistant Professor of Radiology and Radiological Sciences
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Phone: (615)-322-1329
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E-mail: eduard.chekmenev@vanderbilt.edu
Web: www.vuiis.vanderbilt.edu

Iowa State University, Department of Chemistry

Postdoctoral position in biological solid-state NMR

A postdoctoral position is now available for biological solid-state NMR research of membrane proteins and other biomolecules. We seek strongly motivated researchers with experience either in solid-state NMR or in protein solution NMR. Familiarity with protein biochemistry is desirable. My laboratory has full use or significant access to 400 MHz, 600 MHz, and 700 MHz solid-state NMR spectrometers. Interested candidates should send their curriculum vitae (including a list of publications) and the names and addresses of two references to Mei Hong.

Mei Hong, John D. Corbett Professor of Chemistry
Department of Chemistry
Iowa State University
Ames, IA 50011
Tel: 515-294-3521
Fax: 515-294-0105
email: mhong@iastate.edu
http://www.public.iastate.edu/~hongweb/

University of North Florida, Department of Chemistry

Analytical Instrumentation Facility Manager
(PhD analytical/physical chemistry)

http://www.unf.edu/coas/chemistry/

Responsibilities include maintenance and upkeep of the departmental 500 MHz Varian NMR as well as other major instrumentation (both current and future acquisitions) in the Chemistry Department, training faculty and students, providing expertise to faculty and students in utilizing major instrumentation in research and their implementation in instruction, offering service to other departments at UNF and to the outside (academia and industry). Opportunities for collaborative research are available and strongly encouraged. This is a **staff position** tenable from 2010.

Contact Chemistry Department Chairperson:
mailto:kenneth.laali@UNF.edu

Kenneth K. Laali
Professor and Chair
Department of Chemistry
University of North Florida
Science and Engineering Building
1 UNF Drive, Jacksonville, FL 32224, USA
FAX: 904-620-3535
Tel: 904-620-1503

Durham University, Durham, UK

Postdoctoral research associate position in the Solid-State NMR group from early 2010

This 3 year position is the key staff appointment in a significant collaborative project to determine the performance limits of homo- and hetero-nuclear decoupling in organic solid-state NMR, with the goal of understanding and developing methods to maximise performance in state-of-the-art experiments involving high magnetic fields and ultra fast magic-angle spinning. The work in Durham will focus on the acquisition of reference data sets and the development of numerical simulations. This work will be closely coordinated with experimental work based at Warwick (**Dr S. P. Brown**) and theoretical work at ETH Zurich (**Dr M. Ernst**), but will also be integrated with a wider research effort involving groups across Europe (**Emsley, Kentgens**), Canada (**Goward**) and Japan (**Takeda**), as well as the pharmaceutical companies, AstraZeneca and GlaxoSmithKline, plus support from instrument manufacturers (Bruker, Varian). The challenging objectives of the project mean that applicants must have a strong background in solid-state NMR theory and practice. Excellent IT skills are also essential, not only for the development of simulation / analysis software, but also for the maintenance of web-based collaboration tools to co-ordinate information exchange between the project partners. The high profile of the project and the contacts with other internationally leading research groups make this a good position for applicants to develop their prior experience and to demonstrate their abilities to a wider audience.

For further information on the Durham group, go to:
www.dur.ac.uk/solids.nmr

For application information, go to:

https://jobs.dur.ac.uk/jobdtls.asp?Session_in=&Uid=&vref=3515

Paul Hodgkinson (Durham, UK)

Listings of NMR jobs and vacancies

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

NMR Wiki
http://nmrwiki.org/wiki/index.php?title=Category:Jobs

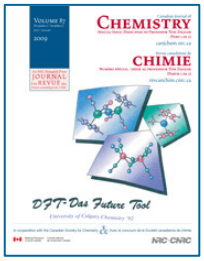
NMR jobs on the NMR Information Server
http://www.spincore.com/nmrjobs/

AMPERE mailing list
https://listes.sc.univ-paris-diderot.fr/sympa/info/nmr

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

Canadian NMR Research Highlights

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



Canadian Journal of Chemistry
volume 87 (#7, #10) 2009

This special issue of *Canadian Journal of Chemistry* is dedicated to Professor **Tom Ziegler** (University of Calgary), a Tier 1 Canada Research Chair in Theoretical Inorganic Chemistry, one of the pioneers of density functional theory (DFT). Prof. Ziegler has made many important contributions to the development of DFT calculations of NMR parameters.

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

This special *CJC* issue is divided in two parts:

Part 1 of 2 (volume 87, # 7, July 2009)
http://pubs.nrc-cnrc.gc.ca/rp-ps/inDetail.jsp?jcode=cjc&lang=eng&vol=87&is=7

Part 2 of 2 (volume 87, # 10, October 2009)
http://pubs.nrc-cnrc.gc.ca/rp-ps/inDetail.jsp?jcode=cjc&lang=eng&vol=87&is=10

Two research papers in *PNAS*

R. Das, I. André, Y. Shen, Y. Wu, A. Lemak, S. Bansal, C.H. Arrowsmith, T. Szyperski and D. Baker, "Simultaneous prediction of protein folding and docking at high resolution," *Proceedings of The National Academy of Sciences of The United States of America* (2009) online.
http://dx.doi.org/10.1073/pnas.0904407106

F.J. Amador, S. Liu, N. Ishiyama, M.J. Plevin, A. Wilson, D.H. Maclennan, M. Ikura, "Crystal structure of type 1 ryanodine receptor amino-terminal beta-trefoil domain reveals a disease-associated mutation "hot spot" loop," *Proceedings of The National Academy of Sciences of The United States of America* **106** (2009) 11040-11044.
http://dx.doi.org/10.1073/pnas.0905186106

Magnetic Resonance in Chemistry Special issue

volume 47, issue S1, 2009
"NMR-based mixture analysis - metabolomics and beyond"
http://www3.interscience.wiley.com/journal/122679447/issue

T. Bezabeh, R.L. Somorjai and I.C.P. Smith, "MR metabolomics of fecal extracts: applications in the study of bowel diseases," *Magnetic Resonance in Chemistry* **47** (2009) S54-S61. **(review)**
http://dx.doi.org/10.1002/mrc.2530

M. Cuperlovi-Culf, N. Belacel, A.S. Culf, I.C. Chute, R.J. Ouellette, I.W. Burton, T.K. Karakach, J.A. Walter, "NMR metabolic analysis of samples using fuzzy K-means clustering," *Magnetic Resonance in Chemistry* **47** (2009) S96-S104.
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T.K. Karakach, R. Knight, E.M. Lenz, M.R. Viant, J.A. Walter, "Analysis of time course ^{1}H NMR metabolomics data by multivariate curve resolution," *Magnetic Resonance in Chemistry* **47** (2009) S105-S117**.**
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Review in *Trends in Biochemical Sciences*

A.K. Mittermaier, L.E. Kay, "Observing biological dynamics at atomic resolution using NMR," *Trends in Biochemical Sciences* (2009) in press. **(review)**
http://dx.doi.org/10.1016/j.tibs.2009.07.004

Review in *Nature Chemical Biology*

A.J. Baldwin, L.E. Kay, "NMR spectroscopy brings invisible protein states into focus," *Nature Chemical Biology* **5** (2009) 808-814.
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Current topic in *Biochemistry*

G. Harauz, V. Ladizhansky, J.M. Boggs, "Structural Polymorphism and Multifunctionality of Myelin Basic Protein," *Biochemistry* **48** (2009) 8094-8104. **(Current Topic)**
http://dx.doi.org/10.1021/bi901005f

Recent NMR Publications

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

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S. Bourbigot, L. Fardy, A.J. Waring, M.R. Yeaman and V. Booth, "Structure of chemokine-derived antimicrobial peptide interleukin-8alpha and interaction with detergent micelles and oriented lipid bilayers," *Biochemistry* **48** (2009) 10509-10521. http://dx.doi.org/10.1021/bi901311p

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