



Canadian NMR News

submitted by Lawrence McIntosh (UBC)

UBC Biomolecular NMR Facility

A new solution/solid-state Bruker **Ascend 850 MHz** NMR spectrometer has been installed in the UBC Biomolecular NMR Facility. The instrument was purchased through funding of the "Advanced Structural Biology for Re-emerging Infectious Diseases" initiative by CFI and BCKDF, with contributions by Bruker Canada. In addition, solution-state **500** and **600 MHz** spectrometers and a solid-state **500 MHz** spectrometer were upgraded with Bruker **Avance III** consoles. The facility is expertly managed by **Mark Okon** with occasional meddling by **Suzana Straus** and **Lawrence McIntosh**.

The solution-state spectrometers are equipped with 5 mm cryogenic xyz-gradient TCI probes for standard triple resonance $^1\text{H}/^{13}\text{C}/^{15}\text{N}$ experiments as well as direct ^{13}C observation. The 600 MHz spectrometer also has a cryogenic QCI probe for $^1\text{H}/^{19}\text{F}/^{13}\text{C}/^{15}\text{N}$ experiments with high sensitivity direct detection of ^1H , ^{19}F , or ^{13}C . Room temperature $^1\text{H}/^{31}\text{P}/^{13}\text{C}/^{15}\text{N}$ QXI probes are available for the 600 and 850 MHz instruments, allowing the extra option of indirect ^{31}P detection experiments for proteins and nucleic acids.

The 850 MHz instrument is equipped with an E-Free triple resonance Magic Angle Spinning solid state NMR probe for biological samples and an E-Free High Power Static Fixed Frequency Triple Resonance Probe for aligned solid biological samples.

We are most willing to help Canadian researchers who could benefit from access to this instrumentation.

<http://otter.biochem.ubc.ca/HOME.html>

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The 850 MHz NMR spectrometer in the basement of the Life Sciences Centre.

Visit "**the Resonance**" (Bruker) for an exiting photo report from the installation to see a 4 ton magnet traveling via an elevator shaft!

<http://tinyurl.com/7qfy8ch>

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

CFI LOF 2012 Competition Results

Gillian Goward (McMaster University) has been awarded \$380,650 towards "In Situ Characterization of Electrochemical Processes in Lithium Ion Batteries".

Mount Allison University (Sackville, NB) has been awarded a \$195,776 equipment grant for a new NMR spectrometer. This new NMR instrument will support research by **Dr. Stephen Westcott**, the Canada Research Chair in Boron Chemistry, and his colleagues at the Chemistry Department.

Read the press release by MTA:
http://www.mta.ca/news/news_display.php?id=3803



ICMRBS 2012 Founders' Medal - Call for Nominations

The International Conference of Magnetic Resonance in Biological Systems (**ICMRBS**) was co-founded by Oleg Jardetzky, Mildred Cohn, and Robert Schulman in 1964. The conference has been organized biannually over the past half century, and currently attracts between 800 and 1,000 scientists to a six-day scientific forum held at different locations across the world.

<http://www.icmrbs.org>

In 2002, the ICMRBS Council established the Founders' Medal to recognize exceptional contributions by young scientists (under 41 years at the time of the award) to the development and/or progress of the field of magnetic resonance in biological systems. An award winner will receive the Medal as well as \$3,000 (in USD), and she or he will be invited to present a lecture at the XXVth ICMRBS meeting, which will be held in Lyon, France, August 19-24, 2012.

Previous Recipients Lewis Kay, Univ. of Toronto, Canada (2002), Nico Tjandra, National Institutes of Health, USA (2005), Marc Baldus, Max-Planck-Institute for Biophysical Chemistry, Germany (2006), Chad Rienstra, Univ. of Illinois, USA (2008), and Mei Hong, Iowa State Univ., USA (2010).

Nomination Procedure Nominations must be submitted by email to the Chair of the ICMRBS Council (2010-2012), **Mitsu Ikura**

E-mail: mikura@uhnres.utoronto.ca

The deadline for nominations is **March 31st, 2012**. The nomination package should include (1) cover letter, (2) outline of the candidate's "exceptional contributions", (3) the candidate's CV and publication list.

Selection Committee Peter Wright (Chair), Marc Baldus, Masatsune Kainosho, Ann McDermott, Thomas Prisner

Raymond Andrew Prize 2012 - Call for nominations

Call for Nominations for the Raymond Andrew Prize for an outstanding Ph.D. thesis in the field of magnetic resonance

For the Raymond Andrew Prize 2012 the AMPERE Prize Committee is seeking your help in searching for qualified candidates who completed their dissertation during the period of 2010/2011. The prize will be presented during the **EUROMAR 2012** in Dublin (Ireland) from 1th to 5th July, 2012.

You are kindly invited to submit nominations by e-mail to

Email: andrewprice@nmr.phys.chem.ethz.ch

Suggestions must be received by **15th February 2012** and should include the following documents: (1) Nomination letter, (2) Curriculum vitae, (3) List of publications and presentations at conferences, (4) PhD thesis in PDF.

The thesis should be written in English. In exceptional cases, the thesis may also be submitted in triplicate as a hardcopy to the AMPERE Secretariat.

Submissions that arrive too late will automatically be transferred to the next year. The prize committee will reconsider excellent contributions for two years in a row.

For a list of past Andrew Prize winners see:

http://www.ampere.ethz.ch/andrew_prize.htm

Gunnar Jeschke

Secretary General, Groupement AMPERE

Special issue of the *Journal of Magnetic Resonance*



Volume 213, Issue 2, Pages 213-574 (December 2011)

Magnetic Moments,

Groundbreaking papers from the pages of the *Journal of Magnetic Resonance* - and recollections from the scientists behind them.

<http://www.sciencedirect.com/science/journal/10907807/213/2>

To celebrate the 2011 International Year of Chemistry *JMR* has assembled a collection of reprints of some of the most significant papers published in the journal since its inception over 40 years ago. These reprints are accompanied by video/audio commentaries by their authors giving a rare "behind the scene" glimpse into magnetic resonance research.

These videos are also available on *YouTube*
<http://www.youtube.com/playlist?list=PL1D790E241B661706>

Halogen bonding

David Bryce (University of Ottawa) reports from the IUPAC sponsored **IUCr Workshop on "Categorizing Halogen Bonding and Other Noncovalent Interactions Involving Halogen Atoms"** which was held in August 20-12, 2011 in Sigüenza, Spain. Dave's participation in this workshop was supported by the 2011 CNC-IUPAC travel award. His recent research in solid-state NMR of quadrupolar halogens shows a great potential for solid-state NMR to contribute to this area of research.

D. Bryce "Halogen Bonding" *Chemistry International* **34** (2012) 27-29.
http://www.iupac.org/publications/ci/2012/3401/cc1_200811.html

suggested by Alexey Denisov (Concordia)

Pharma Industry in Crisis

Elisabeth Pain from *Science's Career Magazine* reviews the current state of the job market in the pharmaceutical industry.

<http://dx.doi.org/10.1126/science.caredit.a1100136>

Solid-state NMR for quantum computing

Recent research by a team from the Institute for Quantum Computing (Waterloo) is highlighted by *PhysOrg*. **Osama Moussa** and colleagues from IQC have used ^{13}C NMR in a single crystal of malonic acid to test error corrections in quantum information processing.

<http://www.physorg.com/news/2011-11-quantum-error-solid-state.html>

O. Moussa, J. Baugh, C.A. Ryan, R. Laflamme, "Demonstration of sufficient control for two rounds of quantum error correction in a solid state ensemble quantum information processor," *Physical Review Letters* **107** (2011) 160501.

<http://dx.doi.org/10.1103/PhysRevLett.107.160501>

"NMR is Good" contest by Cambridge Isotope Laboratories



Have you acquired an NMR spectrum you are really proud of?

Submit - Your favorite NMR spectrum will be showcased on CIL's website and in our Hospitality Suite at **ENC 2012**.

Vote - Vote for your favorite NMR spectra online, April 16th-18th and in person at CIL's ENC Hospitality Suite. All votes will be entered to win an **iPAD2!**

Win - Receive the most votes and win a travel stipend for \$1500 or CIL product in the amount of \$1500.

Dates to remember: Submission starts January 25th and ends March 15th. Voting April 16th-18th. Online or at the ENC Hospitality Suite

To submit your spectrum:

http://www.isotope.com/cil/news/nmr_submission.cfm

NMR on Twitter

List of new solid-state NMR papers updated by Luke O'Dell (NRC-SIMS)

<http://twitter.com/solidstateNMR>

uOttawa NMR by Glenn Facey

<http://twitter.com/uOttawaNMR>

NMR Wiki <http://twitter.com/nmrwiki>

nmr900 <http://twitter.com/nmr900>

Bruker <http://twitter.com/bruker>

Agilent <http://twitter.com/agilent>

Recognition



Recognition: Lewis Kay

Special issue of the *Journal of Biomolecular NMR* on the occasion of **Prof. Lewis E. Kay's 50th birthday**, volume 51, numbers 1-2, September 2011.

Kevin H. Gardner, Anthony Mittermaier

and **Frans A.A. Mulder**, "A tribute to Lewis E. Kay on his 50th birthday" *Journal of Biomolecular NMR* **51** (2011) 3-4. **(Editorial)**
<http://dx.doi.org/10.1007/s10858-011-9561-x>

A fitting collection of 18 research publications by colleagues, friends and former students of Lewis Kay to celebrate his many pioneering contributions to the field of biomolecular NMR spectroscopy.

Read the news story by UofT (photo credit):

http://www.biochemistry.utoronto.ca/research/research_news.html

Dr. Gary Schrobilgen (McMaster) has received the McMaster's 2011 **Distinguished Alumni Award** for the Sciences.

Dr. Schrobilgen is a renowned authority in NMR spectroscopy of noble gases and their compounds. In collaboration with Michael Gerken (Lethbridge) he has written a chapter on the subject for the *Encyclopedia of Magnetic Resonance*

G.J. Schrobilgen and M. Gerken, "Noble Gas Elements", *Encyclopedia of Magnetic Resonance* (2011).
<http://dx.doi.org/10.1002/9780470034590.emrstm0346.pub2>

From the citation: "After earning his undergraduate degree in his native Iowa, Dr. Gary Schrobilgen came to Canada and Brock University for his Master of Science degree and then graduated from McMaster University with his PhD in inorganic chemistry in 1974 under the supervision of Professor Ron Gillespie. Following a postdoctoral fellowship in England, he joined McMaster's Chemistry Department where, in 1988, he became a full professor of inorganic chemistry.

Dr. Schrobilgen's research has focussed on fundamental studies of highly reactive chemical species involving fluorine derivatives of the noble gases and polyatomic anions of main-group elements. He is perhaps best known for his detailed work involving the syntheses and structural characterizations of a large percentage of the known compounds of krypton and xenon, as well as fluoro- and oxofluoro-derivatives of main-group elements and transition metals in their highest oxidation states. His work has had applications in nuclear power generation, photovoltaic and semiconductor materials, refrigerants, advanced rocket propellants and microelectronics.

In addition to leadership in research, Dr. Schrobilgen is an accomplished mentor, having won the McMaster University President's Award for Excellence in Graduate Supervision. Dr. Schrobilgen has dedicated himself not just to research and teaching, but to advancing his profession as well. He has served on the Executive Committee of the Division of Fluorine Chemistry of the American Chemical Society, holding the chairmanship of the committee in 2005.

Dr. Schrobilgen has also collected many of the most prestigious awards in his field. A fellow of the Royal Society of Canada, he has received the American Chemical Society Award for Creative Work in Fluorine Chemistry, the Alcan Lecture Award, the International Award for Pure or Applied Chemistry, the E.W.R. Steacie Award in Chemistry, a Humboldt Research Award from the Alexander von Humboldt Foundation and the Canada Council Killam Research Fellowship."

http://www.mcmaster.ca/ua/alumni/programs_recognition_distalumni.html



See **Dr. Gary Schrobilgen** speak about his research with noble gases in this video by *the Spotlight McMaster* team.

<http://www.youtube.com/watch?v=NSc7gcXHIho>

NMR Theses Recently Defended

Robert Attrell (University of Ottawa),
December 2011

Supervisor: Prof. David Bryce

M.Sc. thesis: "A Solid-State ^{35}Cl and ^{81}Br NMR and Computational Study of Chlorine and Bromine Electric Field Gradient and Chemical Shift Tensors in Haloanilinium Halides"

Becky Chapman (University of Ottawa),
November 2011

Supervisor: Prof. David Bryce

Ph.D. thesis: "Development and Application of Chlorine Solid-State Nuclear Magnetic Resonance and Quantum Chemical Calculations to the Study of Organic and Inorganic Systems"

On the move

Dr. Andy Lo has decided to leave his post as NMR technician at the University of Ottawa to accept a similar position at the University of Guelph. His last day of work at uOttawa was February 3rd. We wish Andy well in his new position and will miss him in our Facility.

Glenn, Dave

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. This report is only available as a PDF version

http://nmr900.ca/annual_e.html

We would like to thank all who contributed to this report, and to acknowledge our many users, clients, partners and funding agencies for continuing support of the 900 project.

Upcoming NMR Events



95th Canadian Chemistry Conference and Exhibition
CALGARY, ALBERTA
May 26-30, 2012 • Energizing Chemistry
CALL for Papers Now Open!

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 take part in 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 tentatively beginning Sunday afternoon, May 27th.

The confirmed invited speakers are Michèle Auger (Laval), Jochen Autscbach (SUNY - Buffalo), Alex Bain (McMaster), Darren Brouwer (Redeemer), David Bryce (Ottawa), Gillian Goward (McMaster), Yining Huang (Western), Scott Kroeker (Manitoba), Andrew MacFarlane (UBC), Karl T. Mueller (PNNL - Richland), Luke O'Dell (NRC Canada), John Ripmeester (NRC Canada), Rob Schurko (Windsor), Victor Terskikh (NRC Canada), Gang Wu (Queen's).

In addition, the conference will feature the usual **poster session**. Finally, on Saturday, May 26th the National Ultrahigh-Field NMR Facility for Solids and Bruker Canada will be hosting the **7th Annual Solid-State NMR Workshop**. I certainly hope that you and your colleagues can attend the workshop.

Please visit the conference web site <http://www.csc2012.ca> for a full list of symposia and for abstract submission instructions. All abstracts must be submitted on-line by Wednesday, **February 15**. The Web site also provides information on the many attractions in the Calgary area.

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>

2012 NMR BOOTCAMP

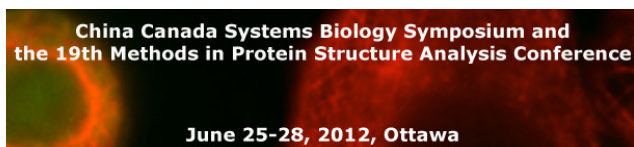
NANUC 2012 Biomolecular NMR BootCamp will be hosted by the NMR Facility in Chemistry at the University of Toronto, June 4th to 9th, 2012 on campus.

Our keynote lecturer this year is Prof. **Chad Reinstra** (UIUC) on BioSolids NMR. We will have Dr. **Frank Delaglio** (NIDDK, NIH) for the NMRPipe Suite; Dr. **Nico Tjandra** (LBPC, NIH) with Dynamics and Relaxation; Dr. **Bruce Johnson** (UMBC) on NMRView; Dr. **Charles Schwieters** (ISL, NIH) demonstrating Xplor-NIH, and one day on pulse sequence programming (**Agilent/Bruker**).

More information will be available soon at <http://www.nanuc.ca/resources/workshops.php>

Please mark your calendars,

Timothy Burrow, University of Toronto
<http://www.chem.utoronto.ca/facilities/nmr/nmr.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>

Biophysical Society 56th Annual Meeting

February 25-29, 2012, San Diego, California
<http://www.biophysics.org/2012meeting>

 **Biophysical Society of Canada Mixer**
Sunday, February 26, 6-7 PM

11th Chemical BioPhysics Symposium

April 13-15, 2012, University of Toronto
<http://www.chembiophys.ca>

53rd ENC


April 15-20, 2012, Miami, Florida
<http://www.enc-conference.org/>

20th ISMRM Scientific Meeting and Exhibition of the International Society for Magnetic Resonance in Medicine


May 5-11, 2012, Melbourne, Australia
<http://www.ismrm.org>


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
<http://www.nanuc.ca/resources/workshops.php>

 **24th CMSC**, Canadian Materials Science Conference
June 5-8, 2012, London, Ontario, Canada
<http://www.eng.uwo.ca/2012cmssc>

 **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 Symposium on Xenon NMR of Materials

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

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

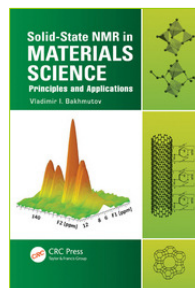
August 19-24, 2012, Lyon, France
<http://www.pasteur.fr/infosci/conf/sb/ICMRBS/>

SMASH 2012 Small Molecule NMR Conference

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

New NMR Books

Solid-State NMR in Materials Science: Principles and Applications



Author: Vladimir Bakhmutov (Texas A&M University)
Hardcover: 280 pages
Publisher: CRC Press; 1st edition (December 19, 2011)
Language: English
ISBN: 978-1439869635

<http://www.amazon.com/dp/1439869634>
<http://www.amazon.ca/dp/1439869634>

CRC: Solid-state NMR is a powerful physical method widely applied in modern fundamental and applied science, medicine, and industry. Its role is particularly valuable in materials chemistry due to the capability of solid-state NMR to rapidly solve tasks connected with structural descriptions of complex systems on macro and/or molecular levels, and the identification of the dynamics often responsible for complex systems mechanical properties.

Written for non-specialists, **Solid-State NMR in Materials Science: Principles and Applications** introduces the general physical principles of pulsed NMR, by including elements of the theory and practice in the registration of NMR signals, and by explaining different NMR equipment.

After the preliminaries, the book covers: The theory and features of solid-state NMR and nuclear relaxation in solids, including dynamics of materials. Different materials, diamagnetic and paramagnetic, from metals and metal clusters to amorphous composites. The methodology of collection and interpretations of solid-state NMR data, including strategies and criteria for structural characterizations of different materials. Practical examples of multinuclear NMR and relaxation experiments as well as interpretations of data obtained. Numerous solid-state NMR experiments performed for various materials to evaluate their structure and dynamics. Written in clear and simple language, this book includes clear illustrations, numerous examples, and detailed bibliographies. It an excellent reference not only for young and experienced researchers, but also for students interested in a future in materials science.

NMR Jobs and Vacancies

Postdoctoral position, NMR Spectroscopy of Lithium Ion Battery Materials

McMaster University, Hamilton, ON

An opening for a Postdoctoral Fellow is available in the **Department of Chemistry and Chemical Biology at McMaster University**. The successful candidate will work in the research group of Dr. Goward and the focus of this industry-funded position will be research on development and application of in situ NMR measurements of electrochemical lithium ion cells, with an aim to understand processes in vehicle batteries. This position is intended for a physical chemist interested in moving into a new research area, or for an NMR spectroscopist, interested in using their NMR expertise in this applied field. (knowledge of electrochemistry and material chemistry is also an asset). This research project will involve close collaboration with material scientists, chemists, and mathematicians, as well as research scientists with our Industrial Partners.

The fellowship is open to candidates of any nationality and selection will be based upon the candidate's research potential. The start date of the position is May 1, 2012. The duration of the position will be initially one year with extension for the second year contingent on satisfactory performance. The annual salary will be \$45,000 CAD. We will begin reviewing applications on **March 1, 2012**. Applications received after this date will be accepted until the position is filled, and to ensure full consideration, applicants are advised to submit all supporting materials by the deadline.

Applicants should provide at least three letters of recommendation. They may be sent directly to:

Dr. Gillian Goward

Department of Chemistry and Chemical Biology
McMaster University

Hamilton, Ontario, CANADA L8S 4M1

Phone: +1 (905) 525 9140 ext. 24176

Fax: +1 (905) 522-2509

Email: goward@mcmaster.ca

<http://www.chemistry.mcmaster.ca/goward>

McMaster is committed to Employment Equity and encourages applications from all qualified candidates, including aboriginal peoples, persons with disabilities, members of visible minorities and women.

University of Wisconsin-Madison, Department of Chemistry

(Instrumentation Technologist)

http://www.ohr.wisc.edu/pvl/pv_072666.html

Kansas State University, KS

(Postdoc in solid-state NMR/crystallography)

http://nmr900.ca/nmr_jobs.html#ksu

University of Delaware

(NMR Spectroscopist)

http://nmr900.ca/nmr_jobs.html#udel

PhD and postdoc solid-state NMR positions (multiple, Europe)

http://nmr900.ca/nmr_jobs.html#europe

University of Connecticut

(NMR Spectroscopist/Manager)

http://nmr900.ca/nmr_jobs.html#uc

Brown University, Providence, RI

(Structural Biology NMR Faculty Position)

http://nmr900.ca/nmr_jobs.html#brown

University of Liege, Belgium

(Postdoc in solid-state NMR of pharmaceuticals)

http://nmr900.ca/nmr_jobs.html#liege

University of Piemonte Orientale, Italy

(Postdoc in solid-state NMR)

http://nmr900.ca/nmr_jobs.html#upo

University of California, Irvine

(NMR Spectroscopist/manager)

http://nmr900.ca/nmr_jobs.html#uci

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&chld=0>

FG-MR Jobs

<http://fgmrjobs.blogspot.com/>

Canadian NMR Research Highlights

Automated Determination of Protein Structures from NMR

Cheryl Arrowsmith (Ontario Cancer Institute, NESG, University of Toronto) is among a large multinational team involved in a feasibility study of the fully automatic NMR determination of protein structures.

A. Rosato, J.M. Aramini, C. Arrowsmith, A. Bagaria, D. Baker, A. Cavalli, J.F. Doreleijers, A. Eletsy, A. Giachetti, P. Guerry, A. Gutmanas, P. Güntert, Y. He, T. Herrmann, Y.J. Huang, V. Jaravine, H.R.A. Jonker, M.A. Kennedy, O.F. Lange, G. Liu, T.E. Malliavin, R. Mani, B. Mao, G.T. Montelione, M. Nilges, P. Rossi, G. van der Schot, H. Schwalbe, T.A. Szyperski, M. Vendruscolo, R. Vernon, W.F. Vranken, S. de Vries, G.W. Vuister, B. Wu, Y. Yang, A.M.J.J. Bonvin "Blind Testing of Routine, Fully Automated Determination of Protein Structures from NMR Data," *Structure* **20** (2012) 227–236.

<http://dx.doi.org/10.1016/j.str.2012.01.002>

Summary

The protocols currently used for protein structure determination by nuclear magnetic resonance (NMR) depend on the determination of a large number of upper distance limits for proton-proton pairs. Typically, this task is performed manually by an experienced researcher rather than automatically by using a specific computer program. To assess whether it is indeed possible to generate in a fully automated manner NMR structures adequate for deposition in the Protein Data Bank, we gathered 10 experimental data sets with unassigned nuclear Overhauser effect spectroscopy (NOESY) peak lists for various proteins of unknown structure, computed structures for each of them using different, fully automatic programs, and compared the results to each other and to the manually solved reference structures that were not available at the time the data were provided. This constitutes a stringent "blind" assessment similar to the CASP and CAPRI initiatives. This study demonstrates the feasibility of routine, fully automated protein structure determination by NMR.

Cover article in the *Journal of the American Chemical Society*



Gang Wu, Zhehong Gan, Irene C. M. Kwan, James C. Fettinger, and Jeffery T. Davis, "High Resolution ^{39}K NMR Spectroscopy of Bio-organic Solids," *J. Am. Chem. Soc.* **133** (2011) 19570–19573. (Cover Article)

<http://dx.doi.org/10.1021/ja2052446>

Edge article in *Chemical Science*

J. Zhu, T. Kurahashi, H. Fujii and G. Wu, "Solid-state ^{17}O NMR and computational studies of terminal transition metal oxo compounds," *Chemical Science* **3** (2012) 391–397. (Edge Article)

<http://dx.doi.org/10.1039/C1SC00725D>



Encyclopedia of Magnetic Resonance: new entries

A. O'Sullivan, D. Avizonis, J.B. German and C.M. Slupsky, "Software Tools for NMR Metabolomics", *Encyclopedia of Magnetic*

Resonance, Wiley (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1232>

N. De Zanche, "Birdcage Volume Coil Design", *Encyclopedia of Magnetic Resonance*, Wiley (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1288>

D.I. Hoult, "Receiver Design for MR", *Encyclopedia of Magnetic Resonance*, Wiley (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1137>

J.W. Zwanziger, "Computing Electric Field Gradient Tensors", *Encyclopedia of Magnetic Resonance*, Wiley (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1208>

D.L. Bryce and R.E. Wasylshen, "Quadrupolar Nuclei in Solids: Influence of Different Interactions on Spectra", *Encyclopedia of Magnetic Resonance*, Wiley (2011).

<http://dx.doi.org/10.1002/9780470034590.emrstm1197>

G. Wu, "Alkali Metal NMR of Biological Molecules", *Encyclopedia of Magnetic Resonance*, Wiley (2011).
<http://dx.doi.org/10.1002/9780470034590.emrstm1210>

T.T. Nakashima and R.E. Wasylishen, "Sensitivity and Resolution Enhancement of Half-integer Quadrupolar Nuclei in Solid-state NMR", *Encyclopedia of Magnetic Resonance*, Wiley (2011).
<http://dx.doi.org/10.1002/9780470034590.emrstm1200>

L.A. O'Dell and C.I. Ratcliffe, "Quadrupolar NMR to Investigate Dynamics in Solid Materials", *Encyclopedia of Magnetic Resonance*, Wiley (2011).
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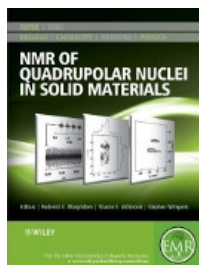
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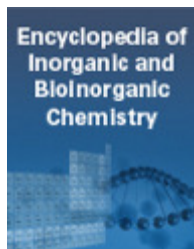
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NMR of Quadrupolar Nuclei in Solid Materials
Roderick E. Wasylishen (Editor)
Sharon E. Ashbrook (Editor)
Stephen Wimperis (Editor)
Hardcover: 584 pages
Publisher: Wiley; July 2012
Language: English
ISBN: 978-0470973981

[http://www.amazon.com/dp/0470973986/](http://www.amazon.com/dp/0470973986)
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