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

Canadian NMR Research News Bulletin #8.4
Fall 2014

Guest Editorial

Bill Reynolds:

Scientific Innovation Versus Corporate Bean Counters

E-mail: wreynold@chem.utoronto.ca

As a regular user of Varian and then Agilent NMR spectrometers from 1960 to the present, I have seen a series of bad business decisions which, cumulatively, have led to yesterday's announcement [*that Agilent Technologies is to exit Nuclear Magnetic Resonance business*]. I thought that this post might provide useful insight into the problems with carrying out scientific innovation in a bottom line-oriented business environment.

From the early 1950 to the mid 1960, Varian Associates was arguably the most innovative scientific instrument company in North America and probably the world. Led by the Varian brothers and senior scientists such as Wes Anderson, Martin Packard and Jim Shoolery, they successively developed the HR line of NMR spectrometers from 30 to 40 to 60 to 100 MHz, followed by the A-60, the HA-100 and finally the HR-200, the first spectrometer with a superconducting solenoid. At the same time, they pioneered a number of the innovations incorporated in these spectrometers, including sample spinning, shims, flux stabilization, spin decoupling, integration and field/frequency locks. What makes this most impressive to me is that, at that stage, Varian had no serious competitors in the field and thus no incentive, other than desire to advance the field of NMR, to so rapidly incorporate improvements.

In This Issue

What I regard as the golden age of Varian Associates was capped in 1966 by the invention by Wes Anderson and Richard Ernst of FT NMR. However, by that time, business-oriented decision making seemed to be taking over at Varian. Instead of immediately proceeding to commercialize FT NMR, they delayed, apparently because Varian was doing so well in marketing existing systems, that they felt no urgency. However, Bruker took advantage of this delay to market the first dedicated FT NMR spectrometer, establishing themselves as a serious player in the NMR field. While Varian quickly followed with the XL-100, this represented the first time that a major commercial NMR innovation hadn't originated with Varian.

In the early 1970, Varian started marketing a superconducting FT spectrometer (the SC-300) in competition with the Bruker HX-270. However, in about 1973, Varian management

made an incredibly stupid business decision. The SC-300 was expensive to build and, concluding that there would be a very limited market for high field spectrometers, they decided to withdraw from the high field NMR market to concentrate on manufacture of their more profitable routine spectrometers (deja vu, anyone?). At that point, a number of their senior scientists, including Ray Freeman, left, I believe in protest to the decision. Before long, it was realized that this had been a bad decision and they moved back into the high field business. However, this left them in a catch up position, with Bruker having already established their dominant role in that NMR area.

A somewhat similar problem occurred in the late 1980 to early 1990. After a He-cooled probe had been demonstrated by scientists at Oxford University in 1984, Howard Hill at Varian set out to develop a commercial cold probe. I recall that at that point Varian had a collaboration with a company (Conductus?) that manufactured superconducting materials that could be used in the probe. At least one prototype was developed and tested. However, this research was not pursued vigorously by Varian (probably due to high development costs and a shortage of capital funds). Instead, once again, Bruker took the lead in this field with a much more extensive line of cryoprobes.

Thus, by the time of takeover of the Varian NMR division by Agilent in 2010, while Varian had some excellent products in their low field line, they were struggling to compete with Bruker in the high field area. Nevertheless, it seemed that Agilent had a lot of confidence in their ability to turn the situation around. For example, an Agilent spokesman gave an enthusiastic talk at an Agilent Users' Meeting before the ENC in 2011 where he stated that it was the Agilent goal to become the dominant player in the NMR field. One argument that he gave was that Agilent's expertise in the electronics field would particularly help in building better spectrometers. This surprised me since I felt that they had inherited an excellent direct drive console plus some superb software including BioPack, but that a lot of effort would be required to catch Bruker in the probe and high field solenoid areas. I later made these comments in an email to him, but I was left concerned that Agilent didn't l really understand the magnitude of the task that they had taken on.

These concerns seemed justified when Agilent somewhat later announced that they were 'temporarily' abandoned marketing ultra-high field spectrometers to concentrate on their lower field lines. From announcements made at the time, it was clear that this move had been catalyzed by poor financial performance in the NMR division which was affecting the profitability of Life Sciences Division which included NMR. However, the problem with that approach was that it raised serious doubts among potential buyers of Agilent's long-term commitment to NMR, decreasing the likelihood that they would buy from Agilent, and thus risking further loss of sales. This was compounded by the fact that Agilent was still investing a significant amount of money in developing NMR probes and other improved components. In any case, the failure of that strategy was confirmed by yesterday's bombshell announcement.

So what went wrong with the takeover? First, as I suggested above, I am convinced that Agilent had not fully appreciated the nature of the problems that they were facing and the difficulty of making a rapid turn around. Second, from a purely business viewpoint, it probably would have made more sense to close the NMR division at the time when they announced the pull-back from the ultra-high field NMR area. That would have saved both operational losses and development costs. However, management may have been very reluctant to do that, since it would have indicated to shareholders that the original takeover decision was a bad one. Finally, there is a real possibility that the new probes, consoles, etc., which have either recently been announced or scheduled to be announced soon could have turned the division to better profitability. Certainly, I detected a lot of

optimism from Agilent NMR people at the time of the recent SMASH meeting, optimism that has now been dashed. I believe that, having kept going this long, it would have made more sense to keep the division running for at least a couple of more years to give it a reasonable opportunity to turn things around and save some of Agilent's investment. As it stands, I am sure that there will be fallout for senior Agilent management, since someone will have to accept responsibility for a business deal that went so wrong.

One might wonder how Bruker has apparently avoided similar problems. The answer is that for much of its existence has been a privately owned company with the Laukien family as principal owners. While hardnosed businessmen, they are also scientists who recognize that it may sometimes be logical to forgo short term profits in favour of investments that will pay off handsomely in the future. Unfortunately this is usually not a viable option for a publicly traded company (like Agilent or Varian in its later years) where shareholders carefully check quarterly reports for profitability. Maybe now that Bruker is publicly traded, it will be more constrained as well. Of course, this also a good reason for them to increase prices to improve their bottom line.

So is there anything meaningful that we can do? I suspect probably not a lot. However, the knowledge that they have angered so many people that are also potential buyers of other Agilent equipment will at least encourage them to provide more than just the minimum required service and support, at least in the near future. Second, making the IP available, maybe to a third party vendor, should make sense to them in terms that they paid for it, either with their original purchase or with development costs and thus could recoup some of their losses. Knowledge that many are interested in keeping it available would help.

MOOT XXVII NMR Symposium, Montréal, Québec, October 18-19, 2014

The 27th MOOT NMR Symposium was held at the Université du Québec à Montréal (UQAM) during the week-end of October 18 to 19 at the Complexe des Sciences in the heart of the city center. The event gathered 104 participants from Ontario to the Atlantic Provinces, as well as from the United States and France.

A total of 19 talks and 41 posters were presented, and the two thirds of these presentations were given by students. The judges had a hard time selecting two best oral presentations and three best posters considering the excellent quality of the work and presentations.

Daryl Good (University of Guelph) and **Rohan Alvares** (University of Toronto) were selected as award winners for the best oral presentation, while **Zoe Reeve** (McMaster University), **Patricia Bouchard** (Université de Montréal) and **Miranda Schmidt** (University of Guelph) received the best poster awards.

left to right: Daryl Good, Rohan Alvares, Zoe Reeve, Patricia Bouchard, Miranda Schmidt

This year, two keynote speakers were invited to share their experience on the Canadian path of solid-state NMR. **Dr. John Ripmeester** launched the symposium on Saturday with an insightful talk on the study of gas hydrates by solid-state NMR, while on Sunday **Dr. James Davis** took us all the way from the first use of quadrupolar echoes in the study of membranes to the investigation of membrane proteins today.

Continued…

UQAM was the last location on the list proposed by enthusiastic volunteers at the banquet of MOOT XXII NMR Symposium in 2009 (Carleton University, Ottawa). Therefore discussions have been going on and another list of enthusiastic volunteers has been created!

The 28th MOOT in 2015 will be organized at McMaster University in Hamilton by Alex Bain, Gillian Goward, Giuseppe Melacini and Bob Berno. Then Chris Kirby (Agriculture and Agri-Food Canada) offered to host the MOOT in Prince Edward Island in 2016. The symposium would then be organized in 2017 at the University of Western Ontario (London) by Mathew Willans and Yining Huang, in 2018 at the Université de Sherbrooke by Pierre Lavigne, in 2019 at the University of Ottawa by Dave Bryce and Natalie Goto, and in 2020 at the University of Guelph by Vladimir Ladizhansky. If all the stars are aligned in the NMR field, we shall all meet at the XXXIIIrd MOOT!

Thanks to everyone for their participation, and we look forward to seeing you in Hamilton next year!

Isabelle Marcotte and Alexandre Arnold
27th MOOT NMR symposium
http://www.mootnmr.org

The MOOT XXVII NMR Symposium was made possible by generous contributions from Bruker, Agilent, New Era Enterprises, ACP Chemicals, Cambridge Isotope Laboratories, MestreLab Research, GRASP (Groupe de recherche axé sur la structure des protéines), UQAM's Department of Chemistry, and the two UQAM's research centers, Pharmaqam and NanoQAM.

GRASP Groupe de Recherche Axé sur la Structure des Protéines
7ème COLLOQUE ANNUEL
7th ANNUAL SYMPOSIUM

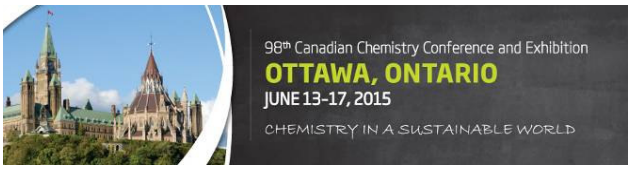
Monday November 24, 2014, 8:00am - 6:30pm, McGill University

Dear Colleagues,

Drs. Kalle Gehring and Albert Berghuis would like to invite you to take part in the seventh scientific symposium of **GRASP.**

Outstanding international speakers - Khan Huy Bui, Werner Kuehlbrandt, Andreas Martin, Helen Saibil, Cynthia Wolberger - poster sessions, exhibitors and short talks will be presented at this auspicious event. Registration is free, thanks to our very generous sponsors.

For more information visit
http://grasp.mcgill.ca/english/symposium/symposium.html



98th Canadian Chemistry Conference and Exhibition (CSC 2015) *"Chemistry in a Sustainable World"* will take place in Ottawa, Ontario from **June 13-17, 2015**. The CSC is the largest annual national event for chemical professionals attracting close to 2500 participants each year.

There will be a one-and-half day symposium on Solid-State NMR as well as a separate symposium on Biomolecular NMR.

Confirmed international speakers for the **Solid-State NMR Symposium** being organized by David Bryce (Ottawa) and Andreas Brinkmann (NRC) include:

Christian Bonhomme (UPMC, France)
Lyndon Emsley (ENS Lyon, France)
Philip Grandinetti (Ohio State University, USA)
Kenneth Harris (Cardiff University, Wales)
Chris Jaroniec (Ohio State University, USA)
Klaus Schmidt-Rohr (Brandeis University, USA)

More details on the symposia, abstract submission and registration will be posted on the conference website at
http://www.csc2015.ca

The abstract submission opens December 15, 2014.

Canada Research Chair in magnetic resonance renewed

In October 2014 the Government of Canada announced an investment of $118 million to fund 137 new or renewed Canada Research Chairs at 34 Canadian universities. This included renewal of one Chair involved in magnetic resonance research.

Lewis Kay (University of Toronto Canada Research Chair Tier 1 in Proteomics, Bioinformatics and Functional Genomics

http://www.chairs-chaires.gc.ca/chairholders-titulaires/profile-eng.aspx?profileId=651

Lewis Kay was also awarded a supplementary infrastructure funding through the Canada Foundation for Innovation (CFI), "NMR Enhancement at Moderate Magnetic Fields" $399,999.

Canada Research Chairs in MR

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

Cheryl Arrowsmith (Toronto) Biochemistry

Bruce Balcom (UNB) Multidisciplinary

Valerie Booth (Memorial) Biochemistry

David Cory *(Waterloo) Quantum Information

Mitsuhiko Ikura (Toronto) Molecular Biology

Lewis Kay (Toronto) Biochemistry

Raymond Laflamme (Waterloo) Physics

Pascale Legault (Montréal) Biochemistry

Younès Messaddeq *(Laval) Photonics

Simon Sharpe (Toronto) Biochemistry

Gary Shaw (Western) Structural Neurobiology

Josef Zwanziger (Dalhousie) Phys Chemistry

* Canada Excellence Research Chairs

Scott Kroeker (Manitoba) is on research leave in Orléans, France until August 2015. Scott is a research fellow at *Le Studium Institute of Advanced Studies*, working in a CNRS Lab "Conditions Extrêmes et Matériaux: Haute Température et Irradiation" (CEMHTI). Scott's research project is focused on high-temperature and high-field NMR studies of nuclear-related glasses.

Theses Defended

Mohammad Mazhab Jafari (University of Toronto) June 2014

Supervisor: Prof. Mitsuhiko Ikura

Ph.D. thesis: "Structure, catalytic mechanism and function of the mTOR activator Rheb in solution and in association with lipid bilayer membranes"

Émile Robert (Université Laval) Fall 2014

Supervisor: Prof. Michèle Auger

M.Sc. thesis: "Étude spectroscopique de la thanatine: Interactions avec des membranes lipidiques modèles"

Alexandrine Huot (Université Laval) Summer 2014

Supervisors: Prof. Michèle Auger & Prof. Michel Pézolet

M.Sc. thesis: "Étude de fibres et de films de soie par spectroscopie de vibration"

Contributed by Darren Brouwer (Redeemer)

NMR Spectroscopy comes to Redeemer

http://cs.redeemer.ca/sciences/?p=83

The Chemistry Department is excited to announce the arrival of an innovative "benchtop" Nuclear Magnetic Resonance (NMR) spectrometer at Redeemer, which will provide new and exciting opportunities for hands-on learning and research for our chemistry, biology, health science, and environmental science students.

NMReady 60 MHz
http://nanalysis.com/

One of the most important tasks in chemistry is determining the molecular structure of chemical compounds. To the naked eye, a chemical compound might just be a clear liquid or a white powder. The ability to deduce the "invisible" molecular-scale structure of matter is of paramount importance in chemistry, biochemistry, and medicine. For example, knowing the molecular structure of a

pharmaceutical compound is vital to understanding its medicinal function.

The most important tool in chemistry for determining molecular structure is a technique called "Nuclear Magnetic Resonance Spectroscopy" (often abbreviated as "NMR spectroscopy").

Up until only a few years ago, obtaining an NMR spectrometer has been prohibitive due to the very high cost, large space demands, and significant maintenance requirements. Through a number remarkable technological innovations, **Nanalysis Corporation** based in Calgary has developed a "benchtop" NMR spectrometer that drastically reduces the cost, space, and maintenance requirements, while maintaining impressive specs for the type of analysis performed in university-level chemistry courses.

The NMR spectrometer will be used extensively in our organic chemistry labs as well as senior research projects. There are also opportunities to disseminate the pedagogical innovations that come out of our labs to other universities through Nanalysis' education program.

The new NMR spectrometer complements the other instrumentation in our well-equipped Chemistry department, including high-performance liquid chromatography (HPLC), gas chromatography (GC), infrared (IR) spectroscopy, UV/visible spectroscopy, and flame and graphite furnace atomic absorption/emission spectrophotometers.

This new acquisition was made possible by a generous targeted donation of a Redeemer supporter and a significant educational discount from the supplier, for which we are deeply grateful.

For further information, please contact

Darren Brouwer

http://www.redeemer.ca/faculty/darren-brouwer.aspx

Contributed by Guy Bernard (Alberta)

New 400 MHz NMR Spectrometer for the Wasylishen Lab at the University of Alberta

After 30 years of faithful service, our Bruker/Oxford 4.7 T wide-bore NMR magnet was decommissioned on July 13, 2014. Installed at Dalhousie University in 1984 with an MSL console, the system was one of the first dedicated solid-state NMR spectrometers with a superconducting magnet in Canada. The MSL console was replaced with a CMX Infinity 200 in 1998. In 2000 both the console and magnet were moved to the University of Alberta.

The magnet was used to acquire thousands of NMR spectra of a significant portion of the NMR-active nuclei with frequencies ranging between those of ^{15}N and ^{205}Tl, in addition to ^{1}H and ^{19}F. It helped train over two dozen graduate students and several post-docs, and was also used by several visiting professors. Data acquired with this magnet have been published in more than 200 journal articles.

The 4.7 T magnet was decommissioned to make room for a **Bruker Avance III HD NMR** system, equipped with a 400 MHz narrow-bore magnet, which was installed in September, 2014. The two-channel system is equipped with a 5 mm double-resonance solenoid probe, with inserts that allow tuning from slightly lower than ^{15}N to above ^{31}P, along with ^{1}H decoupling. Preliminary spectra have been very impressive! A 4 mm double-resonance MAS probe, tuning to a similar frequency range, is expected soon. The NMR system is capable of variable-temperature experiments and, with a suitable probe, solution samples can be examined.

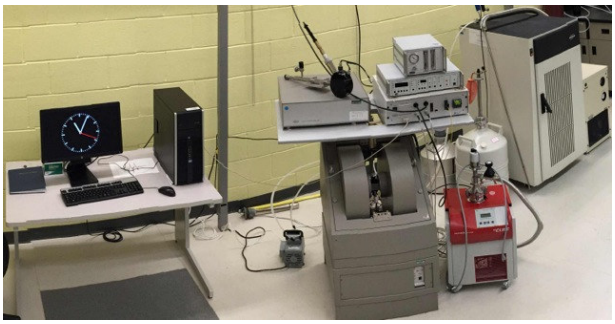
New 400 MHz Bruker NMR system

Funding for the system was kindly provided by **CFI** though a *Leading Edge Grant* to applicants that included **Professors Sylvie Quideau**

(Department of Renewable Resources) and **Rod Wasylishen** (Department of Chemistry). Matching funds were provided by **Alberta Enterprises and Advanced Education** and by **Bruker Biospin**. The system will be used by Sylvie's group to continue their studies of soil organic matter, and by Rod's group in their continuing physical chemistry research.

Contributed by Tim Burrow (Toronto)

Electron Paramagnetic Resonance at the University of Toronto



The Department of Chemistry at the University of Toronto is now equipped with a **Bruker EMX X-band EPR** with an Oxford liquid helium cryostat to acquire spectra from 4 K and higher. There are two VT controllers; the Oxford cryostat and a BVT4131 to give flexibility in cooling or heating. There are two cavities available; **ER4119HS** for routine work and **ER4123D** for biological samples.

If you are interested in using this EPR spectrometer in your research please contact

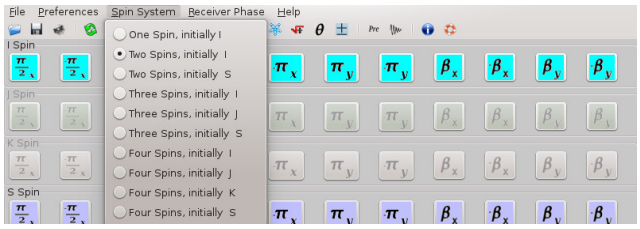
Timothy Burrow, PhD MBA
Facilities Development Manager
e-mail: tim.burrow@utoronto.ca
phone: 416-978-5728
fax: 416-978-8775

Contributed by Keith Brown (Saskatchewan)

WxProdOp Product Operator Calculator

This is to announce a new version of the product operator calculator, **wxProdOp**. Calculations may be done with one, two, three or four spins-1/2. Since complex expressions can result after long strings of operations, the aim of the program is to simplify things as far as possible via trigonometric identities and other methods. The new version of the calculator now includes a 'receiver' section which simulates what the receiver 'sees', both at the beginning of acquisition and at the end.

As with previous versions, there is an extensive manual included with the program.



The program runs under either Windows or Linux and is available at
https://sourceforge.net
http://sourceforge.net/projects/wxprodop/

I hope that you find this useful and would be grateful for any comments and suggestions for improvement.

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

---

from *http://www.theresonance.com*

Bruker announces the launch of a new sharing platform for pulse sequences and programs – **the Resonance Exchange**.

The new platform will enable the exchange and sharing of customer-written sequences and programs, bringing a wealth of expertise and know-how to the Bruker magnetic resonance user communities. The new library will be the prime repository and exchange for your Liquids, Solids, Imaging and EPR sequences, and we have some of the top experts in the field preparing to offer their support to our new platform.

You can begin to support the library with your own submissions right now. To learn more, visit the library at http://bruker.com/ppq

Resonance Exchange Bulletin will provide a regular update from Bruker's library platform and will feature key applications and highlight a selection of new programs and downloads. The first issue of the Bulletin (in pdf) is now online. http://tinyurl.com/lteyngz

http://www.theresonance.com/2014/categories/academics/the-resonance-exchange-bulletin-program-library-update-in-one

---

Special issue of *the Canadian Journal of Chemistry* in honour of Dr. John Ripmeester

The *Canadian Journal of Chemistry* is pleased to announce a call for papers for a special issue in honour of **Dr. John Ripmeester** (NRC) and his outstanding contributions to chemistry.

The deadline for submissions is **December 1, 2014**. The special issue will be published in 2015.

The *Canadian Journal of Chemistry* reports current research findings in all branches of chemistry. It includes the traditional areas of analytical, inorganic, organic, and physical-theoretical chemistry and newer interdisciplinary areas such as materials science, spectroscopy, chemical physics, and biological, medicinal and environmental chemistry.

Please submit your paper at
http://www.nrcresearchpress.com/journal/cjc

The issue will be edited by Yining Huang, Darren Brouwer, and David Bryce.

Prof. David L. Bryce
Department of Chemistry
University of Ottawa

E-mail: dbryce@uottawa.ca
http://mysite.science.uottawa.ca/dbryce/

Special issue of *Acta Crystallographica C:* NMR Crystallography

http://www.iucr.org/resources/commissions/nmr-crystallography

The journal *Acta Crystallographica Section C* is planning a number of special issues with the aim of expanding the scope and authorship of the journal, including one on NMR crystallography.

Guest editors:

Roderick Wasylishen (University of Alberta, Canada) and **Francis Taulelle** (Université de Versailles Saint Quentin en Yvelines, France)

Authors should submit their paper at
http://journals.iucr.org/c/services/specialissues.html

Papers are expected to be submitted by **January 31, 2015.**
http://journals.iucr.org/c/services/nmr_nfa_2015.pdf

Special issue of *Magnetic Resonance in Chemistry* in honour of Prof. William F. Reynolds

Colleagues,

Magnetic Resonance in Chemistry (Wiley) has announced a Special Issue in honour of **Professor William F. Reynolds** (University of Toronto), who has served the Journal as a senior editor for many years. This issue will be co-edited by Alex D. Bain (McMaster) and Raul G. Enriquez (Universidad Nacional Autónoma de México).

Bill has been doing NMR for 50 years and is an international expert in liquid-state NMR pulse sequences and structure elucidation of natural products. Papers from any branch of NMR and natural products chemistry will be welcomed by the editors.

The deadline for submission is **May 1, 2015**. For further information, please contact Alex Bain bain@mcmaster.ca

Author Guidelines for submission can be found at
http://onlinelibrary.wiley.com/doi/10.1002/mrc.v52.9/issuetoc
http://tinyurl.com/orzkfoa

Alex D. Bain
Professor of Chemistry
McMaster University
1280 Main St. W.
Hamilton, ON, CANADA L8S 4M1
E-mail: bain@mcmaster.ca
phone: (905) 525 9140 ext 24524
fax: (905) 522 2509
http://www.chemistry.mcmaster.ca/bain/index.html

Press release
http://www.acdlabs.com/company/media/pr/140924_20years.php

ACD/Labs Celebrates 20 Year Anniversary - From Modest Beginnings to a Global Cheminformatics Operation

Toronto, Canada (September 24, 2014)

ACD/Labs, a leading cheminformatics company, is celebrating their 20th anniversary this month. Two decades of experience have transformed ACD/Labs from a startup chemistry software provider into a successful company that develops and commercializes solutions and services relied upon by R&D researchers worldwide.

In 1994 when chemistry laboratories predominantly used computers as typewriters, a group of young chemists recognized the potential for computer assisted chemistry solutions. Focusing on tools to increase the productivity of a scientist's daily work - chemical structure drawing, NMR predictors and databases, and hydrophobicity predictors resulting in log*D* and pK_a software - they laid the foundation of the company. ACD/Labs' offerings have diversified and grown since, from a handful of desktop products to cheminformatics platforms that can be deployed enterprise-wide.

While the company has grown to a global corporation, it remains under the same private ownership, committed to supporting chemical R&D. ACD/Labs' dedication to chemistry is apparent through academic freeware offerings; affiliations and collaborations with numerous organizations and initiatives (IUPAC, InChI Trust, Open PHACTS, Pistoia Alliance, and the Allotrope Foundation); strategic partnerships; and participation in research projects such as PharmaSea. The long-lasting scientific culture of the company is evident through innovations that include Automated Structure Verification by NMR and the most peer-reviewed Computer Assisted Structure Elucidation software on the market.

"I recall receiving version 2.0 of ACD/Labs software while working in the pharmaceutical industry", says **Duncan Farrant**. "One reason I continue to upgrade more than 17 years on is that I have found that ACD/Labs software handles the structure-spectrum relationship seamlessly. I find that structures are presented efficiently and with an intuitive relationship to spectral data. The capability to create, access, and search well-organized databases of spectral data was one of the reasons I worked to introduce the software when I moved from pharma to polymer research."

"We deployed ACD/Labs to our global chemistry community for analytical problem-solving over 15 years ago because it provided analysts and chemists the ability to process spectral data regardless of the instrument vendor", says **Randy Rutkowske** (Manager of Analytical Chemistry at a major US pharmaceutical company). "The software greatly improves how I do my job and saves me a minimum of 50% of my time so I can concentrate on processing samples, science, and management responsibilities."

"At ACD/Labs, we are thankful to our customers for making this milestone anniversary possible," said **Daria Thorp** (President, ACD/Labs). "Organizations today are asking for solutions to help researchers create knowledge-rich scientific assets and intelligently reuse globally distributed knowledge. 'Silent automation' of scientific processes is also in high demand to improve productivity and give scientists more time to be inventive and insightful. We are aiming present and future developments on helping our customers solve these challenges."

Advanced Chemistry Development, Inc. (ACD/Labs) - Our cheminformatics solutions are used in industries that work with small molecules including pharma/biotech, chemicals, consumer goods, agrochemicals, petrochemicals, academic institutions, and government organizations.

For more information, please visit
http://www.acdlabs.com

Follow us on Twitter
http://twitter.com/ACDLabs

http://www.iucr.org/resources/commissions/nmr-crystallography

The International Union of Crystallography: Commission on NMR Crystallography and Related Methods

The Commission on NMR Crystallography and Related Methods was established at the Montreal General Assembly in August 2014.

Terms of Reference

The Commission on NMR Crystallography and Related Methods was established at the Montreal General Assembly in August 2014. The Commission will serve several useful roles for the community that studies the crystalline state using magnetic resonance, as well as for the larger crystallographic community. The terms of reference are as follows:

Establish, implement and maintain standards

The NMR community already operates under some guidelines put forward by IUPAC. These mostly concern chemical shift referencing – a not unimportant issue for the proper collection, analysis and reporting of spectral data. The proposed Commission will first identify areas in need of common spectral standards, and then serve as a clearinghouse for these issues. Members will be chosen who have familiarity with the technical complexities that arise in this area. The Commission may work toward the development of a common format for sharing magnetic resonance crystal information – modeled on the Crystallographic Information File format – that would keep track of raw NMR data and extracted information. At present, there is no such common standard in the NMR community, though some national crystallographic societies are already active in proposing such extensions. Additionally, integration of NMR data into structure search formats is already under development or may be soon, in packages such as *FOX* and *Jana2006*. Such integration could also be linked to topological crystallography software packages, such as *TOPOS*.

The Commission may undertake the compilation of basic NMR crystallographic knowledge into usable *International Tables* for NMR crystallography. Such a compendium may contain a list of irreducible crystallographic symmetries – akin to listings used in infrared, Raman and UV spectroscopy – as well as symmetries related to NMR pulse sequences used for selective extraction of spin interactions. Another specific contribution would be a section for correspondences between the quantum description of NMR observables and the associated structural parameters. Most of these notions, familiar to spectroscopists manipulating phase coherence, are not commonplace for methods without such phase coherence. The Commission may also endeavour to simplify and systematize the taxonomy (and terminology) to bridge NMR and diffraction based fields. Additionally, cross-Commission efforts should be made to integrate recent developments in other areas. One such example is the incorporation of topological crystallography, which is under the purview of the Commission on Mathematical and Theoretical Crystallography, into NMR crystallography.

Assist journals and editors

As the number of manuscripts submitted to peer-reviewed journals that employ magnetic resonance in the study of the crystalline state rises, editors and referees unfamiliar with NMR may need some guidelines for how to assess the quality of data reported, as well as the level of experimental detail that is commonplace in NMR forums. The proposed Commission could put forward a set of recommendations for journals in the larger crystallographic community. As such, there should be some representation within the Commission from the community of current or former journal editors. This could also provide a fruitful intersection with the existing Commission on Journals. Several leading journals have had recent themed issues on NMR crystallography. The Commission may promote the use of IUCr journals as a stable forum for NMR crystallographic articles, which are currently scattered in many different broad-audience journals.

Help organize conferences and workshops

Conferences in NMR crystallography have already been organized in recent times. The SMARTER series of conferences is the most obvious example with an approximate audience of about 100 participants. This conference has been supported since its birth in 2005 by the IUCr Commission on Inorganic and Mineral Structures. Other conferences, such as the Gordon Research Conference (GRC) on

Computational Aspects – Biomolecular NMR and the Experimental NMR Conference (ENC), have held themed sessions on NMR crystallography. Judging by the recent publication and conference activity, it is clear that the magnetic resonance and crystallographic communities are cross-fertilizing. For graduate students in one area, accessibility to working knowledge in the other field will be critical in their training. There is great potential for targeted workshops to help such students. For example, a hands-on workshop for a graduate student in crystal engineering in solid-state NMR would be of great value. A series of regional workshops, which would reduce travel costs and showcase local NMR capabilities, might cover theory basics and simple data collection. A short course – in the spirit of the Gordon Research Seminars – that precedes a major meeting could also be of useful service to the NMR crystallographic community. Such a mechanism would provide an efficient way to leverage against existing travel plans, and it could serve as an international networking opportunity for young researchers.

Serve as a liaison to commercial vendors

Both diffraction and NMR rely on expensive equipment, which is sold by a handful of vendors that market diffraction and magnetic resonance instruments. The IUCr likely does not want to get involved in the commercial side of crystallography, yet the truth is that researchers in both NMR and diffraction have a symbiotic relationship with the vendors that manufacture and sell the instruments. Researchers rely on healthy Research & Development that stems from friendly competition between the vendors to spur innovation, which, in turn, leads to the next generation of capabilities. The Commission could serve in some capacity as the representative for the research community, giving feedback and gentle encouragement to the vendors as warranted. A working relationship between the Commission and leading vendors can also be tapped to support conferences, workshops and student travel, as the need arises. In NMR, the main vendors are Bruker, Agilent and Jeol, with many small companies providing consoles, magnets, probes, software packages and services. The three main companies in NMR also have a significant presence in the diffraction community.

Other activities

The Commission will tailor its efforts in conjunction with regional and international bodies, such as the International Society for MAgnetic Resonance (ISMAR) or the American Crystallographic Association (ACA), to advance its agenda.

Commission members

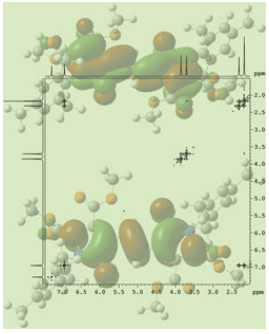
Members of Commissions are elected by the General Assembly for a term of three years, renewable for a maximum of nine years in total (or 12 years if serving the final term as Chair). Subject to the approval of the President, consultants may be appointed at any time to strengthen a Commission. (The immediate past Chair is automatically appointed as a consultant.)

Membership

F. Taulelle (Chair, France)
R.K. Harris (UK)
M.A. Mehta (USA)
T. Polenova (USA)
M.J. Potrzebowski (Poland)
R.E. Wasylishen (Canada)

Special issue of *Acta Crystallographica C*

http://www.iucr.org/resources/commissions/nmr-crystallography



The journal *Acta Crystallographica Section C* is planning a number of special issues with the aim of expanding the scope and authorship of the journal, including one on NMR crystallography.

NMR Crystallography

Guest editors:

Roderick Wasylishen (University of Alberta, Canada) and

Francis Taulelle (Université de Versailles Saint Quentin en Yvelines, France)

Authors should submit their paper via the web at
http://journals.iucr.org/c/services/specialissues.html

Papers are expected to be submitted by **31 January 2015.**
http://journals.iucr.org/c/services/nmr_nfa_2015.pdf

Press release
http://www.agilent.com/about/newsroom/presrel/2014/14oct-gp14028.html

Agilent Technologies to Close Nuclear Magnetic Resonance Business

SANTA CLARA, Calif., Oct. 14, 2014

Agilent Technologies Inc. (NYSE: A) today announced it is exiting its Nuclear Magnetic Resonance business. Agilent entered the NMR business in 2010, with the acquisition of Varian. Since then, the business has not met growth and profitability objectives.

"Today's announcement represents a difficult decision necessary to drive improved profitability," said Mike McMullen, president and chief operating officer, and CEO-elect. "The NMR team has been extremely dedicated and has made many excellent contributions. However, this action is a step in ensuring that our investments are placed on higher-value life sciences, applied markets and diagnostics solutions that will continue to drive growth across the company."

Agilent will stop taking new NMR system orders immediately, but the company will continue to meet customer commitments for orders in progress and for ongoing support contracts. Agilent will continue to provide service on all installed NMR systems.

The company expects that this decision will eliminate about 300 jobs, mostly within the next 12 months. The majority of the affected positions are located in Yarnton, U.K., and Santa Clara, California.

Today's announcement is part of Agilent's strategy to address the business shortfalls of its Research Products Division. In early 2013 Agilent announced its exit of the OEM and Specialty Magnet business and later the MRI business to focus resources on the core NMR portfolio. Despite these adjustments, the NMR business has continued to fall short of growth and profitability objectives.

To cover the cost of exiting this business, Agilent will take an approximate $72 million restructuring charge in the fourth quarter. It expects a $20 million to $30 million decline in revenues in fiscal year 2015 due to the NMR business closure, but a positive impact of about $10 million in operating profit in FY15.

For the fourth quarter of 2014, Agilent anticipates non-GAAP earnings per share of $0.87 to $0.91, and projects revenues to be negatively affected by currency at about $13 million, and lower NMR-related revenues by about $12 million.

Keysight has posted its investor roadshow slide deck on its website at http://www.investor.keysight.com "New Agilent" will post its investor roadshow slide deck on Friday, Oct. 17, after the market closes at http://www.investor.agilent.com

About NMR

Nuclear magnetic resonance (NMR) spectroscopy is an analytical chemistry technique used in quality control and research for determining the content and purity of a sample as well as its molecular structure. It is used primarily in academia and government, the pharmaceutical, biotech and chemical industries.

About Agilent Technologies

Agilent Technologies Inc. (NYSE: A) is the world's premier measurement company and a technology leader in chemical analysis, life sciences, diagnostics, electronics and communications. The company's 20,600 employees serve customers in more than 100 countries. Agilent had revenues of $6.8 billion in fiscal 2013. Information about Agilent is available at http://www.agilent.com

On Sept. 19, 2013, Agilent announced plans to separate into two publicly traded companies through a tax-free spinoff of its electronic measurement business. The new company is named Keysight Technologies, Inc. The separation is expected to be completed in early November 2014.

Forward-Looking Statements

This news release contains forward-looking statements as defined in the Securities Exchange Act of 1934 and is subject to the safe harbors created therein. The forward-looking statements contained herein include, but are not limited to, information regarding the separation of Agilent's electronic measurement business; future revenues, earnings and profitability; the future demand for the company's products and services; and customer expectations. These forward-looking statements involve risks and uncertainties that could cause Agilent's results to differ materially from management's current expectations. Such risks and uncertainties include, but are not limited to, unforeseen changes in the strength of our customers' businesses; unforeseen changes in the demand for current and new products, technologies, and services; customer

purchasing decisions and timing, and the risk that we are not able to realize the savings expected from integration and restructuring activities.

In addition, other risks that Agilent faces include those detailed in Agilent's filings with the Securities and Exchange Commission, including our latest Form 10-K and Form 10-Q. Forward-looking statements are based on the beliefs and assumptions of Agilent's management and on currently available information. Agilent undertakes no responsibility to publicly update or revise any forward-looking statement.

# # #

Contact:
Michele Drake
+1 408 345 8396
michele_drake@agilent.com
Neil Rees (U.K.)
+44 186 529 1472
neil_rees@agilent.com

Investor Contact:
Alicia Rodriguez
+1 408 345 8948
alicia_rodriguez@agilent.com

---

http://www.chem.agilent.com/en-US/Products-Services/Instruments-Systems/Nuclear-Magnetic-Resonance/Pages/default.aspx

Nuclear Magnetic Resonance

October 14, 2014

Dear Agilent Customer,

As you are a valued customer, we want to let you know that in response to certain market conditions, Agilent has made the strategic decision to close its NMR (Nuclear Magnetic Resonance) business.

Effective immediately, Agilent will no longer be accepting orders for NMR systems. We will honor our existing contractual commitments to deliver open orders and fulfill support obligations. **Agilent will continue to provide support for 7 years after product obsolescence, information about our ongoing support offerings can be found here.**

We value your partnership with Agilent and we will do our best to minimize any inconvenience or disruption to your business. For further information please contact us at pdl-nmr@agilent.com

Thank you for your ongoing commitment to Agilent.

Sincerely,

Regina Schuck

VP and GM, Research Products Division, Agilent Technologies

---

http://www.chem.agilent.com/en-US/Technical-Support/Instruments-Systems/Nuclear-Magnetic-Resonance/Pages/nmr-support.aspx

NMR Support Offerings

Dear Valued Agilent Customer,

On October 14, 2014, Agilent Technologies announced that it is closing its NMR (Nuclear Magnetic Resonance) business.

This letter contains useful information about Agilent's continued support commitment for your NMR system(s). Agilent's products are well known for their quality, performance and reliability, and we are committed to ensuring that you have many years of useful service from your instrument.

All existing warranty and standard service obligations for NMR systems will be fully honored and we will continue to renew and offer service contracts just as we do today.

Agilent will continue to provide its Agilent Advantage and other support options for its NMR consoles for seven (7) years after product obsolescence. Therefore, DD2 consoles as well as 400-MR DD2 and ProPulse consoles will reach end of Advantage support on October 14, 2021. DD1 (VNMRS) consoles will reach end of Advantage support on November 1, 2017.

Once NMR systems reach the end of their Advantage support dates Agilent typically provides our Asset Maximization service offering for three (3) years. Asset Maximization provides the same level of service except that parts availability is provided on commercially reasonable effort basis. As end of Agilent Advantage support dates approach, Agilent will review parts availability and Asset Maximization support duration.

Standard production NMR accessories including probes and automation have support for seven (7) years after the end of production. Support for customized products is provided for five (5) years from the date of original customer acceptance. Magnets have a support period of seven (7) years from original customer acceptance of the magnet.

The last commercial Agilent NMR software release is VnmrJ4.2. There will be no further enhancements to this product. Major defects impacting current capabilities in VnmrJ4 will be addressed within reasonable commercial effort through October 2015.

Should you have any questions, please contact your local Agilent Services team. Thank you for your ongoing commitment to Agilent.

Sincerely,

Mark Doak
President, Agilent CrossLab

NMR Events

7th Annual GRASP Symposium

November 24, 2014, McGill University, Montréal, QC, Canada
http://grasp.mcgill.ca/english/symposium/symposium.html

Biophysical Society 59th Annual Meeting

February 7-11, 2015, Baltimore, Maryland
http://www.biophysics.org/2015meeting

Biophysical Society of Canada - Travel Awards and Mixer

PANIC 2015 Practical Applications of NMR in Industry Conference

February 11-13, 2015, La Jolla, CA
http://www.panicnmr.com/

56th ENC

April 19-24, 2015, Asilomar, CA
http://www.enc-conference.org/

26th ISMRM Annual Meeting International Society for Magnetic Resonance in Medicine

May 30 – June 5, 2015, Toronto, ON
http://ismrm.org/15/

Computational Aspects - Biomolecular NMR Gordon Research Seminar & Conference

June 6-12, 2015, Lucca (Barga), Italy
http://www.grc.org/programs.aspx?id=15573
http://www.grc.org/programs.aspx?id=14571

CSC 2015 the 98th Canadian Chemistry Conference and Exhibition

June 13-17, 2015, Ottawa, ON, Canada
http://www.csc2015.ca/

AMPERE NMR School

June 14-20, 2015, Zakopane, Poland
http://www.staff.amu.edu.pl/~school/index.html

EUROMAR 2015

July 5-10, 2015, Prague, Czech Republic
http://www.euromar2015.org/

57th Rocky Mountain Conference on Magnetic Resonance: EPR Symposium

July 26-30, 2015, Snowbird, Utah
http://www.rockychem.com/

ISMAR 2015 19th International Society of Magnetic Resonance Conference

August 16-21, 2015, Shanghai, China
http://ismar2015.ecnu.edu.cn/

9th Alpine Conference on Solid-State NMR

September 13-17, 2015, Chamonix Mont-Blanc, France
http://www.alpine-conference.org

SMASH 2015 Small Molecule NMR Conference

September 20-23, 2015, Baveno, Italy
http://www.smashnmr.org/

MOOT XXVIII NMR Symposium

Fall 2015, McMaster University, Hamilton
http://www.mootnmr.org/

Pacifichem 2015 The International Chemical Congress of Pacific Basin Societies

December 15-20, 2015, Honolulu, Hawaii, USA
http://www.pacifichem.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.pacifichem.org/symposiadesc2015/

ICMRBS 2016 XXVIIth International Conference on Magnetic Resonance in Biological Systems

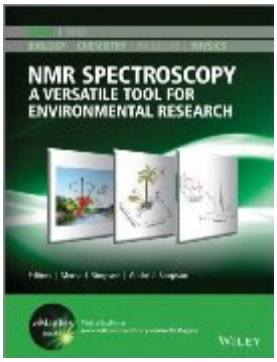
August 21-26, 2016, Kyoto, Japan
http://www.icmrbs2016.org/

ISMAR 2017 20th International Society of Magnetic Resonance Conference

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

New NMR Books

NMR Spectroscopy: A Versatile Tool for Environmental Research



Myrna J. Simpson **(Editor)**
Andre J. Simpson **(Editor)**
Hardcover: 448 pages
Publisher: Wiley; July 2014
Language: English
ISBN: 978-1118616475

http://ca.wiley.com/WileyCDA/WileyTitle/productCd-1118616472.html
http://www.amazon.com/dp/1118616472
http://www.amazon.ca/dp/1118616472

Wiley: The challenges faced by environmental scientists today are vast, complex, and multi-faceted. For instance, predicting the fate of an environmental pollutant or understanding ecosystem responses to climate change, necessitate a firm understanding of molecular structure and dynamics of environmental media as well as the components that exist and interact within this media. Furthermore, linking information obtained at the molecular-scale to ecosystem-level processes is a major pursuit of modern environmental research. As such, NMR spectroscopy and its scalability from the molecular-scale to the macroscopic-scale, is facilitating rapid growth in environmental science. In addition, the versatility of NMR spectroscopy has resulted in the development and implementation of different types of NMR techniques to examine the structure of various types of environmental samples, living and non-living, as well as the study of critical environmental processes. This comprehensive handbook is a collection of chapters that span from methods to how NMR is used in environmental research to gain insight into various ecosystem properties. It is organized into three parts:

Part A focuses on methods used in environmental NMR which span from solution-state to magnetic resonance imaging.

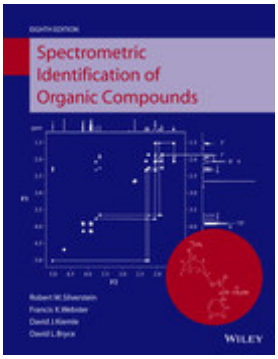
Part B emphasizes how NMR spectroscopy plays an essential role in understanding various types of environmental components and related processes, including different forms of organic matter found in soil, water, and air as well as how NMR is used to probe the fate of water, organic pollutants, and metals in the environment.

Part C focuses on the growing field of environmental metabolomics which uses NMR as its main discovery platform.

This volume highlights the immense potential of NMR spectroscopy to expand our fundamental understanding of environmental processes and how it will continue to do so well into the future.

Table of contents
http://ca.wiley.com/WileyCDA/WileyTitle/productCd-1118616472.html

Spectrometric Identification of Organic Compounds, 8th Edition



Robert M. Silverstein, Francis X. Webster, David Kiemle, David L. Bryce

Paperback: 462 pages
Publisher: Wiley; September 2014
Language: English
ISBN: 978-0470616376

http://ca.wiley.com/WileyCDA/WileyTitle/productCd-EHEP001779.html
http://www.amazon.com/dp/0470616377
http://www.amazon.ca/dp/0470616377

Wiley: First published over 40 years ago, this was the first text on the identification of organic compounds using spectroscopy. This text is now considered to be a classic. The key strength of this text is the extensive set of real-data problems. Even professional chemists use these spectra as reference data. Spectrometric Identification of Organic Compounds is written by and for organic chemists, and emphasizes the synergistic effect resulting from the interplay of the spectra. This book is characterized by its problem-solving approach with extensive reference charts and tables.

The 8th edition of this text maintains its student-friendly writing style – wording throughout has been updated for consistency and to be more reflective of modern usage and methods. Chapter 3 on proton NMR spectroscopy has been overhauled and updated. Also, new information on polymers and phosphorus functional groups has been added to Chapter 2 on IR spectroscopy.

Canadian NMR Research Highlights

NMR of Liquid Crystals

Magnetic Resonance in Chemistry
special issue
October 2014, Volume 52, Issue 10 Pages 531–663

http://onlinelibrary.wiley.com/doi/10.1002/mrc.v52.10/issuetoc

guest-edited by

Ronald Y. Dong (UBC)

Ronald Y. Dong, "MRC special issue on NMR of liquid crystals," **(Editorial)** *Magnetic Resonance in Chemistry* **52** (2014) 531. http://dx.doi.org/10.1002/mrc.4109

Canadian contributions

A.P. Manning, M. Giese, A.S. Terpstra, M.J. MacLachlan, W.Y. Hamad, R.Y. Dong and C.A. Michal, "NMR of guest-host systems: 8CB in chiral nematic porous glasses" *Magnetic Resonance in Chemistry* **52** (2014) 532–539. http://dx.doi.org/10.1002/mrc.4101

A. Ferraz, J. Zhang, P.J. Sebastião, A.C. Ribeiro and R.Y. Dong, "Proton and deuterium nuclear spin relaxation study of the SmA and SmC* phases of BP8Cl-d_{17}: a self-consistent analysis" *Magnetic Resonance in Chemistry* **52** (2014) 546–555. http://dx.doi.org/10.1002/mrc.4107

A.C.J. Weber, D.H.J. Chen, "Conformational problem of alkanes in liquid crystals by NMR spectroscopy" *Magnetic Resonance in Chemistry* **52** (2014) 560–569. **(Review)** http://dx.doi.org/10.1002/mrc.4124

E.E. Burnell, R.Y. Dong, A.C.J. Weber and A. Yethiraj, "NMR of solutes in nematic and smectic A liquid crystals: the anisotropic intermolecular potential," *Magnetic Resonance in Chemistry* **52** (2014) 570–580. **(Review)** http://dx.doi.org/10.1002/mrc.4113

J.L. Figueirinhas, R.Y. Dong, "NMR of bent-core nematogens: a mini-review," *Magnetic Resonance in Chemistry* **52** (2014) 614–624. **(Review)** http://dx.doi.org/10.1002/mrc.4097

Cover article in *the Journal of Physical Chemistry C*

Peng He, Bryan Lucier, Victor Terskikh, Qi Shi, Jinxiang Dong, Yueying Chu, Anmin Zheng, Andre Sutrisno, Yining Huang, "Spies Within Metal Organic Frameworks: Investigating Metal Centers Using Solid-State NMR," *Journal of Physical Chemistry C* **118** (2014) 23728–23744. **(Cover Article)** http://dx.doi.org/10.1021/jp5063868

Solid-state NMR: yielding rich information on local environments of metals within metal-organic frameworks. Solid-state NMR spectroscopy (SSNMR) targeting NMR-active metal centers at natural abundance, in concert with *ab initio* density functional theory calculations and X-ray diffraction, is a powerful tool for elucidating the molecular-level structure of metal-organic frameworks (MOFs). ^{91}Zr, ^{115}In, ^{139}La, $^{47/49}$Ti, and ^{67}Zn SSNMR experiments are sensitive to subtle differences in coordination, bond length distribution, and ligand geometry about the metal center within MOFs. SSNMR spectroscopy of metal centers offers an impressive addition to the arsenal of the techniques for MOF characterization. On the cover, the structure of the MOF MIL-140A is shown at three different magnifications, representing the detailed structural information available from SSNMR experiments. The corresponding ^{91}Zr SSNMR spectrum of MIL-140A acquired at a magnetic field of 21.1 T is shown in the bottom right. The background is a perspective view down one of the channels within the MIL-140A crystal structure.

This cover article features results obtained using the 21.1 T solid-state NMR spectrometer at the National Ultrahigh-Field NMR Facility for Solids.

NMR paper in *Nature Chemical Biology*

L. Freiburger, T. Miletti, S. Zhu, O. Baettig, A. Berghuis, K. Auclair & A. Mittermaier, "Substrate-dependent switching of the allosteric binding mechanism of a dimeric enzyme," *Nature Chemical Biology* **10** (2014) 937-942. http://dx.doi.org/10.1038/nchembio.1626

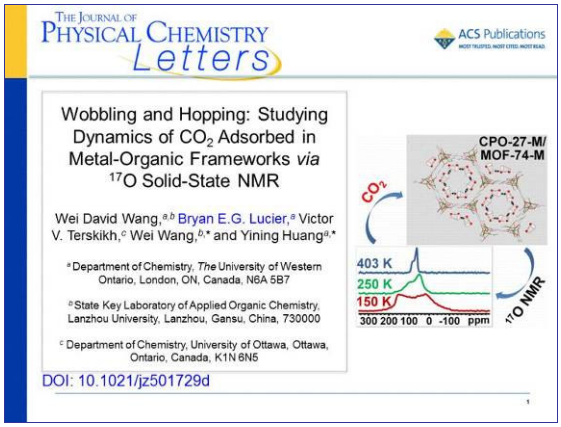
NMR paper in *Nature Communications*

D. Meiri, C.B. Marshall, D. Mokady, J. LaRose, M. Mullin, A.-C. Gingras, M. Ikura and R. Rottapel, "Mechanistic insight into GPCR-mediated activation of the microtubule-associated RhoA exchange factor GEF-H1," *Nature Communications* **5** (2014) 4857. http://dx.doi.org/10.1038/ncomms5857

ACS LiveSlides

http://pubs.acs.org/page/jpclcd/ACSLiveSlides.html

ACS: Welcome to ACS LiveSlides™ for the *Journal of Physical Chemistry Letters*. These slide presentations are created by the authors about their published research in *JPC Letters*, and include the author's own voice describing the research as the slides automatically advance. You can view each ACS LiveSlides™ presentation and then link directly to the full text of the respective article.



http://tinyurl.com/mfzc54e

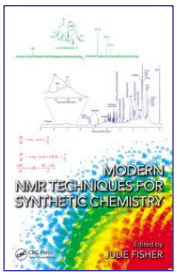
http://pubs.acs.org/iapps/liveslides/pages/index.htm?mscNo=jz501729d

W.D. Wang, B.E.G. Lucier, V.V. Terskikh, W. Wang, and Y. Huang, "Wobbling and Hopping: Studying Dynamics of CO_2 Adsorbed in Metal–Organic Frameworks via ^{17}O Solid-State NMR," *Journal of Physical Chemistry Letters* **5** (2014) 3360–3365. http://dx.doi.org/10.1021/jz501729d

NMR paper in *Angewandte Chemie*

Y. Gao, A. Toubaei, X. Kong and G. Wu, "Acidity and Hydrogen Exchange Dynamics of Iron(II)-Bound Nitroxyl in Aqueous Solution," *Angewandte Chemie International Edition* **53** (2014) 11547–11551. http://dx.doi.org/10.1002/anie.201407018

Modern NMR Techniques for Synthetic Chemistry



CRC Series: New Directions in Organic & Biological Chemistry
Published: October 13, 2014, CRC Press
Content: 363 Pages | 153 B/W Illustrations
Editor: Julie Fisher
Cat/ISBN: K20552 / 9781466592247

http://www.crcpress.com/product/isbn/9781466592247
http://www.crcnetbase.com/isbn/9781466592254

Alex Bain, "Dynamic NMR," **Chapter 2**, pages 15-62, in *"Modern NMR Techniques for Synthetic Chemistry" CRC Series: New Directions in Organic & Biological Chemistry* Published: October 13, 2014 by CRC Press, Editor: Julie Fisher, ISBN: 9781466592247. http://dx.doi.org/10.1201/b17535-3

NMR paper in *PNAS*

P.M. Hwang, F. Cai, S.E. Pineda-Sanabria, D.C. Corson, B.D. Sykes, "The cardiac-specific n-terminal region of troponin I positions the regulatory domain of troponin C," *Proc. Natl. Acad. Sci. USA* **111** (2014) 14412-14417. http://dx.doi.org/10.1073/pnas.1410775111

Press release: "University of Alberta researchers explain 38-year-old mystery of the heart" http://www.eurekalert.org/pub_releases/2014-09/uoaf-uoa092914.php

Biochimica et Biophysica Acta (BBA) - Biomembranes
special issue: Interfacially active peptides and proteins
http://www.sciencedirect.com/science/journal/00052736/1838/9

G. Wang, B. Mishra, R.F. Epand, R.M. Epand, "High-quality 3D structures shine light on antibacterial, anti-biofilm and antiviral activities of human cathelicidin LL-37 and its fragments," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1838** (2014) 2160–2172. **(Review)** http://dx.doi.org/10.1016/j.bbamem.2014.01.016

M. Fillion, M. Noël, A. Lorin, N. Voyer, M. Auger, "Investigation of the mechanism of action of novel amphipathic peptides: Insights from solid-state NMR studies of oriented lipid bilayers," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1838** (2014) 2173–2179. http://dx.doi.org/10.1016/j.bbamem.2014.01.029

Recent NMR Publications

most recent NMR publications by Canadian research groups as they appear on http://nmr900.ca website. This list should not be considered complete. You are encouraged to let us know of your recent publications as they become available.

Memorial University of Newfoundland

E.E. Burnell, R.Y. Dong, A.C.J. Weber and A. Yethiraj, "NMR of solutes in nematic and smectic A liquid crystals: the anisotropic intermolecular potential," *Magnetic Resonance in Chemistry* **52** (2014) 570–580. **(Review)** http://dx.doi.org/10.1002/mrc.4113

Dalhousie University

A. Pandey, M. Sarker, X.-Q. Liu, J.K. Rainey, "Small expression tags enhance bacterial expression of the first three transmembrane segments of the apelin receptor," *Biochemistry and Cell Biology* **92** (2014) 269-278. http://dx.doi.org/10.1139/bcb-2014-0009

University of New Brunswick

S. Vashaee, F. Goora, M.M. Britton, B. Newling, B.J. Balcom, "Mapping B1-induced eddy current effects near metallic structures in MR images: A comparison of simulation and experiment," *Journal of Magnetic Resonance* (2014) online. http://dx.doi.org/10.1016/j.jmr.2014.10.016

A. Arbabi, J. Hall, P. Richard, S. Wilkins, I.V. Mastikhin, "MR relaxometry of micro-bubbles in the vertical bubbly flow at a low magnetic field (0.2 T)," *Journal of Magnetic Resonance* **249** (2014) 16–23. http://dx.doi.org/10.1016/j.jmr.2014.10.001

I. Mastikhin, M. Barnhill, "Sensitization of a stray-field NMR to vibrations: A potential for MR elastometry with a portable NMR sensor," *Journal of Magnetic Resonance* **248** (2014) 1-7. http://dx.doi.org/10.1016/j.jmr.2014.09.003

Université Laval

S.M.C. Gobeil, C.M. Clouthier, J. Park, D. Gagné, A.M. Berghuis, N. Doucet, J.N. Pelletier, "Maintenance of Native-like Protein Dynamics May Not Be Required for Engineering Functional Proteins," *Chemistry & Biology* **21** (2014) 1330–1340. http://dx.doi.org/10.1016/j.chembiol.2014.07.016

M. Gauthier, J. Leclerc, T. Lefèvre, S.M. Gagné, and M. Auger, "Effect of pH on the structure of the recombinant Cterminal domain of *Nephila clavipes* dragline silk protein," *Biomacromolecules* (2014) online. http://dx.doi.org/10.1021/bm501241n

L. Bédard, T. Lefèvre, É. Morin-Michaud, and M. Auger, "Besides fibrillization: putative role of the peptide fragment 71-82 on the structural and assembly behavior of alfa-synuclein," *Biochemistry* **53** (2014) 6463-6472. http://dx.doi.org/10.1021/bi5008707

Université de Sherbrooke

J. He, L. Tremblay, S. Lacelle, Y. Zhao, "How can photoisomerization of azobenzene induce a large cloud point temperature shift of PNIPAM?," *Polymer Chemistry* **5** (2014) 5403-5411. http://dx.doi.org/10.1039/c4py00546e

McGill University

L. Freiburger, T. Miletti, S. Zhu, O. Baettig, A. Berghuis, K. Auclair & A. Mittermaier, "Substrate-dependent switching of the allosteric binding mechanism of a dimeric enzyme," *Nature Chemical Biology* **10** (2014) 937-942. http://dx.doi.org/10.1038/nchembio.1626

Université de Montréal

E. Bonneau and P. Legault, "Nuclear Magnetic Resonance Structure of the III–IV–V Three-Way Junction from the Varkud Satellite Ribozyme and Identification of Magnesium-Binding Sites Using Paramagnetic Relaxation Enhancement," *Biochemistry* **53** (2014) 6264-6275. http://dx.doi.org/10.1021/bi500826n

University of Ottawa

F.A. Perras and D.L. Bryce, "Direct Characterization of Metal-Metal Bonds Between Nuclei with Strong Quadrupolar Interactions via NMR Spectroscopy," *Journal of Physical Chemistry Letters* **5** (2014) 4049-4054.
http://dx.doi.org/10.1021/jz5023448

J. Xu, B.E.G. Lucier, Z. Lin, A. Sutrisno, V.V. Terskikh, and Y. Huang, "New Insights Into the Short-Range Structures of Layered and Microporous Titanosilicates as Revealed by $^{47/49}$Ti, ^{23}Na, ^{39}K, and ^{29}Si Solid-State NMR Spectroscopy," *Journal of Physical Chemistry C* **118** (2014) online.
http://dx.doi.org/10.1021/jp5077966

H.A. Kalviri, F. Gärtner, E. Ye, I. Korobkov and R.T. Baker, "Probing the second dehydrogenation step in ammonia-borane dehydrocoupling: Characterization and reactivity of the key intermediate, B-(cyclotriborazanyl)amine-borane," *Chem. Sci.* (2014) online.
http://dx.doi.org/10.1039/c4sc02710h

X. Kong, A. Tang, R. Wang, E. Ye, V.V. Terskikh, G. Wu, "Are the Amide Bonds in N-Acyl Imidazoles Twisted? A Combined Solid-State ^{17}O NMR, Crystallographic, and Computational Study," *Canadian Journal of Chemistry* **92** (2014) online.
http://dx.doi.org/10.1139/cjc-2014-0397

K.M.N. Burgess and D.L. Bryce, "On the Crystal Structure of the Vaterite Polymorph of $CaCO_3$. A Calcium-43 Solid-State NMR and Computational Assessment," *Solid State Nuclear Magnetic Resonance* (2014) online.
http://dx.doi.org/10.1016/j.ssnmr.2014.08.003

W.D. Wang, B.E.G. Lucier, V.V. Terskikh, W. Wang, and Y. Huang, "Wobbling and Hopping: Studying Dynamics of CO_2 Adsorbed in Metal–Organic Frameworks via ^{17}O Solid-State NMR," *Journal of Physical Chemistry Letters* **5** (2014) 3360–3365.
http://dx.doi.org/10.1021/jz501729d

H. Ghasriani, J.K.-C. Kwok, A.R. Sherratt, A.C.Y. Foo, T. Qureshi, and N.K. Goto, "Micelle-Catalyzed Domain Swapping in the GlpG Rhomboid Protease Cytoplasmic Domain," *Biochemistry* (2014) online.
http://dx.doi.org/10.1021/bi500919v

Z.L. Ma, K.M. Wentz, B.A. Hammann, I-Ya Chang, M.K. Kamunde-Devonish, P.H.-Y. Cheong, D.W. Johnson, V.V. Terskikh, and S.E. Hayes, "Solid State ^{69}Ga and ^{71}Ga NMR study of the nanoscale inorganic cluster $[Ga_{13}(\mu_3\text{-}OH)6(\mu_2\text{-}OH)_{18}(H_2O)_{24}](NO_3)_{15}$," *Chemistry of Materials* **26** (2014) 4978-4983.
http://dx.doi.org/10.1021/cm501862u

P. He, B. Lucier, V. Terskikh, Q. Shi, J. Dong, Y. Chu, A. Zheng, A. Sutrisno, Y. Huang, "Spies Within Metal Organic Frameworks: Investigating Metal Centers Using Solid-State NMR," *Journal of Physical Chemistry C* **118** (2014) 23728–23744. **(Cover Article)**
http://dx.doi.org/10.1021/jp5063868

Health Canada

Y. Aubin, D.I. Freedberg, D.A. Keire, "One- and Two-Dimensional NMR Techniques for Biopharmaceuticals," Chapter 13 in *Biophysical Characterization of Proteins in Developing Biopharmaceuticals* (2015) 341–383.
http://dx.doi.org/10.1016/B978-0-444-59573-7.00013-0

NRC Canada

M.D. Jones, E. Vinogradov, J.F. Nomellini, J. Smit, "The core and O-polysaccharide structure of the *Caulobacter crescentus* lipopolysaccharide," *Carbohydrate Research* (2014) online.
http://dx.doi.org/10.1016/j.carres.2014.10.003

C.A. O'Keefe, K.E. Johnston, K. Sutter, J. Autschbach, R. Gauvin, J. Trébosc, L. Delevoye, N. Popoff, M. Taoufik, K. Oudatchin, and R.W. Schurko, "An Investigation of Chlorine Ligands in Transition-Metal Complexes via ^{35}Cl Solid-State NMR and Density Functional Theory Calculations," *Inorganic Chemistry* **53** (2014) 9581–9597.
http://dx.doi.org/10.1021/ic501004u

Queen's University

Y. Wu, Y. Yang, M. Dong, F. Sauriol, Q. Shi, Y. Gu, C. Huo, "A New Taraxastane-Type Triterpene from the Flowers of *Inula cappa*," *Chemistry of Natural Compounds* **50** (2014) online.
http://dx.doi.org/10.1007/s10600-014-1098-2

X. Kong, A. Tang, R. Wang, E. Ye, V.V. Terskikh, G. Wu, "Are the Amide Bonds in N-Acyl Imidazoles Twisted? A Combined Solid-State ^{17}O NMR, Crystallographic, and Computational Study," *Canadian Journal of Chemistry* **92** (2014) online.
http://dx.doi.org/10.1139/cjc-2014-0397

M.W.A. MacLean, T.K. Wood, G. Wu, R.P. Lemieux, and C.M. Crudden, "Chiral Periodic Mesoporous Organosilicas: Probing Chiral Induction in the Solid State," *Chem. Mater.* **26** (2014) 5852–5859.
http://dx.doi.org/10.1021/cm501826b

Y. Gao, A. Toubaei, X. Kong and G. Wu, "Acidity and Hydrogen Exchange Dynamics of Iron(II)-Bound Nitroxyl in Aqueous Solution," *Angewandte Chemie International Edition* **53** (2014) 11547–11551.
http://dx.doi.org/10.1002/anie.201407018

University of Toronto

D. Meiri, C.B. Marshall, D. Mokady, J. LaRose, M. Mullin, A.-C. Gingras, M. Ikura and R. Rottapel, "Mechanistic insight into GPCR-mediated activation of the microtubule-associated RhoA exchange factor GEF-H1," *Nature Communications* **5** (2014) 4857.
http://dx.doi.org/10.1038/ncomms5857

D. Long, A. Sekhar, L.E. Kay, "Triple resonance-based 13Cα and 13Cβ CEST experiments for studies of ms timescale dynamics in proteins," *Journal of Biomolecular NMR* (2014) online.
http://dx.doi.org/10.1007/s10858-014-9868-5

A. Lemak, B. Wu, A. Yee, S. Houliston, H.-W. Lee, A. Gutmanas, X. Fang, M. Garcia, A. Semesi, Y.-X. Wang, J.H. Prestegard, C.H. Arrowsmith, "Structural Characterization of a Flexible Two-Domain Protein in Solution Using Small Angle X-Ray Scattering and NMR Data," *Structure* (2014) online.
http://dx.doi.org/10.1016/j.str.2014.09.013

A.A. Yee, A. Semesi, M. Garcia, C.H. Arrowsmith, "Screening Proteins for NMR Suitability," in *"Structural Genomics and Drug Discovery" Series: Methods in Molecular Biology* **1140** (2014) 169-178.
http://dx.doi.org/10.1007/978-1-4939-0354-2_13

A.J. Simpson, P.J. Mitchell, H. Masoom, Y.L. Mobarhan, A. Adamo, and A.P. Dicks, "An Oil Spill in a Tube: An Accessible Approach for Teaching Environmental NMR Spectroscopy," *J. Chem. Educ.* (2014) accepted.
http://dx.doi.org/10.1021/ed500364b

S.C. Genest, M.J. Simpson, A.J. Simpson, R. Soong and D.J. McNally, "Analysis of soil organic matter at the solid–water interface by nuclear magnetic resonance spectroscopy," *Environmental Chemistry* **11** (2014) 472-482.
http://dx.doi.org/10.1071/EN14060

J. Hoang and R.S. Prosser, "Conformational Selection and Functional Dynamics of Calmodulin: A ^{19}F NMR Study" *Biochemistry* **53** (2014) 5727–5736.
http://dx.doi.org/10.1021/bi500679c

E.D. de Araujo, V. Kanelis, "Successful development and use of a thermodynamic stability screen for optimizing the yield of nucleotide binding domains," *Protein Expression and Purification* **103** (2014) 38–47.
http://dx.doi.org/10.1016/j.pep.2014.08.006

McMaster University

N.M. DeAlmeida, D.K. Paul, K. Karan and G.R. Goward, "^{1}H Solid State NMR Study of Nanothin Nafion Films," *Journal of Physical Chemistry C* **118** (2014) online.
http://dx.doi.org/10.1021/jp5086747

T.R. Field and A.D. Bain, "Singularities in the lineshape of a second-order perturbed quadrupolar nucleus. The Magic-Angle Spinning Case," *Solid State Nuclear Magnetic Resonance* (2014) online.
http://dx.doi.org/10.1016/j.ssnmr.2014.10.005

A. Bain, "Dynamic NMR," in *"Modern NMR Techniques for Synthetic Chemistry" Series: New Directions in Organic & Biological Chemistry* Published: October 13, 2014 by CRC Press, Editor: Julie Fisher, ISBN: 9781466592247.
http://www.crcnetbase.com/isbn/9781466592254

Redeemer University College

D.H. Brouwer and M. Horvath, "A simulated annealing approach for solving zeolite crystal structures from twodimensional NMR correlation spectra," *Solid State Nuclear Magnetic Resonance* (2014) online.
http://dx.doi.org/10.1016/j.ssnmr.2014.10.004

University of Waterloo

B.D. Adams, R. Black, Z. Williams, R. Fernandes, M. Cuisinier, E.J. Berg, P. Novak, G.K. Murphy and L.F. Nazar, "Towards a Stable Organic Electrolyte for the Lithium Oxygen Battery," *Advanced Energy Materials* (2014) online.
http://dx.doi.org/10.1002/aenm.201400867

University of Western Ontario

J. Xu, B.E.G. Lucier, Z. Lin, A. Sutrisno, V.V. Terskikh, and Y. Huang, "New Insights Into the Short-Range Structures of Layered and Microporous Titanosilicates as Revealed by $^{47/49}$Ti, ^{23}Na, ^{39}K, and ^{29}Si Solid-State NMR Spectroscopy," *Journal of Physical Chemistry C* **118** (2014) online.
http://dx.doi.org/10.1021/jp5077966

W.D. Wang, B.E.G. Lucier, V.V. Terskikh, W. Wang, and Y. Huang, "Wobbling and Hopping: Studying Dynamics of CO_2 Adsorbed in Metal–Organic Frameworks via ^{17}O Solid-State NMR," *Journal of Physical Chemistry Letters* **5** (2014) 3360–3365.
http://dx.doi.org/10.1021/jz501729d

B.J. Malbrecht, J.W. Dube, M.J. Willans, and P.J. Ragogna, "Addressing the Chemical Sorcery of "GaI": Benefits of Solid-State Analysis Aiding in the Synthesis of P-Ga Coordination Compounds," *Inorganic Chemistry* **53** (2014) 9644–9656.
http://dx.doi.org/10.1021/ic501139w

P. He, B. Lucier, V. Terskikh, Q. Shi, J. Dong, Y. Chu, A. Zheng, A. Sutrisno, Y. Huang, "Spies Within Metal Organic Frameworks: Investigating Metal Centers Using Solid-State NMR," *Journal of Physical Chemistry C* **118** (2014) 23728–23744. **(Cover Article)**
http://dx.doi.org/10.1021/jp5063868

University of Windsor

A.J. Rossini, M.P. Hildebrand, P. Hazendonk, and R.W. Schurko, "Multinuclear Solid-State NMR Studies of Polymer Supported Scandium Triflate Catalysts," *J. Phys. Chem. C* **118** (2014) 22649–22662.
http://dx.doi.org/10.1021/jp507470v

C.A. O'Keefe, K.E. Johnston, K. Sutter, J. Autschbach, R. Gauvin, J. Trébosc, L. Delevoye, N. Popoff, M. Taoufik, K. Oudatchin, and R.W. Schurko, "An Investigation of Chlorine Ligands in Transition-Metal Complexes via ^{35}Cl Solid-State NMR and Density Functional Theory Calculations," *Inorganic Chemistry* **53** (2014) 9581–9597.
http://dx.doi.org/10.1021/ic501004u

University of Manitoba

B. Zhou, V.K. Michaelis, Y. Yao, B.L. Sherriff, S. Kroeker and Y. Pan, "Density functional theory study of the magnetic shielding mechanism for ^{11}B in pentaborate minerals: ulexite and probertite," *CrystEngComm* **16** (2014) 10418-10427.
http://dx.doi.org/10.1039/c4ce01749h

University of Saskatchewan

B. Zhou, V.K. Michaelis, Y. Yao, B.L. Sherriff, S. Kroeker and Y. Pan, "Density functional theory study of the magnetic shielding mechanism for ^{11}B in pentaborate minerals: ulexite and probertite," *CrystEngComm* **16** (2014) 10418-10427.
http://dx.doi.org/10.1039/c4ce01749h

University of Alberta

P.M. Hwang, F. Cai, S.E. Pineda-Sanabria, D.C. Corson, B.D. Sykes, "The cardiac-specific n-terminal region of troponin I positions the regulatory domain of troponin C," *Proc. Natl. Acad. Sci. USA* **111** (2014) 14412-14417.
http://dx.doi.org/10.1073/pnas.1410775111

University of Calgary

B.C.H. Chu, R. Otten, K. D. Krewulak, F.A.A. Mulder, and H.J. Vogel, "The Solution Structure, Binding Properties, and Dynamics of the Bacterial Siderophore-binding Protein FepB," *Journal of Biological Chemistry* **289** (2014) 29219-29234.
http://dx.doi.org/10.1074/jbc.M114.564021

M. Arias, K.V. Jensen, L.T. Nguyen, D.G. Storey, H.J. Vogel, "Hydroxy-tryptophan containing derivatives of tritrpticin: Modification of antimicrobial activity and membrane interactions," *Biochimica et Biophysica Acta (BBA) - Biomembranes* (2014) accepted. **(special issue)**
http://dx.doi.org/10.1016/j.bbamem.2014.08.024

H. Ishida, A. Garcia-Herrero, H.J. Vogel, "The Periplasmic Domain of *Escherichia coli* Outer Membrane Protein A can Undergo a Localized Temperature Dependent Structural Transition," *Biochimica et Biophysica Acta (BBA) - Biomembranes* **1838** (2014) 3014–3024.
http://dx.doi.org/10.1016/j.bbamem.2014.08.008

University of Lethbridge

A.J. Rossini, M.P. Hildebrand, P. Hazendonk, and R.W. Schurko, "Multinuclear Solid-State NMR Studies of Polymer Supported Scandium Triflate Catalysts," *J. Phys. Chem. C* **118** (2014) 22649–22662.
http://dx.doi.org/10.1021/jp507470v

University of British Columbia

Y. Sang, A.R. Tait, W.R.P. Scott, A.L. Creagh, P. Kumar, C.A. Haynes, and S.K. Straus, "Probing the Interaction between U24 and the SH3 Domain of Fyn Tyrosine Kinase," *Biochemistry* **53** (2014) online.
http://dx.doi.org/10.1021/bi500945x

E.E. Burnell, R.Y. Dong, A.C.J. Weber and A. Yethiraj, "NMR of solutes in nematic and smectic A liquid crystals: the anisotropic intermolecular potential," *Magnetic Resonance in Chemistry* **52** (2014) 570–580. **(special issue) (Review)**
http://dx.doi.org/10.1002/mrc.4113

A.C.J. Weber, D.H.J. Chen, "Conformational problem of alkanes in liquid crystals by NMR spectroscopy" *Magnetic Resonance in Chemistry* **52** (2014) 560–569. **(special issue) (Review)**
http://dx.doi.org/10.1002/mrc.4124

A.P. Manning, M. Giese, A.S. Terpstra, M.J. MacLachlan, W.Y. Hamad, R.Y. Dong and C.A. Michal, "NMR of guest-host systems: 8CB in chiral nematic porous glasses" *Magnetic Resonance in Chemistry* **52** (2014) 532–539. **(special issue)**
http://dx.doi.org/10.1002/mrc.4101

Contact us

Victor Terskikh, Manager
National Ultrahigh-field NMR Facility for Solids

1200 Montreal Road M-40
Ottawa ON, K1A 0R6
Tel. (613) 998-5552
Fax: (613) 990-1555

Email: nmr.canada@gmail.com

Web: http://nmr900.ca