~~Biological & medical applications of β-NMR spectroscopy~~

Chemical applications of β-detected NMR

Ryan M. L. McFadden

TRIUMF

4004 Wesbrook Mall, Vancouver, BC V6T 2A3

2021-08-16

Agenda

What is β-NMR / why is it useful?

Chemical applications of β-NMR
- Lithium-ion diffusion
- Solvent molecular dynamics
- Magnesium coordination chemistry

Concluding remarks

Solid State Nuclear Magnetic Resonance 68-69 (2015) 1–12

Contents lists available at ScienceDirect

Solid State Nuclear Magnetic Resonance

journal homepage: www.elsevier.com/locate/ssnmr

Trends

Implanted-ion βNMR: A new probe for nanoscience

W.A. MacFarlane

Chemistry Department, University of British Columbia, 2036 Main Mall, Vancouver, Canada V6T 1Z1

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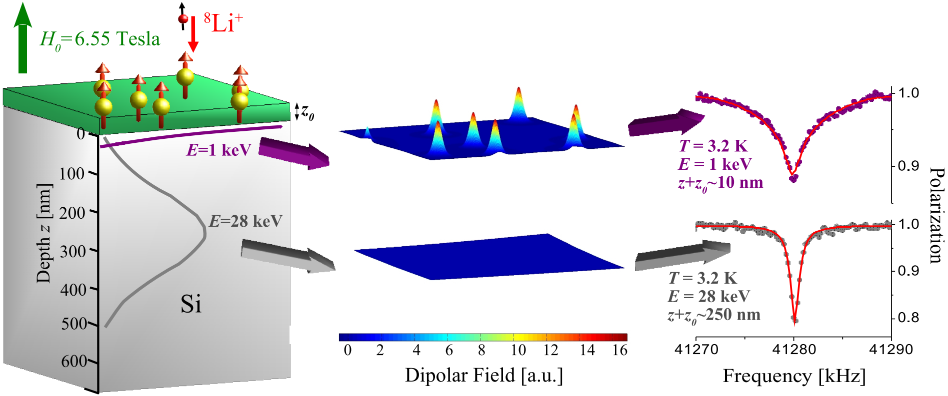
ABSTRACT

NMR detected by radioactive beta decay, β-NMR, is undergoing a renaissance largely due to the availability of high intensity low energy beams of the most common probe ion, $^{8}Li^{+}$, and dedicated facilities for materials research. The radioactive detection scheme, combined with the low energy ion beam, enable depth resolved NMR measurements in crystals, thin films and multilayers on depth scales of 2–200 nm. After a brief historical introduction, technical aspects of implanted-ion β-NMR are presented, followed by a review of recent applications to a wide range of solids.

A “nanoscience”’ example

^{8}Li β-NMR of a monolayer of Mn_{12} single molecule magnets



Z. Salman et al., Nano Lett. **7**, 1551 (2007)

The "killer" features of β-NMR at TRIUMF

- $\sim 10^{10}$ times more sensitive than "conventional" NMR.
- depth resolution on the scale of $\sim 1\,\mathrm{nm}$ to $\sim 500\,\mathrm{nm}$.
- can be used to study (almost) any material.

Raison d'être:

A technique for studying materials / systems that are difficult / inaccessible by conventional means!

What about “chemical” applications of β-NMR?

chem·is·try
noun

1. the branch of science that deals with the identification of the substances of which matter is composed;

   the investigation of their properties and the ways in which they interact, combine, and change;

   and the use of these processes to form new substances.

2. the complex emotional or psychological interaction between two people.

cm CHEMISTRY OF MATERIALS

Article

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Microscopic Dynamics of Li^+ in Rutile TiO_2 Revealed by ^8Li β-Detected Nuclear Magnetic Resonance

Ryan M. L. McFadden,[*,†,‡] Terry J. Buck,[¶] Aris Chatzichristos,[¶,‡] Chia-Chin Chen,[§] Kim H. Chow,[‖] David L. Cortie,[¶,†,‡,■] Martin H. Dehn,[¶,‡] Victoria L. Karner,[†,‡] Dimitrios Koumoulis,[⊥,●] C. D. Philip Levy,[□] Chilin Li,[○] Iain McKenzie,[□,△] Rotraut Merkle,[§] Gerald D. Morris,[□] Matthew R. Pearson,[□] Zaher Salman,[▽] Dominik Samuelis,[§,▲] Monika Stachura,[□] Jiyu Xiao,[†] Joachim Maier,[§] Robert F. Kiefl,[¶,‡,□] and W. Andrew MacFarlane[*,†,‡,□]

[†]Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, BC V6T 1Z1, Canada

[‡]Stewart Blusson Quantum Matter Institute, University of British Columbia, 2355 East Mall, Vancouver, BC V6T 1Z4, Canada

[¶]Department of Physics and Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1, Canada

[§]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart, Germany

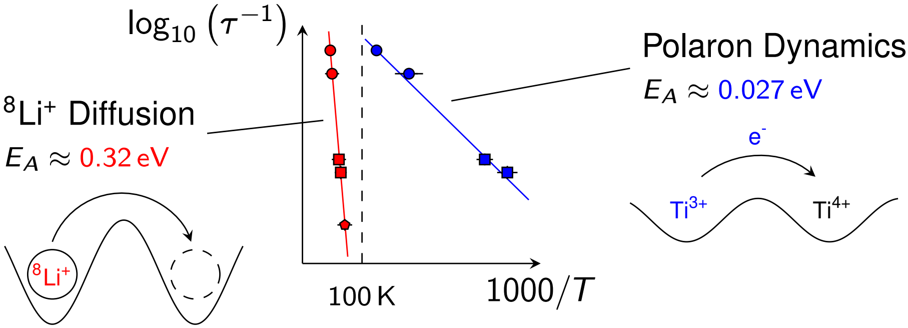
[‖]Department of Physics, University of Alberta, 4-181 CCIS, Edmonton, AB T6G 2E1, Canada

[⊥]Department of Chemistry and Biochemistry, University of California, Los Angeles, 607 Charles E. Young Drive East, Los Angeles, California 90095, United States

[□]TRIUMF, 4004 Wesbrook Mall, Vancouver, BC V6T 2A3, Canada

[○]Shanghai Institute of Ceramics, Chinese Academy of Sciences, 1295 Dingxi Road, Shanghai 200050, P.R. China

^{8}Li β-NMR senses the elementary "hopping" rate τ^{-1} of Li^{+} and e^{-} defects in rutile TiO_2



R. M. L. McFadden et al., Chem. Mater. **29**, 10187 (2017)

CHEMISTRY OF MATERIALS

Article

Cite This: *Chem. Mater.* 2019, 31, 9346−9353

pubs.acs.org/cm

Dynamics of Liquid 1-Ethyl-3-Methylimidazolium Acetate Measured with Implanted-Ion ^{8}Li β-NMR

Derek Fujimoto,[*,†,§] Ryan M. L. McFadden,[‡,§] Martin H. Dehn,[†,§] Yael Petel,[‡] Aris Chatzichristos,[†,§] Lars Hemmingsen,[∥] Victoria L. Karner,[‡,§] Robert F. Kiefl,[†,§] C. D. Philip Levy,[⊥] Iain McKenzie,[⊥,#] Carl A. Michal,[†] Gerald D. Morris,[⊥] Matthew R. Pearson,[⊥] Daniel Szunyogh,[∥] John O. Ticknor,[‡,§] Monika Stachura,[⊥] and W. Andrew MacFarlane[‡,§,⊥]

[†]Department of Physics and Astronomy and [‡]Department of Chemistry, University of British Columbia, Vancouver, BC V6T 1Z1, Canada

[§]Stewart Blusson Quantum Matter Institute, University of British Columbia, Vancouver, BC V6T 1Z4, Canada

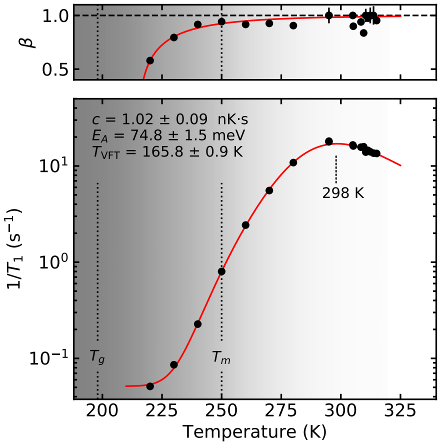
[∥]Department of Chemistry, University of Copenhagen, 2100 Kbenhavn, Denmark

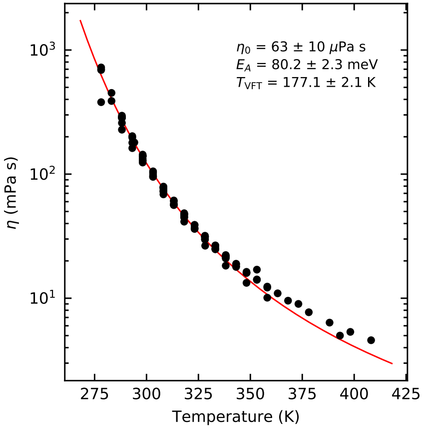
[⊥]TRIUMF, Vancouver, BC V6T 2A3, Canada

[#]Department of Chemistry, Simon Fraser University, Burnaby, BC V5A 1S6, Canada

ABSTRACT: We demonstrate the application of implanted-ion β-detected NMR as a probe of ionic liquid molecular dynamics through the measurement of ^{8}Li spin-lattice relaxation (SLR) and resonance in 1-ethyl-3-methylimidazolium acetate. The motional

^{8}Li β-NMR senses the elementary fluctuations arrising from molecular dynamics of the host solvent





D. Fujimoto et al., Chem. Mater. **31**, 9346 (2019)

Dalton Transactions

ROYAL SOCIETY OF CHEMISTRY

COMMUNICATION

View Article Online
View Journal | View Issue

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rsc.li/dalton

Direct observation of Mg^{2+} complexes in ionic liquid solutions by ^{31}Mg β-NMR spectroscopy†

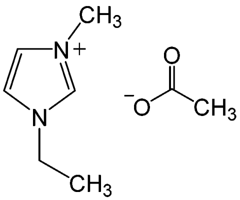
Daniel Szunyogh, ‡[a] Ryan M. L. McFadden, ‡[b,c] Victoria L. Karner,‡[b,c] Aris Chatzichristos,[c,d] Thomas Day Goodacre,[e] Martin H. Dehn,[c,d] Lia Formenti,[f] Derek Fujimoto, [c,d] Alexander Gottberg,[e] Evan Kallenberg,[d] Ildikó Kálomista, [a] Robert F. Kiefl,[c,d] Flemming H. Larsen, [g] Jens Lassen, [e] C. D. Philip Levy,[e] Ruohong Li,[e] W. Andrew MacFarlane,[b,c] Iain McKenzie, [h,i] Gerald D. Morris,[h] Stavroula Pallada,[a] Matthew R. Pearson,[h] Stephan P. A. Sauer, [a] Paul Schaffer,[j] Peter W. Thulstrup, [a] Lars Hemmingsen*[a] and Monika Stachura *[j]

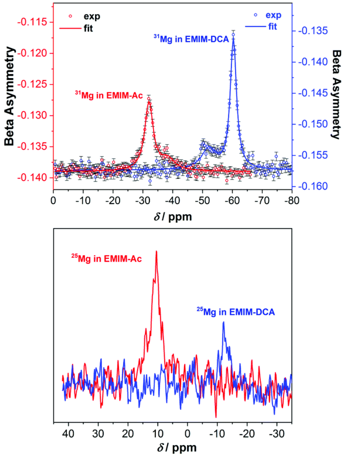
NMR spectra of Mg^{2+} ions in ionic liquids were recorded using a highly sensitive variant of NMR spectroscopy known as β-NMR. The β-NMR spectra of $MgCl_2$ in EMIM-Ac and EMIM-DCA compare favourably with conventional NMR, and exhibit linewidths of

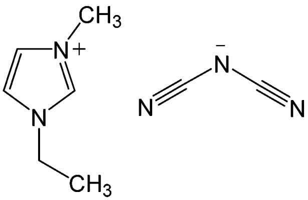
high-intensity radioactive ion beam (RIB) facilities, many new nuclei are available in quantities sufficient for the study of condensed matter. The main challenge to the use of RIBs as probes in liquids is the incompatibility of typical solutions

Resolving different coordination complexes using β-NMR

^{31}Mg β-NMR in two room temprature ionic liquids







D. Szunyogh et al., Dalton Trans. **47**, 14431 (2018)

Some friendly competition from CERN

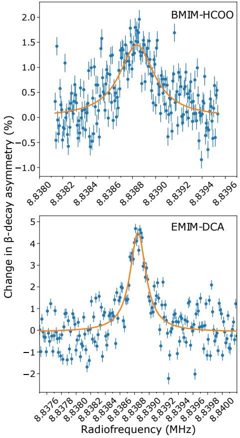
^{26}Na β-NMR in two room temperature ionic liquids

PHYSICAL REVIEW X **10,** 041061 (2020)

Magnetic Moments of Short-Lived Nuclei with Part-per-Million Accuracy: Toward Novel Applications of β-Detected NMR in Physics, Chemistry, and Biology

R. D. Harding,[1,2,†] S. Pallada,[1,‡] J. Croese,[1,3] A. Antušek,[4] M. Baranowski,[5] M. L. Bissell,[6] L. Cerato,[7] K. M. Dziubinska-Kühn,[1,8] W. Gins,[9,§] F. P. Gustafsson,[9] A. Javaji,[1,10,¶] R. B. Jolivet,[3] A. Kanellakopoulos,[9] B. Karg,[3] M. Kempka,[5] V. Kocman,[11] M. Kozak,[5,12] K. Kulesz,[3,1] M. Madurga Flores,[13] G. Neyens,[9,1] R. Pietrzyk,[5] J. Plavec,[11] M. Pomorski,[14,**] A. Skrzypczak,[15] P. Wagenknecht,[1,10,††] F. Wienholtz,[1,‡‡] J. Wolak,[5] Z. Xu,[13] D. Zakoucky,[16] and M. Kowalska[1,3,*]

[1]*Experimental Physics Department, CERN, 1211 Geneva, Switzerland*
[2]*Department of Physics, University of York, YO10 5DD York, United Kingdom*
[3]*Department of Nuclear and Particle Physics, University of Geneva, 1211 Geneva, Switzerland*
[4]*Faculty of Materials Science and Technology, Slovak University of Technology, 917 24 Trnava, Slovak Republic*
[5]*Faculty of Physics, Adam Mickiewicz University, 61-614 Poznań, Poland*
[6]*School of Physics and Astronomy, The University of Manchester, M13 9PL Manchester, United Kingdom*
[7]*Department of Molecular Biology, University of Geneva, 1211 Geneva, Switzerland*
[8]*Institute of Analytical Chemistry, Leipzig University, D-04103 Leipzig, Germany*
[9]*Instituut voor Kern- en Stalingsfysica, KU Leuven, B-3001 Leuven, Belgium*
[10]*Faculty of Mathematics and Natural Sciences, Oldenburg University, 26129 Oldenburg, Germany*
[11]*Slovenian NMR Centre, National Institute of Chemistry, SI-1001 Ljubljana, Slovenia*
[12]*National Synchrotron Radiation Centre SOLARIS, Jagiellonian University, 30-392 Kraków, Poland*
[13]*Department of Physics and Astronomy, University of Tennessee, Knoxville 37996, Tennessee, USA*
[14]*Faculty of Physics, University of Warsaw, 02-093 Warsaw, Poland*
[15]*Faculty of Chemical Technology, Poznan University of Technology, 60-965 Poznań, Poland*
[16]*Nuclear Physics Institute, Czech Academy of Sciences, CZ-25068 Rez, Czech Republic*



R. D. Harding et al., Phys. Rev. X **10**, 041061 (2020)

First results towards studying Mg^{II} biochemistry

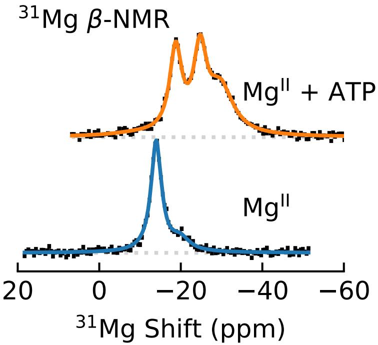
^{31}Mg β-NMR in EMIM-Ac + ATP solutions

Mg^{II} binding to adenosine triphosphate in 1-ethyl-3-methylimidazolium acetate characterized by ^{31}P NMR and ^{31}Mg β-detected NMR

Ryan M. L. McFadden,[1,*] Dániel Szunyogh,[2,*] Nicholas Bravo-Frank,[3] Aris Chatzichristos,[4,5,†] Martin H. Dehn,[4,5] Derek Fujimoto,[4,5] Attila Jancsó,[6] Silke Johannsen,[7] Ildikó Kálomista,[2] Victoria L. Karner,[5,8] Robert F. Kiefl,[1,4,5] Flemming H. Larsen,[9,‡] Jens Lassen,[1,10,11] C. D. Philip Levy,[1] Ruohong Li,[1] Iain McKenzie,[1,12,13] Hannah McPhee,[14,§] Gerald D. Morris,[1] Matthew R. Pearson,[1] Stephan P. A. Sauer,[2] Roland K. O. Sigel,[7] Peter W. Thulstrup,[2] W. Andrew MacFarlane,[1,5,8] Lars Hemmingsen,[2,¶] and Monika Stachura[1,12,**]

[1]*TRIUMF, 4004 Wesbrook Mall, Vancouver, BC V6T 2A3, Canada*
[2]*Department of Chemistry, University of Copenhagen, Universitetsparken 5, 2100 Copenhagen, Denmark*
[3]*Faculty of Engineering, University of Victoria, 3800 Finnerty Road, Victoria, BC V8P 5C2, Canada*
[4]*Department of Physics and Astronomy, 6224 Agricultural Road, University of British Columbia, Vancouver, BC V6T 1Z1, Canada*
[5]*Stewart Blusson Quantum Matter Institute, 2355 East Mall, University of British Columbia, Vancouver, BC V6T 1Z4, Canada*
[6]*Department of Inorganic and Analytical Chemistry, University of Szeged, Dóm tér 7, H-6720 Szeged, Hungary*
[7]*Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH 8057 Zürich, Switzerland*
[8]*Department of Chemistry, 2036 Main Mall, University of British Columbia, Vancouver, BC V6T 1Z1, Canada*
[9]*Department of Food Science, University of Copenhagen, Rolighedsvej 26, 1958 Frederiksberg C, Denmark*
[10]*Department of Physics, Simon Fraser University, 8888 University Drive, Burnaby, BC V5A 1S6, Canada*
[11]*Department of Physics and Astronomy, University of Manitoba, 30A Sifton Road, Winnipeg, MB R3T 2N2, Canada*
[12]*Department of Chemistry, Simon Fraser University, 8888 University Drive, Burnaby, BC V5A 1S6, Canada*
[13]*Department of Physics and Astronomy, University of Waterloo, 200 University Avenue West, Waterloo, ON N2L 3G1, Canada*
[14]*Department of Engineering Physics, McMaster University, 1280 Main Street West, Hamilton, ON L8S 4L7, Canada*

(Dated: June 15, 2021)



R. M. L. McFadden et al. Angew. Chem. Int. Ed. **under review** (2021)

Concluding remarks

- TRIUMF's β-NMR facility is a unique scientific tool with a diverse portfolio of applications.
- TRIUMF is pioneering new applications of β-NMR, with long-term goals of studying biochemistry / medicine.
- The potential for novel discovery is high!

Acknowledgements:

My colleagues at TRIUMF and collaborators at UBC / Copenhagen (whose names populate the author lists of the works presented here)!

Questions?

Science Talk 1

30 points

Scan the QR code from the Game Center tab of the ScanHunt app.

ScanHunt - Event Gamification by ATIVsoftware.com

Technical / scientific reviews of β-NMR at TRIUMF

Hyperfine Interact (2014) 225:173–182
DOI 10.1007/s10751-013-0894-6

β-NMR

Gerald D. Morris

Published online: 23 October 2013

Abstract The β-NMR facility at ISAC is constructed specifically for experiments in condensed matter physics with radioactive ion beams. Using co-linear optical pumping, a $^8Li^+$ ion beam having a large nuclear spin polarisation and low energy (nominally 30 keV) can be generated. When implanted into materials these ions penetrate to shallow depths comparable to length scales of interest in the physics of surfaces and interfaces between materials. Such low-energy ions can be decelerated with simple electrostatic optics to enable depth-resolved studies of near-surface phenomena over the range of about 2–200 nm. Since the β-NMR signal is extracted

G. D. Morris, Hyperfine Interact. **225**, 173 (2014)

Solid State Nuclear Magnetic Resonance 68-69 (2015) 1–12

Contents lists available at ScienceDirect

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Trends

Implanted-ion βNMR: A new probe for nanoscience

W.A. MacFarlane

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Radioactive ion beams
Muon spin rotation

ABSTRACT

NMR detected by radioactive beta decay, β-NMR, is undergoing a renaissance largely due to the availability of high intensity low energy beams of the most common probe ion, $^8Li^+$, and dedicated facilities for materials research. The radioactive detection scheme, combined with the low energy ion beam, enable depth resolved NMR measurements in crystals, thin films and multilayers on depth scales of 2–200 nm. After a brief historical introduction, technical aspects of implanted-ion β-NMR are presented, followed by a review of recent applications to a wide range of solids.

Contents

W. A. MacFarlane, Solid State Nucl. Magn. Reson. **68–69**, 1 (2015)

Development of ^{31}Mg as a β-NMR probe

Hyperfine Interact (2016) 237: 162
DOI 10.1007/s10751-016-1372-8

CrossMark

Development of a polarized $^{31}Mg^{+}$ beam as a spin-1/2 probe for BNMR

C. D. P. Levy[1] · M. R. Pearson[1] · M. H. Dehn[2] · V. L. Karner[3] · R. F. Kiefl[1,4,5] · J. Lassen[1] · R. Li[1] · W. A. MacFarlane[3,4] · R. M. L. McFadden[3] · G. D. Morris[1] · M. Stachura[1] · A. Teigelhöfer[1,6] · A. Voss[7]

Published online: 22 November 2016

Abstract A 28 keV beam of $^{31}Mg^{+}$ ions was extracted from a uranium carbide, proton-beam-irradiated target coupled to a laser ion source. The ion beam was nuclear-spin polarized by collinear optical pumping on the $^{2}S_{1/2}$–$^{2}P_{1/2}$ transition at 280 nm. The polarization was preserved by an extended 1 mT guide field as the beam was transported via electrostatic bends into a 2.5 T longitudinal magnetic field. There the beam was implanted into a single crystal MgO target and the beta decay asymmetry was measured. Both hyperfine ground states were optically pumped with a single frequency light source, using segmentation of the beam energy, which boosted the polarization by approximately 50 %

C. D. P. Levy et al., Hyperfine Interact. **237**, 162 (2016)

Check for updates

Proc. 14th Int. Conf. on Muon Spin Rotation, Relaxation and Resonance (μSR2017)
JPS Conf. Proc. **21**, 011047 (2018)
https://doi.org/10.7566/JPSCP.21.011047

On the Use of ^{31}Mg for β-Detected NMR Studies of Solids

Ryan M. L. McFadden[1,2], Aris Chatzichristos[2,3], Martin H. Dehn[2,3], Derek Fujimoto[2,3], Hiroshi Funakubo[4], Alexander Gottberg[5], Taro Hitosugi[6,7], Victoria L. Karner[1,2], Robert F. Kiefl[2,3], Mao Kurokawa[4], Jens Lassen[5], C. D. Philip Levy[5], Ruohong Li[5], Gerald D. Morris[5], Matthew R. Pearson[5], Susumu Shiraki[6], Monika Stachura[5], Jun Sugiyama[8,9], Dániel M. Szunyogh[10], and W. Andrew MacFarlane[1,2]

[1] *Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, BC V6T 1Z1, Canada*
[2] *Stewart Blusson Quantum Matter Institute, University of British Columbia, 2355 East Mall, Vancouver, BC V6T 1Z4, Canada*
[3] *Department of Physics & Astronomy, University of British Columbia, 6224 Agricultural Road, Vancouver, BC V6T 1Z1, Canada*
[4] *Department of Innovative and Engineered Materials, Tokyo Institute of Technology, J2-1508, 4259 Nagatsuda-cho, Midori-ku, Yokohama 226-8502, Japan*
[5] *TRIUMF, 4004 Wesbrook Mall, Vancouver, BC V6T 2A3, Canada*
[6] *Advanced Institute for Material Research (AIMR), Tohoku University, Sendai, 980-8577, Japan*
[7] *School of Materials and Chemical Technology, Tokyo Institute of Technology, Tokyo, 152-8550, Japan*
[8] *Toyota Central Research & Development Laboratories, Inc., 41-1, Yokomichi, Nagakute, Aichi 480-1192, Japan*
[9] *Advanced Science Research Center, Japan Atomic Energy Agency, Ooaza Shirakata 2-4, Tokai-mura, Naka-gun, Ibaraki-ken 319-1195, Japan*
[10] *Kemisk Institut, Københavns Universitet, Universitetsparken 5, 2100 København, Denmark*

E-mail: rmlm@chem.ubc.ca, wam@chem.ubc.ca

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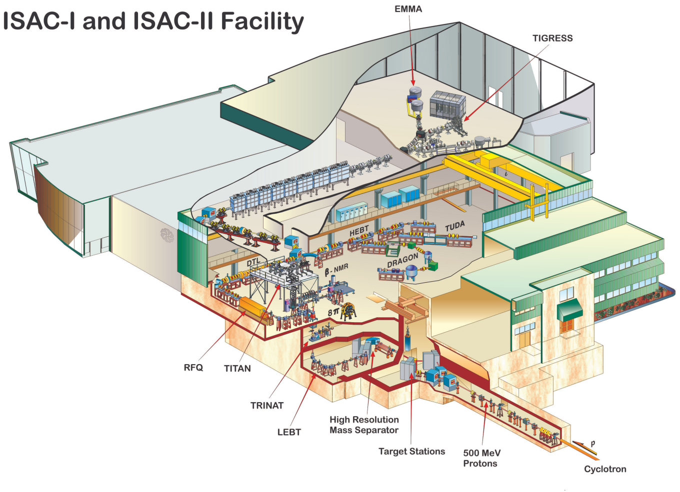
It has long been desirable to develop a spin-1/2 nucleus as a probe for β-detected NMR studies of solid materials. As a *pure* magnetic probe, it would greatly compliment our most extensively used

R. M. L. McFadden et al., JPS Conf. Proc. **21**, 011047 (2018)

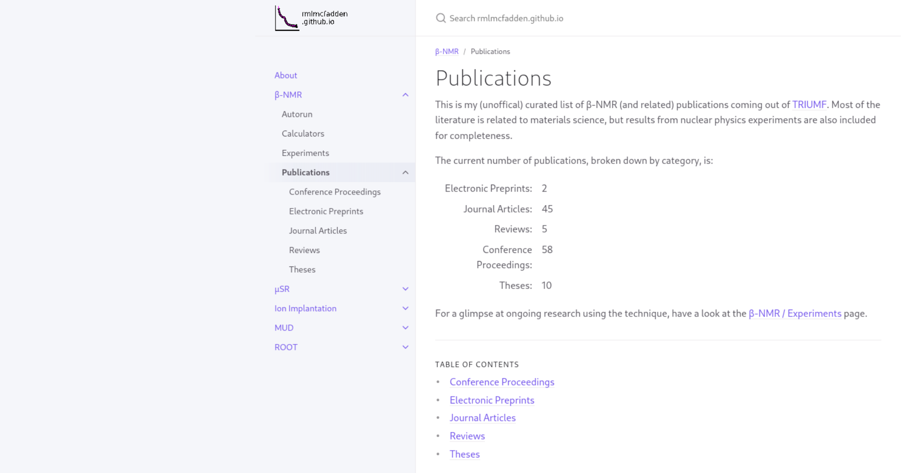
TRIUMF's isotope seperator and accelerator (ISAC) facility



J. Dilling et al., Hyperfine Interact. **225**, 1 (2014)

My list(s) of TRIUMF's β-NMR (and related) publications

https://rmlmcfadden.github.io/bnmr/publications/



rmlmcfadden .github.io

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    - Electronic Preprints
    - Journal Articles
    - Reviews
    - Theses
- μSR
- Ion Implantation
- MUD
- ROOT

β-NMR / Publications

Publications

This is my (unoffical) curated list of β-NMR (and related) publications coming out of TRIUMF. Most of the literature is related to materials science, but results from nuclear physics experiments are also included for completeness.

The current number of publications, broken down by category, is:

Electronic Preprints:	2
Journal Articles:	45
Reviews:	5
Conference Proceedings:	58
Theses:	10

For a glimpse at ongoing research using the technique, have a look at the β-NMR / Experiments page.

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