β-detected Nuclear Magnetic Resonance (β-NMR) Spectroscopy at TRIUMF

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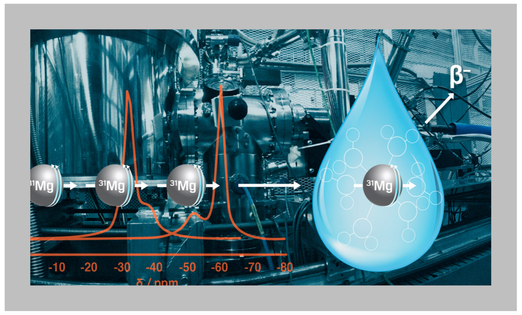
β-NMR in Life Sciences

TRIUMF's Life Sciences has pioneered the use of β-NMR in applications to the characterization of the role of different metal ions in living systems, such as DNA, RNA, beta-amyloid or ATP. In β-NMR, a radioactive isotopes are incorporated into a biomolecule's structure to act as an incredibly sensitive built-in probe transmitting otherwise unattainable information. This is done through the beam implantation of radioactive isotopes, including ^{31}Mg, into solutions of target molecules.



Billion-fold increase in sensitivity of NMR resonances of NMR Mg^{2}+ ions in solution recorded using a specialized version of NMR spectroscopy known as β-NMR.

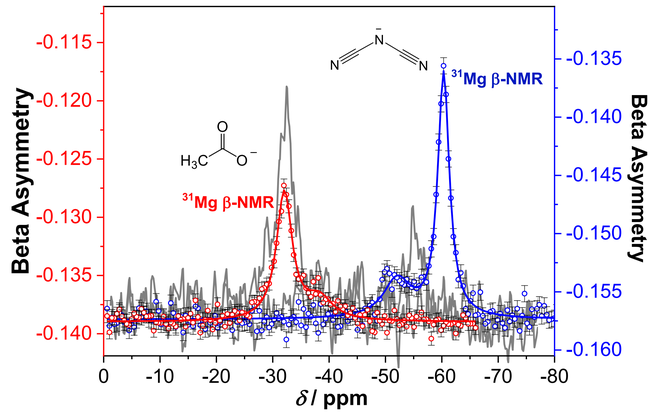
Publications:

1. R. McFadden *et al*. Angew. Chemie, 2021, in revision
2. D. Szunyogh *et al*. Dalton Trans. 2018, **47**, 14431-14435.
3. R. McFadden *et al*. JPS Conf. Proc. 2018, **21**, 011047.
4. M. Stachura *et al*. Hyperfine Interact. 2017, **238**, 32.

Although β-NMR spectroscopy has been applied to nuclear physics and condensed matter over the past five decades, its applications to biology, chemistry and medicine are still fairly uncommon mainly due to technical difficulties in maintaining liquid samples under high vacuum. Over the past 3 years, TRIUMF has not only pioneered technology that overcame this barrier, but also carried out first experiments on liquids and biological samples, moving from proof-of-feasibility to first applications. In April 2017 we have recorded the first ever β-NMR signals originating from oxygen and nitrogen coordinating Mg2+ in typical Mg complexes, illustrating that β-NMR can in fact discriminate between different structures. In July 2018 we have carried out first β-NMR measurements on Mg coordinating to ATP, a molecule that is a biological currency of energy. This achievement marks a milestone in applications of β-NMR into biologically relevant samples, and opens new opportunities in the fields of biology, chemistry and medicine.

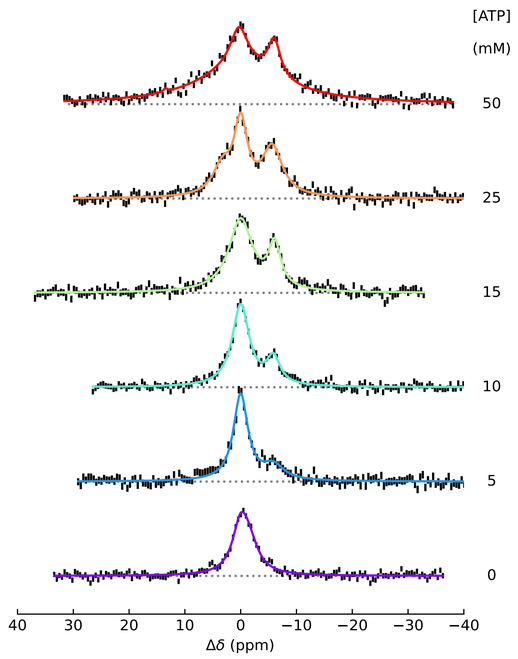
Property	β-NMR
spin	I=1/2
magnetic field	3.2 T
sample volume	3 uL
FWHM	~ 2 ppm
measurement time	20 min

^{31}Mg β-NMR of $MgCl_2$ in Ionic Liquids

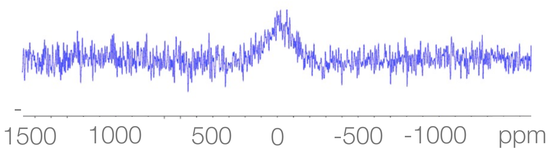


β-NMR	Properties	NMR
^{31}Mg (I=1/2)	Isotope	^{25}Mg (I=5/2)
3.41	Magnetic Field (T)	11.7
22	Temperature (°C)	72
2-4	Sample volume (mL)	550
20 min	Time of meas.	72 hours

^{31}Mg β-NMR of Mg in ATP



^{25}Mg NMR of Mg in ATP



Property	NMR
spin	I=5/2
magnetic field	11.7 T
sample volume	550 mL
FWHM	~ 200 ppm
measurement time	72 h

Discovery, accelerated