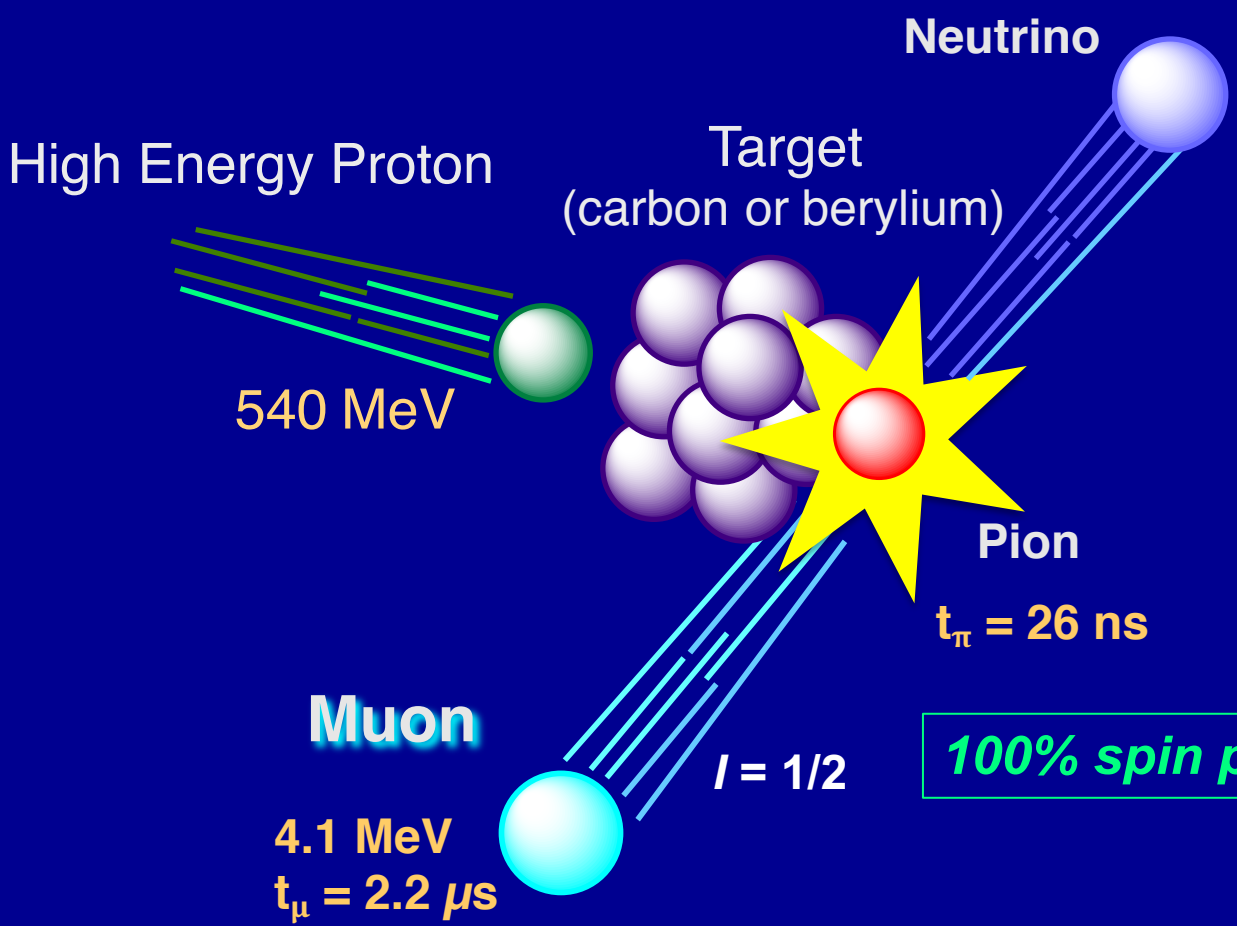
μSR Spectroscopy

The positive muon (μ^+) is an elementary subatomic particle that is assigned as a member of lepton (spin I = 1/2). High-energy beam of proton from accelerators such as cyclotron and synchrotron produce almost fully polarized muons for analyzing the spin characteristics of materials. The muon has one ninth of the proton mass ($0.1126m_p$), and the polarized "ultralight proton" is applicable to similar spectroscopic analyses to electron-spin resonance (ESR) and nuclear magnetic resonance (NMR) without the alternative magnetic resonance techniques. The lifetime of muon is 2.2 microseconds, which is useful for monitoring chemical events such as radical addition within 10 ns.

In contact with matter, the positive muon captures an electron and become a muonium (Mu = [μ^+e^-]) that is a light isotope of hydrogen atom. The muoniums have been utilized for monitoring radical reactions of usual unsaturated organic molecules including benzene, alkene, alkyne, and ketone, and the corresponding radicals via muonium addition can be characterized by muon spin rotation/resonance/relaxation (μSR) spectroscopy based on observation of the positrons from the collapsed (polarized) muons.

What is Muon?

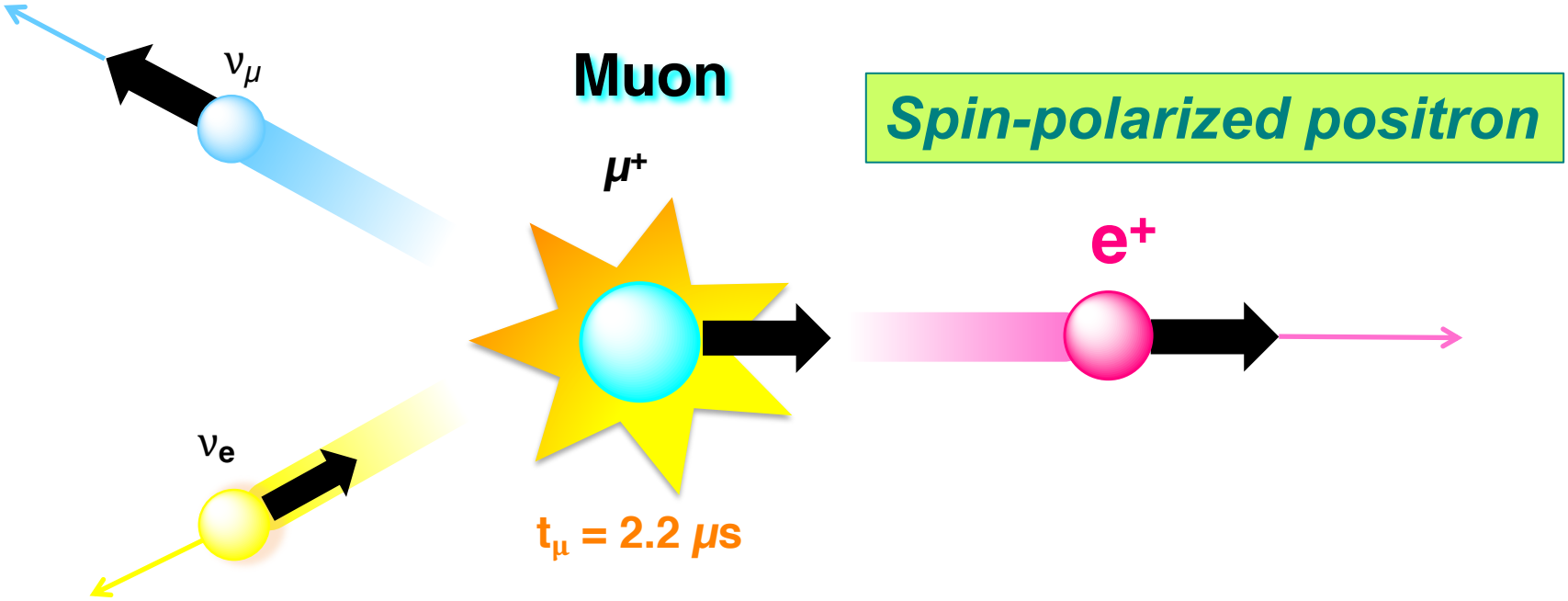


Light isotope of proton ($m_\mu = 0.113 m_p$)

Ref) http://cmms.triumf.ca/intro/musr/cap/musr0097.htm

What is Muon?

(Positive) Muon Decay



$$\mu^+ \longrightarrow e^+ + \nu_e + \nu_\mu$$

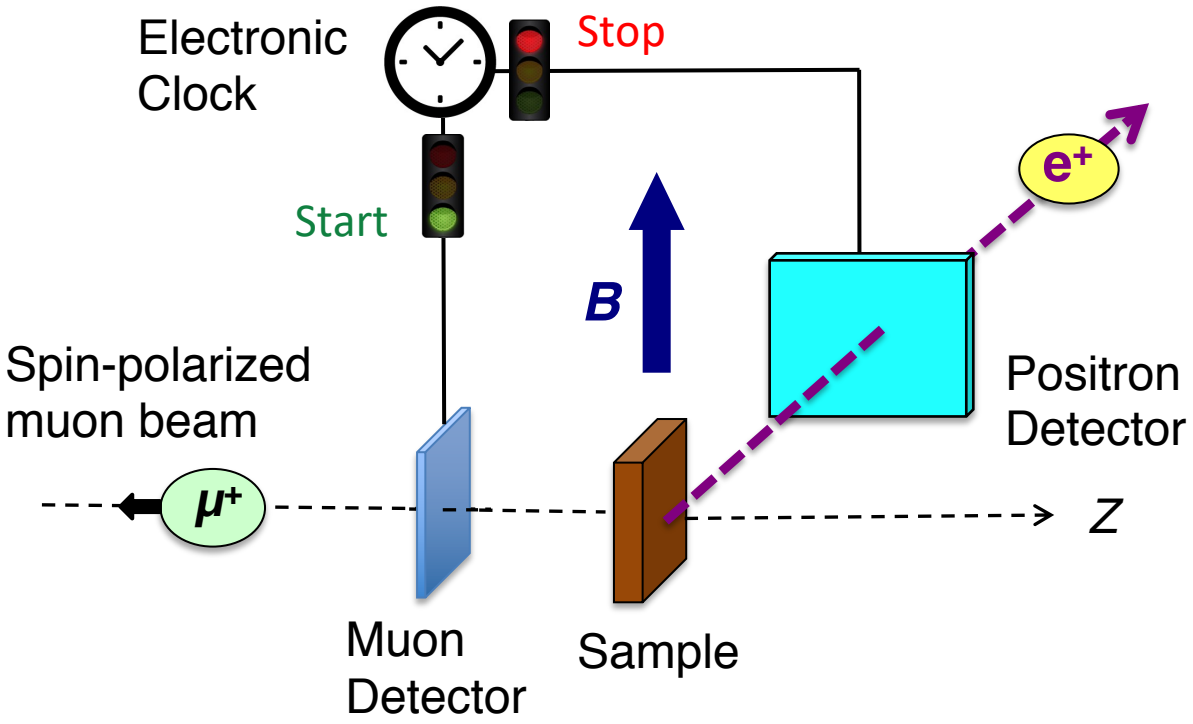
***Muon Spin Rotation / Resonance / Relaxation* (μSR)**

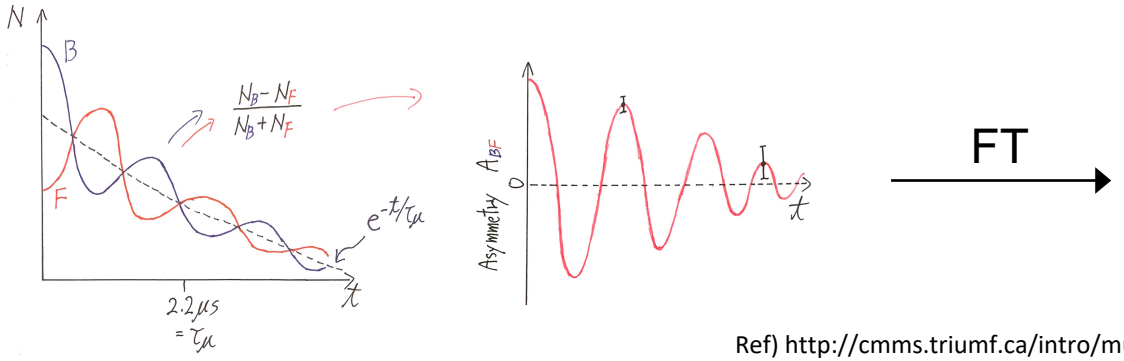
TF-μSR Measurement

Illustration of Experiment

(Transverse-Field Muon Spin Rotation)

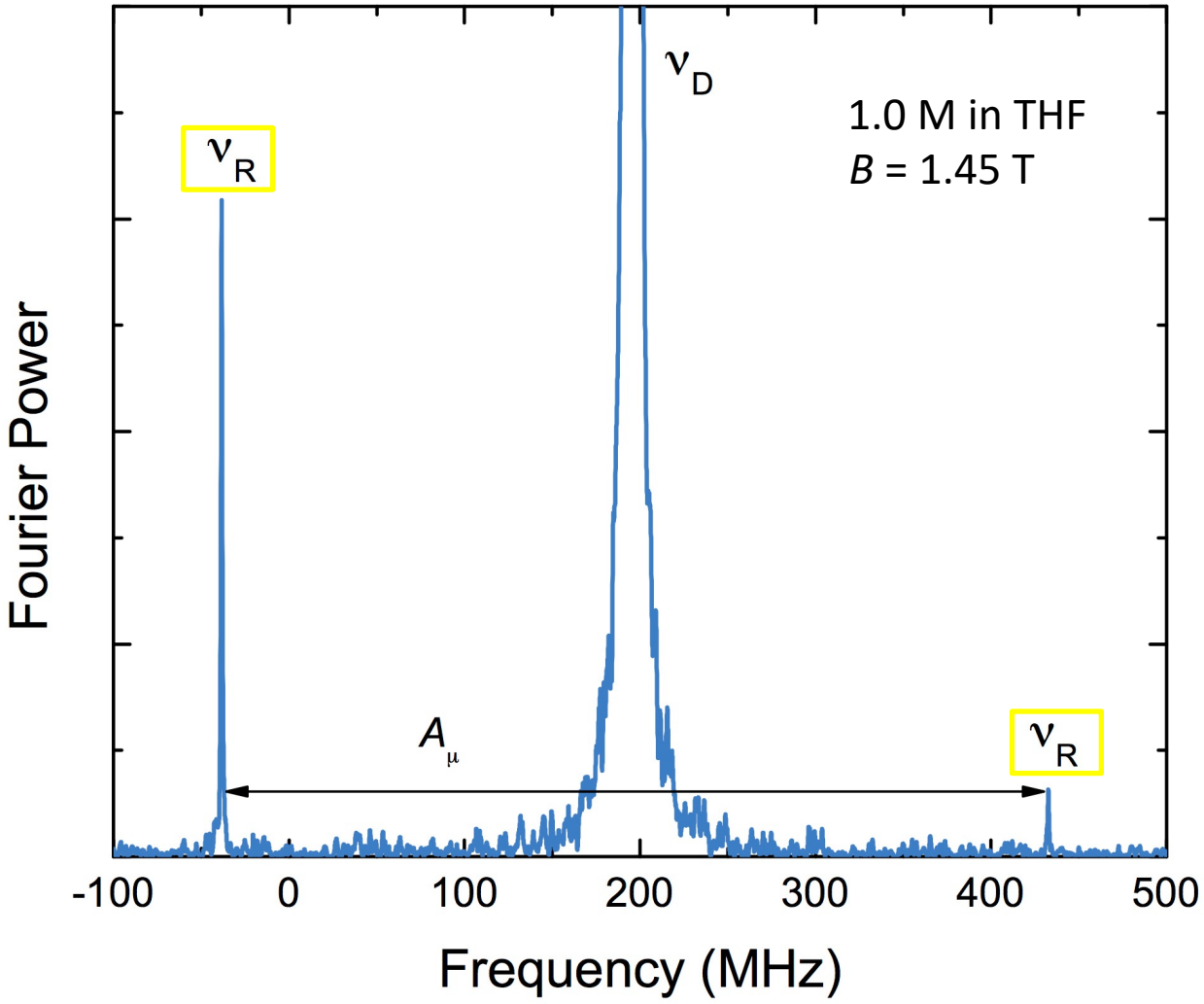
横磁場ミュオンスピン回転

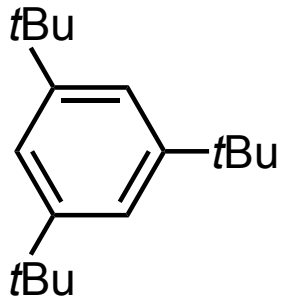




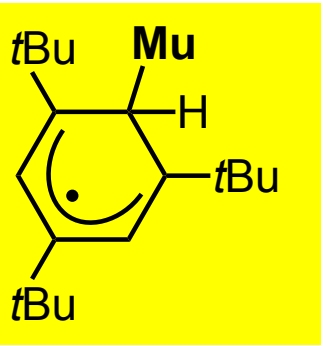
Ref) http://cmms.triumf.ca/intro/musr/cap/musr0097.htm

TF-μSR Study of Mes*H





+ **Mu**



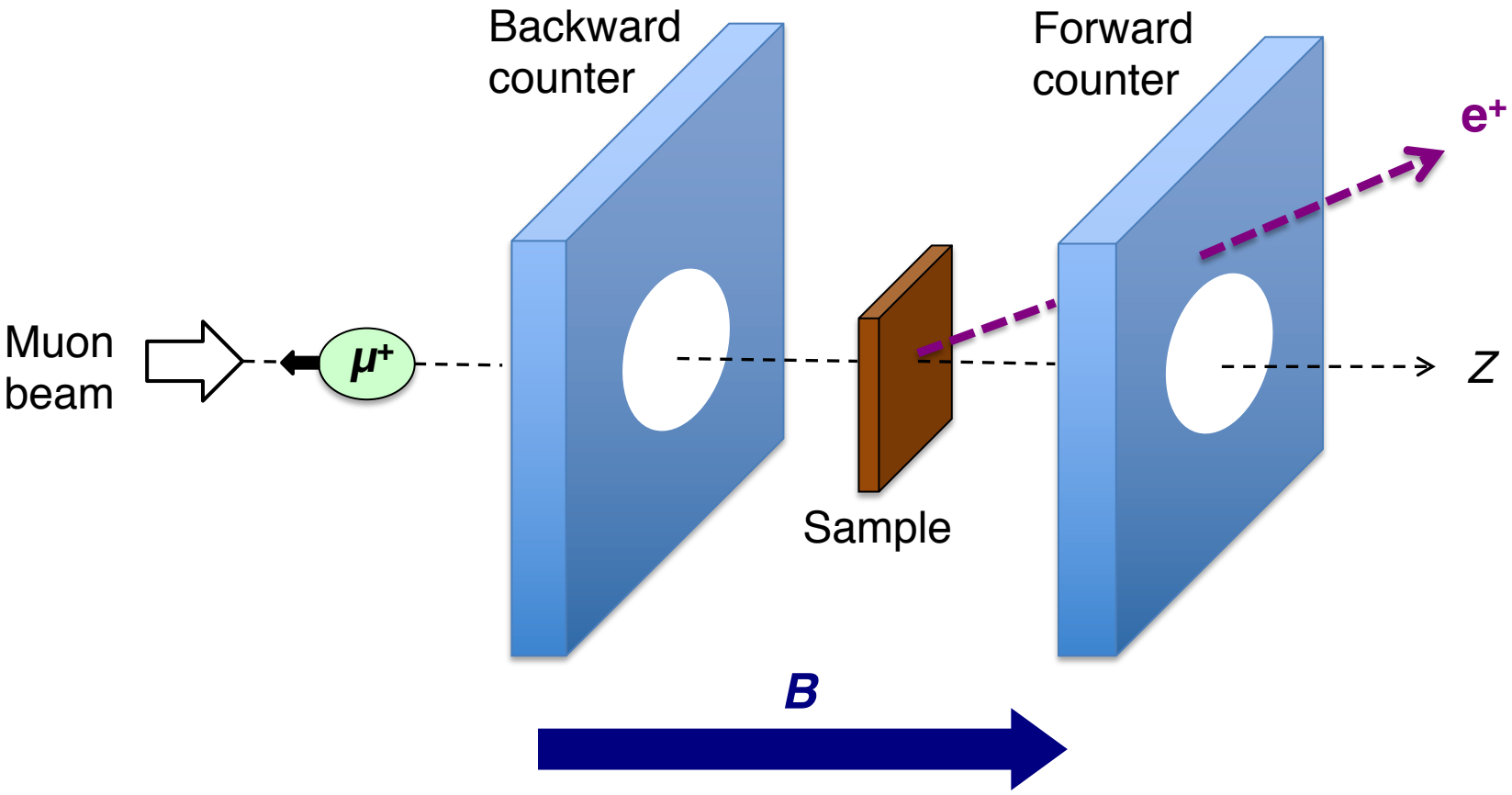
A_μ = 468.4 MHz

μ-LCR Technique

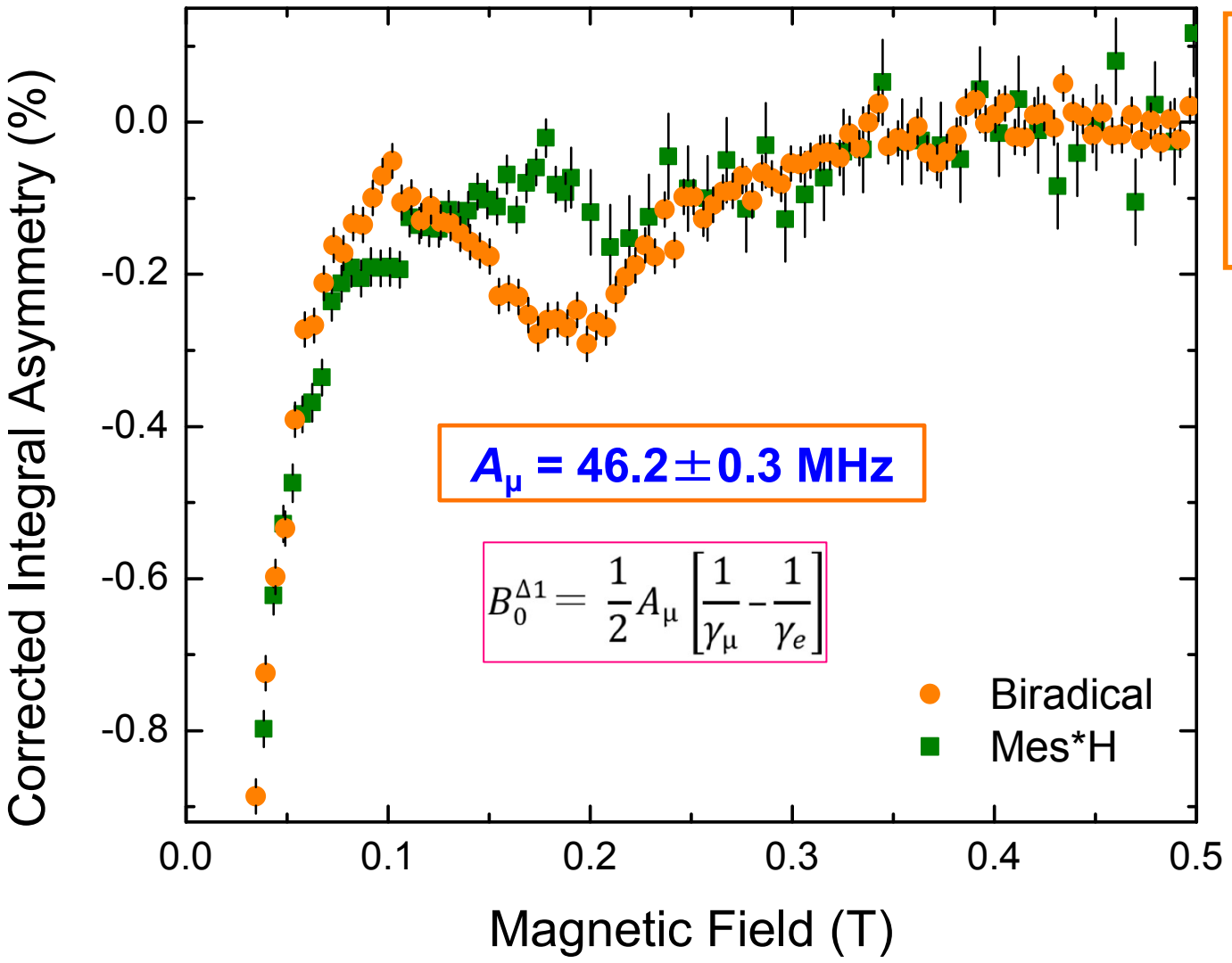
Illustration of Experiment

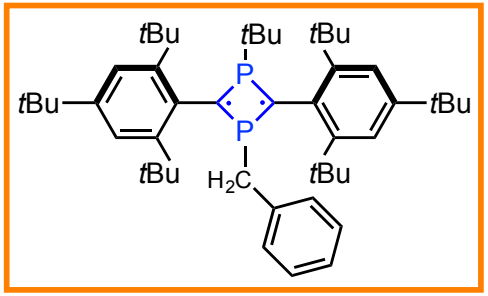
(Muon Level-Crossing Resonance)

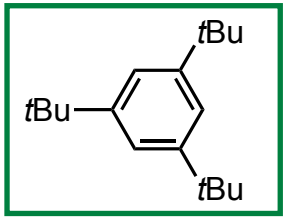
ミュオンエネルギー準位交差共鳴



μ-LCR Study of Biradical Powder

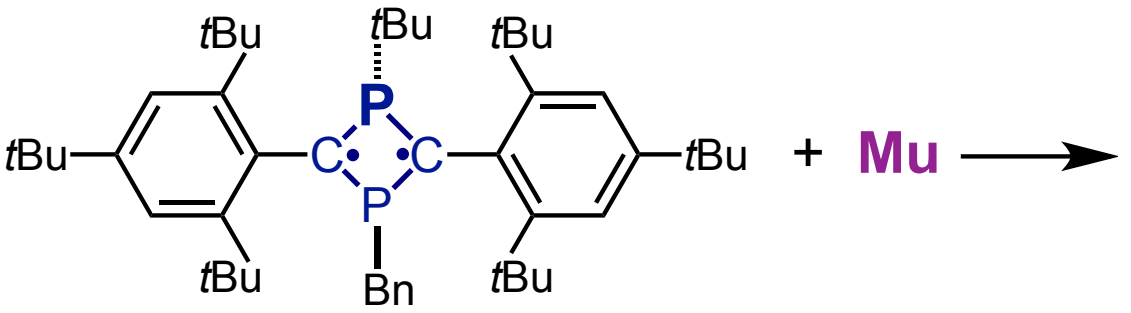


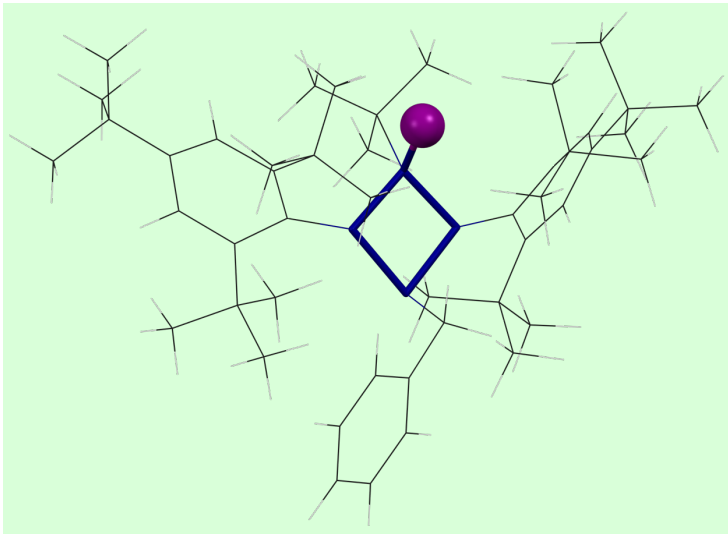




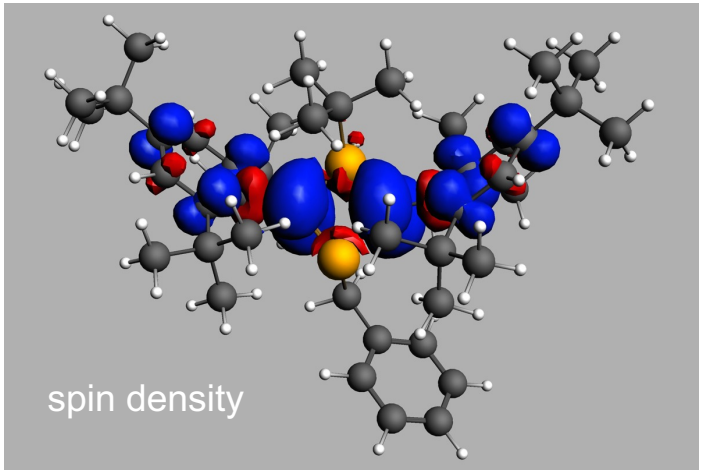
Angew. Chem. Int. Ed. **2018**, *57*, 8608.

μSR of a 1,3-Diphopshacyclobutane-2,4-diyl: Summary





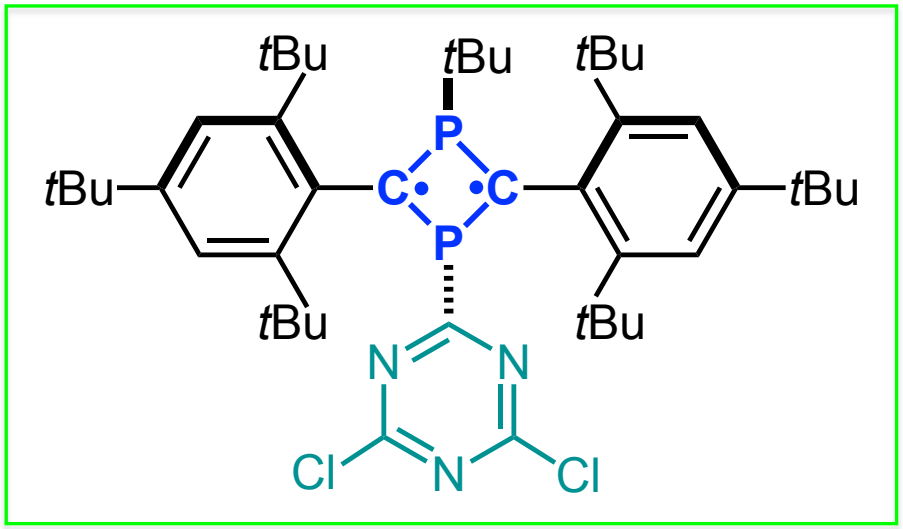
Predominant muoniation over the PCPC cycle was characterized.

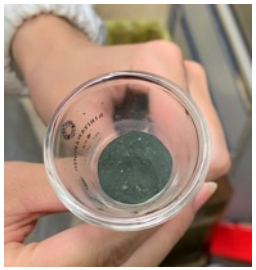


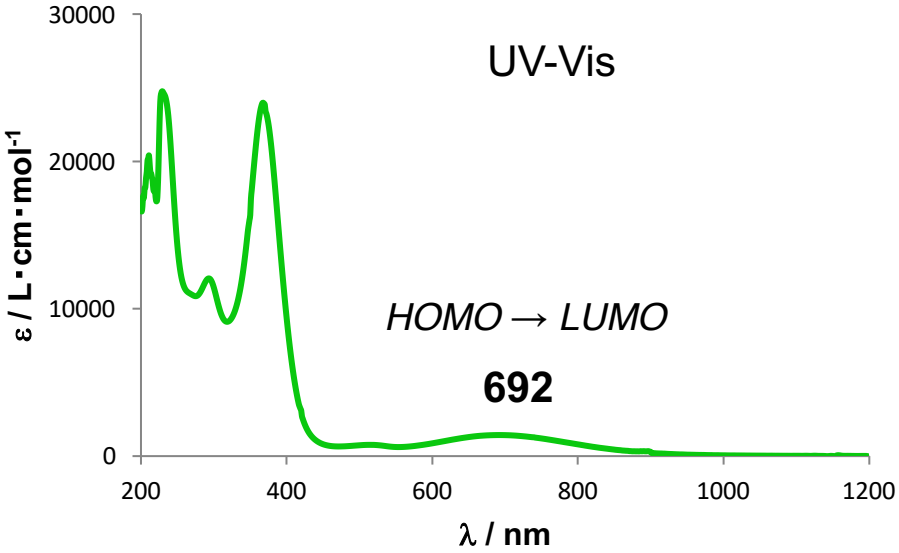
Angew. Chem. Int. Ed. **2018**, *57*, 8608.

Another Muoniated 1,3-Diphopshacyclobutane-2,4-diyl

"Small Band-Gap" Biradical





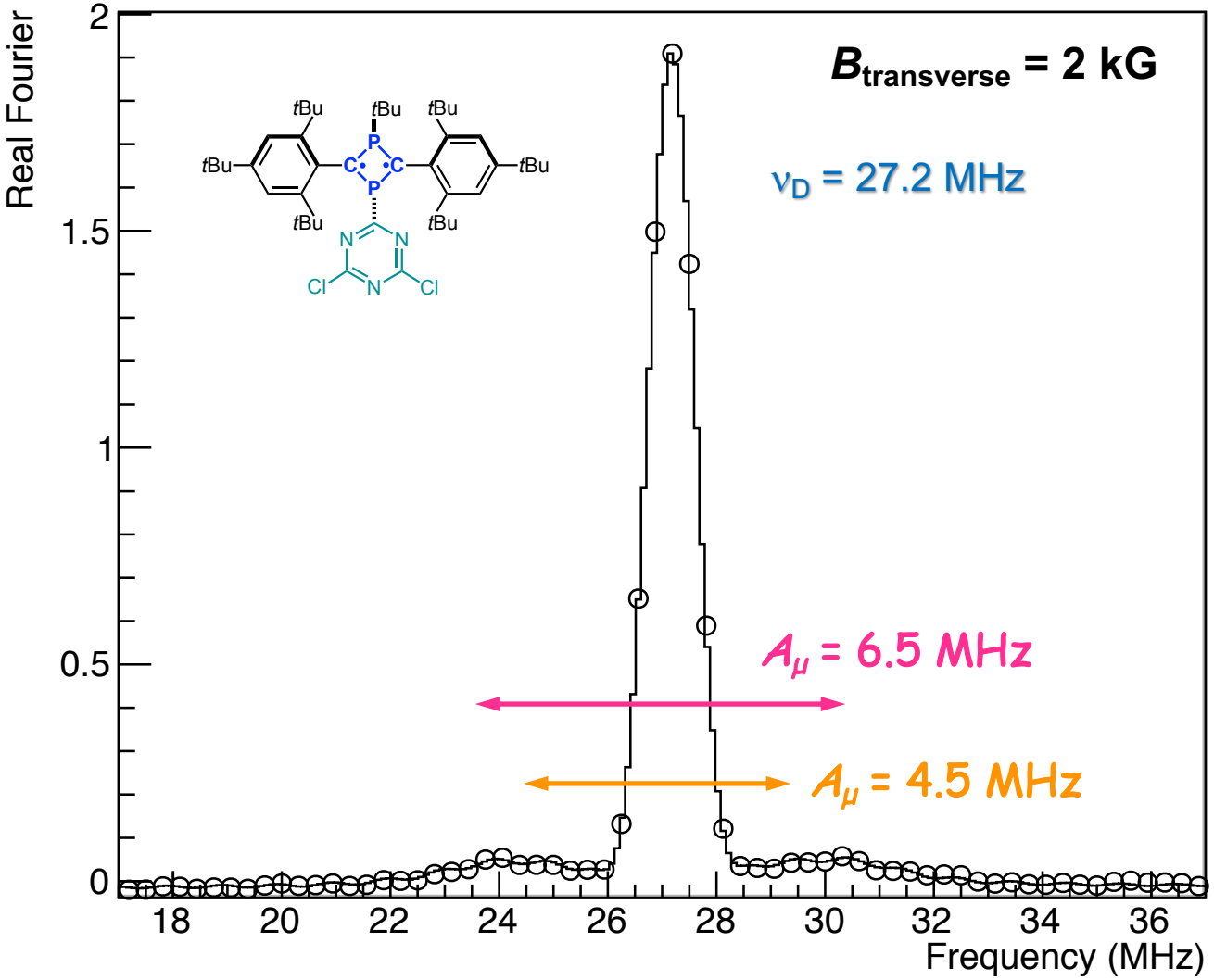


J. Am. Chem. Soc. **2013**, *135*, 17610.

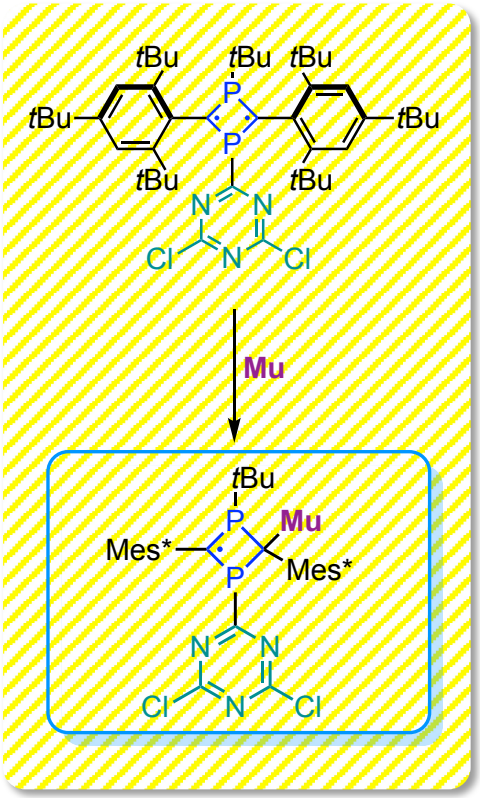
(Review)
Tetrahedron Lett. **2018**, *59*, 1.
Chem. Rec. **2018**, *17*, 445.

Another Muoniated 1,3-Diphopshacyclobutane-2,4-diyl

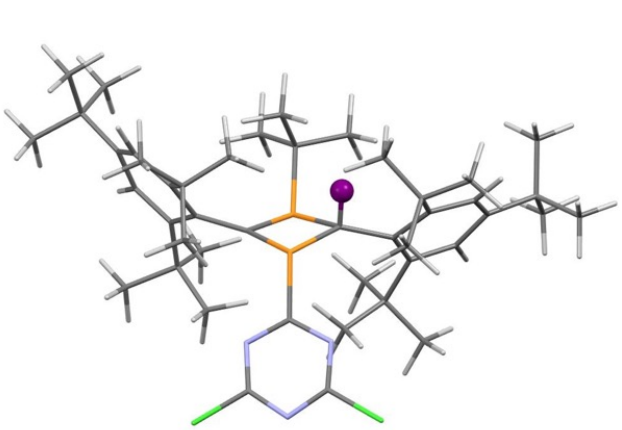
TF-μSR

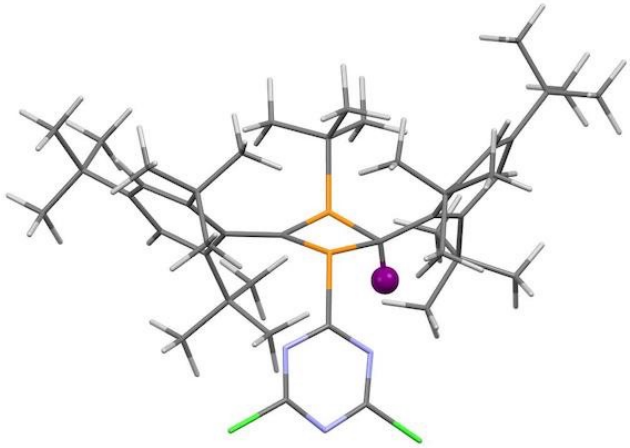


Another Muoniated 1,3-Diphopshacyclobutane-2,4-diyl



DFT Study UBP86-D3(BJ)/TZ2P-J//UwB97XD/6-311G(d,p)





$A(\mu)$ = 7.8 MHz

ΔE = +0.082 eV

$A(\mu)$ = 10.3 MHz

ΔE = 0.0 meV

Two diastereoisomers = *Consistent with the TF-μSR experiment*

Experiment $B_{transverse}$ = 2 kG

A_μ = 4.5 MHz A_μ = 6.5 MHz

Bull Chem. Soc. Jpn. **2021**, *94*, 2970.