



Hyperfine Spectroscopy and Characterization of Muonium Centers in ZnGeP_2

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Overview of MuSR



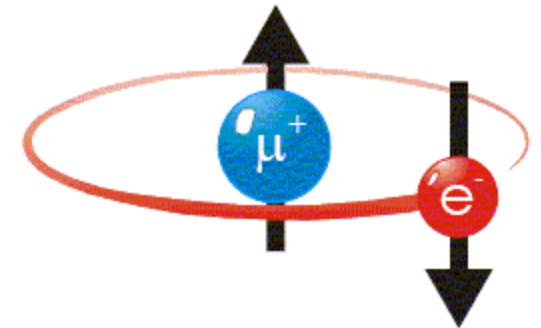
- 📌 MuSR = Muon Spin Research
(Relaxation/Rotation/Resonance)
- 📌 App: Semiconductors – exp. analog for H defects
- 📌 Implant 100% Spin-polarized Muons
- 📌 Spin vector evolves in local magnetic environment
- 📌 e^+ emitted preferentially along spin direction
- 📌 e^+ count information then analyzed

Muonium



	Muon	Proton
Mass (m_p)	0.1126 \approx 1/9	1
Spin	$\frac{1}{2}$	$\frac{1}{2}$
Gyro. Ratio, γ ($s^{-1} T^{-1}$)	8.51607×10^8 $\approx 3.2 \times \gamma_P$	2.67520×10^8
Lifetime, τ (μs)	2.19709	Stable
	Muonium	Hydrogen
Reduced e^- mass (m_e)	0.995187	0.999456
Ground-state Radius (\AA)	0.531736	0.529465
Ground-state Energy (eV)	-13.5403	-13.5984

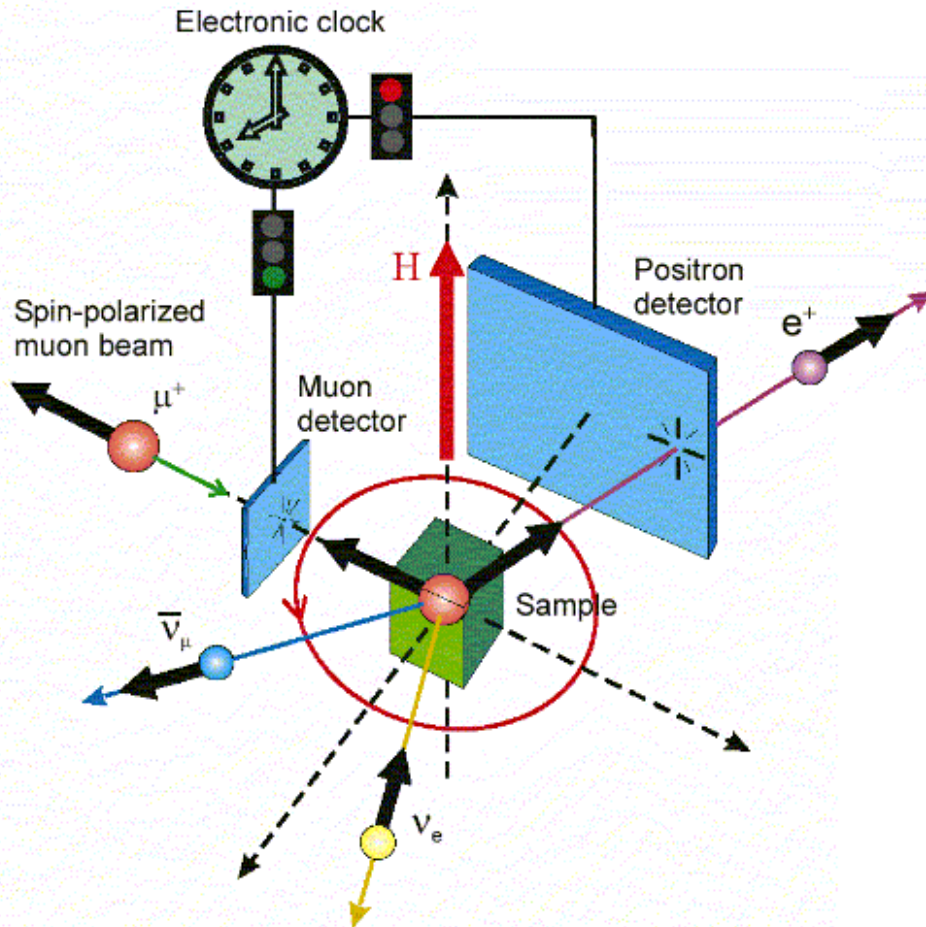
Muonium ($Mu \equiv \mu^+ e^-$)





Overview of MuSR: TF

Transverse Field (TF)- μ SR



Brewer, <http://musr.ca>

Field applied \perp to initial spin polarization
 $\rightarrow \mu^+$ spin precession about applied field

$\text{Mu}^0 = \mu^+ + e^-$
 \rightarrow spin-orbit coupling
 \rightarrow affects local field of μ^+
 \rightarrow diff prec. Freq for:
 $|\uparrow_\mu\rangle + |\uparrow_e\rangle$ & $|\uparrow_\mu\rangle + |\downarrow_e\rangle$

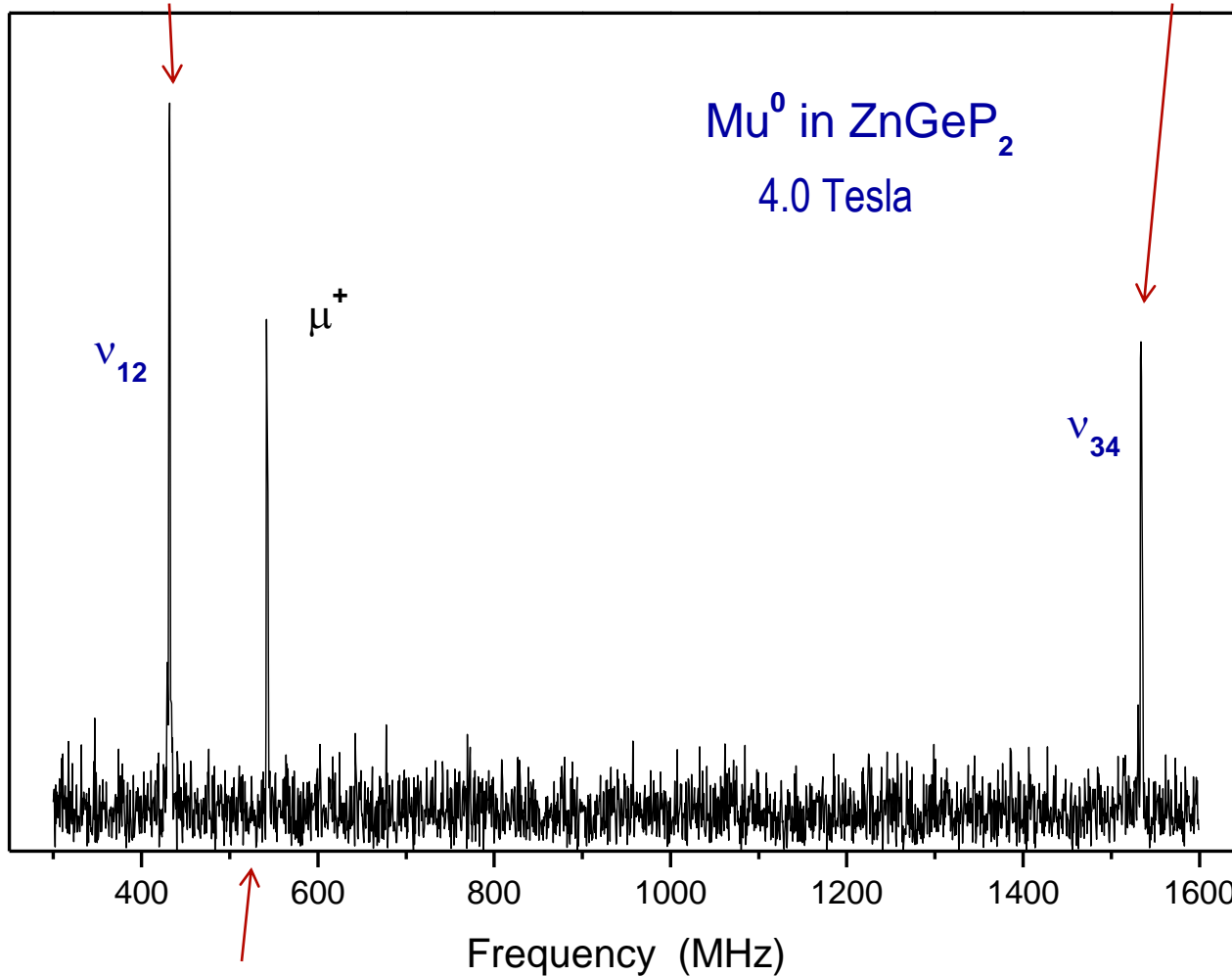
Hyperfine Spectroscopy of ZnGeP_2

(from $TF\text{-}\mu\text{SR}$)



- 431.55 MHz (+/- 0.004)

1534.07 MHz (+/- 0.06)



$$A_1 = \nu_{34} - \nu_{12} \\ = 1965.6 \text{ MHz}$$

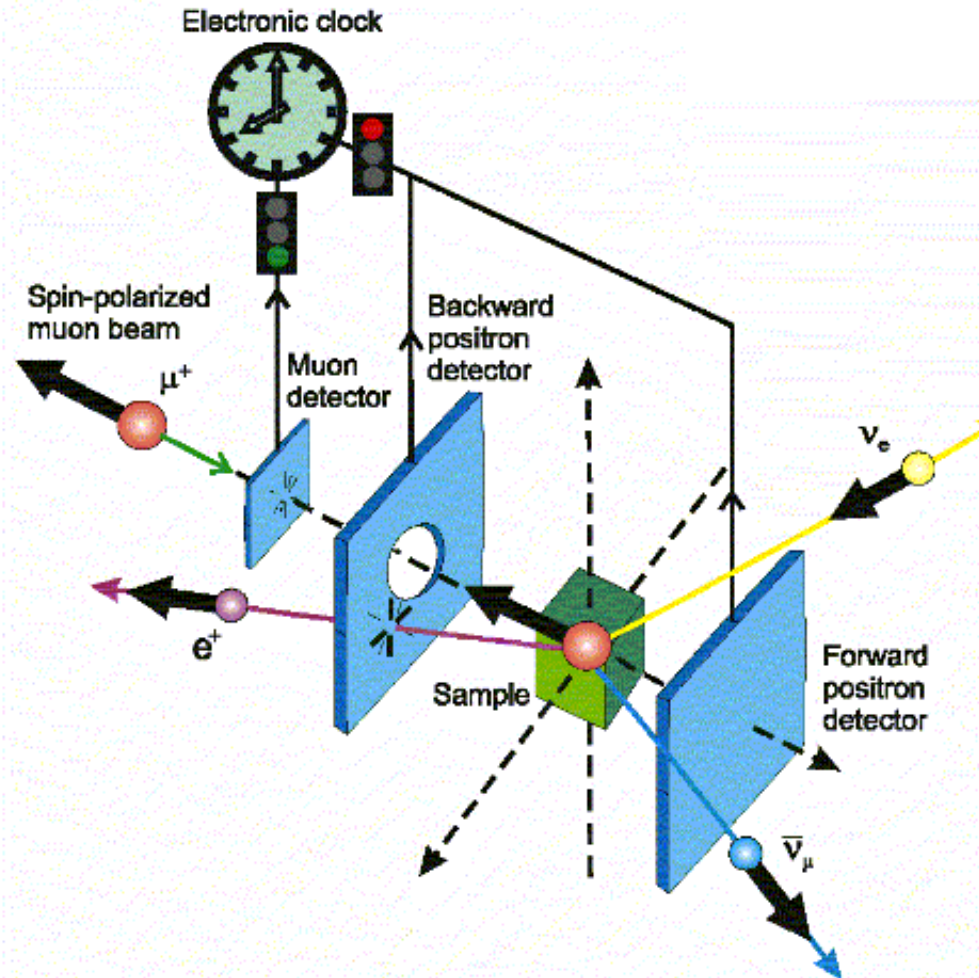
542.16 MHz



Overview of MuSR: LF

B applied \parallel to μ^+ spin pol.
→ breaks HF interaction

⇒ Change in Spin $P(t)$ from:
1) local environment (nearby nuclear moments)
2) muonium motion (e^- spin-flip w/ each site change, transferring back to μ^+ contributing to $\Delta P(t)$)



From LF- μ SR



*HF info from T_1^{-1} depolarization curves
(field dep. of Amp.)

**Current analysis suggests axially symmetric anisotropic
HF interaction with:

→ $A_2 = 3185$ MHz & $D = 374$ MHz

*F.L. Pratt, *Philos. Mag. Lett.* **75** (1997) 371.

**P.W. Mengyan, et. Al., *Physica B* (2009), doi: 10.1016/j.physb.2009.08.212

Note: TF vs LF results for HF term(s)



TF data:

$$A_1 = 1961.8 (+/- 2.3) \text{ MHz}$$

(isotropic – experimental determination)

LF data:

$$A_2 = 3185 \text{ MHz}$$

$$D = 374 \text{ MHz}$$

Why the different HF?



ZnGeP₂: Structure

Chalcopyrite structured
II-IV-V₂ material

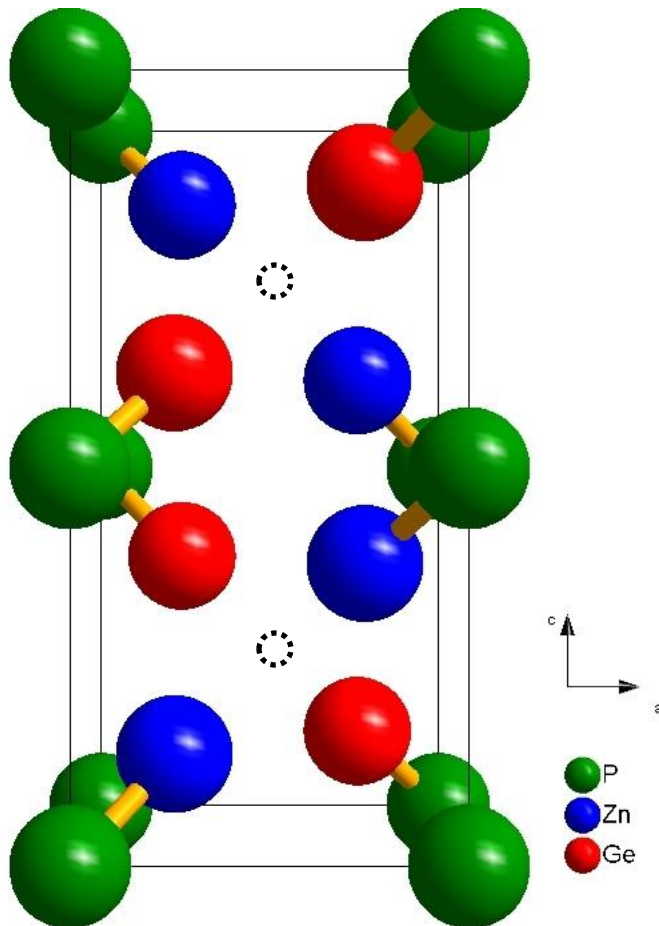
Zincblende structure (c.f. III-V),
doubled unit-cell

III-Sublattice replaced by II-IV
atoms, 1:1

V replaced by V₂

2 T-sites: T_V & T_{II-IV}

ZnGeP₂: II-IV pseudo-T-site



*Unequal charge on Zn (+1.2q_e) & Ge (+1.8q_e)
→ distorted 1s Ψ
→ anisotropy with [110] axial symmetry

$$\vec{E} = \mp \frac{1}{4\pi\epsilon_0} \frac{32\sqrt{3}}{9} (q_{Zn} - q_{Ge}) [110]$$

Seen in LF but not TF
⇒ not promptly formed, but
visited throughout lifetime

The Sample



Single Crystal

Nominally undoped

$7.1 \times 8.5 \times 1.1 \text{ mm}^3$

Orientation: [001]



Summary: Mu⁰ Centers in ZnGeP₂



- 1) Implantation
- 2) Formation of Mu⁰ in T_V
with isotropic: $A_1 = 1961.8$ (+/- 2.3) MHz
(Visible in TF)
- 3) Mu⁰ hops w/ ID change ea. hop (not discussed)
- 4) Mu⁰ in T_{II-IV} with anisotropic:
 $A_2 = 3185$ MHz $D = 374$ MHz (+/- 10%)
(Visible in LF Repolarization data)

Summary



This completes our discussion of the Muonium
centers in ZnGeP_2

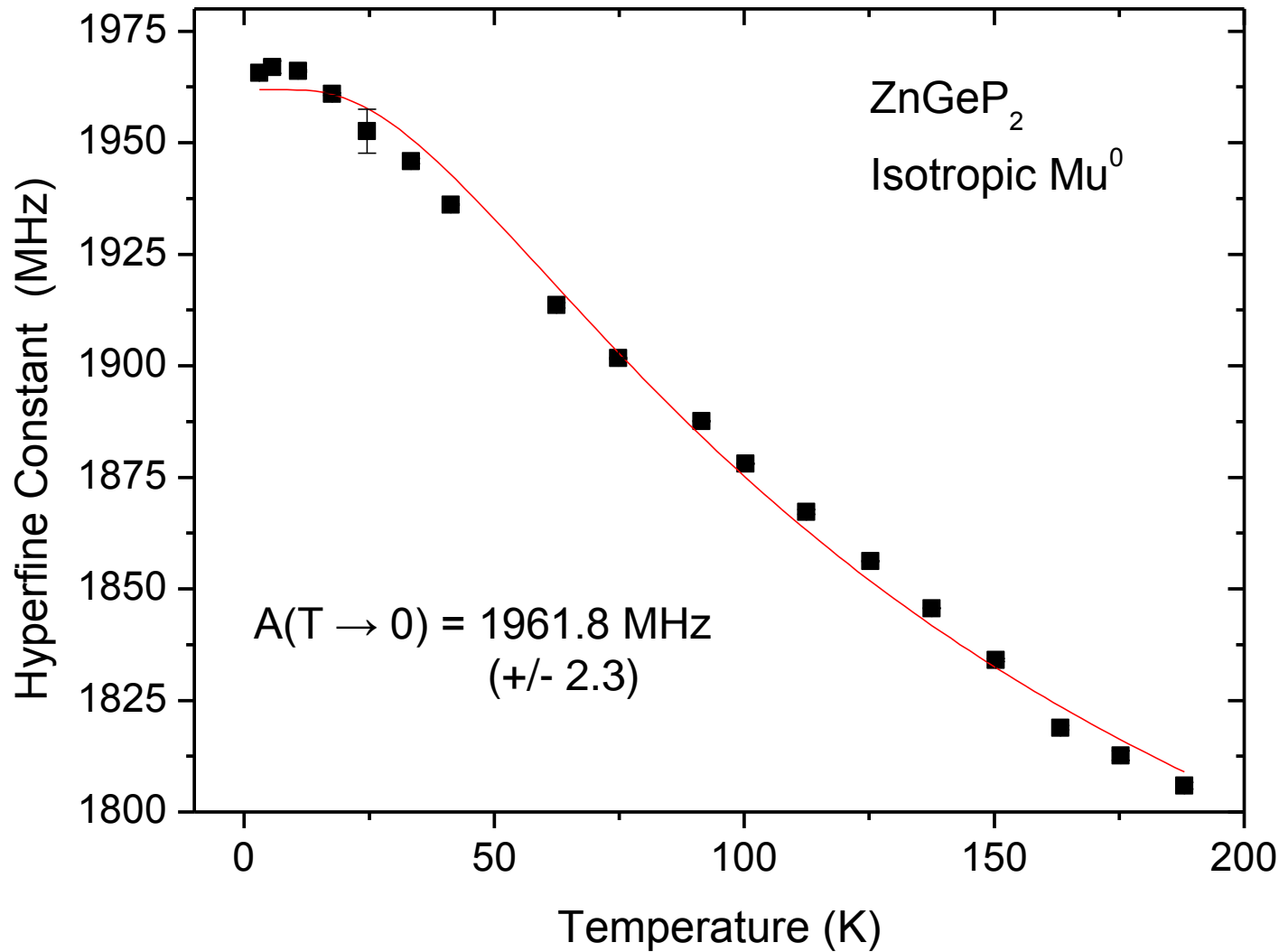
Thank You



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Hyperfine Spectroscopy of ZnGeP_2

(from $TF\text{-}\mu\text{SR}$)



ZnGeP₂: Structure



Chalcopyrite structured
II-IV-V₂ material

Zincblende structure,
doubled unit-cell

III-Sublattice replaced by
II-IV atoms, 1:1

V replaced by V₂

