

Nuclear Magnetic Resonance spectroscopy

Normal Operation Training Course



1. Syllabus

NMR Training, 2024

➤ Training Schedule

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2. Basic principles

3. Pulse sequence

4. Chemical shift

5. Tuning & Matching

Lock & Shim

6. Solid-state NMR

7. Hardware

8. Pre-treatment

9. Operation

10. Processing

11. Technical Knowhow

12. Cautions

13. FAQ

14. Basic information

15. Emergency

16. Case Study

17. References

18. External training

19. Attachments

1. NMR self-user training

- 1) Theory class (Sun-Phil Han, 4174)
- 2) Operation class (Sun-Phil Han, 4174)

2. Practice NMR yourself

- Exercise operation with self-user over 3 times or request to manager by e-mail

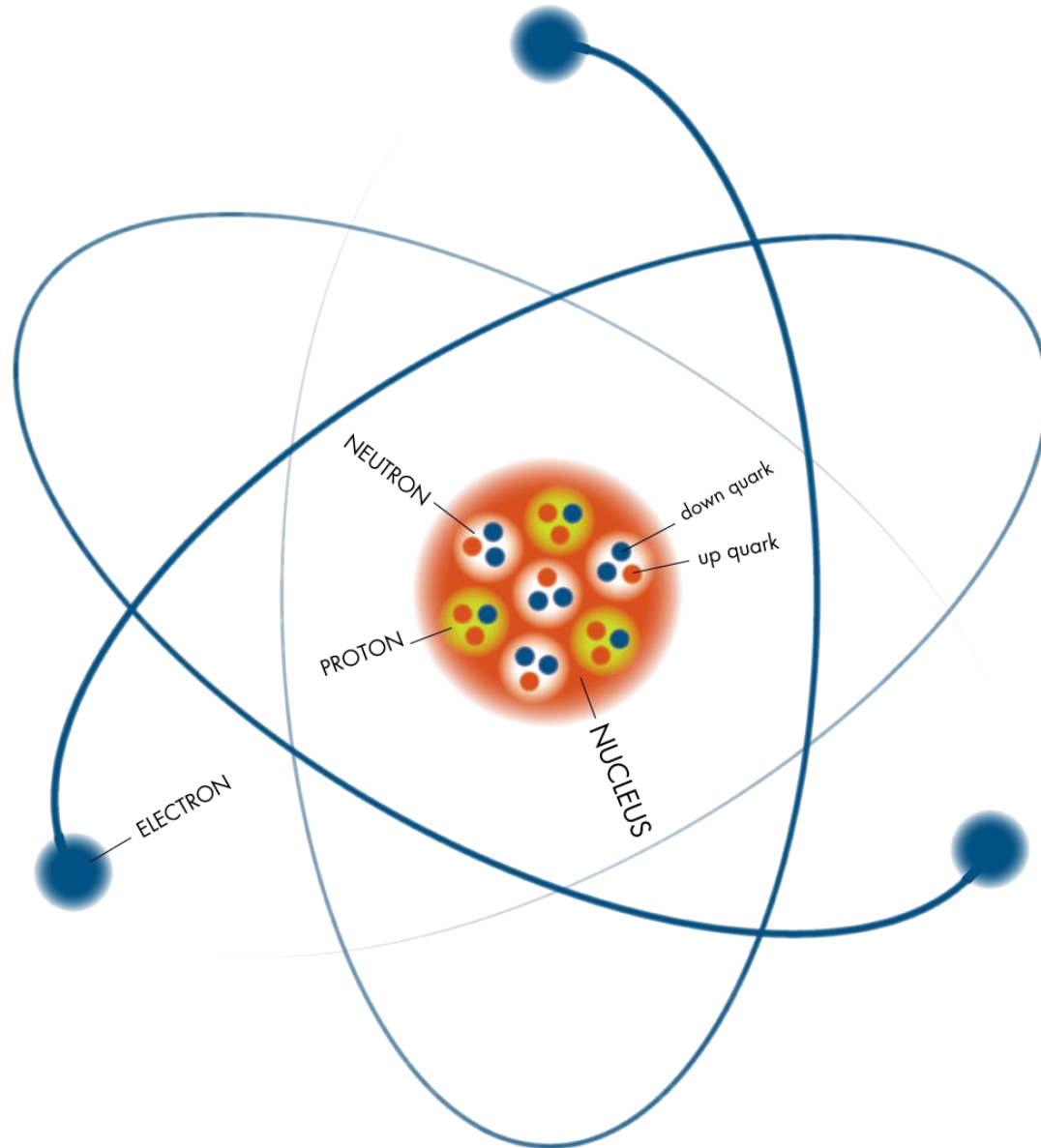
3. Attend the NMR test

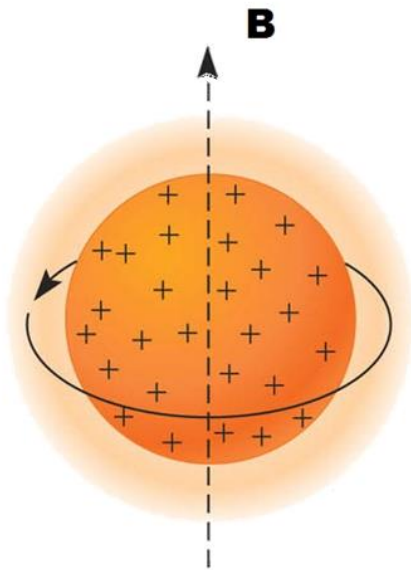
- Request for self-user test by e-mail
- The manager reserves a test time on UNIST portal.
- Test time : 30min
- Explain about NMR principle (2 ~ 3 questions)
- Acquire NMR data by using Bruker automation system(Icon-NMR)
- You have to get a self-user in one month

2. Basic principles

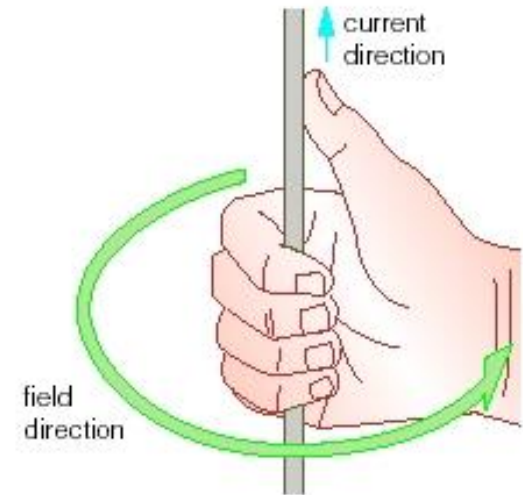
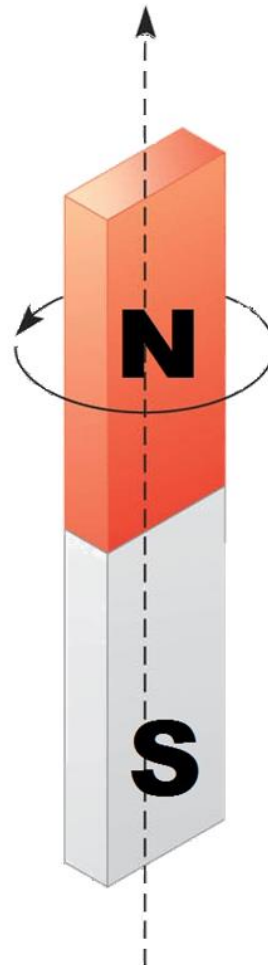
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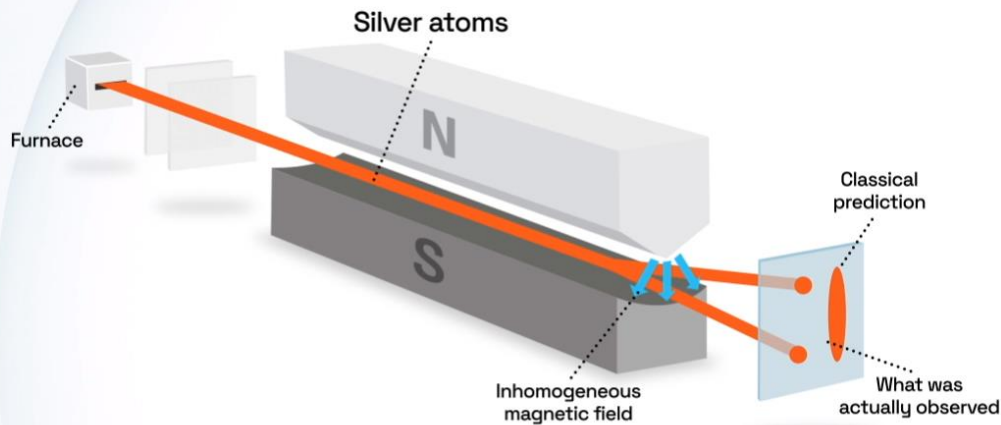


Magnetic moment



Ampere's law

지만 효과 (Zeeman effect)



슈테른 Stern - Gerlach 게를라흐 실험

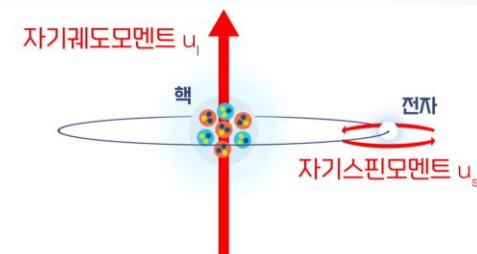
이름	기호	값	물리량
주양자수 (Principal Quantum Number)	n	1, 2, 3, 4 ...	전자 에너지 (오비탈 크기)
각운동량 양자수 (Angular Momentum Quantum Number)	l	0, 1, 2, 3, 4 ...	궤도 각운동량의 크기 (오비탈 모양)
자기양자수 (Magnetic Quantum Number)	m_l	-1, ..., -1, 0, 1, ..., l	궤도 각운동량의 방향 (오비탈 배열)
스핀양자수 (Spin Quantum Number)	m_s	+1/2 (up) -1/2 (down)	전자 스핀 방향

정상 지만 효과

자기장 내에서 spectrum이 홀수개로 갈라짐
 $= 2l + 1$

비정상 지만 효과

스핀양자수(m_s)에 따라 spectrum이 짝수 개로 나뉨
 $= 2m_s + 1$



이름	기호	값	물리량
핵스핀양자수 (Nuclear Spin Quantum Number)		+1/2 (up) -1/2 (down)	핵 스핀 방향

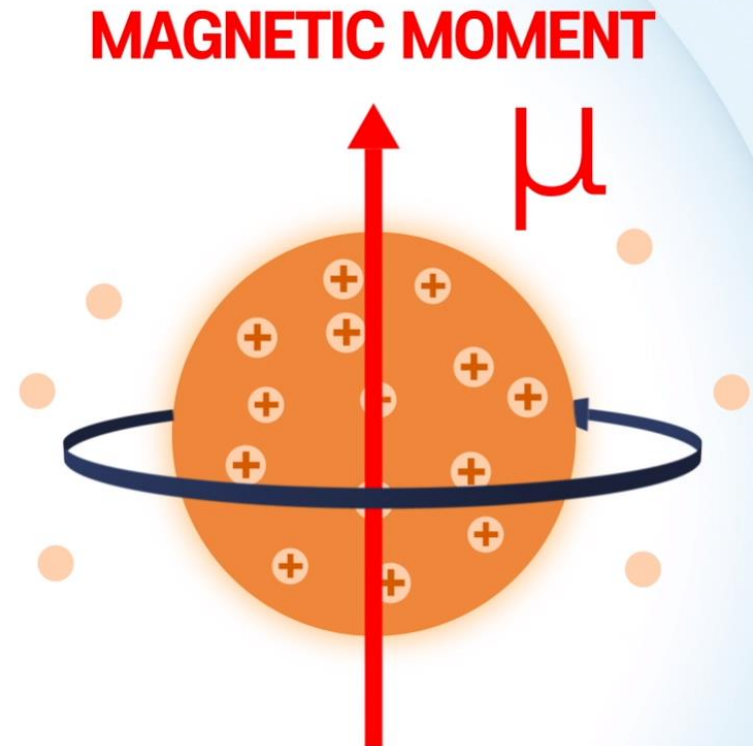
자기 모멘트 (Magnetic moment)

$$\mu = \gamma I$$

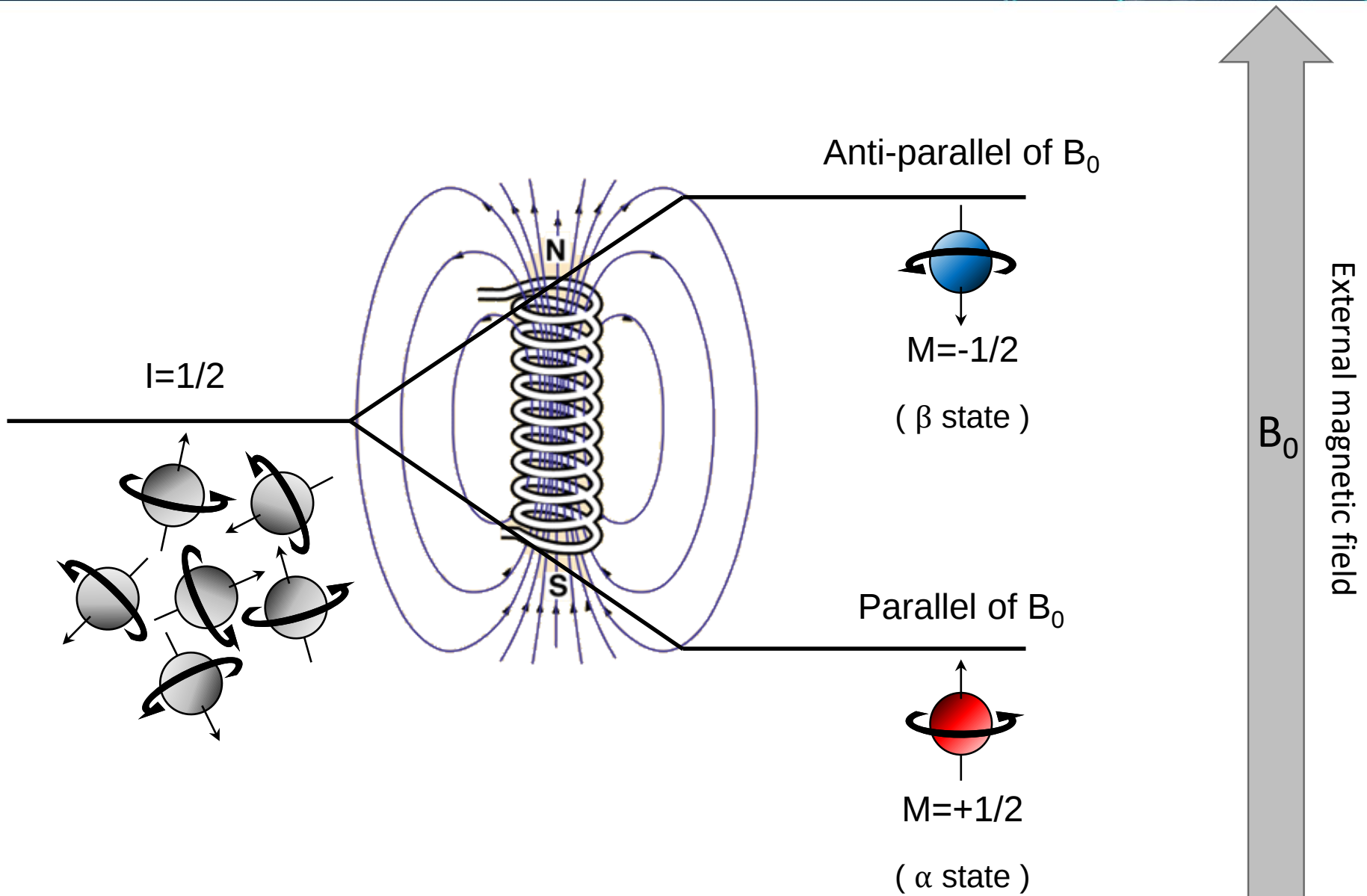
μ : 핵자기모멘트
(Nuclear magnetic moment)

γ : 자기회전비율
(Gyromagnetic moment)

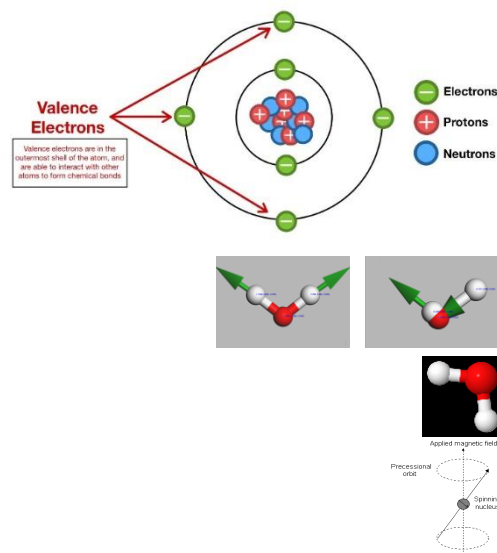
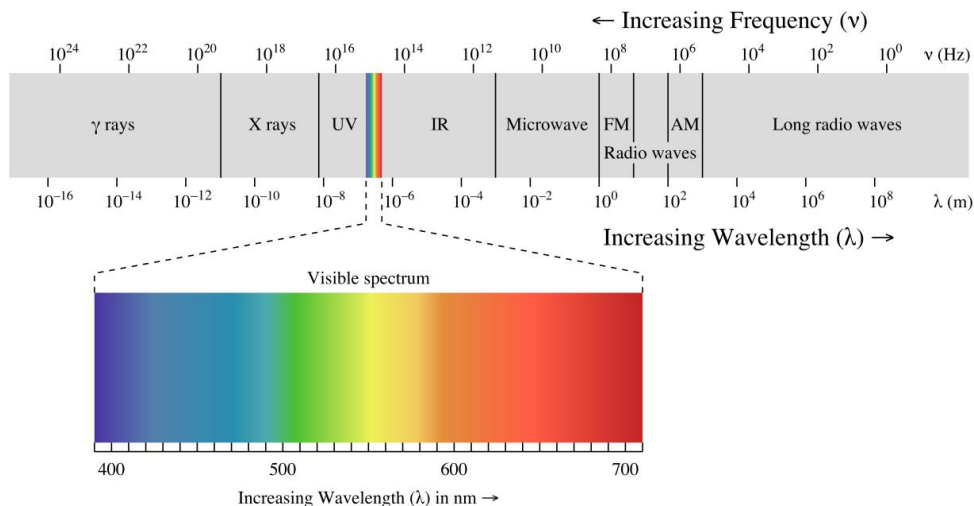
I : 핵스핀양자수
(Nuclear spin quantum number)



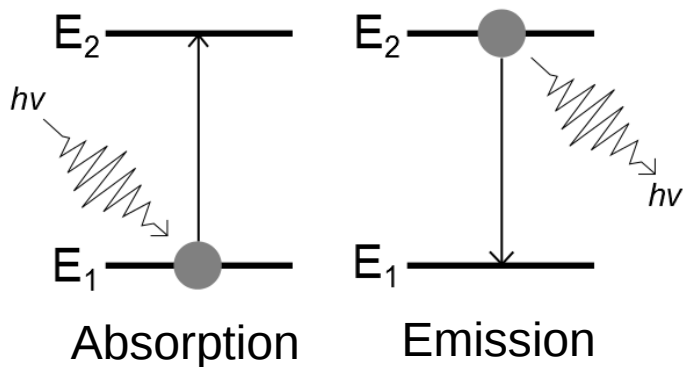
Energy states splitting (B_0)



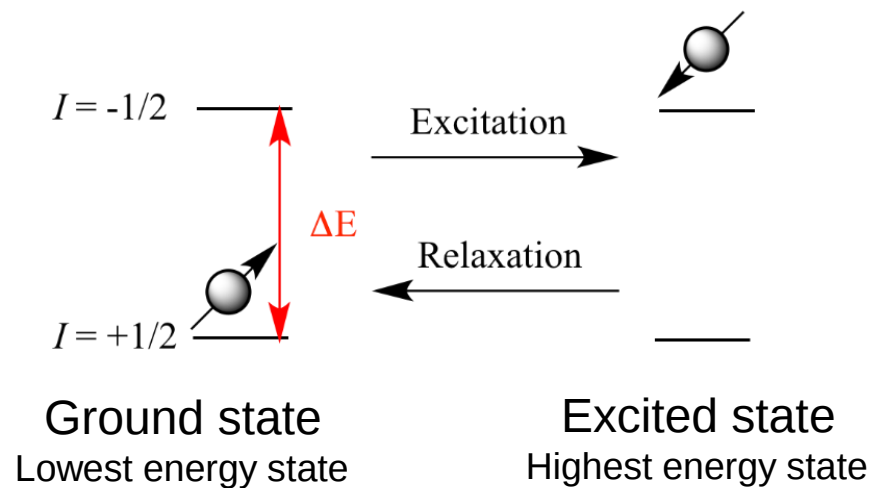
Electromagnetic spectrum



Region of electromagnetic spectrum	Interaction	Spectroscopic technique
Y-ray	Nuclear	Mossbauer spectroscopy
X-ray	Core-level electron	X-ray absorption spectroscopy
Ultraviolet (UV)	Valence electron	UV/Vis spectroscopy
Visible (Vis)	Valence electron	UV/Vis spectroscopy
Infrared (IR)	Molecular vibration	IR spectroscopy Raman spectroscopy
Microwave	Molecular rotation	Microwave spectroscopy
Radio-wave	Nuclear spin	Nuclear magnetic resonance spectroscopy



Spectroscopy



NMR

I (Nuclear spin quantum number)

Table 1. General rules for determination of nuclear spin quantum numbers

Mass Number	Number of Protons	Number of Neutrons	Spin (I)	Example
Even	Even	Even	0	^{16}O
0, 2, 4, 6 ...	Odd	Odd	Integer (1,2,...)	^2H
Odd	Even	Odd	Half-Integer (1/2, 3/2,...)	^{13}C
1, 3, 5, 7 ...	Odd	Even	Half-Integer (1/2, 3/2,...)	^{15}N

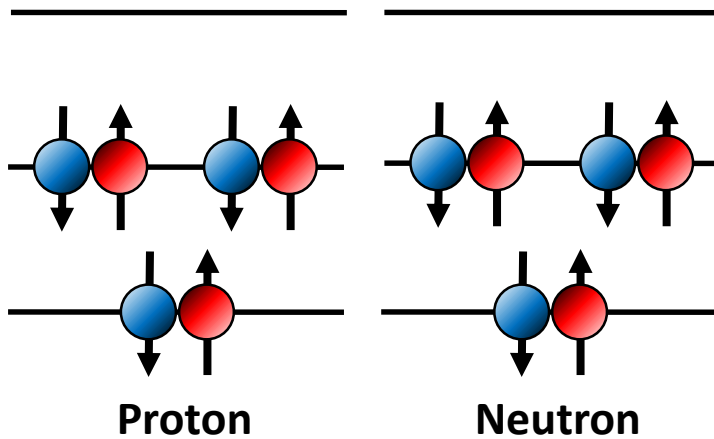
Nucleus	Spin	Resonance frequency (MHz) in field of 2.3487 T	g value
^1H	$\frac{1}{2}$	100.00	5.585
^{10}B	3	10.75	0.6002
^{11}B	$\frac{3}{2}$	32.08	1.792
^{13}C	$\frac{1}{2}$	25.14	1.404
^{14}N	1	7.22	0.4036
^{15}N	$\frac{1}{2}$	10.13	-0.5660
^{17}O	$\frac{5}{2}$	13.56	-0.7572
^{19}F	$\frac{1}{2}$	94.07	5.255
^{29}Si	$\frac{1}{2}$	19.87	-1.110
^{31}P	$\frac{1}{2}$	40.48	2.261
^{35}Cl	$\frac{3}{2}$	9.80	0.5472
^{37}Cl	$\frac{3}{2}$	8.16	0.4555
^{107}Ag	$\frac{1}{2}$	4.05	-0.2260
^{119}Sn	$\frac{1}{2}$	37.27	-2.082
^{127}I	$\frac{5}{2}$	20.00	1.118
^{199}Hg	$\frac{1}{2}$	17.83	0.996

Table 5-2 Quadrupole moments, linewidth factors and receptivities of some spin $>\frac{1}{2}$ nuclides^(a)

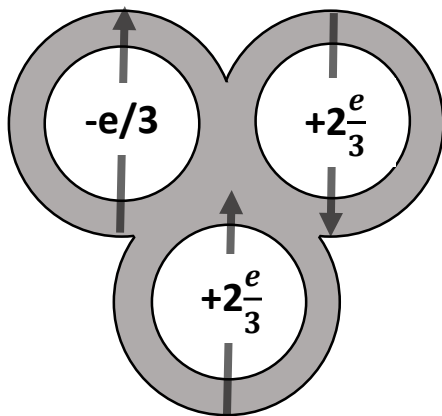
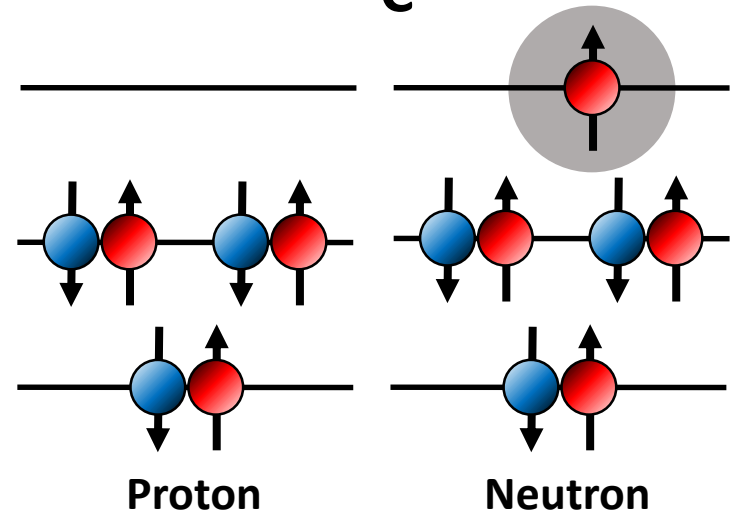
Nuclide	Spin <i>I</i>	Quadrupole moment $Q/10^{-28} \text{ m}^2$	Linewidth factor $10^{56} \ell/\text{m}^4$	Relative receptivity	
				D^p	D^c
^2H	1	2.8×10^{-3}	3.9×10^{-5}	1.45×10^{-6}	8.21×10^{-3}
^6Li	1	-8×10^{-4}	3.2×10^{-6}	6.31×10^{-4}	3.58
^7Li	$\frac{3}{2}$	-4×10^{-2}	2.1×10^{-3}	0.272	1.54×10^3
^{10}B	3	8.5×10^{-2}	1.4×10^{-3}	3.93×10^{-3}	22.3
^{11}B	$\frac{3}{2}$	4.1×10^{-2}	2.2×10^{-3}	0.133	7.52×10^2
^{14}N	1	1×10^{-2}	5×10^{-4}	1.00×10^{-3}	5.69
^{17}O	$\frac{5}{2}$	-2.6×10^{-2}	2.2×10^{-4}	1.08×10^{-5}	6.11×10^{-2}
^{35}Cl	$\frac{3}{2}$	-0.10	1.3×10^{-2}	3.56×10^{-3}	20.2
^{37}Cl	$\frac{3}{2}$	-7.9×10^{-2}	8.3×10^{-3}	6.66×10^{-4}	3.78
^{59}Co	$\frac{7}{2}$	0.38	2.0×10^{-2}	0.277	1.57×10^3
^{75}As	$\frac{3}{2}$	0.29	0.11	2.53×10^{-2}	1.44×10^2
^{127}I	$\frac{5}{2}$	-0.79	0.20	9.50×10^{-2}	5.39×10^2
^{133}Cs	$\frac{7}{2}$	-3×10^{-3}	1.2×10^{-6}	4.82×10^{-2}	2.73×10^2
^{181}Ta	$\frac{7}{2}$	3	1.2	3.65×10^{-2}	2.07×10^2

I (Nuclear spin quantum number)

$I = 0$
 ^{12}C

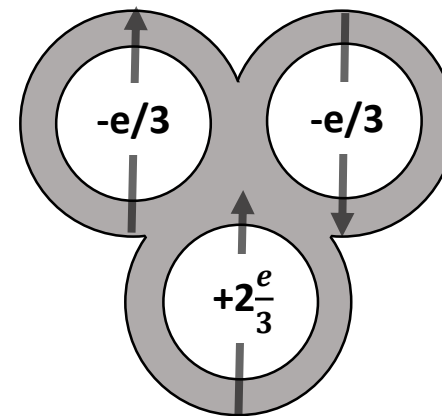


$I = 1/2$
 ^{13}C



Charge = $+e$
Spin = $1/2$

Proton

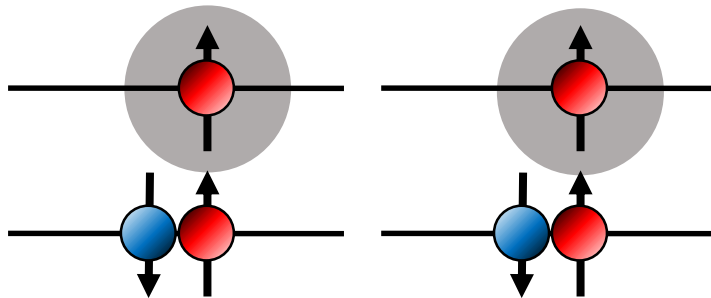


Charge = 0
Spin = $1/2$

Neutron

I (Nuclear spin quantum number)

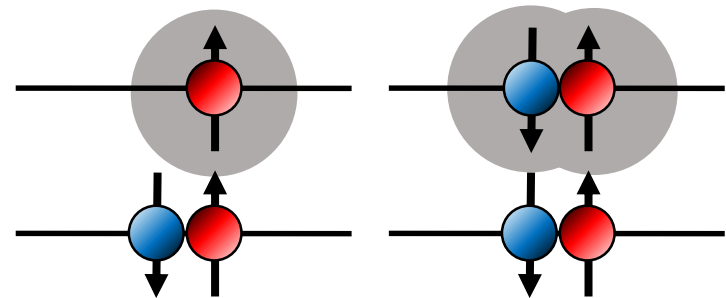
$I = 1$
 ${}^6\text{Li}$



Proton

Neutron

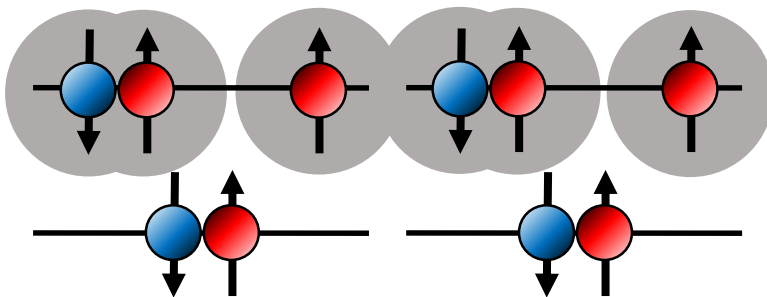
$I = 3/2$
 ${}^7\text{Li}$



Proton

Neutron

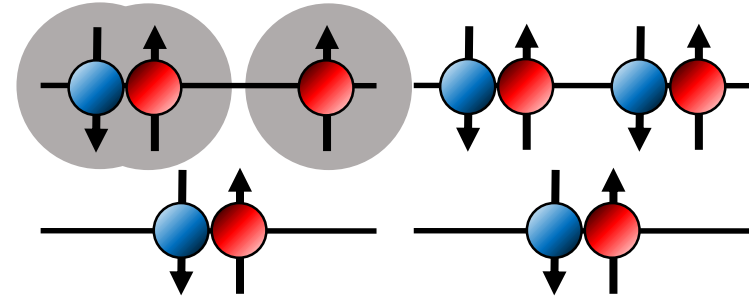
$I = 3$
 ${}^{10}\text{B}$



Proton

Neutron

$I = 3/2$
 ${}^{11}\text{B}$

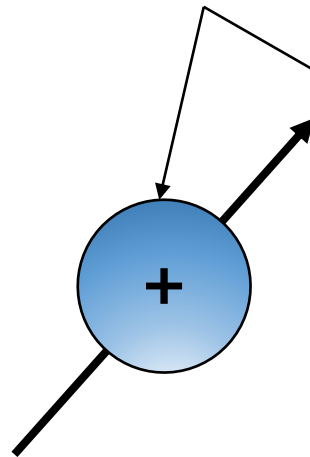


Proton

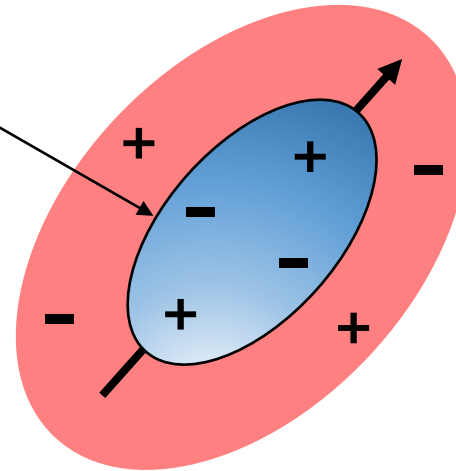
Neutron

I (Nuclear spin quantum number)

Nuclear charge distribution



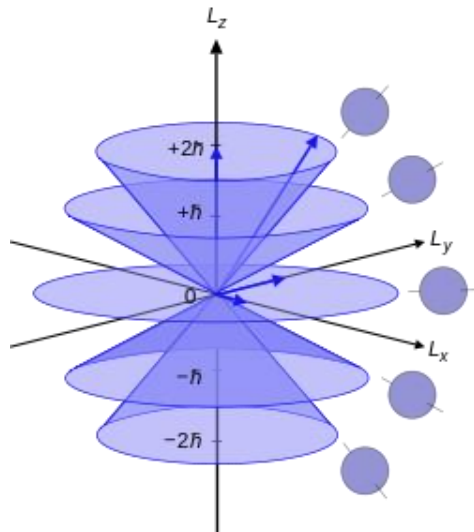
Electrical field gradient



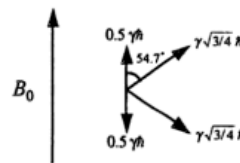
$\langle 2nl+1 \text{ rule} \rangle$

$I = 1/2$

$I > 1/2$

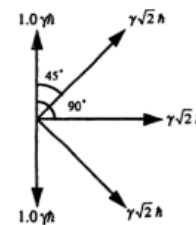


$I=1/2$



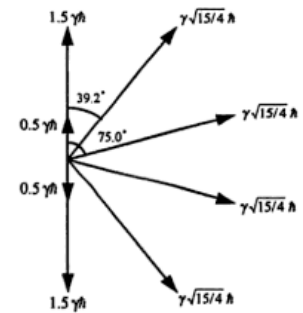
(A)

$I=1$



(B)

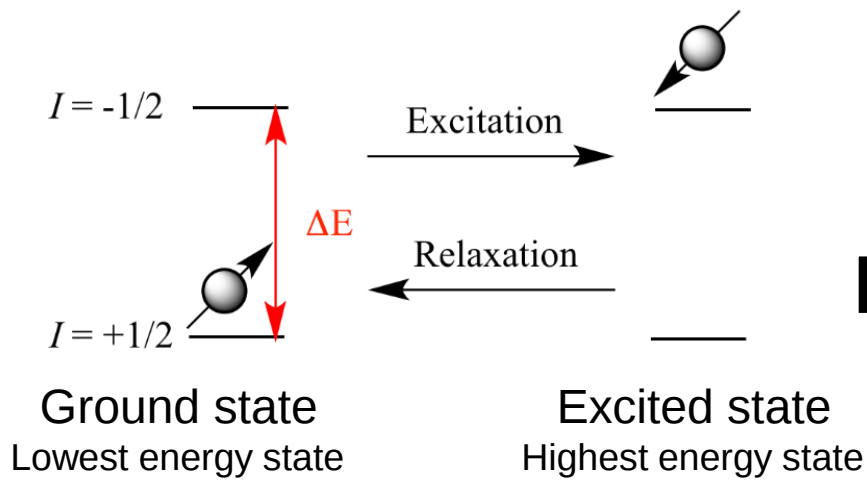
$I=3/2$



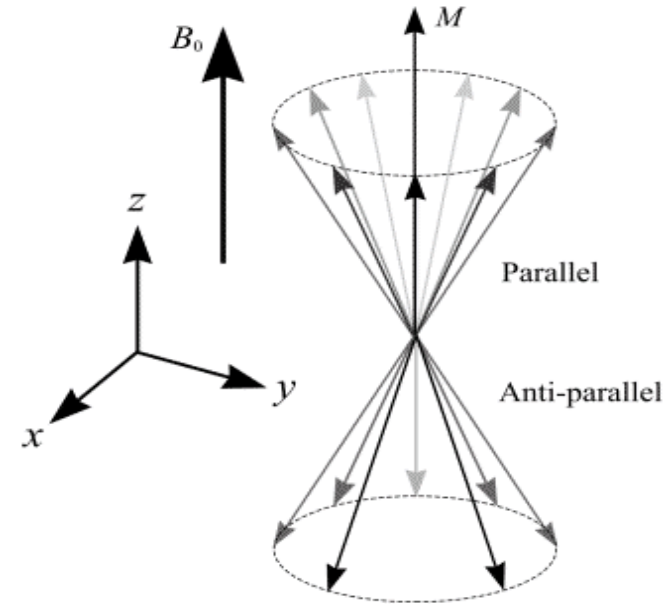
(C)

Figure 1.5 The actual magnitudes of nuclear magnetic moment vectors and their components along the z axis for nuclei with (A) spin- $\frac{1}{2}$, (B) spin-1, and (C) spin- $\frac{3}{2}$.

M_z (Net magnetization)



NMR



M_z (Net magnetization)

Energy term

$$\frac{N^-}{N^+} = \exp\left(\frac{-\Delta U}{kT}\right) = \exp\left(\frac{-\hbar\omega_0}{kT}\right)$$

$$\omega^0 = -\gamma B_0$$

$$\frac{N_{\text{antipar}}}{N_{\text{par}}} = e^{-\frac{\Delta E}{kT}}$$

$$\frac{N_a}{N_b} = e^{-\frac{\gamma \hbar B_0}{kT}}$$

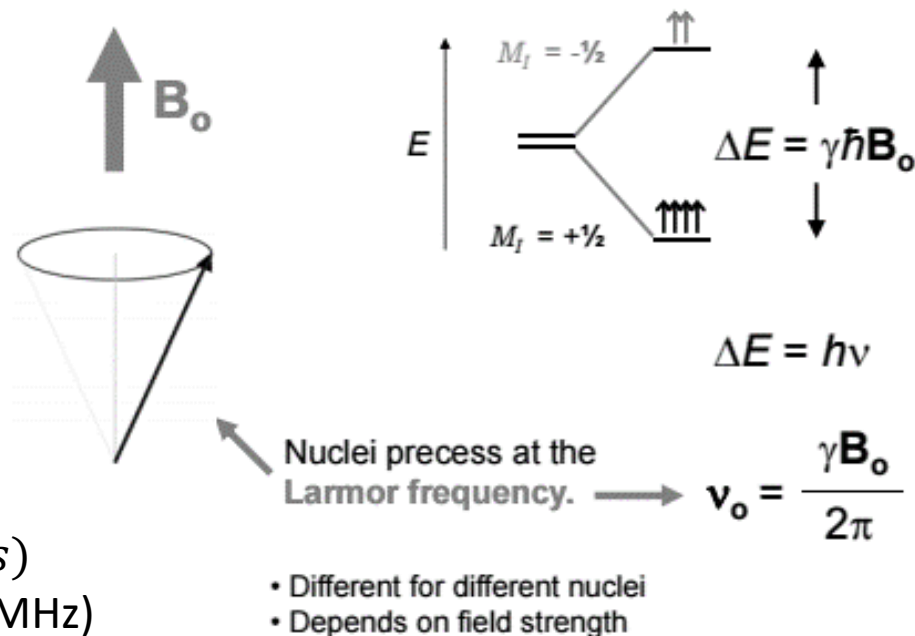
$$E_m = \frac{\gamma \hbar}{2\pi} B_0$$

E_m = Energy of quantum state m (J)

γ = Gyromagnetic ratio ($T^{-1}s^{-1}$)

h = Planck's constant ($6.628 \times 10^{-34} \text{ J s}$)

B_0 = Applied magnetic field (2.35 T = 100MHz)



$$\Delta E_m = \left[\frac{1}{2} - \left(-\frac{1}{2} \right) \right] \frac{\gamma \hbar}{2\pi} B_0 = \frac{\gamma \hbar}{2\pi} B_0$$

$$\Delta E = \frac{(2.68 \times 10^8 \text{ T}^{-1}\text{s}^{-1})(6.628 \times 10^{-34} \text{ J s})(9.38 \text{ T})}{2\pi} = 2.650 \times 10^{-25} \text{ J}$$

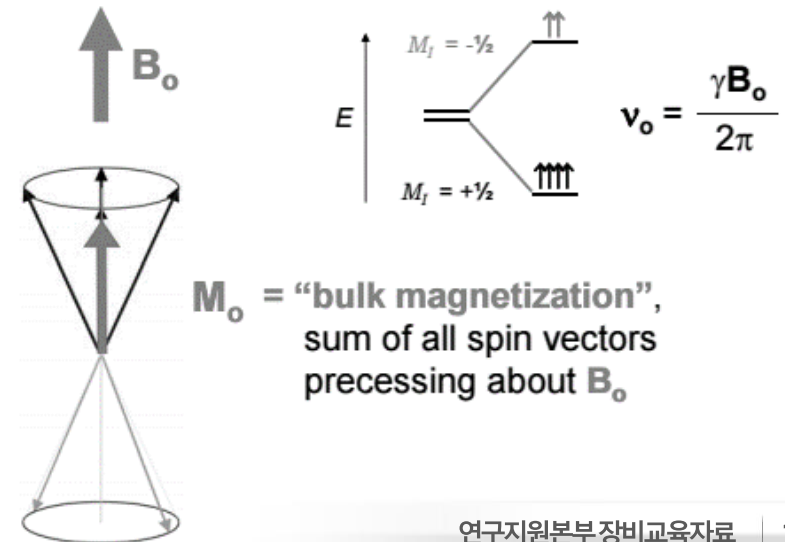
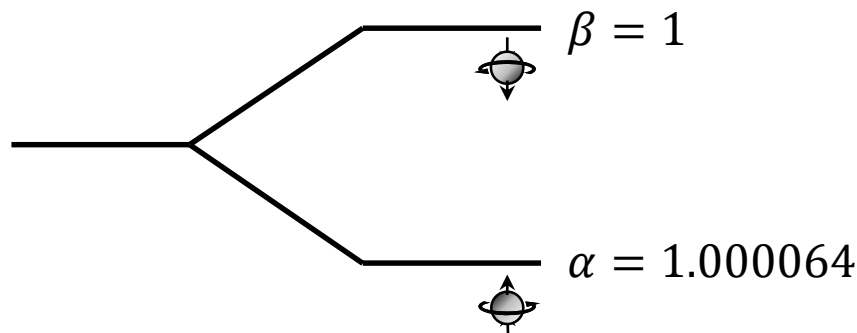
$$\nu = \frac{\Delta E}{h} = \frac{2.650 \times 10^{-25} \text{ J}}{6.626 \times 10^{-34} \text{ J s}} = 400 \times 10^6 \text{ s}^{-1} = \mathbf{400 \text{ MHz}}$$

$$V = \frac{N_\beta}{N_\alpha} = e^{\frac{\Delta E}{kT}}$$

For ^1H in 9.38 T magnet field

$$\frac{N_\beta}{N_\alpha} = e^{\frac{2.650 \times 10^{-25} \text{ J}}{(1.38 \times 10^{-23} \text{ J/K})(298 \text{ K})}} = e^{0.0000403} = 1.000064$$

$\alpha : \beta = 1.000064 : 1 \rightarrow 10^{-5}$ (Thermal Equilibration)

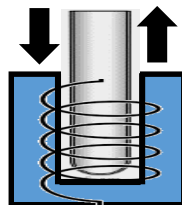


Factors of sensitivity

L-N₂ (77K) -> S/N ratio = 2~3 times

L-He (4K) -> S/N ratio = 4 time

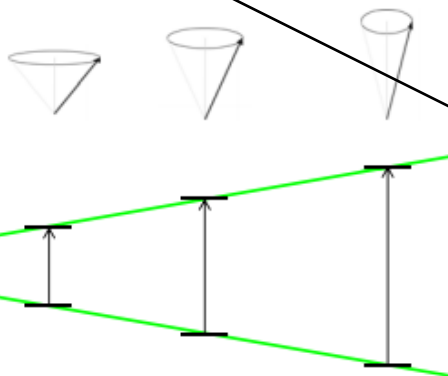
$$\frac{N_\beta}{N_\alpha} = e^{-\left(\frac{\gamma h B_0}{2\pi k T}\right)}$$



To enhance sensitivity

$B_0 \uparrow$ $\gamma \uparrow$ $T \downarrow$

$$\nu_0 = \frac{\gamma B_0}{2\pi}$$



B_0	4.73 T	9.46 T	11.75 T
ν_0 (^1H)	200 MHz	400 MHz	500 MHz
ν_0 (^{13}C)	50 MHz	100 MHz	125 MHz

$$100 \text{ MHz} = 2.35 \text{ T}$$

great nucleus.

not so great.

poor.

also great.

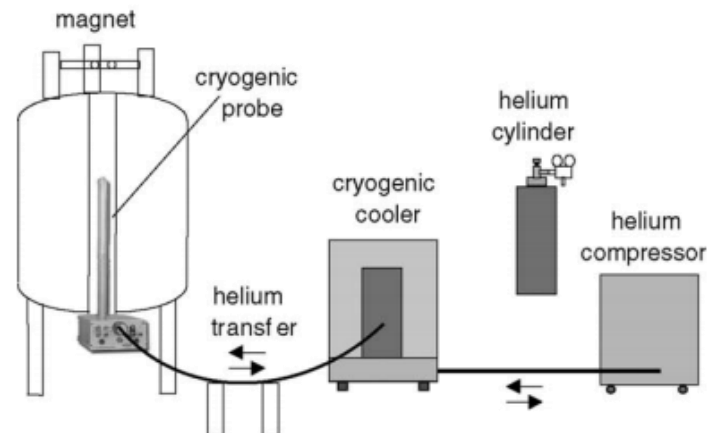
also great.

Nuclei of Major Interest to NMR Spectroscopists							
Isotope	Abundance (%)	Z	Spin	μ^a	$\gamma \times 10^{-8}^b$	Relative ^c sensitivity	ν_0 at 1T (MHz)
^1H	99.9844	1	1/2	2.7927	2.6752	1	42.577
^2H	0.0156	1	1	0.8574	0.4107		6.536
^{10}B	18.83	5	3	1.8006	0.2875		4.575
^{11}B	81.17	5	3/2	2.6880	0.8583		13.660
^{13}C	1.108	6	1/2	0.7022	0.6726	X 32	10.705
^{14}N	99.635	7	1	0.4036	0.1933		3.076
^{15}N	0.365	7	1/2	-0.2830	-0.2711	X 300	3.15
^{19}F	100	9	1/2	2.6273	2.5167	0.83	40.055
^{29}Si	4.70	14	1/2	-0.5548	-0.5316		8.460
^{31}P	100	15	1/2	1.1305	1.0829	6.65×10^{-2}	17.235

^a Magnetic moment in units of the nuclear magneton, $eh/(4\pi m_p c)$.

^b Magnetogyric ratio in SI units.

^c For equal numbers of nuclei at constant field.



S/N (Signal to Noise) ratio

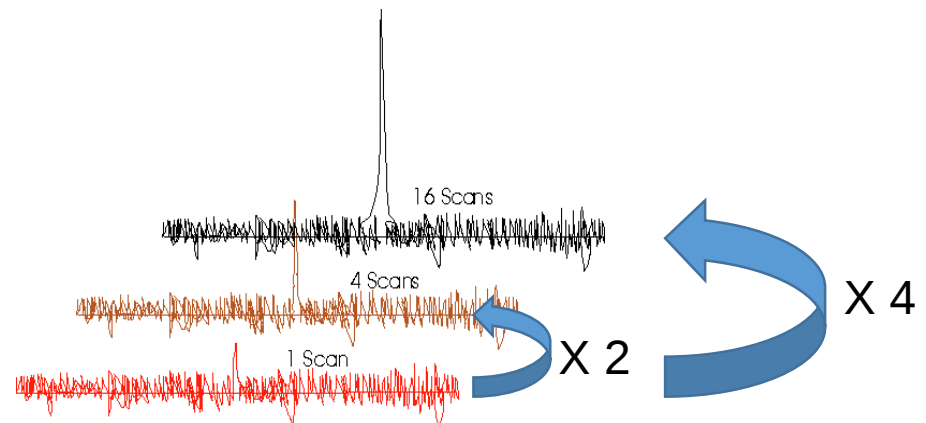
$$S/N \sim n \gamma^{5/2} B_0^{3/2} (NS)^{1/2}$$

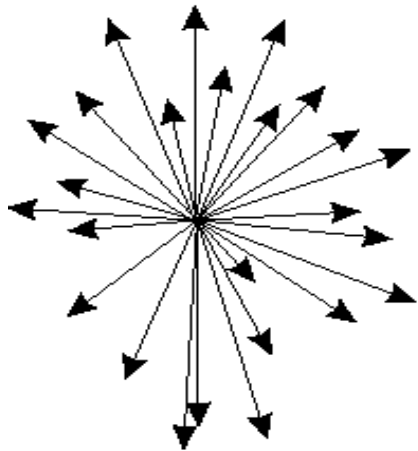
Number of spins Number of scans

1. 핵의 개수에 비례(몰수, 몰농도에 비례)
2. 비교자기장/기존자기장의 3/2 제곱만큼 감도 상승
3. 스캔수의 1/2 제곱

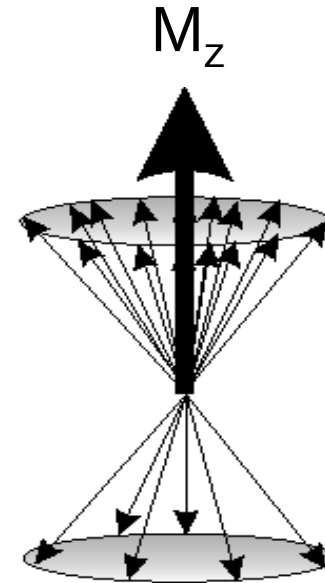
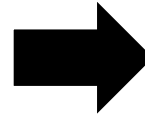
600 MHz + Cryo(N₂) = 950 MHz

$\left(\frac{600}{400}\right)^{3/2}$	S/N ratio	Time
= 1.84		3.38
$\left(\frac{950}{600}\right)^{3/2}$		
= 1.99		3.96
$\left(\frac{950}{400}\right)^{3/2}$		
= 3.66		13.40





No magnetic field (B_0)



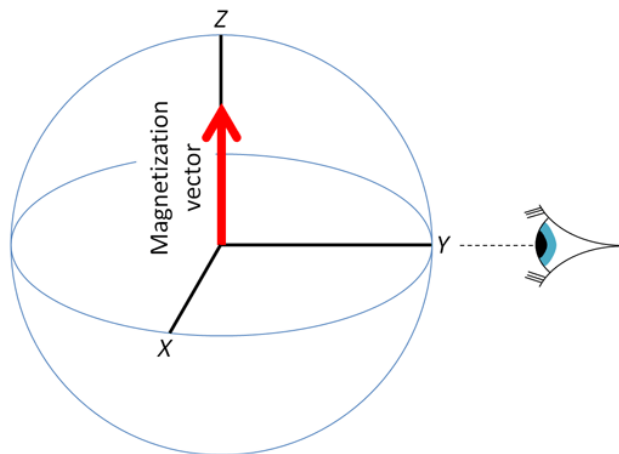
Spins in magnetic field (B_0)

3. Pulse sequence

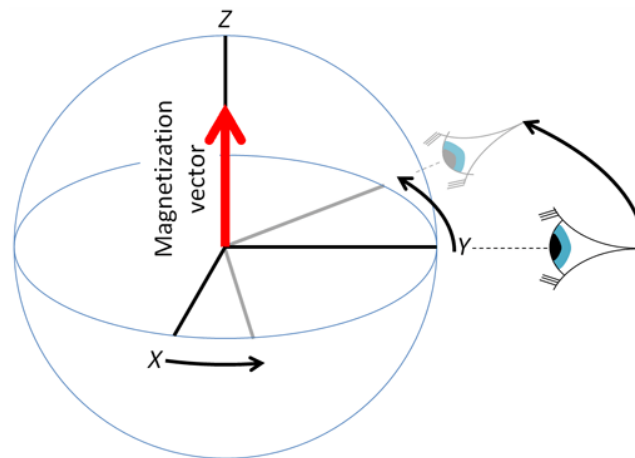
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<Laboratory frame>



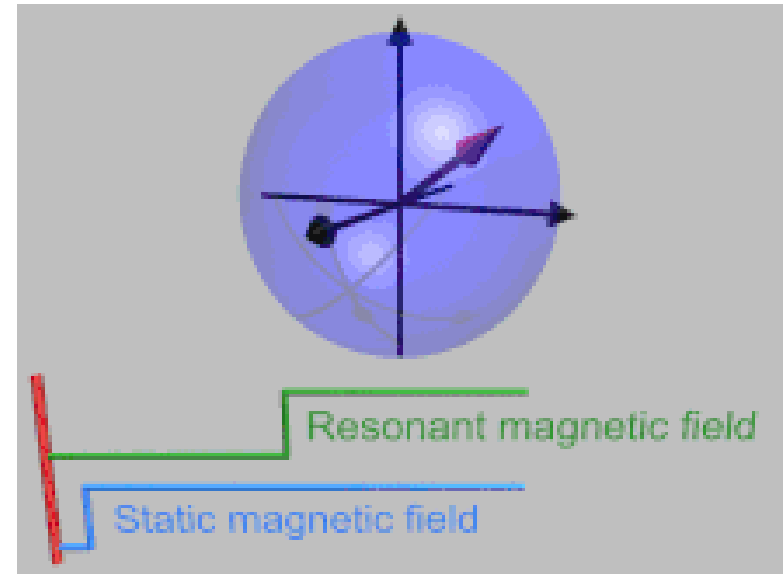
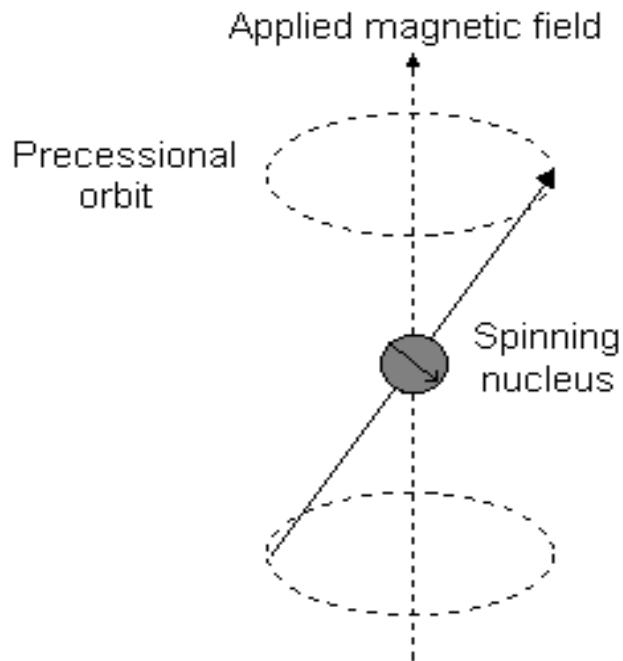
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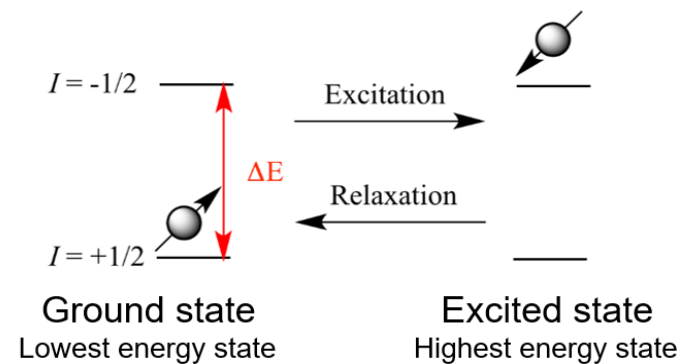
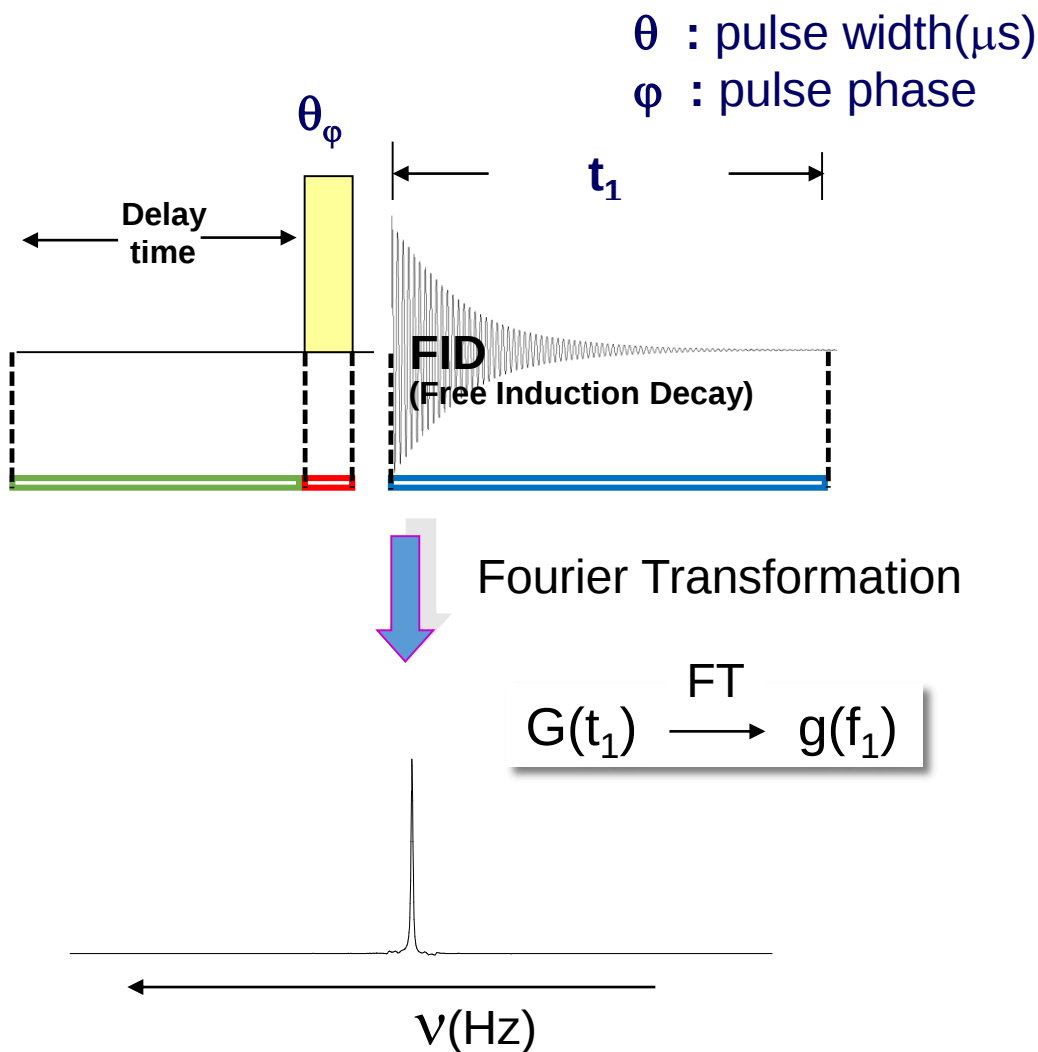
Merry-go-round viewed from the laboratory frame



Merry-go-round viewed from the rotating frame



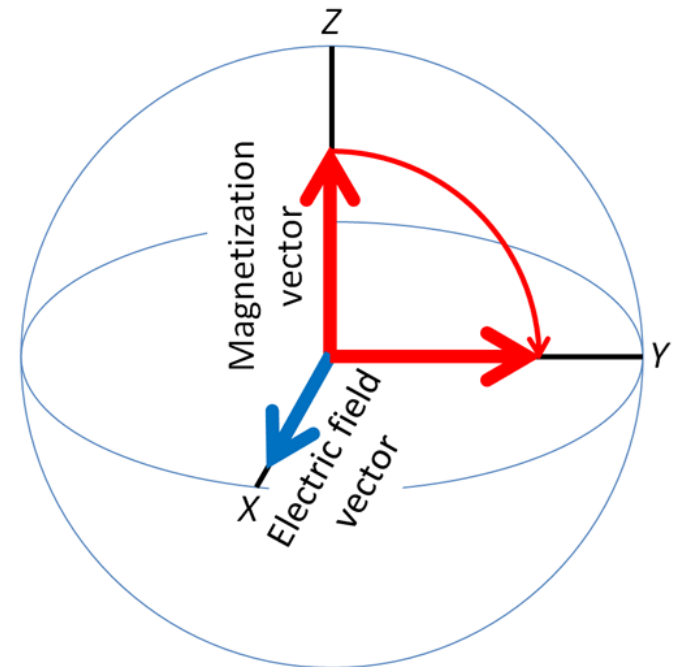
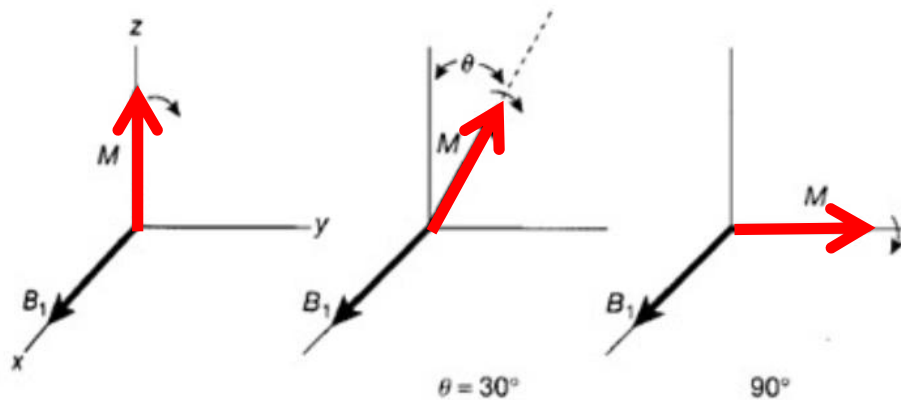
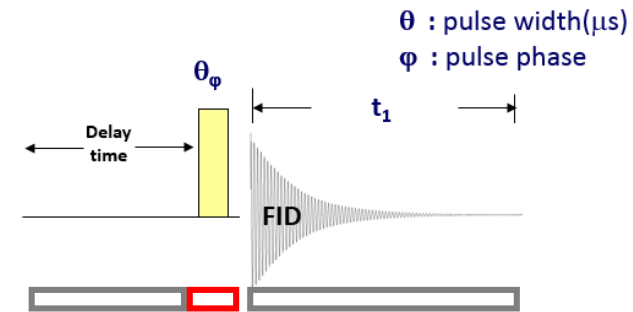
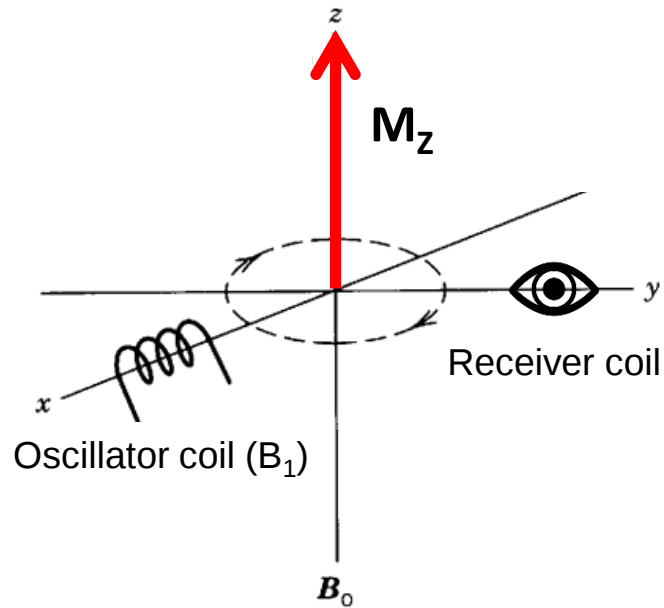
Basic 1D NMR

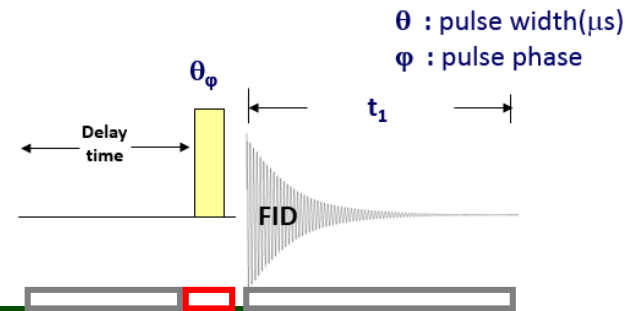


NMR

Parameter

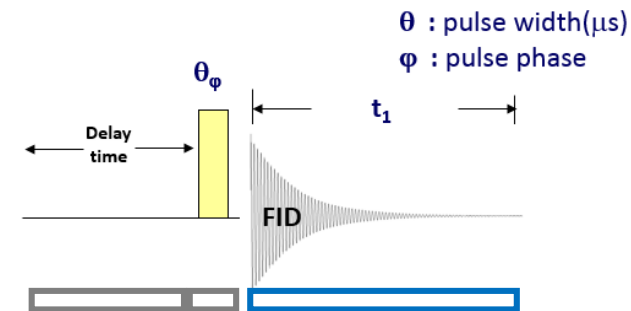
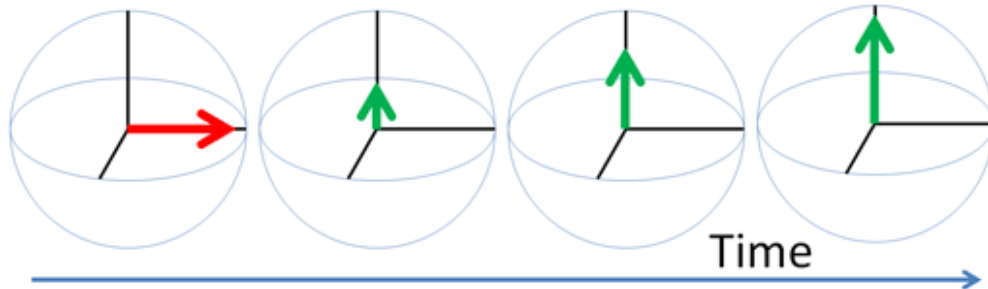
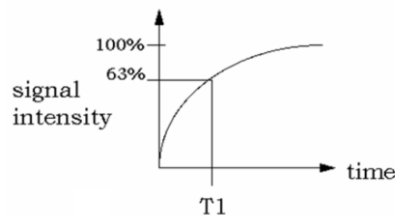
- D1 (Relaxation delay time)
- P1 (Pulse width)
PLW1 (Power level)
- AQ (Acquisition time)





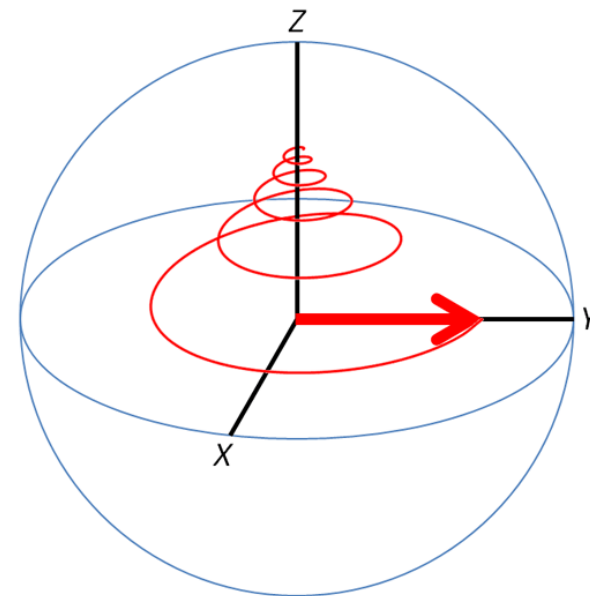
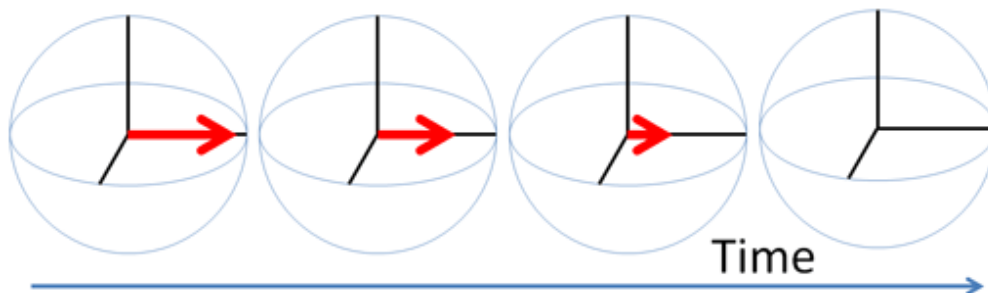
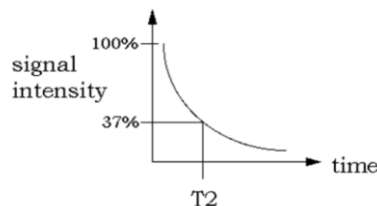
T1 relaxation (recovery)

- longitudinal relaxation
- spin-lattice relaxation



T2 relaxation (decay)

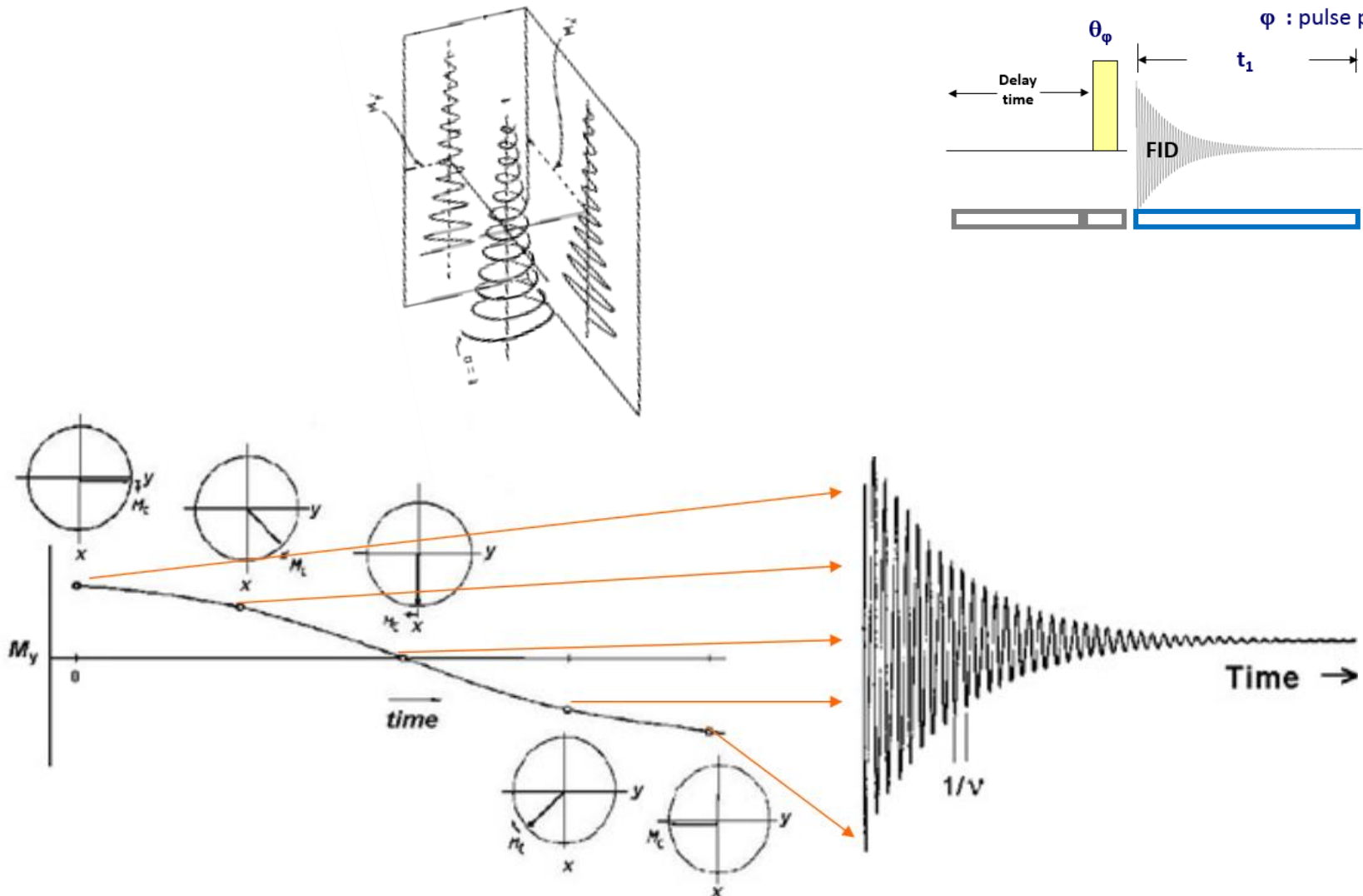
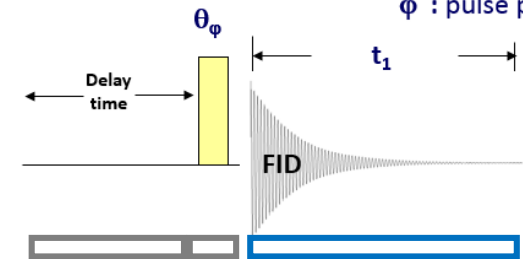
- transverse relaxation
- spin-spin relaxation



FID(Free Induction Decay)

θ : pulse width(μs)

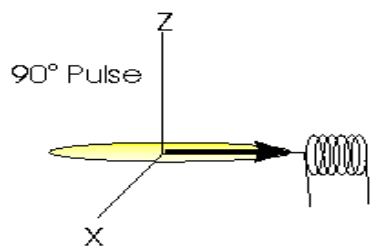
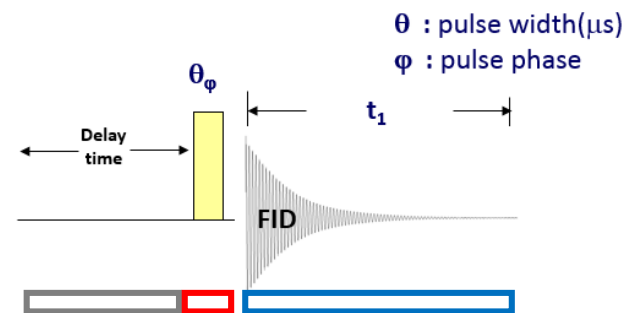
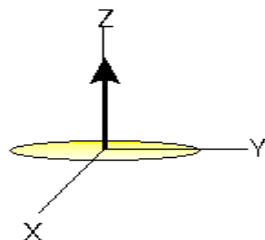
ϕ : pulse phase



Pulse width (pw) 90°



Same as

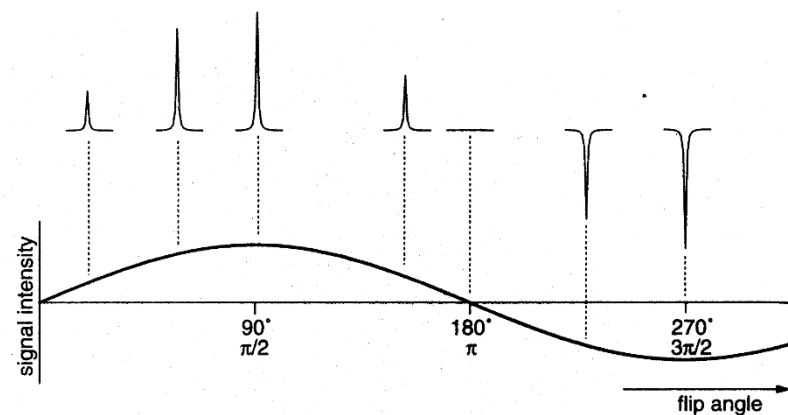
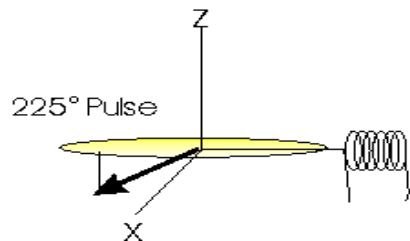
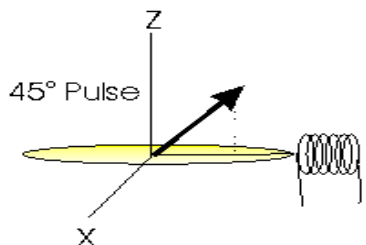
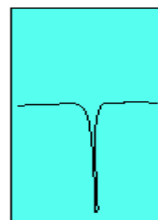
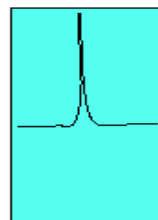
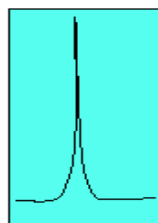


Detected
Signal



FT

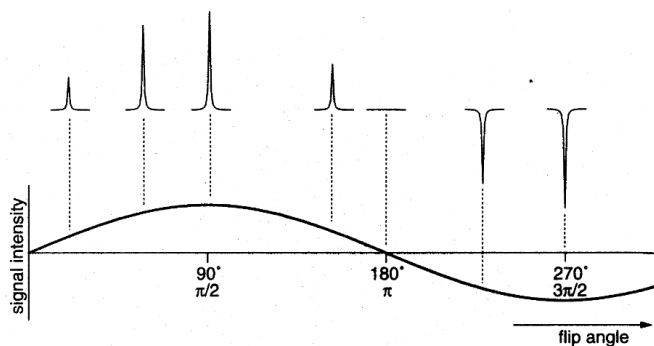
Spectrum



1. Find **P1** (for 90 °, maximum intensity)

1) Find P1 for 180 ° (zero intensity)

2) $\frac{1}{2}$ (P1 for 180 °) = P1 for 90 °



2. Find **D1**

1) $AQ + D1 = T1 * 3 \sim 5$

2) Measure T1 relaxation time

a. t1ir1d (Find D7null, short exp.)

b. t1ir (Find T1, long exp.)

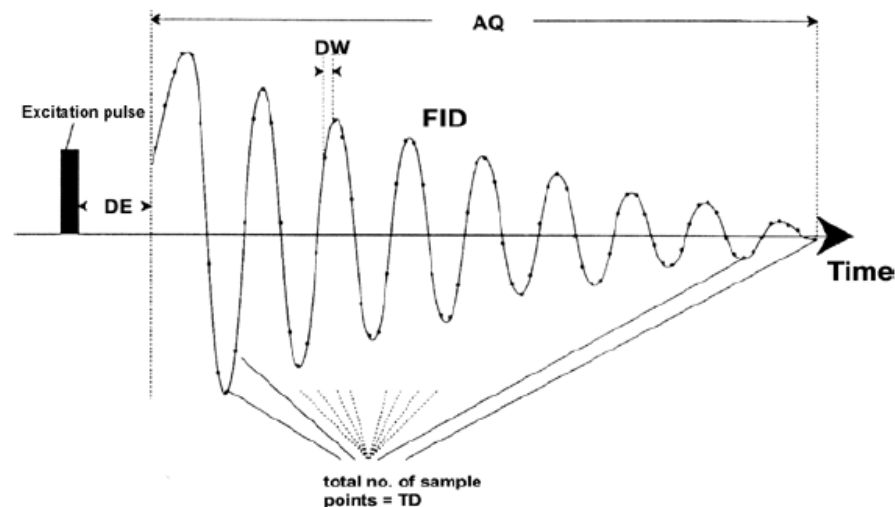
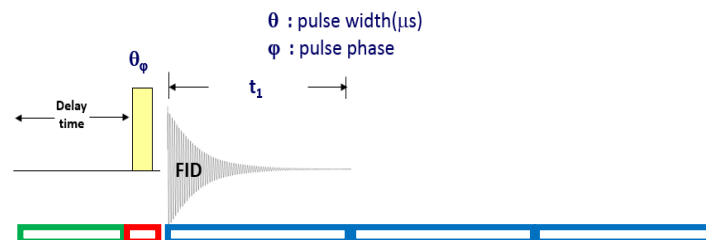
$$T1 * \ln(2) = D7null$$

$$T1 = D7null * 1.443$$

3. Find **AQ**

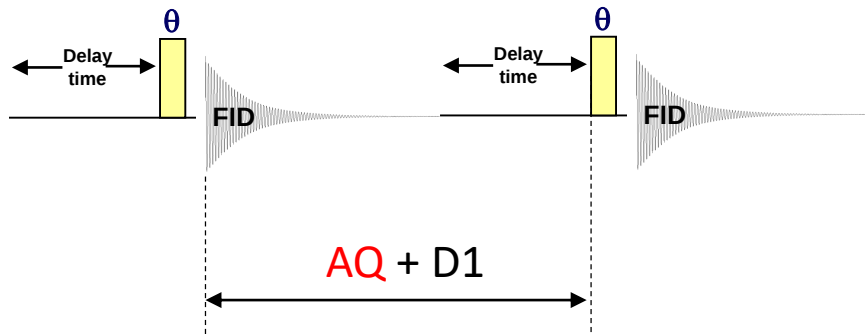
1) **AQ** = FID * 2 - 3

= dwell time * complex point



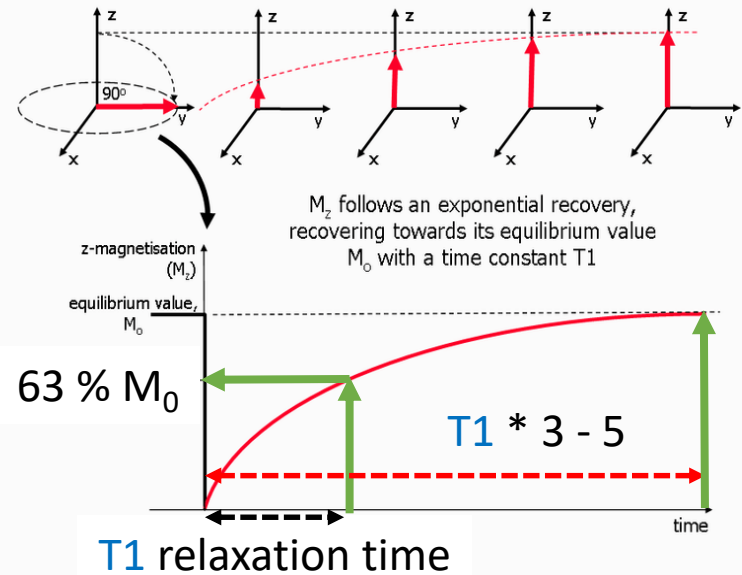
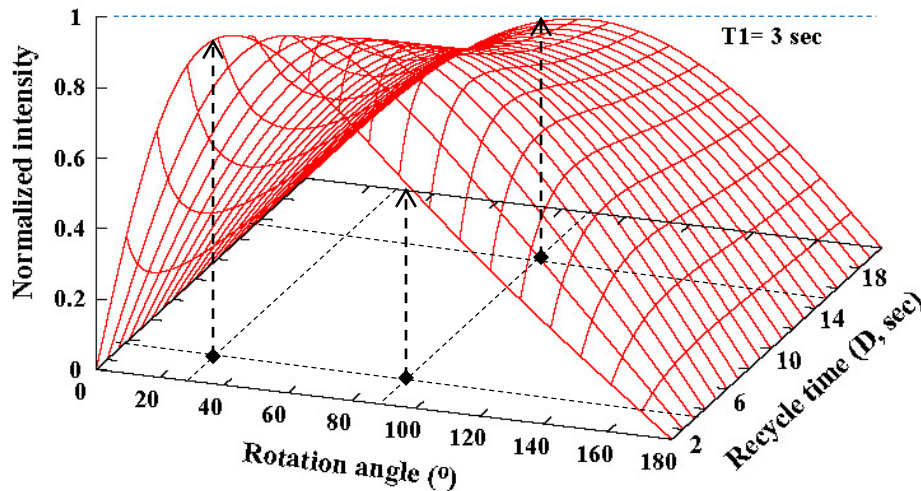
D1 (Recycle delay time for Quantitative NMR)

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$$\begin{aligned}
 \text{AQ} + \text{D1} &= T1 * 1.3 \quad (\text{Maximum S/N ratio}) \\
 &= T1 * 3 \quad (\text{Integration accuracy} = 90 \%) \\
 &= T1 * 5 \quad (\text{Integration accuracy} = 99 \%) \\
 &= T1 * 7 \quad (\text{Integration accuracy} = 99.9 \%)
 \end{aligned}$$

Figure 2: Sensitivity Dependence on Rotation Angle and Recycle Time



$$T1 = 3 \text{ s}$$

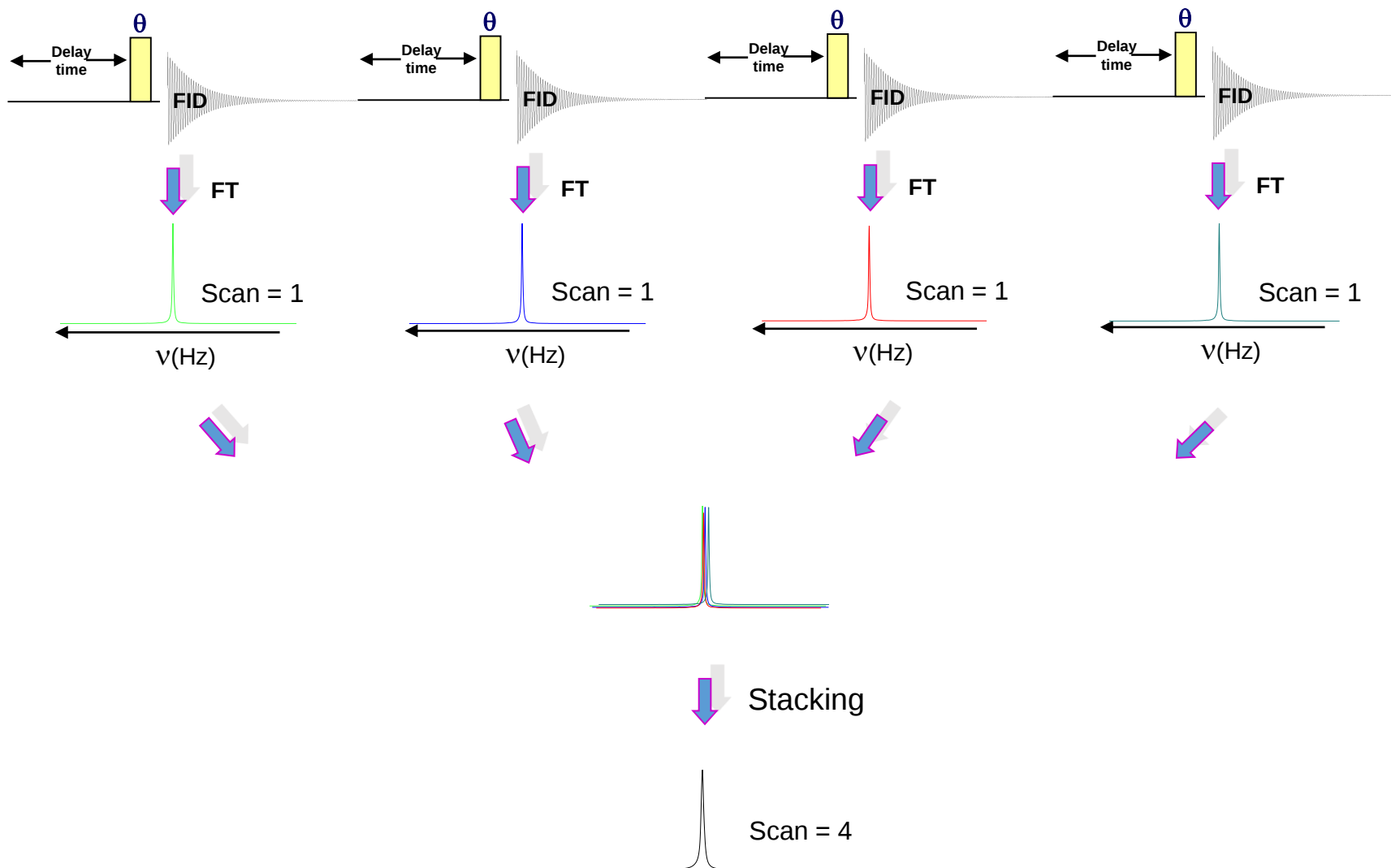
$$\text{AQ} + \text{D1} = T1 * 5$$

$$\text{AQ} + \text{D1} = 15 \text{ s for } 90^\circ$$

$$\text{AQ} + \text{D1} = 5 \text{ s for } 30^\circ [1/3]$$

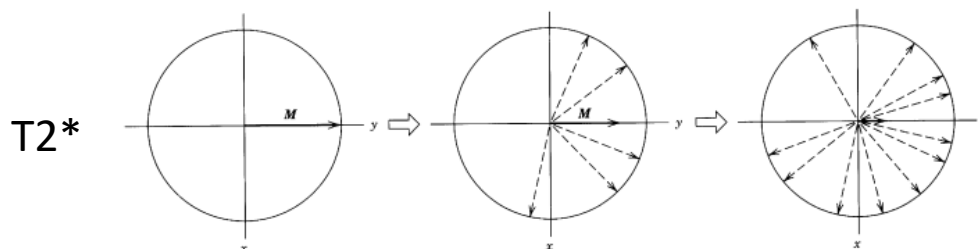
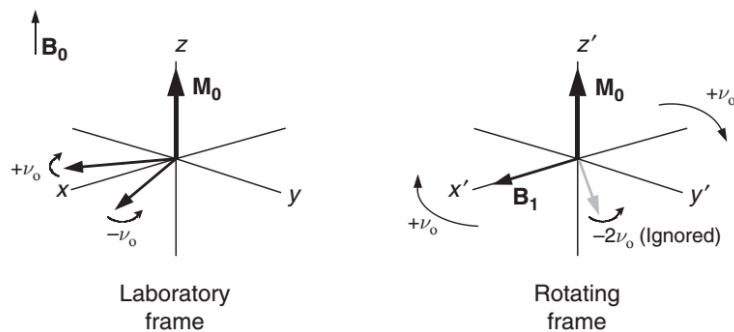
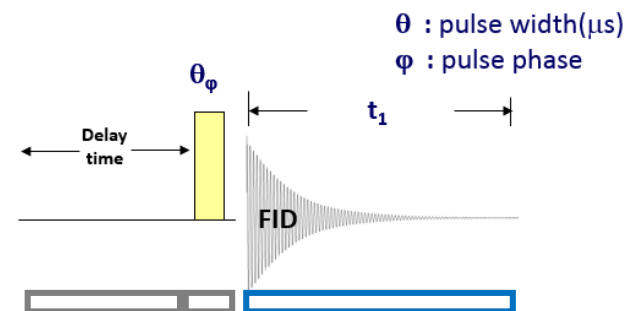
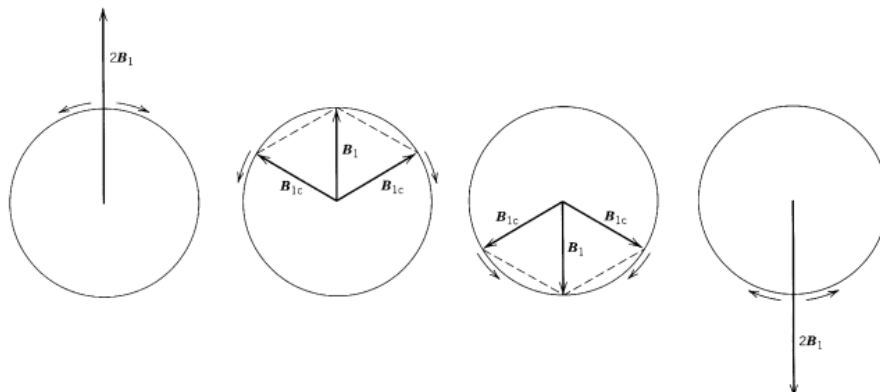
(Low angle = short experiment time)

For example, number of scan = 4

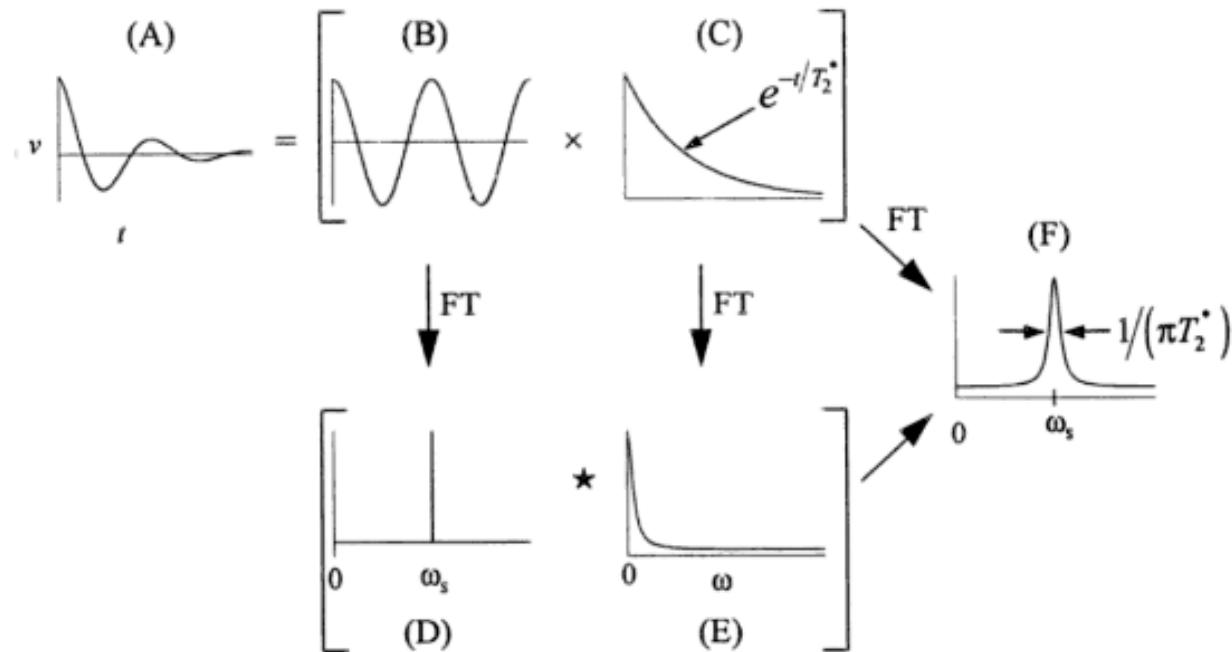


T2 relaxation

T2



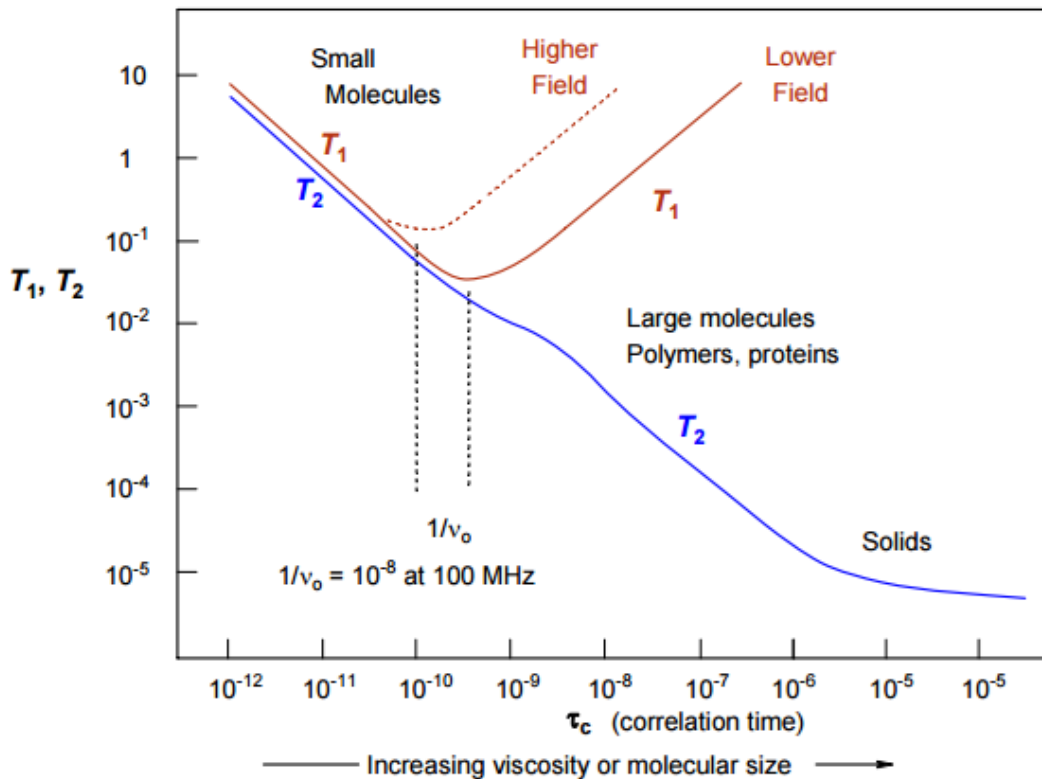
T_2^* relaxation time (T_2 in rotating frame)



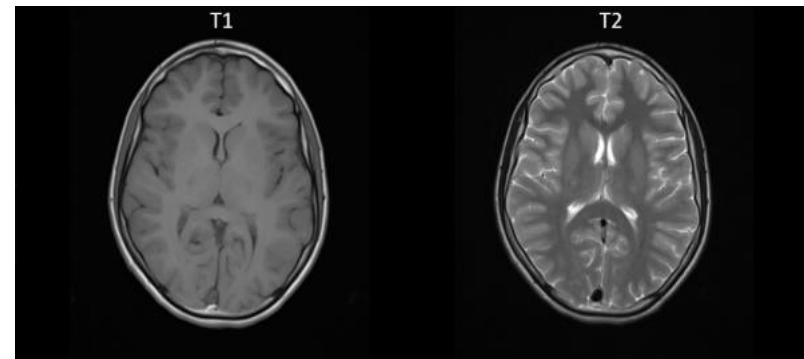
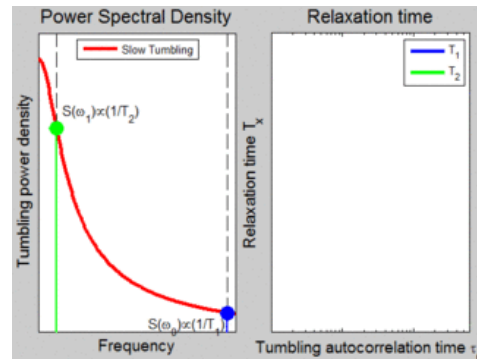
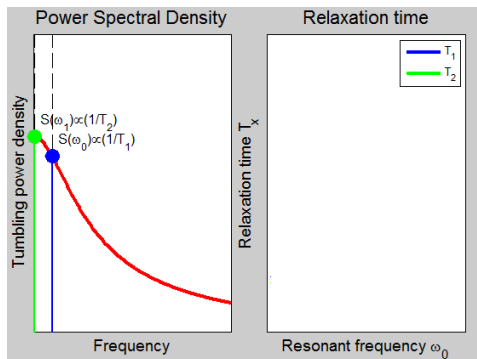
$$\Delta\nu \cdot \Delta t \geq 1$$

If Δt (i.e., T_2^*) is small, then $\Delta\nu$ is large, and the peak is therefore broad. T_2^* , whose major component is field inhomogeneity is the principal determining factor for peak width since T_2^* is always less than T_1 or T_2 .

Tumbling rate vs Magnetic field

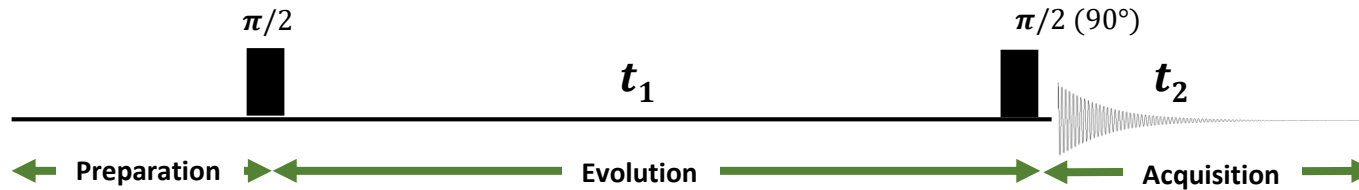


Tissue	T1 (msec)	T2 (msec)
Water/CSF	4000	2000
Gray matter	900	90
Muscle	900	50
Liver	500 Dark	40 Dark
Fat	250 Bright	70 Bright
Tendon	400	5
Proteins	250	0.1- 1.0
Ice	5000	0.001

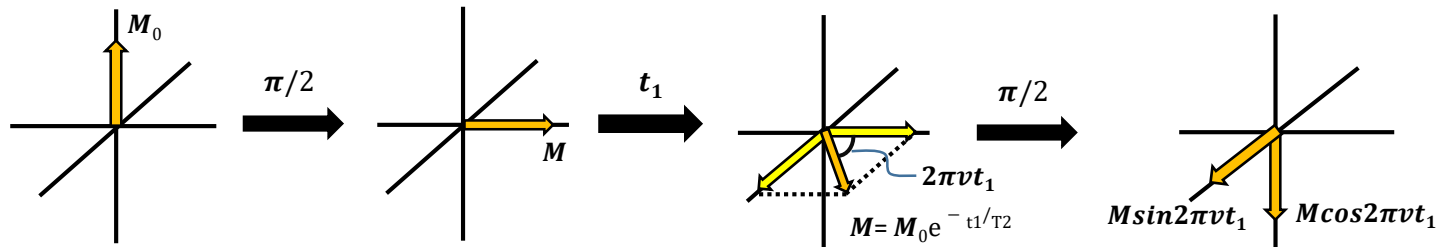


COSY (Correlation SpectroscopY)

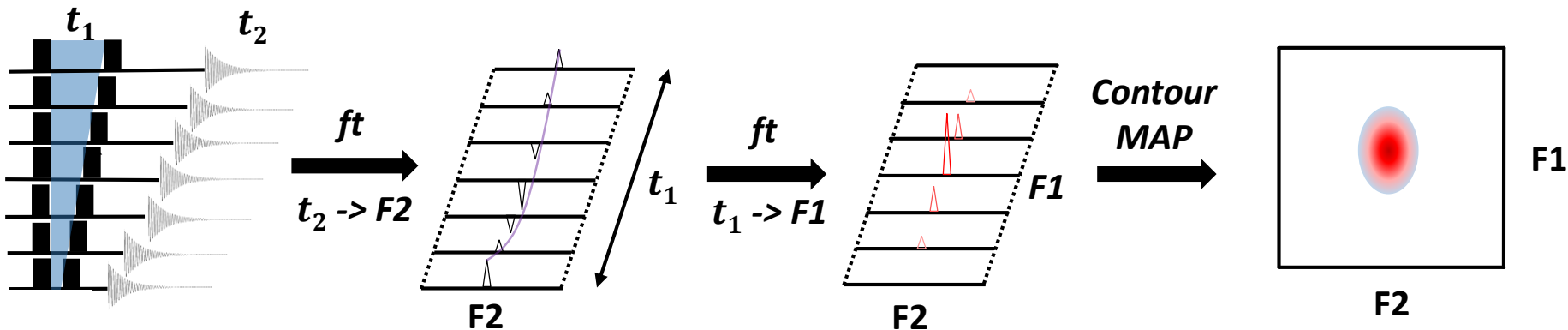
<Pulse sequence of COSY>



<Vector of 2D NMR>

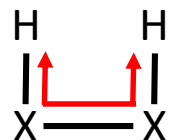


<Example of 2D NMR>



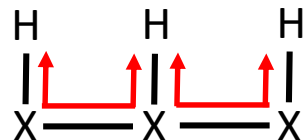
Bonding

Scalar coupling (J Coupling)



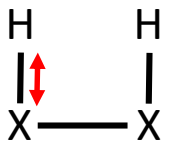
$$J_{2HH} \sim J_{3HH}$$

1H-1H COSY



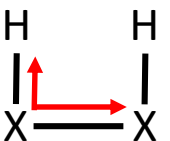
$$J_{2HH} \sim J_{5HH}$$

1H-1H TOCSY



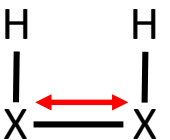
$$J_{1HX}$$

1H-X HSQC
1H-X HMQC
X->1H HETCOR



$$J_{2HX} \sim J_{3HX}$$

1H-X HMBC



$$J_{1XX}$$

X-X COSY
X-X INADEQUATE
H-X-X-H
AQDEQUATE

Space

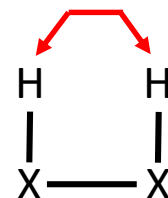
Dipolar coupling

NOESY = Small, Large molecules (along T1)

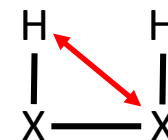
ROESY = Middle molecules (along T2)

Small < 700 Da < Middle < 1.2 kDa < Large

Distance = 3 ~ 5 Å



1H-1H NOESY
1H-1H ROESY



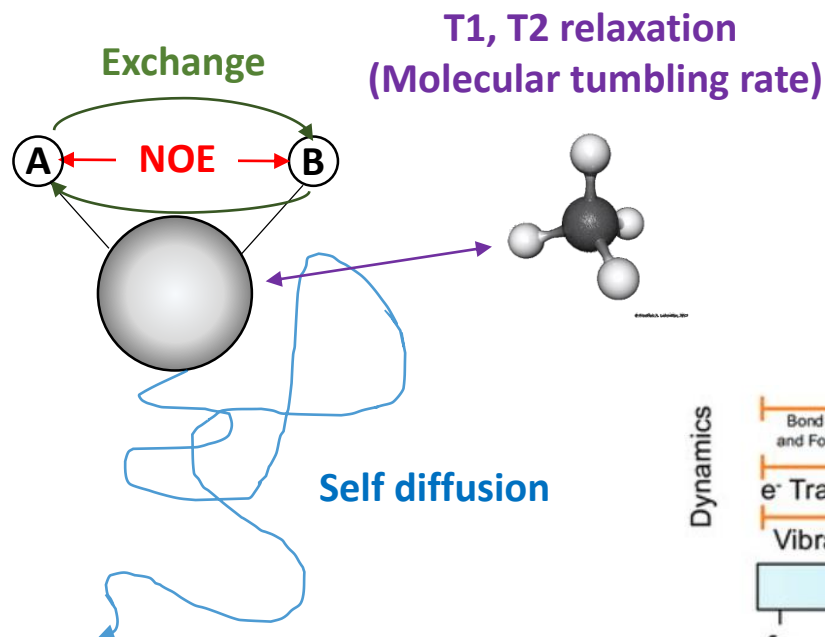
2D HOESY

Motion

Self-Diffusion DOSY (Diffusion)

Tumbling T1 (Inversion recovery)
T2 (CPMG)

Correlation in 2D NMR

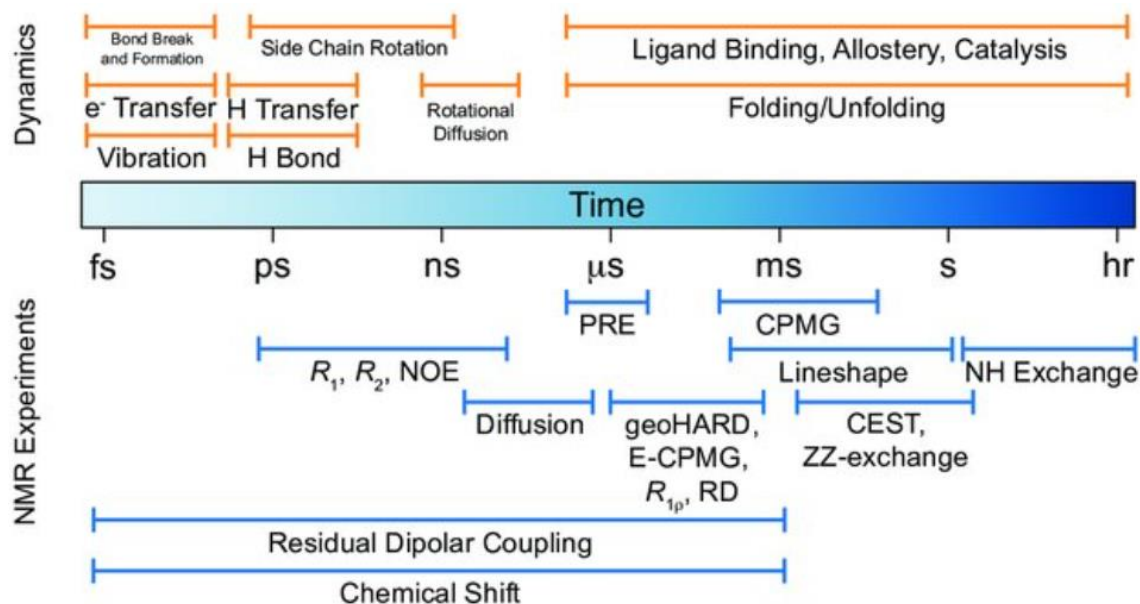


Exchange (EXSY)

NOE (NOESY/ROESY)

Diffusion (DOSY)

T1, T2 (Inversion recovery, CPMG)

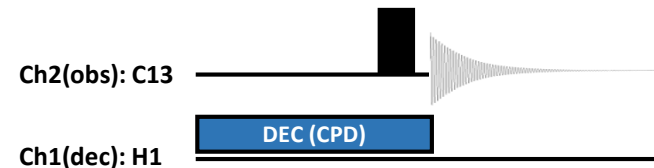


C13 with or without 1H Decoupling

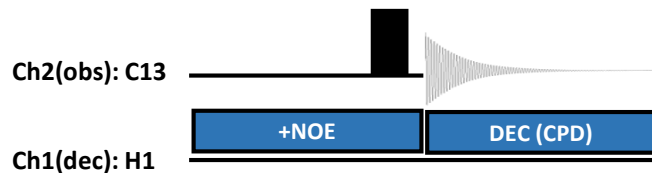
zg (-NOE, -DEC)



zgga (+NOE, -DEC)



zgdc (+NOE, +DEC)

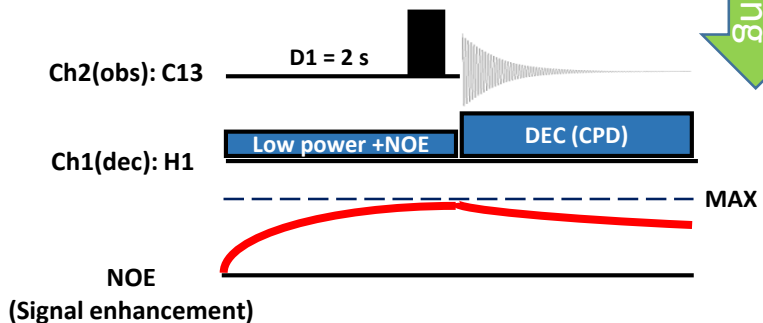


zgca (-NOE, +DEC_CW)



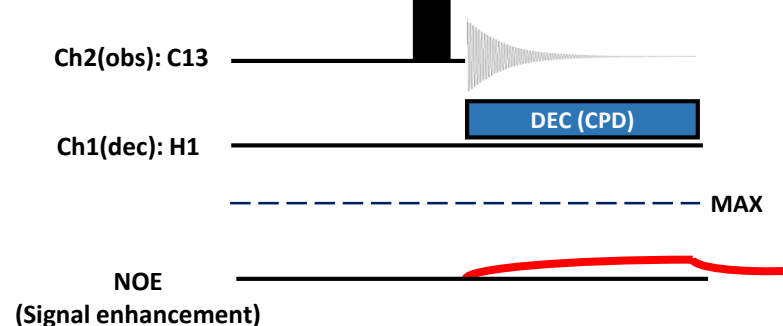
C13CPD

zgpg (+NOE, +DEC_Intensity)



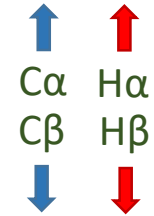
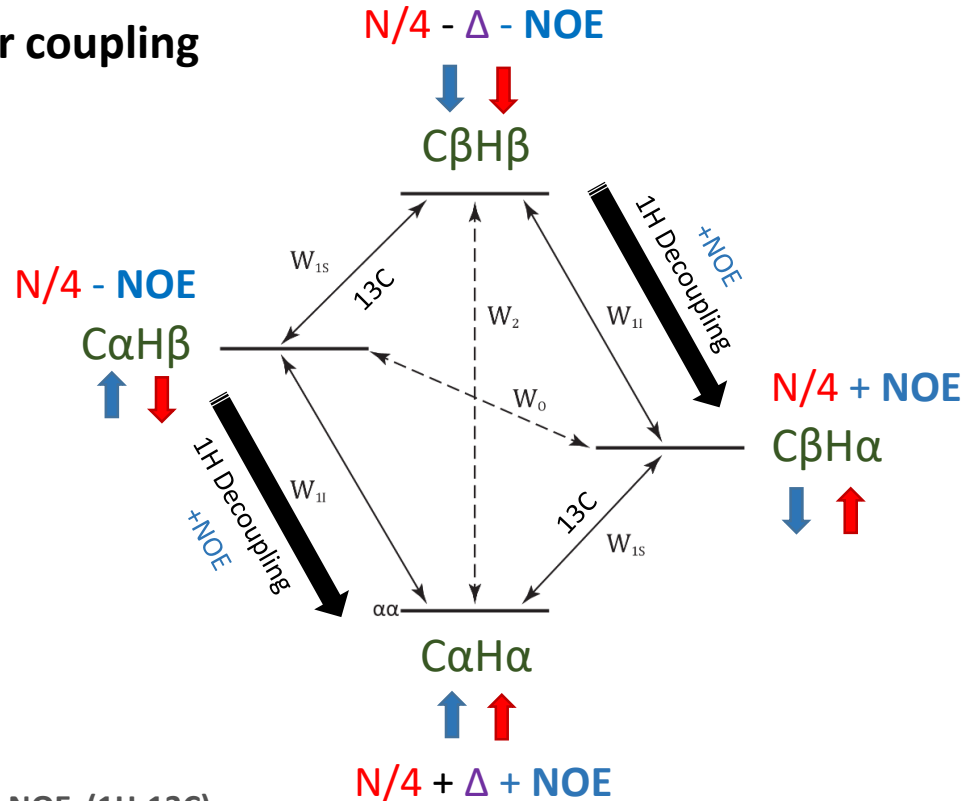
C13IG

zgig (-NOE, +DEC, Integration)



NOE (Nuclear Overhauser Effect)

Dipolar coupling



W (Transition Probability)

W_0 = Zero quantum

W_1 = Single quantum

W_2 = Double quantum

W_{1L} = ^1H transition

W_{1S} = ^{13}C transition

Hetero NOE (^1H - ^{13}C)

$$\text{NOE} = 1 + \frac{1}{2} * \left(\frac{r_H}{r_C} \right)$$

$$\text{NOE} = 1 + 1.998$$

$$\text{NOE} = 3 \text{ (Maximum enhancement)}$$

$$\text{NOE} = 1 + \frac{1}{2} * \frac{W_2 - W_0}{2w_1 + w_2 + w_0} * \left(\frac{r_H}{r_C} \right)$$

Total longitudinal dipolar relaxation rate

N = Total Nucleus

Δ = Population

4. Chemical shift

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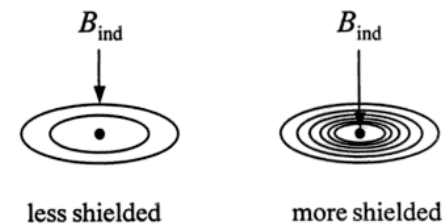
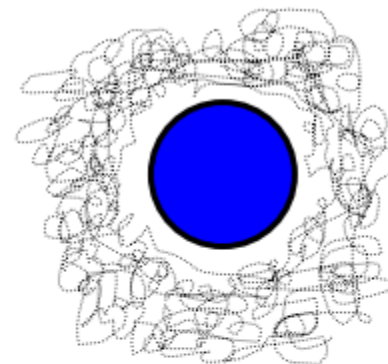


Figure 1.11 Nuclear shielding.



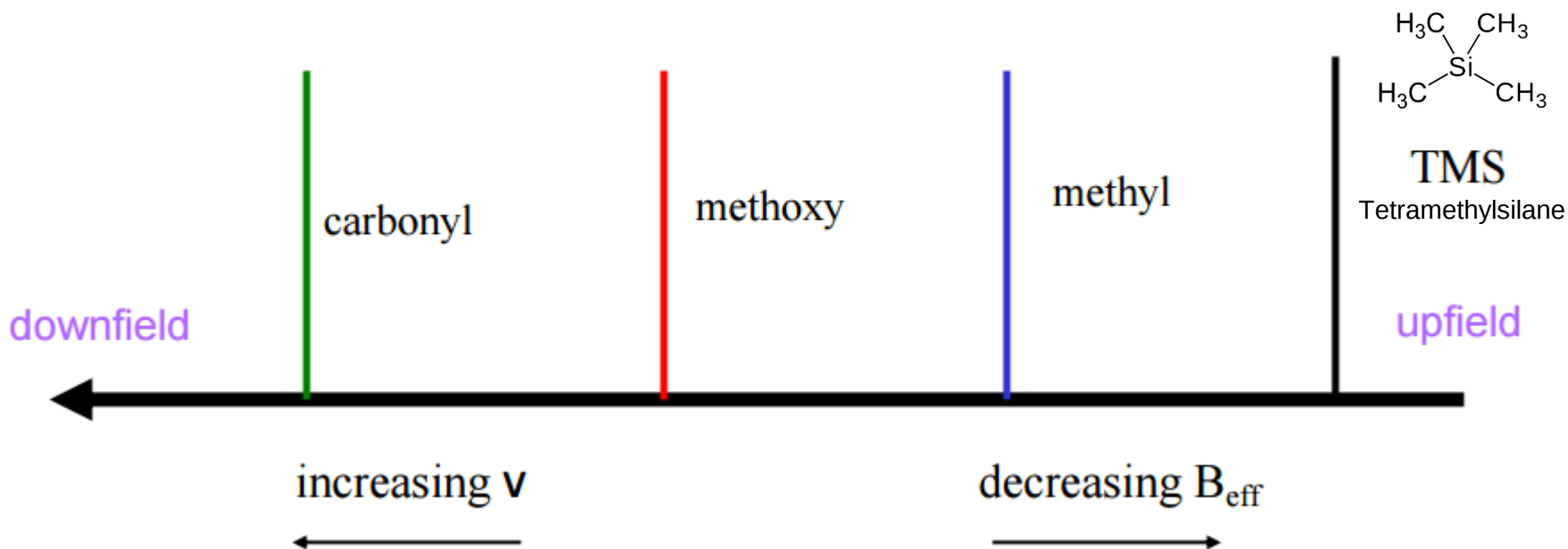
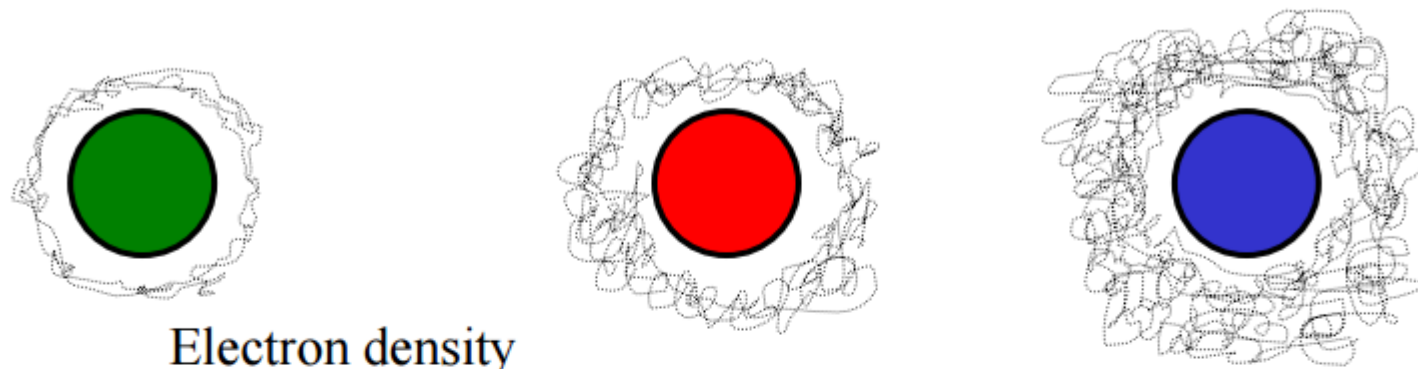
Carbonyl

- Less e^- density
- Nucleus 'deshielded' from B_0
- Feels the field (B_{eff}) more



Methyl

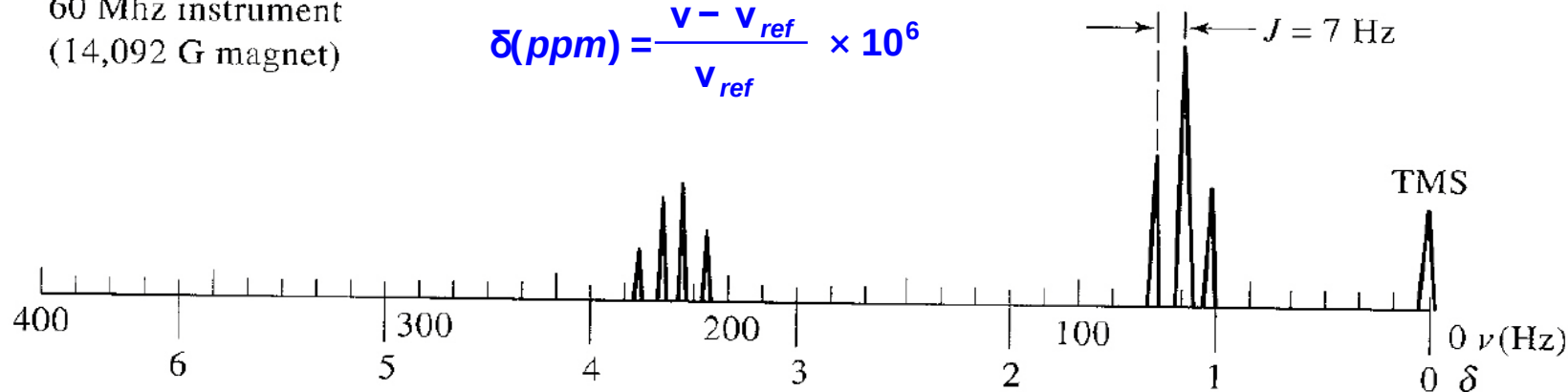
- More e^- density
- Nucleus 'shielded' from B_0 by e^-
- Feels the field (B_{eff}) less



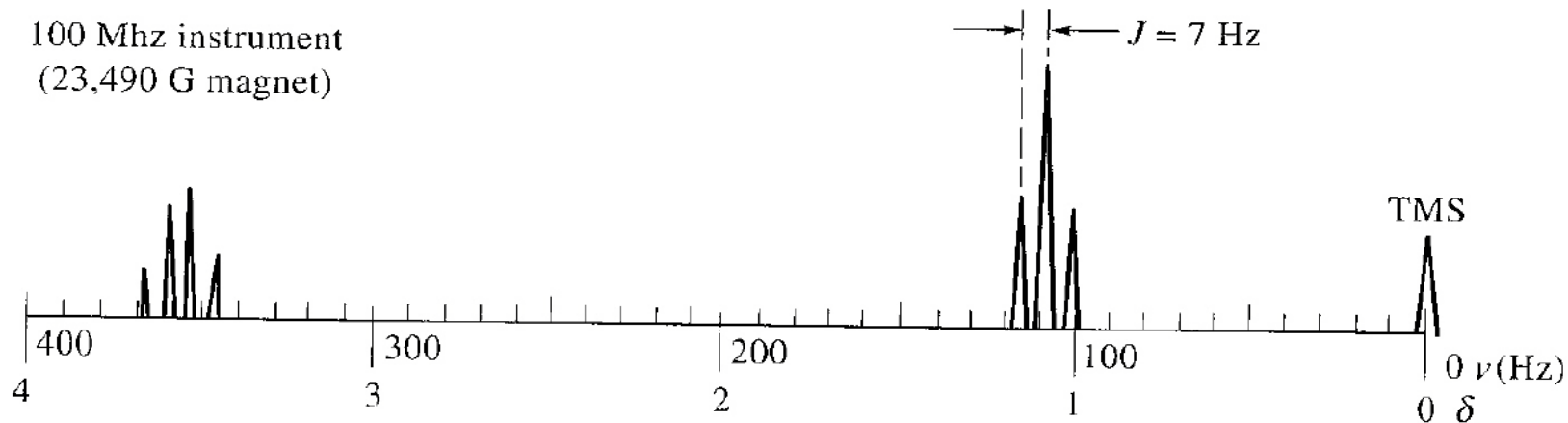
Chemical shift

60 Mhz instrument
(14,092 G magnet)

$$\delta(ppm) = \frac{\nu - \nu_{ref}}{\nu_{ref}} \times 10^6$$



100 Mhz instrument
(23,490 G magnet)



Low field	→	B_0	→	High field
Low shielding				High shielding
High frequency	←	ν	←	Low frequency

胆固醇

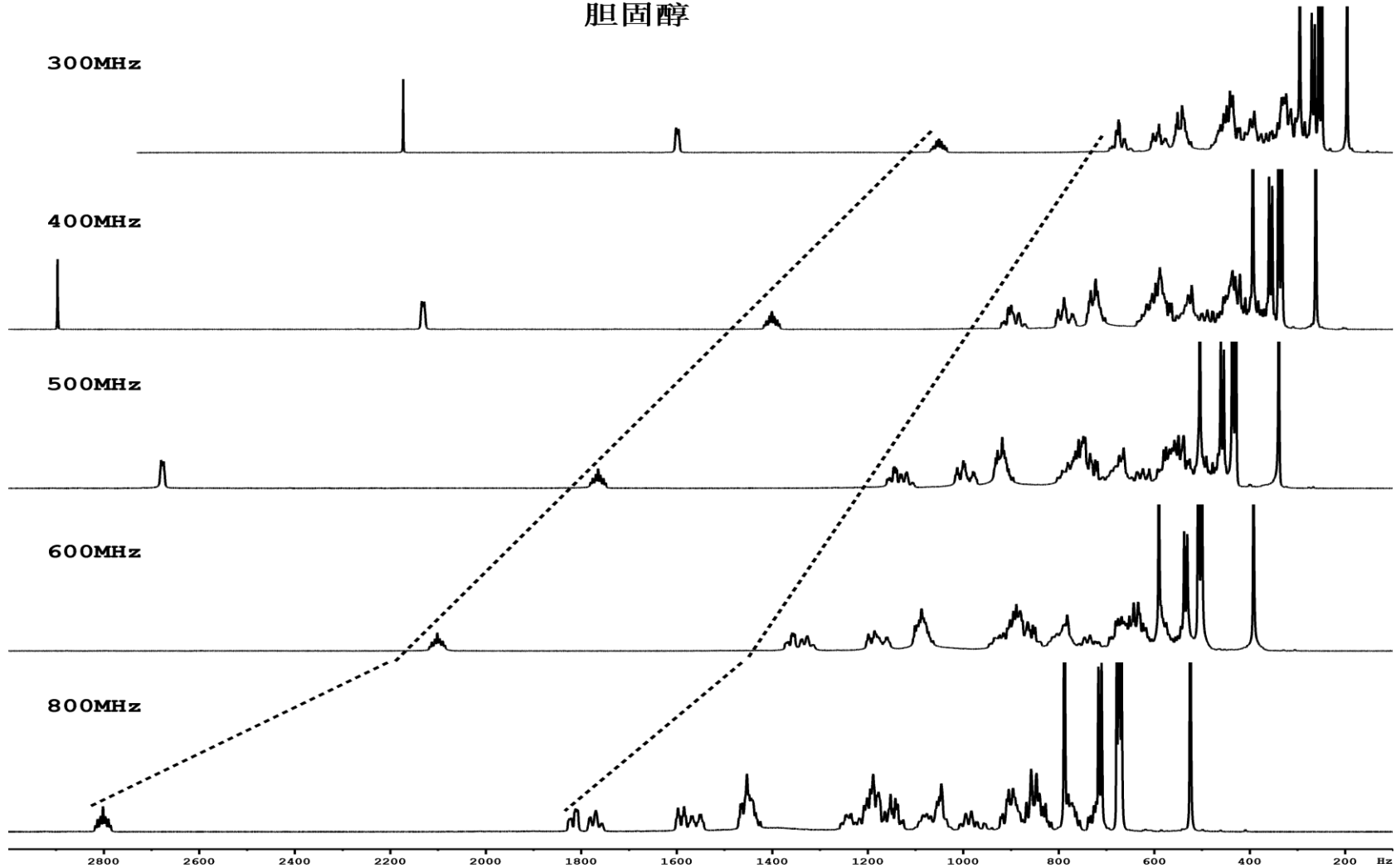


TABLE 13-2 Chemical Shifts of the Chloromethanes

Compound	Chemical Shift	Difference
$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \end{array}$	$\delta 0.2$	
$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{H} \\ \\ \text{H} \end{array}$	$\delta 3.0$	2.8 ppm
$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{Cl} \\ \\ \text{H} \end{array}$	$\delta 5.3$	2.3 ppm
$\begin{array}{c} \text{H} \\ \\ \text{H}-\text{C}-\text{Cl} \\ \\ \text{Cl} \end{array}$	$\delta 7.2$	1.9 ppm

Note: Each chlorine atom added changes the chemical shift of the remaining methyl protons by about 2 to 3 ppm. These changes are nearly additive.

- More electronegative atoms deshield more and give larger shift values.
- Effect decreases with distance.
- Additional electronegative atoms cause increase in chemical shift.

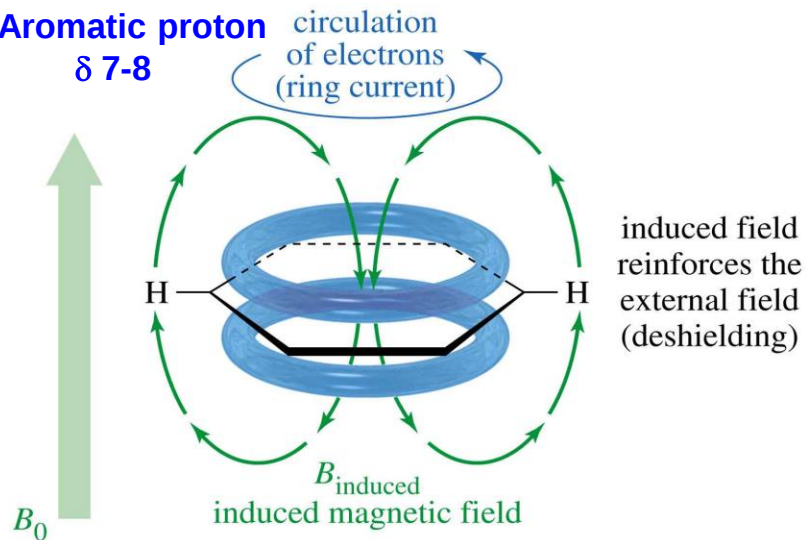
^1H chemical shift

Type of Proton	Approximate δ	Type of Proton	Approximate δ
alkane ($-\text{CH}_3$)	0.9	>C=C<CH_3	1.7
alkane ($-\text{CH}_2-$)	1.3	$\text{Ph}-\text{H}$	7.2
alkane ($-\text{CH}-$)	1.4	$\text{Ph}-\text{CH}_3$	2.3
$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{CH}_3 \end{array}$	2.1	$\text{R}-\text{CHO}$	9–10
$-\text{C}\equiv\text{C}-\text{H}$	2.5	$\text{R}-\text{COOH}$	10–12
$\text{R}-\text{CH}_2-\text{X}$ (X = halogen, O)	3–4	$\text{R}-\text{OH}$	variable, about 2–5
$\begin{array}{c} \diagup \\ \text{C}=\text{C} \\ \diagdown \end{array} \text{H}$	5–6	$\text{Ar}-\text{OH}$	variable, about 4–7
		$\text{R}-\text{NH}_2$	variable, about 1.5–4

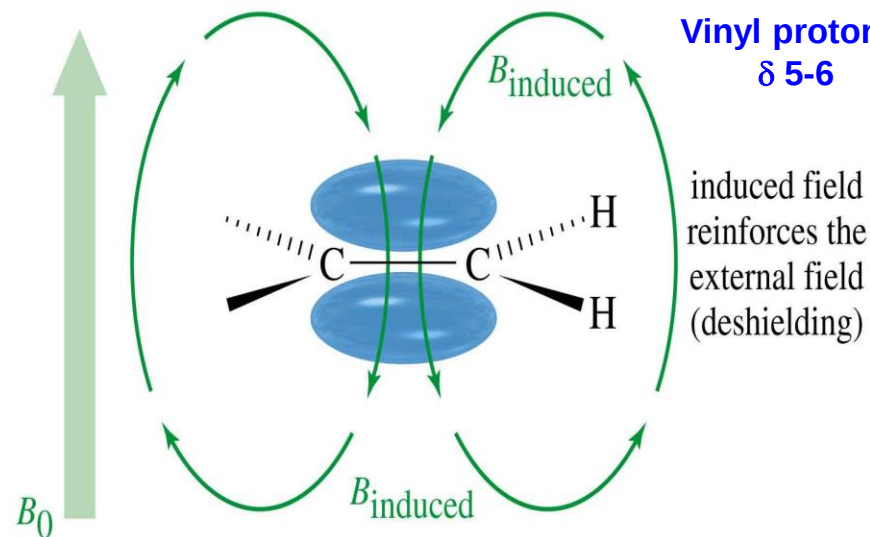
Note: These values are approximate, as all chemical shifts are affected by neighboring substituents. The numbers given here assume that alkyl groups are the only other substituents present. A more complete table of chemical shifts appears in Appendix 1.

^1H chemical shift

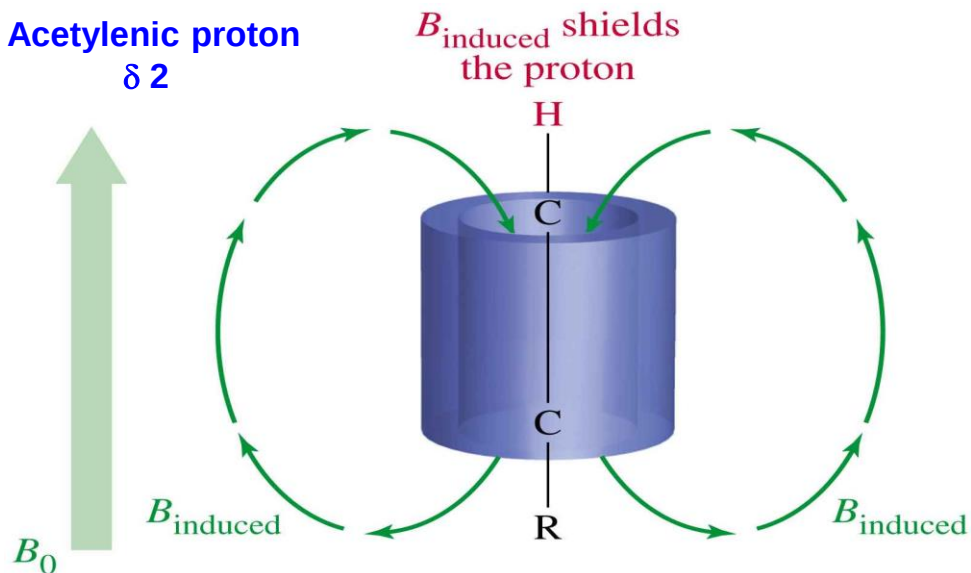
Aromatic proton
 δ 7-8



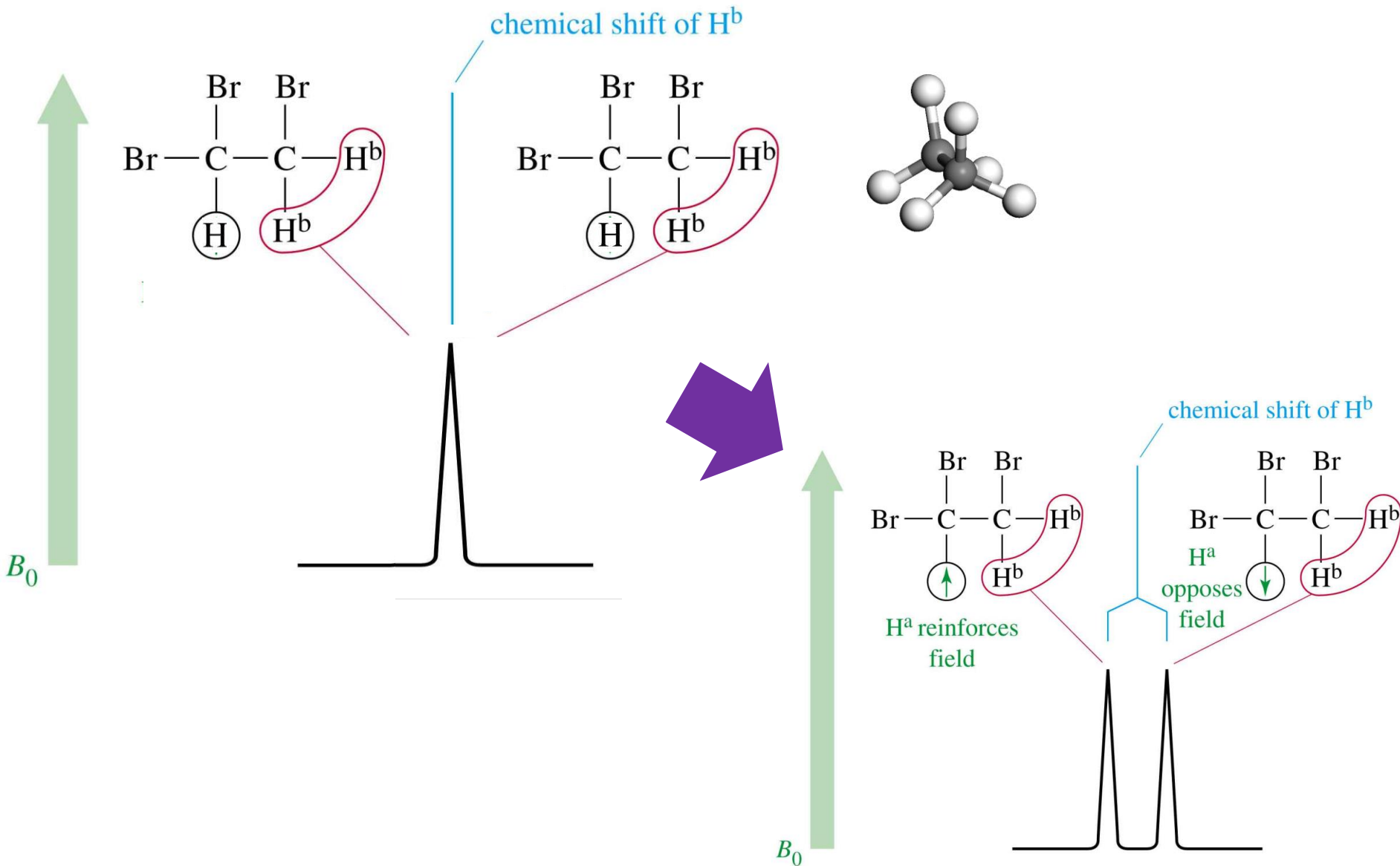
Vinyl proton
 δ 5-6



Acetylenic proton
 δ 2



Spin-Spin (J) coupling



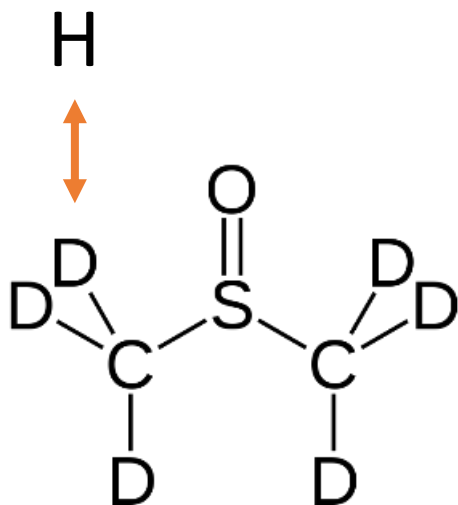
Peak splits by J-coupling → Pascal's triangle

n	n+1	Intensity ratio	Multiplicity
0	1	1	Singlet
1	2	1 1	Doublet
2	3	1 2 1	Triplet
3	4	1 3 3 1	Quartet
4	5	1 4 6 4 1	Quintet
5	6	1 5 10 10 5 1	Sextet

n: number of equivalent neighboring nuclear

H(Proton): $I=1/2$

D(Deuterium): $I=1$



2nI+1 rule

N = Number of neighbor nuclear

I = Nuclear spin quantum number

$$2J_{HD} : 2 * 2 * 1 + 1 = 5 \text{ (Quintet)}$$

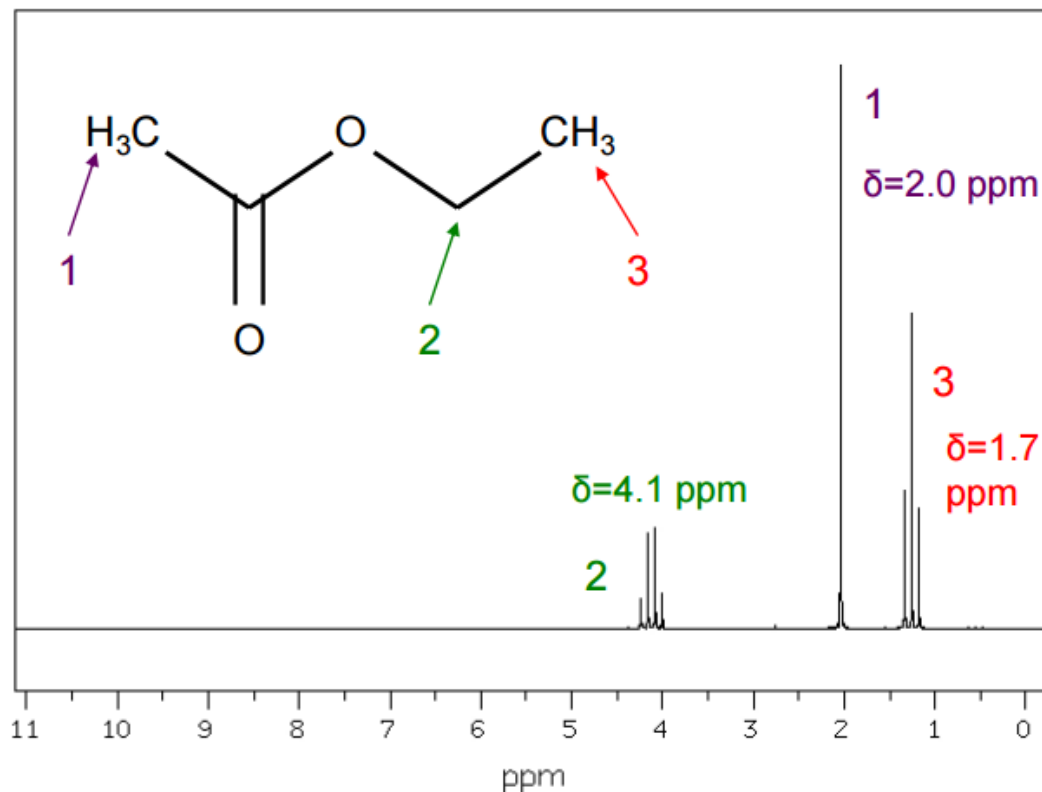
$$2J_{HH} : 2 * 2 * 1/2 + 1 = 3 \text{ (Triplet)}$$

Coupling constant

$$2J_{HD} = \text{Hz}$$

ex) DMSO-D6 $\leftrightarrow$ DMSO-D5+H1 $\leftrightarrow$ DMSO-H6
 None Quintet Triplet

Ethyl acetate



Spin-Spin Splitting patterns

1. **Singlet.** 3 equivalent protons. Not coupled to any neighboring protons.
2. **Quartet.** 2 equivalent protons. Split (1:3:3:1) because coupled to the 3 ¹Hs at the 3 position.
3. **Triplet.** 3 equivalent protons. Split (1:2:1) because coupled to the 2 ¹Hs at the 2 position.

$$\text{Multiplicity} = N (\text{\# of neighbors}) + 1$$

<Data>

1. Chemical shift (shielding/deshielding)
2. Spin-Spin coupling
3. Peak integral
4. Relaxation
5. Diffusion coefficient

<Application>

1. Qualitative/Quantitative
2. Structure assign
3. Dynamics/Kinetics
4. Purification

<Industry>

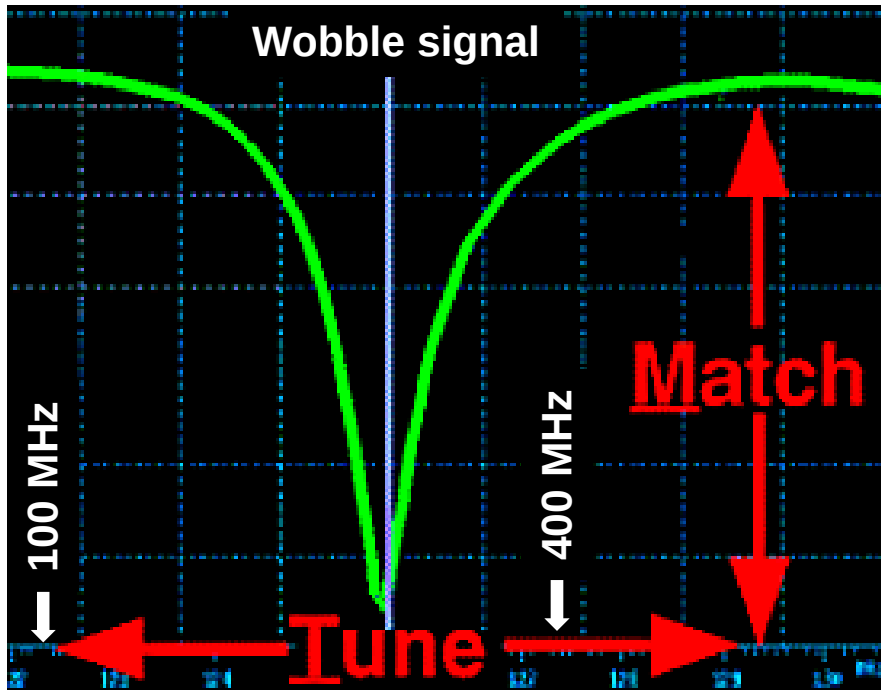
1. Organic chemistry
2. Metabolomics
3. Drug development
4. QC/QA
5. Polymer

5. Tuning & Matching

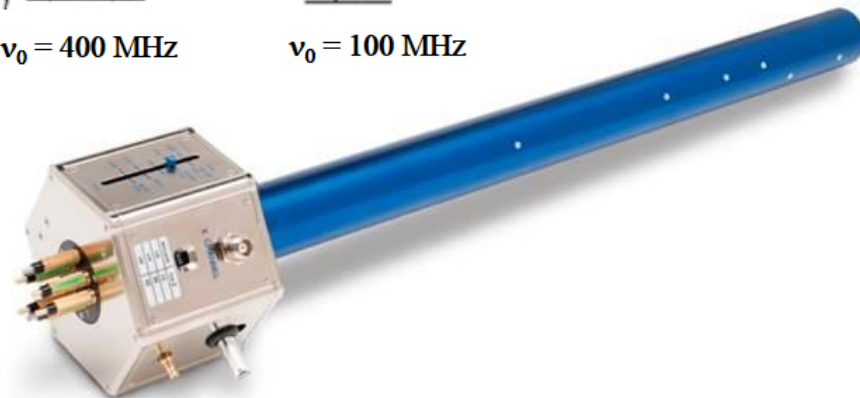
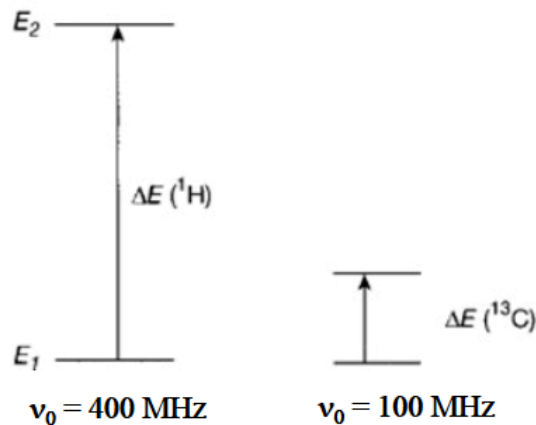
Lock & Shim

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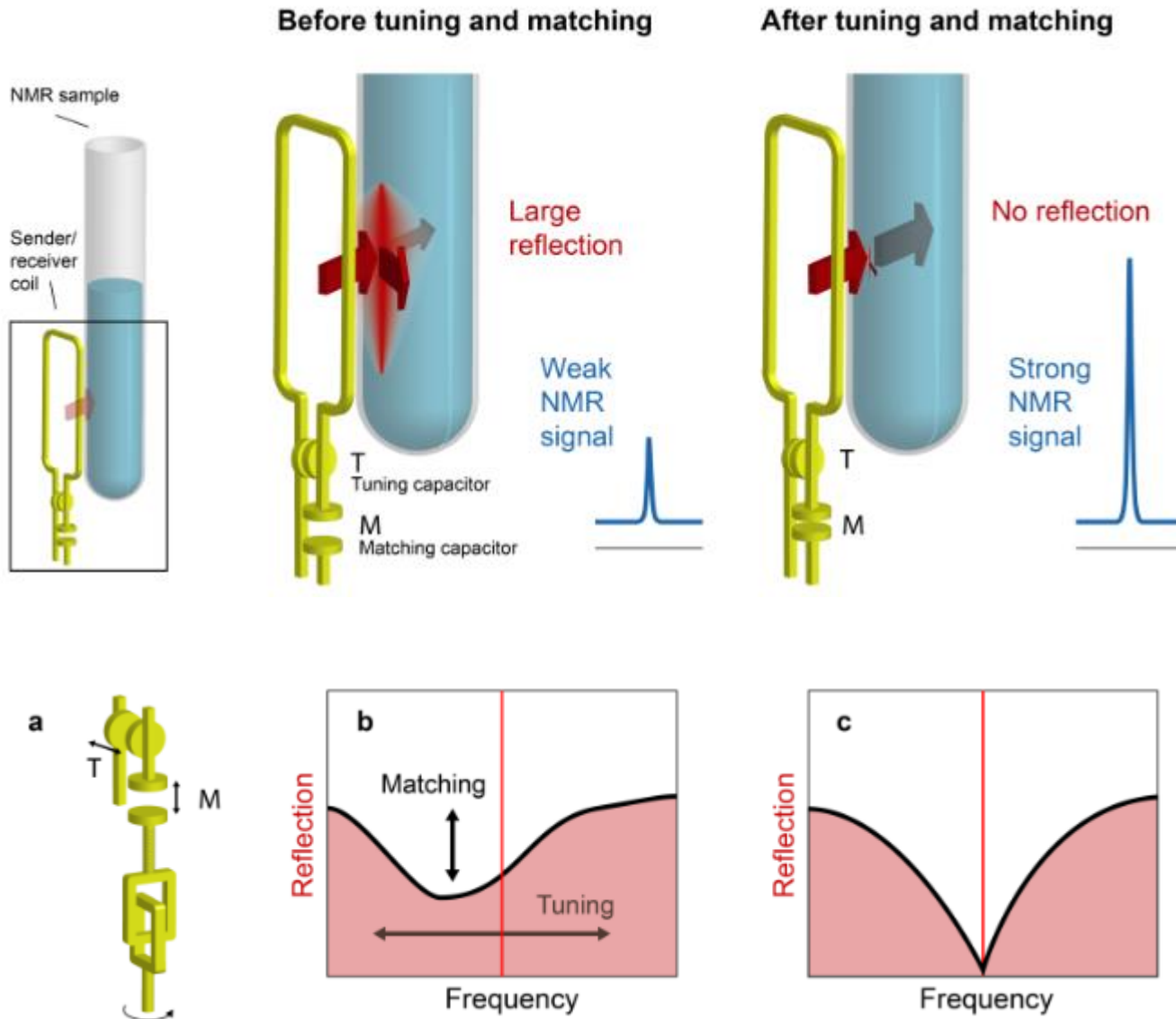


Tuning is the process of adjusting this frequency until it coincides with the frequency of the pulses transmitted to the circuit. For example, the frequency at which the ^1H resonant circuit is most sensitive must be set to **the carrier frequency of the ^1H pulses**.



Matching is the process of adjusting the impedance of the resonant circuit until it corresponds with the impedance of the transmission line connected to it. **This impedance is 50Ω** . Correct matching minimizes the power that is transmitted to the coil

Tuning & Matching



5mm DB auto-X probe (Varian 600) [Tune & Match range = 31P (40%) ~ 15N (10%)]

5mm BBO Probe (Bruker 400) [Tune & Match range = 31P (40%) ~ 15N (10%)]

-> 31P(40%), 13C (25%), 15N(10%), 35Cl(9.7%)

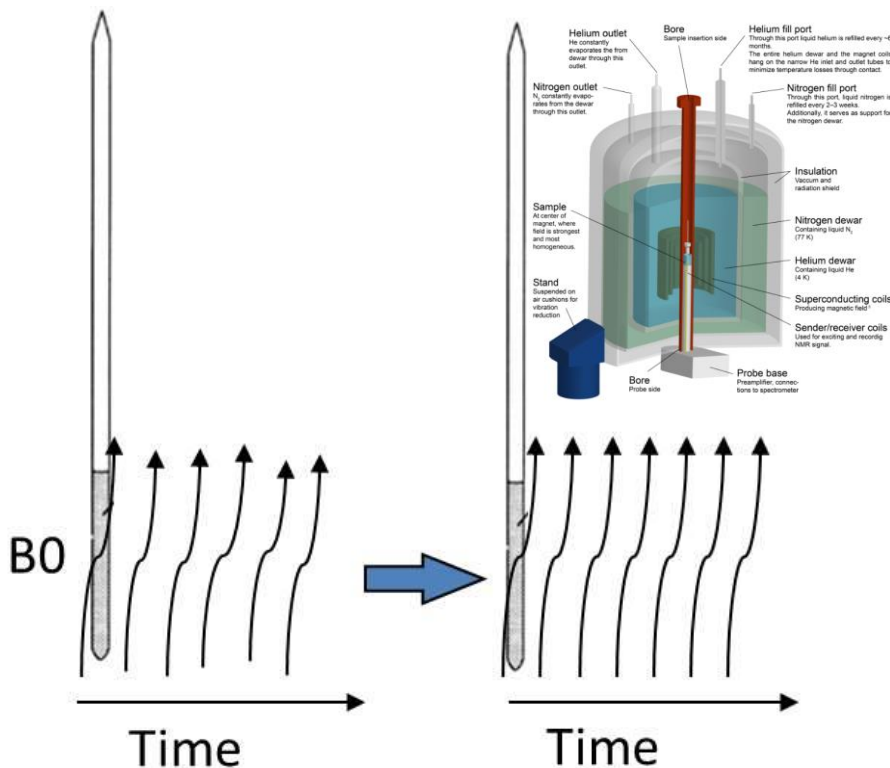
Smart probe or I-probe [Tune & Match range = 31P (40%) ~ 109Ag (4.65%)]

-> 31P(40%), 13C (25%), 15N(10%), 35Cl(9.7%), 33S (7.6%), 14N(7.2%), 25Mg(6.1%), 109Ag (4.65%)

		Theoretical NMR Freq. (free atom)	Molar Receptivity (rel. ¹ H)	Receptivity at Nat. Abund. (rel. ¹³ C)	Reference Sample	Measured. NMR Freq. (rel. ¹ H ref.)
A	Sym	ν_0 [MHz]	$R_M(H)$	$R_{NA}(C)$	Reference	Ξ [MHz]
1	n	68.4979	3.21E-01			
1	H	100.0000	1.00E+00	5.87E+03	1% Me ₄ Si in CDCl ₃	100.000000
2	D	15.3506	9.65E-03	6.52E-03	(CD ₃) ₄ Si neat	15.350609
3	T	106.6640	1.21E+00		TMS-T ₁	106.663974
3	He	76.1767	4.42E-01	3.48E-03	He gas	76.178976
6	Li	14.7170	8.50E-03	3.79E+00	9.7 m LiCl in D ₂ O	14.716086
7	Li	38.8667	2.94E-01	1.59E+03	9.7 m LiCl in D ₂ O	38.863797
9	Be	14.0536	1.39E-02	8.15E+01	0.43 m BeSO ₄ in D ₂ O	14.051813
10	B	10.7456	1.99E-02	2.32E+01	15% BF ₃ ·Et ₂ O in CDCl ₃	10.743658
11	B	32.0897	1.65E-01	7.77E+02	15% BF ₃ ·Et ₂ O in CDCl ₃	32.083974
13	C	25.1504	1.59E-02	1.00E+00	1% Me ₄ Si in CDCl ₃ DSS in D ₂ O	25.145020 25.144953
14	N	7.2285	1.01E-03	5.90E+00	MeNO ₂ + 10% CDCl ₃	7.226317
15	N	10.1398	1.04E-03	2.23E-02	MeNO ₂ + 10% CDCl ₃ liquid NH ₃	10.136767 10.132767
17	O	13.5617	2.91E-02	6.50E-02	D ₂ O	13.556457
19	F	94.0570	8.32E-01	4.89E+03	CCl ₃ F	94.094011
21	Ne	7.8987	2.46E-03	3.91E-02	Neon gas, 1.1 MPa	7.894296
23	Na	26.4683	9.27E-02	5.45E+02	0.1 M NaCl in D ₂ O	26.451900
25	Mg	6.1260	2.68E-03	1.58E+00	11 M MgCl ₂ in D ₂ O	6.121635

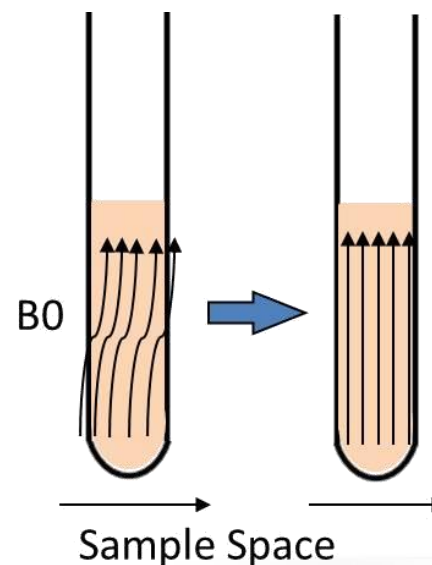
Locking B_0

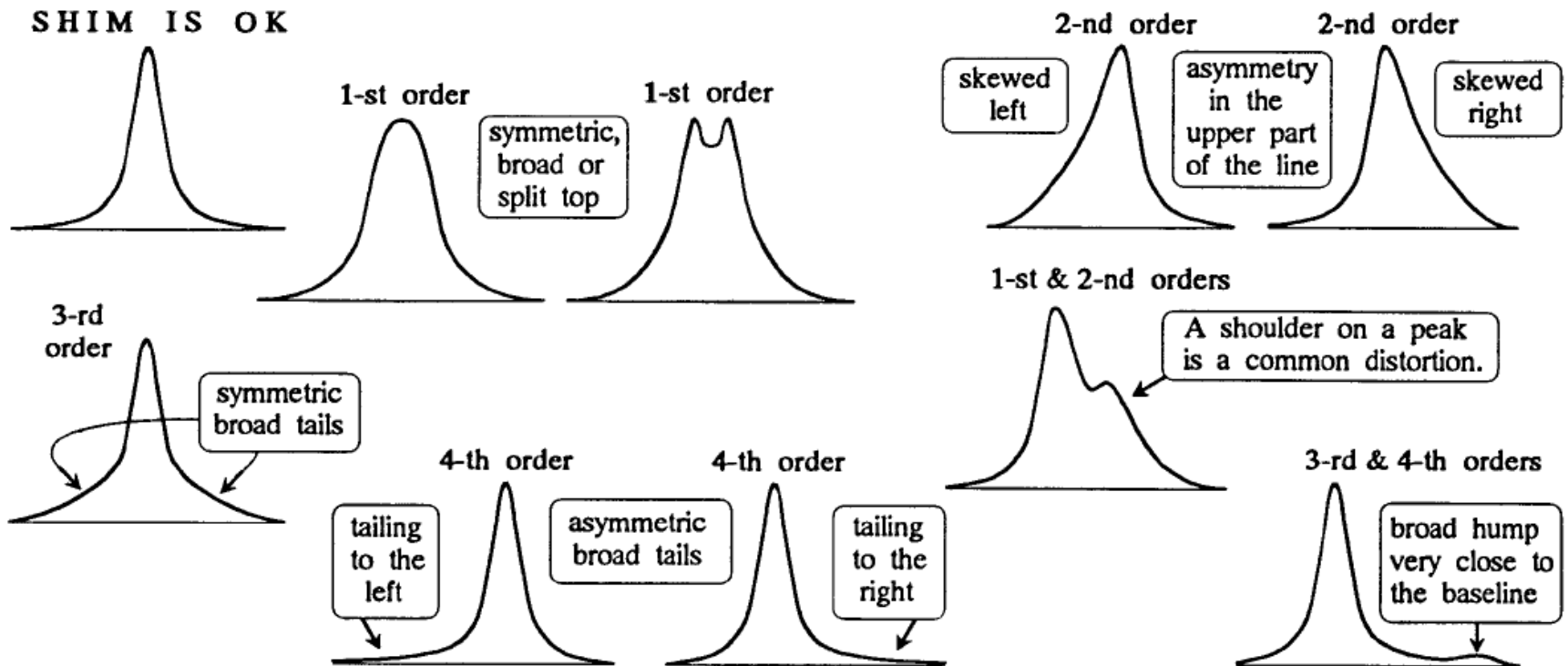
Locking is to stabilize B_0 time to time. When locking is activated, the feedback-control of B_0 is achieved by reading the ^2H signal and adjusting the Z_0 shim.



Shimming B_0

Shimming is to homogenize B_0 in the sample space. Bio-NMR uses about 40 different shims to achieve this goal. The main shim sets that users must check are Z1, Z2, Z3, Z4, X1, Y1, XZ, and YZ.





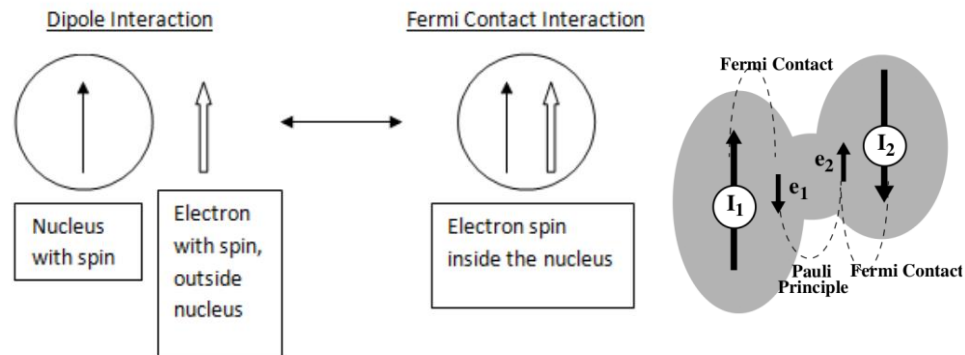
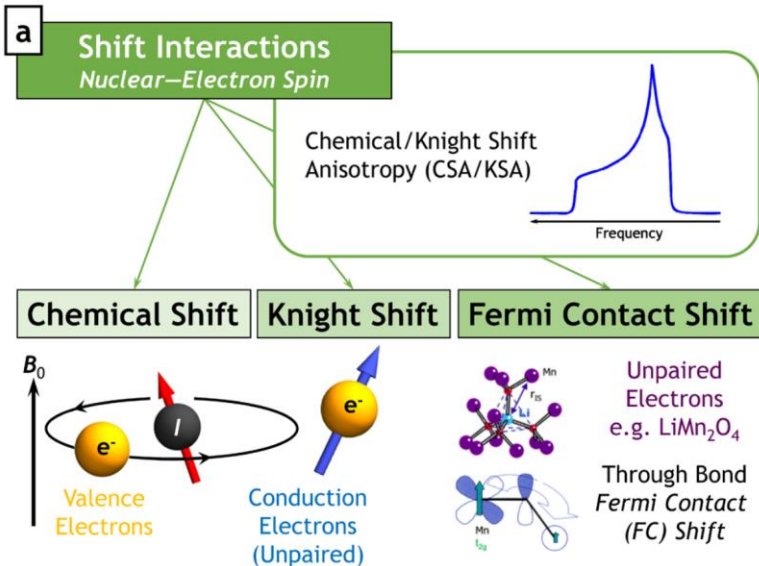
SKETCHES OF LINE DISTORTIONS CAUSED BY VARIOUS GRADIENTS

6. Solid-state NMR

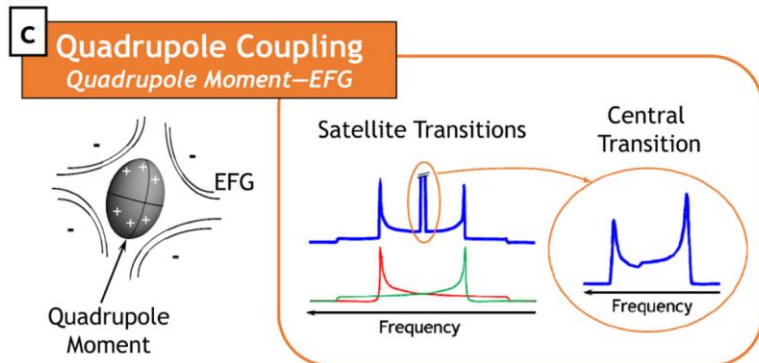
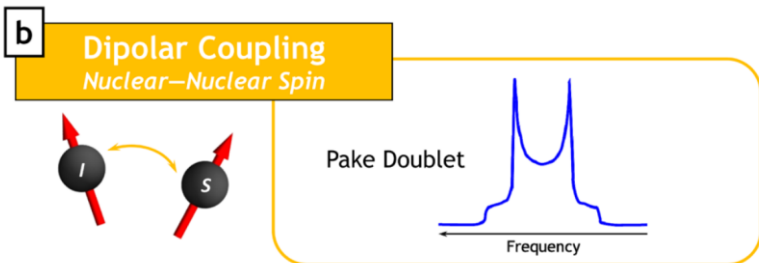
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Interaction in Solid-state NMR



Chemical shift: Interaction for valence electron
Knight shift: Interaction for unpaired electron



Energy state
 $2nI+1 = 4$

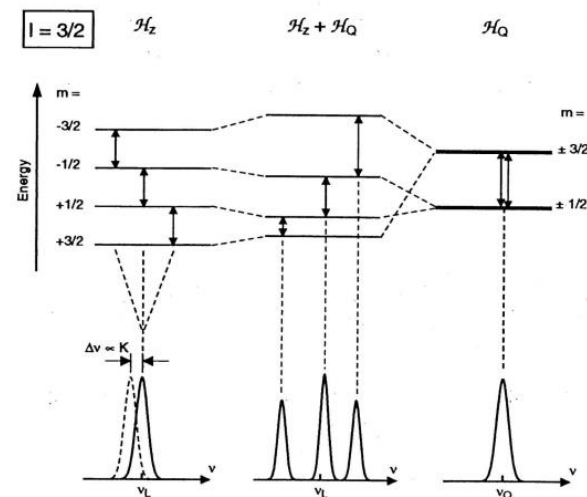
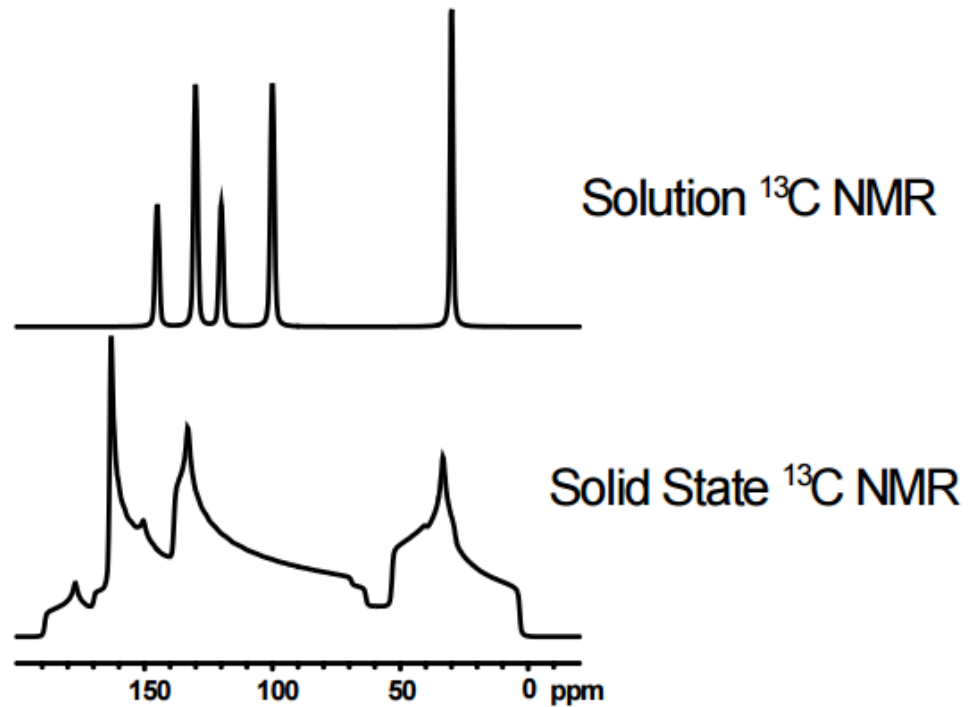
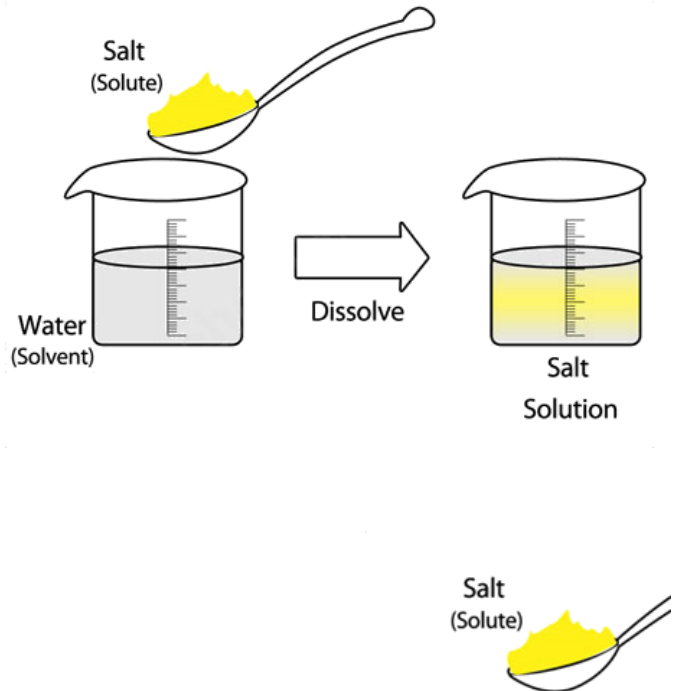


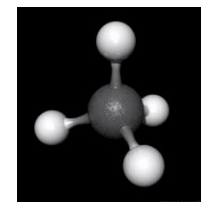
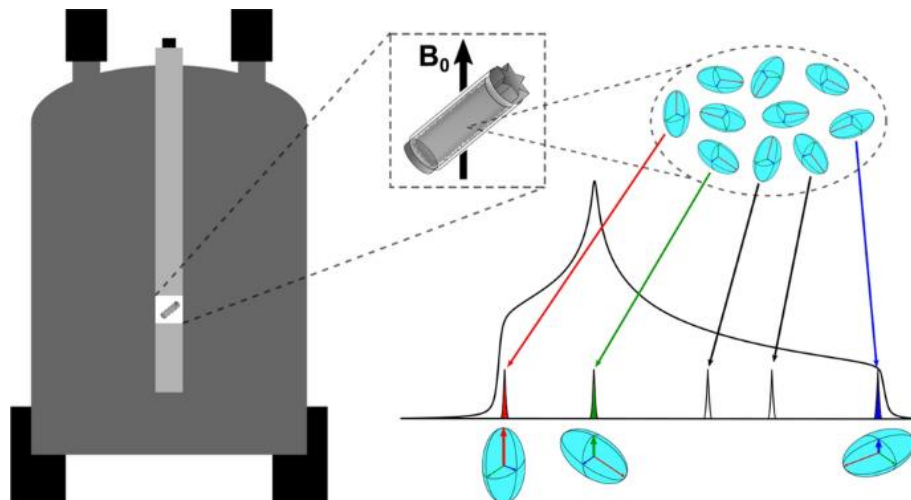
Figure 2.2: Result of the combination of the Zeeman and the quadrupole interaction for a Spin $I = 3/2$ nuclei in an external magnetic field.

$$H_{\text{TOTAL}} = H_Z + H_D + H_{\text{SC}} + H_{\text{CS}} + H_Q + \dots$$

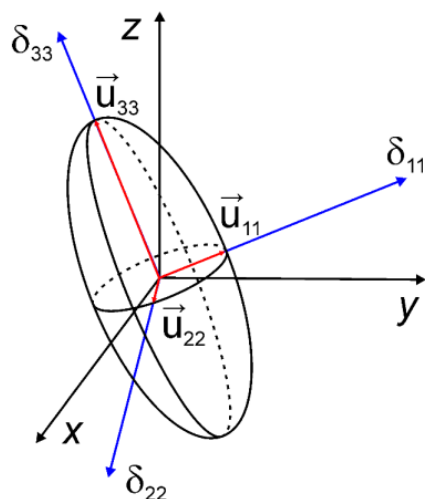
13C NMR At 9.4 T	Zeeman	Dipolar	Scalar (J-coupling)	Chemical shift	Quadrupolar
	H_Z	H_D (Through space between spin)	H_{SC} (Through bond of electrons)	H_{CS}	H_Q
In solution	100 MHz	0 kHz	~ 400 Hz	Isotropic value	0
In solid	100 MHz	Up to 100 kHz	Up to 10 kHz	Up to 100 kHz CSA (Chemical Shift Anisotropy)	Up to MHz
How to remove		Dipolar decoupling	Scalar decoupling	MAS (Magic Angle Spinning)	MAS (Magic Angle Spinning) High field NMR



CSA (Chemical Shift Anisotropy)



**Isotropic value
(Solution)**



$$\hat{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

$$\delta = u^{-1} \cdot \delta_{PAS} \cdot u$$

$$\text{where } \delta_{PAS} = \begin{pmatrix} \delta_{11} & 0 & 0 \\ 0 & \delta_{22} & 0 \\ 0 & 0 & \delta_{33} \end{pmatrix}$$

$$\text{and } u = (\vec{u}_{11}, \vec{u}_{22}, \vec{u}_{33})$$

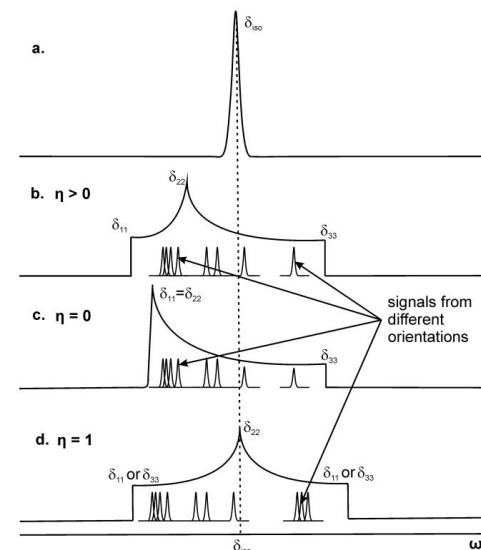


Figure 2.12. The effect of CSA on NMR spectra: a) Isotropic signal in solution-state NMR as a result of rapid motional averaging. b, c and d) Powder patterns observed at different values of the asymmetry parameter η .

asymmetry parameter = η (eta)

Magic Angle Spinning (MAS)

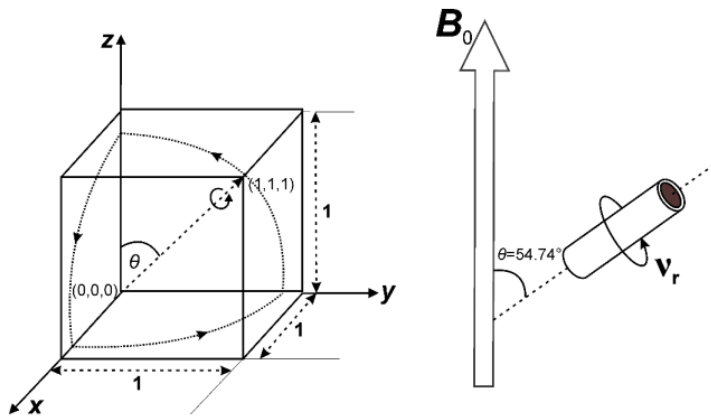


Figure 2.17. The unit cube representation of the magic angle (*left*) and sample rotation at the magic angle with a frequency ν_r (*right*).

Isotropic value

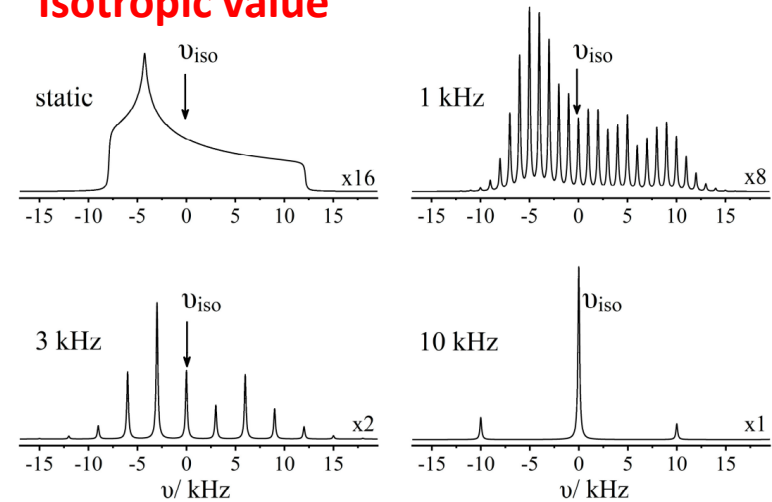


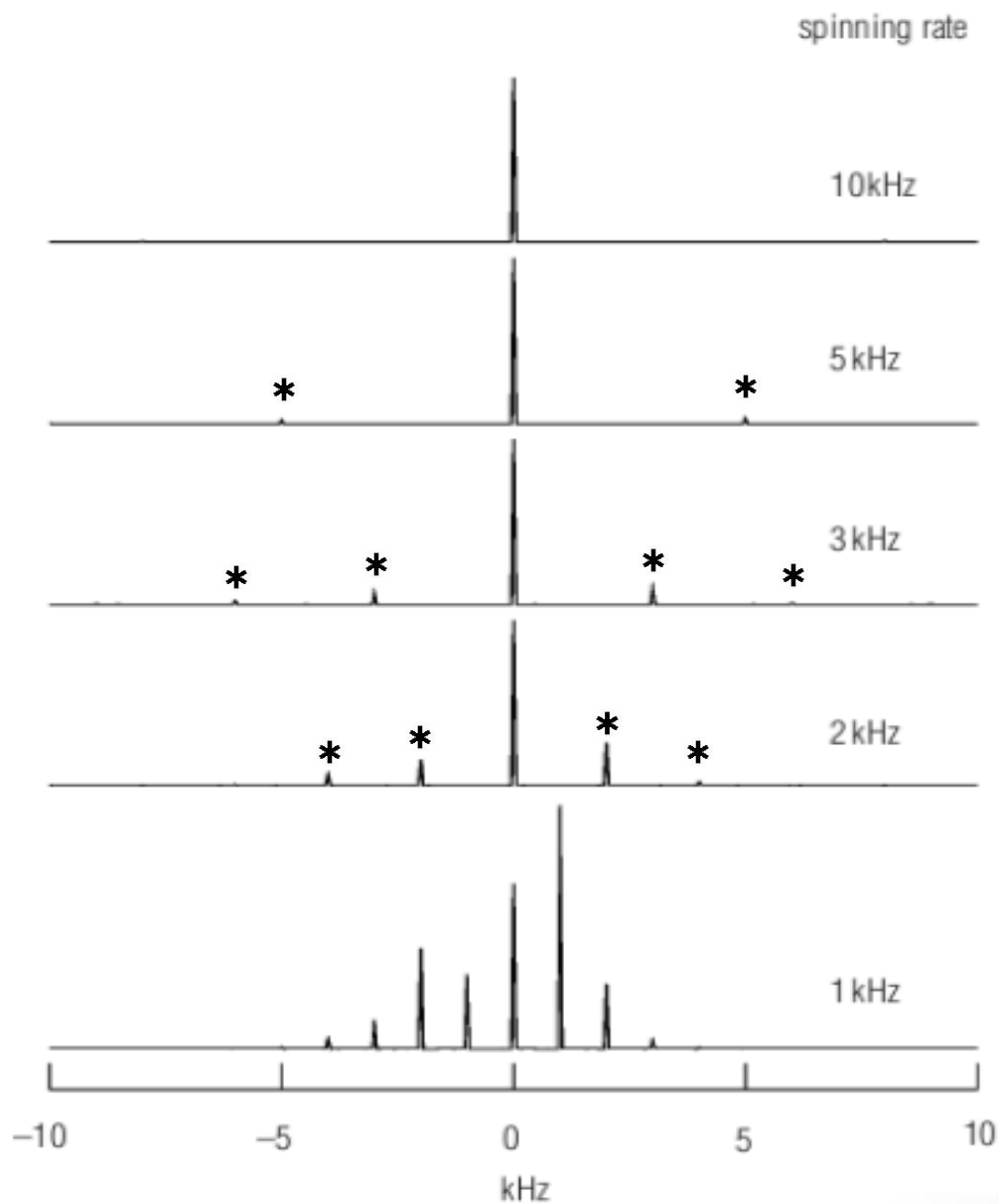
Figure 3. Numerical simulations demonstrating the effect of magic-angle spinning (MAS) upon the solid-state NMR line shape of a spin-1/2 nucleus with dominant line broadening due to the magnetic shielding anisotropy. Spinning sidebands are located at integer multiples of the rotor frequency.

$$\omega_P(\theta) = 2\pi\nu_P(\theta) = \gamma B_0 \left(1 - \sigma_{iso} - \frac{1}{3} \Delta\sigma (3\cos^2\theta - 1) \right)$$

$$\theta = 54.7^\circ$$

$$3\cos^2\theta - 1 = 0$$

Spinning side-band



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Organic complexes

Inorganic complexes

Zeolites

Mesoporous solids

Microporous solids

Aluminosilicates/phosphates

Minerals

Biological molecules

Glasses

Cements

Food products

Wood

Ceramics

Bones

Semiconductors

Metals and alloys

Archaeological specimens

Polymers

Resins

Surfaces

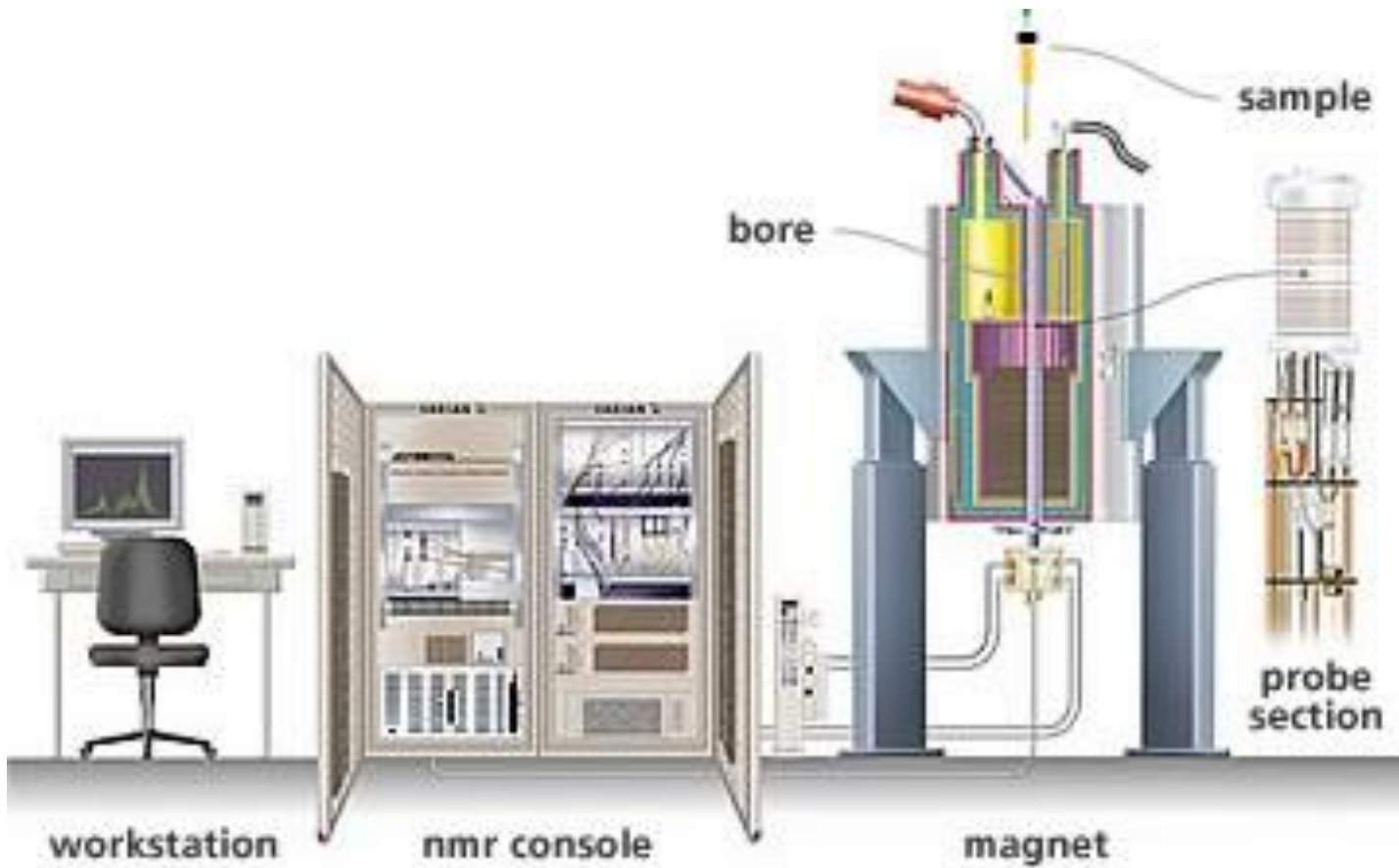
But, Fine particle + at least 20mg

7. Hardware

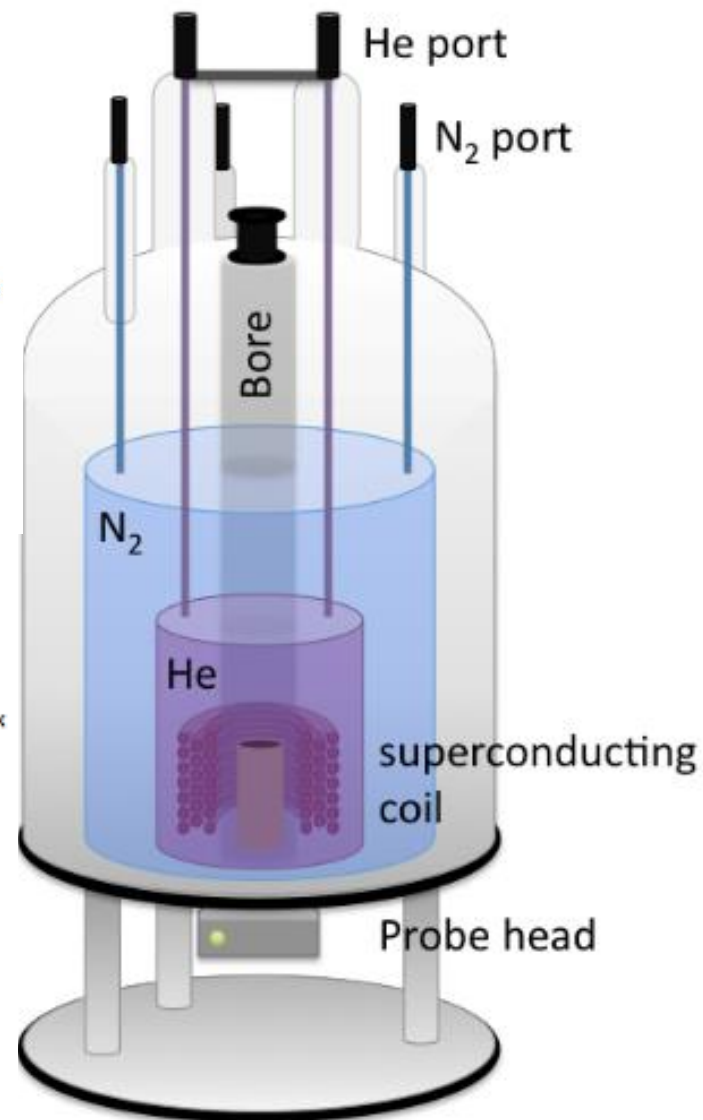
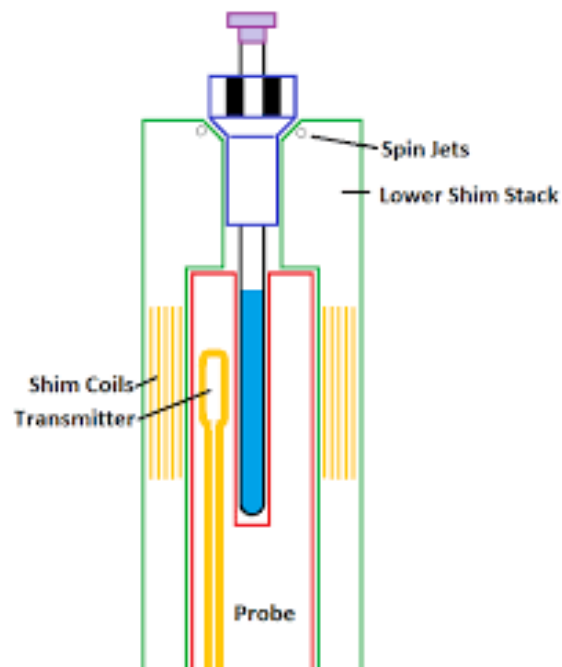
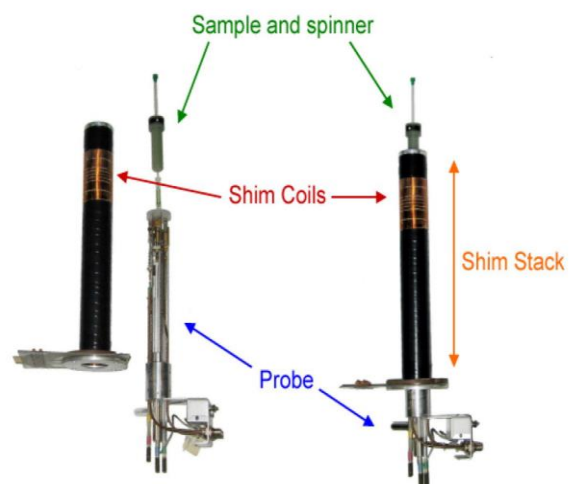
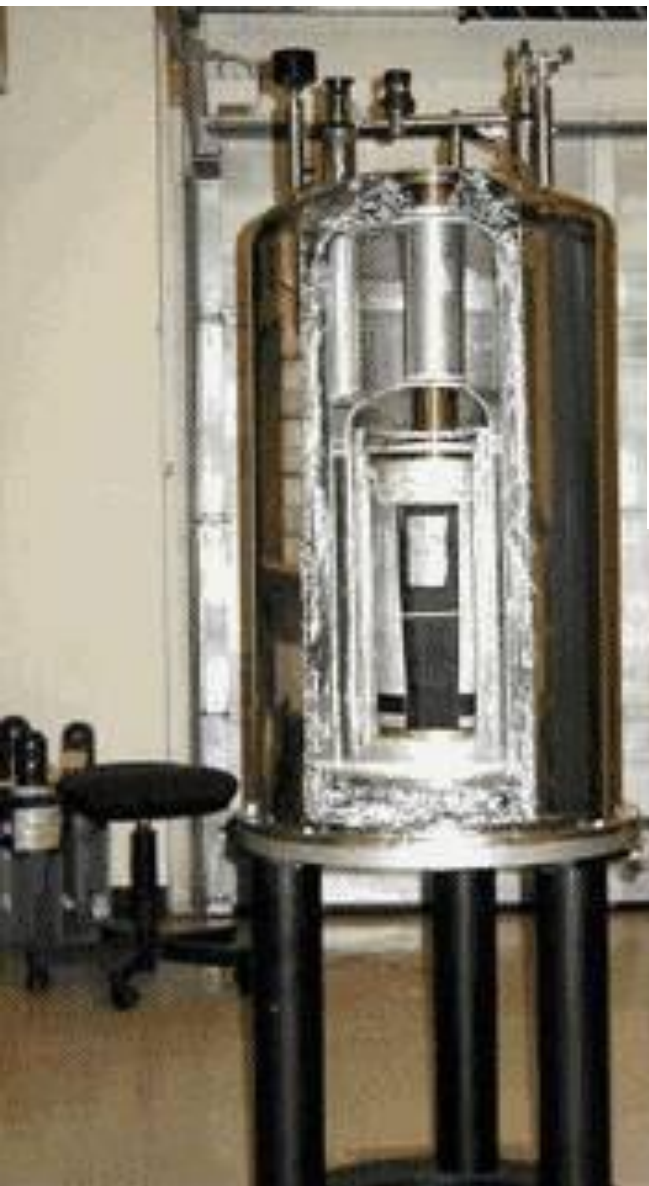
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NMR diagram



Magnet diagram



Varian 600 MHz NMR



	600 MHz NMR
Location	102-B119
Measurement Type	Self / Request
Model	VNMRS 600 (Varian)
Magnet	14.1 T
Channel	3 channel
Probe	5 mm PFG Auto X DB probe 5 mm Automated triple resonance probe 4 mm Nano TM probe 1.6 mm triple resonance HXY MAS solid probe 5 mm double resonance MAS solid probe
Auto-sampler	X
Auto-tuning & matching	-
Power	100 W / 300 W / 300 W
Channel	Ch1 : ^1H , ^{19}F Ch2 : 170MHz(^{31}P) ~ 150 MHz (^{13}C) Ch3 : 150MHz(^{13}C) ~ 60 MHz (^{15}N)
Temperature	-60 ~ 100 °C

Bruker 400 MHz NMR

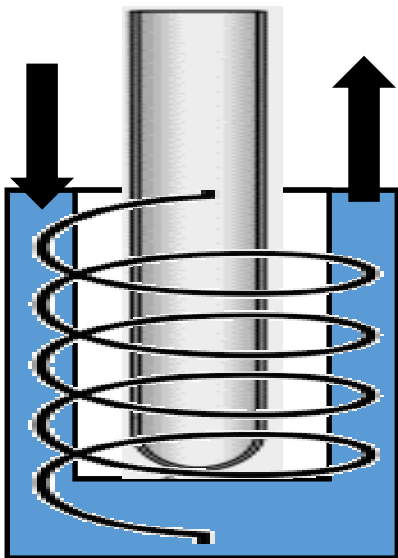


	400 MHz NMR
Location	102-B119
Measurement Type	Self / Request
Model	AVANCE III HD (Bruker)
Magnet	9.4 T
Channel	2 channel
Probe	BBO probe
Auto-sampler	O
Auto-tuning & matching	O
Power	100 W / 500 W
Channel	Ch1 : ^1H , ^{19}F Ch2 : 160MHz(^{13}C) ~ 49 MHz (^{15}N)
Temperature	-150 (20) ~ 150 °C

Cryogenic Bruker 600 MHz NMR (Jan, 2023)



L-N₂ (77K) -> S/N ratio 2~3배
L-He (4K) -> S/N ratio 4배



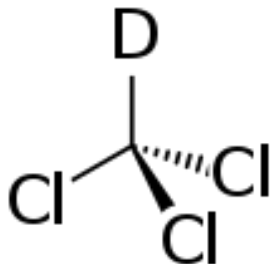
	600 MHz NMR
Location	102-B119
Measurement Type	Self / Request
Model	AVANCE NEO
Magnet	14.1 T
Channel	2 channel
Probe	5 mm Cryo-probe 5 mm I-probe
Auto-sampler	O
Auto-tuning & matching	O
Power	300 W / 500 W
Channel	Ch1 : ¹ H Ch2 : 240MHz(³¹ P) ~ 27.6 MHz (¹⁰⁹ Ag), ¹⁹ F
Temperature	-150 ~ 150 °C

8. Pre-treatment

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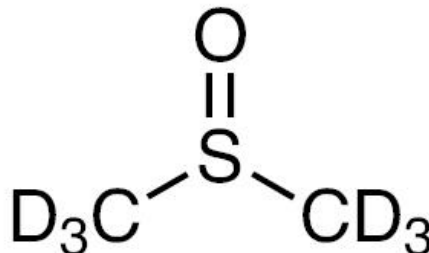
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Dielectric constant : **Polar** > 20 > **Non-polar**



CDCl₃

- Dielectric constant: 4.8
- Advantage:
 - Cheap,
 - Easily Removed
- Disadvantage:
 - Light sensitive(Contain HCl)
 - Toxic, carcinogenic
 - Weak lock signal
 - Easily evaporated

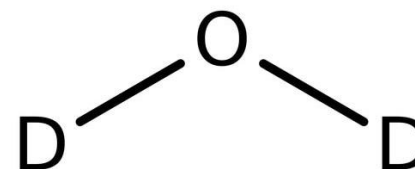


DMSO-D₆

- Dielectric constant: 46.7
- Advantage:
 - Strong lock signal
- Disadvantage:
 - High price
 - Highly viscosity
 - Easily contain water
 - M.P.: 20 ~ 22 °C (Freeze RT)
 - Hard removed

NMR Solvent Storage

Avoid light & moisture: All NMR solvent
Store refrigerator (4°C): CDCl₃, THF-D₈

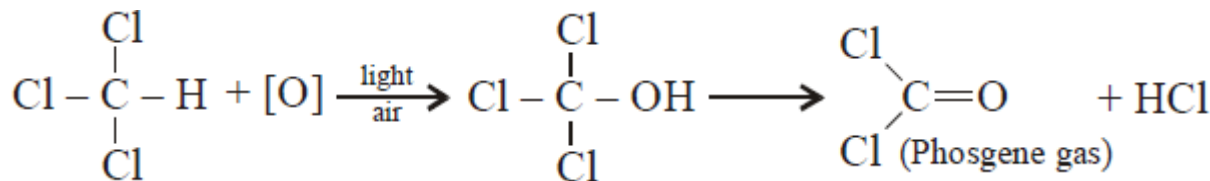


D₂O

- Dielectric constant: 78.5
- Advantage:
 - Cheap
- Disadvantage:
 - Exchange OH and NH
 - Easily contain water
 - Chemical shift (Temp. dependent)
 - Hard removed

CDCl₃ + Light -> HCl

- Use silver foil
(Stabilizer, radical scavenger)
- Use molecular sieve
(Eliminate H₂O)



Change of chemical shift

- Temperature
- pH
- Concentration

HOD peaks

- Related residual H₂O
- Slow exchange H₂O and HOD
→ two peaks
(singlet H₂O, 1:1:1 triplet HOD)
- Hydrogen bond
→ Broad peak of HOD

How to remove residual water

→ Use Molecular Sieve 3~5 g in 100g (CDCl₃)

- 3 Å: Adsorption of polar liquid (NH₃, H₂O)
- 4 Å: Adsorption of Non-polar liquid
(H₂O, CO₂, SO₂, H₂S, C₂H₄, C₂H₆, C₃H₆, EtOH)
- 5 Å: Adsorption of Linear C_xH_x to n-C₄H₁₀
Alcohols to C₄H₉OH
C₄H₉SH

Thin wall (Precision-Glass)

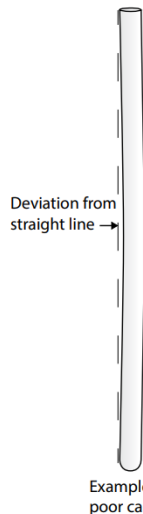
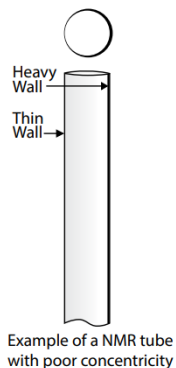
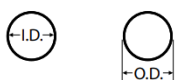
- **Temp 120 °C**
- Critical shimming quality (low Fe₂O₃)
- **Good volume reproducibility**
- High sample volume in RF coil
- 535-PP-7 (600 MHz grade, \$40)
- 527-PP-7 (400 MHz grade, \$25)

Economy (Middle MW)

- **MW<1500**, RT
- WG-1241-7 (600 MHz grade, \$10)
- WG-1228-7 (400 MHz grade, \$9)

High-Throughput (low MW)

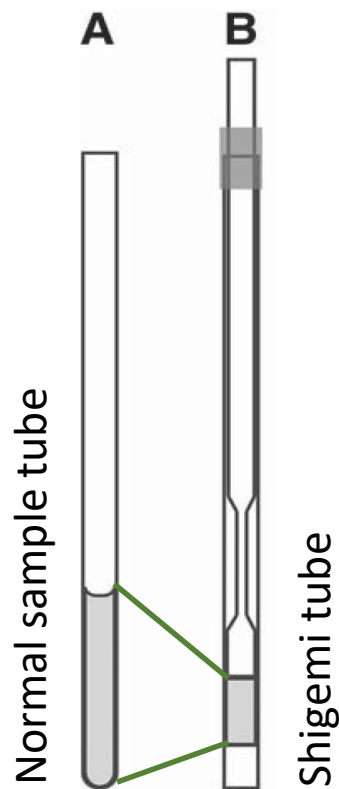
- up to 600 MHz, **MW<250**, RT
- WG-1000 (\$2)



5mm Thin-Wall NMR Tube Comparison Table

	High-Throughput	Economy	Precision (Glass)	Precision (Quartz)	Precision (Suprasil)
Material	Type 1 Class B Borosilicate Glass	Type 1 Class B Borosilicate Glass	Type 1 Class A Borosilicate Glass	Clear Fused Quartz	Synthetic Quartz
Impact On Shimming Quality By Paramagnetic Impurities	Medium (1200ppm Fe ₂ O ₃)	Medium (1200ppm Fe ₂ O ₃)	Small (400ppm Fe ₂ O ₃)	None (0.5ppm Fe ₂ O ₃)	None (<0.005ppm Fe ₂ O ₃)
Maximum Working Temperature	Ambient	Ambient	230° C	1300° C	1300° C
Sample Volume Reproducibility	10%	10%	0.5%	0.5%	0.5%
Recommended Applications	Small molecule experiments up to 600 MHz (MW<250)	1D NMR experiments with small organic molecules (MW<1500)	Experiments requiring critical shimming quality (high-field, multi-dimension, multi-nuclei)	¹¹ B NMR, rapid cooling/heating experiments, photochemistry studies	Photochemistry studies with deep UV light source

Special purpose sample tube

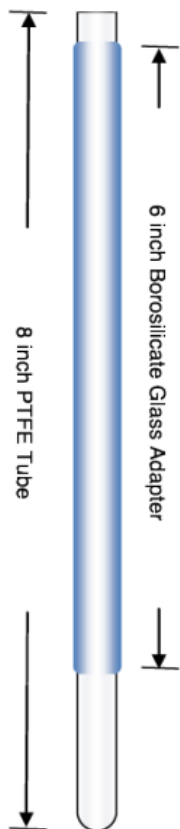


Reduce sample volume (1/3)

Shigemi tube

\$ 300 - 400

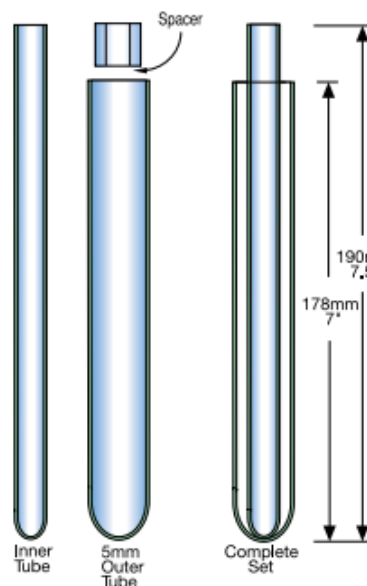
- Increase 16% SNR
- Low con. or low volume



PTFE tube

\$ 60

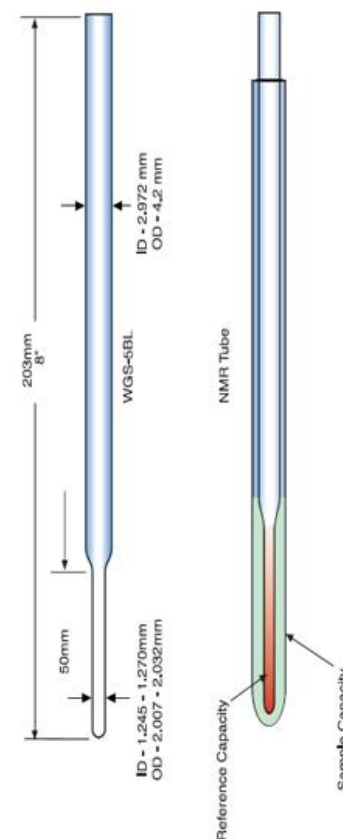
- HF or ^{29}Si NMR



Coaxial tube

\$ 40 - 50 (+ \$ 50)

- Non-deuterated sample
- Quantitative NMR
- Referencing



Stem Coaxial tube

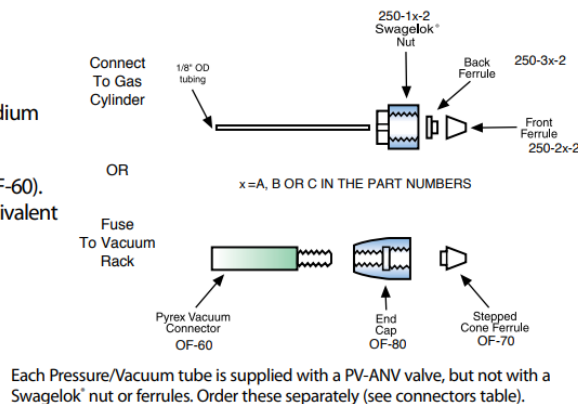
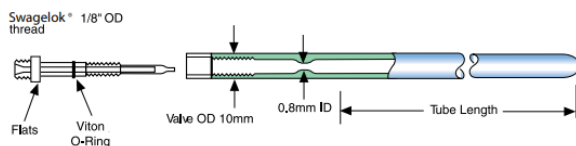
\$ 40 - 50 (+ \$ 50)

- Non-deuterated sample
- Quantitative NMR
- Referencing

Special purpose tube & cap

Pressure/Vacuum Sample Tube

Wilmad's Pressure/Vacuum Tube is the most reliable NMR tube for medium range pressure (<300 psi) experiments in the market. It is designed to connect to a 1/8" metal (stainless steel or brass) vacuum line using SwageLok® fittings or a rubber vacuum hose and a glass connector (OF-60). The PV-ANV valve is made of PTFE and all other parts are Pyrex® or equivalent glass. Valve is opened simply by turning counterclockwise.



Each Pressure/Vacuum tube is supplied with a PV-ANV valve, but not with a Swagelok® nut or ferrules. Order these separately (see connectors table).

Low Pressure/Vacuum Tubes

Wilmad's Low Pressure/Vacuum (LPV) tube is ideal for anaerobic and gas-tight NMR experiments, and offers a convenient flame-free sealing solution for air sensitive or volatile liquid samples.

- Robust sealing system allows pressure build-up inside the sample
- Greaseless PTFE piston provides a 100% contamination-free seal
- Redesigned with a 4X larger sealing surface; eliminates leaks and greatly increases lifetime when compared to traditional J. Young tubes
- Axial symmetric design guarantees application in spinning experiments
- Due to the nature of glass, Extreme Caution should be exercised when using at elevated or reduced pressures since a tiny scratch on the glass surface would significantly lower the tensile strength. Adequate safety shielding should always be used when working in these conditions.



Ethyl Vinyl Acetate Cap

- Cheap
- Avoid CDCl₃, Acetone-D₆



Ethyl Vinyl Acetate Cap + Teflon tape

- Cheap
- Use CDCl₃, Acetone-D₆



PTFE Cap

\$ 16 (or \$ 5 economy ver.)

- Use CDCl₃, Acetone-D₆, HF

- Sample volume = 500 ul (400 ~ 700 ul)
- Sample concentration
 1. ^1H : 0.05 mM ~ 10 mM (Too high concentration cause Line-broadening effect)
 2. ^{13}C , 2D NMR(COSY, NOESY, TOCSY, etc.): 10 mM ~ 100 mM
 3. ^{15}N , ^{17}O , Hetero 2D NMR (HSQC, HMBC, HMQC, etc.): 100 mM < Highest concentration
 - ex) Sample A (MW=200), 0.05 mg / 500 ul = 0.5 mM = 100 ppm
 - Sample A (MW=200), 1 mg / 500 ul = 10 mM = 2000 ppm
 - Sample B (MW=500), 25 mg / 500 ul = 100 mM

<Internal reference>

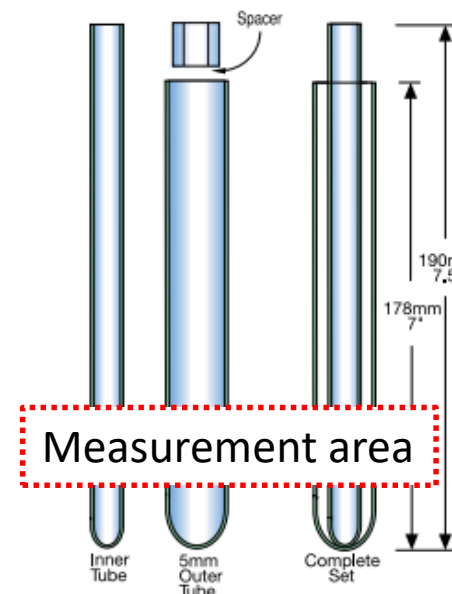
1. Sample + NMR solvent (CDCl₃, D₂O, DMSO-D₆, etc.) + reference compound (TMS, DSS)

<External reference>

- 2-1. Sample + NMR solvent (CDCl₃, D₂O, DMSO-D₆, etc.)
- 2-2. Reference sample (P31: TPP = -17.57 ppm, F19: TFT: -63.72 ppm)

3. Coaxial sample tube (Evans method)

- Inner tube: NMR solvent or Reference
- Outer tube: Sample



- None deuterated solvent condition -> No Lock / No auto shim -> Poor or not easy measurement
- NMR solvent and Referencing (+Quantitative NMR)

- Degassing

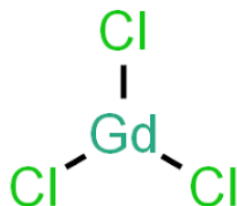
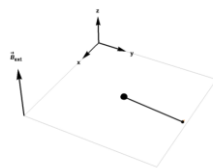
Oxygen (Paramagnetic) -> Short T1&T2 relaxation-> **Quench** for NMR signal -> Purge N2 or Ar gas

- Doping agent (Use Paramagnetic agent)

- Reduce T1 & T2 -> Short experiment time

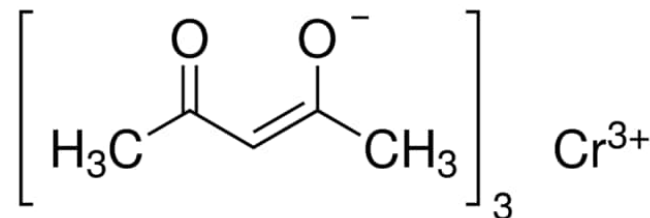
- Line broadening effect (poor shimming)

- Add paramagnetic material concentration: 1 mM (1H), 25 mM – 50 mM (13C)



GdCl3

Gadolinium(III) chloride



Cr(acac)3

Chromium(III) acetylacetonate

or

CuSO4, MnCl2, NiCl2

Dielectric constant : **Polar** > 20 > **Non-polar**

- Wash sample tube to acetone or ethanol.

Cheap sample tube dry-situation tilted state in oven make possible bending
(Sample tube bending test → rolls the ground If bending sample tube spins, quartz glass in probe has some damage.)



Probe Bottom

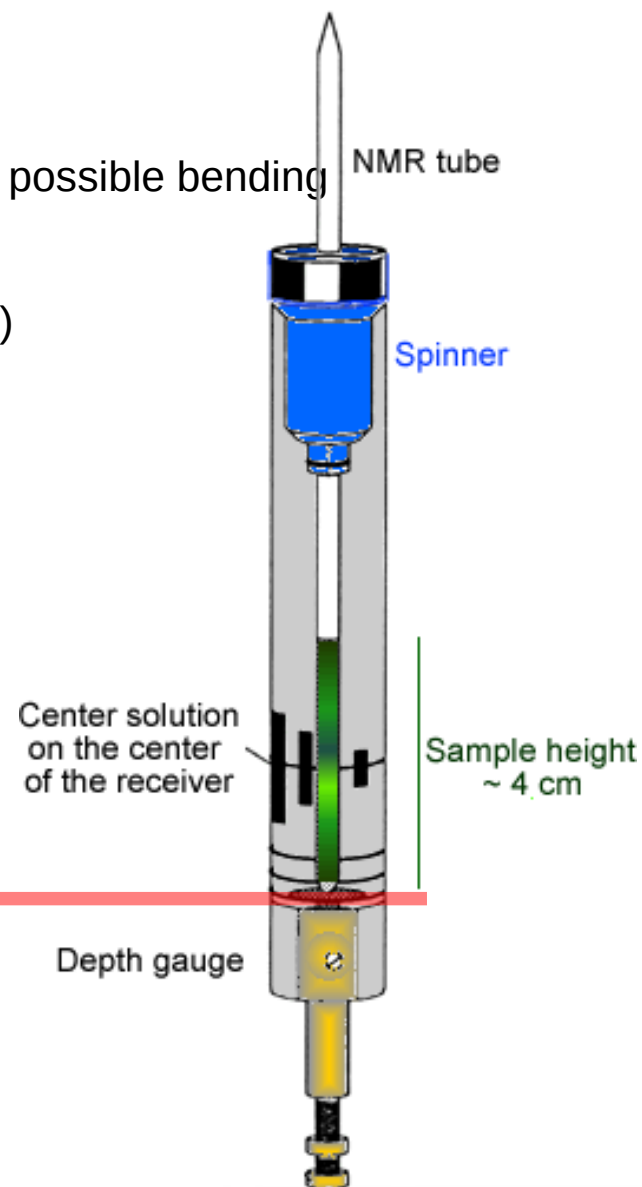
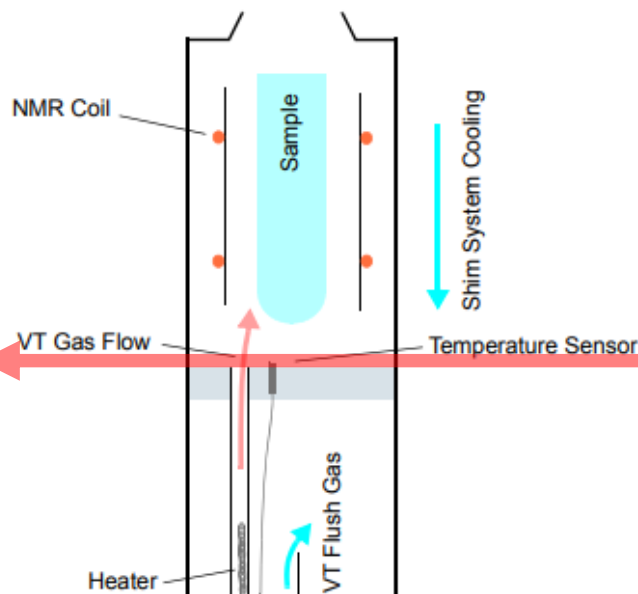
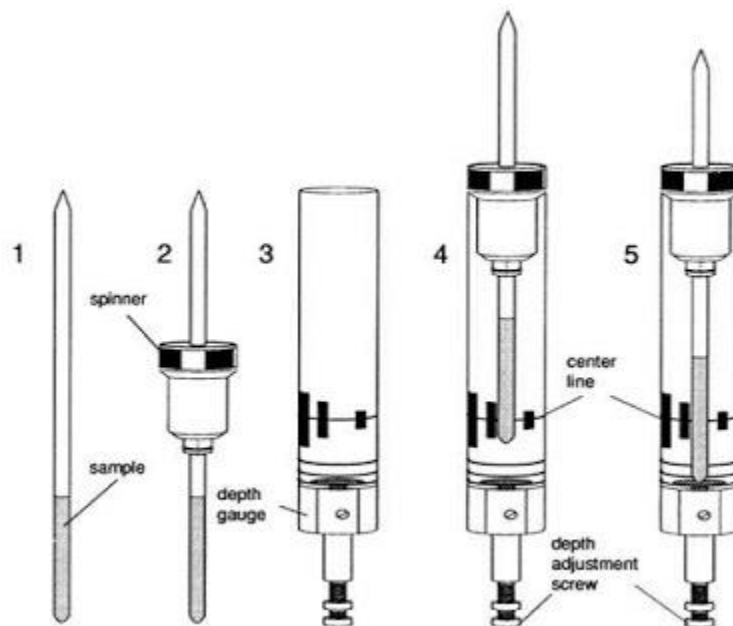
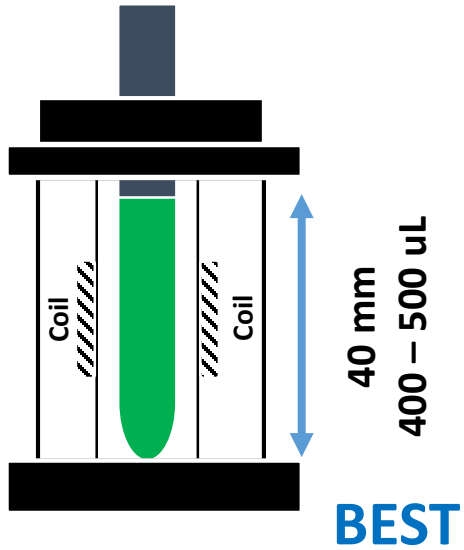
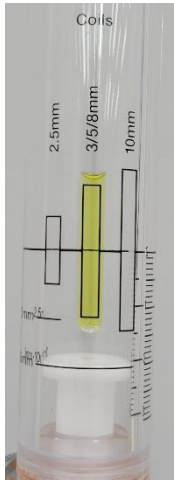


Figure 3.1 Sketch of sample temperature control in a NMR probe

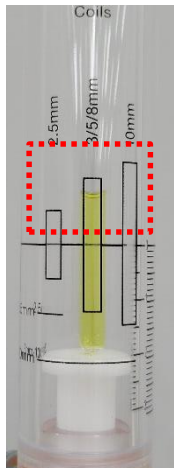
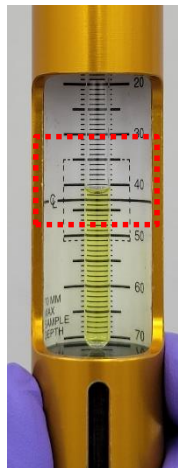
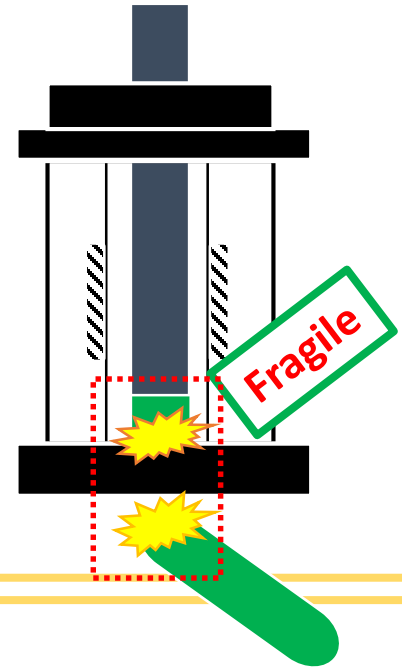
1. Perfect solution sample filters syringe filter.
(If your sample has insolubility, It makes low resolution and sensitivity about peak)
2. 5 mm sample tube inserts sample 0.5 ml (500 μ l, 4cm)
3. Spinner placed on depth gauge insert sample tube
(※ Don't touch O-ring)
4. Check location depth gauge center (dash line square) with sample tube
5. Remove depth gauge.



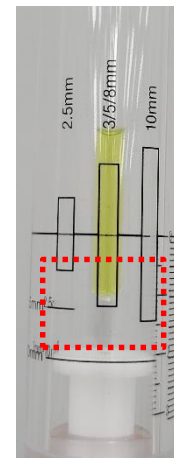
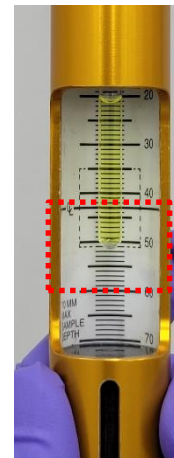
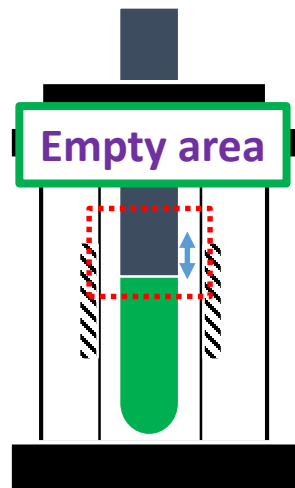
Sample volume and height



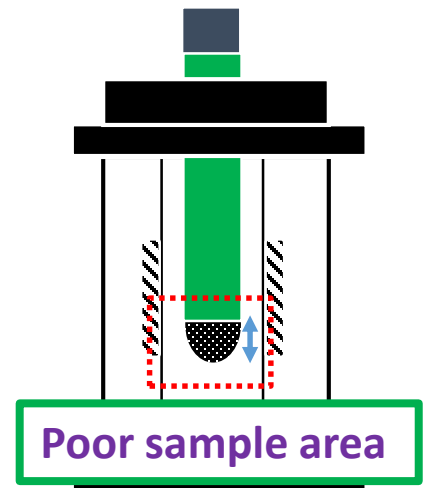
Worst



Bad shim

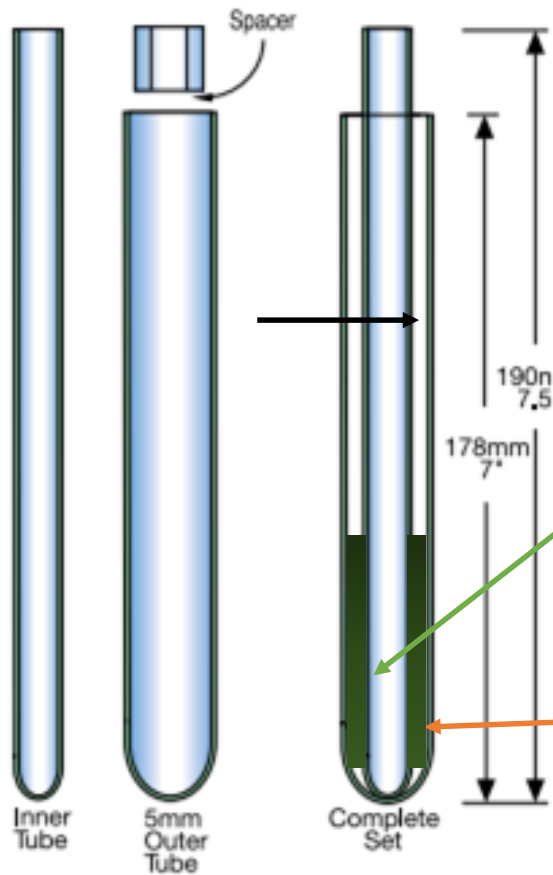


Bad shim

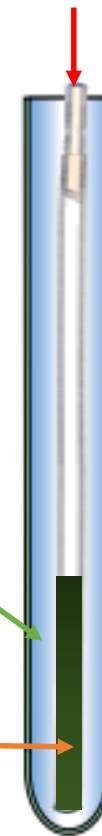


Sampling for PF6 or Toxic sample

Standard Evans method



PTFE tube



Reference
(NMR solvent, Standard)

Sample

Coaxial tube

9. Operation Manual

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9-1. Manually Operation

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1. Create Dataset



Click **Create Dataset** (edc) - Start tab.
Insert parameter value.

Prepare for a new experiment by creating a new data set and initializing its NMR parameters according to the selected experiment type. For multi-receiver experiments several datasets are created. Please define the number of receivers in the box below.

NAME	proton_exp
EXPNO	1
PROCNO	1
DIR	C:\data3.0
Solvent	DMSO
Experiment Dirs.	C:\Bruker\TopSpin3.0.b.40\exp\stan\nmr\par
Experiment	PROTON
TITLE	1D- Proton experiment 30 mg Menthyl Anthranilate in DMSO-d6

☐ Show new dataset in new window

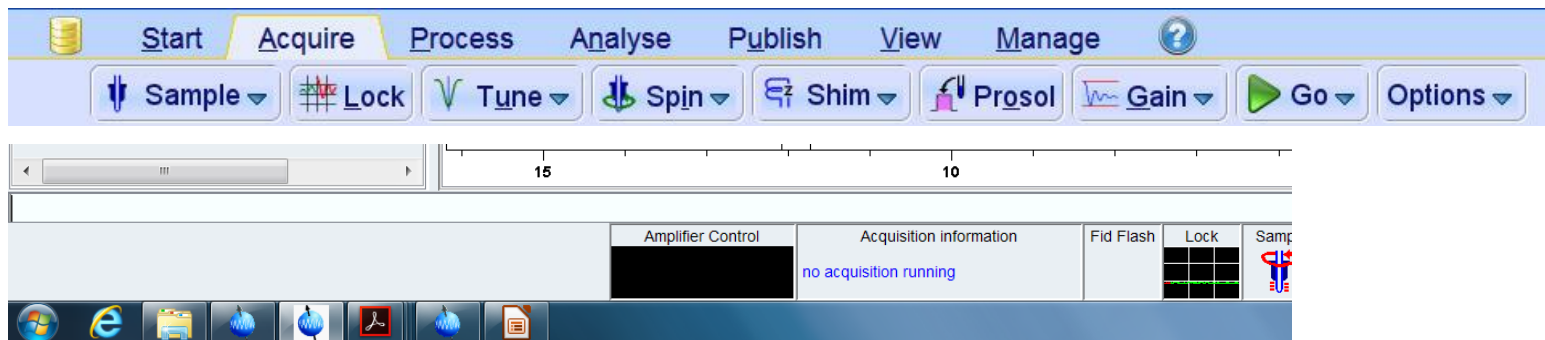
1 Receivers (1,2, ...16)

OK Cancel More Info... Help

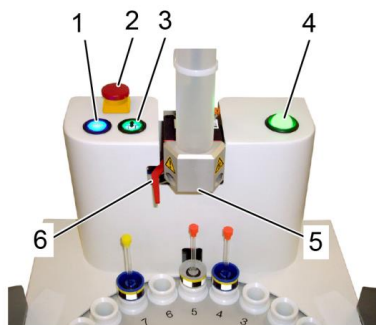
Experiment name : ex) 20160908_Test_1
Experiment number : ex) 1(1H), 2(13C), 10(2D) (1~999)
Processing number: ex) 1
Data save route ex) \ data
NMR solvent

Parameter set
ex) proton - PROTON, carbon - C13CPD
Direct type or select
Sample information.

2. Sample insertion into the magnet



Insert : Prompt types **sx #** (sample holder number)
Eject : Prompt types **sx ej**



1. Rotate carousel clockwise blue push button (enabled)
2. Emergency stop button
3. Inject/Eject green push button (enabled)
4. State LED (green showing *idle* state)
5. Sample gate (open)
6. Sample over length latch



- Press the blue button to rotate the carousel so that the sample carrier to measure next is below the Transport tube gate.



- When pressing the Inject/Eject button the sample carrier below the Transport tube gate will be lifted towards the magnet bore and transported to the magnet bore.



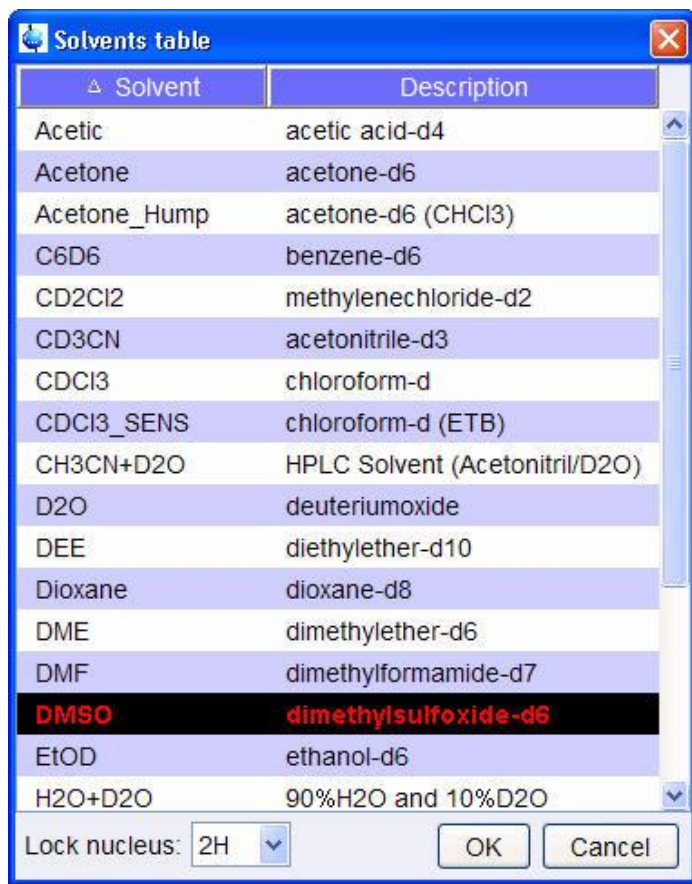
- When pressing the Inject/Eject button a second time the sample carrier will be removed from the magnet bore and transported to the SampleCase and placed in the holder below the Transport tube gate.

※ (XXX) or bold character are command. Could use command line.

3. Lock



Click  (lock) - Acquire tab

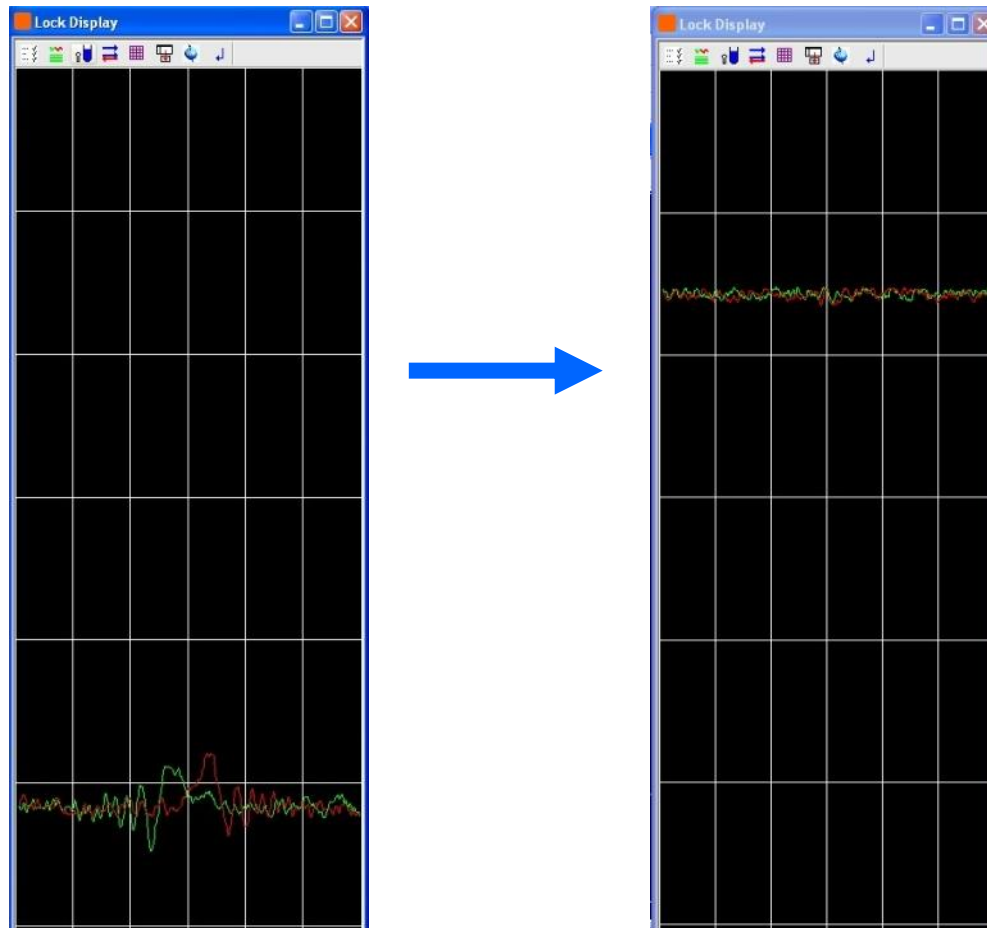


Choice lock solvent
(or, "lock used-NMR-solvent" ex) **lock DMSO**).

3. Lock

Lock-complete condition display lock level on state line.

If lock level is so high, control lock power or lock gain. (proper lock level = 50 ~ 60)





4. Tune

Click  (atma)

5. Spinning

Click  (ro on)

6. Shimming

Click  (tg)

7. Prosol

Click  (getprosol)

8. Receiver gain

Click  (rga)



9. Parameter

Number of scan : Prompt types **ns** (edit #)

Relaxation delay : Prompt types **de** (edit #)

10. Acquisition

Click  (zg)

Experiment end



Click



- Turn sample rotation on (ro on)
- Turn sample rotation off (ro off)
- Change sample rotation rate (ro)
- MAS Pneumatic Unit (masdisp)

Stop sample rotation (ro off) spinning

Type **bsmsdisp** on command line

Click lock On-Off (Stop lock)



To use manually operation

- 1) **sx #** - Insert sample into magnet
- 2) **edc** - Create new experiments room
- 3) **rsh** - Refresh optimized shim-map
- 4) **ro on** – spinning on
- 5) **lock** - Locking
- 6) **atma** - Auto tuning & matching
- 7) **getprosol** - Update standard parameter [ex, p1, plw1]
- 8) **ased** - Change parameter [ex, ns(number of scan), d1(delay time)]
- 9) **topshim** - shimming
- 10) **rga** - Auto-adjust receiver gain
- 11) **zg** - start experiment
- 12) **efp** - Fourier transformation
- 13) **apk** - auto-phase correction
- 14) **absn** - auto-baseline correction
- 15) **ro off** – spinning off
- 1) **sx ej** – sample eject

If automation system is connecting,
sx command is not working.

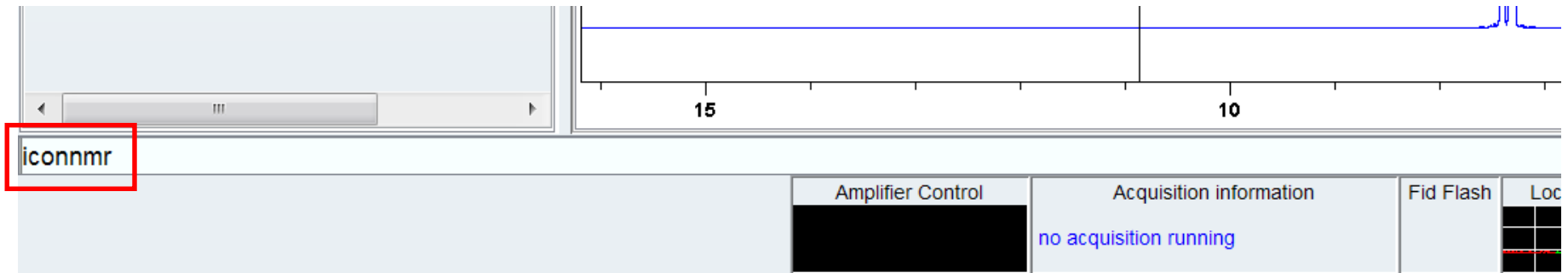


9-2. Automation (Icon-NMR)

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1. Open Icon-NMR

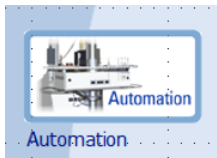


To open Icon-NMR : Prompt types **iconnmr**



2. Automation

Click



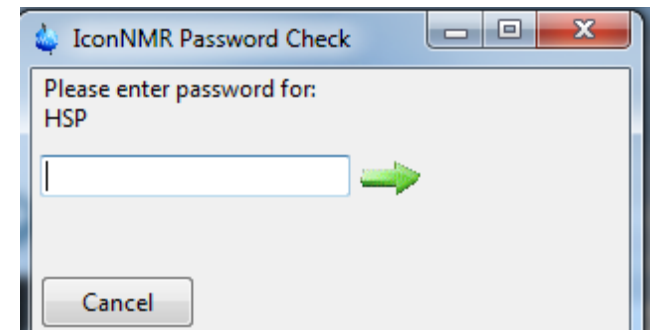
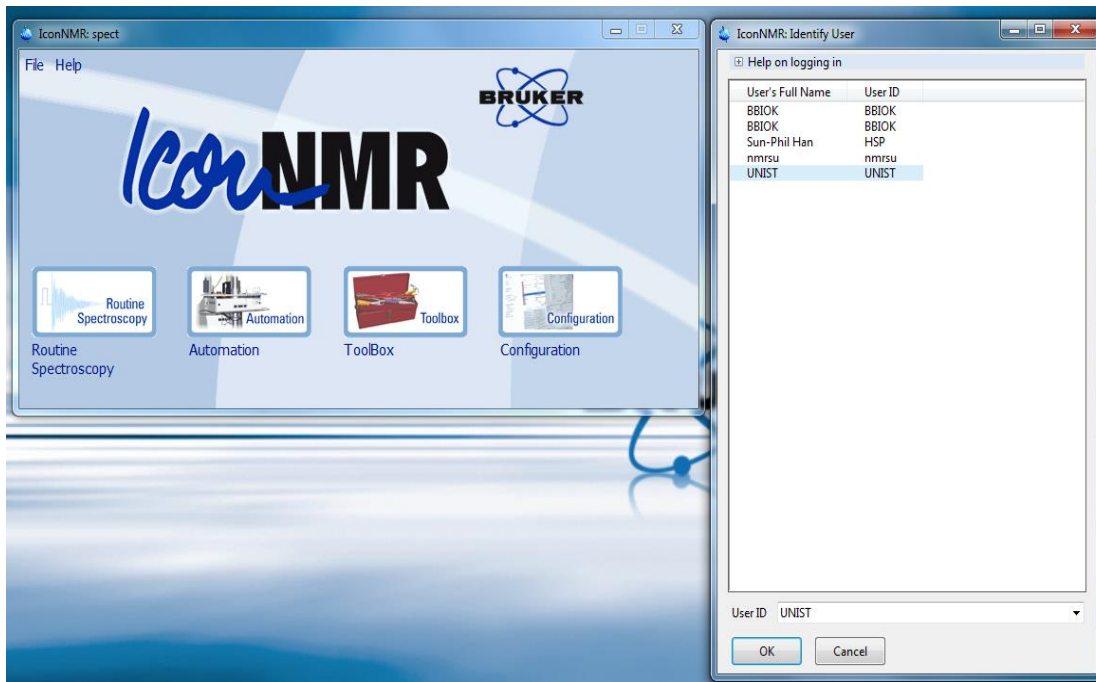
Automation



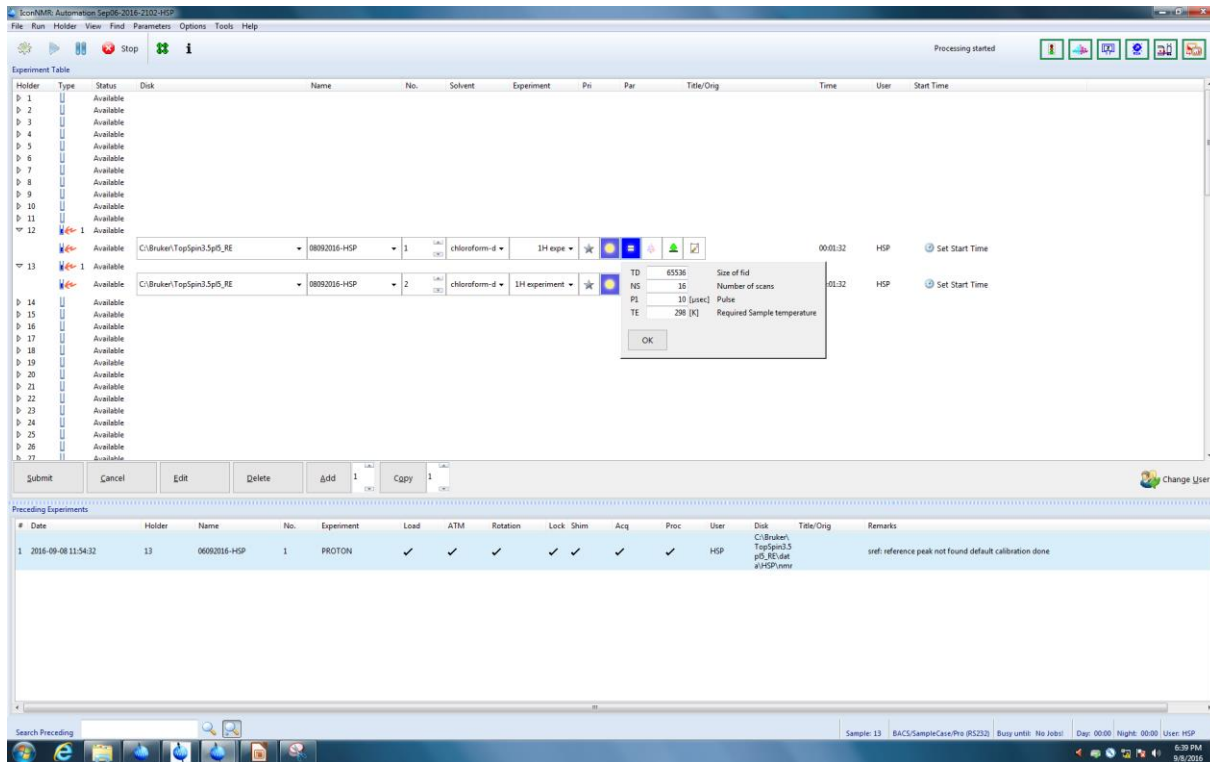
3. Login

Select user ID

Insert password



4. Experiment Table



1) Check holder status

2) Double click
empty holder (1~24)

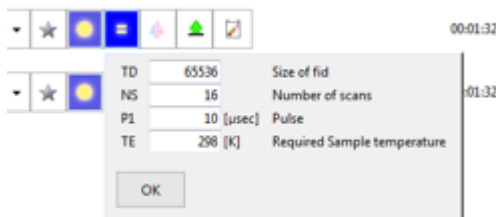
3) Type sample name

4) Change No.
(experiments number)

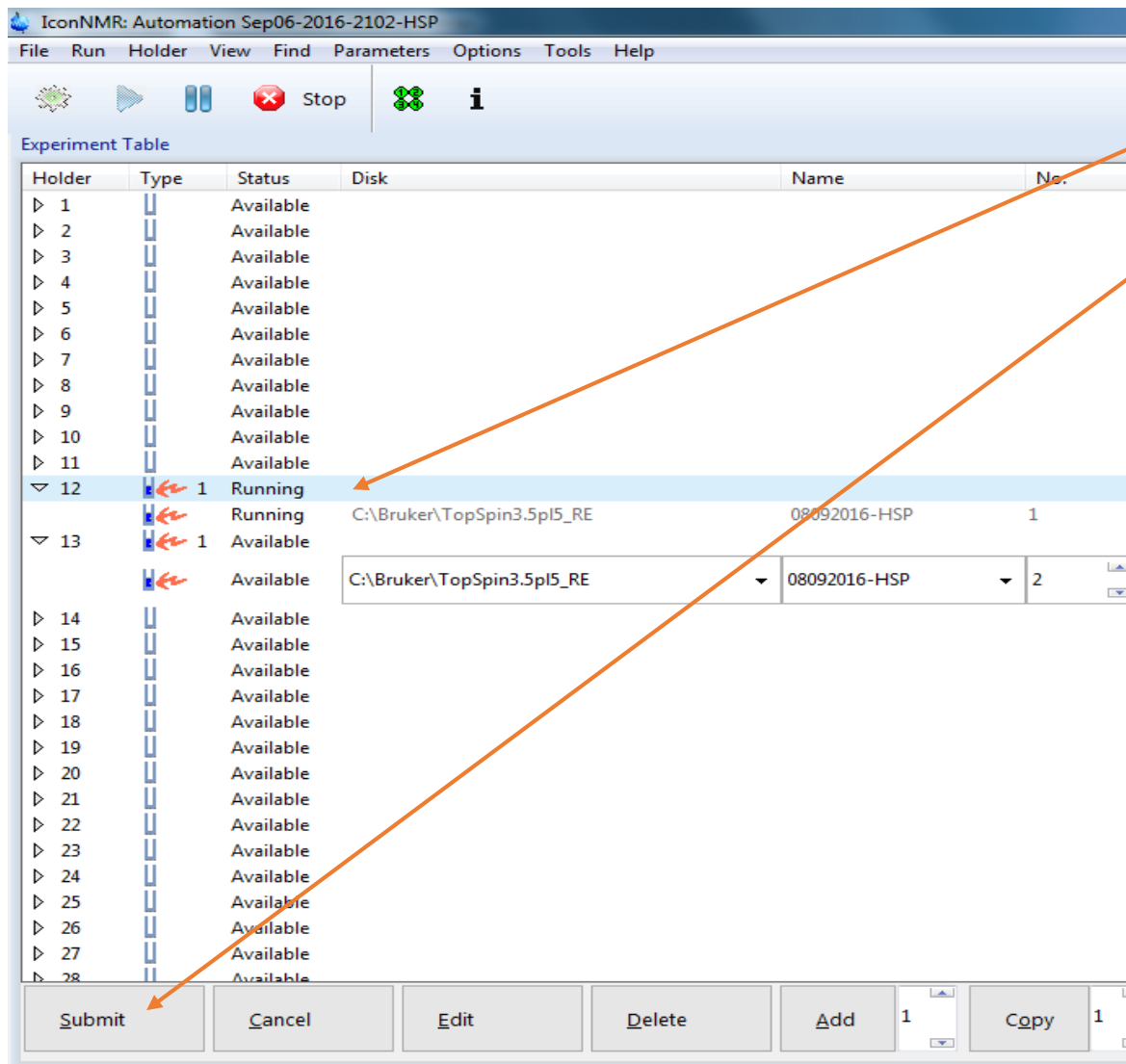
5) Select NMR solvent

6) Choice Experiment
(Proton, 13CCPD, 13CIG, etc.)

7) Change parameter value
(ns, p1, d1 .. etc) 



5. Acquisition



5) Choice experiment holder

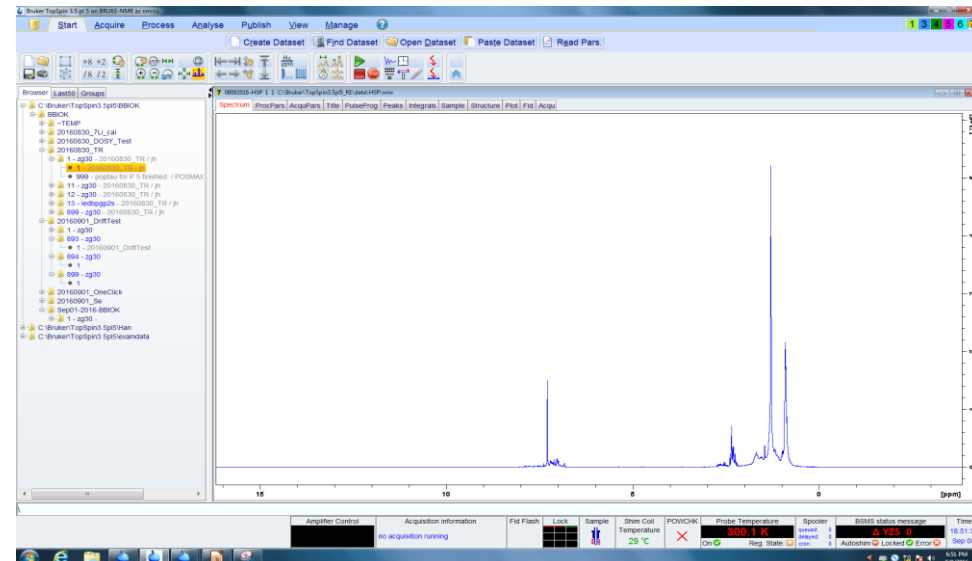
6) Click submit

6. Check NMR data

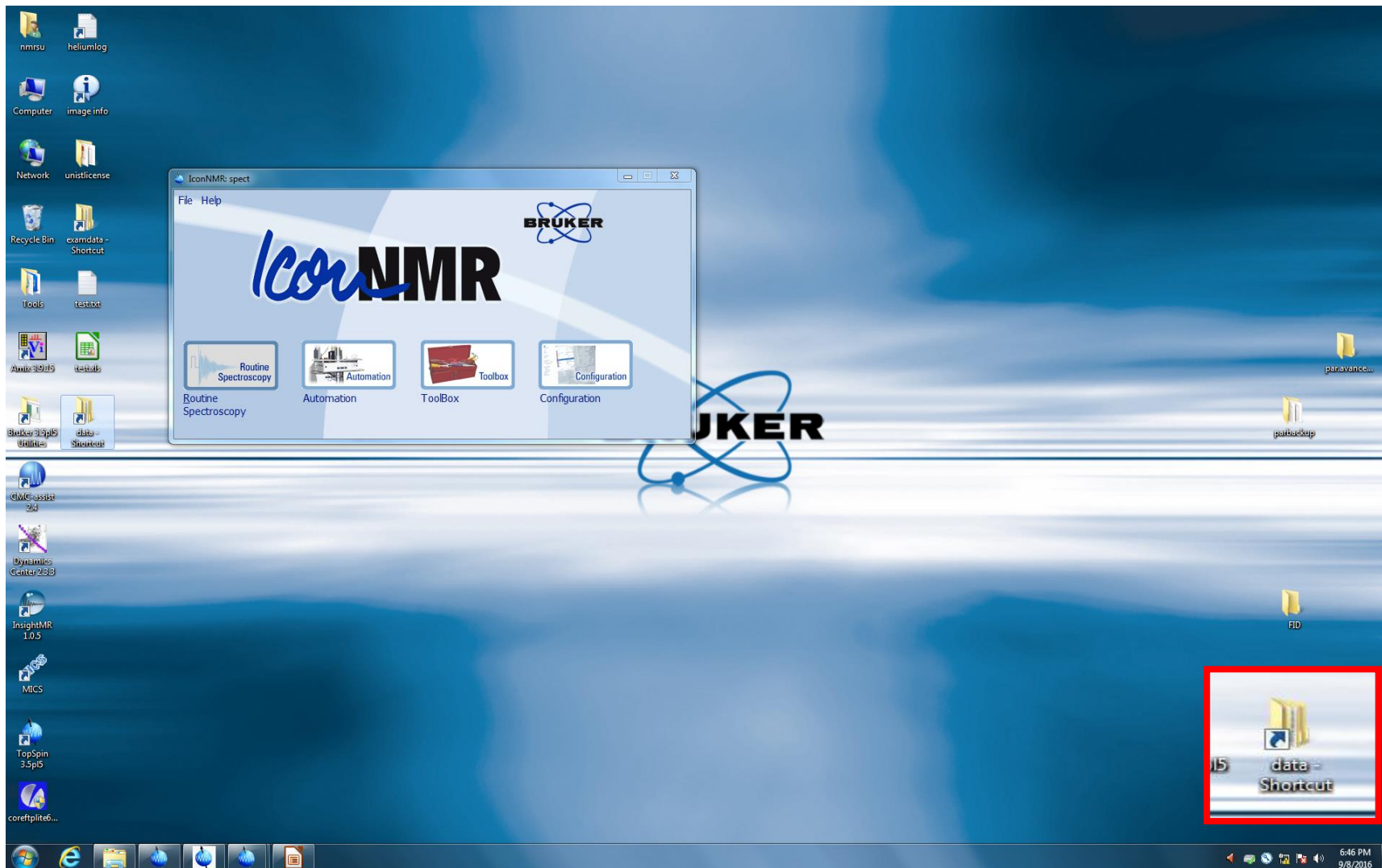
#	Date	Holder	Name	No.	Experiment	Load	ATM	Rotation	Lock	Shim	Acq	Proc	User	Disk	Title/Orig
2	2016-09-08 18:44:37	12	08092016-HSP	1	PROTON								HSP	C:\Bruker\TopSpin3.5 p05_RE\data a\HSP\nmr	
1	2016-09-08 11:54:32	13	06092016-HSP	1	PROTON	✓	✓	✓	✓	✓	✓	✓	HSP	C:\Bruker\TopSpin3.5 p05_RE\data a\HSP\nmr	

7) Double-Click
Preceding Experiments tap

8) Show NMR-spectrum



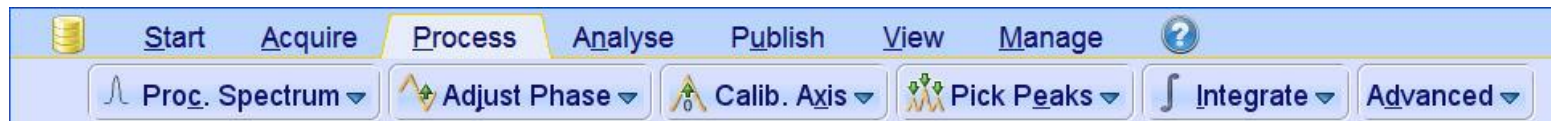
7. Data Route (FID)



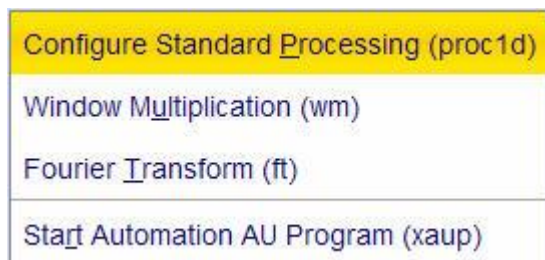
10. Processing

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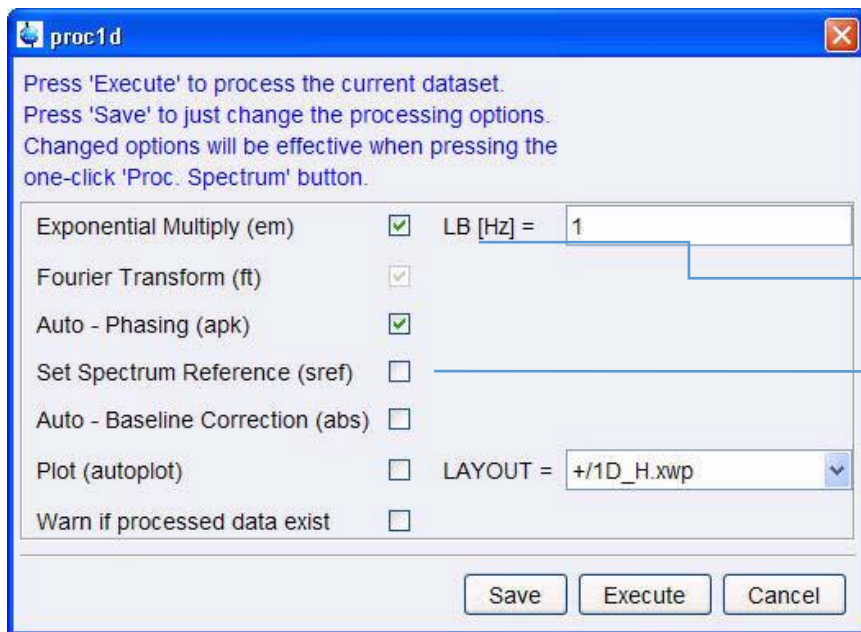
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Click **Proc. Spectrum** down arrow



Click Configure Standard Processing (proc1d)

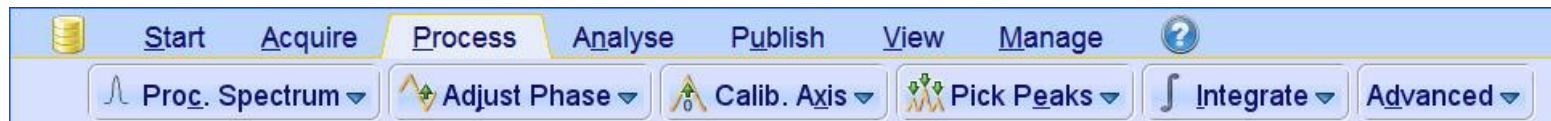


LB $\uparrow$ $\rightarrow$ sensitivity $\uparrow$, resolution $\downarrow$
 Default 0.3 (^1H)
 Sensitivity 1 ~ 3 (^{13}C)

If reference use TMS, check TMS.
 TMS - chemical shift = 0 (Automation)

* To save

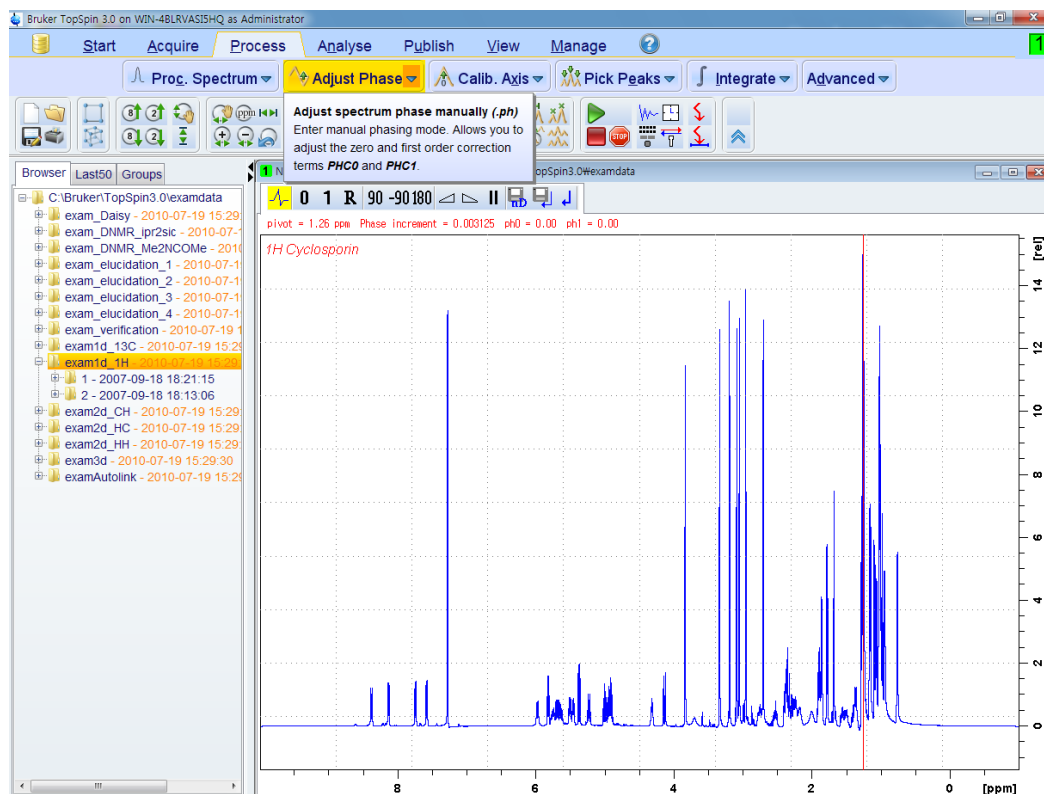
Click **Proc. Spectrum**



Process tab

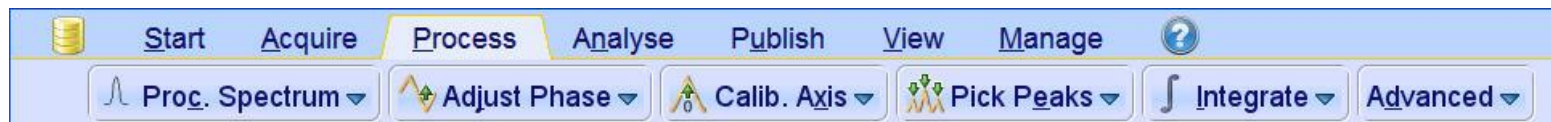


After **apk**(Auto – Phasing), phase-correction through manual phasing

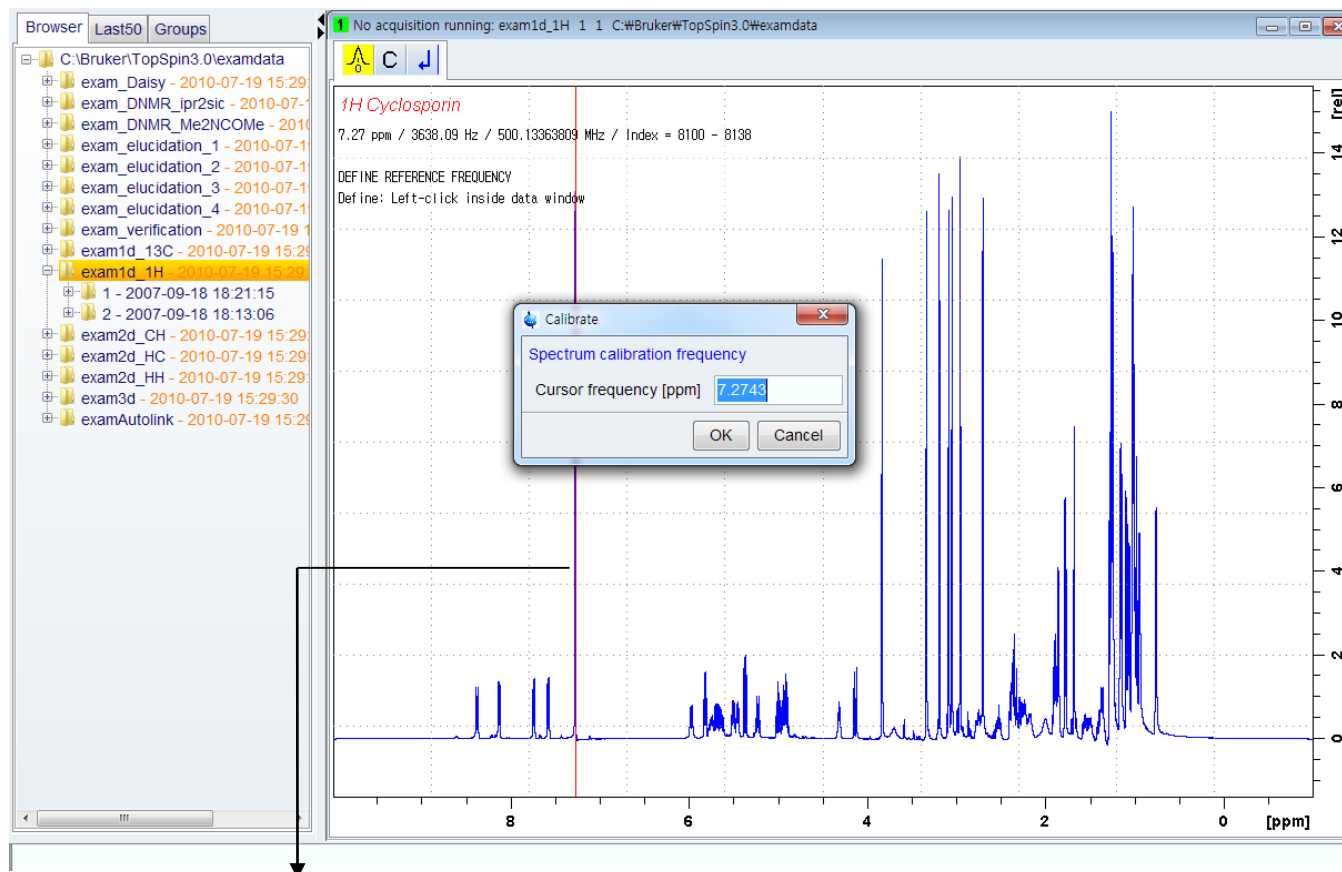


Spectrum moves like a seesaw shape

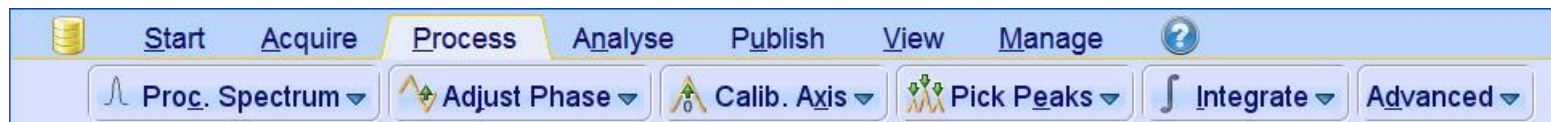
Spectrum move uniform



Click **Calib. Axis**. Change chemical shift.



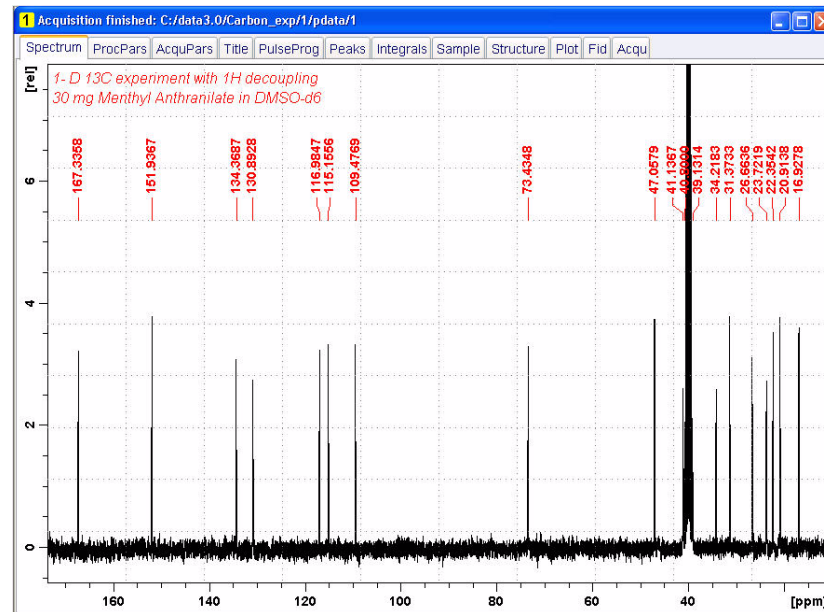
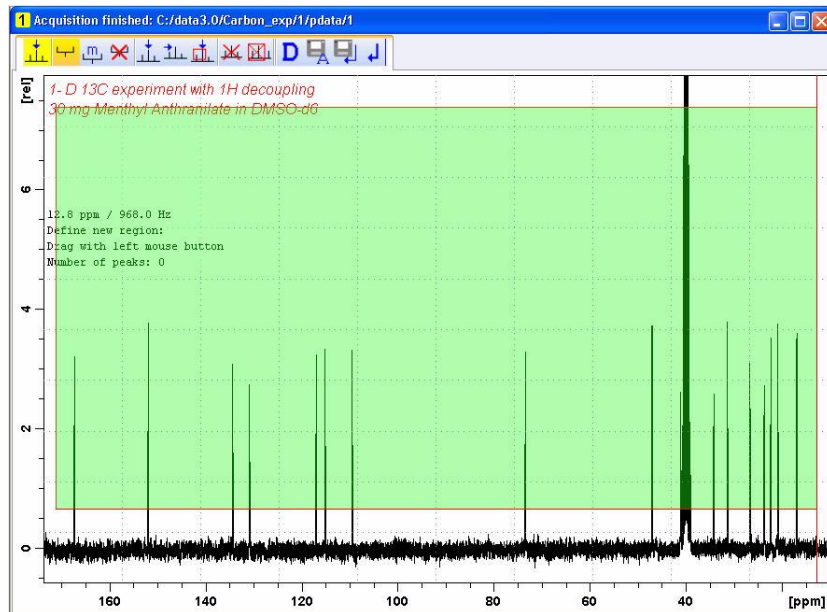
마우스 왼쪽 버튼을 이용하여 알고 있는 **peak**를 클릭 하고 정확한 값을 넣어 준다.

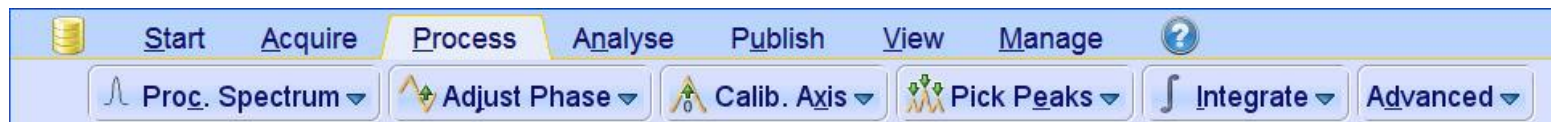


Click  **Pick Peaks**

Click 

Drag left-mouse. (Peak located on square box)





Click  Pick Peaks

Control threshold and choice peak

ex) 0.5 higher than peak picking

> mi 0.5

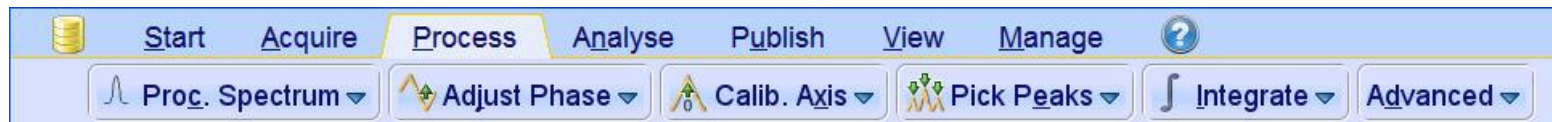
> pps



Plus one peak.

Modify selection area.

Select peak about square box



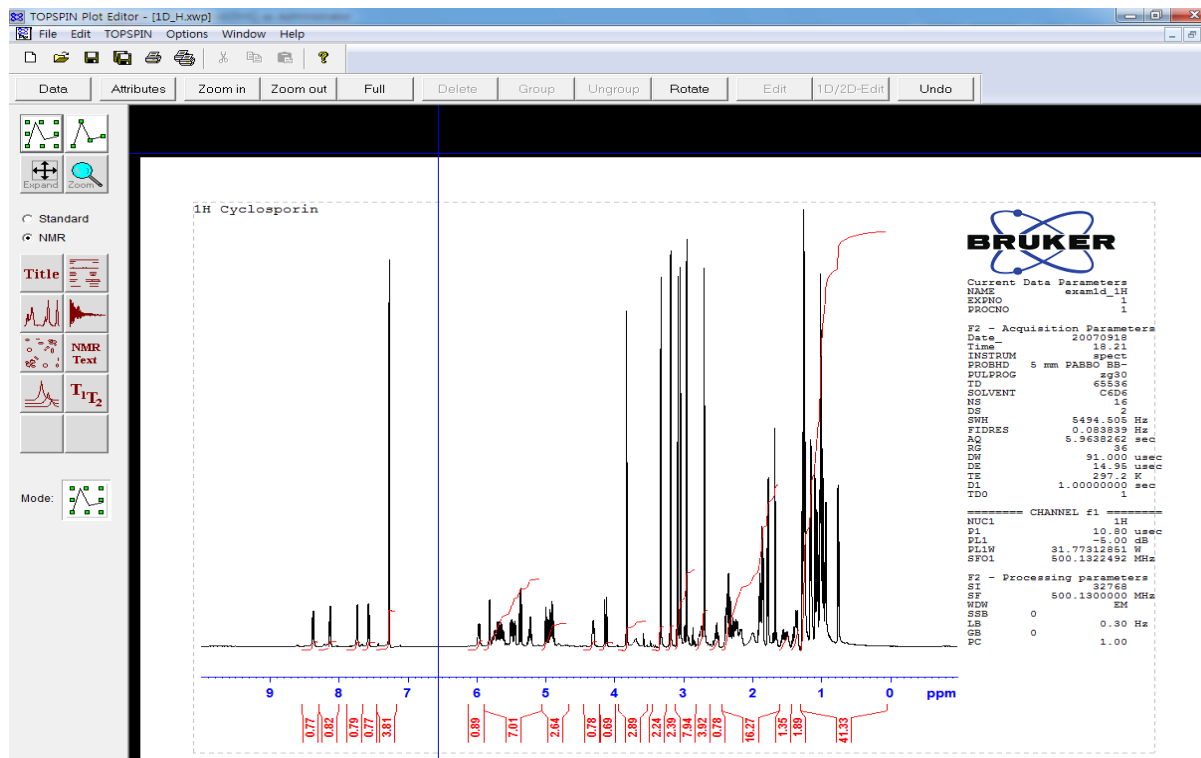
Click  **Integrate**



 → **Select integration about square box**
 → **Divide overlapped peak**
 → **Modify selection area**



Click  Plot Layout ▼

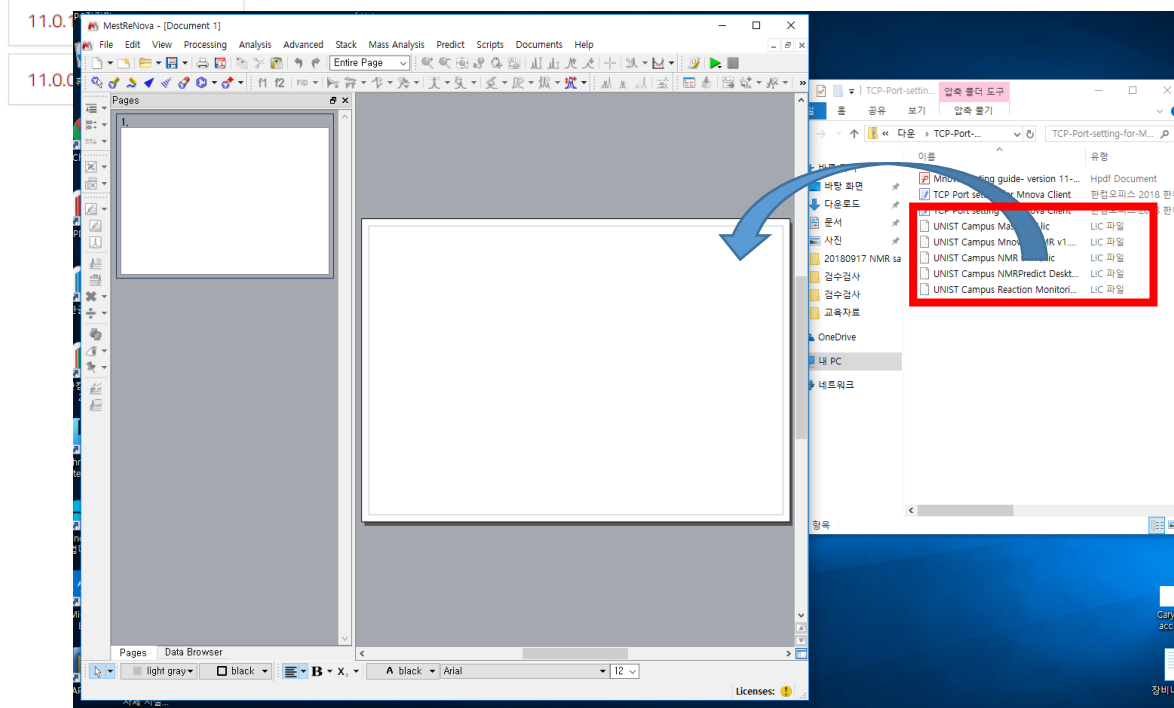


<https://ucrf.unist.ac.kr/en/mnova-installation/>

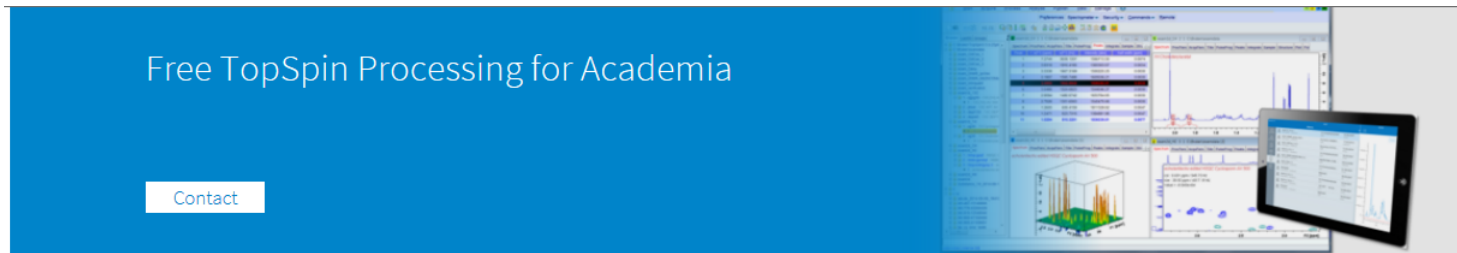
Download previous versions.

If you hold an old Mnova license we really encourage you to update it. However if you need an older installer, here is a full list of releases:

12.0.2 ▼	11.0.4 ▼	10.0.2 ▼	9.1.0 ▼
12.0.1 ▼	11.0.3 ▼	10.0.1 ▼	9.0.1 ▼
12.0.0 ▼	11.0.2 ▼	10.0.0 ▼	9.0.0 ▼



<https://www.bruker.com/nc/service/support-upgrades/software-downloads/nmr/free-topspin-processing/download-page.html>



Home - Service - Support & Upgrades - Software Downloads - NMR - Free TopSpin processing - Download Page

Free TopSpin processing software for academia

TopSpin processing software is free for academia and governmental institutions only

In order to provide students, researchers and teachers with unlimited access to the best tools for off-line NMR processing, Bruker is making their market leading NMR processing software TopSpin available free of charge for all academic users. In addition to Bruker NMR data, the software is able to process data acquired on Agilent, Varian and Jeol systems, as well as read any data provided in JCAMP format.

Access to the download section

Please note: Access to this download section is restricted to academic customers.

[Please register for a customer account here.](#)

In case you already have an account on bruker.com please [log in](#) to download the TopSpin processing package. By downloading the free TopSpin processing software, you confirm that you are employed by- or studying at an academic- or governmental institution and that you use the software exclusively in this context.

As a registered academic or governmental customer, you will have access to software updates and patches for:

- Free TopSpin processing software for Windows, Linux and MAC OS X
- Free Dynamics Center for Windows, Linux and MAC

Disclaimer

The download and use of the free software for commercial organizations or companies is prohibited. To download software for a commercial organization, please follow [this link](#).

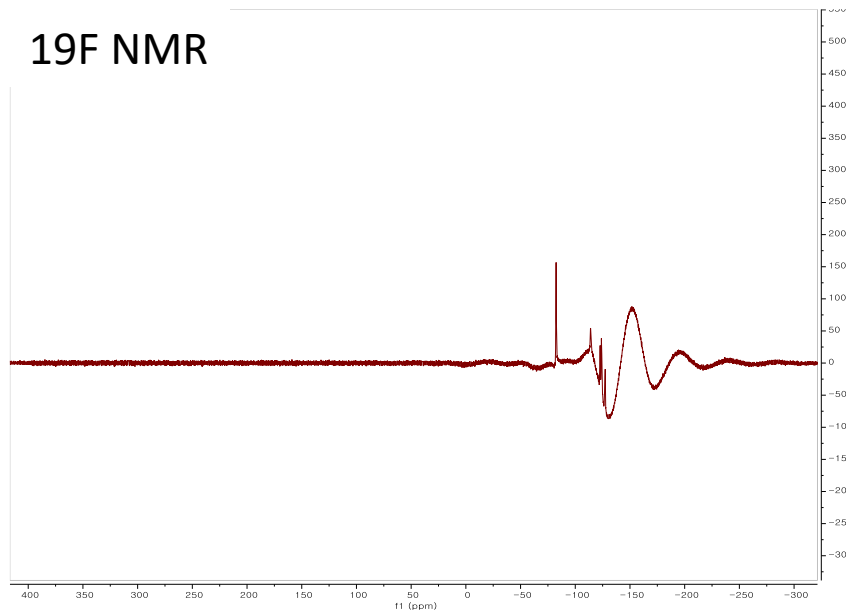
11. Technical Knowhow

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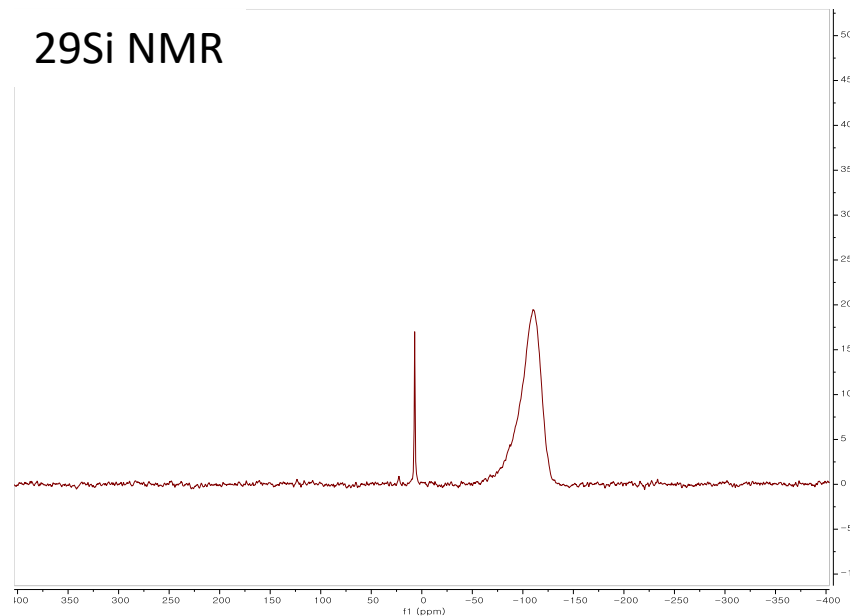
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Poor background

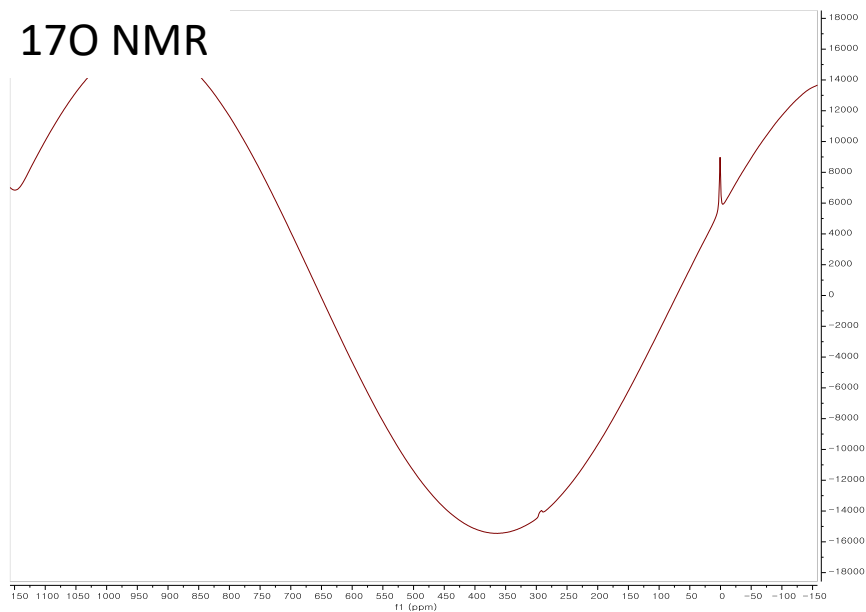
^{19}F NMR



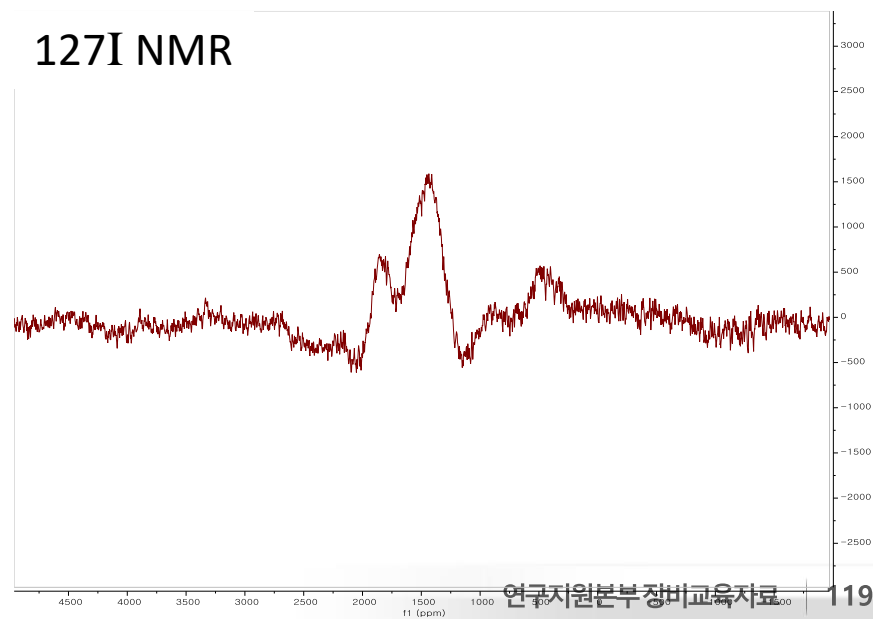
^{29}Si NMR



^{17}O NMR



^{127}I NMR



Poor background signal in NMR

Sample signal

- 1) Background
- 2) Ringing

1) Material

Borosilicate
Background: ^{11}B , ^{17}O , ^{29}Si



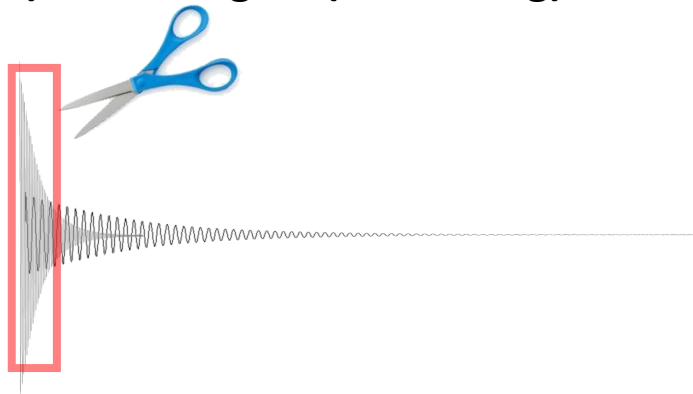
PTFE (Teflon)
Background: ^1H , ^{13}C , ^{19}F

2) Ringing

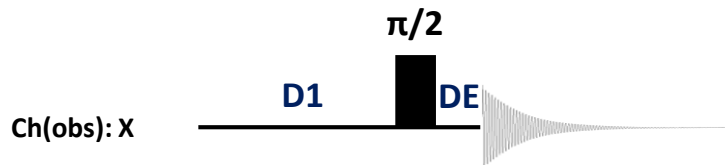


How to remove background signal

1) Cut off signal (Processing)



2) Prescan Delay (DE)



DE = 30 - 40 μ s (Normally 4 - 25 μ s)

For suppress "bad background signal"

1) Probe materials (Solid signal)

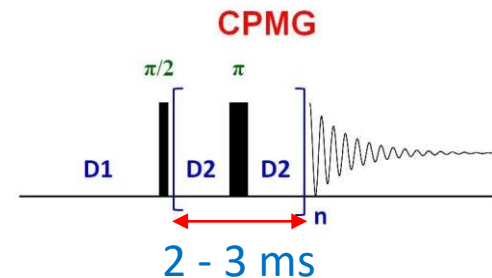
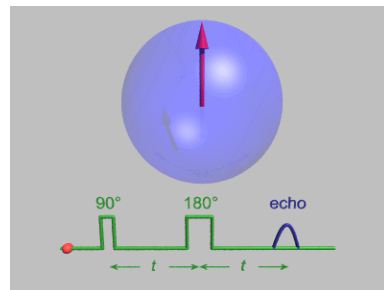
2) Ringing

-> Short D1 ex. 17O -> D1 = 0.1 - 0.2 s

<Solution NMR>

3) CPMG (Spin echo)

- Suppress magnetic field inhomogeneous (T2)

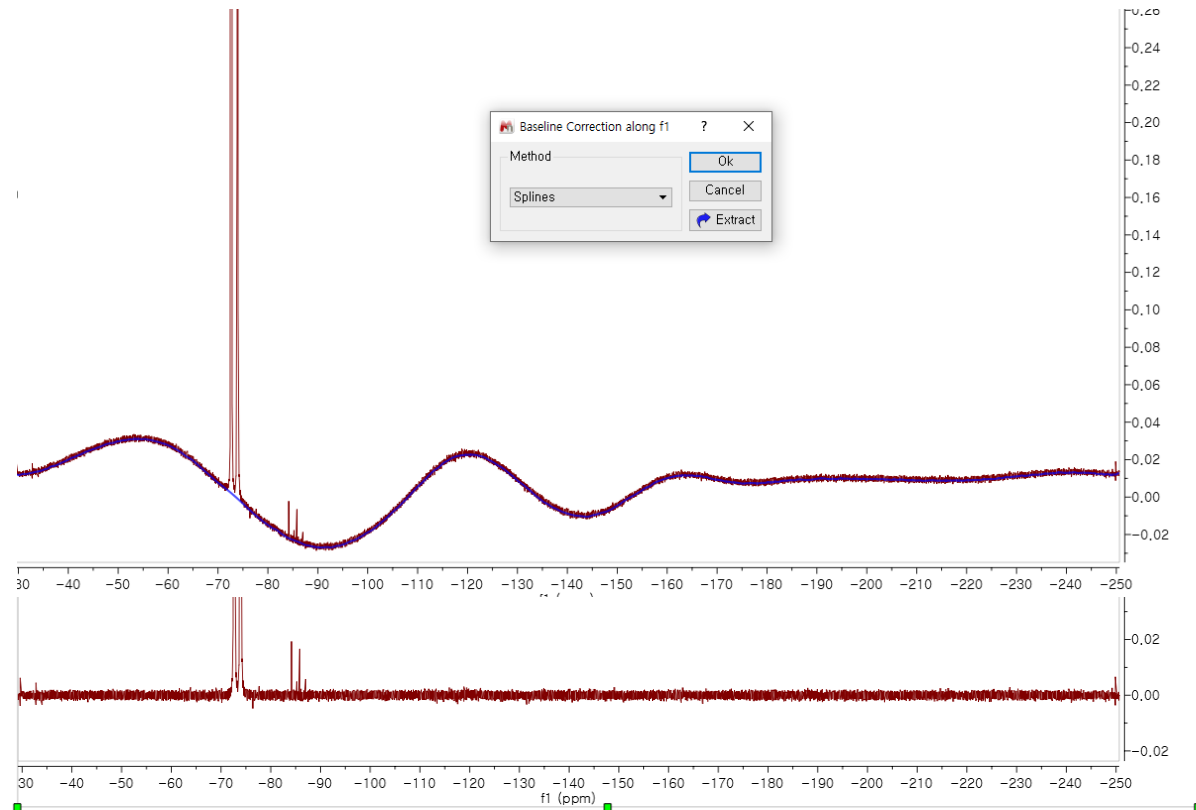
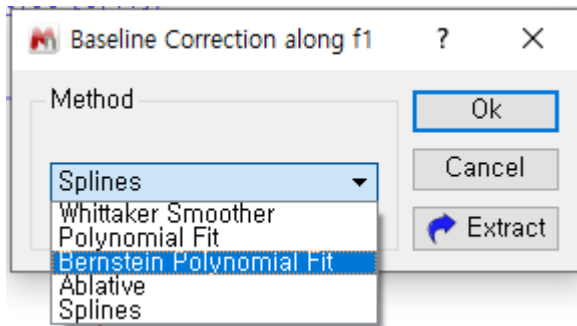


D2 = 1 ms (0.001 s)

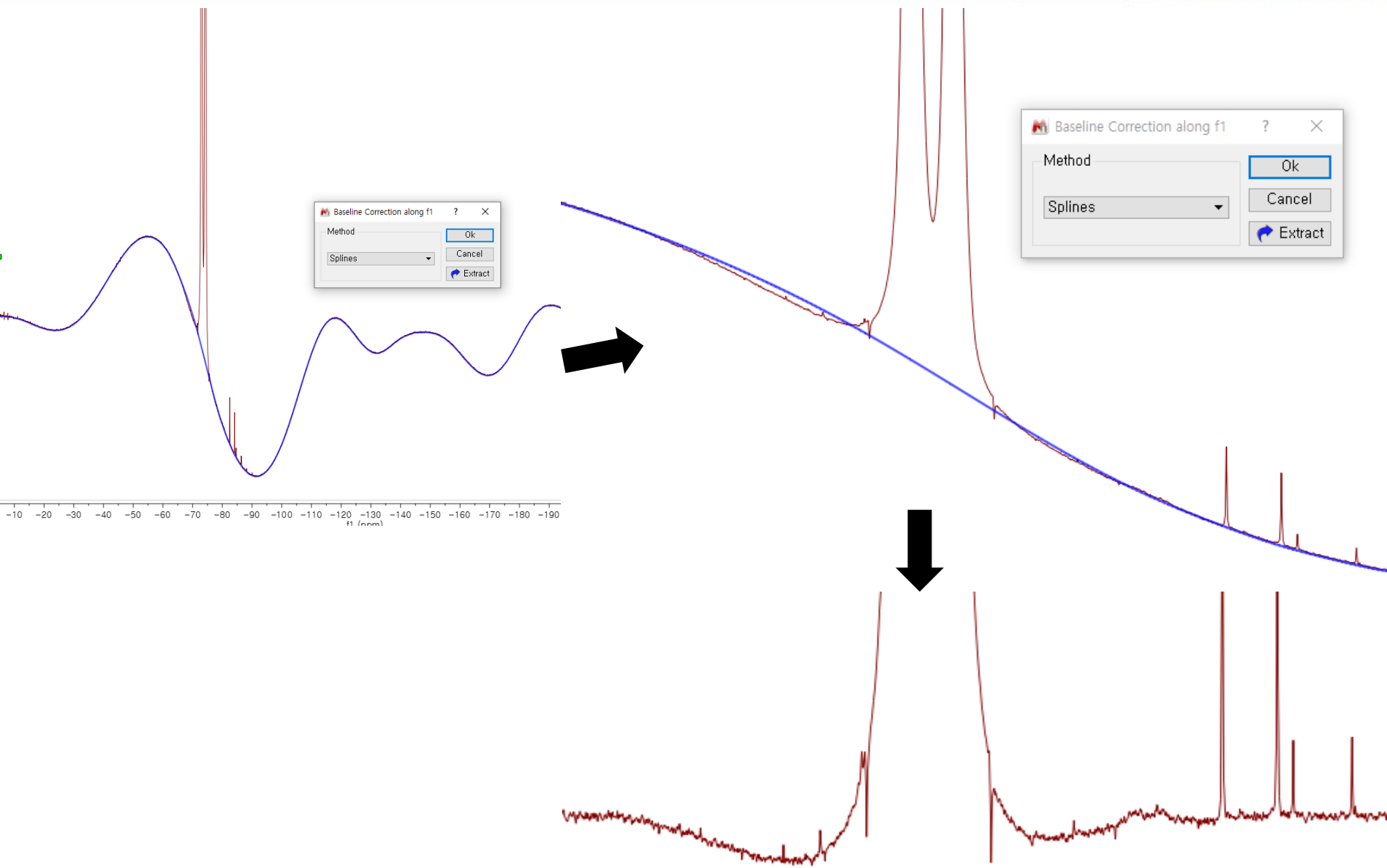
Teflon decay time < 1 ms

Baseline correction (Processing)

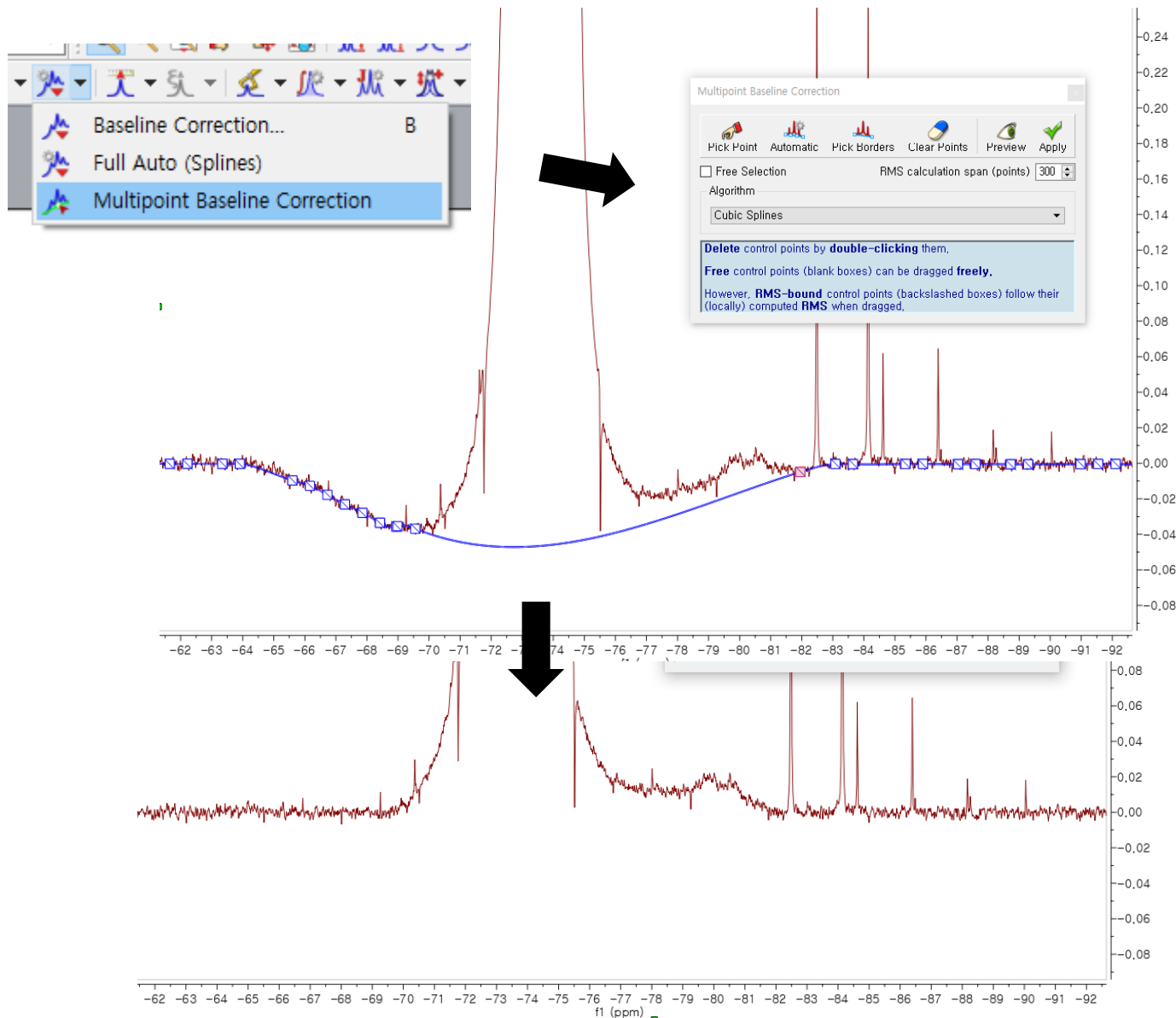
Polynomial Fit = 2 - 3
(or Bernstein Polynomial Fit)



Baseline correction (Processing)



Multipoint baseline correction (Processing)

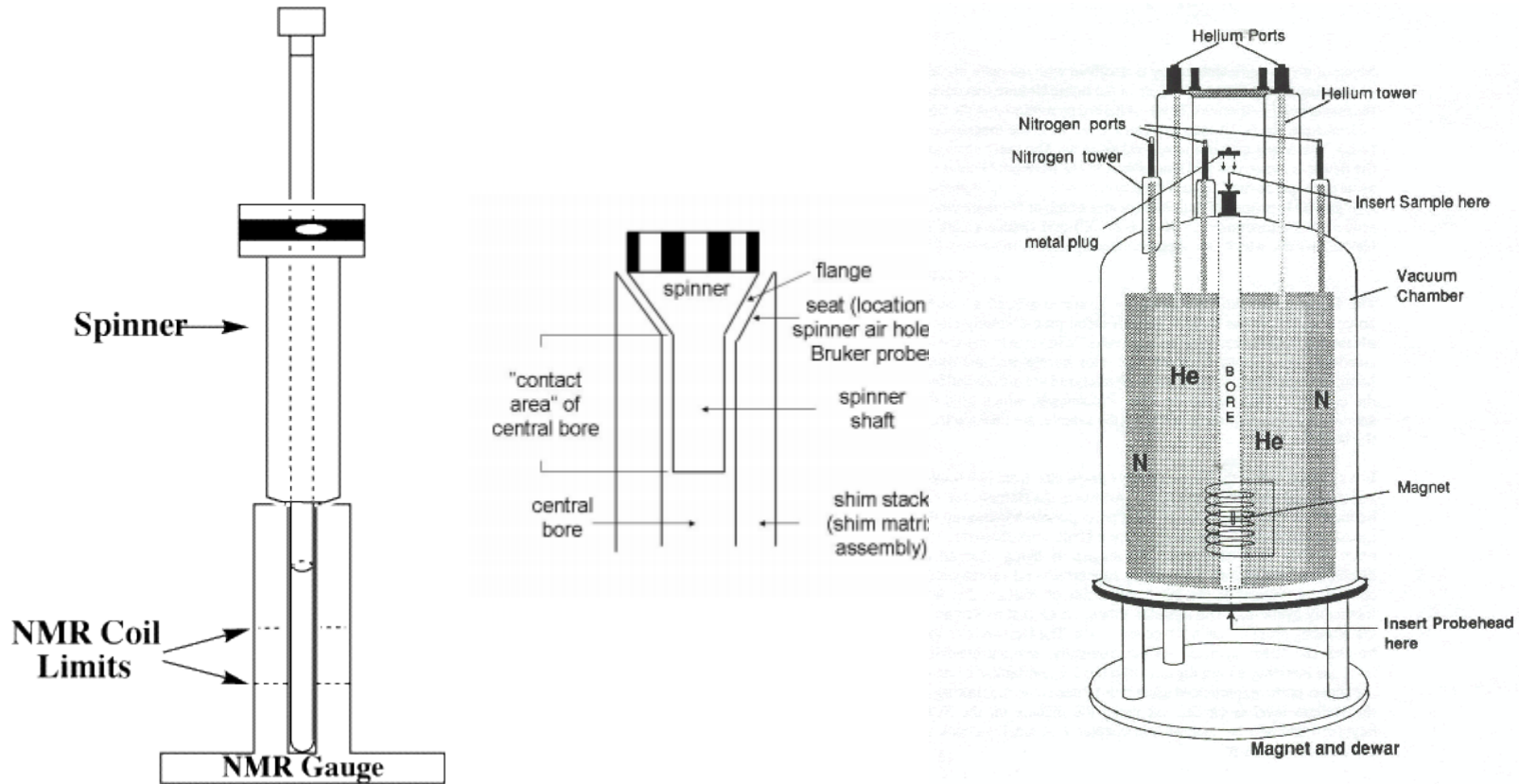


12. Caution

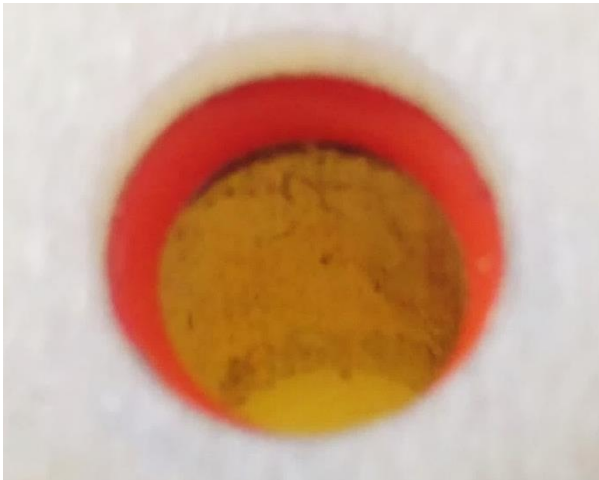
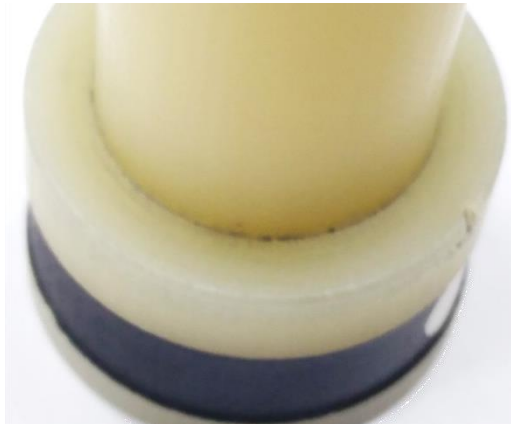
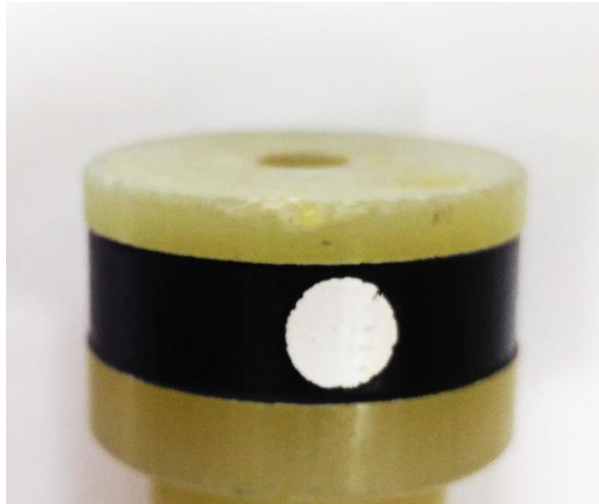
UNIST

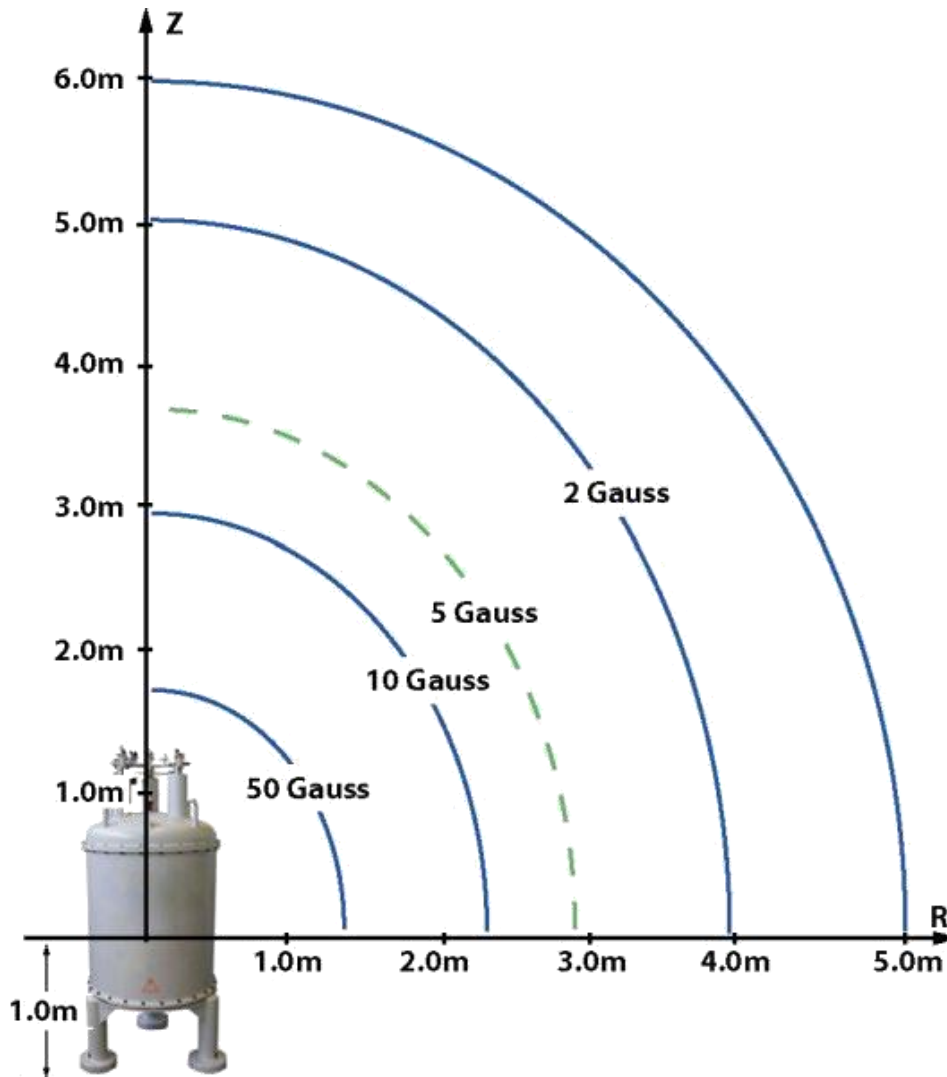
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Consist of magnet



Spinner damage

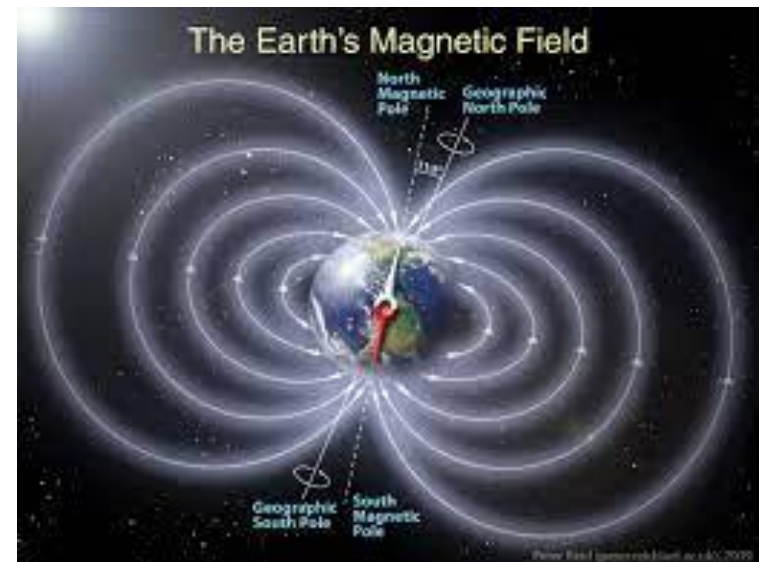




5 Gauss line

‘Safe’ levels of static magnetic field exposure for general purpose

Earth`s Magnetic field = **0.5 gauss**



Warning Signs



Caution: Extremely high magnetic stray fields.



Caution: Watches and electronic or electro-mechanical devices may be damaged.



Danger: No entrance for people carrying pace-makers.



Caution: Credit cards, magnetic storage media as tapes, floppy disks or hard disks, may be damaged.



Danger: No entrance for people carrying medical implants.

0.5 Gauss

= Average earth
magnetic field

5 Gauss line

= MR safety standard



Credit
card



earphon
e

10 Gauss line



Watch,
Key

5 Gauss line



Metallic
tool



Hand
cart



Scissors,
pen



Gas
containe
r

Human Body react to Oxygen-Deficiency

O2 Concentration
21%

Symptoms
Natural air



O2 Concentration
18%

Symptoms
Limit level for not causing serious health problems. Continuous ventilation is required



O2 Concentration
16%-12%

Symptoms
Rapid breathing,
Increase in pulse rate,
Loss of concentration,
Headache, Nausea,
Ear ringing



O2 Concentration
14%-9%

Symptoms
Stupor, Headache,
Nausea, Cyanosis,
Faintness on the entire
body



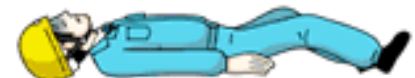
O2 Concentration
10%-6%

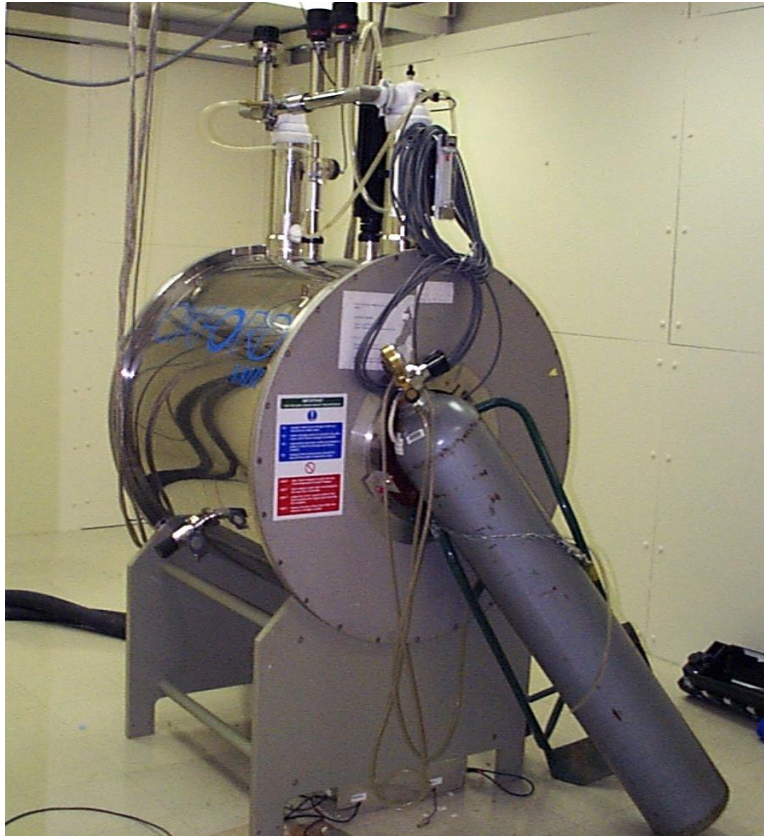
Symptoms
Comatose, Loss of consciousness,
Muscle spasm on the entire body



O2 Concentration
6% or less

Symptoms
Unconsciousness, Comatose,
Cessation of breathing,
Cardiac arrest, Die in 6 minutes







Agilent Confidential

<https://www.youtube.com/watch?v=4dbQxyrhZ2A&t=63s>

https://youtu.be/d-G3Kg-7n_M?t=5

13. FAQ

-자주 하는 질문

-장비 이용료

UNIST

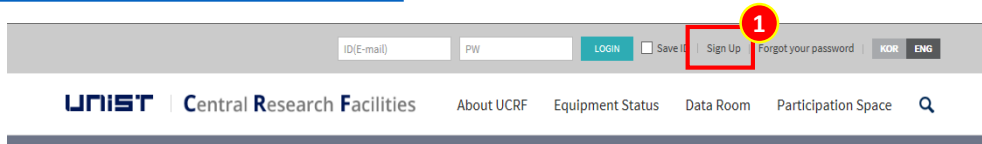
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Equipment fee

Model	Reservation time unit	Daily maximum reservation time	Cancelable timing	Fee	
600 MHz NMR	10 min.	unlimited	1.0 hr	Client	10,000/10min
				Self-user	5,000/10min
				Acc. used	3,000/10min
400 MHz NMR	10 min.	1 hr (2 PM to 8 PM, weekdays)	1.0 hr	Client	5,000/10min
				Self-user	2,500/10min
				Acc. used	3,300/10min

Create Account

www.ucrf.unist.ac.kr



The screenshot shows the top navigation bar of the UNIST UCRF website. It includes input fields for 'ID(E-mail)' and 'PW', a 'LOGIN' button, a 'Save ID' checkbox, and a 'Sign Up' link highlighted with a red box and the number 1. Other links include 'Forgot your password', 'KOR', and 'ENG'. Below the navigation bar is a horizontal menu with links: 'UNIST | Central Research Facilities', 'About UCRF', 'Equipment Status', 'Data Room', and 'Participation Space'.

1. Click [Sign up].
2. Click [UNIST Member].
3. Input [Portal id/pw]_Click [Confirm].
Please check your information.
4. Input professor name in [Principal investigation]
_Click [Professor search]_Click professor name.
5. Click [Create Account].



The screenshot shows the account creation form on the UNIST UCRF website. It has a tabbed interface with 'UNIST member' (highlighted with a red box and number 2), 'Industry member', and 'External member'. The form fields include: 'ID/E-mail' (m*k*m @unist.ac.kr), 'Password' (masked with asterisks, with a 'Confirm' button highlighted by a red box and number 3), 'Name' (홍길동), 'Department' (연구지원본부), 'Student ID No. / Professor ID No. / Staff ID No.' (20*39), 'Contact' (Extension: 4064, Cell phone: 010-**-****), and 'Principal Investigator' (김교수, with a 'Professor Search' button highlighted by a red box and number 4). At the bottom is a 'Create Account' button highlighted by a red box and number 5.

Request for Self-user

www.ucrf.unist.ac.kr

Welcome 손선헌 | LOGOUT | **My Page** | Edit profile | KOR | ENG

F Equipment Status Data Room Participation Space 🔍

My Page
UNIST Central Research Facilities

- Request for Self-user** ▼
- Status of analysis request ▼
- Status of settlements ▼
- Status of education application ▼
- Status of tour application ▼
- Status of access permissions application ▼
- Status of penalty ▼

Home > MY PAGE > Status of analysis request

Status of analysis request

Equipment	Status	Application date	Result of analysis
-----------	--------	------------------	--------------------

Request for Self-user

4-1 Materials Characterization Lab ▼

4-2 Surface Analysis ▼

4-3 Confocal Raman ▼

4-4 **Apply**

After pass the test,

1. Login UCRF website.
2. Click [My Page].
3. Click [Request for Self user].
4. Select the equipment.
 - 1) Select [Materials Characterization Lab].
 - 2) Select [Surface Analysis].
 - 3) Select [Confocal Raman].
 - 4) Click [Apply].

portal.unist.ac.kr – Research Equipment– Equipment reservation/input result

Equipment Reservation

Detailed Navigation

- Equipment Reservation
- Equipment Reservation List
- Equipment Status

Favorite

Equipment reservation

Search condition

Reservation date: 2015.01.01 ~ 2015.08.26

☒ Reservation ☐ Input result ☐ Completed ☐ All

1st classification:

2nd classification:

Equipment name:

Equipment booking list

Select	Status	Sortation	Equipment name	Chief of research	Reservation date	Reservation time	Fee	1st classification	2nd classification name	Application date	Free_Test	Free_Longterm	Memo
☐	Reservation	Admin	Confocal Raman	김영기	2015.08.17	13:00~16:30	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.04 18:44	☐	☐	
☐	Reservation	Admin	AFM-Raman	김영기	2015.08.17	13:00~16:30	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.10 16:27	☐	☐	
☐	Reservation	Admin	Confocal Raman	김영기	2015.08.17	09:00~11:30	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.04 18:44	☐	☐	
☐	Reservation	Admin	AFM-Raman	김영기	2015.08.17	09:00~11:30	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.10 16:27	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.08.13	15:00~18:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.08.07 10:53	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.08.13	13:30~15:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.08.07 10:52	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.08.13	09:00~12:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.08.07 08:57	☐	☐	
☐	Reservation	Admin	Confocal Raman	김영기	2015.08.12	15:30~17:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.07 17:15	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.08.12	10:30~11:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.08.07 14:57	☐	☐	
☐	Reservation	Admin	Confocal Raman	김영기	2015.08.12	09:00~10:30	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.06 13:21	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.08.11	14:30~18:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.08.07 08:57	☐	☐	
☐	Reservation	Admin	Confocal Raman	김영기	2015.08.11	13:30~14:30	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.05 11:42	☐	☐	
☐	Reservation	Admin	Confocal Raman	김영기	2015.08.11	09:00~10:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.08.10 13:04	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.08.11	09:00~12:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.08.07 10:56	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.07.29	09:30~10:30	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.07.28 13:26	☐	☐	
☐	Reservation	Admin	FT-IR	김영기	2015.07.17	16:00~17:00	0.00	UMAL - 기기분석실	Spectroscopic Analysis	2015.07.17 18:00	☐	☐	

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 help

 Inquiry

Inquiry

Reservation date: 2015.01.01 ~ 2015.08.04

1st classification: 2nd classification: Equipment name:

Application

Application

Select	Status	Reservation	Reservation	Chief of research	Reservation date	Reservation time	Fee	1st classification	2nd classification name	Application date	Free_Test	Free_Longterm	Memo
☐	Reservation	Self	AFM-Raman	김영기	2015.07.24	14:00~15:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.07.17 11:08	☐	☐	
☐	Reservation	Self	Confocal Raman	김영기	2015.07.24	14:00~15:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.07.17 11:07	☐	☐	
☐	Reservation	Self	FT-IR	김영기	2015.07.23	13:30~17:00	0.00	UMAL - 기기분석실	Spectroscopic Analys	2015.07.17 11:05	☐	☐	
☐	Reservation	Self	Confocal Raman	김영기	2015.07.22	13:00~14:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.07.20 11:20	☐	☐	
☐	Reservation	Self	Fluorometer	김영기	2015.07.20	14:00~14:30	0.00	UMAL - 기기분석실	Spectroscopic Analys	2015.07.17 11:03	☐	☐	
☐	Reservation	Self	Fluorometer	김영기	2015.07.20	13:30~14:00	0.00	UMAL - 기기분석실	Spectroscopic Analys	2015.07.16 16:55	☐	☐	
☐	Reservation	Self	FT-IR	김영기	2015.07.17	16:00~17:00	0.00	UMAL - 기기분석실	Spectroscopic Analys	2015.07.17 18:00	☐	☐	

3

1

2

[illegible]

1. Select the classification and equipment
2. Select the time you want on white box.
Yellow box : my reservation
Red box : others reservation
3. Click [Application].

Reservation cancel

Equipment reservation

Search condition

 Inquiry

Reservation date: 2015.01.01 ~ 2015.08.04

1st classification: UMAL - 기기분석실

2nd classification: Surface Analysis

Equipment name: Confocal Raman

☒ Reservation ☐ Input result ☐ Completed ☐ All

Equipment Reservation cancel

 Application  Reservation cancel  Input result

Select	Status	Sortation	Equipment name	Chief of research	Reservation date	Reservation time	Fee	1st classification	2nd classification name
☒	Reservation	Self	Confocal Raman	김영기	2015.07.24	14:00~15:00	0.00	UMAL - 기기분석실	Surface Analysis
☐	Reservation	Self	Confocal Raman	김영기	2015.07.22	13:00~14:00	0.00	UMAL - 기기분석실	Surface Analysis

1. Select the reservation.
2. Click the [Reservation cancel].

Input result

After measurement, you have to input result instead of filling in log sheet

Equipment reservation

Search condition

Inquiry

Reservation date: 2015.01.01 ~ 2015.08.04

1st classification: UMAL - 기기분석실

2nd classification: Surface Analysis

Equipment name: Confocal Raman

Reservation ☒ Input result ☐ Completed ☐ All

Equipment booking list

Input result

Application Reservation cancel **Input result**

Select	Status	Sortation	Equipment name	Chief of research	Reservation date	Reservation time	Fee	1st classification	2nd classification name	Application date	Free_Test	Free_Longterm	Memo
☒	Reservation	Self	Confocal Raman	김영기	2015.07.24	14:00~15:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.07.17 11:07	☐	☐	
☐	Reservation	Self	Confocal Raman	김영기	2015.07.22	13:00~14:00	0.00	UMAL - 기기분석실	Surface Analysis	2015.07.20 11:20	☐	☐	

1. Select the reservation.
2. Click the [Input result].
3. Check the information and click [Save].

Reservation information

Reservation number: 2015001217

Reservation date: 2015.07.24

Application date: 2015.07.17

Reservation time: 14:00~15:00

Client authorization: Self

Rate: 50

Equipment name: Confocal Raman

Project information

Chief of research	Chief of research	Detail project number	detailed item	Executable amount		
20032	김영기			0	0	0

Fee

Cost	Unit quantity	Unit	unit amount	discount applying	Option applying	Amount	Fee	Rate	Amount
기본공정료	0.5	H	12,500	☒		1.0	25,000	50	12,500
합계							25,000		12,500

Process condition

equipment status (problem and repair)

• 벌점 부과 기준

No.	벌점 부과 내용	벌점
[장비 사용 자격]		
1	해당 장비에 대하여 직접 사용이 허가 되지 않은 사용자가 기기를 사용	5
2	장비 예약하지 않고 장비 사용	3
3	장비 예약자 본인이 아닌 자가 장비를 사용	3
[장비 사용 예약]		
4	허용시간 이외의 시간에 장비 예약 및 사용	1
5	장비 예약시간을 초과하여, 예약시간 종료 전에 초과시간에 대한 예약없이 장비 사용	1
6	장비 예약 취소 사실 통보 없이 해당 시간에 장비 사용하지 않은 경우	3
7	「연구지원본부 운영지침」제7조의 내용을 기준으로, 장비 예약 취소 기한이 지나서 예약을 취소한 경우	1
8	예약 후 장비담당자에게 통보하지 않고 기기 사용	1
[부주의한 행동]		
9	장비 사용 중 허용되지 않은 기능 조작	3
10	장비 사용 중 장비의 이상이나 고장 발견 후 담당자에게 즉시 고지하지 않은 경우	3
11	사용자 부주의로 기기 손상 및 고장	5
12	사용자 부주의로 장비 부속품 분실 또는 파손	5
13	장비 사용 후 장비사용일지를 작성하지 않거나 허위 작성 또는 일부만 작성	1
14	담당자가 장비 또는 시설의 정상적인 작동과 안전을 유지하는 데에 반드시 파악해야할 시료의 정보를 제공하지 않아 장비 손상 및 고장을 초래	3
15	야간 또는 장비 담당자의 정규 근무시간이 아닌 때에 장비 사용 후 소등, 출입문단속, 주변 정리 등을 확인하지 않고 퇴실	3
16	유독 물질 및 가스의 누출 또는 화재 발생의 위험을 초래	5
17	타인의 개인물품(분석 및 공정 소모품 및 기자재)을 사전 동의 없이 사용하거나 훔치는 행위	5

Penalty points for users of equipment

- Penalty points criteria

No.	Behaviors subject to penalty points	Penalty pts.
[Eligibility to use equipment]		
1	Unauthorized use of equipment without permission	5
2	Use of equipment without a reservation	3
3	Someone other than the equipment lessee used the equipment	3
[Reservations for using equipment]		
4	Reserved and used equipment outside of permitted hours	1
5	Use of equipment beyond the time reserved without making another reservation beforehand for extra time	1
6	Failed to use the equipment during the reserved time and did not cancel reservation in advance	3
7	Cancelling reservations for equipment after the cancellation deadline, under Article 7, Guideline for the Operation of the UNIST Central Research Facilities (UCRF)	1
8	Use of any equipment without giving a prior notice to the equipment manager, after making a reservation	1
[Careless behaviors]		
9	Using functions on the equipment that are not permitted	3
10	Failure to promptly notify the manager of any errors or failures detected during use	3
11	Negligence that resulted in damages or failure to the equipment	5
12	Negligence that resulted in loss or damage to an equipment component or part	5
13	Failure to record in the equipment usage log after using any equipment, or misrepresentation or partial representation of the facts	1
14	Failure to provide specimen information required by the equipment manager to ensure normal operations and safety of equipment or facilities, thus resulting in damage or failure to the equipment	3
15	Leaving the laboratory without putting the laboratory back in order, without turning off the lights, or without properly locking the entrance door, after using equipment at nighttime or during the equipment manager's off-hours	3
16	Causing leakage of toxic substances, gases, or causing risk of fire	5
17	Using or stealing someone's personal items (e.g. supplies, equipment or materials for analysis and process) without prior consent	5

- Follow-up Actions after Imposing Penalty Points

구분	벌점	조치내용
[장비사용자 개인]		
개인에게 부과된 벌점 합산	≥ 5 points	장비 담당자가 사용자 및 지도교수에게 이메일로 통보(벌점 8점 이상일 시 장비 사용이 3개월간 금지됨을 공지)하고 해당 사용자의 벌점 내역을 기기실에 게시
	≥ 8 points	장비 담당자가 사용자 및 지도교수에게 사용자의 해당 장비 사용이 3개월간 금지되고 재교육 후 사용이 가능함을 이메일로 통보하고 지도교수에게 공문 발송, 해당 사용자의 벌점 내역을 기기실에 게시
(사용자 소속 연구실)		
동일 연구실에서 동일 장비에 대하여 연구실 소속 학생들에게 부과된 벌점 합산	≥ 12 points	장비 담당자가 지도교수와 해당 사용자에게 벌점 15점 이상일 시 해당 연구실의 해당 장비 사용이 3개월간 금지됨을 이메일로 통보
	≥ 15 points	장비 담당자가 지도교수에게 해당 연구실의 해당 장비 사용이 3개월간 금지됨을 이메일로 통보, 지도교수에게 공문 발송, 해당 사용자의 벌점 내역을 기기실에 게시
동일 연구실에서 연구지원본부 전체 장비에 대하여 연구실 소속 학생들에게 부과된 벌점 합산	≥ 20 points	연구지원본부에서 지도교수와 소속 학생에게 벌점 25점 이상일 시 해당 연구실의 연구지원본부 전체 장비 사용이 1개월간 금지됨을 이메일로 통보
	≥ 25 points	연구지원본부에서 지도교수와 소속 학생에게 해당 연구실의 연구지원본부 전체 장비 사용이 1개월간 금지됨을 이메일로 통보, 지도교수에게 공문 발송, 해당 벌점 내역을 연구지원본부 게시판에 게시

Penalty points for users of equipment

- Follow-up Actions after Imposing Penalty Points

Classification	Penalty pts.	Follow-up actions
(Individual users of equipment)		
Sum up penalty points imposed to individuals	≥ 5 points	Equipment manager will notify user(s) and their supervising professor by e-mail of their penalty points total, and shall post the details of their penalty points on the bulletin board of the equipment room. Users with penalty points 8 points or higher may not use the relevant equipment for 3 months.
	≥ 8 points	Equipment manager will notify user(s) and their supervising professor by e-mail that the user(s) may not use the relevant equipment for 3 months until they complete their orientation course. They will also forward an official notice to their supervising professor; and will post details of their penalty points on the bulletin board of the equipment room.
(User's laboratory)		
Sum up penalty points imposed on the students in the laboratory for the same equipment in the same laboratory	≥ 12 points	Equipment manager will notify the user(s) and their supervising professor by e-mail that the user(s) with penalty points 15 points or higher may not use the relevant equipment in the laboratory for 3 months.
	≥ 15 points	Equipment manager will e-mail the supervising professor to inform that the user(s) may not use the relevant equipment in the laboratory for 3 months. They will also forward an official notice to their supervising professor; and will post the details of their penalty points on the bulletin board of the equipment room.
Sum up penalty points imposed on the students in the laboratory for all UCRF equipment in the same laboratory	≥ 20 points	UCRF will notify students and their supervising professor by e-mail that the user(s) with 25 penalty points or higher may not use any UCRF equipment in the laboratory for 1 month.
	≥ 25 points	UCRF will notify students and their supervising professor by e-mail that the user(s) may not use any UCRF equipment in the laboratory for 1 month. They will also forward official notice to their supervising professor; and will post details of their penalty points on the bulletin board of UCRF.

14. Basic information

UNIST

ULSAN NATIONAL INSTITUTE OF
SCIENCE AND TECHNOLOGY

NMR Specifications

	Varian 600 MHz NMR	Bruker 600 MHz NMR	Bruker 400 MHz NMR
Location	102-B119	102-B119	102-B119
Measurement Type	Self / Request	Self / Request	Self / Request
Model	VNMRS 600 (Varian)	AVANCE NEO (Bruker)	AVANCE III HD (Bruker)
Magnet	14.1 T	9.4 T	9.4 T
Channel	3 channel	2 channel	2 channel
Probe	5 mm PFG Auto X DB probe 5 mm Automated triple resonance probe 4 mm Nano TM probe 1.6 mm triple resonance HXY MAS solid probe 5 mm double resonance MAS solid probe	- Prodigy probe 5 mm i-probe	BBO probe
Auto-sampler	X	O	O
Auto-tuning & matching	O	O	O
Power	100 W / 300 W / 300 W	100 W / 500 W	100 W / 500 W
Channel	- Ch1 : ^1H, ^{19}F - Ch2 : 170MHz(^{31}P) ~ 150 MHz (^{13}C) - Ch3 : 150MHz(^{13}C) ~ 60 MHz (^{15}N)	- Ch1: ^1H, ^{19}F - Ch2: 170MHz(^{31}P) ~ 150 MHz (^{13}C)	- Ch1: ^1H, ^{19}F - Ch2 160MHz(^{13}Q) ~ 49 MHz (^{15}N)
Temperature	- 80 ~ 90 °C	- 40 ~ 150 °C - 150 ~ 150 °C	- 150(20) ~ 150 °C

5mm PFG Auto X DB



5mm PFG Auto Triple



5 mm Double MAS [Solid]



1.6 mm Triple MAS [Solid]



102-B119

의뢰 / 자율사용 가능

Solution NMR

^1H - ^{19}F / ^{15}N - ^{31}P
(56 ~ 155 MHz)

-80 ~ 130 °C

X Broad-Band experiment

20 Hz

5 mm sample tube

500 μl 이상

102-B119

의뢰 / 자율사용 가능

Solution NMR

^1H / ^{13}C / ^{15}N

-20 ~ 80 °C

Triple resonance experiment

20 Hz

5 mm sample tube

500 μl 이상

102-B119

의뢰가능

Solid-state NMR

^1H - ^{19}F / ^{15}N - ^{31}P

RT.

One-pulse, CP-MAS

5-12 kHz

5 mm rotor

Fine powder 1 g 이상

102-B119

의뢰가능

Solid-state NMR

^1H - ^{19}F / ^{15}N - ^{31}P / ^{15}N - ^{31}P

-50 ~ 50 °C

One-pulse, CP-MAS

8-40 kHz

1.6 mm rotor

Fine powder 20 mg 이상

4mm Nano-probe



XR-401



5 mm One probe [Solution]



5 mm BBO probe [Solution]



102-B119

의뢰가능

HR-MAS NMR

^1H - ^{19}F / ^{15}N - ^{31}P

0 ~ 50 °C

HR-MAS experiment

2.5 kHz

4 mm sampling tube

100 μl 이상

102-B119

의뢰가능

Temperature control unit

^1H / ^{13}C / ^{15}N

-40(-60) ~ 100 °C

Temperature control

-

-

-

102-B119

의뢰 / 자율사용가능

Solution NMR (Agilent 400)

^1H - ^{19}F / ^{15}N - ^{31}P

-80 ~ 130 °C

X Broad-Band experiment

20 Hz

5 mm sample tube

500 μl 이상

102-B119

의뢰 / 자율사용가능

Solution NMR (Bruker 400)

^1H - ^{19}F / ^{15}N - ^{31}P

0 ~ 50 °C

X Broad-Band experiment

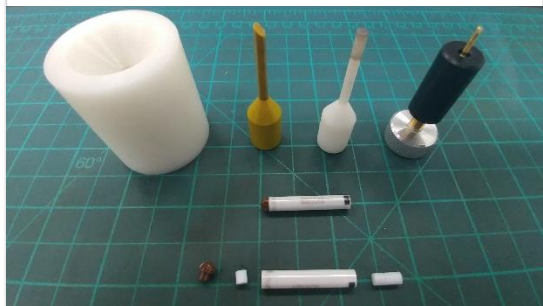
20 Hz

5 mm sample tube

500 μl 이상

NMR sample preparation

5 mm rotor



1.6 mm rotor

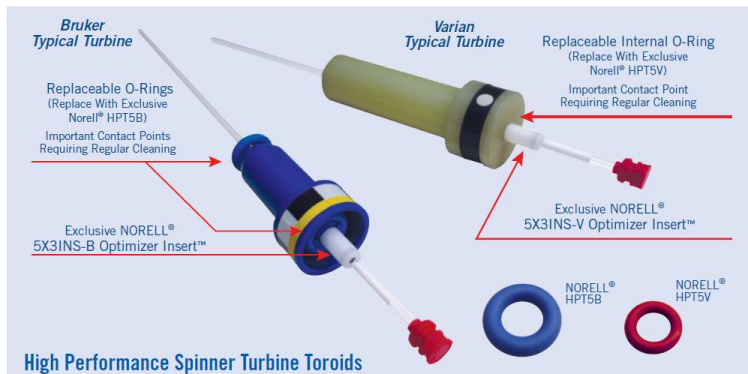


4 mm sampling tube



NMR spinner

Standard Sample Holder



Temperature limit



Ceramic
Variable



STV-5
-40 ~ 60 °C



POM
0 ~ 80 °C



Ceramic
-150 ~ 180 °C

15. Emergency

- 장비 작동
- 연락 체계

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SCIENCE AND TECHNOLOGY

연구실 번호
(Laboratory No.)

자연과학관
B119호

연구실명
(Laboratory Name)

핵자기공명분광기실
NMR Laboratory

연구실
안전담당자
(Safety Manager)

Sun-Phil Han 내선(Extension) (4174)

★ Please do not hesitate to contact "Safety Manager", if you have any queries or urgent business.

(문의 사항 또는 급한 용무가 있을 시, "연구실 안전담당자"에게 연락 요망)

원외 주요 연락처
External Main Telephone

소방서 Fire Station 119
경찰서 Police Station 112
중은삼성병원 052)220-7500
Hospital



화재, 폭발, 가스 · 화학약품 누

출 등 응급상황 발생시

Fire, Explosion, Gas and

Chemical Leak etc.

응급상황 발생시
Emergency Call

052) 217-
0119

16. Case Study

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Li salt & Electrolyte

리튬이온전지 리튬염 종류 및 특징

종류	분자량 (MW)	녹는점 (°C)	분해온도 (°C)	이온전도도(mS/cm)	
				In PC	In EC/DMC
LiPF ₆	151.9	200	80	5.8	10.7
LiBF ₄	93.9	293	100	3.4	4.9
LiAsF ₆	195.9	340	100	5.7	11.1
LiClO ₄	106.4	236	100	5.6	8.4
LiCF ₃ SO ₃	155.9	300	100	1.7	-

자료: 전자부품연구원

전해질 종류 및 특징

	액체 전해질		겔 폴리머 전해질	고체 전해질	
	유기 전해질	이온성 액체		폴리머 전해질	무기 전해질
구성	유기용매 + 리튬염	이온성 액체 + 리튬염	폴리머 + 유기용매 + 리튬염	폴리머(가교제 + 가소제) + 리튬염	산화계 황화계
이온전도도	$\sim 10^{-2}$ (S/cm)	$\sim 10^{-3}$ (S/cm)	$\sim 10^{-3}$ (S/cm)	$\sim 10^{-5}$ (S/cm)	$\sim 10^{-3}$ (S/cm)
저온 특성	중음	중음	중음	나쁨	중음
고온 안정성	나쁨	아주 좋음	중음	아주 좋음	아주 좋음
예	LiPF ₆ in EC/DEC	LiTFSI in EMITFSI	LiPF ₆ + PVdF-HFP + EC/DEC	LiTFSI + PEGDME + BPA	Li _{1+x} Al _x Ge _{2-x} (PO ₄) ₃ Li ₂ S-P ₂ S ₅

자료: 한국화학연구원

Solution NMR

1D NMR: ¹H, ¹³C, ¹⁷O, ¹⁹F, ³¹P, ³³S
T1/T2 analysis
DOSY NMR

HR-MAS NMR

Solid-state NMR

1D NMR: ¹H, ¹³C, ¹⁷O, ¹⁹F, ³¹P, ³³S
T1/T2 analysis
Solid DOSY NMR
2D NMR: MQ-MAS

P(Phosphorus): $I=1/2$

F(Fluorine): $I=1/2$

2nI+1 rule

N = Number of neighbor nuclear

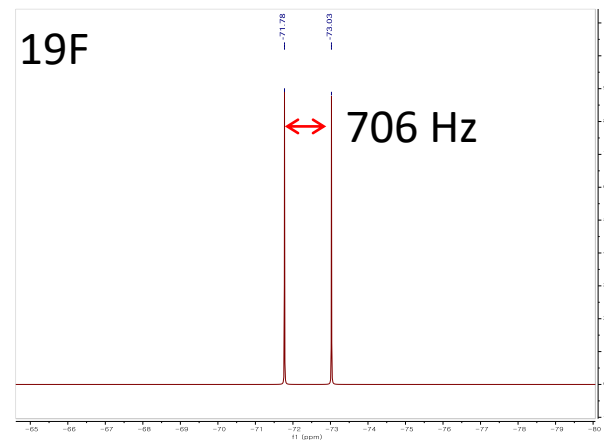
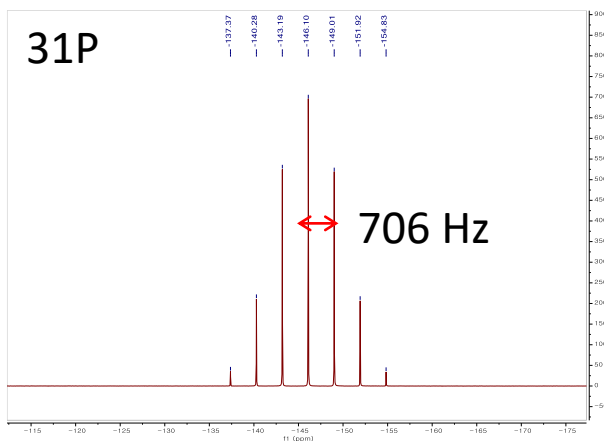
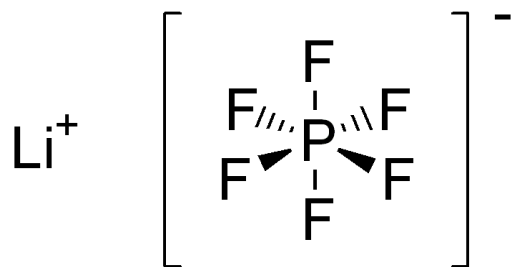
I = Nuclear spin quantum number

$$1J_{PF}: 2 * 6 * 1/2 + 1 = 7 \text{ (Septet)}$$

$$1J_{FP}: 2 * 1 * 1/2 + 1 = 2 \text{ (Doublet)}$$

Coupling constant

$$1J_{PF} = 1J_{FP} = 706 \text{ Hz}$$



29Si

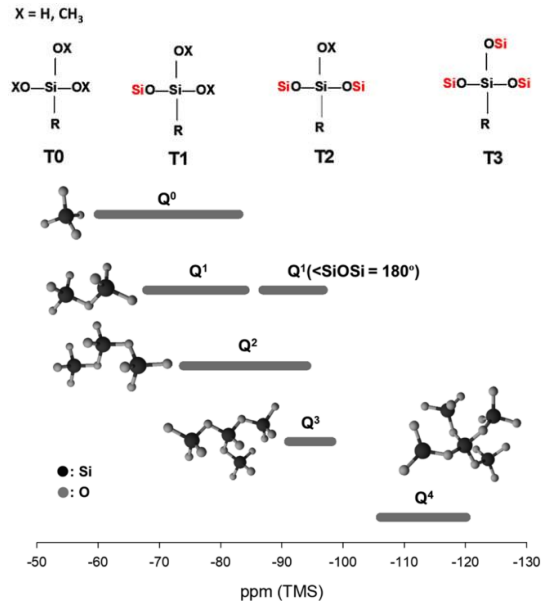


Fig. 2. Classification of silicate minerals according to the degree of polymerization of SiO₄ and their chemical shifts in ²⁹Si NMR (adapted from Magi et al. [31]).

13C

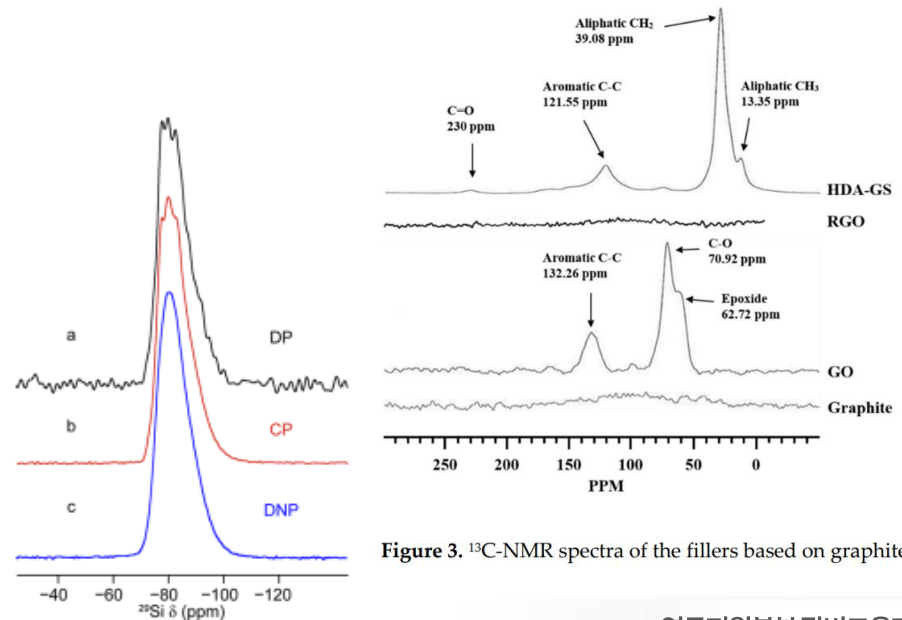
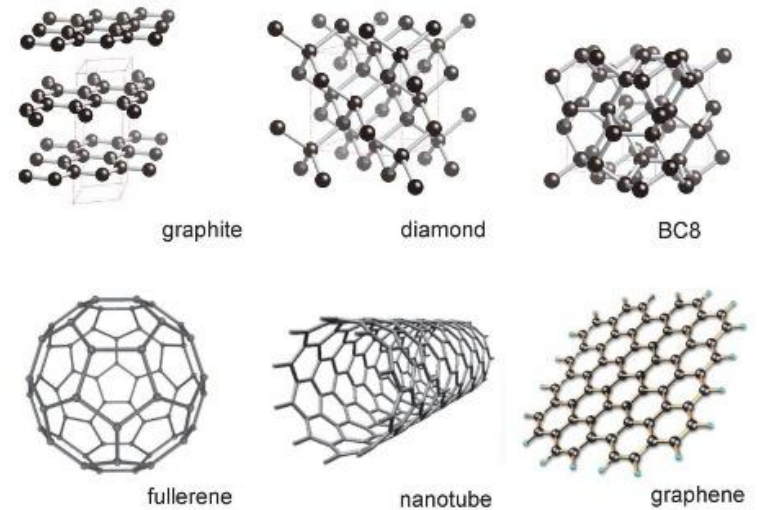
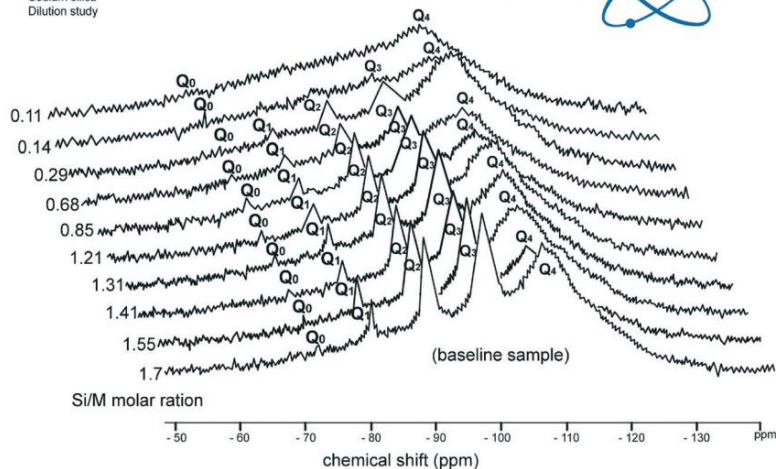
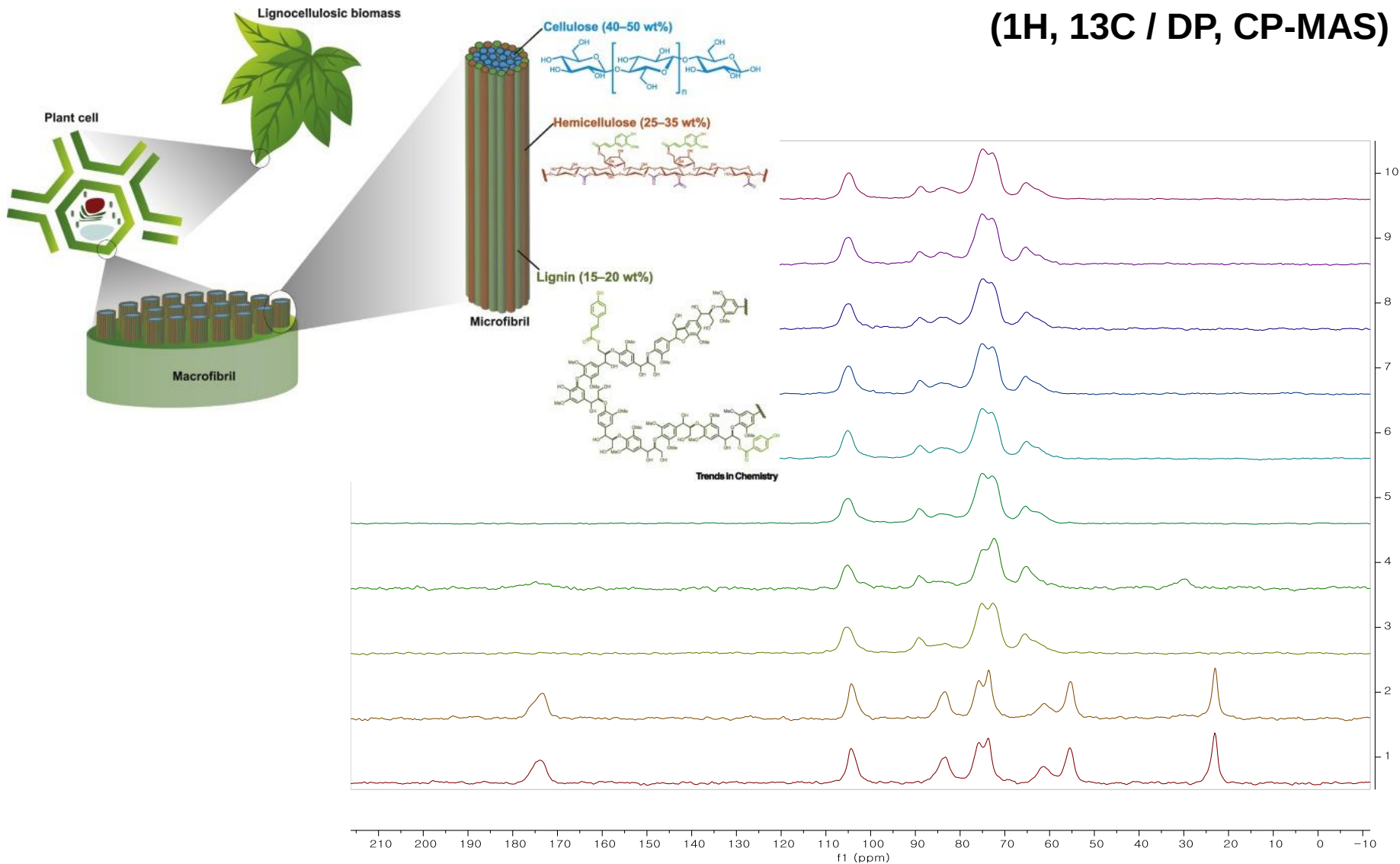


Figure 3. ¹³C-NMR spectra of the fillers based on graphite.

VUT Bruker DPX300 Spectrometer
29S1 NMR Spectrum 5mm BBIZ
Sodium silica
Dilution study



Solid-state NMR (¹H, ¹³C / DP, CP-MAS)



G-quadruplex 가 Li ion의 이동속도를 향상시킴

G-quadruplex의 이온채널 형성 분석

ScienceAdvances
AAAS

Manuscript
Template

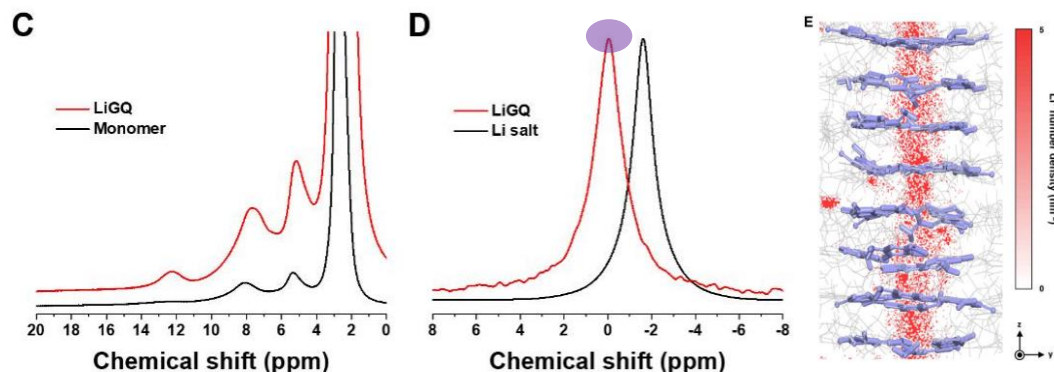
FRONT MATTER

Title

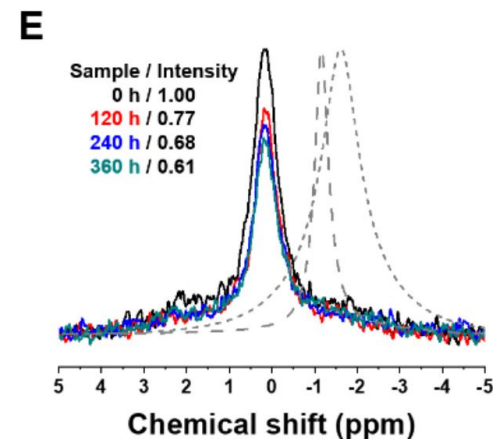
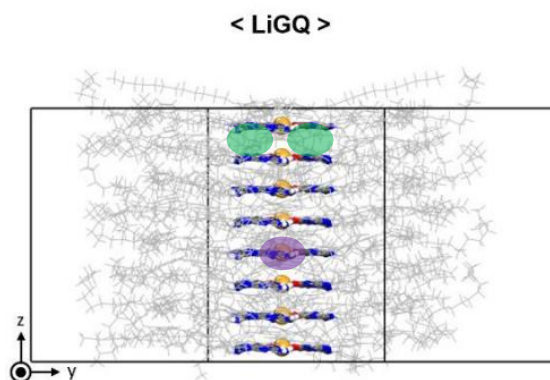
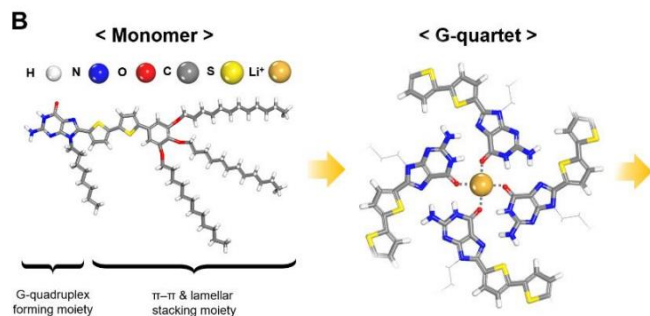
Ion slippage through Li⁺-centered G-quadruplex

Authors

Seok-Kyu Cho,^{1†} Kyung Min Lee,^{2†} So-Huei Kang,^{2,3†} Kihun Jeong,⁴ Sun-Phil Han,⁵ Ji Eun Lee,² Seungho Lee,⁶ Tae Joo Shin,³ Ja-Hyoung Ryu,⁶ Changduk Yang,^{2*} Sang Kyu Kwak,^{2*} Sang-Young Lee^{4*}



shows a π - π stacking distance of ~ 3.4 Å. MAS (C) ¹H and (D) ⁷Li NMR spectra of the LiGQ. A characteristic ¹H NMR peak at 12 ppm exhibits the Hoogsteen hydrogen bond of G-quartet assembly. The deshielded singlet ⁷Li NMR peak at -0.044 ppm reveals the isolation of Li⁺ from its counter anion. (E) Contour plot of Li⁺ number density of the LiGQ under an electric field. Red bar indicates the 2D number density of Li⁺ projected to the yz-plane.



이온전도 메커니즘 확인

고체 전해질 첨가제 분석

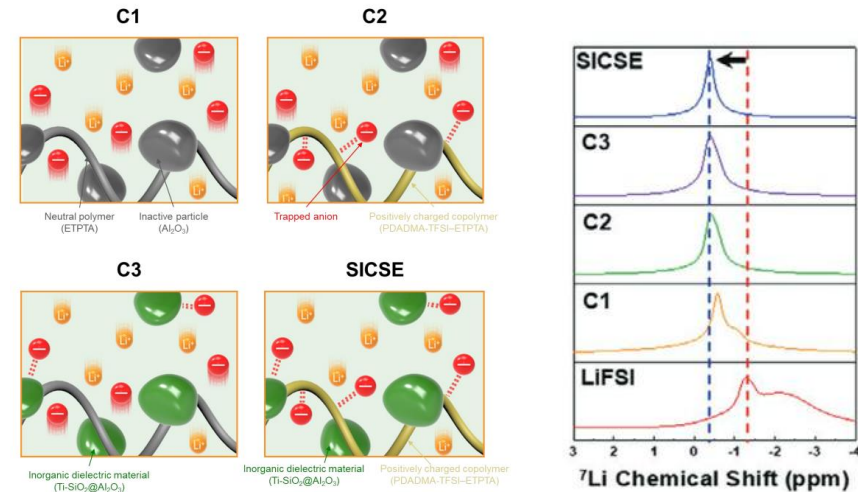
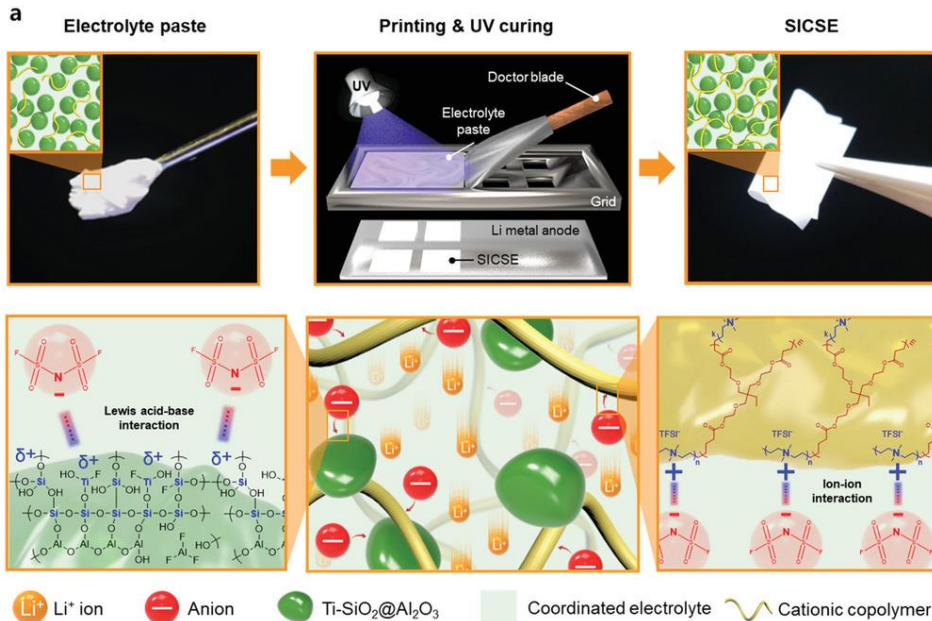
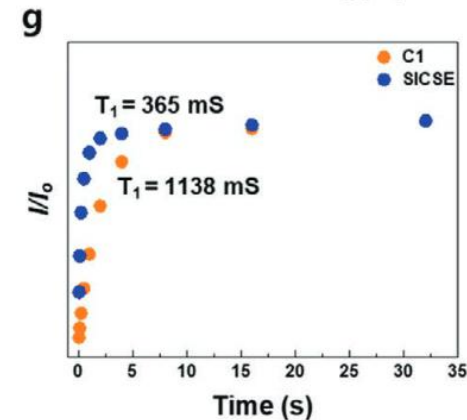
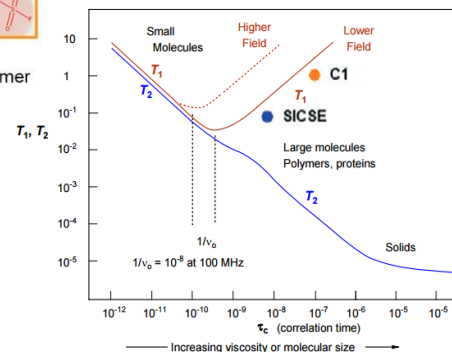


Figure S9. Conceptual illustration depicting the ion transport phenomena of the control samples (C1, C2, and C3) and SICSE, along with their chemical structure and anion trapping sites.

d) 7Li NMR spectra of the SICSE, control samples (C1, C2, and C3), and LiFSI



g) Inversion–recovery plots obtained from 7Li MAS NMR spectra.

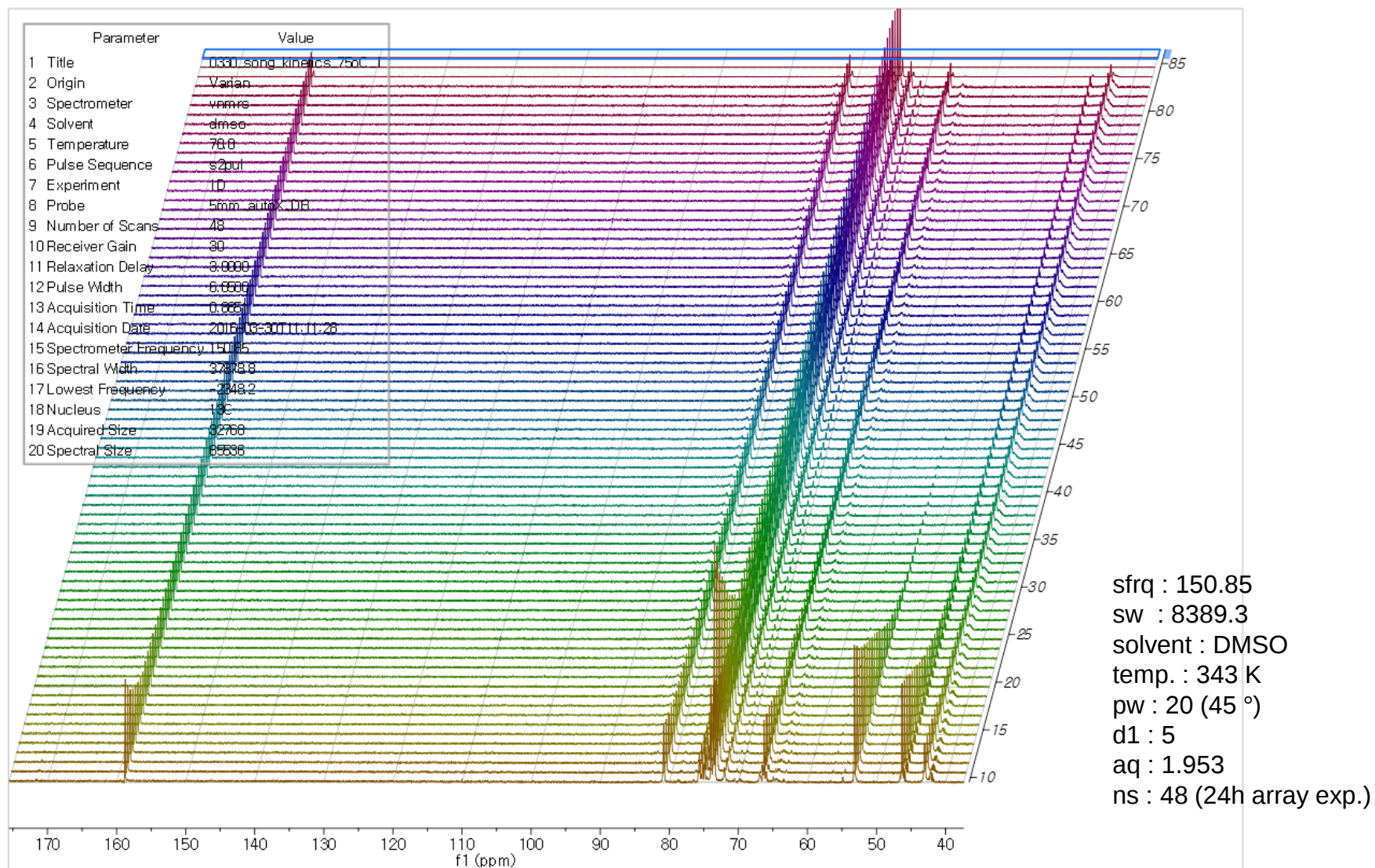
ADVANCED ENERGY MATERIALS

Research Article | Full Access

Single-Ion Conducting Soft Electrolytes for Semi-Solid Lithium Metal Batteries Enabling Cell Fabrication and Operation under Ambient Conditions

Kyeong-Seok Oh, Jung-Hui Kim, Se-Hee Kim, Dongrak Oh, Sun-Phil Han, Kwangeun Jung, Zhuyi Wang, Liyi Shi, Yongxiang Su, Taeun Yim, Shuai Yuan, Sang-Young Lee

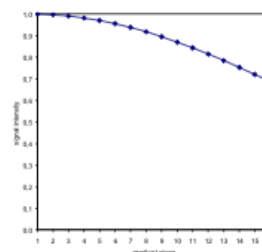
First published: 08 August 2021 | <https://doi.org/10.1002/aenm.202101813> | Citations: 3



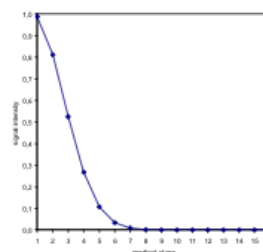
Diffusion Ordered Spectroscopy

$$D = \frac{kT}{6\pi\eta r_s}$$

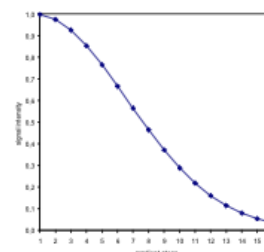
$$I/I_0 = e^{(-Dg^2\delta^2\sigma^2g^2\Delta')}$$



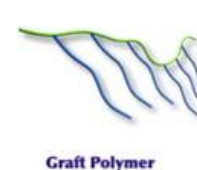
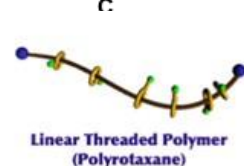
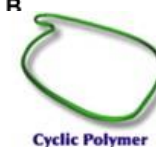
A



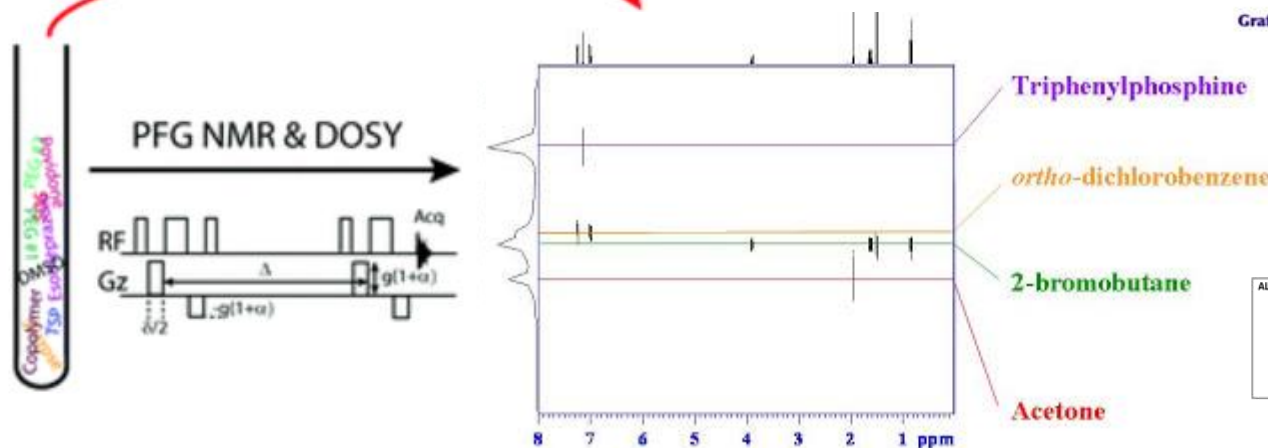
B



C

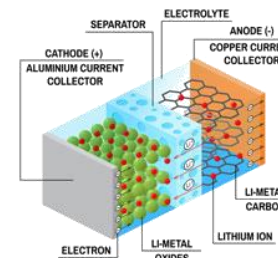


Unravelling mixture

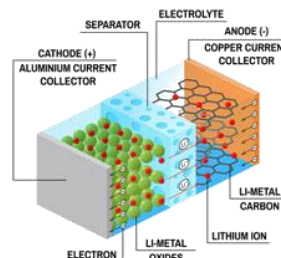


LITHIUM-ION BATTERY

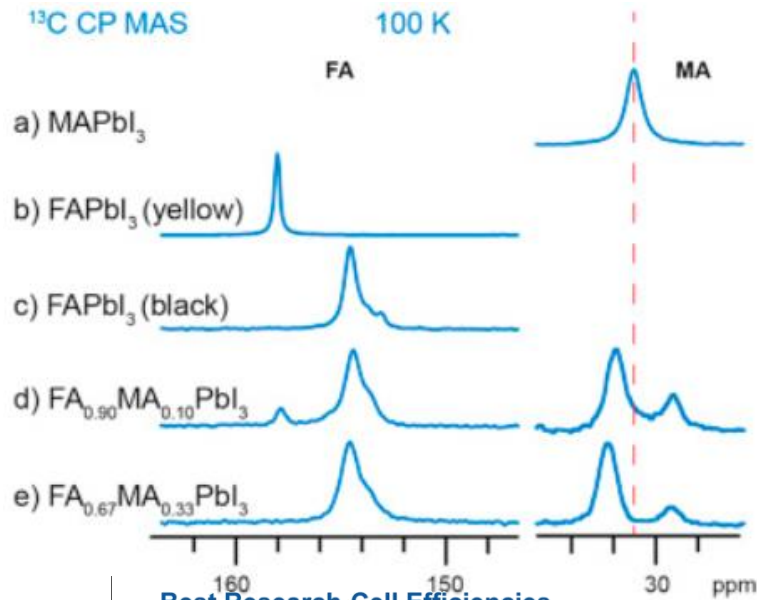
DISCHARGE



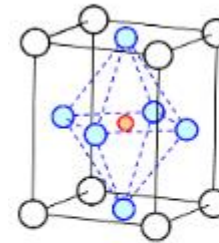
CHARGE



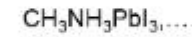
Solid-state NMR (Perovskite)



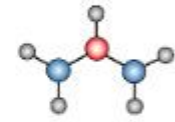
Metal halide perovskite



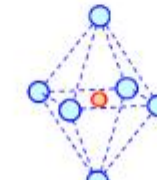
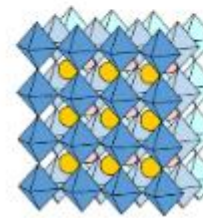
- A (organic cation, Cs⁺)
- B (Pb²⁺, Sn²⁺, ...)
- X (I⁻, Cl⁻, Br⁻)



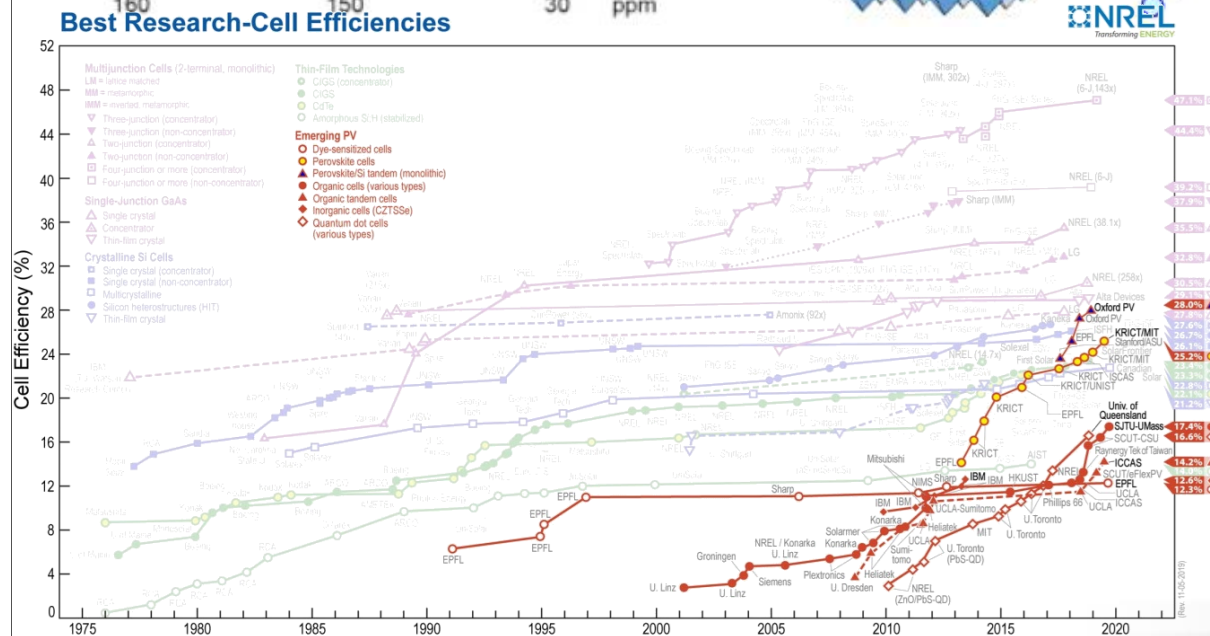
methylammonium (CH₃NH₃)⁺



formamidinium (NH₂CHNH₂)⁺



BX₆ octahedron



^{13}C Solid-state NMR (CP-MAS)

20160428-Styrene-CPMAS-C13_3h

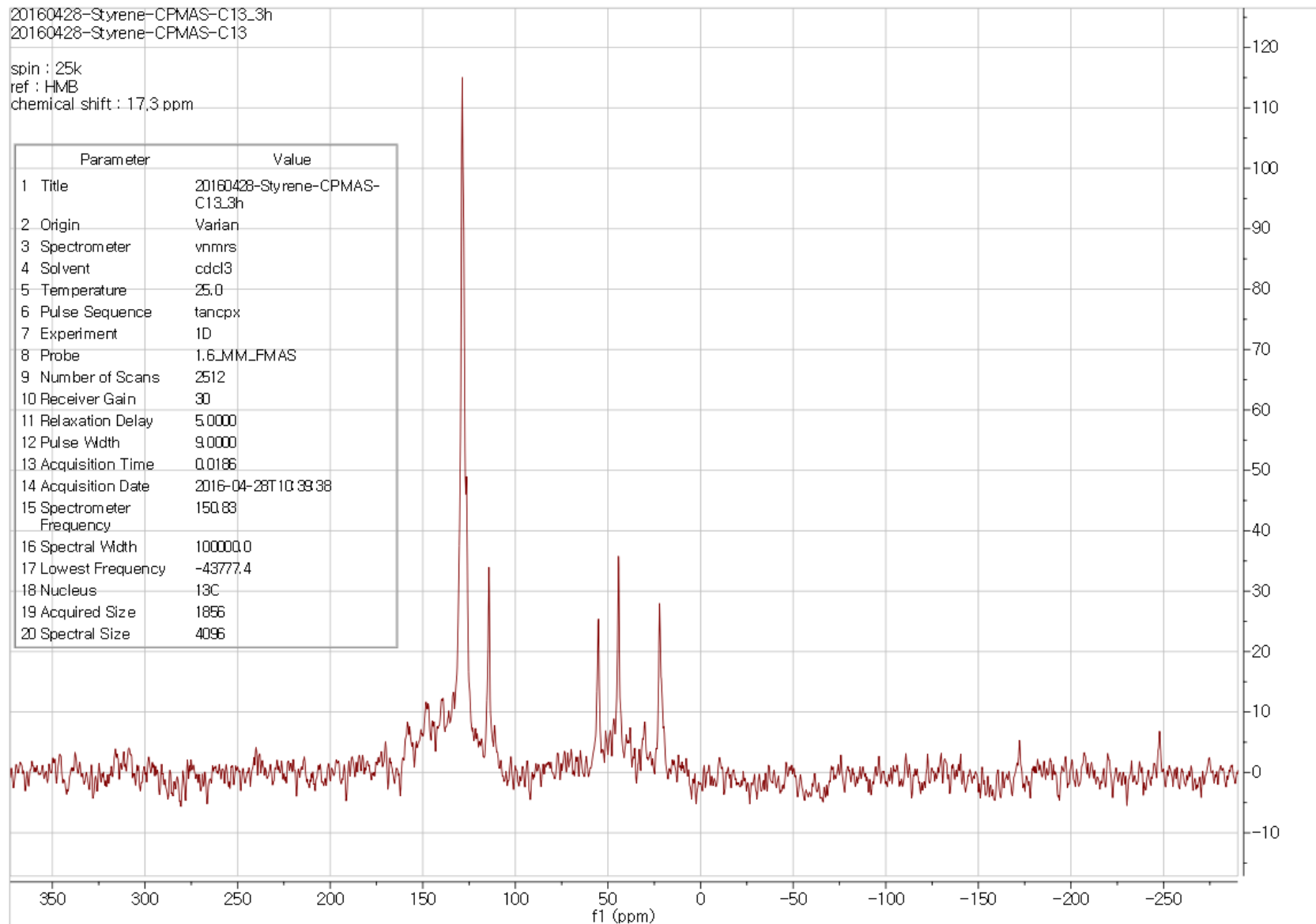
20160428-Styrene-CPMAS-C13

spin : 25k

ref : HMB

chemical shift : 17,3 ppm

Parameter	Value
1 Title	20160428-Styrene-CPMAS-C13_3h
2 Origin	Varian
3 Spectrometer	nmr5
4 Solvent	cdcl3
5 Temperature	25.0
6 Pulse Sequence	tanpax
7 Experiment	1D
8 Probe	1.6_MM_FMAS
9 Number of Scans	2512
10 Receiver Gain	30
11 Relaxation Delay	5.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.0186
14 Acquisition Date	2016-04-28T10:39:38
15 Spectrometer Frequency	150.83
16 Spectral Width	100000.0
17 Lowest Frequency	-43777.4
18 Nucleus	^{13}C
19 Acquired Size	1856
20 Spectral Size	4096





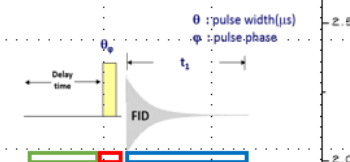
NMR을 이용한 Pulverized Coal 조성분석

One-Pulse

Table 2. Structure parameters and assignment for the ^{13}C -NMR spectra of coal [84,86-88].

Parameter	Assignment	Chemical Shift (ppm)
f_{CH}	CH_3 carbon ¹	0-25
f_{CH}	CH/CH_2 carbon + quaternary carbon ²	25-51
f_{CH}	aliphatic carbon bonded to oxygen ³	51-90
$f_{\text{H+8}}$	protonated aromatic carbon + aromatic bridgehead carbon	90-137
f_{H}	protonated aromatic carbon	90-129
f_{N}	non-protonated aromatic carbon	129-165
$f_{\text{N+5}}$	aromatic carbon bonded to carbon	129-150
f_{H}	aromatic bridgehead carbon	129-137
f_{H}	alkylated aromatic carbon	137-150
f_{H}	phenolic ethers	150-165
f_{C}	carbonyl/ carboxyl carbon ⁴	165-220
f_{CP}	aromaticity	90-165
f_{H}	aliphatic carbon	0-90
f_{H}	aromatic carbon	90-220
X_{H}	ratio of aromatic bridgehead carbon to aromaticity	(129-137)/(90-165)

¹ Aliphatic CH_3 carbon (0-25 ppm), aromatic CH_3 carbon (25-36 ppm), quaternary carbon (36-51 ppm). ² CH/CH_2 carbon (25-36 ppm), quaternary carbon (36-51 ppm). ³ Methoxy/aromatic methoxy (51-75 ppm), aliphatic carbon bonded to oxygen in cyclic hydrocarbon (75-90 ppm). ⁴ Carboxyl carbon (165-185 ppm), carbonyl carbon (185-220 ppm).



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Model: Varian

Magnet: 600 MHz

Pulse: One-Pulse

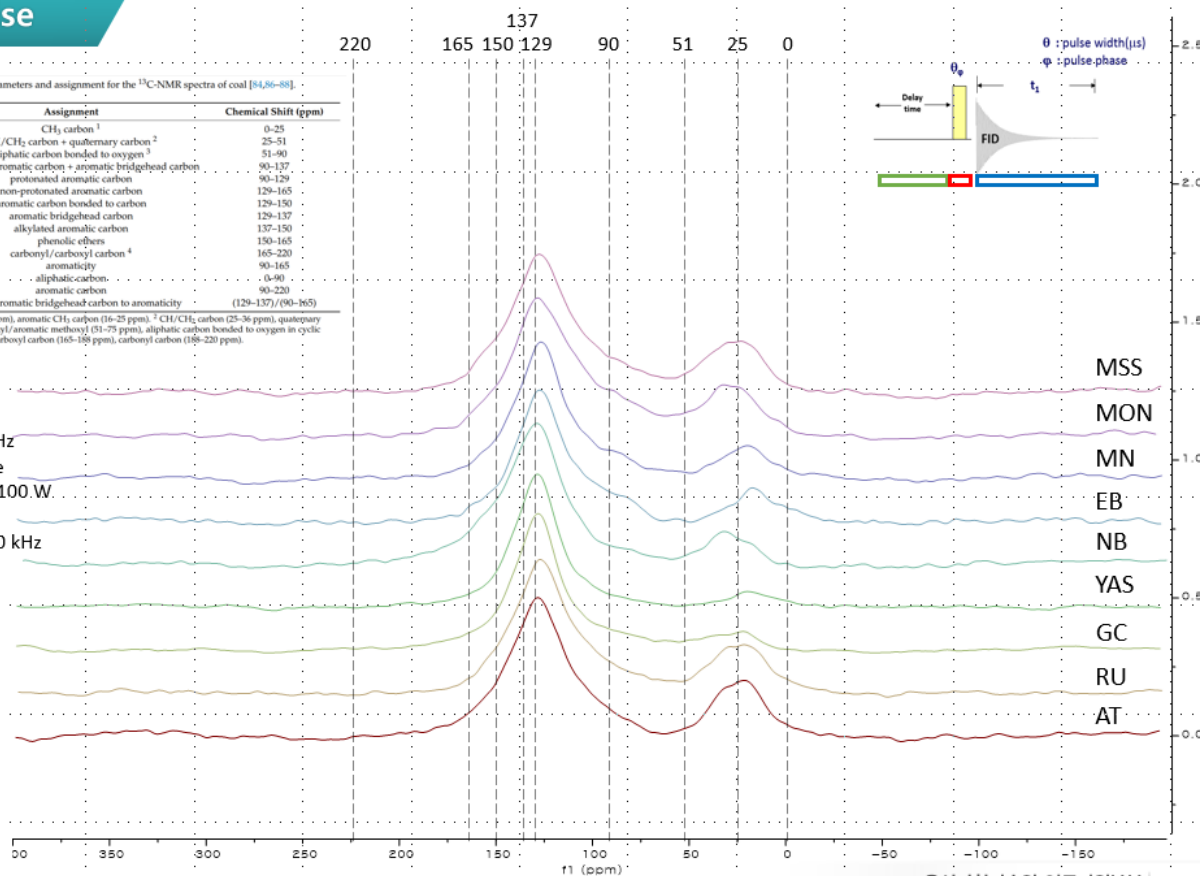
^1H Decoupling: 100.W

Rotor: 1.6 mm

Spinning rate: 40 kHz

NS: 1024

D1: 60

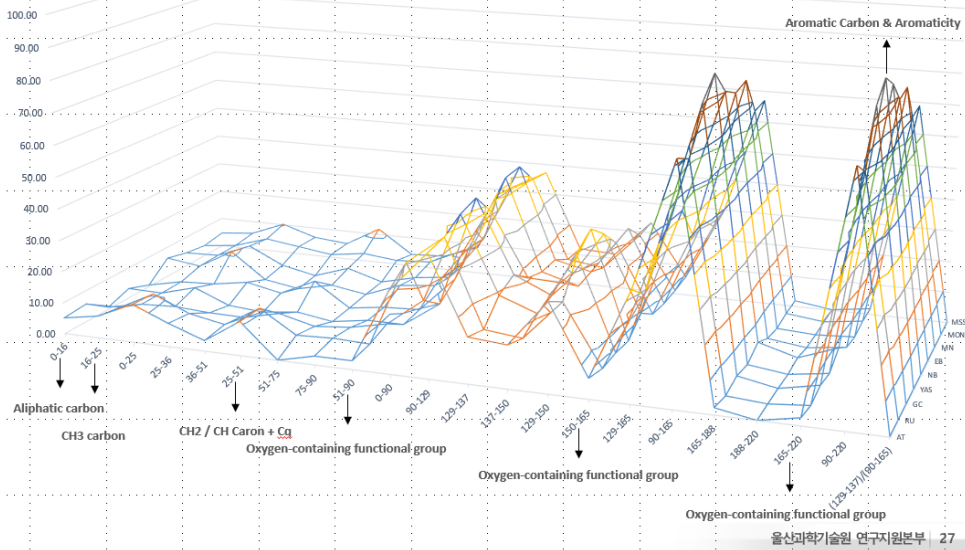


울산과학기술원 연구지원본부 18

^{13}C Solid-state NMR (Coal)

NMR을 이용한 Pulverized Coal 조성분석

NMR data

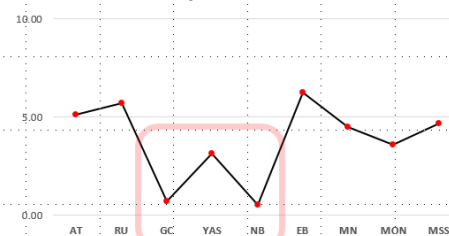


NMR을 이용한 Pulverized Coal 조성분석

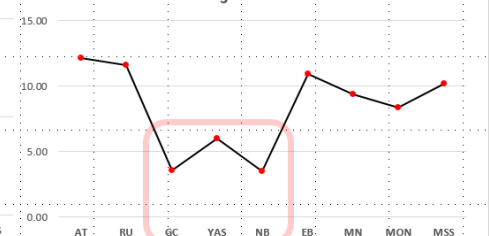
NMR data

결과: YAS, GC의 휘발분 함량이 적음

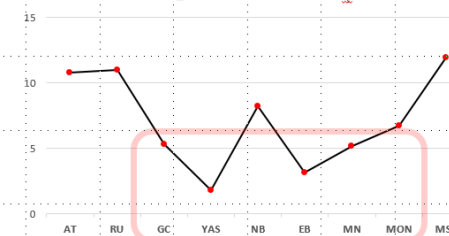
Aliphatic carbon



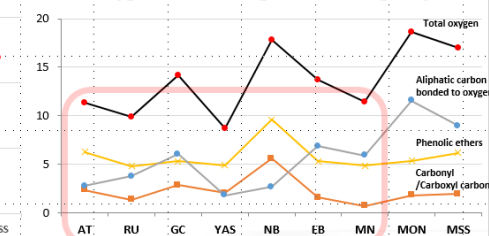
CH₃ carbon



CH₂ / CH Carbon + C_q



Oxygen-containing functional group

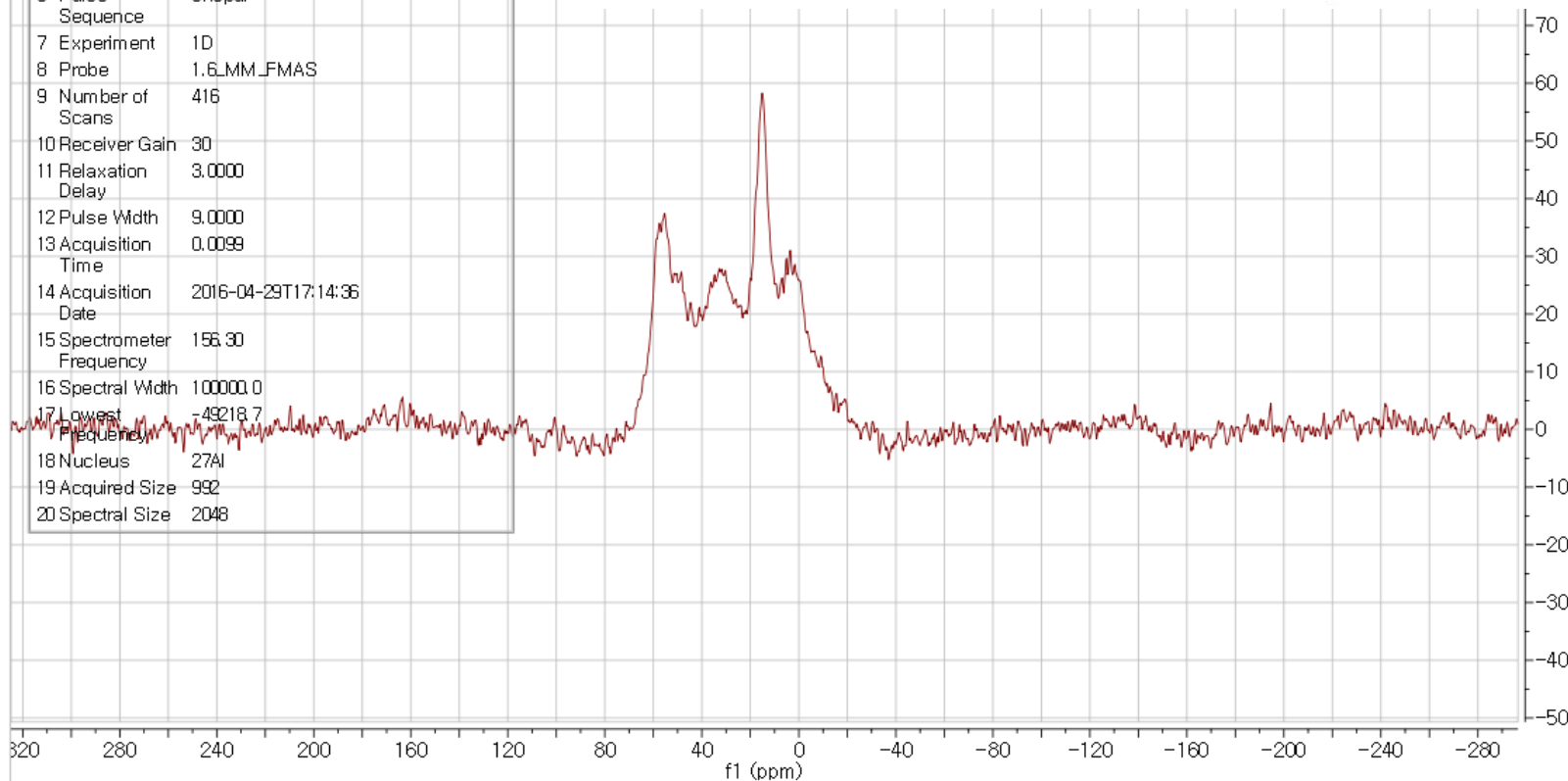
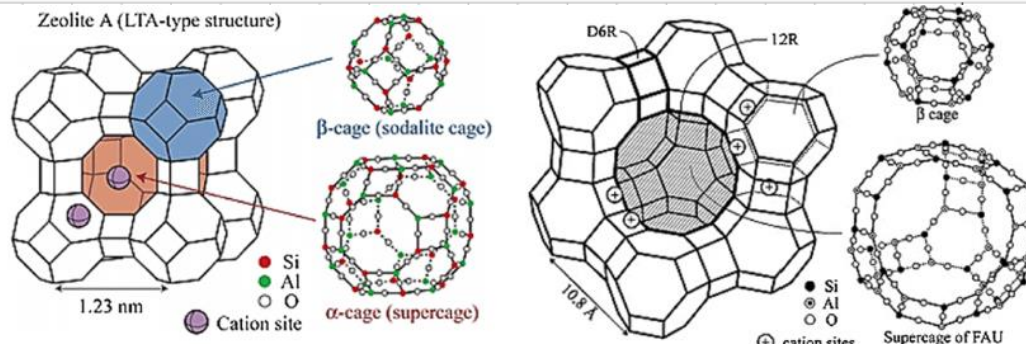


^{27}Al Solid-state NMR (Zeolite)

20160429-#160422_HLform_49C_750C_20h_AI27
20160429-#160422_HLform_49C_750C_20h_AI27

ref : 1.1M $\text{Al}(\text{NO}_3)_3$
chemical shift : 0 ppm

Parameter	Value
1 Title	20160429- #160422_HLform_49C_750C_20h_AI27
2 Origin	Varian
3 Spectrometer	nmr
4 Solvent	cdcl3
5 Temperature	25.0
6 Pulse Sequence	onepul
7 Experiment	1D
8 Probe	1.6_MM_FMAS
9 Number of Scans	416
10 Receiver Gain	30
11 Relaxation Delay	3.0000
12 Pulse Width	9.0000
13 Acquisition Time	0.0099
14 Acquisition Date	2016-04-29T17:14:36
15 Spectrometer Frequency	156.30
16 Spectral Width	100000.0
17 Lowest Frequency	-49218.7
18 Nucleus	^{27}Al
19 Acquired Size	992
20 Spectral Size	2048



Organic complexes

Inorganic complexes

Zeolites

Mesoporous solids

Microporous solids

Aluminosilicates/phosphates

Minerals

Biological molecules

Glasses

Cements

Food products

Wood

Ceramics

Bones

Semiconductors

Metals and alloys

Archaeological specimens

Polymers

Resins

Surfaces

But, Fine particle + at least 20mg

17. References

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- 참고논문
- 웹사이트

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<Solid-state NMR>

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2) Biological Solids, Membrane Proteins, Drugs, Lipid Assemblies

- a. Solid state NMR Spectroscopy for Biopolymers by H. Saito et al, 2007, Springer
- b. NMR spectroscopy of Biological Solids by A. Ramamoorthy, 2006, CRC Press

18. Attachments

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CAMPUS MAP

- ① 102동 자연과학관
- ② 104동 제1공학관
- ③ 106동 제2공학관
- ④ 114동 경영관
- ⑤ 201동 대학본부
- ⑥ 202동 학술정보관
- ⑦ 203동 학생회관
- ⑧ 205동 실내체육관
- ⑨ 정단소재연구관
- ⑩ 출기세포연구관
- ⑪ 기기기술동
- ⑫ 301~309동 학생기숙사
- ⑬ 교수아파트
- ⑭ 저차원 탄소 혁신소재 연구관

11 기기기술동

- 기기기술실

10 출기세포연구관

- 생체효능검증실

9 정단소재연구관

14 저차원 탄소 혁신소재 연구관

1 102동 자연과학관

- 기기분석실
- 나노소재공정실
- 환경분석실
- 방사선안전관리실

2 104동 제1공학관

- 바이오메드이미징실

3 104동 제1공학관

- 바이오메드이미징실

- 기기분석실
- 나노소재공정실
- 환경분석실
- 방사선안전관리실

4 114동 경영관

- 경영관리실

5 201동 대학본부

- 대학본부

6 202동 학술정보관

- 학술정보관

7 203동 학생회관

- 학생회관

8 205동 실내체육관

- 실내체육관

9 정단소재연구관

- 정단소재연구관

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- 기기기술실

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- 학생기숙사

13 교수아파트

- 교수아파트



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