北京大学
PEKING UNIVERSITY

北京核磁共振中心
Beijing NMR Center, Peking University

核磁共振上机培训

李红卫

2020-10

核磁共振上机基础

李红卫

2020-10-25

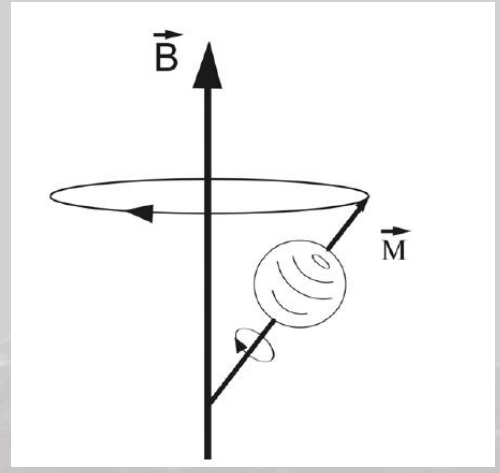
基本原理

基本条件：
稳定磁场B_0

核 磁 共振

检测对象：自旋量子数I不为0

自旋量子数(I)	示例
半整数（1/2，3/2…）	^{1}H, ^{13}C, ^{15}N
整数（1，2，…）	^{2}D, ^{14}N



检测内容：
原子核进动频率

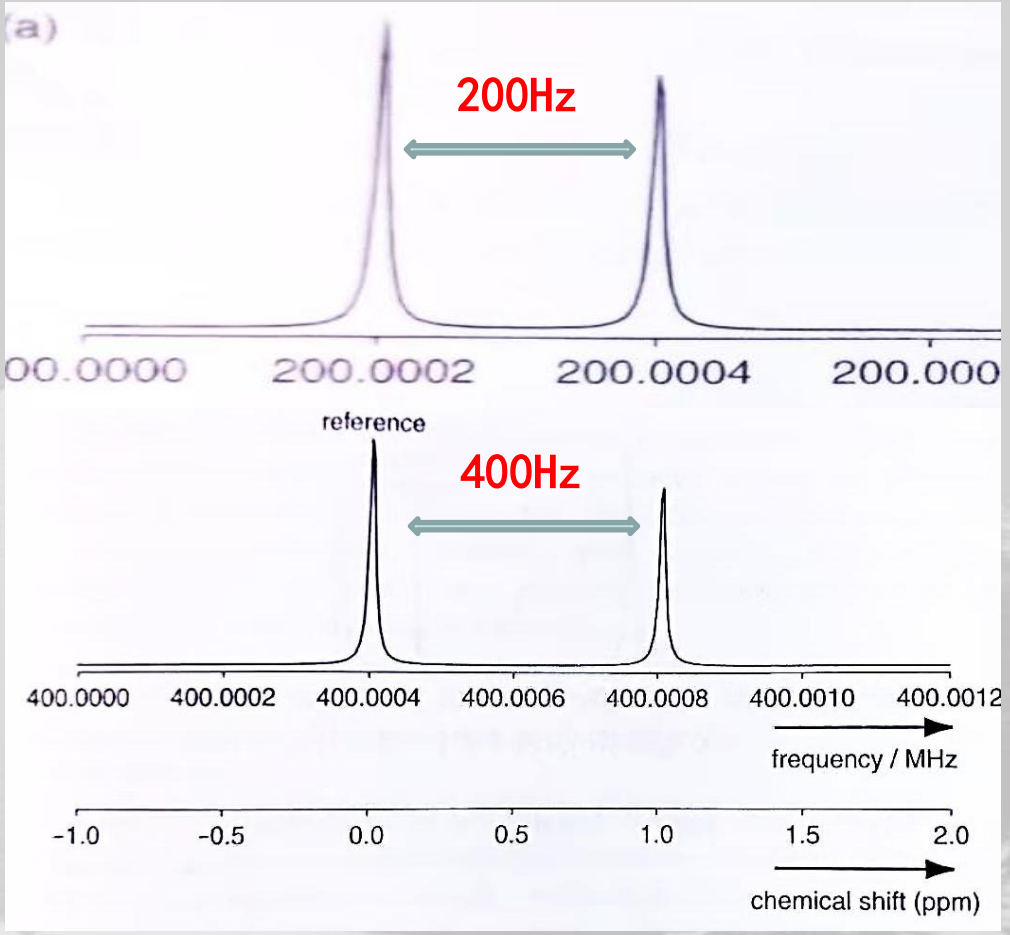
$$\upsilon = \frac{\gamma B_0}{2\pi}$$

γ：旋磁比，与不同原子核的性质相关；

υ: 进动频率；B_0：磁场强度；

- Spin，Precession and Larmor frequency

化学位移及分辨率

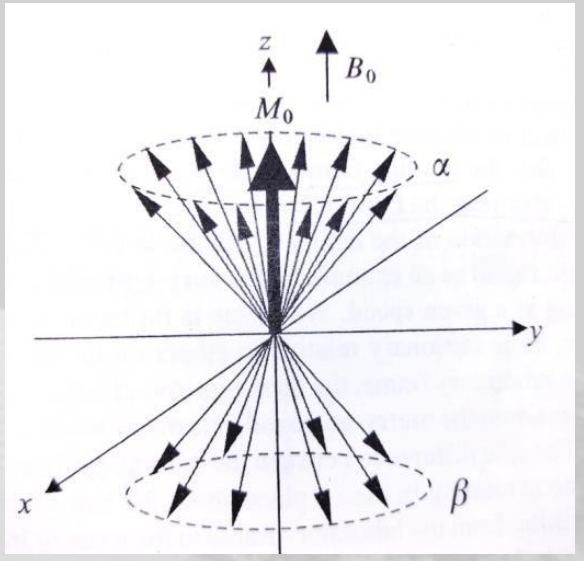


$$\upsilon_{real} = \frac{\gamma B_{eff}}{2\pi}$$

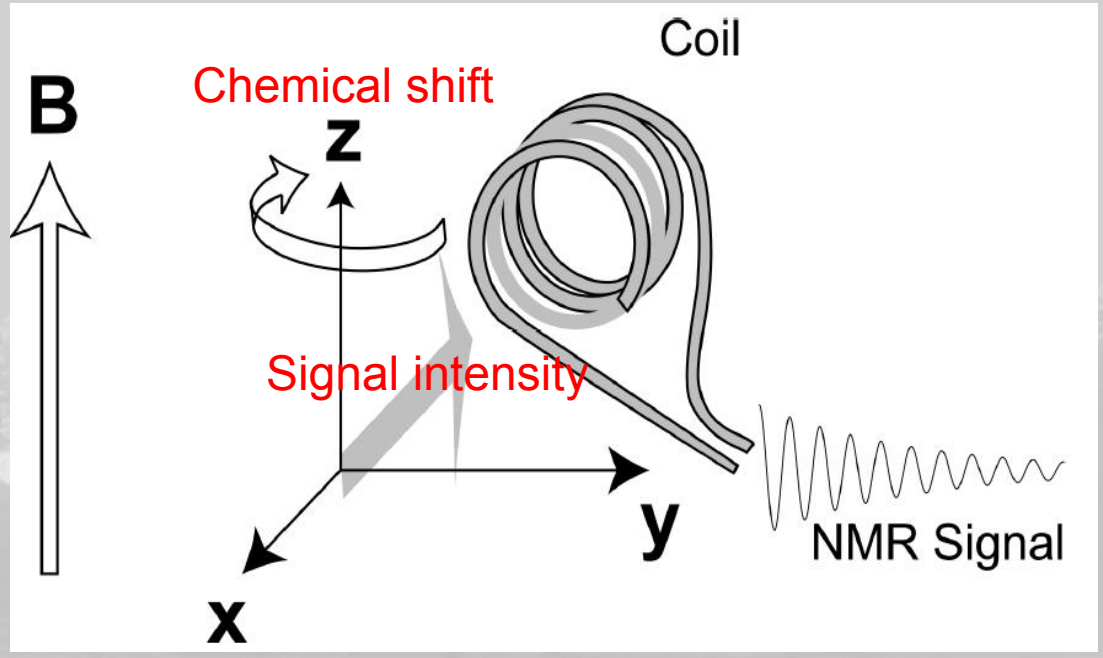
$$\delta(ppm) = \frac{\upsilon - \upsilon_{ref}}{\upsilon_{BF1}} \times 10^6$$

场强越高，分辨率越高

核磁共振信号产生

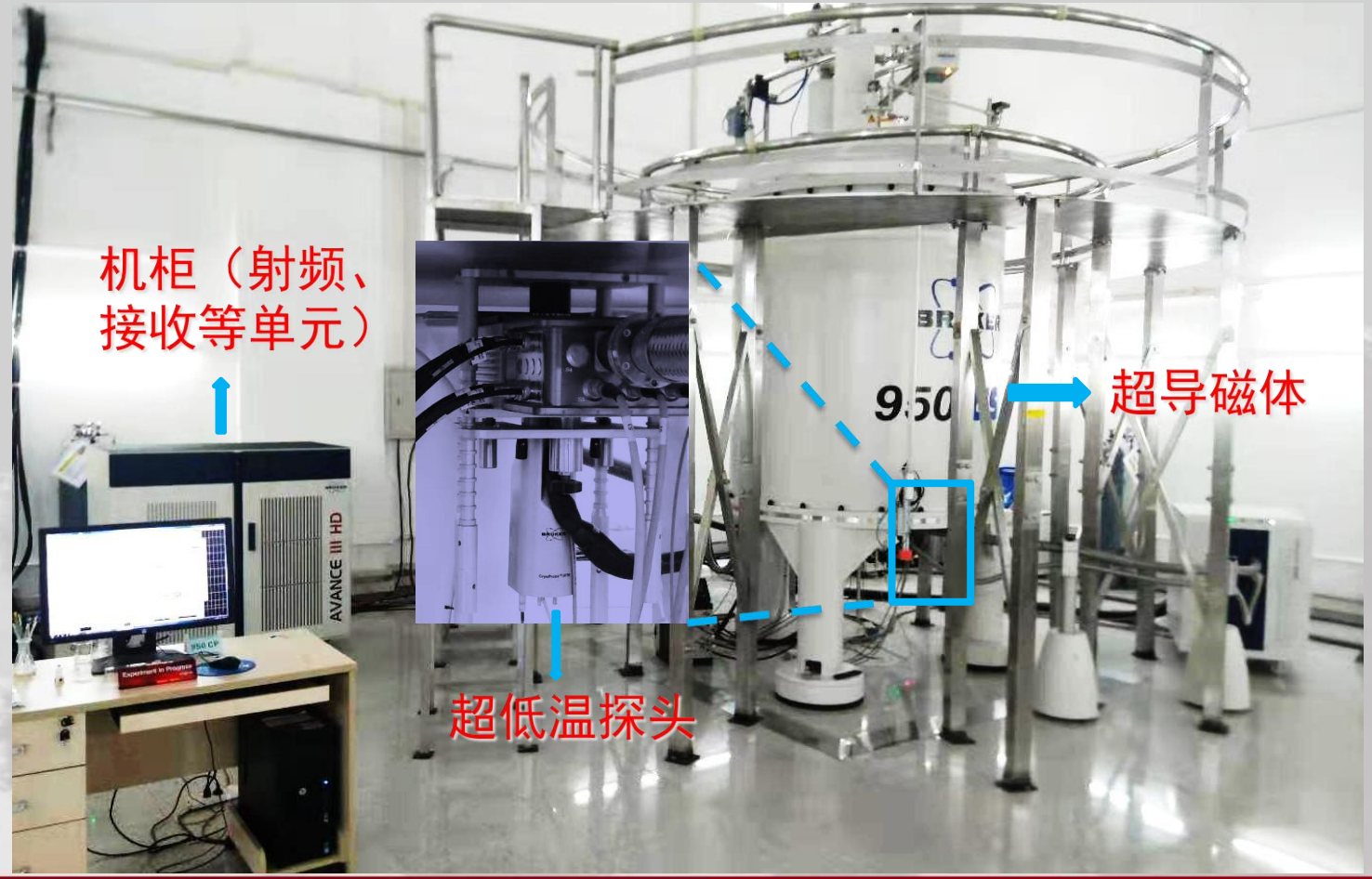


Bulk Magnetization

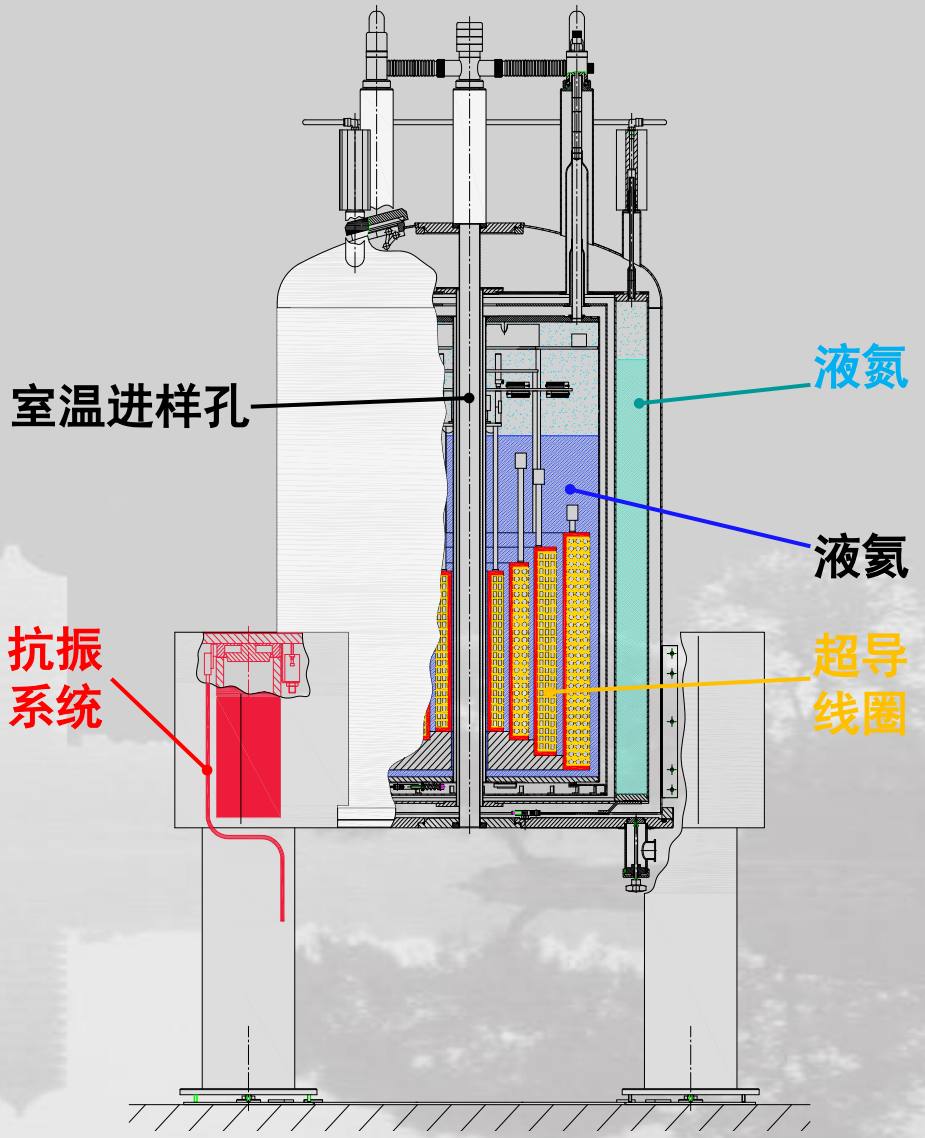


1D experiments:

核磁共振仪器及注意事项



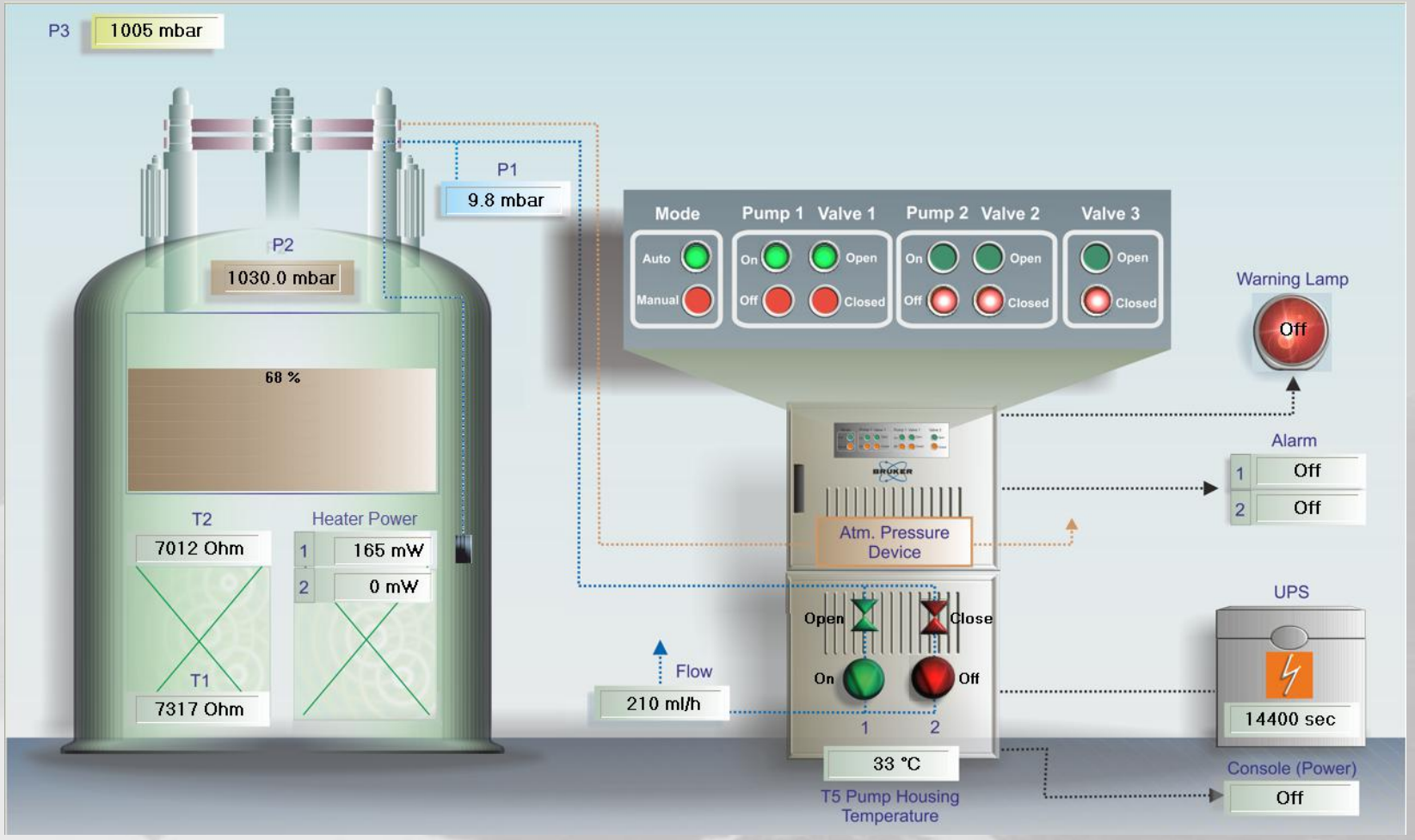
磁体



Attention

- 使用心脏起搏器和体内有金属植入者禁止进入核磁共振实验室。
- 严禁携带以下物品进入核磁共振仪器实验室：铁磁性物质（铁制工具，钥匙等），电子设备（手机，手表等），电子卡片（银行卡等），除核磁样品以外的化学品，食品和饮料。
- 磁体处于悬浮状态，上样时禁止触碰磁体

2K磁体


P3
1005 mbar
P1
9.8 mbar
P2
1030.0 mbar
68 %
T2
7012 Ohm
T1
7317 Ohm
Heater Power
1
165 mW
2
0 mW
Mode
Pump 1
Valve 1
Pump 2
Valve 2
Valve 3
Auto
Manual
On
Off
Open
Closed
Warning Lamp
Off
Alarm
1
Off
2
Off
Atm. Pressure Device
Open
Close
On
Off
1
2
Flow
210 ml/h
33 °C
T5 Pump Housing Temperature
UPS
14400 sec
Console (Power)
Off

探头

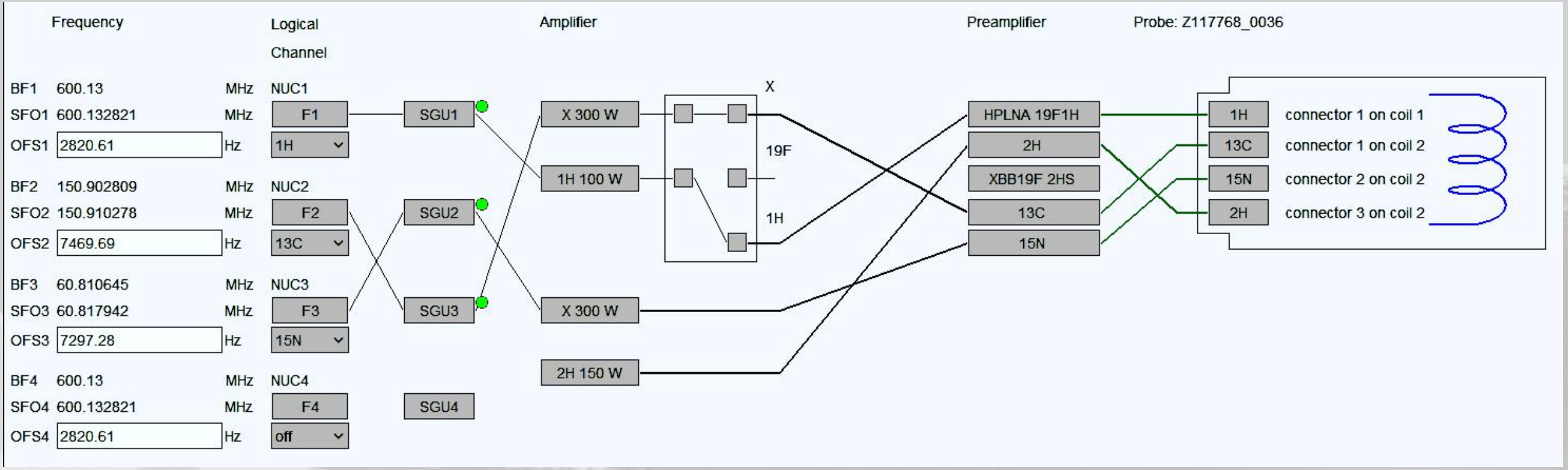
Attention

- 使用完好无损的核磁管
- 无自动上样器的仪器，上样前需确认Lift气流
- 上样前要将核磁管擦拭干净，特别是刚从低温取出的样品
- 使用合适的脉冲功率

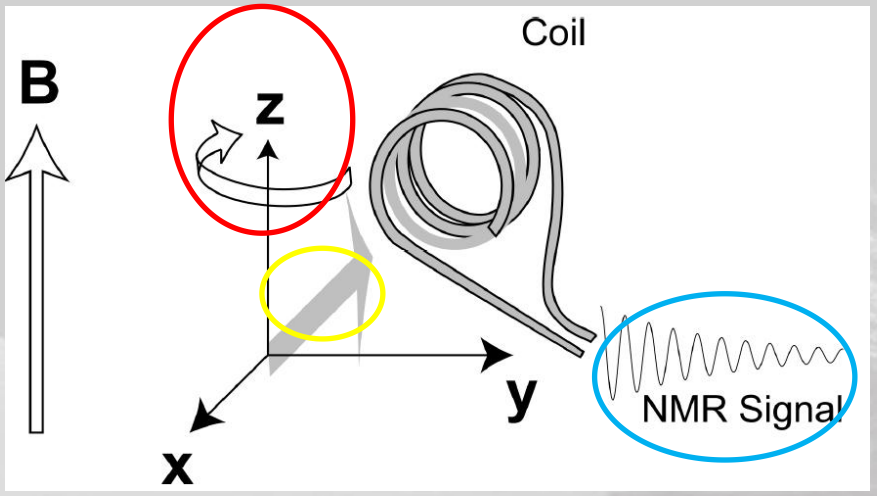
进入核磁实验室对仪器的任何操作都需要具有核磁上机权限的人陪同

控制器

信号通路


Frequency
Logical Channel
Amplifier
Preamplifier
Probe: Z117768_0036
BF1 600.13 MHz
SFO1 600.132821 MHz
OFS1 2820.61 Hz
NUC1
F1
1H
SGU1
BF2 150.902809 MHz
SFO2 150.910278 MHz
OFS2 7469.69 Hz
NUC2
F2
13C
SGU2
BF3 60.810645 MHz
SFO3 60.817942 MHz
OFS3 7297.28 Hz
NUC3
F3
15N
SGU3
BF4 600.13 MHz
SFO4 600.132821 MHz
OFS4 2820.61 Hz
NUC4
F4
off
SGU4
X 300 W
1H 100 W
X 300 W
2H 150 W
X
19F
1H
HPLNA 19F1H
2H
XBB19F 2HS
13C
15N
1H
13C
15N
2H
connector 1 on coil 1
connector 1 on coil 2
connector 2 on coil 2
connector 3 on coil 2

实验操作流程



Sample preparation

Field preparation（lock, atmm, topshim）

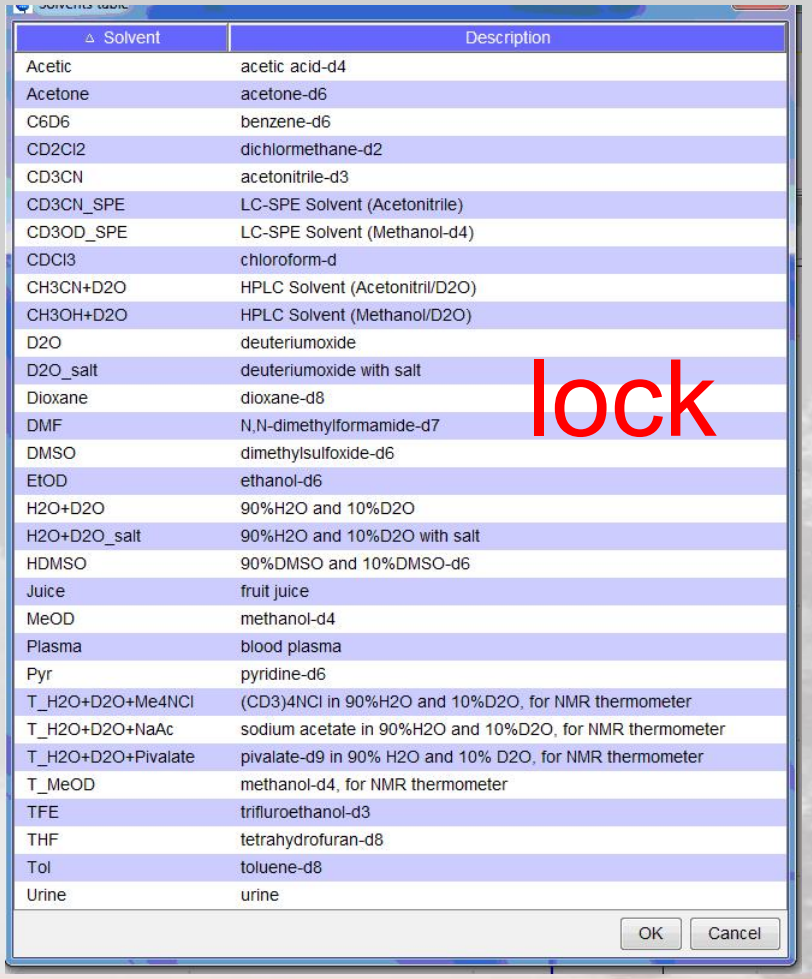
Pulse calibration

Experiment-related parameter

样品准备

- 样品的制备
  - 非标记样品；^{15}N 标记样品；^{15}N 和^{13}C标记样品；其他特殊标记样品；
  - 样品浓度：~mM量级;
  - 溶剂的体积为450-550 μl；
  - 选择合适的缓冲体系，pH<7.5；DSS；D_2O；
  - 核磁管一般为5mm内径的核磁管；
- 进样与出样
  - Bruker 自动进样系统
  - Lift命令进样

磁场准备

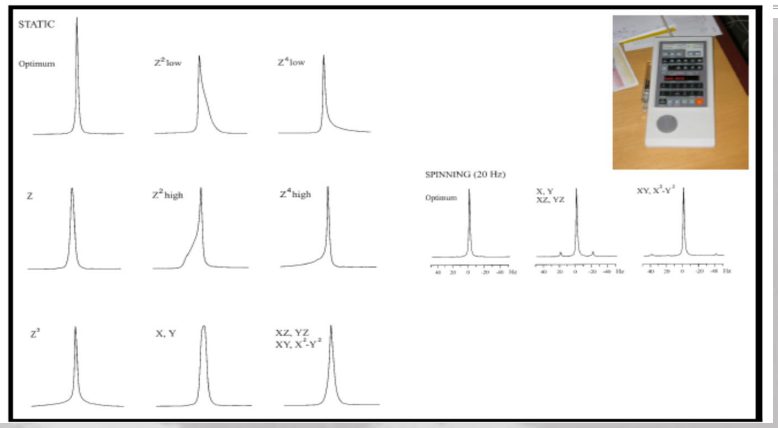


Solvent	Description
Acetic	acetic acid-d4
Acetone	acetone-d6
C6D6	benzene-d6
CD2Cl2	dichlormethane-d2
CD3CN	acetonitrile-d3
CD3CN_SPE	LC-SPE Solvent (Acetonitrile)
CD3OD_SPE	LC-SPE Solvent (Methanol-d4)
CDCl3	chloroform-d
CH3CN+D2O	HPLC Solvent (Acetonitril/D2O)
CH3OH+D2O	HPLC Solvent (Methanol/D2O)
D2O	deuteriumoxide
D2O_salt	deuteriumoxide with salt
Dioxane	dioxane-d8
DMF	N,N-dimethylformamide-d7
DMSO	dimethylsulfoxide-d6
EtOD	ethanol-d6
H2O+D2O	90%H2O and 10%D2O
H2O+D2O_salt	90%H2O and 10%D2O with salt
HDMSO	90%DMSO and 10%DMSO-d6
Juice	fruit juice
MeOD	methanol-d4
Plasma	blood plasma
Pyr	pyridine-d6
T_H2O+D2O+Me4NCl	(CD3)4NCl in 90%H2O and 10%D2O, for NMR thermometer
T_H2O+D2O+NaAc	sodium acetate in 90%H2O and 10%D2O, for NMR thermometer
T_H2O+D2O+Pivalate	pivalate-d9 in 90% H2O and 10% D2O, for NMR thermometer
T_MeOD	methanol-d4, for NMR thermometer
TFE	trifluroethanol-d3
THF	tetrahydrofuran-d8
Tol	toluene-d8
Urine	urine

OK Cancel

lock

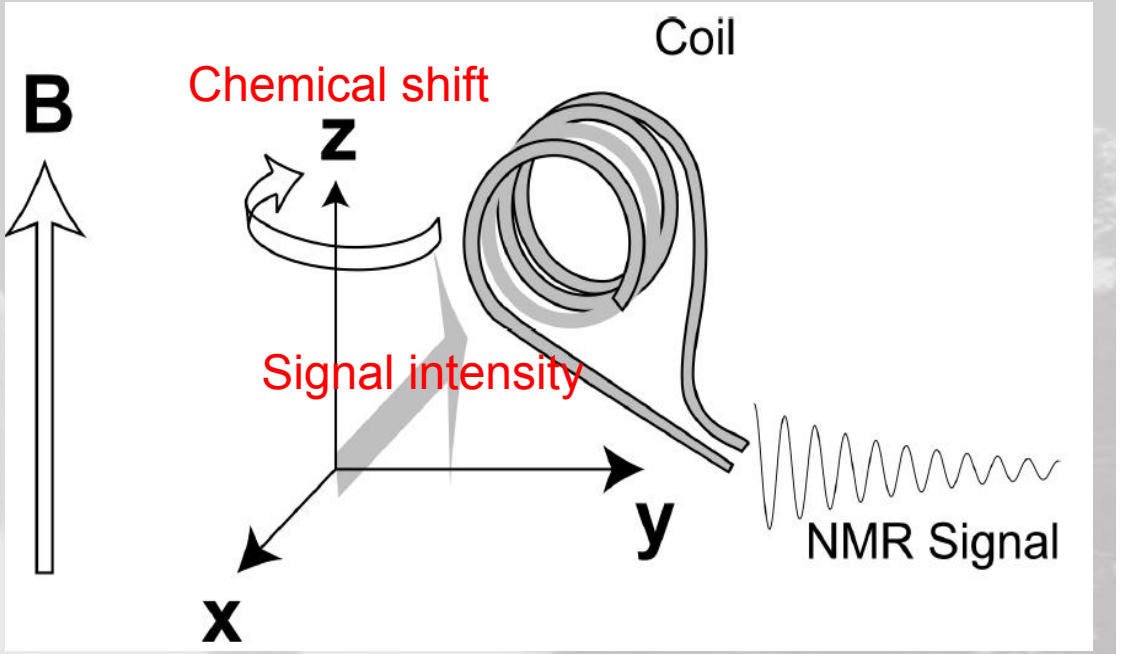
atmm

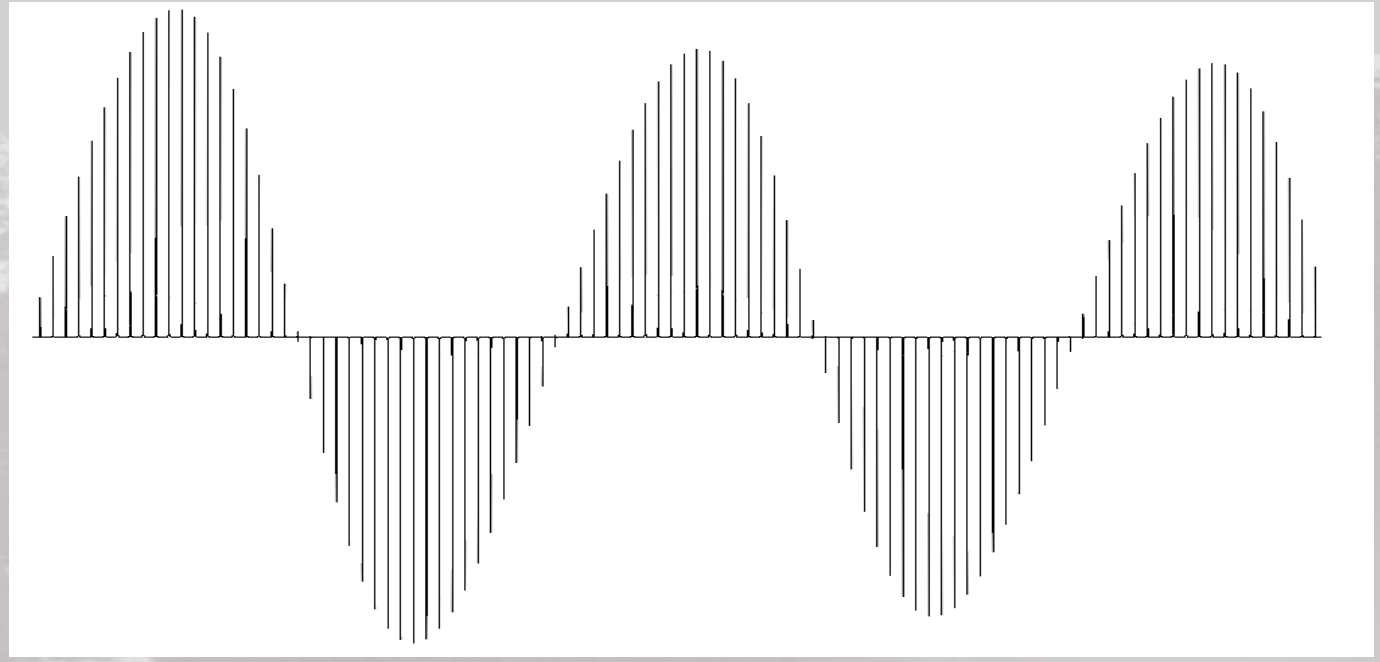


topshim

^{1}H的刻度

利用360°信号最弱的原理来刻度90°脉冲长度：p1和plw1



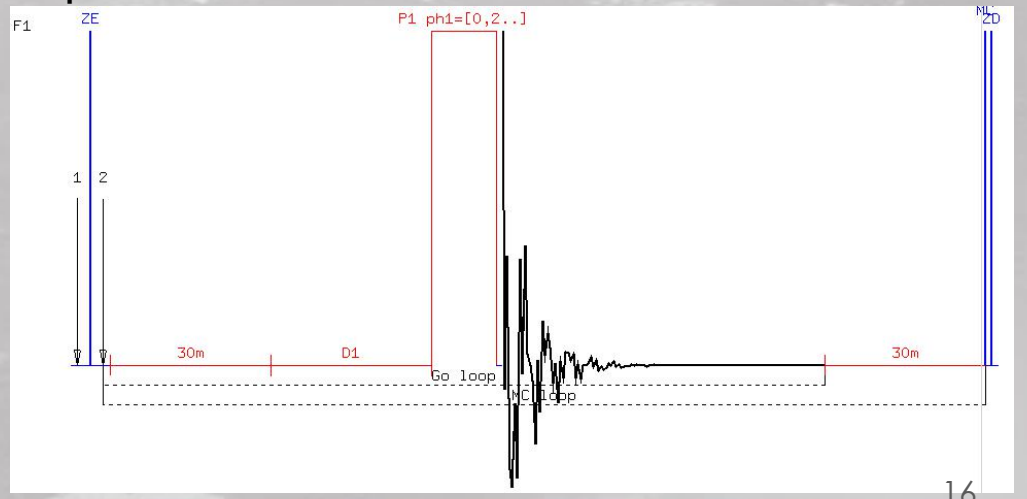


^{1}H的刻度实验

```
;zg
;avance-version (12/01/11)
;1D sequence
;
;$CLASS=HighRes
;$DIM=1D
;$TYPE=
;$SUBTYPE=
;$COMMENT=

#include <Avance.incl>

"acqt0=-p1*2/3.1416"
```

```
1 ze
2 30m
  d1      recycle delay
  p1 ph1     pulses
  go=2 ph31
  30m mc #0 to 2 F0(zd)     detection
exit


ph1=0 2 2 0 1 3 3 1
ph31=0 2 2 0 1 3 3 1
```

```
;pl1 : f1 channel - power level for pulse (default)
;p1 : f1 channel -  high power pulse
;d1 : relaxation delay; 1-5 * T1
;ns: 1 * n, total number of scans: NS * TD0

;$Id: zg,v 1.10.8.1 2012/01/31 17:56:41 ber
Exp $
```



^{1}H的刻度实验具体参数

Spectrum | ProcPars | AcquPars | Title | PulseProg | Peaks | Integrals | Sample | Structure | Plot | Fid

Probe: not defined

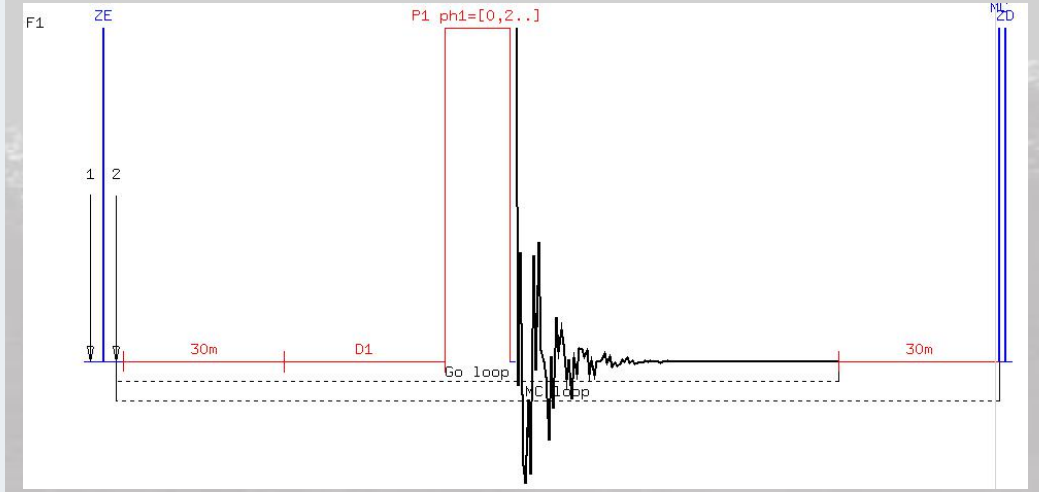
General
Channel f1

General

PULPROG	zg	... E	Pulse program for acquisition
TD	65536		Time domain size
SWH [Hz, ppm]	8012.82	20.0254	Sweep width
AQ [sec]	4.0894465		Acquisition time
RG	16		Receiver gain
DW [µsec]	62.400		Dwell time
DE [µsec]	10.00		Pre-scan-delay
D1 [sec]	1.00000000		Relaxation delay; 1-5 * T1
DS	0		Number of dummy scans
NS	1		1 * n, total number of scans: NS * TD0
TD0	1		Dimension of accumulation loop

Channel f1

SFO1 [MHz]	400.1318700		Frequency of ch. 1
O1 [Hz, ppm]	1869.97	4.673	Frequency of ch. 1
NUC1	1H Edi...		Nucleus for channel 1
P1 [µsec]	8.61		F1 channel - high power pulse
PLW1 [W, -dBW]	12.589	-11.00	F1 channel - power level for pulse (default)



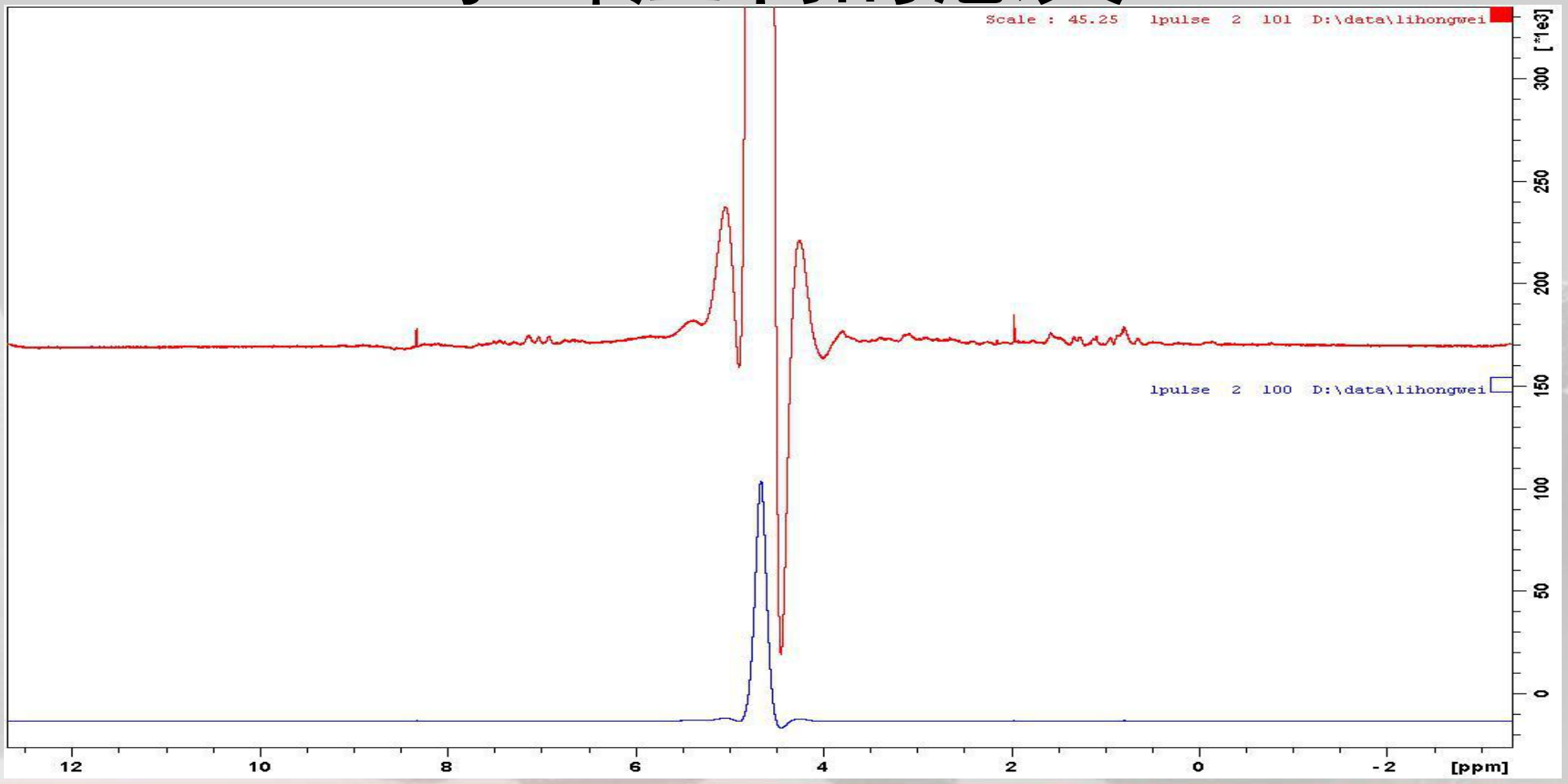
上机练习核磁实验基本流程和 ^{1}H脉冲刻度

水峰压制的^{1}H谱

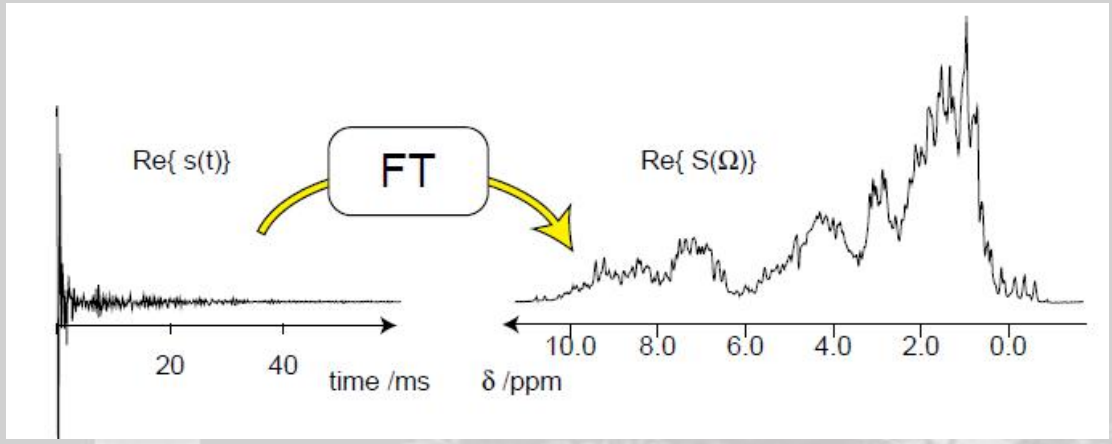
李红卫

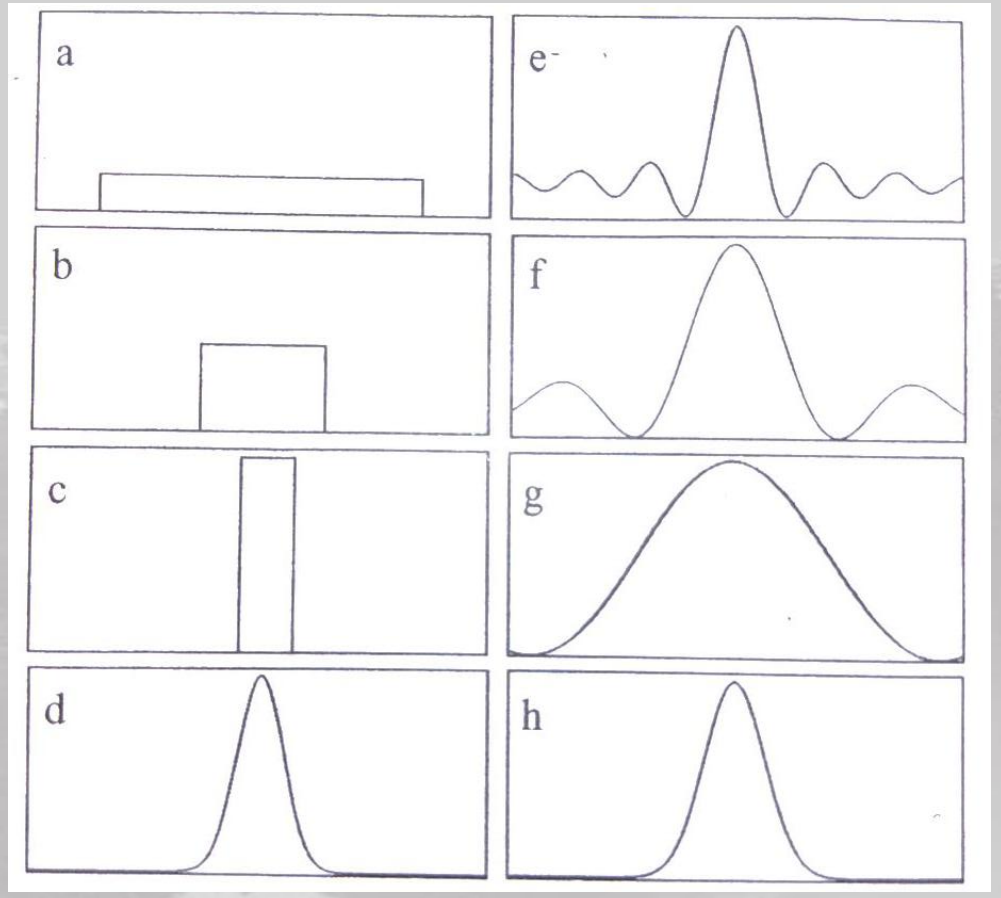
2020-11-01

水峰压制的意义


Scale : 45.25 1pulse 2 101 D:\data\lihongwei
1pulse 2 100 D:\data\lihongwei
300
250
200
150
100
50
0
[*1e3]
12
10
8
6
4
2
0
-2
[ppm]

不同脉冲及激发范围差异





脉冲功率和时间的不同导致其激发的化学位移范围不同

edprosol

File Edit View Help

Modified Observe and Saved Decouple Prosol Parameter Set for:

Probe: Z118687_0006 CP TCI 500S2 H-C/N-D-05 Z | Select ...

Solvent: generic

Observe Nucleus: 1H | Decouple Nucleus: 13C

Observe Comment: Default 1H obs 500

Decouple Comment: Default 13C dec 500

90 deg. Pulses | HR Square Pulses | HR Shape Pulses | Others

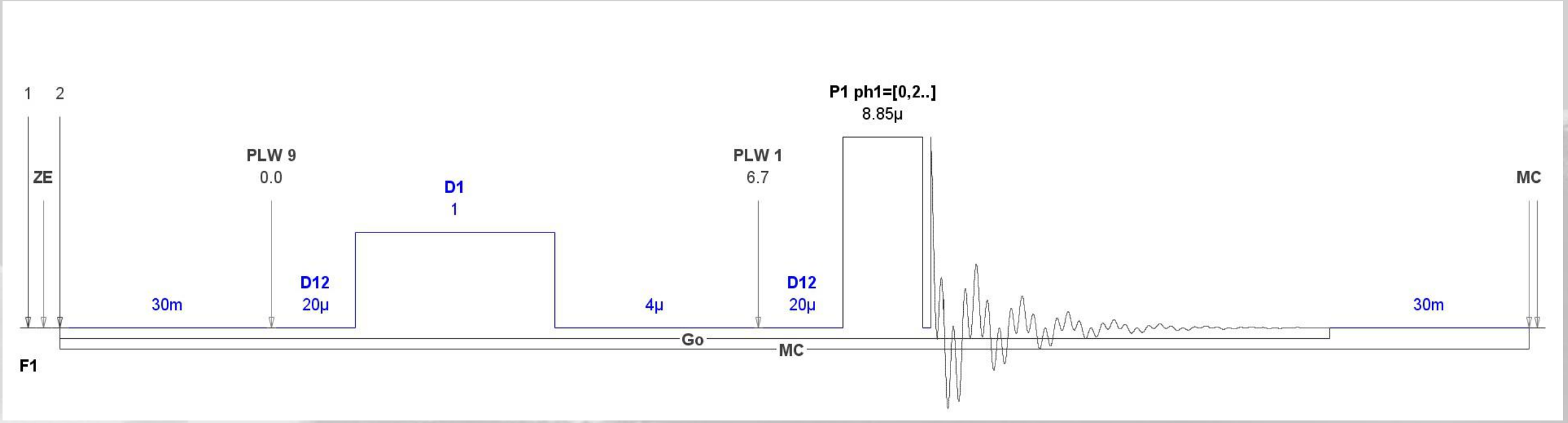
	Observe			Decouple			
Nucleus	Pulse Width[μs]	Att. Lvl.[dB]	Set	Pulse Width[μs]	Att. Lvl.[dB]	Set	Nucleus
1H	11.45	-8.26		8.00	-8.26		1H
2H	67.80	-16.23		67.80	-16.23		2H
13C	12.00	-19.68		12.00	-19.68		13C
15N	25.00	-21.52		25.00	-21.52		15N
Nucleus	Pulse Width[μs]	Att. Lvl.[dB]	Set	Pulse Width[μs]	Att. Lvl.[dB]	Set	Nucleus

Last Save | Print | Copy to Solvent | Copy to Probe | Save

Observe			#	Decouple		
	PuW[µs]	A[dB]			PuW[µs]	A[dB]
cpd	45.00	3.63	0	cpd	75.00	-3.71
TOCSY spinlock	25.00	-1.48	1	TOCSY spinlock	25.00	-13.31
ROESY spinlock (cw, RF fiel	110.00	11.39	2	ROESY spinlock	125.00	0.67
presat. (cw irradiation, RF fi	5000.00	44.54	3	presat. (cw irradiation, RF fi	250.00	6.69
			4	2nd cpd (power gated)	98.70	-1.38
			5	low power cpd	140.00	1.65
			6	bilev cpd (cw part)	35.00	-10.39
TOCSY/hetero T. (med. sele	52.00	4.88	7	TOCSY/hetero T. (med. sele	52.00	-6.95
TOCSY/hetero T. (high sele	78.00	8.40	8	TOCSY/hetero T. (high sele	78.00	-3.43
			9	TOCSY/hetero T. (very high	250.00	6.69
cleanex spinlock	52.00	4.88	10			
ROESY pulsed (90°)	108.00	11.23	11			
low power presat. (cw irrad.,	25000.00	58.52	12	low power presat. (cw irrad.,		
			13			
			14	homodecoupling	750.00	16.23
			15			
			16			
			17	low power cpd (2)	480.00	12.36
			18	180° (matched field for Calp	128.90	-5.08
			19			
			20			
			21			
			22			
			23			

Observe				#	Decouple			
	Filename	PuW[µs]	A[dB]			Filename	PuW[µs]	A[dB]
selective excitation	Gaus1_270.1000	80000.00	51.37	0	selective excitation	Q5.1000	40000.00	25.50
selective refocussing	Gaus1_180r.1000	80000.00	54.89	1	select. inversion/refocussing	Q3_surbop.1	40000.00	26.37
bandsel. excitation	Q5.1000	10000.00	25.29	2	bandsel. excitation	Q5.1000	3600.00	4.59
bandsel. inv./refoc.	Q3.1000	10000.00	28.15	3	bandsel. inv./refoc.	Q3_surbop.1	3792.00	5.91
off-resonance presat. (powe	Squa100.1000	100000.00	70.56	4	adiabatic inversion	Crp60,0.5,20.1	500.00	-13.11
90° flip back (H2O)	Squa100.1000	1000.00	30.56	5	adiabatic refocussing	Crp60comp.4	2000.00	-13.11
2nd 90° flip back (H2O)	Sinc1.1000	4000.00	38.01	6	Cali/CO 90°	Q5.1000	384.00	-14.85
90° WET	Sinc1.1000	20000.00	51.98	7	Cali/CO 90° timerev.	Q5tr.1000	384.00	-14.85
120° NH region	Pc9_4_120.1000	2880.00	19.19	8	Cali/CO 180°	Q3.1000	307.00	-13.94
180° NH region I	Rsnob.1000	960.00	10.78	9	Calpha sel. 90°	Q5.1000	1800.00	-1.43
90° NH region I	Pc9_4_90.1000	2640.00	20.93	10	Calpha sel. 90° timerev.	Q5tr.1000	1800.00	-1.43
90° NH region I timerev.	Pc9_4_90.1000	2640.00	20.93	11	Calpha sel. 180°	Q3.1000	1000.00	-3.68
180° NH region II	Reburp.1000	1680.00	7.09	12	adiabatic decoupling	Crp32,1.5,20.2	1500.00	-3.39
90° NH region II	Eburp2.1000	2040.00	12.47	13	adiab. decoupling (bilev par	Crp32,1.5,20.2	750.00	-9.41
90° NH region II timerev.	Eburp2tr.1000	2040.00	12.47	14	180° short broadband	Bip720,100,10.1	192.00	-13.66
180° broadband	Bip720,50,20.1	240.00	0.11	15	180° medium selectivity	Q3_surbop.1	888.00	-6.70
cleanex 90° (H2O)	Gaus1_90.1000	5000.00	36.83	16	180° high selectivity	Q3_surbop.1	2520.00	2.36
cleanex 180° (H2O)	Gaus1_180r.1000	7500.00	34.33	17	90° high selectivity	Q5.1000	4440.00	6.41
z-spoil (adiabatic)	Crp60,20,20.10	20000.00	14.74	18	90° high selectivity timerev.	Q5tr.1000	4440.00	6.41
180° H1' (na_)	Reburp.1000	3960.00	14.54	19	x-filter (adiabatic 180)	Crp60_xfilt.2	1895.00	-6.93
				20	Ca or CO decoupling	Q3_surbop.1	972.00	-5.92
180° H2O (selective)	Gaus1_180i.1000	120000.00	58.42	21	simult. Ca + CO selective	Q3Ca_CaCO.1000	922.00	-10.41
180° Halpha sel.	Reburp.1000	1920.00	8.25	22	Cbeta decoupling			
90° Hmethyl sel.	Pc9_4_90.1000	7200.00	29.65	23	na_: 90°	Q5.1000	1200.00	-4.96

presat压水（zgpr）



PULPROG	zgpr ... E		Pulse program for acquisition
TD	32768		Time domain size
SWH [Hz, ppm]	8012.82	16.0214	Sweep width
AQ [sec]	2.0447233		Acquisition time
RG	1		Receiver gain
DW [µsec]	62.400		Dwell time
DE [µsec]	10.00		Pre-scan-delay
D1 [sec]	1.000000000		Relaxation delay; 1-5 * T1
d12 [sec]	0.00002000		Delay for power switching [20 usec]
DS	0		Number of dummy scans
NS	1		1 * n, total number of scans: NS * TD0
TD0	1		Number of averages in 1D

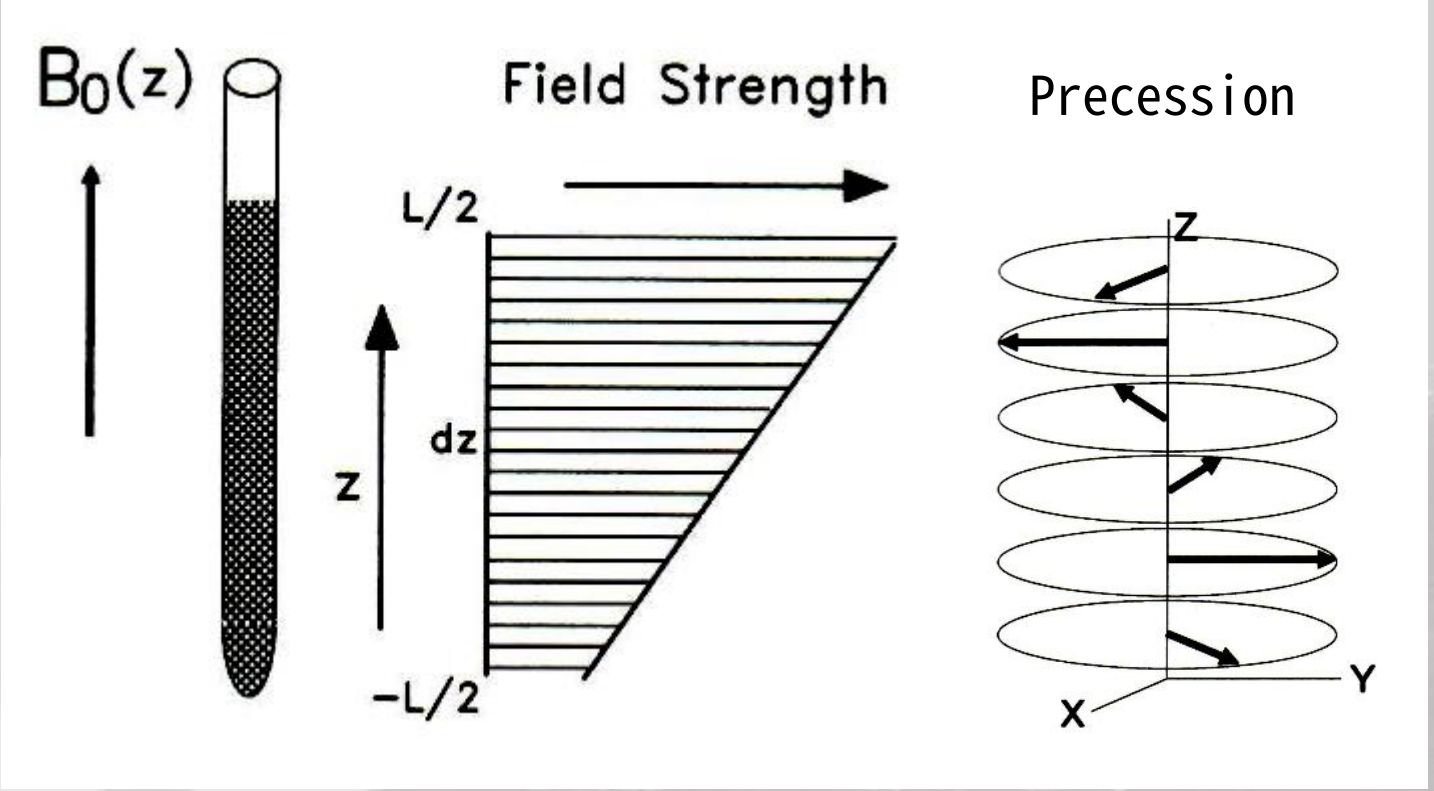
预饱和压水时间

Channel f1

SFO1 [MHz]	500.1323366		Frequency of ch. 1
O1 [Hz, ppm]	2336.61	4.672	Frequency of ch. 1
NUC1	1H Edit...		Nucleus for channel 1
P1 [µsec]	8.000		F1 channel - 90 degree high power pulse
PLW1 [W, dB]	6.7	8.26	F1 channel - power level for pulse (default)
PLW9 [W, dB]	1.7152e-005	47.66	F1 channel - power level for presaturation

预饱和压水功率

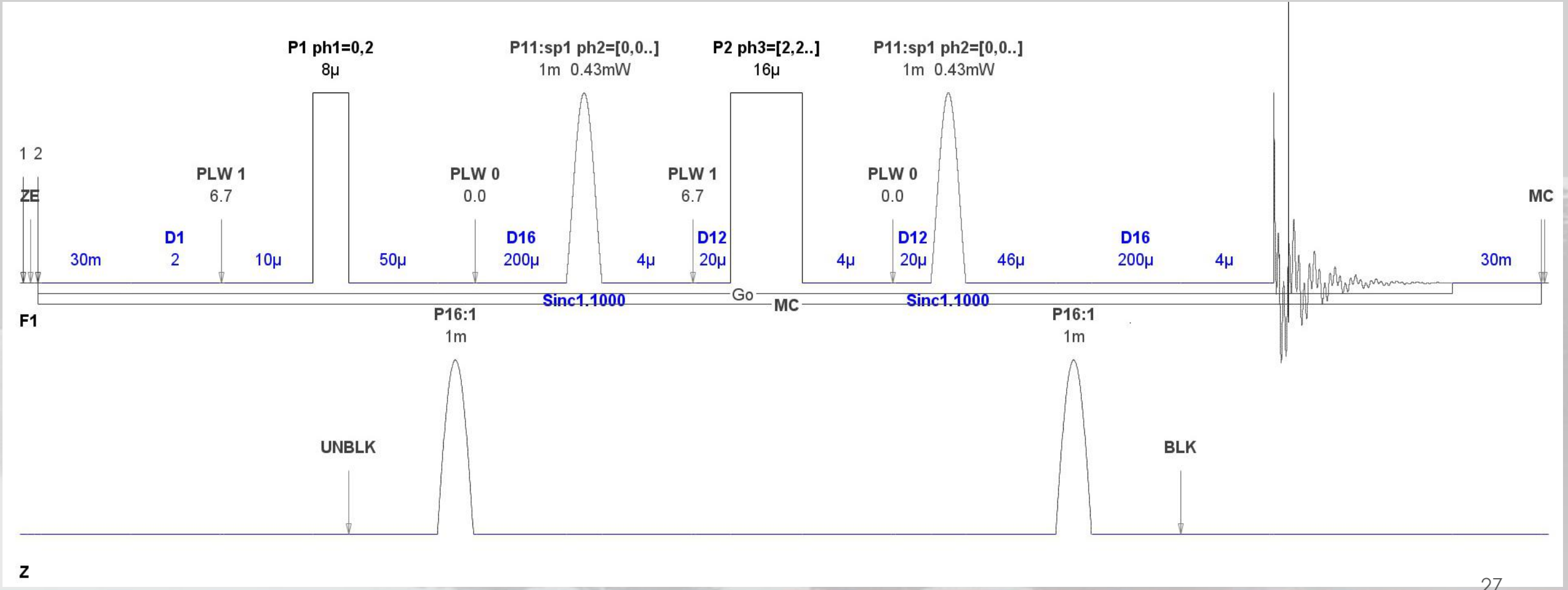
脉冲梯度场



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

消除不需要的信号

watergate压水（zggpwg）



PULPROG	zggpwg	... E	Pulse program for acquisition
TD	32768		
SWH [Hz, ppm]	8012.82	16.0214	
AQ [sec]	2.0447233		
RG	203		
DW [µsec]	62.400		
DE [µsec]	10.00		
D1 [sec]	2.000000000		
d12 [sec]	0.00002000		
D16 [sec]	0.000200000		
DS	4		
NS	8		
TD0	1		

Channel f1

SFO1 [MHz]	500.1323506		Frequency of ch. 1
O1 [Hz, ppm]	2350.61	4.700	Frequency of ch. 1
NUC1	1H Edit...		Nucleus for channel 1
P1 [µsec]	8.000		F1 channel - 90 degree high power pulse
p2 [µsec]	16.00		F1 channel - 180 degree high power pulse
P11 [µsec]	1000.000		F1 channel - 90 degree shaped pulse
PLW0 [W, dB]	0	1000.00	0W
PLW1 [W, dB]	6.7	-8.26	F1 channel - power level for pulse (default)
SPNAM 1	Sinc1.1000 ... E		File name for SP1
SPOAL1	0.500		Phase alignment of freq. offset in SP1
SPOFFS1 [Hz]	0		Offset frequency for SP1
SPW1 [W, -dBW]	0.0004288	33.68	F1 channel - shaped pulse 90 degree

水的选择性激发

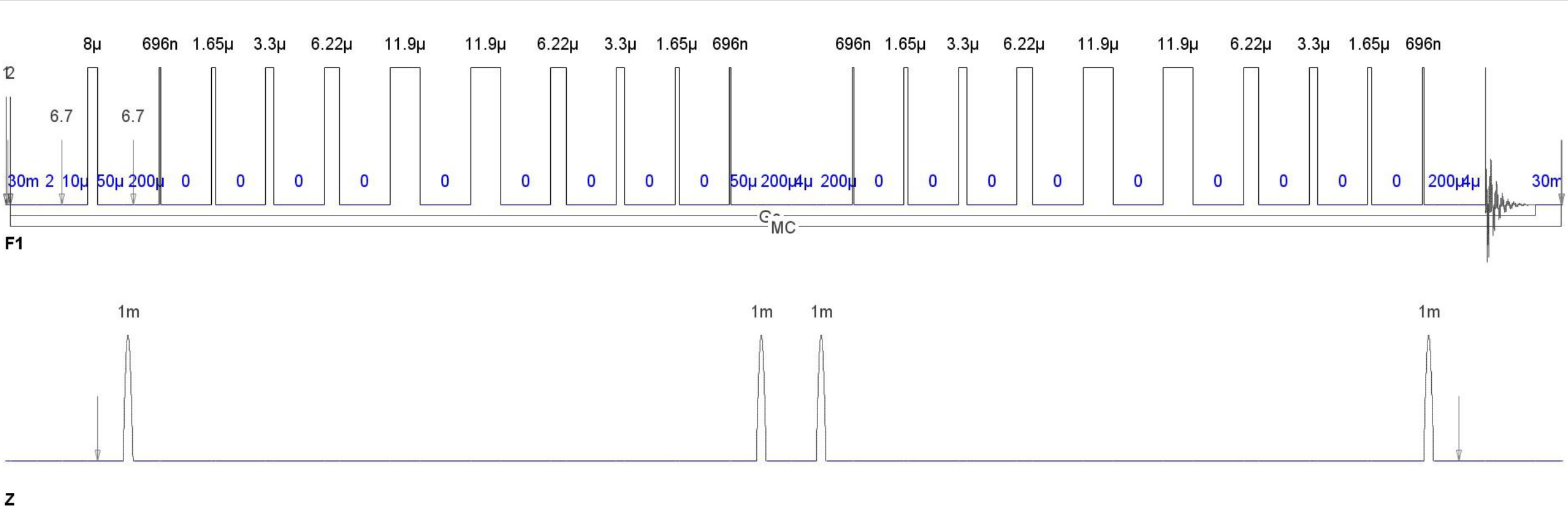
Gradient channel

GPNAM 1	SMSQ10.100 ... E		SMSQ10.100
GPZ1 [%]	20.00		20%
P16 [µsec]	1000.000		Homospoil/gradient pulse

压水梯度场

watergate

组合脉冲压水watergate w5 pulse



PULPROG	zggpw5 ... E		Pulse program for acquisition
TD	32768		Time domain size
SWH [Hz, ppm]	8012.82	16.0214	Sweep width
AQ [sec]	2.0447233		Acquisition time
RG	203		Receiver gain
DW [µsec]	62.400		Dwell time
DE [µsec]	10.00		Pre-scan-delay
D1 [sec]	2.000000000		
D16 [sec]	0.000200000		
D19 [sec]	0		
DS	4		
NS	8		
TD0	1		

组合脉冲时间间隔

Channel f1

SFO1 [MHz]	500.1323506		Frequency of ch. 1
O1 [Hz, ppm]	2350.61	4.700	Frequency of ch. 1
NUC1	1H Edit...		Nucleus for channel 1
P1 [µsec]	8.000		F1 channel - 90 degree high power pulse
P27 [µsec]	8.000		F1 channel - 90 degree pulse at pl18
PLW1 [W, dB]	6.7	-8.26	F1 channel - power level for pulse (default)
PLW18 [W, dB]	6.7	-8.26	F1 channel - power level for 3-9-19-pulse (watergate)

组合脉冲脉宽和功率

Gradient channel

GPNAM 1	SMSQ10.100 ... E	SMSQ10.100
GPZ1 [%]	34.00	34%
GPNAM 2	SMSQ10.100 ... E	SMSQ10.100
GPZ2 [%]	22.00	22%
P16 [µsec]	1000.000	Homospoil/gradient pulse

压水梯度场

watergate W5

上机练习压水^{1}H谱
zggpw5和zgpr

2D谱……

- J coupling
- T1 and T2
- INEPT
- NHSQC

上机练习^{1}H-^{15}N HSQC

3D三共振实验

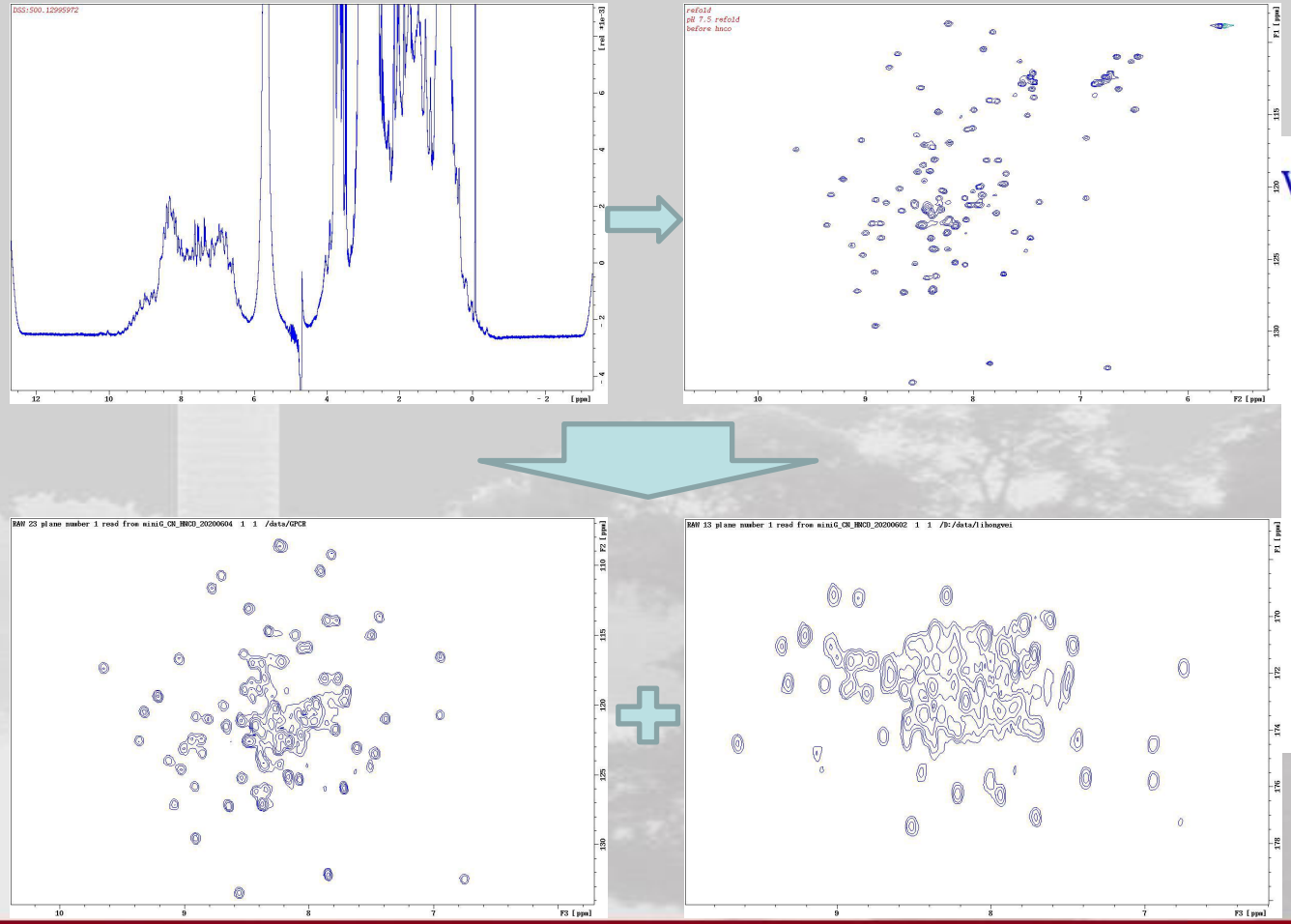
李红卫

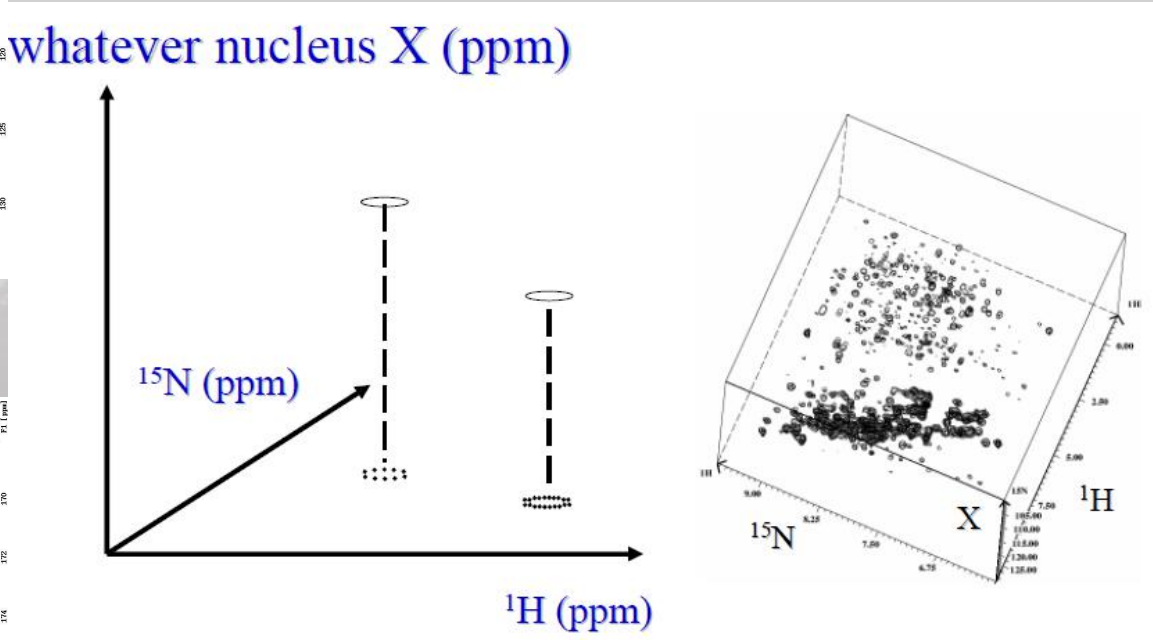
2020-11-15

脉冲构成基本模块

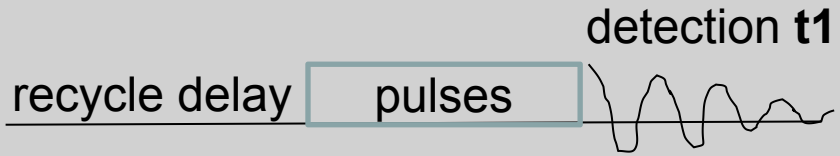
- Hard pulse
- Shape pulse
- Composed pulse
- Gradient
- Delay and coupling
- Phase cycle

1D-2D-3D实验





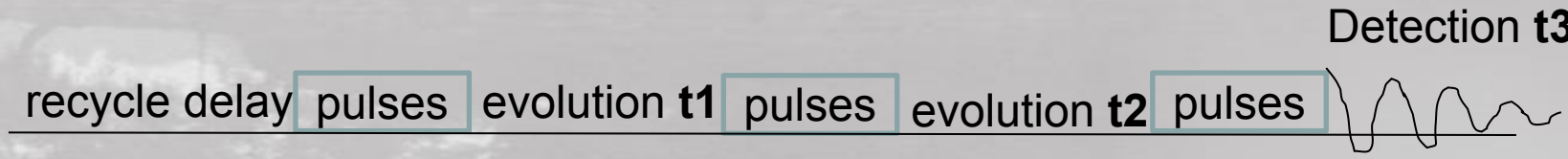
1D experiments:



2D experiments:

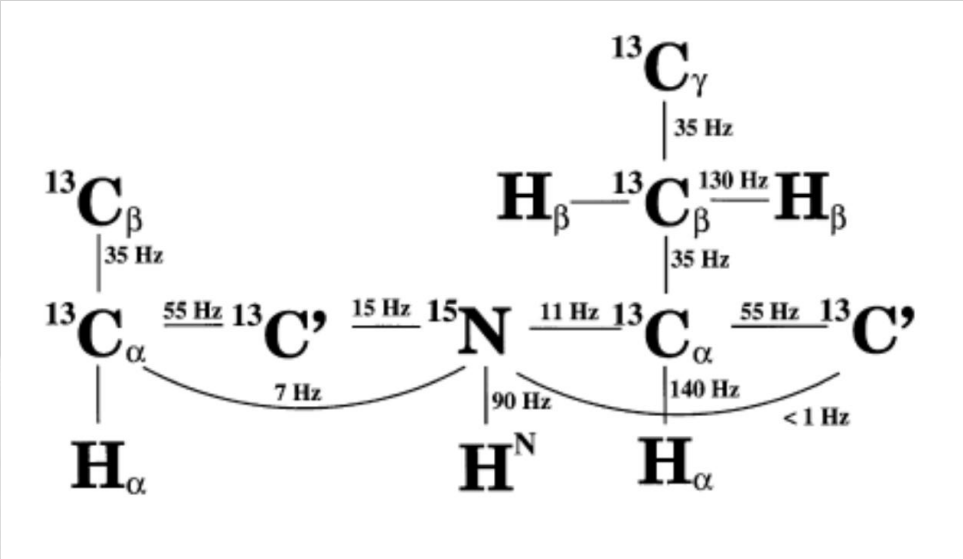
1D: ~min;
2D: ~hours;
3D: ~days

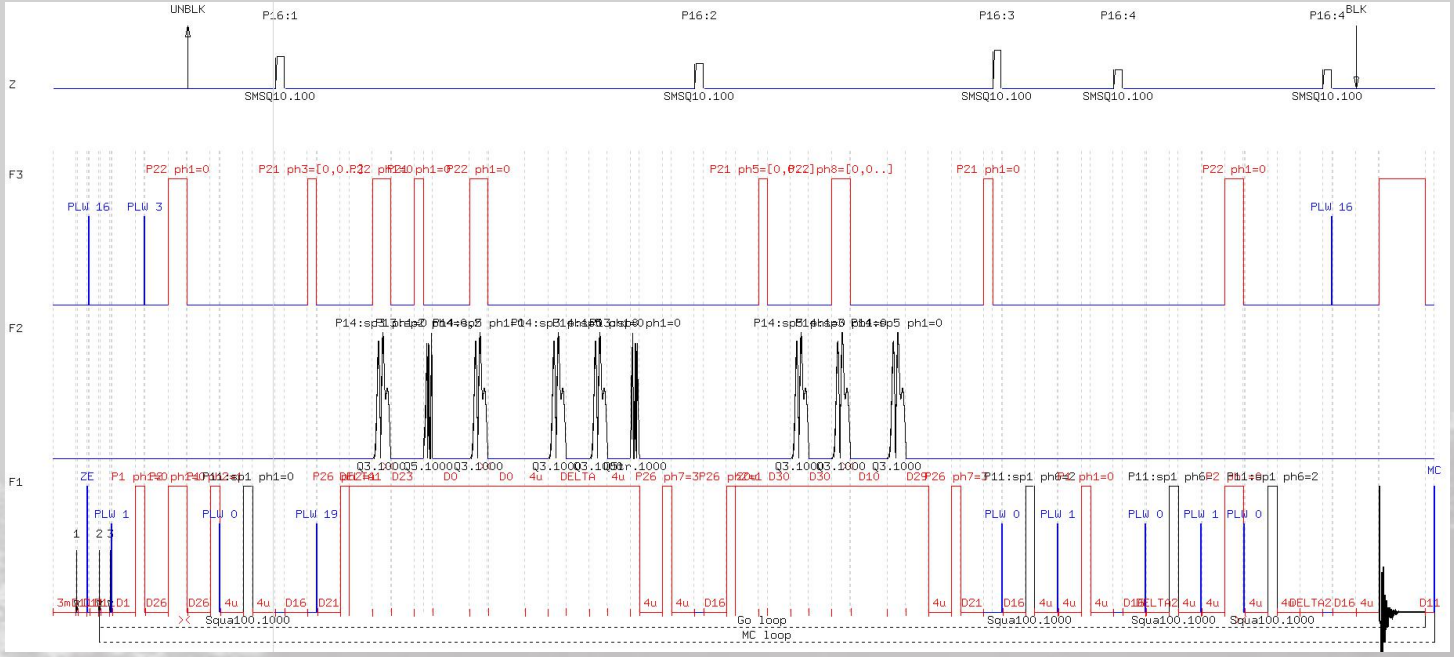
3D experiments:



Multidimention: Cycles=n1*n2*…..

J-coupling：





1、磁矩传递
2、化学位移标记
3、化学位移标记时去耦
4、去除水和其他不需要的信号

General

PULPROG	hncagpwg3d		d10 [sec]	0.00584650		incremented delay (F2 in 3D) = d23/2-p14/2	
TD	1024		d11 [sec]	0.03000000		Delay for disk I/O	[30 msec]
SWH [Hz, ppm]	6009.62	12.0161	D16 [sec]	0.000200000		Delay for homospoil/gradient recovery	
AQ [sec]	0.0851968		d21 [sec]	0.00550000		1/(2J(NH)	[5.5 msec]
RG	512		d23 [sec]	0.01200000		1/(4J(NCa)	[12 msec]
DW [µsec]	83.200		d26 [sec]	0.00230000		1/(4J'(NH)	[2.3 msec]
DE [µsec]	20.00		d29 [sec]	0.00029750		incremented delay (F2 in 3D) = d23/2-p14/2-p26-d21-4u	
d0 [sec]	0.00000300		d30 [sec]	0.00584650		decremented delay (F2 in 3D) = d23/2-p14/2	
D1 [sec]	1.100000024		DELTA [sec]	0.00000600		DELTA=d0*2+larger(p14,p22)-p14	
			DELTA1 [sec]	0.00645500		DELTA1=d23-d21-p26	
			DELTA2 [sec]	0.00008800		DELTA2=d26-p16-d16-p11-12u	
			DS	32		>= 16	
			in0 [sec]	0.00012420		1/(2 * SW(Ca)) = DW(Ca)	
			in10 [sec]	0.00018970		1/(4 * SW(N)) = (1/2) DW(N)	
			in29 [sec]	0.00018970		= in10	
			in30 [sec]	0.00018970		= in10	
			INF1 [µsec]	248.40		1/SW(Ca) = 2 * DW(Ca)	
			INF2 [µsec]	758.80		1/SW(N) = 2 * DW(N)	
			NS	32		8 * n	
			TDav	0		Number of averages in nD	

General Parameter

Channel f1

SFO1 [MHz]	500.1323506		Frequency of ch. 1
O1 [Hz, ppm]	2350.61	4.700	Frequency of ch. 1
NUC1	1H Edit...		Nucleus for channel 1
CPDPRG 1	waltz65 ... E		File name for cpd1
P1 [µsec]	11.700		F1 channel - 90 degree high power pulse
p2 [µsec]	23.40		F1 channel - 180 degree high power pulse
P11 [µsec]	1000.000		F1 channel - 90 degree shaped pulse [1 msec]
P26 [µsec]	45.000		F1 channel - 90 degree pulse at pl19
PCPD1 [µsec]	45.00		F1 channel - 90 degree pulse for decoupling sequence
PLW0 [W, dB]	0	1000.00	0W
PLW1 [W, dB]	6.2	-7.92	F1 channel - power level for pulse (default)
PLW19 [W, dB]	0.4	3.98	F1 channel - power level for CPD/BB decoupling
SPNAM 1	Squa100.1000 ... E		File name for SP1
SPOAL1	0.500		Phase alignment of freq. offset in SP1
SPOFFS1 [Hz]	0		Offset frequency for SP1
SPW1 [W, -dBW]	0.00079433	31.00	F1 channel - shaped pulse 90 degree (H2O on resonance)

1H Parameter：
45us ~ plw9

Channel f2

SFO2 [MHz]	125.7645794		Frequency of ch. 2
O2 [Hz, ppm]	6790.92	54.000	Frequency of ch. 2
NUC2	13C Edit...		Nucleus for channel 2
CNST21	174.0000000		CO chemical shift (offset, in ppm)
P13 [µsec]	384.000		F2 channel - 90 degree shaped pulse
P14 [µsec]	307.000		F2 channel - 180 degree shaped pulse
PLW2 [W, dB]	0	1000.00	Power PLW2
SPNAM 2	Q5.1000 . . E		File name for SP2
SPOAL2	1.000		Phase alignment of freq. offset in SP2
spoffs2 [Hz]	0		spoffs2=0
SPW2 [W, -dBW]	26.95	-14.31	F2 channel - shaped pulse 90 degree (Ca on resonance)
SPNAM 3	Q3.1000 . . E		File name for SP3
SPOAL3	0.500		Phase alignment of freq. offset in SP3
spoffs3 [Hz]	0		spoffs3=0
SPW3 [W, -dBW]	21.84	-13.39	F2 channel - shaped pulse 180 degree (Ca on resonance)
SPNAM 5	Q3.1000 . . E		File name for SP5
SPOAL5	0.500		Phase alignment of freq. offset in SP5
spoffs5 [Hz]	15090.93		spoffs5=bf2*(cnst21/1000000)-o2
SPW5 [W, -dBW]	21.84	-13.39	f2 channel - shaped pulse 180 degree (C=O off resonance)
SPNAM 8	Q5tr.1000 . . E		File name for SP8
SPOAL8	0		Phase alignment of freq. offset in SP8
spoffs8 [Hz]	0		spoffs8=0
SPW8 [W, -dBW]	26.95	-14.31	F2 channel - shaped pulse 90 degree (Ca on resonance)

13C Parameter

```
(center (p14:sp3 ph1):f2 (p22 ph1):f3 )
d23
(p21 ph1):f3

(p13:sp2 ph4):f2
d0
(center (p14:sp5 ph1):f2 (p22 ph8):f3 )
d0
4u
(p14:sp3 ph1):f2
DELTA
(p14:sp5 ph1):f2
4u
(p13:sp8 ph1):f2

4u do:f1
(p26 ph7):f1
4u
p16:gp2
d16
(p26 ph2):f1
20u cpds1:f1 ph1
```

Channel f3

SFO3 [MHz]	50.6838141		Frequency of ch. 3
O3 [Hz, ppm]	6081.33	120.000	Frequency of ch. 3
NUC3	15N Edit...		Nucleus for channel 3
CPDPRG 3	garp ... E		File name for cpd3
P21 [µsec]	25.000		F3 channel - 90 degree high power pulse
p22 [µsec]	50.00		F3 channel - 180 degree high power pulse
PCPD3 [µsec]	190.00		F3 channel - 90 degree pulse for decoupling sequence
PLW3 [W, dB]	135	-21.30	F3 channel - power level for pulse (default)
PLW16 [W, dB]	2.34	-3.69	F3 channel - power level for CPD/BB decoupling

Gradient channel

GPNAM 1	SMSQ10.100 ... E		SMSQ10.100
GPZ1 [%]	50.00		50%
GPNAM 2	SMSQ10.100 ... E		SMSQ10.100
GPZ2 [%]	40.00		40%
GPNAM 3	SMSQ10.100 ... E		SMSQ10.100
GPZ3 [%]	60.00		60%
GPNAM 4	SMSQ10.100 ... E		SMSQ10.100
GPZ4 [%]	30.00		30%
P16 [µsec]	1000.000		Homospoil/gradient pulse [1 msec]

15N and Gradient Parameter

Experiment

PULPROG	hncagpwg3d ... E			Current pulse program
AQ_mod	DQD			Acquisition mode
FnTYPE	traditional(planes)			nD acquisition mode for 3D etc.
FnMODE		States-TPPI	States-TPPI	Acquisition mode for 2D, 3D etc.
ProjAngle [degree]		0		Angle for projection-spectroscopy
TD	1024	52	64	Size of fid
DS	32			Number of dummy scans
NS	32			Number of scans
TD0	1			Loop count for 'td0'
TDav	0			Average loop counter for nD experiments

Width

SW [ppm]	12.0161	26.0000	32.0000	Spectral width
SWH [Hz]	6009.615	1317.779	4024.467	Spectral width
IN_F [µsec]		758.85	248.48	Increment for delay
AQ [sec]	0.0851968	0.0197302	0.0079514	Acquisition time
FIDRES [Hz]	11.737530	50.683815	125.764580	Fid resolution
FW [Hz]	125000.000			Filter width

Experiment Parameter

上机练习HNCA

谢谢大家！