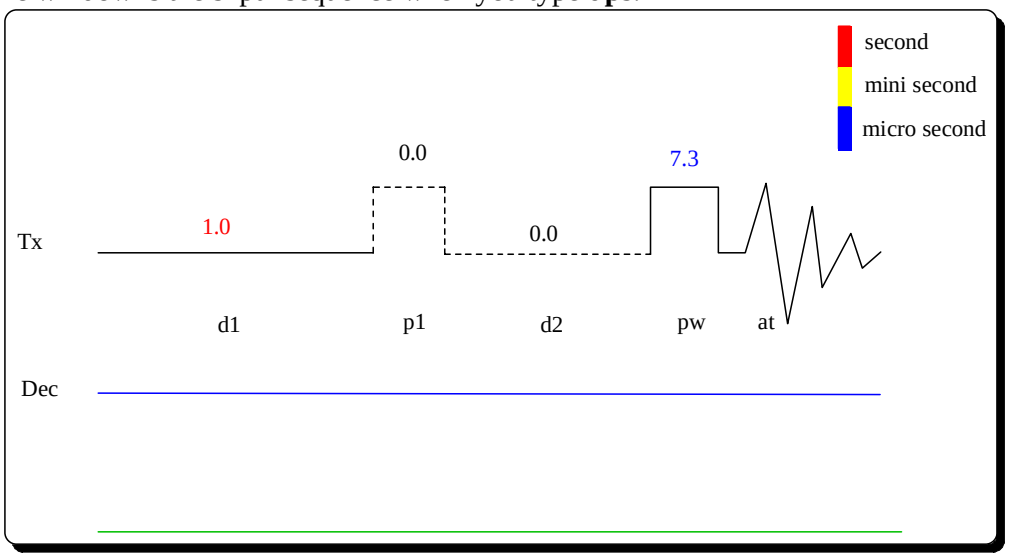
1. What is Probe?

The probe transmits RF to the sample and detects minute voltages in return. RF = radio frequency. The probe is kind expensive. So be careful to setup the parameters. Tpwr, dpwr….

2. The s2pul sequence

The window is the s2pul sequence when you type **dps**.



3. So how can you start your H1 NMR experiment?

1. log in and open the NMR window by clicking the NMR icon at the bottom.
2. click **Main Manu**, **set up**, **H1**, **solvent D2O** buttons and type **su** if necessary.
3. click **acqi** button at the upper right corner., lock the magnetic field. By changing the lock level.
4. shim the magnetic field using gradient shimming as follows: type **gshmstr**, then click **Gradient shim on z**, wait until shim is converged, type **gshmend**.(In this step, nt is set to 8, you can type **nt=4** to shorten your time). If you want to run the expt with spin off, click **acqi**, and then click **lock**, then click **off** for spin.
5. type **dps** to display the pulse sequence which is shown above. This is the default pulse for most of the proton NMR.

6. You type **dg** to view the parameters.

The following is a table of parameters when you type **dg**.

acquisition		sample		processing		flags	
sfrq	399.73	date	mar 8, 2004	lb	not used	il	n
tn	h1	solvent	D_2O	sb	not used	in	n
at	3.744	file	exp	gf	not used	dp	y
np	44932	decoupling		awc	not used	hs	nn
sw	6000	dn	h1	lsfid	not used	special	
fb	3000	dof	0	phfid	not used	temp	not used
bs	16	dm	nnn	wtfile			
ss	0	dmm	c	proc	ft		
tpwr	60	dmf	11148	fn	not used		
pw	7.3	dpwr	42	math	f		
p1	0						
d1	1.000			werr			
d2	0			wexp			
tof	0			wbs			
nt	32			wnt			
ct	0						

sfrq: resonance frequency of the machine. 400 mHz machine, sfrq=400.

tn: transmitter nucleus, tn=H1; tn=C13; or tn=P31….

at: acquisition time(in seconds), at=3.7, 0.8.
(at too small can cause wiggles around the peak). to change **at**, you need to do the following things:(type **dg**, type **nt=1**, type **ga**, type **aph**, type **df** to view fid. click or type **dscale** to view the **at** at which you got the spectrum. watch the decay of the fid to find the ideal **at**).

np: number of data points. np=2*at*sw

sw: spectrum width(Hz). in 400 mHz machine, sw=6000.
the ppm(parts per million of the spectrum is 6000/400=15 ppm.
you can move **sw** by setting the two cursors on both sides of the spectrum and type **movesw**. then type **nt=32**(or whatever you want and then type **ga** to get the ideal spectrum.

fb: filter bandwidth(Hz). when you set sw=6000, the computer uses the data about 0.6*SW to remove the 5% of the field at both ends,

bs: block size. the computer saves the data in blocks. so if you set **bs=32**, and you run a spectrum with **nt=64**. you want to take a look at your spectrum when you see that there are already 16 ct, you can't! type **wft** helps nothings. but if **bs=4**, then you can.

ss: steady state .

pw: pulse width, (micro seconds). indicates the energy to force the magnet tip to 90 degree to z axis. the time(pw) is related to the degree the magnet is bent to x-axis. if it is =pw90, then the tip is 90 degree.

tpwr: transmitter power(db). (the value is between 0~63 db)

p1: first pulse delay(sec).

d1: (first delay , after p1(-Z), the magnet has to take some time to back to +Z(equiblirium)(there are –Z and +Z).

d2: second delay (sec). after the pw, the time for the magnet to go back to Z.

tof: transmitter offset(Hz). the center of the spectrum. for h1 spectrum, tof=0 indicates the center position is 5.5 ppm.; so, the very right position is 5.5-7.5=-2 ppm. and the very left is 5.5+7.5=13 ppm.

if you want to see a peak at –3 ppm, you need to move tof to the right for 1 ppm at least. tof=-400 for the 400 mHz machine.

nt: number of transients. This is the data between 1 to 10^9.

ct: completed transients.

dn: decoupler nuclei.

dof: decoupler offset. This is the frequency of a specific peak. You place the cursor at this peak so that the peak can be decoupled. Then type SD(=set decoupler). The computer will automatically find the frequency of the peak.

dm: decoupler mode. “n”, ‘y”’ n means decoupler mode close.

dmm: decoupler modulation mode, “c” means continuous wave modulation.

dmf: decoupler modulation frequency(Hz).

dpwr: decoupler power(dB). For 200, 300 and 400 MHz systems, the maximum is set to 49.Too high a **dpwr** might cause probe damage.

lb: line broadwidth(Hz). When you type wft, the machine will give a value. You can also type a specific data.
Large **lb** will increase sensitivity and decrease the resolution.

sb: sine bell constant. If you type wti, you open the window function.
If you place the top of sin function at the beginning of FID, you would enhance the sensitivity.
If you place the top of sine bell at the end of FID, you would enhance the resolution.

gf: Gaussian Function. By changing this you can see the change of your spectrum.

fn: fourier number. The value is a data of 2^n which is somewhere close to **np**.
If fn > np, the computer will put in zeros. This is called zero filling.

4. What is going on with the 90 pulse?

Go to my homepage to view the 90 pulse
http://www.chem.uky.edu/research/miller/cungen_homepage.htm