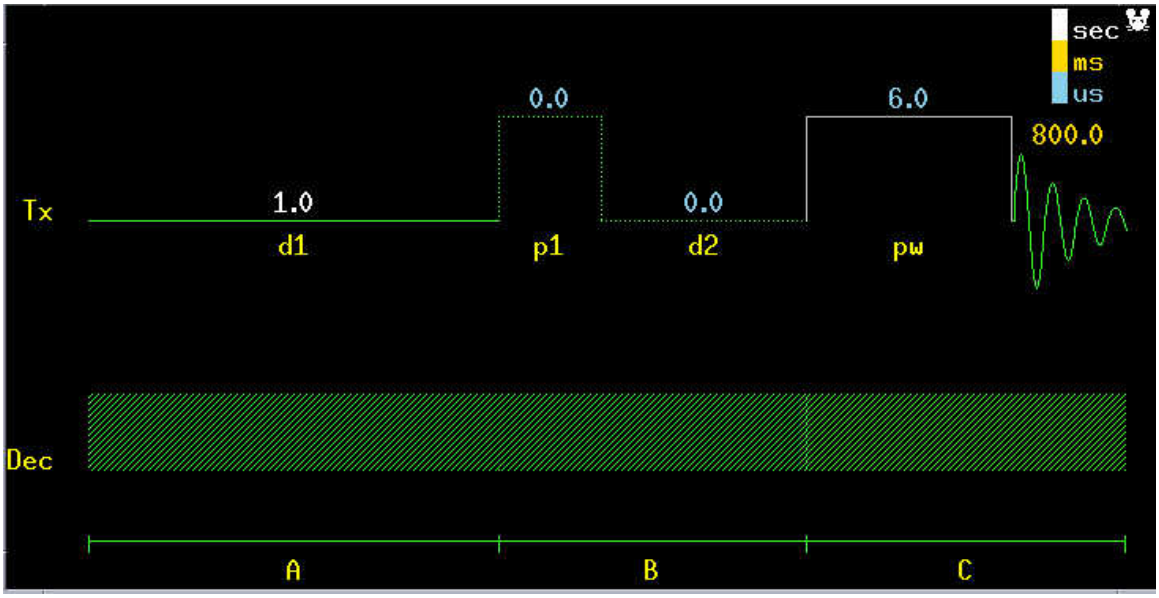
DEPT experiment

Distortionless Enhancement by Polarization Transfer, DEPT is the most widely used experiment in C-13 spectroscopy.

1. Basic C-13 NMR

To set up a DEPT experiment, first set up a carbon experiment.
MAIN MANU→ SET UP → C13, CDCL3
dps ↵ you will see the following sequence.



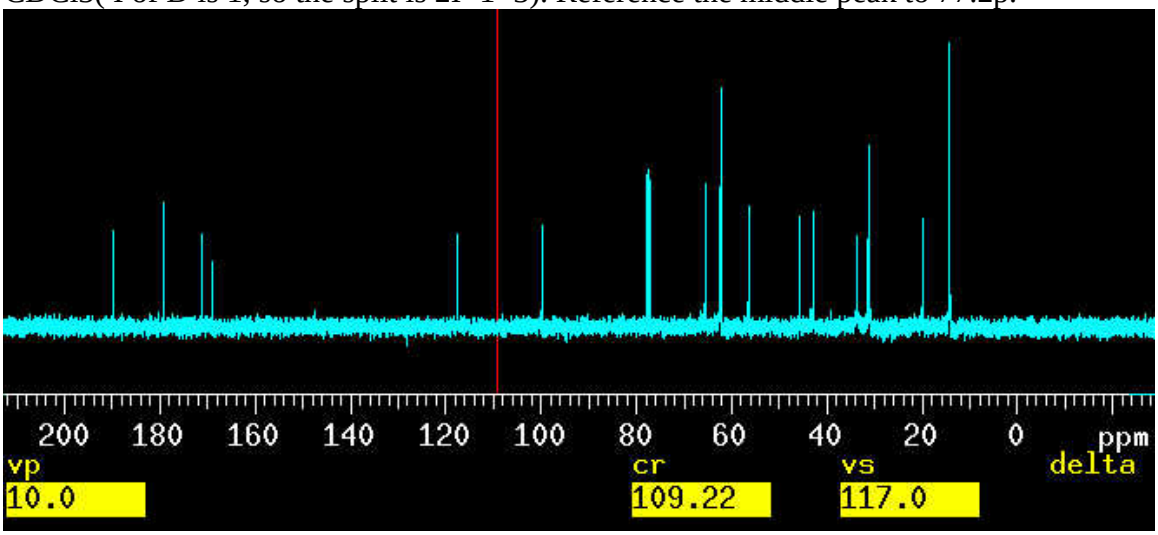
dg ↵ you will see the following parameters.

ACQUISITION		SAMPLE		PROCESSING		FLAGS	
sfrq	100.521	date	May 20 2004	lb	1.00	il	n
tn	C13	solvent	CDCl3	sb	not used	in	n
at	0.800	file	exp	gf	not used	dp	y
np	40000	DECOUPLING		awc	not used	hs	nn
sw	25000.0	dn	H1	lsfid	not used	SPECIAL	
fb	14000	dof	0	phfid	not used	temp	not used
bs	16	dm	yyy	wtfile			
ss	0	dmm	w	proc	ft		
tpwr	57	dmf	11148	fn	not used		
pw	6.0	dpwr	42	math	f		
p1	0						
d1	1.000			werr			
d2	0			wexp			
tof	0			wbs			
nt	1024			wnt			
ct	15						

dm=yyy indicates that decoupling is on in all three sections, ***A***, ***B***, and ***C*** as shown in the sequence.

Now type **ga** ↵

You can view your spectrum when 16 scans are done because ***bs=16***.
wft ↵ to see your C-13 spectrum.
aph ↵
use the middle mouse button to increase/decrease the peaks.
dscale ↵ to view the scales and you should see that at ~77 ppm, the 3-peak signal is CDCl3(I of D is 1, so the split is 2I+1=3). Reference the middle peak to 77.2p.

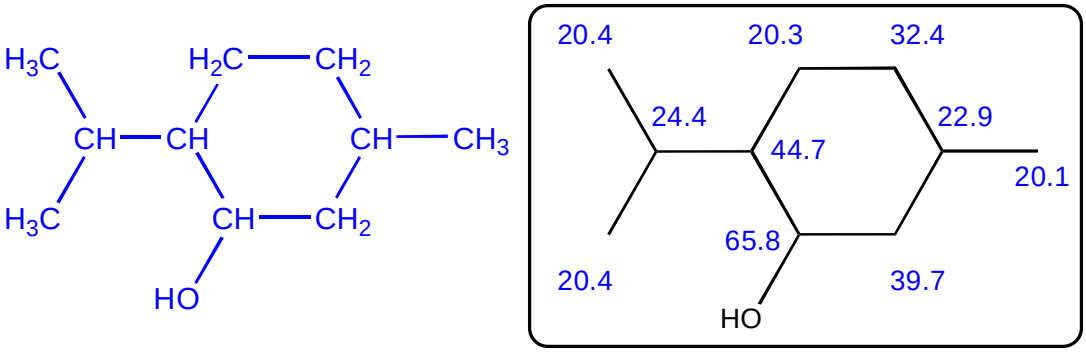


2. calibrate the pw90 for C-13 spectrum

This is similar to H1-NMR. The pw in the above text window is a default number which is set up by the manager. This number is normally somewhere between pw45 and pw60.

3. DEPT C-13 NMR

When you have a nice basic C-13 NMR spectrum, your parameters will be automatically applied to the DEPT experiment if you just calibrated the pw90 for C-13. Now let us use a concentrated sample, menthol in C_6D_6.



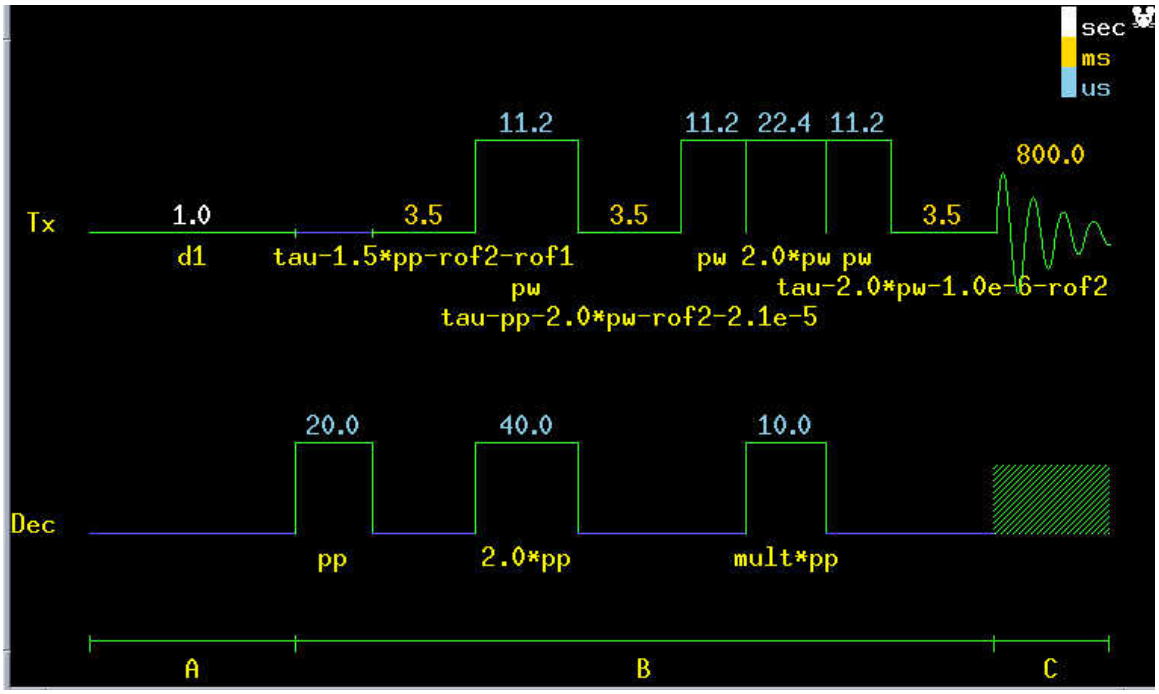
In this manual, concentrated menthol in C6D6 is used for DEPT experiment.

DEPT ↵

ACQUISITION		TRANSMITTER		DEPT		PROCESSING	
seqfil	DEPT	tn	C13	j1xh	140.0	lb	1.00
sw	25000.0	sfrq	100.521	mult	arrayed	sb	not used
at	0.800	tof	0	SPECIAL		gf	not used
np	40000	tpwr	57	temp	not used	awc	not used
fb	14000	pw	11.200	spin	not used	lsfid	not used
bs	16	DECOUPLER		gain	54	fn	not used
ss	-4	dn	H1	hst	0.008	FLAGS	
d1	1.000	dof	0	pw90	11.200	il	n
nt	8	dm	nny	alfa	20.000	in	n
ct	8	dmm	ccw			dp	y
SAMPLE		pplvl	56			hs	n
date	May 27 2004	pp	20.000				
solvent	Benzene	dpwr	42				
sample	undefined	dmf	11148				

In the DEPT, **pw** is set to **pw90,** which you just calibrated.

dps ↵ to view the sequence



From the text window, you see that ***j1xh=140***, here ***x*** is Carbon. This is a default number. **mult** means multiplicity, indicating the pulse width.

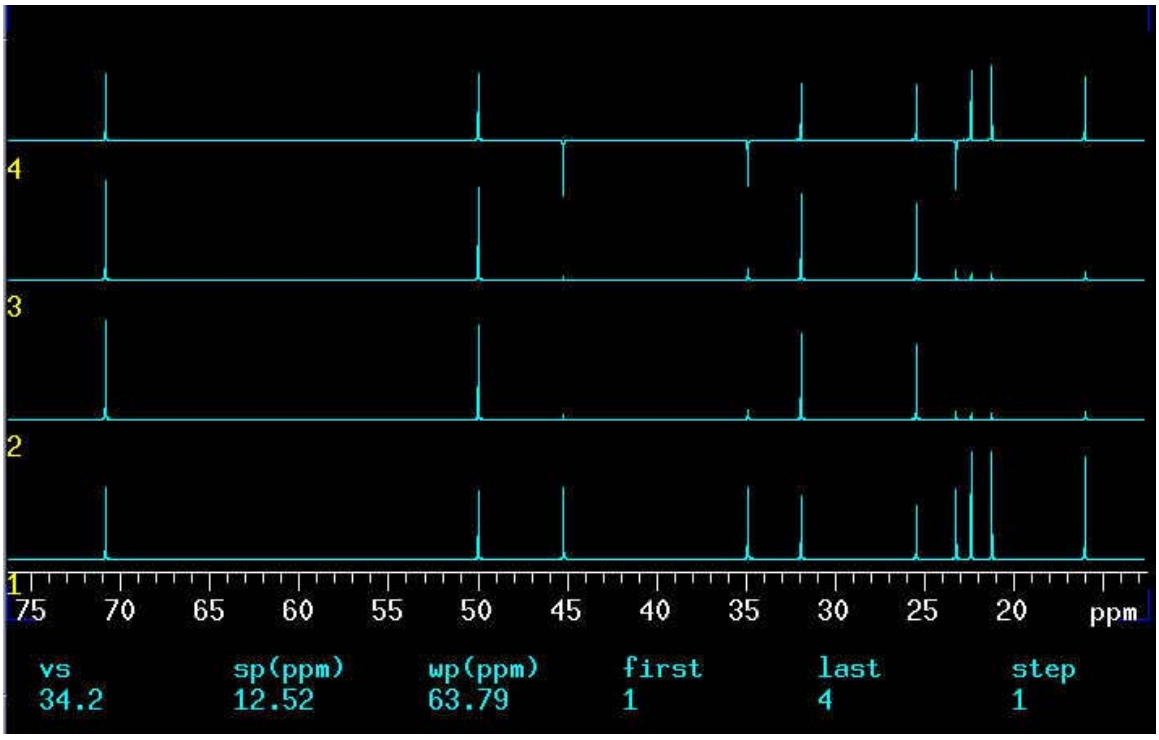
You also need to calibrate the ***pp,*** which is the same as ***pw*** in Proton NMR. Here pp is set to pw60. **pp** can be calibrated using **d2pul** sequence, which means you have to spend more time on doing other job. So just set pp=pw60. You can vary pp somewhere around pw60. You can also array **pp** by setting **mult=0.5**.

In DEPT, ***mult*pp = θ pulse***
Mult is arrayed so as to have a series pulses. ***mult=0.5, 1.0, 1.0, 1.5.*** This can be seen by typing **da**↵.
mult=0.5 45° pulse, all C atoms, up;
mult=1.0, 90° pulse, CH carbons, up;
mult=1.5, 135° pulse, CH2 carbons, down; others, up.

nt=8↵ because this sample is concentrated. You should set an nt based on your sample.

ga ↵.
When the experiment is done, type **ds(1) aph**↵

Click th and adjust the level to select all the C-13 peaks.
dssa dssl↵.



It is easy to analyze the data.
adept ↵

The following is the text window which tells you how many CH3, CH2 and CH groups in the molecule.

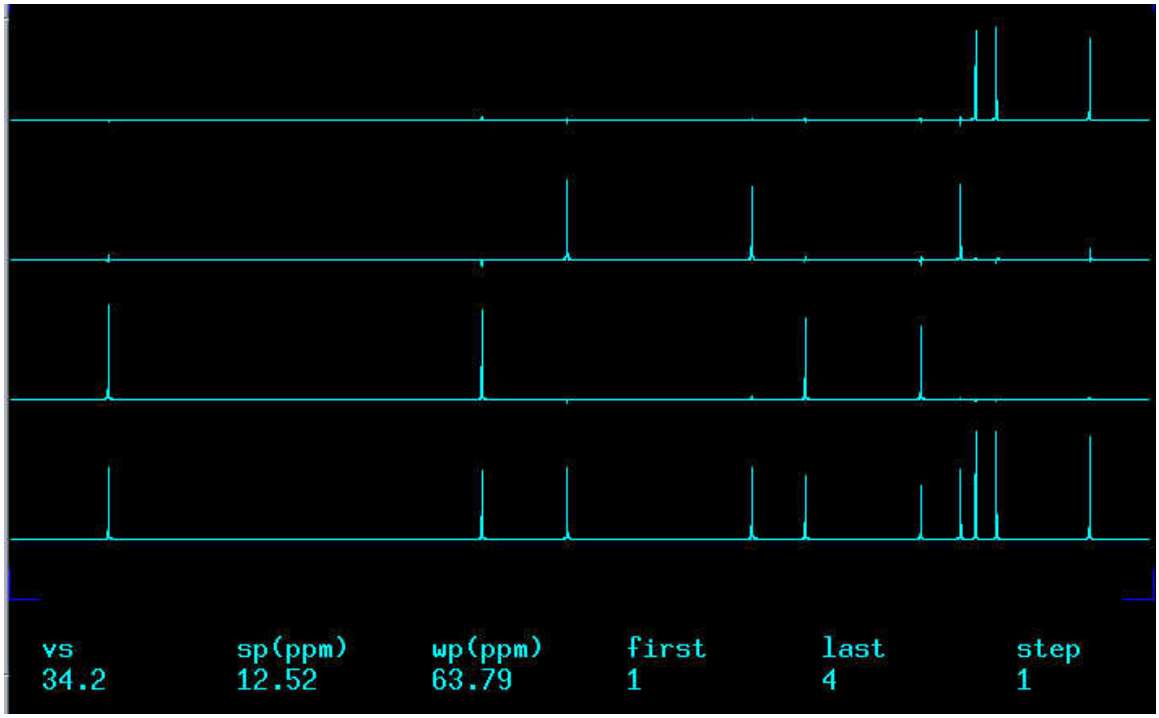
```
sample   undefined  dmf          11148
ADEPT SPECTRUM ANALYSIS

index        frequency       ppm        intensity
   1 D        7118.8        70.819        60.651
   2 D        5019.9        49.939        57.236
   3 T        4540.0        45.165        51.429
   4 T        3502.4        34.842        47.048
   5 D        3201.8        31.852        52.658
   6 D        2551.0        25.378        46.861
   7 T        2328.2        23.161        48.053
   8 Q        2243.5        22.319        57.771
   9 Q        2126.8        21.157        59.769
  10 Q        1602.6        15.943        52.600

Number of protonated carbons: 10

CH :    4
CH2:    3
CH3:    3
```

dssa ↵ This time you see the spectra after analysis.



Good luck! If you need further help, let me know. Cungen Zhang at UK