# C8953
# NMR structural analysis - seminar
## Vector model & edited $^{13}C$ NMR spectra

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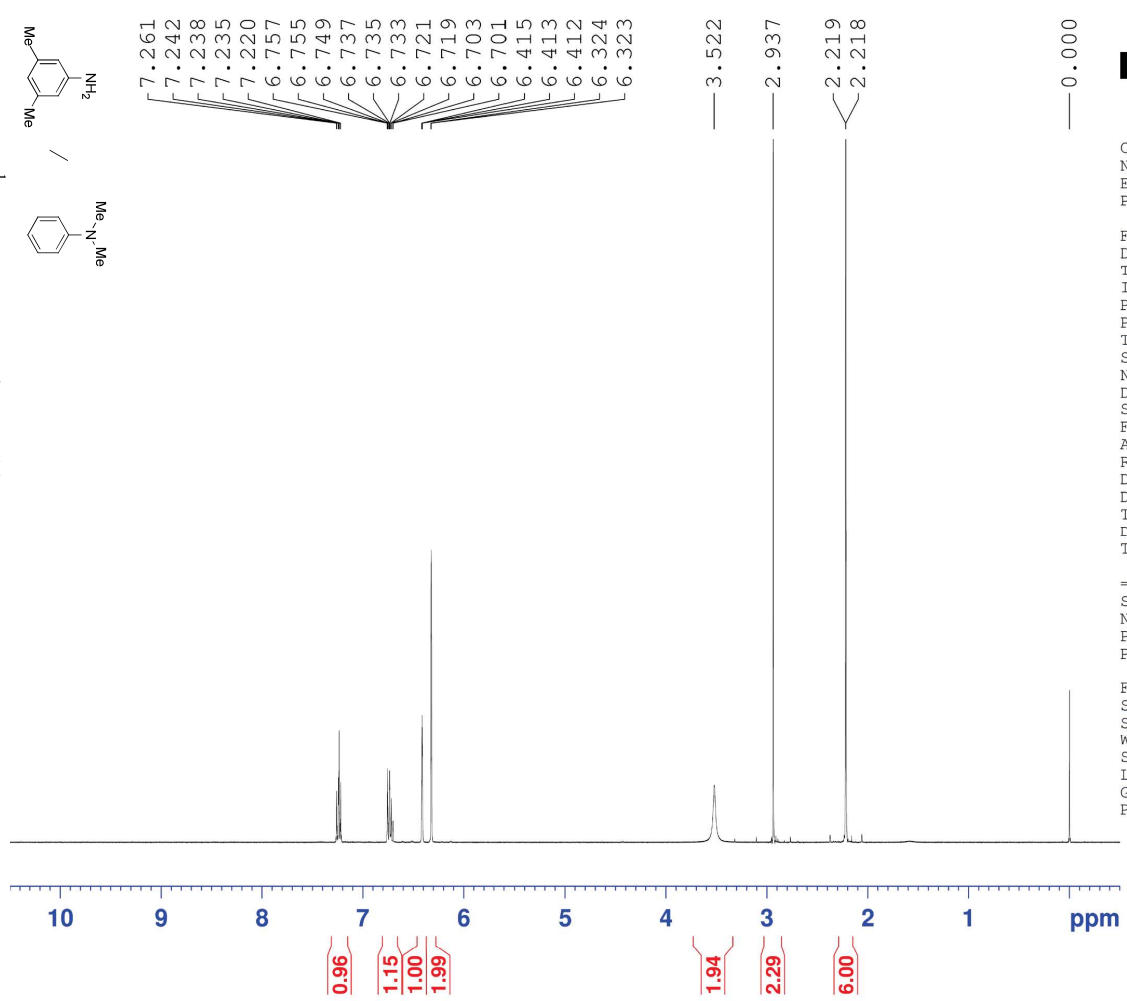
# Determine percentage of dominant regioisomer in attached $^{1}$H spectrum:

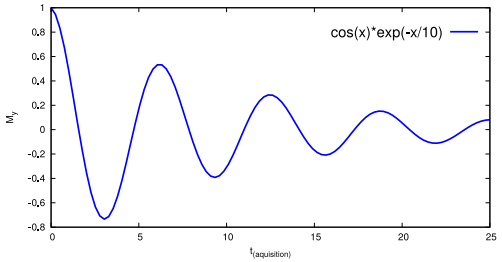


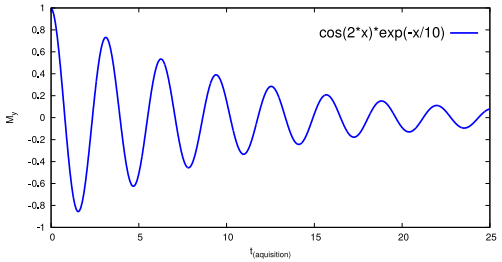

Spectrum S-23: $^{1}$H NMR spectrum from Table 3.

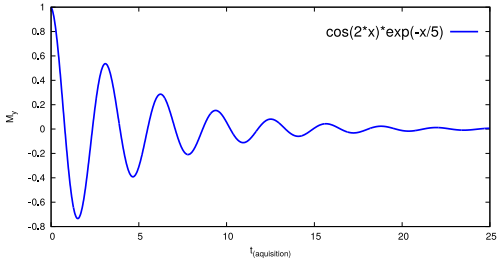
BRUKER

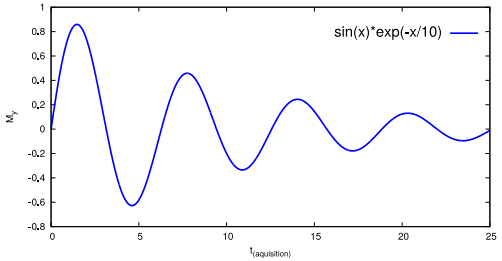
```
Current Data Parameters
NAME         DALO-V-108R
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20131026
Time              13.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    1
DS                    0
SWH            5597.015 Hz
FIDRES         0.085404 Hz
AQ             5.8545995 sec
RG                87.49
DW               89.333 usec
DE                6.50 usec
TE                298.1 K
D1           30.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.2224013 MHz
NUC1                 1H
P1                16.00 usec
PLW1         12.00000000 W

F2 - Processing parameters
SI                65536
SF           400.2200196 MHz
WDW                  EM
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

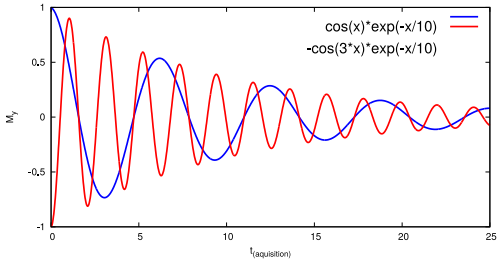
# Processing simulated NMR signal:



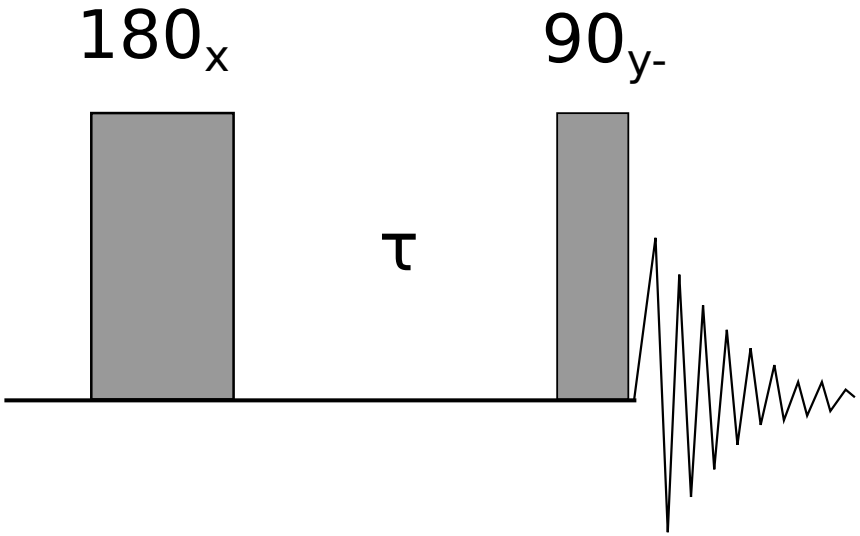



# $T_1$ relaxation

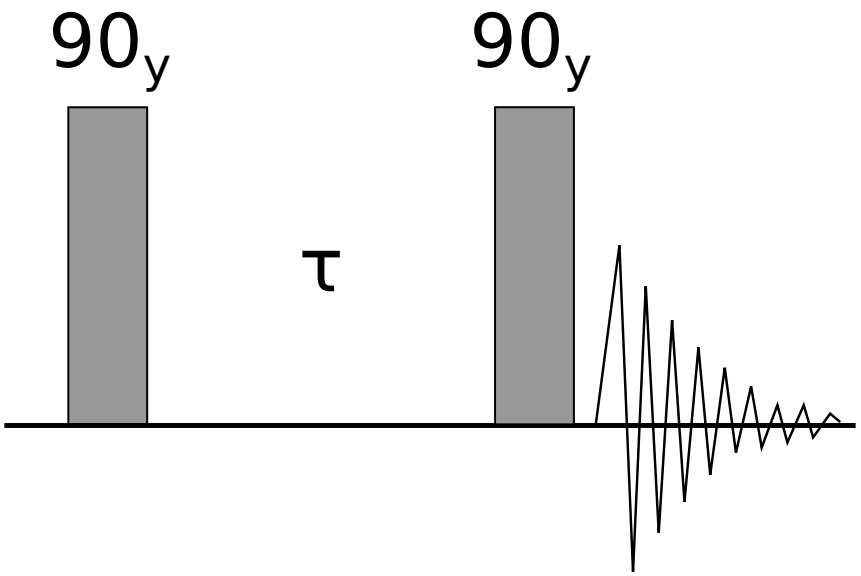
Apply following sequence (inversion recovery) to isolated spin characterized by **a)** $\tau = 2 * T_1$ and **b)** $\tau = 0.2 * T_1$. Draw semi-quantitatively resulting spectrum.



# 1-$\bar{1}$ sequence

Draw the evolution of macroscopic magnetization through the sequence:
**90(y) - $\tau$ - 90(y) - aq**
Consider the evolution of an isolated spin due to the chemical shift.

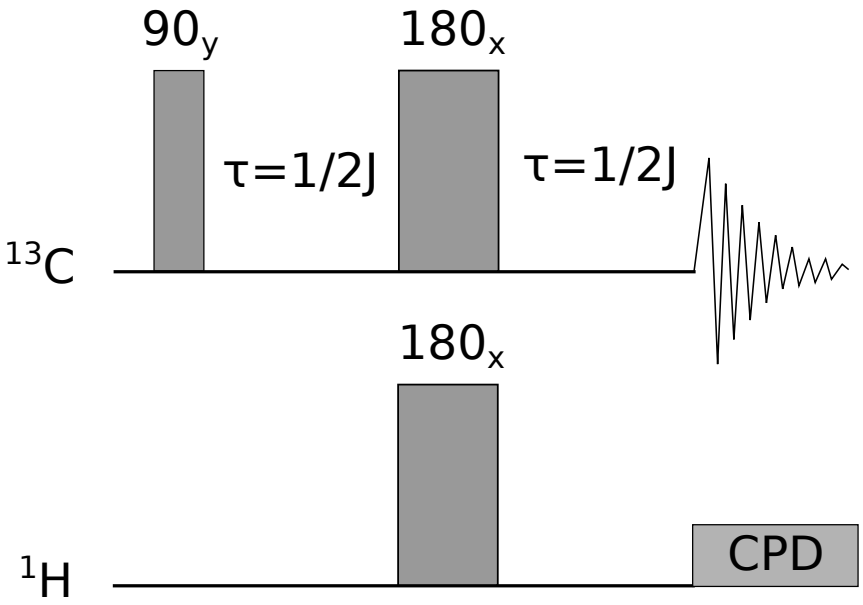
1. How does the result differ for the following offsets: $\Omega\tau = 0, \pi/2, \pi$.
2. Draw lineshapes of resulting signal assuming the a) $y+$ b) $x+$ corresponds to zero phase of receiver (prior phase correction).



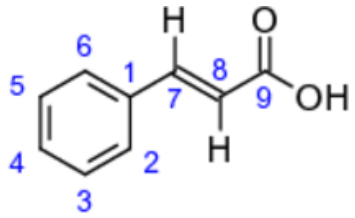
# Heteronuclear spin echo

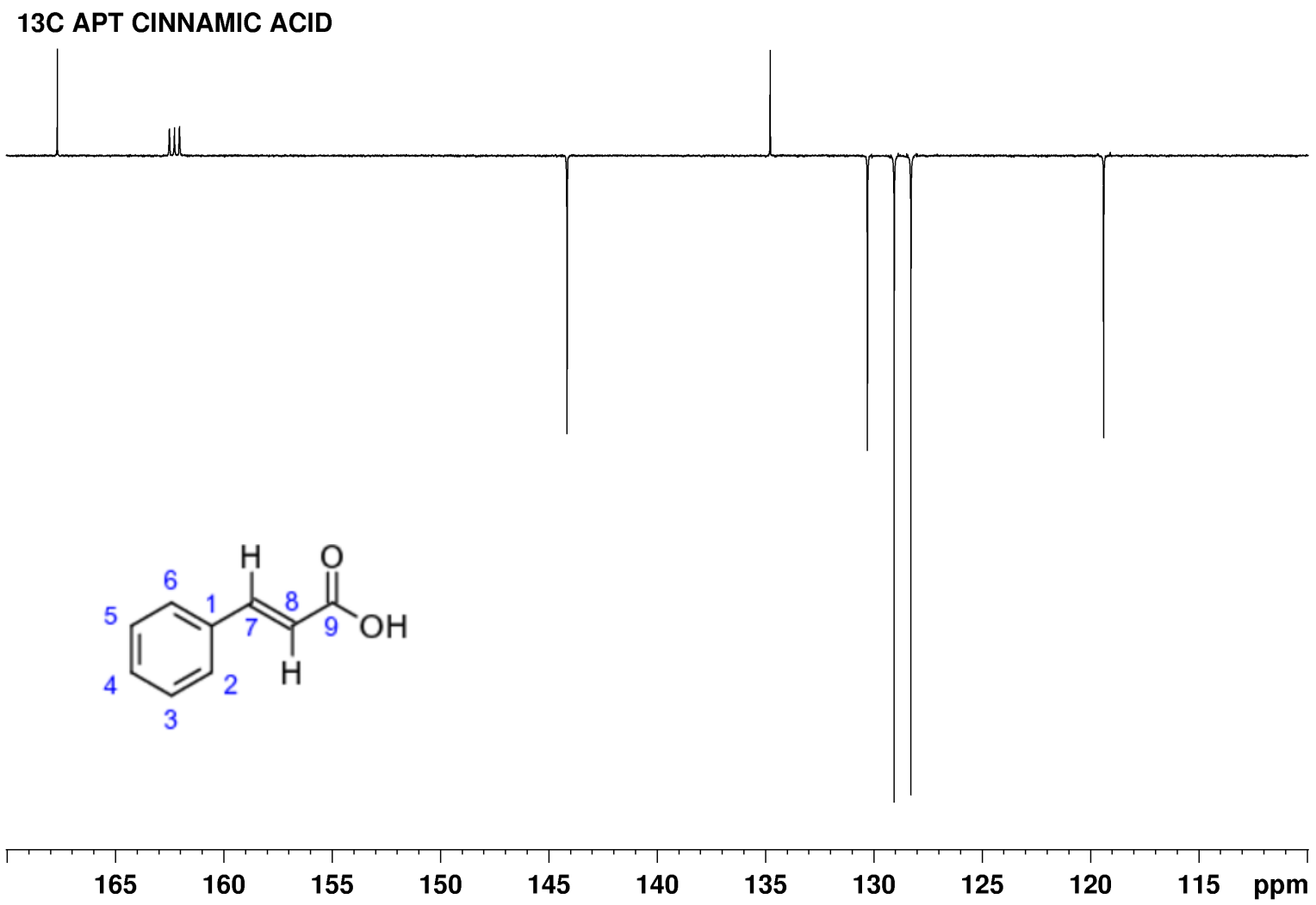
By using vector diagrams determine the result of attached pulse sequence.

1. **Ignore 180 pulse** in hydrogen channel for isolated spin systems **a)** $^{13}C$-$^{1}H$ and **b)** $^{13}C$-$^{1}H_2$. Explain the role of CPD block.
2. Lets consider **the complete sequence** and isolated spin systems **a)** $^{13}C$-$^{1}H$ and **b)** $^{13}C$-$^{1}H_2$.

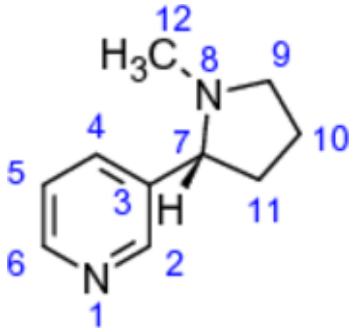


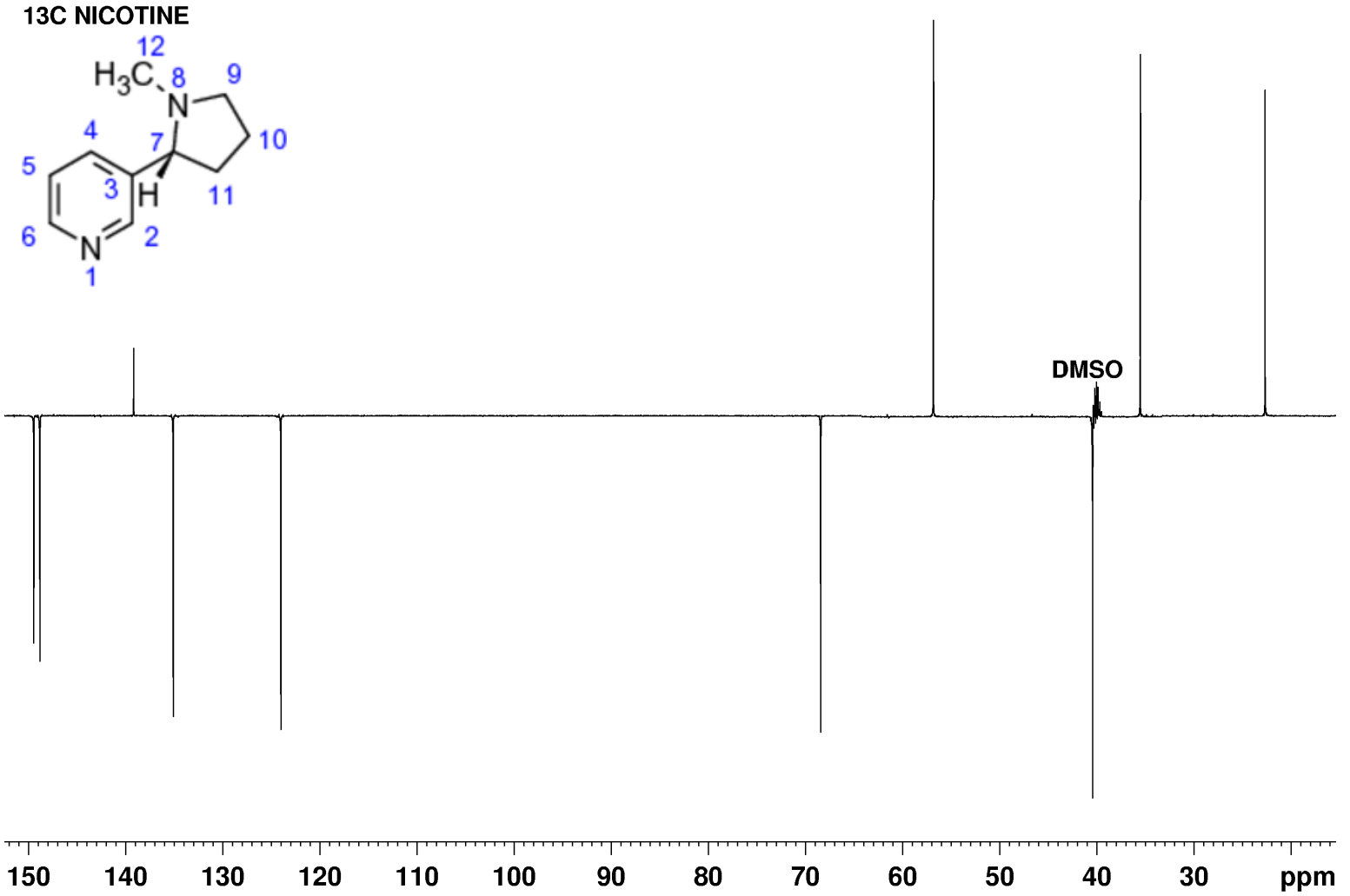
# $^{13}$C APT Cinnamic acid



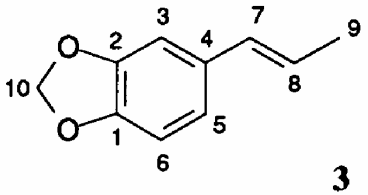



# $^{13}$C APT Nicotine

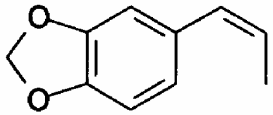


# DEPT experiment




**3**



**4**

Which is the major product? Assign the signals as far as possible. Why does the signal at $\delta = 100.8$ exist in the spectrum 3.3.c, although its intensity should be zero?

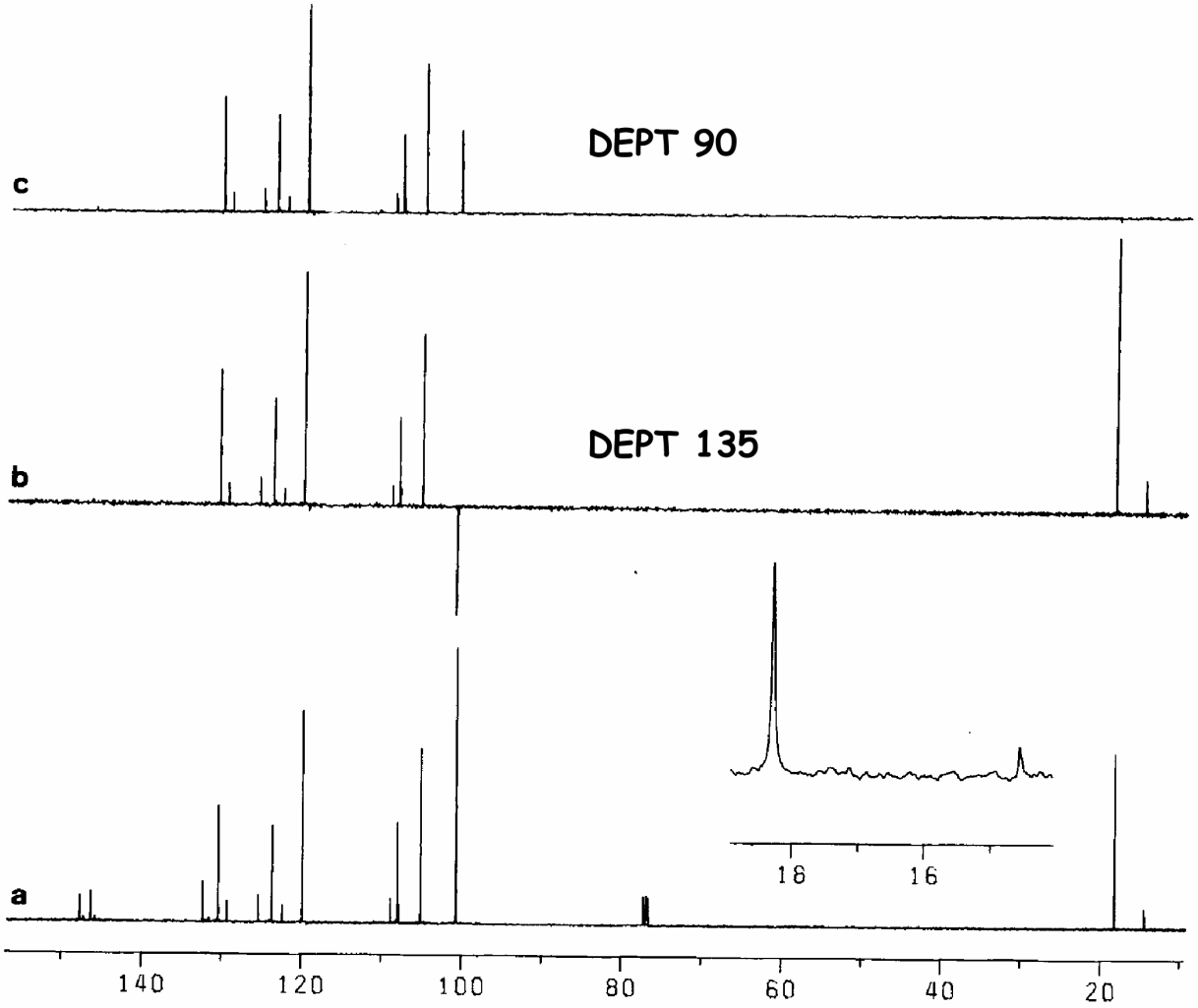



**Fig. 3.3.** (a) $^{1}H$ broad-band decoupled $^{13}C$ NMR spectrum of a mixture of **3** and **4** in $CDCl_3$. Traces (b) and (c) are DEPT spectra