Nuclear Magnetic Resonance
Part 3
Carbon - 13

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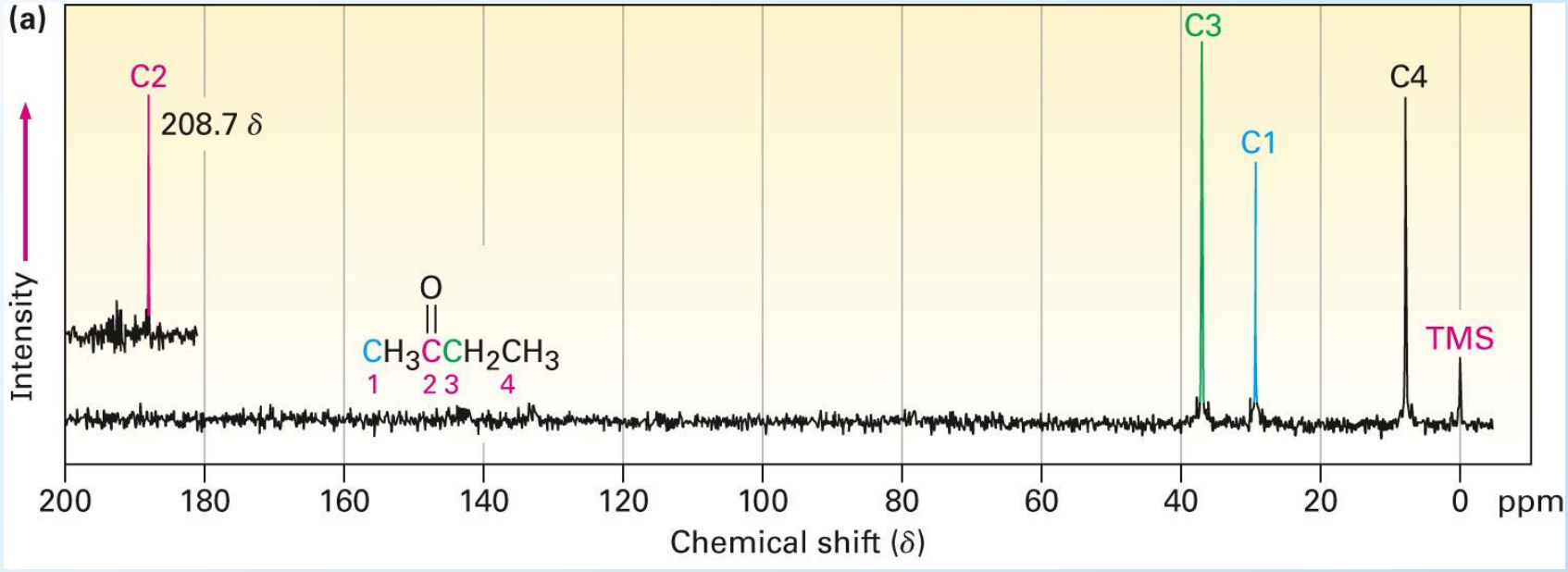
Carbon-13

- ^{12}C has no magnetic spin.
- ^{13}C has a magnetic spin, but is only 1% of the carbon in a sample.
- Signals are weak, getting lost in noise.
- Hundreds of spectra are taken, averaged.
- Below is the spectrum for **2- butanone**

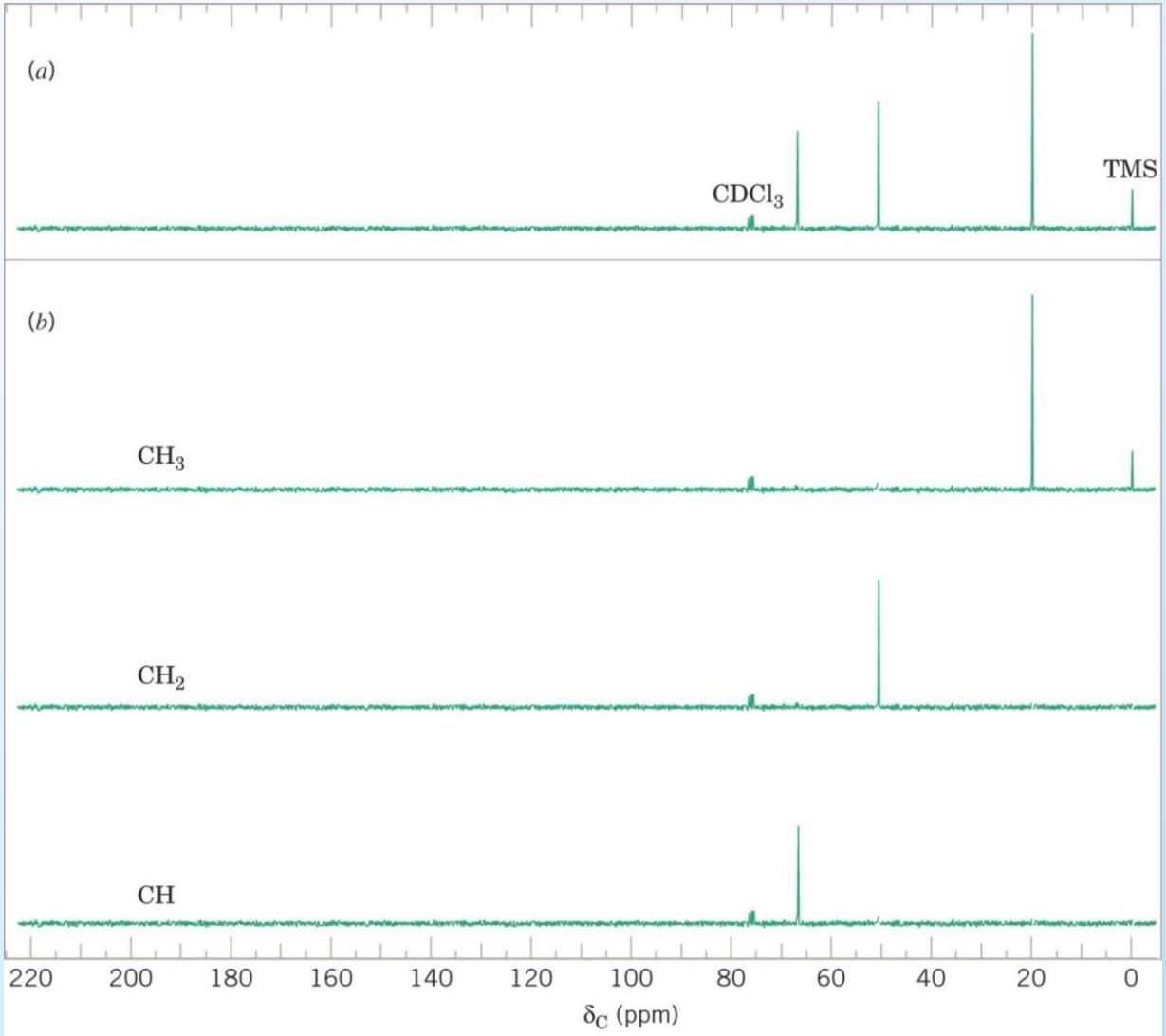


DEPT for C-13

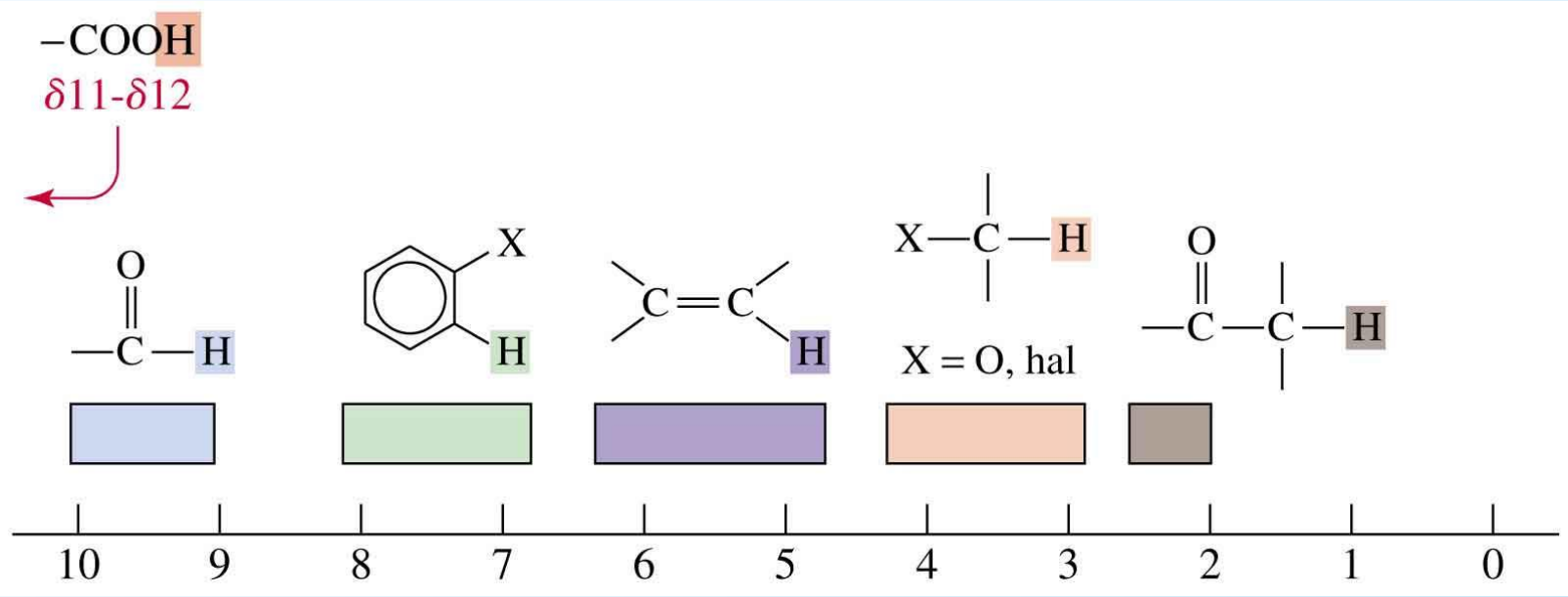
Example: 1-chloro-2-propanol

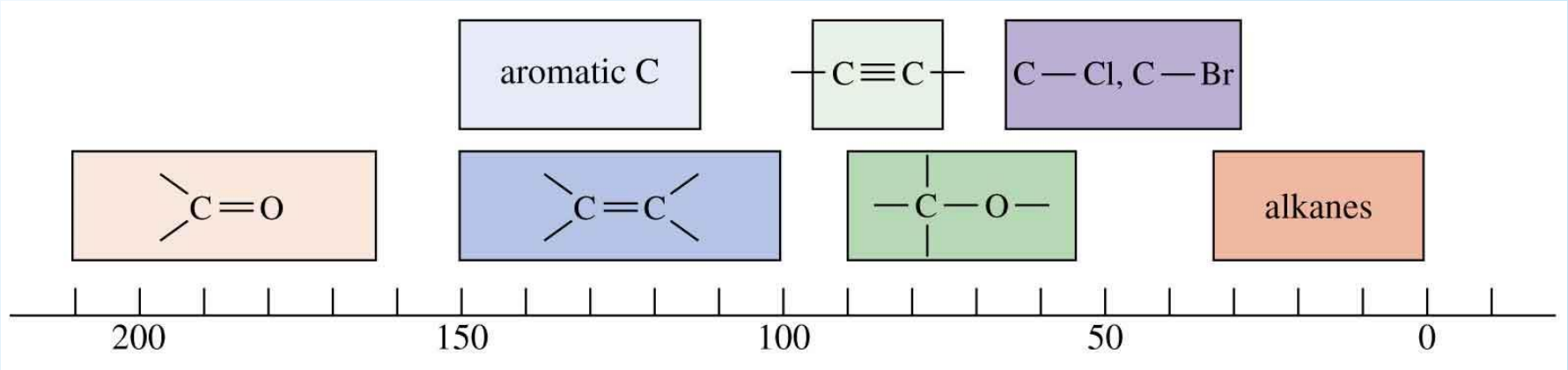
(a) The broadband decoupled spectrum and

(b) a set of DEPT spectra showing the separate CH, CH_2, and CH_3 signals

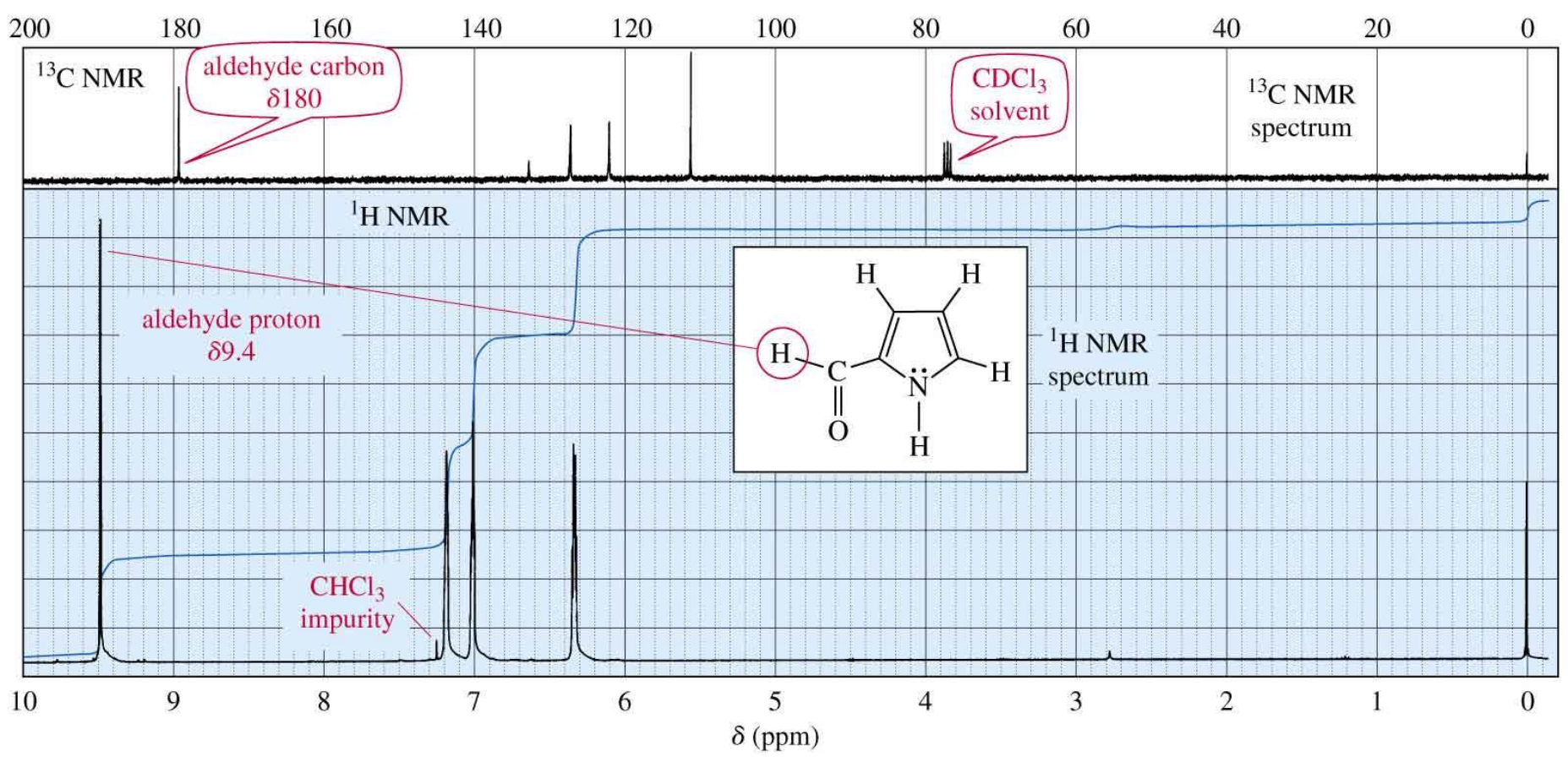


Hydrogen and Carbon Chemical Shifts

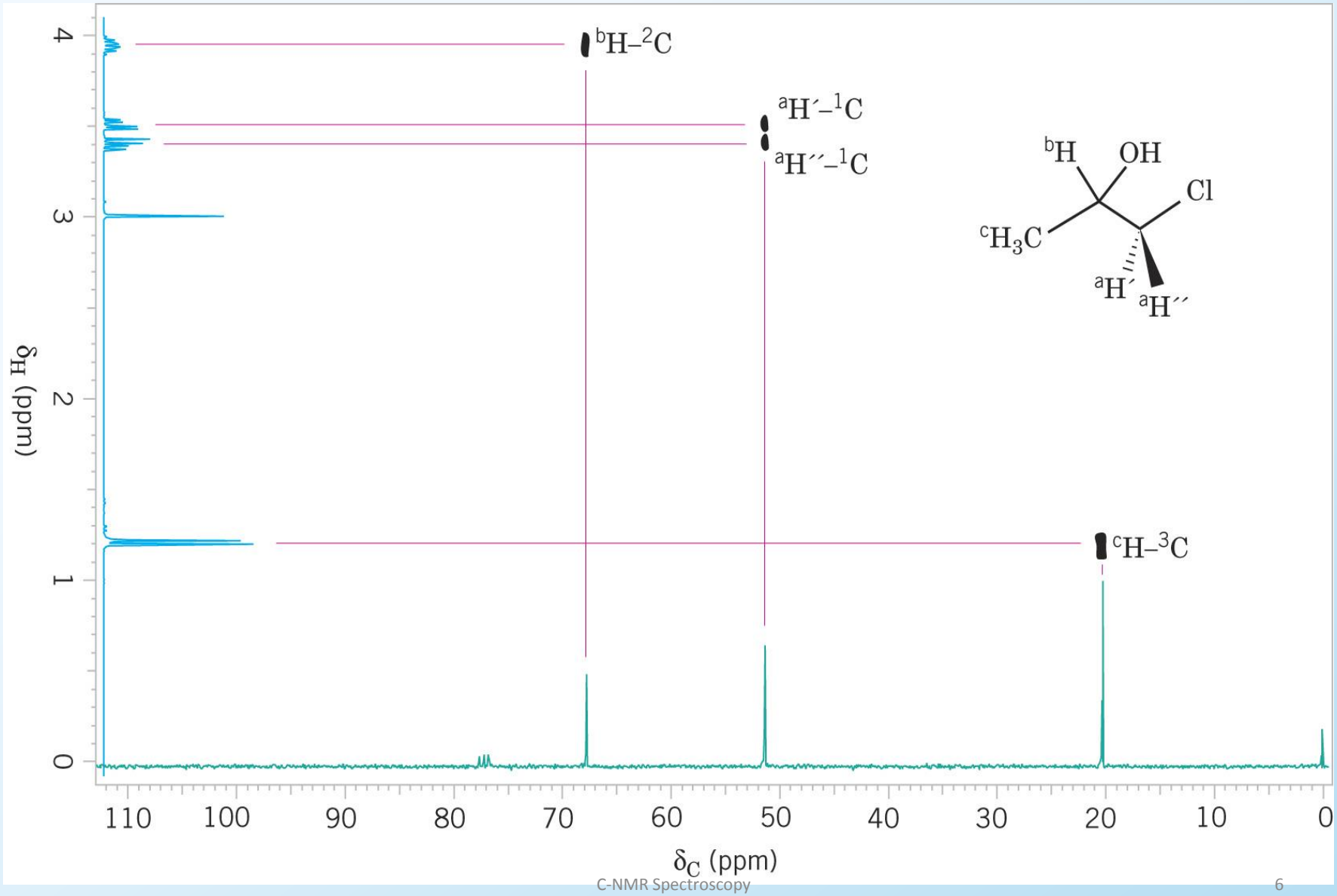




Combined ^{13}C and ^{1}H Spectra



H and C coupled NMR (HETCOR)



Spin-Spin Splitting

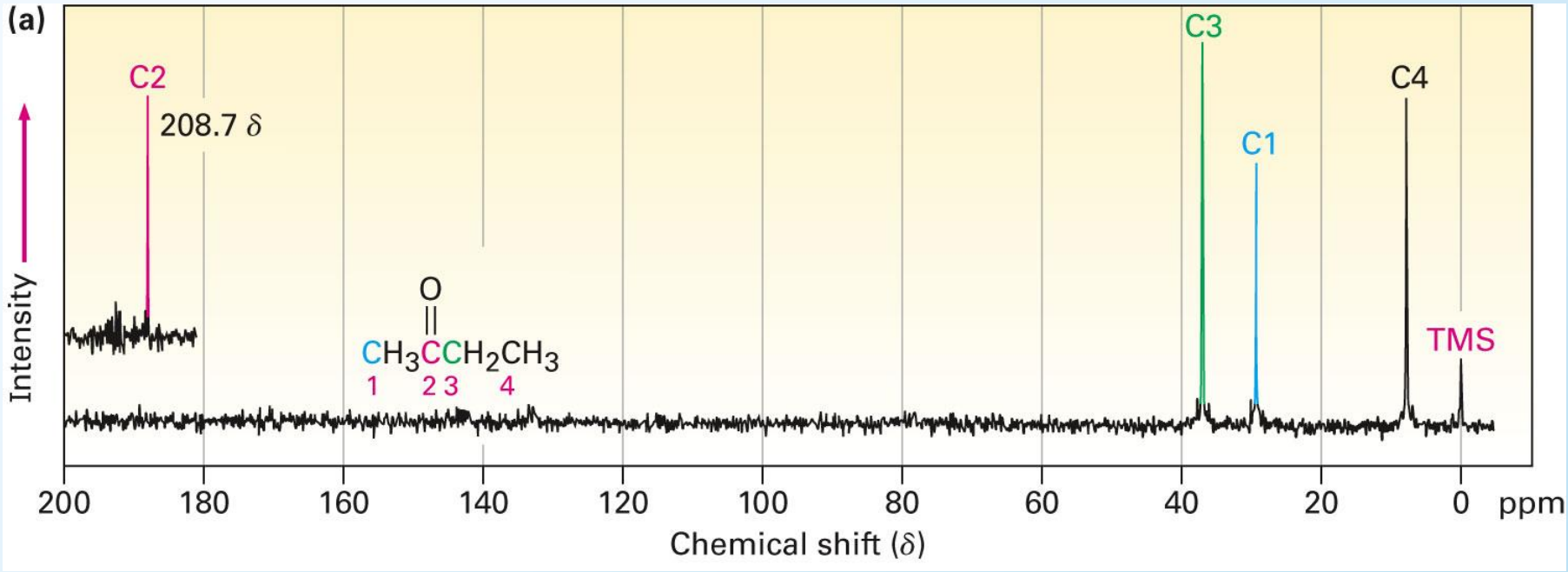
- It is unlikely that a ^{13}C would be adjacent to another ^{13}C, so splitting by carbon is negligible.
- ^{13}C will magnetically couple with attached protons and adjacent protons.
- These complex splitting patterns are difficult to interpret.

Interpreting ^{13}C NMR

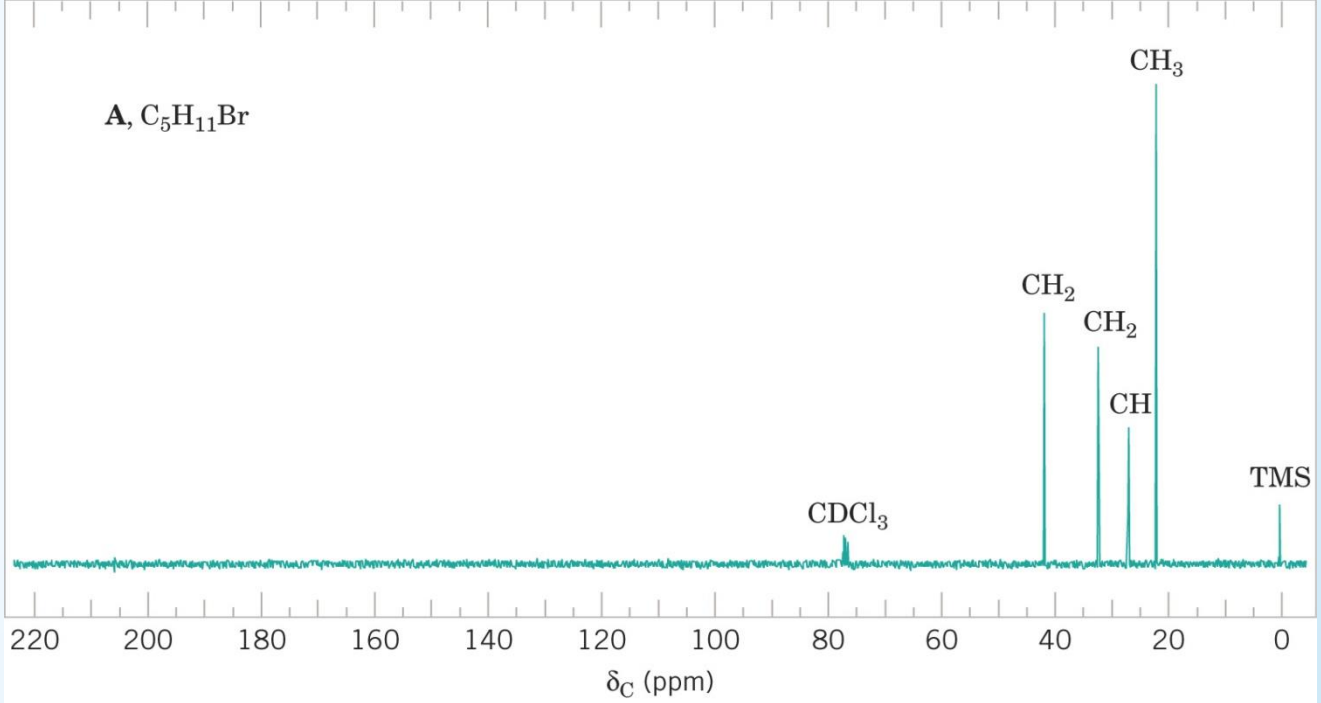
- The number of different signals indicates the number of different kinds of carbon.
- The location (chemical shift) indicates the type of functional group.
- The peak area indicates the numbers of carbons (if integrated).
- The splitting pattern of off-resonance decoupled spectrum indicates the number of protons attached to the carbon.

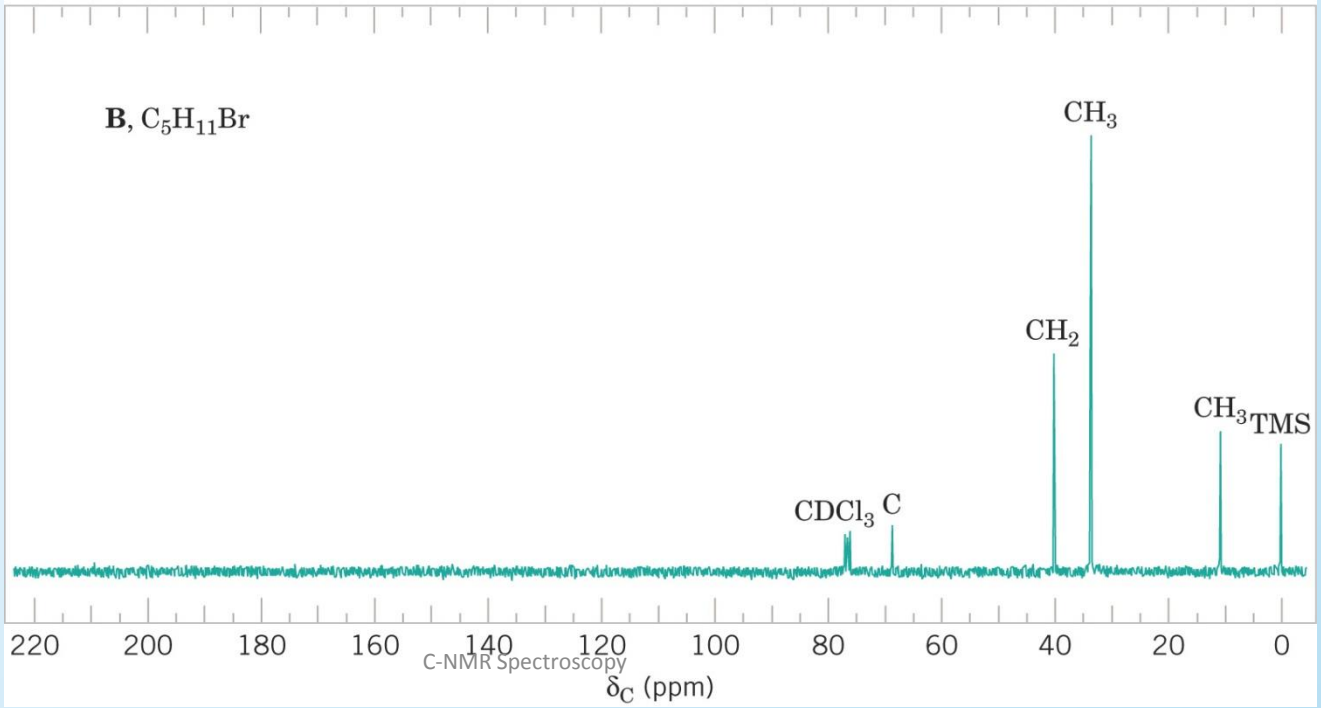
C-13 NMR of 2-butanone

- $CH_3COCH_2CH_3$
- Shows the carbon of C=O (carbonyl) group on the left, and the alkyl carbons on the right – upfield.

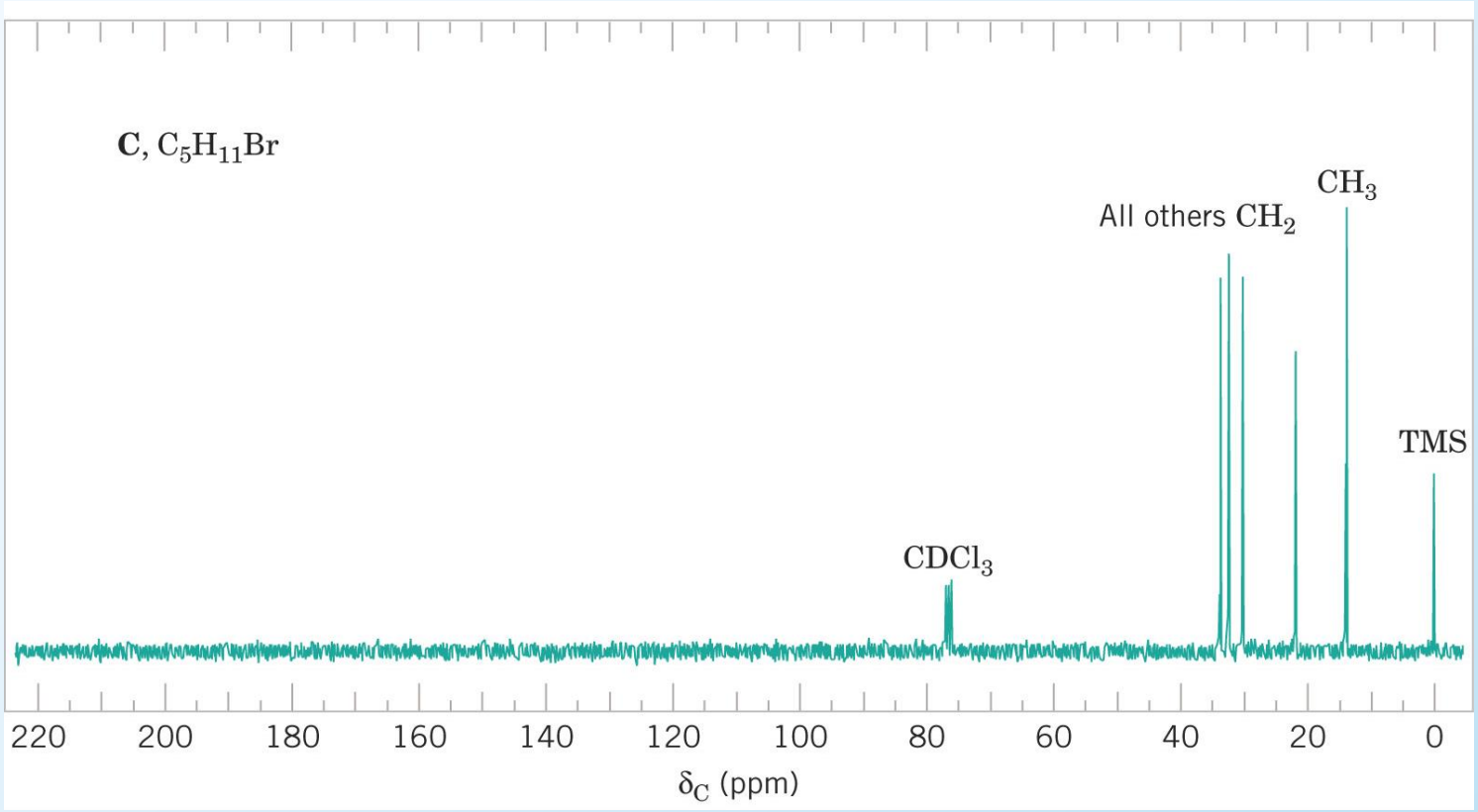


Problems


A, $C_5H_{11}Br$
CH_3
CH_2
CH_2
CH
TMS
$CDCl_3$
220 200 180 160 140 120 100 80 60 40 20 0
δ_C (ppm)

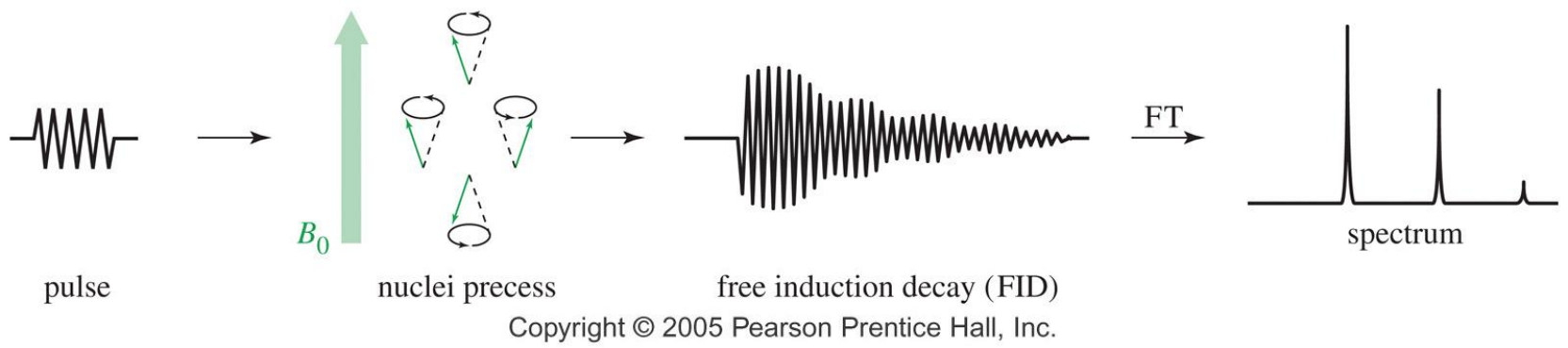

B, $C_5H_{11}Br$
CH_3
CH_2
CH_3
TMS
$CDCl_3$
C
220 200 180 160 140 120 100 80 60 40 20 0
δ_C (ppm)

Problem


C, $C_5H_{11}Br$
CH_3
All others CH_2
TMS
$CDCl_3$
220
200
180
160
140
120
100
80
60
40
20
0
δ_C (ppm)

Fourier Transform NMR

- Radio-frequency pulse given.
- Nuclei absorb energy and precess (spin) like little tops.
- A complex signal is produced, then decays as the nuclei lose energy.
- Free induction decay is converted to spectrum.



Key Concepts

- Chemical shifts
- Interpret a C-13 NMR
- Predict signals for C-13 NMR for a compound