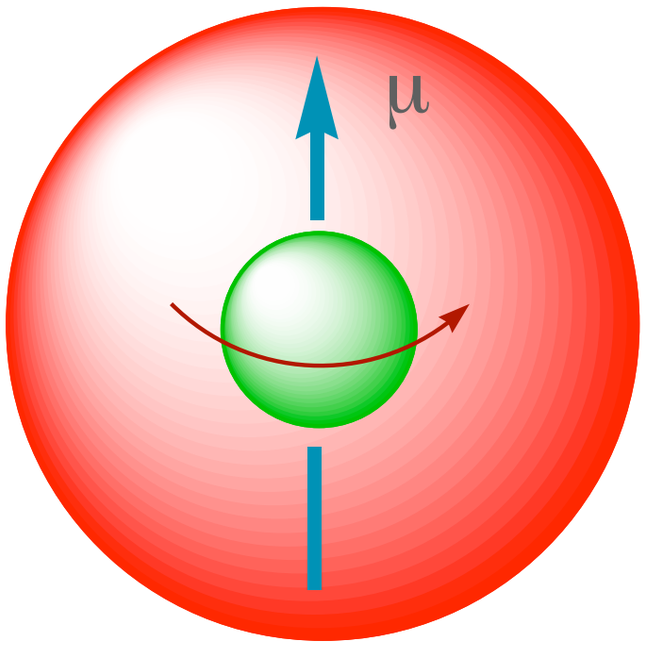
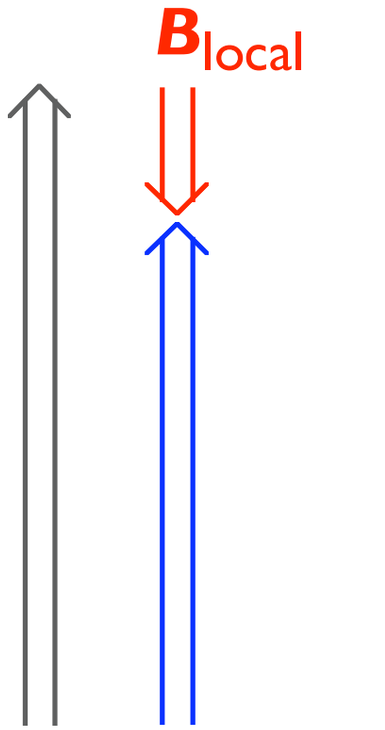
From Last Lecture

Electronic Sheilding





$B_{effective} = B_0 - B_{local}$

Actual magnetic field felt by the nucleus

From Last Lecture

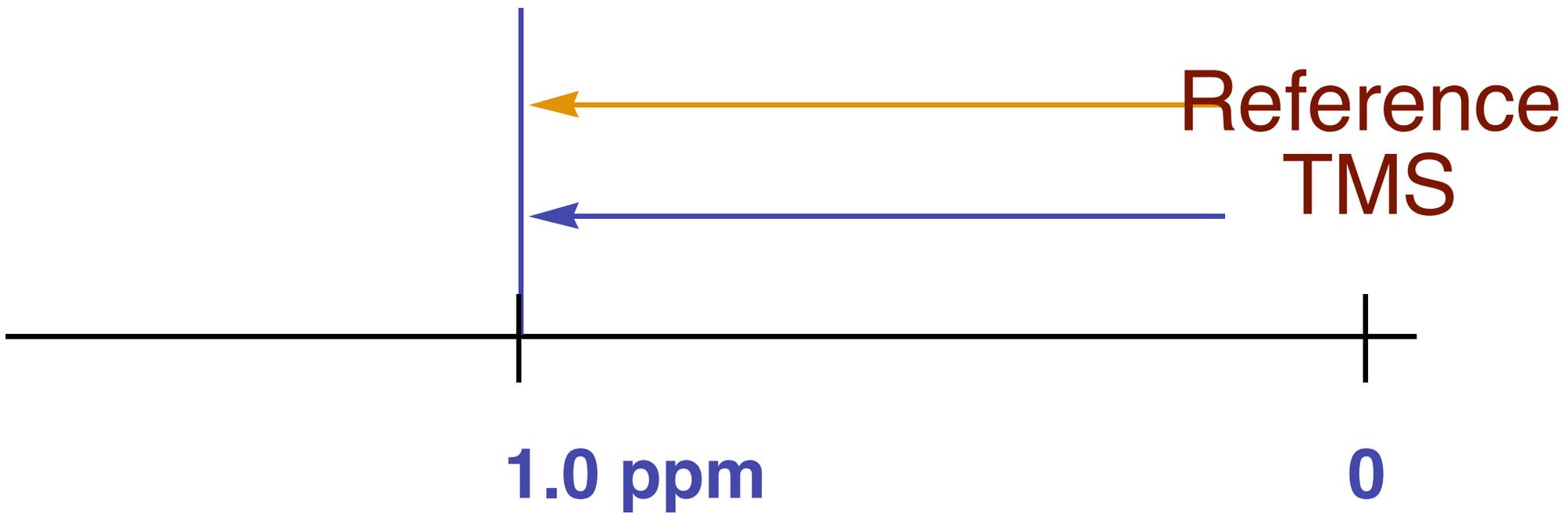
- δ = ppm = $\dfrac{\text{Chemical Shift from TMS (Hz)}}{\text{Spectrometer Frequency (MHz)}}$

100 MHz NMR

$$\frac{100\ \text{Hz}}{100\ \text{MHz}} = 1.0\ \text{ppm}$$

300 MHz NMR

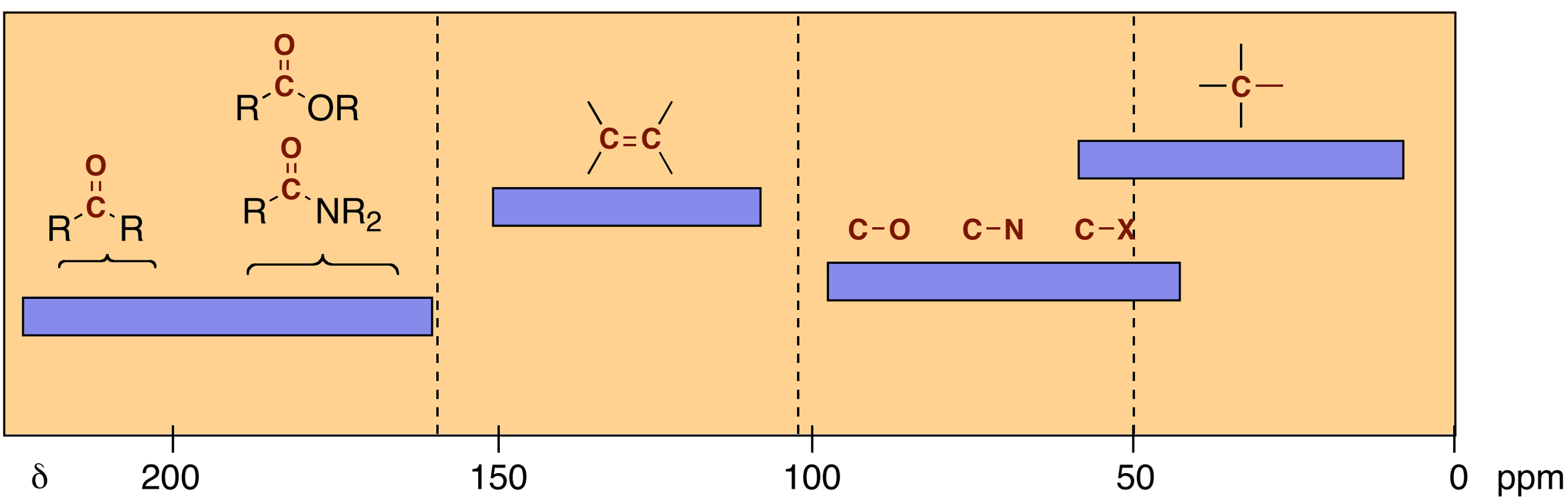
$$\frac{300\ \text{Hz}}{300\ \text{MHz}} = 1.0\ \text{ppm}$$



From Last Lecture

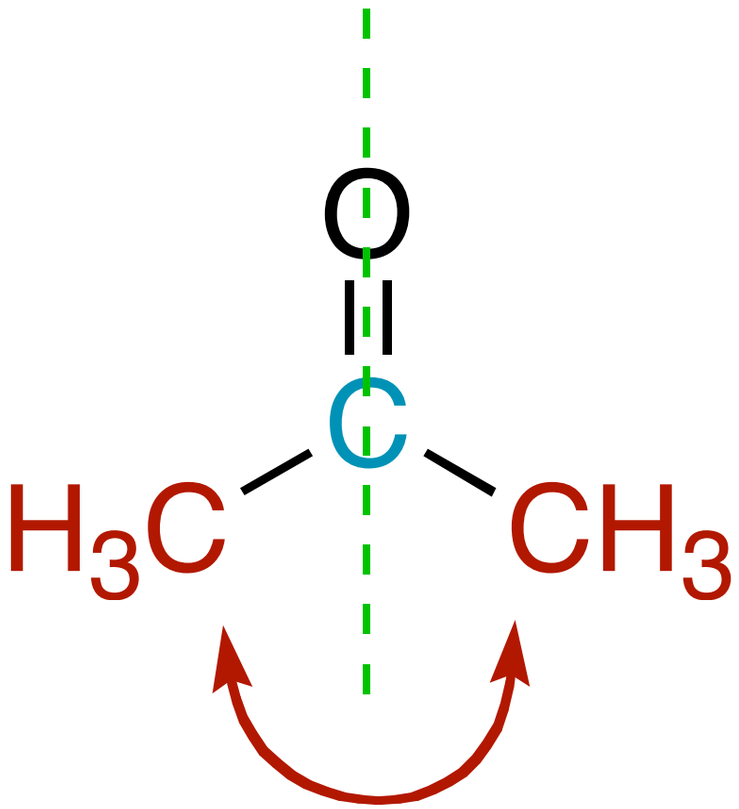
- Difficult - Carbon 13 only 1.1% of all carbon.
- Number of different carbons
- Functional Group Regions

^{13}C NMR

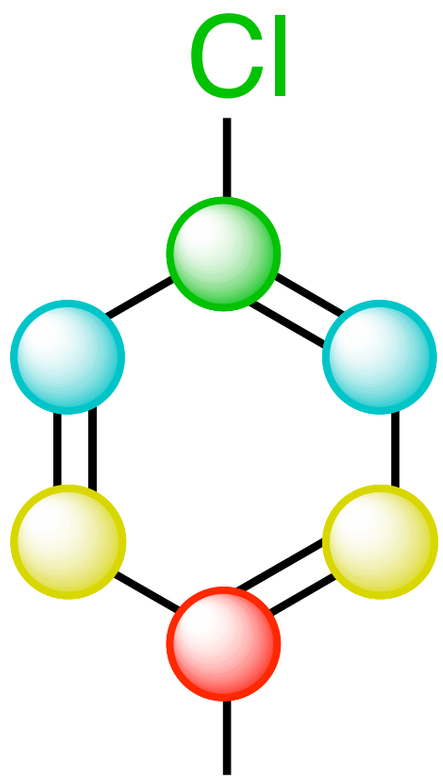


From Last Lecture

- Symmetry in molecules can make carbons "Chemically Equivalent"

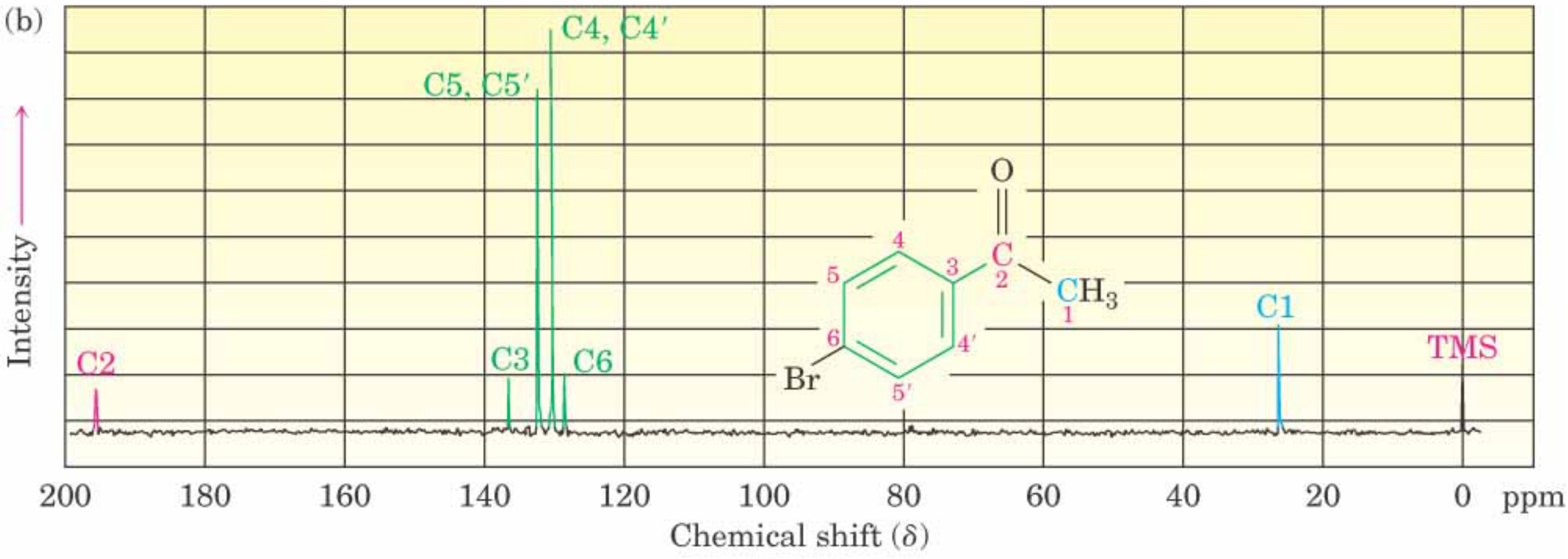


same electronic environment



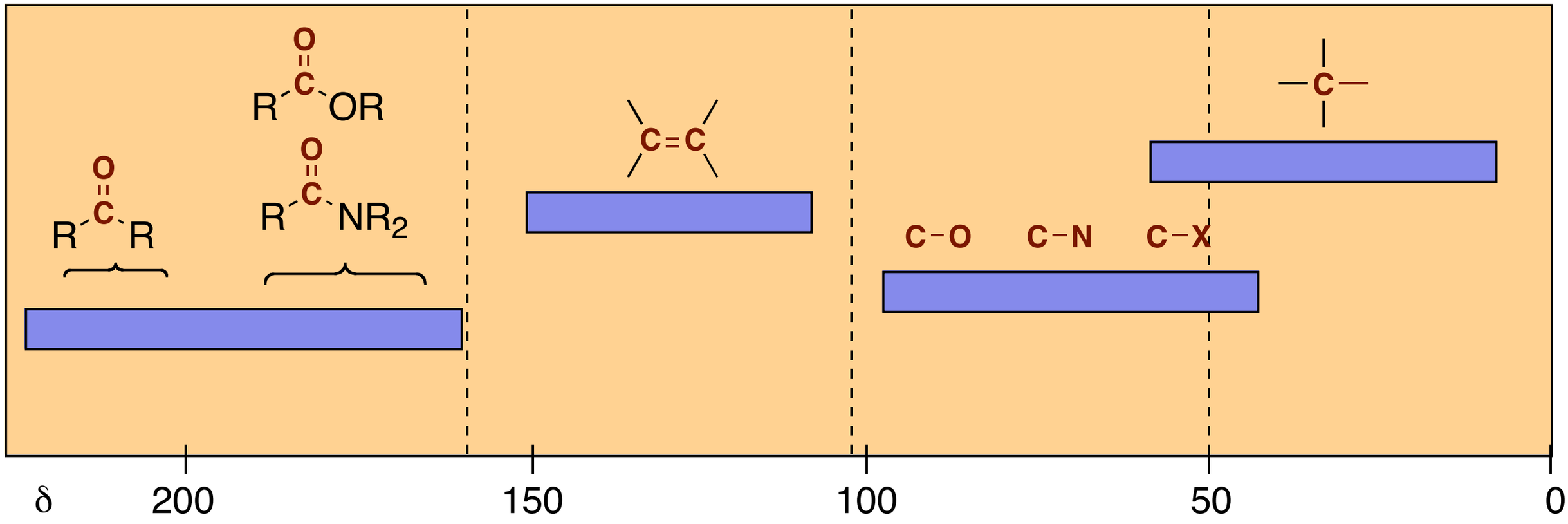
Substitution of Carbon

- The intensity of the peaks roughly correlates with the number of hydrogens on the carbon.

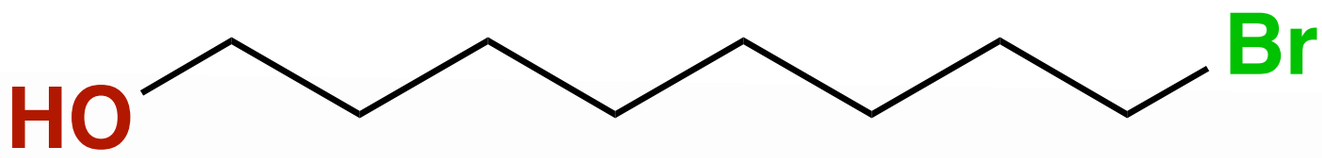


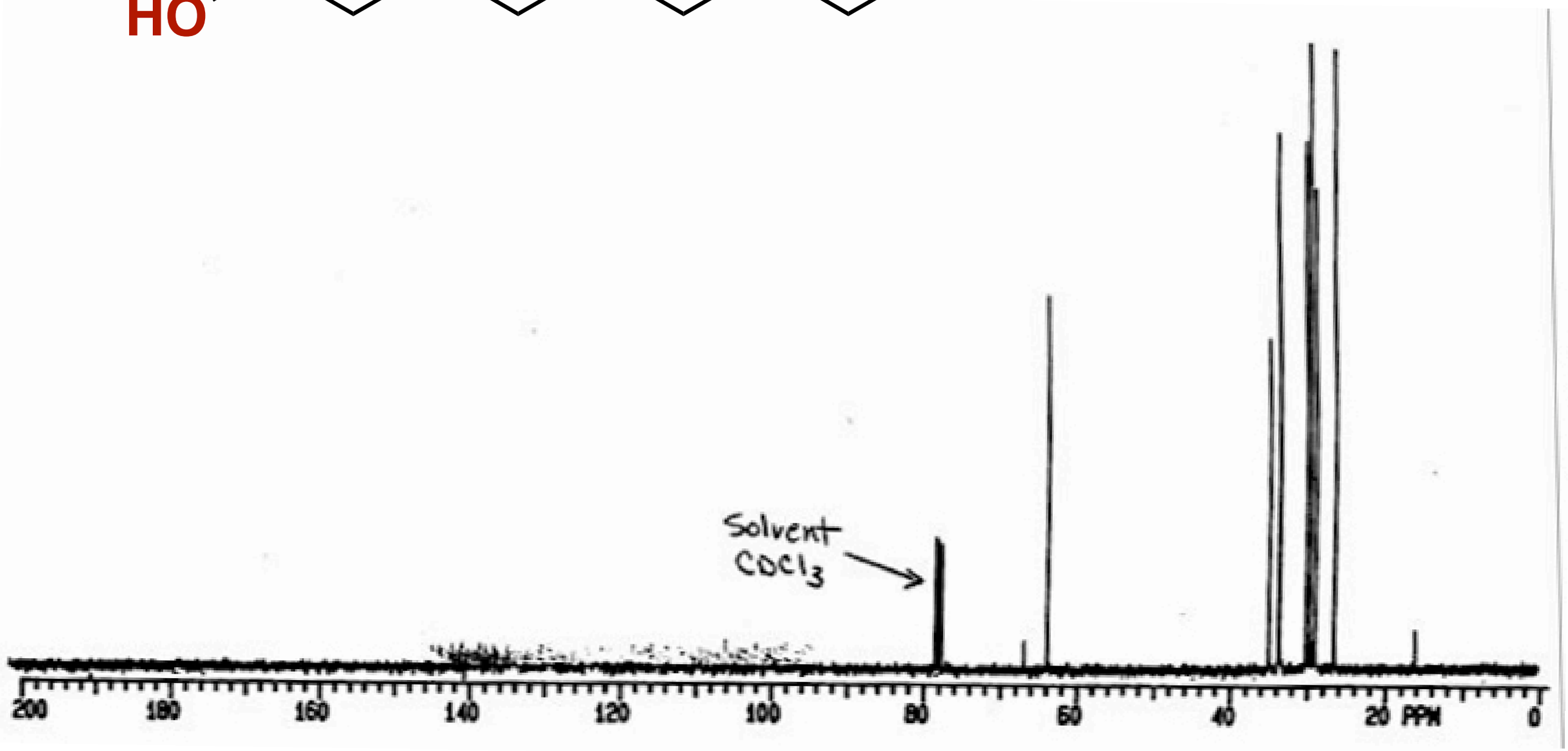
C13 NMR Regions

^{13}C NMR

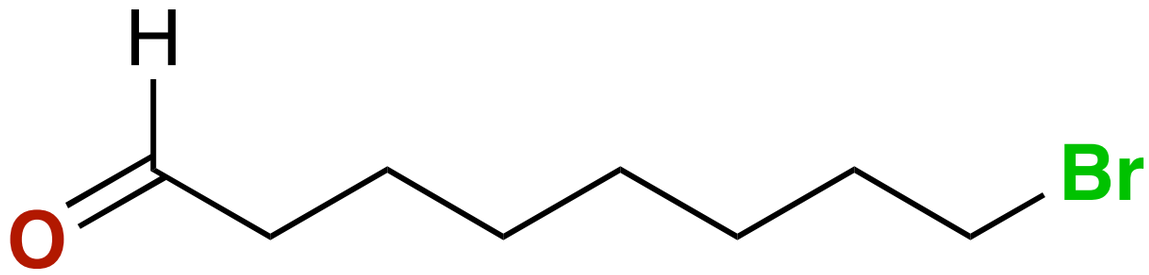


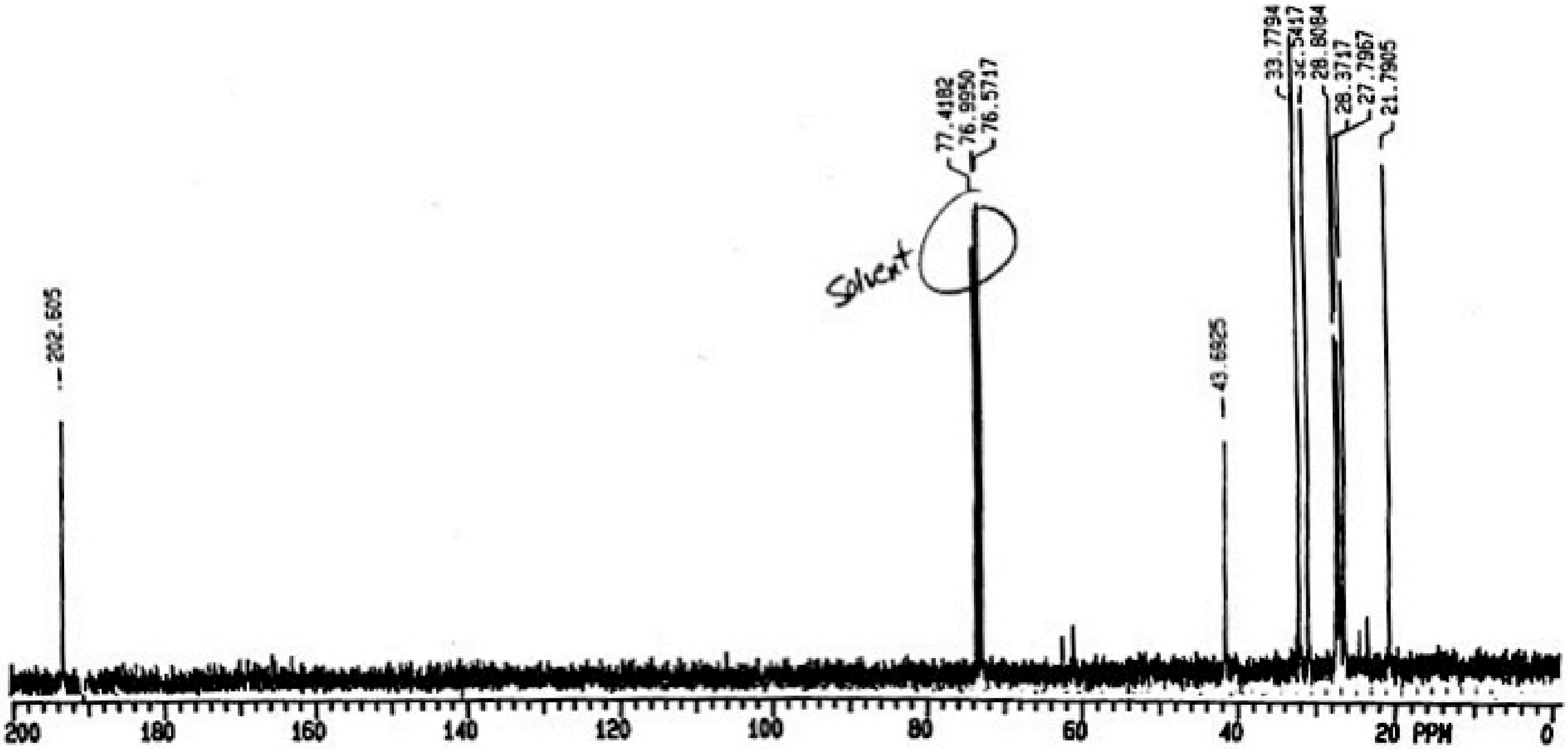
Bromooctanol



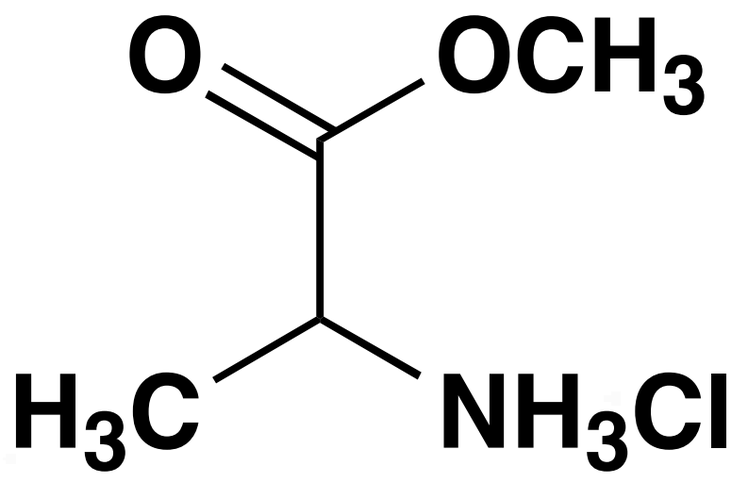


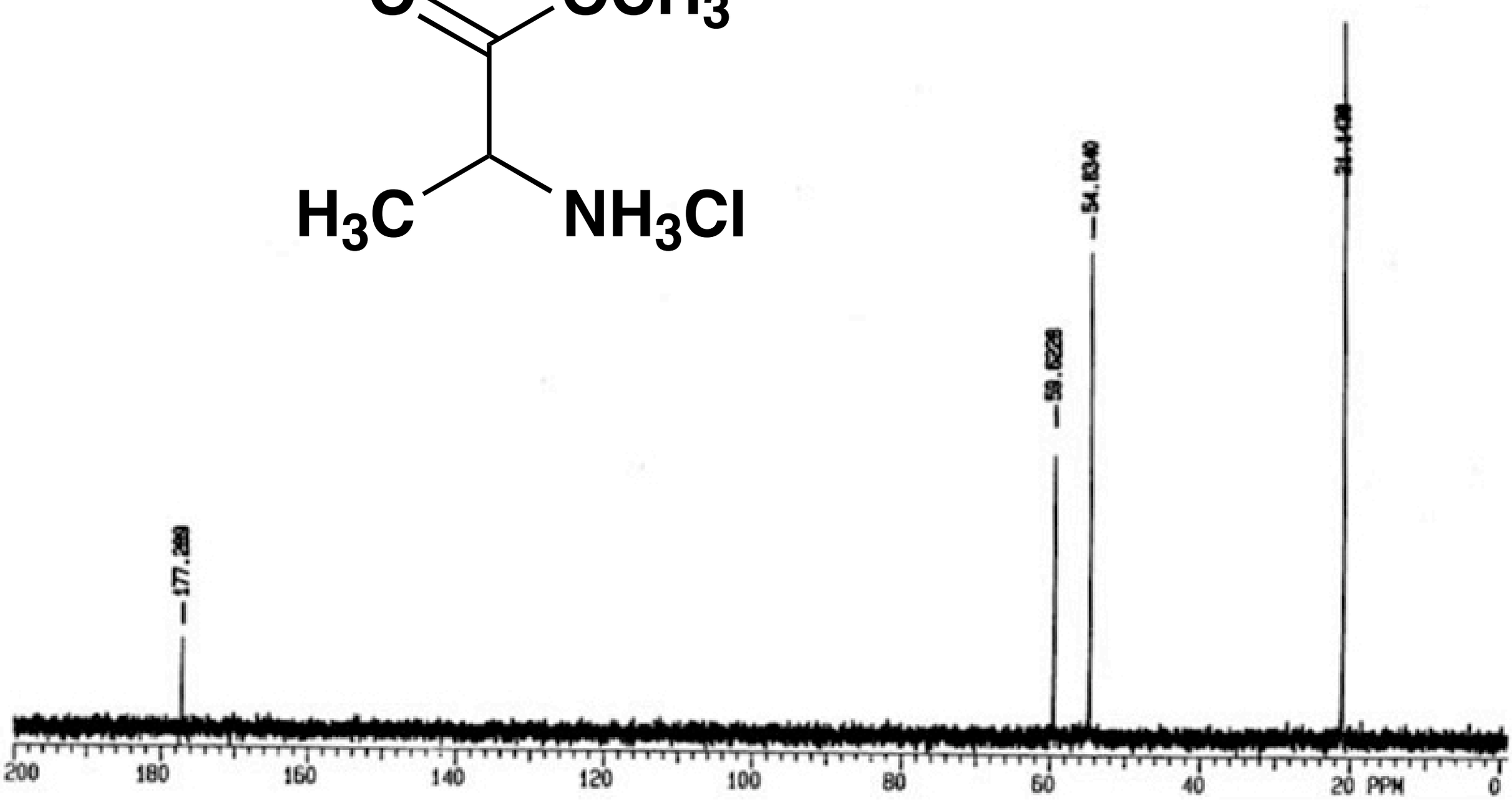
Bromooctanal



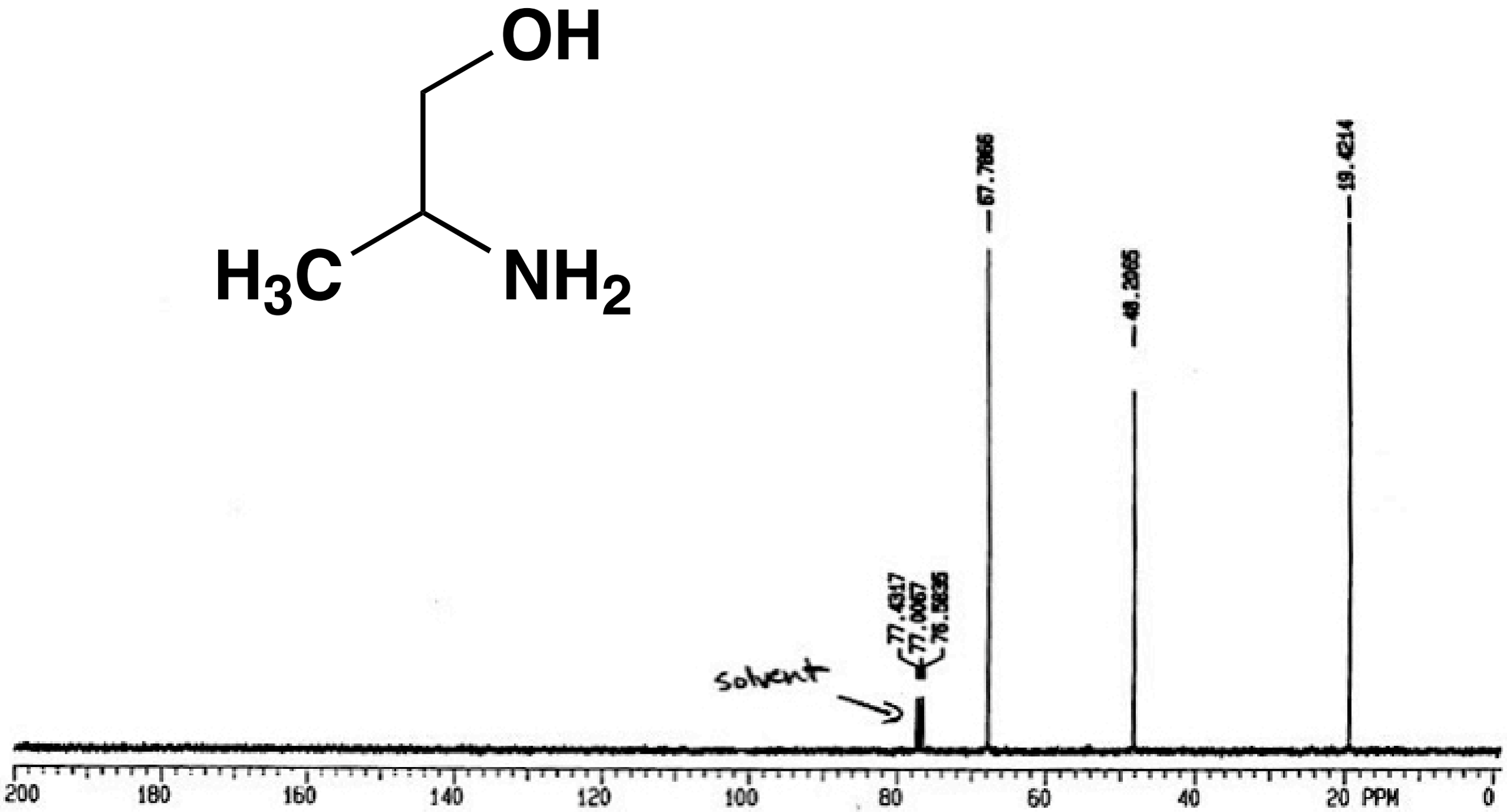


Alanine Me-Ester HCl

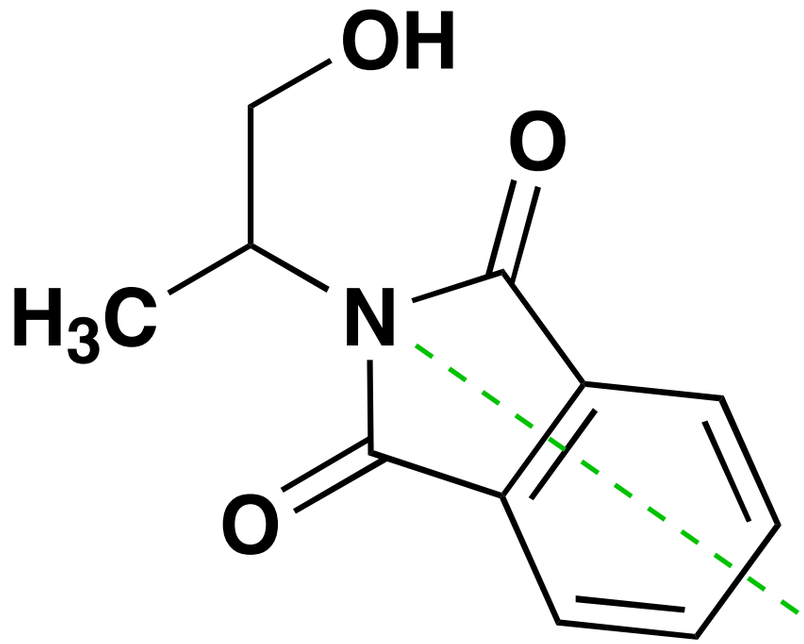


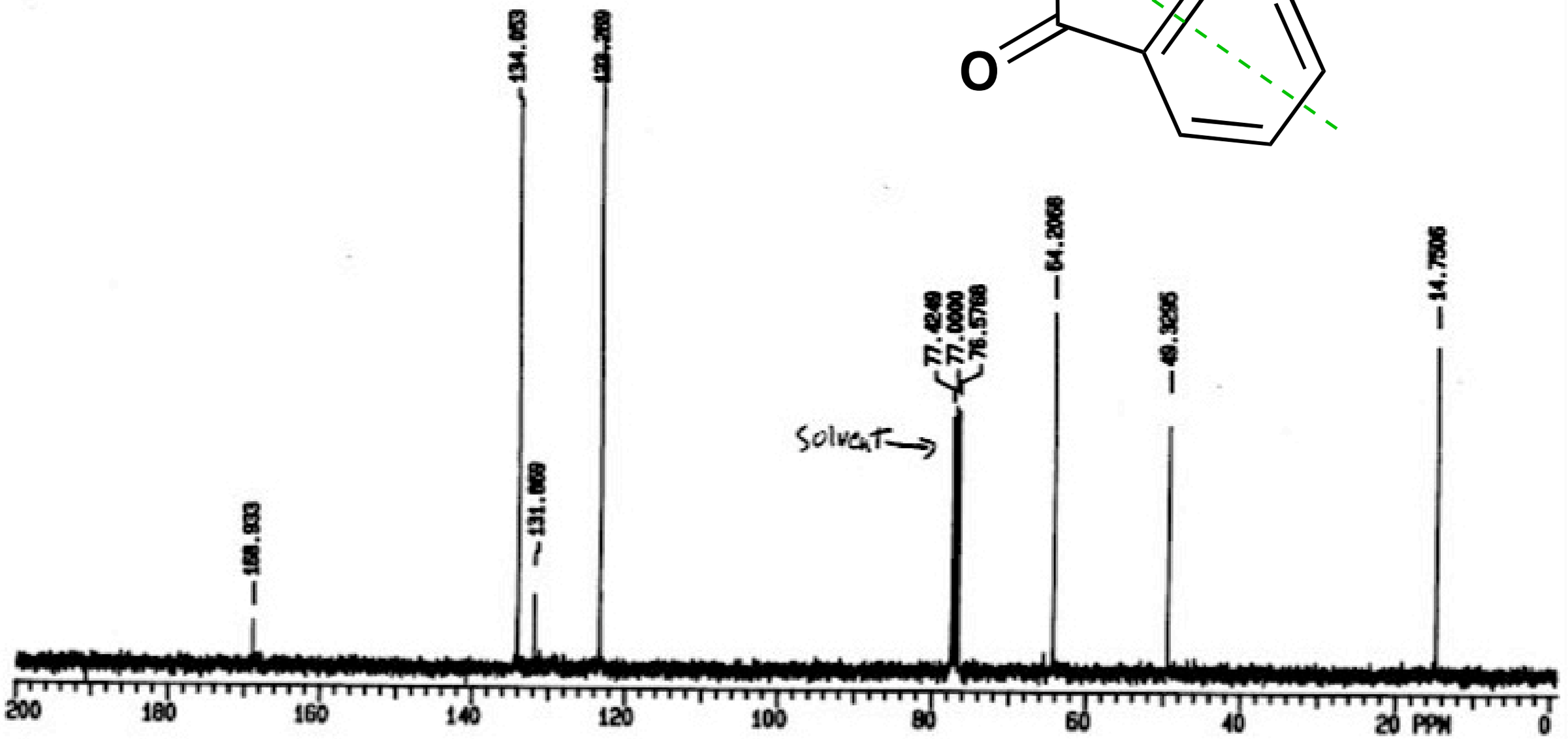


Alaninol

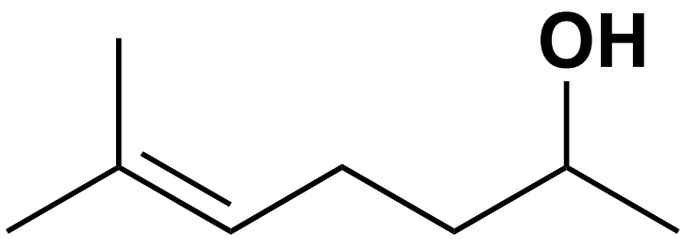

OH
H3C
NH2
67.7686
49.2935
19.4214
77.4917
77.0067
76.5835
Solvent
200
180
160
140
120
100
80
60
40
20
PPM
0

Alaninol - phthalimide

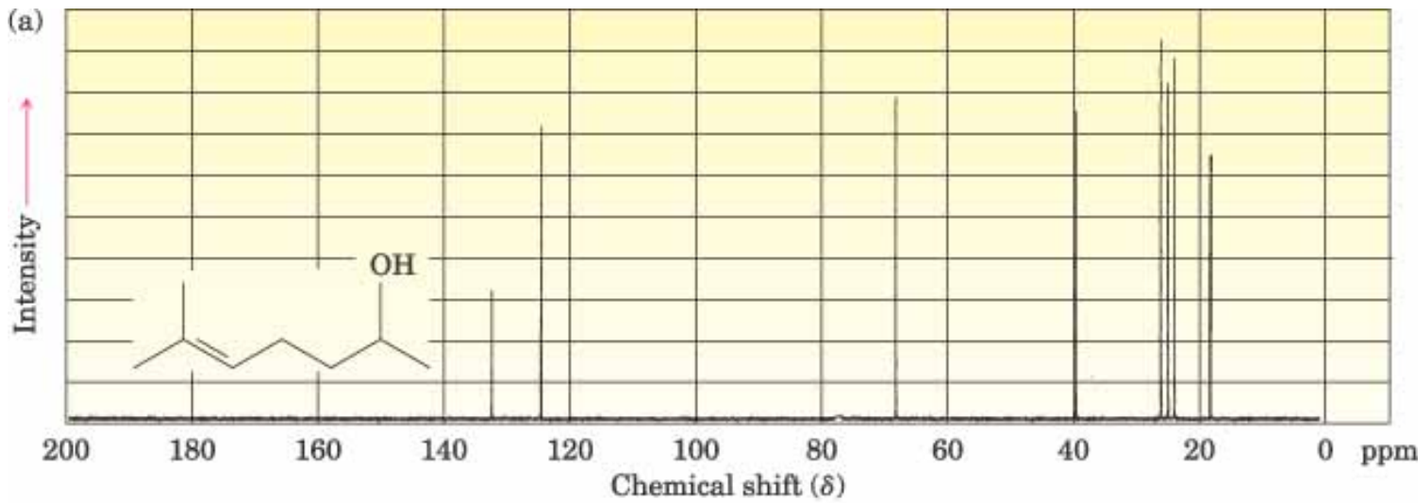


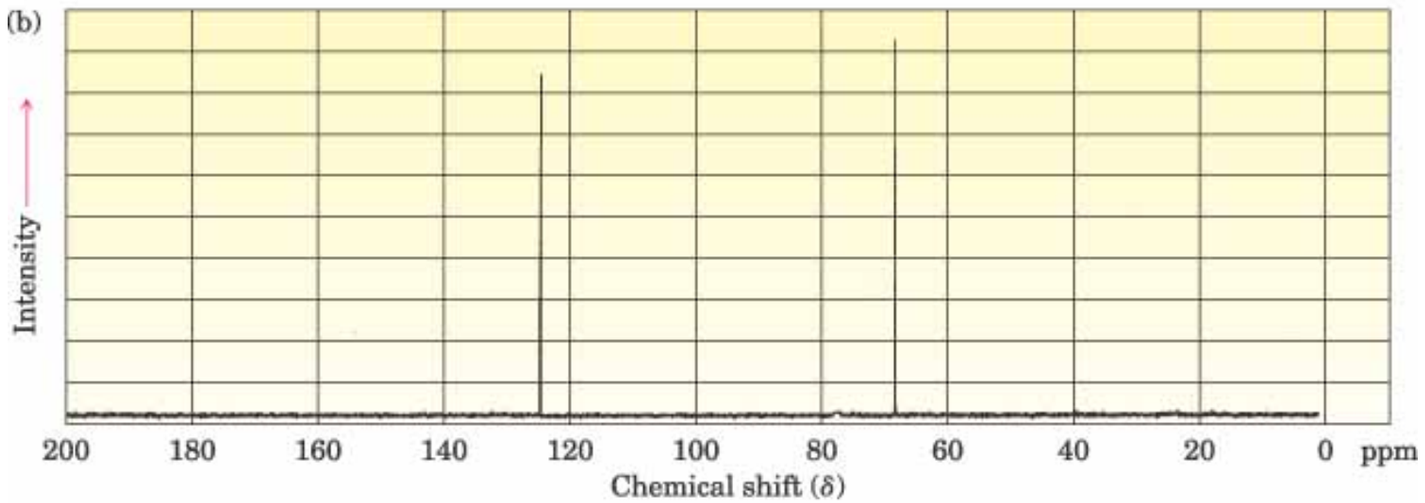


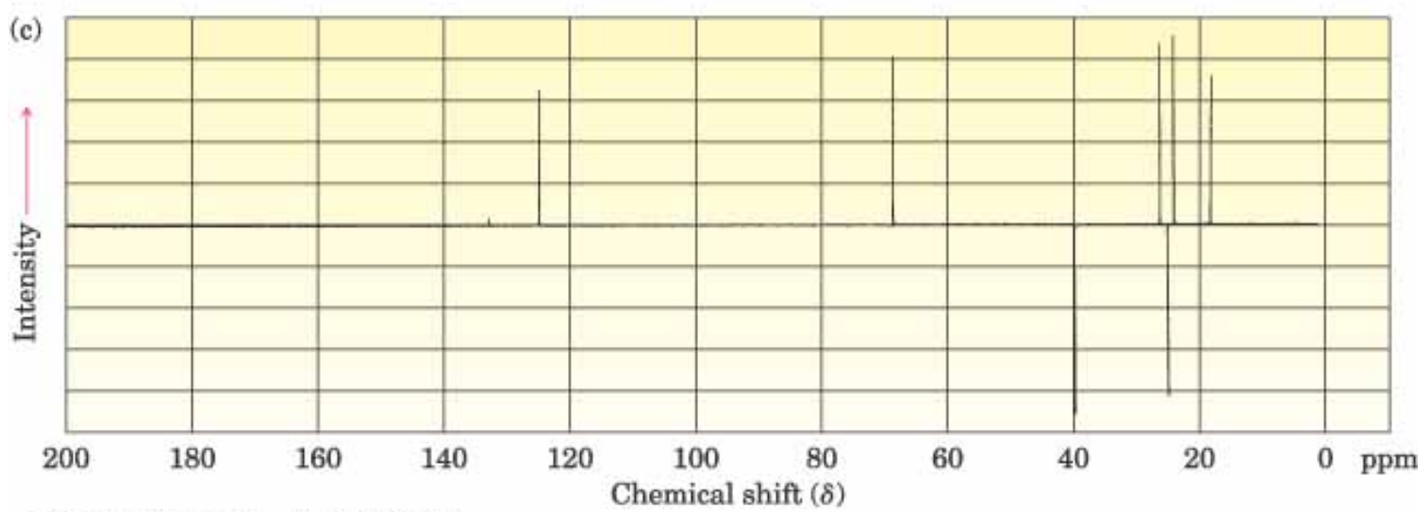
DEPT-C13



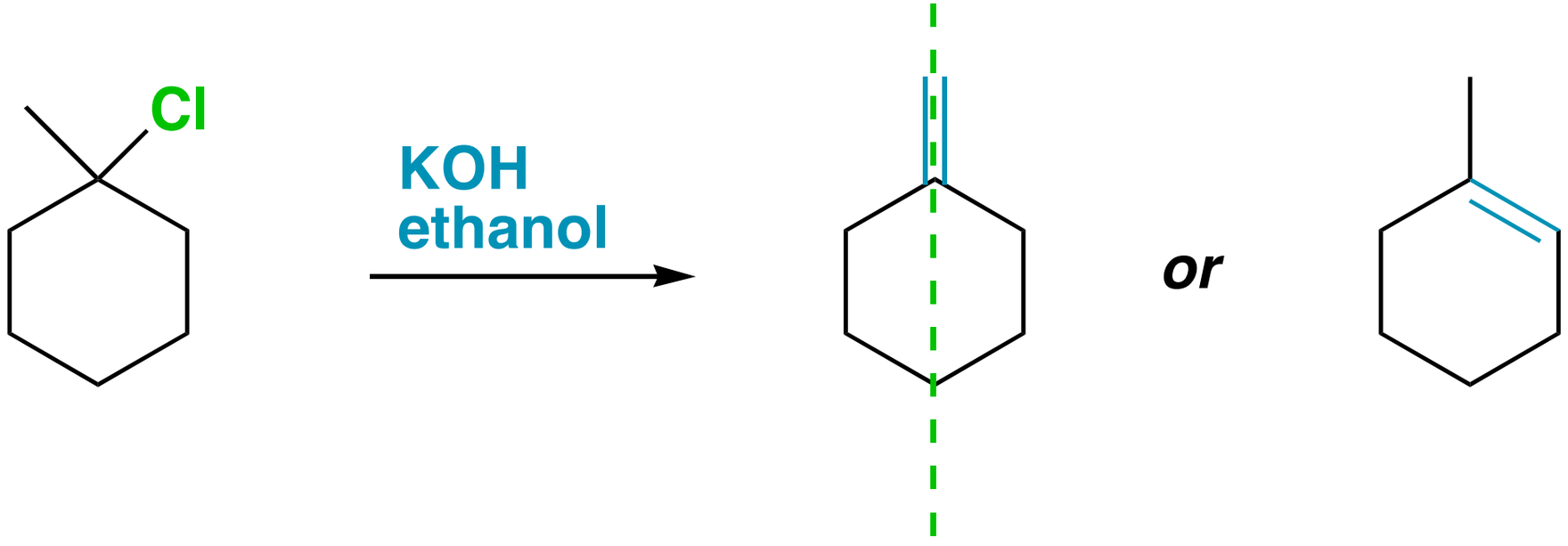
- A - normal C13
- B - CH carbons only
- C - Odd # up (CH3 and CH) Even # down (CH2)

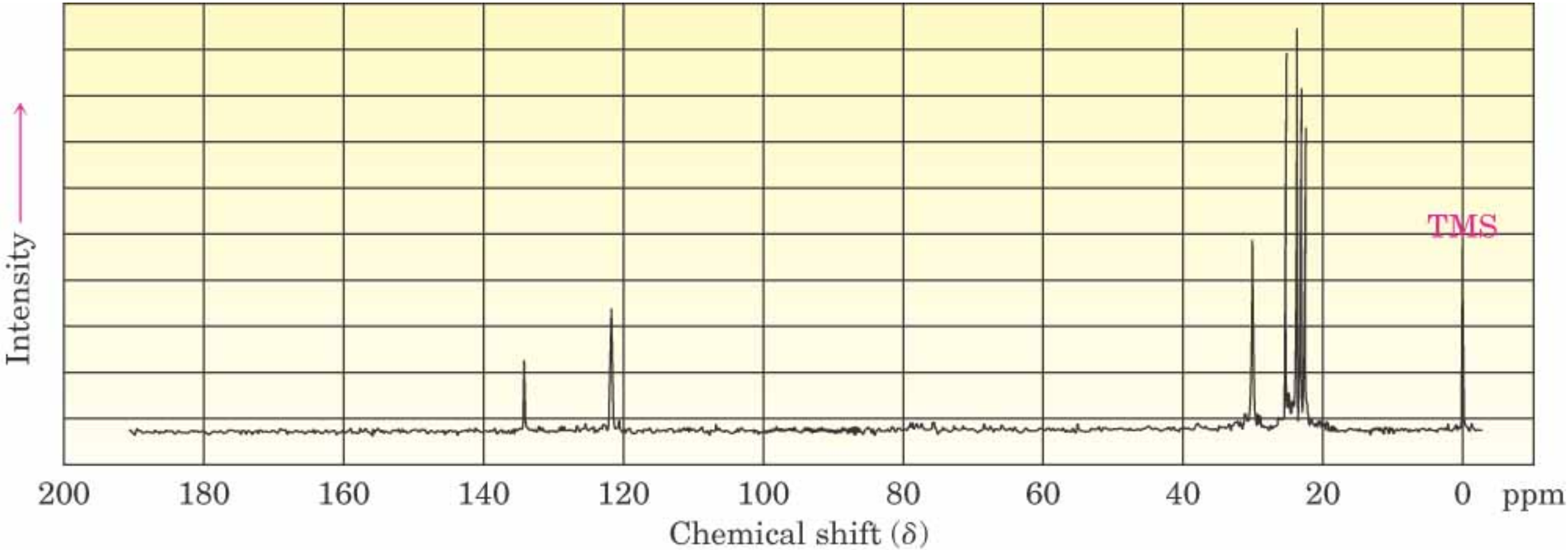




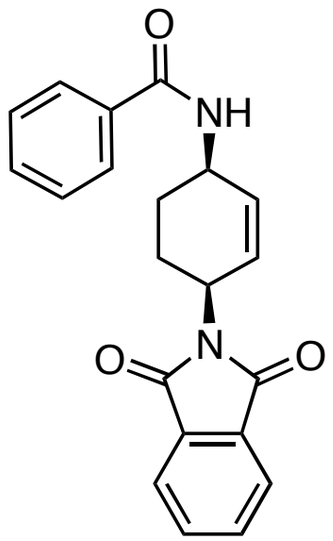


Example from 13.7

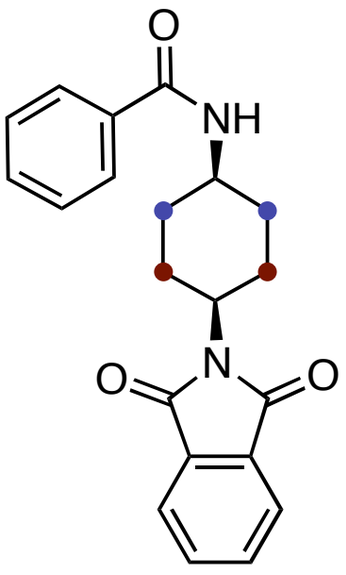




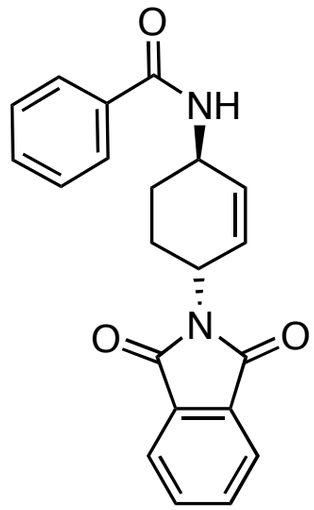
A Real Example



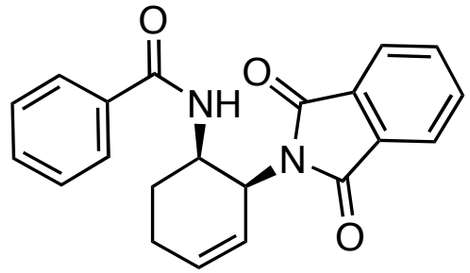
H_2, Pd/C



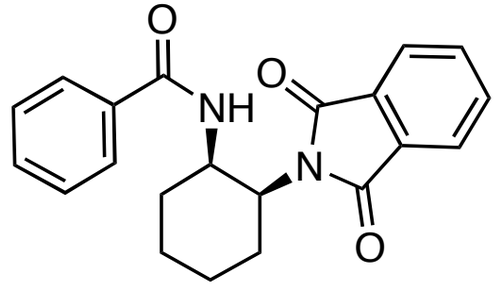
In the alkane region there would only be 4 peaks due to symmetry



OR

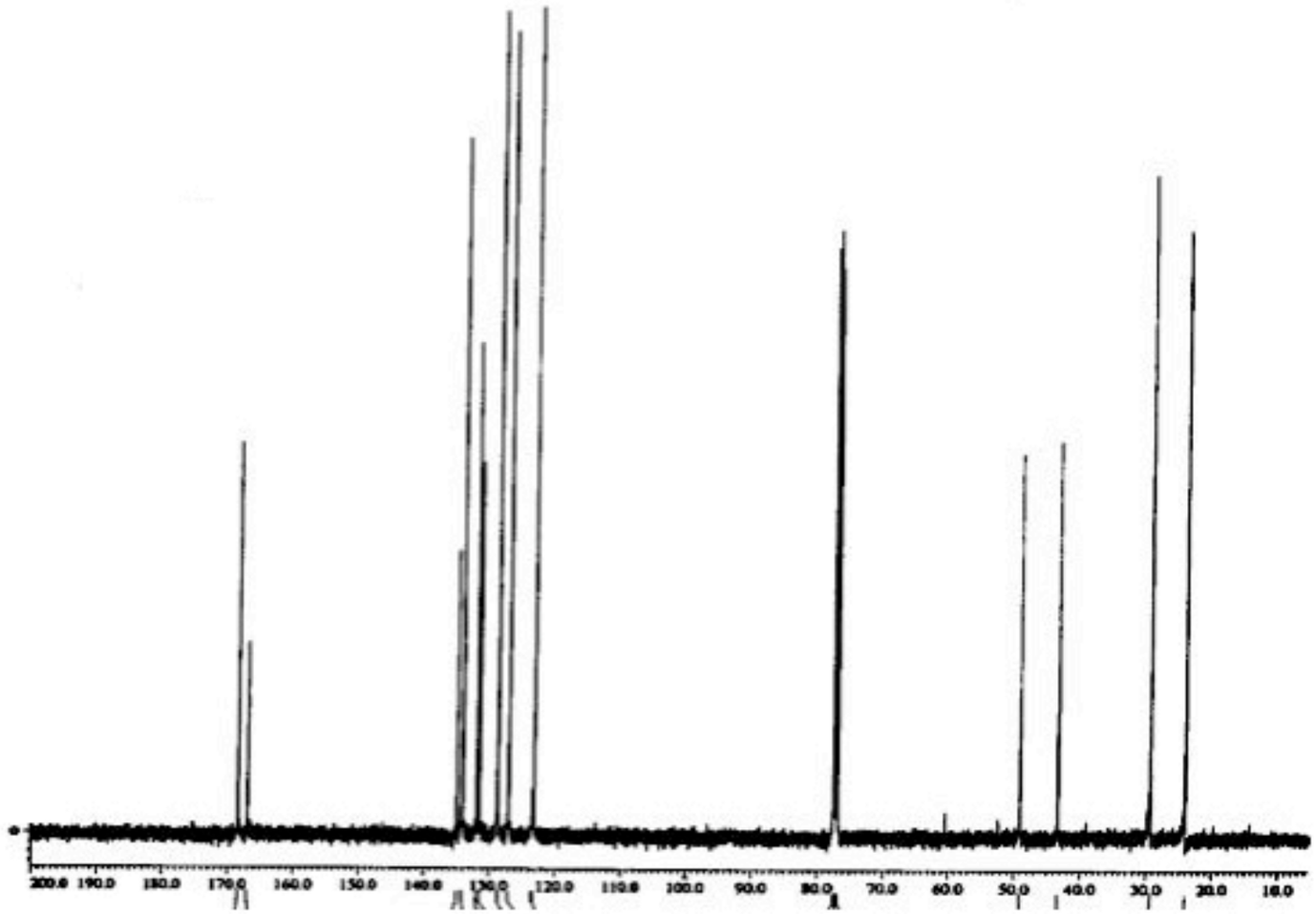


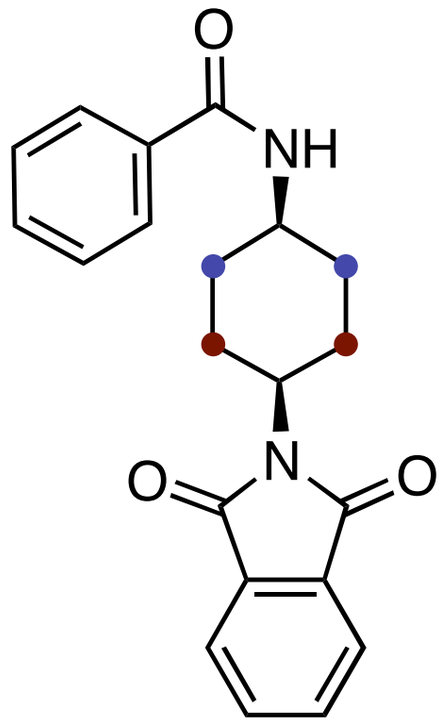
H_2, Pd/C

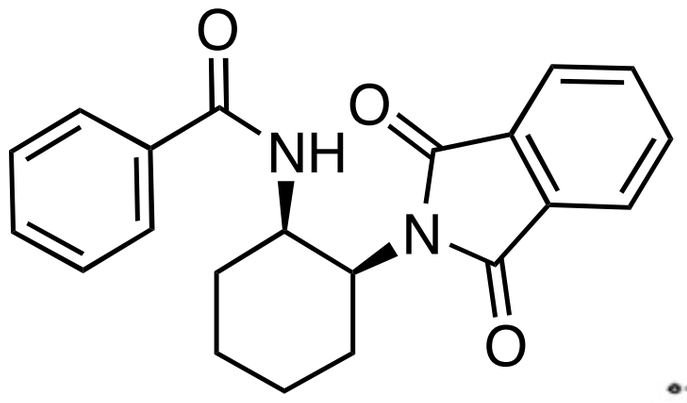


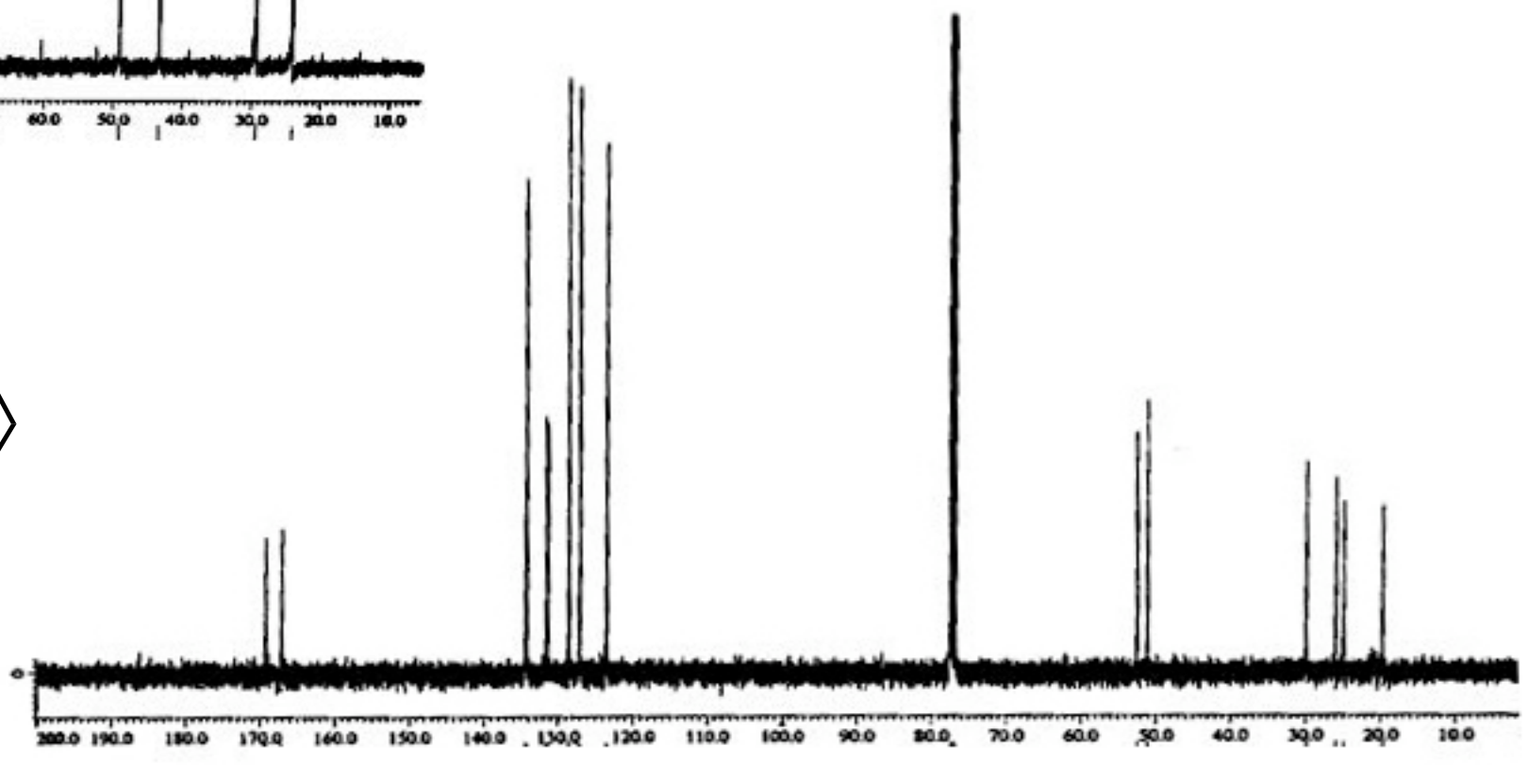
In the alkane region there would be 6 different peaks

The Answer Is . . .







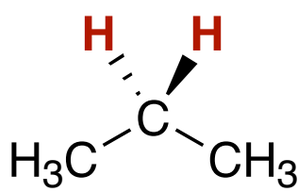


Proton NMR

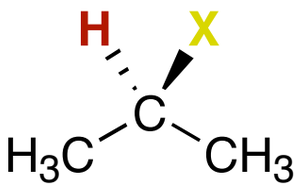
- Number of chemically different hydrogens
- Relative Ratios of protons (peak size)
- How many neighboring hydrogens
- Chemical shifts and functional groups

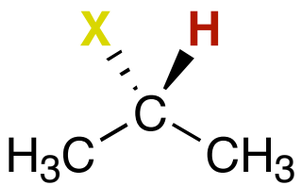
Proton Equivalency

Homotopic

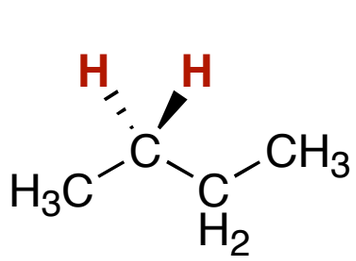


replace H's - same

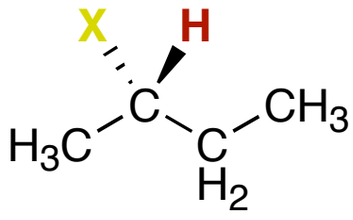


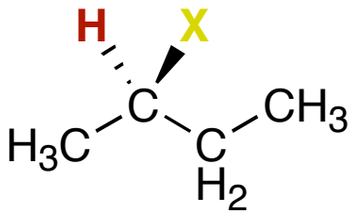


Enantiotopic

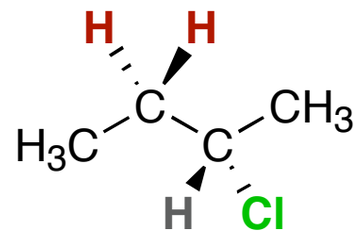


replace H's - enantiomers

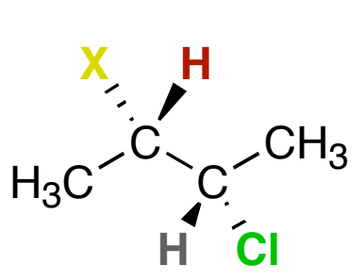


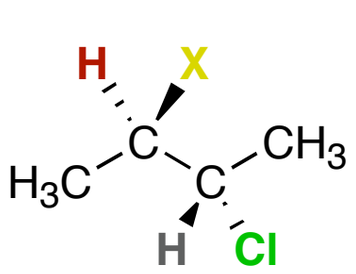


Diastereotopic



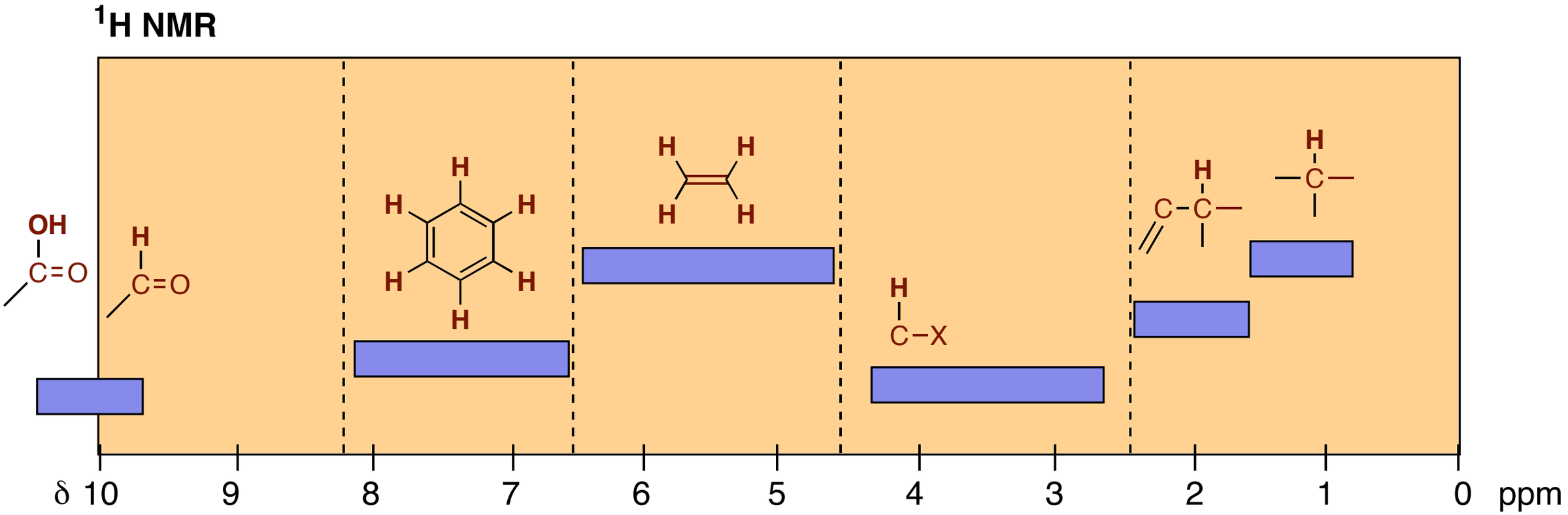
replace H's - diastereomers





Proton NMR Scale

Range 0-10 ppm



Methyl Acetate

Area under peak corresponds to the number of H's for that resonance