13.18 Carbon-13 NMR

SALIENT FACTS ABOUT ^{13}C NMR

^{12}C is not NMR-active I = 0

however….

^{13}C does have spin, I = 1/2 (odd mass)

^{13}C signals are 6000 times weaker than ^{1}H because:

1. Natural abundance of ^{13}C is small (1.08% of all C)
2. Magnetic moment of ^{13}C is small

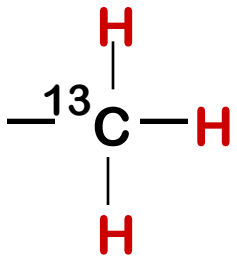
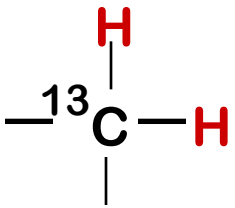
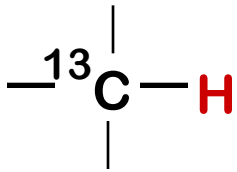
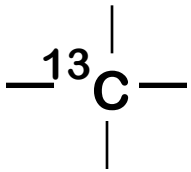
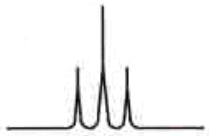
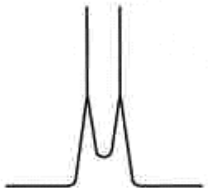
PULSED FT-NMR IS REQUIRED

The chemical shift range is larger than for protons

0 - 220 ppm

COUPLING TO ATTACHED PROTONS

COUPLING TO ATTACHED PROTONS

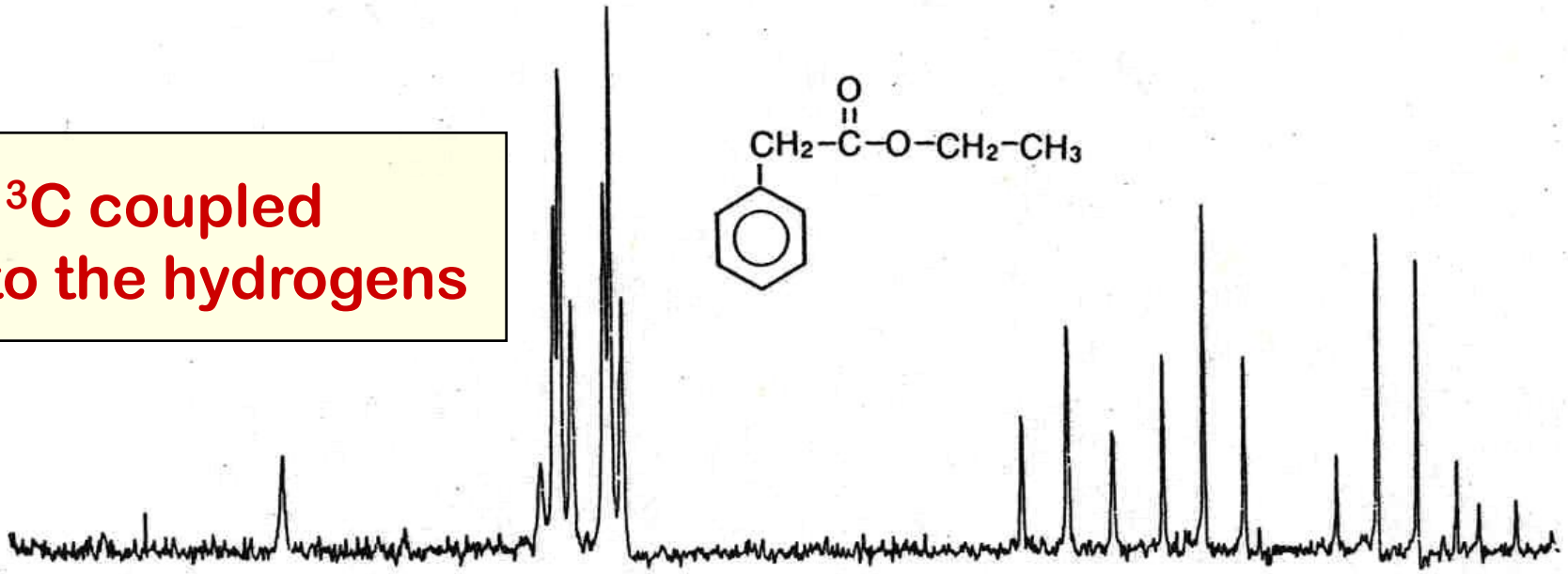
3 protons	2 protons	1 proton	0 protons
			
n+1 = 4	n+1 = 3	n+1 = 2	n+1 = 1
			
Methyl carbon	Methylene carbon	Methine carbon	Quaternary carbon

The effect of attached protons on ^{13}C resonances

(n+1 rule applies) (J's are large ~ 100 - 200 Hz)

ETHYL PHENYLACETATE

^{13}C coupled to the hydrogens

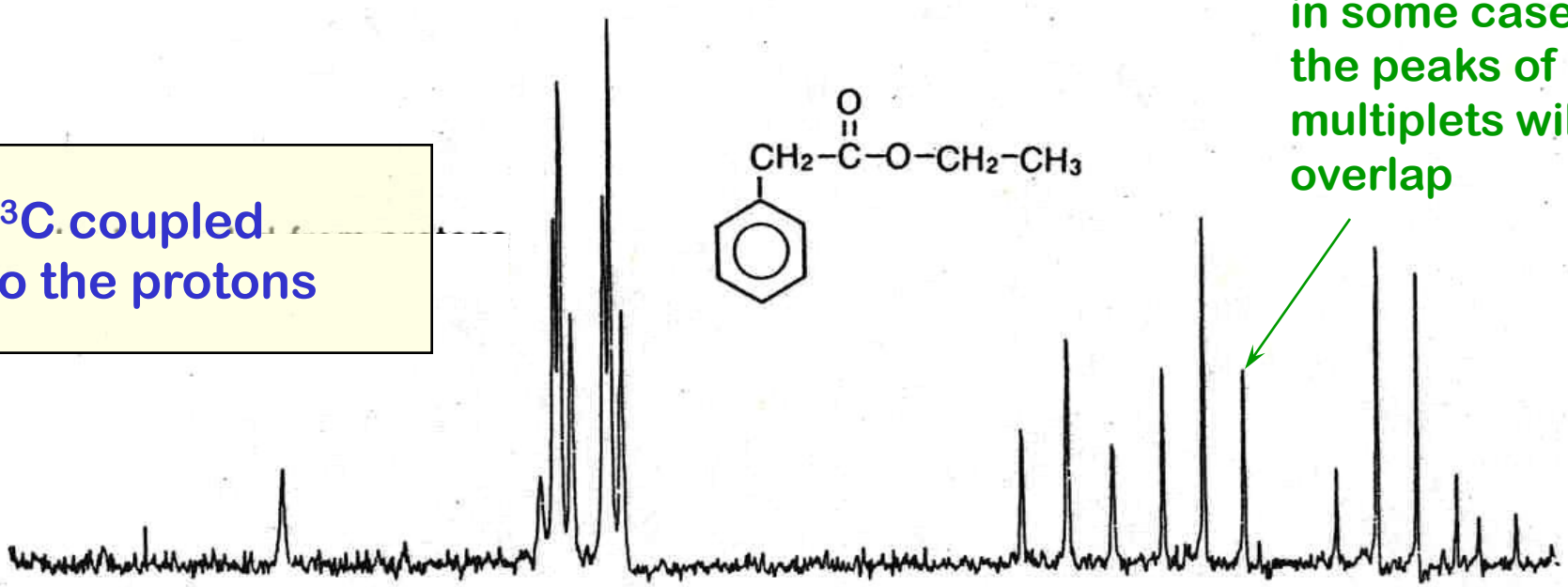


DECOUPLED SPECTRA

ETHYL PHENYLACETATE

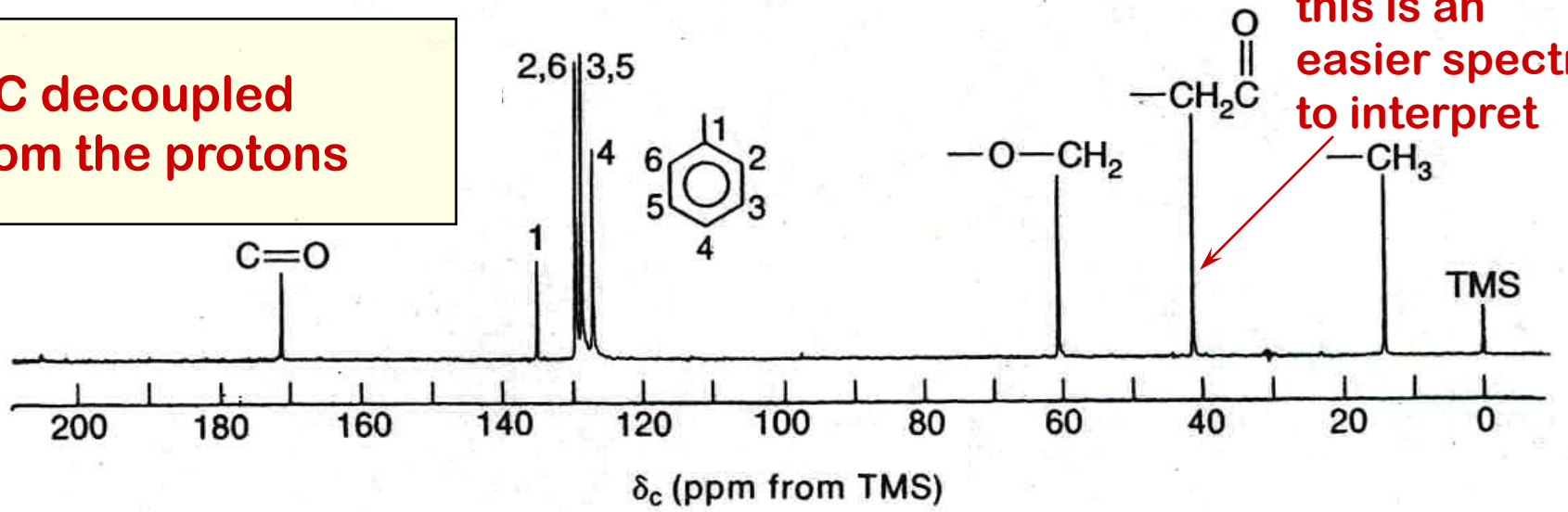
^{13}C coupled to the protons

in some cases the peaks of the multiplets will overlap

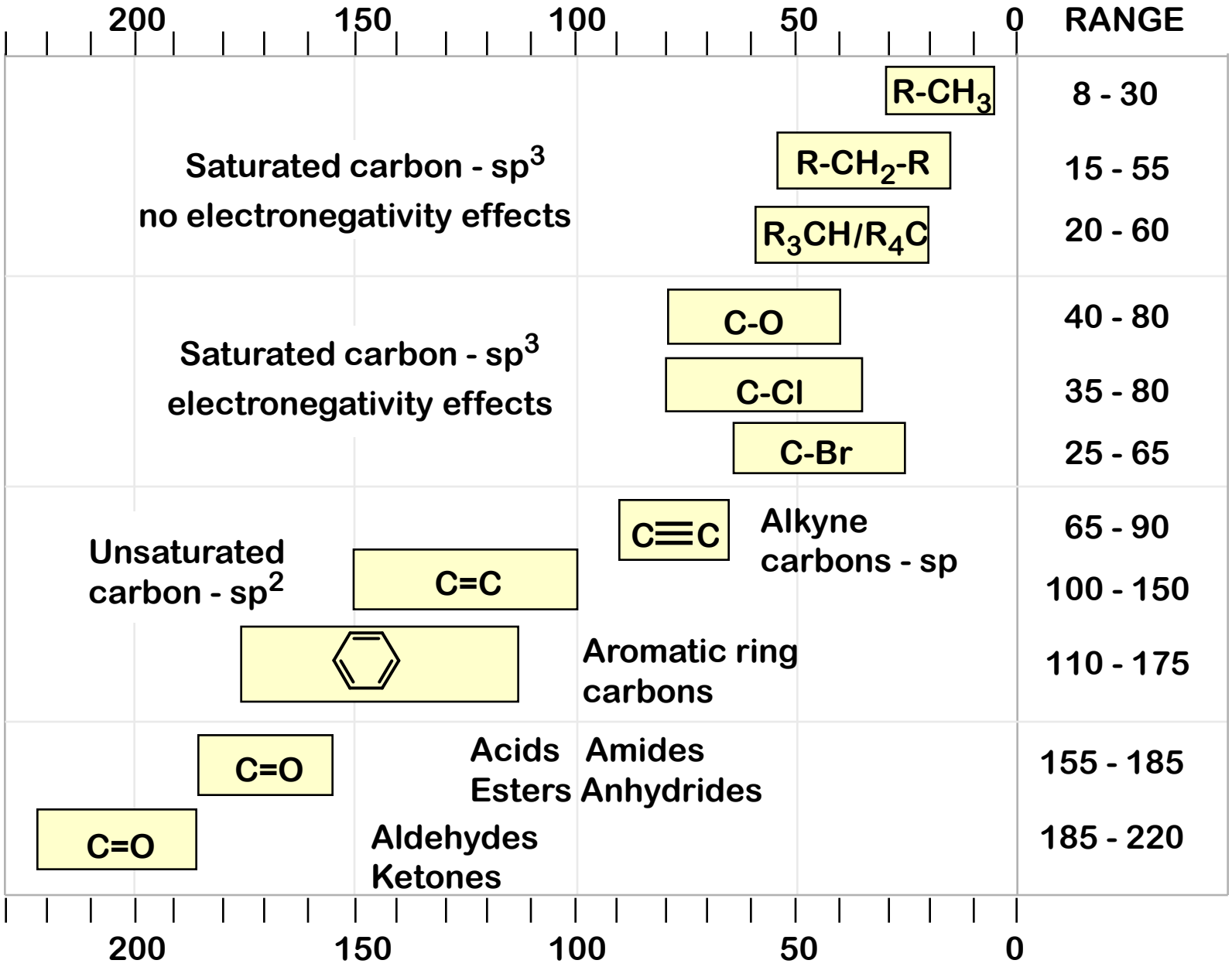


^{13}C decoupled from the protons

this is an easier spectrum to interpret



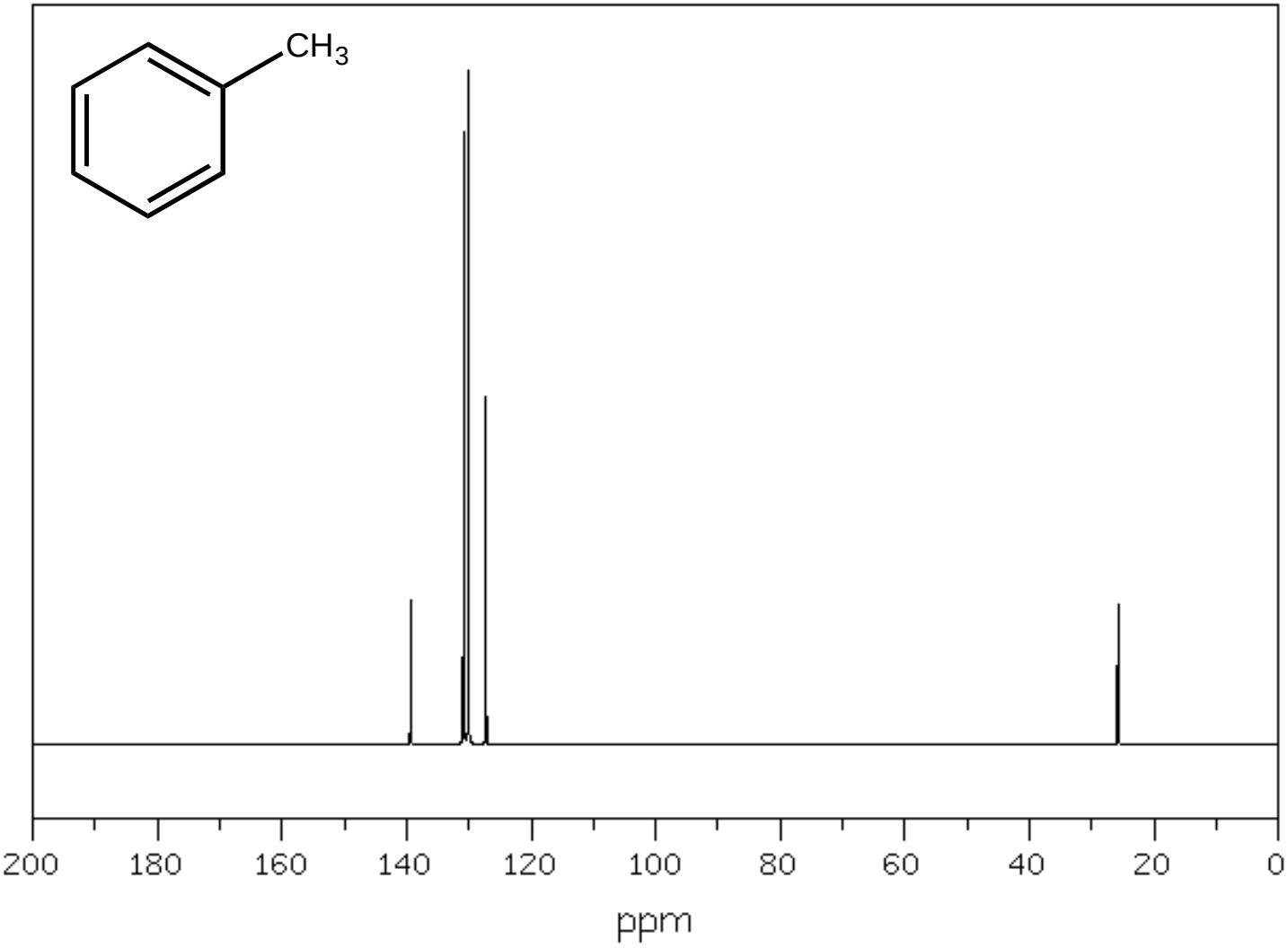
CHEMICAL SHIFTS OF ^{13}C ATOMS



Correlation chart for ^{13}C Chemical Shifts (ppm)

SPECTRA

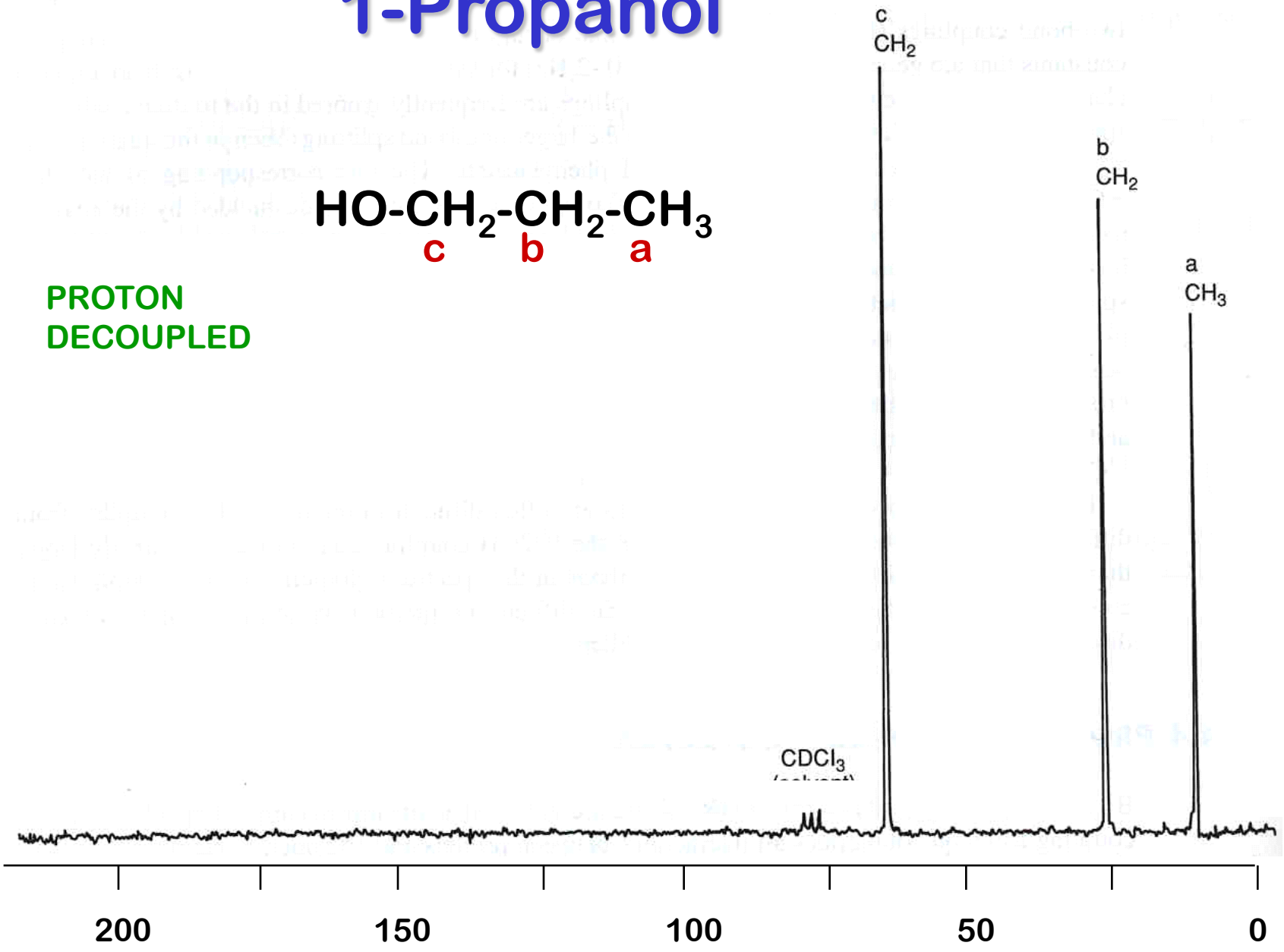
Toluene



1-Propanol

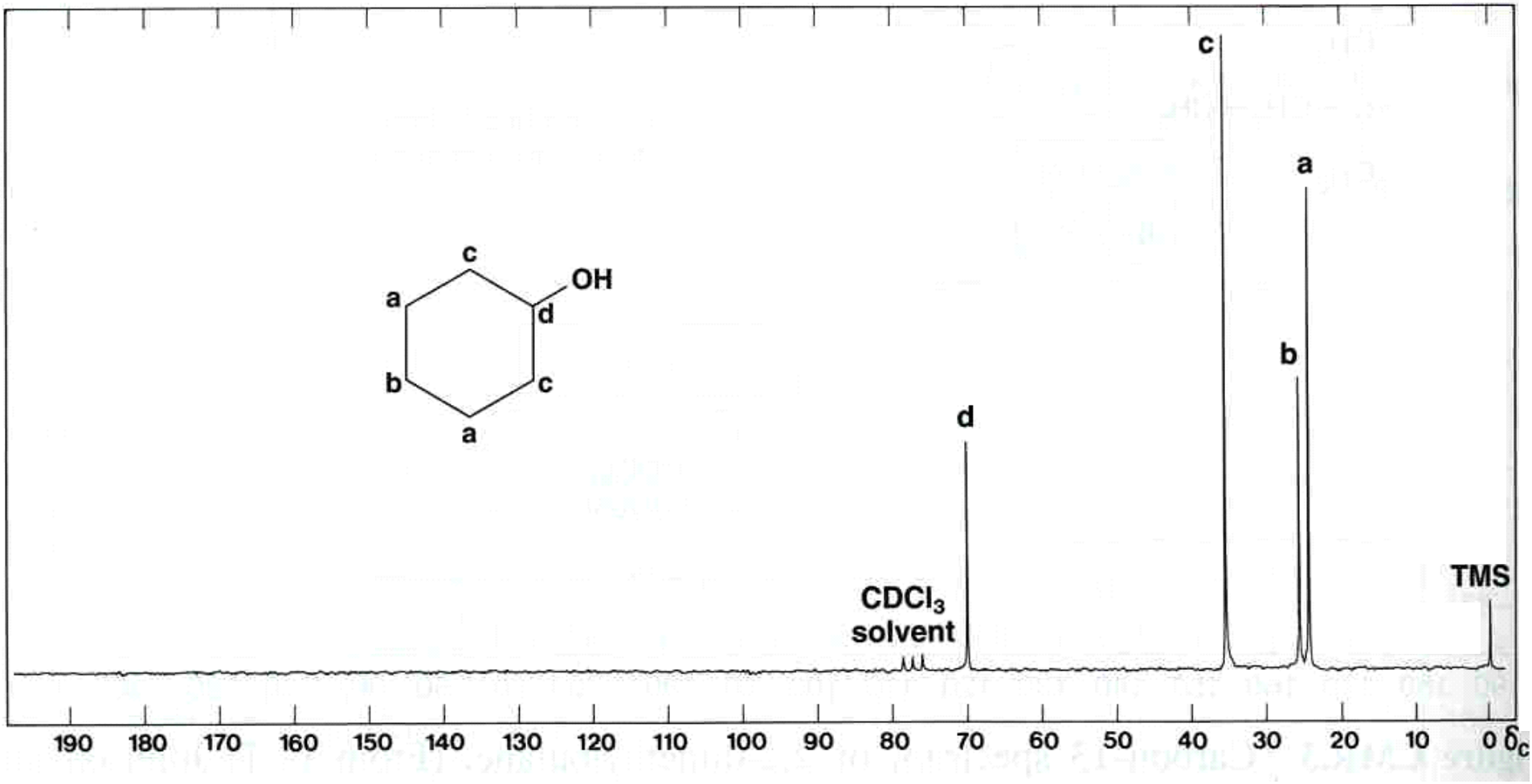
$HO\text{-}\underset{c}{CH_2}\text{-}\underset{b}{CH_2}\text{-}\underset{a}{CH_3}$

PROTON DECOUPLED

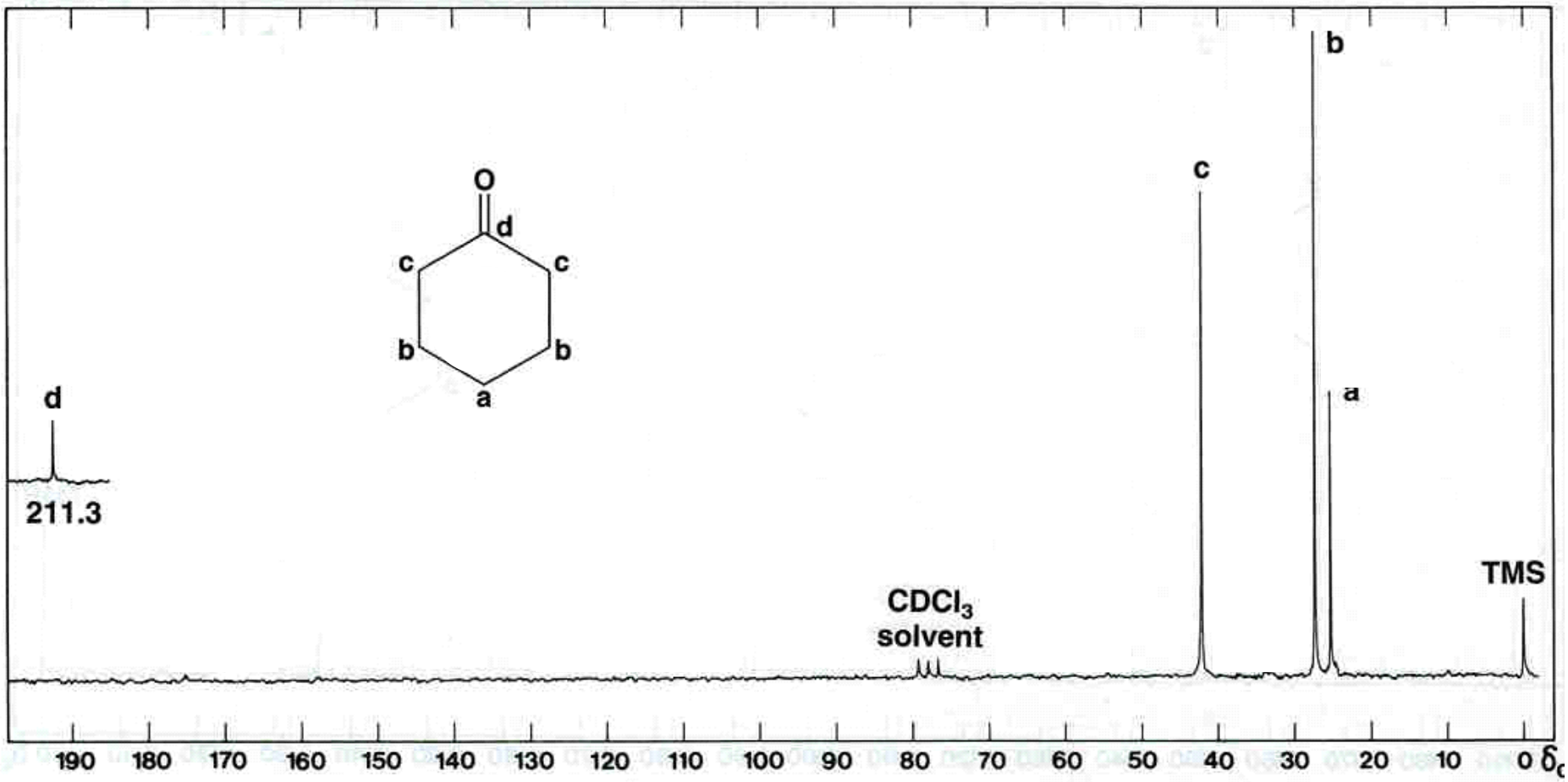


Proton-decoupled 13C spectrum of 1-propanol (22.5 MHz)

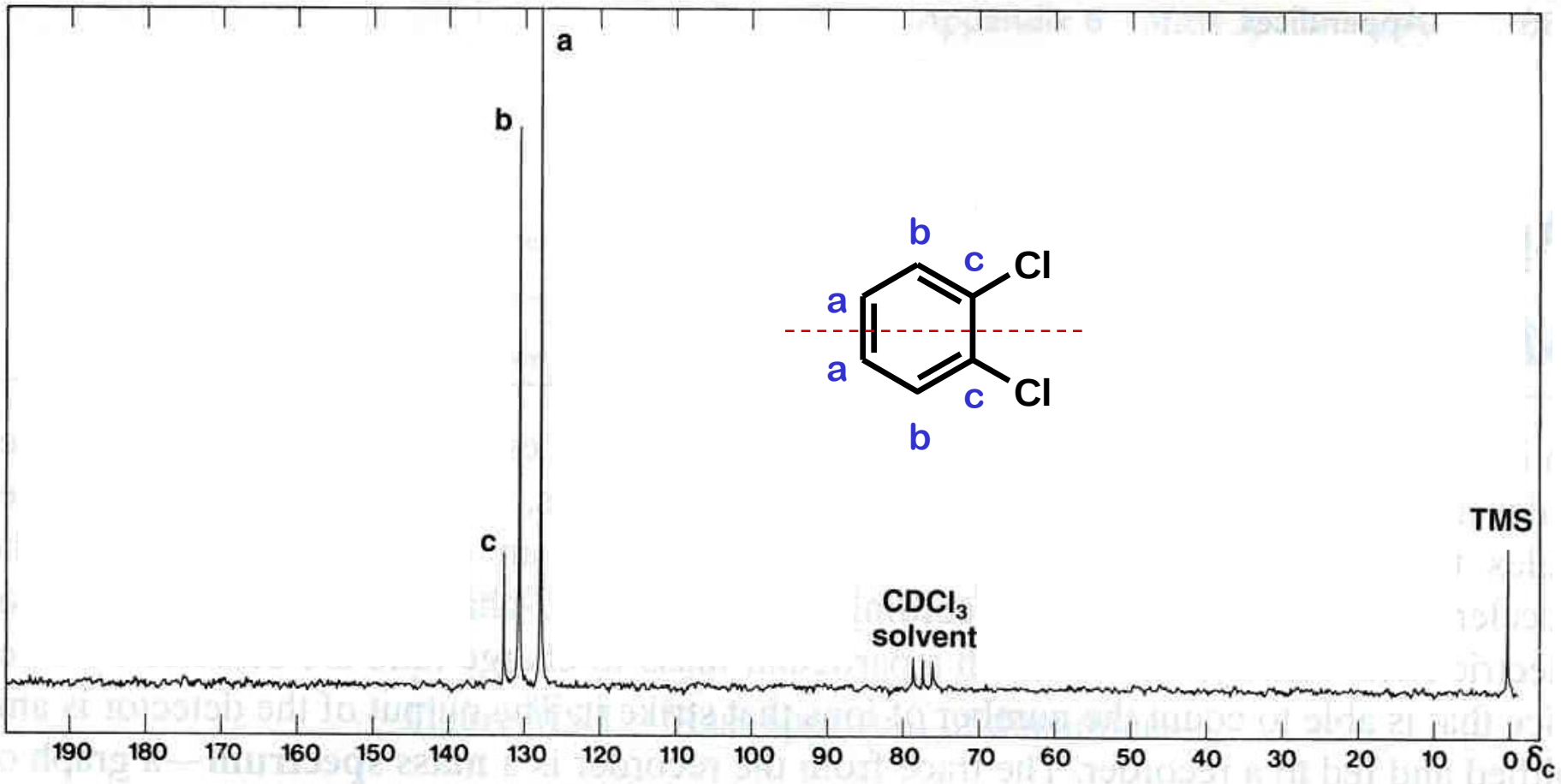
Cyclohexanol



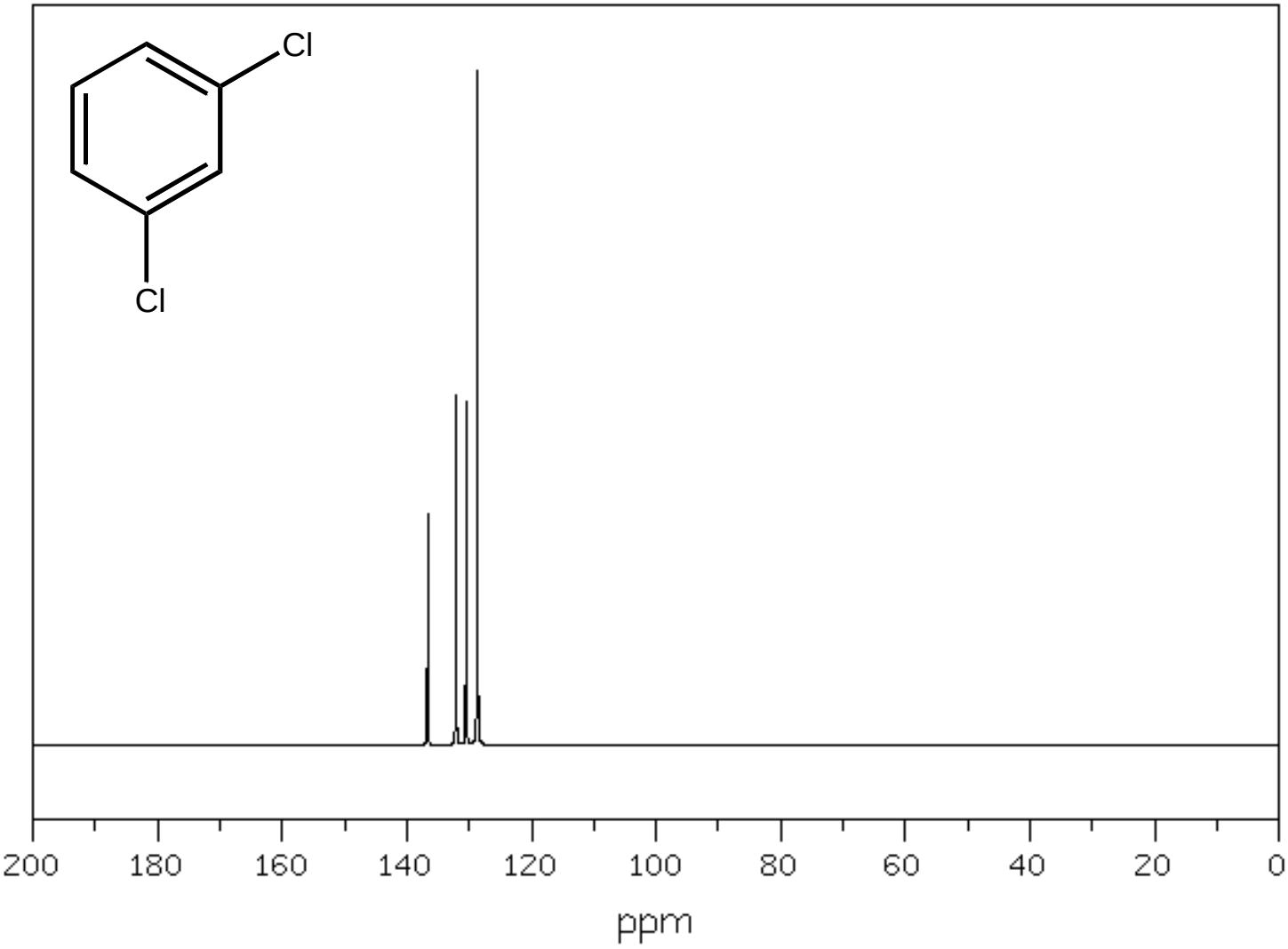
Cyclohexanone



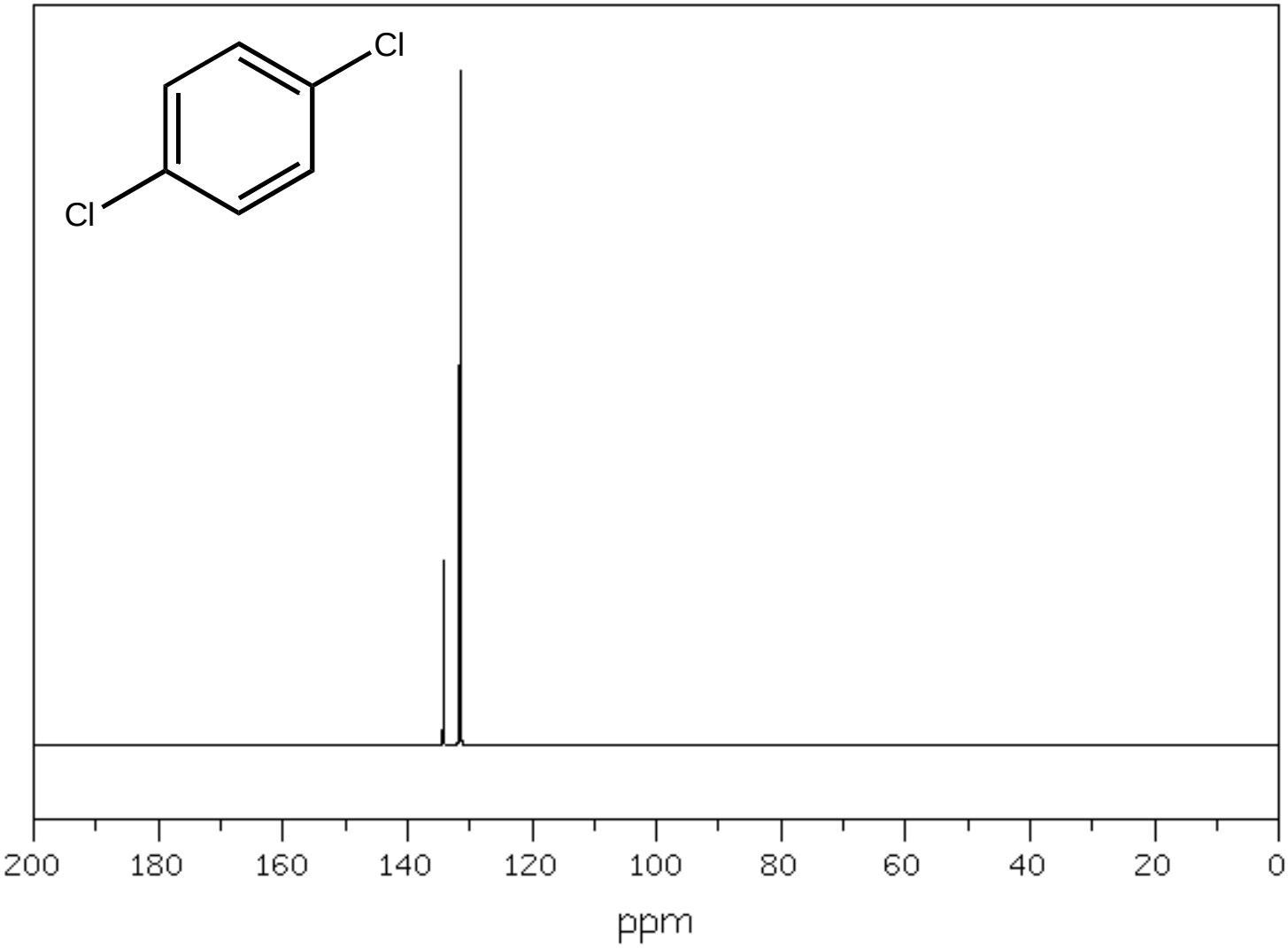
1,2-Dichlorobenzene



1,3-Dichlolrobenzene



1,4-Dichlorobenzene



Exercício

	Composto A	Composto B	Composto C
Fórmula Molecular	$C_7H_{14}O$	$C_6H_{14}O$	$C_5H_6N_2$
Deslocamento químico (ppm), multiplicidade e quantidade	23, q (2)	11, q (2)	16, t (2)
	28, d	23, t (2)	22, t
	29, q	44, d	119, s
	33, t	65, t	
	42, t		
	206, s		