Qualitative Organic Analysis – CH 351

NMR Spectroscopy - 2

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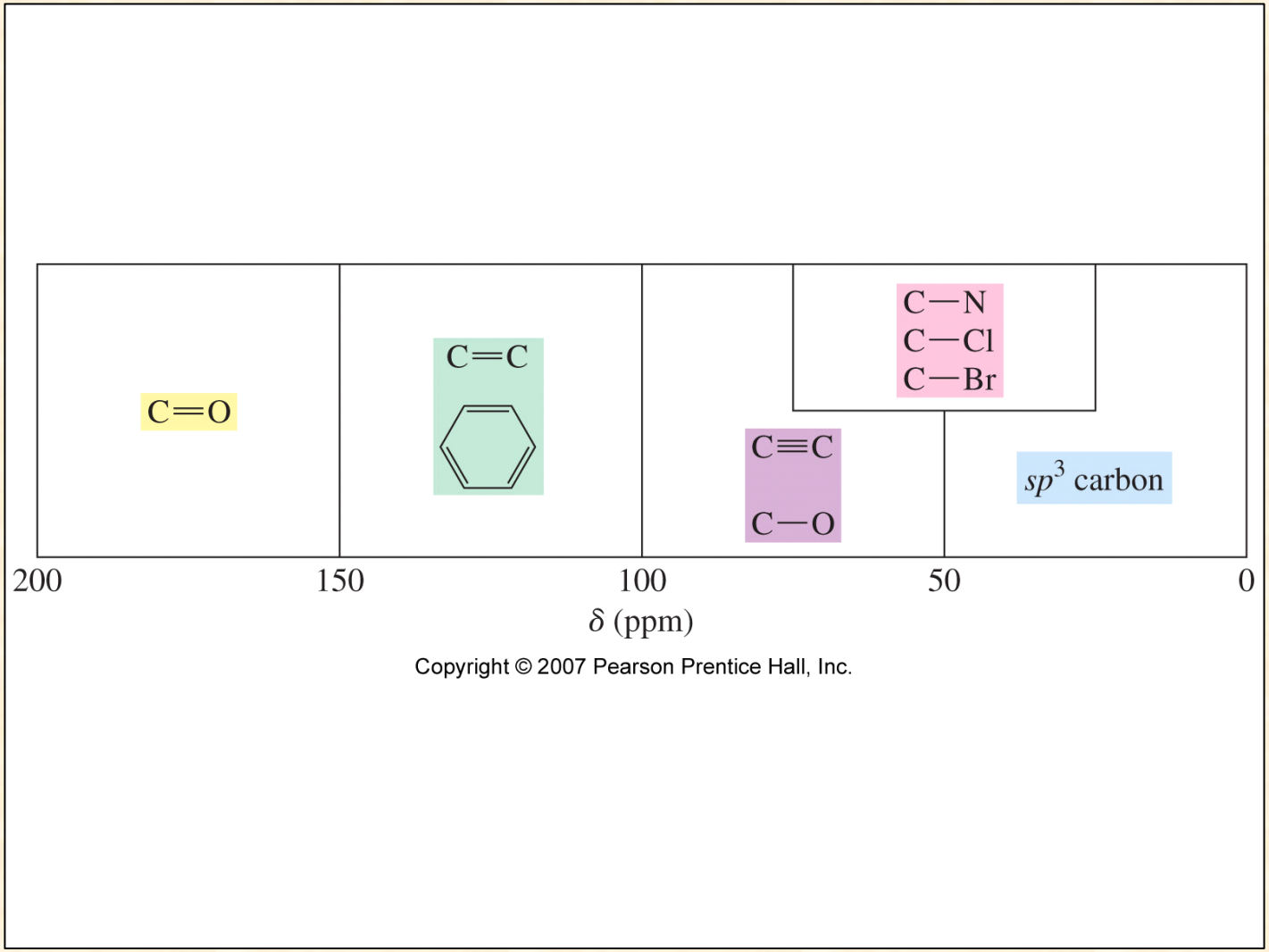
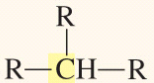
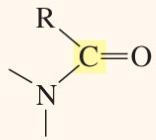
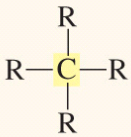
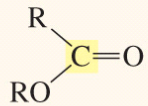
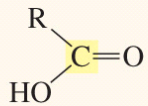
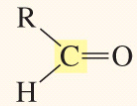
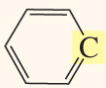
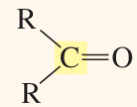
^{13}C-NMR Spectroscopy

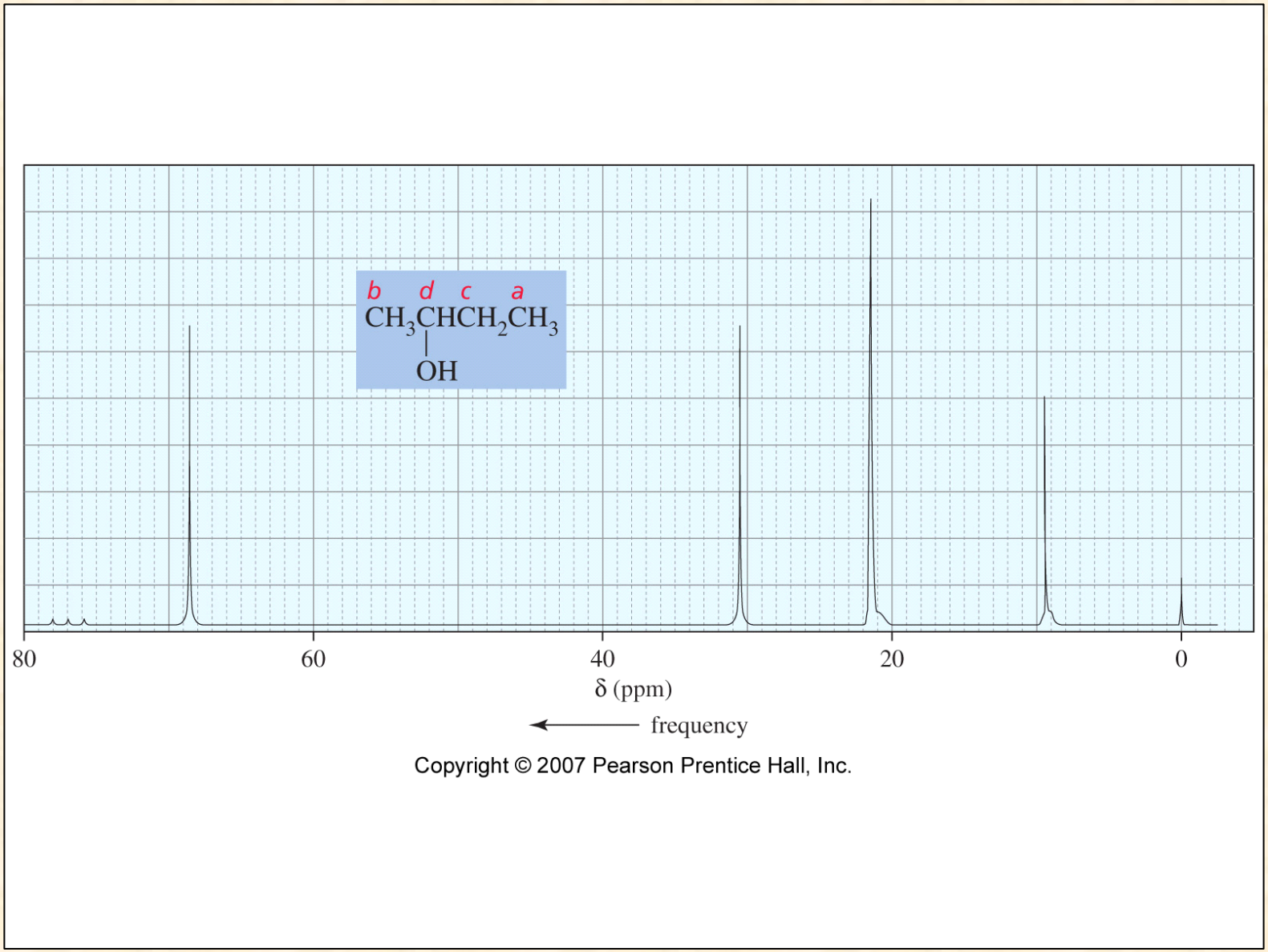


^{13}C-NMR Spectroscopy

Table 13.4 Approximate Values of Chemical Shifts for ^{13}C NMR

Type of carbon	Approximate chemical shift (ppm)	Type of carbon	Approximate chemical shift (ppm)
$(CH_3)_4Si$	0	C—I	0–40
R—CH_3	8–35	C—Br	25–65
R—CH_2—R	15–50	C—Cl C—N C—O	35–80 40–60 50–80
	20–60		165–175
	30–40		165–175
≡C	65–85		175–185
=C	100–150		190–200
	110–170		205–220

^{13}C-NMR Spectroscopy



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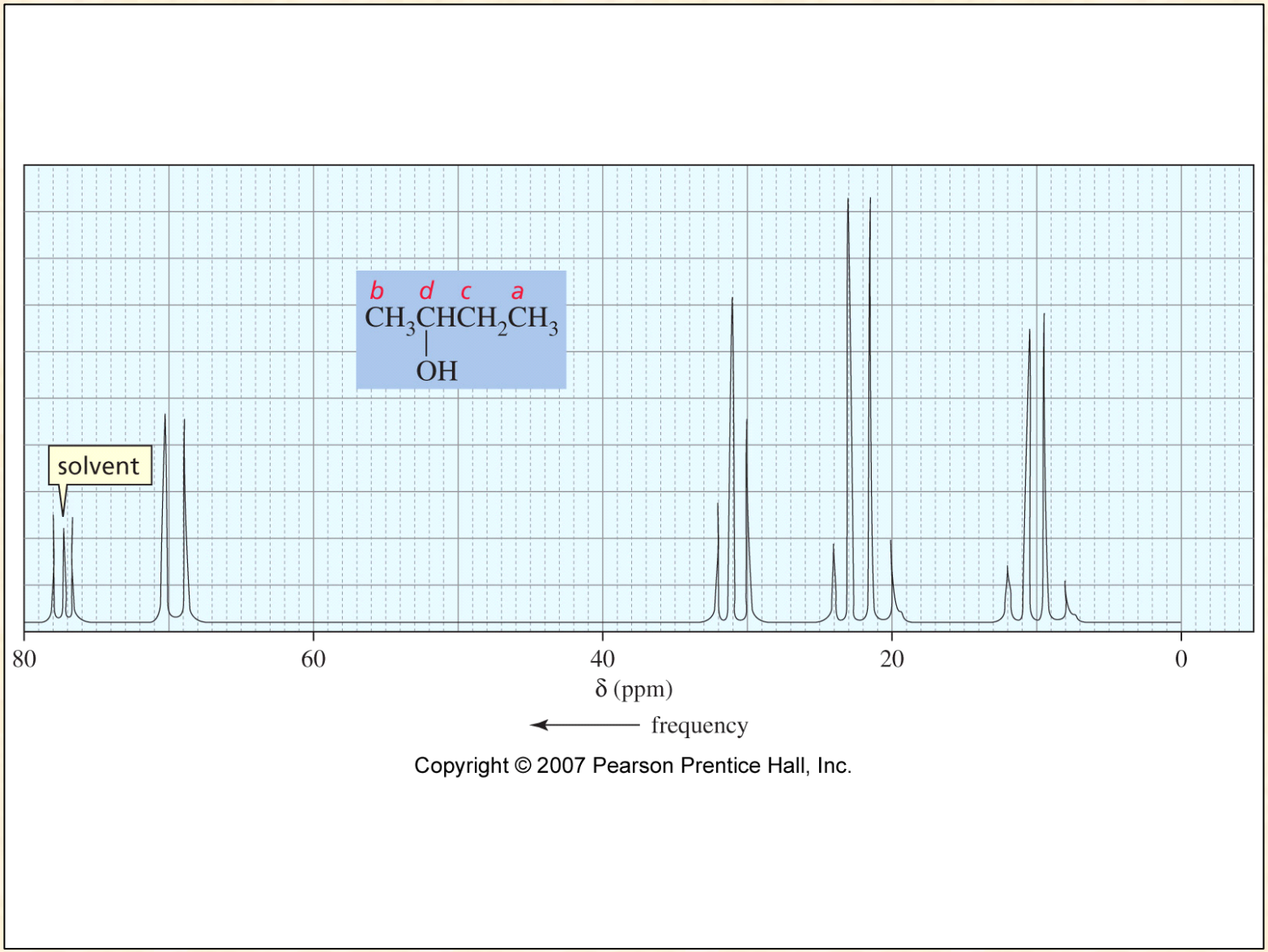

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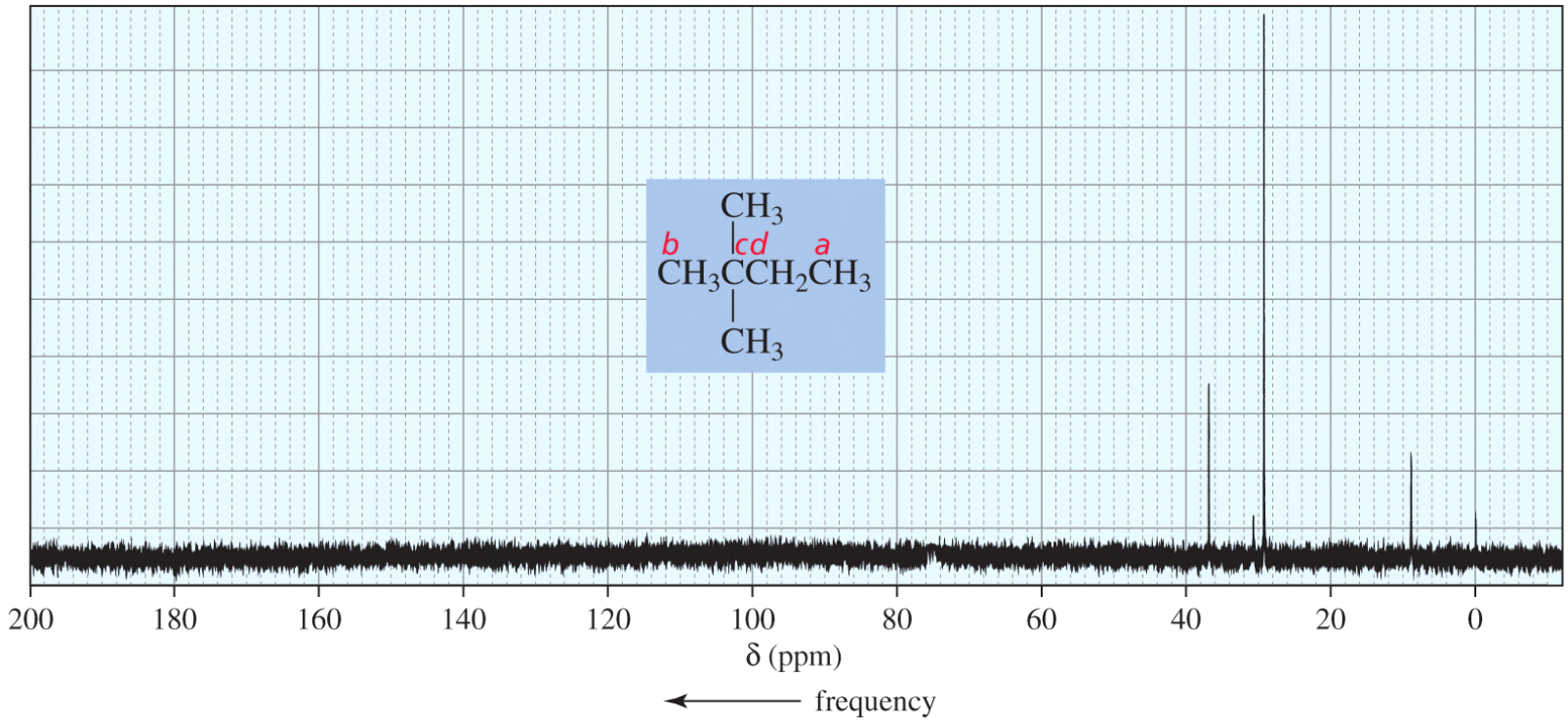

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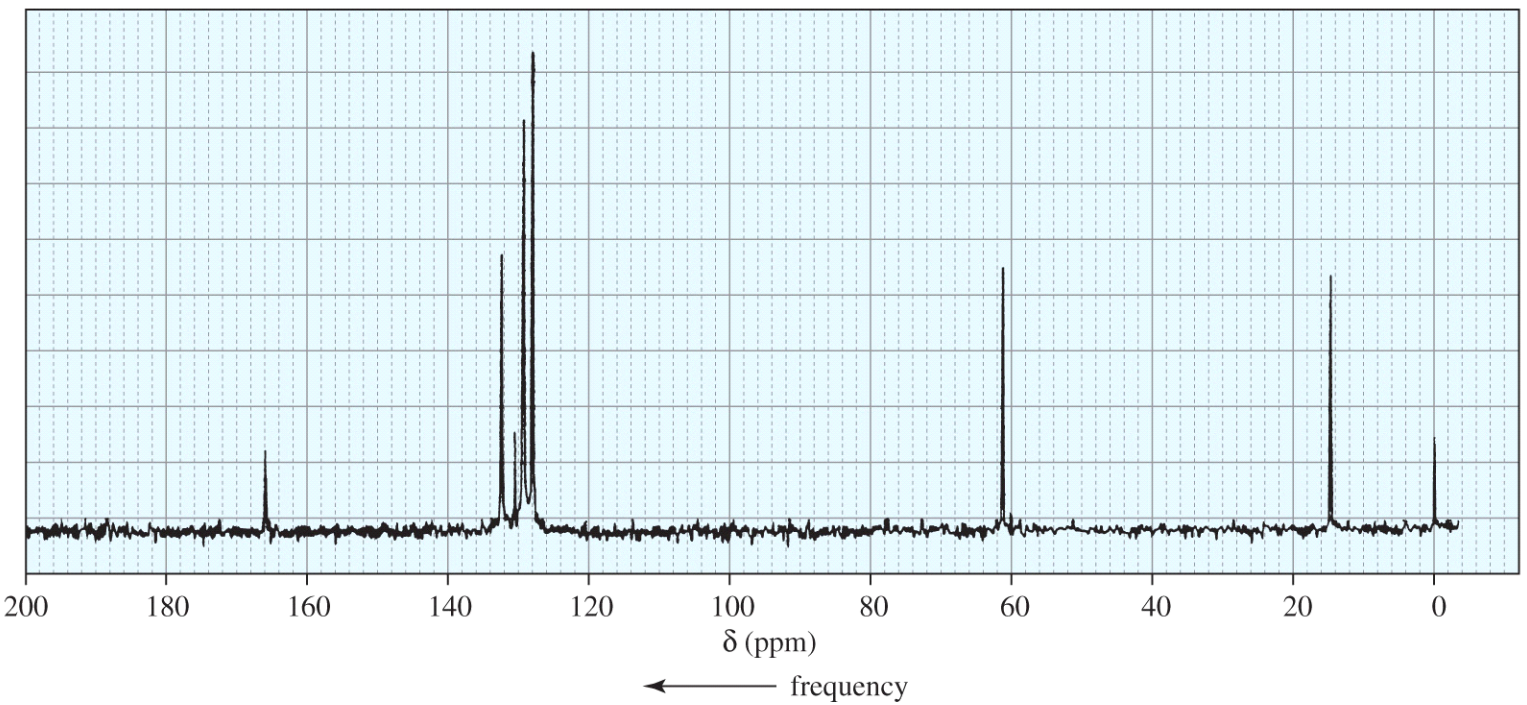

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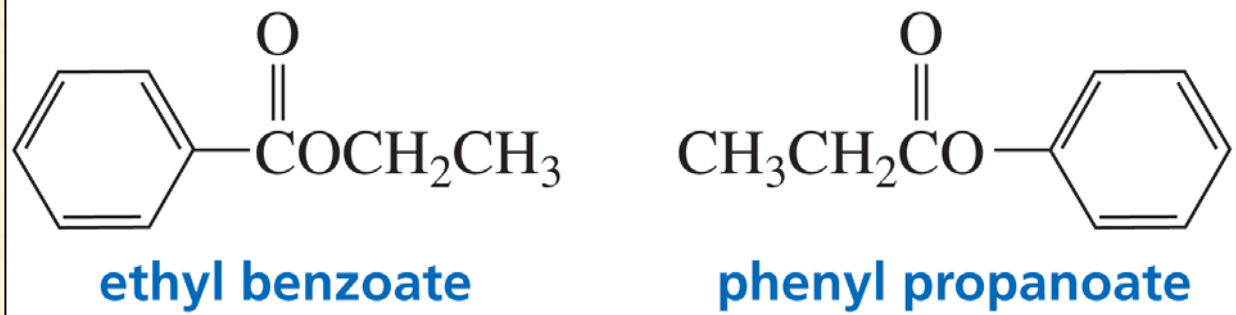


ethyl benzoate phenyl propanoate

^{19}F-NMR Spectroscopy

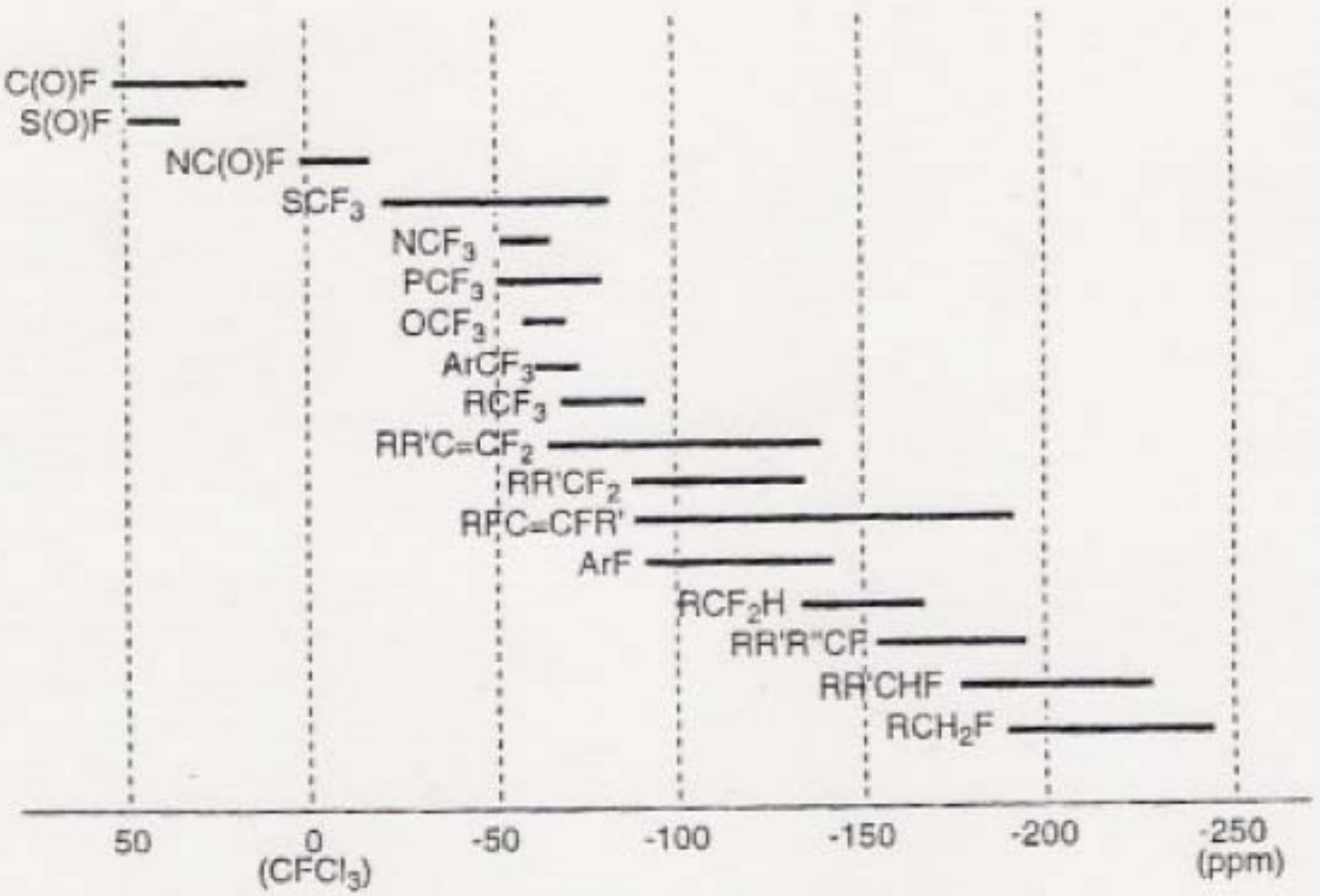


Fig. 1.15. ^{19}F-NMR chemical shifts of fluorine substituents

^{19}F-NMR Spectroscopy

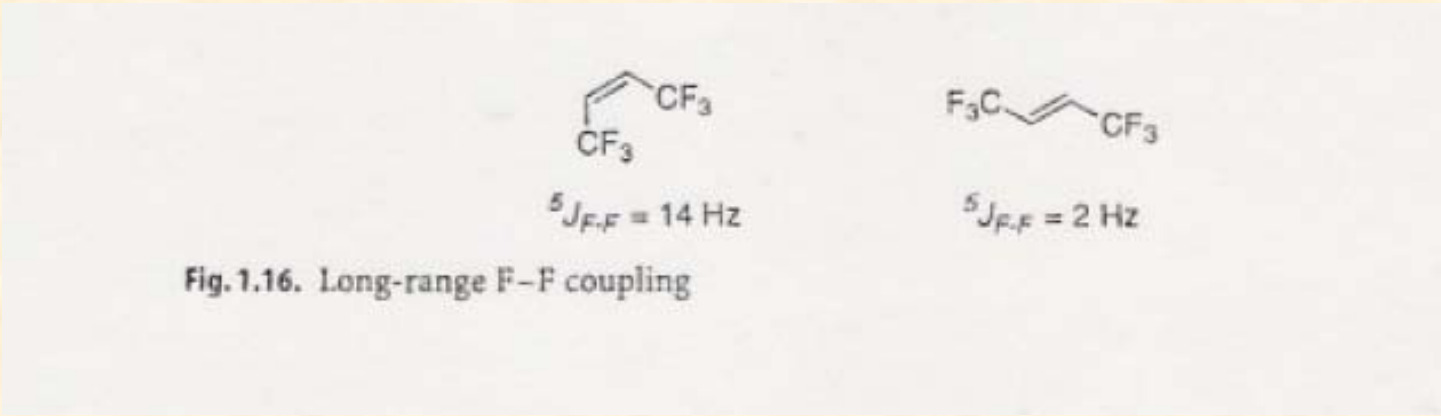
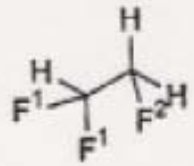


Fig. 1.16. Long-range F–F coupling

^{19}F-NMR Spectroscopy

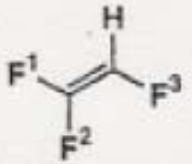
- Fluoroalkane



F^1; -129.9 ppm ($^2J_{H\text{-}F}$ = 55 Hz, $^3J_{F\text{-}F}$ = 18 Hz, $^3J_{H\text{-}F}$ = 13 Hz)

F^2; -288.9 ppm ($^2J_{H\text{-}F}$ = 46 Hz, $^3J_{F\text{-}F}$ = 18 Hz, $^3J_{H\text{-}F}$ = 6 Hz)

- Fluoroalkene



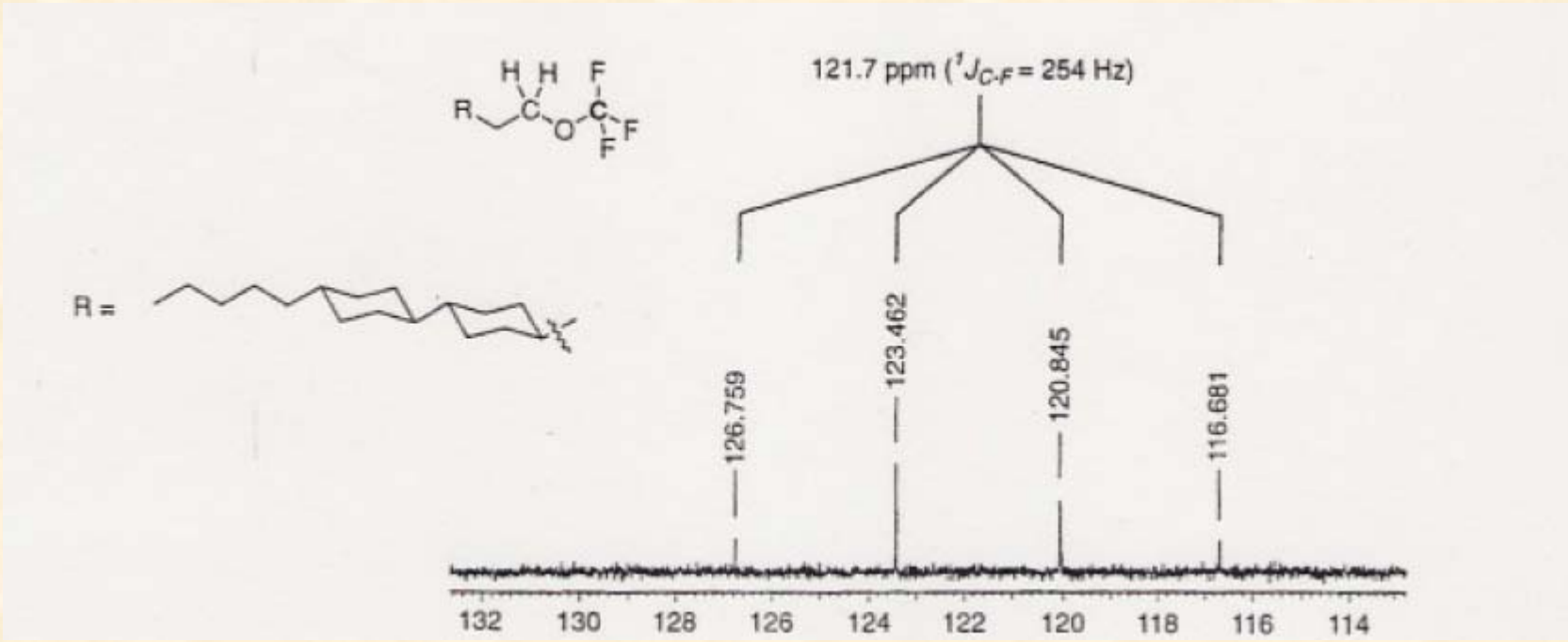
F^1: -125.7 ppm ($^2J_{F\text{-}F}$ = 87 Hz, $^3J_{F\text{-}F\,(trans\text{-})}$ = 119 Hz, $^3J_{H\text{-}F\,(cis\text{-})}$ = 4 Hz)

F^2: -99.7 ppm ($^2J_{F\text{-}F}$ = 87 Hz, $^3J_{F\text{-}F\,(cis\text{-})}$ = 33 Hz, $^3J_{H\text{-}F\,(trans\text{-})}$ = 13 Hz)

F^3: -205.0 ppm ($^2J_{H\text{-}F}$ = 71 Hz, $^3J_{F\text{-}F\,(cis\text{-})}$ = 33 Hz, $^3J_{F\text{-}F\,(trans\text{-})}$ = 119 Hz)

Fig. 1.18. ^{19}F-NMR data of fluoroalkanes and -alkenes

^{19}F-NMR Spectroscopy



^{19}F-NMR Spectroscopy

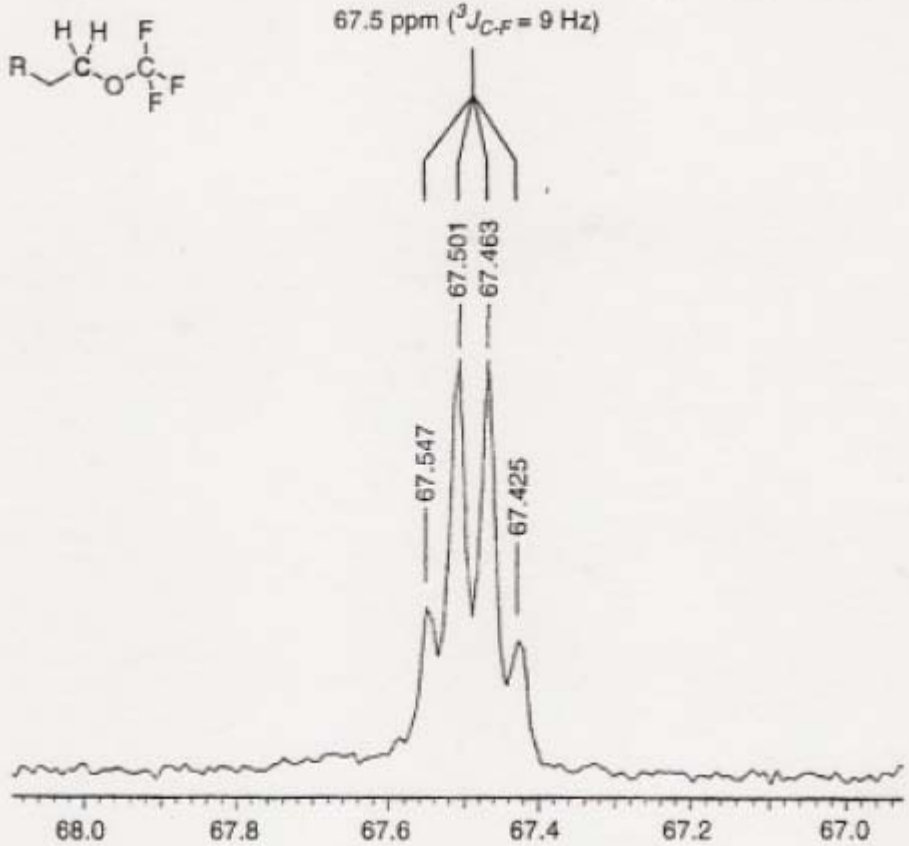


Fig. 1.17. ^{13}C-NMR spectra of C–F coupling