



Qualitative Organic Analysis – CH 351

NMR Spectroscopy - 2

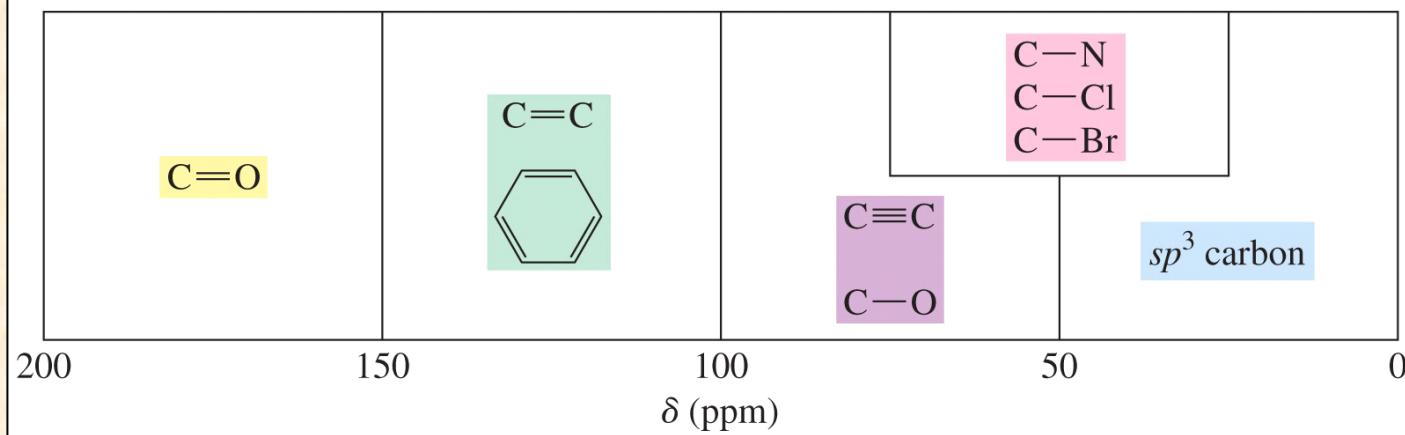
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^{13}C -NMR Spectroscopy



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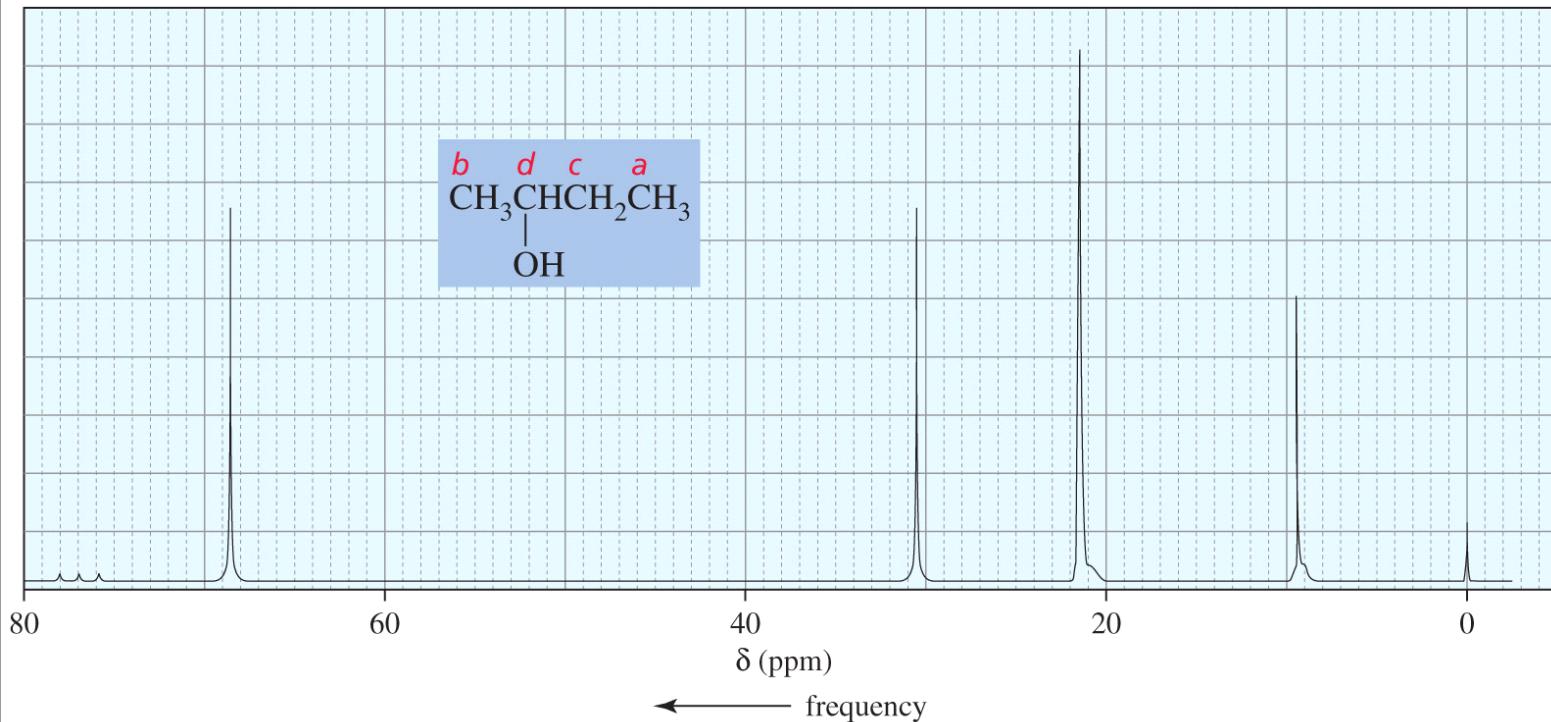
¹³C-NMR Spectroscopy



Table 13.4 Approximate Values of Chemical Shifts for ¹³C NMR

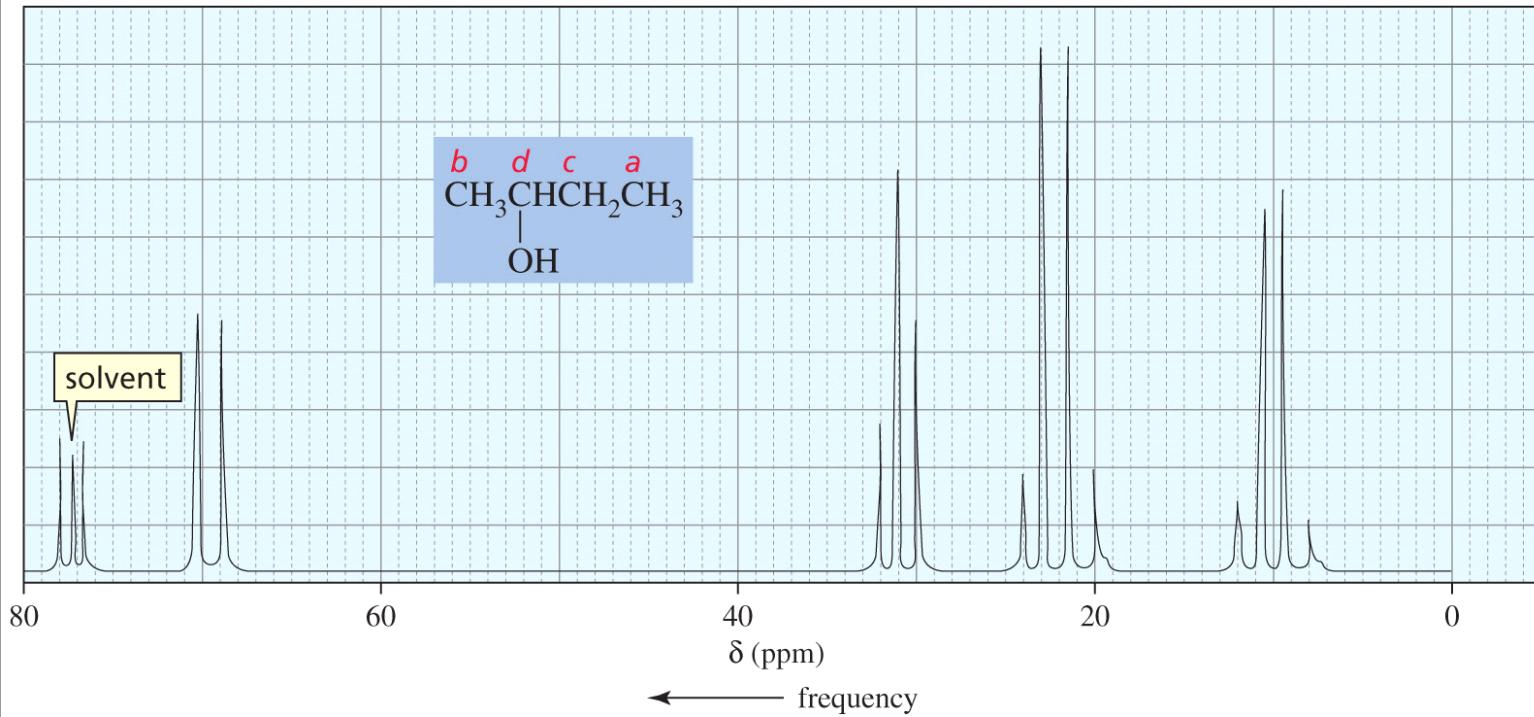
Type of carbon	Approximate chemical shift (ppm)	Type of carbon	Approximate chemical shift (ppm)
(CH ₃) ₄ Si	0	C—I	0–40
R—CH ₃	8–35	C—Br	25–65
R—CH ₂ —R	15–50	C—Cl C—N C—O	35–80 40–60 50–80
$\begin{array}{c} R \\ \\ R—CH—R \end{array}$	20–60	$\begin{array}{c} R \\ \\ R—C=O \\ \\ N \\ \end{array}$	165–175
$\begin{array}{c} R \\ \\ R—C—R \\ \\ R \end{array}$	30–40	$\begin{array}{c} R \\ \\ R—C=O \\ \\ RO \end{array}$	165–175
≡C	65–85	$\begin{array}{c} R \\ \\ R—C=O \\ \\ HO \end{array}$	175–185
=C	100–150	$\begin{array}{c} R \\ \\ R—C=O \\ \\ H \end{array}$	190–200
$\begin{array}{c} \text{C} \\ \\ \text{C}_6\text{H}_5 \end{array}$	110–170	$\begin{array}{c} R \\ \\ R—C=O \end{array}$	205–220

^{13}C -NMR Spectroscopy



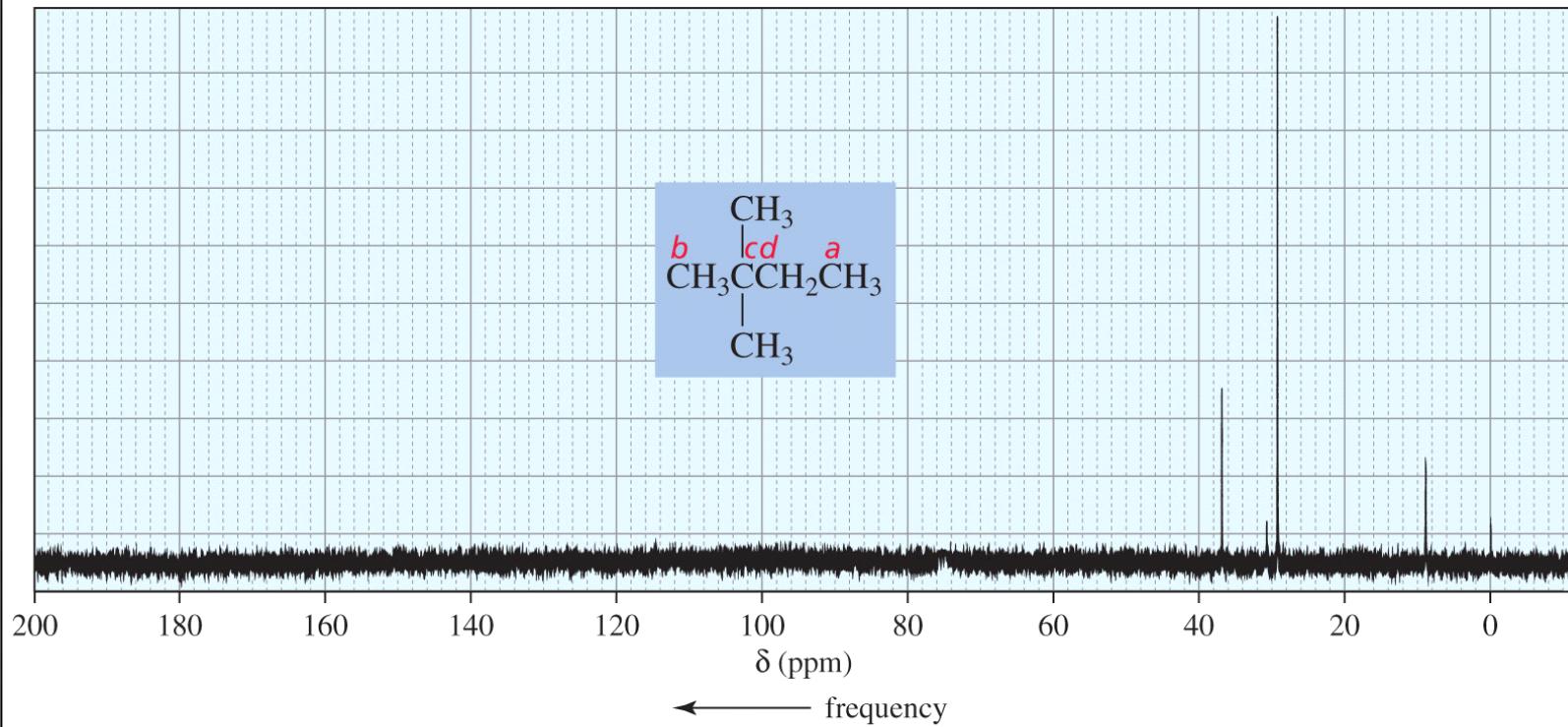
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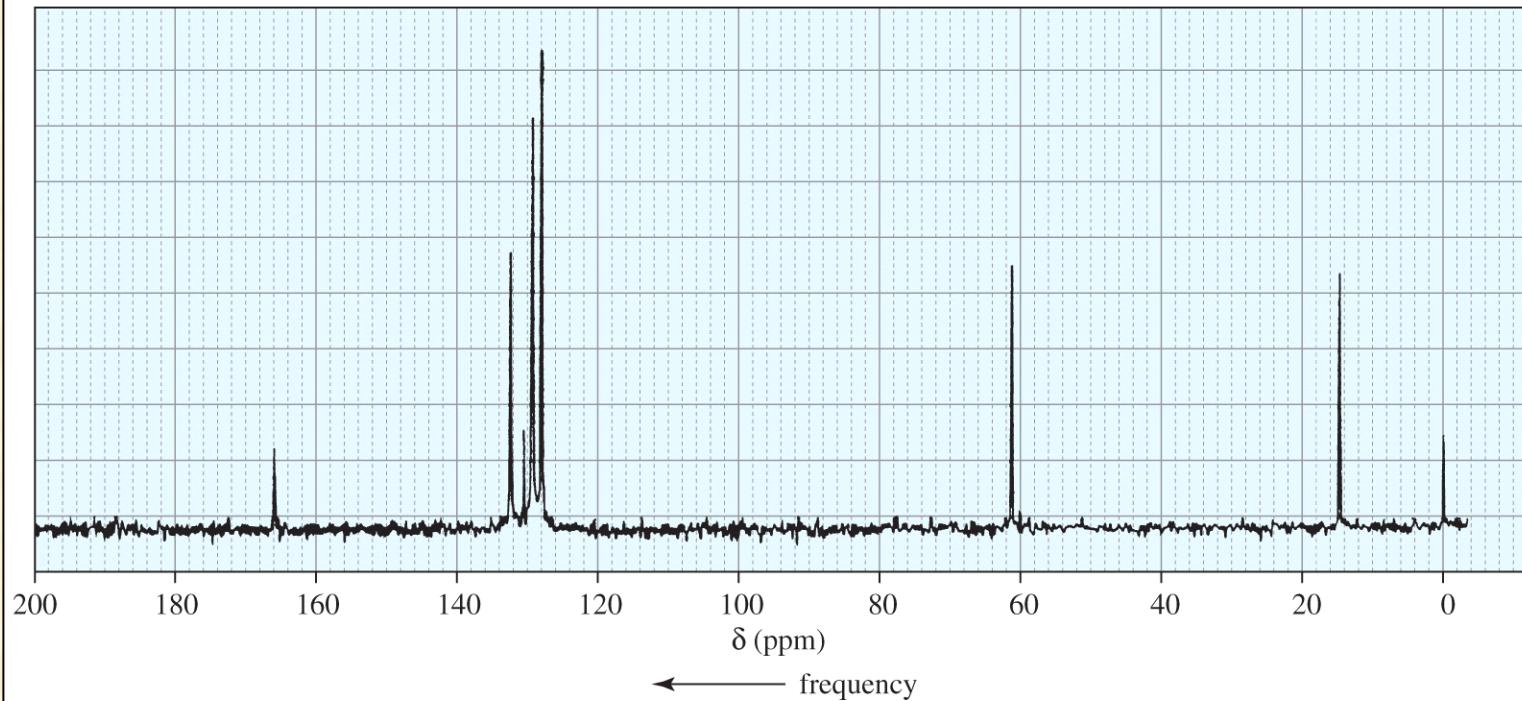
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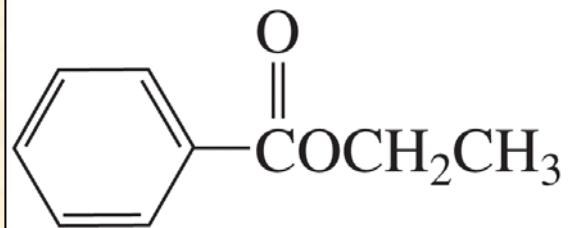
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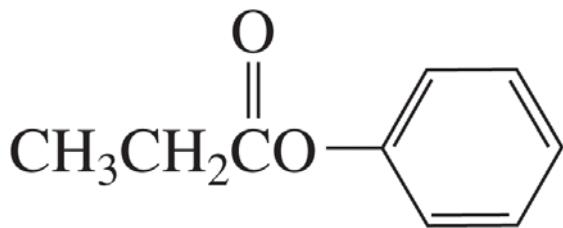


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ethyl benzoate



phenyl propanoate

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¹⁹F-NMR Spectroscopy

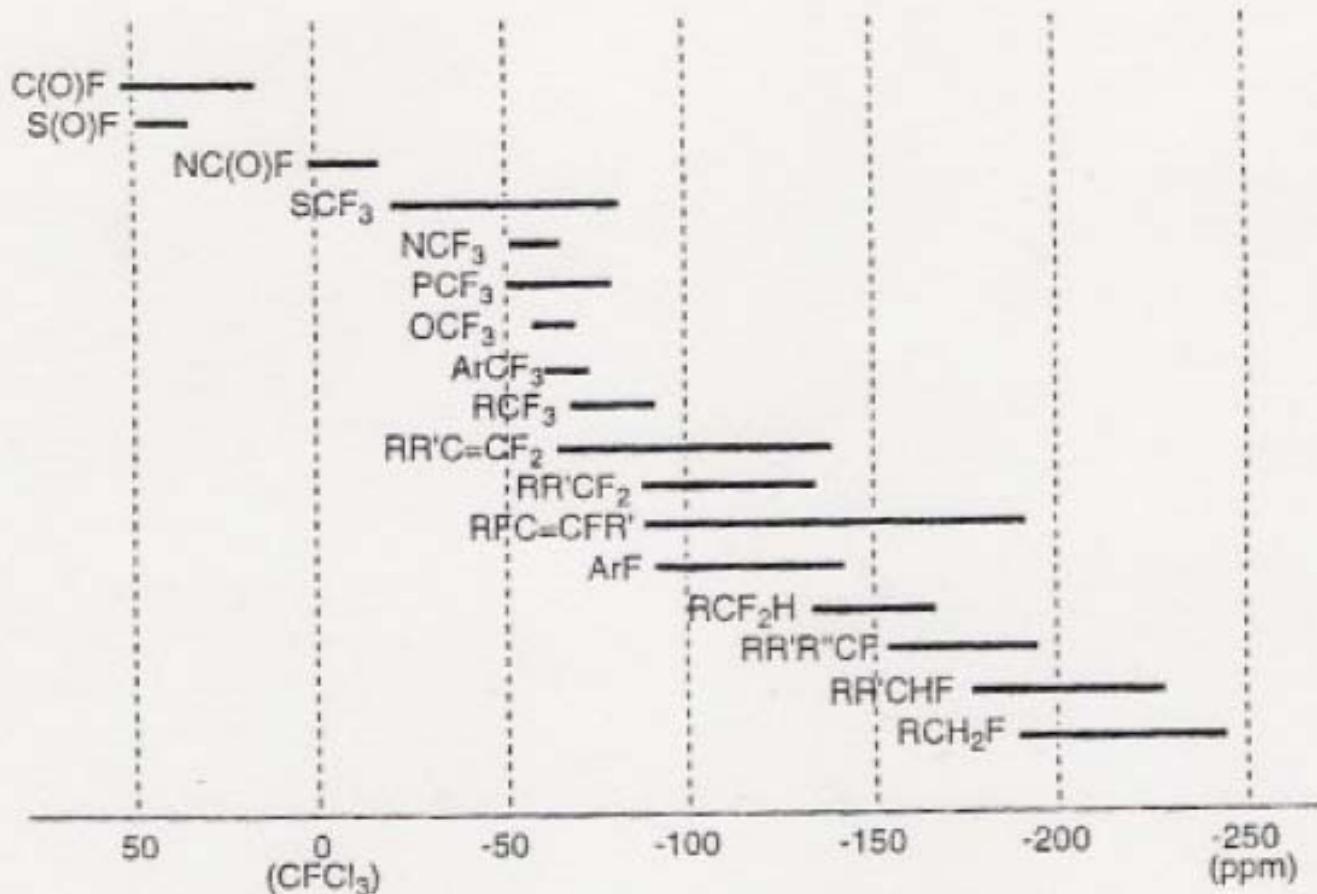
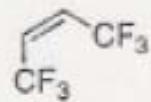


Fig. 1.15. ¹⁹F-NMR chemical shifts of fluorine substituents

¹⁹F-NMR Spectroscopy



$$^5J_{F,F} = 14 \text{ Hz}$$

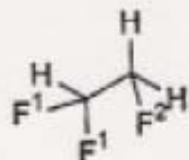


$$^5J_{F,F} = 2 \text{ Hz}$$

Fig. 1.16. Long-range F–F coupling

¹⁹F-NMR Spectroscopy

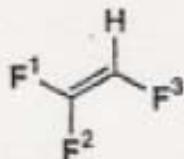
- Fluoroalkane



F¹; -129.9 ppm (²J_{H,F} = 55 Hz, ³J_{F,F} = 18 Hz, ³J_{H,F} = 13 Hz)

F²; -288.9 ppm (²J_{H,F} = 46 Hz, ³J_{F,F} = 18 Hz, ³J_{H,F} = 6 Hz)

- Fluoroalkene



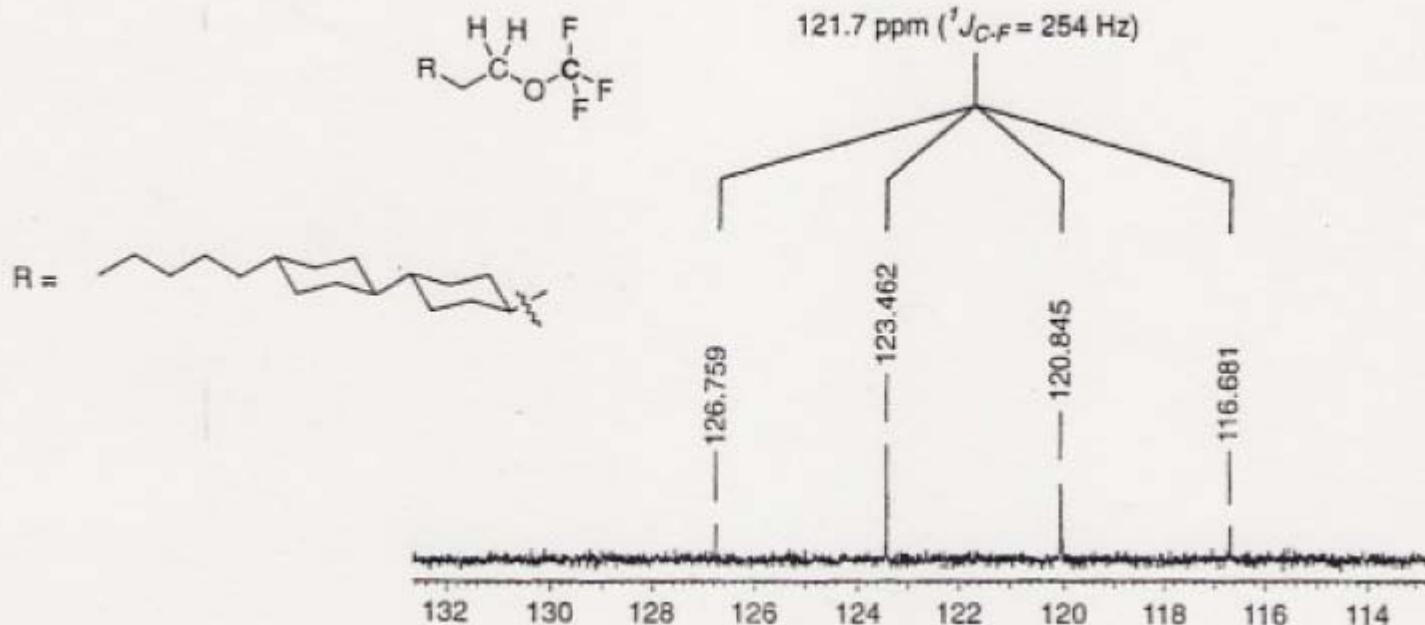
F¹; -125.7 ppm (²J_{F,F} = 87 Hz, ³J_{F,F (trans)} = 119 Hz, ³J_{H,F (cis)} = 4 Hz)

F²; -99.7 ppm (²J_{F,F} = 87 Hz, ³J_{F,F (cis)} = 33 Hz, ³J_{H,F (trans)} = 13 Hz)

F³; -205.0 ppm (²J_{H,F} = 71 Hz, ³J_{F,F (cis)} = 33 Hz, ³J_{F,F (trans)} = 119 Hz)

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

¹⁹F-NMR Spectroscopy



¹⁹F-NMR Spectroscopy

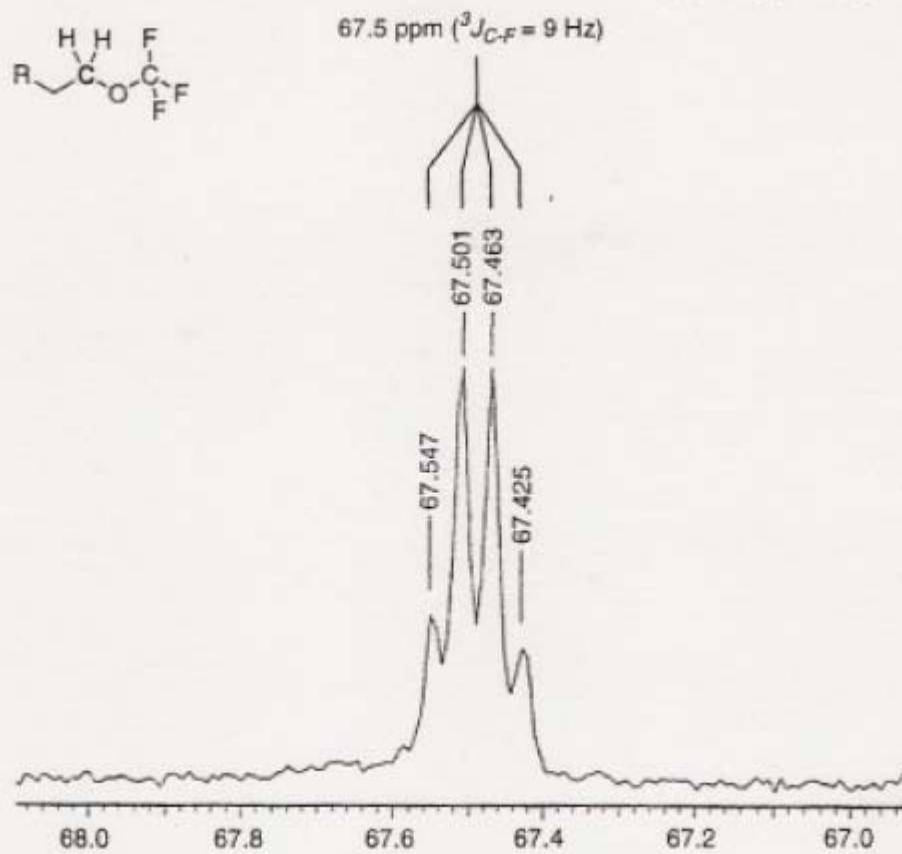


Fig. 1.17. ¹³C-NMR spectra of C-F coupling