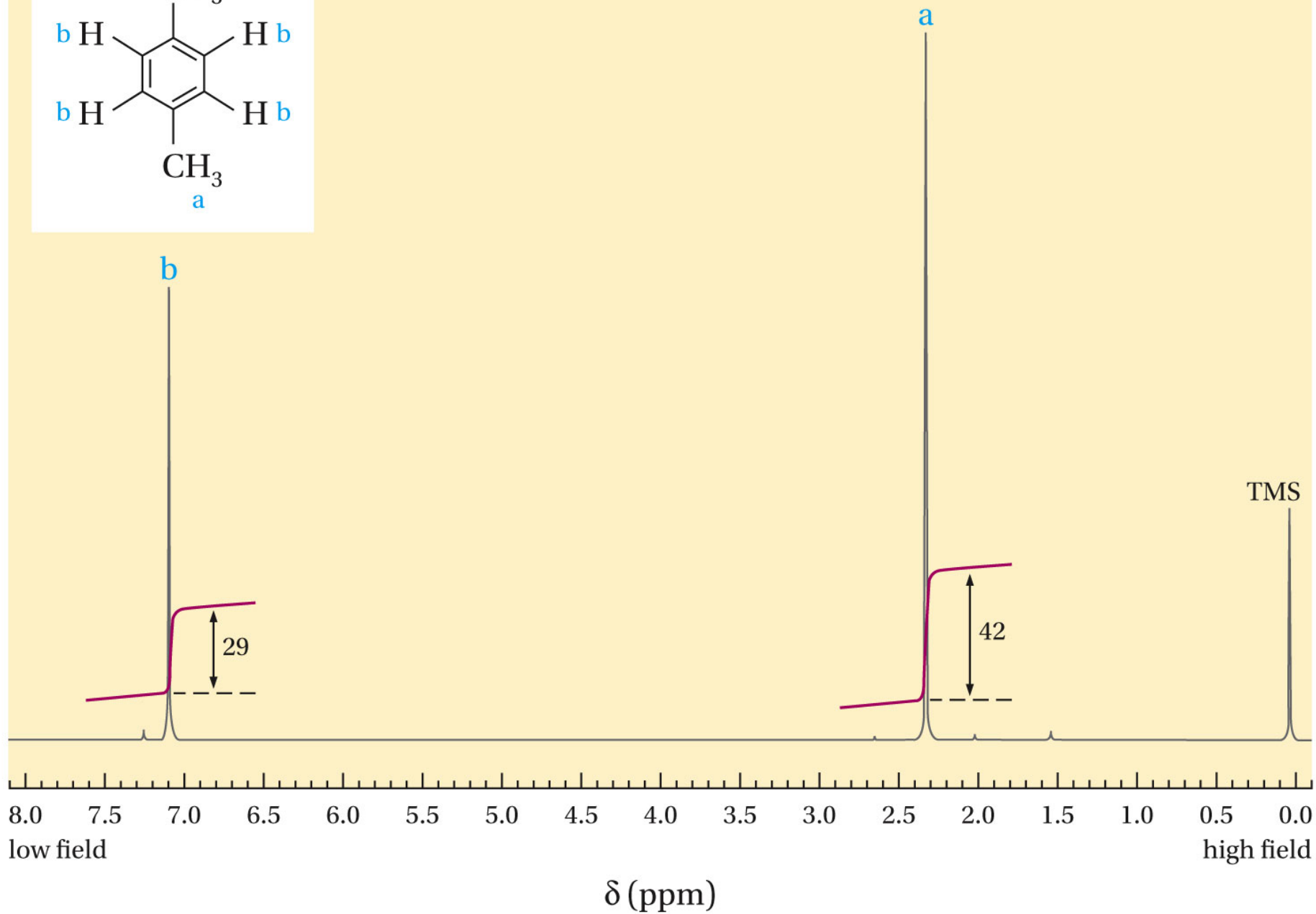
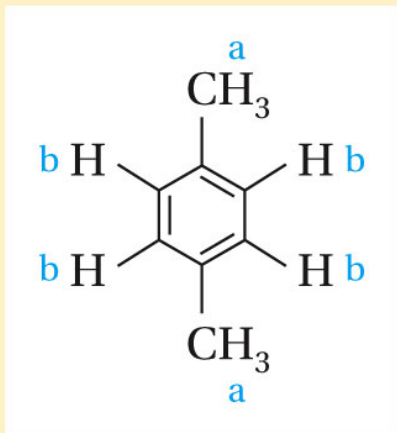
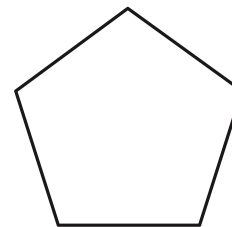
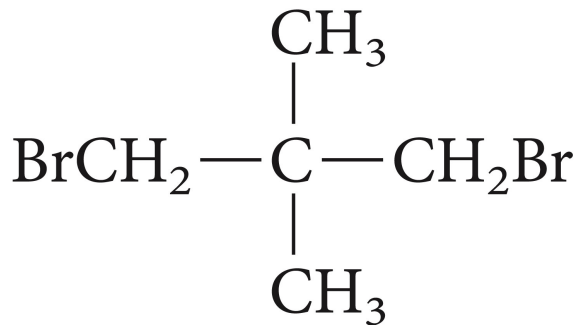
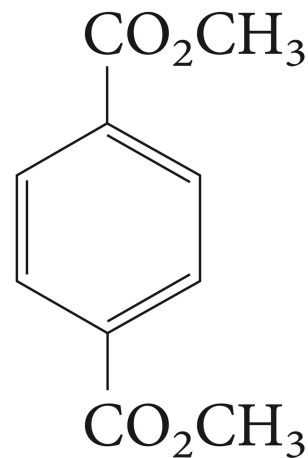
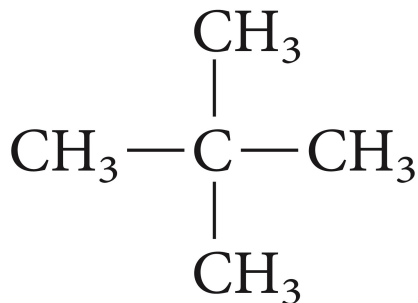


Spectroscopy

^1H NMR



How many peaks do you expect to see in the ^1H NMR spectrum of each of the Following compounds?



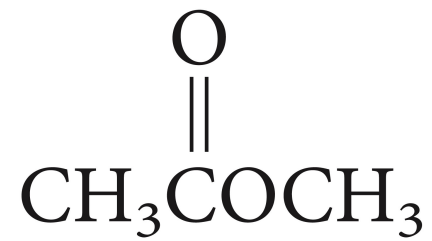
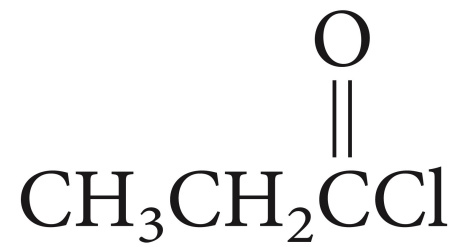
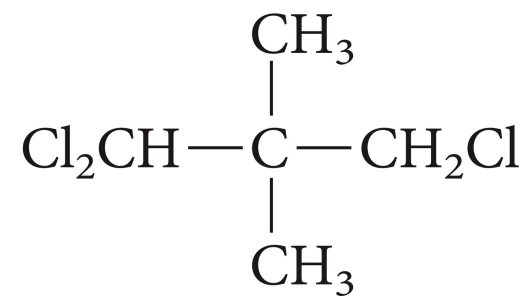
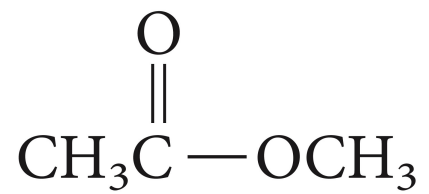
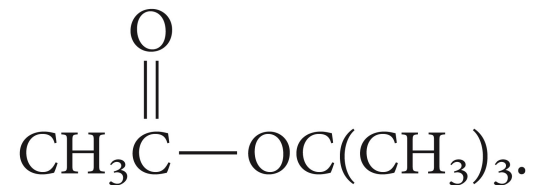
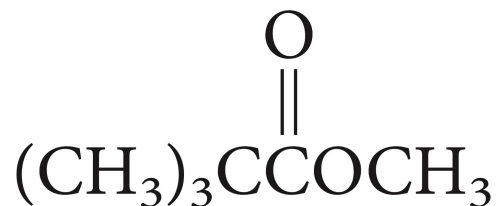


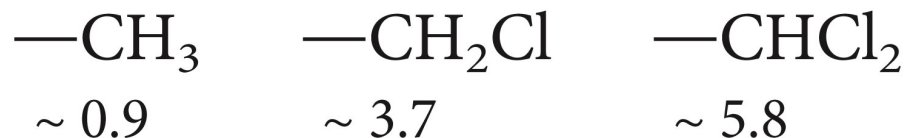
Table 12.2 Typical ^1H Chemical Shifts (Relative to Tetramethylsilane)

Type of ^1H	δ (ppm)	Type of ^1H	δ (ppm)
$\text{C}-\text{CH}_3$	0.85–0.95	$-\text{CH}_2-\text{F}$	4.3–4.4
$\text{C}-\text{CH}_2-\text{C}$	1.20–1.35	$-\text{CH}_2-\text{Br}$	3.4–3.6
		$-\text{CH}_2-\text{I}$	3.1–3.3
$\begin{array}{c} \text{C} \\ \\ \text{C}-\text{CH}-\text{C} \end{array}$	1.40–1.65	$\text{CH}_2=\text{C}$	4.6–5.0
$\text{CH}_3-\text{C}=\text{C}$	1.6–1.9	$-\text{CH}=\text{C}$	5.2–5.7
CH_3-Ar	2.2–2.5	$\text{Ar}-\text{H}$	6.6–8.0
$\begin{array}{c} \text{CH}_3-\text{C}=\text{O} \\ \end{array}$	2.1–2.6	$-\text{C}\equiv\text{C}-\text{H}$	2.4–2.7
$\text{CH}_3-\text{N} \begin{array}{l} \diagup \\ \diagdown \end{array}$	2.1–3.0	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{H} \end{array}$	9.5–9.7
$\text{CH}_3-\text{O}-$	3.5–3.8	$\begin{array}{c} \text{O} \\ \\ -\text{C}-\text{OH} \end{array}$	10–13
$-\text{CH}_2-\text{Cl}$	3.6–3.8	$\text{R}-\text{OH}$	0.5–5.5
$-\text{CHCl}_2$	5.8–5.9	$\text{Ar}-\text{OH}$	4–8





An ester is suspected to have either of the two structures. Its ^1H NMR Spectrum consists of two peaks at $\delta=0.9$ and $\delta=3.6$ (with relative areas 3:1) which compound is it. Describe the spectrum that would be expected if it had the other ester.



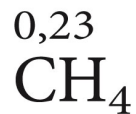
Electron withdrawing groups generally cause a downfield chemical shift.

This is because the electron withdrawing groups “deshields” the nucleus allowing it to flip its spin at a lower applied external field or lower frequency.

Predict the order of chemical shift of the various ^1H signals of 1-bromopropane

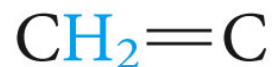


Compare and explain the following chemical shifts





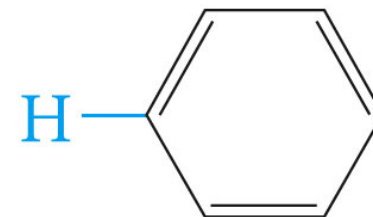
δ 1.2–1.35



4.6–5.0



5.2–5.7

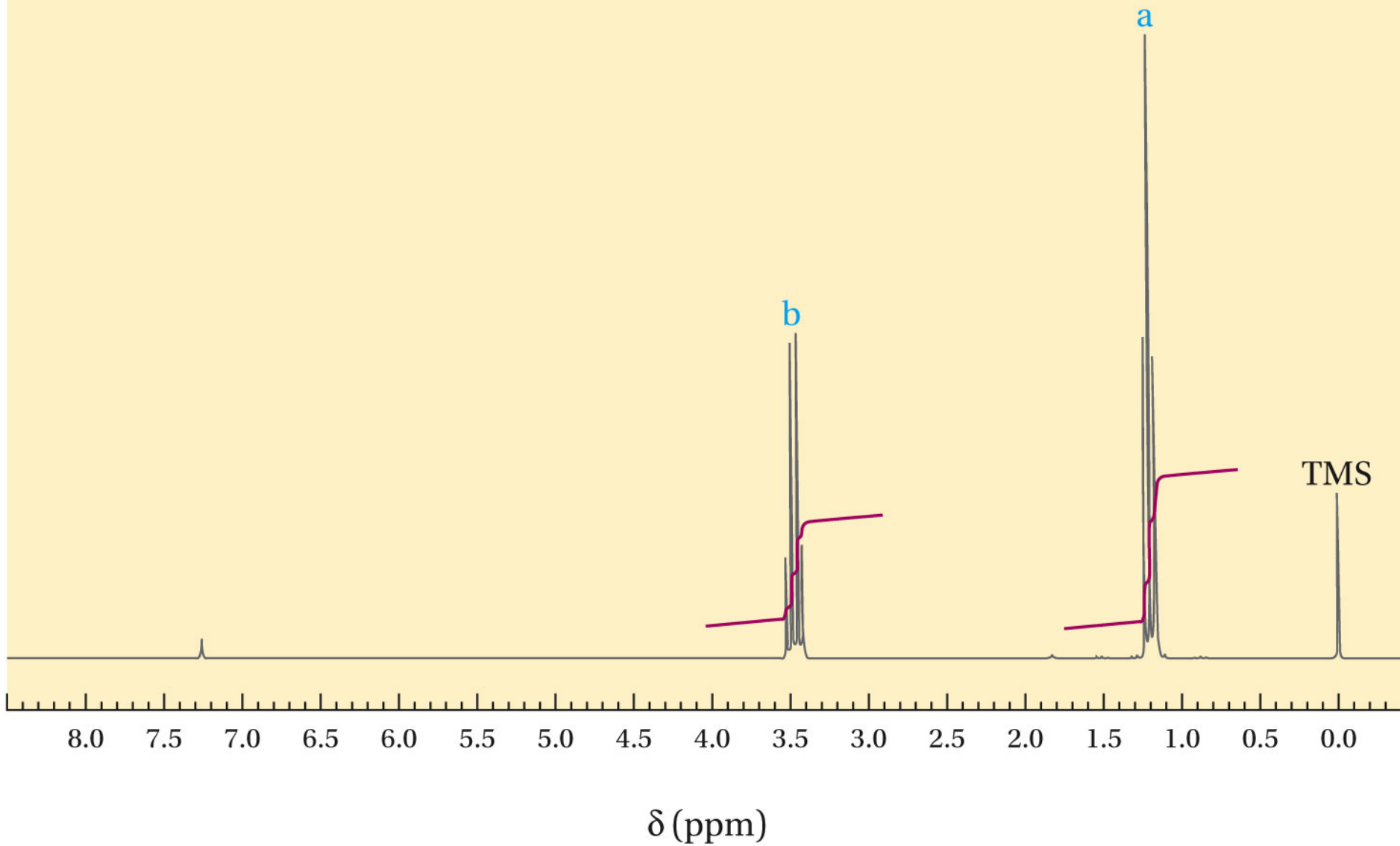


6.6–8.0

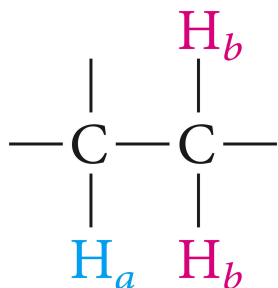
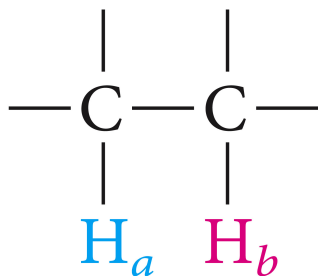
The other factor affecting the chemical shifts is the presence of pi electrons

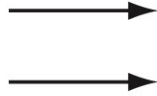


Spin-Spin Splitting



To predict the splitting pattern, the *n+1 rule* is applied





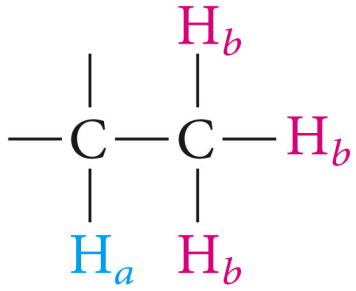
both aligned
with the field



one with and
one against the
field



both aligned
against the field



or

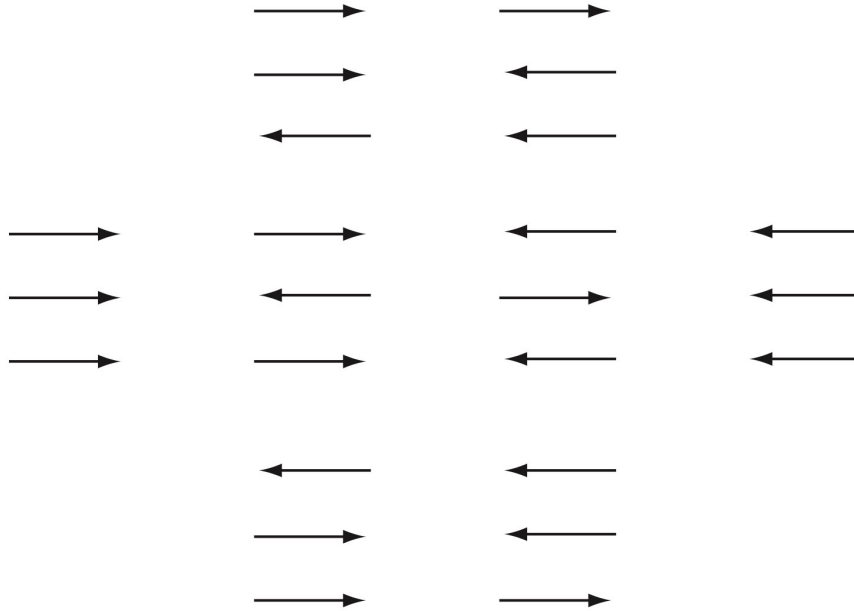
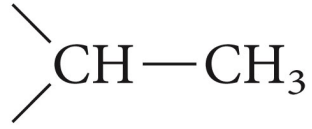


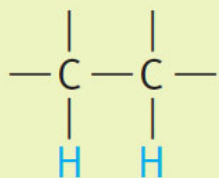
Table 12.3 ▀ **Some Typical Coupling Constants**

Group

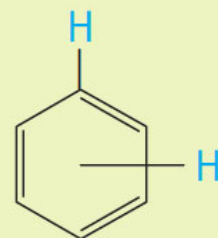
***J* (Hz)**

Group

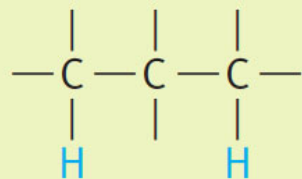
***J* (Hz)**



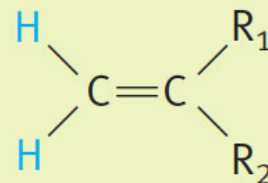
6–8



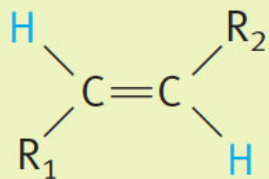
ortho: 6–10
meta: 1–3
para: 0–1



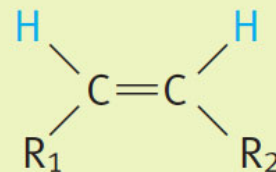
0–1



0–3



12–18



6–12

