IR

Table 25.1 *A simplified correlation table*

	Type of Vibration		*Frequency (cm^{-1})*	*Intensity*[a]
C—H	Alkanes	(stretch)	3000–2850	s
	—CH_3	(bend)	1450 and 1375	m
	—CH_2—	(bend)	1465	m
	Alkenes	(stretch)	3100–3000	m
		(bend)	1700–1000	s
	Aromatics	(stretch)	3150–3050	s
		(out-of-plane bend)	1000–700	s
	Alkyne	(stretch)	ca. 3300	s
	Aldehyde		2900–2800	w
			2800–2700	w
C—C	Alkane	Not interpretatively useful		
C=C	Alkene		1680–1600	m–w
	Aromatic		1600–1400	m–w
C≡C	Alkyne		2250–2100	m–w
C=O	Aldehyde		1740–1720	s
	Ketone (acyclic)		1725–1705	s
	Carboxylic acid		1725–1700	s
	Ester		1750–1730	s
	Amide		1700–1640	s
	Anhydride		ca. 1810	s
			ca. 1760	s
C—O	Alcohols, ethers, esters, carboxylic acids		1300–1000	s
O—H	Alcohol, phenols			
	Free		3650–3600	m
	H-Bonded		3400–3200	m
	Carboxylic acids		3300–2500	m
N—H	Primary and secondary amines		ca. 3500	m
C≡N	Nitriles		2260–2240	m
N=O	Nitro (R—NO_2)		1600–1500	s
			1400–1300	s
C—X	Fluoride		1400–1000	s
	Chloride		800–600	s
	Bromide, iodide		<600	s

[a]s, strong; m, medium; w, weak.

Table 25.2 *Base values for absorptions of bonds*

O—H	3400 cm^{-1}	C≡C	2150 cm^{-1}
N—H	3500 cm^{-1}	C=O	1715 cm^{-1}
C—H	3000 cm^{-1}	C=C	1650 cm^{-1}
C≡N	2250 cm^{-1}	C—O	1100 cm^{-1}

IR

IR

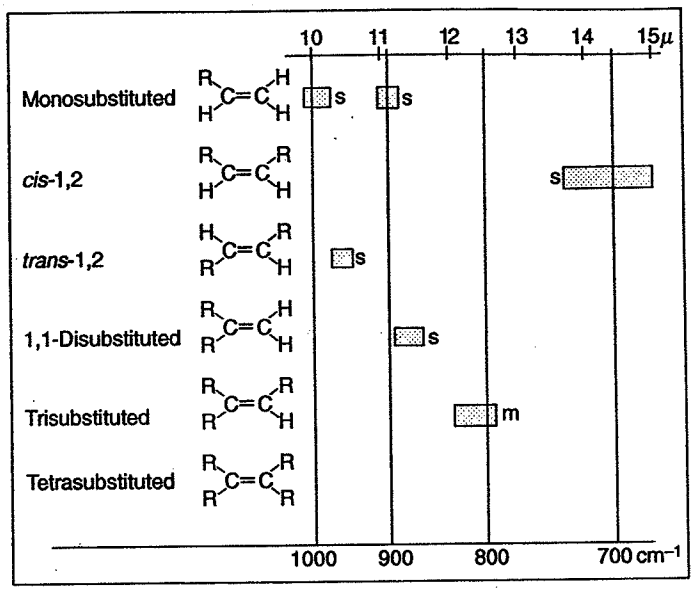
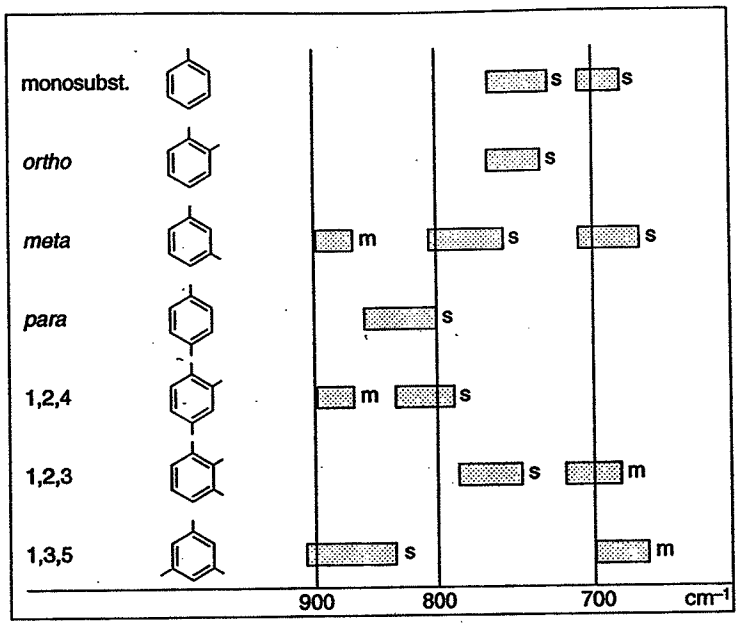
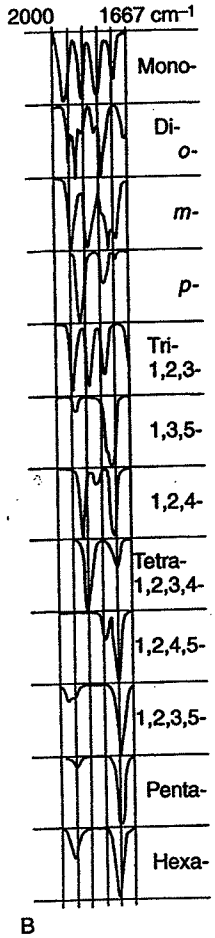


Figure 25.16
The C—H out-of-plane bending vibrations for substituted alkenes.



A



B

^1H-NMR

TABLE 9.1 Approximate Proton Chemical Shifts

Type of Proton	Chemical Shift (δ, ppm)	Type of Proton	Chemical Shift (δ, ppm)
1° Alkyl, RCH_3	0.8–1.2	Alkyl bromide, RCH_2Br	3.4–3.6
2° Alkyl, RCH_2R	1.2–1.5	Alkyl chloride, RCH_2Cl	3.6–3.8
3° Alkyl, R_3CH	1.4–1.8	Vinylic, $R_2C{=}CH_2$	4.6–5.0
Allylic, $R_2C{=}C(R){-}CH_3$	1.6–1.9	Vinylic, $R_2C{=}CH(R)$	5.2–5.7
Ketone, $RCCH_3$ (=O)	2.1–2.6	Aromatic, ArH	6.0–8.5
Benzylic, $ArCH_3$	2.2–2.5	Aldehyde, RCH (=O)	9.5–10.5
Acetylenic, $RC{\equiv}CH$	2.5–3.1	Alcohol hydroxyl, ROH	0.5–6.0[a]
Alkyl iodide, RCH_2I	3.1–3.3	Amino, $R{-}NH_2$	1.0–5.0[a]
Ether, $ROCH_2R$	3.3–3.9	Phenolic, ArOH	4.5–7.7[a]
Alcohol, $HOCH_2R$	3.3–4.0	Carboxylic, $RCOH$ (=O)	10–13[a]

[a]The chemical shifts of these protons vary in different solvents and with temperature and concentration.

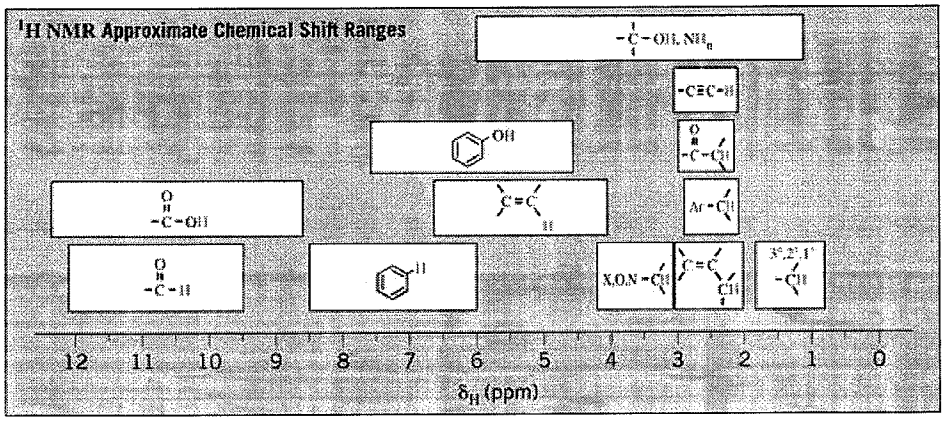


FIGURE 9.2 Approximate proton chemical shifts.

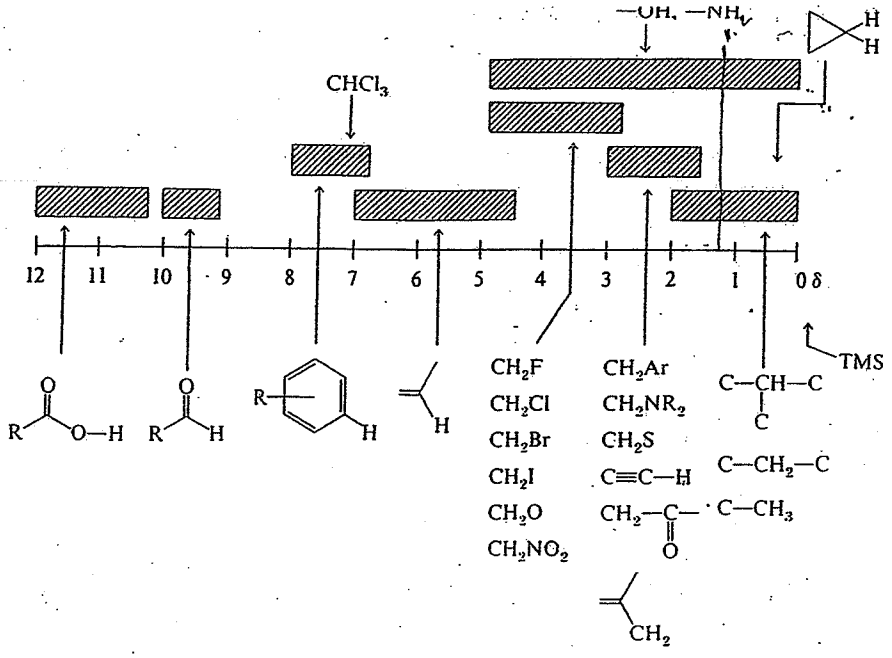


Figure 26.7
A simplified correlation chart for proton chemical shift values.

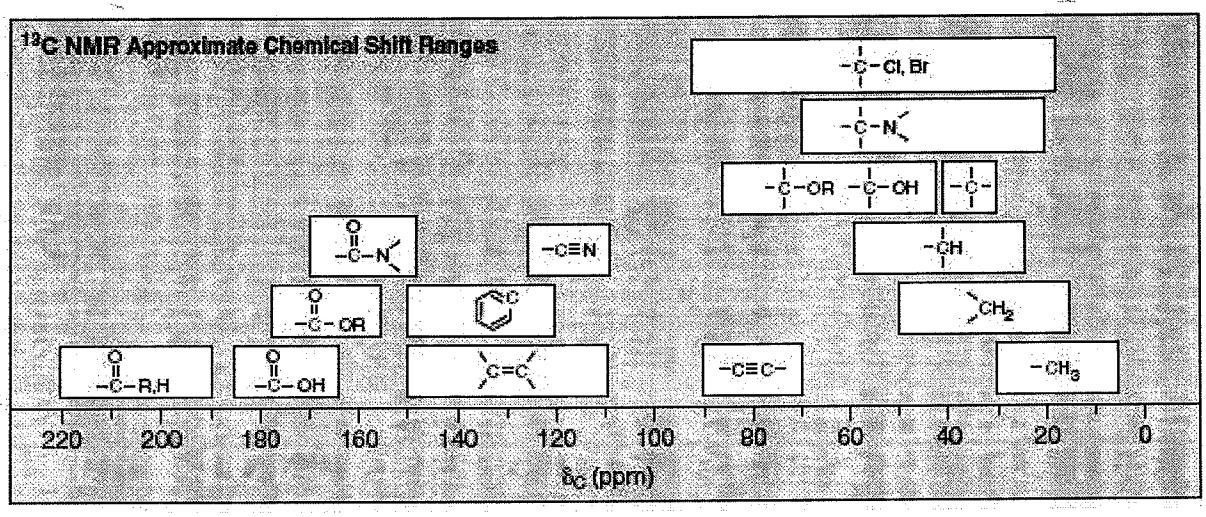
Table 26.5 *Proton chemical shifts in p-disubstituted benzene compounds*

Substituent X	*δ (ppm)*	
—OCH_3	6.80	Electron donating (shielding)
—OH	6.60	
—NH_2	6.36	
—CH_3	7.05	
—H	7.32	
—COOH	8.20	Electron withdrawing (deshielding)
—NO_2	8.48	

Table 26.4 *Representative coupling constants and approximate values (Hz)*

H H C—C	^3J	6–8		*ortho*			a,a	8–14
	$^3J_{trans}$	11–18		^3J	6–10		^3J a,e	0–7
	$^3J_{cis}$	6–15		*meta*			e,e	0–5
	$^2J_{gem}$	0–5		^4J	1–4		^3J *cis*	6–12
	^3J	4–10		*para*			*trans*	4–8
H—C≡C—C—H	^4J	0–3		^5J	≈0		^3J *cis*	2–5
				^3J	8–11		*trans*	1–3
							^3J	5–7

^{13}C-NMR


13C NMR Approximate Chemical Shift Ranges
-C-Cl, Br
-C-N
-C-OR
-C-OH
-C-
-C≡N
-CH
CH2
-CH3
-C≡C-
C=C
-C-R,H
-C-OH
-C-OR
-C-N
220
200
180
160
140
120
100
80
60
40
20
0
δC (ppm)