TABLE 13.4 Infrared Absorption Frequencies of Some Common Structural Units

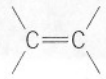
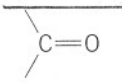
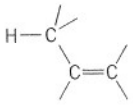
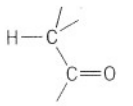
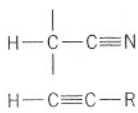
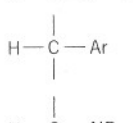
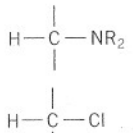
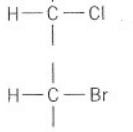
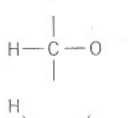
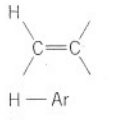
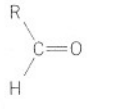
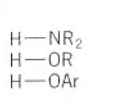
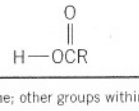
Structural unit	Frequency, cm^{-1}	Structural unit	Frequency, cm^{-1}
Stretching vibrations			
Single bonds		**Double bonds**	
—O—H (alcohols)	3200–3600		1620–1680
—O—H (carboxylic acids)	2500–3600		
	3350–3500	Aldehydes and ketones	1710–1750
sp C—H	3310–3320	Carboxylic acids	1700–1725
sp^2 C—H	3000–3100	Acid anhydrides	1800–1850 and 1740–1790
sp^3 C—H	2850–2950	Acyl halides	1770–1815
sp^2 C—O	1200	Esters	1730–1750
sp^3 C—O	1025–1200	Amides	1680–1700
		Triple bonds	
		—C≡C—	2100–2200
		—C≡N	2240–2280
Bending vibrations of diagnostic value			
Alkenes:		***Substituted derivatives of benzene:***	
$RCH=CH_2$	910, 990	Monosubstituted	730–770 and 690–710
$R_2C=CH_2$	890	Ortho-disubstituted	735–770
cis-RCH=CHR′	665–730	Meta-disubstituted	750–810 and 680–730
trans-RCH=CHR′	960–980	Para-disubstituted	790–840
$R_2C=CHR'$	790–840		

TABLE 13.3 Chemical Shifts of Representative Carbons

Type of carbon	Chemical shift (δ) ppm*	Type of carbon	Chemical shift (δ) ppm*
Hydrocarbons		**Functionally substituted carbons**	
RCH_3	0–35	RCH_2Br	20–40
R_2CH_2	15–40	RCH_2Cl	25–50
R_3CH	25–50	RCH_2NH_2	35–50
R_4C	30–40	RCH_2OH and RCH_2OR	50–65
RC≡CR	65–90	RC≡N	110–125
	110–175		190–220
$R_2C=CR_2$	100–150		160–185

*Approximate values relative to tetramethylsilane.

TABLE 13.1 Approximate Chemical Shifts of Representative Protons

Compound class or type of proton		Chemical shift (δ), ppm*
Protons bonded to carbon		
Alkane	RCH_3, R_2CH_2, R_3CH	0.9–1.8
Allylic		1.5–2.6
C—H adjacent to C=O		2.0–2.5
C—H adjacent to C≡N		2.1–2.3
Alkyne	H—C≡C—R	2.5
Benzylic		2.3–2.8
Amine		2.2–2.9
Alkyl chloride		3.1–4.1
Alkyl bromide		2.7–4.1
Alcohol or ether		3.3–3.7
Vinylic		4.5–6.5
Aryl	H—Ar	6.5–8.5
Aldehyde		9–10
Protons bonded to nitrogen or oxygen		
Amine	$H—NR_2$	1–3†
Alcohol	H—OR	0.5–5†
Phenol	H—OAr	6–8†
Carboxylic acid		10–13†

*Approximate values relative to tetramethylsilane; other groups within the molecule can cause a proton signal to appear outside of the range cited.
†The chemical shifts of O—H and N—H protons are temperature- and concentration-dependent.