

Table 1. Characteristic IR Absorption Peaks of Functional Groups\*

Vibration	Position (cm <sup>-1</sup> )	Intensity*	Notes
<b>Alkanes</b>			
C-H stretch	2990 – 2850	m to s	
<b>Alkenes</b>			
=C-H stretch	3100 – 3000	m	
C=C stretch	1680 – 1620 (sat.) 1650 – 1600 (conj.)	w to m	
=C-H bend	995 – 685	s	See Table 2 for detail
<b>Alkynes</b>			
≡C-H stretch	3310 – 3200	s	
C≡C stretch	2250 – 2100	m to w	
<b>Aromatic Compounds</b>			
C-H stretch	3100 – 3000	m to w	
C=C stretch	1625 – 1440	m to w	Hidden in fingerprint region
C-H bend	900 – 680	s	See Table 2 for detail
<b>Alcohols**</b>			
O-H stretch	3550 – 3200	br, s	Hydrogen bonded (typical)
<b>Amines</b>			
N-H stretch	3550 – 3250	br, m	Primary (two bands) Secondary (one band)
<b>Nitriles</b>			
C≡N stretch	2280 – 2200	s	
<b>Aldehydes</b>			
C-H stretch	2900 – 2800 & 2800 – 2700	s	H-C=O Fermi doublet
C=O stretch	1740 – 1720 (sat.) 1715 – 1680 (conj.)	s	
<b>Ketones</b>			
C=O stretch	1750 – 1705 (sat.) 1700 – 1665 (conj.)	s	
<b>Esters**</b>			
C=O stretch	1765 – 1735 (sat.) 1730 – 1715 (conj.)	s	
<b>Carboxylic Acids**</b>			
O-H stretch	3200 – 2500	br, m to w	
C=O stretch	1725 – 1700 (sat.) 1715 – 1680 (conj.)	s	
<b>Amides</b>			
N-H stretch	3500 – 3150	m	Primary (two bands) Secondary (one band)
C=O stretch	1700 – 1630	s	

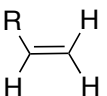
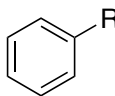
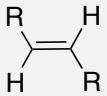
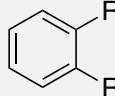
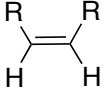
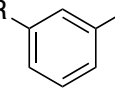
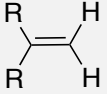
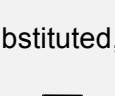
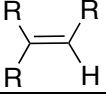
Table 1 cont'd

Vibration	Position (cm <sup>-1</sup> )	Intensity	Notes
<b>Anhydrides**</b>			
C=O stretch	1850 – 1800 & 1790 – 1740	s	
<b>Acid Chlorides</b>			
C=O stretch	1815 – 1770	s	
<b>Nitro Compounds</b>			
NO <sub>2</sub> stretch	1570 – 1490 & 1390 – 1300	s	
<b>Thiols†</b>			
R-S-H stretch	2550 – 2600		
<b>Alkyl &amp; Aryl Halides†</b>			
C-F stretch	1000 – 1400		Hidden in fingerprint region
C-Cl stretch	< 600 – 840		
C-Br stretch	< 700		
C-I stretch	< 600		

\* Abbreviations: s = strong; m = medium; w = weak; br = broad; sat. = saturated; conj. = conjugated

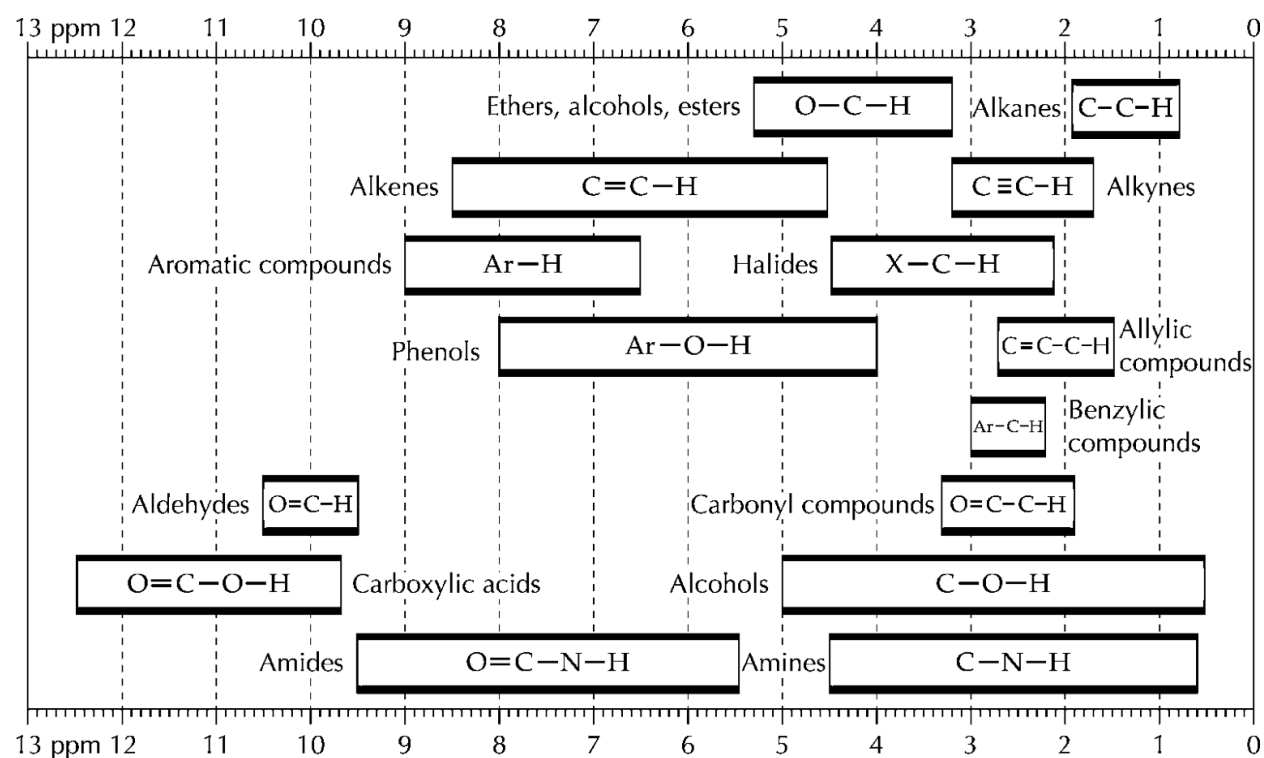
\*\* Alcohols, Esters, Carboxylic Acids, and Anhydrides also absorb in the fingerprint region due to the C-O stretch (1300 – 1000, s).

Table 2. Out-of-Plane C-H Bending Vibrations in Alkenes and Aromatics

Alkene Structure	Position (cm <sup>-1</sup> )	Phenyl Structure	Position (cm <sup>-1</sup> )
Mono-substituted 	997 – 985 & 915 – 905	Mono-substituted 	770 – 730 & 720 – 680
Disubstituted, <i>trans</i> 	980 – 960	Disubstituted, <i>ortho</i> 	770 – 735
Disubstituted, <i>cis</i> 	730 – 665	Disubstituted, <i>meta</i> 	810 – 750 & 725 – 680
Disubstituted, <i>symm.</i> 	895 – 885	Disubstituted, <i>para</i> 	860 – 800
Trisubstituted 	840 – 790		

\* Adapted from...Mohrig, J. R.; Hammond, C. N.; Schatz, P. F. "Infrared Spectroscopy" in *Techniques in Organic Chemistry*. Freeman: New York, 2006.

† Palleros, D. R. "Infrared Spectroscopy" in *Experimental Organic Chemistry*. Wiley: New York, 2000. p. 688.



**FIGURE 22.13** Approximate regions of chemical shifts for different types of protons in organic compounds.

**TABLE 22.2** Characteristic  $^1\text{H}$  NMR chemical shifts in  $\text{CDCl}_3$

Compound	Chemical shift ( $\delta$ , ppm)
TMS	0.0
Alkanes (C-C-H)	0.8–1.9
Amines (C-N-H)	0.6–4.5
Alcohols (C-O-H)	0.5–5.0
Alkenes <sup>a</sup> (C=C-C-H)	1.5–2.6
Alkynes (C≡C-H)	1.7–3.1
Carbonyl compounds (O=C-C-H)	1.9–3.3
Halides (X-C-H)	2.1–4.5
Aromatic compounds <sup>b</sup> (Ar-C-H)	2.2–3.0
Alcohols, esters, ethers (O-C-H)	3.2–5.3
Alkenes (C=C-H)	4.5–8.5
Phenols (Ar-O-H)	4.0–8.0
Amides (O=C-N-H)	5.5–9.5
Aromatic compounds (Ar-H)	6.5–9.0
Aldehydes (O=C-H)	9.5–10.5
Carboxylic acids (O=C-O-H)	9.7–12.5

a. Allylic protons.

b. Benzylic protons.

**TABLE 22.4 Additive parameters for predicting NMR chemical shifts of aromatic protons in  $\text{CDCl}_3$**

Group	Base value		
	<i>ortho</i>	<i>meta</i>	<i>para</i>
$-\text{CH}_3$	-0.18	-0.11	-0.21
$-\text{CH}(\text{CH}_3)_2$	-0.14	-0.08	-0.20
$-\text{CH}_2\text{Cl}$	0.02	-0.01	-0.04
$-\text{CH}=\text{CH}_2$	0.04	-0.04	-0.12
$-\text{CH}=\text{CHAr}$	0.14	-0.02	-0.11
$-\text{CH}=\text{CHCO}_2\text{H}$	0.19	0.04	0.05
$-\text{CH}=\text{CH}(\text{C}=\text{O})\text{Ar}$	0.28	0.06	0.05
Group	<i>ortho</i>	<i>meta</i>	<i>para</i>
$-\text{Ar}$	0.23	0.07	-0.02
$-(\text{C}=\text{O})\text{H}$	0.53	0.18	0.28
$-(\text{C}=\text{O})\text{R}$	0.60	0.10	0.20
$-(\text{C}=\text{O})\text{Ar}$	0.45	0.12	0.23
$-(\text{C}=\text{O})\text{CH}=\text{CHAr}$	0.67	0.14	0.21
$-(\text{C}=\text{O})\text{OCH}_3$	0.68	0.08	0.19
$-(\text{C}=\text{O})\text{OCH}_2\text{CH}_3$	0.69	0.06	0.17
$-(\text{C}=\text{O})\text{OH}$	0.77	0.11	0.25
$-(\text{C}=\text{O})\text{Cl}$	0.76	0.16	0.33
$-(\text{C}=\text{O})\text{NH}_2$	0.46	0.09	0.17
$-\text{C}\equiv\text{N}$	0.29	0.12	0.25
$-\text{F}$	-0.32	-0.05	-0.25
$-\text{Cl}$	-0.02	-0.07	-0.13
$-\text{Br}$	0.13	-0.13	-0.08
$-\text{OH}$	-0.53	-0.14	-0.43
$-\text{OR}$	-0.45	-0.07	-0.41
$-\text{OAr}$	-0.36	-0.04	-0.28
$-\text{O}(\text{C}=\text{O})\text{R}$	-0.27	0.02	-0.13
$-\text{O}(\text{C}=\text{O})\text{Ar}$	-0.14	0.07	-0.09
$-\text{NH}_2$	-0.71	-0.22	-0.62
$-\text{N}(\text{CH}_3)_2$	-0.68	-0.15	-0.73
$-\text{NH}(\text{C}=\text{O})\text{R}$	0.14	-0.07	-0.27
$-\text{NO}_2$	0.87	0.20	0.35

a. Base value is the measured chemical shift of benzene in  $\text{CDCl}_3$  (1% solution).

**TABLE 22.3 Additive parameters for predicting NMR chemical shifts of alkyl protons in  $\text{CDCl}_3$ <sup>a</sup>**

Group (Y)	Base values		
	Alpha ( $\alpha$ ) substituent	Beta ( $\beta$ ) substituent	Gamma ( $\gamma$ ) substituent
	Methyl	0.9 ppm	
	Methylene	1.2 ppm	
	Methine	1.5 ppm	
	$\text{H}-\underset{\text{C}}{\overset{\text{C}}{\text{C}}}-\text{Y}$	$\text{H}-\underset{\text{C}}{\overset{\text{C}}{\text{C}}}-\underset{\text{C}}{\overset{\text{C}}{\text{C}}}-\text{Y}$	$\text{H}-\underset{\text{C}}{\overset{\text{C}}{\text{C}}}-\underset{\text{C}}{\overset{\text{C}}{\text{C}}}-\underset{\text{C}}{\overset{\text{C}}{\text{C}}}-\text{Y}$
—R	0.0	0.0	0.0
—C=C	0.8	0.2	0.1
—C=C—Ar <sup>b</sup>	0.9	0.1	0.0
—C=C(C=O)OR	1.0	0.3	0.1
—C≡C—R	0.9	0.3	0.1
—C≡C—Ar	1.2	0.4	0.2
—Ar	1.4	0.4	0.1
—(C=O)OH	1.1	0.3	0.1
—(C=O)OR	1.1	0.3	0.1
—(C=O)H	1.1	0.4	0.1
—(C=O)R	1.2	0.3	0.0
—(C=O)Ar	1.7	0.3	0.1
—(C=O)NH <sub>2</sub>	1.0	0.3	0.1
—(C=O)Cl	1.8	0.4	0.1
—C≡N	1.1	0.4	0.2
—Br	2.1	0.7	0.2
—Cl	2.2	0.5	0.2
—OH	2.3	0.3	0.1
—OR	2.1	0.3	0.1
—OAr	2.8	0.5	0.3
—O(C=O)R	2.8	0.5	0.1
—O(C=O)Ar	3.1	0.5	0.2
—NH <sub>2</sub>	1.5	0.2	0.1
—NH(C=O)R	2.1	0.3	0.1
—NH(C=O)Ar	2.3	0.4	0.1

a. There may be differences of 0.1–0.5 ppm in the chemical shift values calculated from this table and those measured from individual spectra.

b. Ar = aromatic group.

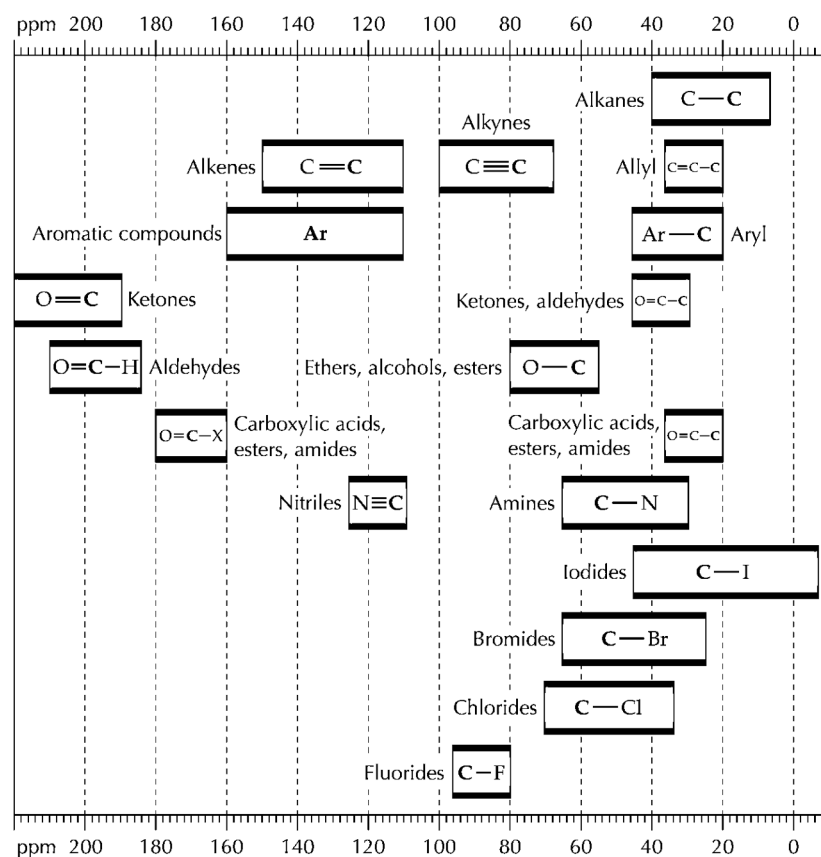


FIGURE 23.4 Approximate regions of  $^{13}\text{C}$  chemical shifts for different types of carbon atoms in organic compounds.

TABLE 23.1 Characteristic  $^{13}\text{C}$  NMR chemical shifts in  $\text{CDCl}_3$

Compound	Chemical shift (ppm)
TMS	0.0
$\text{CDCl}_3$ (t)	77
Alkane (C— $\text{CH}_3$ )	7–30
Alkane (C— $\text{CH}_2$ )	15–40
Alkane (C—CH) and (C—C)	15–40
Carboxylic acids, esters, and amides (C—C=O)	20–35
Allyl (C—C=C)	20–35
Arene (C—Ar)	20–45
Ketones, aldehydes (C—C=O)	30–45
Amines (C—N)	30–65
Iodides (C—I)	-5–45
Bromides (C—Br)	25–65
Chlorides (C—Cl)	35–70
Fluorides (C—F)	80–95
Alcohols (C—OH), ethers (C—OR), esters (C—O[C=O]R)	55–80
Alkyne (C≡C)	70–100
Alkene (C=C)	110–150
Aromatic	110–160
Nitriles (C≡N)	110–125
Carboxylic acids, esters, and amides (C=O)	160–180
Aldehydes (C=O)	185–210
Ketones (C=O)	190–220