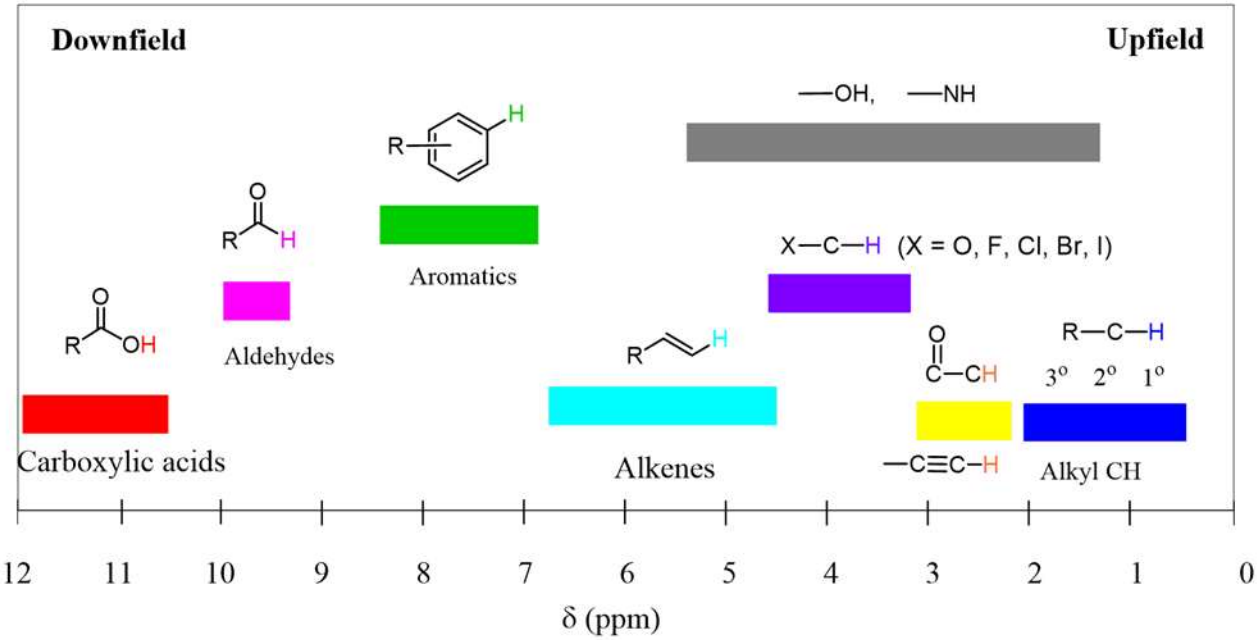
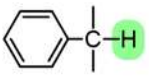
^{1}H NMR chemical shift values

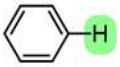


R-CH_3	**0.7 - 1.3**
R-CH_2-R	**1.2 - 1.4**
R_3CH	**1.4 - 1.7**
R–C=C–CH_3	**1.6 - 2.6**
R–C(=O)–CH_3	2.1 - **2.5**
RO–C(=O)–CH_3	**2.1 - 2.6**
N≡C–CH_3	**2.1 - 3.0**
	**2.3 - 2.7**
R–≡–H	**1.7 - 2.7**
R–N–C–H	**2.2 - 2.9**
R–S–C–H	**2.0 - 3.0**

R= H or alkyl

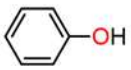
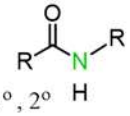
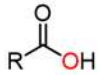
I–C–H	**2.0 - 4.0**
Br–C–H	**2.7 - 4.1**
Cl–C–H	**3.1 - 4.1**
RO–C–H	**3.2 - 3.8**

R= H or alkyl

R–C(=O)–O–C–H	**3.5 - 4.8**
O_2N–C–H	**4.1 - 4.3**
F–C–H	**4.2 - 4.8**
[1] R–C=C–H	4.5 - **6.5**
	**6.5 - 8.0**
R–C(=O)–H	9.0 - **10**

NH and OH peaks are most often broad or may as well be missing completely unless the sample is very dry.

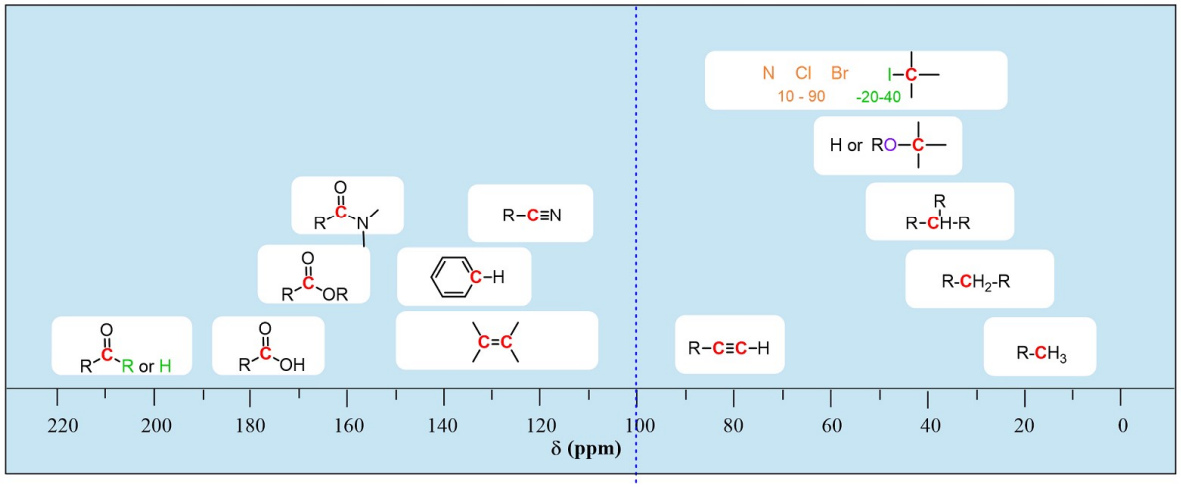
This is also true for any proton capable of making hydrogen bonding:

R–SH R = alkyl or aryl	1.0 - **5.0**
$R–NH_2$ 1°, 2°	1.0 - **5.0**
R–OH 1°, 2°, 3°	1.0 - **5.0**
	**4.0 – 12.0**
 1°, 2°	**5.0 - 9.0**
	**10.0 – 13.5**

Downfield shifts more common

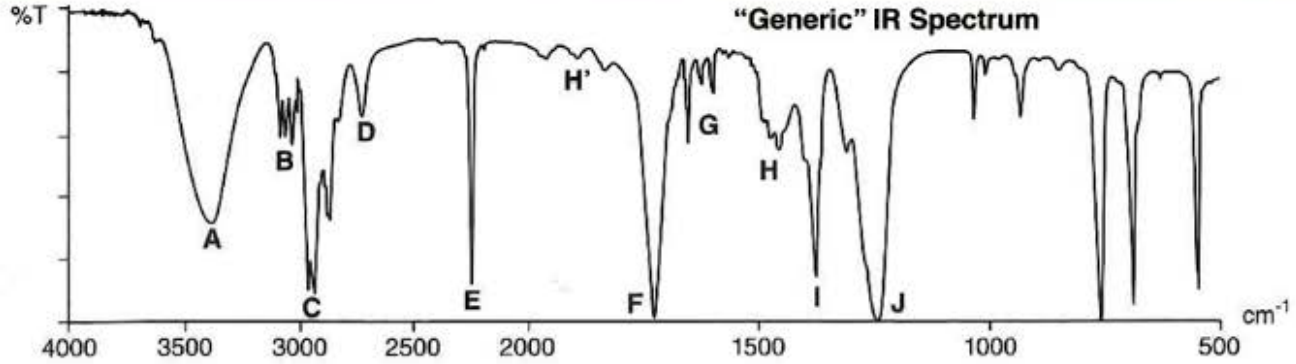
[1] Moves to downfield if conjugated

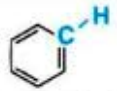
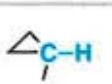
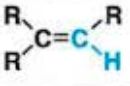
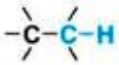
^{13}C NMR Chemical Shift Values

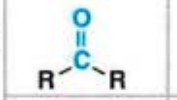
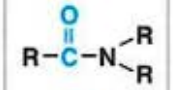
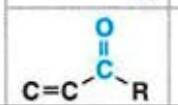


Type of carbon	δ (ppm)	Description of carbon
$R-CH_3$	10-30	primary alkyl (methyl)
$R-CH_2-R$	15-55	secondary alkyl (methylene)
R_3C-H $R-\overset{R}{\underset{R}{C}}-R$	20-60	tertiary or quaternary alkyl
C–I	0-40	attached to iodine
C–Br	25-65	attached to bromine
C–N	40-60	attached to nitrogen
C–Cl	35-80	attached to chlorine
C–O	40-80	attached to oxygen
RC≡CR	65-90	alkynyl
$R_2C=CR_2$	100-150	alkenyl
	110-170	aromatic (phenyl ring C)
$R-\overset{O}{\overset{\|}{C}}-OH$ $R-\overset{O}{\overset{\|}{C}}-OR$ $R-\overset{O}{\overset{\|}{C}}-NH_2$	165-185	C=O, carboxylic acid, ester, amide
$R-\overset{O}{\overset{\|}{C}}-R$ $R-\overset{O}{\overset{\|}{C}}-H$	185-220	C=O, ketone or aldehyde

IR Interpretation Guide



O-H N-H stretch	A	R–O–H	3600–3200	Phenols 3500
		–N–H	3500–3290 1° 3400–3340 2°	1°→2 peaks 2°→1 peak med. to weak
		–C(=O)–O–H	3550–2500	Broad & often "monstrous"
C-H stretch	B	R–C≡C–H	3300	
			3300–3000	No peaks in this area means no aromatic!
			3300–3100	
			3300–3000	No peaks in this area means no alkene!
	C		2960–2850	In "all" IR spectra
	D	R–C(=O)–H	2820 & 2720	2720 is key peak

C≡N C≡C	E	R–C≡C–R'	2260–2190	Weak to none if symmetrical
		R–C≡N	2250 aliph. 2230 arom.	
		R–C≡C–H	2140–2100	
C=O	F		1785 4-ring 1750 5-ring 1715 6-ring	Depends on size of ring
		R–C(=O)–O–R	1735 aliph. 1720 arom.	
		R–C(=O)–H	1730–1705	1730 aliphatic 1703 conjugated
			~1715 cm-1	1685 conjugated
		R–C(=O)–O–H	~1710	1680 conjugated
			1690 1° 1680 2° 1650 3°	Aromatic amides 1675 1°
			1685	Aromatic 1690

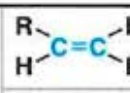
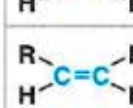
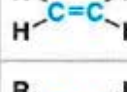
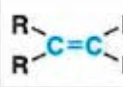
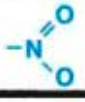
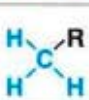
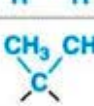
C=C	G		1675	
			1658	Tri- & tetra-substituted ~1670
			~1653	
			~1645	
	H H'		1600, 1580, 1500, 1450	Move and vary in intensity; H' = overtones 2000–1650
nitro	H I		1550–1490 1355–1315	Aromatic nitro Both strong
C–C & C–H bend	I		1490–1440	Scissor bend
			1470–1430 & 1380–1370	Umbrella bend
			1390–1375 & 1370–1360	t-butyl ~1365
C–O	J	C–O ethers esters	1150–1060 alkyl ethers and esters	1270–1200 aryl & vinyl ethers 1285 acids
		C–O alcohols	1150 3° 1100 2° 1050 1°	Tertiary Secondary Primary

Table 1. Characteristic IR Absorption Peaks of Functional Groups*

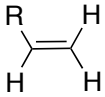
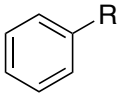
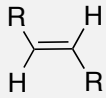
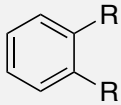
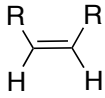
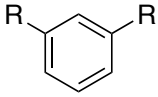
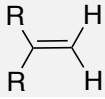
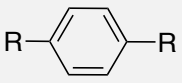
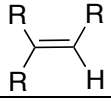
Vibration	Position (cm^{-1})	Intensity*	Notes
Alkanes			
C-H stretch	2990 – 2850	m to s	
Alkenes			
=C-H stretch	3100 – 3000	m	
C=C stretch	1680 – 1620 (sat.) 1650 – 1600 (conj.)	w to m	
=C-H bend	995 – 685	s	See Table 2 for detail
Alkynes			
≡C-H stretch	3310 – 3200	s	
C≡C stretch	2250 – 2100	m to w	
Aromatic Compounds			
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
Alcohols**			
O-H stretch	3550 – 3200	br, s	Hydrogen bonded (typical)
Amines			
N-H stretch	3550 – 3250	br, m	Primary (two bands) Secondary (one band)
Nitriles			
C≡N stretch	2280 – 2200	s	
Aldehydes			
C-H stretch	2900 – 2800 & 2800 – 2700	s	H-C=O Fermi doublet
C=O stretch	1740 – 1720 (sat.) 1715 – 1680 (conj.)	s	
Ketones			
C=O stretch	1750 – 1705 (sat.) 1700 – 1665 (conj.)	s	
Esters**			
C=O stretch	1765 – 1735 (sat.) 1730 – 1715 (conj.)	s	
Carboxylic Acids**			
O-H stretch	3200 – 2500	br, m to w	
C=O stretch	1725 – 1700 (sat.) 1715 – 1680 (conj.)	s	
Amides			
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^{-1})	Intensity	Notes
Anhydrides**			
C=O stretch	1850 – 1800 & 1790 – 1740	s	
Acid Chlorides			
C=O stretch	1815 – 1770	s	
Nitro Compounds			
NO_2 stretch	1570 – 1490 & 1390 – 1300	s	
Thiols†			
R-S-H stretch	2550 – 2600		
Alkyl & Aryl Halides†			
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^{-1})	Phenyl Structure	Position (cm^{-1})
Mono-substituted 	997 – 985 & 915 – 905	Mono-substituted 	770 – 730 & 720 – 680
Disubstituted, *trans* 	980 – 960	Disubstituted, *ortho* 	770 – 735
Disubstituted, *cis* 	730 – 665	Disubstituted, *meta* 	810 – 750 & 725 – 680
Disubstituted, symm. 	895 – 885	Disubstituted, *para* 	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.