

Useful Spectroscopic Data

Important Infrared Absorptions

<i>Type of Absorption</i>	<i>Frequency, cm^{-1}, (Intensity)</i>	<i>Comment</i>
C-H stretch	2850–3000 (m)	Alkanes occurs in all compounds with aliphatic C-H bonds
C=C stretch		Alkenes
$\begin{array}{l} \text{-CH=CH}_2 \\ \\ \text{C=CH}_2 \end{array}$	1640 (m)	
$\begin{array}{l} \text{C=CH}_2 \\ / \end{array}$	1655 (m)	
others	1660–1675 (w)	not observed if alkene is symmetrical
=C-H stretch	3000–3100 (m)	
=C-H bend		
$\begin{array}{l} \text{-CH=CH}_2 \\ \\ \text{C=CH}_2 \end{array}$	910–990 (s)	
$\begin{array}{l} \text{C=CH}_2 \\ / \end{array}$	890 (s)	
$\begin{array}{c} \text{H} \\ \\ \text{C}=\text{C} \\ / \quad \backslash \\ \text{H} \quad \text{H} \end{array}$	960–980 (s)	
$\begin{array}{c} \text{H} \quad \text{H} \\ \quad \\ \text{C}=\text{C} \\ / \quad \backslash \\ \text{H} \quad \text{H} \end{array}$	675–730 (s)	position is highly variable
$\begin{array}{c} \text{H} \\ \\ \text{C}=\text{C} \\ / \quad \backslash \\ \quad \quad \end{array}$	800–840 (s)	
O-H stretch	3200–3400 (s)	Alcohols and Phenols
C-O stretch	1050–1250 (s)	also present in other compounds with C-O bonds: ethers, esters, etc.
C≡C stretch	2100–2200 (m)	Alkynes not present or weak in many internal alkynes
≡C-H stretch	3300 (s)	present only in terminal alkynes
C=C stretch	1500, 1600 (s)	Aromatic Compounds two absorptions
C-H bend	650–750 (s)	
overtone	1660–2000 (w)	
C=O stretch		Aldehydes
ordinary	1720–1725 (s)	
α,β-unsaturated	1680–1690 (s)	
benzaldehydes	1700 (s)	
C-H stretch	2720 (m)	
C=O stretch		Ketones
ordinary	1710–1715 (s)	increases with decreasing ring size
α,β-unsaturated	1670–1680 (s)	
aryl ketones	1680–1690 (s)	

Important Infrared Absorptions (continued...)

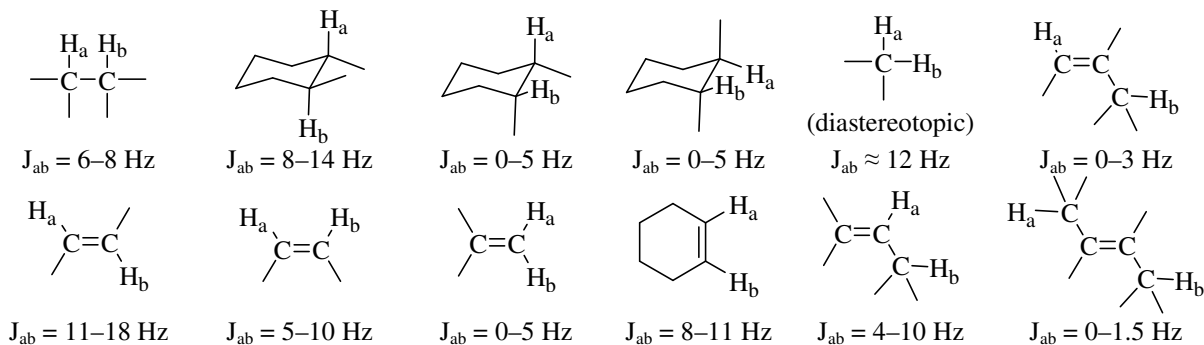
		Carboxylic Acids
C=O stretch		
ordinary	1710 (s)	
benzoic acids	1680–1690 (s)	
O–H stretch	2400–3000 (s)	very broad
		Esters and Lactones
C=O stretch	1735 (s)	increases with decreasing ring size
		Acid Chlorides
C=O stretch	1800 (s)	second weaker band sometimes observed at 1700–1750
		Acid Anhydrides
C=O stretch	1760, 1820 (s)	two bands; increases with decreasing ring size in cyclic anhydrides
		Amides and Lactams
C=O stretch	1650–1655 (s)	increases with decreasing ring size
N–H bend	1640 (s)	
N–H stretch	3200–3400 (m)	doublet absorption observed for some primary amides
		Nitriles
C≡N stretch	2200–2250 (m)	
		Amines
N–H stretch	3200–3375 (m)	several absorptions sometimes observed, especially for primary amines

Characteristic ¹H NMR Chemical Shifts

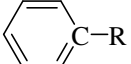





<i>Type of Hydrogen</i> (<i>R = alkyl, Ar = aryl</i>)	<i>Chemical Shift (δ)*</i>	<i>Type of Hydrogen</i> (<i>R = alkyl, Ar = aryl</i>)	<i>Chemical Shift (δ)*</i>
(CH ₃) ₄ Si	0 (by definition)	$\begin{array}{c} \text{O} \\ \\ \text{RCCH}_2\text{R} \end{array}$	2.2–2.6
RCH ₃	0.8–1.0	$\begin{array}{c} \text{O} \\ \\ \text{RCOCH}_3 \end{array}$	3.7–3.9
RCH ₂ R	1.2–1.4	$\begin{array}{c} \text{O} \\ \\ \text{RCOCH}_2\text{R} \end{array}$	4.1–4.7
R ₃ CH	1.4–1.7	RCH ₂ I	3.1–3.3
R ₂ C=CRCHR ₂	1.6–2.6	RCH ₂ Br	3.4–3.6
RC≡CH	2.0–3.0	RCH ₂ Cl	3.6–3.8
ArCH ₃	2.2–2.5	RCH ₂ F	4.4–4.5
ArCH ₂ R	2.3–2.8	ArOH	4.5–4.7
ROH	0.5–6.0	R ₂ C=CH ₂	4.6–5.0
RCH ₂ OH	3.4–4.0	R ₂ C=CHR	5.0–5.7
RCH ₂ OR	3.3–4.0	ArH	6.5–8.5
R ₂ NH	0.5–5.0	$\begin{array}{c} \text{O} \\ \\ \text{RCH} \end{array}$	9.5–10.1
$\begin{array}{c} \text{O} \\ \\ \text{RCCH}_3 \end{array}$	2.1–2.3	$\begin{array}{c} \text{O} \\ \\ \text{RCOH} \end{array}$	10–13

*Values are relative to TMS. Other nearby functional groups may cause the signal to appear outside of these general ranges.

Characteristic ¹H NMR Coupling Constants



Characteristic ¹³C NMR Chemical Shifts

Type of Carbon (<i>R</i> = alkyl, <i>Ar</i> = aryl)	Chemical Shift (δ)*	Type of Carbon (<i>R</i> = alkyl, <i>Ar</i> = aryl)	Chemical Shift (δ)*
(CH ₃) ₄ Si	0 (by definition)	RC≡CR	65-85
RCH ₃	10-40	R ₂ C=CR ₂	100-150
RCH ₂ R	15-55		110-160
R ₃ CH	20-60		160-180
RCH ₂ I	0-40		165-180
RCH ₂ Br	25-65		165-185
RCH ₂ Cl	35-80		180-215
R ₃ COH	40-80		180-215
R ₃ COR	40-80		

*Values are relative to TMS. Other nearby functional groups may cause the signal to appear outside of these general ranges.