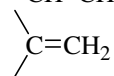
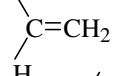
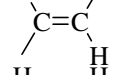
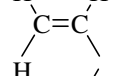
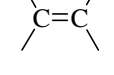


Useful Spectroscopic Data

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
–CH=CH ₂	1640 (m)	
	1655 (m)	
others	1660–1675 (w)	not observed if alkene is symmetrical
=C–H stretch	3000–3100 (m)	
=C–H bend		
–CH=CH ₂	910–990 (s)	
	890 (s)	
	960–980 (s)	
	675–730 (s)	position is highly variable
	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 overtone	650–750 (s) 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...)

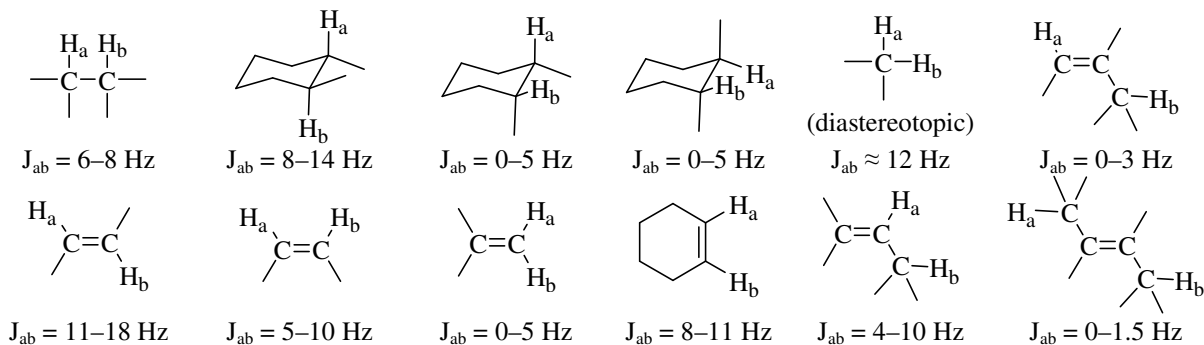
		Carboxylic Acids
C=O stretch		
ordinary	1710 (s)	
benzoic acids	1680–1690 (s)	
O–H stretch	3400–3000 (s)	very broad
		Esters and Lactones
C=O stretch	1735 (s)	increases with decreasing ring size
		Acid Chlorides
C=O stretch	1800 (s)	second weaker band sometimes observed at 1700–1750
		Acid Anhydrides
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.