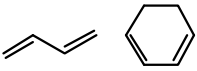
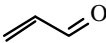



Infrared Absorption Assignments Functional Groups

wavenumber (cm ⁻¹)	structure
3600-3200 (broad)	O-H
3500-3200 (broad)	N-H
3300 (very narrow)	alkyne C-H
3100-3000 (m)	aromatic C-H
3080-3020 (m)	alkene C-H
3000-2800	alkane C-H
3000-2500 (broad)	acid O-H
2260-2210 (m)	nitrile C≡N
2260-2100 (v)	alkyne C≡C
1760-1690	C=O
1680-1640 (v)	alkene C=C
1600 and 1500 (v)	aromatic C=C
1560-1515 and 1385-1345	nitro N-O
1470-1350	C-H
1300-1080	C-N
1300-1000	C-O
1000-675	alkene C-H
870-675	aromatic C-H

*Absorption is strong unless marked otherwise:
(m) moderate, (w) weak, (v) variable

UV Chromophores

Structure	$\pi \rightarrow \pi^*$	$n \rightarrow \pi^*$
C=C	(165 nm)	-
	214/256	-
C=O	(150)	280
	215	320
	(180), 208, 260 (w)	-
-NO ₂	210	280

Exact Masses of Common Isotopes

Element	Abundance	Mass
¹ H	100	1.00783
² H	0.016	2.01410
¹² C	100	12.0000
¹³ C	1.11	13.00336
¹⁴ N	100	14.0031
¹⁵ N	0.38	15.0001
¹⁶ O	100	15.9949
¹⁷ O	0.04	16.9991
¹⁸ O	0.20	17.9992
¹⁹ F	100	18.9984
²⁸ Si	100	27.9769
²⁹ Si	5.10	28.9765
³⁰ Si	3.35	29.9738
³¹ P	100	30.9738
³² S	100	31.9721
³³ S	0.78	32.9715
³⁴ S	4.40	33.9679
³⁵ Cl	100	34.9689
³⁷ Cl	32.5	36.9659
⁷⁹ Br	100	78.9183
⁸¹ Br	98	80.9163
¹²⁷ I	100	126.9045

Additional Infrared Assignments, by Chemical Classes

Typical Position (cm ⁻¹)	Structure
<u>Hydrocarbons</u> (C-H bend)	
1450	-CH ₂ -
1450 and 1380	-CH ₃
1380 doublet	geminal dimethyl, R ₂ C(CH ₃) ₂
1000 and 915	RCH=CH ₂
890	R ₂ C=CH ₂
970	-CH=CH- <i>trans</i>
700	-CH=CH- <i>cis</i>
800	R ₂ C=CHR
~750 and ~700	monosubstituted aromatic
800-850	<i>p</i> - disubstituted aromatic
750-805	<i>m</i> - disubstituted aromatic
730-760	<i>o</i> - disubstituted aromatic

Alcohols and Phenols

3600 (v)	O-H, free
3200-3600 (broad)	O-H, H-bonded
1230	C-O, phenol
1150	C-O, 3° alcohol
1100	C-O, 2° alcohol
1050	C-O, 1° alcohol

Carboxylic Acids

3000 (broad)	O-H
1710	C=O, H-bonded
1250	C-O
920	O-H

Aldehydes and Ketones

2720	C-H, aldehyde
1720	C=O

Amines

3300 (v)	N-H
3300 (doublet)	1° amine -NH ₂
1600 (broad)	N-H
1360-1080	C-N
850 (broad)	N-H

Carbon-halogen

C-F	1100
C-Cl	800
C-Br	600
C-I	500

NMR Characteristic Chemical Shifts, δ , ppm

Description	Formula Type	^{13}C	^1H
Hydrocarbons			
Primary	$-\text{CH}_3$	8-30	0.7-1.3
Secondary	$-\text{CH}_2-$	15-55	1.2-1.4
Tertiary	$\begin{array}{c} \text{H} \\ \\ -\text{C}- \\ \end{array}$	20-60	1.4-1.7
Quaternary	$\begin{array}{c} \\ -\text{C}- \\ \end{array}$	30-50	
Vinyl	$\begin{array}{c} \text{H} \\ \diagdown \\ \text{C}=\text{C} \\ \diagup \end{array}$	100-150	4.5-6.5
Alkynyl	$\text{H}-\text{C}\equiv\text{C}-$	65-85	2.5-2.7
Aromatic	$\text{H}-\text{Ar}$	110-160	6.5-8.0
Allylic	$\begin{array}{c} \text{H}_3\text{C} \\ \diagdown \\ \text{C}=\text{C} \\ \diagup \end{array}$	10-35	1.7-2.0
Benzylic	CH_3Ar	10-35	2.0-3.0
CH_3 Adjacent to an Electronegative Group			
Fluorine	CH_3F	75	4.3
Chlorine	CH_3Cl	25	3.1
Bromine	CH_3Br	10	2.7
Iodine	CH_3I	21	2.2
Oxygen	$\text{CH}_3-\text{O}-$	50-60	3.2
Carbonyl	$\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{C} \\ \diagdown \end{array}$	25-35	2.0-2.7
Nitrogen	$\text{CH}_3-\text{N}-$	25-50	2.1
Functional Groups			
Hydroxyl	$\text{H}-\text{O}-$		2.5-5.0
Phenol	$\text{H}-\text{O}-\text{Ar}$		4.0-12.0
Enol	$\begin{array}{c} \text{H}-\text{O} \\ \diagdown \\ \text{C}=\text{C} \\ \diagup \end{array}$		15.0-17.0
Aldehyde	$-\text{CHO}$	190-215	9.0-10.0
Ketone	$\begin{array}{c} \text{O} \\ \\ \text{C} \\ \diagdown \end{array}$	180-220	
Carboxylic Acid	$-\text{COOH}$	150-185	10.5-12.0
Amine	$-\text{NH}-$		1.0-5.0