

## Infrared Absorption Bands


### Important OH, NH and CH Single Bond Stretching Absorptions

Bond Type	Family	Frequency Range, $\text{cm}^{-1}$	Comments
$\text{O}-\text{H}$	Alcohols	3600 – 3200	Strong, broad
$\text{N}-\text{H}$	Amines, amides	3500 – 3200	Weak – medium. 1°: 2 bands; 2°: 1 band; 3°: no bands
$\text{O}-\text{H}$	Carboxylic acid	3300 – 2500	Strong; <u>very broad</u> . Usually strongest at ~3000 with gradual tapering to 2500
$\text{spC}-\text{H}$	Alkyne	3320 – 3300	Strong – medium
$\text{sp}^2\text{C}-\text{H}$	Alkene, aromatic	3100 – 3000	Medium – weak. May be shoulder on stronger $\text{sp}^3\text{C}-\text{H}$ band
$\text{sp}^3\text{C}-\text{H}$	Alkane	3000 – 2800	Weak-medium. Intensity proportional to number of C-H alkane bonds
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$	Aldehyde	2850 – 2700	Weak to medium, <u>usually two sharp bands</u>

### Important CC and CN Triple Bond Stretching Absorptions

Bond Type	Family	Frequency Range, $\text{cm}^{-1}$	Comments
$\text{C}\equiv\text{C}$	Alkyne	2260 – 2100	Weak – medium
$\text{C}\equiv\text{N}$	Nitrile	2260 – 2220	Medium


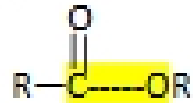
### Important CC, CN and CO Double Bond Stretching Absorptions

Bond Type	Family	Frequency Range, $\text{cm}^{-1}$	Comments
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{H}$	Aldehyde	1740 – 1685	Strong
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{R}$	Ketone	1750 – 1660	Strong
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$	Carboxylic Acid	1725 – 1665	Strong
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{OR}$	Ester	1775 – 1715	Strong
$\text{R}-\overset{\text{O}}{\parallel}{\text{C}}-\text{N}$	Amide	1695 – 1615	Strong
$\text{R}-\text{C}=\text{N}-\text{R}'$	Imine	1650 – 1550	Medium
$\text{C}=\text{C}$	Alkene	1680 – 1600	Medium – weak; narrow
	Aromatic	~1600 and ~1500 – 1430	Medium – weak

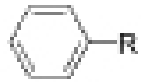

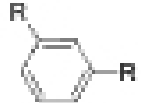

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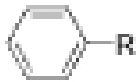




### Important **CO Single Bond Stretching** Absorptions

Bond Type	Family	Frequency Range, $\text{cm}^{-1}$	Comments
$\text{RH}_2\text{C}-\text{OH}$	Primary Alcohol	1075 – 1000	Strong – medium
$\text{R}_2\text{HC}-\text{OH}$	Secondary Alcohol	1130 – 1000	Strong – medium
$\text{R}_3\text{C}-\text{OH}$	Tertiary Alcohol	1210 – 1100	Strong – medium
	Phenol	1260 – 1180	Strong
	Ester	1310 – 1160	Strong, broad

### Important **CH Bending** Absorptions




Bond Type	Family	Frequency Range, $\text{cm}^{-1}$	Comments
$\text{sp}^3\text{C}-\text{H}$	Alkane	1480 – 1430 1395 – 1340	Weak – medium
$\text{RCH}=\text{CH}_2$	Monosubstituted Alkene	997 – 985 and 915 – 905	Medium
$\text{R}_2\text{C}=\text{CH}_2$	Disubstituted terminal Alkene	895 – 885	Usually strong
$\text{cis-RCH}=\text{CHR}'$	<i>cis</i> -Alkene	730 – 665	Usually strong
$\text{trans-RCH}=\text{CHR}'$	<i>trans</i> -Alkene	980 – 960	Usually strong
$\text{R}_2\text{C}=\text{CHR}'$	Trisubstituted Alkene	840 – 790	Usually strong
	Monosubstituted Benzene	770 – 730 and 720 – 680	Usually strong
	<i>ortho</i> -Disubstituted Benzene	770 – 735	Usually strong
	<i>meta</i> -Disubstituted Benzene	810 – 750 and 725 – 680	Usually strong
	<i>para</i> -Disubstituted Benzene	860 – 800	Usually strong

### Miscellaneous Diagnostic Absorptions

Bond Type	Family	Frequency Range, $\text{cm}^{-1}$	Typical Absorption Pattern	Comments
	Monosubstituted Benzene	2000 – 1650		Weak; multiple bands. Not always present.
	<i>ortho</i> -Disubstituted Benzene	2000 – 1650		Weak; multiple bands. Not always present.
	<i>meta</i> -Disubstituted Benzene	2000 – 1650		Weak; multiple bands. Not always present.
	<i>para</i> -Disubstituted Benzene	2000 – 1650		Weak; multiple bands. Not always present.

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**CHARACTERISTIC CHEMICAL SHIFT VALUES FOR  $^1\text{H}$  NMR**  
**Tabular Display**

Type of Proton	Structure	Chemical Shift, ppm
Cyclopropane	$\text{C}_3\text{H}_6$	0.2
Primary	$\text{R}-\text{CH}_3$	0.9
Secondary	$\text{R}_2-\text{CH}_2$	1.3
Tertiary	$\text{R}_3-\text{C}-\text{H}$	1.5
Allylic	$\text{C}=\text{C}-\text{CH}_3$	1.7
Carbonyl Compounds	$\text{H}-\text{C}-\text{C}=\text{O}$	2 – 2.7
Acetylenic	$\text{C}\equiv\text{C}-\text{H}$	2 – 3
Benzylic	$\text{Ar}-\text{C}-\text{H}$	2 – 2.3
Esters	$\text{H}-\text{C}-\text{CO}_2\text{R}$	2 – 2.2
Acids	$\text{H}-\text{C}-\text{CO}_2\text{H}$	2 – 2.6
Ethers	$\text{H}-\text{C}-\text{OR}$	3.3 – 4
Alcohols	$\text{H}-\text{C}-\text{OH}$	3.4 – 4
Esters	$\text{RCO}_2-\text{C}-\text{H}$	3.7 – 4.1
Iodides	$\text{H}-\text{C}-\text{I}$	2 – 4
Bromides	$\text{H}-\text{C}-\text{Br}$	2.5 – 4
Chlorides	$\text{H}-\text{C}-\text{Cl}$	3 – 4
Fluorides	$\text{H}-\text{C}-\text{F}$	4 – 4.5
Vinylic	$\text{C}=\text{C}-\text{H}$	4.6 – 5.9
Aromatic	$\text{Ar}-\text{H}$	6 – 8.5
Amino	$\text{R}-\text{NH}_2$	1 – 5, variable*
Hydroxylic	$\text{R}-\text{C}-\text{OH}$	1 – 5.5, variable*
Phenolic	$\text{Ar}-\text{OH}$	4 – 7, variable*
Aldehydes		9 - 10
Carboxylic Acids		10 – 12, variable*
Amides		5 – 8, variable*

\* = Exchanges with  $\text{D}_2\text{O}$

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