

## General Infrared Absorption Ranges of Various Functional Groups

Bond	Type of Compound	Frequency Range cm <sup>-1</sup>	Intensity
C—H	Alkanes	2850-2970	Strong
		1340- 1470	Strong
C—H	Alkenes	3010-3095	Medium
		675-995	Strong
C—H	Alkynes	3300	Strong
C—H	Aromatic rings	3010-3100	Medium
		690-900	Strong
O—H	Monomeric alcohols, phenols	3590-3650	Variable
	Hydrogen-bonded alcohols, phenols	3200-3600	Variable, sometimes broad
	Monomeric carboxylic acids	3500-3650	Medium
	Hydrogen-bonded carboxylic acids	2500-2700	Broad
N—H	Amines, amides	3300-3500	Medium
C=C	Alkenes	1610-1680	Variable
C=C	Aromatic rings	1500-1600	Variable
C≡C	Alkynes	2100-2260	Variable
C—N	Amines, amides	1180-1360	Strong
C≡N	Nitriles	2210-2280	Strong
C—O	Alcohols, ethers, carboxylic acids, esters	1050-1300	Strong
C=O	Aldehydes, ketones, carboxylic acids, esters	1690-1760	Strong
NO <sub>2</sub>	Nitro compounds	1500-1570	Strong
		1300- 1370	Strong

### *Characteristic IR Absorption Frequencies*

***The hydrogen stretch region (3600-2500 cm<sup>-1</sup>).*** Absorption in this region is associated with the stretching vibration of hydrogen atoms bonded to carbon, oxygen and nitrogen. Care should be exercised in the interpretation of very weak bands because these may be overtones of strong bands occurring at frequencies one-half the value of the weak absorption; that is, 1800-1250 cm<sup>-1</sup>. Overtones of bands near 1650 cm<sup>-1</sup> are particularly common.

$\nu$ (cm <sup>-1</sup> )	Functional Group	Comments
(1) 3600-3400	O—H stretching Intensity: variable	3600 cm <sup>-1</sup> (sharp) unassociated O-H, 3400 cm <sup>-1</sup> (broad) associated O-H; both bands frequently present in alcohol spectra; with strongly associated O-H (CO <sub>2</sub> H or enolized, -dicarbonyl compound) band is very broad (about 500 cm <sup>-1</sup> with its center at 2900-3000 cm <sup>-1</sup> ).
(2) 3400-3200	N—H stretching Intensity: medium	3400 cm <sup>-1</sup> (sharp) unassociated N-H, 3200 cm <sup>-1</sup> (broad) associated N-H; an NH <sub>2</sub> group usually appears as a doublet (separation about 50 cm <sup>-1</sup> the N-H of a secondary amine is often very weak.
(3) 3300  (4) 3080-3010	C—H stretching of an alkyne Intensity: strong  C—H stretching of an alkene Intensity: strong to medium	The complete absence of absorption in this region, 3300-3000 cm <sup>-1</sup> , indicates the absence of hydrogen atoms bonded to C=C or C-C and <i>usually</i> indicates the lack of unsaturation in the molecule. Because this absorption may be very weak in large molecules, some care should be exercised in this interpretation. In addition to the absorption at about 3050 cm <sup>-1</sup> , aromatic compounds will frequently show <i>sharp</i> bands of medium intensity at about 1500 <i>and</i> 1600 cm <sup>-1</sup> .
(5) 3050	C—H stretching of an aromatic compound Intensity: variable; usually medium to weak	

(6) 3000-2600	OH strongly hydrogen-bonded Intensity: medium	A very broad band in this region superimposed on the C-H stretching frequencies is characteristic of carboxylic acids (see 1).
(7) 2980-2900	C—H stretching of an aliphatic compound Intensity: strong	Just as in the previous C-H entries (3-5), <i>complete</i> absence of hydrogen atoms bonded to tetravalent carbon atoms. The tertiary C-H absorption is weak.
(8) 2850-2760	C—H stretching of an aldehyde Intensity: weak	Either one or two bands may be found in this region for a single aldehyde function in the molecule.

**The triple bond region (2300—2000  $\text{cm}^{-1}$ ).** Absorption in this region is associated with the stretching vibration of triple bonds.

$\nu$ ( $\text{cm}^{-1}$ )	Functional Group	Comments
(1) 2260-2215	C N Intensity: strong	Nitriles conjugated with double bonds absorb at lower end of frequency range; nonconjugated nitriles appear at upper end of range.
(2) 2150-2100	C C Intensity: strong in <i>terminal</i> alkynes. variable in others.	This band will be absent if the alkyne is symmetrical, and will be very weak or absent if the alkyne is nearly symmetrical.

**The double-bond region (1900—1550  $\text{cm}^{-1}$ ).** Absorption in this region is *usually* associated with the stretching vibration of carbon-carbon, carbon-oxygen and carbon-nitrogen double bonds.

$\nu$ ( $\text{cm}^{-1}$ )	Functional Group	Comments
(1) 1815-1770	C=O stretching of an acid chloride Intensity: strong	Conjugated and nonconjugated carbonyls absorb at the lower and upper ends, respectively, of the range.
(2) 1870-1800 and 1790-1740	C=O stretching of an acid anhydride Intensity: strong	<i>Both bands</i> are present; <i>each band</i> is altered by ring size and conjugation to approximately the same extent noted for ketones (see 4)
(3) 1750-1735	C=O stretching of an ester or lactone Intensity: very strong	This band is subject to all the structural effects discussed in 4: thus, a conjugated ester absorbs at about 1710 $\text{cm}^{-1}$ and a $\gamma$ -lactone (gamma lactone) absorbs at about 1780 $\text{cm}^{-1}$ .

(4) 1725-1705	C=O stretching of an aldehyde or ketone Intensity: very strong	<p>This value refers to the carbonyl absorption frequency of an acyclic, nonconjugated aldehyde or ketone in which no electronegative groups, for example, halogens, are near the carbonyl group: because this frequency is altered in a predictable way by structural alterations, the following generalizations may be drawn:</p> <p><i>(a) Effect of conjugation:</i> Conjugation of the carbonyl group with an aryl ring or carbon-carbon double or triple bond lowers the frequency by about <math>30\text{ cm}^{-1}</math>. If the carbonyl group is part of a cross-conjugated system (unsaturation on each side of the carbonyl group), the frequency is lowered by about <math>50\text{ cm}^{-1}</math>.</p> <p><i>(b) Effect of ring size:</i> Carbonyl groups in six-membered and larger rings exhibit approximately the same absorption as acyclic ketones; carbonyl groups contained in rings smaller than six absorb at higher frequencies, for example, a cyclopentanone absorbs at about <math>1745\text{ cm}^{-1}</math> and a cyclobutanone absorbs at about <math>1780\text{ cm}^{-1}</math>. The effects of conjugation and ring size are additive, for example, a 2-cyclopentenone absorbs at about <math>1710\text{ cm}^{-1}</math>.</p> <p><i>(c) Effect of electronegative atoms:</i> An electronegative atom (especially oxygen or halogen) bonded to the <math>\alpha</math>-carbon atom of an aldehyde or ketone may raise the position of the carbonyl absorption frequency by about <math>20\text{ cm}^{-1}</math>.</p>
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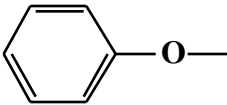
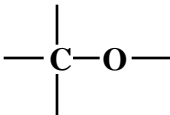

(5) 1700	C=O stretching of an acid Intensity: strong	This absorption frequency is lowered by conjugation, as noted under entry 4.
(6) 1690-1650	C=O stretching of an amide or lactam Intensity: strong	This band is lowered in frequency by about 20 $\text{cm}^{-1}$ by conjugation. The frequency of the band is raised about 35 $\text{cm}^{-1}$ in $\beta$ -lactams and 70 $\text{cm}^{-1}$ in $\gamma$ -lactams.
(7) 1660-1600	C=C stretching of an alkene Intensity: variable	Nonconjugated alkenes appear at upper end of range, and absorptions are usually weak; conjugated alkenes appear at lower end of range, and absorptions are medium to strong. The absorption frequencies of these bands are raised by ring strain but to a lesser extent than noted with carbonyl functions (see 4).
(8) 1680-1640	C=N stretching Intensity: variable	This band is usually weak and difficult to assign.

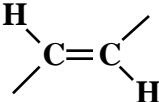
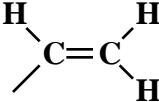
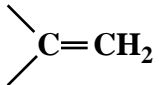
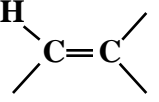
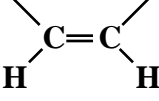
***The hydrogen bending region (1600-1250  $\text{cm}^{-1}$ ).*** Absorption in this region is commonly due to bending vibration of hydrogen atoms attached to carbon and to nitrogen. These bands generally do not provide much useful structural information. In the listing, the bands that are most useful for structural assignment have been marked with an asterisk (\*).

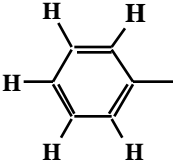
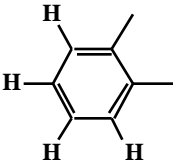
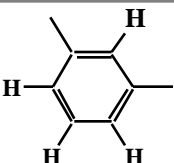
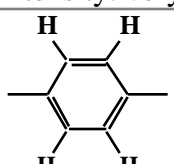
$\nu$ ( $\text{cm}^{-1}$ )	Functional Group	Comments
(1) 1600	-NH <sub>2</sub> bending Intensity: strong to medium	This band in conjunction with bands in the 3300 $\text{cm}^{-1}$ region is often used to characterize primary amines and unsubstituted amides.
(2) 1540	-NH- bending Intensity: generally weak	This band in conjunction with bands in the 3300 $\text{cm}^{-1}$ region is often used to characterize secondary amines and monosubstituted amines. In the case of secondary amines this band. Like the N-H stretching band in the 3300 $\text{cm}^{-1}$ region, may be very weak.
(3) *1520 and 1350	NO <sub>2</sub> coupled stretching bands Intensity: strong	This pair of bands is usually very intense.
(4) 1465	-CH <sub>2</sub> -bending Intensity: variable	The intensity of this band varies according to the number of methylene groups present: the more such groups, the more intense the absorption.

(5) 1410	-CH <sub>2</sub> - bending of carbonyl-containing component Intensity: variable	This absorption is characteristic of methylene groups adjacent to carbonyl functions: its intensity depends on the number of such groups present in the molecule.
(6) *1450 and 1375	-CH <sub>3</sub> Intensity: strong	The band of lower frequency (1375 cm <sup>-1</sup> ) is usually used to characterize a methyl group. If two methyl groups are bonded to one carbon atom, a characteristic doublet (1385 and 1365 cm <sup>-1</sup> ) will be present.
(7) 1325	-CH- bending Intensity: weak	This band is weak and often unreliable.

**The fingerprint region (1250-600 cm<sup>-1</sup>).** The fingerprint region of the spectrum is generally rich in detail, with many bands appearing. This region is particularly diagnostic for determining whether an unknown substance is identical with a known substance, the IR spectrum of which is available. It is not practical to make assignments to all these bands because many of them represent combination frequencies and therefore are very sensitive to the total molecular structure; moreover, many single bond stretching vibrations and a variety of bending vibrations also appear in this region. Suggested structural assignments in this region must be regarded as tentative and are generally taken as corroborative evidence in conjunction with assignments of bands at higher frequencies.

$\nu$ (cm <sup>-1</sup> )	Functional Group	Comments
(1) 1200	 Intensity: strong	It is not certain whether these strong bands arise from C-O bending or C-O stretching vibrations. One or more strong bands are found in this region in the spectra of alcohols, ethers and esters. The relationship indicated between structure and band location is only approximate and any structural assignment based on this relationship must be regarded as tentative. Esters often exhibit one or two strong bands between 1170 and 1270 cm <sup>-1</sup> .
(2) 1150	 Intensity: strong	
(3) 1100	 Intensity: strong	
(4) 1050	-CH <sub>2</sub> -O- Intensity: strong	

(5) 965	 C-H bending Intensity: strong	This strong band is present in the spectra of trans-1,2-disubstituted ethylenes.
(6) 985 and 910	 C-H bending Intensity: strong	The lower frequency band of these two strong bands is used to characterize a terminal vinyl group.
(7) 890	 C-H bending Intensity: strong	This strong band, used to characterize a methylene group, may be raised by 20-80 cm <sup>-1</sup> if the methylene group is bonded to an electronegative group or atom.
(8) 810-840	 Intensity: strong	Very unreliable; this band is not always present and frequently seems to be outside this range, since substituents are varied.
(9) 700	 Intensity: variable	This band, attributable to a cis-1,2-disubstituted ethylene, is unreliable because it is frequently obscured by solvent absorption or other bands.

(10) 750 and 690	 <p>C-H bending Intensity: strong</p>	<p>These bands are of limited value because they are frequently obscured by solvent absorption or other bands. Their usefulness will be most important when independent evidence leads to a structural assignment complete except for position of aromatic substituents.</p>
(11) 750	 <p>C-H bending Intensity: very strong</p>	
(12) 780 and 700	 <p>Intensity: very strong</p>	
(13) 825	 <p>Intensity: very strong</p>	



(14) 1400-1000	C-F Intensity: strong	The position of these bands is quite sensitive to structure. As a result, they are not particularly useful because the presence of halogen is more easily detected by chemical methods. The bands are usually strong.
(15) 800-600	C-Cl Intensity: strong	
(16) 700-500	C-Br Intensity: strong	
(17) 600-400	C-I Intensity: strong	

