Alkenes are compounds that have a carbon-carbon double bond, \(-\text{C}≡\text{C}\). The stretching vibration of the \(\text{C}≡\text{C}\) bond usually gives rise to a moderate band in the region 1680-1640 cm\(^{-1}\).

Stretching vibrations of the \(-\text{C}=\text{C}=\text{H}\) bond are of higher frequency (higher wavenumber) than those of the \(-\text{C}–\text{C}–\text{H}\) bond in alkanes.

This is a very useful tool for interpreting IR spectra: Only alkenes and aromatics show a C-H stretch slightly higher than 3000 cm\(^{-1}\). Compounds that do not have a \(\text{C}=\text{C}\) bond show C-H stretches only below 3000 cm\(^{-1}\).

The strongest bands in the spectra of alkenes are those attributed to the carbon-hydrogen bending vibrations of the \(\text{=C–H}\) group. These bands are in the region 1000-650 cm\(^{-1}\) (Note: this overlaps the fingerprint region).

Summary:

- C=C stretch from 1680-1640 cm\(^{-1}\)
- \(=\text{C}=\text{H}\) stretch from 3100-3000 cm\(^{-1}\)
- \(=\text{C}–\text{H}\) bend from 1000-650 cm\(^{-1}\)

The IR spectrum of 1-octene is shown below. Note the band greater than 3000 cm\(^{-1}\) for the \(=\text{C–H}\) stretch and the several bands lower than 3000 cm\(^{-1}\) for \(-\text{C–H}\) stretch (alkanes). The C=C stretch band is at 1644 cm\(^{-1}\). Bands for C-H scissoring (1465) and methyl rock (1378) are marked on this spectrum; in routine IR analysis, these bands are not specific to an alkene and are generally not noted because they are present in almost all organic molecules (and they are in the fingerprint region). The bands at 917 cm\(^{-1}\) and 1044 cm\(^{-1}\) are attributed to \(=\text{C}–\text{C}\&\text{Mac173};\text{H}\) bends.
It is interesting to overlay a spectrum of 1-octene with octane (shown below). Note how similar they are, except for the bands due to C=C or C=C–H stretches/bends.
IR Spectroscopy Tutorial: Alkynes

Alkynes are compounds that have a carbon-carbon triple bond (\(-\text{C}≡\text{C}-\)). The \(-\text{C}≡\text{C}-\) stretch appears as a weak band from 2260-2100 cm\(^{-1}\). This can be an important diagnostic tool because very few organic compounds show an absorption in this region.

A terminal alkyne (but not an internal alkyne) will show a \(\text{C-H}\) stretch as a strong, narrow band in the range 3330-3270 cm\(^{-1}\). (Often this band is indistinguishable from bands resulting from other functional groups on the same molecule which absorb in this region, such as the O-H stretch.)

A terminal alkyne will show a \(\text{C-H}\) bending vibration in the region 700-610 cm\(^{-1}\).

**Summary:**

- \(-\text{C}≡\text{C}-\) stretch from 2260-2100 cm\(^{-1}\)
- \(-\text{C}≡\text{C-H}\): \(\text{C-H}\) stretch from 3330-3270 cm\(^{-1}\)
- \(-\text{C}≡\text{C-H}\): \(\text{C-H}\) bend from 700-610 cm\(^{-1}\)

The spectrum of 1-hexyne, a terminal alkyne, is shown below. Note the \(\text{C-H}\) stretch of the \(\text{C-H}\) bond adjacent to the carbon-carbon triple bond (3324), the carbon-carbon triple bond stretch (2126), and the \(\text{C-H}\) bend of the \(\text{C-H}\) bond adjacent to the carbon-carbon triple bond (636). The other bands noted are \(\text{C-H}\) stretch, scissoring, and methyl rock bands from the alkane portions of the molecule.
IR Spectroscopy Tutorial: Aromatics

The $\equiv$C–H stretch in aromatics is observed at 3100-3000 cm$^{-1}$. Note that this is at slightly higher frequency than is the –C–H stretch in alkanes.

This is a very useful tool for interpreting IR spectra: Only alkenes and aromatics show a C–H stretch slightly higher than 3000 cm$^{-1}$. Compounds that do not have a C=C bond show C–H stretches only below 3000 cm$^{-1}$.

Aromatic hydrocarbons show absorptions in the regions 1600-1585 cm$^{-1}$ and 1500-1400 cm$^{-1}$ due to carbon-carbon stretching vibrations in the aromatic ring.

Bands in the region 1250-1000 cm$^{-1}$ are due to C–H in-plane bending, although these bands are too weak to be observed in most aromatic compounds.

Besides the C–H stretch above 3000 cm$^{-1}$, two other regions of the infrared spectra of aromatics distinguish aromatics from organic compounds that do not have an aromatic ring:

- 2000-1665 cm$^{-1}$ (weak bands known as "overtones")
- 900-675 cm$^{-1}$ (out-of-plane or "oop" bands)

Not only do these bands distinguish aromatics, but they can be useful if you want to determine the number and positions of substituents on the aromatic ring. The pattern of overtone bands in the region 2000-1665 cm$^{-1}$ reflect the substitution pattern on the ring. The pattern of the oop C–H bending bands in the region 900-675 cm$^{-1}$ are also characteristic of the aromatic substitution pattern. Details of the correlation between IR patterns in these two regions and ring substitution are available in the literature references linked in the left frame (especially the books by Shriner and Fuson, Silverstein et. al., and the Aldrich Library of IR Spectra).

In some instances, it is useful to remember that aromatics in general show a lot more bands than compounds that do not contain an aromatic ring. If you are presented with two spectra and told that one is aromatic and one is not, a quick glance at the sheer multitude of bands in one of the spectra can tell you that it is the aromatic compound.

Summary:

- C–H stretch from 3100-3000 cm$^{-1}$
- overtones, weak, from 2000-1665 cm$^{-1}$
- C–C stretch (in-ring) from 1600-1585 cm$^{-1}$
- C–C stretch (in-ring) from 1500-1400 cm$^{-1}$
- C–H "oop" from 900-675 cm$^{-1}$

The spectrum of toluene is shown below. Note the $\equiv$C–H stretches of aromatics (3099, 3068, 3032) and the

http://orgchem.colorado.edu/hndbk/support/ir/tutor/tutorial.html
C–H stretches of the alkyl (methyl) group (2925 is the only one marked). The characteristic overtones are seen from about 2000-1665. Also note the carbon-carbon stretches in the aromatic ring (1614, 1506, 1465), the in-plane C–H bending (1086, 1035), and the C–H oop (738).
Alcohols have characteristic IR absorptions associated with both the O-H and the C-O stretching vibrations. When run as a thin liquid film, or "neat", the O-H stretch of alcohols appears in the region 3500-3200 cm\(^{-1}\) and is a very intense, broad band. The C-O stretch shows up in the region 1260-1050 cm\(^{-1}\).

- O-H stretch, hydrogen bonded 3500-3200 cm\(^{-1}\)
- C-O stretch 1260-1050 cm\(^{-1}\) (s)

The spectrum of ethanol is shown below. Note the very broad, strong band of the O-H stretch (3391) and the C-O stretches (1102, 1055).
**IR Spectroscopy Tutorial: Ketones**

The carbonyl stretching vibration band $\text{C}=\text{O}$ of saturated aliphatic ketones appears at 1715 cm$^{-1}$. Conjugation of the carbonyl group with carbon-carbon double bonds or phenyl groups, as in alpha, beta-unsaturated aldehydes and benzaldehyde, shifts this band to lower wavenumbers, 1685-1666 cm$^{-1}$. See also:

- carbonyl stretching frequencies
- unsaturation/saturation refresher

**Summary:**

- C=O stretch:
  - aliphatic ketones 1715 cm$^{-1}$
  - $\alpha,\beta$-unsaturated ketones 1685-1666 cm$^{-1}$

The spectrum of 2-butanone is shown below. This is a saturated ketone, and the C=O band appears at 1715. Note the C–H stretches (around 2991) of alkyl groups. It's usually not necessary to mark any of the bands in the fingerprint region (less than 1500 cm$^{-1}$).
IR Spectroscopy Tutorial: Aldehydes

The carbonyl stretch $\text{C}=\text{O}$ of saturated aliphatic aldehydes appears from 1740-1720 cm$^{-1}$. As in ketones, if the carbons adjacent to the aldehyde group are unsaturated, this vibration is shifted to lower wavenumbers, 1710-1685 cm$^{-1}$. See also:

- carbonyl stretching frequencies
- unsaturation/saturation refresher

Another useful diagnostic band for aldehydes is the $\text{O}=$$\text{C}$$-\text{H}$ stretch. This band generally appears as one or two bands of moderate intensity in the region 2830-2695 cm$^{-1}$. Since the band near 2830 cm$^{-1}$ is usually indistinguishable from other $\text{C}$$-\text{H}$ stretching vibration bands (recall that the $\text{C}$$-\text{H}$ stretches of alkanes appear from 3000-2850 cm$^{-1}$), the presence of a moderate band near 2720 cm$^{-1}$ is more likely to be helpful in determining whether or not a compound is an aldehyde.

If you suspect a compound to be an aldehyde, always look for a peak around 2720 cm$^{-1}$; it often appears as a shoulder-type peak just to the right of the alkyl $\text{C}$$-\text{H}$ stretches.

Summary:

- $\text{H}=$$\text{C}$$=\text{O}$ stretch 2830-2695 cm$^{-1}$
- $\text{C}=\text{O}$ stretch:
  - aliphatic aldehydes 1740-1720 cm$^{-1}$
  - alpha, beta-unsaturated aldehydes 1710-1685 cm$^{-1}$

The spectra of benzaldehyde and butyraldehyde are shown below. Note that the $\text{O}=$$\text{C}$ stretch of the alpha, beta-unsaturated compound -- benzaldehyde -- is at a lower wavenumber than that of the saturated butyraldehyde.

Note the $\text{O}=$$\text{C}$$-\text{H}$ stretches in both aldehydes in the region 2830-2695 cm$^{-1}$, especially the shoulder peak at 2725 cm$^{-1}$ in butyraldehyde and 2745 cm$^{-1}$ in benzaldehyde.
Carboxylic acids show a strong, wide band for the O–H stretch. Unlike the O–H stretch band observed in alcohols, the carboxylic acid O–H stretch appears as a very broad band in the region 3300-2500 cm⁻¹, centered at about 3000 cm⁻¹. This is in the same region as the C–H stretching bands of both alkyl and aromatic groups. Thus a carboxylic acid shows a somewhat "messy" absorption pattern in the region 3300-2500 cm⁻¹, with the broad O–H band superimposed on the sharp C–H stretching bands. The reason that the O–H stretch band of carboxylic acids is so broad is because carboxylic acids usually exist as hydrogen-bonded dimers.

The carbonyl stretch C=O of a carboxylic acid appears as an intense band from 1760-1690 cm⁻¹. The exact position of this broad band depends on whether the carboxylic acid is saturated or unsaturated, dimerized, or has internal hydrogen bonding. See also:

- carbonyl stretching frequencies

The C–O stretch appears in the region 1320-1210 cm⁻¹, and the O–H bend is in the region 1440-1395 cm⁻¹ and 950-910 cm⁻¹, although the 1440-1395 band may not be distinguishable from C–H bending bands in the same region.

Summary:

- O–H stretch from 3300-2500 cm⁻¹
- C=O stretch from 1760-1690 cm⁻¹
- C–O stretch from 1320-1210 cm⁻¹
- O–H bend from 1440-1395 and 950-910 cm⁻¹

The spectrum of hexanoic acid is shown below. Note the broad peak due to O–H stretch superimposed on the sharp band due to C–H stretch. Note the C=O stretch (1721), C–O stretch (1296), O–H bends (1419, 948), and C–O stretch (1296).
hexanoic acid

2971
O-H stretch
(and C-H stretch)

1419
O-H bend

1296
C-O stretch

948
O-H bend

1721
C=O stretch

Wavenumbers (cm⁻¹)

%Transmittance

back to
IR Tutorial
Contents

http://orgchem.colorado.edu/hndbksupport/irtutor/tutorial.html
IR Spectroscopy Tutorial: Esters

The carbonyl stretch $\text{C=O}$ of aliphatic esters appears from 1750-1735 cm$^{-1}$; that of $\alpha, \beta$-unsaturated esters appears from 1730-1715 cm$^{-1}$. See also:

- **carbonyl stretching frequencies**

The $\text{C-O}$ stretches appear as two or more bands in the region 1300-1000 cm$^{-1}$.

Summary:

- $\text{C=O}$ stretch
  - aliphatic from 1750-1735 cm$^{-1}$
  - $\alpha, \beta$-unsaturated from 1730-1715 cm$^{-1}$
- $\text{C-O}$ stretch from 1300-1000 cm$^{-1}$

The spectra of ethyl acetate and ethyl benzoate are shown below. Note that the $\text{C=O}$ stretch of ethyl acetate (1752) is at a higher wavelength than that of the $\alpha, \beta$-unsaturated ester ethyl benzoate (1726). Also note the $\text{C-O}$ stretches in the region 1300-1000 cm$^{-1}$.
IR Spectroscopy Tutorial

back to
IR Tutorial
Contents

http://orgchem.colorado.edu/hndbksupport/irtutorial/tutorial.html
IR Spectroscopy Tutorial: Amines

The N–H stretches of amines are in the region 3300-3000 cm\(^{-1}\). These bands are weaker and sharper than those of the alcohol O–H stretches which appear in the same region. In primary amines (RNH\(_2\)), there are two bands in this region, the asymmetrical N–H stretch and the symmetrical N–H stretch.

Secondary amines (R\(_2\)NH) show only a single weak band in the 3300-3000 cm\(^{-1}\) region, since they have only one N–H bond. Tertiary amines (R\(_3\)N) do not show any band in this region since they do not have an N–H bond.

(A shoulder band usually appears on the lower wavenumber side in primary and secondary liquid amines arising from the overtone of the N–H bending band: this can confuse interpretation. Note the spectrum of aniline, below.)

The N–H bending vibration of primary amines is observed in the region 1650-1580 cm\(^{-1}\). Usually, secondary amines do not show a band in this region and tertiary amines never show a band in this region. (This band can be very sharp and close enough to the carbonyl region to cause students to interpret it as a carbonyl band.)

Another band attributed to amines is observed in the region 910-665 cm\(^{-1}\). This strong, broad band is due to N–H wag and observed only for primary and secondary amines.

The C–N stretching vibration of aliphatic amines is observed as medium or weak bands in the region 1250-1020 cm\(^{-1}\). In aromatic amines, the band is usually strong and in the region 1335-1250 cm\(^{-1}\).

Summary:

- N–H stretch 3400-3250 cm\(^{-1}\)
  - 1° amine: two bands from 3400-3300 and 3330-3250 cm\(^{-1}\)
  - 2° amine: one band from 3350-3310 cm\(^{-1}\)
  - 3° amine: no bands in this region
- N–H bend (primary amines only) from 1650-1580 cm\(^{-1}\)
- C–N stretch (aromatic amines) from 1335-1250 cm\(^{-1}\)
- C–N stretch (aliphatic amines) from 1250-1020 cm\(^{-1}\)
- N–H wag (primary and secondary amines only) from 910-665 cm\(^{-1}\)

The spectrum of aniline is shown below. This primary amine shows two N–H stretches (3442, 3360); note the shoulder band, which is an overtone of the N–H bending vibration. The C–N stretch appears at 1281 rather than at lower wavenumbers because aniline is an aromatic compound. Also note the N–H bend at

http://orgchem.colorado.edu/hndbksupport/irtutor/tutorial.html
IR Spectroscopy Tutorial: Amines

The N-H stretches of amines are in the region 3300-3000 cm\(^{-1}\). These bands are weaker and sharper than those of the alcohol O-H stretches which appear in the same region. In primary amines (RNH\(_2\)), there are two bands in this region, the asymmetrical N-H stretch and the symmetrical N-H stretch.

Secondary amines (R\(_2\)NH) show only a single weak band in the 3300-3000 cm\(^{-1}\) region, since they have only one N-H bond. Tertiary amines (R\(_3\)N) do not show any band in this region since they do not have an N-H bond.

(A shoulder band usually appears on the lower wavenumber side in primary and secondary liquid amines arising from the overtone of the N-H bending band: this can confuse interpretation. Note the spectrum of aniline, below.)

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The C-N stretching vibration of aliphatic amines is observed as medium or weak bands in the region 1250-1020 cm\(^{-1}\). In aromatic amines, the band is usually strong and in the region 1335-1250 cm\(^{-1}\).

Summary:

- N-H stretch 3400-3250 cm\(^{-1}\)
  - 1\(^{\circ}\) amine: two bands from 3400-3300 and 3330-3250 cm\(^{-1}\)
  - 2\(^{\circ}\) amine: one band from 3350-3310 cm\(^{-1}\)
  - 3\(^{\circ}\) amine: no bands in this region
- N-H bend (primary amines only) from 1650-1580 cm\(^{-1}\)
- C-N stretch (aromatic amines) from 1335-1250 cm\(^{-1}\)
- C-N stretch (aliphatic amines) from 1250-1020 cm\(^{-1}\)
- N-H wag (primary and secondary amines only) from 910-665 cm\(^{-1}\)

The spectrum of aniline is shown below. This primary amine shows two N-H stretches (3442, 3360); note the shoulder band, which is an overtone of the N-H bending vibration. The C-N stretch appears at 1281 rather than at lower wavenumbers because aniline is an aromatic compound. Also note the N-H bend at

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The spectrum of diethylamine is below. Note that this secondary amine shows only one N–H stretch (3288). The C–N stretch is at 1143, in the range for non-aromatic amines (1250-1020). Diethylamine also shows an N–H wag (733).
Triethylamine is a tertiary amine and does not have an N–H stretch, nor an N–H wag. The C–N stretch is at 1214 cm$^{-1}$ (non-aromatic).
Note the absence of a N-H stretch in this compound, a tertiary amine.

Triethylamine

H₃C-N-CH₂CH₃

C-N stretch

Wavenumbers (cm⁻¹)