Common Group Frequencies Summary

When analyzing an IR spectrum, it is helpful to overlay the diagram below onto the spectrum with our mind to help recognize functional groups.

![Diagram of Group Frequency and Fingerprint Regions](image)

Figure 1. Group frequency and fingerprint regions of the mid-infrared spectrum

The region of the infrared spectrum from 1200 to 700 cm\(^{-1}\) is called the fingerprint region. This region is notable for the large number of infrared bands that are found there. Many different vibrations, including C-O, C-C and C-N single bond stretches, C-H bending vibrations, and some bands due to benzene rings are found in this region. The fingerprint region is often the most complex and confusing region to interpret, and is usually the last section of a spectrum to be interpreted. However, the utility of the fingerprint region is that the many bands there provide a fingerprint for a molecule.

Group Frequencies - a closer look

Detailed information about the infrared absorptions observed for various bonded atoms and groups is usually presented in tabular form. The following table provides a collection of such data for the most common functional groups. Following the color scheme of the chart, stretching absorptions are listed in the blue-shaded section and bending absorptions in the green shaded part. More detailed descriptions for certain groups (e.g. alkenes, arenes, alcohols, amines & carbonyl compounds) may be viewed by clicking on the functional class name. Since most organic compounds have C-H bonds, a useful rule is that absorption in the 2850 to 3000 cm\(^{-1}\) is due to sp\(^3\) C-H stretching; whereas, absorption above 3000 cm\(^{-1}\) is from sp\(^2\) C-H stretching or sp C-H stretching if it is near 3300 cm\(^{-1}\).

<table>
<thead>
<tr>
<th>Functional Class</th>
<th>Stretching Vibrations</th>
<th>Bending Vibrations</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Range (cm(^{-1}))</td>
<td>Intensity</td>
</tr>
<tr>
<td>Alkanes</td>
<td>2850-3000</td>
<td>str</td>
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<td></td>
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<tr>
<td>Alkenes</td>
<td>3020-3100</td>
<td>med</td>
</tr>
<tr>
<td></td>
<td>1630-1680</td>
<td>var</td>
</tr>
<tr>
<td><strong>Group</strong></td>
<td><strong>Wavenumbers</strong></td>
<td><strong>Int.</strong></td>
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<td>------------------------</td>
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<tr>
<td><strong>Alkynes</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1900-2000</td>
<td>str</td>
<td></td>
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<tr>
<td>3300</td>
<td>str</td>
<td></td>
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<tr>
<td>2100-2250</td>
<td>var</td>
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<td><strong>Arenes</strong></td>
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<tr>
<td>3030</td>
<td>var</td>
<td></td>
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<tr>
<td>1600 &amp; 1500</td>
<td>med-wk</td>
<td></td>
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<tr>
<td><strong>Alcohols &amp; Phenols</strong></td>
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<tr>
<td>3580-3650</td>
<td>var</td>
<td></td>
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<tr>
<td>3200-3550</td>
<td>str</td>
<td></td>
</tr>
<tr>
<td>970-1250</td>
<td>str</td>
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<tr>
<td><strong>Amines</strong></td>
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<tr>
<td>3400-3500 (dil. soln.)</td>
<td>wk</td>
<td></td>
</tr>
<tr>
<td>3300-3400 (dil. soln.)</td>
<td>wk</td>
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<tr>
<td>1000-1250</td>
<td>med</td>
<td></td>
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<tr>
<td><strong>Aldehydes &amp; Ketones</strong></td>
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<tr>
<td>2690-2840 (2 bands)</td>
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<td></td>
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<tr>
<td>1720-1740</td>
<td>str</td>
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<td>1710-1720</td>
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<tr>
<td>1350-1360</td>
<td>str</td>
<td></td>
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<tr>
<td>1400-1450</td>
<td>str</td>
<td></td>
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<tr>
<td>1100</td>
<td>str</td>
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<tr>
<td>1350-1360</td>
<td>str</td>
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<tr>
<td>1400-1450</td>
<td>str</td>
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<tr>
<td><strong>Carboxylic Acids &amp;</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Derivatives</td>
<td>2500-3300 (acids) overlap</td>
<td></td>
</tr>
<tr>
<td></td>
<td>C-H</td>
<td></td>
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<tr>
<td></td>
<td>C=O (H-bonded)</td>
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<tr>
<td></td>
<td>O-C (sometimes 2-peaks)</td>
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</table>
Recognizing Group Frequencies in IR Spectra - a very close look

Hydrocarbons

Hydrocarbons compounds contain only C-H and C-C bonds, but there is plenty of information to be obtained from the infrared spectra arising from C-H stretching and C-H bending.

In alkanes, which have very few bands, each band in the spectrum can be assigned:

- C–H stretch from 3000–2850 cm\(^{-1}\)
- C–H bend or scissoring from 1470-1450 cm\(^{-1}\)
- C–H rock, methyl from 1370-1350 cm\(^{-1}\)
- C–H rock, methyl, seen only in long chain alkanes, from 725-720 cm\(^{-1}\)

Figure 3. shows the IR spectrum of octane. Since most organic compounds have these features, these C-H vibrations are usually not noted when interpreting a routine IR spectrum. Note that the change in dipole moment with respect to distance for the C-H stretching is greater than that for others shown, which is why the C-H stretch band is the more intense.

![Infrared Spectrum of Octane](image)

In alkenes compounds, each band in the spectrum can be assigned:
• C=C stretch from 1680-1640 cm\(^{-1}\)
• =C–H stretch from 3100-3000 cm\(^{-1}\)
• =C–H bend from 1000-650 cm\(^{-1}\)

Figure 4. shows the IR spectrum of 1-octene. As alkanes compounds, these bands are not specific and are generally not noted because they are present in almost all organic molecules.

Figure 4. Infrared Spectrum of 1-Octene

In alkynes, each band in the spectrum can be assigned:

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

The spectrum of 1-hexyne, a terminal alkyne, is shown below.

Figure 5. Infrared Spectrum of 1-Hexyne
In aromatic compounds, each band in the spectrum can be assigned:

- 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\(^{-1}\)

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\(^{-1}\).

Figure 6. shows the spectrum of toluene.

![Infrared Spectrum of Toluene](image)

**Functional Groups Containing the C-O Bond**

Alcohols have IR absorptions associated with both the O-H and the C-O stretching vibrations.

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

Figure 7. shows the spectrum of ethanol. Note the very broad, strong band of the O–H stretch.
The carbonyl stretching vibration band C=O of saturated aliphatic ketones appears:

- C=O stretch - aliphatic ketones 1715 cm\(^{-1}\)
- ?, ?-unsaturated ketones 1685-1666 cm\(^{-1}\)

Figure 8. shows the spectrum of 2-butanone. This is a saturated ketone, and the C=O band appears at 1715.

If a compound is suspected to be an aldehyde, a peak always appears around 2720 cm\(^{-1}\) which often appears as a shoulder-type peak just to the right of the alkyl C–H stretches.

Figure 8. Infrared Spectrum of 2-Butanone
• H–C=O stretch 2830-2695 cm⁻¹
• C=O stretch:
  ◦ aliphatic aldehydes 1740-1720 cm⁻¹
  ◦ alpha, beta-unsaturated aldehydes 1710-1685 cm⁻¹

Figure 9. shows the spectrum of butyraldehyde.

![Infrared Spectrum of Butyraldehyde](image)

Figure 9. Infrared Spectrum of Butyraldehyde

The carbonyl stretch C=O of esters appears:

• C=O stretch
  ◦ aliphatic from 1750-1735 cm⁻¹
  ◦ ?, ?,-unsaturated from 1730-1715 cm⁻¹
• C–O stretch from 1300-1000 cm⁻¹

Figure 10. shows the spectrum of ethyl benzoate.
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.

- 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\(^{-1}\)

Figure 11. shows the spectrum of hexanoic acid.
Organic Nitrogen Compounds

- N–O asymmetric stretch from 1550-1475 cm\(^{-1}\)
- N–O symmetric stretch from 1360-1290 cm\(^{-1}\)

Organic Compounds Containing Halogens

Alkyl halides are compounds that have a C–X bond, where X is a halogen: bromine, chlorine, fluorene, or iodine.

- C–H wag (\(-\text{CH}_2\text{X}\)) from 1300-1150 cm\(^{-1}\)
- C–X stretches (general) from 850-515 cm\(^{-1}\)
  - C–Cl stretch 850-550 cm\(^{-1}\)
  - C–Br stretch 690-515 cm\(^{-1}\)

The spectrum of 1-chloro-2-methylpropane are shown below.
Figure 13. Infrared Spectrum of 1-chloro-2-methylpropane

For more Infrared spectra Spectral database of organic molecules is introduced to use free database. Also, the infrared spectroscopy correlation table is linked on bottom of page to find other assigned IR peaks.

Exercise

1. What functional groups give the following signals in an IR spectrum?

   A) 1700 cm$^{-1}$
   
   B) 1550 cm$^{-1}$
   
   C) 1700 cm$^{-1}$ and 2510-3000 cm$^{-1}$

2. How can you distinguish the following pairs of compounds through IR analysis?

   A) CH$_3$OH (Methanol) and CH$_3$CH$_2$OCH$_2$CH$_3$ (Diethylether)
   
   B) Cyclopentane and 1-pentene.
   
   C)
3. The following spectra is for the accompanying compound. What are the peaks that you can identify in the spectrum?

![Spectral Image]

Source: SDBSWeb: [http://sdbs.db.aist.go.jp](http://sdbs.db.aist.go.jp) (National Institute of Advanced Industrial Science and Technology, 2 December 2016)

4. What absorptions would the following compounds have in an IR spectra?

(A) ![Compounds Image A]

(B) ![Compounds Image B]

(C) ![Compounds Image C]

**Answer**

1. [Blank Line]


2.

A) A OH peak will be present around 3300 cm\(^{-1}\) for methanol and will be absent in the ether.

B) 1-pentene will have an alkene peak around 1650 cm\(^{-1}\) for the C=C and there will be another peak around 3100 cm\(^{-1}\) for the sp\(^2\) C-H group on the alkene.

C) Cannot distinguish these two isomers. They both have the same functional groups and therefore would have the same peaks on an IR spectra.

3.

**Frequency (cm\(^{-1}\)) Functional Group**

- 3200 C≡C-H
- 2900-3000 C-C-H, C=C-H
- 2100 C≡C
- 1610 C=C

(There is also an aromatic undertone region between 2000-1600 which describes the substitution on the phenyl ring.)

4.

A)

**Frequency (cm\(^{-1}\)) Functional Group**
2900-3000 C-C-H, C=C-H  
1710 C=O  
1610 C=C  
1100 C-O  

**B)**

Frequency (cm⁻¹) Functional Group

3200 C≡C-H  
2900-3000 C-C-H, C=C-H  
2100 C≡C  
1710 C=O  

**C)**

Frequency (cm⁻¹) Functional Group

3300 (broad) O-H  
2900-3000 C-C-H, C=C-H  
2000-1800 Aromatic Overtones  
1710 C=O  
1610 C=C  

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**Contributors and Attributions**

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