How to Interpret an IR Spectrum

Don’t be overwhelmed when you first view IR spectra or this document. We have simplified the interpretation by having you only focus on 4/5 regions of the spectrum. Do not try to examine and identify each and every peak within the entire spectrum. Instead, sequentially look at each of the designated 4/5 regions. You can ignore all the areas outside of these 4/5 regions. While each and every bond will give a peak, many of these peaks are not very useful. Therefore only focus on these 4/5 regions. Yes, you are expected memorize the exact location for each of these regions and to know the distinctive peak shape for the N-H/O-H region. To start to analyze a spectrum, first determine if there is a substantial absorbance present in each of the designated regions. Then determine which bond types are present. From the bond types, determine which functional group is responsible for that particular combination. That is the functional group of the molecule. You need to know your functional groups to be able to do this successfully.

N-H/OH Bonds. This is toward the far left of the spectra. (3200-3500 cm⁻¹)
The shape and exact location define which group is present.
- O-H 3200-3500 cm⁻¹ Alcohol; Broad, rounded and distinct
- NH₂ 3200-3500 cm⁻¹ Primary Amine; Sharp double point
- N-H 3200-3500 cm⁻¹ Secondary Amine; Sharp single point
- COO-H 2500-3500 cm⁻¹ Carboxylic Acid; Very broad. Extends outside designated region.

CH Bonds The exact location defines which group is present. (2800-3100 cm⁻¹)
sp³-C-H 2800-3000 cm⁻¹ sp³ Carbon-Hydrogen; Multi-peaked, strong. Almost always present
sp²-C-H 3000-3100 cm⁻¹ sp² Carbon-Hydrogen; Usually a shoulder on left of sp³ C-H absorbance.
sp-C-H 3300 cm⁻¹ Terminal Alkyne: Icicle-like within typical ‘NH/OH’ region

Triple Bonds Two types of bonds overlap. (2100-2300 cm⁻¹)
C≡N 2200-2300 cm⁻¹ Nitrile;
C≡C 2100-2250 cm⁻¹ Terminal alkyne; weak (often not seen at all for internal alkynes.)

Double Bonds Two types of bonds overlap. The shape and exact location defines which group is present. (1620-1800 cm⁻¹)
C=O 1650-1800 cm⁻¹ Carbonyl; Strong distinct absorbance.
C=C 1620-1680 cm⁻¹ Alkene; Sharp medium size

Fingerprint Region This area is used to confirm identity but is not very useful for assigning identity.
C-O 1000-1300 cm⁻¹. This area is difficult to distinguish. Use only when necessary. This area will be necessary to distinguish between an alkane and an ether, and between a ketone and an ester.
<table>
<thead>
<tr>
<th>Functional Groups</th>
<th>Position (cm$^{-1}$)</th>
<th>Shape</th>
</tr>
</thead>
<tbody>
<tr>
<td>O-H/ NH (Hydrogen bonded to Nitrogen &amp; Oxygen)</td>
<td>3200-3500</td>
<td>strong, rounded</td>
</tr>
<tr>
<td>-O-H</td>
<td>3200-3600</td>
<td>medium, pointed</td>
</tr>
<tr>
<td>-N-H, -NH$_2$</td>
<td>3200-3500</td>
<td>medium, pointed</td>
</tr>
<tr>
<td>-COOH</td>
<td>2500-3500</td>
<td>very broad</td>
</tr>
<tr>
<td>C-H (Hydrogen bonded to Carbon)</td>
<td>2800-3100, 3300</td>
<td></td>
</tr>
<tr>
<td>sp $\equiv$C-H</td>
<td>3300</td>
<td>strong, narrow, pointed</td>
</tr>
<tr>
<td>sp$^2$ =C-H</td>
<td>3000-3100</td>
<td>medium, shoulder</td>
</tr>
<tr>
<td>sp$^3$ C-H</td>
<td>2800-3000</td>
<td>multi-peaked</td>
</tr>
<tr>
<td>$\equiv$ (Triple Bond; Carbon to carbon and carbon to nitrogen)</td>
<td>2100-2300</td>
<td></td>
</tr>
<tr>
<td>C≡N</td>
<td>2200-2300</td>
<td>weak sharp</td>
</tr>
<tr>
<td>C≡C-H</td>
<td>2100-2250</td>
<td>very weak sharp</td>
</tr>
<tr>
<td>= (Double Bond; Carbon to )</td>
<td>1620-1800</td>
<td></td>
</tr>
<tr>
<td>C=O</td>
<td>1650-1800</td>
<td>strong</td>
</tr>
<tr>
<td>C=C</td>
<td>1620-1680</td>
<td>medium, sharp</td>
</tr>
<tr>
<td>Fingerprint</td>
<td>&lt;1600</td>
<td>limited value</td>
</tr>
<tr>
<td>-C-O-</td>
<td>1000-1300</td>
<td>use only when necessary</td>
</tr>
</tbody>
</table>

Note: All spectra from SDBSWeb: [http://sdbs.db.aist.go.jp](http://sdbs.db.aist.go.jp) (National Institute of Advanced Industrial Science and Technology, August 31, 2016)
3200-3500 cm\(^{-1}\) Oxygen-hydrogen, nitrogen-hydrogen (and sp hybridized carbon-hydrogen bonds). **Shape dependent.**

Alcohols, Carboxylic Acids, Amines, Terminal Alkynes.

**ALCOHOLS** have very distinctive **broad rounded** absorbance between 3200 and 3600 cm\(^{-1}\). There is a distinct break between the \(-\text{OH}\) absorbance and the sp\(^3\)CH absorbance.

**CARBOXYLIC ACID**- The \(-\text{OH}\) of a carboxylic acid **shifts over toward 3000 cm\(^{-1}\)**. This is a **very broad** absorbance 2500 to 3500 cm\(^{-1}\) which spills over the sp\(^3\)CH absorbance.

**TERMINAL ALKYNES**- The terminal C-H bond of \(\equiv\text{C}-\text{H}\) has a **very sharp** \(\text{‘icicle’ like absorbance around 3300 cm}^{-1}\).**

**PRIMARY AMINES**- Show **TWO** short pointed absorbances between 3200-3500 cm\(^{-1}\).

**SECONDARY AMINES**- Shows one short pointed absorbance between 3200-3500 cm\(^{-1}\).

**TERTIARY AMINES**- There are no N-H bonds, so no \(-\text{N-H}\) absorbance.
Pattern differences between Carboxylic Acids, Alcohols, Terminal Alkynes and Amines

- **Carboxylic acid**
  - O-H
  - C=O

- **Alcohol**
  - O-H

- **Internal alkyne or nitrile**
  - C≡C/C≡N

- **Terminal Alkyne**
  - H-C≡C

- **Secondary Amine**
  - N

- **Primary Amine**
  - N

Chemical structures and peaks indicating differences in spectroscopic properties.
2800-3100 cm\(^{-1}\). \(\text{sp}^3\) and \(\text{sp}^2\) carbon-hydrogen bonds.

Virtually every organic molecule will have an absorbance in this region. Alkanes have little discernible difference in IR and this area is of little valuable to help distinguish similar structures. Alkanes (\(\text{sp}^3\) 2800-3000 cm\(^{-1}\)), alkenes (\(\text{sp}^2\) 3000-3100 cm\(^{-1}\)), alkynes (sp \(\sim\) 3300 cm\(^{-1}\)). If alkene \(\equiv\text{C-H}\) is present it will often look like shoulder to left of regular \(\equiv\text{C-H}\) absorbance around 3100. Aromatic C-H tend to be a bit weaker.

\[
\begin{align*}
\text{Alkane, Pentane} & \quad \text{Alkene, 1-pentene} & \quad \text{Aromatic, toluene}
\end{align*}
\]

2100-2300 cm\(^{-1}\). Triple bonds. -C≡N or C≡C.

ALKYNES and NITRILES have an absorbance in a usually barren area of 2100-2300 cm\(^{-1}\). The nitrile peak is usually stronger than alkyne and between 2200 and 2300 cm\(^{-1}\). The alkyne is normally between 2100-2300 cm\(^{-1}\) and is only readily apparent for terminal alkynes. The terminal \(\equiv\text{C-H}\) bond will show an additional absorbance around 3300 cm\(^{-1}\).

\[
\begin{align*}
\text{R-C≡N nitrile} & \quad \text{-C≡CH alkyne}
\end{align*}
\]
1620-1680 cm\(^{-1}\) & 1650-1800 cm\(^{-1}\) Carbonyl (C=O) and Alkene (C=C)

Carbonyl groups have very distinctive and strong absorbance between 1650-1800 cm\(^{-1}\). Alkene C=C, absorb between 1620 and 1680 cm\(^{-1}\). Alkenes tend to be sharper and less intense (weaker).

1000-1300 cm\(^{-1}\). C-O stretch.

This is a difficult to correctly interpret region. Use this region only when necessary, such as when trying to distinguish an ether from an alkane or between an ester from a ketone. This is the least important IR.

Sizable strong absorbance little or weak absorbance
Alkane. Only sp\(^3\) C-H at 2800-3000 cm\(^{-1}\).

Alkene. Sp\(^2\) C-H at 3100 cm\(^{-1}\), sp\(^3\) C-H at 2800-3000 cm\(^{-1}\), C=C at 1620 cm\(^{-1}\).

Primary Amine, NH\(_2\) at 3400 cm\(^{-1}\), sp\(^3\) C-H at 2800-3000 cm\(^{-1}\).

Secondary Amine, NH at 3400 cm\(^{-1}\), sp\(^3\) C-H at 2800-3000 cm\(^{-1}\).
Carboxylic Acid. VERY BROAD —O-H which spills over into normal sp\(^3\) C-H at 2800-3000cm\(^{-1}\) region, C=O at 1710cm\(^{-1}\),

\[ \text{[X] 3200-3500cm}^{-1}(\text{O--H,N-H}) \]
\[ \text{[X] 3000-3100 cm}^{-1}(=\text{C-H}) \]
\[ \text{[X] 2800-3000 cm}^{-1}(\text{C-H}) \]
\[ \text{[ ] 2100-2300 cm}^{-1}(≡) \]
\[ \text{[X ] 1650-1800 cm}^{-1}(\text{C=O}) \]
\[ \text{[ ] 1620-1680 cm}^{-1}(\text{C=C}) \]
\[ \text{[x ] 1000-1300 cm}^{-1}(\text{C-O}) \]

Alcohol. -O-H broad at 3300cm\(^{-1}\), sp\(^3\) C-H at 2800-3000cm\(^{-1}\), (-C-O at 1100cm-1),

\[ \text{[X] 3200-3500cm}^{-1}(\text{O--H,N-H}) \]
\[ \text{[ ] 3000-3100 cm}^{-1}(=\text{C-H}) \]
\[ \text{[X] 2800-3000 cm}^{-1}(\text{C-H}) \]
\[ \text{[ ] 2100-2300 cm}^{-1}(≡) \]
\[ \text{[ ] 1650-1800 cm}^{-1}(\text{C=O}) \]
\[ \text{[ ] 1620-1680 cm}^{-1}(\text{C=C}) \]
\[ \text{[X ] 1000-1300 cm}^{-1}(\text{C-O}) \]

Internal alkyne or nitrile sp\(^3\) C-H at 2800-3000cm\(^{-1}\), C≡C or C≡N at 2250cm⁻¹,

\[ \text{[ ] 3200-3500cm}^{-1}(\text{O--H,N-H}) \]
\[ \text{[ ] 3000-3100 cm}^{-1}(=\text{C-H}) \]
\[ \text{[X] 2800-3000 cm}^{-1}(\text{C-H}) \]
\[ \text{[X ] 2100-2300 cm}^{-1}(≡) \]
\[ \text{[ ] 1650-1800 cm}^{-1}(\text{C=O}) \]
\[ \text{[ ] 1620-1680 cm}^{-1}(\text{C=C}) \]
\[ \text{[ ] 1000-1300 cm}^{-1}(\text{C-O}) \]

terminal alkyne Sp C-H at 3300cm\(^{-1}\), sp\(^3\) C-H at 2800-3000cm\(^{-1}\), C≡C or C≡N at 2250cm⁻¹,

\[ \text{[X] 3200-3500cm}^{-1}(\text{O--H,N-H}) \]
\[ \text{[ ] 3000-3100 cm}^{-1}(=\text{C-H}) \]
\[ \text{[X] 2800-3000 cm}^{-1}(\text{C-H}) \]
\[ \text{[X ] 2100-2300 cm}^{-1}(≡) \]
\[ \text{[ ] 1650-1800 cm}^{-1}(\text{C=O}) \]
\[ \text{[ ] 1620-1680 cm}^{-1}(\text{C=C}) \]
\[ \text{[ ] 1000-1300 cm}^{-1}(\text{C-O}) \]
**Ketone or Aldehyde**, sp\(^3\) C-H at 2800-3000 cm\(^{-1}\), C=O at 1730 cm\(^{-1}\),

\[ \begin{align*}
&[\ ] 3200-3500 \text{ cm}^{-1} (\text{O-H,N-H}) \\
&[\ ] 3000-3100 \text{ cm}^{-1} (\text{C-H}) \\
&[X] 2800-3000 \text{ cm}^{-1} (\text{C-H}) \\
&[\ ] 2100-2300 \text{ cm}^{-1} (\equiv) \\
&[X] 1650-1800 \text{ cm}^{-1} (\text{C}=\text{O}) \\
&[\ ] 1620-1680 \text{ cm}^{-1} (\text{C}=\text{C}) \\
&[\ ] 1000-1300 \text{ cm}^{-1} (\text{C-O})
\end{align*} \]

**Ester**, sp\(^3\) C-H at 2800-3000 cm\(^{-1}\), C=O at 1750 cm\(^{-1}\), (-C-O at 1250 cm\(^{-1}\))

\[ \begin{align*}
&[\ ] 3200-3500 \text{ cm}^{-1} (\text{O-H,N-H}) \\
&[\ ] 3000-3100 \text{ cm}^{-1} (\text{C-H}) \\
&[X] 2800-3000 \text{ cm}^{-1} (\text{C-H}) \\
&[\ ] 2100-2300 \text{ cm}^{-1} (\equiv) \\
&[X] 1650-1800 \text{ cm}^{-1} (\text{C}=\text{O}) \\
&[\ ] 1620-1680 \text{ cm}^{-1} (\text{C}=\text{C}) \\
&[X] 1000-1300 \text{ cm}^{-1} (\text{C-O})
\end{align*} \]

**Amide**, -NH\(_2\) at 3300 cm\(^{-1}\), sp\(^3\) C-H at 2800-3000 cm\(^{-1}\), C=O at 1750 cm\(^{-1}\),

\[ \begin{align*}
&[X] 3200-3500 \text{ cm}^{-1} (\text{O-H,N-H}) \\
&[\ ] 3000-3100 \text{ cm}^{-1} (\text{C-H}) \\
&[X] 2800-3000 \text{ cm}^{-1} (\text{C-H}) \\
&[\ ] 2100-2300 \text{ cm}^{-1} (\equiv) \\
&[X] 1650-1800 \text{ cm}^{-1} (\text{C}=\text{O}) \\
&[\ ] 1620-1680 \text{ cm}^{-1} (\text{C}=\text{C}) \\
&[\ ] 1000-1300 \text{ cm}^{-1} (\text{C-O})
\end{align*} \]

**Ether**, sp\(^3\) C-H at 2800-3000 cm\(^{-1}\), (-C-O at 1150 cm\(^{-1}\)),

\[ \begin{align*}
&[\ ] 3200-3500 \text{ cm}^{-1} (\text{O-H,N-H}) \\
&[\ ] 3000-3100 \text{ cm}^{-1} (\text{C-H}) \\
&[X] 2800-3000 \text{ cm}^{-1} (\text{C-H}) \\
&[\ ] 2100-2300 \text{ cm}^{-1} (\equiv) \\
&[\ ] 1650-1800 \text{ cm}^{-1} (\text{C}=\text{O}) \\
&[\ ] 1620-1680 \text{ cm}^{-1} (\text{C}=\text{C}) \\
&[X] 1000-1300 \text{ cm}^{-1} (\text{C-O})
\end{align*} \]
### IR absorbance regions based on Functional Groups

<table>
<thead>
<tr>
<th>Functional Groups</th>
<th>Alkane</th>
<th>Alkene</th>
<th>Terminal alkyne</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amide</td>
<td>[ ] 3200-3500 cm⁻¹(O-H,N-H)</td>
<td>[ ] 3200-3500 cm⁻¹(O-H,N-H)</td>
<td>[X] 3300 cm⁻¹(≡C-H)</td>
</tr>
<tr>
<td></td>
<td>[ ] 3000-3100 cm⁻¹(≡C-H)</td>
<td>[X] 3000-3100 cm⁻¹(≡C-H)</td>
<td>[ ] 3000-3100 cm⁻¹(≡C-H)</td>
</tr>
<tr>
<td>Ketone and aldehydes</td>
<td>[X] 2800-3000 cm⁻¹(C=H)</td>
<td>[X] 2800-3000 cm⁻¹(C=H)</td>
<td>[X] 2800-3000 cm⁻¹(C-H)</td>
</tr>
<tr>
<td></td>
<td>[ ] 2100-2300 cm⁻¹(≡)</td>
<td>[ ] 2100-2300 cm⁻¹(≡)</td>
<td>[X] 2100-2300 cm⁻¹(C≡C)</td>
</tr>
<tr>
<td></td>
<td>[ ] 1650-1800 cm⁻¹(C=O)</td>
<td>[ ] 1650-1800 cm⁻¹(C=O)</td>
<td>[ ] 1650-1800 cm⁻¹(C=O)</td>
</tr>
<tr>
<td></td>
<td>[X] 1620-1680 cm⁻¹(C=C)</td>
<td>[X] 1620-1680 cm⁻¹(C=C)</td>
<td>[X] 1620-1680 cm⁻¹(C=C)</td>
</tr>
<tr>
<td></td>
<td>[ ] 1000-1300 cm⁻¹(C-O)</td>
<td>[ ] 1000-1300 cm⁻¹(C-O)</td>
<td>[ ] 1000-1300 cm⁻¹(C-O)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Nitrile or internal Alkyne</th>
<th>Alcohol</th>
<th>Ether</th>
</tr>
</thead>
<tbody>
<tr>
<td>C≡C≡N or Nitrile</td>
<td>[ ] 3300 cm⁻¹(≡C-H)</td>
<td>[X] 3100-3500 cm⁻¹(=O-H)</td>
</tr>
<tr>
<td>C≡C≡C</td>
<td>[ ] 3000-3100 cm⁻¹(=C-H)</td>
<td>[ ] 3000-3100 cm⁻¹(=C-H)</td>
</tr>
<tr>
<td></td>
<td>[X] 2800-3000 cm⁻¹(C=H)</td>
<td>[X] 2800-3000 cm⁻¹(C-H)</td>
</tr>
<tr>
<td></td>
<td>[X] 2100-2300 cm⁻¹(C≡N, C≡C)</td>
<td>[X] 2100-2300 cm⁻¹(C≡N)</td>
</tr>
<tr>
<td></td>
<td>[ ] 1650-1800 cm⁻¹(C=O)</td>
<td>[ ] 1650-1800 cm⁻¹(C=O)</td>
</tr>
<tr>
<td></td>
<td>[X] 1620-1680 cm⁻¹(C≡C)</td>
<td>[X] 1620-1680 cm⁻¹(C≡C)</td>
</tr>
<tr>
<td></td>
<td>[ ] 1000-1300 cm⁻¹(C-O)</td>
<td>[X] 1000-1300 cm⁻¹(C-O)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Ketone and aldehydes</th>
<th>Ester</th>
<th>Carboxylic Acid</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[ ] 3200-3500 cm⁻¹(O-H)</td>
<td>[ ] 3200-3500 cm⁻¹(O-H)</td>
</tr>
<tr>
<td></td>
<td>[X] 2800-3100 cm⁻¹(C=H)</td>
<td>[X] 2800-3100 cm⁻¹(C=H)</td>
</tr>
<tr>
<td></td>
<td>[X] 2100-2300 cm⁻¹(≡)</td>
<td>[X] 2100-2300 cm⁻¹(≡)</td>
</tr>
<tr>
<td></td>
<td>[X] 1650-1800 cm⁻¹(C=O)</td>
<td>[X] 1650-1800 cm⁻¹(C=O)</td>
</tr>
<tr>
<td></td>
<td>[X] 1620-1680 cm⁻¹(C≡C)</td>
<td>[X] 1620-1680 cm⁻¹(C≡C)</td>
</tr>
<tr>
<td></td>
<td>[ ] 1000-1300 cm⁻¹(C-O)</td>
<td>[X] 1000-1300 cm⁻¹(C-O)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Amine</th>
<th>Amide</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>[X] 3200-3500 cm⁻¹(N-H)</td>
</tr>
<tr>
<td></td>
<td>[X] 2800-3100 cm⁻¹(C=H)</td>
</tr>
<tr>
<td></td>
<td>[X] 2100-2300 cm⁻¹(≡)</td>
</tr>
<tr>
<td></td>
<td>[X] 1650-1800 cm⁻¹(C=O)</td>
</tr>
<tr>
<td></td>
<td>[X] 1620-1680 cm⁻¹(C≡C)</td>
</tr>
<tr>
<td></td>
<td>[ ] 1000-1300 cm⁻¹(C-O)</td>
</tr>
</tbody>
</table>