**IR Spectroscopy Tutorial: How to analyze IR spectra**

If you have followed this tutorial group-by-group, you will realize that in even rather simple, mono-functional molecules there are so many IR bands that it is not feasible to assign every band in an IR spectrum. Instead, look for tell-tale bands -- the region from 4000-1300 cm-1 is particularly useful for determining the presence of specific functional groups. You can rely on the [IR correlation charts](http://orgchem.colorado.edu/Spectroscopy/specttutor/irchart.html) (linked in the left frame), but we recommend (in fact, in organic chem 1 lab, we *require*) that you memorize the distinctive bands of the common functional bands:

|  |  |  |
| --- | --- | --- |
| 3500-3300 cm-1 | N–H stretch | 1&Mac251;, 2&Mac251; amines |
| 3500-3200 cm-1 | O–H stretch | alcohols, a broad, strong band |
| 3100-3000 cm-1 | C–H stretch | alkenes |
| 3000-2850 cm-1 | C–H stretch | alkanes |
| 1760-1665 cm-1 | C=O stretch | ketones, aldehydes, esters |
| 1680-1640 cm-1 | C=C stretch | alkenes |

Begin by looking in the region from 4000-1300. Look at the C–H stretching bands around 3000:

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| --- | --- |
|  | *Indicates:* |
| Are any or all to the right of 3000? | alkyl groups (present in most organic molecules) |
| Are any or all to the left of 3000? | a C=C bond or aromatic group in the molecule |

Look for a carbonyl in the region 1760-1690. If there is such a band:

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| --- | --- |
|  | *Indicates:* |
| Is an O–H band also present? | a carboxylic acid group |
| Is a C–O band also present? | an ester |
| Is an aldehydic C–H band also present? | an aldehyde |
| Is an N–H band also present? | an amide |
| Are none of the above present? | a ketone |

(also check the [exact position of the carbonyl band](http://orgchem.colorado.edu/Spectroscopy/irtutor/carbonylsir.html) for clues as to the type of carbonyl compound it is)

Look for a broad O–H band in the region 3500-3200 cm-1. If there is such a band:

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| --- | --- |
|  | *Indicates:* |
| Is an O–H band present? | an alcohol or phenol |

Look for a single or double sharp N–H band in the region 3400-3250 cm-1. If there is such a band:

|  |  |
| --- | --- |
|  | *Indicates:* |
| Are there two bands? | a primary amine |
| Is there only one band? | a secondary amine |

Other structural features to check for:

|  |  |
| --- | --- |
|  | *Indicates:* |
| Are there C–O stretches? | an ether (or an ester if there is a carbonyl band too) |
| Is there a C=C stretching band? | an alkene |
| Are there aromatic stretching bands? | an aromatic |
| Is there a C≡C band? | an alkyne |
| Are there -NO2 bands? | a nitro compound |

If there is an absence of major functional group bands in the region 4000-1300 cm-1 (other than C–H stretches), the compound is probably a strict hydrocarbon.

Also check the region from 900-650 cm-1. Aromatics, alkyl halides, carboxylic acids, amines, and amides show moderate or strong absorption bands (bending vibrations) in this region.

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| As a beginning student, you should not try to assign or interpret every peak in the spectrum. Concentrate on learning the major bands and recognizing their presence and absence in any given spectrum. |

In the organic chem teaching labs, you usually know what compound you started with and what compound you are trying to make. For instance, if you are oxidizing an alcohol to a ketone, your product should show a carbonyl band but no hydroxyl band. If no carbonyl band is present, the experiment was not successful. If both carbonyl and hydroxyl bands are present, the product is not pure.