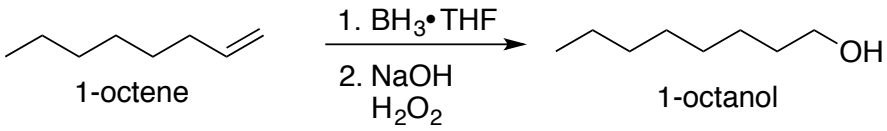
Chemistry 233

Infrared Spectroscopy
Spring 2018

Consider Lab 9 – Hydroboration/Oxidation:
How do we know that the reaction has occurred as expected?

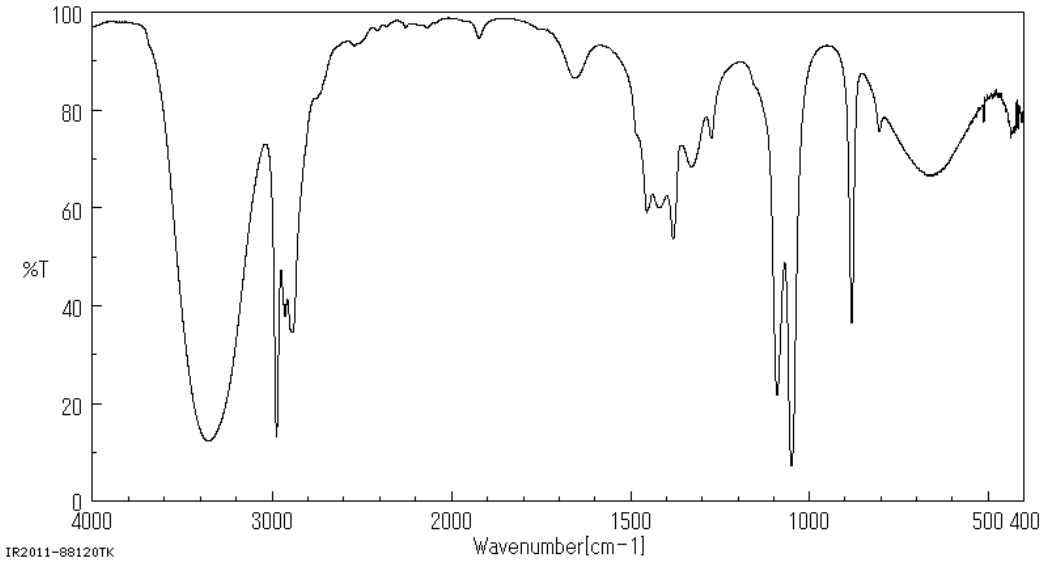


Infrared Spectroscopy

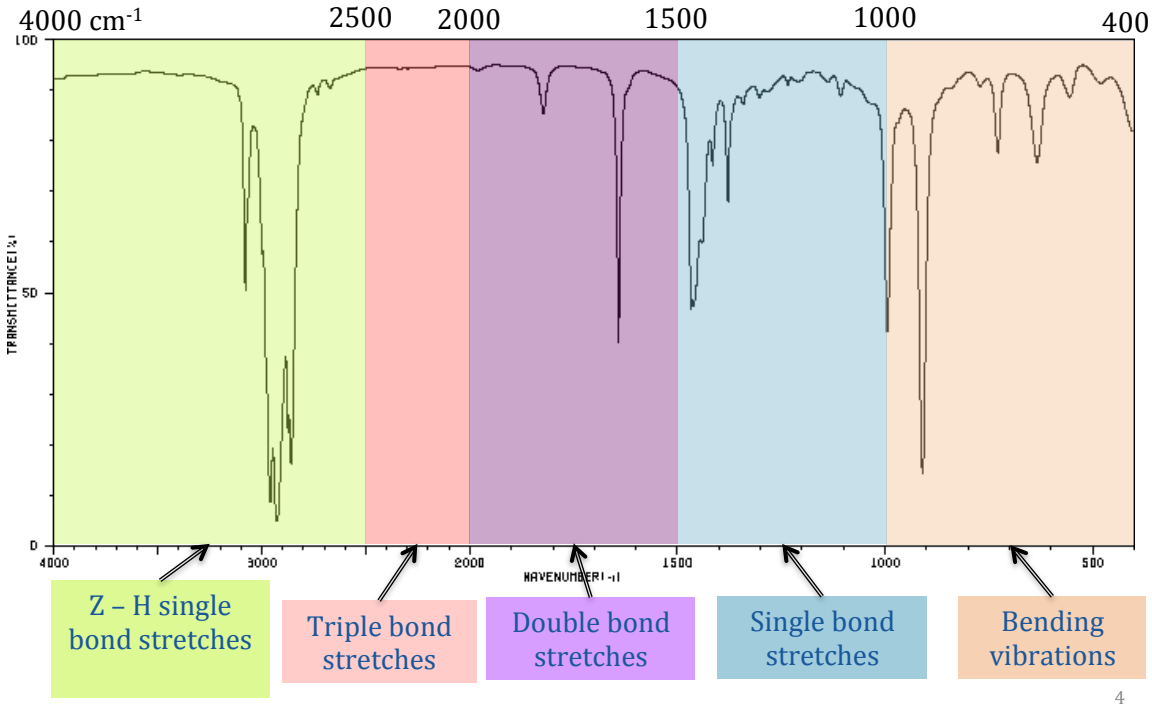
- **Main Purpose = determination of functional groups in a molecule.**
- **Generally can not deduce an entire structure from IR.**

- **When IR light is passed through a molecule, the bonds will absorb IR light causing the bonds to stretch or bend.**
- **This energy absorption can be seen on the IR spectrum.**

Sample IR Spectrum

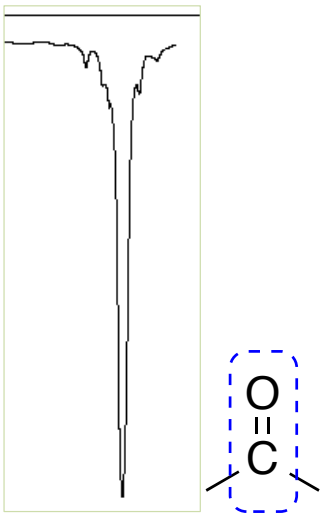


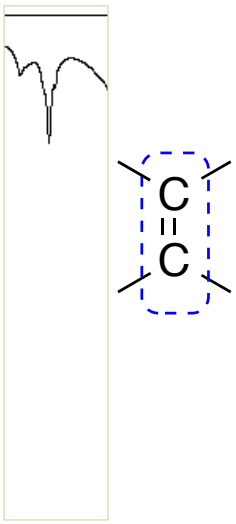
General IR Regions



Signal Intensity

A more polar bond will have a stronger absorption than a less polar bond.

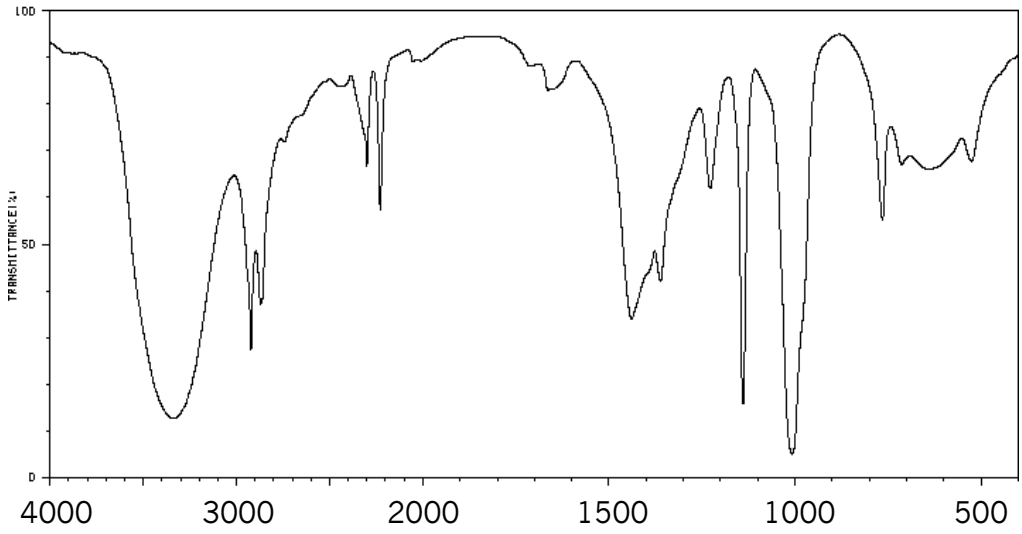




Key Functional Groups to Look For

1) Alcohol O-H Stretch

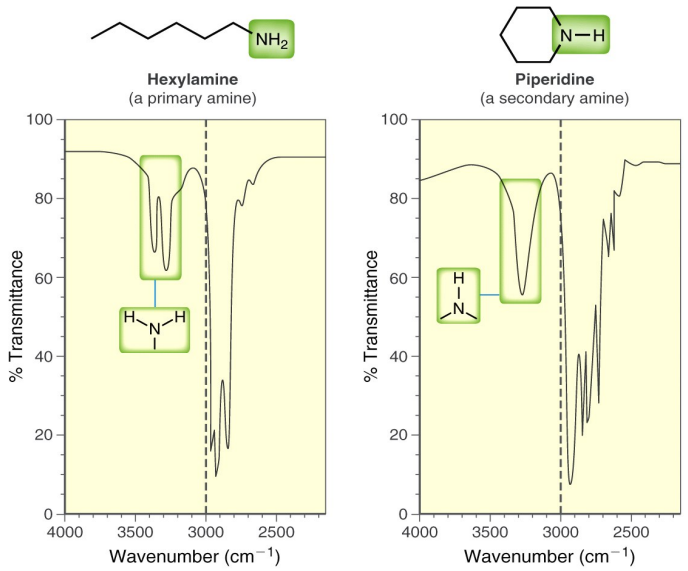
Broad Stretch, 3200-3600 cm^{-1}



Key Functional Groups to Look For

2) Amine/Amide N-H Stretch

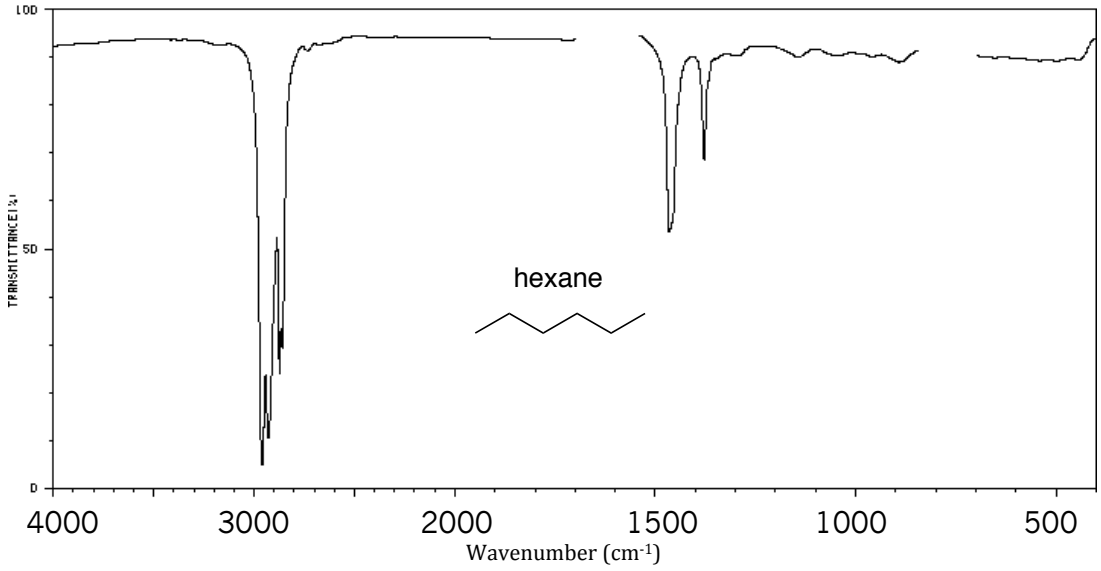
Medium Stretch, 3300-3500 cm^{-1}



Key Functional Groups to Look For

3) Alkane – Csp^3-H Stretch

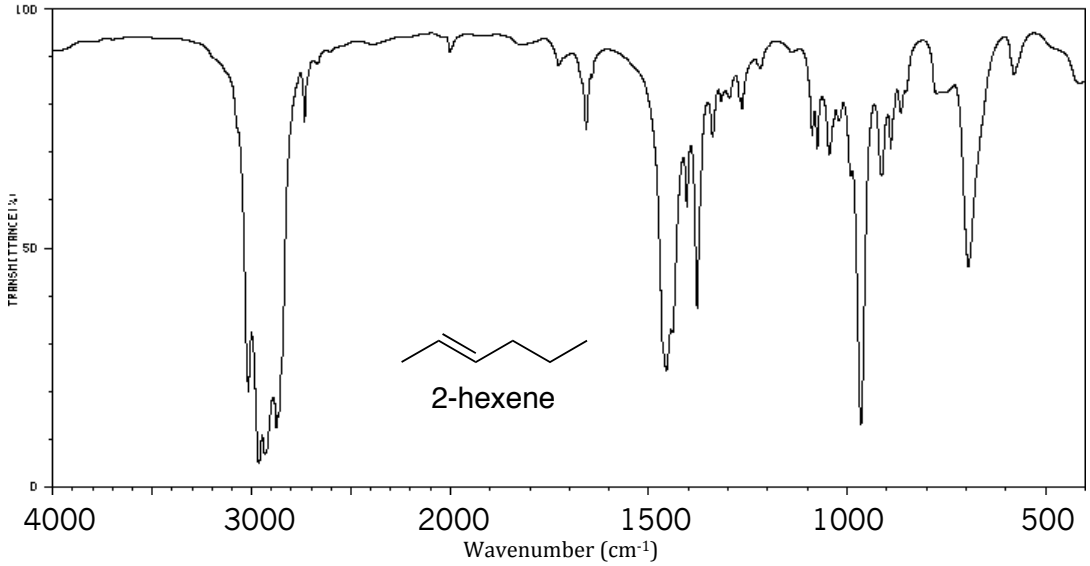
Stretches just below 3000 cm^{-1}



Key Functional Groups to Look For

4) Alkene *Csp^2-H just above 3000 cm^{-1}*

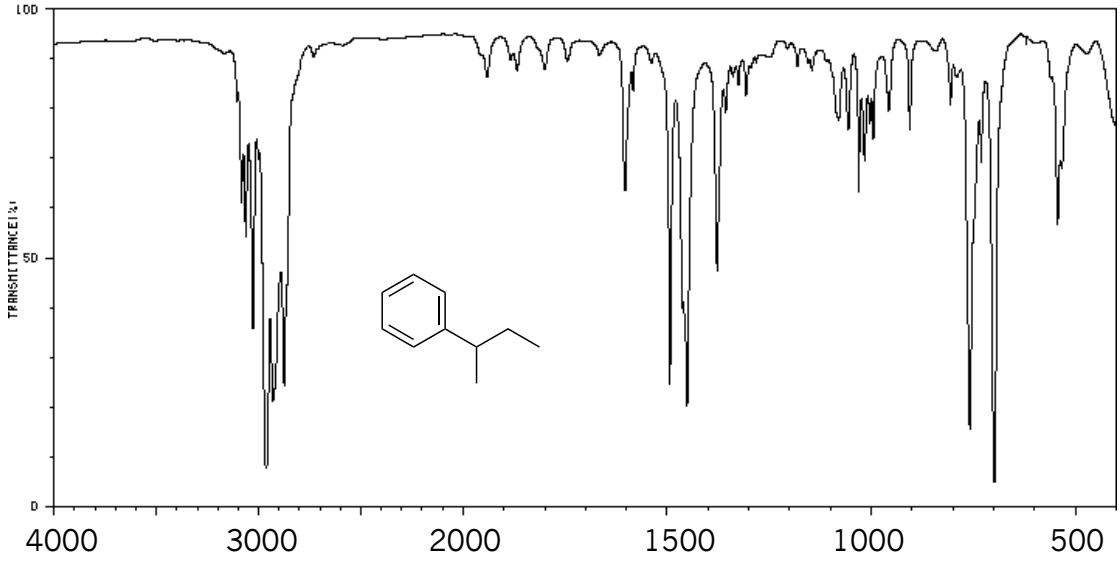
C=C stretch 1600-1700 cm^{-1}



Key Functional Groups to Look For

5) Arene *Csp^2-H just above 3000 cm^{-1}*

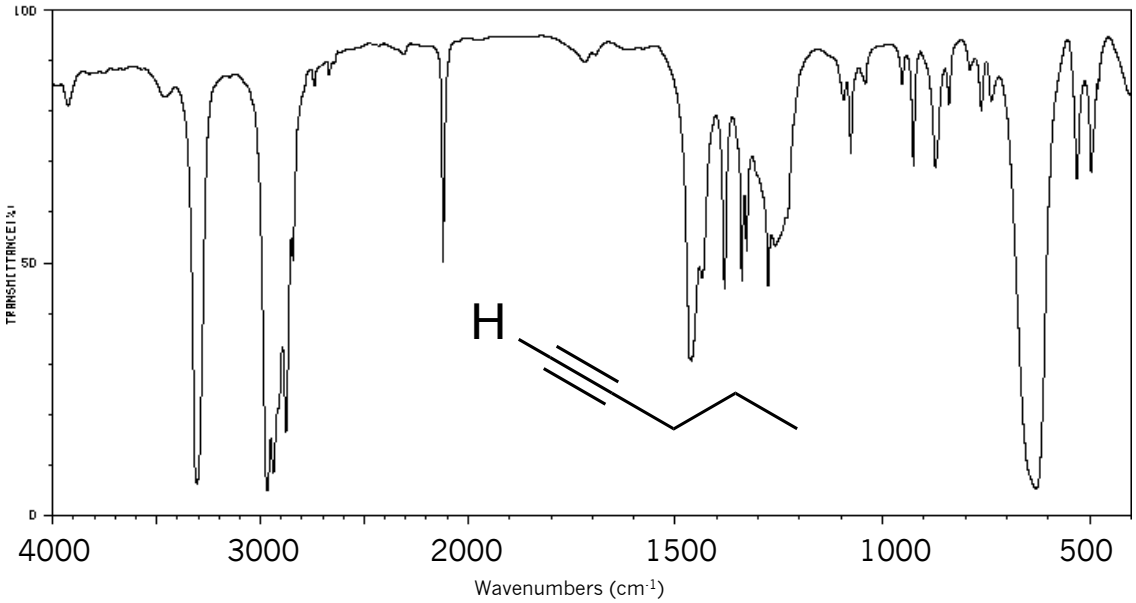
Arene stretches 1600, 1500, <1500 cm^{-1}



Key Functional Groups to Look For

6) Alkyne *Csp-H ~3300 cm^{-1} (terminal alkyne)*

C≡C stretch ~2150 cm^{-1}



Key Functional Groups to Look For

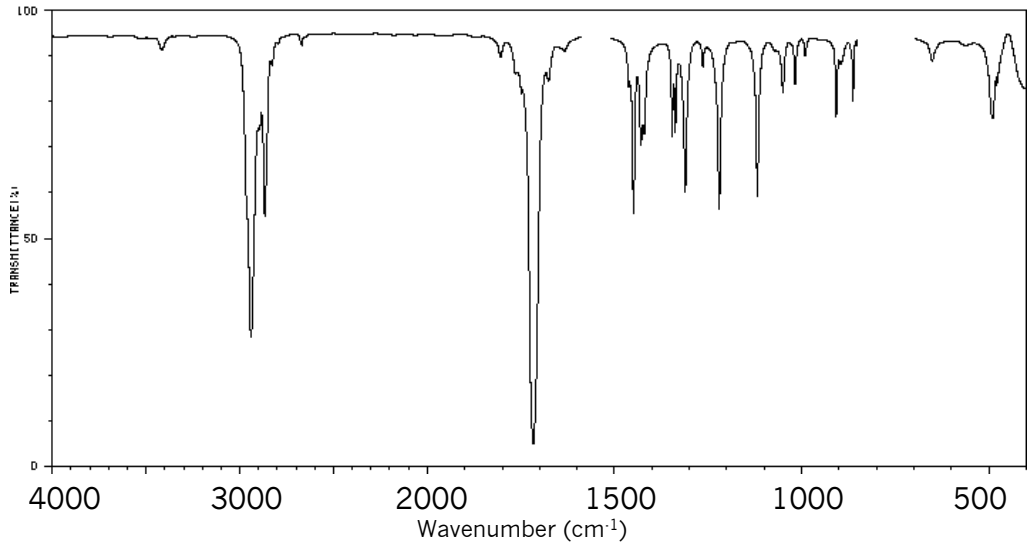
7) Carbonyl Groups

Look for the C=O functional group in the 1650 – 1750 cm^{-1} region.

Use other features to distinguish the various carbonyl groups from one another.

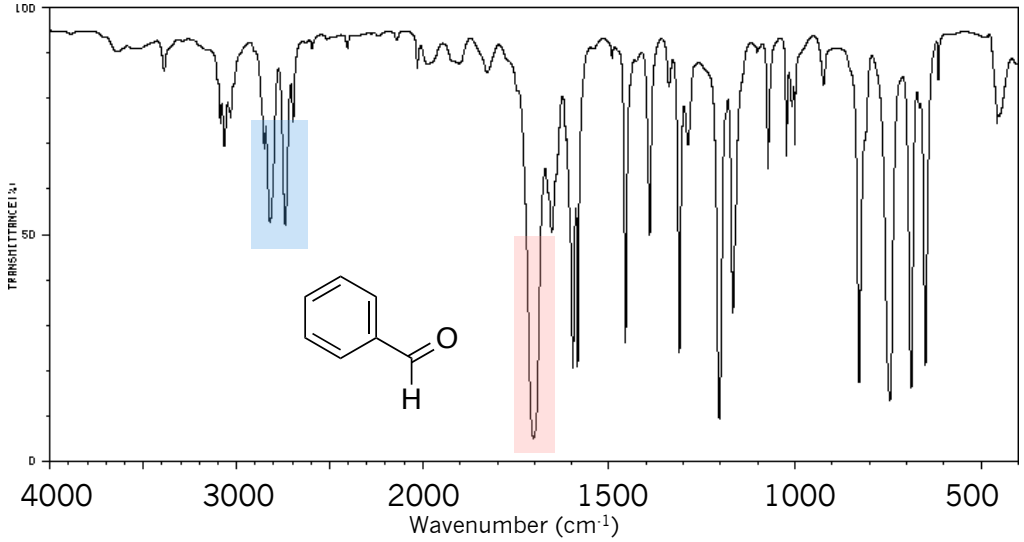
A Ketone

Strong sharp stretch ~1700 cm^{-1}



An Aldehyde

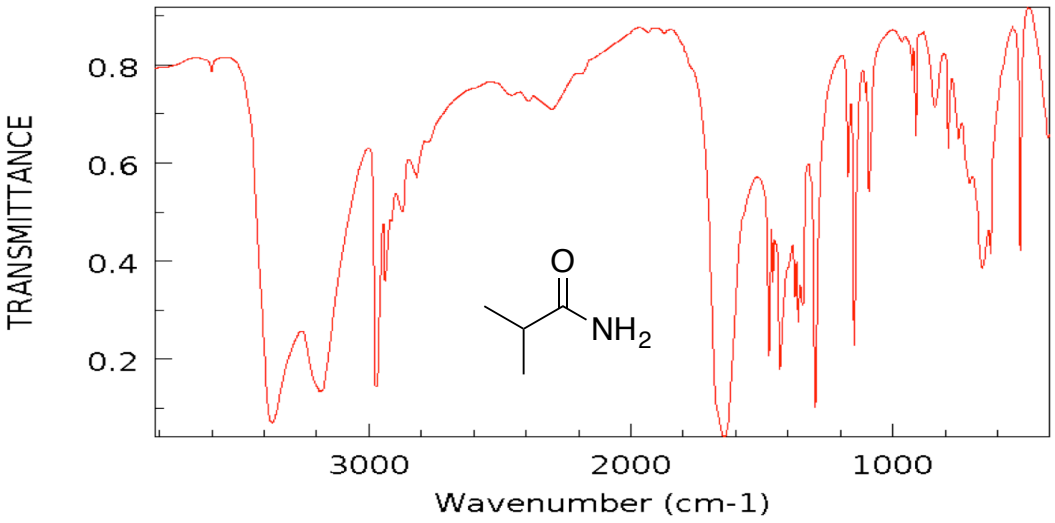
In aldehydes, look for specific aldehyde C-H stretches at ~2720 and ~2820 cm^{-1}.



An Amide

Look for the C=O stretch ~1650 cm^{-1}

Also look for N-H stretches above 3000 cm^{-1}

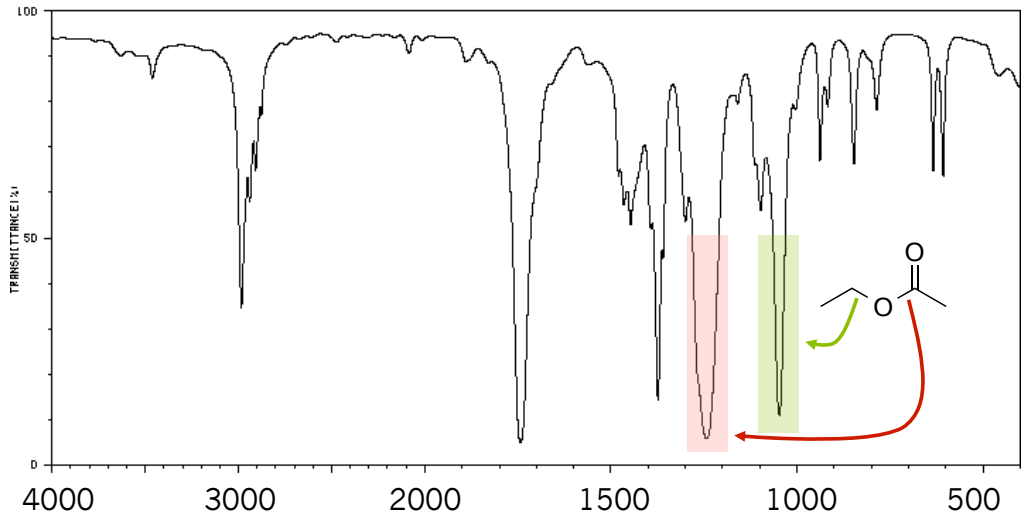


An Ester

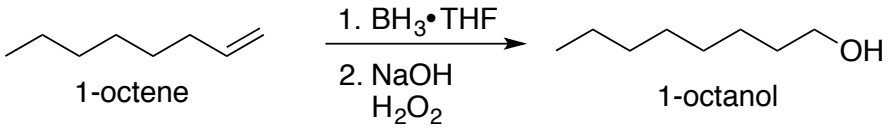
Look for the C=O stretch ~1750 cm^{-1}

Csp^3-O stretch: 1000-1100 cm^{-1}

Csp^2-O stretch: 1200-1300 cm^{-1}



Hydroboration Reaction



1-octene

1-octanol