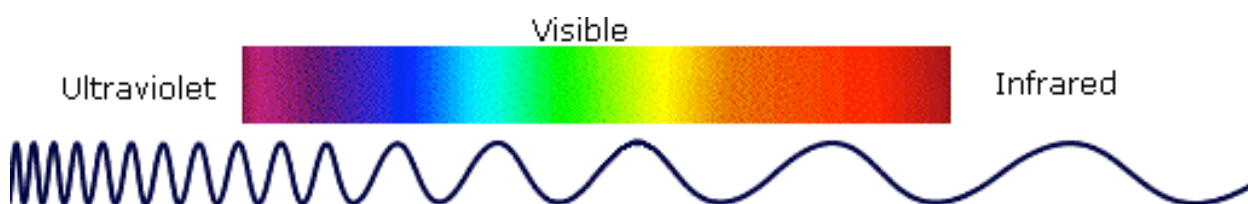


IR Spectra: Tricks for Identifying the 5 Zones

It's easier than you think! 😊

Introduction: The light our eyes see is a small part of a broad spectrum of electromagnetic radiation. On the immediate high energy side of the visible spectrum is the ultraviolet, and on the low energy side is the infrared. The portion of the infrared region is used for analysis of organic compounds.



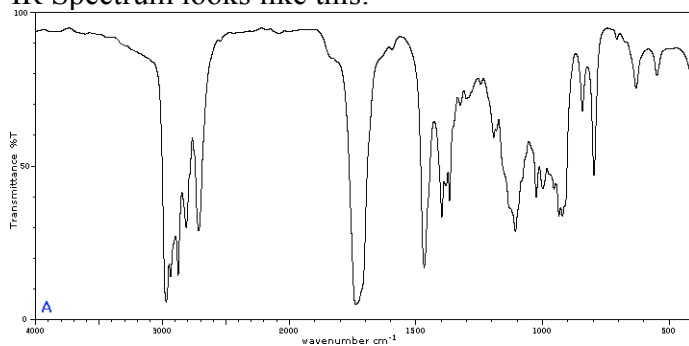
Why is it useful? Infrared (IR) spectroscopy is one of the most common spectroscopic techniques used by organic and inorganic chemists. Simply, it is the absorption measurement of different IR frequencies by a sample positioned in the path of an IR beam. The main goal of IR spectroscopic analysis is to determine the **chemical functional groups** in the sample. Different functional groups absorb characteristic frequencies of IR radiation.

Basically: We use the IR Spectrum to identify Functional Groups that are present within a molecule. This is important because knowing the functional groups present brings us closer to identifying an unknown substance and molecule.

Infrared Spectrum: is the plot of photon energy (x axis) versus the amount of photons (y axis)

• X axis: the stretching frequency • Y axis: the amount of photons absorbed

IR Spectrum looks like this:



The IR Spectrum is divided into 5 Zones and a Fingerprint Region. As Chemistry 14C students we do not need to know how to interpret the Fingerprint region.

FIVE ZONES

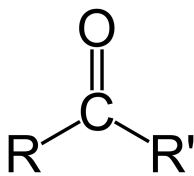
- Each zone has a characteristic frequency and in each zone specific bonds have very specific peak intensities. Looking at the peak determines what functional group is present.

Characteristic Stretching Frequencies: The Five Zones (Table)

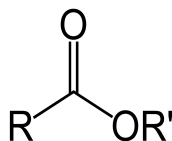
Bond	Stretching Frequency (cm ⁻¹)	Intensity and Shape
ZONE 1: 3700-3200 cm⁻¹		
Alcohol O-H	3650-3200 cm ⁻¹	Usually strong and broad
Alkyne ≡C-H	3340-3250	Usually strong and sharp
Amine or Amide N-H	3500-3200	Medium; often broad
ZONE 2: 3200-2700 cm⁻¹		
Aryl or Vinyl sp ² C-H	3100-3000	Variable
Alkyl sp ³ C-H	2960-2850	Variable
Aldehyde	~2900 and ~2700	Medium; two peaks
Carboxylic Acid O-H	3000-2500	Usually strong; very broad
ZONE 3: 2300-2000 cm⁻¹		
Alkyne C≡C	2260-2000	Variable and sharp
Nitrile C≡N	2260-2220	Variable and sharp
ZONE 4: 1850-1650 cm⁻¹		
Ketone C=O	1750-1705	Strong
Ester C=O	1750-1735	Strong
Aldehyde C=O	1740-1720	Strong
Carboxylic Acid C=O	1725-1700	Strong
Amide C=O	1690-1650	Strong
ZONE 5: 1680-1450 cm⁻¹		
Alkene C=C	1680-1620	Variable
Benzene Ring C=C	~1600 and ~1500	~1600 often has 2 peaks

Attention: The functional group **BOLDED** are the ones that appear in more than one zone. They must be present in all characteristic zones to exist.

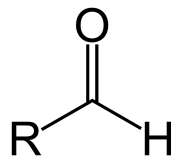
Functional Groups ☺: Here's a quick recap of some functional groups in case you forgot.



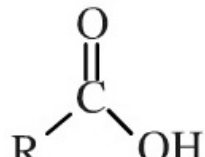
Ketone



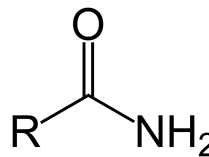
Ester



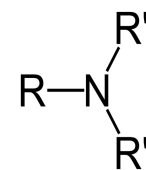
Aldehyde



Carboxylic Acid



Amide



Amine

Tricks for Remembering the FUNCTIONAL GROUPS

A Ketone is CoCy (Cocky) KETONE COC

Ester is a cooc (Cook) ESTER COOC

Al Cohs (A man named Al Coughs) Aldehyde COH

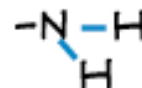
Tricks for Identifying the Zones



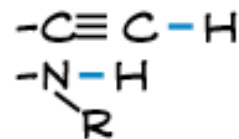
A SMOOTH TONGUE
MEANS AN **ALCOHOL**.



VAMPIRE FANGS MEANS
A **PRIMARY AMINE**...



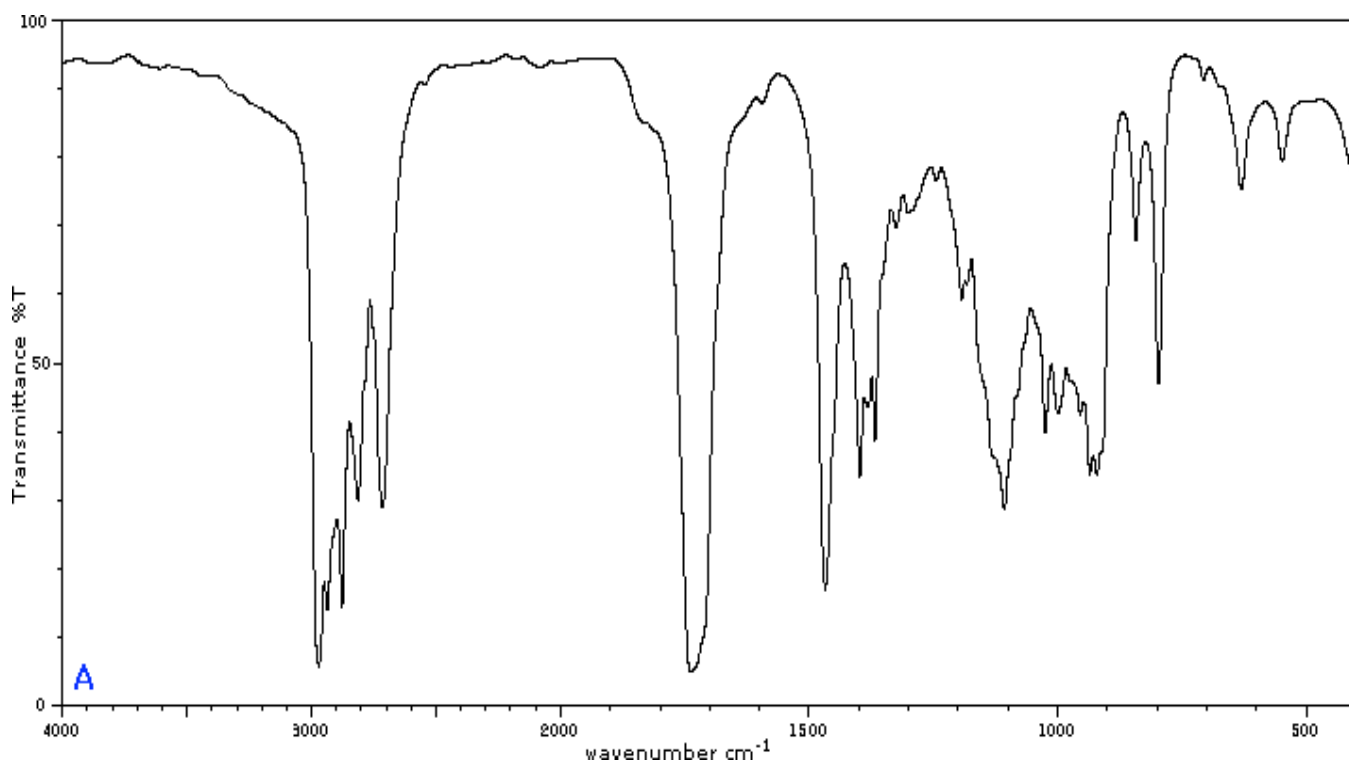
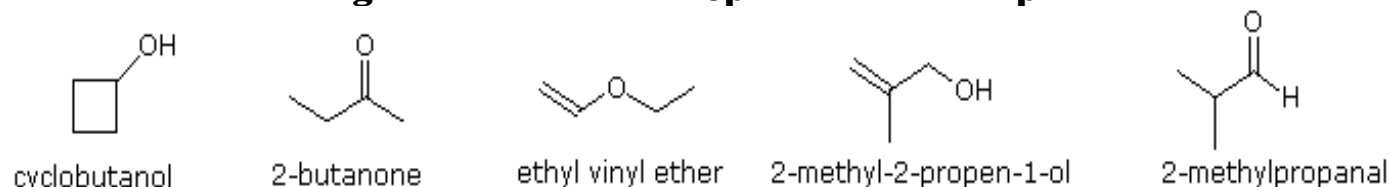
ONE KNOCK-OUT FANG
MEANS A **2° AMINE**,
OR A **TERMINAL ALKYNE**.



HAIRY BEARD IS A SIGN FOR
A **CARBOXYLIC ACID**.



Practice Problem: Using what you have just learned. Decide which of the following 5 molecules the IR Spectrum below depicts.

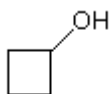


Solution: You can solve this problem by process of elimination.

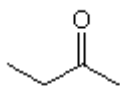
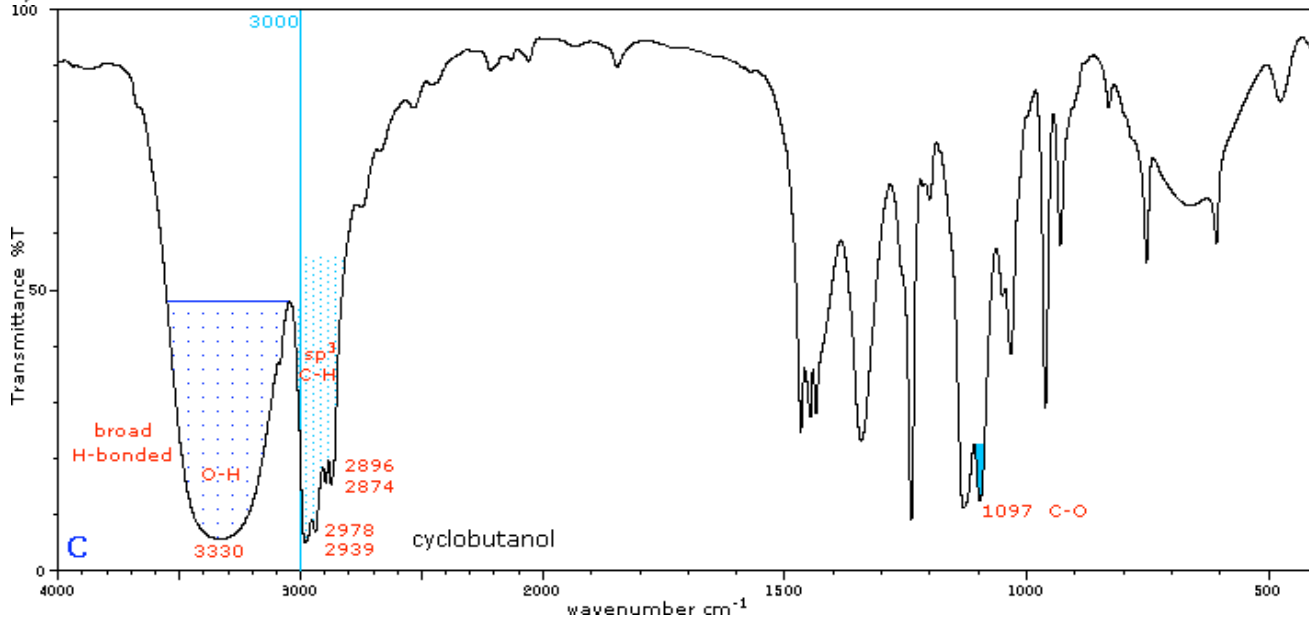
1. By looking at the IR Spectrum you can eliminate all molecules with an alcohol in it (cyclobutanol and 2-methyl-2-propen-1-ol). This is because the IR spectrum does not show an alcohol present. (Remember: You need a broad peak at about 3300. Hint: Alcohol peak looks like a tongue.)
2. Now you have three choices left. 2-butanone has a ketone present in the molecule. (Remember: A ketone is a Carbon double bonded to an oxygen. The carbon is bonded to two other Carbons). Ethyl Vinyl Ether has an ether present in the molecule (An ether is one functional group that is not identified on within the 5 zones so move on to the next molecule). 2-methylpropanal has an aldehyde in its molecule. (Remember: An aldehyde is a carbon double bonded to oxygen. The carbon is bonded to a carbon and hydrogen).
3. So by looking at the IR Spectrum above, do you see a ketone or an aldehyde present? We can immediately tell that the molecule portrayed by the IR spectrum must be the last molecule (2-methylpropanal) because the IR spectrum has a peak in Zone 2 at 2700 and 2900. This signifies that an Aldehyde is present.

Answer: 2-methylpropanal ☺

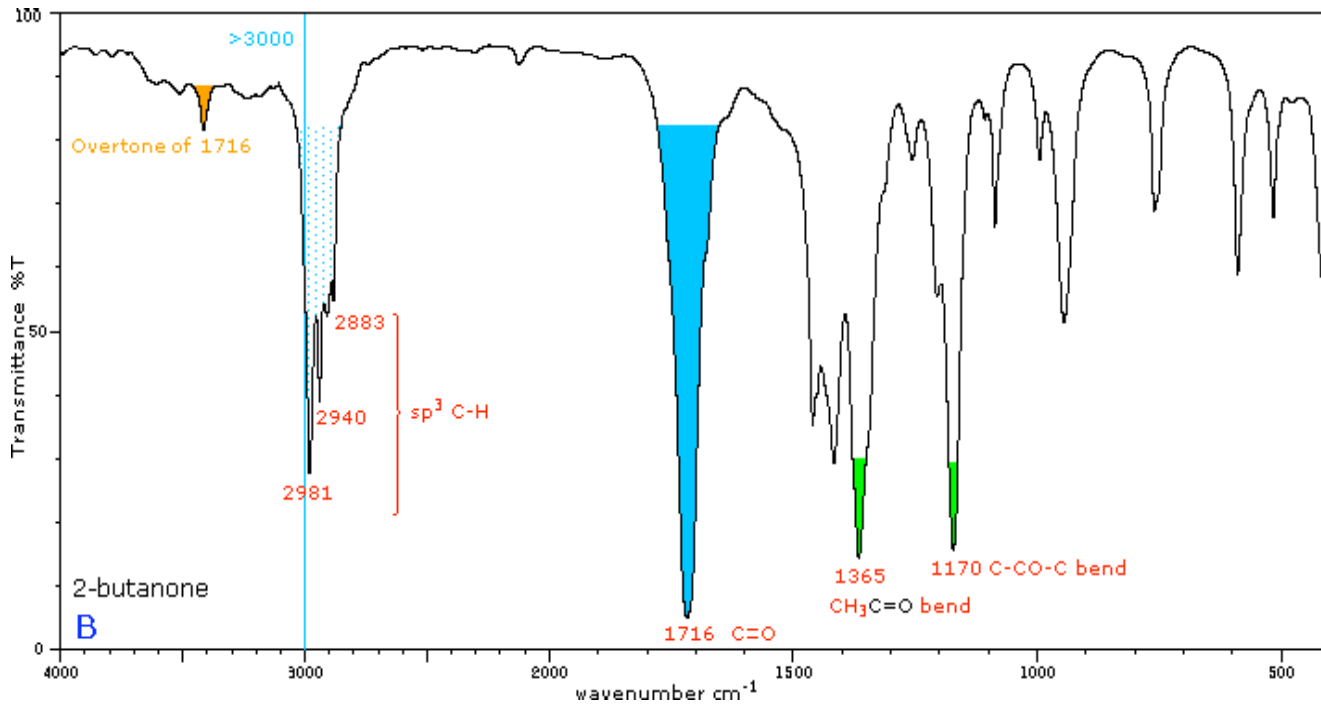
The IR spectrums for the remaining choices would look like this:

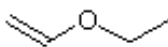


cyclobutanol

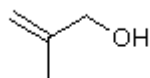
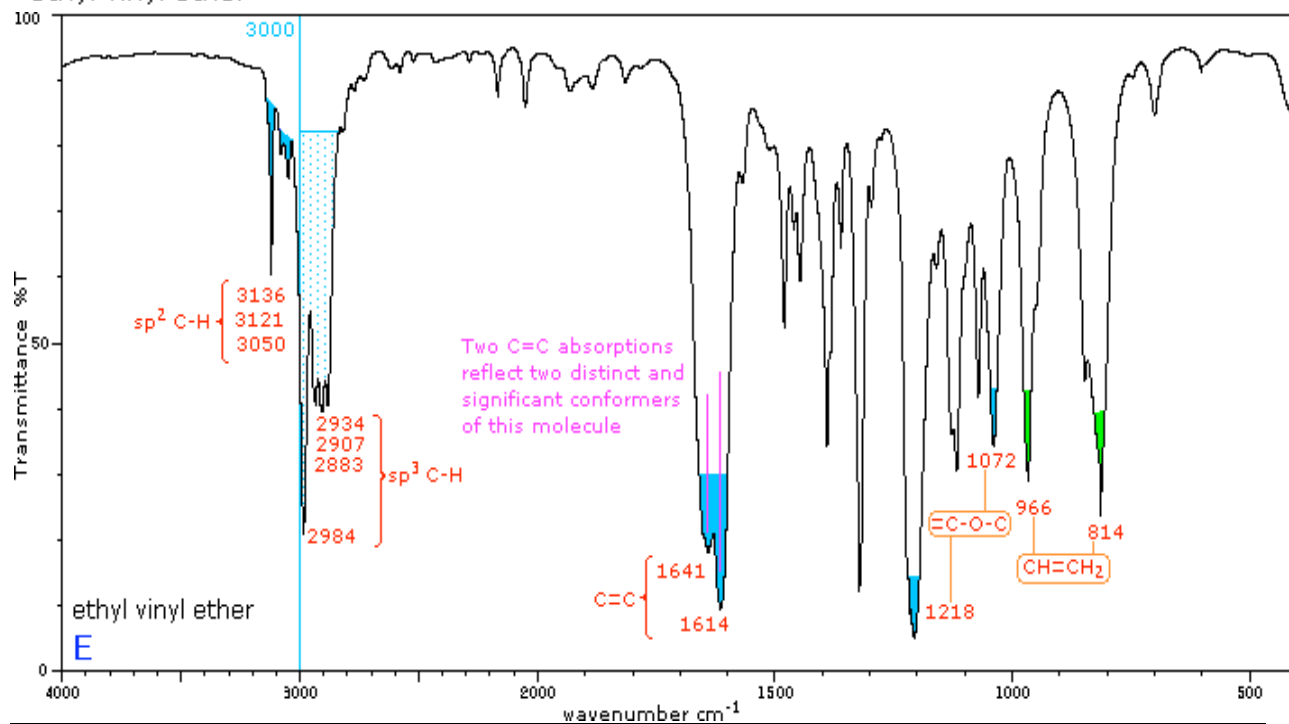


2-butanone

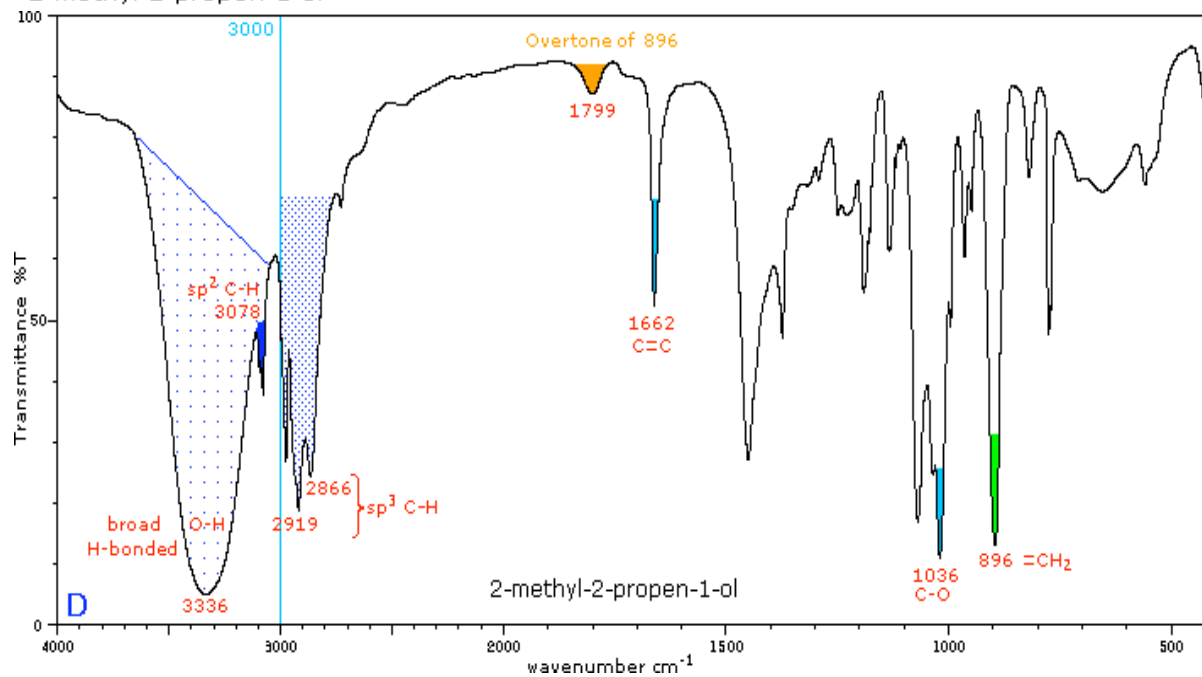




ethyl vinyl ether



2-methyl-2-propen-1-ol



Sources:

Dr. Hardinger's Chem 14C Lecture Supplement

<http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm>

<http://www.prenhall.com/settle/chapters/ch15.pdf>

Images:

All images of Functional Groups (Ketone, Ester, Aldehyde, Carboxylic Acid, Amine, Amide) were taken from Wikipedia.

http://en.wikipedia.org/wiki/Functional_group

<http://toeholds.files.wordpress.com/2010/09/ir-illustrated.pdf>

Spectral Graphs:

(<http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/Spectrpy/InfraRed/infrared.htm>)