IR SPECTROSCOPY BASICS

A BIT ABOUT INFRARED….

An infra-red (IR) spectrometer passes a beam of infra-red radiation through an organic sample and the chemical bonds in the sample are able to absorb some of the wavelengths of infra-red radiation, with **different bonds absorbing different wavelengths**.

The x axis demonstrates the infra-red wavelengths being absorbed, measured as **wavenumbers** (units = cm^{-1}) – DIFFERENT WAVELENGTHS ARE ABSORBED BY DIFFERENT FUNCTIONAL GROUPS

The y axis measures how much infra-red radiation is being absorbed at each wavenumber as **transmittance**. When the line is at the top of the spectrum this indicates 100% transmittance of IR (so no absorption). THIS IS NOT SO IMPORTANT TO US

WHAT DO WE WANT TO KNOW?

We want to know how the structure is related to the energy that is absorbed.

WHY SHOULD I CARE?

This will let us make conclusions about the structure.

WHAT DOES AN IR SPECTRUM SHOW US?

FUNCTIONAL GROUPS!!! (or absence of…)

WHAT ARE WE LOOKING FOR?

PEAKS! We are looking for downward spikes in the graph.

WHY ARE SOME PEAKS BIGGER THAN OTHERS?

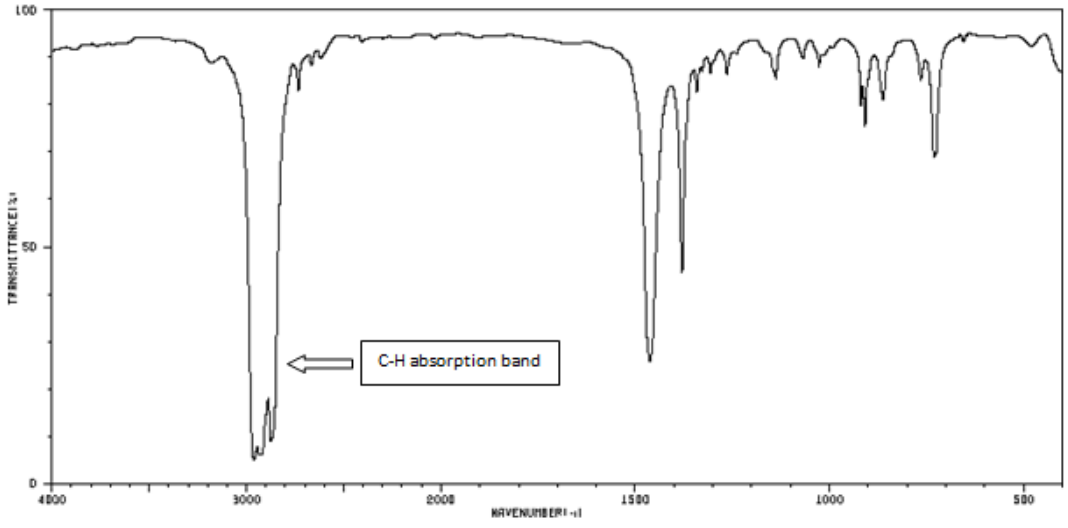
Polarity determines the peak's strength. The more polar a molecule is, the stronger the peak is.
Repetition can also determine strength; many of the same functional group leads to a larger peak. (BUT AGAIN, DO NOT WORRY TOO MUCH ABOUT THIS)

Interpreting an IR spectrum

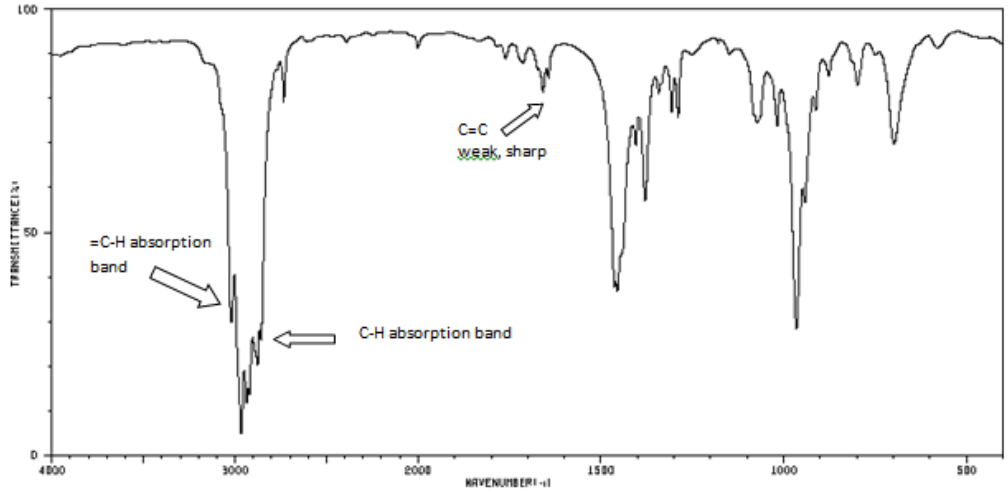
Group	Bonds	Absorption
Alkanes	C-H	2850-3000 cm^{-1}, multiple peaks forming strong & sharp band of peaks
Alkenes	C=C =C-H	1600-1700 cm^{-1} medium, sharp ~3100 cm^{-1} weak, sharp band
Alcohols	O-H C-O	3200-3600 cm^{-1} strong, broad 1000-1100 cm^{-1} strong, sharp
Haloalkanes	C-X C-Br C-Cl	500-600 cm^{-1} sharp, medium/strong 600-800 cm^{-1} sharp, medium/strong
Amines	N-H C-N	3350-3500 cm^{-1} weak/medium, sharp 1000-1200 cm^{-1} weak/medium
Aldehydes	C=O C-H (of aldehyde)	1680-1750 cm^{-1} strong, sharp 2750-2850 cm^{-1} medium
Ketones	C=O	1680-1750 cm^{-1} strong, sharp
Carboxylic Acids	C=O O-H C-O	1700-1750 cm^{-1} strong, sharp 2200-3600 cm^{-1} strong, broad 1200-1320 cm^{-1} medium, weak
Amides	C=O N-H	1650-1700 cm^{-1} strong, sharp 3350-3500 cm^{-1}, variable
Acid Chlorides	C=O C-X	1750-1850 cm^{-1} strong, sharp (see haloalkanes above)
Esters	O=C-O-C O=C-O-C O=C-O-C	1700-1750 cm^{-1} strong, sharp 1250-1350 cm^{-1} strong 1000-1100 cm^{-1} strong

Examples of spectra for each functional group

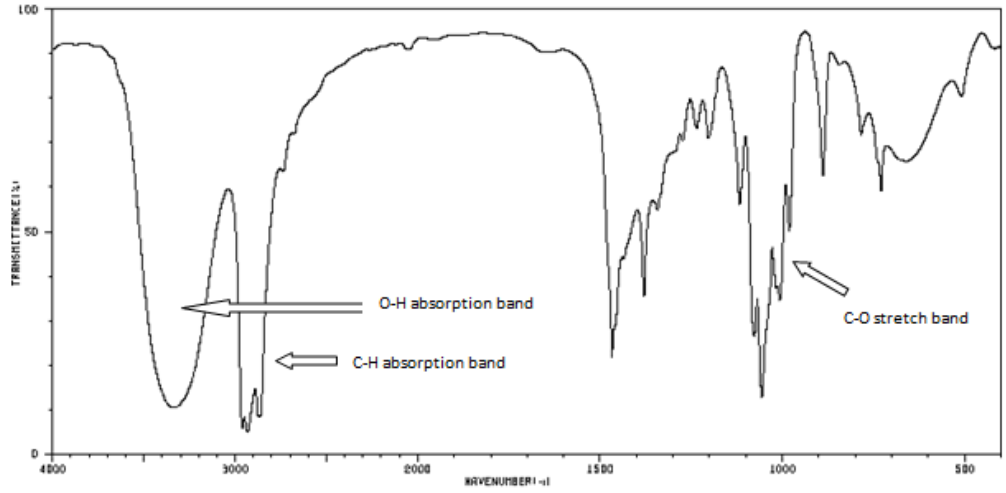
Alkane (pentane)



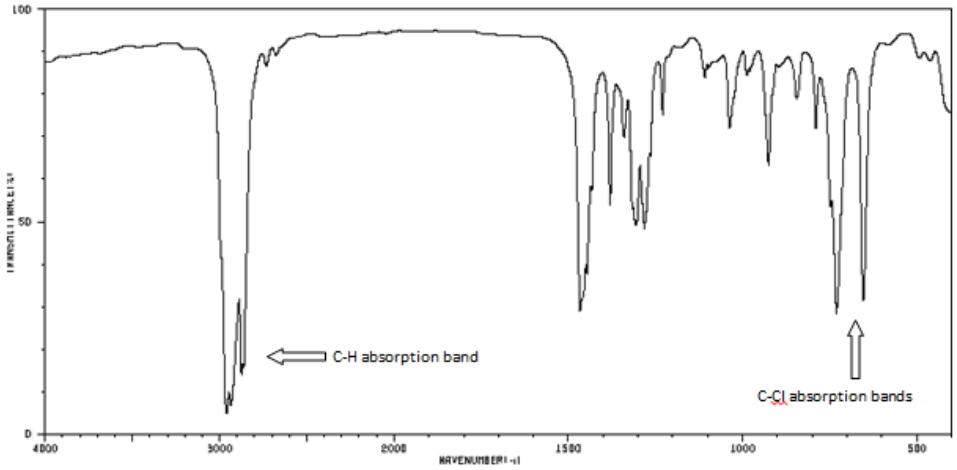
ALKENE (2-PENTENE)



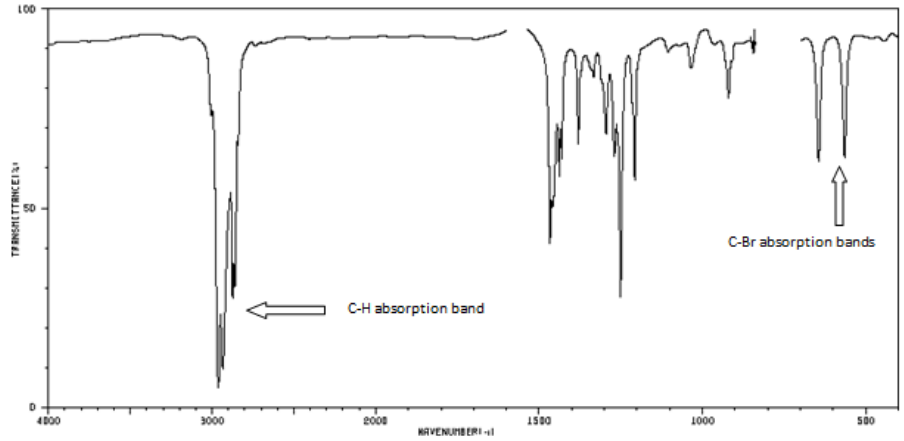
ALCOHOL (PENTAN-1-OL)



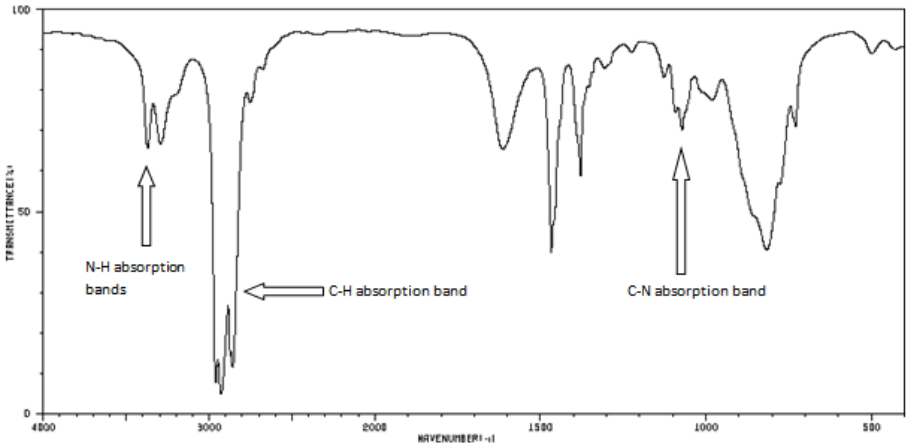
HALOALKANE (1-CHLOROPENTANE)



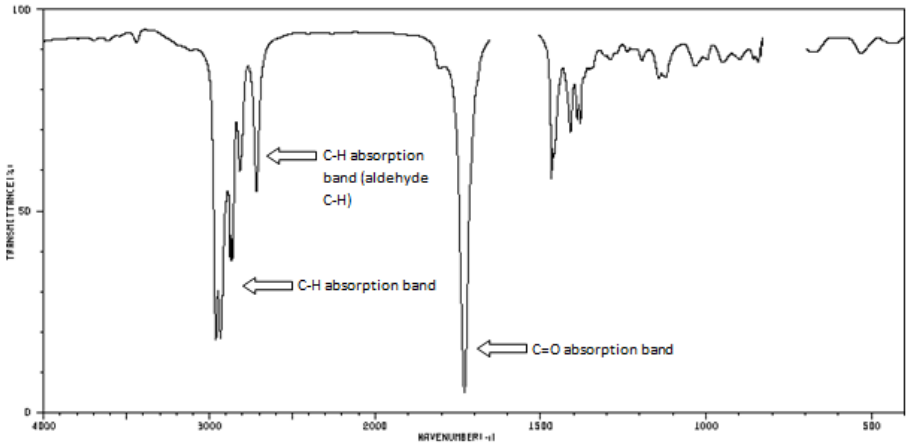
HALOALKANE (1-BROMOPENTANE)



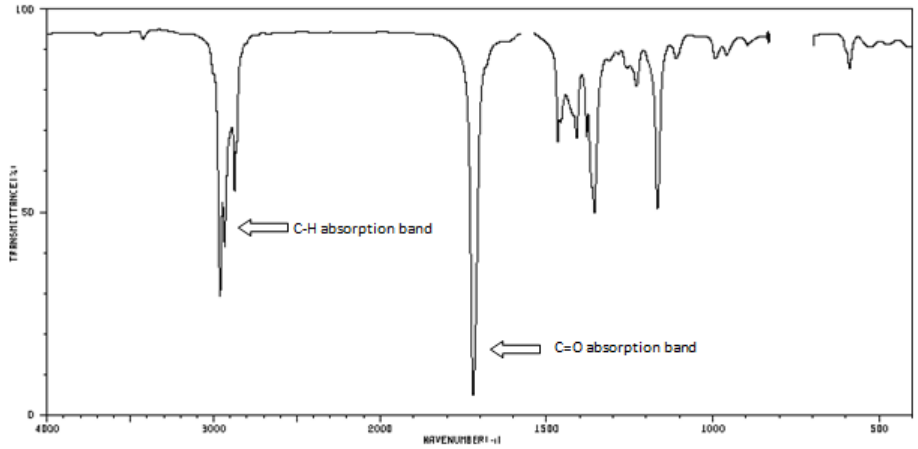
AMINE (1-PENTANAMINE)



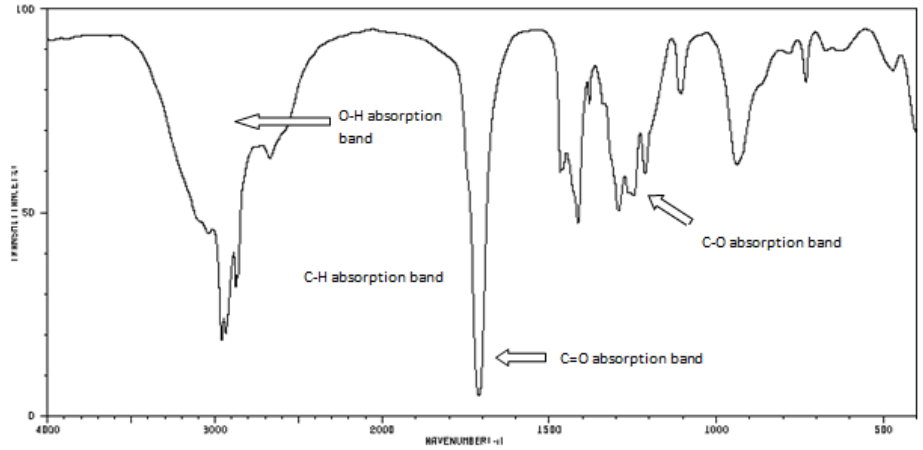
ALDEHYDE (HEXANAL)



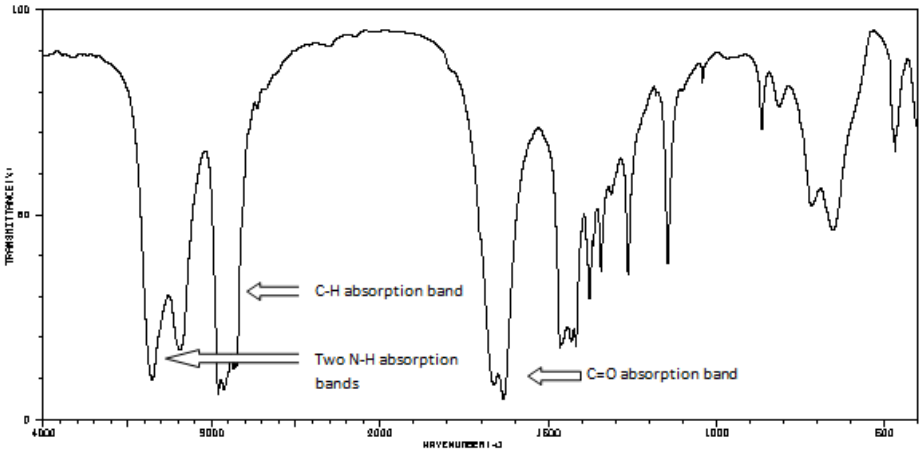
KETONE (2-HEXANONE)



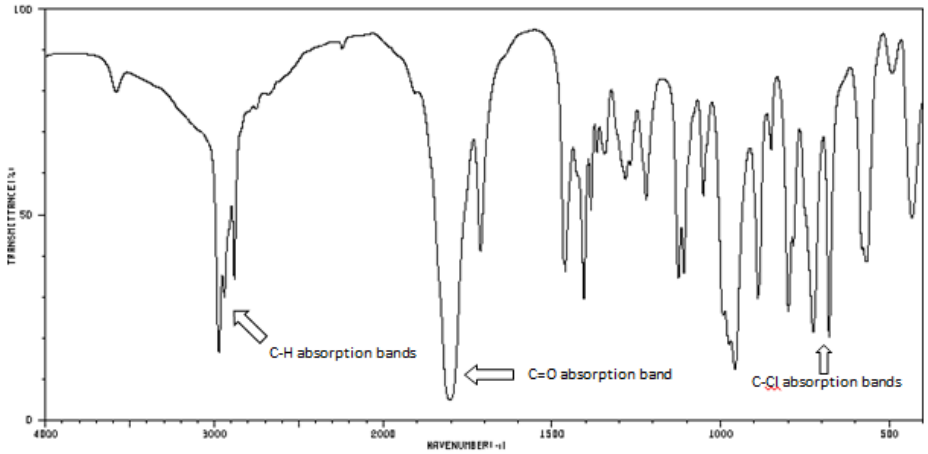
CARBOXYLIC ACID (HEXANOIC ACID)



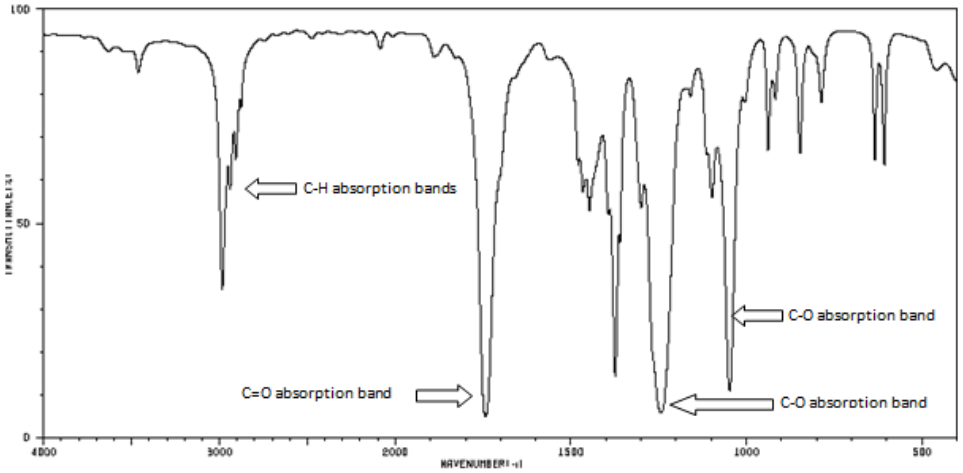
AMIDE (BUTANAMIDE)



Acyl chloride (butanoyl chloride)



Ester (ethylethanoate)



Now go and look at the bubbl.us decision chart and the practice questions and answers!