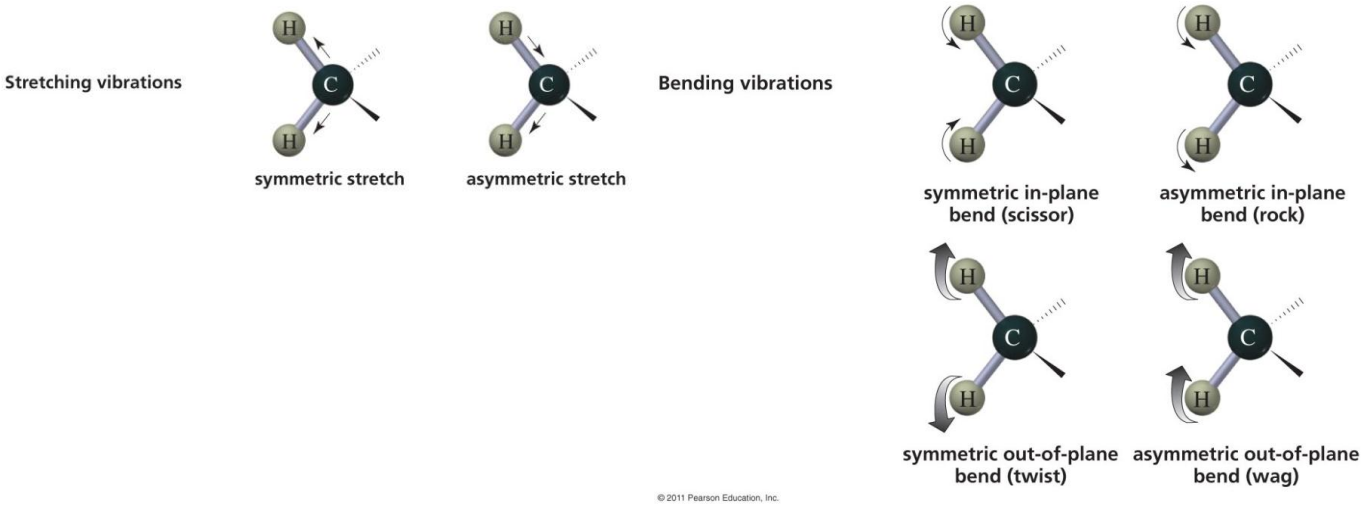
Analysis of Functional Groups using Infrared (IR) Spectroscopy

INTRODUCTION

Infrared spectroscopy is a technique that can be used to identify which functional groups are present in a compound. The bonds in a molecule can stretch, bend and wag, similar to balls that are attached to springs.

Here are some different types of bond movements.



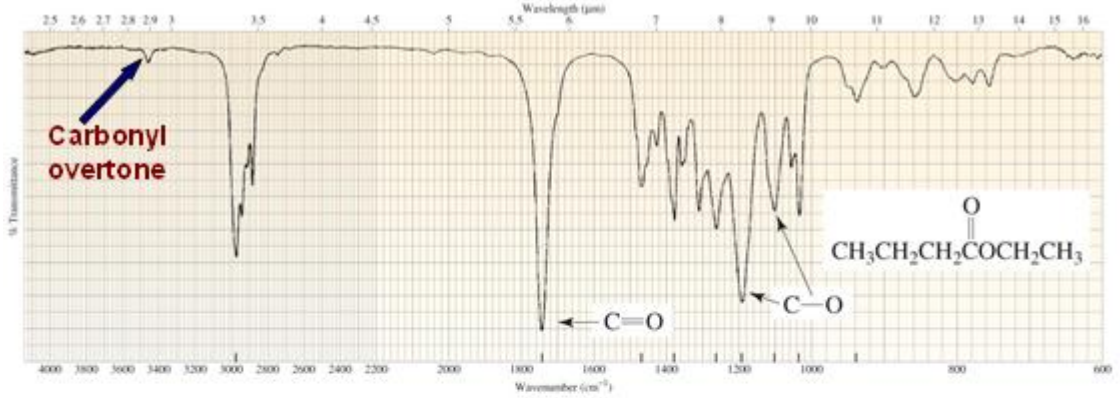
When a light wave of a correct frequency (measured in cm^{-1}) is in resonance with a bond motion and transfers its energy to this motion (like a parent pushing a swinging child), then we say that the light is **absorbed** by the molecule. The frequency absorbed will depend on the type of bonds present, and can actually indicate which functional groups are present.

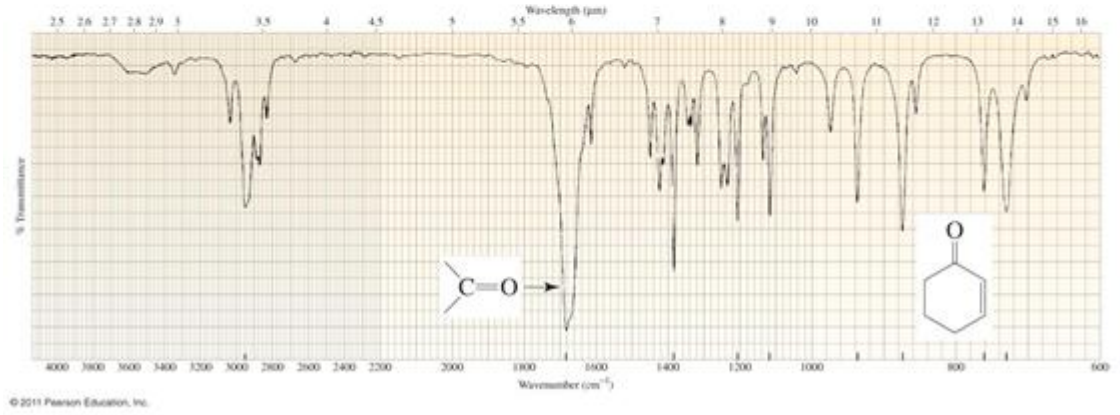
The following table shows which functional groups can be detected at which particular wavelength.

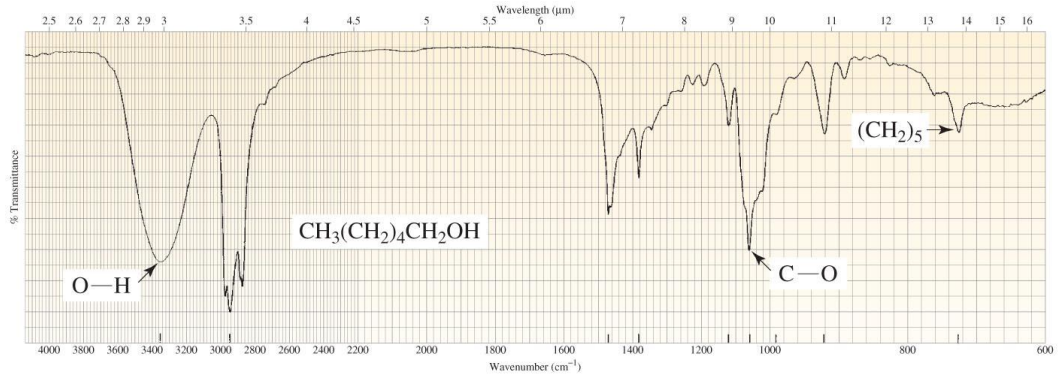
Table 13.4 Frequencies of Important IR Stretching Vibrations

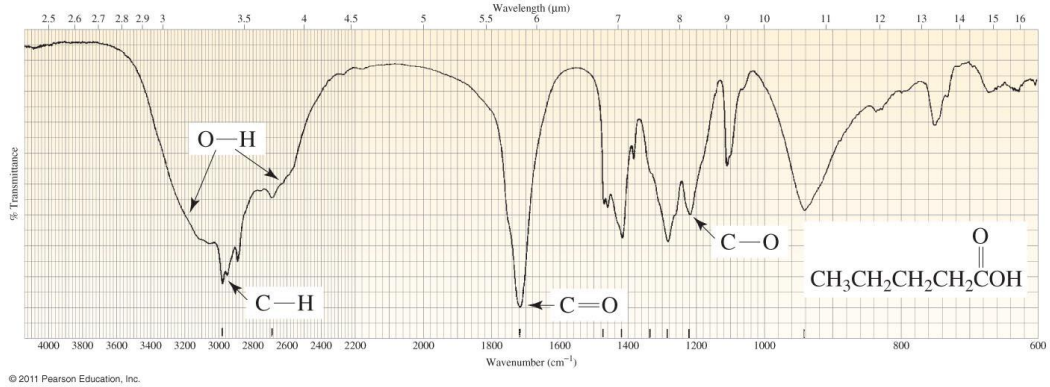
Type of bond	Wavenumber (cm^{-1})	Intensity
C≡N	2260–2220	medium
C≡C	2260–2100	medium to weak
C=C	1680–1600	medium
C=N	1650–1550	medium
	~1600 and ~1500–1430	strong to weak
C=O	1780–1650	strong
C—O	1250–1050	strong
C—N	1230–1020	medium
O—H (alcohol)	3650–3200	strong, broad
O—H (carboxylic acid)	3300–2500	strong, very broad
N—H	3500–3300	medium, broad
C—H	3300–2700	medium

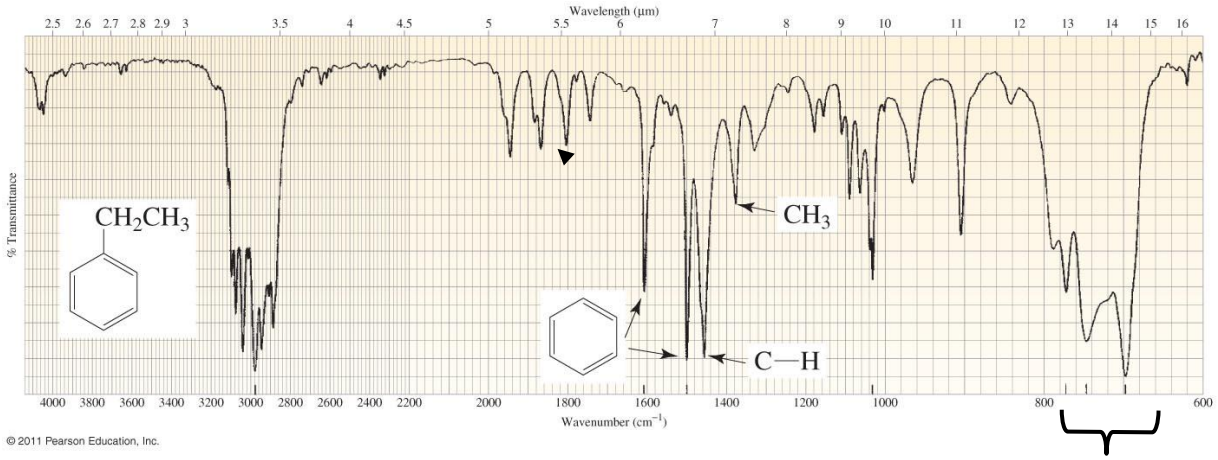
Below are the IR spectra of an ester, a ketone, an alcohol, a carboxylic acid and an aromatic are provided. Note the characteristic absorption peak for each functional group that is present. Can you find the C-H peak in each one?











Benzene in-plane and
out-of-plane C—H bends

EXPERIMENTAL SET-UP:
You will be provided with one vial of each of the following known compounds: cyclohexanone, methyl benzoate, cyclohexanol, ethyl acetoacetate, o-xylene and octane. Obtain an IR spectrum of each of these known compounds.

You will also be given one vial containing an unknown compound. Obtain an IR spectrum of your unknown compound and compare it to the spectra of the known compounds to determine the identity of your unknown.

PRE-LAB EXERCISE:
For each compound, draw its structural formula and indicate the types of bonds and corresponding wavelengths of the predicted peaks in its IR spectra. (Refer to the table in the Introduction.)

cyclohexanone structure	types of bonds & peaks (cm^{-1})	methyl benzoate structure	types of bonds & peaks (cm^{-1})
cyclohexanol structure	types of bonds & peaks (cm^{-1})	ethyl acetoacetate structure	types of bonds & peaks (cm^{-1})
o-xylene structure	types of bonds & peaks (cm^{-1})	octane structure	types of bonds & peaks (cm^{-1})

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Name: _____

Lab Partner: _____

LAB REPORT SHEET

1. Unknown number:_____
2. Include the infrared spectrum of your unknown.
3. Data: List the significant peaks in the spectrum by wavenumber (cm^{-1}) and indicate the structural features associated with each absorption.

Wavenumber of significant peaks	Structural feature

4. Conclusion:

   a) Give the name and draw the structure of your unknown compound.

   b) Justify your conclusion.