ACTIVITY

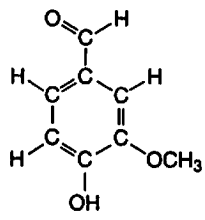
Can We Identify Unknown Plastics Using Infrared Spectroscopy?

LEARNING GOALS

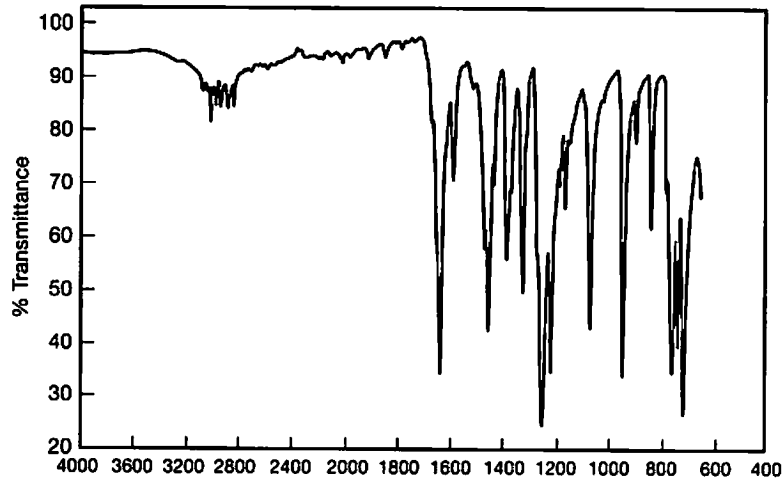
- To become familiar with infrared (IR) spectroscopy
- To relate IR spectra to the bonds present in different polymers
- To identify polymers based on their IR spectra

INTRODUCTION

Infrared spectroscopy is based on the premise that when light of a particular frequency is directed at a molecule, it may stimulate the vibration of a particular type of bond within the molecule. If this occurs, that particular frequency of light will be absorbed and the amount of absorption can be measured using an infrared spectrophotometer. The frequency of light that is absorbed depends on two factors: the masses of the atoms involved and the relative stiffness of the bonds. Thus, by determining the frequency of light absorbed by the molecule, we can determine the types of bonds in a molecule. Infrared spectra are typically plotted as percent transmittance on the *y*-axis and wavenumbers on the *x*-axis. (A wavenumber is the inverse of the wavelength of light involved, and thus is related to the frequency of the light.)



Vanillin



Infrared spectrum of vanillin

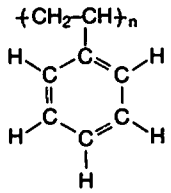
As an example, the infrared spectrum of vanillin is shown above. In regions where the percent transmittance is high, light is not absorbed. In regions where light is absorbed, there are valleys in the spectrum. The deeper the valley, the greater the absorption. The valleys in an infrared spectrum are often referred to as "peaks."

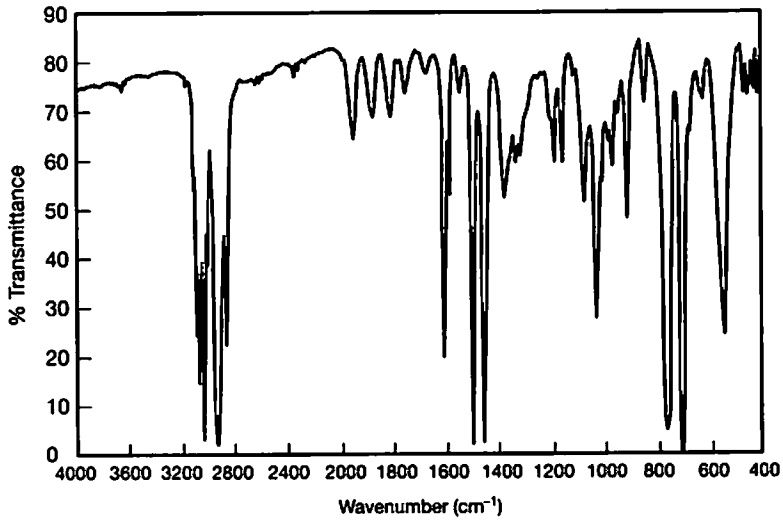
As described previously, certain portions of the IR spectrum are associated with particular molecular vibrations. The table here gives some specific examples of the portion of the spectrum associated with certain types of bonds. For example, because the energy absorbed by a C = C bond (~1650 cm^{-1}) is different from that absorbed by C ≡ C bond (~2175 cm^{-1}), it is possible to use infrared spectroscopy to determine which type of bond is present in a molecule. In this laboratory data analysis exercise, you will use infrared spectroscopy to identify the bonds present in a variety of different molecules including plastics.

IMPORTANT INFRARED BANDS

TYPE OF BOND	WAVENUMBER (cm^{-1})	INTENSITY
N≡C	2260–2220	Medium
C≡C	2260–2100	Medium
C=C	1680–1600	Medium
 Benzene	~1230 and ~1500	Strong
C=O	1780–1650	Strong
C–O	1250–1050	Strong
C–N	1230–1020	Medium
O–H (alcohol)	3650–3200	Strong, broad
O–H (acid)	3300–2500	Strong, very broad
N–H	3500–3300	Medium, broad
C–H	3300–2700	Medium

1. Polystyrene is a polymer with the following structural formula and infrared spectrum:



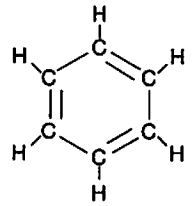


Infrared spectrum of polystyrene

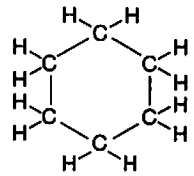
a) Which peak(s) in the spectrum of polystyrene correspond to the benzene ring in polystyrene?

b) What bond(s) cause the peaks near wavenumber 3000 cm^{-1}?

2. The structures of benzene and cyclohexane are shown here.



Benzene



Cyclohexane

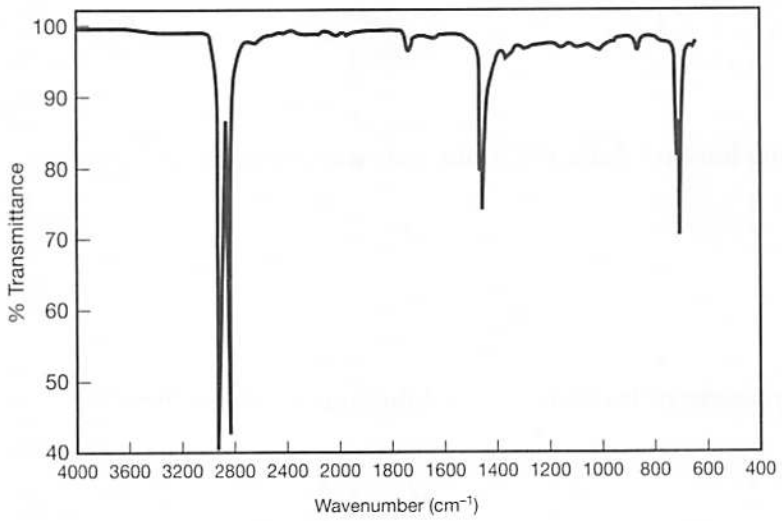
a) What peak(s) would you expect benzene and cyclohexane to have in common?

b) How would you expect the spectra of benzene and cyclohexane to differ? Give specific peak wavenumbers in your response.

3. Ethylene ($H_2C{=}CH_2$) is the monomer used to produce polyethylene, $-(H_2C{-}CH_2)_n$

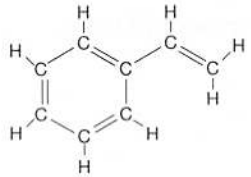
a) Would you expect the major peak(s) in the spectrum of ethylene to be the same as those in polyethylene? Why or why not?

b) The spectrum of either ethylene or polyethylene is given here. Which is it? Explain your reasoning.

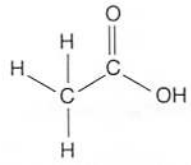


4. Where would you expect to find peaks in the spectrum of the following molecules?

a) Styrene



b) Acetic acid



5. Three IR spectra appear here. They are for the compounds:

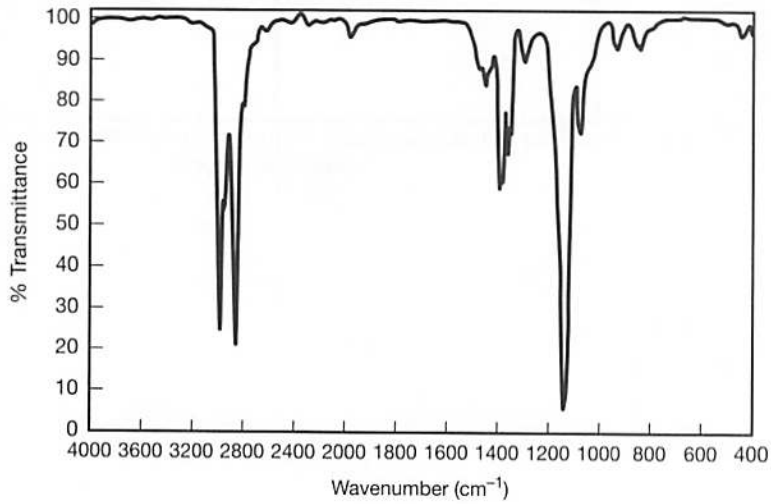
   Methyl ethyl ketone, $CH_3COCH_2CH_3$

   1-Butanol, $CH_3CH_2CH_2CH_2OH$

   Diethyl ether, $CH_3CH_2OCH_2CH_3$

   Draw the structural formula for the proper compound next to the corresponding infrared spectrum, and label the major peaks with the type of bond being stretched.

a)



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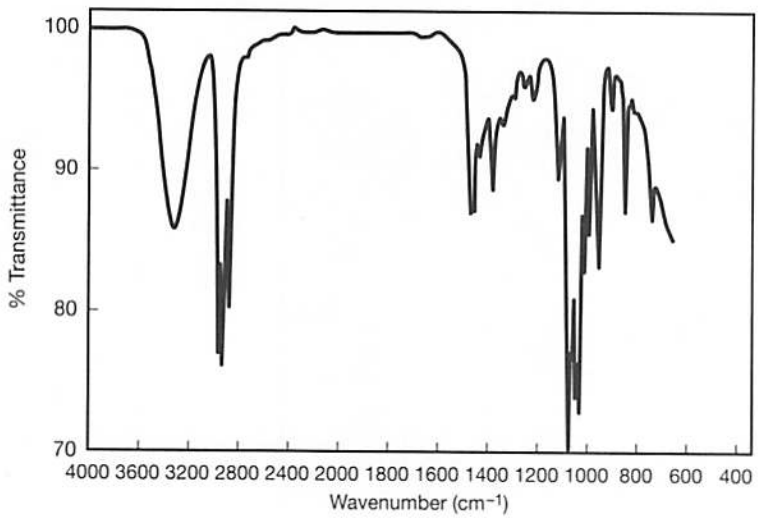
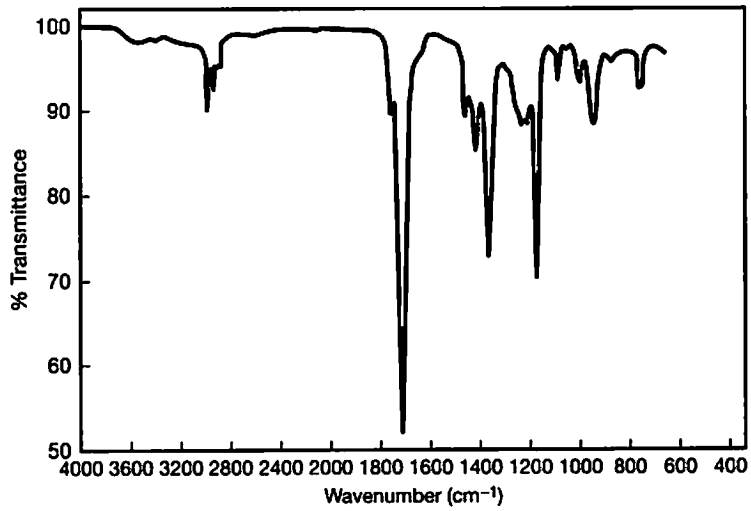


c)



Adapted by Sharon Anthony, Karen Harding, and Kim Kostka from the ChemConnections module "How Do We Get from Bonds to Bags, Bottles, and Backpacks?" by Karen Harding and Sharon Anthony.