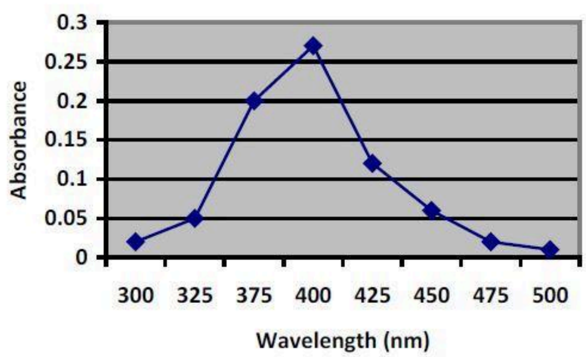
Intermolecular Forces and Properties
3.11 Spectroscopy and the Electromagnetic Spectrum
3.13 Beer-Lambert Law
Worksheet Key

1) What factors are necessary in order to cause an electron transition during an ultraviolet/visual (UV/Vis) spectroscopy experiment?

The energy contained by the incident photons must be exactly the same as the difference in energy between the two MOs in order for the photons to be absorbed by electrons and transmit the electrons to the higher energy MO.
The molecule must have π-orbitals (which means that it must contain double or triple bonds within its structure) or it must have non-bonding MOs (which means it must contain MOs with lone pairs). Light between the wavelength of 200 nm and 800 nm can only transmit electrons from π (bonding orbitals) to π^* (anti-bonding orbitals), or from non-bonding orbitals to a π^* (anti-bonding orbitals) or σ^* (anti-bonding orbitals).

2) Use the UV/Vis spectra below to determine which wavelength of light is experiencing the highest degree of absorbance by the molecules in the sample under investigation.

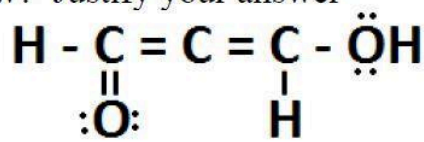


400 nm

3) Explain what happens within the structure of a molecule during an ultraviolet/visual (UV/Vis) spectroscopy experiment.

A photon absorbs an electron for a π (bonding orbital) and transmits it to a π^* (anti-bonding orbital); or a photon absorbs an electron from a non-bonding MO and transmits it to a π^* (anti-bonding orbital) or σ^* (anti-bonding orbital). The photon must contain the same amount of energy as the difference in energy between the two MOs.

4) Would it be possible to conduct an UV/Vis spectroscopy experiment on a sample of the compound below? Justify your answer



It would be possible to conduct a UV/Vis spectroscopy experiment on a sample of this compound, as it has π-orbitals associated with its double bonds and non-bonding MOs (lone pairs). Light between the wavelength of 200 nm and 800 nm can only transmit electrons from π (bonding orbitals) to π^* (anti-bonding orbitals), or from non-bonding orbitals to a π^* (anti-bonding orbitals) or σ^* (anti-bonding orbitals).

5) Would it be possible to conduct an UV/Vis spectroscopy experiment on a solution containing a colored compound? Justify your answer.

It is possible to conduct UV/Vis spectroscopy experiments on solutions containing colored compounds, as all colored compounds absorb light in the visual spectrum.

6) Would it be possible to conduct an UV/Vis spectroscopy experiment on a solution containing a colorless compound? Justify your answer.

It is possible to conduct UV/Vis spectroscopy experiments on solutions containing colorless compounds, as some colorless compounds absorb light in the ultraviolet spectrum.

7) A UV/Vis spectrometer was used to determine the concentration of an unknown colored compound in solution. The cuvette had a path length of 1.00 cm and the molar absorptivity was found to be 0.296 $M^{1}\text{cm}^{-1}$. Find the concentration of the unknown compound in solution if the absorbance was measured to be 0.314 A.

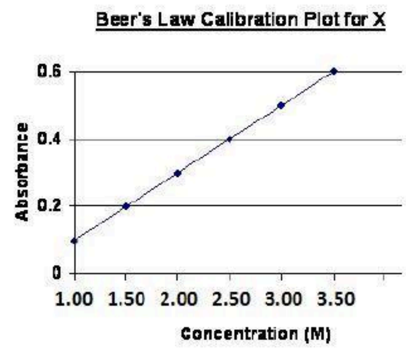
$$A = abc$$

$$c = \frac{A}{ab} = \frac{0.314}{\left(0.296M^{-1}\text{cm}^{-1}\right)\left(1.00\text{ cm}\right)}$$

$$c = 1.06M$$

8) A spectrometer with a 1.00 cm path length cuvette was used to measure the absorbance of a solution containing an unknown colored compound. At 624 nm the absorbance was measured to be 0.400 A.

a) Use the Beer's Law plot below to find the molar absorptivity of the solution.



$$A = abc$$
$$a = \frac{A}{bc} = \frac{0.400}{(1.00\text{ cm})(2.50M)}$$
$$a = 0.160M^{-1}\text{cm}^{-1}$$

b) Find the concentration if the absorbance was 0.684 A.

$$A = abc$$
$$c = \frac{A}{ab} = \frac{0.684}{(0.160M^{-1}\text{cm}^{-1})(1.00\text{ cm})}$$
$$c = 4.28M$$

9) Explain how absorption of electromagnetic radiation occurs in infrared (IR) spectroscopy experiments.

Different types of covalent bonds in molecules vibrate at different frequencies, which are within the IR spectrum, and IR radiation of the exact same frequency is absorbed by those covalent bonds.

10) If you were to design an experiment to determine the differences between some of the energy levels in a pure sample of a molecular compound, would you choose to use an infrared (IR) spectrometer or an ultraviolet/visual (UV/Vis) spectrometer? Justify your answer.

One would use an ultraviolet/visual (UV/Vis) spectrometer. In UV/Vis spectroscopy, photons cause electrons to move from lower energy MOs to higher energy MOs. For this to happen, the difference between the energy levels of the two MOs must be exactly the same as the energy contained by the photon. After one has determined the frequencies of electromagnetic radiation that are being absorbed by the sample, the energy contained by the photons in that electromagnetic radiation can be calculated using $E = hv$.

11) If you were to design an experiment to determine the different types of atoms and bonds that make up a pure sample of an unknown compound, would you choose to use an infrared (IR) spectrometer or an ultraviolet/visual (UV/Vis) spectrometer? Justify your answer.

One would use an IR spectrometer. In IR spectroscopy, different frequencies of electromagnetic radiation in the IR spectrum are absorbed by different types of bonds in the molecule that vibrate at the same frequencies as the radiation. The spectrum that is obtained from these experiments can be used to identify the different types of bonds in the structure and the elements that are involved in those bonds.

12) If you were to design an experiment to identify an unknown compound, would you choose to use an infrared (IR) spectrometer or an ultraviolet/visual (UV/Vis) spectrometer? Justify your answer.

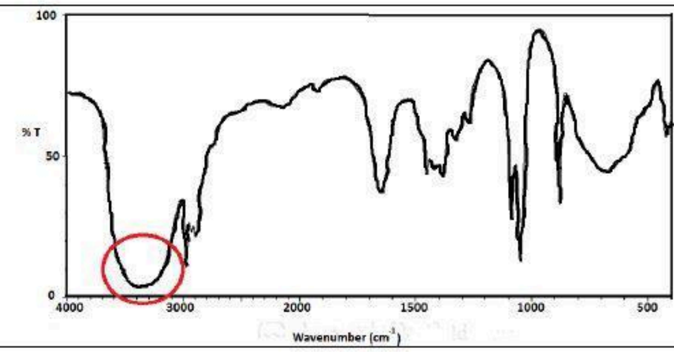
One would use an IR spectrometer. In IR spectroscopy, different frequencies of electromagnetic radiation in the IR spectrum are absorbed by different types of bonds in the molecule that vibrate at the same frequencies. The spectrum that is obtained from these experiments can be used to identify the different types of bonds in the structure and elements that are involved in those bonds. The spectrum for a compound also provides a 'fingerprint' that can be used to identify it.

13) If you were to design an experiment to find the concentration of a compound in solution, would you choose to use an infrared (IR) spectrometer or an ultraviolet/visual (UV/Vis) spectrometer? Justify your answer.

One would use an UV/Vis spectrometer. If the molar absorptivity, a, of the compound at the wavelength being used in the experiment is known, one can use an UV/Vis spectrometer to measure the absorbance, A, of a sample of the solution. The concentration of the solutions can then be calculated using the Beer-Lambert law equation: $A = abc$. In this equation 'b' is the path length of the curvette, which would be known, and 'c' is the concentration of the solution.

14) Below is an infrared spectrum of ethanol, CH_3CH_2OH. The functional group for alcohols (-OH) always peaks between wavenumbers 3650 cm^{-1} and 2500 cm^{-1}.

a. Identify the peak that is associated with the –OH group.



b. Do the peaks on infrared spectra point up or down? Justify your answer.

They point down, as percent transmittance is on the y-axis. If the bond is absorbing most of the light, only a very small amount is transmitted through the sample.