Learning Objectives and Worksheet XI

Chemistry 1B-AL Fall 2016

~~Lectures~~ (19-20) Spectroscopy

The material on spectroscopy will be taken from a number of sources and will not specifically follow the presentation in Zumdahl. It will be especially important to pay close attention to the handouts, worksheets, videos, and class presentations.

Understanding the electronic structure of atoms and bonding in molecules has been a primary focus of our work so far in Chemistry 1B. It is a very, very, nice story, but how can one experimentally verify that these abstract concepts actually occur in nature? Spectroscopy provides a primary experimental tool for investigating molecular structure. Additionally, other phenomena arising from the interaction of light (radiation) with matter are of wide ranging importance.

I. Basic Concepts of Spectroscopy

1. Know the names of the major types of electromagnetic radiation ranging from long wavelengths, corresponding to _____ frequencies, to short wavelengths corresponding to _____ frequencies.

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i.
ii.
iii.
iv.
v.
vi.

long λ

short λ

2. The relationship between the wavelength and frequency of electromagnetic radiation is: _____ .

3. The energy of a quantum of radiation is related to its frequency and wavelength by _____.

Related videos: https://youtu.be/OQwTcl9TeUM

4. The position and intensity of a spectral absorption cannot only reveal information about the structure of a molecule, but the intensity contains information on the _____ of the compound (think Beer's Law).

II. Types of spectroscopy corresponding to differing regions of the electromagnetic spectrum

1. X-rays
   i. Generally, what two things might occur when x-rays interact with a molecule

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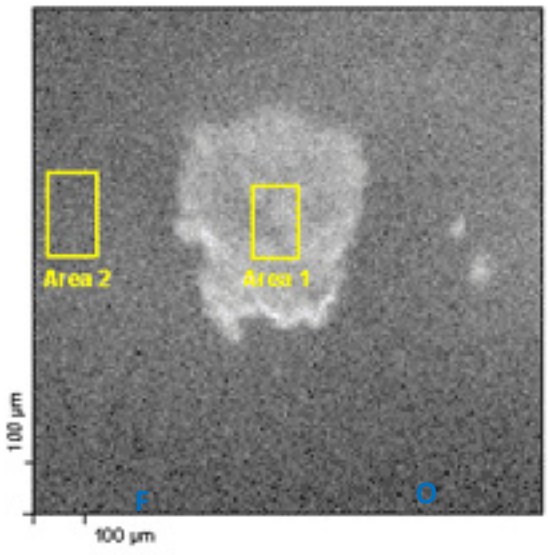
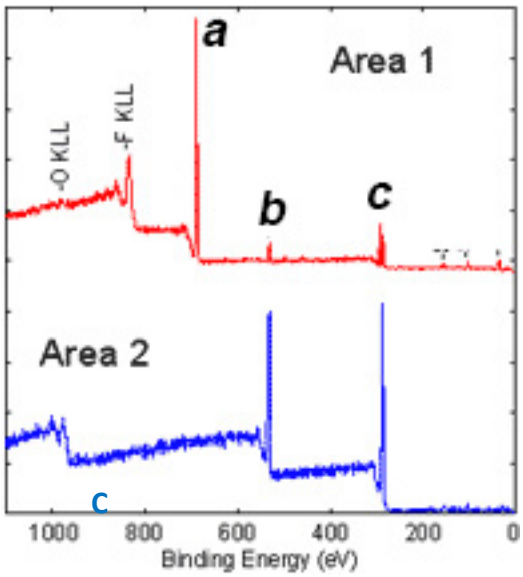
   ii. In _____ spectroscopy, the binding energy of an inner shell electron is determined by knowing the energy of the X-ray photon and measuring the _____ of the inner shell electron which is ejected.
   iii. This type of spectroscopy is used to _____ .
   iv. ESCA spectra were obtained for a surface putatively containing only carbon and oxygen compounds. However fluorine contamination was observed in Area 1, while Area 2 remained uncontaminated. In the ESCA spectrum for Area 1, identify which peak corresponds to ejection of 1s inner shell electrons from **O, F, or C**:

a. _____ b. _____ c. _____





Why does the atom that you identified for peak **a** have the greatest 1s binding energy (~650 eV)? _____
_____.

2. Far Ultraviolet
   i. Semantically, why is the spectral region with λ≅30 nm called the **'far' ultraviolet** vis a vis the '**near' ultraviolet** with λ≅300 nm?
   _____.

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ii. Semantically, why is spectroscopy using far ultraviolet wavelengths call **vacuum UV spectroscopy**? _____
_____.

iii. What type of electronic excitations are caused by absorption of far UV radiation? _____

3. Near Ultraviolet

i. What type of electronic excitations are caused by radiation in the near ultraviolet (~300 nm) ? _____

4. Visible

i. What wavelengths correspond to the visible region of the spectrum? _____

ii. These wavelengths are 'visible' because they interact with the molecule _____ found in the _____ of the human eye. When light is absorbed initiates a _____ (geomteric change) in the retinal moiety found in this molecule.

iii. For a compound to appear colored it must have

iv. Two general classes of molecules that appear colored are glazes of transition metal complexes and molecules with extended chains of conjugated double bonds. The types of electronic transition that gives rise to color in these compounds are:

a. transition metal complexes (e.g. an octahedral complex) _____

b. conjugated polyenes _____

5. Infrared

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i. Absorption of infrared light results in _____ excitations.

ii. The energy required to excite a given bond (i.e. the energy or wave number of the infrared absorption) depends on the _____ of the atoms and the _____ of the bond.

iii. A higher bond order implies a _____ value of $\tilde{\nu}$ for the absorption frequency (wave number) of the bond. Which molecule C_2H_2, C_2H_4, or C_2H_6 will have the smallest $\tilde{\nu}$ for excitation of its carbon-carbon bond? _____

iv. Know how to use group vibrational frequencies to distinguish molecules on the basis of their IR spectra.

6. Microwave
   i. Radiation in the microwave region induces _____ transitions in molecules.
   ii. In a microwave oven these absorptions in _____ are very effective in heating up the food.
   iii. Microwaves are also used in _____ spectroscopy where they have an appropriate energy to flip the magnet associated with _____ placed in an external magnetic field.
7. Radiowave
   i. _____ is the major type of spectroscopy that utilizes radiowave frequencies.
   ii. In this spectroscopy radiowaves have an appropriate energy to flip the magnet associated with _____ placed in an external magnetic field.
   iii. Hydrogen nuclei in differing molecular environments will absorb radiowaves of _____ .
   iv. Know how to use NMR spectra to distinguish molecules having differing numbers of non-equivalent hydrogen nuclei.

III. Vocabulary

1. Losss of energy in return to ground state
   i. After excitation there are three types of processes by which an excited state molecule can lose energy in returning to the ground state. These are:

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   ii. in _ _ a photon of higher frequency than in _
   iii. ____ _____ is the slower emission process since it involves flipping an _ _____ during return to the ground state.
2. The chemical reaction reactants ⟶ (products)* ⟶ products + h represents _____ ___ .