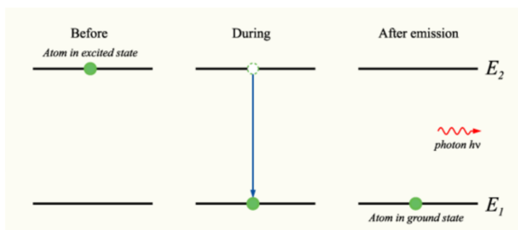
1.3: Introduction to Molecular Spectroscopy

Objectives

After completing this section, you should be able to

- Understand how an organic molecule interacts with electromagnetic radiation.
- Understand how different frequencies affect organic molecules.

Now that we we have discussed electromagnetic radiation and what it is, let's look at how it can interact with organic molecules. As was discussed in the last section, electromagnetic radiation can either acts as a wave or a particle, a photon. As a wave, it is represented by velocity, wavelength, and frequency. Light is an electromagnetic wave since the speed of electromagnetic waves is the same as the speed of light. As a particle, electromagnetic radiation is represented as a photon, which transports energy. When a photon is absorbed, the electron can be moved up or down an energy level. When it moves up, it absorbs energy, when it moves down, energy is released as is shown in the diagram below. Thus, since each atom has its own distinct set of energy levels, each element emits and absorbs different frequencies. Photons with higher energies produce shorter wavelengths and photons with lower energies produce longer wavelengths.

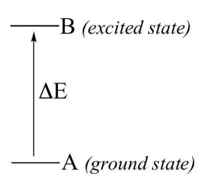


Electromagnetic radiation is also categorized into two groups based, ionizing and non-ionizing, on the severity of the radiation. Ionizing radiation holds a great amount of energy to remove electrons and cause the matter to become ionized. Thus, higher frequency waves such as the X-rays and gamma-rays have ionizing radiation. However, lower frequency waves such as radio waves, do not have ionizing radiation and are grouped as non-ionizing.

Molecular spectroscopy – the basic idea

In a spectroscopy experiment, electromagnetic radiation of a specified range of wavelengths is allowed to pass through a sample containing a compound of interest. The sample molecules absorb energy from some of the wavelengths, and as a result jump from a low energy ‘ground state’ to some higher energy ‘excited state’. Other wavelengths are *not* absorbed by the sample molecule, so they pass on through. A detector on the other side of the sample records which wavelengths were absorbed, and to what extent they were absorbed.

Here is the key to molecular spectroscopy: *a given molecule will specifically absorb only those wavelengths which have energies that correspond to the energy difference of the transition that is occurring.* Thus, if the transition involves the molecule jumping from ground state A to excited state B, with an energy difference of **Δ**E, the molecule will specifically absorb radiation with wavelength that corresponds to **Δ**E, while allowing other wavelengths to pass through unabsorbed.



By observing which wavelengths a molecule absorbs, and to what extent it absorbs them, we can gain information about the nature of the energetic transitions that a molecule is able to undergo, and thus information about its structure. If a sample is irradiated with energy of many wavelengths and determine which are absorbed and which are transmitted, the absorption spectrum of the compound can be measured. The energy the molecule gains when it absorbs radiation must be distributed over the molecule in some way. The different types of radiation cause different ways of interacting with the electromagnetic radiation. With infrared radiation, the energy absorbed by a molecule causes bonds to bend and stretch. With ultraviolet radiation, the energy absorbed causes an electron to jump from a lower energy orbital to a higher energy orbital. With these different frequencies interacting differently with the molecule, different types of structural information can be gleaned as you interpret the results of absorption spectra.

These generalized ideas may all sound quite confusing at this point, but things will become much clearer as we begin to discuss specific examples. In the upcoming chapters, ultraviolet spectroscopy, infrared spectroscopy, and nuclear magnetic resonance spectroscopy will be discussed in greater detail.

? Exercise 1.3.1

Knowing that infrared radiation causes bonds to bend and stretch more vigorously. Would you expect this type of radiation to be ionizing or non-ionizing?

Answer

The photons of infrared radiation absorbed do have enough energy to cause an increase in the amplitude of bond vibrations (bending/stretching), but not enough energy to break a covalent bond.

? Exercise 1.3.2

The **Δ**E (energy gap) has in inverse dependance on wavelength.

E=hc/λ

Therfore, a smaller gap leads to a longer or shorter wavelength?

Answer

The smaller the energy gap, the longer the wavelength of light that will be absorbed in the electronic transition.

Contributors and Attributions

- Dr. Dietmar Kennepohl FCIC (Professor of Chemistry, Athabasca University)
- Prof. Steven Farmer (Sonoma State University)
- William Reusch, Professor Emeritus (Michigan State U.), Virtual Textbook of Organic Chemistry

---