3.S: Summary

Concepts & Vocabulary

3.1 Chapter Objectives and Preview of Ultraviolet Spectroscopy

- Ultraviolet (UV) spectroscopy is a technique that is only applicable to conjugated compounds giving information on the nature of the conjugated pi electron system.

3.2 Conjugated Dienes

- A diene is a hydrocarbon chain that has two double bonds that may or may not be adjacent to each other.
- The arrangements of these double bonds can have varying affects on the compounds reactivity and stability.
- A molecule is defined as conjugated when there is a system of connected p orbitals where electron density can be shared across the system.
- Enones are a type of conjugated diene.
- Polyenes are compounds that have more than two double bonds present in the molecule.

3.3 Electronic Transitions

- When both electrons are paired in the lower-energy bonding orbital – this is the Highest Occupied Molecular Orbital (HOMO). The antibonding σ* orbital, in turn, is the Lowest Unoccupied Molecular Orbital (LUMO).
- If the molecule is exposed to light of a wavelength with energy equal to ΔE, the HOMO-LUMO energy gap, this wavelength will be absorbed and the energy used to bump one of the electrons from the HOMO to the LUMO.
- π- π* energy gaps are narrower than σ - σ***** gaps.
- Where UV-vis spectroscopy becomes useful to most organic and biological chemists is in the study of molecules with conjugated pi systems.
- In these groups, the energy gap for π -π* transitions is smaller than for isolated double bonds, and thus the wavelength absorbed is longer.

3.4 Ultraviolet Absorption

- To understand why some compounds are colored and others are not, and to determine the relationship of conjugation to color, we must make accurate measurements of light absorption at different wavelengths in and near the visible part of the spectrum.
- The visible region of the spectrum comprises photon energies of 36 to 72 kcal/mol, and the near ultraviolet region, out to 200 nm, extends this energy range to 143 kcal/mol.
- When sample molecules are exposed to light having an energy that matches a possible electronic transition within the molecule, some of the light energy will be absorbed as the electron is promoted to a higher energy orbital.

3.5 UV- Visible Spectrometer

- UV-Vis spectrometers have a light source (usually a deuterium or tungsten lamp), a sample holder and a detector.
- UV-vis spectroscopic data can give qualitative and quantitative information of a given compound or molecule.
- For a sample, it is important to use a reference cell to zero the instrument for the solvent the compound is in.
- For quantitative information on the compound, calibrating the instrument using known concentrations of the compound in question in a solution with the same solvent as the unknown sample would be necessary for accurate results.
- UV-vis spectroscopy works well on liquids and solutions, but if the sample is more of a suspension of solid particles in liquid, the sample will scatter the light more than absorb the light and the data will be very skewed.
- Every solvent has a UV-vis absorbance cutoff wavelength, which is the wavelength below which the solvent itself absorbs all of the light.

3.6 Interpreting Ultraviolet Spectra

- The basic setup is: radiation with a range of wavelengths is directed through a sample of interest, and a detector records which wavelengths were absorbed and to what extent the absorption occurred.
- Some UV spectra have only one broad peak, although many molecules have more than one broad peak.
- The convention in UV-vis spectroscopy is to show the baseline at the bottom of the graph with the peaks pointing up. Wavelength values on the x-axis are generally measured in nanometers (nm).

- There are two things that we look for and record from a UV-Vis spectrum. The first is lambda max (λ_{max}), which is the wavelength at maximal light absorbance and the secon is to record how much light is absorbed at λ_{max}.

3.7 Conjugation and the Absorption of Light in the Real World

- Light influence our everyday lives.
- Eyes receive light energy then transfer and passing the energy into neural impulses to brain.
- As an energy wave, energy is passed on through light at different wavelength.
- Light energy can convert chemicals to other forms.
- In human eyes, rod and cones react to light stimulation, and a series of chemical reactions happen in cells.

Skills to Master

- Skill 3.1 Distinguish between different types of dienes.
- Skill 3.2 Compare molecules to determine if there is a larger or smaller energy gap.
- Skill 3.3 Understand which molecules will absorb longer wavelengths.
- Skill 3.4 Calculate the energy to excite a molecule from HOMO to LUMO.
- Skill 3.5 Understand how the spectrometer works.
- Skill 3.6 Understand the limitations of a spectrometer.
- Skill 3.7 Determine λ_{max}.
- Skill 3.8 Gather information from a UV-vis spectrum.
- Skill 3.9 Understand why humans see different colors.

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