1.S Summary of Organic Spectroscopy

Concepts & Vocabulary

1.1: Chapter Objectives and Preview of Spectroscopy

- Modern spectroscopic techniques have reduced the time it once took for structure determination.
- Spectroscopic techniques are based on the absorption of radiation from the electromagnetic spectrum.
- The different spectroscopic techniques can give different snapshots of the molecule's structure and lending insight to properties the molecule may have.

1.2 The Nature of Radiant Energy and Electromagnetic Radiation

- Electromagnetic radiation is composed of electrical and magnetic waves which oscillate on perpendicular planes.
- Electron radiation is released as photons, which are bundles of light energy that travel at the speed of light as quantized harmonic waves.
- The amplitude is basically the height of the wave. Larger amplitude means higher energy and lower amplitude means lower energy.
- Amplitude is important because it tells you the intensity or brightness of a wave in comparison with other waves.
- The different properties of the various types of electromagnetic radiation are due to differences in their wavelengths, and the corresponding differences in their energies: *shorter wavelengths correspond to higher energy.*
- Longer waves have lower frequencies, and shorter waves have higher frequencies.
- The full range of electromagnetic radiation wavelengths is referred to as the electromagnetic spectrum.
- The different types of electromagnetic radiation shown in the electromagnetic spectrum consists of radio waves, microwaves, infrared waves, visible light, ultraviolet radiation, X-rays, and gamma rays.

1.3 Introduction to Spectroscopy

- 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.
- Since each atom has its own distinct set of energy levels, each element emits and absorbs different frequencies.
- Electromagnetic radiation is also categorized into two groups based, ionizing and non-ionizing, on the severity of the radiation.
- In spectroscopic techniques, 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’.
- 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.*
- 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.

1.4 Time-resolved vs. Frequency-resolved

- Spectroscopic measurements are typically taken in one of two domains: frequency or time.
- Frequency is used to represent the number of cycles occurring in a given time period.
- The frequency domain is the most familiar domain in spectroscopy.
- UV/visible, infrared, photoelectron, microwave, and X-ray spectroscopy all have applications in the frequency domain.
- The results of these spectroscopic techniques are typically given in some form of intensity versus wavelength.
- Rather than acquiring spectra by averaging data over a relatively long time range, data is acquired over discrete time intervals or, in some cases, continuously. This may be done over one or many wavelengths.
- Time resolved spectroscopy observes the change in eigen states with respect to time.
- In order for data from time-resolved spectroscopy to be useful, the spectroscopy must be suited to the time scale of the process of interest.
- Time resolved spectroscopy can be used to study kinetics, reactions, and lifetimes.
- Some spectroscopies yield data in both time and frequency domains. The most prominent of these techniques is time-resolved laser spectroscopy.

1.5 The Power of the Fourier Transform for Spectroscopists

- Fourier transform is a mathematical technique that can be used to transform a function from one real variable to another.
- Fourier transform from time domain to frequency domain is the essential process that enable us to translate raw data to readable spectra.
- The nature of trigonometric function enables Fourier transform to convert a function from the domain of one variable to another and reconstruct it later on.
- This is a robust mathematical tool to process data in different domains under different circumstances.
- Fourier transform are widely involved in spectroscopy in all research areas that require high accuracy, sensitivity, and resolution.
- By definition, Fourier transform spectroscopy is a spectroscopic technique where interferograms are collected by measurements of the coherence of an electromagnetic radiation source in the time-domain or space-domain, and translated into frequency domain through Fourier transform.
- With a Fourier transform spectrometer equipped with an interferometer, we can easily vary the parameter in time domain or spatial domain by changing the position of the movable mirror.
- An interferometer can let through a beam with the whole wavelength range at once, and measure the intensity of the total beam at that optical path difference.
- If the beam is modified for each new data point by scanning the moving mirror along the axis of the moving arm, a series of intensity versus each optical path length difference are collected.
- Fourier transform spectroscopy can be applied to a variety of regions of spectroscopy and it continues to grow in application and utilization including optical spectroscopy, infrared spectroscopy (IR), nuclear magnetic resonance, electron paramagnetic resonance spectroscopy, mass spectrometry, and magnetic resonance spectroscopic imaging (MRSI).

1.6 Upcoming Spectroscopy Techniques

- Ultra-violet spectroscopy shows absorption only if conjugated π electron systems are present.
- Infrared spectroscopy allows for the identification of functional groups present in a molecule.
- Nuclear magnetic resonance distinguishes and counts atoms in different locations in the molecule.

Skills to Master

- Skill 1.1 Be able to manipulate the equations to calculate frequency or energy.
- Skill 1.2 Determine which frequency or wavelength is a higher energy.
- Skill 1.3 Understand how an organic molecule interacts with electromagnetic radiation.
- Skill 1.4 Determine how an energy gap will lead to longer or shorter wavelength.
- Skill 1.5 Know why some spectrometers use frequency domain and others use time domain.
- Skill 1.6 Perform a Fourier transform to show how to extract spectrum from the raw data.
- Skill 1.7 Compare an interferometer with a monochromator.
- Skill 1.8 Know the important components to make Fourier transform spectrometer practical and what are they used for.
