4.S Summary

Concepts & Vocabulary

4.2 Theory

- Molecules can absorb light energy by three different processes and IR absorptions occur with small differences between the rotational and vibrational modes.
- IR absorption is a net change in dipole moment in a molecule as it vibrates or rotates.
- The absorption of IR radiation by a molecule can be likened to two atoms attached to each other by a massless spring often based using Hooke's Law.
- The bond of a molecule experiences various types of vibrations and rotations since they are not stationary and to fluctuate continuously, which are defined by stretching and bending modes.
- A molecule consisting of (N) number of atoms has a total of 3N degrees of freedom, corresponding to the Cartesian coordinates of each atom in the molecule.
- The larger the molecule, the more complex the vibrational modes.

4.3 Instrumentation

- There are two types of instruments used to measure IR absorption: Fourier transform (FT) spectrometers and dispersive spectrometers.
- The basic components of a dispersive IR spectrometer include a radiation source, monochromator, and detector.
- Dispersive spectrometers have a double-beam design with two equivalent beams from the same source passing through the sample and reference chambers as independent beams.
- A common FTIR spectrometer consists of a source, interferometer, sample compartment, detector, amplifier, A/D convertor, and a computer.
- The major difference between an FTIR spectrometer and a dispersive IR spectrometer is the Michelson interferometer.
- The Michelson interferometer, which is the core of FTIR spectrometers, is used to split one beam of light into two so that the paths of the two beams are different.
- IR spectra can be obtained from solid, liquid, or gas samples.

4.4 The IR Spectrum

- The IR spectrum is a graph where the x-axis is frequency and is labeled as wavenumber (cm^{-1}).
- The y-axis is the amount of light absorbed and labeled as Transmittance (%).
- The spectrum is measuring how much light has been transmitted at a particular frequency.
- Bond strength and reduced mass are the two molecular properties determine the wavenumber at which a molecule will absorb infrared light.
- No two chemical substances in the universe have the same force constants and atomic masses, which is why the infrared spectrum of each chemical substance is unique.
- Peak intensity is determined by dipole moment and the concentration of the sample.
- The width of infrared bands for solid and liquid samples is determined by the number of chemical environments which is related to the strength of intermolecular interactions such as hydrogen bonding.
- An important observation made by early researchers is that many functional group absorb infrared radiation at about the same wavenumber, regardless of the structure of the rest of the molecule.

4.5 IR Data Table

- Since similar functional groups appear at similar frequencies, a data table was curated for scientists to use as a guide for where they would expect certain peaks.

4.6 Interpretation

- The hydrogen bond region falls from 4000 to 2500 cm^{-1}. This is the area you will find all of your O-H, N-H, and C-H bonds that typically appear in organic molecules.
- The next region is the triple bond region (2500 - 2000 cm^{-1}), where the C≡C and C≡N bonds commonly found in organic molecules will absorb.
- The double bond region (2000 - 1500 cm^{-1}). Here you will find the C=C, C=O, and C=N bonds.

- The fingerprint region is 1500 - 600 cm^{-1}, where all the single bonds will be found with the exception of some of the bonds to hydrogen that are found in the hydrogen bond region.
- You are looking to determine what functional groups are a part of a molecule.
- You do NOT need to analyze every single peak.

4.7 Identifying Characteristic Functional Groups

- Ethers have IR absorptions associated with both the C-O stretching vibrations.
- Alcohols have IR absorptions associated with both the O-H and the C-O stretching vibrations.
- Ketones have IR absorptions associated with the C=O bond.
- Aldehydes have IR absorptions associated with the C=O bond and the aldehydic proton.
- Carboxylic acids have IR absorptions associated with the C=O bond and the carboxylic acid proton.
- Esters have IR absorptions associated with the C=O bond and the C-O bond.
- Amines have IR absorptions associated with the N-H bond. There is a C-N peak as well, but it is often buried in the fingerprint region and difficult to discern.
- Nitriles have IR absorptions associated with the C≡N bond. There is a C-N peak as well, but it is often buried in the fingerprint region and difficult to discern.
- IR spectroscopy can prove to be a very valuable tool, given the information it provides about the presence or absence of key functional groups.

4.9 Application

- The most common application of IR spectroscopy is determining the functional groups present or absent in a molecule.
- Environmental scientists use IR for detecting industrial pollutants.
- In art conservation, IR spectroscopy is used to help identify what pigments, adhesives, fibers, plastics, and binders were used.
- IR spectroscopy is used in a wide variety of industries.

Skills to Master

- Skill 4.1 Distinguish between different types of stretching.
- Skill 4.2 Determine the number of vibrational modes molecules may have.
- Skill 4.3 Understand the instrumentation used to obtain IR spectra.
- Skill 4.4 Orient oneself with an IR spectrum.
- Skill 4.5 Be able to read a data table for IR spectroscopy.
- Skill 4.6 Determine functional groups present in the molecule based on an IR spectrum.