Chapter 15

Understanding How to Analyze Structures of Products (Part 2): Infrared Spectroscopy (IR), Polarimetry, and Ultraviolet-Visible Spectrophotometry (UV-Vis)

Key Concepts

IR:

Infrared spectroscopy works on the principle that electromagnetic radiation is absorbed when the frequency of bond vibration matches the frequency of the radiation. This happens in the IR portion of the electromagnetic spectrum.

The shorter the bond, the faster it vibrates, and therefore, the higher the frequency of radiation that is absorbed.

Since hydrogen has only 1 shell, it forms the shortest covalent bond. As a result, a bond to hydrogen absorbs radiation with the highest wavenumber (2500–3500 cm^{-1}) of any bond in an organic molecule. Triple bonds that exist between carbon and/or nitrogen atoms are the next shortest (2000–2500 cm^{-1}), followed by double bonds between carbon, nitrogen, and/or oxygen (1500–2000 cm^{-1}). Bonds that are part of a resonance system and therefore are in-between double and single bonds absorb radiation at an even lower frequency than double bonds (1400–1500 cm^{-1}). Since oxygen and nitrogen are slightly smaller than carbon, a bond between carbon and oxygen or nitrogen has a slightly higher vibrational frequency than a comparable bond between carbon atoms.

To simplify analysis of IR data, focus on bands above 1700 cm^{-1}. Use bands below 1600 cm^{-1} as needed to confirm known data, or to narrow down possibilities.

Another important concept is that the more intensely a bond vibrates, the more radiation it absorbs. Because electronegativity differences cause electrons to be yanked toward the more electronegative atom, it means that the greater the electronegativity difference, the more pronounced the vibration, and therefore the more radiation that is absorbed.

Polarimetry:

Chiral compounds rotate plane-polarized light. Since each molecule in an enantiomer pair rotates light the same number of degrees, but in opposite directions, polarimetry can be used to determine the purity of a chiral compound.

UV-Visible Spectrophotometry:

The greater the amount of resonance, the lower the energy of UV-visible light a molecule absorbs. Since absorbance and concentration are proportional for a given compound, the concentration of a compound in a solution can be calculated based on its UV-Vis absorbance.

What You Need to Learn, Understand, and Apply

1. **The types of information gained when analyzing a sample using infrared spectroscopy.**
2. **The general theory of infrared spectroscopy.**
3. **The ability to identify unique IR absorption bands for alcohols, amines, alkynes, alkenes, carboxylic acids, aldehydes, nitriles, carbonyl compounds, benzenes, esters, and ethers.**
4. **The ability to confirm IR absorption bands.**
5. **The ability to determine whether a molecule rotates plane-polarized light.**
6. **The ability to do calculations related to polarimetry.**
7. **A working knowledge of the general theory and use of UV-Vis spectroscopy**
8. **The skills needed to apply the material and avoid common errors.**