1.6: Upcoming Spectroscopy Techniques

Learning Objectives

- Have a brief introduction to each of the techniques to be discussed in upcoming chapters
- Understand what type of information each technique gives to help with structure determination

To "see" a molecule, we must use light having a wavelength smaller than the molecule itself (roughly 1 to 15 angstroms). Such radiation is found in the X-ray region of the spectrum, and the field of **X-ray crystallography** yields remarkably detailed pictures of molecular structures amenable to examination. The chief limiting factor here is the need for high quality crystals of the compound being studied. The methods of X-ray crystallography are too complex to be described here; nevertheless, as automatic instrumentation and data handling techniques improve, it will undoubtedly prove to be the procedure of choice for structure determination. The spectroscopic techniques described below do not provide a three-dimensional picture of a molecule, but instead yield information about certain characteristic features. A brief summary of this information follows:

- **Ultraviolet-Visible Spectroscopy**: Absorption of this relatively high-energy light causes electronic excitation. The easily accessible part of this region (wavelengths of 200 to 800 nm) shows absorption only if conjugated π electron systems are present.
- **Infrared Spectroscopy**: Absorption of this lower energy radiation causes vibrational and rotational excitation of groups of atoms. within the molecule. Because of their characteristic absorptions, identification of functional groups is easily accomplished.
- **Nuclear Magnetic Resonance (NMR) Spectroscopy**: Absorption in the low-energy radio-frequency part of the spectrum causes excitation of nuclear spin states. NMR spectrometers are tuned to certain nuclei (e.g. ^{1}H, ^{13}C, ^{19}F & ^{31}P). For a given type of nucleus, high-resolution spectroscopy distinguishes and counts atoms in different locations in the molecule.