Realizing that light may be considered to have both wave-like and particle-like characteristics, it is useful to consider that a given frequency or wavelength of light is associated with a "light quanta" of energy we now call a photon. As noted in the following equations, frequency and energy change proportionally, but wavelength has an inverse relationship to these quantities.

\[ \nu = \frac{c}{\lambda} \]

and

\[ \Delta E = h\nu \]

with

- \( \nu \) is the frequency of light
- \( \lambda \) is the wavelength of light
- \( c \) is the speed of light \((3 \times 10^8 \text{ m/sec})\)
- \( \Delta E \) is the transition energy (difference of energies between the initial and final states)
- \( h \) is Planck's constant \((6.626069 \times 10^{-34} \text{ J s})\)

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 \( \pi \) 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. \(^1\text{H}, ^{13}\text{C}, ^{19}\text{F} \) & \(^{31}\text{P}\)). For a given type of nucleus, high-resolution spectroscopy distinguishes and counts atoms in different locations in the molecule.

Contributors