6 chapter

Basic Principles of Spectroscopy

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6.1 INTRODUCTION

Spectroscopy deals with the production, measurement, and interpretation of spectra arising from the *interaction of electromagnetic radiation with matter*. There are many different spectroscopic methods available for solving a wide range of analytical problems. The methods differ with respect to the species to be analyzed (such as molecular or atomic spectroscopy), the type of radiation-matter interaction to be monitored (such as absorption, emission, or diffraction), and the region of the electromagnetic spectrum used in the analysis. Spectroscopic methods are very informative and widely used for both quantitative and qualitative analyses. Spectroscopic methods based on the absorption or emission of radiation in the *ultraviolet* (UV), *visible* (Vis), *infrared* (IR), and radio (*nuclear magnetic resonance*, *NMR*) frequency ranges are most commonly encountered in traditional food analysis laboratories. Each of these methods is distinct in that it monitors different types of molecular or atomic transitions. The basis of these transitions is explained in the sections below.

6.2 LIGHT

6.2.1 Properties

Light may be thought of as particles of energy that move through space with wavelike properties. This image of light suggests that the energy associated with a ray of light is not distributed continuously through space along the wave's associated electric and magnetic fields but rather that it is concentrated in discrete packets. Light is therefore said to have a dual nature: *particulate* and *wavelike*. Phenomena associated with light propagation, such as interference, diffraction, and refraction, are most easily explained using the wave theory of electromagnetic radiation. However, the interaction of light with matter, which is the basis of absorption and emission spectroscopy, may be best understood in terms of the particulate nature of light. Light is not unique in possessing both wavelike and particulate properties. For example, fundamental particles of matter, such as electrons, protons, and neutrons, are known to exhibit wavelike behavior.

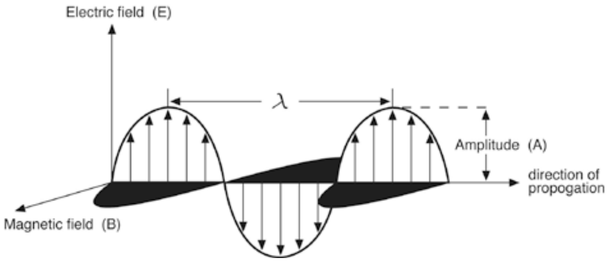
The wave properties of electromagnetic radiation are described in terms of the wave's frequency, wavelength, and amplitude. A graphical representation of a plane-polarized electromagnetic wave is given in Fig. 6.1. The wave is plane polarized in that the oscillating electric and magnetic fields making up the wave are each limited to a single plane. The *frequency* (ν, the lower case Greek letter *nu*) of a wave is defined as the number of oscillations the wave will make at a given point per second. This is the reciprocal of the *period* (p) of a wave, which is the time in seconds required for successive maxima of the wave to pass a fixed point. The *wavelength* (λ) represents the distance between successive maxima on any given wave. The units used in reporting wavelengths will depend on the region of electromagnetic radiation used in the analysis. Spectroscopic data sometimes are reported with respect to *wave numbers* ($\bar{v}$), which are reciprocal wavelengths in units of cm^{-1}. Wave numbers are encountered most often in IR spectroscopy. The *velocity of propagation* (v_i) of an electromagnetic wave, in units of distance per second, in any given medium "i" can be calculated by taking the product of the frequency of the wave, in cycles per second, and its wavelength in that particular medium:

$$v_i = \nu\lambda_i \tag{6.1}$$

where:

v_i = velocity of propagation in medium i
ν = frequency (of associated wave)
λ_i = wavelength in medium i

The frequency of an electromagnetic wave is determined by the source of the radiation, and it remains constant as the wave traverses different media. However, the velocity of propagation of a wave will vary slightly depending on the medium through which the light is propagated. The wavelength of the radiation will change in proportion to changes in wave velocity as defined by Eq. 6.1. The *amplitude of the wave* (A) represents the magnitude of the electric vector at the wave maxima. The *radiant power* (P) and *radiant intensity* (I) of

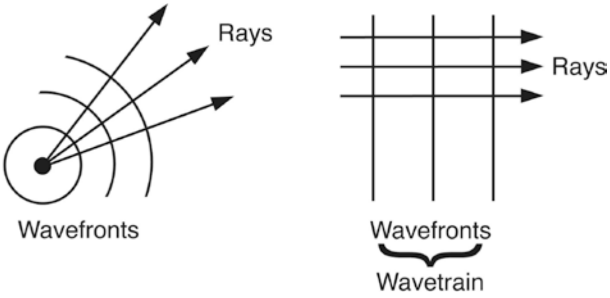


6.1 figure

Representation of plane-polarized electromagnetic radiation propagating along the *x*-axis. The electric and magnetic fields are in phase, perpendicular to each other and to the direction of propagation a beam of radiation are proportional to the square of the amplitude of the associated waves making up that radiation. Figure 6.1 indicates that electromagnetic waves are composed of *oscillating magnetic* and *electric fields*, the two of which are mutually perpendicular, in phase with each other, and perpendicular to the direction of wave propagation. As drawn, the waves represent changes in the respective field strengths with time at a fixed location or changes in the respective field strengths over distance at a fixed time. The electrical and magnetic components of the waves are represented as a series of vectors whose lengths are proportional to the magnitude of the respective field. It is the oscillating electric field that is of most significance to spectroscopic phenomena such as absorption, transmission, and refraction. However, a purely electric field, without its associated magnetic field, is impossible.

6.2.2 Terminology

The propagation of electromagnetic waves is often described in terms of wave fronts or trains of waves (Fig. 6.2). A *wave front* represents the locus of a set of points, all of which are in phase. For a point source of light, a concentric ring that passes through the maxima of adjacent light rays will represent a wave front. The entire ring need not be drawn in all cases, such that wave fronts may represent planes of light in cases where the observation is sufficiently removed from the point source that the curved surface appears planar. Wave fronts are most typically drawn by connecting maxima, minima, or both for adjacent rays. If maxima are used for depicting wave fronts, then each of the wave fronts will be separated by one wavelength. A *train of waves*, or *wave train*, refers to a series of wave fronts, all of which are in phase, that is, each individual wave will have a maximum amplitude at the same location in space. A wave train also may be represented by a series of light rays. Rays of light are used generally with reference to the corpuscular nature of light, representing the path of photons. A wave train would indicate that a series of photons, all in phase, followed the same path.



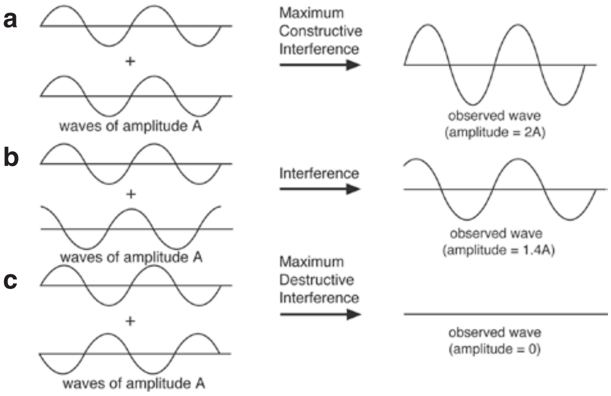
6.2 figure

Wave fronts, wave trains, and rays (From Hugh D. Young, *University Physics* (8th. Ed.) (p. 947), © 1992 by Addison-Wesley, Reading, MA. Courtesy of the publisher)

6.2.3 Interference

Interference is the term used to describe the observation that when two or more wave trains cross one another, they result in an instantaneous wave, at the point of intersection, whose amplitude is the algebraic sum of the amplitudes of the individual waves at the point of intersection. The law describing this wave behavior is known as the *principle of superposition*. Superposition of sinusoidal waves is illustrated in Fig. 6.3. Note that in all cases, the effective amplitude of the perceived wave at the point in question is the combined effect of each of the waves that crosses that point at any given instant. In spectroscopy, the amplitude of most general interest is that corresponding to the magnitude of the resulting electric field intensity. *Maximum constructive interference* of two waves occurs when the waves are completely in phase (i.e., the maxima of one wave align with the maxima of the other wave), while *maximum destructive interference* occurs when waves are 180° out of phase (the maxima of one wave align with the minima of the other wave). This concept of interference is fundamental to the interpretation of diffraction data, which represents a specialized segment of qualitative spectroscopy. Interference phenomena also are widely used in the design of spectroscopic instruments that require the dispersion or selection of radiation, such as those instruments employing grating monochromators or interference filters, as described in Chap. 7.

Interference phenomena are best rationalized by considering the wavelike nature of light. However,



6.3 figure

Interference of identical waves that are (**a**) in phase, (**b**) 90° out of phase, and (**c**) 180° out of phase

6.1 table Properties of light

Symbols/terms	*Relationship*	*Frequently used units*
λ = wavelength	$\lambda_i \nu = v_i$ ($v_i = c$ *in a vacuum*)	nm (nanometers, 10^{-9} m) Å (Ångstrom units, 10^{-10} m) µm (microns, 10^{-6} m) mµ (millimicrons, 10^{-9} m)
ν = frequency		Hz (hertz, 1 Hz = 1 oscillation per second)
c = speed of light		2.9979×10^{8} m s^{-1} in vacuum
$\bar{\upsilon}$ = wave number	$=1/\lambda$	cm^{-1} kK (kilokayser, 1 kK = 1,000 cm^{-1})
p = period	$p = 1/\nu$	s
E = energy	$E = h\nu$ $= hc/\lambda$ $= hc\bar{\upsilon}$	J (1 J = 1 kg m^2 s^{-2}) cal (calorie, 1 cal = 4.184 J) erg (1 erg = 10^{-7} J) eV (1 eV = 1.6022×10^{-19} J)
h = Planck's constant		6.6262×10^{-34} J s
P = radiant power	Amount of energy striking a given unit area per unit time	(Joules) $(m^2)^{-1}(s)^{-1}$

phenomena such as the absorption and emission of radiation are more easily understood by considering the particulate nature of light. The particles of energy that move through space with wavelike properties are called *photons*. The energy of a photon can be defined in terms of the frequency of the wave with which it is associated (Eq. 6.2):

$$E = h\nu \tag{6.2}$$

where:

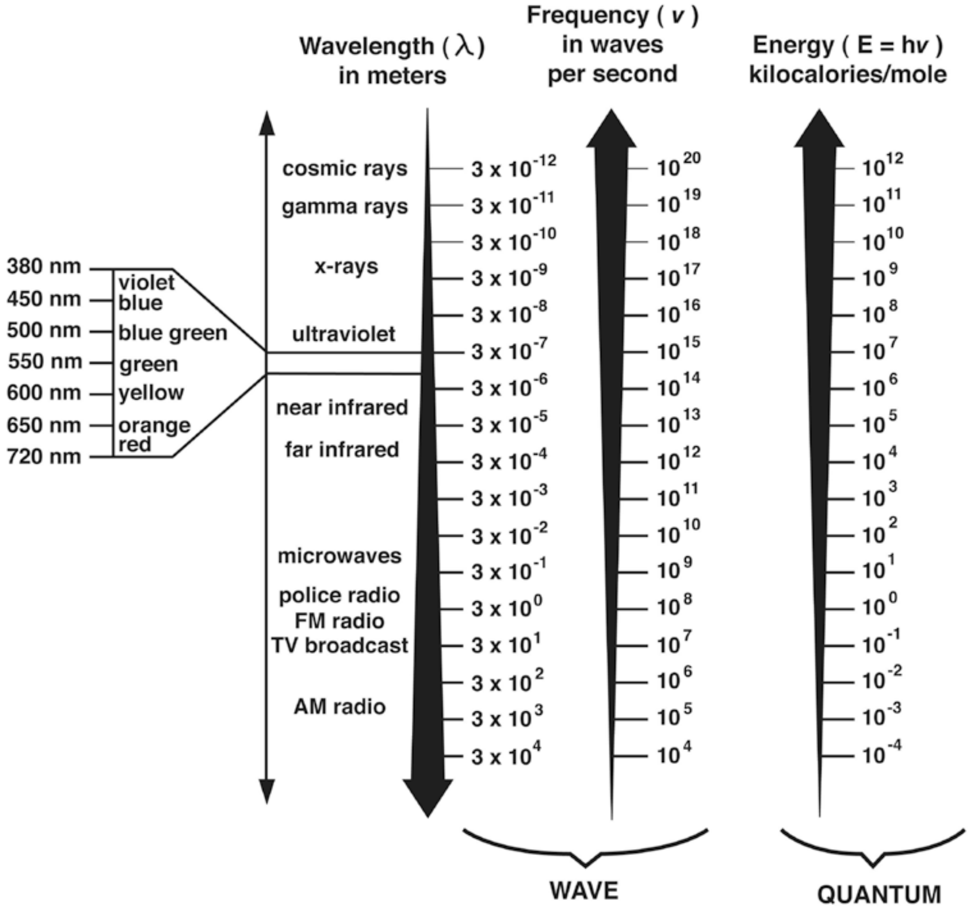
E = energy of a photon
h = Planck's constant
ν = frequency (of associated wave)

This relationship indicates that the photons making up *monochromatic light*, which is electromagnetic radiation composed of waves having a single frequency and wavelength, are all of equivalent energy. Furthermore, just as the frequency of a wave is a constant determined by the radiation source, the energy of associated photons also will be unchanging. The brightness of a beam of monochromatic light, when expressed in terms of the particulate nature of light, will be the product of the photon flux and the energy per photon. The *photon flux* refers to the number of photons flowing across a unit area perpendicular to the beam per unit time. It follows that to change the brightness of a beam of monochromatic light will require a change in the photon flux. In spectroscopy, the term *brightness* is generally not used, but rather one refers to the *radiant power* (P) or the *radiant intensity* (I) of a beam of light. Radiant power and radiant intensity often are used synonymously when referring to the amount of radiant energy striking a given area per unit time. In terms of International System of Units (SI) (time, seconds; area, meters; energy, joules), radiant power equals the number of joules of radiant energy impinging on a 1 m^2 area of detector per second. The basic interrelationships of light-related properties and a general scheme of the electromagnetic spectrum are presented in Table 6.1 and Fig. 6.4, respectively.

6.3 ENERGY STATES OF MATTER

6.3.1 Quantum Nature of Matter

The energy content of matter is quantized. Consequently, the potential or internal energy content of an atom or molecule does not vary in a continuous manner but rather in a series of discrete steps. Atoms and molecules, under normal conditions, exist predominantly in the *ground state*, which is the state of lowest energy. Ground-state atoms and molecules can gain energy, in which case they will be elevated to one of their higher energy states, referred to as *excited states*. The quantum nature of atoms and molecules puts limitations on the energy levels that are available to these species. Consequently, there will be specific "allowed" *internal energy levels* for each atomic or molecular species. Internal energy levels not corresponding to an allowed value for that particular species are unattainable. The set of available energy levels for any given atom or molecule will be distinct for that species. Similarly, the potential energy spacings between allowed internal energy levels will be characteristic of a species. Therefore, the set of potential energy spacings for a species may be used qualitatively as a distinct fingerprint. Qualitative absorption



6.4 figure

The electromagnetic spectrum (From Milton [1], p. 3. Courtesy of Milton Roy Company, Rochester, NY, a subsidiary of Sundstrand Corporation)

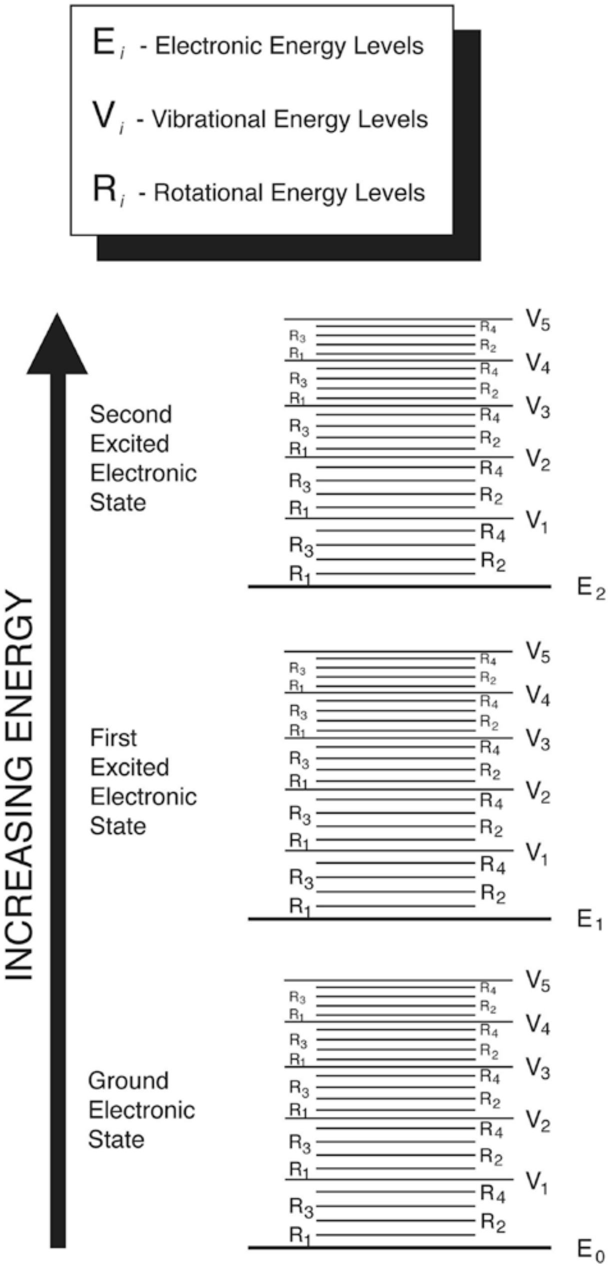
and emission spectroscopy make use of this phenomenon in that these techniques attempt to determine an unknown compound's relative energy spacings by measuring transitions between allowed energy levels.

6.3.2 Electronic, Vibrational, and Rotational Energy Levels

The relative *potential energy* of an atom or molecule corresponds to the energy difference between the energy state in which the species exists and that of the ground state. Figure 6.5 is a partial molecular energy-level diagram depicting potential energy levels for an organic molecule. The lowest energy state in the figure, bottom line in bold, represents the ground state. There are three *electronic energy states* depicted, each with its corresponding vibrational and rotational energy levels. Each of the electronic states corresponds to a given *electron orbital*. Electrons in different orbitals are of different potential energy. When an electron changes orbitals, such as when absorbing or emitting a photon of appropriate energy, it is termed an *electronic transition* since it is the electron that is changing energy levels. However, any change in the potential energy of an electron will, by necessity, result in a corresponding change in the potential energy of the atom or molecule that the electron is associated with.

Atoms are like *molecules* in that only specific energy levels are allowed for atomic electrons. Consequently, an energy-level diagram of an atom would consist of a series of electronic energy levels. In contrast to molecules, the electronic energy levels of atoms have no corresponding vibrational and rotational levels and, hence, may appear less complicated. Atomic energy levels correspond to allowed electron shells (orbits) and corresponding subshells (i.e., 1s, 2s, 2p, etc.). The magnitude of the energy difference between the ground state and first excited states for valence electrons of atoms and bonding electrons of molecules is generally of the same range as the energy content of photons associated with UV and Vis radiation.

The wider lines within each electronic state of Fig. 6.5 depict the species' *vibrational energy levels*. The atoms that comprise a molecule are in constant motion,



6.5 figure Partial molecular energy-level diagram depicting three electronic states

vibrating in many ways. However, in all cases the energy associated with this vibrational motion corresponds to defined quantized energy levels. The energy differences between neighboring vibrational energy levels are much smaller than those between adjacent electronic energy levels. Therefore, it is common to consider that several vibrational energy levels are superimposed on each of the molecular electronic energy levels. Energy differences between allowed vibrational energy levels are of the same magnitude as the energy of photons associated with radiation in the IR region. Vibrational energy levels would not be superimposed on an atomic potential energy-level diagram since this vibrational motion does not exist in a single atom. In this respect, the potential energy diagram for an atom is less complex than that for a molecule, the atomic energy-level diagram having fewer energy levels.

The potential energy of a molecule also is quantized in terms of the energy associated with the rotation of the molecule about its center of gravity. These *rotational energy levels* are yet more closely spaced than the corresponding vibrational levels, as depicted by the narrow lines within each electronic state shown in Fig. 6.5. Hence, it is customary to consider several rotational energy levels superimposed on each of the permitted vibrational energy levels. The energy spacings between rotational energy levels are of the same magnitude as the energy associated with photons of microwave radiation. Microwave spectroscopy is not commonly used in food analysis laboratories; however, the presence of these different energy levels will impact the spectrum observed in other forms of spectroscopy, as will be discussed later. Similar to the situation of vibrational energy levels, rotational energy levels are not of consequence to atomic spectroscopy.

In summation, the internal energy of an *atom* is described in terms of its *electronic energy levels*, while the internal energy of a *molecule* is dependent on its *electronic*, *vibrational*, and *rotational energies*. The algebraic form of these statements follows:

$$E_{\text{atom}} = E_{\text{electronic}} \tag{6.3}$$

$$E_{\text{molecule}} = E_{\text{electronic}} + E_{\text{vibrational}} + E_{\text{rotational}} \tag{6.4}$$

The spectroscopist makes use of the fact that each of these associated energies is quantized and that different species will have somewhat different energy spacings.

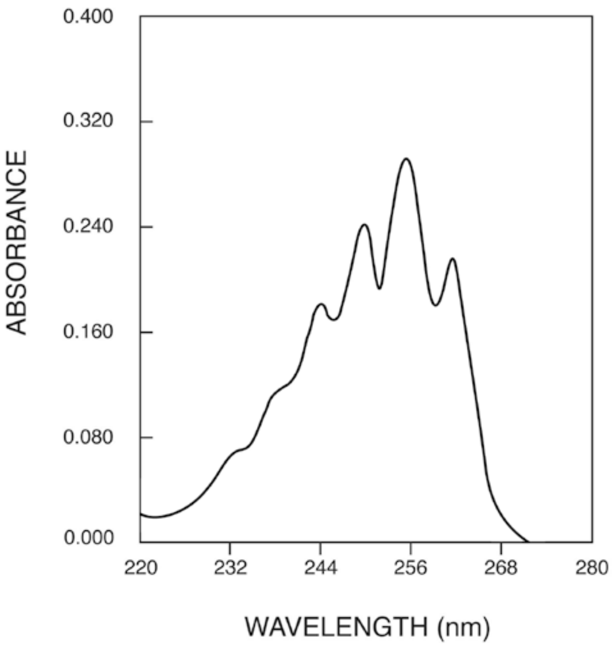
6.3.3 Nuclear Energy Levels in Applied Magnetic Fields

NMR spectroscopy makes use of yet another type of quantized energy level. The energy levels of importance to NMR spectroscopy differ with respect to those described above in that they are relevant only in the presence of an applied external *magnetic field*. The basis for the observed energy levels may be rationalized by considering that the nuclei of some atoms behave as tiny bar magnets. Hence, when the atoms are placed in a magnetic field, their nuclear magnetic moment will have a preferred orientation, just as a bar magnet would behave. The NMR-sensitive nuclei of general relevance to the food analyst have two permissible orientations. The energy difference between these allowed orientations depends on the effective magnetic field strength that the nuclei experience. The effective magnetic field strength will itself depend on the strength of the applied magnetic field and the chemical environment surrounding the nuclei in question. The applied magnetic field strength will be set by the spectroscopist, and it is essentially equivalent for each of the nuclei in the applied field. Hence, differences in energy spacings of NMR-sensitive nuclei will depend solely on the identity of the nucleus and its environment. In general, the energy spacings between permissible nuclear orientations, under usable external magnetic field strengths, are of the same magnitude as the energy associated with radiation in the radio frequency range.

6.4 ENERGY-LEVEL TRANSITIONS IN SPECTROSCOPY

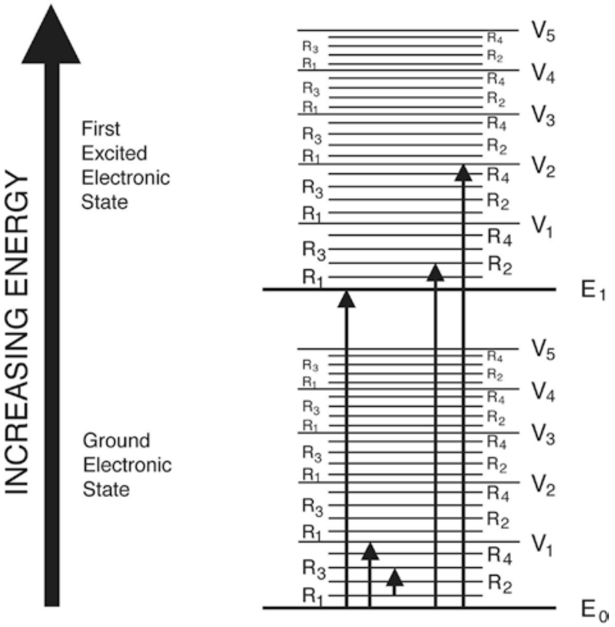
6.4.1 Absorption of Radiation

The *absorption of radiation* by an atom or molecule is that process in which energy from a photon of electromagnetic radiation is transferred to the absorbing species. When an atom or molecule absorbs a photon of light, its internal energy increases by an amount equivalent to the amount of energy in that particular photon. Therefore, in the process of absorption, the species goes from a lower energy state to a more *excited state*. In most cases, the species is in the *ground state* prior to absorption. Since the absorption process may be considered quantitative (i.e., all of the photon's energy is transferred to the absorbing species), the photon being absorbed must have an energy content that exactly matches the energy difference between the energy levels across which the transition occurs. This must be the case due to the quantized energy levels of matter, as discussed previously. Consequently, if one plots photon energy versus the relative absorbance of radiation uniquely composed of photons of that energy, one observes a characteristic *absorption spectrum*, the shape of which is determined by the relative absorptivity of photons of different energy. The *absorptivity* of a compound is a wavelength-dependent proportionality constant that relates the absorbing species concentration to its experimentally measured absorbance under defined conditions. A representative absorption spectrum covering a portion of the UV radiation range is presented in Fig. 6.6. The independent variable of an absorption spectrum is most commonly expressed in terms of the wave properties (wavelength, frequency, or wave numbers) of the radiation, as in Fig. 6.6, rather than the energy of the associated photons.



6.6 figure

Absorption spectrum of a 0.005 *M* benzene in water solution



6.7 figure

Partial molecular energy-level diagram including electronic, vibrational, and rotational transitions

Various molecular transitions resulting from the absorption of photons of different energy are shown schematically in Fig. 6.7. The transitions depicted represent those that may be induced by absorption of UV, Vis, IR, and microwave radiation. The figure also includes transitions in which the molecule is excited from the ground state to an exited electronic state with a simultaneous change in its vibrational or rotational energy levels. Although not shown in the figure, the absorption of a photon of appropriate energy also may

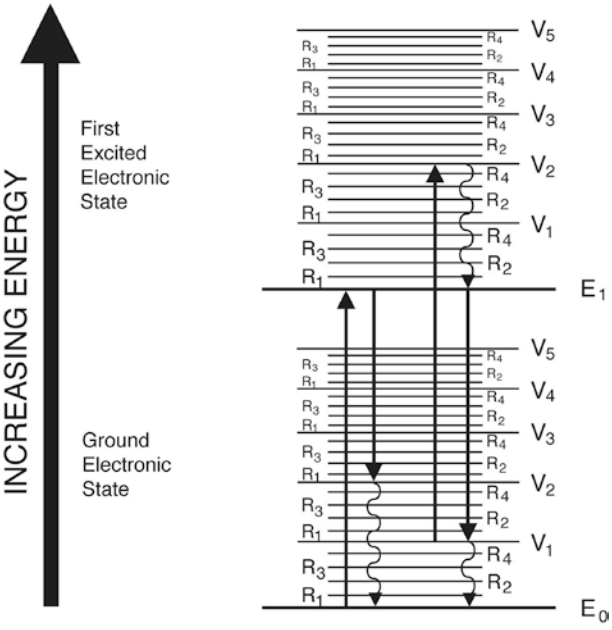
6.2 table Wavelength regions, spectroscopic methods, and associated transitions

Wavelength region	*Wavelength limits*	*Type of spectroscopy*	*Usual wavelength range*	*Types of transitions in chemical systems with similar energies*
Gamma rays	0.01–1 Å	Emission	<0.1 Å	Nuclear proton/neutron arrangements
X-rays	0.1–10 nm	Absorption, emission, fluorescence, and diffraction	0.1–100 Å	Inner-shell electrons
Ultraviolet	10–380 nm	Absorption, emission, and fluorescence	180–380 nm	Outer-shell electrons in atoms, bonding electrons in molecules
Visible	380–750 nm	Absorption, emission, and fluorescence	380–750 nm	Same as ultraviolet
Infrared	0.075–1000 μm	Absorption	0.78–300 μm	Vibrational position of atoms in molecular bonds
Microwave	0.1–100 cm	Absorption	0.75–3.75 mm	Rotational position in molecules
		Electron spin resonance	3 cm	Orientation of unpaired electrons in an applied magnetic field
Radio wave	1–1000 m	Nuclear magnetic resonance	0.6–10 m	Orientation of nuclei in an applied magnetic field

cause simultaneous changes in electronic, vibrational, and rotational energy levels. The ability of molecules to have simultaneous transitions between the different energy levels tends to broaden the peaks in the UV-Vis absorption spectrum of molecules relative to those peaks observed in the absorption spectrum of atoms. This would be expected when one considers that vibrational and rotational energy levels are absent in an atomic energy-level diagram. The depicted transitions between vibrational energy levels, without associated electronic transitions, are induced by radiation in the IR region. Independent transitions between allowed rotational energy levels also are depicted, these resulting from the absorption of photons of microwave radiation. A summary of transitions relevant to atomic and molecular absorption spectroscopy, including corresponding wavelength regions, is presented in Table 6.2.

6.4.2 Emission of Radiation

Emission is essentially the reverse of the absorption process, occurring when energy from an atom or molecule is released in the form of a photon of radiation. A molecule raised to an excited state will typically remain in the excited state for a very short period of time before relaxing back to the ground state. There are several *relaxation processes* through which an excited molecule may dissipate energy. The most common relaxation process is for the excited molecule to dissipate its energy through a series of small steps brought on by collisions with other molecules. The energy is thus converted to kinetic energy, the net result being the dissipation of the energy as heat. Under normal conditions, the dissipated heat is not enough to measurably affect the system. In some cases, molecules excited by the absorption of UV or Vis light will lose a portion of their excess energy through the emission of a photon. This emission process is referred to as either *fluorescence* or *phosphorescence*, depending on the nature of the excited state. In molecular fluorescence spectroscopy, the photons emitted from the excited species generally will be of lower energy and longer wavelength than the corresponding photons that were absorbed in the excitation process. The reason is that, in most cases, only a fraction of the energy difference between the excited and ground states is lost in the emission process. The other fraction of the excess energy is dissipated as heat during vibrational relaxation. This process is depicted in Fig. 6.8, which illustrates that the excited species undergoes vibrational relaxation down to the lowest vibrational energy level within the excited electronic state, and then undergoes a transition to the ground electronic state through the emission of a photon. The photon emitted will have an energy that equals the energy difference between the lowest vibrational level of the excited electronic state and the ground electronic state level it descends to. The fluorescing molecule may descend to any of the vibrational levels within the ground electronic state. If the fluorescence transition is to an excited vibrational level within the ground electronic state, then it will quickly return to the ground state (lowest energy



6.8 figure Partial molecular energy-level diagram including absorption, vibrational relaxation, and fluorescence relaxation

level) via vibrational relaxation. In yet other cases, an excited species may be of sufficient energy to initiate some type of photochemistry that ultimately leads to a decrease in the system's potential energy. In all cases, the relaxation process is driven by the tendency for a species to exist at its lowest permissible internal energy level. The relaxation process that dominates a system will be the one that minimizes the lifetime of the excited state. Under normal conditions, the relaxation process is so rapid that the population of molecules in the ground state is essentially unchanged.

6.4.3 Population of Energy Levels

The preceding text discussed the existence and quantum nature of molecular, atomic, and nuclear energy levels. It is now relevant to ask how a population of particles is likely to be distributed among their permissible energy levels, i.e., the relative population of the different energy levels. This is important to consider because the intensity of the signal generated in a spectroscopic method is a function of the number of particles in the energy level corresponding to the origin of the signal. For example, when doing traditional molecular absorption spectroscopy, one is measuring the excitation of molecules in the ground state (Chap. 7); when doing atomic emission spectroscopy, one is measuring photons emitted by atoms in an excited state (Chap. 9). In the former case, the observed signal will be a function of the number of molecules in the ground state; in the latter case the signal will be a function of the number of molecules in the appropriate excited state. For a given collection of particles, the relative population of the different energy levels is described by the Boltzmann distribution. The *Boltzmann distribution* is a probability distribution or frequency distribution; when applied to a group of particles, it describes the average number of particles to be found in the different energy levels available to those particles (assuming the system is in thermal equilibrium). The Boltzmann distribution law may be expressed as follows:

$$\left(p' / p\right) = e^{-(E'-E)/kT} \tag{6.5}$$

where:

p' = probability of finding particle in energy level E'
p = probability of finding particle in energy level E
E' = energy corresponding higher energy level
E = energy corresponding to lower energy level
k = Boltzmann constant
T = absolute temperature

The equation indicates that the fraction of molecules in the higher energy state (E') decreases exponentially with increasing ΔE (i.e., $E'-E$). In UV-Vis spectroscopy, the vast majority of the molecules are in the ground state since the energy difference between the ground state and the first excited state is relatively large. In nuclear magnetic resonance spectroscopy, the populations in the two energy states are nearly identical due to the relatively small energy difference between the lower and higher energy states (the lower energy state being slightly more populated). These relationships are consistent with UV-Vis spectroscopy being significantly more sensitive than nuclear magnetic resonance spectroscopy. The equation also illustrates that increasing the temperature of a system will increase the fraction of molecules in the higher energy state. This is relevant to atomic emission spectroscopy where molecules in the excited state are emitting the detected signal. At room temperature there are insufficient neutral atoms in the excited state to do atomic emission spectroscopy. However, as one continues to raise the temperature of the analyte mixture, the fraction of atoms in the excited state increases to the point that atomic emission spectroscopy becomes feasible.

6.5 SUMMARY

Spectroscopy deals with the interaction of electromagnetic radiation with matter. Spectrochemical analysis, a branch of spectroscopy, encompasses a wide range of techniques used in analytical laboratories for the qualitative and quantitative analysis of the chemical composition of foods. Common spectrochemical analysis methods include UV, Vis, and IR absorption spectroscopy, molecular fluorescence spectroscopy, and NMR spectroscopy. In each of these methods, the analyst attempts to measure the amount of radiation either absorbed or emitted by the analyte. All of these methods make use of the facts that the energy content of matter is quantized and that photons of radiation may be absorbed or emitted by matter if the energy associated with the photon equals the energy difference for allowed transitions of that given species. The above methods differ from each other with respect to the radiation wavelengths used in the analysis or the molecular vs. atomic nature of the analyte.

6.6 STUDY QUESTIONS

1. Which phenomena associated with light are most readily explained by considering the wave nature of light? Explain these phenomena based on your understanding of interference.
2. Which phenomena associated with light are most readily explained by considering the particulate nature of light? Explain these phenomena based on your understanding of the quantum nature of electromagnetic radiation.
3. What does it mean to say that the energy content of matter is quantized?
4. Molecular absorption of radiation in the UV-Vis range results in transitions between what types of energy levels?
5. Molecular absorption of radiation in the IR range results in transitions between what types of energy levels?
6. Why is an applied magnetic field necessary for NMR spectroscopy?
7. How do the allowed energy levels of molecules differ from those of atoms? Answer with respect to the energy-level diagram depicted in Fig. 6.5.
8. In fluorescence spectroscopy, why is the wavelength of the emitted radiation longer than the wavelength of the radiation used for excitation of the analyte?

RESOURCE MATERIALS

- Atkins P, de Paulo J (2012) Elements of physical chemistry 6th ed, W.H. Freeman, New York
- Ball DW (2001) The basics of spectroscopy. Society of Photo-optical Instrumentation Engineers, Bellingham, WA
- Currell G (2000) Analytical instrumentation – performance characteristics and quality. Wiley, New York, pp 67–91
- Duckett 2 (2000) Foundations of spectroscopy. Oxford University Press, New York
- Harris DC (2015) Quantitative chemical analysis, 9th edn. WH Freeman, New York
- Harris DC, Bertolucci MD (1989) Symmetry and spectroscopy. Dover, Mineola, NY
- Harwood LM, Claridge TDW (1997) Introduction to organic spectroscopy. Oxford University Press, New York
- Ingle JD Jr, Crouch SR (1988) Spectrochemical analysis. Prentice Hall, Englewood Cliffs, NJ
- Meyers RA (ed) (2000) Encyclopedia of analytical chemistry: applications, theory, and instrumentation. 5, 2857–4332
- Milton Roy educational manual for the SPECTRONIC® 20 & 20D spectrophotometers (1989) Milton Roy Co., Rochester, NY
- Pavia DL, Lampman GM, Kriz GS Vyvyan JA (2015) Introduction to spectroscopy. 5th Edition, Cengage Learning, Independence, KY
- Robinson JW, Frame EMS, Frame GM II (2014) Undergraduate instrumental analysis. 7th edn. Marcel Dekker, New York
- Young HD, Freedman RA (2011) Sears and Zemansky's university physics, vol. 2, 13th edn. Addison-Wesley, Boston
- Skoog DA, Holler FJ, Crouch SR (2007) Principles of instrumental analysis, 6th edn. Brooks/Cole, Pacific Grove, CA