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Introduction to Infrared Spectroscopy

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1.1 Introduction

Infrared spectroscopy is a useful tool for molecular structural studies, identification, and quantitative analyses of materials. The advantage of this technique lies in its wide applicability to various problems in both the condensed phase and gaseous state. As described in the later chapters of this book, infrared spectroscopy is used in chemical, environmental, life, materials, pharmaceutical, and surface sciences, as well as in many technological applications. The purpose of this book is to provide readers with a practical guide to the experimental aspects of this versatile method.

In this chapter, introductory explanations are given on an infrared absorption spectrum and related basic subjects, which readers should understand before reading the later chapters, on the assumption that the readers have no preliminary knowledge of infrared spectroscopy.

As is well known, visible light is absorbed by various materials and the absorption of visible light is associated with the colors of materials. Blue materials absorb radiation with a red color, and red materials absorb radiation with a blue color. The wavelengths of radiation with a red color are longer than those with a blue color. A diagram showing quantitatively the absorption of visible light at different wavelengths from violet to red is called a visible absorption spectrum. The visible absorption spectrum closely reflects the color of the material from which the spectrum is measured.

The wavelengths of infrared radiation are longer than those of radiation with red color. Radiation with red color has the longest wavelengths among visible light, the wavelength of which increases from violet to red. Infrared radiation, though not detectable by human eyes, is absorbed by almost all materials. An infrared spectrum is a plot quantitatively showing the absorption of infrared radiation against the wavelength of infrared radiation.
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It is usually possible to observe an infrared absorption spectrum from any material except metals, regardless of whether the sample is in the gaseous, liquid, or solid state. This advantage makes infrared spectroscopy a most useful tool, utilized for many purposes in various fields.

Measurements of infrared spectra are mostly done for liquid and solid samples. In the visible absorption spectra of liquids and solids, only one or two broad bands are typically observed but infrared absorption spectra show at least several, often many relatively sharp absorption bands. Most organic compounds have a significant number of infrared absorption bands. This difference between the visible and infrared absorption spectra is due to the different origins for the two kinds of spectra. Visible absorption is associated with the states of electrons in a molecule. By contrast, infrared absorptions arise from the vibrational states of atoms in a molecule. In other words, the visible absorption spectrum is an electronic spectrum and the infrared spectrum is a vibrational spectrum. Vibrational motions of atoms in a molecule are called molecular vibrations.

At present, measurements of infrared spectra are widely performed in materials science, life science, and surface science. In these fields, the states of targets of research are usually liquids or solids. This book primarily aims at describing the fundamentals of infrared spectroscopy and practical methods of measuring infrared spectra from various samples in the liquid and solid states.

1.2 Fundamentals of Infrared Spectroscopy

A basic knowledge of infrared spectroscopy that readers should have before performing infrared measurements is briefly described in this section.

1.2.1 The Ordinate and Abscissa Axes of an Infrared Spectrum

It has been known for a long time that vapors, liquids, crystals, powder, glass, and many other substances absorb infrared radiation. The wavelength region of infrared radiation is not strictly defined but the wavelength regions generally accepted for near-infrared, mid-infrared, and far-infrared radiation are as follows: 700 nm to 2.5 μm for near-infrared, 2.5–25 μm for mid-infrared, and 25 μm to 1 mm for far-infrared.

The absorption intensity is taken as the ordinate axis of an infrared spectrum. The wavelength can be used as the abscissa axis of an infrared spectrum. At present, however, it is customary, in the mid-infrared region in particular, to use the wavenumber as the abscissa axis instead of the wavelength. The wavenumber is the number of light waves per unit length (usually 1 cm) and corresponds to the reciprocal of the wavelength. The wavenumber used as the abscissa axis of an infrared spectrum is always expressed in units of cm\(^{-1}\). In this book, the abscissa axis of an infrared spectrum is always designated as “Wavenumber/cm\(^{-1}\).” It should be mentioned, however, that the wavelength is often used as the abscissa axis in the near-infrared region, if a near-infrared spectrum is measured as an extension of a visible absorption spectrum.

There are publications in which the higher wavenumber (corresponding to the shorter wavelength) is placed on the left side of a spectrum, whereas it is placed on the right side in other cases. This inconsistency has occurred because infrared spectra published
before the 1950s used the wavelength as the abscissa axis and placed the longer wavelength (corresponding to the lower wavenumber) on the right side. Following this tradition, many infrared spectra published since the 1960s also have placed the higher wavenumber on the left side and the lower wavenumber on the right side. In recent years, however, infrared spectra in publications which feature the direction of the abscissa axis oppositely have been increasing in number.

The wavenumber, which is the number of light waves per centimeter as mentioned above, corresponds to the frequency divided by the speed of light. Therefore, the wavenumber is proportional to the energy $E$ of a photon as expressed in the following equation:

$$E = h\tilde{\nu}$$

where $h$ is the Planck constant, $c$ the speed of light, and $\tilde{\nu}$ the wavenumber of infrared radiation. This proportionality between $E$ and $\tilde{\nu}$ is the reason why the wavenumber is now used as the abscissa axis of an infrared spectrum. In Appendix A relations closely associated with Equation (1.1) are explained in detail.

The above-mentioned wavelength regions of infrared radiation correspond to the wavenumber regions of about $14000–4000\text{ cm}^{-1}$ for near-infrared, $4000–400\text{ cm}^{-1}$ for mid-infrared, and $400–10\text{ cm}^{-1}$ for far-infrared.

The wavenumber region of $400–10\text{ cm}^{-1}$ for far-infrared corresponds to the frequency region of $(12 - 0.3) \times 10^{12}\text{ Hz}$ or $12 - 0.3\text{ THz}$. This means that the far-infrared region approximately coincides with the terahertz frequency region. For this reason, the term terahertz spectroscopy is recently being increasingly used in place of far-infrared spectroscopy. However, the term far-infrared spectroscopy is considered a better designation because of its consistency with other optical spectroscopies.

1.2.2 The Intensity of Infrared Radiation

As infrared radiation is an electromagnetic wave, electromagnetic theory is applicable to it. In this theory, the intensity of an electromagnetic wave irradiating an area is defined as the average energy of radiation per unit area per unit time. In this book, according to the tradition of spectroscopy, the term intensity is used for this quantity. It is worth pointing out, however, that the term irradiance is increasingly used in other fields instead of “intensity.” This quantity is given in units of $\text{W m}^{-2}$ (= $\text{J s}^{-1} \text{ m}^{-2}$), although its absolute value is rarely discussed in infrared spectroscopy except when lasers are involved. The intensity $I$ is proportional to the time average of the square of the amplitude of the electric field $E$. In vacuum, $I$ is expressed as

$$I = \varepsilon_0 c_0 \langle E^2 \rangle_t$$

where $\varepsilon_0$ and $c_0$ denote, respectively, the electric constant and the speed of light in vacuum, and the symbol $\langle \rangle_t$ means time average. This relationship will be mentioned later in Section 1.2.4.

1.2.3 Lambert–Beer’s Law

Let us consider the absorption of infrared radiation which occurs when an infrared beam passes through a sample layer. As shown in Figure 1.1, a collimated infrared beam with
intensity $I_0$ at wavenumber $\tilde{\nu}$ irradiates a sample with thickness $l$ at right angles to its surface. If the sample is transparent to the infrared beam, the infrared beam passes through the sample without losing its intensity. Here, reflection of the infrared beam at the surface of the sample is not considered. If the sample absorbs the infrared radiation of wavenumber $\tilde{\nu}$, the infrared intensity decreases as the beam passes through the sample. If the amount of the absorption by the thin layer $dl$ in Figure 1.1 is expressed by $-dI$ (the minus sign reflects the fact that $dl$ is a negative quantity corresponding to an intensity decrease), the following equation holds.

$$-dI = \alpha dl$$ \hspace{1cm} (1.3)

where $\alpha$ is a proportionality constant representing the magnitude of absorption (called the absorption coefficient) and $I$ is the intensity of the beam entering the thin layer $dl$. Integration of Equation (1.2) gives the following equation.

$$\ln I = -\alpha l + a$$ \hspace{1cm} (1.4)

where the integration constant $a$ must be equal to $\ln I_0$ ($I_0$ is the intensity at $l = 0$). Then, the following two equations are derived.

$$\ln \left(\frac{I_0}{I}\right) = \alpha l$$ \hspace{1cm} (1.5)

$$I = I_0 \exp(-\alpha l)$$ \hspace{1cm} (1.6)

It should be remembered that each of $I_0$, $I$, and $\alpha$ is a function of $\tilde{\nu}$ and, strictly speaking, should be expressed, respectively, as $I_0(\tilde{\nu})$, $I(\tilde{\nu})$, and $\alpha(\tilde{\nu})$. Equation (1.5) means that the absorption intensity expressed as $\ln(I_0/I)$ is proportional to the thickness of the sample. This relation is known as Lambert’s law. The quantity $\ln(I_0/I)$ is called absorbance (denoted by $A$) or optical density (OD). The quantity $I/I_0$ expressed in a percentage scale is called transmittance (“transmission factor” is also recommended by IUPAC [1]). It is also used to express the absorption intensity. The absorption intensity expressed in either absorbance or transmittance is taken as the ordinate axis of an infrared spectrum.

If the sample is a solution, the absorption coefficient $\alpha$ in Equations (1.3)–(1.6) should be replaced by $\varepsilon c_s$, where $\varepsilon$, a function of $\tilde{\nu}$, is a proportionality constant and $c_s$ is the concentration of a solute in the solution. This means that the absorbance is proportional to both the thickness (sometimes called the cell pathlength) of the solution and the concentration of the solute. This relation, known as Lambert–Beer’s law, holds for most dilute
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solutions, but deviations from this law may occur in various cases, particularly in concentrated solutions (see Section 3.6.5). In practice, the natural (or Napierian) logarithm in Equation (1.5) is often replaced by the common (or decadic) logarithm, as will be described in Section 3.4.1. The relation that the absorbance is proportional to the concentration of the solute is called Beer’s law.

1.2.4 Complex Refractive Index

The relation in Equation (1.6) can also be derived in the following way. The electric field $E$ of an electromagnetic wave (or an infrared beam) traveling in the $x$ direction in vacuum may be expressed as

$$E = A \exp \left( \frac{x}{\lambda} - vt \right)$$  \hspace{1cm} (1.7)

where $A$ is a vector representing the amplitude of the light wave, $v$ the frequency of the light wave, $t$ time, and $\lambda$ the wavelength of the light wave. In Appendix B the meaning of the right-hand side of Equation (1.7) (and a closely related form of $A \exp 2\pi i(\nu t - x/\lambda)$) is discussed in more detail.

If the light wave travels in a medium other than vacuum, it is necessary to introduce the complex refractive index $\hat{n}$ defined as

$$\hat{n} = n + ik$$  \hspace{1cm} (1.8)

where $n$ is the (real) refractive index, and $k$, which is called the absorption index or the imaginary refractive index, is a constant to express the absorption of light by the medium. The wavelength $\lambda$ in the medium is related to the wavelength $\lambda_0$ in vacuum by the equation $\lambda = \lambda_0/\hat{n}$. By substituting $\lambda_0/\hat{n}$ for $\lambda$ in Equation (1.7), the following equation is derived.

$$E = A \exp \left( -\frac{2\pi kx}{\lambda_0} \right) \exp 2\pi i \left( \frac{nx}{\lambda_0} - vt \right)$$  \hspace{1cm} (1.9)

As is clear from Equation (1.9), the amplitude of the light wave decreases in proportion to the factor $\exp \left( -\frac{2\pi kl}{\lambda_0} \right)$. Since the intensity is proportional to the square of the amplitude of the electric field, the ratio of the intensity $I$ at $x = l$ to $I_0$ at $x = 0$ is given by the following equation.

$$\frac{I}{I_0} = \left[ |A| \exp(-2\pi kl/\lambda_0) \right]^2$$

$$= \exp \left( -\frac{4\pi kl}{\lambda_0} \right)$$  \hspace{1cm} (1.10)

If $4\pi k/\lambda_0$ in Equation (1.10) is equated with $\alpha$, Equation (1.10) is identical with Equation (1.6). In some literature, the complex refractive index is defined as $\hat{n} = n - ik$. In this case, the right side of Equation (1.7) should be given as $E = A \exp 2\pi i(\nu t - x/\lambda)$.

The complex refractive index is an important quantity. It shows that refraction and absorption are closely related with each other and these should always be treated as a pair. It may be said that the purpose of experimental spectroscopy is to determine quantitatively the real and imaginary parts of the complex refractive index for any material. However, this
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Purpose is not easy to fulfill, because it is experimentally difficult to separate absorption from reflection (and refraction) completely. For example, a cell is usually used to measure a transmission infrared spectrum from a liquid or solution. In this case, reflection occurs at the cell window surfaces, making the determination of $I_0$ difficult. If the sample is a dilute solution, this problem may be solved by using a cell containing solvent only and measuring the intensity of infrared radiation transmitted from this cell. The intensity measured in this way may be used as $I_0$. There is no convenient, reliable method applicable to concentrated solutions, liquids, solid films, and so on. In most practical applications, however, measurements of absorption in a qualitative manner give useful information, so that the quantitative determination of the complex refractive index is usually set aside.

1.2.5 Signal-to-Noise Ratio

Here, mention is made of the measure of rating the quality of an observed spectrum. The purpose of spectral measurements is to determine the quantity of the radiation absorbed, reflected, or emitted by the sample. This quantity is called the signal. In practice, the signal is always accompanied by noise arising from various sources. The magnitudes of the signal and noise are usually denoted by $S$ and $N$, respectively. The signal-to-noise ratio of an observed band, which is often abbreviated as the $S/N$ ratio, SN ratio, or SNR, is used to rate the quality of an observed spectrum; that is, a spectrum with a higher signal-to-noise ratio has a higher quality.

1.3 Origin of Infrared Absorption

According to quantum mechanics, a molecule has discrete energy levels for electronic motions, molecular vibrations, and molecular rotations. If the molecule is irradiated by electromagnetic waves ranging from ultraviolet light to microwaves, the molecule absorbs the energies of the electromagnetic waves and undergoes a transition from a state of a lower energy to another state of a higher energy. Such a transition by absorbing the energy of an electromagnetic wave (or a photon) must satisfy certain conditions. The energy of a photon given in Equation (1.1) should coincide with the energy difference between an energy level of the molecule (usually the ground-state level) and a higher energy level (an excited-state level). In addition to this requirement for the coincidence of energy, whether the transition in the molecule occurs by interaction with the electromagnetic wave is governed by specific rules based on quantum mechanics and group theory, which are called selection rules [2–4]. Due to the selection rules, transitions in a molecule are grouped into allowed and forbidden cases, and only allowed transitions give rise to absorptions of the electromagnetic waves including infrared radiation.

Almost all infrared absorptions arise from the transitions between the energy levels of molecular vibrations. In this sense, infrared absorption spectra, together with Raman spectra and neutron inelastic scattering spectra, constitute vibrational spectra. Infrared absorption spectra observed from gases are accompanied by fine structures due to the transitions associated with rotational energy levels. As a result, vibration—rotation spectra are observed from gaseous samples. In liquids and solids, free rotation of molecules
does not occur, so that infrared spectra observed from liquids and solids are “pure” vibrational spectra.

Infrared absorption occurs by electric interaction of molecules with infrared radiation. If the dipole moment of a molecule changes with a molecular vibration, infrared radiation with the frequency equal to the frequency of the molecular vibration is absorbed by the molecule. In quantum mechanical terms, a molecular vibration has energy levels specified by the vibrational quantum number \( v \), and usually the transition from the ground vibrational state \( (v = 0) \) to the first excited vibrational state \( (v = 1) \) occurs with an infrared absorption. In other words, the molecule is vibrationally excited by absorbing the energy of infrared radiation. The absorption arising from the \( \nu = 0 \) to \( \nu = 1 \) transition is called the fundamental tone. Overtones correspond to the transitions from \( \nu = 0 \) to \( \nu = 2, 3, 4, \ldots \), but the probabilities for these transitions are small. Generally, the overtone absorptions are much weaker in intensity than the fundamental absorption. It should be mentioned, however, that near-infrared absorptions arise from either overtones or combination tones, the latter being transitions from the ground state to excited vibrational states involving two or more vibrations of a polyatomic molecule. Absorptions corresponding to transitions between excited vibrational states are called hot bands. Unless the temperature of the sample is very high, hot bands are not observed.

1.4 Normal Vibrations and Their Symmetry

If an atom in a molecule is displaced from its equilibrium position, a force is exerted on the atom to help it restore to its equilibrium position. This restoring force is closely approximated by the Hooke’s-law force in most cases; the restoring force is proportional to the displacement in magnitude and works in the direction of decreasing the displacement. A vibration in such a force field (harmonic force field) is called a harmonic vibration. A molecule consisting of \( N \) atoms has \((3N - 6)\) degrees of vibrational freedom \((3N - 5)\) for a linear molecule. Molecular mechanics shows that there are \((3N - 6)\) or \((3N - 5)\) molecular vibrations which are independent of each other and have no contribution from either the translation or rotation of the molecule as a whole. These are called normal vibrations. The frequencies and patterns of normal vibrations can be calculated if the molecular structure and force constants are known [3–5]. At present, such calculations are performed by using an appropriate program package of quantum chemical computations [6].

If a molecule has any symmetry, its normal vibrations are classified by the symmetry. To discuss in detail the relationship between molecular symmetry and normal vibrations, group theoretical analysis is required. Each molecule belongs to one of about 20 point groups. Each point group has symmetry species specified by symmetry operations, and normal vibrations are classified into symmetry species. Whether or not the normal vibrations of a molecule belonging to a symmetry species of a point group have possibilities of absorbing infrared radiation is determined by group theory. If a normal vibration has a possibility of absorbing infrared radiation, it is called an infrared-active vibration (or mode). In other words, it is an allowed case and gives rise to an infrared absorption. If a normal vibration has no such possibility, it is an infrared-inactive vibration; it is forbidden in infrared absorption.
In most applications of infrared spectroscopy, materials to be studied seldom contain molecules of high symmetry. It may therefore seem that the group theoretical analysis is of little value in practice. However, many molecules have substructures which are nearly symmetric. It may be worth pointing out that the group theoretical analysis helps understand the spectral feature due to the vibrations occurring mainly in such a substructure.

Normal vibrations form a solid basis for understanding molecular vibrations. It should be remembered, however, that they are conceptual entities in that they are derived from the harmonic approximation which assumes a harmonic force field for molecular vibrations. Deviations from this approximation (i.e., deviations from Hooke’s law) exist in real molecules, and the energy levels of a molecular vibration are determined by not only the harmonic term but also higher-order terms (anharmonicities) in the force field function. Although the effects of anharmonicities on molecular vibrational frequencies are relatively small in most molecules, normal (vibrational) frequencies derived in the harmonic approximation do not completely agree with observed frequencies of fundamental tones (fundamental frequencies). However, a fundamental frequency is frequently treated as a normal frequency on the assumption that the difference between them must be negligibly small.

1.5 Group Vibrations and Characteristic Absorption Bands

In theory, a normal vibration involves vibrational motions of all atoms in a molecule. In many cases, however, the contribution of a vibration localized within a particular group of atoms in a molecule is dominant in a normal vibration. Such a vibration is called a group vibration or a characteristic vibration (of the group). The frequency of a group vibration, being essentially free from the effect of neighboring groups, occurs within a relatively narrow range. If an absorption due to such a group vibration has a high intensity, it is called a characteristic absorption band, which indicates the presence of the group. Some representative group vibrations and the approximate wavenumbers of the infrared absorption bands arising from them are listed in Table 1.1. The characteristic absorption bands provide clues for identifying compounds or their substructures by infrared spectroscopy [7–9].

1.6 Brief History of Infrared Spectroscopy

In this section, how infrared spectrometry (the method of measuring infrared spectra) has been developed since the beginning of the twentieth century is briefly described. Further information may be found elsewhere [10].

1.6.1 Before the Mid-1960s

Development of a reliable method of measuring infrared spectra was an important subject of research in physics in the beginning of the twentieth century. William W. Coblentz (1873–1962) made a major contribution to the instrumentation of early infrared spectrometers and the compilation of the infrared spectra of many organic compounds in the period before 1930. At that time, alkali halide crystals were used as the prism for dispersing infrared radiation.
### Table 1.1  Group vibrations and their characteristic absorption wavenumber.

<table>
<thead>
<tr>
<th>Group vibration</th>
<th>Classification</th>
<th>Wavenumber/cm⁻¹</th>
</tr>
</thead>
<tbody>
<tr>
<td>OH stretch</td>
<td>Free</td>
<td>3600</td>
</tr>
<tr>
<td></td>
<td>H-bonded</td>
<td>3000–2500</td>
</tr>
<tr>
<td>CH stretch</td>
<td>Olefin</td>
<td>3080</td>
</tr>
<tr>
<td></td>
<td>Methyl</td>
<td>2960, ~2870</td>
</tr>
<tr>
<td></td>
<td>Methylene</td>
<td>2925, ~2850</td>
</tr>
<tr>
<td>SH stretch</td>
<td></td>
<td>2600–2550</td>
</tr>
<tr>
<td>C=O stretch</td>
<td>Acyl chloride</td>
<td>1810</td>
</tr>
<tr>
<td></td>
<td>Ester</td>
<td>1735</td>
</tr>
<tr>
<td></td>
<td>Aliphatic aldehyde</td>
<td>1730</td>
</tr>
<tr>
<td></td>
<td>Aliphatic ketone</td>
<td>1715</td>
</tr>
<tr>
<td></td>
<td>Aromatic aldehyde</td>
<td>1705</td>
</tr>
<tr>
<td></td>
<td>Carboxylic acid</td>
<td>1700</td>
</tr>
<tr>
<td></td>
<td>Amide (peptide)</td>
<td>1700–1630</td>
</tr>
<tr>
<td></td>
<td>Aromatic ketone</td>
<td>1690</td>
</tr>
<tr>
<td></td>
<td>Quinone</td>
<td>1670</td>
</tr>
<tr>
<td>Benzene ring stretch</td>
<td></td>
<td>1610–1590</td>
</tr>
<tr>
<td>CCl stretch</td>
<td>RCH₂Cl</td>
<td>760–700 or 690–650</td>
</tr>
<tr>
<td></td>
<td>R₁R₂CHCl</td>
<td>700–670 or 640–600</td>
</tr>
<tr>
<td></td>
<td>R₁R₂R₃CCl</td>
<td>640–610 or 580–550</td>
</tr>
<tr>
<td>CH₃ bend</td>
<td>Asymmetric or degenerate</td>
<td>1460</td>
</tr>
<tr>
<td></td>
<td>Symmetric</td>
<td>1380</td>
</tr>
<tr>
<td>CH₂ bend</td>
<td>Scissor</td>
<td>1450</td>
</tr>
<tr>
<td>CH out-of-plane bend</td>
<td>RHC=CH₂</td>
<td>990, ~910</td>
</tr>
<tr>
<td></td>
<td>RHC=CHR (trans)</td>
<td>960</td>
</tr>
<tr>
<td></td>
<td>R₁R₂C=CH₂</td>
<td>890</td>
</tr>
<tr>
<td></td>
<td>R₁R₂C=CHR₃</td>
<td>820</td>
</tr>
<tr>
<td></td>
<td>Monosubstituted benzene</td>
<td>740</td>
</tr>
<tr>
<td></td>
<td>Disubstituted benzene (o-)</td>
<td>750</td>
</tr>
<tr>
<td></td>
<td>Disubstituted benzene (p-)</td>
<td>800</td>
</tr>
</tbody>
</table>

During World War II, great progress was made in infrared-related technology, particularly in electronics and detectors. This resulted in the commercial production of recording infrared spectrophotometers. In the postwar period, the recording infrared spectrophotometer soon became an instrument indispensable for chemical research in not only universities but also research laboratories of industrial companies. In recognition of Coblentz’s early contributions to infrared spectroscopy as well as to foster the understanding and application of infrared spectroscopy, the Coblentz Society was formed in 1954 in USA. This Society is still active and now has members from all over the world. In the mid-1950s, the use of gratings as the dispersive element began, and gratings replaced prisms by the mid-1960s.

#### 1.6.2 After the Mid-1960s

Spectrometry using prisms and/or gratings as the means for dispersing radiation of continuously varying wavelengths is called *dispersive spectrometry*. At present,
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this type of spectrometry is not used in the infrared region (particularly in the mid-infrared region), except in special cases (see Section 1.6.3). Instead, interferometric (or interferometer-based) spectrometry is common in the infrared, and it is usually referred to as Fourier transform infrared (FT-IR) spectrometry, because the Fourier transform of an interferogram measured by the interferometer is an infrared spectrum. The principle of FT-IR spectrometry was established by the 1950s, but its practical use had to wait for the advent of high-speed computers, which enabled the fast Fourier transform. In the mid-1960s, the first commercial FT-IR spectrometer became available, and it was after the mid-1970s that FT-IR spectrometers became widely used. As will be discussed in Chapters 4–6 the advantages of FT-IR spectrometry over dispersive spectrometry are now well established from the viewpoint of instrumentation theory. From a practical viewpoint, the greatest advantage is the high reproducibility of observed interferograms, which ensures high S/N ratios of an observed spectrum through accumulation of the observed interferograms. As a result of this advantage, minute spectral differences of $10^{-4}$ or less in the absorbance scale between two spectra can easily be detected. In this book, most chapters deal with FT-IR spectrometry and its applications to various methods of infrared spectroscopic measurements. Only terahertz spectrometry in Chapter 19 and a large part of time-resolved infrared spectrometry in Chapter 20 are laser-based measurements. This shows how widely FT spectrometry is used at present in the measurements of vibrational spectra.

1.6.3 Future

Although it is not easy to foresee future developments in infrared spectrometry, there is a possibility of revival of dispersive spectrometry in which a grating is combined with a planar array detector. Such a spectrometer is expected to be handy and small in size, as it needs no mechanism for moving an optical component. In fact, spectrometers in this category are already being produced and may become a convenient tool for practical analysis in various fields. Finally, a completely new type of spectrometry may happen if a laser widely tunable in the infrared and easy to operate should come into existence.

References


