*Chapter 6*

# *Near-infrared spectroscopy*

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## 6.1 INTRODUCTION

The near-infrared portion of the electromagnetic spectrum is located between the visible and mid-range infrared (MIR) sections, roughly 750–2500 nm or 13,333–4000 $cm^{-1}$ (see Fig. 6.1). It consists (mainly) of overtones and combinations of the bands found in the mid-range infrared region (4000–200 $cm^{-1}$). The region was discovered by Sir William Herschel in 1800 [1]. Sir William was attempting to discover the color of light that carried the heat of sunlight. He used a glass prism to split the colors from white light and arranged a series of thermometers, wrapped in dark cloth, such that they would each be exposed to a different colored light.

Not much happened in the visible region, but as he allowed the thermometer to be located next to the red band, he noticed a dramatic

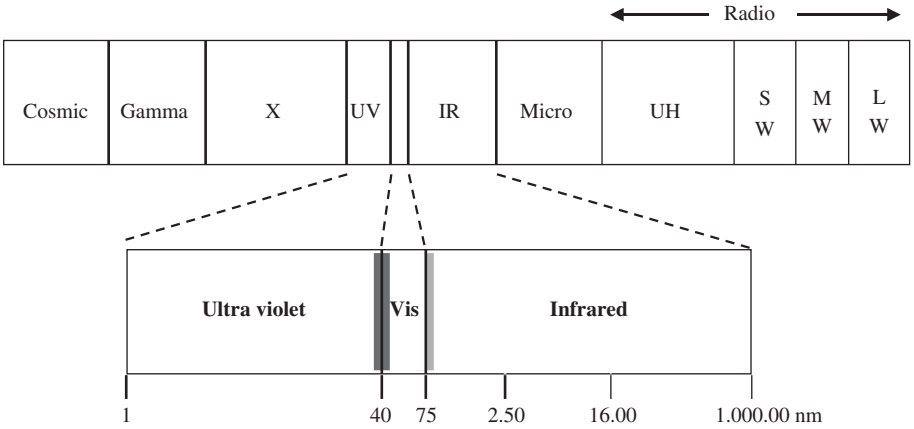


Fig. 6.1. Electromagnetic spectrum in wavelength.

*Comprehensive Analytical Chemistry 47*
S. Ahuja and N. Jespersen (Eds)
Volume 47 ISSN: 0166-526X DOI: 10.1016/S0166-526X(06)47006-9
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increase in temperature. He (correctly) assumed there was a type of light, which, while invisible to the naked eye, was capable of carrying heat. Since it was ''beyond the red'' portion, he named it ''infrared.'' The truth be told, mid-range infrared radiation does not penetrate glass (re: your car in summertime), so what he discovered was the *near*-infrared (NIR). The significance of the discovery was that it was the first evidence of ''light'' (now called electromagnetic radiation) outside the visible region.

In 1881, Abney and Festing [2], using newly developed photographic plates, recorded the spectra of organic liquids in the 1–2$\mu$ range. Inspired by this work, W. W. Coblentz built a rock salt spectrometer with a sensitive thermopile connected to a mirror galvanometer [3]. While it took a day to produce a single spectrum, he managed to produce several hundred spectra of organic compounds, publishing his results in a series of papers in 1905. The regions of the spectrum related to groups, such as –OH, became apparent, although, he discovered that no two compounds had the same spectrum.

While good, commercial instruments were not generally available, research was being performed in the near-infrared (NIR). One of the first quantitative measurements was at Mount Wilson observatory in 1912; F. E. Fowler measured the moisture in the atmosphere [4]. Later, in 1938, Ellis and Bath [5] measured the amount of water in gelatin. During the early 1940s, Barchewitz [6] performed analyses of fuels, and Barr and Harp [7] published the spectra of vegetable oils. Later in the 1940s, Harry Willis of ICI characterized polymers and used NIR to measure the thickness of polymer films. WW II emphasized the use of mid-range IR for synthetic rubber, pushing the instrument manufacturers to commercialize IR spectrometers.

In general, NIR papers did not begin in earnest until the 1970s, when commercial instruments became easily available because of the work of the US Department of Agriculture (USDA)[8–12]. Some of these developments will be discussed in Section 6.3. After the success of the USDA, food producers, chemical producers, polymer manufacturers, gasoline producers, etc. picked up the ball and ran with it. The last to become involved, mainly for regulatory reasons, are the pharmaceutical and biochemical industries.

In number of labs, the NIR is a rapid, non-destructive test. It is used (everywhere) for water determination. For the petroleum industry, it is routinely used for octane and betaine values, to determine levels of additives, and as a test for unsaturation. The polymer companies, in addition to identification, use NIR for molecular weight, cross-linking, iodine value (unsaturation) block copolymer ratios, and numerous

physical attributes. Thus, it is logical that textiles are also analyzed using NIR: sizing, coatings, heat-treatments, dyes, and blend levels (cotton, Dacron, polyester, etc.) are all measured.

In agriculture and food, NIR has been a powerful tool for decades. All shipments of grain leaving US ports are analyzed for moisture, fat, protein, and starch via NIR. Processed foods are also a prime venue for NIR: percent of fat in cheese spread, hardness of wheat, and freshness of meats are just some of the applications in food.

In pharmaceuticals, NIR is used for, of course, moisture, polymorphic (drug) forms, percent crystallinity, isomer purity, tablet/capsule assay, coating levels, evaluation of dissolution times, and numerous process tests. It is a rapid means for the Food and Drug Administration to check for counterfeit drugs, and for the Drug Enforcement Agency to ascertain what type of materials are impounded in "drug raids."

## 6.2 BASIC THEORY

In short, near-infrared spectra arise from the same source as mid-range (or "normal") infrared spectroscopy: vibrations, stretches, and rotations of atoms about a chemical bond. In a classical model of the vibrations between two atoms, Hooke's Law was used to provide a basis for the math. This equation gave the lowest or base energies that arise from a harmonic (diatomic) oscillator, namely:

$$v = 1/2\pi(k/\mu)^{1/2} \tag{6.1}$$

where $v$ is the vibrational frequency; $k$ the classical force constant and $\mu$ reduced mass of the two atoms.

This gives a reasonable approximation of the fundamental vibrational frequency of a simple diatomic molecule. Indeed, it is quite close to the average value of a two-atom stretching frequency within a polyatomic molecule. Since NIR is based upon the hydrogen-X bands within a molecule, this simplified equation would lead to reduced masses for CH, OH, and NH or 0.85, 0.89, and 0.87, respectively. It would seem, based upon these values, that there would be no differentiation among moieties. However, with actual electron donating and withdrawing properties of adjacent atoms, hydrogen bonding, and van der Waal's forces actually changing these values, spectra certainly do exist.

Since we recognize that the allowed energy levels for molecular vibrations are not a continuum, but have distinct values, the manner in which we calculate them is slightly more complex.

The energy levels are described by quantum theory and may be found by solving the time-independent Schroedinger equation by using the vibrational Hamiltonian for a diatomic molecule [13,14].

$$\frac{-h^2\delta^2\psi(X)}{2m\delta(X)} + V(X)\psi(X) = E\psi(X) \tag{6.2}$$

Solving this equation gives complicated values for the ground and excited states, as well. Using a simplified version of the equation, more "usable" levels may be discerned (here, the "echoes" of Hooke's Law are seen)

$$E_v = (v + 1/2)h/2\pi(k/\mu)^{1/2} \qquad (v = 0, 1, 2 \ldots) \tag{6.3}$$

Rewriting this equation, substituting the quantum term $hv$, the equation becomes

$$E_v = (v + 1/2)hv \qquad (v = 0, 1, 2 \ldots) \tag{6.4}$$

Polyatomic molecules, with the many layers of vibrational levels, can be treated, to a first approximation, as a series of diatomic, independent, and harmonic oscillators. This general equation may be expressed as

$$E(v_1, v_2, v_3, \ldots) = \sum_{i=1}^{3N-6} (v_i + 1/2)hv \quad (v_1, v_2, v_3, \ldots = 0, 1, 3 \ldots) \tag{6.5}$$

In a case where the transition of an energy state is from 0 to 1 in any one of the vibrational states ($v_1$,$v_2$,$v_3$, ... ), the transition is considered as *fundamental* and is allowed by selection rules. When a transition is from the ground state to $v_i = 2, 3, \ldots$, and all others are zero, it is known as an *overtone*. Transitions from the ground state to a state for which $v_i = 1$ and $v_j = 1$ simultaneously are known as *combination bands*. Other combinations, such as $v_i = 1$, $v_j = 1$, $v_k = 1$, or $v_i = 2$, $v_j = 1$, etc., are also possible. In the strictest form, overtones and combinations are not allowed, however they do appear (weaker than fundamentals) due to anharmonicity or Fermi resonance.

In practice, the harmonic oscillator has limits. In the "ideal" case, the two atoms can approach and recede with no change in the attractive force and without any repulsive force between electron clouds. In reality, the two atoms will dissociate when far enough apart, and will be repulsed by van der Waal's forces as they come closer. The net effect is the varying attraction between the two in the bond. When using a quantum model, the energy levels would be evenly spaced, making the overtones forbidden.

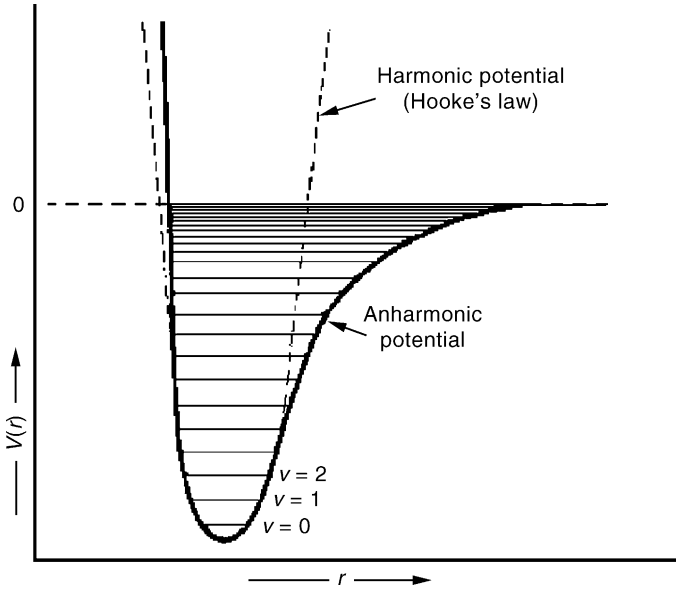


Fig. 6.2. Energy curve for Hooke's law versus Quantum Model of harmonic oscillator.

In the actual (working) model (see Fig. 6.2), the levels become closer as the vibrational number increases. It is this "anharmonicity" that allows the overtones to exist. The equation describing this phenomenon is

$$E_v = (v + 1/2)h\omega_e - (v + 1/2)^2\omega_e X_e + \text{higher terms} \tag{6.6}$$

where $\omega_e = (1/2\pi)(K_e/\mu_e)^{1/2}$ is a vibrational frequency; $\omega_e X_e$ the anharmonicity constant (this is usually between 1 and 5%); $K_e$ the harmonic force constant ($K = \sim 5 \times 10^5$ dyn/cm for single bonds, $\sim 10 \times 10^5$ dyn/cm for double bonds, and $\sim 15 \times 10^5$ dyn/cm for triple bonds); and $\mu_e$ the reduced mass of the two atoms.

Using these factors and a fundamental vibration at 3500 nm, the first overtone would be

$$n = 3500/2 + (3500 \times [0.01, 0.02, \ldots]) \tag{6.7}$$

This equation will give values from 1785 to 1925 nm. In reality, the first overtone would likely be at 3500/2 $\pm$ several nanometers, usually to a longer wavelength. The anharmonicity gives rise to varying distances between overtones. As a consequence, two overlapping peaks may be separated at a higher overtone.

To make the spectrum more complicated, *Combination Bands* also exist. These are simply two or more bands that are physically adjacent or nearby on a molecule that add or subtract their energies (in the frequency domain) to produce a new or separate band. For example, the molecule $SO_2$, according to the formula for allowed bands,

$$\#\text{bands} = 3N - 6 \tag{6.8}$$

should have three absorption bands, where $N$ are the number of atoms. Those are the symmetric stretch (at 1151 $cm^{-1}$), the asymmetric stretch (1361 $cm^{-1}$), and the O–S–O bend (519 $cm^{-1}$). These are allowed by Group Theory. However, four other bands appear in the $SO_2$ spectrum: 606, 1871, 2305, and 2499 $cm^{-1}$.

These may be explained in the following manner. One band is explained as the anharmonic overtone of the symmetric stretch at 1151 $cm^{-1}$, occurring at 2305 $cm^{-1}$, with the 3 $cm^{-1}$ difference attributed to the anharmonic constant. The other three bands may be explained as combination bands.

Since two bands may combine as $\nu_a - \nu_b$ or $\nu_a + \nu_b$ to create a new band. Using these concepts, the band assignments for $SO_2$ may be seen as [15],

| $\nu$ ($cm^{-1}$) | Assignment |
|---|---|
| 519 | $\nu_2$ |
| 606 | $\nu_1 - \nu_2$ |
| 1151 | $\nu_1$ |
| 1361 | $\nu_3$ |
| 1871 | $\nu_2 + \nu_3$ |
| 2305 | $2\nu_1$ |
| 2499 | $\nu_1 + \nu_3$ |

Any unknown (isolated) band may be deduced from first principles; unfortunately, there is considerable overlap in the NIR region, but this is where Chemometrics will be discussed. An idealized spectrum of combinations and overtones is seen in Fig. 6.3.

Another potential source of peaks in the NIR is called *Fermi resonance*. This is where an overtone or combination band interacts strongly with a fundamental band. The math is covered in any good theoretical spectroscopy text, but, in short, the two different-sized, closely located peaks tend to normalize in size and move away from one another. This leads to difficulties in "first principle" identification of peaks within complex spectra.

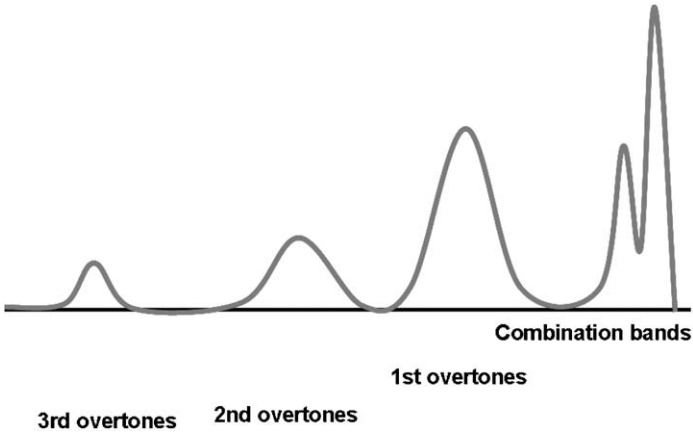


Fig. 6.3. Idealized NIR spectrum.

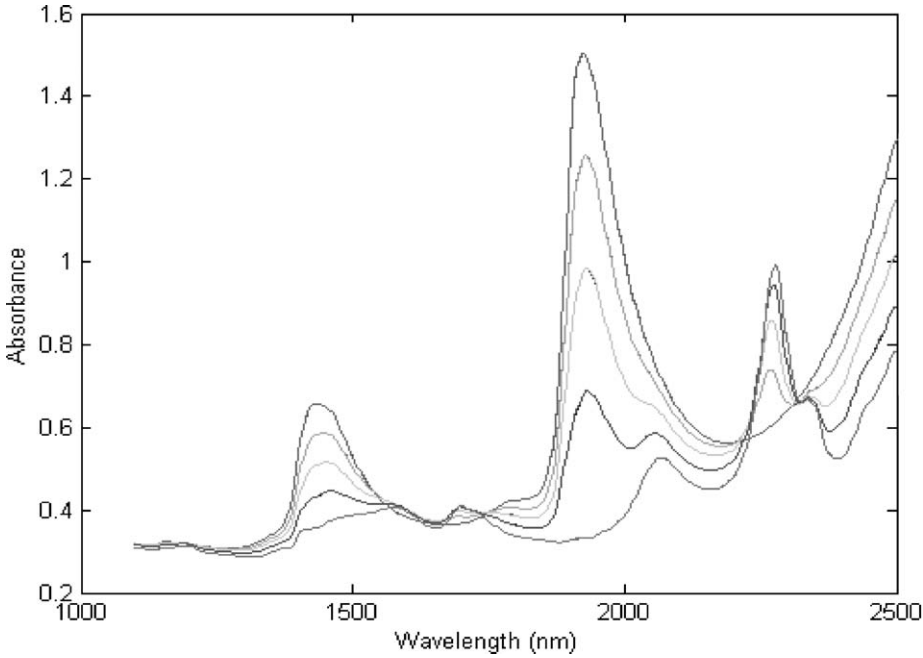


Fig. 6.4. Spectra of water–methanol mixtures.

Figure 6.4 shows the spectra of a series of water/methanol mixtures. In reality, NIR is used for often complex mixtures relying on chemometrics in lieu of actual spectral interpretation. Thus, while based on ‘‘real’’ spectroscopic principles, NIR is seldom about spectroscopy.

The skills needed to master NIR are physics, statistics, chemometrics, and optics.

## 6.3 INSTRUMENTATION

Since NIR was developed by the USDA for food products, the first (commercial) mode developed was diffuse reflection. The earliest work was performed on instruments which had, in essence, NIR as an "extra." The UV/Vis hardware (e.g., Cary model 10) had an additional detector and could be used through the NIR. This one fact explains why so much literature uses nanometers for units instead of wave numbers.

Another reason for nm instead of $cm^{-1}$ is that mid-IR spectroscopists use the energy (wave numbers) to do spectral interpretation. With the massive overlapping in the NIR, coupled with hydrogen bonding, the NIR spectra are not easily "interpreted," so nanometers tend to remind us of that fact.

The first NIR instruments were, in reality, developed for the UV and Vis regions of the spectrum. They were made by seven companies: Beckman, Cary (now owned by Varian), Coleman, Perkin-Elmer, Shimadzu, Unicam, and Zeiss. Based on the work of Karl Norris and coworkers in the USDA, the Illinois Department of Agriculture solicited bids from companies to produce a "pure" NIR instrument, capable of measuring protein, oil, and moisture in soybeans.

The first commercial unit was produced by Dickey-John. It contained a tungsten-halogen lamp, six interference filters, and uncooled lead sulfide (PbS) detectors, using a 0–45° geometry. That is, the light struck the sample straight on and the light was collected at 45° to the normal.

The samples had dry matter over 85% and were ground to pass through a 1 mm screen and then packed in a quartz-windowed cup. The unit was demonstrated at the 1971 Illinois State Fair. After the success of this instrument, Neotec (later Pacific Scientific, then NIR Systems, then Perstorp, then FOSS) built a rotating (tilting) filter instrument. Both instruments were dedicated, analog systems, neither of which was considered "user-friendly."

In the middle of the 1970s, Technicon Instruments had Dickey-John produce a filter instrument for them, named the InfraAlyzer. The first, numbered 2.5, featured dust proof optics and internal temperature control. This improved stability and ruggedness made it practical for consumers to operate. Technicon also introduced the gold plated integrating sphere.

Since the 1980s, numerous instruments with varied construction have been introduced. In most spectroscopic techniques there are just a few technologies involved. In mid-range IR, there remain a number of grating type monochromators used, but in the whole, interferometers rule. The so-called ''FT-(Fourier Transform) IRs'' are the standard for the mid-range IR. For UV and Visible, gratings (either scanning or fixed with diode arrays) are the norm. However, with NIR, a plethora of wavelength selections are available.

In addition to interference filters, NIR manufacturers use holographic gratings (moving and fixed), interferometers, polarization interferometers, diode arrays, acoustic-optic tunable filters, as well as some specialty types.

While most other techniques use a limited amount of detectors (e.g., silica for visible, photomultipliers for UV) and MIR has a small number, NIR uses many types of semiconductors for detectors. The original PbS detectors are still one of the largest used in NIR, however, indium gallium arsenide (InGaAs), indium arsenide (InAs), indium antimonide (InSb), and lead selenide (PbSe) are among the semiconductor combinations used, both cooled and ambient.

Most samples analyzed by NIR are ''as is'' samples, typical of agriculture, now food, polymers, and pharmaceuticals. Because of this a large number of sample presentation techniques have been developed: cups, dipping fiber optics, spinning cups, flow-through cells, paired fiber probes, cuvettes, windows in production systems, and non-contact systems. In fact, much of the engineering goes into sample presentation. This places a lot of the system's success or failure on features having little to do with spectroscopy.

The size, speed, noise levels, precision, accuracy, and cost vary among the instruments. Higher cost does not necessarily mean better performance. Unlike ''typical'' spectroscopy, where the sample is reduced and, often, diluted in a non-interfering matrix, samples in NIR are read ''as is'' and one size instrument does NOT fit all. The application will determine the instrument (an idea that escapes many instrument salespeople).

As a general statement, the one thing that all NIR spectrometers, built in the past 25 years, have in common is that they are all single beam. This means that periodic wavelength, noise, and linearity checks must be made. In typical chemical or instrumental analyses (i.e. titrations or HPLC), a standard is run in parallel with an unknown and the result calculated from the response of the two. This is defined as an analysis or assay.

In NIR, a series of samples are scanned and then analyzed by a referee method. An equation is generated and used for future unknowns. This equation is used after the instrument is checked for compliance with initial performance criteria (at the time of the equation calibration). No standard is available for process or "natural" samples. The value(s) is gleaned from chemometric principles. This is defined as a prediction.

Thus, while a well-maintained instrument is important for any chemical/physical measurement, in NIR, without a concurrent standard for comparison, it is critical that the instrument be continuously calibrated and maintained. Since the major manufacturers of equipment have worked with the pharmaceutical industry, this has been formalized into what is called IQ/OQ/PQ, or Instrument Qualification, Operational Qualification, and Performance Qualification. The first is routinely performed (at first) by the manufacturer in the lab/process location, the second *in situ* by the user with help from the manufacturer, and the third is product/use dependent. These formal tests apply to all instruments in any industry.

## 6.4 MATH TREATMENTS

Since most quantitative applications are on mixtures of materials, complex mathematical treatments have been developed. The most common programs are Multiple Linear Regression (MLR), Partial Least Squares (PLS), and Principal Component Analyses (PCA). While these are described in detail in another chapter, they will be described briefly here.

MLR is based on classical least squares regression. Since "known" samples of things like wheat cannot be prepared, some changes, demanded by statistics, must be made. In a Beer's law plot, common in calibration of UV and other solution-based tests, the equation for a straight line

$$Y = mX + b \tag{6.9}$$

represents the line where $Y$ is the absorbance generated by the corresponding concentration, $X$. Since we are considering a "true" Beer's law plot, zero concentration has zero absorbance, so that the "$b$" or intercept is always zero. In this case, the better known or least error-prone values, by convention, plotted along the $X$-axis, are the concentrations of materials. This is simply because a balance and volumetric

glassware are used to make the solutions and, in this case, the absorbance is less accurate and is plotted on the $Y$-axis.

In most NIR measurements, the sample is not a simple solution, but either a complex solution or a complex solid. In this case, the material (or property) being assessed is measured by a referee method, not weighed into a flask from a balance. As a consequence, the more reliable (accurate) measurement is the absorbance. Thus, the "Inverse Beer's Law" equation becomes

$$A = \xi bc \tag{6.10}$$

where $A$ is the absorbance measured at a specific wavelength; $\xi$ the molar absorptivity (at that wavelength in $\mathrm{L\,mol^{-1}cm^{-1}}$); $b$ the path length (in cm); $c$ the concentration (in $\mathrm{mol\,L^{-1}}$); and but is now written as

$$C = b_1 A + b_0 \tag{6.11}$$

where $A$ is the absorbance measured at a specific wavelength; $C$ the concentration; $b_1$ the constant that incorporates $\xi$ and $b$; and $b_0$ the intercept of the calibration line.

Since there are few clear absorbance peaks in a complex mixture, because of the overlap several wavelengths are often needed to generate a linear, descriptive equation. The equation then takes on the form of

$$C = b_1 A_1 + b_2 A_2 + \cdots + b_n A_n + b_0 \tag{6.12}$$

where $C$ is the concentration; $b_1, \ldots, b_n$ are constants for wavelengths 1 through $n$; and $A_1, \ldots, A_n$ are absorbance at wavelengths 1 through $n$.

If an MLR equation needs more than five wavelengths, it is often better to apply one of the other multivariate algorithms mentioned above. Since the information which an analyst seeks is spread throughout the sample, methods such as PLS and PCA use much or all of the NIR spectra to determine the information sought.

One example of MLR is seen in Figs. 6.5 and 6.6. Figure 6.5 shows the second derivative spectra of various combinations of two polymorphic forms of a crystalline drug substance. Since the chemistry is identical, only hydrogen bonding differences affect the spectra. The wavelength where the calibration is made is highlighted. The resulting calibration curve (two wavelength MLR equation) is seen in Fig. 6.6.

The differences of consequence will be highlighted here. Both show the variances within a set of spectra and attempt to define it. How they are developed and applied is slightly different, however.

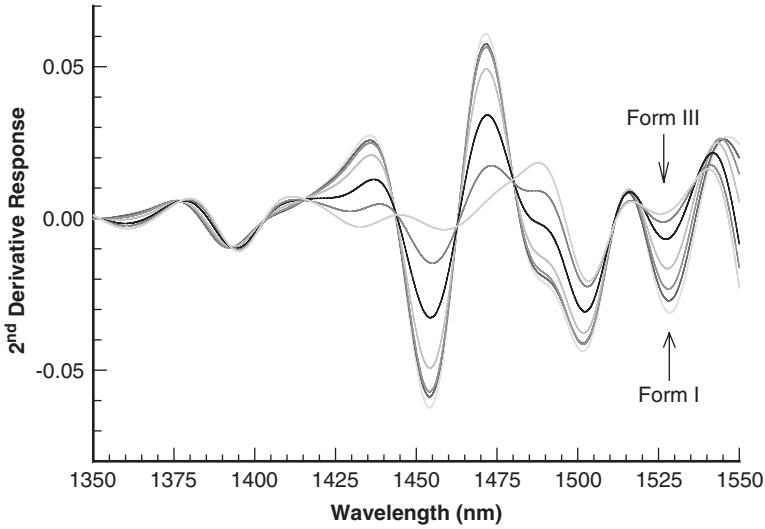


Fig. 6.5. Second derivative spectra of polymorphic mixtures.

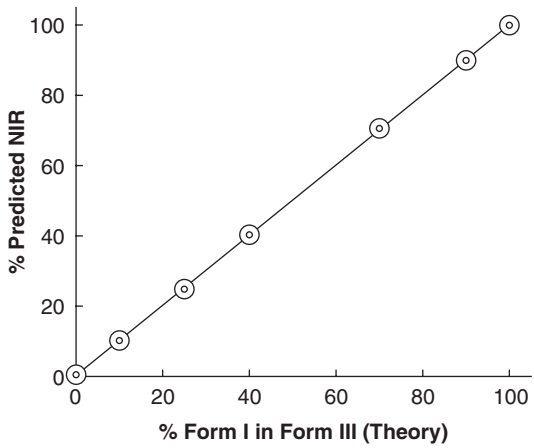


Fig. 6.6. Calibration curve for polymorph determination.

PCA is based only on the variances among spectra. No content information is used to generate the preliminary factors. In a series of mixtures of water and methanol (shown in Fig. 6.3), for instance, the first Principal Component (see Fig. 6.7) shows the positive and negative ‘‘lobes’’ representing the shifting of water in a positive direction and methanol in a negative direction. This is based solely on the change in

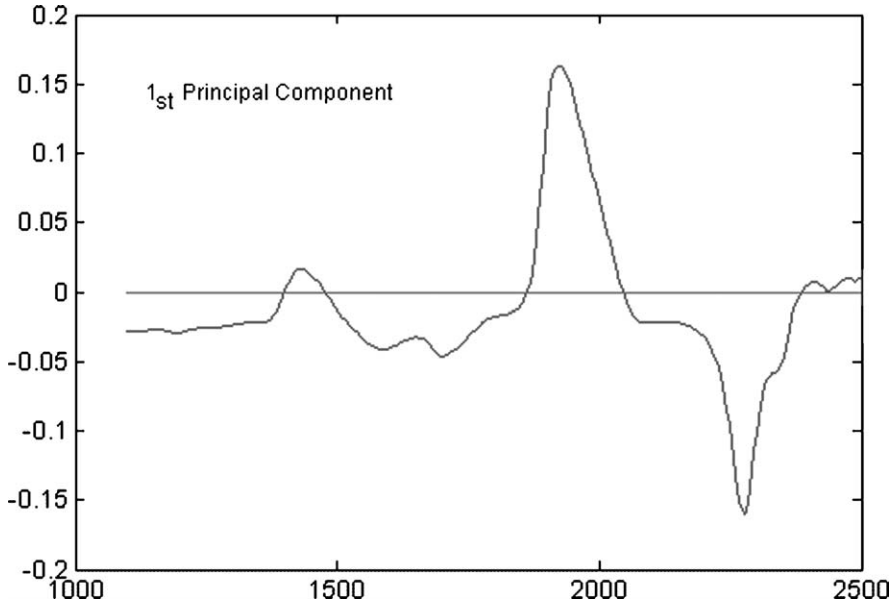


Fig. 6.7. First principal component of water–methanol mixture in Fig. 6.4.

spectra; no assay values have been given. Since the introduction of PLS, PCA has been used almost entirely in qualitative analyses, where numbers may not be available or relevant (which is the ''better'' lactose for production use?). In a purely qualitative use, PCA is used to show both differences and similarities among groups of materials. Figure 6.8 shows two groups of sample tablets, ''clustered'' purely on physical differences.

More definitive information may also be gleaned from PCA. In Fig. 6.9, three principal component scores are graphed to show how the amount of roasting in coffee beans may be ascertained.

In PLS, the variance is generated using the quantities generated by the referee analytical method. Therefore, the factors in a PLS analysis (especially the first) resemble the spectrum of the active ingredient (assuming a quantitative analysis of a constituent). When measuring a physical attribute (hardness, polymorphic form, elasticity), the PLS factor may not resemble any of the materials present in the mixture.

The first PLS factor represents the manner in which the spectra change with respect to the analytical values attached. That is (for normal spectra, not derivatives) as the correlation between change in absorbance and constituent value is greatest, there is a large ''peak'' or

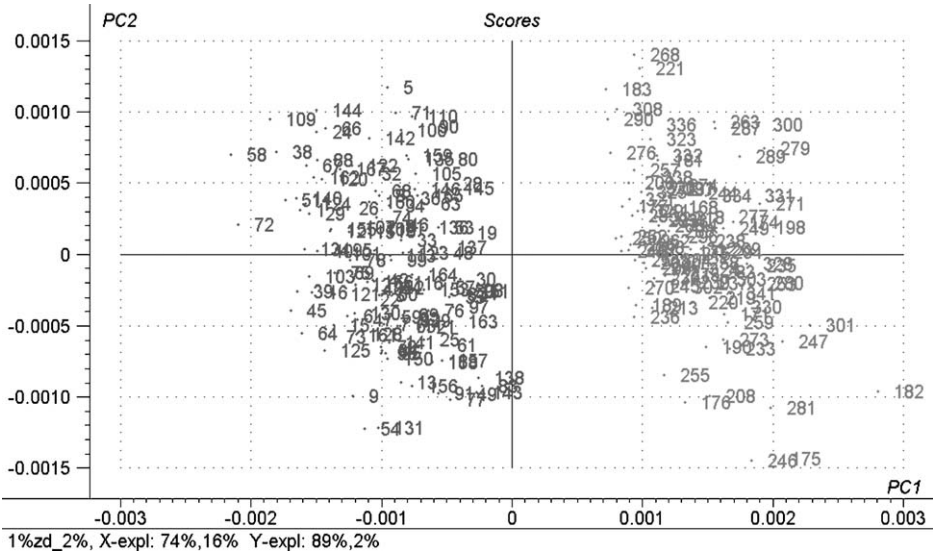


Fig. 6.8. Two-dimensional graph of PC scores of two groups of pharmaceutical tablets.

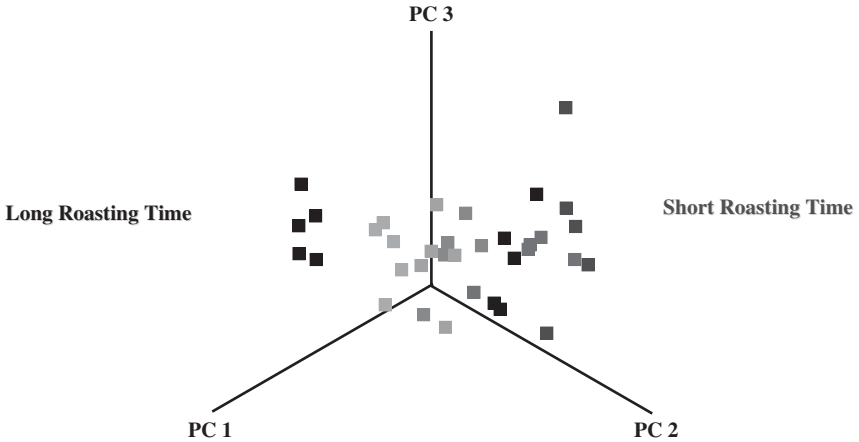


Fig. 6.9. Three-dimensional representation of PC scores for roasted coffee beans, roasted for varying amounts of time.

upswing in the factor (in the positive direction). A negative correlation brings about a negative swing. [This factor may even be used to uncover wavelengths for MLR equations.] Since this relationship exists, PLS is primarily a quantitative algorithm.

## 6.5 APPLICATIONS

The largest bodies of references for NIR applications are in the fields of agriculture and food. Following closely behind are chemicals, petrochemicals, and polymers. Only recently has the pharmaceutical industry recognized the potential of NIR. Because of its ability to make rapid, non-destructive, and non-invasive measurements, NIR is widely used in process analyses.

In agricultural applications, the most commonly analyzed constituents are water, protein, starch, sugars, and fiber [16–20]. Such physical or chemical functions such as hardness of wheat, minerals, and food values have no actual relation to chemicals seen in the NIR. These are usually done by inferential spectroscopy. That is, the effect of minerals or the relationship of the spectra to *in vitro* reactions is used *in lieu* of chemical analyses to NIR active constituents. Considering that all shipments of grain from the US since the 1980s have been cleared by NIR, it can be argued that this is a critical application of the technique.

The same functions used in agriculture can be applied to processed foods. In baked goods, wheat gluten, various additives, starch damage, and water absorption are just some of the parameters measured [21–24]. Dairy products are also important and often analyzed by NIR. Moisture, fat, protein, lactose, lactic acid, and ash are common analytes in the dairy industry [25–28].

Other food/agricultural applications are in the beverage and fabrics/wool industries. Wood fibers are easily analyzed for lignin, wool and cotton for ability to accept dyes, and beverages, both soft and hard, may be analyzed for contents.

Polymers may be analyzed from the synthesis stage (reaction monitoring) through blending and actual fabrication of plastic end products [29–35]. The molecular weight, degree of polymerization and cross-linking, hydroxyl values, acid number, and saponification values are just some of the values monitored (non-destructively, in real time). A major polymer company in Delaware is said to have as many as 1200 units throughout its plants.

The most recent converts are in the health care industry. Pharmaceutical and biological applications have become myriad since the early 1980s. The first widespread application was for the identification/qualification of incoming raw materials. Since then, applications have appeared for moisture (bound and free), blend uniformity of powders, tablet and capsule assays, counterfeiting, polymorphism, degree of crystallinity, hardness (of tablets), dissolution prediction, isomerism, as

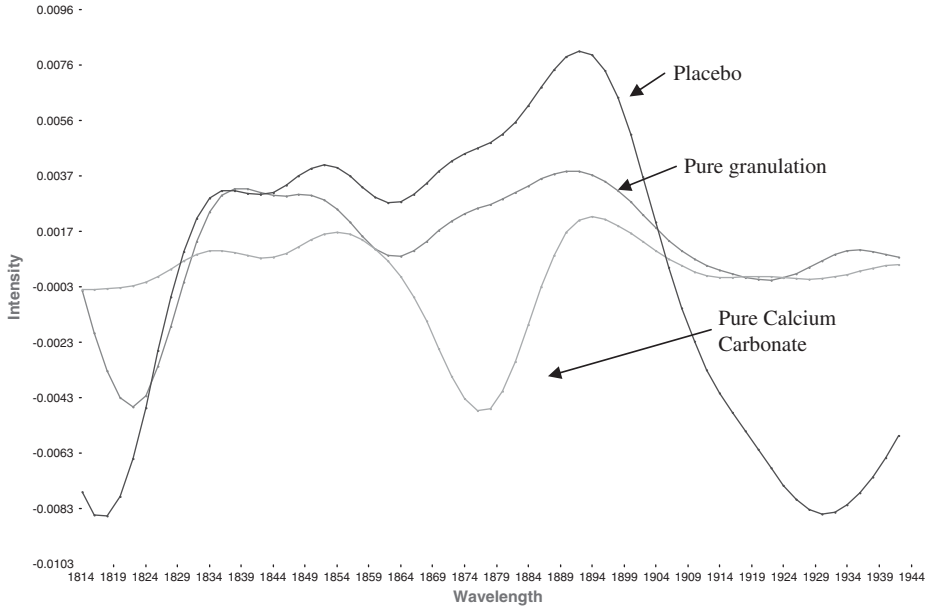


Fig. 6.10. Overlay of spectra of typical pharmaceutical ingredients for a tablet mixture

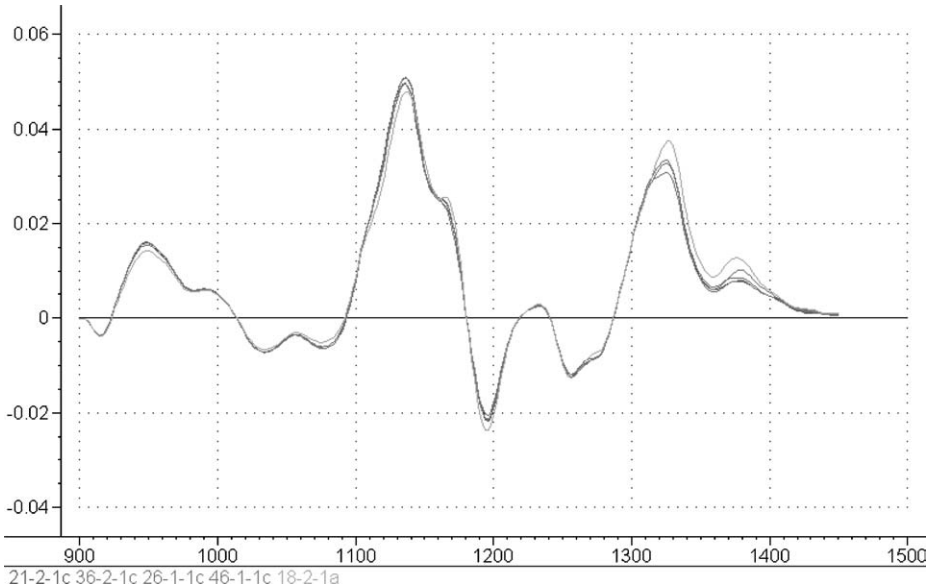


Fig. 6.11. Overlay of spectra for several tablets on a conveyor belt

well as synthesis monitoring [36–44]. Figure 6.10 shows the overlay of several components of a tablet mixture. The regions of interest are easily discerned for analysis.

In the process setting, NIR is fast enough to capture information at amazing speeds. Figure. 6.11 shows the spectra of tablets, generated as

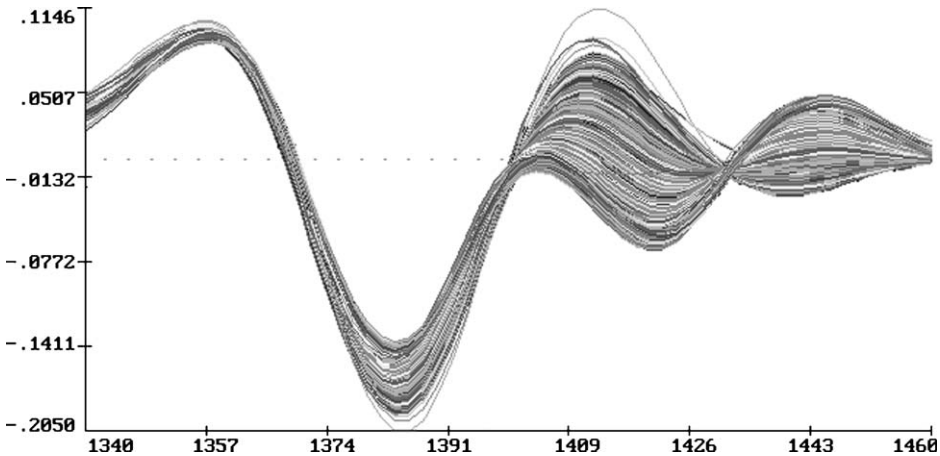


Fig. 6.12. Spectra from a granulation drying process. The bound and free water are seen at ~1420 and ~1440 nm, respectively.

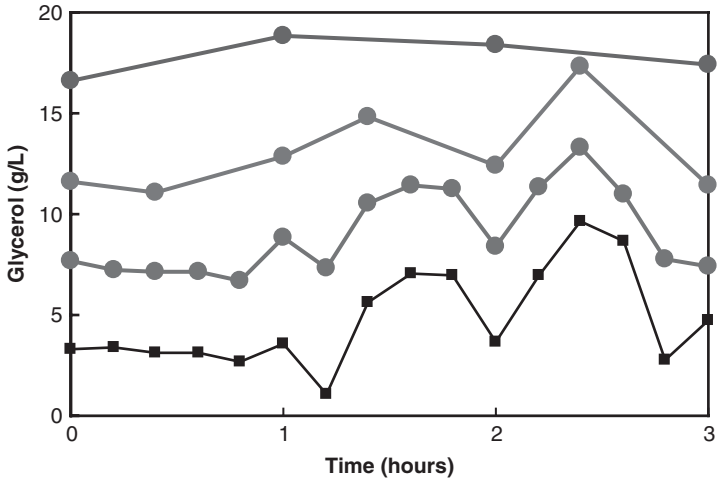


Fig. 6.13. Comparison of rates of sampling for a bioprocess (fermentation); the ability of NIR to measure in real time is compared with discrete sampling techniques.

they pass through the beam at conveyor-belt speeds. Medical and biological applications include skin and tissue monitoring, blood analysis, and fermentation of biologics [45–50]. Figure 6.12 shows the advantage of NIR in rapid sampling and analysis of glycerol in a fermentation process. The sampling rate for a bioprocess may be greatly increased with a NIR probe, as seen in Fig. 6.13, where manual and instrumental rates are compared.

Some of the more esoteric applications include currency counterfeiting, determining the quality of bowling alley floors, and watching crops ripen on the vine. In essence, any materials containing hydrogen are candidates for NIR analyses. It is fast, sensitive, rugged, accurate, and non-destructive. It may be used in contact or from a distance, making it one of the more versatile analytical applications today.

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## REVIEW QUESTIONS

1. When and how was near-infrared discovered?
2. What are some of the unique features of NIR?
3. What is the basis of absorption of light in the NIR region?
4. How many types of NIR instruments are in use today?
5. Why are Chemometrics necessary for most NIR measurements?
6. Why would NIR be more affected by hydrogen bonding than mid-range infrared?
7. Name three industrial applications where NIR would have an advantage over ‘‘classical’’ analyses.
8. Why would you guess that NIR instruments are so varied when compared with other spectroscopic methods?