WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
SJIF Impact Factor 8.453
Volume 13, Issue 13, 89-107. Review Article ISSN 2277–7105

# SPECTROSCOPIC TECHNIQUES

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Article Received on
12 May 2024,

Revised on 02 June 2024,
Accepted on 22 June 2024

DOI: 10.20959/wjpr202413-32173

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## INTRODUCTION

Spectroscopy is the study of the interaction between matter and electromagnetic radiation as a function of the wavelength or frequency of the radiation. In simpler terms, spectroscopy is the precise study of color as generalized from visible light to all bands of the electromagnetic spectrum; indeed, historically, spectroscopy originated as the study of the wavelength dependence of the absorption by gas phase matter of visible light dispersed by a prism. Matter waves and acoustic waves can also be considered forms of radiative energy, and recently gravitational waves have been associated with a spectral signature in the context of the Laser Interferometer Gravitational-Wave Observatory (LIGO).

Spectroscopy, primarily in the electromagnetic spectrum, is a fundamental exploratory tool in the fields of physics, chemistry, and astronomy, allowing the composition, physical structure and electronic structure of matter to be investigated at the atomic, molecular and macro scale, and over astronomical distances. Important applications arise from biomedical spectroscopy in the areas of tissue analysis and medical imaging.

Spectroscopy and spectrography are terms used to refer to the measurement of radiation intensity as a function of wavelength and are often used to describe experimental spectroscopic methods. Spectral measurement devices are referred to as spectrometers, spectrophotometers, spectrographs or spectral analyzers. Daily observations of color can be related to spectroscopy. Neon lighting is a direct application of atomic spectroscopy. Neon and other noble gases have characteristic emission frequencies (colors). Neon lamps use collision of electrons with the gas to excite these emissions. Inks, dyes and paints include chemical compounds selected for their spectral characteristics in order to generate specific colors and hues.

A commonly encountered molecular spectrum is that of nitrogen dioxide. Gaseous nitrogen dioxide has a characteristic red absorption feature, and this gives air polluted with nitrogen dioxide a reddish-brown color. Rayleigh scattering is a spectroscopic scattering phenomenon that accounts for the color of the sky. Spectroscopic studies were central to the development of quantum mechanics and included Max Planck's explanation of blackbody radiation, Albert Einstein's explanation of the photoelectric effect and Niels Bohr's explanation of atomic structure and spectra. Spectroscopy is used in physical and analytical chemistry because atoms and molecules have unique spectra. As a result, these spectra can be used to detect, identify and quantify information about the atoms and molecules. Spectroscopy is also used in astronomy and remote sensing on Earth. Most research telescopes have spectrographs. The measured spectra are used to determine the chemical composition and physical properties of astronomical objects (such as their temperature and velocity).

An example of spectroscopy: a prism analyses white light by dispersing it into its component colors.

## Theory

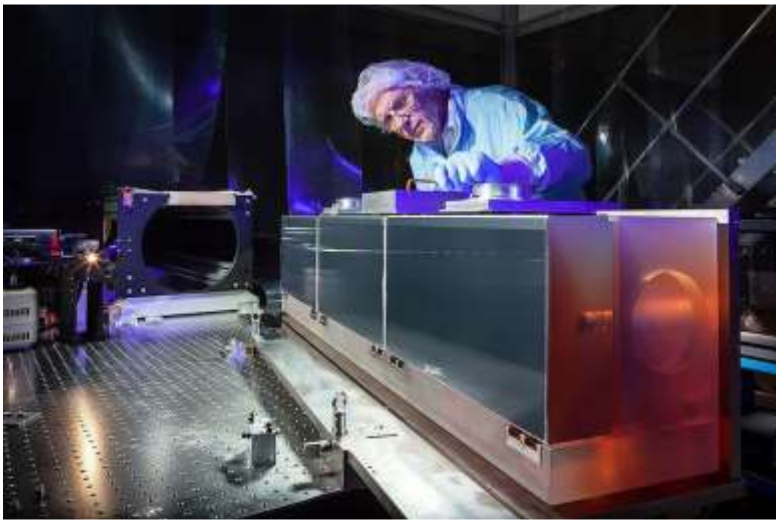
One of the central concepts in spectroscopy is a resonance and its corresponding resonant frequency. Resonances were first characterized in mechanical systems such as pendulums. Mechanical systems that vibrate or oscillate will experience large amplitude oscillations when they are driven at their resonant frequency. A plot of amplitude vs. excitation frequency will have a peak centered at the resonance frequency. This plot is one type of spectrum, with the peak often referred to as a spectral line, and most spectral lines have a similar appearance. In quantum mechanical systems, the analogous resonance is a coupling of two quantum mechanical stationary states of one system, such as an atom, via an oscillatory source of energy such as a photon. The coupling of the two states is strongest when the energy of the source matches the energy difference between the two states.

The energy E of a photon is related to its frequency ν by E = hν where h is Planck's constant, and so a spectrum of the system response vs. photon frequency will peak at the resonant frequency or energy. Particles such as electrons and neutrons have a comparable relationship, the de Broglie relations, between their kinetic energy and their wavelength and frequency and therefore can also excite resonant interactions. Spectra of atoms and molecules often consist of a series of spectral lines, each one representing a resonance between two different quantum states. The explanation of these series, and the spectral patterns associated with them, were one of the experimental enigmas that drove the development and acceptance of quantum mechanics.

The hydrogen spectral series in particular was first successfully explained by the Rutherford–Bohr quantum model of the hydrogen atom. In some cases spectral lines are well separated and distinguishable, but spectral lines can also overlap and appear to be a single transition if the density of energy states is high enough. Named series of lines include the principal, sharp,diffuse and fundamental series.

## Classification of Methods

Spectroscopy is a sufficiently broad field that many sub-disciplines exist, each with numerous implementations of specific spectroscopic techniques. The various implementations and techniques can be classified in several ways.



A huge diffraction grating at the heart of the ultra-precise ESPRESSO spectrograph.

### 1) Ultraviolet–visible spectroscopy

Ultraviolet–visible spectroscopy or ultraviolet–visible spectrophotometry (UV–Vis or UV/Vis) refers to absorption spectroscopy or reflectance spectroscopy in part of the ultraviolet and the full, adjacent visible regions of the electromagnetic spectrum.

### Principle of ultraviolet–visible absorption

Molecules containing bonding and non-bonding electrons (n-electrons) can absorb energy in the form of ultraviolet or visible light to excite these electrons to higher anti-bonding molecular orbitals. The more easily excited the electrons (i.e. lower energy gap between the HOMO andthe LUMO), the longer the wavelength of light it can absorb. There are four possible types of transitions (π–π*, n–π*, σ–σ*, and n–σ*), and they can be ordered as follows: σ–σ* > n–σ* > π– π* > n–π*.

### Applications

UV/Vis spectroscopy is routinely used in analytical chemistry for the quantitative determination of different analytes, such as transition metal ions, highly conjugated organic compounds, and biological macromolecules. Spectroscopic analysis is commonly carried out in solutions but solids and gases may also be studied.

- Solutions of transition metal ions can be colored (i.e., absorb visible light) because d electrons within the metal atoms can be excited from one electronic state to another. The colour of metal ion solutions is strongly affected by the presence of other species, such as certain anions or ligands. For instance, the colour of a dilute solution of copper sulfate is a very light blue; adding ammonia intensifies the colour and changes the wavelength of maximum absorption (λmax).

- Organic compounds, especially those with a high degree of conjugation, also absorb light in the UV or visible regions of the electromagnetic spectrum. The solvents for these determinations are often water for water-soluble compounds, or ethanol for organic-soluble compounds. (Organic solvents may have significant UV absorption; not all solvents are suitable for use in UV spectroscopy. Ethanol absorbs very weakly at most wavelengths.) Solvent polarity and pH can affect the absorption spectrum of an organic compound. Tyrosine, for example, increases in absorption maxima and molar extinction coefficient when pH increases from 6 to 13 or when solvent polarity decreases. While charge transfer complexes also give rise to colours, the colours are often too intense to be used for quantitative measurement.

### Ultraviolet–visible spectrophotometer

The instrument used in ultraviolet–visible spectroscopy is called a UV/Vis spectrophotometer. It measures the intensity of light after passing through a sample (I), and compares it to the intensityof light before it passes through the sample (Io). The ratio I/Io is called the transmittance, and is usually expressed as a percentage (%T). The absorbance, A, is based on the transmittance:

$A = -\log(\%T/100\%)$.

### 2) Fluorescence spectroscopy

Fluorescence spectroscopy is a type of electromagnetic spectroscopy that analyzes fluorescence from a sample. It involves using a beam of light, usually ultraviolet light, that excites the electrons in molecules of certain compounds and causes them to emit light; typically, but not necessarily, visible light. A complementary technique is absorption spectroscopy. In the special case of single molecule fluorescence spectroscopy, intensity fluctuations from the emitted light are measured from either single fluorophores, or pairs of fluorophores.

Devices that measure fluorescence are called fluorometers.

### Instrumentation

Two general types of instruments exist: filter fluorometers that use filters to isolate the incident light and fluorescent light and spectrofluorometers that use a diffraction grating monochromators to isolate the incident light and fluorescent light.

Both types use the following scheme: the light from an excitation source passes through a filteror monochromator, and strikes the sample. A proportion of the incident light is absorbed by the sample, and some of the molecules in the sample fluoresce. The fluorescent light is emitted in all directions. Some of this fluorescent light passes through a second filter or monochromator and reaches a detector, which is usually placed at 90° to the incident light beam to minimize the risk of transmitted or reflected incident light reaching the detector.

Various light sources may be used as excitation sources, including lasers, LED, and lamps; xenon arcs and mercury-vapor lamps in particular. A laser only emits light of high irradiance at a very narrow wavelength interval, typically under 0.01 nm, which makes an excitation monochromator or filter unnecessary. The disadvantage of this method is that the wavelength of a laser cannot be changed by much. A mercury vapor lamp is a line lamp, meaning it emits light near peak wavelengths. By contrast, a xenon arc has a continuous emission spectrum with nearly constant intensity in the range from 300-800 nm and a sufficient irradiance for measurements down to just above 200 nm.

Filters and/or monochromators may be used in fluorimeters. A monochromator transmits light of an adjustable wavelength with an adjustable tolerance. The most common type of monochromator utilizes a diffraction grating, that is, collimated light illuminates a grating and exits with a different angle depending on the wavelength. The monochromator can then be adjusted to select which wavelengths to transmit. For allowing anisotropy measurements, the addition of two polarization filters is necessary: One after the excitation monochromator or filter,and one before the emission monochromator or filter.

As mentioned before, the fluorescence is most often measured at a 90° angle relative to the excitation light. This geometry is used instead of placing the sensor at the line of the excitation light at a 180° angle in order to avoid interference of the transmitted excitation light. No monochromator is perfect and it will transmit some stray light, that is, light with other wavelengths than the targeted. An ideal monochromator would only transmit light in the specified range and have a high wavelength-independent transmission. When measuring at a 90° angle, only the light scattered by the sample causes stray light. This results in a better signal-to- noise ratio, and lowers the detection limit by approximately a factor 10000, when compared to the 180° geometry. Furthermore, the fluorescence can also be measured from the front, which is often done for turbid or opaque samples.

The detector can either be single-channeled or multichanneled. The single-channeled detector can only detect the intensity of one wavelength at a time, while the multichanneled detects the intensity of all wavelengths simultaneously, making the emission monochromator or filter unnecessary. The different types of detectors have both advantages and disadvantages.

The most versatile fluorimeters with dual monochromators and a continuous excitation light source can record both an excitation spectrum and a fluorescence spectrum. When measuring fluorescence spectra, the wavelength of the excitation light is kept constant, preferably at a wavelength of high absorption, and the emission monochromator scans the spectrum. For measuring excitation spectra, the wavelength passing through the emission filter or monochromator is kept constant and the excitation monochromator is scanning. The excitation spectrum generally is identical to the absorption spectrum as the fluorescence intensity is proportional to the absorption.

### Applications

- Fluorescence spectroscopy is used in, among others, biochemical, medical, and chemical research fields for analyzing organic compounds. There has also been a report of its use in differentiating malignant skin tumors from benign.
- Atomic Fluorescence Spectroscopy (AFS) techniques are useful in other kinds of analysis/measurement of a compound present in air or water, or other media, such as CVAFS which is used for heavy metals detection, such as mercury.
- Fluorescence can also be used to redirect photons, see fluorescent solar collector.
- Additionally, Fluorescence spectroscopy can be adapted to the microscopic level using microfluorimetry
- In analytical chemistry, fluorescence detectors are used with HPLC.
- In the field of water research, fluorescence spectroscopy can be used to monitor water quality by detecting organic pollutants. Recent advances in computer science and machine learning have even enabled detection of bacterial contamination of water.

### 3) Infrared spectroscopy

Infrared spectroscopy is the measurement of the interaction of infrared radiation with matter by absorption, emission, or reflection. It is used to study and identify chemical substances or functional groups in solid, liquid, or gaseous forms. It can be used to characterize new materials or identify and verify known and unknown samples. The method or technique of infrared spectroscopy is conducted with an instrument called an infrared spectrometer (or spectrophotometer) which produces an infrared spectrum. An IR spectrum can be visualized in a graph of infrared light absorbance (or transmittance) on the vertical axis vs. frequency or wavelength on the horizontal axis. Typical units of frequency used in IR spectra are reciprocal centimeters (sometimes called wave numbers), with the symbol $cm^{-1}$. Units of IR wavelength are commonly given in micrometers (formerly called "microns"), symbol μm, which are related to wave numbers in a reciprocal way. A common laboratory instrument that uses this technique is a Fourier transform infrared (FTIR) spectrometer. Two-dimensional IR is also possible as discussed below.

## Applications

- Infrared spectroscopy is a simple and reliable technique widely used in both organic and inorganic chemistry, in research and industry. It is used in quality control, dynamic measurement, and monitoring applications such as the long-term unattended measurement of $CO_2$ concentrations in greenhouses and growth chambers by infrared gas analyzers.
- It is also used in forensic analysis in both criminal and civil cases, for example in identifying polymer degradation. It can be used in determining the blood alcohol content of a suspected drunk driver.
- IR-spectroscopy has been successfully used in analysis and identification of pigments in paintings and other art objects such as illuminated manuscripts.
- A useful way of analyzing solid samples without the need for cutting samples uses ATR or attenuated total reflectance spectroscopy. Using this approach, samples are pressed against the face of a single crystal. The infrared radiation passes through the crystal and only interacts with the sample at the interface between the two materials.
- With increasing technology in computer filtering and manipulation of the results, samples in solution can now be measured accurately (water produces a broad absorbance across the range of interest, and thus renders the spectra unreadable without this computer treatment).
- Some instruments also automatically identify the substance being measured from a store of thousands of reference spectra held in storage.
- Infrared spectroscopy is also useful in measuring the degree of polymerization in polymer manufacture. Changes in the character or quantity of a particular bond are

assessed by measuring at a specific frequency over time. Modern research instruments can take infrared measurements across the range of interest as frequently as 32 times a second. This can be done whilst simultaneous measurements are made using other techniques. This makes the observations of chemical reactions and processes quicker and more accurate.

- Infrared spectroscopy has also been successfully utilized in the field of semiconductor microelectronics: for example, infrared spectroscopy can be applied to semiconductors like silicon, gallium arsenide, gallium nitride, zinc selenide, amorphous silicon, silicon nitride, etc.
- Another important application of Infrared Spectroscopy is in the food industry to measure the concentration of various compounds in different food products
- The instruments are now small, and can be transported, even for use in field trials.
- Infrared Spectroscopy is also used in gas leak detection devices such as the DP-IR and Eye CGAs. These devices detect hydrocarbon gas leaks in the transportation of natural gas and crude oil.
- In February 2014, NASA announced a greatly upgraded database, based on IR spectroscopy, for tracking polycyclic aromatic hydrocarbons (PAHs) in the universe. According to scientists, more than 20% of the carbon in the universe may be associated with PAHs, possible starting materials for the formation of life. PAHs seem to have been formed shortly after the Big Bang, are widespread throughout the universe, and are associated with new stars and exoplanets. Infrared spectroscopy is an important analysis method in the recycling process of household waste plastics, and a convenient stand-off method to sort plastic of different polymers (PET, HDPE)
- Recent developments include a miniature IR-spectrometer that's linked to a cloud based database and suitable for personal everyday use, and NIR-spectroscopic chips that can be embedded in smartphones and various gadgets.

### 4) Atomic absorption spectroscopy

Atomic absorption spectroscopy (AAS) and atomic emission spectroscopy (AES) is a spectroanalytical procedure for the quantitative determination of chemical elements using the absorption of optical radiation (light) by free atoms in the gaseous state. Atomic absorption spectroscopy is based on absorption of light by free metallic ions.

In analytical chemistry the technique is used for determining the concentration of a particular element (the analyte) in a sample to be analyzed. AAS can be used to determine over 70 differentelements in solution, or directly in solid samples via electrothermal vaporization and is usedin pharmacology, biophysics, archaeology and toxicology research.

Atomic emission spectroscopy was first used as an analytical technique, and the underlying principles were established in the second half of the 19th century by Robert Wilhelm Bunsen and Gustav Robert Kirchhoff, both professors at the University of Heidelberg, Germany.

The modern form of AAS was largely developed during the 1950s by a team of Australian chemists. They were led by Sir Alan Walsh at the Commonwealth Scientific and Industrial Research Organisation (CSIRO), Division of Chemical Physics, in Melbourne, Australia.

Atomic absorption spectrometry has many uses in different areas of chemistry such as clinical analysis of metals in biological fluids and tissues such as whole blood, plasma, urine, saliva, brain tissue, liver, hair, muscle tissue. Atomic absorption spectrometry can be used in qualitative and quantitative analysis.

### Principles

The technique makes use of the atomic absorption spectrum of a sample in order to assess the concentration of specific analytes within it. It requires standards with known analyte content to establish the relation between the measured absorbance and the analyte concentration and relies therefore on the Beer–Lambert law.

### Instrumentation

In order to analyze a sample for its atomic constituents, it has to be atomized. The atomizers most commonly used nowadays are flames and electrothermal (graphite tube) atomizers. The atoms should then be irradiated by optical radiation, and the radiation source could be an element-specific line radiation source or a continuum radiation source. The radiation then passes through a monochromator in order to separate the element-specific radiation from any other radiation emitted by the radiation source, which is finally measured by a detector.

### Atomizers

The atomizers most commonly used nowadays are (spectroscopic) flames and electrothermal (graphite tube) atomizers. Other atomizers, such as glow-discharge atomization, hydride atomization, or cold-vapor atomization, might be used for special purposes.

### 1. Flame atomizers

The oldest and most commonly used atomizers in AAS are flames, principally the air-acetylene flame with a temperature of about 2300 °C and the nitrous oxide system ($N_2O$)-acetylene flame with a temperature of about 2700 °C. The latter flame, in addition, offers a more reducing environment, being ideally suited for analytes with high affinity to oxygen.

### 2. Electrothermal Atomizers

Electrothermal AAS (ET AAS) using graphite tube atomizers was pioneered by Boris V. L’vov at the Saint Petersburg Polytechnical Institute, Russia, since the late 1950s, and investigated in parallel by Hans Massmann at the Institute of Spectrochemistry and Applied Spectroscopy(ISAS) in Dortmund, Germany.

### 3. Specialized atomization techniques

While flame and electrothermal vaporizers are the most common atomization techniques, severalother atomization methods are utilized for specialized use.

### 4. Glow-discharge atomization

A glow-discharge device (GD) serves as a versatile source, as it can simultaneously introduce and atomize the sample. The glow discharge occurs in a low-pressure argon gas atmosphere between 1 and 10 torr. In this atmosphere lies a pair of electrodes applying a DC voltage of 250 to 1000 V to break down the argon gas into positively charged ions and electrons. These ions, under the influence of the electric field, are accelerated into the cathode surface containing the sample, bombarding the sample and causing neutral sample atom ejection through the process known as sputtering.

### 5. Hydride atomization

Hydride generation techniques are specialized in solutions of specific elements. The technique provides a means of introducing samples containing arsenic, antimony, selenium, bismuth, and lead into an atomizer in the gas phase. With these elements, hydride atomization enhances detection limits by a factor of 10 to 100 compared to alternative methods.

### Radiation Sources

We have to distinguish between line source AAS (LS AAS) and continuum source AAS (CS

AAS). In classical LS AAS, as it has been proposed by Alan Walsh, the high spectral resolution required for AAS measurements is provided by the radiation source itself that emits the spectrum of the analyte in the form of lines that are narrower than the absorption lines. Continuum sources, such as deuterium lamps, are only used for background correction purposes. The advantage of this technique is that only a medium-resolution monochromator is necessary for measuring AAS; however, it has the disadvantage that usually a separate lamp is required for each element that has to be determined. In CS AAS, in contrast, a single lamp, emitting a continuum spectrum over the entire spectral range of interest is used for all elements. Obviously, a high-resolution monochromator is required for this technique, as will be discussed later.

### 1. Hollow cathode lamps

Hollow cathode lamps (HCL) are the most common radiation source in LS AAS. Inside the sealed lamp, filled with argon or neon gas at low pressure, is a cylindrical metal cathode containing the element of interest and an anode. A high voltage is applied across the anode and cathode, resulting in an ionization of the fill gas. The gas ions are accelerated towards the cathode and, upon impact on the cathode, sputter cathode material that is excited in the glow discharge to emit the radiation of the sputtered material, i.e., the element of interest.

### 2. Electrodeless discharge lamps

Electrodeless discharge lamps (EDL) contain a small quantity of the analyte as a metal or a salt in a quartz bulb together with an inert gas, typically argon gas, at low pressure. The bulb is inserted into a coil that is generating an electromagnetic radio frequency field, resulting in a low- pressure inductively coupled discharge in the lamp. The emission from an EDL is higher than that from an HCL, and the line width is generally narrower, but EDLs need a separate power supply and might need a longer time to stabilize.

### 3. Deuterium lamps

Deuterium HCL or even hydrogen HCL and deuterium discharge lamps are used in LS AAS for background correction purposes. The radiation intensity emitted by these lamps decreases significantly with increasing wavelength, so that they can be only used in the wavelength range between 190 and about 320 nm.

### 4. Continuum sources

When a continuum radiation source is used for AAS, it is necessary to use a high-resolution monochromator, as will be discussed later. In addition, it is necessary that the lamp emits radiation of intensity at least an order of magnitude above that of a typical HCL over the entire wavelength range from 190 nm to 900 nm. A special high-pressure xenon short arc lamp, operating in a hot-spot mode has been developed to fulfill these requirements.

### 5. Spectrometer

As already pointed out above, there is a difference between medium-resolution spectrometers that are used for LS AAS and high-resolution spectrometers that are designed for CS AAS. The spectrometer includes the spectral sorting device (monochromator) and the detector.

### 6. Spectrometers for LS AAS

In LS AAS the high resolution that is required for the measurement of atomic absorption is provided by the narrow line emission of the radiation source, and the monochromator simply has to resolve the analytical line from other radiation emitted by the lamp. This can usually be accomplished with a band pass between 0.2 and 2 nm, i.e., a medium-resolution monochromator.

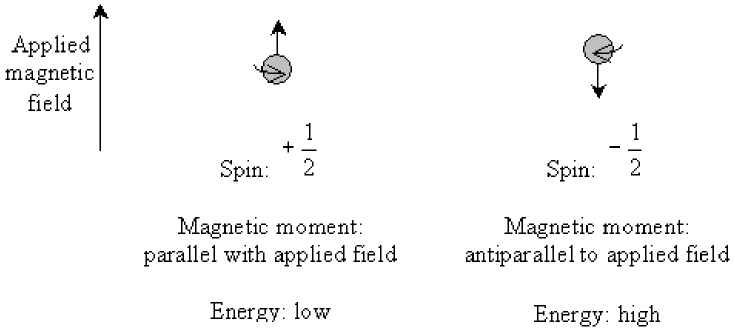
Another feature to make LS AAS element-specific is modulation of the primary radiation and the use of a selective amplifier that is tuned to the same modulation frequency, as already postulated by Alan Walsh. This way any (unmodulated) radiation emitted for example by the atomizer can be excluded, which is imperative for LS AAS. Simple monochromators of the Littrow or (better) the Czerny-Turner design are typically used for LS AAS. Photomultiplier tubes are the most frequently used detectors in LS AAS, although solid state detectors might be preferred because of their better signal-to-noise ratio.

### 7. Spectrometers for CS AAS:

When a continuum radiation source is used for AAS measurement it is indispensable to work with a high-resolution monochromator. The resolution has to be equal to or better than the half width of an atomic absorption line (about 2 pm) in order to avoid losses of sensitivity and linearity of the calibration graph. The research with high-resolution (HR) CS AAS was pioneered by the groups of O'Haver and Harnly in the US, who also developed the (up until now) only simultaneous multi-element spectrometer for this technique. The breakthrough, however, came when the group of Becker-Ross in Berlin, Germany, built a spectrometer entirely designed for HR-CS AAS.

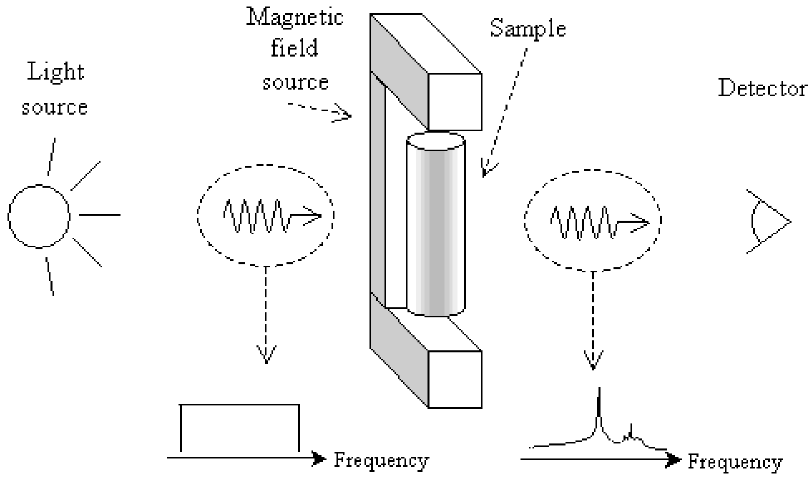
### 5) Nuclear magnetic resonance (NMR)

**Nuclear magnetic resonance (NMR)** spectroscopy takes advantage of the spin states of protons (and, to some extent, other nuclei) to identify a compound. Electrons can have one of two spin quantum states. These spin states have equal energy in the absence of an applied magnetic field. Likewise, protons also have two spin states (with the same designations) of equal energy. When a magnetic field is applied, the protons tend to align their magnetic moments (a vector associated with the "spin" of the particle) parallel with the field-this is the low-energy state. But the protons can also align their magnetic moments antiparallel to the magnetic field-this is the high-energy state. The stronger the magnetic field, the larger the energy difference between the parallel and antiparallel aligned states.



To complicate matters (and to make NMR spectroscopy possible), electrons in the molecule cause "shielding" effects that reduce the magnitude of the magnetic field felt by the protons. Thus, for instance, a compound containing a highly electronegative atom would tend to leave thehydrogen nuclei (protons) more exposed to the magnetic field because the electronegative atom "hogs" the electrons. Conversely, a compound without a highly electronegative atom would tend to allow greater shielding of protons by electrons. Less shielded protons (which are moreexposed to the applied field) thus have a greater difference between high-energy and low-energy spin states, whereas more-shielded protons have a lesser difference between the spin states.

As with IR spectroscopy, NMR spectroscopy passes light through a sample and looks at the spectrum that is transmitted. In this case, however, absorption occurs at frequencies corresponding to the energy difference between two spin states of a proton in the compound. A slightly revised (but still simple) view of NMR spectroscopy is depicted below.

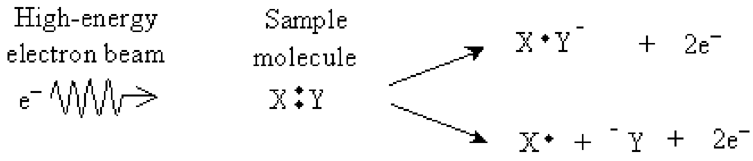


NMR spectra are typically displayed as a series of peaks, such as the sketch shown below (not necessarily representative of any existing compound).

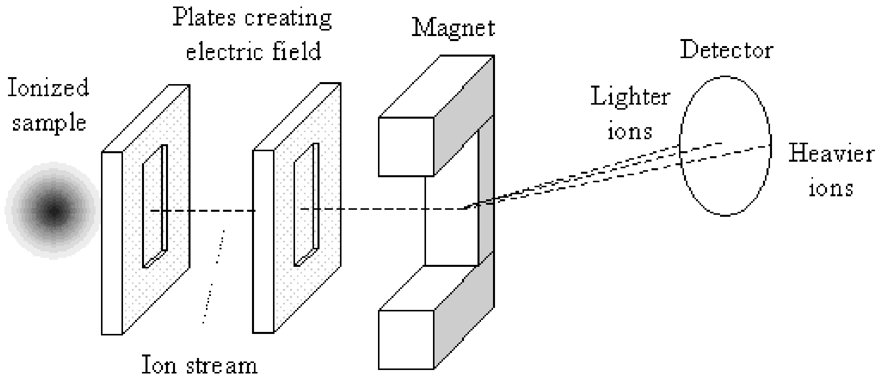
Instead of displaying the peaks on a frequency (or wave number) scale, however, the horizontal axis is often displayed according to **chemical shift,** which is a number proportional to the difference in frequency between the sample peak and a reference peak (typically tetramethylsilane, or (CH3)4Si). Although we will not delve much further into the details of NMRspectra, we can note that we can interpret these spectra by way of the number of peaks (indicating the number of different proton types in the compound), the peak heights (indicating the relative numbers of proton types), and peak splitting (indicating the number of protons near the one creating the peak). Thus, NMR is useful for determining the structure of a sample.

### 6) Mass Spectroscopy

It is nevertheless another instrumental method that chemists use to analyze compounds. Fundamentally, mass spectrometry involves ionization of a sample through bombarding it with high-energy electrons. When these electrons collide with a molecule in the sample, they can dislodge an electron, creating either a cation radical or a cation and a neutral radical.



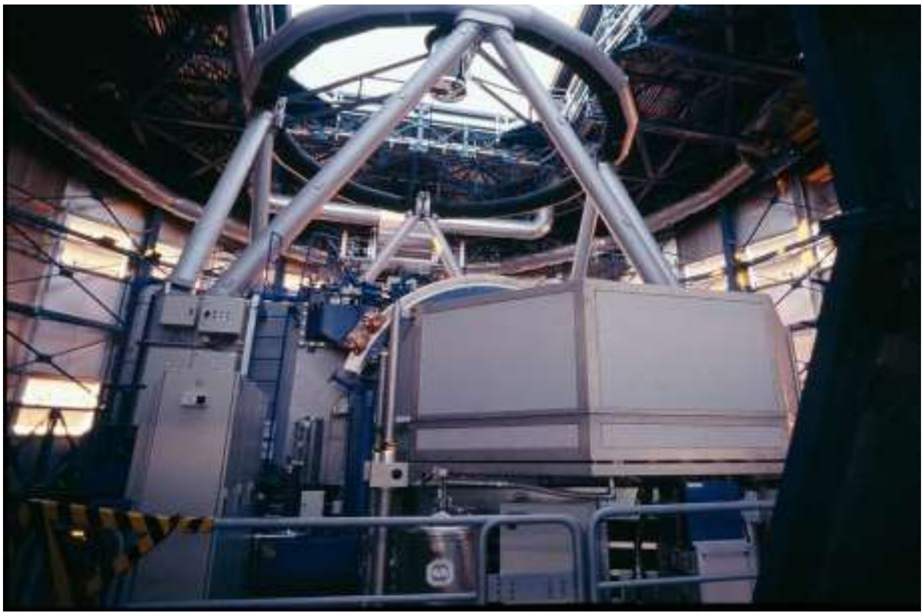
The result is a number of charged particles that can be accelerated by an electric field and then deflected by a magnetic field as shown in the diagram sketched below.



Lighter ions (relative to their respective charges) will be deflects more by the magnetic field than will heavier ions (also relative to their respective charges). Thus, the detector can identify different ion masses (actually, mass-to-charge ratios) by the amount of deflection they undergo, and chemists can use this information to identify the type of compound in the sample. An example mass spectrometry spectrum is shown below. (Again, this spectrum is for illustration; it does not necessarily correspond to an actual compound.) Mass-to-charge ratios are often calculated as the atomic weight (essentially the number of protons and neutrons in the nucleus of an atom) of the entire molecule divided by the charge (in the number of missing electrons).

## Applications

There are several applications to spectroscopy in the field of medicine, physics, chemistry, and astronomy. Taking advantage of the properties of absorbance, spectroscopy can be used to identify certain states of nature. Such examples include.



UVES is a high-resolution spectrograph on the Very Large Telescope.

1. Cure monitoring of composites using optical fibers.
2. Estimate weathered wood exposure times using near infrared spectroscopy.
3. Measurement of different compounds in food samples by absorption spectroscopy both in visible and infrared spectrum.
4. Measurement of toxic compounds in blood samples.
5. Non-destructive elemental analysis by X-ray fluorescence.
6. Electronic structure research with various spectroscopes.
7. Radar to determine the speed and velocity of a distant object.
8. Finding the physical properties of a distant star or nearby exoplanet using the Relativistic Doppler effect.
9. In-ovo sexing: spectroscopy allows to determine the sex of the egg while it is hatching. Developped by French and German companies, both countries decided to ban chick culling, mostly done through a macerator, in 2022.

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